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Conformers of Gaseous Threonine

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Abstract

Following an extensive search on the potential energy surfaces (PES) of the natural amino acid L-threonine (Thr) and its allotropic form L-allo-threonine (aThr), 56 and 61 conformers of Thr and aThr, respectively, have been located with the help of density functional theory (DFT). Accurate structures, relative energies, rotational as well as quartic and sextic centrifugal distortion constants, dipole moments, ¹⁴N nuclear quadrupole coupling constants, anharmonic vibrational frequencies and double-harmonic infrared intensities have been determined from ab initio electronic structure calculations for the five most stable Thr and aThr conformers. The global minimum, **Thr-I**, has a cyclic triple H-bond motif with strong OH^{...}N, C=O^{...}HO, and a weaker NH^{...}OH H-bond, where the latter two involves the side chain OH, and an energetically unfavorable trans -COOH arrangement. The best relative energies of the conformers, accurate within $\pm 1 \text{ kJ mol}^{-1}$, have been determined through the first-principles composite focal-point analysis (FPA) approach. There are four and three conformers of Thr and aThr, respectively, within a relative energy of 5 kJ mol⁻¹. Similarly to other amino acids investigated, lower levels of electronic structure theory, especially the Hartree-Fock level, are unable to determine the correct relative energies of the conformers. The rotational, the quartic and sextic centrifugal distortion, and the ¹⁴N nuclear quadrupole coupling constants as well as the anharmonic vibrational fundamentals and double-harmonic infrared intensities, all determined using DFT, should aid identification and characterization of the conformers of threonine and allo-threonine by rotational and vibrational spectroscopies, respectively.

Keywords: neutral L-threonine • neutral L-allo-threonine • amino acids • *ab initio* calculations • conformational analysis • structure elucidation

This paper is dedicated to Professor Fritz Schaefer on the occasion of his 65th birthday.

I. INTRODUCTION

During the last decades, determination and characterization of the structures of biomolecules, in particular those of proteins and peptides, have been in the focal point of experimental and theoretical research. Since amino acids (AA) are the building blocks of these biopolymers, the structural investigation of AAs, extending from solids to the gas phase, also received considerable attention. Experimental and theoretical structural investigations related to AAs, executed prior to 1999, have been reviewed in ref. 1. During the last decade a considerable number of novel experimental and first-principles computational investigations have been performed on different aspects of the structures of amino acids [2-4], peptides [5,6], and their various complexes [7]. The review of all these studies is out of the scope of the present study and thus only a small number of high-level computational studies originating from our own group are mentioned.

There is only a limited number of natural amino acids and the relatively small size of these molecules allows the application of highly sophisticated experimental and computational techniques during studies related to their equilibrium and dynamical structures usually investigated through their rotational-vibrational spectra. Consequently, we have a detailed understanding of the basics of the structural characteristics of AAs. AAs are chiral, with the sole exception of glycine. In solution and in the solid state, AAs are found in different zwitterionic forms. In the gas phase, however, AAs exist in their neutral form. Furthermore, as AAs are very flexible molecules, all of them exhibit a large number of low-energy conformers and a complex, highly structured potential energy surface (PES). Due partially to the low volatility of AAs and their tendency to decomposition when heated, most of these conformers are not amenable to experimental scrutiny but they can be subjected to detailed quantum chemical investigations. Characterization of the complex PESs of amino acids should precede and supplement related experimental structural studies.

Chiral AAs can play a role in chirally selective organocatalysis, the most important amino acid in this respect appears to be proline (Pro) [8]. As to other applicatons of AAs in chemistry, one may mention functionalization of fullerenes, carbon nanotubes and semiconductor quantum dots with amino acids [9]. Search for signs of life in the universe is also based principally on structural and spectroscopic characterization of Aas [10]. As of today, it seems that none of the AAs have been found outside of our own planet. Threonine, being an essential amino acid is involved in many studies with biochemical importance, for which the present conformational results could prove useful. As examples, we mention the

Molecular Physics

studies of metallic complexes of threonine [11-13] and the possible use of Thr and its derivatives in organocatalysis [14].

The number of local minima on the respective PESs and the structural properties of the related conformers, including accurate relative energy estimates, are available for a number of amino acids [1]. The most accurate relative energies, mostly obtained within the focal-point analysis (FPA) approach [15,16], are available for the amino acids glycine (Gly) [4,17-19], alanine (Ala) [18,20], and proline (Pro) [1-3]. The present computational study expands the list of structurally particularly well characterized amino acids by establishing all of the lowerenergy and almost all of the higher-energy conformers of L-threonine (see Figure 1), one of the two amino acids, the other one being isoleucine, exhibiting two chirality centers. This feature of threonine was one of the reasons for performing this study. The two diastereomers need to be examined separately during conformational and spectroscopic studies as for all practical purposes they appear as two distinct molecules. Obviously, both L-threonine and Lallo-threonine has an enantiomer pair, D-threonine and D-allo-threonine, respectively. In what follows, L-threonine and L-allo-threonine will be abbreviated as Thr and aThr, respectively. In the biosphere only Thr is abundant. Detailed structural characterization of the lowest-energy conformers of these diastereomers was another important aim of the present study. The present study yielded, as primary information, equilibrium structures, relative energies, and a large number of spectroscopic molecular parameters related to the vibrational and rotational spectra of the most important conformers of the two forms of threonine, Thr and aThr. The computational results obtained should help identification of at least some of the conformers of threonine by means of rotational and vibrational spectroscopies.





Figure 1. Pictorial representation of the five lowest-energy conformers of L-threonine (Thr) and L-allo-threonine (aThr)

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II. COMPUTATIONAL DETAILS

Most of the atom-centered Gaussian basis sets selected for the electronic structure computations of this study contain both polarization and diffuse functions, as they are both needed for the determination of accurate structures and relative energies for H-bonded systems [21]. The subcompact 3-21G basis [22] lacks these functions and thus it has been used only for pre-screening the conformers at the Hartree-Fock [23] level of electronic structure theory. The 6-31G* [24] and 6-311++G** [25] bases, used in this study extensively for geometry optimizations and subsequent force field determinations, contain 260 and 369 contracted Gaussian functions (CGFs), respectively, for threonine. The correlation-consistent, polarized-valence (aug)-cc-p(C)VnZ, n = 2 (D), 3 (T), 4 (Q) basis sets of Dunning and coworkers [26,27] have been employed extensively for single-point energy calculations within the FPA approach. (Note that only the augmented (aug) basis set contains diffuse functions, while tight functions, necessary for calculation of core correlation [28] and relativistic effects [29] are only part of core-polarized (C) basis sets.) For Thr, the aug-cc-pVDZ, ccpVTZ, cc-pCVTZ, aug-cc-pVTZ, and aug-cc-pVQZ basis sets contain 265, 366, 470, 575, and 1054 CGFs, respectively. Only the pure spherical harmonics have been employed in the cc basis sets used in this study.

Electronic wave functions have been determined in this study by the singleconfiguration, self-consistent-field, restricted Hartree–Fock (RHF) method [23,30,31], by second-order Møller–Plesset perturbation theory, *i.e.*, MP2 [32], by coupled cluster (CC) methods [33] including all single and double excitations (CCSD) [34] and in cases, additionally, a perturbative correction for contributions from connected triple excitations [CCSD(T)] [35], and by a hybrid density functional theory (DFT) approach usually abbreviated as B3LYP [36]. The T_1 diagnostic values of coupled cluster theory [37] are around 0.013 for the different conformers of Thr, suggesting that they can adequately be described by single-reference-based electron correlation methods. The eight lowest 1s-like core orbitals were kept frozen in all post-Hartree–Fock treatments unless otherwise noted.

Rotation barriers corresponding to the methyl group were computed via restricted optimizations [38-40], fixing the methyl torsional coordinate, at the MP2/cc-pVDZ level.

The electronic structure program packages Gaussian03 [41] and MOLPRO [42] have been used extensively during this study. The package MAB-ACESII [43] was employed for the methyl rotational barrier computations.

II.1. Geometry optimizations

Similarly to a scheme first employed for glycine [17], the conformers of Thr and aThr determined in this study are numbered by Roman numerals (see Figure 1) and reflect the energy order of the conformers determined at the B3LYP/6-311++G** level.

Initial structures for the geometry optimizations of the conformers of Thr and aThr were generated by replacing the appropriate H atom of the global minimum of serine with a CH₃ group followed by an optimization at the HF/3-21G level. Then, 5 of the 6 torsional angles characterizing threonine, CCOH (carboxyl), CCC=O, CCNH, CCC-O, and CCOH (side chain), were modified systematically by 60 degrees. This resulted in 6⁵ = 7776 initial structures for one diastereomer. Initial geometry optimizations on the 7776 structures were performed for each diastereomer at the inexpensive RHF/3-21G level. This simple level of electronic structure theory was chosen for the prescreening of the conformers as it was widely assumed [1] that the RHF/3-21G PESs of amino acids and peptides are more structured than their counterparts determined at more sophisticated, and thus computationally more demanding levels of electronic structure theory. Further optimizations were executed at the more reliable B3LYP/6-31G*, B3LYP/6-311++G**, and MP2/aug-cc-pVTZ levels. Initial structures for the latter optimizations were the local minima found on the RHF/3-21G PES of Thr and aThr.

Relative energies of the lowest-energy conformers of Thr and aThr, obtained by geometry optimizations at the HF/3-21G, DFT(B3LYP)/6-31G*, DFT(B3LYP)/6-311++G**, and MP2/aug-cc-pVTZ levels, are given in Table 1. Cartesian coordinates of the optimized structures and energies of all the conformers found in this study are provided as Supplementary Material.



Molecular Physics

Table 1. Relative energies $(kJ mol^{-1})$ of the most stable L-threonine and L-allo-threonine
conformers obtained from geometry optimizations performed at the MP2/aug-cc-pVTZ,
DFT(B3LYP)/6-311++G**, DFT(B3LYP)/6-31G*, and RHF/3-21G levels ^[a]

Conformer	MP2/	DFT(B3LYP)/	DFT(B3LYP)/	RHF/
	aug-cc-pVTZ	6-311++G**	6-31G*	3-21G
Thr-I	0.00	0.00	0.00	0.00
Thr-II	2.54	1.34	3.18	4.24
Thr-III	4.29	4.33	7.15	-0.96
Thr-IV	4.41	4.80	1.38	3.54
Thr-V	6.77	5.34	9.07	7.69
Thr-VI		7.30		2.68
Thr-VII		7.86		9.95
Thr-VIII		8.06		11.16
Thr-IX		10.82		24.21
Thr-X		11.34		-0.71
Thr-XI		11.47		4.49
Thr-XII		11.91		14.07
aThr-I	0.00	0.00	0.00	0.00
aThr-II	-1.13	0.64	5.48	-0.30
aThr-III	3.18	4.13	4.27	1.39
aThr-IV	5.79	6.43	8.77	1.87
aThr-V	3.50	7.08	13.65	12.53
aThr-VI		7.23		13.02
aThr-VII		7.30		8.32
aThr-VIII		7.42		14.56
aThr-IX		8.11		7.36
aThr-X		8.21		5.62
aThr-XI		10.01		7.81
aThr-XII		10.10		19.49
aThr-XIII		10.13		0.34

^[a] The relative energies of conformer **aThr-I** with respect to conformer **Thr-I** at the MP2, B3LYP/6-311++G**, B3LYP/6-31G*, and RHF levels is 3.67, 2.20, -1.06, and 2.37 kJ mol⁻¹, respectively.

II.2. Focal-point analysis (FPA)

In order to obtain accurate estimates of the relative energies of the conformers of Thr and aThr with corresponding uncertainties, the FPA approach [15,16] was utilized for both diastereomers. The five lowest-energy structures of Thr and aThr (Figure 1), obtained at the B3LYP/6-311++G** level, were included in this investigation.

Extrapolation of the energies to the complete basis set (CBS) limit at the RHF and MP2 levels was performed, as part of the FPA approach, using the formulas $E_n = E_{\text{CBS}} + A(n+1)\exp(-9\sqrt{n})$ [44] and $\varepsilon_n = \varepsilon_{\text{CBS}} + Bn^{-3}$ [45], respectively. In these formulas *n* is the cardinal number of the augmented, correlation-consistent basis sets aug-cc-pVnZ ($n \in \{3,4\}$), *A* and *B* are parameters, E_n is the RHF energy, and ε_n is the MP2 correlation energy increment, and CBS refers to the complete basis set limit. Energy corrections were treated additively, taking advantage of the fact that the contribution of higher-level electron correlation to the requested relative energies does not change significantly with the size of the basis set. CCSD and CCSD(T) correlation energy increments were calculated using the cc-pVTZ basis set.

From the auxiliary corrections needed to be determined within the FPA approach, the core correction was obtained at the MP2/cc-pCVTZ level as the difference between explicit frozen-core (fc) and all-electron (ae) energy computations. The relativistic contributions to the relative energies were estimated within the Douglas-Kroll (DK) formalism [46], as implemented in MOLPRO, at the MP2(ae)/cc-pCVTZ level. After deemed to be unimportant even at the level of precision of this study, the diagonal Born–Oppenheimer corrections (DBOC) [47] were not computed and thus were completely neglected. Zero-point vibrational energies (ZPVE) were obtained as harmonic and anharmonic correction values at the B3LYP/6-311++G** and B3LYP/6-31G* levels, respectively.

The resulting composite single-point relative energies are shown in Tables 2 and 3 for Thr and aThr, respectively.

Molecular Physics

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Table 2. FPA relative energies and energy increments (δ), all in kJ mol⁻¹, for the 5 lowest-energy conformers of L-threonine^[a]

Energy term	Basis	Thr-I	Thr-II	Thr-III	Thr-IV	Thr-V
RHF	aug-cc-pVDZ	0.00	-3.14	-2.01	7.52	0.42
	aug-cc-pVTZ	0.00	-3.01	-2.11	7.80	0.72
	aug-cc-pVQZ	0.00	-2.99	-2.20	7.80	0.77
	CBS	0.00	-2.99	-2.21	7.79	0.78
δ[MP2]	aug-cc-pVDZ	0.00	4.60	6.25	-2.48	5.05
	aug-cc-pVTZ	0.00	5.36	6.47	-3.43	5.90
	aug-cc-pVQZ	0.00	5.36	6.43	-3.47	5.94
	CBS	0.00	5.36	6.39	-3.49	5.98
δ[CCSD]	cc-pVTZ	0.00	-0.74	-1.38	0.66	-0.93
δ [CCSD(T)]	cc-pVTZ	0.00	0.93	1.35	-1.08	1.19
MP2(ae) – MP2(fc)	cc-pCVTZ	0.00	0.08	0.00	0.04	0.08
Relativistic	cc-pCVTZ	0.00	-0.05	0.00	0.03	-0.04
ZPVE(harm)		0.00	-0.41	-1.05	0.68	-0.72
ZPVE(anharm) – ZPVE(harr	n)	0.00	0.14	0.20	-0.21	0.44
FPA relative energies		0.00	2.32	3.30	4.42	6.77

^[a] All the FPA energy computations were performed employing the fully optimized B3LYP/6-311++G** structures as references. Energy increments (δ) refer to the previous level of theory, MP2 to RHF, CCSD to MP2, and CCSD(T) to CCSD. The abbreviations (fc) and (ae) show that the correlated-level electronic structure computations were done with the frozen core approximation or with all electrons, respectively. The ZPVE(harm)s (harmonic zero-point vibrational energies) correspond to B3LYP/6-311++G** harmonic frequencies. The ZPVE(anharm)s (anharmonic zeropoint vibrational energies) were obtained at the B3LYP/6-31G* level based on quartic normal coordinate force fields and second-order vibrational perturbation theory (VPT2).

Energy term	Basis	aThr-I	aThr-II	aThr-III	aThr-IV	aThr-V
RHF	aug-cc-pVDZ	0.00	-8.53	2.19	-3.63	4.70
	aug-cc-pVTZ	0.00	-8.55	2.22	-3.17	4.66
	aug-cc-pVQZ	0.00	-8.42	2.40	-2.98	4.88
	CBS	0.00	-8.41	2.43	-2.95	4.91
δ[MP2]	aug-cc-pVDZ	0.00	6.46	0.47	7.56	-1.77
	aug-cc-pVTZ	0.00	7.94	1.18	9.11	-0.66
	aug-cc-pVQZ	0.00	8.25	1.41	9.39	-0.29
	CBS	0.00	8.48	1.57	9.60	-0.01
δ[CCSD]	cc-pVTZ	0.00	-1.54	-0.68	-2.32	0.26
δ [CCSD(T)]	cc-pVTZ	0.00	2.14	0.53	1.89	0.89
MP2(ae) – MP2(fc)	cc-pCVTZ	0.00	-0.01	0.04	0.08	-0.04
Relativistic	cc-pCVTZ	0.00	-0.05	-0.03	-0.06	-0.02
ZPVE(harm)		0.00	-1.40	-0.53	-0.85	-0.91
ZPVE(anharm) – ZPVE(harm)		0.00	-0.01	0.09	-0.02	0.13
FPA rel. energies		0.00	-0.80	3.42	5.37	5.21

Table 3. FPA relative energies and energy increments (δ), all in kJ mol⁻¹, for the 5 lowest-energy conformers of L-allo-threonine.^[a]

^[a] See footnote [a] to Table 2. The relative energy of conformer **aThr-I** with respect to conformer

Thr-I is 3.07 kJ mol^{-1} .

II.3. Spectroscopic parameters

For all local minima, quadratic force constants were computed at the B3LYP/6-311++G** level using the B3LYP/6-311++G** optimized structures, thus avoiding the nonzero-force dilemma [48]. For the five lowest-energy conformers of Thr and aThr quartic force fields in normal coordinate space have been determined at the B3LYP/6-31G* level, again at the fully optimized B3LYP/6-31G* structure. The related harmonic and anharmonic vibrational fundamentals of Thr and aThr are reported in Tables 4 and 5, respectively. No scaling of the force fields or of the resulting vibrational wavenumbers has been attempted. The anharmonic vibrational fundamentals were obtained through second-order vibrational perturbation theory (VPT2) [49].

The optimized structures determine the equilibrium rotational constants, while the quadratic and cubic force fields yield the equilibrium quartic and sextic centrifugal distortion constants in the *A*-reduced representation. The anharmonic force fields determined also allow the calculation of vibrationally averaged ground-state rotational constants. For the five lowest-energy Thr and aThr conformers these spectrosopic constants are reported in Tables 6 and 7, respectively.

The ¹⁴N nuclear quadruple coupling constants, resulting from the non-spherical distribution of the nuclear charge, have been determined at the B3LYP/6-311++G** level.

Table 4. Harmonic vibrational fundamentals (ω), their VPT2 anharmonic corrections (Δv), and double-harmonic vibrational intensities (*I*) of the 5 lowest energy conformers of L-threonine^[a]

		Thr-I			Thr-II			Thr-III			Thr-IV	7		Thr-V	
number	ω	Δv	Ι	ω	Δv	Ι	ω	Δv	Ι	ω	Δv	Ι	ω	Δv	Ι
1	3819	-177	46.8	3742	-186	64.9	3762	-188	84.1	3705	-195	131.3	3758	-187	78.7
2	3595	-181	15.3	3708	-199	91.8	3713	-196	60.9	3600	-182	16.1	3718	-198	84.5
3	3495	-108	11.1	3582	-181	12.1	3612	-183	21.9	3518	-129	1.1	3592	-181	11.8
4	3455	-262	277.5	3497	-191	6.2	3516	-142	18.8	3467	-259	264.4	3511	-105	4.8
5	3114	-142	18.4	3115	-142	18.9	3109	-148	23.5	3114	-143	15.6	3113	-143	18.3
6	3098	-141	28.9	3109	-143	24.4	3095	-135	35.2	3086	-113	26.6	3107	-143	24.9
7	3055	-131	9.9	3085	-139	8.3	3078	-130	2.0	3055	-138	5.1	3092	-141	5.7
8	3041	-119	7.7	3040	-133	13.2	3023	-160	23.0	3034	-144	29.1	3038	-134	11.9
9	3033	-132	13.5	2959	-106	38.3	3000	-137	19.8	3021	-165	21.4	2964	-109	39.5
10	1824	-31	324.4	1800	-31	296.8	1808	-33	304.2	1808	-31	287.4	1811	-29	321.0
11	1651	-50	32.9	1662	-31	39.5	1642	-58	77.4	1658	-48	38.1	1659	-57	36.8
12	1503	-42	4.4	1502	-36	3.2	1501	-73	4.8	1502	-51	9.7	1502	-39	4.0
13	1484	-9	6.7	1484	-20	6.0	1489	-39	6.0	1491	-48	5.5	1483	-19	3.6
14	1430	-34	6.3	1441	-46	54.3	1431	-30	55.5	1445	-39	16.5	1439	-47	44.4
15	1418	-40	427.2	1425	-32	4.4	1416	-44	23.4	1419	-45	232.8	1409	-32	29.7
16	1409	-34	9.6	1404	-34	23.6	1401	-17	5.6	1409	-33	215.9	1400	-36	0.9
17	1387	-36	4.9	1375	-5	20.3	1370	-34	11.6	1394	-39	21.4	1377	-5	3.6
18	1359	-35	8.0	1339	-19	31.8	1337	-4	24.0	1371	-33	41.7	1333	-14	53.6
19	1280	-32	57.0	1311	-11	81.1	1302	-30	3.1	1311	-30	18.0	1309	-26	59.6
20	1276	-37	0.4	1265	-39	7.5	1258	-31	21.0	1270	-23	2.5	1289	-29	14.8
21	1209	-40	21.5	1226	-33	20.0	1221	-35	49.2	1220	-46	23.6	1229	-18	17.5
22	1197	-37	9.7	1158	-34	75.1	1162	-33	112.9	1192	-36	9.6	1163	-37	213.1
23	1151	-29	24.6	1136	-31	167.6	1136	-32	154.5	1140	-32	8.9	1138	-31	43.8
24	1084	-24	14.4	1113	-40	54.7	1104	-28	27.3	1106	-31	50.5	1110	-37	7.7
25	1052	-18	55.9	1074	-29	12.9	1076	-30	52.8	1090	-31	79.6	1072	-31	14.8
26	1017	-24	11.5	1052	-21	35.6	1026	-22	25.2	1045	-21	5.2	1050	-19	31.7
27	984	-35	88.3	958	-41	46.6	937	-28	0.7	968	-32	23.1	932	-41	16.9
28	909	-24	54.3	925	-22	35.3	892	-45	77.0	903	-41	84.1	921	-23	88.3
29	878	-47	103.5	872	-29	38.8	869	-24	23.9	872	-40	83.5	868	-20	36.4
30	854	-26	51.0	854	-14	98.7	830	-27	75.8	837	-52	61.4	831	-21	92.2
31	822	-18	13.7	742	-19	37.1	728	-14	28.6	799	-18	26.7	752	-16	24.0
32	/51	-15	6.7	666	-16	17.3	659	-3	34.0	/54	-10	3.1	643	-20	58.8
33	650	-11	8.9	610	-41	108.9	630	-31	58.1	609	-29	18.0	595	-46	56.3
34	559	-12	9.3	601	-18	125.4	575	-41	163.9	575	-19	117.5	586	-19	160.0
35	532	-23	3.9	543	-11	1.0	545	-12	22.0	549	-11	3.8	548	-11	6.9
36	453	-50	/.9	469	-1	8.8	4/6	-10	28.5	491	-5	7.3	467	0	10.6
3/	403	-11	88.0	385	-6	21.8	450	-3	4.6	456	-6	3.1	396	-8	6./
38	368	-17	34.8	366	-3	6.3	349	-4	3.3	377	-5	7.8	365	-3	9.4
<i>3</i> 9	336	-7	24.7	307	-/	4.1	301	-3	0.5	337	-11	18.2	309	-8	8.3
40	510	-2	5./ 12.6	290	-21	1.4	270	-8	0.0	298	-29	13.0	291	-2	2.5
41	251	-2	12.0	207	-3 F	5.2 0.5	240	-12	0.9	251	-10	5.5	260	-1	1.5
42	225	-19	1.2	230	5	0.5	215	-25	11.8	245	-12	5.0	221	-4	0.6
45	1/9	-1	5.4 2 1	1/1	-1	1.0	181	-1	0.5	203	-11	ð.U 2 0	102	-1	0.7
44 15	80 51	-5	5.1 5.7	84 47	0	5.5	ð1 60	2	1.2	111 67	-9	5.U	80 41	-2	3.3 1.6
45	51	-4	5.7	4/	-2	0.9	69	/	2.2	0/	-9	1.2	41	-3	1.6

^[a] Harmonic frequencies and intensities were calculated at the B3LYP/6-311++G^{**} level, while anharmonic corrections correspond to the B3LYP/6-31G^{*} level of theory. Frequencies and intensities are given in cm⁻¹ and in km⁻¹, respectively.

1 2 3 4 5 6 7 8 9 1 1 1

Table 5. Harmoni	ic vibrationa	l fundamen	tals	(@)	, the	ir `	VPT2 a	nharmon	ic correction	s (2	1v), and
double-harmonic	vibrational	intensities	(<i>I</i>)	of	the	5	lowest	energy	conformers	of	L-allo-
threonine ^[a]											

9 10			aThr-	ĺ		aThr-I	I		aThr-I	II		aThr-I	V		aThr-	V
11 12	number	ω	Δv	Ι	ω	Δv	Ι	ω	Δv	Ι	ω	Δv	Ι	ω	Δv	Ι
13	1	3690	-197	191.6	3751	-186	70.1	3789	-182	38.5	3752	-190	56.6	3837	-175	35.5
14	2	3596	-180	12.5	3718	-196	67.3	3586	-182	14.0	3740	-186	85.5	3574	-182	19.3
15	3	3506	-125	1.6	3589	-182	13.4	3493	-103	9.8	3595	-182	12.3	3507	-100	1.4
16	4	3464	-263	268.4	3512	-188	6.8	3455	-265	279.7	3505	-131	4.9	3453	-251	273.3
17	5	3114	-142	16.0	3111	-142	20.3	3128	-141	7.0	3110	-142	20.6	3112	-143	15.5
18	6	3101	-141	27.5	3096	-137	36.5	3095	-137	25.1	3094	-128	32.1	3092	-137	22.6
19	7	3041	-140	7.3	3076	-138	9.1	3043	-106	19.6	3066	-133	7.3	3049	-132	20.6
20	8	3034	-117	15.4	3068	-130	1.6	3035	-116	24.0	3059	-136	13.2	3037	-128	5.6
21	9	2937	-85	50.2	3029	-101	13.8	3032	-128	14.0	3028	-151	13.8	3031	-121	15.2
22	10	1808	-21	307.4	1804	-33	299.0	1821	-28	305.2	1780	-34	279.2	1834	-30	338.2
23	11	1660	-45	32.5	1672	-8	40.7	1653	-45	35.2	1643	-80	39.6	1668	-33	45.6
24	12	1501	-37	5.5	1503	-100	5.0	1507	-69	3.5	1505	-68	5.9	1501	-42	10.3
25	13	1488	-6	4.0	1489	17	5.1	1490	11	13.0	1493	-40	10.4	1497	-43	3.5
26	14	1446	-54	11.0	1429	-30	45.2	1429	-46	174 .6	1444	-39	31.2	1426	-58	128.5
27	15	1416	-52	435.3	1425	-35	26.8	1415	-41	158.8	1412	-14	14.9	1417	-20	232.0
28	16	1405	-30	61.4	1412	-19	13.8	1408	-30	107.8	1395	-54	19.3	1405	-46	30.6
29	17	1385	-38	12.3	1377	-40	7.6	1400	-36	42.5	1394	-41	31.4	1384	-33	5.3
30	18	1369	-5	0.3	1330	-28	36.2	1352	-34	14.5	1343	-32	12.7	1364	-39	14.6
31	19	1315	-1	76.0	1295	-27	16.1	1316	-34	7.6	1317	-34	9.3	1317	-41	1.5
32	20	1269	-32	4.4	1263	-33	9.6	1267	-39	4.5	1285	-35	2.9	1260	-34	11.6
33	21	1216	-42	36.9	1215	-36	31.0	1204	-41	27.4	1212	-34	10.7	1228	-36	14.4
34	22	1189	-28	4.8	1173	-35	14.3	1194	-32	19.2	1147	-37	243.0	1192	-34	25.8
35	23	1152	-31	15.1	1130	-34	250.5	1141	-30	33.6	1143	-30	129.4	1125	-30	34 .9
36	24	1111	-31	26.0	1111	-28	98.6	1091	-27	34 .9	1090	-26	11.2	1109	-28	79.0
37	25	1084	-32	57.0	1072	-29	18.5	1074	-25	8.9	1080	-34	19.9	1063	-27	4.7
38	26	1056	-30	10.9	1027	-28	17.7	1035	-21	42.3	1045	-22	32.6	1021	-29	37.4
39	27	975	-28	26.3	958	-39	30.9	973	-36	106.9	943	-23	7.8	964	-34	109.8
40	28	919	-34	78.2	921	-20	48.2	915	-26	46.6	901	-42	32.5	930	-26	42.1
40	29	884	-29	63.6	850	-41	131.1	880	-45	110.3	829	-52	136.2	883	-56	72.8
42	30	847	-62	18.9	828	-18	4.7	860	-23	38.2	816	-23	25.2	867	-25	25.9
42	31	840	-14	102.8	723	-21	19.4	813	-17	8.7	771	-17	34.4	829	-15	8.9
43 ΔΔ	32	736	-12	5.8	650	-13	15.8	754	-14	8.2	709	-9	9.6	731	-10	17.0
45 45	33	631	-20	126.3	644	-8	78.3	607	-9	0.6	629	-30	99.3	648	-13	16.6
46	34	591	-9	3.9	570	-64	20.4	552	-34	11.0	569	-49	207.7	623	-10	8.5
40 //7	35	571	-8	5.7	549	-21	152.0	524	-27	11.6	531	-9	19.6	495	-7	0.6
47 18	36	485	-1	15.6	457	-5	25.9	476	-15	20.1	498	-5	6.9	424	-5	11.7
40	37	406	-10	1.6	414	-2	4.0	437	-9	102.2	391	-2	0.9	362	-10	12.1
49 50	38	357	-10	10.2	362	-5	7.2	366	-18	31.0	358	-6	26.1	325	-32	5.6
50	39	347	-32	25.7	302	-10	5.1	349	-6	9.7	324	-3	14.7	306	-7	38.7
51	40	331	-7	3.7	255	-19	1.7	331	-3	8.0	269	-4	3.7	280	3	73.4
52	41	302	-13	10.6	249	-2	3.2	241	-1	3.0	241	-7	0.2	272	1	25.4
00 54	42	235	-18	6.2	228	-18	8.6	229	-1	5.1	230	-6	3.6	248	-11	0.3
04 55	43	208	-7	6.7	166	0	1.9	199	0	5.5	187	-5	3.6	174	-1	10.5
00 50	44	94	-2	0.9	82	-1	6.0	86	-2	4.1	120	-6	3.5	86	-7	3.9
00 57	45	71	-8	2.0	62	1	0.9	47	-4	5.1	45	-5	0.6	80	-4	2.2
58	^[a] See	footnote	e [a] to t	table 4.												

^[a] See footnote [a] to table 4.

III. CONFORMATIONAL ANALYSIS

III.1. Preliminary tests

The method described in section II.1 for studying the conformational space of Thr and aThr systematically was tested on the neutral amino acids glycine (Gly) and L-alanine (Ala), where the number of conformers are well established as a result of previous high-level first-principles studies [17-20].

At the RHF/3-21G level, only 6 of the 8 and 11 of the 13 conformers were found for Gly and Ala, respectively. The RHF/3-21G optimizations failed to yield the high-energy conformers **Gly-VIIp** and **Gly-VIIIn** for Gly. The most stable conformers **{Gly-Ip,Gly-IIn**} [4] were obtained {28,49} times out of a total of 216 initial structures. Using the same conformational search but this time at the RHF/6-31G** level, all Gly conformers were found. These observations show the possible dangers of using RHF/3-21G optimizations for prescreening the possible conformers of amino acids (and most likely peptides). It is comforting, nevertheless, that RHF/3-21G optimizations always missed only the highest-energy conformers.

The discrepancies obtained for the amino acids Gly and Ala based on the initial prescreening of the conformers at the RHF/3-21G level led us to an extended study of the role of initial geometry optimizations. Taking the Thr conformers determined at the B3LYP/6-311++G** level, preliminary optimizations at the RHF/3-21G, RHF/3-21G**, and RHF/3-21+G** levels were done, continued by B3LYP/6-311++G** level optimizations. It was found that the final B3LYP/6-311++G** structures were often different from the initial B3LYP/6-311++G** structures when using the different basis sets for the preoptimizations at the RHF level. Thus, the conformers found on the PES corresponding to the final optimization level depend somewhat on the level of the initial optimizations. Since the conformers found by only one of the methods were of high relative energy (above 15 kJ mol⁻¹ in all cases), it is safely concluded that this effect is due to the fine structure of the high-energy regions of the different PESs. While this observation is certainly somewhat disturbing, it seems to be not relevant for the low-energy conformers, of highest relevance for practical applications.

III.2. Initial optimizations

Using the inexpensive RHF/3-21G method, 68 and 66 conformers were found for Lthreonine and L-allo-threonine, respectively. When B3LYP/6-311++G** geometry optimizations were performed, using the RHF/3-21G conformers as initial structures, some of the higher-energy RHF/3-21G conformers disappeared, thus finally 56 and 61 conformers were found this way for Thr and aThr, respectively. Of the 7776 initial structures for each diastereomer, {202, 455, 328, 78, 146} and {220, 422, 534, 336, 131} ended up as {**Thr-I**, **Thr-II**, **Thr-III**, **Thr-IV**, **Thr-V**} and {**aThr-I**, **aThr-II**, **aThr-II**, **aThr-IV**, **aThr-V**}, respectively. This clearly shows that these lowest-energy conformers have substantial catchment regions. The smallest region corresponds to **Thr-XV** with only 12 initial structures ending up at that conformer.

III.3. Comparison with the study of Zhang and Lin [50]

The recent investigation of Zhang and Lin [50] is similar to our work in many respect. An important distinction is that in that paper only the L-threonine diastereomer was considered. For L-Thr, Zhang and Lin found 71 conformers at the B3LYP/6-311++G** level, while, as stated above, we found only 56 conformers. This result is the more curious as their grid for the initial optimization was somewhat less systematic, it was based partially on chemical intuition, and they included much less (only 1296) initial points than the grid corresponding to the present study contains (7776). The difference is due to the different theoretical levels used for the initial optimizations, and in this case show that the RHF/3-21G PES is less structured (68 conformers found) than the PES obtained at the B3LYP/6-311++G** level (71 conformers found). Overall, Zhang and Lin obtained 16 conformers which were not found and missed one conformer which was found in the present study. Since the dependence of the results of the conformational search on the method of initial optimization seems to be only relevant for higher-energy conformers, it is important to stress that all conformers of L-Thr up to a relative energy of 19 kJ mol⁻¹ agree in the two studies.

IV. STRUCTURES

The MP2 and DFT(B3LYP) levels of electronic structure theory yield equilibrium structures which may suffer from different problems. It is the intramolecular basis set superposition error (BSSE) that can be quite significant at the MP2 level, especially when smaller basis sets are used, hindering the determination of truly accurate equilibrium structures. By design, this is much less of a problem at the DFT levels. The usual functionals of DFT theory, like B3LYP, suffer, however, from the inability to describe dispersion effects. Therefore, it is comforting to note that the RHF, DFT(B3LYP), and MP2 levels produce the same minima for the five lowest-energy conformers of Thr and aThr. This means that the structures predicted for the lowest-energy conformers are as dependable as can be expected at these levels of electronic structure theory.

It is of fundamental interest to investigate which intramolecular factors (electronic effects including exchange, electrostatic, and hyperconjugative interactions, steric repulsion, H-bonding capabilities, and dispersive interactions) lead to stabilization of the many possible conformers of Thr and aThr. Most of these effects are operative in stabilizing the configurations resulting from rotations around the appropriate single bonds of these molecules.

Threonine is a representative of the three hydroxyamino acids whereby the OH group in the side chain is capable of strong intramolecular H-bonds. The subsequent increase in the number of low-energy conformations has been proved in this study. The presence of NH, carboxylic OH, and side-chain OH H-bond donors and N, C=O, carboxylic OH, and sidechain OH H-bond acceptors allow for the existence of the following types of H-bonds: (a) bifurcated H-bonds between NH₂ and C=O, similar to that found in the most stable conformers of glycine [4,17] and alanine [18,20]; (b) simple H-bonds, like N-H to side-chain OH, carboxylic O–H, and C=O; (c) carboxylic O–H to C=O, side-chain O–H, and NH₂; and (d) side-chain O–H to carbonyl oxygen, nitrogen, and carboxylic OH.

The structure of the global minimum, **Thr-I**, is stabilized by strong OH[…]N, OH[…]O=C and weaker NH[…]O H-bonds, whereby the COOH, NH₂, and the side-chain OH functional groups are interconnected via the three intramolecular H-bonds, while the –COOH group is in an energetically unfavorable trans conformation. In the case of **Thr-II**, although the –COOH group is now in the favorable cis conformation, this substantial energy gain, on the order of 20 kJ mol⁻¹, is not able to compensate for the energy difference between the H-bonds in **Thr-I** and **Thr-II**. **Thr-II** exhibits weaker NH[…]O=C and OH[…]N H-bonds. The H-bond arrangements in the most stable conformers of Thr are completely different from those for

Molecular Physics

glycine and α -alanine, where the global minima have a cis –COOH arrangement with a bifurcated (and thus less strong) NH^{...}O=C H-bonds, while the second lowest energy conformers have a trans –COOH arrangement and strong OH^{...}N H-bonds. This shows, and this conclusion is similar to that obtained in a MW study on the conformers of cysteine [51], that the presence of a polar side chain has a major effect on the conformational preferences of amino acids.

In the case of L-allo-threonine, the global minimum, **aThr-I**, is stabilized, very similarly to **Thr-I**, by strong OH^{...}O=C and OH^{...}N H-bonds, while the –COOH group is again in the less favorable trans conformation. As to **aThr-II**, the –COOH group is in a cis conformation, while OH^{...}N and NH^{...}O=C H-bonds can be found.

A number of different secondary structural effects characterize the other conformers. Among them one can find the OH^{...}NH^{...}O=C structural motif in **Thr-III** whereby the same NH group is included in a H-bond chain. In **Thr-IV**, the stability is due to the OH^{...}O=C and OH^{...}N bonds. While **aThr-III** has the same H-bonds as **Thr-I**, the change in chirality causes the methyl group to be in a highly unfavorable position. Furthermore, **aThr-IV** is stabilized by a sequential NH^{...}OH^{...}O=C H-bond arrangement involving NH^{...}OH and OH^{...}O=C Hbond, including the same side-chain OH group.

In all five low-energy Thr and aThr conformers, the methyl group is found in a staggered position with respect to the β -carbon atom. One can compute straightforwardly the pure (vibrationless) internal rotation barrier of the CH₃ group in Thr and aThr. This was done in the present study at the MP2(fc)/cc-pVDZ level. The rotation barriers determined for the methyl group in Thr and aThr are between 1100 and 1300 cm⁻¹. Furthermore, note that for the three lowest-energy conformers of alanine [20], the methyl rotation barrier is also about 1200 cm⁻¹, computed, as part of this study, at the same level of theory. The characteristic increase of the rotation barrier in these natural amino acids with respect to ethane, where the barrier is 1140 cm⁻¹ at this level [16], originates most probably from increased hyperconjugation, due to the presence of CC and CX (X = O, N) bonds. Note also that the internal rotation barrier of the methyl group can be substantially smaller than the barriers reported; for example, it is only about 400 cm^{-1} in acetaldehyde [40] and much smaller in toluene. Observation of transitions between the energy levels under the slightly different barriers, aimedcompounded by different reduced masses due to the structural differences of the conformers, should help identification of the low-energy conformers of Thr and Ala, as well.

Note, finally, that the only threonine conformer considered by Lakard [52] in a study of the vibrational fundamentals of hydroxyamino acids at the harmonic level, though the figure included in that paper is not particularly instructive, is definitely not the global minimum and it is not even among the five most stable conformers.

V. RELATIVE ENERGIES

As observed repeatedly for amino acids, the introductory Hartree-Fock level of electronic structure theory, independently of the basis set used, is unable to yield the correct relative energies of the conformers of Thr and aThr (see Tables 2 and 3). At the extrapolated RHF/CBS level, **Thr-II** and **Thr-III** both have lower energies than **Thr-I**, while **Thr-IV** has a very high relative energy. These RHF/CBS results clearly show the inadequacy of this level of theory in predicting relative conformational energies for this class of compounds due to its inadequacy in describing fine electrostatic and H-bonding effects. The MP2 level of theory stabilizes Thr-IV substantially, while it destabilizes all the other conformers considered. For Thr, the explicit MP2/aug-cc-pVQZ and the extrapolated MP2/CBS relative energies deviate at most by 0.04 kJ mol⁻¹, an excellent agreement indeed, contributing greatly to the overall accuracy of the FPA relative conformational energies. For aThr, the extrapolation contributions are larger by almost an order of magnitude but they are still surprisingly small on an absolute scale; consequently, the error due to MP2 extrapolation remains a small factor of the overall estimated precision of the FPA relative energies. Compared to δ [MP2], the δ [CCSD] and δ [CCSD(T)] energy increments are relatively small though can affect relative energies by at most 2 kJ mol⁻¹. Overall, it seems safe to attribute about 0.7 kJ mol⁻¹ accuracy to the CCSD(T)/CBS limit FPA relative energies. Based on the CCSD – HF and CCSD(T) – CCSD increments, the relative energy corrections due to electron correlation effects beyond CCSD(T) are estimated to be considerably less than 0.5 kJ mol⁻¹, thus these missing corrections should not affect significantly the CCSD(T)/CBS limit FPA relative energies and their uncertainty estimates.

The DFT(B3LYP) level performs reasonably well, the FPA relative energies, including the ZPVE corrections, are quite similar to the B3LYP/6-311++ G^{**} relative energies. This shows again the utility of the DFT approach for conformational energy studies.

Interestingly, but again in line with our study on the conformers of Pro [2], the relative energies are barely affected by consideration of the core-core and core-valence correlation

Molecular Physics

and the relativistic effects. Even the largest change is smaller than 0.1 kJ mol⁻¹. This is comforting and makes accurate relative energy predictions for the conformers of the building blocks of biopolymers considerably less expensive.

ZPVE corrections are substantial and can affect relative energies on the order of 2 $kJ mol^{-1}$. It is also of general interest to compare harmonic and anharmonic ZPVE corrections to the relative energies. The anharmonic contributions to relative energies of the Thr conformers are on the order of 0.5 $kJ mol^{-1}$. This is significant but not substantial given the other sources of error in the present computations contributing to the final FPA relative energy estimates.

The above statements nearly stand for aThr, as well. The RHF level of theory gives relative energies with considerable error, underestimating the relative energies of **aThr-II** and **aThr-IV**. The MP2 increment compensates most of this error by destabilizing these conformers. Compared to MP2, ∂ [CCSD] and ∂ [CCSD(T)] energy corrections are fairly small yet can affect relative energies by over 2 kJ mol⁻¹. Core correlation and relativistic effects are on the order of 0.01 kJ mol⁻¹, while ZPVE corrections can reach nearly 1.5 kJ mol⁻¹.

In the case of aThr, the B3LYP/6-311++ G^{**} level gives a different relative energy order than the FPA approach. In the cases of **aThr-I** and **aThr-II**, this is due to the ZPVE corrections, which shows the importance of including ZPVE for conformational studies. It is interesting to find that the FPA relative energies give the same relative energy order as the MP2/aug-cc-pVTZ level for the optimized structures.

Since the FPA energy difference between **aThr-I** and **aThr-II** is only 0.8 kJ mol⁻¹ and the assumed uncertainty of the present FPA relative energies is ± 1 kJ mol⁻¹, even the present extensive computations are insufficient to determine the lowest-energy conformer of aThr. Similarly, the small FPA energy difference between **aThr-IV** and **aThr-V** does not allow an unambiguous determination of their energy order.

In order to estimate the uncertainty on the FPA energies resulting from the choice of reference structures, MP2/aug-cc-pVTZ//B3LYP/6-311++G** relative energies were compared to MP2/aug-cc-pVTZ//MP2/aug-cc-pVTZ energies. The average effect is 0.1 and 0.3 kJ mol⁻¹ for Thr and aThr, respectively, suggesting that the DFT reference structures chosen are appropriate for the purposes of the present study.

VI. VIBRATIONAL FUNDAMENTALS

Many vibrational fundamentals are found to be characteristic for some of the conformers of Thr and aThr (*cf.* Tables 4 and 5). One of the most useful fundamentals characterizing the conformers is the intense streching vibrational motion of the carboxyl group, ω_{10} , at about 1 800 cm⁻¹. The spread in ω_{10} is substantial, from 1780 (**aThr-IV**) to 1834 cm⁻¹ (**aThr-V**). The anharmonic corrections alter this picture only slightly as all the VPT2 corrections are between 28 and 34 cm⁻¹. When the C=O group is not involved in H-bonding, *e.g.*, for **Thr-V**, the fundamental is at a high wavenumber, while a strong H-bond between C=O and the side-chain OH results in a substantially lower wavenumber, as for **aThr-IV**. The exact wavenumber of this fundamental should also depend on the cis *vs* trans arrangement of the carboxylic group, though this effect cannot be seen clearly from the data of Tables 4 and 5.

Other simple nuclear motions, such as OH stretching (ω_1 , ω_2) and NH stretching (ω_3 , ω_4), should also be discussed. The OH stretching motion characterizes conformers by intensity ratios (I_1/I_2) varying from 0.7 to 15.3, and by frequency differences ($\omega_1 - \omega_2$) varying between 12 and 263 cm⁻¹, with anharmonic corrections altering only slightly these differences. Correlation between the H-bond structure and the OH band origins cannot be so easily used for identification purposes as ω_{10} . Nearly the same stands for the NH stretching motion. The NH stretches also characterize conformers by their relative intensities (I_3/I_4) and frequency differences ($\omega_3 - \omega_4$). Interestingly, in most cases the $\omega_3 - \omega_4$ frequency differences are considerably modified by the anharmonic corrections.

Various other fundamentals, including ω_{14} , ω_{15} , ω_{18} , ω_{21} , ω_{22} , ω_{24} , and ω_{26} , can also be found where the intensities or the wavenumbers are characteristic of the different conformers. Nevertheless, in these cases the use of this information to identify conformers based on the availability of the infrared spectrum, for example in a matrix isolation study, is not straightforward due to the presence of nearby fundamentals of similar energies.

VII. ROTATIONAL SPECTRA

There are three possible routes to identify conformers via rotational spectroscopy if results from related electronic structure computations are available. The most obvious route is based on the comparison of measured effective rotational constants with equilibrium or vibrationally averaged computed rotational constants. The second route uses the information contained in computed dipole moments and selection rules and thus allows interpretation of measured relative intensities of rotational lines. In the case of amino acids a third route is also open, namely one can use computed ¹⁴N nuclear quadruple coupling constants for the identification of a conformer.

At the B3LYP/6-311+++G^{**} level, the rotational constants corresponding to the optimized equilibrium structures are accurate enough to be useful to deduce the presence of most of the conformers when evaluating experimental data of microwave and millimeterwave spectroscopic studies. Furthermore, some of the conformers (*e.g.*, **Thr-I** and **Thr-IV**, as well as **aThr-I**) have substantial dipole moments thus helping the observation of the related rotational transitions. Nevertheless, given the limited accuracy of the rotational constants obtained at the B3LYP and MP2 levels, in certain cases it might be quite difficult to distinguish the conformers of Thr and aThr based on this information alone. This holds, for example, for **Thr-II** and **Thr-V**. Unfortunately, in this case the ¹⁴N nuclear quadruple coupling constants are also rather similar, hindering further the unequivoval identification of these conformers. In contrast, while the rotational constants of **Thr-II** and **Thr-III** are rather similar, in this case the ¹⁴N nuclear quadruple coupling constants allow for an easy distinction between the measured spectroscopic data of the two conformers.

The relatively accurate rotational and quartic centrifugal distortion (QCD) constants determined should facilitate the observation of the low-energy conformers of L-Thr and L-aThr, especially **Thr-I** and **aThr-I**. The sextic centrifugal distortion constants are so small (they are given in mHz units in Tables 6 and 7) that it is unlikely that they could be determined experimentally with any reasonable certainty. Their smallness also means that the experimental spectrum could straightforwardly be fitted with just the effective rotational and quartic centrifugal distortion constants.

Table 6. Equilibrium rotational constants (A_e , B_e , C_e), their vibrational corrections (ΔA , ΔB , ΔC) leading to ground-state rotational constants A_0 , B_0 , and C_0 , A-reduced quartic (Δ_J , Δ_K , Δ_{JK} , δ_J , δ_J , δ_K) and sextic (Φ_J , Φ_K , Φ_{JK} , Φ_{KJ} , ϕ_j , ϕ_k , ϕ_{jk}) centrifugal distortion constants, ¹⁴N nuclear quadrupole coupling tensor elements (χ_{aa} , χ_{bb} , χ_{cc}), and total dipole moments (μ_{total}) of the five lowest-energy conformers of L-threonine^[a]

	Thr-I	Thr-II	Thr-III	Thr-IV	Thr-V
Ae	3 201.77	2 865.57	3 128.28	2 679.22	2 882.14
ΔA	-32.91	-24.61	-38.07	-27.82	-25.09
Be	1 498.69	1 587.52	1 476.30	1 749.67	1 549.45
ΔB	-25.80	-13.55	-14.75	-17.45	-17.18
$C_{\rm e}$	1 256.81	1 194.30	1 294.91	1 354.93	1 222.85
ΔC	-8.64	-10.49	-9.29	-10.67	-6.24
Δ_J	0.258	0.270	0.172	0.211	0.300
Δ_K	-0.017	-0.142	-0.118	0.192	-0.526
Δ_{JK}	0.404	0.269	0.723	0.006	0.697
δ_J	0.065	0.052	0.020	0.035	0.069
δ_{K}	0.155	0.620	-1.217	-0.028	-0.727
\varPhi_J	-0.15	-0.10	0.08	-0.02	-0.15
Φ_{K}	20.45	13.57	-1.49	-0.20	61.88
Φ_{JK}	6.61	4.77	-4.70	0.10	26.28
Φ_{KJ}	-27.18	-18.09	5.05	-0.47	-87.56
ϕ_{j}	-0.08	-0.04	0.02	0.00	-0.04
ϕ_k	70.70	27.48	-59.03	1.89	138.08
ϕ_{jk}	-0.36	-1.23	2.03	-0.06	-1.54
Xaa	-4.08	-4.83	-0.94	-4.51	-4.80
Хbb	2.12	2.92	3.24	2.66	2.84
Xcc	1.96	1.90	-2.30	1.85	1.95
$\mu_{ ext{total}}$	4.37	2.36	3.02	5.14	3.00

Table 6. cont.

^[a] The equilibrium rotational and quartic centrifugal distortion constants, given in MHz and kHz, respectively, correspond to the parent isotopologue, and were determined at the B3LYP/6-311++G** level. Vibrational corrections and sextic centrifugal distortion constants, given in MHz and mHz, respectively, were determined from anharmonic force fields obtained at the B3LYP/6-31G* level. The nuclear quadrupole coupling tensor elements given correspond to the ¹⁴N nucleus (in MHz). Dipole moments are given in debye.

Je he pa Vibrational κ ad mHz, respective. JSLYP/6-31G* level. pond to the ¹⁴N nucleus (in Mt

Table 7. Equilibrium (A_e , B_e , C_e) rotational constants, their vibrational corrections (ΔA , ΔB , ΔC) leading to ground-state rotational constants A_0 , B_0 , and C_0 , A-reduced quartic (Δ_J , Δ_K , Δ_{JK} , δ_J , δ_K) and sextic (Φ_J , Φ_K , Φ_{JK} , Φ_{KJ} , ϕ_j , ϕ_k , ϕ_{jk}) centrifugal distortion constants, ¹⁴N nuclear quadrupole coupling constants (χ_{aa} , χ_{bb} , χ_{cc}), and total dipole moments (μ_{total}) of the five lowest-energy conformers of L-allo-threonine^[a]

	aThr-I	aThr-II	aThr-III	aThr-IV	aThr-V
$A_{ m e}$	3 076.01	3 019.18	2 773.73	2 738.22	3 059.09
ΔA	-25.24	-29.23	-29.65	-24.31	-28.66
Be	1 639.65	1 464.42	1 702.83	1 627.34	1 483.53
ΔB	-15.83	-9.65	-15.32	-17.21	-14.60
$C_{ m e}$	1 117.74	1 316.22	1 341.31	1 417.04	1 336.00
ΔC	-9.71	-16.16	-13.67	-15.98	-14.96
Δ_J	0.102	0.278	0.250	0.277	0.244
Δ_K	0.248	0.084	0.157	0.909	0.055
Δ_{JK}	0.027	0.170	0.438	0.226	0.190
δ_J	0.032	0.048	0.060	0.016	0.030
δ_{K}	0.170	2.004	-1.337	-0.661	1.386
$arPhi_J$	0.00	-0.13	0.03	-0.11	0.01
Φ_{K}	-0.37	28.67	1.20	7.30	18.87
Φ_{JK}	-0.06	11.43	-0.45	4.46	6.76
Φ_{KJ}	0.10	-40.04	-1.50	-16.01	-25.65
ϕ_{j}	0.00	0.01	0.04	0.03	0.04
ϕ_k	0.00	117.36	-1.27	20.51	89.59
ϕ_{jk}	0.00	-5.55	1.60	-6.23	-1.09
Xaa	-4.64	-5.02	-4.65	-0.34	-0.21
χbb	2.67	3.02	2.75	0.67	2.86
χ_{cc}	1.97	2.00	1.90	-0.33	-2.65
$\mu_{ ext{total}}$	5.31	1.85	4.41	2.75	4.57

^[a] See footnote [a] to Table 6.

Molecular Physics

VIII. SUMMARY

Following an extensive search utilizing $6^5 = 7776$ initial structures for each diastereomer, 68 and 66 conformers (local minima on their related PESs) were found for Lthreonine and L-allo-threonine, respectively, at the RHF/3-21G level of electronic structure theory. After geometry optimizations at the B3LYP/6-311++ G^{**} level, 56 and 61 conformers remained for L-threonine and L-allo-threonine, respectively, within an energy range of 51 and 52 kJ mol⁻¹, respectively. The PESs of the Thr and aThr molecules clearly depend on the level of theory used for their determination. Lacking high-level definitive computational studies, only conformers obtained at several medium theoretical levels should be considered as ones whose likely existence is confirmed by theory. Fortunately, the results obtained show that the conformers found in the lower-energy regions of the PESs have the same bonding arrangements at the HF, DFT(B3LYP), and MP2 levels of theory, thus these conformers should in fact exist.

Following the FPA approach, relative energy predictions with an accuracy of ± 1 kJ mol⁻¹ were determined for the five lowest-energy conformers of both diastereomers of Thr. The computations clearly predict the global minimum for Thr, called **Thr-I**. However, for aThr the relative energies of two conformers, aThr-I and aThr-II are the same within the uncertainty of the FPA approach. In contrast to the global minimum of Gly and Ala, Thr-I contains an energetically unfavorable trans carboxylic group, and it is stabilized by strong OH^{...}N, OH^{...}O=C and weaker NH^{...}O H-bonds, whereby the COOH, NH₂, and the side-chain OH functional groups are interconnected via three intramolecular H-bonds. aThr-I is stabilized, very similarly to Thr-I, by strong OH...O=C and OH...N H-bonds, while the COOH group, to allow for these bonds, is again in the less favorable trans conformation. Thr-II and aThr-II also have similar structures, with energetically favorable cis carboxylic groups, but weaker H-bonds, NH^{...}O=C and OH^{...}N for both **Thr-II** and **aThr-II**. The structural differences between the most stable conformers of Gly and Ala and those of Thr and aThr are clearly due to the presence of the polar side chain. The side chain's significant effect on conformer stability was already observed for cysteine [51]. In the notation of Alonso et al., the presence of OH and SH polar side chains favor type-III conformers over type-I conformers known as global minima for Gly and Ala. As expected, the methyl group is in a staggered conformation for all the low-energy conformers of Thr and aThr, with rotational barriers varying between 1100 and 1300 cm^{-1} .

Spectroscopic parameters (harmonic and anharmonic frequencies, double-harmonic vibrational intensities, rotational constants with corresponding vibrational corrections, A-

reduced quartic and sextic centrifugal distortion constants, dipole moments and nuclear quadrupole coupling constants) were calculated for the conformers of Thr and aThr. Several of these parameters show the possibility for the experimental distinction of the conformers. Most important are the characteristic streching C=O (ω_{10}), NH (ω_3 , ω_4) and OH (ω_1 , ω_2) vibrational fundamentals if the vibrational spectra of the conformers were available. Assignment of the conformers based on pure rotational spectra can be based on rotational constant (equilibrium, A_e , B_e , and C_e , as well as vibrationally averaged A_0 , B_0 , and C_0 constants are provided), A-reduced quartic centrifugal distortion constants (Δ_J , Δ_K , Δ_{JK} , δ_J , and δ_K) and nuclear quadrupole coupling constants (χ_{aa} , χ_{bb} , and χ_{cc}) corresponding to the ¹⁴N nucleus. It seems feasible that conformers of Thr (and similarly those of Ala) could be identified if transitions between the energy levels corresponding to internal rotation characterized by slightly different methyl rotation barriers became available.

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Supplementary material to

Conformers of Gaseous Threonine

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Coordinates and energies are given in angstroms and Hartrees, respectively.

Molecular Physics					
B3LYP/6-	311++G** geomet	ry and energy	of conformer:	Thr	
Ν	-0.0533470	1.7038990	0.2314590		
Н	0.3590150	1.5838260	1.1539310		
С	-0.0442190	0.4246410	-0.4896880		
H	-0.0363780	0.6334110	-1.5655940		
C	1.1430510	-0.503/890	-0.1593510		
U U	-1.3815210	-0.3070190	-0.22/5860		
	1 1738110	-1.4445550	-0.0929990		
0	-1.5379430	-1.4843320	-0.4334870		
Н	0.5281650	-1.4335760	1.4592670		
0	-2.3522510	0.4880920	0.2309000		
H	-1.9233980	1.3640610	0.3658960		
Н	0.4619530	2.4261160	-0.2564510		
С	2.4888610	0.0865890	-0.5502360		
Н	2.6921460	1.0080080	0.0020550		
Н	3.2850080	-0.6229850	-0.3194590		
Н	2.5202000	0.3067220	-1.6209910		
Energy:	-438.426915844				
MP2/aug-	cc-pVTZ geometr	y and energy o	of conformer:	Thr-	
N	-0.0228480	1.6903810	0.2688530		
Н	0.3571380	1.5014330	1.1926450		
С	-0.0325080	0.4464470	-0.4999460		
Н	-0.0298410	0.6933330	-1.5652570		
С	1.1266340	-0.5049620	-0.2019770		
С	-1.3566840	-0.2788850	-0.2338380		
Н	0.9942280	-1.3951460	-0.8198310		
0	1.0926700	-0.8586950	1.1824380		
5	-1.5115450	-1.4644300	-0.4282970		
П	-2 325/110	-1.5121760	1.2099200		
н	-1 8749420	1 3828820	0.3633260		
Н	0.5611700	2.3913320	-0.1672090		
C	2.4747650	0.1241160	-0.4701750		
Н	2.6378010	0.9763930	0.1888130		
Н	3.2640720	-0.6010270	-0.2850380		
Н	2.5423180	0.4597270	-1.5052230		
Energy:	-437.569506052				

1					
2					
3	B3LYP/6-	311++G** geome	try and energy	of conformer:	Thr-II
4					
5	Ν	0.1698080	1.9023870	-0.2684410	
6	Н	-0.2646530	2.2031330	0.6005130	
7	С	0.0095320	0.4556970	-0.4335040	
8	H	0.1436610	0.2014940	-1.4869980	
9	С	1.1509880	-0.2394760	0.3675790	
10	С	-1.3579540	-0.0283770	0.0303600	
11	Н	0.9800490	-0.0154010	1.4325370	
12	0	2.3843380	0.3221540	-0.0481070	
13	0	-1.9633040	0.4334080	0.9670390	
14	H	2.2258460	1.2/62680	-0.1233500	
15	0	-1.8319130	-1.0523370	-0./148490	
16	H	-2.6858660	-1.3164590	-0.3376500	
17	H	-0.2/36900	2.4134800	-1.0233540	
18	C	1.2294720	-1./442590	0.1/110/0	
19	H	2.0924090	-2.1322/30	0.7155260	
20	H	0.3336330	-2.2460040	0.5428480	
21	Н	1.354/640	-1.9882530	-0.8868970	
22		400 40000			
23	Energy:	-438.42640584.	2		
24	MD2 / aur	an num anomati	and another	of conformer.	The TT
25	MPZ/aug-	-cc-pviz geomet.	ry and energy (or conformer:	1111-11
26	N	0 2150230	1 8995500	_0 2575850	
27	н	-0 1945680	2 1704510	0.6322350	
28	C	0.1255610	0 4647260	-0 4423400	
29	н	0.0255010	0.2119030	-1 4929450	
30	C	1 1255050	-0 2468140	0 3655030	
31	C	-1 3322570	-0.0060160	0.0244210	
32	Н	0.9583930	0.0023120	1 4228040	
33	0	2.3791580	0.2520800	-0.0617590	
34	0	-1.9065580	0.4302560	0.9989700	
35	H	2.2461020	1.2094890	-0.1537030	
36	0	-1.8337900	-0.9937040	-0.7499910	
37	H	-2.6799650	-1.2499270	-0.3476670	
38	Н	-0.2729080	2,4221520	-0.9748690	
39	С	1.1348810	-1.7470710	0.1852070	
40	H	1.9852550	-2.1657050	0.7198930	
41	Н	0.2231230	-2.1980880	0.5736040	
42	Н	1.2312190	-1.9974390	-0.8707660	
43					
44	Energy:	-437.56853718	3		
45					
46					
47					
48					
49					
50					
51					
52					
53					
54					

DOLLIYO	SIIIIG geome	ery and energy	or conformer.		
N	0.2094330	1.7152330	-0.1760860		
н С	-0.00000070	2.1553/50	0.0824120		
н	-0.0118720	0.3237980	-0.3081810		
С	1.0858580	-0.5745470	0.0705780		
C	-1.4037190	-0.1054630	-0.1245350		
Н	0.7987080	-1.6203050	-0.0509580		
0	1.1203250	-0.3330130	1.4690640		
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0	-1.6434660	-1.4057260	-0.3949310		
Н	-2.5376390	-1.6066530	-0.0800330		
Н	0.646/190	2.2569870	-0.9096480		
с н	2.4509340 3 1000520	-U.34152UU _A Q50821A	-U.5/682/U -0 0783840		
Н	2.4364200	-0.6061270	-0.0703040 -1.6392160		
H	2.7584420	0.7036820	-0.4798050		
Energy:	-438.425267223	2			
MP2/aug-	-cc-pVTZ geomet:	ry and energy	of conformer:	Thr-III	
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Н	-0.6354210	2.1587430	0.0954840		
С	0.0053990	0.3490860	-0.5806540		
H	0.0293140	0.2596820	-1.6725250		
C	1.0622810	-0.5943080	0.0167490		
C	-1.3/68040	-0.0776380	-0.1403450		
П	0.7963960	-1.6228230	-0.2230430		
0	-2 1809450	0.4070430	0 4151040		
Н	0.9905650	0.4688270	1.6009130		
0	-1.6271430	-1.3628440	-0.4648840		
Н	-2.5218930	-1.5520120	-0.1410080		
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	3.1775120	-0.9316470	-0.0533970		
H	0 1001000	0 1 20260	-1.60054/0		
H H	2.4894600	-0.4120200	0.0015170		
H H H	2.4894600 2.7157510	0.7557890	-0.2815170		
H H H Energy:	2.4894600 2.7157510 -437.56787161	0.7557890	-0.2815170		
H H H Energy:	2.4894600 2.7157510 -437.56787161	0.7557890	-0.2815170		
H H Energy:	2.4894600 2.7157510 -437.56787161	0.7557890	-0.2815170		
H H Energy:	2.4894600 2.7157510 -437.56787161	-0.4120280 0.7557890 7	-0.2815170		
H H Energy:	2.4894600 2.7157510 -437.56787161	-0.4120280 0.7557890 7	-0.2815170		
H H Energy:	2.4894600 2.7157510 -437.56787161	7	-0.2815170		
H H Energy:	2.4894600 2.7157510 -437.56787161	7	-0.2815170		
H H Energy:	2.4894600 2.7157510 -437.56787161	7	-0.2815170		
H H Energy:	2.4894600 2.7157510 -437.56787161	7	-0.2815170		
H H Energy:	2.4894600 2.7157510 -437.56787161	7	-0.2815170		
H H Energy:	2.4894600 2.7157510 -437.56787161	7	-0.2815170		
H H Energy:	2.4894600 2.7157510 -437.56787161	7	-0.2815170		
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2		211	two and another	of conforman.	The TV
4	BSLIP/0-	SII++G^^ geome	try and energy	or contormer:	
5	Ν	-0.8186040	1.7821470	-0.3309400	
6	Н	-0.4205930	2.2264530	0.4902180	
7	С	-0.1907550	0.4827140	-0.6154870	
8	Н	-0.2403160	0.3129490	-1.6958070	
9	С	1.3049830	0.3558530	-0.2214000	
10	С	-1.0409900	-0.6447280	0.0052240	
11	Н	1.8278280	1.1798690	-0.7182750	
12	0	1.8587050	-0.8277410	-0.7734890	
13	0	-0.6466930	-1.7830180	0.1086290	
14	H	1.2999960	-1.5654680	-0.481/550	
15	0	-2.25/8630	-0.26/1330	0.398/980	
16	п u	-2.2900430	2 /259210	0.2224050 -1.1077820	
17	II C	1 5543040	0 4490370	1 2868790	
18	Н	2.6267670	0.3784660	1,4762780	
19	Н	1.2076150	1.3994270	1.7078940	
20	Н	1.0601870	-0.3668810	1.8205460	
21					
22	Energy:	-438.42508780	6		
23					
25	MP2/aug-	cc-pVTZ geomet	ry and energy o	of conformer:	Thr-IV
26	N	_0 8469700	1 7575370	_0 3515190	
27	н	-0 4202520	2 2160600	0.4449560	
28	C	-0.1880080	0.4816160	-0.6407020	
29	H	-0.2058270	0.3118280	-1.7189970	
30	С	1.2812450	0.3921050	-0.1960970	
31	С	-0.9985460	-0.6609140	-0.0233860	
32	Н	1.8031190	1.2381650	-0.6495230	
33	0	1.8855410	-0.7690010	-0.7349080	
34	0	-0.5854010	-1.8013960	0.0445680	
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37	Н	-2.2366340	0.6681460	0.2544960	
30 20	H	-0.7843440	2.3915280	-1.1365740	
39 40	C	1.4380670	0.4501610	1.31/0880	
40 //1	H	2.4963/30	U.4107630 1 2695400	1.5663950	
41	п	1.0200300	-0 /017230	1 7837030	
43	11	0.9430730	0.4017250	1.7037030	
44	Energy:	-437.56810939	8		
45	21				
46					
47					
48					
49					
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51					
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54					

B3LYP/6-311++G** geometry and energy of conformer: N 0.0878610 1.8845440 -0.2474540 H -0.3917680 2.3981650 -0.9779090 C 0.107380 0.4342910 -0.4629700 H 0.1992680 0.2340690 -1.5192340 C 1.1514520 -0.2329730 0.3539300 C 1.3471450 -0.1754040 -0.1421140 H 0.9439590 -0.0532130 1.4202630 O 1.9674510 -0.9263050 -0.8509510 H 2.1852190 1.3350420 -0.0707650 O 1.9674510 -0.2244507 1.2184650 O 1.2860290 -1.265050 0.1067550 H -2.6616110 -0.2041570 1.2184650 C 1.2860290 -1.265050 0.1067550 H 2.1362480 -2.1122220 0.6723260 Energy: -438.424882619 MP2/aug-cc-pVT2 geometry and energy of conformer: N 0.1323170 1.8850100 -0.9373440 C 0.0255380 0.4460660 -0.4714850 H 0.3321450 1.245050 0.3339410 C 1.224650 -0.3398100 0.3339410 C 1.224550 -0.3398100 0.3339410 C 1.224550 -0.3398100 0.3339410 C 1.224550 -0.32170 1.4133990 O 2.3721180 0.3202020 -0.0177380 O 1.3554290 -0.0342170 1.4133990 O 2.3721180 0.3202020 0.0177380 C 1.22667270 1.2729040 -0.8526950 H 2.2067770 1.2729040 0.085950 O -1.7604520 0.2515710 1.0750780 H -2.615570 -0.1864530 1.2124170 H -2.621590 -1.7306230 0.1205030 H -2.201570 -0.1864530 1.2124170 H -0.2221950 -1.7306230 0.1205030 H 2.20231640 -2.4187700 0.6826920 Energy: -437.566928008	B3LYP/6-311++G** geometry and energy of conformer: N 0.0878610 1.8845440 -0.2474540 H -0.3917680 2.3981650 -0.9779090 C 0.0107380 0.2340690 -1.5192340 C 1.1514520 -0.2329730 0.35339300 C 1.3471450 -0.1754040 -0.1421140 H 0.9439590 -0.0532130 1.4202630 O 2.3757110 0.3865930 -0.0067480 O -1.9674510 -0.9263050 -0.8509510 H 2.1852190 1.3350420 -0.0707650 O -1.8030990 0.224500 1.0760170 H -2.6616110 -0.2041570 1.2184690 H 0.33901020 -2.2680380 0.4198280 H 0.33901020 -2.2680380 0.4198280 H 1.4616040 -1.9248700 -0.9535260 H 2.1362480 -2.1122220 0.6723260 Energy: -438.424882619 MP2/aug-cc-pVTZ geometry and energy of conformer: N 0.1323170 1.8850100 -0.2398030 C 0.0255380 0.4460660 -0.4714850 H 0.2324190 0.2429400 1.5234790 C 1.2246025380 0.4460660 -0.4714850 H 0.9202350 -0.332170 1.4133990 O .23721180 0.320200 0.3539410 C 1.1249450 -0.2390800 0.3539410 C 1.3254930 -0.1491490 -0.1490500 H 0.9202350 -0.332170 1.4133990 O 2.3721180 0.320200 -0.0177380 O -1.9554290 -0.957310 -0.8526960 H 2.2067270 1.2729040 -0.975950 O -1.7604520 0.2515710 1.0750780 H -2.6155270 -0.1864530 1.2124170 H 0.22031640 -2.118770 0.6826920 Energy: -437.566928008 Energy: -437.566928008
B3LYP/6-311++G** geometry and energy of conformer N 0.0878610 1.8845440 -0.2474540 H 0.3917680 2.3981650 -0.9779090 C 0.0107380 0.4342910 -0.4629700 H 0.1992680 0.2340690 -1.5192340 C 1.1514520 -0.2329730 0.3539300 C -1.3471450 -0.1754040 -0.1421140 H 0.9439590 -0.0532130 1.4202630 0 2.3757110 0.3865930 -0.0677480 0 -1.9674510 -0.9263050 -0.8509510 H 2.1852190 1.3350420 -0.07076550 0 -1.8030990 0.2224500 1.0760170 H -2.6616110 -0.2041570 1.21846990 CC 1.2860290 -1.7265050 0.1067550 H 0.3301020 -2.2680380 0.4198280 CC 1.2860290 -1.7265050 0.1067550 H 2.1362480 -2.1122220 0.6723260 Energy: -438.424882619 MP2/aug-cc-pVTZ geometry and energy of conformer: N 0.1323170 1.885010 -0.2398030 C 0.0255380 0.4460660 -0.4714850 H 0.2234190 0.2429400 -1.5234790 C 1.3254930 -0.1491490 -0.1490500 H 0.9202350 -0.0342170 1.413399410 C -1.3254930 -0.1491490 -0.1490500 H 0.9202350 -0.0342170 1.41339940 C -1.3254930 -0.2398080 0.3539410 C -1.3254930 -0.2398080 0.3539410 C -1.3254930 -0.2398080 0.3539410 C -1.3254930 -0.2492400 -1.5234790 C 1.1905500 -1.770940 -0.17780 O 2.3721180 0.3200200 -0.0177880 O -1.9554290 -0.239630 1.2124170 H 0.2214950 -0.2351510 -0.8526960 H 2.2067270 1.2729040 -0.0975950 H -2.6155270 -0.1864530 1.2124170 H -0.2621800 2.1194620 0.6649800 H 1.3476350 -1.9355180 -0.9379430 H 0.2719570 -2.2211660 0.4408660 H 1.3476350 -1.9355180 -0.9379430 H 0.2719570 -2.2211660 0.4408660 H 1.3476350 -1.9355180 -0.9379430 H 0.2719570 -2.2211660 0.4408600 H 1.3476350 -1.9355180 -0.9379430 H 0.2719570 -2.211660 0.4408600 H 1.3476350 -1.9355180 -0.9379430 H 0.2719570 -2.211660 0.4408600 H 0.2719570 -2.211660 0.4408600 H 0.2719570 -2.211660 0.4408600 H 0.2719570 -2.21487700 0.6826920 Energy: -437.566928008	BJLYP/6-311++6** geometry and energy of conformer: N 0.0878610 1.8845440 -0.2474540 H -0.3917680 2.3981650 -0.9779090 C 0.0107380 0.4342910 -0.4629700 C 1.1514520 -0.2329730 0.3539300 C 1.3471450 -0.1754040 -0.1421140 0 2.3757110 0.3865930 -0.067480 0 -1.9674510 -0.9263050 -0.8509510 H 2.1852190 1.3350420 -0.07707650 0 -1.8030990 0.2224500 1.0760170 H -2.6616110 -0.2041570 1.2184650 C 1.2860290 -1.7265050 0.4198280 H 0.3901020 -2.2680380 0.4198280 H 2.1362480 -2.1122220 0.6723260 Energy: -438.424882619 MP2/aug-cc-pVTZ geometry and energy of conformer: N 0.1323170 1.8850100 -0.2398030 H 0.2325380 0.4460660 -0.4714850 C 1.224500 0.2429400 -1.5234790 C 1.224950 -0.2398080 0.3539410 C 1.224950 -0.2398080 0.3539410 C 1.224950 -0.2398080 0.3539410 C 1.224950 -0.3251810 -0.9373440 C 1.224950 -0.3251810 -0.9373440 C 1.224950 -0.329020 0.3539410 C 1.224950 -0.329020 0.3539410 C 1.224950 -0.329020 0.3539410 C 1.224950 -0.390800 0.3539410 C 1.224950 -0.390820 0.3539410 C 1.224950 -0.390820 0.3539410 C 1.1249550 -0.132170 1.413999 O 2.3721180 0.320020 -0.0177380 O 1.9554290 -0.9057310 -0.8526950 H 2.2067270 1.2729040 -0.0975950 O -1.7604520 0.2515710 1.0750780 H -2.6155270 -0.1864530 1.2124170 H -2.6251800 2.1194620 0.66249800 C 1.1905960 -1.7306230 0.1205030 H 0.2219570 -2.221160 0.4408660 C 1.1905960 -1.7305310 -0.8526950 D -1.7604520 0.2515710 1.0750780 H 2.0231640 -2.1487700 0.6826920 Energy: -437.566928008
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H -2.6155270 -0.1864530 1.2124170 H -0.2621800 2.1194620 0.6649800 C 1.1905960 -1.7306230 0.1205030 H 0.2719570 -2.2211660 0.4408860 H 1.3476350 -1.9355180 -0.9379430 H 2.0231640 -2.1487700 0.6826920 Energy: -437.566928008	H -2.6155270 -0.1864530 1.2124170 H -0.2621800 2.1194620 0.6649800 C 1.1905960 -1.7306230 0.1205030 H 0.2719570 -2.2211660 0.4408860 H 1.3476350 -1.9355180 -0.9379430 H 2.0231640 -2.1487700 0.6826920 Energy: -437.566928008
H -0.2621800 2.1194620 0.6649800 C 1.1905960 -1.7306230 0.1205030 H 0.2719570 -2.2211660 0.4408860 H 1.3476350 -1.9355180 -0.9379430 H 2.0231640 -2.1487700 0.6826920 Energy: -437.566928008	H -0.2621800 2.1194620 0.6649800 C 1.1905960 -1.7306230 0.1205030 H 0.2719570 -2.2211660 0.4408860 H 1.3476350 -1.9355180 -0.9379430 H 2.0231640 -2.1487700 0.6826920 Energy: -437.566928008
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H 0.2719570 -2.2211660 0.4408860 H 1.3476350 -1.9355180 -0.9379430 H 2.0231640 -2.1487700 0.6826920 Energy: -437.566928008	H 0.2719570 -2.2211660 0.4408860 H 1.3476350 -1.9355180 -0.9379430 H 2.0231640 -2.1487700 0.6826920 Energy: -437.566928008
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Energy: -437.566928008	Energy: -437.566928008

-0.1205910 0.6843540 0.0453620 0.1076370 -1.1634380 1.3463630 -0.9657120 -1.3228340 1.4524000 -0.5447420 2.4247430	try and energy -1.3994510 -1.9870540 -0.6034940 -1.2881030 0.3346920 0.2005650 0.9360790 1.1989520 1.3773840	of conformer: 0.9934550 1.1766820 -0.2238470 -1.0755180 -0.4254480 -0.1861960 -1.3234400 0.7008040	Thr-
$\begin{array}{c} -0.1205910\\ 0.6843540\\ 0.0453620\\ 0.1076370\\ -1.1634380\\ 1.3463630\\ -0.9657120\\ -1.3228340\\ 1.4524000\\ -0.5447420\\ 2.4247430\\ \end{array}$	-1.3994510 -1.9870540 -0.6034940 -1.2881030 0.3346920 0.2005650 0.9360790 1.1989520 1.3773840	0.9934550 1.1766820 -0.2238470 -1.0755180 -0.4254480 -0.1861960 -1.3234400 0.7008040	
0.6843540 0.0453620 0.1076370 -1.1634380 1.3463630 -0.9657120 -1.3228340 1.4524000 -0.5447420 2.4247430	-1.9870540 -0.6034940 -1.2881030 0.3346920 0.2005650 0.9360790 1.1989520 1.3773840	1.1766820 -0.2238470 -1.0755180 -0.4254480 -0.1861960 -1.3234400 0.7008040	
0.0453620 0.1076370 -1.1634380 1.3463630 -0.9657120 -1.3228340 1.4524000 -0.5447420 2.4247430	$\begin{array}{c} -0.6034940 \\ -1.2881030 \\ 0.3346920 \\ 0.2005650 \\ 0.9360790 \\ 1.1989520 \\ 1.3773840 \\ 1.7724370 \end{array}$	-0.2238470 -1.0755180 -0.4254480 -0.1861960 -1.3234400 0.7008040	
$\begin{array}{c} 0.1076370 \\ -1.1634380 \\ 1.3463630 \\ -0.9657120 \\ -1.3228340 \\ 1.4524000 \\ -0.5447420 \\ 2.4247430 \end{array}$	-1.2881030 0.3346920 0.2005650 0.9360790 1.1989520 1.3773840	-1.0755180 -0.4254480 -0.1861960 -1.3234400 0.7008040	
-1.1634380 1.3463630 -0.9657120 -1.3228340 1.4524000 -0.5447420 2.4247430	0.3346920 0.2005650 0.9360790 1.1989520 1.3773840	-0.4254480 -0.1861960 -1.3234400 0.7008040	
$\begin{array}{c} 1.3463630\\ -0.9657120\\ -1.3228340\\ 1.4524000\\ -0.5447420\\ 2.4247430\end{array}$	0.2005650 0.9360790 1.1989520 1.3773840	-0.1861960 -1.3234400 0.7008040	
-0.9657120 -1.3228340 1.4524000 -0.5447420 2.4247430	0.9360790 1.1989520 1.3773840	-1.3234400 0.7008040	
-1.3228340 1.4524000 -0.5447420 2.4247430	1.1989520 1.3773840	0.7008040	
1.4524000 -0.5447420 2.4247430	1.3773840		
-0.5447420 2.4247430	1 7704070	0.0802880	
2.4247430	1.//243/0	0.7281070	
	-0.5770420	-0.4372330	
3.2153660	-0.0241560	-0.3365820	
-0.2848060	-0.7932050	1.7912620	
-2.4662010	-0.4274630	-0.6119270	
-2.4117260	-1.0770210	-1.4898120	
-2.6786830	-1.0439070	0.2621090	
-3.2845380	0.2809320	-0.7533560	
-438.42413392	2		
811++C** deame	try and energy	of conformer.	Thr.
JIIII geome	ery and energy	of conformer.	TIIT
-0.2126490	-1.8206810	0.2695310	
0.0903080	-2.23/1360	0.0915470	
-0.0388390	-0.3743000	1 5409580	
1 1198260	-0.1107090	-0.3520380	
-1 3643260	0.3376500	0.0770720	
0.8613840	0.0300670	-1,4131850	
2.2224130	-0.7126690	-0.0397190	
-1.6463270	1.4582080	0.4133890	
2.9926440	-0.4272070	-0.5413650	
-2.1464320	-0.4043400	-0.7179290	
-1.6964710	-1.2791270	-0.7789300	
-0.6015280	-2.2763270	1.0887040	
1.4670790	1 6123580	0 0711460	
	1.0120000	-0.0/11400	
0.6175860	2.2674990	-0.2664390	
0.6175860	2.2674990	-0.2664390 0.9722120	
0.6175860 1.7673000 2.2979840	2.2674990 1.7364090 1.9276830	-0.2664390 0.9722120 -0.7100800	
	-2.4002010 -2.4117260 -2.6786830 -3.2845380 -438.42413392 -438.42413392 -438.42413392 -438.42413392 -0.2126490 0.6963680 -0.0588590 0.1337270 1.1198260 -1.3643260 0.8613840 2.2224130 -1.6463270 2.9926440 -2.1464320 -1.6964710 -0.6015280	-2.4002010 -2.4117260 -2.6786830 -1.0770210 -2.6786830 -1.0439070 -3.2845380 0.2809320 -438.424133922 -438.424133922 -438.424133922 -0.2126490 0.6963680 -2.2371360 -0.0588590 -0.3743060 0.1337270 -0.1187090 1.1198260 0.3376500 0.8613840 0.3376500 0.8613840 0.3376500 0.8613840 0.3376500 0.8613840 0.3376500 0.8613840 0.3376500 0.8613840 0.3376500 0.8613840 0.3376500 0.8613840 0.3376500 0.8613840 0.3376500 0.8613840 0.300670 2.2224130 -0.7126690 -1.6463270 1.4582080 2.9926440 -0.4272070 -2.1464320 -0.4043400 -1.6964710 -1.2791270 -0.6015280 -2.2763270 1.6122580	-2.4002010 -0.4274030 -0.0119270 -2.4117260 -1.0770210 -1.4898120 -2.6786830 -1.0439070 0.2621090 -3.2845380 0.2809320 -0.7533560 -438.424133922 -0.7533560 -438.424133922 -0.2126490 -1.8206810 0.6963680 -2.2371360 0.0915470 -0.0588590 -0.3743060 0.4934350 0.1337270 -0.1187090 1.5409580 1.1198260 0.1563020 -0.3520380 -1.3643260 0.3376500 0.0770720 0.8613840 0.0300670 -1.4131850 2.2224130 -0.7126690 -0.0397190 -1.6463270 1.4582080 0.4133890 2.9926440 -0.4272070 -0.5413650 -2.1464320 -0.4043400 -0.7179290 -1.6964710 -1.2791270 -0.7789300 -0.6015280 -2.2763270 1.0887040

О О Н О Н Н С Н Н Н Н	2.2620890 -1.6539280 2.7424990 -2.1450690 -1.6980480 0.6994060 1.4647860 0.6032420 1.7896870 2.2751070	-0.6977210 1.4500480 -0.3963070 -0.4006600 -1.2759530 -2.2316040 1.6096880 2.2577260 1.7492970 1.9206650	-0.1707490 0.4350620 0.6088270 -0.7198480 -0.7845350 0.0752000 -0.1035720 -0.2648960 0.9339650 -0.7662380	
Energy:	-438.423845140	C		
B3LYP/6-3	311++G** geomet	try and energy	of conformer:	Thr-IX
	2	1 51		
N H C H C H O H H H H Energy:	-0.0413720 -0.4512880 0.0489910 0.1221530 -1.1244190 1.3669610 -0.8688630 -1.3193560 1.5026810 -0.4926710 2.3929550 3.1961640 -0.6188080 -2.4390040 -3.2299950 -2.3656490 -2.7268480 -438.422793907	-1.2438400 -0.5827480 -0.6334050 -1.4314140 0.3107930 0.1376410 0.8061800 1.2905110 1.2866770 1.7887950 -0.5994420 -0.0599000 -2.0753080 -0.4345690 0.2721390 -1.1788380 -0.9367590	$\begin{array}{c} 1.2151860\\ 1.8688640\\ -0.1137760\\ -0.8563140\\ -0.4859690\\ -0.1436700\\ -1.4346770\\ 0.5314350\\ 0.2175540\\ 0.6097410\\ -0.6046390\\ -0.5337760\\ 1.1987160\\ -0.6583710\\ -0.9154470\\ -1.4561210\\ 0.2686250\end{array}$	
B3LYP/6-7	311++G** geomet	try and energy	of conformer.	Thr-X
N H C H C C H O O H O H H C	-0.7159900 -1.6256120 -0.2274210 -0.2443500 1.2519180 -1.1431430 1.7960570 1.7132030 -2.2010150 2.5869850 -0.7044020 0.2085550 -0.8149610 1.4653320	1.8667120 1.8132780 0.5196140 0.2711770 0.4003020 -0.5226050 1.1940310 -0.8796130 -0.2314190 -1.0707420 -1.7898210 -1.8088900 2.4009910 0.5363510	-0.3779960 0.0724060 -0.6370400 -1.7078130 -0.1951320 0.0383960 -0.7177100 -0.6972480 0.5339270 -0.3407960 0.0132530 -0.3413880 -1.2315750 1.3051990	
H H	2.5324730 1.0589610	0.5170550 1.4912200	1.5479870 1.6428960	
	O O H H C H H H Energy: B3LYP/6-3 N H C C H O O H O H H C H H C H H C H H H Energy: S S LYP/6-3 N H C C H H C H H H C H H H C H H H C H H H C H H H H C H H H H C H H H C H H H H C H H H C H H H C H H H C H H H C H H H C H H H C H H H C H H H C H H H C H H H C H H C H H C H C H H H C H C H H C H C H H C H C H H C C H H C C H H C C H H C C H H C C H H C C H H C C H H C C H H C C H H C C H H C C H H C C H H C C H H C C H C H C C H H C C H C H C C H H C C H H C C H H C C H H C C H H C C H H C C H H C C H H H C C H H H C C H H H C C H H H C C H H H C C H H H C C H H H C C H H H H C C H	O 2.2620890 O -1.6539280 H 2.7424990 O -2.1450690 H -1.6980480 H 0.6994060 C 1.4647860 H 0.6032420 H 1.7896870 H 2.2751070 Energy: -438.423845144 B3LYP/6-311++G** geomet N -0.0413720 H -0.4512880 C 0.0489910 H 0.1221530 C -1.1244190 C 1.3669610 H -0.8688630 O -1.3193560 O 1.5026810 H -0.4926710 O 2.3929550 H 3.1961640 H -0.6188080 C -2.4390040 H -3.2299950 H -2.3656490 H -2.7268480 Energy: -438.42279390 ³ B3LYP/6-311++G** geomet N -0.7159900 H -2.7268480 Energy: -438.42279390 ³ B3LYP/6-311++G** geomet N -0.7159900 H -2.7268480 Energy: -438.42279390 ³ H -2.7268480 Energy: -438.42279390 ³ H -2.7268480 Energy: -438.42279390 ³ H -2.7268480 Energy: -438.42279390 ³ B3LYP/6-311++G** geomet N -0.7159900 H -2.7268480 Energy: -438.42279390 ³ B3LYP/6-311++G** geomet N -0.7159900 H -2.7268480 Energy: -438.42279390 ³ H -2.326550 H -0.8149610 C 1.4653320 H -2.5324730 H 1.0589610	0 2.2620890 -0.6977210 0 -1.6539280 1.4500480 H 2.7424990 -0.3963070 0 -2.1450690 -0.4006600 H -1.6980480 -1.2759530 H 0.6994060 -2.2316040 C 1.4647860 1.6096880 H 0.6032420 2.2577260 H 1.7896870 1.7492970 H 2.2751070 1.9206650 Energy: -438.423845140 M -0.4512880 -0.5827480 C 0.0489910 -0.6334050 H 0.1221530 -1.4314140 C 1.3669610 0.1376410 H -0.8688630 0.8061800 0 -1.3193560 1.2905110 0 1.5026810 1.2866770 H -0.4926710 1.7887950 0 2.3929550 -0.5994420 H 3.1961640 -0.0599000 H -0.6188080 -2.0753080 C -2.4390040 -0.4345690 H -3.229950 0.2721390 H -2.3656490 -1.1788380 H -2.3656490 -1.1788380 H -2.7268480 -0.9367590 Energy: -438.422793907 B3LYP/6-311++G** geometry and energy N -0.7159900 1.8667120 H -2.3656490 -1.1788380 H -2.7268480 -0.9367590 Energy: -438.422793907	0 2.2620890 -0.6977210 -0.1707490 0 -1.6539280 1.4500480 0.4350620 H 2.7424990 -0.3963070 0.6088270 0 -2.1450690 -0.4006600 -0.7198480 H -1.6980480 -1.2759530 -0.7845350 H 0.6994060 -2.2316040 0.0752000 C 1.4647860 1.6096880 -0.1035720 H 0.6032420 2.2577260 -0.2648960 H 1.7896870 1.7492970 0.9339650 H 2.2751070 1.9206650 -0.7662380 Energy: -438.423845140 E3LYP/6-311++G** geometry and energy of conformer: N -0.0413720 -1.2438400 1.2151860 H 0.1221530 -0.6334050 -0.1137760 H 0.1221530 -1.4314140 -0.8563140 C 1.3669610 0.1376410 -0.1436770 O 1.305601 1.2905110 0.5314350 C 1.669610 0.1376410 -0.1436770 O -1.3193660 1.2905110 0.5314350 C 1.6026810 1.2866770 0.2175540 H 0.4925710 1.789750 0.6097410 O 2.392550 -0.5994420 -0.664390 H 3.1961640 -0.599000 -0.5337760 H 3.1961640 -0.599000 -0.5337760 H -0.6188080 -2.0753080 1.1987160 C 2.439004 -0.4345690 -0.6633710 H -2.7266480 -0.394670 0.2175540 H -2.7266480 -0.3967590 0.2686250 Energy: -438.422793907 E3LYP/6-311++G** geometry and energy of conformer: N -0.7159900 1.8667120 -0.3779960 H -2.7266480 -0.9367590 0.2686250 Energy: -438.422793907 E3LYP/6-311++G** geometry and energy of conformer: N -0.7159900 1.8667120 -0.3779960 H -2.7266480 -0.9367590 0.2686250 Energy: -438.422793907 E3LYP/6-311++G** geometry and energy of conformer: N -0.7159900 1.8667120 -0.3779960 H -2.7266480 -0.9367590 0.2686250 Energy: -438.422793907 E3LYP/6-311++G** geometry and energy of conformer: N -0.7159900 1.8667120 -0.3779960 H -2.7266480 -0.9367590 0.2686250 Energy: -438.422793907 E3LYP/6-311++G** geometry and energy of conformer: N -0.7159900 1.8667120 -0.3779960 H -2.7266480 -0.171770 -0.3479960 H -0.2443500 0.2711770 -1.707130 C 1.2519180 0.4003020 -0.1951320 C -1.431430 -0.5226050 0.0333960 H -0.2443500 0.2711770 -1.707130 C 1.2519180 0.4003020 -0.1951320 C -1.453320 0.536510 1.3051990 H 2.56324730 0.5170550 1.5479870 C 1.4653320 0.5365510 1.3051990 H 2.5324730 0.5170550 1.5479870

Energy:	-438.42259687	9		
B3LYP/6-	-311++G** geome	try and energy	of conformer:	Thr-XI
N	0.2721470	1.7740430	-0.1393730	
Н	-0.4706620	2.3967660	-0.4377880	
С	-0.0160480	0.4107210	-0.5430580	
Н	-0.0100170	0.3536420	-1.6383150	
С	1.0771350	-0.5531780	-0.0418440	
С	-1.4075120	-0.0760430	-0.1107240	
Н	0.8021700	-1.5640000	-0.3625790	
0	1.0197440	-0.4778630	1.3906870	
0	-2.2209430	0.5799150	0.4862410	
Н	1./380740	-0.9988080	1./621040	
U H	-1.634963U -2 5/87/00	-1.5733900	-0.3230130 -0.3230130	
11 H	-2.040/490 0 304/390	1 8222200	-U.Z34U88U A 874798A	
C	2.4625120	-0.2056670	-0.5753600	
Н	3.2066290	-0.9019880	-0.1746780	
Н	2.4863000	-0.2915600	-1.6655790	
Н	2.7395710	0.8123810	-0.3008560	
Energy.	-138 12251551	7		
Eller gy.	-430.42234334	1		
B3LYP/6-	-311++G** geome	try and energy	of conformer:	Thr-XI
B3LYP/6- N	-311++G** geome -0.3918680	try and energy -1.8080200	of conformer: 0.0591660	Thr-XI
B3LYP/6- N H	-311++G** geome -0.3918680 0.2072020	try and energy -1.8080200 -2.4092460	of conformer: 0.0591660 0.6133980	Thr-XI
B3LYP/6- N H C	-311++G** geome -0.3918680 0.2072020 -0.0940770	try and energy -1.8080200 -2.4092460 -0.3946940	of conformer: 0.0591660 0.6133980 0.3435790	Thr-XI
B3LYP/6- N H C H	-311++G** geome -0.3918680 0.2072020 -0.0940770 0.0322280	-1.8080200 -2.4092460 -0.3946940 -0.3089030	of conformer: 0.0591660 0.6133980 0.3435790 1.4295700	Thr-XII
B3LYP/6- N H C H C	-311++G** geome -0.3918680 0.2072020 -0.0940770 0.0322280 1.1925940	<pre>try and energy -1.8080200 -2.4092460 -0.3946940 -0.3089030 0.1328910 0.4462220</pre>	of conformer: 0.0591660 0.6133980 0.3435790 1.4295700 -0.3226840	Thr-XII
B3LYP/6- N H C H C C	-311++G** geome -0.3918680 0.2072020 -0.0940770 0.0322280 1.1925940 -1.3475190 1.0098620	<pre>try and energy -1.8080200 -2.4092460 -0.3946940 -0.3089030 0.1328910 0.4463280 0 2263600</pre>	of conformer: 0.0591660 0.6133980 0.3435790 1.4295700 -0.3226840 0.0038290 -1.4036040	Thr-XII
B3LYP/6- N H C H C C H C C H	-311++G** geome -0.3918680 0.2072020 -0.0940770 0.0322280 1.1925940 -1.3475190 1.0098690 2.1675350	<pre>try and energy -1.8080200 -2.4092460 -0.3946940 -0.3089030 0.1328910 0.4463280 0.2263680 -0 9003230</pre>	of conformer: 0.0591660 0.6133980 0.3435790 1.4295700 -0.3226840 0.0038290 -1.4036040 -0.0999060	Thr-XII
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<pre>C</pre>	C	1 1 6 4 2 0 2 0	0.2021320	-0.1024140	
H 1.9153/90 1.0352330 -0.6604630 0 1.8202810 -0.9690960 -0.6604630 0 -2.0967840 -0.0082680 0.6809700 H 1.2333110 -1.6835630 -0.3847850 0 -0.8992500 -1.6951330 -0.1933110 H -1.5737260 -2.2049340 0.2825270 H -1.2235650 2.1996050 -1.1702620 C 1.4548000 0.3706860 1.3545110 H 0.8641450 -0.3922640 1.8726270 H 2.5015340 0.2302420 1.6303540 H 1.1374230 1.3534360 1.7139430 Energy: -438.421670064 B3LYP/6-311++G** geometry and energy of conformer: Thr-XV N -0.5212800 1.9195560 -0.3539110 H -1.4085510 2.1468730 -0.7876350 C -0.1467790 0.5362390 -0.6136420 H -0.1970690 0.3730820 -1.6967470 C 1.3370160 0.2839400 -0.2277290 C -1.0622550 -0.5410210 -0.0179100 H 1.9017020 1.0668540 -0.7374530 0 1.8064530 -0.9417070 -0.7728690 0 -0.7584980 -1.7042820 0.1308880 H 1.2328330 -1.6470070 -0.4412700		-1.1642830	-0.3/32//0	0.0134630	
O 1.8202810 -0.9690960 -0.6604630 O -2.0967840 -0.0082680 0.6809700 H 1.2333110 -1.6835630 -0.3847850 O -0.8992500 -1.6951330 -0.1933110 H -1.5737260 -2.2049340 0.2825270 H -1.2235650 2.1996050 -1.1702620 C 1.4548000 0.3706860 1.3545110 H 0.8641450 -0.3922640 1.8726270 H 2.5015340 0.2302420 1.6303540 H 1.1374230 1.3534360 1.7139430 Energy: -438.421670064 B3LYP/6-311++G** geometry and energy of conformer: Thr-XV N -0.5212800 1.9195560 -0.3539110 H -1.4085510 2.1468730 -0.7876350 C -0.1467790 0.5362390 -0.6136420 H -0.1970690 0.3730820 -1.6967470 C 1.3370160 0.2839400 -0.2277290 C -1.0622550 -0.5410210 -0.0179100 H 1.9017020 1.0668540 -0.7374530 O 1.8064530 -0.9417070 -0.7728690 O -0.7584980 -1.7042820 0.1308880 H 1.2328330 -1.6470070 -0.4412700	H	1.9153790	1.0352330	-0.6370180	
$\begin{array}{llllllllllllllllllllllllllllllllllll$	0	1.8202810	-0.9690960	-0.6604630	
H 1.2333110 -1.6835630 -0.3847850 O -0.8992500 -1.6951330 -0.1933110 H -1.5737260 -2.2049340 0.2825270 H -1.2235650 2.1996050 -1.1702620 C 1.4548000 0.3706860 1.3545110 H 0.8641450 -0.3922640 1.8726270 H 2.5015340 0.2302420 1.6303540 H 1.1374230 1.3534360 1.7139430 Energy: -438.421670064 B3LYP/6 $-311++G^{**}$ geometry and energy of conformer: Thr-XV N -0.5212800 1.9195560 -0.3539110 H -1.4085510 2.1468730 -0.7876350 C -0.1467790 0.5362390 -0.6136420 H -0.1970690 0.3730820 -1.6967470 C 1.3370160 0.2839400 -0.2277290 C -1.0622550 -0.5410210 -0.0179100 H 1.9017020 1.0668540 -0.774530 O 1.8064530 -0.9417070 -0.7728690 O -0.7584980 -1.7042820 0.1308880 H 1.2328330 -1.6470070 -0.4412700	0	-2.0967840	-0.0082680	0.6809700	
O -0.8992500 -1.6951330 -0.1933110 H -1.5737260 -2.2049340 0.2825270 H -1.2235650 2.1996050 -1.1702620 C 1.4548000 0.3706860 1.3545110 H 0.8641450 -0.3922640 1.8726270 H 2.5015340 0.2302420 1.6303540 H 1.1374230 1.3534360 1.7139430 Energy: -438.421670064 B3LYP/6-311++G** geometry and energy of conformer: Thr-XV N -0.5212800 1.9195560 -0.3539110 H -1.4085510 2.1468730 -0.7876350 C -0.1467790 0.5362390 -0.6136420 H -0.1970690 0.3730820 -1.6967470 C 1.3370160 0.2839400 -0.2277290 C -1.0622550 -0.5410210 -0.0179100 H 1.9017020 1.0668540 -0.7374530 O 1.8064530 -0.9417070 -0.7728690 O -0.7584980 -1.7042820 0.1308880 H 1.232830 -1.6470070 -0.4412700	Н	1.2333110	-1.6835630	-0.3847850	
H -1.5737260 -2.2049340 0.2825270 H -1.2235650 2.1996050 -1.1702620 C 1.4548000 0.3706860 1.3545110 H 0.8641450 -0.3922640 1.8726270 H 2.5015340 0.2302420 1.6303540 H 1.1374230 1.3534360 1.7139430 Energy: -438.421670064 B3LYP/6-311++G** geometry and energy of conformer: Thr-XV N -0.5212800 1.9195560 -0.3539110 H -1.4085510 2.1468730 -0.7876350 C -0.1467790 0.5362390 -0.6136420 H -0.1970690 0.3730820 -1.6967470 C 1.3370160 0.2839400 -0.2277290 C -1.0622550 -0.5410210 -0.0179100 H 1.9017020 1.0668540 -0.7374530 O 1.8064530 -0.9417070 -0.7728690 O -0.7584980 -1.7042820 0.1308880 H 1.2328330 -1.6470070 -0.4412700	0	-0.8992500	-1.6951330	-0.1933110	
H -1.2235650 2.1996050 -1.1702620 C 1.4548000 0.3706860 1.3545110 H 0.8641450 -0.3922640 1.8726270 H 2.5015340 0.2302420 1.6303540 H 1.1374230 1.3534360 1.7139430 Energy: -438.421670064 B3LYP/6-311++G** geometry and energy of conformer: Thr-XV N -0.5212800 1.9195560 -0.3539110 H -1.4085510 2.1468730 -0.7876350 C -0.1467790 0.5362390 -0.6136420 H -0.1970690 0.3730820 -1.6967470 C 1.3370160 0.2839400 -0.2277290 C -1.0622550 -0.5410210 -0.0179100 H 1.9017020 1.0668540 -0.7374530 O 1.8064530 -0.9417070 -0.7728690 O -0.7584980 -1.7042820 0.1308880 H 1.2328330 -1.6470070 -0.4412700	Н	-1.5737260	-2.2049340	0.2825270	
C 1.4548000 0.3706860 1.3545110 H 0.8641450 -0.3922640 1.8726270 H 2.5015340 0.2302420 1.6303540 H 1.1374230 1.3534360 1.7139430 Energy: -438.421670064 B3LYP/6-311++G** geometry and energy of conformer: Thr-XV N -0.5212800 1.9195560 -0.3539110 H -1.4085510 2.1468730 -0.7876350 C -0.1467790 0.5362390 -0.6136420 H -0.1970690 0.3730820 -1.6967470 C 1.3370160 0.2839400 -0.2277290 C -1.0622550 -0.5410210 -0.0179100 H 1.9017020 1.0668540 -0.7374530 O 1.8064530 -0.9417070 -0.7728690 O -0.7584980 -1.7042820 0.1308880 H 1.2328330 -1.6470070 -0.4412700	Н	-1.2235650	2.1996050	-1.1702620	
H 0.8641450 -0.3922640 1.8726270 H 2.5015340 0.2302420 1.6303540 H 1.1374230 1.3534360 1.7139430 Energy: -438.421670064 B3LYP/6-311++G** geometry and energy of conformer: Thr-XV N -0.5212800 1.9195560 -0.3539110 H -1.4085510 2.1468730 -0.7876350 C -0.1467790 0.5362390 -0.6136420 H -0.1970690 0.3730820 -1.6967470 C 1.3370160 0.2839400 -0.2277290 C -1.0622550 -0.5410210 -0.0179100 H 1.9017020 1.0668540 -0.7374530 O 1.8064530 -0.9417070 -0.7728690 O -0.7584980 -1.7042820 0.1308880 H 1.2328330 -1.6470070 -0.4412700	С	1.4548000	0.3706860	1.3545110 🧹	
H 2.5015340 0.2302420 1.6303540 H 1.1374230 1.3534360 1.7139430 Energy: -438.421670064 B3LYP/6-311++G** geometry and energy of conformer: Thr-XV N -0.5212800 1.9195560 -0.3539110 H -1.4085510 2.1468730 -0.7876350 C -0.1467790 0.5362390 -0.6136420 H -0.1970690 0.3730820 -1.6967470 C 1.3370160 0.2839400 -0.2277290 C -1.0622550 -0.5410210 -0.0179100 H 1.9017020 1.0668540 -0.7374530 O 1.8064530 -0.9417070 -0.7728690 O -0.7584980 -1.7042820 0.1308880 H 1.2328330 -1.6470070 -0.4412700	Н	0.8641450	-0.3922640	1.8726270	
H 1.1374230 1.3534360 1.7139430 Energy: -438.421670064 B3LYP/6-311++G** geometry and energy of conformer: Thr-XV N -0.5212800 1.9195560 -0.3539110 H -1.4085510 2.1468730 -0.7876350 C -0.1467790 0.5362390 -0.6136420 H -0.1970690 0.3730820 -1.6967470 C 1.3370160 0.2839400 -0.2277290 C -1.0622550 -0.5410210 -0.0179100 H 1.9017020 1.0668540 -0.7374530 O 1.8064530 -0.9417070 -0.7728690 O -0.7584980 -1.7042820 0.1308880 H 1.2328330 -1.6470070 -0.4412700	Н	2.5015340	0.2302420	1.6303540	
Energy: -438.421670064 B3LYP/6-311++G** geometry and energy of conformer: Thr-XV N -0.5212800 1.9195560 -0.3539110 H -1.4085510 2.1468730 -0.7876350 C -0.1467790 0.5362390 -0.6136420 H -0.1970690 0.3730820 -1.6967470 C 1.3370160 0.2839400 -0.2277290 C -1.0622550 -0.5410210 -0.0179100 H 1.9017020 1.0668540 -0.7374530 O 1.8064530 -0.9417070 -0.7728690 O -0.7584980 -1.7042820 0.1308880 H 1.2328330 -1.6470070 -0.4412700	Н	1.1374230	1.3534360	1.7139430	
Energy: -438.421670064 B3LYP/6-311++G** geometry and energy of conformer: Thr-XV N -0.5212800 1.9195560 -0.3539110 H -1.4085510 2.1468730 -0.7876350 C -0.1467790 0.5362390 -0.6136420 H -0.1970690 0.3730820 -1.6967470 C 1.3370160 0.2839400 -0.2277290 C -1.0622550 -0.5410210 -0.0179100 H 1.9017020 1.0668540 -0.7374530 O 1.8064530 -0.9417070 -0.7728690 O -0.7584980 -1.7042820 0.1308880 H 1.2328330 -1.6470070 -0.4412700					
B3LYP/6-311++G** geometry and energy of conformer: Thr-XV N -0.5212800 1.9195560 -0.3539110 H -1.4085510 2.1468730 -0.7876350 C -0.1467790 0.5362390 -0.6136420 H -0.1970690 0.3730820 -1.6967470 C 1.3370160 0.2839400 -0.2277290 C -1.0622550 -0.5410210 -0.0179100 H 1.9017020 1.0668540 -0.7374530 O 1.8064530 -0.9417070 -0.7728690 O -0.7584980 -1.7042820 0.1308880 H 1.2328330 -1.6470070 -0.4412700	Energy:	-438.42167006	4		
B3LYP/6-311++G** geometry and energy of conformer: Thr-XV N -0.5212800 1.9195560 -0.3539110 H -1.4085510 2.1468730 -0.7876350 C -0.1467790 0.5362390 -0.6136420 H -0.1970690 0.3730820 -1.6967470 C 1.3370160 0.2839400 -0.2277290 C -1.0622550 -0.5410210 -0.0179100 H 1.9017020 1.0668540 -0.7374530 O 1.8064530 -0.9417070 -0.7728690 O -0.7584980 -1.7042820 0.1308880 H 1.2328330 -1.6470070 -0.4412700					
B3LYP/6-311++G** geometry and energy of conformer: Thr-XV N -0.5212800 1.9195560 -0.3539110 H -1.4085510 2.1468730 -0.7876350 C -0.1467790 0.5362390 -0.6136420 H -0.1970690 0.3730820 -1.6967470 C 1.3370160 0.2839400 -0.2277290 C -1.0622550 -0.5410210 -0.0179100 H 1.9017020 1.0668540 -0.7374530 O 1.8064530 -0.9417070 -0.7728690 O -0.7584980 -1.7042820 0.1308880 H 1.2328330 -1.6470070 -0.4412700					
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N -0.5212800 1.9195560 -0.3539110 H -1.4085510 2.1468730 -0.7876350 C -0.1467790 0.5362390 -0.6136420 H -0.1970690 0.3730820 -1.6967470 C 1.3370160 0.2839400 -0.2277290 C -1.0622550 -0.5410210 -0.0179100 H 1.9017020 1.0668540 -0.7374530 O 1.8064530 -0.9417070 -0.7728690 O -0.7584980 -1.7042820 0.1308880 H 1.2328330 -1.6470070 -0.4412700		SII G GCOME	ery and energy	or contormer.	TIT 37 A
H-1.40855102.1468730-0.7876350C-0.14677900.5362390-0.6136420H-0.19706900.3730820-1.6967470C1.33701600.2839400-0.2277290C-1.0622550-0.5410210-0.0179100H1.90170201.0668540-0.7374530O1.8064530-0.9417070-0.7728690O-0.7584980-1.70428200.1308880H1.2328330-1.6470070-0.4412700	N	-0.5212800	1.9195560	-0.3539110	
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H-0.19706900.3730820-1.6967470C1.33701600.2839400-0.2277290C-1.0622550-0.5410210-0.0179100H1.90170201.0668540-0.7374530O1.8064530-0.9417070-0.7728690O-0.7584980-1.70428200.1308880H1.2328330-1.6470070-0.4412700	С	-0.1467790	0.5362390	-0.6136420	
C1.33701600.2839400-0.2277290C-1.0622550-0.5410210-0.0179100H1.90170201.0668540-0.7374530O1.8064530-0.9417070-0.7728690O-0.7584980-1.70428200.1308880H1.2328330-1.6470070-0.4412700	Н	-0.1970690	0.3730820	-1.6967470	
C-1.0622550-0.5410210-0.0179100H1.90170201.0668540-0.7374530O1.8064530-0.9417070-0.7728690O-0.7584980-1.70428200.1308880H1.2328330-1.6470070-0.4412700	С	1.3370160	0.2839400	-0.2277290	
H1.90170201.0668540-0.7374530O1.8064530-0.9417070-0.7728690O-0.7584980-1.70428200.1308880H1.2328330-1.6470070-0.4412700	С	-1.0622550	-0.5410210	-0.0179100	
01.8064530-0.9417070-0.77286900-0.7584980-1.70428200.1308880H1.2328330-1.6470070-0.4412700	Н	1.9017020	1.0668540	-0.7374530	
O -0.7584980 -1.7042820 0.1308880 H 1.2328330 -1.6470070 -0.4412700	0	1.8064530	-0.9417070	-0.7728690	
Н 1.2328330 -1.6470070 -0.4412700	0	-0.7584980	-1.7042820	0.1308880	
	Н	1.2328330	-1.6470070	-0.4412700	

0	-2.2863880	-0.0781620	0.3159760	
Н	-2.7965040	-0.8339630	0.6471060	
Н	-0.6232490	2.0984370	0.6392250	
С	1.6039220	0.3789600	1.2759790	
Н	1.0468580	-0.3812500	1.8317710	
Н	2.6675240	0.2186430	1.4617960	
Н	1.3414620	1.3659440	1.6684320	
Energy:	-438.42154158	1		
21				
B3LYP/6-	311++G** geome	etry and energy	of conformer:	Thr-XVI
N	-0.5784370	1.9273800	-0.3001630	
Н	-1.5639310	1.9610530	-0.0624250	
С	-0.1618670	0.5658300	-0.6153250	
Н	-0.1575770	0.3509260	-1.6947020	
С	1.3032400	0.3231520	-0.1345260	
С	-1.1604060	-0.4132230	-0.0195820	
Н	1.8698550	1.1737450	-0.5220660	
0	1.8822860	-0.8134290	-0.7654910	
0	-2.2139900	-0.1214550	0.4850880	
Н	1.3800660	-1.5932590	-0.5006030	
0	-0.7477020	-1.7048750	-0.1311570	
Н	-1.4365850	-2.2635080	0.2607090	
н	-0 4038050	2 5579800	-1 0721420	
C	1 4435010	0 2902270	1 3847650	
ч	0 9/65270	_0 5871630	1 811/230	
и П	2 1005710	0.2429680	1 6573180	
п	2.4995740	1 1077500	1 02/1070	
п	1.0033700	1.10//300	1.0241070	
Energy:	-438.42149829	7		
B3LYP/6-	311++G** geome	etry and energy	of conformer:	Thr-XVII
N	0.1925480	1.7437770	-0.1447390	
Н	-0.5504030	2.3440600	-0.4826600	
С	-0.0084330	0.3694890	-0.5689890	
Н	0.0439780	0.3267250	-1.6628590	
С	1.1174410	-0.5363630	-0.0338600	
С	-1.3566760	-0.2851970	-0.2228820	
Н	0.8860490	-1.5606770	-0.3458350	
0	1.0254870	-0.4406310	1.3969590	
0	-1.6657180	-1.4048070	-0.5485520	
н	1.7152420	-0.9816570	1.7928540	
0	-2 1919900	0 5317220	1 4580840	
ц	-3 0027250 -3 0027250	0.000500	0.400040	
ц	-J.0037230 0 1012040	U.UZOZJOU 1 7057720	0.0233100 0.8687170	
п	U.IJIJJ4U 2 1067000	1.133113U	U.000/4/U 0 5/26070	
	2.430/300	-U.I34030U	-U.J4200/U	
п	3.20329UU 3.5510050	-U./03112U	-U.LU8852U	
н	2.5510850	-U.2432930	-1.6298490	
н	2./183000	0.900/690	-0.2833100	
Energy:	-438.42139539	7		

N -0 H 0 C 0 H 0 C -1 C -1 C -1 H -0 O -1 N -0 H -0 O 2 H -0 C -2 H -2	.2129830 .5188070 .0265030 .0102800 .0985340 .4190500 .8162340 .2696890 .3385430 .4479210 .5504410 .4644810 .3111580 .4403560 .7207720 .2060500 .3948850 8.421382922 +G** geomet .5696310 .5710780 .1522570 .2093940 .3336840 .0591820 .8968610 .8244570 .7348240	-1.0623770 -1.6573580 -0.6918630 -1.5990650 0.2484450 -0.1000950 0.5952760 1.3717290 -0.6609470 1.8772640 1.1615820 1.4448560 -0.2398700 -0.4649240 -0.8558160 0.2376930 -1.2946280 2 2 2 2 2 2 2 2 2 2 2 2 2	<pre>1.3729630 1.7433640 -0.0182400 -0.6270800 -0.5228210 -0.2463730 -1.5273860 0.3430670 -0.7850040 0.3501910 0.2656620 0.1089310 1.9584330 -0.6019200 0.3767910 -0.9358340 -1.3118270</pre>	Thr-XIX
H 0 C 0 H 0 C -1 C -1 C -1 C -1 H -0 O -1 O 2 H -0 O 1 H -0 C -2 H -0 C -1 H -1 C -0 H -1 C -1 H -0 C -1 H -1 C -0 H -1 C -1 H -1 C -0 H -1 C -1 H -0 C -1 H -1 C -0 H -1 C -1 H -0 C -1	.5188070 .0265030 .0102800 .0985340 .4190500 .8162340 .2696890 .3385430 .4479210 .5504410 .4644810 .3111580 .4403560 .7207720 .2060500 .3948850 8.421382922 +G** geomet .5696310 .5710780 .1522570 .2093940 .3336840 .0591820 .8968610 .8244570 .7348240	-1.6573580 -0.6918630 -1.5990650 0.2484450 -0.1000950 0.5952760 1.3717290 -0.6609470 1.8772640 1.1615820 1.4448560 -0.2398700 -0.4649240 -0.8558160 0.2376930 -1.2946280 2 2 2 2 2 3 3 4 4 4 4 8 5 5 8 1.8862950 2.0111070 0.5515110 0.4004490 0.2989270 -0.5347480 1.1266370 -0.8656270	1.7433640 -0.0182400 -0.6270800 -0.5228210 -0.2463730 -1.5273860 0.3430670 -0.7850040 0.3501910 0.2656620 0.1089310 1.9584330 -0.6019200 0.3767910 -0.9358340 -1.3118270 By of conformer: -0.1508650 -0.2426360 -0.5758770 -1.6680100 -0.1978800 -0.0200670 -0.6414560	Thr-XIX
C 0 H 0 C -1 C 1 H -0 O -1 O 2 H -0 O 1 H -0 O 1 H -0 C -2 H -0 C -2 H -1 C -0 H -1 C -1 H -1 C -0 H -1 C -1 H -1 C -0 H -1 C -1 H -1 C -0 H -1 C -1 H -1 C -1 H -2 H -2	.0265030 .0102800 .0985340 .4190500 .8162340 .2696890 .3385430 .4479210 .5504410 .4644810 .3111580 .4403560 .7207720 .2060500 .3948850 8.421382922 +G** geomet .5696310 .5710780 .1522570 .2093940 .3336840 .0591820 .8968610 .8244570 .7348240	-0.6918630 -1.5990650 0.2484450 -0.1000950 0.5952760 1.3717290 -0.6609470 1.8772640 1.1615820 1.4448560 -0.2398700 -0.4649240 -0.8558160 0.2376930 -1.2946280 2 2 2 2 2 2 2 2 2 2 2 2 2	-0.0182400 -0.6270800 -0.2463730 -1.5273860 0.3430670 -0.7850040 0.3501910 0.2656620 0.1089310 1.9584330 -0.6019200 0.3767910 -0.9358340 -1.3118270 By of conformer: -0.1508650 -0.2426360 -0.5758770 -1.6680100 -0.1978800 -0.0200670 -0.6414560	Thr-XIX
H 0 C -1 C 1 H -0 O -1 O 2 H -0 O 2 H -0 C -2 H -0 C -2 H -2	.0102800 .0985340 .4190500 .8162340 .2696890 .3385430 .4479210 .5504410 .4644810 .3111580 .4403560 .7207720 .2060500 .3948850 8.421382922 +G** geomet .5696310 .5710780 .1522570 .2093940 .3336840 .0591820 .8968610 .8244570 .7348240	-1.5990650 0.2484450 -0.1000950 0.5952760 1.3717290 -0.6609470 1.8772640 1.1615820 1.4448560 -0.2398700 -0.4649240 -0.8558160 0.2376930 -1.2946280 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2	-0.6270800 -0.5228210 -0.2463730 -1.5273860 0.3430670 -0.7850040 0.3501910 0.2656620 0.1089310 1.9584330 -0.6019200 0.3767910 -0.9358340 -1.3118270 By of conformer: -0.1508650 -0.2426360 -0.5758770 -1.6680100 -0.1978800 -0.0200670 -0.6414560	Thr-XIX
C -1 C 1 H -0 O -1 O -1 O -1 O -1 O -1 O -1 O -1 H -0 C -2 H -0 C -0 H -0 C -1 H -2 H	.0985340 .4190500 .8162340 .2696890 .3385430 .4479210 .5504410 .4644810 .3111580 .4403560 .7207720 .2060500 .3948850 8.421382922 +G** geomet .5696310 .5710780 .1522570 .2093940 .3336840 .0591820 .8968610 .8244570 .7348240	0.2484450 -0.1000950 0.5952760 1.3717290 -0.6609470 1.8772640 1.1615820 1.4448560 -0.2398700 -0.4649240 -0.8558160 0.2376930 -1.2946280 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2	-0.5228210 -0.2463730 -1.5273860 0.3430670 -0.7850040 0.3501910 0.2656620 0.1089310 1.9584330 -0.6019200 0.3767910 -0.9358340 -1.3118270 angle angle angle angle angle angle angle and angle angl	Thr-XIX
C 1 H -0 O -1 O 2 H -0 O 2 H -0 O 1 H -2 H -3 H -2 H -2 H -2 H -2 H -2 H -3 H -2 H -1 C -0 H -1 C -0 H -0 C -1 H -1 C -0 H -0 C -1 H -0 C -1 H -1 C -0 H -0 C -1 H -0 C -1 H -0 C -1 H -2 H -2 H -2 H -2 H -2 H -0 C -1 H -0 C -2 H -0 C -1 H -0 C -2 H -0 C -1 H -1	.4190500 .8162340 .2696890 .3385430 .4479210 .5504410 .4644810 .3111580 .4403560 .7207720 .2060500 .3948850 8.421382922 +G** geomet .5696310 .5710780 .1522570 .2093940 .3336840 .0591820 .8968610 .8244570 .7348240	-0.1000950 0.5952760 1.3717290 -0.6609470 1.8772640 1.1615820 1.4448560 -0.2398700 -0.4649240 -0.8558160 0.2376930 -1.2946280 2 2 2 2 2 2 2 2 2 2 2 2 2	-0.2463730 -1.5273860 0.3430670 -0.7850040 0.3501910 0.2656620 0.1089310 1.9584330 -0.6019200 0.3767910 -0.9358340 -1.3118270 by of conformer: -0.1508650 -0.2426360 -0.5758770 -1.6680100 -0.1978800 -0.0200670 -0.6414560	Thr-XIX
H -0 O -1 O 2 H -0 O 1 H -0 O 1 H -0 C -2 H -1 C -0 H -1 C -0 H -1 C -0 H -1 C -0 H -1 C -0 H -1 C -1 H -2 H -	.8162340 .2696890 .3385430 .4479210 .5504410 .4644810 .3111580 .4403560 .7207720 .2060500 .3948850 8.421382922 +G** geomet .5696310 .5710780 .1522570 .2093940 .3336840 .0591820 .8968610 .8244570 .7348240	0.5952760 1.3717290 -0.6609470 1.8772640 1.1615820 1.4448560 -0.2398700 -0.4649240 -0.8558160 0.2376930 -1.2946280 2 2 2 2 2 2 2 2 2 2 2 2 2	-1.5273860 0.3430670 -0.7850040 0.3501910 0.2656620 0.1089310 1.9584330 -0.6019200 0.3767910 -0.9358340 -1.3118270 90 of conformer: -0.1508650 -0.2426360 -0.5758770 -1.6680100 -0.1978800 -0.0200670 -0.6414560	Thr-XIX
0 -1 0 2 H -0 0 1 H -0 O 1 H -0 C -2 H -2 H -2 H -2 H -2 H -2 H -2 Energy: -438 B3LYP/6-311+- 0 N -0 H -1 C -0 H -1 C -0 H -0 C 1 H 1 H 1 H 1 H 1 H 1 H 1 H	.2090890 .3385430 .4479210 .5504410 .4644810 .3111580 .4403560 .7207720 .2060500 .3948850 8.421382922 +G** geomet .5696310 .5710780 .1522570 .2093940 .3336840 .0591820 .8968610 .8244570 .7348240	-0.6609470 1.8772640 1.1615820 1.4448560 -0.2398700 -0.4649240 -0.8558160 0.2376930 -1.2946280 2 2 1.8862950 2.0111070 0.5515110 0.4004490 0.2989270 -0.5347480 1.1266370 -0.8656270	0.3430670 -0.7850040 0.3501910 0.2656620 0.1089310 1.9584330 -0.6019200 0.3767910 -0.9358340 -1.3118270 90 of conformer: -0.1508650 -0.2426360 -0.5758770 -1.6680100 -0.1978800 -0.0200670 -0.6414560	Thr-XIX
H -0 H -0 H -0 H -0 H -0 H -2 H -1 C -0 H -0 C -1 H -0 C -1 H -0 C -1 H -1 C -0 H -0 C -1 H -1 C -0 H -1 C -0 H -0 C -1 H -2 H	.4479210 .5504410 .4644810 .3111580 .4403560 .7207720 .2060500 .3948850 8.421382922 +G** geomet .5696310 .5710780 .1522570 .2093940 .3336840 .0591820 .8968610 .8244570 .7348240	1.8772640 1.1615820 1.4448560 -0.2398700 -0.4649240 -0.8558160 0.2376930 -1.2946280 2 2 1.8862950 2.0111070 0.5515110 0.4004490 0.2989270 -0.5347480 1.1266370 -0.8656270	<pre>0.3501910 0.2656620 0.1089310 1.9584330 -0.6019200 0.3767910 -0.9358340 -1.3118270</pre>	Thr-XIX
O 1 M -0 H -2 H -2 H -2 H -2 H -2 Energy: -438 B3LYP/6-311+- N -0 H -1 C -0 H -1 C -0 H -1 C -1 H -0 C 1 O -0 H 1 O -0 H -1 O -0 H 1 H -2 H -0 C 1 H -2 H -2 H -2 H 1 H 1 H 1 H 1 H 1 H 1 H 1 H 1	<pre>+479210 .5504410 .4644810 .3111580 .4403560 .7207720 .2060500 .3948850 8.421382922 +G** geomet .5696310 .5710780 .1522570 .2093940 .3336840 .0591820 .8968610 .8244570 .7348240</pre>	1.1615820 1.4448560 -0.2398700 -0.4649240 -0.8558160 0.2376930 -1.2946280 2 2 2 2 2 2 2 2 2 2 2 2 2	0.2656620 0.1089310 1.9584330 -0.6019200 0.3767910 -0.9358340 -1.3118270 y of conformer: -0.1508650 -0.2426360 -0.5758770 -1.6680100 -0.1978800 -0.0200670 -0.6414560	Thr-XIX
H 2 H -0 C -2 H -2 H -2 H -2 H -2 H -3 H -2 Energy: -438 B3LYP/6-311+- N -0 H -1 C -1 H -1 C -0 H -1 C -1 H -1 C -0 H -1 C -1 H -1 C -0 H -0 C -1 H -1 C -0 H -1 C -1 H -1 C -0 H -1 C -1 H -1 C -0 H -1 C -1 H -1 C -0 H -2 H -2 H -2 H -2 H -2 H -2 H -2 H -0 C -1 H -1 H -2 H -1 H -2 H -1 H -2 H -1 H -	.4644810 .3111580 .4403560 .7207720 .2060500 .3948850 8.421382922 +G** geomet .5696310 .5710780 .1522570 .2093940 .3336840 .0591820 .8968610 .8244570 .7348240	1.4448560 -0.2398700 -0.4649240 -0.8558160 0.2376930 -1.2946280 2 2 1.8862950 2.0111070 0.5515110 0.4004490 0.2989270 -0.5347480 1.1266370 -0.8656270	0.1089310 1.9584330 -0.6019200 0.3767910 -0.9358340 -1.3118270 y of conformer: -0.1508650 -0.2426360 -0.5758770 -1.6680100 -0.1978800 -0.0200670 -0.6414560	Thr-XIX
H -0 C -2 H -2 H -2 H -3 H -2 Energy: -438 B3LYP/6-311+- N -0 H -1 C -1 H -1 C -0 H -1 C -0 H -1 C -1 H -1 C -0 H -1 C -1 H -1 C -1 H -1 C -0 H -1 C -1 H -1 C -1 H -1 C -1 H -1 C -1 H -1 C -0 H -1 C -1 H -2 H -2 H -2 H -2 H -2 H -2 H -2 H -1 H -1 C -1 H -1 C -1 H -1 C -1 H -2 H -2 H -2 H -2 H -2 H -2 H -2 H -2 H -2 H -1 H -1 H -1 H -1 H -2 H -1 H -2 H -1 H -2 H -1 H	.3111580 .4403560 .7207720 .2060500 .3948850 8.421382922 +G** geomet .5696310 .5710780 .1522570 .2093940 .3336840 .0591820 .8968610 .8244570 .7348240	-0.2398700 -0.4649240 -0.8558160 0.2376930 -1.2946280 2 2 1.8862950 2.0111070 0.5515110 0.4004490 0.2989270 -0.5347480 1.1266370 -0.8656270	1.9584330 -0.6019200 0.3767910 -0.9358340 -1.3118270 y of conformer: -0.1508650 -0.2426360 -0.5758770 -1.6680100 -0.1978800 -0.0200670 -0.6414560	Thr-XIX
C -2 H -2 H -2 H -3 H -2 Energy: -438 B3LYP/6-311+- N -0 H -1 C -1 C -1 H -2 H -2	.4403560 .7207720 .2060500 .3948850 8.421382922 +G** geomet .5696310 .5710780 .1522570 .2093940 .3336840 .0591820 .8968610 .8244570 .7348240	-0.4649240 -0.8558160 0.2376930 -1.2946280 2 2 1.8862950 2.0111070 0.5515110 0.4004490 0.2989270 -0.5347480 1.1266370 -0.8656270	-0.6019200 0.3767910 -0.9358340 -1.3118270 By of conformer: -0.1508650 -0.2426360 -0.5758770 -1.6680100 -0.1978800 -0.0200670 -0.6414560	Thr-XIX
H -2 H -3 H -2 Energy: -438 B3LYP/6-311+- N -0 H -1 C -1 Energy: -438 H -1 C -1 H -1 C -1 Energy: -438 H -1 C -1 H -1 C -1 C -1 Energy: -438 H -1 C -1 Energy: -438 H -1 C -1 Energy: -438 H -1 C -1 Energy: -438 H -1 Energy: -438 H -1 Energy: -438 H -1 Energy: -438 H -1 Energy: -438	.7207720 .2060500 .3948850 8.421382922 +G** geomet .5696310 .5710780 .1522570 .2093940 .3336840 .0591820 .8968610 .8244570 .7348240	-0.8558160 0.2376930 -1.2946280 2 2 1.8862950 2.0111070 0.5515110 0.4004490 0.2989270 -0.5347480 1.1266370 -0.8656270	0.3767910 -0.9358340 -1.3118270 by of conformer: -0.1508650 -0.2426360 -0.5758770 -1.6680100 -0.1978800 -0.0200670 -0.6414560	Thr-XIX
H -3 H -2 Energy: -438 B3LYP/6-311+- N -0 H -1 C -0 H -1 C -0 H -0 C 1 H 1 O 1 O -0 H 1 O -0 H -1 C -1 H 2 H -1 Energy: -438	.2060500 .3948850 8.421382922 +G** geomet .5696310 .5710780 .1522570 .2093940 .3336840 .0591820 .8968610 .8244570 .7348240	0.2376930 -1.2946280 2 2 1.8862950 2.0111070 0.5515110 0.4004490 0.2989270 -0.5347480 1.1266370 -0.8656270	-0.9358340 -1.3118270 yy of conformer: -0.1508650 -0.2426360 -0.5758770 -1.6680100 -0.1978800 -0.0200670 -0.6414560	Thr-XIX
H -2 Energy: -438 B3LYP/6-311+- N -0 H -1 C -0 H -1 C -0 H -1 C -1 H 1 O 1 O -2 H -2	.3948850 8.421382922 +G** geomet .5696310 .5710780 .1522570 .2093940 .3336840 .0591820 .8968610 .8244570 .7348240	-1.2946280 2 2 1.8862950 2.0111070 0.5515110 0.4004490 0.2989270 -0.5347480 1.1266370 -0.8656270	-1.3118270 y of conformer: -0.1508650 -0.2426360 -0.5758770 -1.6680100 -0.1978800 -0.0200670 -0.6414560	Thr-XIX
Energy: -438 B3LYP/6-311+- N -0 H -1 C -0 H -0 C 1 C -1 H 1 O 1 O -0 H 1 O -0 H 1 H 2 H -1 Energy: -438	<pre>8.421382922 +G** geomet .5696310 .5710780 .1522570 .2093940 .3336840 .0591820 .8968610 .8244570 .7348240</pre>	2 2 1.8862950 2.0111070 0.5515110 0.4004490 0.2989270 -0.5347480 1.1266370 -0.8656270	y of conformer: -0.1508650 -0.2426360 -0.5758770 -1.6680100 -0.1978800 -0.0200670 -0.6414560	Thr-XIX
B3LYP/6-311+- N -0 H -1 C -0 H -0 C 1 C 1 C -1 H 1 O 1 O -0 H 1 O -2 H -2 H -2 H -2 H -2 H -2 H -2 H -0 C 1 Energy: -438	+G** geomet .5696310 .5710780 .1522570 .2093940 .3336840 .0591820 .8968610 .8244570 .7348240	1.8862950 2.0111070 0.5515110 0.4004490 0.2989270 -0.5347480 1.1266370 -0.8656270	yy of conformer: -0.1508650 -0.2426360 -0.5758770 -1.6680100 -0.1978800 -0.0200670 -0.6414560	Thr-XIX
H -1 C -0 H -0 C 1 C 1 C -1 H 1 O 1 O -0 H 1 O -0 H 1 O -2 H -2 H -2 H -2 H -2 H -2 H -2 H -1 Energy: -438	.5710780 .1522570 .2093940 .3336840 .0591820 .8968610 .8244570 .7348240	2.0111070 0.5515110 0.4004490 0.2989270 -0.5347480 1.1266370 -0.8656270	-0.2426360 -0.5758770 -1.6680100 -0.1978800 -0.0200670 -0.6414560	
C -0 H -0 C 1 C -1 H 1 O 1 O -0 H 1 O -0 H 1 O -2 H -2 H -2 H -2 H -2 H -2 H -2 H -2 H -2 H -1 Energy: -438	.1522570 .2093940 .3336840 .0591820 .8968610 .8244570 .7348240	0.5515110 0.4004490 0.2989270 -0.5347480 1.1266370 -0.8656270	-0.5758770 -1.6680100 -0.1978800 -0.0200670 -0.6414560	
H -0 C 1 C -1 H 1 O 1 O -0 H 1 O -2 H -2 H -2 H -2 H -2 H -2 H -2 H 1 Energy: -438	.2093940 .3336840 .0591820 .8968610 .8244570 .7348240	0.4004490 0.2989270 -0.5347480 1.1266370 -0.8656270	-1.6680100 -0.1978800 -0.0200670 -0.6414560	
C 1 C -1 H 1 O 1 O -0 H 1 O -0 H 1 O -2 H -2 H -0 C 1 H 1 H 2 H 1 Energy: -438	.3336840 .0591820 .8968610 .8244570 .7348240	0.2989270 -0.5347480 1.1266370 -0.8656270	-0.1978800 -0.0200670 -0.6414560	
C -1 H 1 O 1 O -0 H 1 O -0 H 1 O -2 H -2 H -0 C 1 H 1 H 2 H 1 Energy: -438	.0591820 .8968610 .8244570 .7348240	-0.5347480 1.1266370 -0.8656270	-0.0200670 -0.6414560	
H I O 1 O -O H 1 O -O H 1 H -2 H -0 C 1 H 1 H 2 H 1 Energy: -438	.8968610 .8244570 .7348240	1.1266370 -0.8656270	-0.6414560	
0 -0 H 1 O -2 H -2 H -2 H -2 H -0 C 1 H 2 H 1 H 2 H 1 Energy: -438	.8244570 .7348240	-0.8656270	0 0 1 0 7 0 1 0	
H 1 O -2 H -2 H -0 C 1 H 1 H 2 H 1 Energy: -438	. / 540240	_1 60001/0	-0.848/910	
O -2 H -2 H -2 H -0 C 1 H 1 H 2 H 1 Energy: -438	2963020	-1.6908140 -1.6117610	-0.5327560	
H -2 H -0 C 1 H 1 H 2 H 1 Energy: -438	.3110320	-0.1028440	0.2416540	
H -0 C 1 H 1 H 2 H 1 Energy: -438	.8232490	-0.8662890	0.5502290	
C 1 H 1 H 2 H 1 Energy: -438	.1119810	2.5931520	-0.7162030	
H 1 H 2 H 1 Energy: -438	.5928720	0.2824840	1.3075740	
H 2 H 1 Energy: -438	.1042200	-0.5727850	1.7822870	
н 1. Energy: -438	.6663120	0.2023140	1.4900590	
Energy: -438	.2199140	1.1983370	1.7707060	
	8.421129086	5		
B3LYP/6-311+-	+G** geomet	ery and energ	y of conformer:	Thr-XX
N -0	.7308580	1.8669150	-0.3601330	
H -1.			0 0 0 1 - 1 1 1	
u -0.	.6534570	1.8017010	0.0615410	

Η

1.8113110 1.2031620 -0.6714560

1					
2					
3	0	1.7894760	-0.8786780	-0.5895420	
4	0	-2.2222220	-0.2589620	0.4762090	
5	Н	2.0945190	-0.8200270	-1.5009370	
6	0	-0.6704930	-1.7866820	0.0312010	
1	Н	0.2600400	-1.7900010	-0.2772600	
8	H	-0.8053110	2.4195510	-1.2044330	
9	С	1.4446210	0.5224260	1.3319580	
10	Н	2.5077960	U.SI/0690	1.5785010	
11	H U	1.0000950	1.454/610 _0.3116/90	1 85//030	
12	п	0.9000370	-0.3110490	1.0344930	
14	Enerav:	-438.421075307			
15	- 51 -				
16					
17					
18	/				_, _,
19	B3LYP/6-3	11++G** geomet:	ry and energy	of conformer:	Thr-XXI
20	NT	0 1102650	1 2422200	1 1260700	
21	N U	-0.1193630	-1.2422200	1 1012910	
22	C	0 0657780	-0.6525800	-0 2053300	
23	Н	0.0930950	-1.4052590	-1.0012280	
24	C	-1.0959750	0.3286130	-0.4698970	
25	C	1.4563490	0.0192130	-0.2394780	
26	Н	-0.8754030	0.9044240	-1.3728620	
27	0	-1.1315500	1.2969050	0.5950170	
28	0	2.4368950	-0.5963240	-0.5696990	
29	Н	-1.1403550	0.7782500	1.4164830	
3U 21	0	1.5240350	1.3032300	0.1397980	
31 22	Н	0.6327720	1.6133520	0.4136110	
32	Н	0.7547210	-1.6216240	1.4865990	
3/	С	-2.4455210	-0.3617540	-0.6339720	
35	Н	-3.2215390	0.3827010	-0.8204340	
36	H	-2.4251390	-1.05/9320	-1.4775960	
37	Н	-2.7238110	-0.9160590	0.2671200	
38	Energy.	-438.420967528			
39	HHGT GY.	130.120907320			
40					
41					
42					
43	B3LYP/6-3	11++G** geomet:	ry and energy	of conformer:	Thr-XXII
44					
45	N	0.1782550	1.7228290	0.2842200	
46	H	-0.6668530	2.2807450	0.3206010	
47	C	-0.0392250	0.4883760	-0.4518520	
48	н С	-0.06/23/0	0.6306060	-1.5468320	
49	C	-1 4107930	-0.0678890	-0.2017100	
50	H	0.8946880	-1.4207490	-0.7753650	
51 52	0	2.2625080	0.1367780	-0.7610310	
52 53	0	-2.2905550	0.5491840	0.4347260	
54	Н	3.0496880	-0.3488870	-0.4963900	
55	0	-1.5753610	-1.3417690	-0.5425510	
56	Н	-2.4864820	-1.5973140	-0.3326620	
57	Н	0.9279740	2.2566180	-0.1373290	
58	С	1.3134620	-0.8632360	1.2677040	
59	H	0.4443980	-1.3956850	1.6643090	
60	H	2.1782030	-1.5253940	1.3813450	
	Н	1.4/06580	0.0397710	1.8581780	

Molecular Physics

Energy: -438.420596988

	j	1 51		
N	0.0120870	1.9356770	-0.3341160	
Н	-0.3803690	2.2146210	0.5608410	
С	0.0014210	0.4814200	-0.4447510	
Н	0.1248570	0.2008000	-1.4964290	
С	1.1377810	-0.2121200	0.3696660	
С	-1.3554650	-0.0168880	0.0213570	
Н	1.0035400	0.0601490	1.4204530	
0	2.3872280	0.3820180	0.0007360	
0	-1.9293540	0.3867380	1.0022350	
Н	2.6817810	-0.0087930	-0.8301520	
0	-1.8542620	-0.9951490	-0.7680010	
Н	-2.7049560	-1.2656010	-0.3882800	
Н	0.9723890	2.2634540	-0.3721110	
С	1.1824480	-1.7285930	0.2222510	
H	0.2711830	-2.1973010	0.6001650	
Н	1.2910510	-2.0191660	-0.8287740	
Н	2.0299150	-2.1296730	0.7821950	
Energy:	-438.42053440	9		
B31 VD/6-	-311++C** decme	try and energy	of conformer:	Thr-XXII
B3LYP/6-	-311++G** geome	try and energy	of conformer:	Thr-XXI
B3LYP/6- N	-311++G** geome 0.0119250	try and energy 1.9373550	of conformer: -0.3075720	Thr-XXI
B3LYP/6- N H	-311++G** geome 0.0119250 -0.2756370	try and energy 1.9373550 2.2039380	of conformer: -0.3075720 0.6298530	Thr-XXI
B3LYP/6- N H C	-311++G** geome 0.0119250 -0.2756370 0.0074290	try and energy 1.9373550 2.2039380 0.4839820	of conformer: -0.3075720 0.6298530 -0.4356370	Thr-XXI
B3LYP/6- N H C H	-311++G** geome 0.0119250 -0.2756370 0.0074290 0.1266720	etry and energy 1.9373550 2.2039380 0.4839820 0.2233540	of conformer: -0.3075720 0.6298530 -0.4356370 -1.4904560	Thr-XXI
B3LYP/6- N H C H C	-311++G** geome 0.0119250 -0.2756370 0.0074290 0.1266720 1.1383400	try and energy 1.9373550 2.2039380 0.4839820 0.2233540 -0.2289210	<pre>of conformer: -0.3075720 0.6298530 -0.4356370 -1.4904560 0.3504060</pre>	Thr-XXI
B3LYP/6- N H C H C C	-311++G** geome 0.0119250 -0.2756370 0.0074290 0.1266720 1.1383400 -1.3473670	etry and energy 1.9373550 2.2039380 0.4839820 0.2233540 -0.2289210 -0.0157720	<pre>of conformer: -0.3075720 0.6298530 -0.4356370 -1.4904560 0.3504060 0.0411010</pre>	Thr-XXI
B3LYP/6- N H C H C C H	-311++G** geome 0.0119250 -0.2756370 0.0074290 0.1266720 1.1383400 -1.3473670 1.0170610	etry and energy 1.9373550 2.2039380 0.4839820 0.2233540 -0.2289210 -0.0157720 0.0255590	<pre>-0.3075720 0.6298530 -0.4356370 -1.4904560 0.3504060 0.0411010 1.4123780</pre>	Thr-XXI
B3LYP/6- N H C H C C H O	-311++G** geome 0.0119250 -0.2756370 0.0074290 0.1266720 1.1383400 -1.3473670 1.0170610 2.3440630	try and energy 1.9373550 2.2039380 0.4839820 0.2233540 -0.2289210 -0.0157720 0.0255590 0.3653650	<pre>of conformer: -0.3075720 0.6298530 -0.4356370 -1.4904560 0.3504060 0.0411010 1.4123780 -0.1502420</pre>	Thr-XXI
B3LYP/6- N H C H C C H O O	-311++G** geome 0.0119250 -0.2756370 0.0074290 0.1266720 1.1383400 -1.3473670 1.0170610 2.3440630 -1.8764470	try and energy 1.9373550 2.2039380 0.4839820 0.2233540 -0.2289210 -0.0157720 0.0255590 0.3653650 0.3305740	<pre>of conformer: -0.3075720 0.6298530 -0.4356370 -1.4904560 0.3504060 0.0411010 1.4123780 -0.1502420 1.0681020</pre>	Thr-XXI
B3LYP/6- N H C H C C H O O H	-311++G** geome 0.0119250 -0.2756370 0.0074290 0.1266720 1.1383400 -1.3473670 1.0170610 2.3440630 -1.8764470 3.0886180	try and energy 1.9373550 2.2039380 0.4839820 0.2233540 -0.2289210 -0.0157720 0.0255590 0.3653650 0.3305740 0.0467400	<pre>of conformer: -0.3075720 0.6298530 -0.4356370 -1.4904560 0.3504060 0.0411010 1.4123780 -0.1502420 1.0681020 0.3691960</pre>	Thr-XXI
B3LYP/6- N H C H C H O O H O O H	-311++G** geome 0.0119250 -0.2756370 0.0074290 0.1266720 1.1383400 -1.3473670 1.0170610 2.3440630 -1.8764470 3.0886180 -1.9031380	etry and energy 1.9373550 2.2039380 0.4839820 0.2233540 -0.2289210 -0.0157720 0.0255590 0.3653650 0.3305740 0.0467400 -0.9129260	<pre>-0.3075720 0.6298530 -0.4356370 -1.4904560 0.3504060 0.0411010 1.4123780 -0.1502420 1.0681020 0.3691960 -0.8025300</pre>	Thr-XXIV
B3LYP/6- N H C H C H O O H O H	-311++G** geome 0.0119250 -0.2756370 0.0074290 0.1266720 1.1383400 -1.3473670 1.0170610 2.3440630 -1.8764470 3.0886180 -1.9031380 -2.7533580	try and energy 1.9373550 2.2039380 0.4839820 0.2233540 -0.2289210 -0.0157720 0.0255590 0.3653650 0.3305740 0.0467400 -0.9129260 -1.1802360	<pre>-0.3075720 0.6298530 -0.4356370 -1.4904560 0.3504060 0.0411010 1.4123780 -0.1502420 1.0681020 0.3691960 -0.8025300 -0.4193160</pre>	Thr-XXIV
B3LYP/6- N H C H C H O O H H H H	-311++G** geome 0.0119250 -0.2756370 0.0074290 0.1266720 1.1383400 -1.3473670 1.0170610 2.3440630 -1.8764470 3.0886180 -1.9031380 -2.7533580 0.9543590	etry and energy 1.9373550 2.2039380 0.4839820 0.2233540 -0.2289210 -0.0157720 0.0255590 0.3653650 0.3305740 0.0467400 -0.9129260 -1.1802360 2.2806180	<pre>-0.3075720 0.6298530 -0.4356370 -1.4904560 0.3504060 0.0411010 1.4123780 -0.1502420 1.0681020 0.3691960 -0.8025300 -0.4193160 -0.4612160</pre>	Thr-XXI
B3LYP/6- N H C H C C H O O H H C	-311++G** geome 0.0119250 -0.2756370 0.0074290 0.1266720 1.1383400 -1.3473670 1.0170610 2.3440630 -1.8764470 3.0886180 -1.9031380 -2.7533580 0.9543590 1.1577340	try and energy 1.9373550 2.2039380 0.4839820 0.2233540 -0.2289210 -0.0157720 0.0255590 0.3653650 0.3305740 0.0467400 -0.9129260 -1.1802360 2.2806180 -1.7445970	<pre>-0.3075720 0.6298530 -0.4356370 -1.4904560 0.3504060 0.0411010 1.4123780 -0.1502420 1.0681020 0.3691960 -0.8025300 -0.4193160 -0.4612160 0.1751410</pre>	Thr-XXI
B3LYP/6- N H C H C H O O H H C H H	-311++G** geome 0.0119250 -0.2756370 0.0074290 0.1266720 1.1383400 -1.3473670 1.0170610 2.3440630 -1.8764470 3.0886180 -1.9031380 -2.7533580 0.9543590 1.1577340 0.2548410	try and energy 1.9373550 2.2039380 0.4839820 0.2233540 -0.2289210 -0.0157720 0.0255590 0.3653650 0.3305740 0.0467400 -0.9129260 -1.1802360 2.2806180 -1.7445970 -2.2063460	<pre>-0.3075720 0.6298530 -0.4356370 -1.4904560 0.3504060 0.0411010 1.4123780 -0.1502420 1.0681020 0.3691960 -0.8025300 -0.4193160 -0.4612160 0.1751410 0.5830840</pre>	Thr-XXI
B3LYP/6- N H C H C C H O H H C H H H	-311++G** geome 0.0119250 -0.2756370 0.0074290 0.1266720 1.1383400 -1.3473670 1.0170610 2.3440630 -1.8764470 3.0886180 -1.9031380 -2.7533580 0.9543590 1.1577340 0.2548410 1.2380620	try and energy 1.9373550 2.2039380 0.4839820 0.2233540 -0.2289210 -0.0157720 0.0255590 0.3653650 0.3305740 0.0467400 -0.9129260 -1.1802360 2.2806180 -1.7445970 -2.2063460 -2.0100760	<pre>-0.3075720 0.6298530 -0.4356370 -1.4904560 0.3504060 0.0411010 1.4123780 -0.1502420 1.0681020 0.3691960 -0.8025300 -0.4193160 -0.4612160 0.1751410 0.5830840 -0.8819350</pre>	Thr-XXI
B3LYP/6- N H C H C H O O H O H H H H H H	-311++G** geome 0.0119250 -0.2756370 0.0074290 0.1266720 1.1383400 -1.3473670 1.0170610 2.3440630 -1.8764470 3.0886180 -1.9031380 -2.7533580 0.9543590 1.1577340 0.2548410 1.2380620 2.0132750	try and energy 1.9373550 2.2039380 0.4839820 0.2233540 -0.2289210 -0.0157720 0.0255590 0.3653650 0.3305740 0.0467400 -0.9129260 -1.1802360 2.2806180 -1.7445970 -2.2063460 -2.0100760 -2.1772930	<pre>-0.3075720 0.6298530 -0.4356370 -1.4904560 0.3504060 0.0411010 1.4123780 -0.1502420 1.0681020 0.3691960 -0.8025300 -0.4193160 -0.4612160 0.1751410 0.5830840 -0.8819350 0.7027090</pre>	Thr-XXIV
B3LYP/6- N H C C H C H O O H H C H H H Energy:	-311++G** geome 0.0119250 -0.2756370 0.0074290 0.1266720 1.1383400 -1.3473670 1.0170610 2.3440630 -1.8764470 3.0886180 -1.9031380 -2.7533580 0.9543590 1.1577340 0.2548410 1.2380620 2.0132750 -438.42053260	try and energy 1.9373550 2.2039380 0.4839820 0.2233540 -0.2289210 -0.0157720 0.0255590 0.3653650 0.3305740 0.0467400 -0.9129260 -1.1802360 2.2806180 -1.7445970 -2.2063460 -2.0100760 -2.1772930	<pre>-0.3075720 0.6298530 -0.4356370 -1.4904560 0.3504060 0.0411010 1.4123780 -0.1502420 1.0681020 0.3691960 -0.8025300 -0.4193160 -0.4612160 0.1751410 0.5830840 -0.8819350 0.7027090</pre>	Thr-XXIV
B3LYP/6- N H C H C H O O H O H H H Energy:	-311++G** geome 0.0119250 -0.2756370 0.0074290 0.1266720 1.1383400 -1.3473670 1.0170610 2.3440630 -1.8764470 3.0886180 -1.9031380 -2.7533580 0.9543590 1.1577340 0.2548410 1.2380620 2.0132750 -438.42053260	etry and energy 1.9373550 2.2039380 0.4839820 0.2233540 -0.2289210 -0.0157720 0.0255590 0.3653650 0.3305740 0.0467400 -0.9129260 -1.1802360 2.2806180 -1.7445970 -2.2063460 -2.0100760 -2.1772930	<pre>-0.3075720 0.6298530 -0.4356370 -1.4904560 0.3504060 0.0411010 1.4123780 -0.1502420 1.0681020 0.3691960 -0.8025300 -0.4193160 -0.4612160 0.1751410 0.5830840 -0.8819350 0.7027090</pre>	Thr-XXIV

 B3LYP/6-311++G**
 geometry and energy of conformer:
 Thr-XXV

 N
 -0.0982090
 -0.9222640
 1.5056010

 H
 -0.4033540
 -0.0727720
 1.9712700

 C
 0.0241960
 -0.6964720
 0.0660630

 H
 -0.0069430
 -1.6612420
 -0.4428670

1					
2					
3	С	-1.0699750	0.2239260	-0.5571600	
4	С	1.4178810	-0.1519790	-0.2274710	
5	Н	-0.7621570	0.4686480	-1.5845570	
6	0	-1.2291980	1.4238350	0.1999730	
1	0	2.2628330	-0.6897130	-0.8921060	
8	Н	-0.3823340	1.8864730	0.2251450	
9	0	1.6133590	1.0745110	0.3401930	
10	Н	2.5212570	1.3481780	0.1375670	
11	H	-0.7767400	-1.6484490	1.7007460	
12	С	-2.4306990	-0.4553140	-0.5986290	
13	H	-2./618690	-0./198500	0.408/850	
14	H	-3.1688490	0.2253430	-1.0263690	
15	Н	-2.3959110	-1.3605100	-1.2102240	
16	-	400 40005505	2		
17	Energy:	-438.42025585	3		
18					
19					
20					
21		211	tau and anonau	of conformor.	The VVVT
22	R3TIL/0-	sii++G^^ geome	try and energy	of conformer:	IUL-XXVI
23	N	0 0633420	1 8760450	_0 8002950	
24	ц	-0 6911350	2 2811890	-0.8002950 -1.3437440	
25	C	-0.0618980	0 4246150	-0 7404920	
26	н	-0 2839710	0.0592170	-1 7473250	
27	C	1 2982590	-0.2071300	-0 3158400	
28	C	-1, 1897900	-0.0476620	0.1774590	
29	н	2 0078960	0 0821460	-1 1011540	
30	0	1.2036510	-1.6294900	-0.2295240	
31	0	-1.5031670	0.4832820	1.2141990	
32	H	0.8956790	-1.9844830	-1.0702380	
33	0	-1.8235030	-1.1400740	-0.3082810	
34	Н	-2.4854800	-1.4087570	0.3478570	
35	Н	0.0023140	2.2714150	0.1334010	
36	С	1.8210300	0.2769900	1.0274330	
37	Н	2.7765770	-0.2096730	1.2322450	
38	Н	1.9845790	1.3559740	1.0136360	
39	Н	1.1286850	0.0300450	1.8348720	
40					
41	Energy:	-438.41993422	4		
42					
43					
44					
45			_		
46	B3LYP/6-3	311++G** geome	try and energy	of conformer:	Thr-XXVII
47					
48	N	-0.1477480	-1.2451090	1.2118140	
49	H	0.5851420	-1.90/5620	1.4414960	
50		0.0718540	-0.6/50820	-0.1209180	
51	п	1 0005260	-1.4996220	-0.0339000	
52	C	-1.0990000 1.1566050	0.2391090	-0.3133370	
53	ч	_0 8773570	0.0029070	-U.244/22U _1 /087020	
54	0	-1 1125680	1 2122150	1.10/920	
55	0	2 <u>4141490</u>	-0 5827170	-0 6802200	
56	ч	_1 8417980	1 9129960	0 2790870	
57	0	1.5649110	1.2627530	0.2257370	
58	H	0.6808940	1.5922380	0.4806670	
59	Н	-0.1570900	-0.5225230	1.9244680	
60	С	-2.4393920	-0.4807500	-0.5560590	
	Н	-2.6576680	-0.9415590	0.4072180	

- 3 4	Н Н	-3.2413630	0.2181820	-0.8141730	
5	11	2.4240010	1.2012510	1.5214540	
6	Energy:	-438.41981170	1		
7					
8					
9					
10		211	+		
11	B3LIP/0-	-311++G^^ geome	try and energy	of conformer:	TUL-XXVIII
12	N	-0.6588050	1.8625360	-0.5595770	
14	H	-0.8737180	2.1075010	0.4000050	
15	С	-0.1266380	0.5143400	-0.6877920	
16	Н	-0.0600670	0.2732550	-1.7542180	
17	С	1.3184760	0.2840640	-0.1258770	
18	С	-1.0548320	-0.5348160	-0.1000970	
19	H	1.9287600	1.0845780	-0.5567530	
20	0	1.8/53450	-0.9201020	-0.6324910	
21	н	1 2382390	-1.6322210	-0.1781370	
22	0	-2.1114040	-0.0377660	0.5676020	
23	Н	-2.6090450	-0.7930570	0.9182420	
24 25	Н	-0.0077870	2.5449210	-0.9316010	
20	С	1.4101950	0.3578180	1.3984430	
20	Н	0.8479970	-0.4538100	1.8703310	
28	H	2.4534480	0.2621220	1.7046720	
29	Н	1.029/100	1.310/010	1.//80340	
30	Energy.	-438 41961825	9		
31	LINCL GY .	100.11001020			
32					
33					
33 34 25					
33 34 35 36	B3LYP/6-	-311++G** geome	try and energy	of conformer:	Thr-XXIX
33 34 35 36 37	B3LYP/6-	-311++G** geome	try and energy	of conformer:	Thr-XXIX
33 34 35 36 37 38	B3LYP/6- N	-311++G** geome -0.0871570 0.8440900	try and energy 1.9085340 2.3005820	of conformer: -0.3383170	Thr-XXIX
33 34 35 36 37 38 39	B3LYP/6- N H C	-311++G** geome -0.0871570 0.8440900 -0.0019850	try and energy 1.9085340 2.3005820 0.4566440	of conformer: -0.3383170 -0.4424250 -0.4779060	Thr-XXIX
33 34 35 36 37 38 39 40	B3LYP/6- N H C H	-311++G** geome -0.0871570 0.8440900 -0.0019850 0.1923090	try and energy 1.9085340 2.3005820 0.4566440 0.2206870	of conformer: -0.3383170 -0.4424250 -0.4779060 -1.5288930	Thr-XXIX
33 34 35 36 37 38 39 40 41	B3LYP/6- N H C H C	-311++G** geome -0.0871570 0.8440900 -0.0019850 0.1923090 1.1339210	try and energy 1.9085340 2.3005820 0.4566440 0.2206870 -0.1940040	of conformer: -0.3383170 -0.4424250 -0.4779060 -1.5288930 0.3705940	Thr-XXIX
33 34 35 36 37 38 39 40 41 42	B3LYP/6- N H C H C C	-311++G** geome -0.0871570 0.8440900 -0.0019850 0.1923090 1.1339210 -1.3450910	try and energy 1.9085340 2.3005820 0.4566440 0.2206870 -0.1940040 -0.1778920	of conformer: -0.3383170 -0.4424250 -0.4779060 -1.5288930 0.3705940 -0.1611230	Thr-XXIX
33 34 35 36 37 38 39 40 41 42 43	B3LYP/6- N H C H C C H	-311++G** geome -0.0871570 0.8440900 -0.0019850 0.1923090 1.1339210 -1.3450910 0.9463610	try and energy 1.9085340 2.3005820 0.4566440 0.2206870 -0.1940040 -0.1778920 0.0433070	of conformer: -0.3383170 -0.4424250 -0.4779060 -1.5288930 0.3705940 -0.1611230 1.4218420	Thr-XXIX
33 34 35 36 37 38 39 40 41 42 43 44	B3LYP/6- N H C H C H C	-311++G** geome -0.0871570 0.8440900 -0.0019850 0.1923090 1.1339210 -1.3450910 0.9463610 2.3638060	try and energy 1.9085340 2.3005820 0.4566440 0.2206870 -0.1940040 -0.1778920 0.0433070 0.4730740	of conformer: -0.3383170 -0.4424250 -0.4779060 -1.5288930 0.3705940 -0.1611230 1.4218420 0.0648070	Thr-XXIX
33 34 35 36 37 38 39 40 41 42 43 44 45	B3LYP/6- N H C H C C H O O	-311++G** geome -0.0871570 0.8440900 -0.0019850 0.1923090 1.1339210 -1.3450910 0.9463610 2.3638060 -1.8944520 2.7266250	try and energy 1.9085340 2.3005820 0.4566440 0.2206870 -0.1940040 -0.1778920 0.0433070 0.4730740 -1.0257130 0.0244400	of conformer: -0.3383170 -0.4424250 -0.4779060 -1.5288930 0.3705940 -0.1611230 1.4218420 0.0648070 -0.8164930 -0.7442420	Thr-XXIX
33 34 35 36 37 38 39 40 41 42 43 44 45 46 47	B3LYP/6- N H C H C C H O O H	-311++G** geome -0.0871570 0.8440900 -0.0019850 0.1923090 1.1339210 -1.3450910 0.9463610 2.3638060 -1.8944520 2.7266250 -1.8615880	try and energy 1.9085340 2.3005820 0.4566440 0.2206870 -0.1940040 -0.1778920 0.0433070 0.4730740 -1.0257130 0.0944400 0.2943260	of conformer: -0.3383170 -0.4424250 -0.4779060 -1.5288930 0.3705940 -0.1611230 1.4218420 0.0648070 -0.8164930 -0.7443420 1.0021790	Thr-XXIX
33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48	B3LYP/6- N H C H C C H O O H O H	-311++G** geome -0.0871570 0.8440900 -0.0019850 0.1923090 1.1339210 -1.3450910 0.9463610 2.3638060 -1.8944520 2.7266250 -1.8615880 -2.7138580	try and energy 1.9085340 2.3005820 0.4566440 0.2206870 -0.1940040 -0.1778920 0.0433070 0.4730740 -1.0257130 0.0944400 0.2943260 -0.1457640	of conformer: -0.3383170 -0.4424250 -0.4779060 -1.5288930 0.3705940 -0.1611230 1.4218420 0.0648070 -0.8164930 -0.7443420 1.0021790 1.1410130	Thr-XXIX
33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49	B3LYP/6- N H C H C H O O H O H H	-311++G** geome -0.0871570 0.8440900 -0.0019850 0.1923090 1.1339210 -1.3450910 0.9463610 2.3638060 -1.8944520 2.7266250 -1.8615880 -2.7138580 -0.4192310	try and energy 1.9085340 2.3005820 0.4566440 0.2206870 -0.1940040 -0.1778920 0.0433070 0.4730740 -1.0257130 0.0944400 0.2943260 -0.1457640 2.1558790	of conformer: -0.3383170 -0.4424250 -0.4779060 -1.5288930 0.3705940 -0.1611230 1.4218420 0.0648070 -0.8164930 -0.7443420 1.0021790 1.1410130 0.5889780	Thr-XXIX
33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50	B3LYP/6- N H C H C H O O H O H C	-311++G** geome -0.0871570 0.8440900 -0.0019850 0.1923090 1.1339210 -1.3450910 0.9463610 2.3638060 -1.8944520 2.7266250 -1.8615880 -2.7138580 -0.4192310 1.2605670	try and energy 1.9085340 2.3005820 0.4566440 0.2206870 -0.1940040 -0.1778920 0.0433070 0.4730740 -1.0257130 0.0944400 0.2943260 -0.1457640 2.1558790 -1.7019010	of conformer: -0.3383170 -0.4424250 -0.4779060 -1.5288930 0.3705940 -0.1611230 1.4218420 0.0648070 -0.8164930 -0.7443420 1.0021790 1.1410130 0.5889780 0.1872100	Thr-XXIX
33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51	B3LYP/6- N H C H C C H O O H O H H C H	-311++G** geome -0.0871570 0.8440900 -0.0019850 0.1923090 1.1339210 -1.3450910 0.9463610 2.3638060 -1.8944520 2.7266250 -1.8615880 -2.7138580 -0.4192310 1.2605670 0.3531380	try and energy 1.9085340 2.3005820 0.4566440 0.2206870 -0.1940040 -0.1778920 0.0433070 0.4730740 -1.0257130 0.0944400 0.2943260 -0.1457640 2.1558790 -1.7019010 -2.2245160	of conformer: -0.3383170 -0.4424250 -0.4779060 -1.5288930 0.3705940 -0.1611230 1.4218420 0.0648070 -0.8164930 -0.7443420 1.0021790 1.1410130 0.5889780 0.1872100 0.4975750	Thr-XXIX
33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52	B3LYP/6- N H C H C C H O H H C H H H	-311++G** geome -0.0871570 0.8440900 -0.0019850 0.1923090 1.1339210 -1.3450910 0.9463610 2.3638060 -1.8944520 2.7266250 -1.8615880 -2.7138580 -0.4192310 1.2605670 0.3531380 1.4391160	try and energy 1.9085340 2.3005820 0.4566440 0.2206870 -0.1940040 -0.1778920 0.0433070 0.4730740 -1.0257130 0.0944400 0.2943260 -0.1457640 2.1558790 -1.7019010 -2.2245160 -1.9549470	of conformer: -0.3383170 -0.4424250 -0.4779060 -1.5288930 0.3705940 -0.1611230 1.4218420 0.0648070 -0.8164930 -0.7443420 1.0021790 1.1410130 0.5889780 0.1872100 0.4975750 -0.8639970	Thr-XXIX
33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53	B3LYP/6- N H C H C C H O O H O H H C H H H H	-311++G** geome -0.0871570 0.8440900 -0.0019850 0.1923090 1.1339210 -1.3450910 0.9463610 2.3638060 -1.8944520 2.7266250 -1.8615880 -2.7138580 -0.4192310 1.2605670 0.3531380 1.4391160 2.0949480	try and energy 1.9085340 2.3005820 0.4566440 0.2206870 -0.1940040 -0.1778920 0.0433070 0.4730740 -1.0257130 0.0944400 0.2943260 -0.1457640 2.1558790 -1.7019010 -2.2245160 -1.9549470 -2.0799850	of conformer: -0.3383170 -0.4424250 -0.4779060 -1.5288930 0.3705940 -0.1611230 1.4218420 0.0648070 -0.8164930 -0.7443420 1.0021790 1.1410130 0.5889780 0.1872100 0.4975750 -0.8639970 0.7818750	Thr-XXIX
33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54	B3LYP/6- N H C H C H O O H O H H H H H H	-311++G** geome -0.0871570 0.8440900 -0.0019850 0.1923090 1.1339210 -1.3450910 0.9463610 2.3638060 -1.8944520 2.7266250 -1.8615880 -2.7138580 -0.4192310 1.2605670 0.3531380 1.4391160 2.0949480	try and energy 1.9085340 2.3005820 0.4566440 0.2206870 -0.1940040 -0.1778920 0.0433070 0.4730740 -1.0257130 0.0944400 0.2943260 -0.1457640 2.1558790 -1.7019010 -2.2245160 -1.9549470 -2.0799850	of conformer: -0.3383170 -0.4424250 -0.4779060 -1.5288930 0.3705940 -0.1611230 1.4218420 0.0648070 -0.8164930 -0.7443420 1.0021790 1.1410130 0.5889780 0.1872100 0.4975750 -0.8639970 0.7818750	Thr-XXIX
33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55	B3LYP/6- N H C H C C H O O H O H H C H H H Energy:	-311++G** geome -0.0871570 0.8440900 -0.0019850 0.1923090 1.1339210 -1.3450910 0.9463610 2.3638060 -1.8944520 2.7266250 -1.8615880 -2.7138580 -0.4192310 1.2605670 0.3531380 1.4391160 2.0949480 -438.41948404	try and energy 1.9085340 2.3005820 0.4566440 0.2206870 -0.1940040 -0.1778920 0.0433070 0.4730740 -1.0257130 0.0944400 0.2943260 -0.1457640 2.1558790 -1.7019010 -2.2245160 -1.9549470 -2.0799850 9	of conformer: -0.3383170 -0.4424250 -0.4779060 -1.5288930 0.3705940 -0.1611230 1.4218420 0.0648070 -0.8164930 -0.7443420 1.0021790 1.1410130 0.5889780 0.1872100 0.4975750 -0.8639970 0.7818750	Thr-XXIX
33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 7	B3LYP/6- N H C C H O O H O H H C H H H Energy:	-311++G** geome -0.0871570 0.8440900 -0.0019850 0.1923090 1.1339210 -1.3450910 0.9463610 2.3638060 -1.8944520 2.7266250 -1.8615880 -2.7138580 -0.4192310 1.2605670 0.3531380 1.4391160 2.0949480 -438.41948404	try and energy 1.9085340 2.3005820 0.4566440 0.2206870 -0.1940040 -0.1778920 0.0433070 0.4730740 -1.0257130 0.0944400 0.2943260 -0.1457640 2.1558790 -1.7019010 -2.2245160 -1.9549470 -2.0799850 9	of conformer: -0.3383170 -0.4424250 -0.4779060 -1.5288930 0.3705940 -0.1611230 1.4218420 0.0648070 -0.8164930 -0.7443420 1.0021790 1.1410130 0.5889780 0.1872100 0.4975750 -0.8639970 0.7818750	Thr-XXIX
33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58	B3LYP/6- N H C H C H O O H O H H H H Energy:	-311++G** geome -0.0871570 0.8440900 -0.0019850 0.1923090 1.1339210 -1.3450910 0.9463610 2.3638060 -1.8944520 2.7266250 -1.8615880 -2.7138580 -0.4192310 1.2605670 0.3531380 1.4391160 2.0949480 -438.41948404	try and energy 1.9085340 2.3005820 0.4566440 0.2206870 -0.1940040 -0.1778920 0.0433070 0.4730740 -1.0257130 0.0944400 0.2943260 -0.1457640 2.1558790 -1.7019010 -2.2245160 -1.9549470 -2.0799850 9	of conformer: -0.3383170 -0.4424250 -0.4779060 -1.5288930 0.3705940 -0.1611230 1.4218420 0.0648070 -0.8164930 -0.7443420 1.0021790 1.1410130 0.5889780 0.1872100 0.4975750 -0.8639970 0.7818750	Thr-XXIX
33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58	B3LYP/6- N H C H C H O H O H H C H H H Energy:	-311++G** geome -0.0871570 0.8440900 -0.0019850 0.1923090 1.1339210 -1.3450910 0.9463610 2.3638060 -1.8944520 2.7266250 -1.8615880 -2.7138580 -0.4192310 1.2605670 0.3531380 1.4391160 2.0949480 -438.41948404	try and energy 1.9085340 2.3005820 0.4566440 0.2206870 -0.1940040 -0.1778920 0.0433070 0.4730740 -1.0257130 0.0944400 0.2943260 -0.1457640 2.1558790 -1.7019010 -2.2245160 -1.9549470 -2.0799850 9	of conformer: -0.3383170 -0.4424250 -0.4779060 -1.5288930 0.3705940 -0.1611230 1.4218420 0.0648070 -0.8164930 -0.7443420 1.0021790 1.1410130 0.5889780 0.1872100 0.4975750 -0.8639970 0.7818750	Thr-XXIX
33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60	B3LYP/6- N H C C H O O H H C H H H Energy: B3LYP/6-	-311++G** geome -0.0871570 0.8440900 -0.0019850 0.1923090 1.1339210 -1.3450910 0.9463610 2.3638060 -1.8944520 2.7266250 -1.8615880 -2.7138580 -0.4192310 1.2605670 0.3531380 1.4391160 2.0949480 -438.41948404	try and energy 1.9085340 2.3005820 0.4566440 0.2206870 -0.1940040 -0.1778920 0.0433070 0.4730740 -1.0257130 0.0944400 0.2943260 -0.1457640 2.1558790 -1.7019010 -2.2245160 -1.9549470 -2.0799850 9	of conformer: -0.3383170 -0.4424250 -0.4779060 -1.5288930 0.3705940 -0.1611230 1.4218420 0.0648070 -0.8164930 -0.7443420 1.0021790 1.1410130 0.5889780 0.1872100 0.4975750 -0.8639970 0.7818750 of conformer:	Thr-XXIX
33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60	B3LYP/6- N H C H C C H O O H O H H H Energy: B3LYP/6-	-311++G** geome -0.0871570 0.8440900 -0.0019850 0.1923090 1.1339210 -1.3450910 0.9463610 2.3638060 -1.8944520 2.7266250 -1.8615880 -2.7138580 -0.4192310 1.2605670 0.3531380 1.4391160 2.0949480 -438.41948404 -311++G** geome	try and energy 1.9085340 2.3005820 0.4566440 0.2206870 -0.1940040 -0.1778920 0.0433070 0.4730740 -1.0257130 0.0944400 0.2943260 -0.1457640 2.1558790 -1.7019010 -2.2245160 -1.9549470 -2.0799850 9 try and energy	of conformer: -0.3383170 -0.4424250 -0.4779060 -1.5288930 0.3705940 -0.1611230 1.4218420 0.0648070 -0.8164930 -0.7443420 1.0021790 1.1410130 0.5889780 0.1872100 0.4975750 -0.8639970 0.7818750 of conformer:	Thr-XXIX

Н	-0.3394860	2.1550230	0.6266150	
C	0.0020860	0.4569830	-0.4730680	
Н	0.1949150	0.2311420	-1.5244370	
2	1.1319070	-0.2085120	0.3550460	
C	-1.3445060	-0.1710060	-0.1495830	
H	0.9485110	0.0075140	1.4169540	
0	2.3226510	0.4689490	-0.0699170	
0	-1.9255980	-0.9801220	-0.8250050	
н	3.0684270	0.1400290	0.4412950	
0	-1.8296330	0.2700200	1.0397620	
Н	-2.6914500	-0.1521820	1.1750310	
Н	0.8253190	2.3116030	-0.5171120	
C	1.2462170	-1,7147260	0.1400390	
Н	0.3470720	-2.2376420	0.4754280	
Н	1,4024770	-1.9410030	-0.9175840	
H	2.0919340	-2.1172240	0.7062960	
Energy:	-438.41944597	3		
21				
B3LYP/6-	-311++G** geome	try and energy	of conformer: T	hr-XXX
N	0.0226880	1.8829110	-0.7477320	
Н	-0.0475930	2.2518860	0.1961090	
С	-0.0780880	0.4250940	-0.7315620	
Н	-0.3173430	0.0781800	-1.7377690	
С	1.2917580	-0.1916710	-0.3632020	
С	-1.1765330	-0.0745510	0.2105690	
Н	1.9746650	0.1220520	-1.1627080	
0	1.1024600	-1.6101060	-0.4094690	
0	-1.3502240	0.3354120	1.3341080	
Н	1.9148880	-2.0402240	-0.1257220	
0	-1.9709380	-1.0041770	-0.3579820	
Н	-2.6198160	-1.2768510	0.3094590	
Н	-0.7344130	2.2887150	-1.2864540	
С	1.8584040	0.2592780	0.9793800	
Н	1.1961620	-0.0108780	1.8036750	
Н	2.8334410	-0.2111340	1.1445750	
Н	2.0175620	1.3399410	0.9885940	
Energy:	-438.41917785	8		
B3LYP/6-	-311++G** geome	try and energy	of conformer: T	hr-XXX
N	0.2123150	1.7949590	-0.3540140	
Н	-0.6767870	2.2832420	-0.3203950	
С	0.0569650	0.4803330	0.2767830	
Н	-0.0193580	0.5335320	1.3775230	
С	-1.2174430	-0.1968910	-0.2613670	
С	1.3191750	-0.3137730	-0.0449410	
Н	-1.1067690	-0.3137230	-1.3410020	
0	-2.3212590	0.7096960	-0.0993030	
0	1.4054250	-1.2877890	-0.7470460	
Н	-2.6666440	0.6159610	0.7955320	
0	2.3952080	0.2415500	0.5669980	
Н	3.1774180	-0.2592300	0.2892040	

Н	0.9145200	2.3493500	0.1220400	
С	-1.5167480	-1.5426150	0.3866820	
Н	-0.7189440	-2.2590610	0.1894470	
Н	-1.6275550	-1.4392730	1.4731840	
Н	-2.4487760	-1.9454950	-0.0155640	
Energy:	-438.41874399	7		
B3LYP/6-	-311++G** geome	try and energy	of conformer:	Thr-XXXII
Ν	0.1397450	1.8101650	-0.2514790	
Н	-0.0758470	1.9704100	0.7270110	
С	-0.0141670	0.4038760	-0.5759280	
Н	0.0054740	0.2835100	-1.6651870	
С	1.0553640	-0.5714780	-0.0099780	
С	-1.3937160	-0.0493330	-0.1107970	
H	0.7677450	-1.5828450	-0.3236360	
0	0.9793940	-0.4663570	1.4144760	
U	-2.1132080	0.5439400	0.6462270	
п	1.7270600	-1.0/12/90	L.809/940	
U Ц	-1.121969U	-1.24/9100	-U.030391U _0 2061720	
п u	-2.3939090	-1.4910460	-0.2961730	
C	2 4603480	-0 2720870	-0 5254650	
Н	2.7932880	0.7235320	-0.2209950	
Н	3.1748030	-0.9969400	-0.1233010	
Н	2.5001960	-0.3416580	-1.6164960	
	120 11061772	-		
Energy:	-430.41001//3	Ţ		
Energy:	-430.41001//3	1	62	
B3LYP/6-	-438.41881773 -311++G** geome	l try and energy	of conformer:	Thr-XXXIV
Energy: B3LYP/6- N	-438.41861773 -311++G** geome -0.0864220	1 try and energy 1.8827520	of conformer: -0.3881530	Thr-XXXIV
Energy: B3LYP/6- N H	-438.41861773 -311++G** geome -0.0864220 -0.2161500	1 try and energy 1.8827520 2.1985570	<pre>v of conformer: -0.3881530 0.5669810</pre>	Thr-XXXIV
Energy: B3LYP/6- N H C	-438.41861773 -311++G** geome -0.0864220 -0.2161500 -0.0010770	1 try and energy 1.8827520 2.1985570 0.4273660	<pre>v of conformer: -0.3881530 0.5669810 -0.4907660</pre>	Thr-XXXIV
Energy: B3LYP/6- N H C H	-438.41861773 -311++G** geome -0.0864220 -0.2161500 -0.0010770 0.1749660	1 try and energy 1.8827520 2.1985570 0.4273660 0.1758490	<pre>of conformer: -0.3881530 0.5669810 -0.4907660 -1.5384330</pre>	Thr-XXXIV
Energy: B3LYP/6- N H C H C	-438.41861773 -311++G** geome -0.0864220 -0.2161500 -0.0010770 0.1749660 1.1311440	1 try and energy 1.8827520 2.1985570 0.4273660 0.1758490 -0.2344060	<pre>v of conformer: -0.3881530 0.5669810 -0.4907660 -1.5384330 0.3526040</pre>	Thr-XXXIV
Energy: B3LYP/6- N H C H C C	-438.41861773 -311++G** geome -0.0864220 -0.2161500 -0.0010770 0.1749660 1.1311440 -1.3535260	1 try and energy 1.8827520 2.1985570 0.4273660 0.1758490 -0.2344060 -0.1684670	<pre>v of conformer: -0.3881530 0.5669810 -0.4907660 -1.5384330 0.3526040 -0.1313090</pre>	Thr-XXXIV
Energy: B3LYP/6- N H C C H	-438.41861773 -311++G** geome -0.0864220 -0.2161500 -0.0010770 0.1749660 1.1311440 -1.3535260 0.9098310	1 try and energy 1.8827520 2.1985570 0.4273660 0.1758490 -0.2344060 -0.1684670 -0.0636140	<pre>v of conformer: -0.3881530 0.5669810 -0.4907660 -1.5384330 0.3526040 -0.1313090 1.4151150</pre>	Thr-XXXIV
Energy: B3LYP/6- N H C H C H O O	-438.41861773 -311++G** geome -0.0864220 -0.2161500 -0.0010770 0.1749660 1.1311440 -1.3535260 0.9098310 2.3847960	1 try and energy 1.8827520 2.1985570 0.4273660 0.1758490 -0.2344060 -0.1684670 -0.0636140 0.3704120	<pre>v of conformer: -0.3881530 0.5669810 -0.4907660 -1.5384330 0.3526040 -0.1313090 1.4151150 0.0237010</pre>	Thr-XXXIV
Energy: B3LYP/6- N H C H C C H O O	-438.41861773 -311++G** geome -0.0864220 -0.2161500 -0.0010770 0.1749660 1.1311440 -1.3535260 0.9098310 2.3847960 -1.9740550	1 try and energy 1.8827520 2.1985570 0.4273660 0.1758490 -0.2344060 -0.1684670 -0.0636140 0.3704120 -0.9640620	<pre> of conformer: -0.3881530 0.5669810 -0.4907660 -1.5384330 0.3526040 -0.1313090 1.4151150 0.0237010 -0.7870780 0.4110010 -0.41100010 -0.41100 -0.411000 -0.411000 -0.411000 -0.411000</pre>	Thr-XXXIV
Energy: B3LYP/6- N H C C H C H O O H	-438.41861773 -311++G** geome -0.2161500 -0.0010770 0.1749660 1.1311440 -1.3535260 0.9098310 2.3847960 -1.9740550 2.4158190	1 try and energy 1.8827520 2.1985570 0.4273660 0.1758490 -0.2344060 -0.1684670 -0.0636140 0.3704120 -0.9640620 1.2504100	<pre> of conformer: -0.3881530 0.5669810 -0.4907660 -1.5384330 0.3526040 -0.1313090 1.4151150 0.0237010 -0.7870780 0.4118210 1.07267222 -0.13120 1.07267222 -0.13120 -0.7870780 0.4118210 1.0726722 -0.13120 1.0726722 -0.13120 -</pre>	Thr-XXXIV
Energy: B3LYP/6- N H C C H C C H O O H O U	-438.41861773 -311++G** geome -0.2161500 -0.0010770 0.1749660 1.1311440 -1.3535260 0.9098310 2.3847960 -1.9740550 2.4158190 -1.7894910	1 try and energy 1.8827520 2.1985570 0.4273660 0.1758490 -0.2344060 -0.1684670 -0.0636140 0.3704120 -0.9640620 1.2504100 0.2860150	<pre> of conformer: -0.3881530 0.5669810 -0.4907660 -1.5384330 0.3526040 -0.1313090 1.4151150 0.0237010 -0.7870780 0.4118210 1.0726780 1.2206000 </pre>	Thr-XXXIV
Energy: B3LYP/6- N H C H C C H O O H O H	-438.41861773 -311++G** geome -0.0864220 -0.2161500 -0.0010770 0.1749660 1.1311440 -1.3535260 0.9098310 2.3847960 -1.9740550 2.4158190 -1.7894910 -2.6553420 0.7242820	1 try and energy 1.8827520 2.1985570 0.4273660 0.1758490 -0.2344060 -0.1684670 -0.0636140 0.3704120 -0.9640620 1.2504100 0.2860150 -0.1165290 2.3317070	<pre>v of conformer: -0.3881530 0.5669810 -0.4907660 -1.5384330 0.3526040 -0.1313090 1.4151150 0.0237010 -0.7870780 0.4118210 1.0726780 1.2386080 -0.786020</pre>	Thr-XXXIV
Energy: B3LYP/6- N H C H C C H O O H O H C	-438.41861773 -311++G** geome -0.0864220 -0.2161500 -0.0010770 0.1749660 1.1311440 -1.3535260 0.9098310 2.3847960 -1.9740550 2.4158190 -1.7894910 -2.6553420 0.7242920 1.2769300	1 try and energy 1.8827520 2.1985570 0.4273660 0.1758490 -0.2344060 -0.1684670 -0.0636140 0.3704120 -0.9640620 1.2504100 0.2860150 -0.1165290 2.3317870 -1.7244850	<pre> of conformer: -0.3881530 0.5669810 -0.4907660 -1.5384330 0.3526040 -0.1313090 1.4151150 0.0237010 -0.7870780 0.4118210 1.0726780 1.2386080 -0.7964030 0.0857050 0.0857050 </pre>	Thr-XXXIV
Energy: B3LYP/6- N H C H C C H O O H O H H C H H C H	-438.41861773 -311++G** geome -0.0864220 -0.2161500 -0.0010770 0.1749660 1.1311440 -1.3535260 0.9098310 2.3847960 -1.9740550 2.4158190 -1.7894910 -2.6553420 0.7242920 1.2769300 1.5242280	1 try and energy 1.8827520 2.1985570 0.4273660 0.1758490 -0.2344060 -0.1684670 -0.0636140 0.3704120 -0.9640620 1.2504100 0.2860150 -0.1165290 2.3317870 -1.7244850 -1.8972410	<pre> of conformer: -0.3881530 0.5669810 -0.4907660 -1.5384330 0.3526040 -0.1313090 1.4151150 0.0237010 -0.7870780 0.4118210 1.0726780 1.2386080 -0.7964030 0.0857050 -0.9649690 -0.96496</pre>	Thr-XXXIV
Energy: B3LYP/6- N H C H C H O H H C H H H	-438.41861773 -311++G** geome -0.0864220 -0.2161500 -0.0010770 0.1749660 1.1311440 -1.3535260 0.9098310 2.3847960 -1.9740550 2.4158190 -1.7894910 -2.6553420 0.7242920 1.2769300 1.5242280 2.0815620	1 try and energy 1.8827520 2.1985570 0.4273660 0.1758490 -0.2344060 -0.1684670 -0.0636140 0.3704120 -0.9640620 1.2504100 0.2860150 -0.1165290 2.3317870 -1.7244850 -1.8972410 -2.1339670	<pre> of conformer: -0.3881530 0.5669810 -0.4907660 -1.5384330 0.3526040 -0.1313090 1.4151150 0.0237010 -0.7870780 0.4118210 1.0726780 1.2386080 -0.7964030 0.0857050 -0.9649690 0.6989200 </pre>	Thr-XXXIV
Energy: B3LYP/6- N H C C H C C H O O H H C H H H H	-438.41861773 -311++G** geome -0.0864220 -0.2161500 -0.0010770 0.1749660 1.1311440 -1.3535260 0.9098310 2.3847960 -1.9740550 2.4158190 -1.7894910 -2.6553420 0.7242920 1.2769300 1.5242280 2.0815620 0.3549300	1 try and energy 1.8827520 2.1985570 0.4273660 0.1758490 -0.2344060 -0.1684670 -0.0636140 0.3704120 -0.9640620 1.2504100 0.2860150 -0.1165290 2.3317870 -1.7244850 -1.8972410 -2.1339670 -2.2634800	<pre> of conformer: -0.3881530 0.5669810 -0.4907660 -1.5384330 0.3526040 -0.1313090 1.4151150 0.0237010 -0.7870780 0.4118210 1.0726780 1.2386080 -0.7964030 0.0857050 -0.9649690 0.6989200 0.3136280 </pre>	Thr-XXXIV
Energy: B3LYP/6- N H C C H O O H O H H C H H H Energy:	-438.41861773 -311++G** geome -0.0864220 -0.2161500 -0.0010770 0.1749660 1.1311440 -1.3535260 0.9098310 2.3847960 -1.9740550 2.4158190 -1.7894910 -2.6553420 0.7242920 1.2769300 1.5242280 2.0815620 0.3549300 -438.41855534	1 try and energy 1.8827520 2.1985570 0.4273660 0.1758490 -0.2344060 -0.1684670 -0.0636140 0.3704120 -0.9640620 1.2504100 0.2860150 -0.1165290 2.3317870 -1.7244850 -1.8972410 -2.1339670 -2.2634800 1	<pre> of conformer: -0.3881530 0.5669810 -0.4907660 -1.5384330 0.3526040 -0.1313090 1.4151150 0.0237010 -0.7870780 0.4118210 1.0726780 1.2386080 -0.7964030 0.0857050 -0.9649690 0.6989200 0.3136280 -0.3136280 -0.3126280 -0.3136280</pre>	Thr-XXXIV
Energy: B3LYP/6- N H C C H O O H H C H H H Energy: B3LYP/6-	-438.41861773 -311++G** geome -0.0864220 -0.2161500 -0.0010770 0.1749660 1.1311440 -1.3535260 0.9098310 2.3847960 -1.9740550 2.4158190 -1.7894910 -2.6553420 0.7242920 1.2769300 1.5242280 2.0815620 0.3549300 -438.41855534 -311++G** geome	1 try and energy 1.8827520 2.1985570 0.4273660 0.1758490 -0.2344060 -0.1684670 -0.0636140 0.3704120 -0.9640620 1.2504100 0.2860150 -0.1165290 2.3317870 -1.7244850 -1.8972410 -2.1339670 -2.2634800 1 try and energy	<pre> of conformer: -0.3881530 0.5669810 -0.4907660 -1.5384330 0.3526040 -0.1313090 1.4151150 0.0237010 -0.7870780 0.4118210 1.0726780 1.2386080 -0.7964030 0.0857050 -0.9649690 0.6989200 0.3136280 v of conformer: </pre>	Thr-XXXIV
Energy: B3LYP/6- N H C C H C C H O O H H C H H E nergy: B3LYP/6- N	-438.41861773 -311++G** geome -0.0864220 -0.2161500 -0.0010770 0.1749660 1.1311440 -1.3535260 0.9098310 2.3847960 -1.9740550 2.4158190 -1.7894910 -2.6553420 0.7242920 1.2769300 1.5242280 2.0815620 0.3549300 -438.41855534 -311++G** geome 0.0917630	1 try and energy 1.8827520 2.1985570 0.4273660 0.1758490 -0.2344060 -0.1684670 -0.0636140 0.3704120 -0.9640620 1.2504100 0.2860150 -0.1165290 2.3317870 -1.7244850 -1.8972410 -2.1339670 -2.2634800 1 try and energy 1.6853540	<pre> of conformer: -0.3881530 0.5669810 -0.4907660 -1.5384330 0.3526040 -0.1313090 1.4151150 0.0237010 -0.7870780 0.4118210 1.0726780 1.2386080 -0.7964030 0.0857050 -0.9649690 0.6989200 0.3136280 v of conformer: -0.2798000</pre>	Thr-XXXI Thr-XXXV

ч	_0 /573790	2 2698680	_0 9028850	
C	-0.0286220	0.2636940	-0.6443290	
H	0.0338930	0.0834860	-1.7237960	
С	1.0799940	-0.5797020	0.0323560	
C	-1.4007230	-0.2774530	-0.2038580	
н	0.8497840	-1.6226300	-0.1935980	
0	1.0101390	-0.4903110	1.4529150	
0	-1.8562380	-1.2992030	-0.6415960	
Н	1,1248270	0.4298200	1,7167150	
0	-2.0433920	0.4716800	0.7065130	
H	-1.4565220	1.2216190	0.9216580	
Н	1.0504170	2.0097190	-0.3530370	
С	2.4818140	-0.2565940	-0.4865930	
H	3.2025490	-0.9315590	-0.0218990	
Н	2.5402450	-0.3805410	-1.5715970	
Н	2.7909960	0.7657420	-0.2410720	
Energy:	-438.41854432	5		
/ c				_,
B3LYP/6-	311++G** geome	try and energy	of conformer:	Thr-XXXV1
N	0.0708310	1.7809980	-0.1976800	
Н	0.0381060	1.8727830	0.8122810	
С	-0.0054870	0.3829930	-0.5890670	
Н	0.0662670	0.3254570	-1.6797750	
С	1.0896840	-0.5581780	-0.0195660	
С	-1.3608240	-0.2378110	-0.2528200	
Н	0.8456220	-1.5733960	-0.3543720	
0	0.9684250	-0.4745010	1.4062670	
0	-1.7204550	-1.3074780	-0.6828650	
H	1.5656060	-1.1104280	1.8115760	
0	-2.1098740	0.5017770	0.5853340	
H	-2.9204380	-0.0015630	0.7557710	
Н	0.9318380	2.2026780	-0.5260350	
С	2.4941150	-0.1908780	-0.4875280	
H	3.2286470	-0.8853190	-0.0687510	
Н	2.5702870	-0.2492170	-1.5774300	
Н	2.7685560	0.8168790	-0.1655030	
Energy:	-438.41843498	8		
B3LYP/6-	311++G** geome	try and energy	of conformer:	Thr-XXXVII
N	0.1090110	1,9085680	-0.2778820	
Н	-0.3578410	2.1975030	0.5789480	
С	-0.0143240	0.4593990	-0.4314020	
Н	0.1500950	0.2129880	-1.4866650	
С	1.1425100	-0.1986680	0.3784840	
С	-1.3823120	-0.0619370	0.0293890	
Н	0.9671800	0.0404480	1.4388440	
0	2.3633750	0.3772310	-0.0516370	
0	-2.0275380	0.4690960	0.8914280	
Н	2.1914600	1.3290880	-0.1272750	
0	-1.8428990	-1.1886880	-0.5711610	
Н	-1.2186910	-1.4986880	-1.2390940	
Н	-0.3412570	2.4005820	-1.0417190	
3	1.2544310	-1.7061750	0.2142150	

Н	0.3869450	-2.2252250	0.6278000	
Н	1.3719730	-1.9740750	-0.8411230	
Н	2.1417280	-2.0594170	0.7423000	
Energy:	-438.41826893	57		
B3LYP/6-	311++G** geome	etry and energy	of conformer:	Thr-2
Ν	-0.0445150	1.8411230	-0.8161040	
Н	-0.0854710	2.2370770	0.1167920	
С	-0.0751130	0.3824500	-0.7732460	
Н	-0.2465950	0.0247420	-1.7923700	
С	1.3084440	-0.1752870	-0.3296780	
С	-1.2177640	-0.2315310	0.0386100	
Н	2.0057670	0.1160630	-1.1257520	
0	1.2658630	-1.5965570	-0.2013670	
0	-1.9137270	-1.1417590	-0.3353580	
Н	0.9285230	-1.9878970	-1.0146650	
0	-1.3906670	0.3723350	1.2411960	
Н	-2.1212720	-0.0818210	1.6879910	
Н	-0.8311320	2.2083060	-1.3400340	
С	1.8274690	0.3648290	0.9943180	
Н	1.1554670	0.1140490	1.8169030	
Н	2.8026100	-0.0815240	1.1987580	
Н	1.9537470	1.4482280	0.9493130	
Energy:	-438.41821867	7		
Energy: B3LYP/6-	-438.41821867 311++G** geome	7 etry and energy	of conformer:	Thr-
Energy: B3LYP/6- N	-438.41821867 311++G** geome -0.0830810	7 etry and energy 1.8518360	of conformer: 0.3146390	Thr-
Energy: B3LYP/6- N H	-438.41821867 311++G** geome -0.0830810 -0.7244710	27 etry and energy 1.8518360 2.4595480	of conformer: 0.3146390 -0.1843000	Thr-
Energy: B3LYP/6- N H C	-438.41821867 311++G** geome -0.0830810 -0.7244710 -0.0226530	etry and energy 1.8518360 2.4595480 0.5332950	of conformer: 0.3146390 -0.1843000 -0.3298020	Thr-
Energy: B3LYP/6- N H C H	-438.41821867 311++G** geome -0.0830810 -0.7244710 -0.0226530 0.1033300	27 etry and energy 1.8518360 2.4595480 0.5332950 0.5918830	of conformer: 0.3146390 -0.1843000 -0.3298020 -1.4199590	Thr-
Energy: B3LYP/6- N H C H C	-438.41821867 311++G** geome -0.0830810 -0.7244710 -0.0226530 0.1033300 1.1584090	27 etry and energy 1.8518360 2.4595480 0.5332950 0.5918830 -0.2637270	of conformer: 0.3146390 -0.1843000 -0.3298020 -1.4199590 0.2390910	Thr-
Energy: B3LYP/6- N H C H C C	-438.41821867 311++G** geome -0.0830810 -0.7244710 -0.0226530 0.1033300 1.1584090 -1.3827400	27 etry and energy 1.8518360 2.4595480 0.5332950 0.5918830 -0.2637270 -0.1201750	of conformer: 0.3146390 -0.1843000 -0.3298020 -1.4199590 0.2390910 -0.1003520	Thr-
Energy: B3LYP/6- N H C H C C H H	-438.41821867 311++G** geome -0.0830810 -0.7244710 -0.0226530 0.1033300 1.1584090 -1.3827400 1.0219930	27 etry and energy 1.8518360 2.4595480 0.5332950 0.5918830 -0.2637270 -0.1201750 -0.3505930	of conformer: 0.3146390 -0.1843000 -0.3298020 -1.4199590 0.2390910 -0.1003520 1.3222030	Thr-
Energy: B3LYP/6- N H C H C C H O	-438.41821867 311++G** geome -0.0830810 -0.7244710 -0.0226530 0.1033300 1.1584090 -1.3827400 1.0219930 2.3102310	27 etry and energy 1.8518360 2.4595480 0.5332950 0.5918830 -0.2637270 -0.1201750 -0.3505930 0.5542040	of conformer: 0.3146390 -0.1843000 -0.3298020 -1.4199590 0.2390910 -0.1003520 1.3222030 -0.0344630	Thr-
Energy: B3LYP/6- N H C H C C H O O	-438.41821867 311++G** geome -0.0830810 -0.7244710 -0.0226530 0.1033300 1.1584090 -1.3827400 1.0219930 2.3102310 -2.3156460	27 2.4595480 0.5332950 0.5918830 -0.2637270 -0.1201750 -0.3505930 0.5542040 -0.0052540	<pre>of conformer: 0.3146390 -0.1843000 -0.3298020 -1.4199590 0.2390910 -0.1003520 1.3222030 -0.0344630 -0.8557080</pre>	Thr-
Energy: B3LYP/6- N H C C H C C H O O H	-438.41821867 311++G** geome -0.0830810 -0.7244710 -0.0226530 0.1033300 1.1584090 -1.3827400 1.0219930 2.3102310 -2.3156460 3.0688680	27 2.4595480 0.5332950 0.5918830 -0.2637270 -0.1201750 -0.3505930 0.5542040 -0.0052540 0.1872910	<pre>of conformer: 0.3146390 -0.1843000 -0.3298020 -1.4199590 0.2390910 -0.1003520 1.3222030 -0.0344630 -0.8557080 0.4293310</pre>	Thr-
Energy: B3LYP/6- N H C C H C C H O O O H O O	-438.41821867 311++G** geome -0.0830810 -0.7244710 -0.0226530 0.1033300 1.1584090 -1.3827400 1.0219930 2.3102310 -2.3156460 3.0688680 -1.4680440	27 etry and energy 1.8518360 2.4595480 0.5332950 0.5918830 -0.2637270 -0.1201750 -0.3505930 0.5542040 -0.0052540 0.1872910 -0.8050750	<pre> of conformer: 0.3146390 -0.1843000 -0.3298020 -1.4199590 0.2390910 -0.1003520 1.3222030 -0.0344630 -0.8557080 0.4293310 1.0623800 </pre>	Thr-
Energy: B3LYP/6- N H C H C C H O O H O H	-438.41821867 311++G** geome -0.0830810 -0.7244710 -0.0226530 0.1033300 1.1584090 -1.3827400 1.0219930 2.3102310 -2.3156460 3.0688680 -1.4680440 -2.3826060	27 etry and energy 1.8518360 2.4595480 0.5332950 0.5918830 -0.2637270 -0.1201750 -0.3505930 0.5542040 -0.0052540 0.1872910 -0.8050750 -1.1161140	<pre>of conformer: 0.3146390 -0.1843000 -0.3298020 -1.4199590 0.2390910 -0.1003520 1.3222030 -0.0344630 -0.8557080 0.4293310 1.0623800 1.1440460</pre>	Thr-
Energy: B3LYP/6- N H C H C C H O O H H O H H	-438.41821867 311++G** geome -0.0830810 -0.7244710 -0.0226530 0.1033300 1.1584090 -1.3827400 1.0219930 2.3102310 -2.3156460 3.0688680 -1.4680440 -2.3826060 0.8412870	27 etry and energy 1.8518360 2.4595480 0.5332950 0.5918830 -0.2637270 -0.1201750 -0.3505930 0.5542040 -0.0052540 0.1872910 -0.8050750 -1.1161140 2.2700580	<pre>of conformer: 0.3146390 -0.1843000 -0.3298020 -1.4199590 0.2390910 -0.1003520 1.3222030 -0.0344630 -0.8557080 0.4293310 1.0623800 1.1440460 0.2776170</pre>	Thr-
Energy: B3LYP/6- N H C C H C C H O O H H O H H C	-438.41821867 311++G** geome -0.0830810 -0.7244710 -0.0226530 0.1033300 1.1584090 -1.3827400 1.0219930 2.3102310 -2.3156460 3.0688680 -1.4680440 -2.3826060 0.8412870 1.3094350	27 etry and energy 1.8518360 2.4595480 0.5332950 0.5918830 -0.2637270 -0.1201750 -0.3505930 0.5542040 -0.0052540 0.1872910 -0.8050750 -1.1161140 2.2700580 -1.6443720	<pre>of conformer: 0.3146390 -0.1843000 -0.3298020 -1.4199590 0.2390910 -0.1003520 1.3222030 -0.0344630 -0.8557080 0.4293310 1.0623800 1.1440460 0.2776170 -0.3930080</pre>	Thr-
Energy: B3LYP/6- N H C H C C H O O H O H H C H H	-438.41821867 311++G** geome -0.0830810 -0.7244710 -0.0226530 0.1033300 1.1584090 -1.3827400 1.0219930 2.3102310 -2.3156460 3.0688680 -1.4680440 -2.3826060 0.8412870 1.3094350 0.4419370	27 etry and energy 1.8518360 2.4595480 0.5332950 0.5918830 -0.2637270 -0.1201750 -0.3505930 0.5542040 -0.0052540 0.1872910 -0.8050750 -1.1161140 2.2700580 -1.6443720 -2.2737740	<pre>of conformer: 0.3146390 -0.1843000 -0.3298020 -1.4199590 0.2390910 -0.1003520 1.3222030 -0.0344630 -0.8557080 0.4293310 1.0623800 1.1440460 0.2776170 -0.3930080 -0.1816120</pre>	Thr-
Energy: B3LYP/6- N H C H C C H O O H O H C H H C H H H	-438.41821867 311++G** geome -0.0830810 -0.7244710 -0.0226530 0.1033300 1.1584090 -1.3827400 1.0219930 2.3102310 -2.3156460 3.0688680 -1.4680440 -2.3826060 0.8412870 1.3094350 0.4419370 1.4348690	27 etry and energy 1.8518360 2.4595480 0.5332950 0.5918830 -0.2637270 -0.1201750 -0.3505930 0.5542040 -0.0052540 0.1872910 -0.8050750 -1.1161140 2.2700580 -1.6443720 -2.2737740 -1.5600170	<pre>of conformer: 0.3146390 -0.1843000 -0.3298020 -1.4199590 0.2390910 -0.1003520 1.3222030 -0.0344630 -0.8557080 0.4293310 1.0623800 1.1440460 0.2776170 -0.3930080 -0.1816120 -1.4755450</pre>	Thr-
Energy: B3LYP/6- N H C C H C C H O O H O H H C H H H H	-438.41821867	27 etry and energy 1.8518360 2.4595480 0.5332950 0.5918830 -0.2637270 -0.1201750 -0.3505930 0.5542040 -0.0052540 0.1872910 -0.8050750 -1.1161140 2.2700580 -1.6443720 -2.2737740 -1.5600170 -2.1522550	<pre>of conformer: 0.3146390 -0.1843000 -0.3298020 -1.4199590 0.2390910 -0.1003520 1.3222030 -0.0344630 -0.8557080 0.4293310 1.0623800 1.1440460 0.2776170 -0.3930080 -0.1816120 -1.4755450 0.0125080</pre>	Thr-
Energy: B3LYP/6- N H C C H C C H O O O H O O H C H H C H H C H E nergy:	-438.41821867	27 etry and energy 1.8518360 2.4595480 0.5332950 0.5918830 -0.2637270 -0.1201750 -0.3505930 0.5542040 -0.0052540 0.1872910 -0.8050750 -1.1161140 2.2700580 -1.6443720 -2.2737740 -1.5600170 -2.1522550	<pre>of conformer: 0.3146390 -0.1843000 -0.3298020 -1.4199590 0.2390910 -0.1003520 1.3222030 -0.0344630 -0.8557080 0.4293310 1.0623800 1.1440460 0.2776170 -0.3930080 -0.1816120 -1.4755450 0.0125080</pre>	Thr-
Energy: B3LYP/6- N H C C H O O H O H H H Energy: B3LYP/6-	-438.41821867 311++G** geome -0.0830810 -0.7244710 -0.0226530 0.1033300 1.1584090 -1.3827400 1.0219930 2.3102310 -2.3156460 3.0688680 -1.4680440 -2.3826060 0.8412870 1.3094350 0.4419370 1.4348690 2.1893350 -438.41802090 311++G** geome	<pre>27 etry and energy 1.8518360 2.4595480 0.5332950 0.5918830 -0.2637270 -0.1201750 -0.3505930 0.5542040 -0.0052540 0.1872910 -0.8050750 -1.1161140 2.2700580 -1.6443720 -2.2737740 -1.5600170 -2.1522550 22 etry and energy</pre>	<pre>of conformer: 0.3146390 -0.1843000 -0.3298020 -1.4199590 0.2390910 -0.1003520 1.3222030 -0.0344630 -0.8557080 0.4293310 1.0623800 1.1440460 0.2776170 -0.3930080 -0.1816120 -1.4755450 0.0125080</pre>	Thr-
Energy: B3LYP/6- N H C C H O O H O H H C H H H Energy: B3LYP/6-	-438.41821867 311++G** geome -0.0830810 -0.7244710 -0.0226530 0.1033300 1.1584090 -1.3827400 1.0219930 2.3102310 -2.3156460 3.0688680 -1.4680440 -2.3826060 0.8412870 1.3094350 0.4419370 1.4348690 2.1893350 -438.41802090 311++G** geome	<pre>27 etry and energy 1.8518360 2.4595480 0.5332950 0.5918830 -0.2637270 -0.1201750 -0.3505930 0.5542040 -0.0052540 0.1872910 -0.8050750 -1.1161140 2.2700580 -1.6443720 -2.2737740 -1.5600170 -2.1522550 22 etry and energy 1.8585250</pre>	<pre>of conformer: 0.3146390 -0.1843000 -0.3298020 -1.4199590 0.2390910 -0.1003520 1.3222030 -0.0344630 -0.8557080 0.4293310 1.0623800 1.1440460 0.2776170 -0.3930080 -0.1816120 -1.4755450 0.0125080</pre>	Thr-
Energy: B3LYP/6- N H C C H O O H O H H C H H H Energy: B3LYP/6- N H	-438.41821867 311++G** geome -0.0830810 -0.7244710 -0.0226530 0.1033300 1.1584090 -1.3827400 1.0219930 2.3102310 -2.3156460 3.0688680 -1.4680440 -2.3826060 0.8412870 1.3094350 0.4419370 1.4348690 2.1893350 -438.41802090 311++G** geome -0.1612090 -0.2908270	<pre>27 27 2.1.8518360 2.4595480 0.5332950 0.5918830 -0.2637270 -0.1201750 -0.3505930 0.5542040 -0.0052540 0.1872910 -0.8050750 -1.1161140 2.2700580 -1.6443720 -2.2737740 -1.5600170 -2.1522550 22 2.273740 2.1522550 2.2675740 2.267575 2.26757 2.2675740 2.267575 2.267575 2.267575 2.267575 2.26757 2.2675</pre>	<pre>of conformer: 0.3146390 -0.1843000 -0.3298020 -1.4199590 0.2390910 -0.1003520 1.3222030 -0.0344630 -0.8557080 0.4293310 1.0623800 1.1440460 0.2776170 -0.3930080 -0.1816120 -1.4755450 0.0125080</pre>	Thr-
Energy: B3LYP/6- N H C C H O O H H C H H H Energy: B3LYP/6- N H C	-438.41821867 311++G** geome -0.0830810 -0.7244710 -0.0226530 0.1033300 1.1584090 -1.3827400 1.0219930 2.3102310 -2.3156460 3.0688680 -1.4680440 -2.3826060 0.8412870 1.3094350 0.4419370 1.4348690 2.1893350 -438.41802090 311++G** geome -0.1612090 -0.2908270 -0.0719470	<pre>27 27 2.1.8518360 2.4595480 0.5332950 0.5918830 -0.2637270 -0.1201750 -0.3505930 0.5542040 -0.0052540 0.1872910 -0.8050750 -1.1161140 2.2700580 -1.6443720 -2.2737740 -1.5600170 -2.1522550 22 2.2675740 0.4070660</pre>	<pre>of conformer: 0.3146390 -0.1843000 -0.3298020 -1.4199590 0.2390910 -0.1003520 1.3222030 -0.0344630 -0.8557080 0.4293310 1.0623800 1.1440460 0.2776170 -0.3930080 -0.1816120 -1.4755450 0.0125080</pre>	Thr-
Energy: B3LYP/6- N H C C H O O H O O H O O H O O H O O H O C H H C H H Energy: B3LYP/6- N H C C H H C C H O O O H O O N H C C N H C C N H C C N H C C N H C C N H C C N H C C N H C C N H C C N H C C N H C C N H C C N H C C N H C C N H C C N H C C N H C C N H C C N H O O O N H C C N H O O N H C C N H C C N H C C N H O O N H C C N H C C N H C C N H C C N H C C N H C C N H C C N H C C N H O O N H C C N H O O N H C C N H C C N H C N H C C N H O O N H C C N H O O N H C C N H N H C C N H N H C C N H N H	-438.41821867 311++G** geome -0.0830810 -0.7244710 -0.0226530 0.1033300 1.1584090 -1.3827400 1.0219930 2.3102310 -2.3156460 3.0688680 -1.4680440 -2.3826060 0.8412870 1.3094350 0.4419370 1.4348690 2.1893350 -438.41802090 311++G** geome -0.1612090 -0.2908270 -0.0719470 -0.2420690	<pre>27 27 2.1.8518360 2.4595480 0.5332950 0.5918830 -0.2637270 -0.1201750 -0.3505930 0.5542040 -0.0052540 0.1872910 -0.8050750 -1.1161140 2.2700580 -1.6443720 -2.2737740 -1.5600170 -2.1522550 22 2.2675740 0.4070660 -0.0169090 </pre>	<pre>of conformer: 0.3146390 -0.1843000 -0.3298020 -1.4199590 0.2390910 -0.1003520 1.3222030 -0.0344630 -0.8557080 0.4293310 1.0623800 1.1440460 0.2776170 -0.3930080 -0.1816120 -1.4755450 0.0125080 of conformer: -0.8496080 0.0700790 -0.7559960 -1.7519930</pre>	Thr-

С	1.3092720	-0.1388770	-0.2645430	
С	-1.1976090	-0.0803980	0.1421810	
Н	2.0437980	0.2427830	-0.9914770	
0	1.3369470	-1.5651060	-0.2603410	
0	-1.5739050	0.4855770	1.1379730	
Н	1.0143320	-1.8980920	-1.1048840	
0	-1.7295370	-1.2433400	-0.2904530	
H	-2.3948350	-1.51///50	0.3596680	
H	0.6/10300	2.2549010	-1.2/24080	
С	1.7203040	0.3100540	1.1293340	
H	1.01/0000	-0.0498200	1.8826770	
H	2.7078920	-0.0951210	1.35/9690	
Н	1.7739890	1.3986/90	1.1943340	
Energy:	-438.41786911	.1		
B3LYP/6-	311++G** geome	etry and energy	of conformer:	Thr-XLI
Ν	-0.0324190	1.8809760	0.2178140	
Н	0.9174830	2.2371620	0.2617440	
С	-0.0102640	0.5346410	-0.3572560	
Н	0.1228490	0.5293260	-1.4499360	
С	1.1478610	-0.2671260	0.2737380	
С	-1.3777240	-0.1002820	-0.1168230	
Н	1.0090450	-0.2649770	1.3560960	
0	2.3755060	0.4448480	0.0638300	
0	-2.2342510	-0.2074120	-0.9598840	
Н	2.6717170	0.2893440	-0.8405110	
0	-1.5506410	-0.5192870	1.1561710	
Н	-2.4564920	-0.8566440	1.2268390	
Н	-0.5859150	2.5130440	-0.3499110	
С	1.2422390	-1.6966610	-0.2461360	
Н	1.3817710	-1.7127060	-1.3331180	
Н	2.0902380	-2.2044780	0.2175360	
Н	0.3386540	-2.2655300	-0.0155120	
Fneray.	-438 41773384	6		
Lifer gy .	100.11770001			
B3LYP/6-	311++G** geome	try and energy	of conformer:	Thr-XLII
Ν	-0.1222980	1.8873060	-0.6396680	
Н	-0.9207210	2.2735960	-1.1306130	
С	-0.1057810	0.4266650	-0.7363740	
Н	-0.3007800	0.1536900	-1.7742100	
С	1.2991960	-0.1167110	-0.3963820	
С	-1.2320710	-0.2469870	0.0532940	
Н	1.9536850	0.2695470	-1.1885170	
0	1.1888910	-1.5395840	-0.5044280	
0	-2.1162890	-0.9078920	-0.4258930	
Н	2.0349580	-1.9367710	-0.2766300	
0	-1.1830250	0.0428670	1.3828920	
Н	-1.9451560	-0.3911980	1.7953530	
Н	-0.1740100	2.1940600	0.3259880	
С	1.8713840	0.3069440	0.9536610	
Н	1.2604830	-0.0579250	1.7798680	
Н	2.8845130	-0.0937390	1.0639980	
Н	1.9501240	1.3950000	1.0166830	

Molecular Physics

Energy: -438.416965250

NN -0.1884010 1.8592180 -0.8039330 H -0.1763880 2.2626160 0.1269550 C -0.0866920 0.4043140 -0.7457610 H -0.2827200 -0.034590 -1.7391440 C 1.3024700 -0.1417190 -0.3132850 C -1.1871910 -0.0894740 0.185540 H 2.0128020 0.2516140 -1.0572480 O 1.2184370 -1.5635710 -0.4432620 O -1.3958530 0.3624570 -0.1303880 O -1.9183050 -1.0843050 -0.3492670 H 2.0395800 -1.9559420 -0.1303880 O -1.9183050 -1.0843050 -0.3492670 H 2.5748520 -1.3471760 0.3144420 H 0.5650520 2.2627820 -1.3494770 C 1.7707250 0.2713900 1.0785380 H 1.0997700 -0.1051910 1.85520370 H 2.7758950 -0.1222930 1.2622740 H 1.8295590 1.3588160 1.1699600 Energy: -438.416792867 B3LYP/6-311++6** geometry and energy of conformer: Thr-XLIV N -0.2539740 1.8118220 -0.8630330 H -0.2459270 2.2387700 0.0565390 C -0.0767670 0.3649860 -0.7832200 H -0.1973930 -0.0377650 -1.793440 C 1.33197120 -0.1199840 -0.2759520 C -1.2101560 -0.2684040 0.0115920 H 2.0404690 0.2451540 -1.0250510 O -1.3789220 -1.5431340 -0.261510 D -1.7867480 -1.2273090 -0.303450 H 0.9824640 -1.9282970 -0.9956810 O -1.4976270 0.4183110 1.1431320 H 0.9824640 -1.9282970 -0.9956810 O -1.4976270 0.4183110 1.1431320 H 0.4970620 2.2372700 -1.4232810 C 1.7377930 0.3991930 1.0918970 H 2.223180 -0.0470505 1.5866210 H 2.2288430 0.0087860 1.3312460 H 0.4770620 2.237270 -1.4232810 C 1.7377930 0.3991930 1.0918970 H 1.0432690 0.0726330 1.8678610 H 2.7288430 0.0087860 1.3312460 H 1.7923410 1.4899920 1.1026350 Energy: -438.416053844 B3LYP/6-311++G** geometry and energy of conformer: Thr-XLV N 0.1630950 1.7075640 -0.0322460 H 0.4646500 2.2990720 -0.6956160 C -0.0323770 0.350890 -0.5364590 H 0.4467800 1.275240 -0.123270 D -0.5364590 H 0.04636500 2.2990720 -0.6956160 C -0.0323770 0.5501540 -0.122550 C -1.4378860 -0.1215240 -0.1233730	-0.1884010 1.8592180 -0.8039330 -0.1763880 2.2626160 0.1269550 -0.0866920 0.4043140 -0.7457610 -0.2827200 -0.0034590 -1.7391440 1.3024700 -0.1417190 -0.3132850 -1.1871910 -0.0894740 0.185540 2.0128020 0.2516140 -1.0572480 1.2184370 -1.5635710 -0.4432620 -1.3958530 0.3624570 1.2860100 2.0395800 -1.9559420 -0.1303880 -1.9183050 -1.0843050 -0.3492670 -2.5748250 -1.3471760 0.314420 0.5650520 2.2627820 -1.3494770 1.7707250 0.2713900 1.0785380 1.0997700 -0.1051910 1.8520370 2.7758950 -0.1222930 1.2622740 1.8295590 1.3588160 1.1699600 mergy: -438.416792867 3LYP/6-311++G** geometry and energy of conformer: Thr-XLI -0.2539740 1.8118220 -0.8630330 -0.2459270 2.2387700 0.0565390 -0.0767670 0.3649860 -0.7832200 -0.1973930 -0.0377650 -1.7938440 1.3197120 -0.1199840 -0.2759520 -1.2101560 -0.2684040 0.0115920 2.0404690 0.2451540 -1.0250510 1.3789220 -1.5431340 -0.2061510 -1.7867480 -1.2773090 -0.3034450 0.982460 -1.9239790 -0.9956810 -1.4976270 0.4183110 1.1431320 -2.2231820 -0.0470650 1.5866210 0.7786740 0.3991930 1.0918970 1.0432690 0.0726830 1.8678610 2.7288430 0.0087860 1.3312460 1.7923410 1.4699920 1.1026350 mergy: -438.416053844 3LYP/6-311++G** geometry and energy of conformer: Thr-XLV 0.1630950 1.7075640 -0.0322460 0.6465600 2.2990720 -0.6956160 -0.0323770 0.3308990 -0.3364590 -0.0323770 0.3508990 -0.5364590 -0.0323770 0.3508990 -0.5364590 -0.0323770 0.3508990 -0.5364590 -0.0323770 0.3508990 -0.5364590 -0.0323770 0.3508990 -0.5364590 -0.0323770 0.3508990 -0.5364590 -0.012220 0.2965400 -1.6335640	B3LYP/6-	-311++G** geome	try and energy	of conformer:	Thr-XLI
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	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C	1 1270060	0.1015040	0.0122200	
	0.902/210 -1.60523/0 -0.2222/20		-1.43/000U	-U.IZIJZ4U	-0.1233/30	

1					
2					
3	0	1.1227050	-0.4729230	1.4261710	
4	0	-2.2778080	0.6232810	0.3020840	
5	Н	1.0406050	0.4712750	1.6354030	
6	0	-1.7249500	-1.4252630	-0.3255160	
7	Н	-0.9362300	-1 9165780	-0.5858770	
8	U U	-0.7359660	2 1251710	0.1899360	
0	II C	-0.7559000	2.1231710	0.1099300	
9	C	2.4618020	-0.1940/90	-0.5961350	
10	H	3.2345380	-0.8329170	-0.1648/00	
11	Н	2.4612040	-0.3342800	-1.6819950	
12	Н	2.7228330	0.8443880	-0.3760850	
13					
14	Energy:	-438.415737637			
15					
16					
10					
17	B3IVD/6_3	211C** goomet:	ry and energy	of conformer.	Thr_VI VI
18	DOLIE/0-2	JII++G geomet.	ry and energy	or contormer.	THT -VPAT
19	NT	0 0500000	1 1004500	1 2522400	
20	N	-0.0508300	-1.1284500	1.3522490	
21	H	-0.6861400	-1.9103200	1.4493350	
22	С	0.0711170	-0.6923310	-0.0389100	
23	Н	0.0900770	-1.5796180	-0.6728010	
23	С	-1.0662360	0.2298520	-0.5392520	
24	С	1.4626880	-0.0503900	-0.2307850	
25	н	-0 7933010	0 6024960	-1 5352830	
26	\cap	_1 0968310	1 3452070	0 3845800	
27	0	-1.0900510	1.3432070	0.3043000	
28	0	2.3657060	-0.6138380	-0.7865340	
29	Н	-1./358810	2.0007760	0.08/6010	
20	0	1.6209510	1.1885430	0.2828700	
30	Н	0.7556060	1.5358060	0.5672710	
31	Н	-0.3629500	-0.3778700	1.9583500	
32	С	-2.4219130	-0.4597790	-0.6051170	
33	Н	-3.1953000	0.2378440	-0.9401650	
34	Н	-2.3951920	-1 2888550	-1 3176150	
35	н	-2 7136560	-0 8445110	0 3746140	
36	11	2.7130300	0.0110110	0.3710110	
37	Enonerre	120 115255600			
38	Ellergy:	-430.413333000			
20					
40					
40			_		
41	B3LYP/6-3	311++G** geomet:	ry and energy	of conformer:	Thr-XLVII
42					
43	Ν	-0.1393770	-1.2392960	1.1878900	
44	Н	-0.3759920	-0.5238630	1.8692910	
45	С	0.0673120	-0.6225140	-0.1232850	
46	Н	0.1245600	-1.4196460	-0.8763400	
47	С	-1.1396880	0.2800330	-0.4790320	
48	С	1.3687840	0.1981300	-0.1669470	
10	H	-0.9078410	0.7730600	-1.4337810	
49	0	-1 3412220	1 2622190	0 5326770	
50	0	1 /511120	1 2507170	0.1476100	
51	0	1.4311120	1.3307170	0.14/0190	
52	H	-0.5372540	1.8011280	0.5688900	
53	0	2.4918700	-0.4744940	-0.5292080	
54	H	2.2734510	-1.3720590	-0.8091390	
55	Н	0.6729020	-1.7485960	1.5174310	
56	С	-2.4327160	-0.5075230	-0.6253210	
57	Н	-3.2466560	0.1773170	-0.8700350	
57	Н	-2.3487600	-1.2473270	-1.4261320	
58	ц	-2 67/9960	-1.0252380	0.3033930	
50	11	2.0/4//00	T • O O O O O O O O O O	• • • • • • • • • • • • • •	
59	11	2.0749900	1.0202000	0.0000000	
59 60	II Energy:	-438 414630711	1.0202000		

-0.3093120 -0.2057330 -0.2057330 -0.2361820 1.3125220 -1.2294770 2.0031750 1.3047620 -1.9866440 2.1526800 -1.3149460 -2.0754660 0.3338500 1.7646010 1.1241500	try and energy 1.8173620 2.2298510 0.3707870 -0.0079360 -0.0918840 -0.2713500 0.3357620 -1.5160080 -1.1099910 -1.8621870 0.2418950 -0.1803350 2.2725790 0.3529890	-0.7919380 0.1281830 -0.7688310 -1.7828960 -0.3201590 0.0324150 -1.0639610 -0.4408370 -0.3741840 -0.1453820 1.2901770 1.7176260 -1.4301000	Thr-XL
$\begin{array}{c} -0.3093120\\ -0.2057330\\ -0.0999250\\ -0.2361820\\ 1.3125220\\ -1.2294770\\ 2.0031750\\ 1.3047620\\ -1.9866440\\ 2.1526800\\ -1.3149460\\ -2.0754660\\ 0.3338500\\ 1.7646010\\ 1.1241500\end{array}$	1.8173620 2.2298510 0.3707870 -0.0079360 -0.0918840 -0.2713500 0.3357620 -1.5160080 -1.1099910 -1.8621870 0.2418950 -0.1803350 2.2725790 0.3529890	-0.7919380 0.1281830 -0.7688310 -1.7828960 -0.3201590 0.0324150 -1.0639610 -0.4408370 -0.3741840 -0.1453820 1.2901770 1.7176260 -1.4301000	
$\begin{array}{c} -0.2057330\\ -0.0999250\\ -0.2361820\\ 1.3125220\\ -1.2294770\\ 2.0031750\\ 1.3047620\\ -1.9866440\\ 2.1526800\\ -1.3149460\\ -2.0754660\\ 0.3338500\\ 1.7646010\\ 1.1241500\end{array}$	2.2298510 0.3707870 -0.0079360 -0.0918840 -0.2713500 0.3357620 -1.5160080 -1.1099910 -1.8621870 0.2418950 -0.1803350 2.2725790 0.3529890	0.1281830 -0.7688310 -1.7828960 -0.3201590 0.0324150 -1.0639610 -0.4408370 -0.3741840 -0.1453820 1.2901770 1.7176260 -1.4301000	
$\begin{array}{c} -0.0999250\\ -0.2361820\\ 1.3125220\\ -1.2294770\\ 2.0031750\\ 1.3047620\\ -1.9866440\\ 2.1526800\\ -1.3149460\\ -2.0754660\\ 0.3338500\\ 1.7646010\\ 1.1241500\end{array}$	0.3707870 -0.0079360 -0.0918840 -0.2713500 0.3357620 -1.5160080 -1.1099910 -1.8621870 0.2418950 -0.1803350 2.2725790 0.3529890	-0.7688310 -1.7828960 -0.3201590 0.0324150 -1.0639610 -0.4408370 -0.3741840 -0.1453820 1.2901770 1.7176260 -1.4301000	
$\begin{array}{c} -0.2361820\\ 1.3125220\\ -1.2294770\\ 2.0031750\\ 1.3047620\\ -1.9866440\\ 2.1526800\\ -1.3149460\\ -2.0754660\\ 0.3338500\\ 1.7646010\\ 1.1241500 \end{array}$	-0.0079360 -0.0918840 -0.2713500 0.3357620 -1.5160080 -1.1099910 -1.8621870 0.2418950 -0.1803350 2.2725790 0.3529890	-1.7828960 -0.3201590 0.0324150 -1.0639610 -0.4408370 -0.3741840 -0.1453820 1.2901770 1.7176260 -1.4301000	
$\begin{array}{c} 1.3125220\\ -1.2294770\\ 2.0031750\\ 1.3047620\\ -1.9866440\\ 2.1526800\\ -1.3149460\\ -2.0754660\\ 0.3338500\\ 1.7646010\\ 1.1241500\end{array}$	-0.0918840 -0.2713500 0.3357620 -1.5160080 -1.1099910 -1.8621870 0.2418950 -0.1803350 2.2725790 0.3529890	-0.3201590 0.0324150 -1.0639610 -0.4408370 -0.3741840 -0.1453820 1.2901770 1.7176260 -1.4301000	
-1.2294770 2.0031750 1.3047620 -1.9866440 2.1526800 -1.3149460 -2.0754660 0.3338500 1.7646010 1.1241500	-0.2713500 0.3357620 -1.5160080 -1.1099910 -1.8621870 0.2418950 -0.1803350 2.2725790 0.3529890	0.0324150 -1.0639610 -0.4408370 -0.3741840 -0.1453820 1.2901770 1.7176260 -1.4301000	
2.0031750 1.3047620 -1.9866440 2.1526800 -1.3149460 -2.0754660 0.3338500 1.7646010 1.1241500	0.3357620 -1.5160080 -1.1099910 -1.8621870 0.2418950 -0.1803350 2.2725790 0.3529890	-1.0639610 -0.4408370 -0.3741840 -0.1453820 1.2901770 1.7176260 -1.4301000	
$\begin{array}{c} 1.3047620 \\ -1.9866440 \\ 2.1526800 \\ -1.3149460 \\ -2.0754660 \\ 0.3338500 \\ 1.7646010 \\ 1.1241500 \end{array}$	-1.5160080 -1.1099910 -1.8621870 0.2418950 -0.1803350 2.2725790 0.3529890	-0.4408370 -0.3741840 -0.1453820 1.2901770 1.7176260 -1.4301000	
-1.9866440 2.1526800 -1.3149460 -2.0754660 0.3338500 1.7646010 1.1241500	-1.1099910 -1.8621870 0.2418950 -0.1803350 2.2725790 0.3529890	-0.3741840 -0.1453820 1.2901770 1.7176260 -1.4301000	
2.1526800 -1.3149460 -2.0754660 0.3338500 1.7646010 1.1241500	-1.8621870 0.2418950 -0.1803350 2.2725790 0.3529890	-0.1453820 1.2901770 1.7176260 -1.4301000	
-1.3149460 -2.0754660 0.3338500 1.7646010 1.1241500	0.2418950 -0.1803350 2.2725790 0.3529890	1.2901770 1.7176260 -1.4301000	
-2.0754660 0.3338500 1.7646010 1.1241500	-0.1803350 2.2725790 0.3529890	1.7176260 -1.4301000	
0.3338500 1.7646010 1.1241500	2.2725790 0.3529890	-1.4301000	
1.7646010 1.1241500	0.3529890	1 0000000	
1.1241500		1.0682660	
	-0.0610000	1.8476480	
2.7923170	0.0187060	1.2443580	
1.7646980	1.4425990	1.1567000	
-438.41428376	9		
-311++G** geome	try and energy	of conformer:	Thr-XL
0.0188040	1.8879400	0.0602360	
-0.5314530	2.4781900	-0.5539310	
-0.0264390	0.4795030	-0.3705270	
0.1084390	0.4689370	-1.4534090	
1.1736440	-0.2618220	0.2594430	
-1.3957570	-0.1640140	-0.1133930	
1.0365350	-0.2901230	1.3597310	
2.3587350	0.4569650	-0.0276790	
-2.2322540	-0.3006710	-0.9614520	
2.1259980	1.3965790	0.0348010	
-1.6698960	-0.5232730	1.1736700	
-0.8831860	-0.4457880	1.7293170	
0.0001000	0.110,000		
-0.3321940	2.0166600	1.0051110	
-0.3321940 1.3369480	2.0166600	1.0051110 -0.2537480	
-0.3321940 1.3369480 1.4735680	2.0166600 -1.6842380 -1.6795700	1.0051110 -0.2537480 -1.3377740	
-0.3321940 1.3369480 1.4735680 2.2195680	2.0166600 -1.6842380 -1.6795700 -2.1392410	1.0051110 -0.2537480 -1.3377740 0.1990630	
-0.3321940 1.3369480 1.4735680 2.2195680 0.4680530	2.0166600 -1.6842380 -1.6795700 -2.1392410 -2.3019720	1.0051110 -0.2537480 -1.3377740 0.1990630 -0.0115240	
	-438.41428376 -438.41428376 0.0188040 -0.5314530 -0.0264390 0.1084390 1.1736440 -1.3957570 1.0365350 2.3587350 -2.2322540 2.1259980 -1.6698960	-438.414283769 -438.414283769 311++G** geometry and energy 0.0188040 1.8879400 -0.5314530 2.4781900 -0.0264390 0.4795030 0.1084390 0.4689370 1.1736440 -0.2618220 -1.3957570 -0.1640140 1.0365350 -0.2901230 2.3587350 0.4569650 -2.2322540 -0.3006710 2.1259980 1.3965790 -1.6698960 -0.5232730	-438.414283769 -438.414283769 -438.414283769 -438.414283769 -438.414283769 -0.0188040 -0.5314530 -0.0264390 -0.4795030 -0.3705270 0.1084390 1.1736440 -0.2618220 0.2594430 -1.4534090 1.1736440 -0.2618220 0.2594430 -1.3957570 -0.1640140 -0.1133930 1.0365350 -0.2901230 1.3597310 2.3587350 0.4569650 -0.0276790 -2.2322540 -0.3006710 -0.9614520 2.1259980 1.3965790 0.0348010 -1.6698960 -0.5232730 1.1736700

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2					
3	0	-1.8122780	0.2717380	1.1399960	
4	Н	3.0780050	0.0978320	0.3706940	
6	U U	-Z.UZ8858U	-0.8953150	-0./341/80	
7	п	-1.3003320	-0.9920420	-1.3734600	
8	н С	1 1505470	2.20/0000	-0.4322790	
9	U U	1.1303470	-2 195/970	0.1793100	
3 10	н	1 2375320	-2.0083120	-0.8766420	
10	н	2 0063500	-2 1679780	0.0700420	
12	11	2.0003300	2.10/9/00	0.1002150	
13	Energy:	-438.412787935			
14					
15					
16					
17	B3LYP/6-	311++G** geomet:	ry and energy	of conformer:	Thr-LI
18					
19	Ν	-0.5499040	1.8495380	0.1823190	
20	Н	-0.0445280	2.6264980	-0.2302400	
21	С	-0.1538490	0.5868590	-0.4496230	
22	Η	-0.2720030	0.6103460	-1.5498140	
23	С	1.3446910	0.3140810	-0.1723850	
24	С	-1.1011110	-0.5257980	-0.0040250	
25	H	1.8557720	1.2563750	-0.4261020	
26	0	1.8486280	-0.7301690	-1.0040560	
27	0	-0.8150630	-1.6338890	0.35/1310	
28	Н	1.7896270	-0.4590360	-1.9259660	
29	U	-2.3956750	-0.1113140	-0.1141420	
30	п	-2.9562550	-0.8303220	0.1658840	
31	C C	1 6794420	-0.0382060	1 2687200	
32	Н	1.2878900	-1.0241720	1 5170040	
33	H	2.7633910	-0.0489780	1.3990150	
34	Н	1.2488460	0.7031260	1.9445180	
35					
36	Energy:	-438.412520745			
37					
38					
39					
40	B3LYP/6-	311++G** geomet:	ry and energy	of conformer:	Thr-LII
41				0.1155500	
42	N	0.2369850	1.7669510	-0.1157790	
43	H	0.2444820	1.8058290	0.8996530	
44	C	-0.0356190	0.4048080	-0.5330590	
40	н С	-0.0339100	-0 5364620	-1.0310030	
40	C	-1 /372/10	-0.09/3320	-0.0974050	
47	н	0 8829370	-1 5551740	-0 4236540	
40	0	1.0122230	-0.5341990	1,3717490	
49 50	0	-2.2380670	0.5957790	0.4653890	
51	H	1.7946760	-0.9600330	1.7355520	
52	0	-1.7673000	-1.3651360	-0.4534940	
53	Н	-1.0163640	-1.8135060	-0.8609330	
54	Н	-0.5136290	2.3788050	-0.4179000	
55	С	2.4664660	-0.1225380	-0.5617240	
56	Н	3.2306520	-0.8089680	-0.1825880	
57	Н	2.5021720	-0.1599360	-1.6541430	
58	Н	2.7008570	0.8928550	-0.2430900	
59	-	400 4100000000			
60	Energy:	-438.412327313			

N H C H C C H O O H O U	-0.0157450 0.9425150 -0.0158390 0.1186900 1.1299630 -1.3684510 0.9882930 2.3744590 -1.8472690 2.6899450	1.9284530 2.2644440 0.4747840 0.1948500 -0.2047700 -0.0339030 0.0659390 0.3975370 0.3249370	-0.3551070 -0.3771390 -0.4465130 -1.5023330 0.3631430 0.0573790 1.4127010 -0.0057140	
H C C C H O O H	0.9425150 -0.0158390 0.1186900 1.1299630 -1.3684510 0.9882930 2.3744590 -1.8472690 2.6899450	2.2644440 0.4747840 0.1948500 -0.2047700 -0.0339030 0.0659390 0.3975370 0.3249370	-0.3771390 -0.4465130 -1.5023330 0.3631430 0.0573790 1.4127010 -0.0057140	
С Н С С Н О О Н	-0.0158390 0.1186900 1.1299630 -1.3684510 0.9882930 2.3744590 -1.8472690 2.6899450	0.4747840 0.1948500 -0.2047700 -0.0339030 0.0659390 0.3975370 0.3249370	-0.4465130 -1.5023330 0.3631430 0.0573790 1.4127010 -0.0057140	
H C C H O O H	0.1186900 1.1299630 -1.3684510 0.9882930 2.3744590 -1.8472690 2.6899450	0.1948500 -0.2047700 -0.0339030 0.0659390 0.3975370 0.3249370	-1.5023330 0.3631430 0.0573790 1.4127010 -0.0057140	
С С Н О Н О	1.1299630 -1.3684510 0.9882930 2.3744590 -1.8472690 2.6899450	-0.2047700 -0.0339030 0.0659390 0.3975370 0.3249370	0.3631430 0.0573790 1.4127010 -0.0057140	
С Н О О Н О	-1.3684510 0.9882930 2.3744590 -1.8472690 2.6899450	-0.0339030 0.0659390 0.3975370 0.3249370	0.0573790 1.4127010 -0.0057140	
н О О Н О	0.9882930 2.3744590 -1.8472690 2.6899450	0.0659390 0.3975370 0.3249370	1.4127010 -0.0057140	
0 0 H 0	2.3744590 -1.8472690 2.6899450	0.3975370 0.3249370	-0.0057140	
0 H 0	-1.8472690 2.6899450	0.3249370		
H O	2.6899450		1.0974490	
0		-0.0091940	-0.8209040	
TT	-2.0025540	-0.9595760	-0.7047700	
п	-1.5308170	-1.0890570	-1.5363530	
Н	-0.4294060	2.2119870	0.5289950	
C	1.1782850	-1.7214480	0.2168190	
Н	0.2673790	-2.1918950	0.5950210	
Н	1.2992960	-2.0137530	-0.8338880	
Н	2.0234900	-2.1236540	0.7789650	
Energy: -	438.41198888	8		
B3LYP/6-31	1++G** geome	try and energy	of conformer:	Thr-LIV
N	0.0406680	1,9300640	-0.1267260	
Н	0.8995460	2.3176010	-0.4983940	
C	-0.0186320	0.5051050	-0.3983340	
H	0.1265710	0.2537380	-1.4657010	
C	1.1322660	-0.1816700	0.3724040	
C	-1.3863840	-0.0457010	0.0328150	
Н	1.0330280	0.1279170	1.4188160	
0	2.3222680	0.3924520	-0.1922470	
0	-2.0734610	0.4245080	0.8916290	
Н	3.0523630	0.2677310	0.4216880	
0	-1.8035300	-1.1529370	-0.6434010	
Н	-1.1673720	-1.3880820	-1.3302720	
Н	-0.7545930	2.4290070	-0.5067970	
С	1.1693010	-1.7035160	0.2692830	
Н	0.2937940	-2.1644340	0.7324840	
Н	1.2368310	-2.0247000	-0.7749220	
Н	2.0536300	-2.0867110	0.7853140	

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2					
3	0	-1.8655080	-1.2888320	-0.5103240	
4	Н	-1.2568720	-1.6726490	-1.1530050	
5	Н	1.0706490	2.0700050	-0.4541640	
6	С	2.4547590	-0.2890290	-0.5180950	
7	Н	3.1844500	-0.9626690	-0.0587450	
8	Н	2.4836260	-0.4576530	-1.5985310	
9	Н	2.7771010	0.7347090	-0.3122020	
10					
11	Energy:	-438.40798347	9		
12					
13					
14					
15	B3LYP/6-	-311++G** geome	try and energy	of conformer:	Thr-LV1
16		0,0000000	1 0001000	0 0000400	
17	N	0.0930600	1.9231390	-0.0296460	
18	H	1.04/9800	2.23/1380	-0.1661680	
19	C	-0.0137050	0.5165040	-0.3/55210	
20	H	0.0834070	0.3232590	-1.4628520	
21	C	1.1342270	-0.2502140	0.32/9310	
22	C	-1.3654200	-0.0382280	0.1110090	
23	H	1.0294650	-0.0553320	1.3968950	
24	0	2.3839230	0.3411080	-0.0395730	
25	U	-1.7407760	0.0029640	1.240000	
26	п	2.0/39000	-0.0359060	-0.0700200	
27	U U	-2.1340300	-0.0301730	-0.8438090	
28	11 Ч	-0 5335310	2 5085680	-0 5689720	
29	II C	1 1251160	_1 7/03860	-0.5009720	
30	ч	1 2180240	-1.960/610	-1 0153740	
31	н	1 9642800	-2 2220950	0 5710840	
32	H	0 2049640	-2 2164690	0.4159390	
33	11	0.2019010	2.2101090	0.11333390	
34	Energy:	-438.40746769	6		
35			-		
36					
37					
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39					
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			Mole	ecular Physics	
1					
2 3 4	B3LYP/6-	-311++G** geomet	try and energy	of conformer:	aThr-I
 ↓ 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 	N H C H C H O H H C H H	0.2923440 0.0289510 0.0568290 -0.0800310 -1.1837500 1.3458670 -1.0098190 -1.3712230 1.3762730 -0.5259760 2.4389950 2.1233100 -0.2275260 -2.4695860 -2.6399370 -2.4542010	1.8515520 2.0580980 0.4377930 0.3642720 -0.2176340 -0.3568710 -0.2383200 -1.5348850 -1.5610510 -2.0018520 0.3972740 1.3260630 2.4764410 0.5477090 0.6192240	0.0058230 -0.9537200 0.3400420 1.4251160 -0.3222290 0.0329220 -1.4117690 0.1653400 -0.0738490 0.0657870 -0.0854610 -0.0065920 0.6096490 -0.0373330 1.0409560 -0.4640690	
20 21	н Н	-2.4542010 -3.3096980	0.0054080	-0.4747620	
22 23	Energy:	-438.426076096	5		
24 25	MP2/aug-	-cc-pVTZ geometi	ry and energy	of conformer:	aThr-I
26 27 28 29 30 31 32 33 45 36 37 38 39 40 41 42 43 44 50 51 52 53 45 56 57 58 59	N H C H C H O H H C H H H Energy:	0.2779100 0.0219000 0.0504700 -0.0983050 -1.1651990 1.3314440 -0.9799290 -1.3534250 1.3699800 -0.4906890 2.4182540 2.0755600 -0.2853630 -2.4433220 -2.5984810 -2.4271300 -3.2817580 -435.933243196	1.8412290 2.0222540 0.4334780 0.3549570 -0.2188160 -0.3491660 -0.2326860 -1.5333810 -1.5584090 -1.9749690 0.4132350 1.3332470 2.4505600 0.5407600 0.6093950 1.5425680 -0.0030290	0.0116870 -0.9537360 0.3478070 1.4284760 -0.3265250 0.0377150 -1.4114700 0.1594760 -0.0706310 0.0787340 -0.0918330 -0.0058470 0.5896710 -0.0398110 1.0375240 -0.4658640 -0.4705160	
00		UR	L: http://mc.manu	uscriptcentral.com	l/tandf/tmph

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2					e The TT
4	B3L1P/6	311++G^^ geomet	ry and energy	of conformer:	ainr-ii
5	Ν	0.3845910	1.7459650	0.1091240	
6	Н	-0.0076120	1.8208290	1.0430750	
7	С	-0.0023820	0.4823340	-0.5098950	
8	Н	-0.0121850	0.6105720	-1.5953050	
9	С	1.0913670	-0.5924520	-0.2199330	
10	С	-1.3845200	0.0038690	-0.0869770	
11	Н	0.8795460	-1.4680330	-0.8372570	
12	0	2.3333930	-0.0789570	-0.6746890	
13	0	-2.0387470	0.4683270	0.8134310	
14	Н	2.3787120	0.8301190	-0.3403510	
15	0	-1.8044800	-1.0422640	-0.8358020	
16	Н	-2.6737640	-1.3113630	-0.5009800	
17	Н	0.0344840	2.5356120	-0.4203560	
18	С	1.1635060	-1.0059530	1.2505090	
19	Н	1.9840080	-1.7134110	1.3829300	
20	Н	1.3567510	-0.1432830	1.8944120	
21	H	0.2387730	-1.4864350	1.5842230	
22		400 40500005			
23	Energy:	-438.425833825			
24	MD2/aug	a nutra acomotr	u and onergu	of conformar.	oThr TT
25	MPZ/aug-	de-pviz geometr	y and energy (or contormer:	aini-ii
26	N	0 4252700	1 7279270	0 0802170	
27	Н	0.0052150	1.8007140	1.0015020	
28	C	0.0140320	0.4777880	-0.5389850	
29	H	0.0133340	0.5931430	-1.6230830	
30	С	1.0628600	-0.6080150	-0.2122960	
31	С	-1.3582370	0.0215490	-0.1021900	
32	Н	0.8484860	-1.4893660	-0.8162380	
33	0	2.3283540	-0.1285860	-0.6299060	
34	0	-2.0001310	0.5004240	0.8064990	
35	Н	2.3531660	0.7904650	-0.3172260	
36	0	-1.7805750	-1.0365590	-0.8313230	
37	Н	-2.6448750	-1.2891150	-0.4685780	
38	Η	0.0771310	2.5161590	-0.4503700	
39	С	1.0708360	-0.9743800	1.2627500	
40	Н	1.8646780	-1.6953590	1.4465340	
41	Н	1.2658770	-0.0925510	1.8739110	
42	H	0.1219680	-1.4134730	1.5741970	
43		427 560540604			
44	Energy:	-43/.568540604			
45					
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			Mole	cular Physics	
1					
2 3 4	B3LYP/6-	311++G** geomet	ry and energy	of conformer:	aThr-III
4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21	N H C H C C H O O H O H H H H H	-0.9006290 -0.6137430 -0.1875900 -0.1835870 1.2722380 -1.0282340 1.7022080 1.2802490 -0.5803840 1.0651210 -2.3148780 -2.3802580 -0.7090630 2.1481710 3.1679950 1.7698160 2.1785030	1.7481870 2.0552030 0.5111930 0.4335630 0.4666440 -0.6883160 1.4472520 0.4061520 -1.7937070 -0.4986610 -0.3914370 0.5818950 2.4992030 -0.6083830 -0.5168610 -1.6072410 -0.4865580	-0.2100110 0.7168340 -0.5698130 -1.6630430 -0.0591800 -0.0699370 -0.2879700 1.3696180 0.1077570 1.6300760 0.1338070 0.0004750 -0.8627630 -0.6969090 -0.3163470 -0.4775380 -1.7840710	
21 22	Energy:	-438.424501996		1.,010,10	
23 24	MP2/aug-	cc-pVTZ geometr	v and energy o	of conformer:	aThr-III
26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53	N H C H C H O H H C H H H Energy:	-0.9211890 -0.6547970 -0.1861370 -0.1727840 1.2509350 -0.9952070 1.6698990 1.2223290 -0.5186200 0.9784000 -2.2918140 -2.3581610 -0.6841900 2.1425890 3.1506690 1.7656160 2.1854330 -437.566898070	$\begin{array}{c} 1.7352070\\ 1.9815240\\ 0.5300810\\ 0.4844290\\ 0.4858440\\ -0.6850570\\ 1.4823170\\ 0.3330430\\ -1.7837330\\ -0.5877200\\ -0.4223490\\ 0.5531170\\ 2.5181670\\ -0.5374470\\ -0.4583060\\ -1.5444030\\ -0.3517910\\ \end{array}$	-0.1692450 0.7804080 -0.5660090 -1.6583880 -0.0925070 -0.1922880 1.3840800 0.0919080 1.5545360 0.0948870 -0.0294690 -0.7647840 -0.7122100 -0.3087350 -0.5502960 -1.7862180	
54 55 56 57 58 59 60		UR	L: http://mc.manu	scriptcentral.com	ı/tandf/tmph

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2					
3 1	B3LYP/6-	311++G** geomet	ry and energy	of conformer:	aThr-IV
- 5	NT	0 2002000	1 0/0/700	0 1/07250	
6	IN H	-1.3630650	2 2121010	-0.2407070	
7	II C	-1.3030030	0 5713100	-0.5719860	
8	ч	-0.1302020	0.5120350	-1 6485280	
9	C	1 3359430	0.2164080	-0 2936370	
10	C	-1.0971610	-0.3984880	0.1209660	
10	н	1 9254210	1 0006590	-0 7751470	
12	0	1.6341190	0.3370720	1,0967300	
12	0	-0.8841980	-1.0018660	1.1498550	
14	н	1.0848210	-0.3093910	1.5626510	
14	0	-2.2873330	-0.4716000	-0.5179610	
16	Н	-2.8675950	-1.0442020	0.0082530	
17	Н	-0.1034020	2.0691190	0.8262380	
10	C	1.7475030	-1.1443130	-0.8542200	
10	H	1.1907290	-1.9588570	-0.3827620	
19	Н	1.5802620	-1.1908490	-1.9347820	
20	Н	2.8100860	-1.3083240	-0.6658000	
21					
22	Energy:	-438.423629378			
23	21				
24 25	MP2/aug-	cc-pVTZ geometr	y and energy o	of conformer:	aThr-IV
26					
20	Ν	-0.3790920	1.9401160	-0.1350980	
28	H	-1.3619210	2.1786020	-0.1948500	
20	С	-0.1361750	0.5698900	-0.5795430	
30	Н	-0.3283600	0.5140030	-1.6518560	
31	С	1.3248370	0.2154370	-0.3096790	
32	С	-1.0760710	-0.3933950	0.1202200	
33	H	1.9206620	0.9816240	-0.8071580	
34	0	1.6271250	0.3510920	1.0752350	
35	0	-0.8475650	-1.0032430	1.1478020	
36	H	1.0600390	-0.28/3130	1.5333150	
37	0	-2.2/43230	-0.4559280	-0.5027490	
38	H	-2.8354310	-1.0309440	0.0432130	
30	H	-0.0834380	2.0268120	0.8320320	
40	U	1.0904820	-1.1380140	-0.840/310	
40	H	1.12/19/0	-1.93/5410	-0.3339980	
41	П U	2 7548810	-1.2242700	-1.9123370	
42	11	2.7340010	-1.3400400	-0.0003720	
43	Eneray.	-437.565902301			
45	LINCI GY.	137.303902301			
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		Mol	ecular Physics	
B3LYP/6-	311++G** geome	try and energy	of conformer:	aThr-V
N	0.1053490	1.7111100	0.1581730	
Н	1.0854160	1.8783950	0.3668560	
С	-0.0393510	0.4423970	-0.5739110	
H	-0.012/820	0.5804690	-1.6593570	
C	-1 3942710	-0.2099300	-0.2238400 -0.2411520	
Н	0.9531240	-1.4190970	-0.8614810	
0	2.3017990	0.1453140	-0.6037880	
0	-1.8242730	-1.1610560	-0.8398760	
Н	3.0564300	-0.4151700	-0.3967810	
0	-2.0341380	0.3603780	0.7885420	
H	-1.4518760	1.1001040	1.0774480	
H	-0.20/6160	2.4909730	-0.4107310	
с н	T.T33/700	-U.9/18500 -1 5187110	1.2393900 1.5139360	
H	1.9877770	-1.6432220	1.4051720	
 H	1.2477870	-0.1151550	1.9084820	
Energy:	-438.42338082	9		
MP2/aug-	cc-pVTZ geomet	ry and energy	of conformer: a	aThr-V
N	0.1575090	1.6961910	0.1338620	
H	1.150/150	1.8483260	0.2/8/810	
н	-0.0287130	0.4433130	-0.8003700	
C.	1.0655250	-0.5594850	-0.2244650	
C	-1.3735630	-0.1825210	-0.2475020	
H	0.9077530	-1.4438650	-0.8462870	
0	2.2921070	0.0872120	-0.5783160	
0	-1.8372570	-1.1236860	-0.8481290	
H	3.0186070	-0.4872490	-0.3119620	
U U	-1.96/48/0	0.3//8160	0.8156470	
п H	-1.3307070 -0.1774380	2 4784930	-0.4160750	
C	1.0498910	-0.9506280	1.2428630	
H	0.1217560	-1.4618460	1.4974000	
Н	1.8734260	-1.6350450	1.4502990	
H	1.1586800	-0.0753150	1.8813740	
Energy:	-437.56677789	5		

B3LYP/6	-311++G** geome	etry and energy	of conformer:	aThr-VI
N	-0.0955450	1.7052140	0.3193320	
п	-0.0726050	2.4074000	-0.1340140	
Ч	-0.0720030	0.4494920	-0.4424330	
C	1 1660500	-0 1130630	-1.3029330	
C	-1 381/260	-0.3300020	-0.2019370	
с ц	-1.3014200	-0.3300020 -1.3050670	-0.2002930	
0	2 2670620	-1.3030070	-0.6976100	
0	-1 5236910	-1 4897210	-0.4952410	
H	3.0725230	-0.1617450	-0.6601850	
0	-2.3635310	0.4165420	0.3158280	
Н	-1.9670610	1.3036330	0.4661020	
Н	0.2796840	1.5796930	1.2549450	
С	1.3732850	-0.9397380	1.1771510	
Н	0.5289080	-1.5519480	1.5021080	
Н	2.2705950	-1.5630170	1.2320000	
Н	1.5105320	-0.1113850	1.8784040	
Energy:	-438.42332051	.1		
B3LYP/6	5-311++G** geome	try and energy	of conformer:	aThr-VII
	2			
N	0.3060560	1.7244680	0.1537380	
Н	-0.1197550	2.5140820	-0.3165110	
С	0.0042770	0.4681200	-0.5281790	
Н	0.0490430	0.6474130	-1.6051200	
С	1.1338870	-0.5646780	-0.2303070	
С	-1.3627410	-0.1561850	-0.2693680	
Н	0.9785260	-1.4255290	-0.8836850	
0	2.3685730	0.0158680	-0.6187760	
0	-1.8233390	-1.0663460	-0.9112650	
H	2.3554670	0.9213590	-0.2/26940	
0	-2.0152340	0.3964180	0.7843780	
H	-2.8531700	-0.0812000	0.8831160	
п	-0.0324240	1.0202620	1.1093950	
U U	T.T072200	-1.UZ&363U	1.2269U3U	
п u	0.2330000	-1.33/4ZIU	1.3U013/U	
п Н	Z.UIU8/UU 1 3081070	-1./U9423U _0 1850180	1.304311U 1.9096770	
11	T.30013/0	-0.1030100	1.3030//0	
Enerav:	-438.42329450	4		
2	100,1202,100	-		
B3LYP/6	-311++G** geome	etry and energy	of conformer:	aThr-VIII
NT	0 1001050	1 7100500	0 1000000	
IN LI	U.1061950	1./130560 2.4012620	U.LU89890	
11 C	-0.0383120 -0.1331330	2,401202U 0 1031050	-U.4/0913U _0 570/570	
U U	-U.USOSISU	U,4Z34Z3U 0 59/1/50	-U.J/343/U _1 6710700	
п С	-0.0144300 1 1022820	0.5241030 -0 5531940	-1.0/12/00 -0 18505/0	
C	_1 3076000	-0.21/8360	-0.1030340	
Ч	1.3970000 0.9465960	-1 4692210	-0 7630410	
0	2 3680850	0 0337640	-0 5154930	
0	-1 8281630	-1.1729800	-0.8291910	
~	T.0201000	- · · · 2 / 0 0 0	· · · · · · · · · · · · · · · · · · ·	

2 3 4 5 5 7 3 3 9	Н О Н С Н Н Н	2.4833750 -2.0386790 -1.4611440 1.0816620 1.1502810 0.2271110 1.9825600 1.3002780	0.0216670 0.371110 1.1180690 1.8813750 -0.8954490 -1.3841240 -1.5764890 -0.0029870	-1.4715890 0.7783210 1.0548850 0.3382470 1.2981160 1.6161150 1.4822410 1.9098790	
11 12 13	Energy:	-438.423250569)		
13 14 15 16 17					
19	B3LYP/6-	311++G** geomet	ry and energy	of conformer:	aThr-IX
20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38	N H C H C C H O O H O H H C H H H 1 Energy:	-0.4700340 -1.4462760 -0.1257190 -0.1321780 1.3210010 -1.1790270 1.9279470 1.3624510 -2.1056740 0.9028030 -0.9978990 -1.7060930 -0.2695600 1.9286460 1.4156750 1.8801800 2.9773190 -438.422988926	1.8581390 1.9687400 0.4457680 0.1326500 0.2523440 -0.3999110 0.9503350 0.6402260 0.0418210 1.4924160 -1.7232300 -2.1812740 2.4092260 -1.1343720 -1.8533090 -1.4887520 -1.0905170	-0.5036360 -0.2517430 -0.6907120 -1.7441580 -0.1432150 0.0137780 -0.7419440 1.2200270 0.6466070 1.2653450 -0.1820470 0.2962030 -1.3285370 -0.2701480 0.3676070 -1.3033210 0.0310880	
39 40	21				
41 42 43	B3LYP/6-	311++G** geomet	ry and energy	of conformer:	aThr-X
44	N	-0.0706400	1.8513750	0.4304850	
45 46	н С	-0.8015610	2.4343/20	0.0385110	
40 17	Н	0.0760400	0.7191310	-1.3115900	
48	С	1.2292760	-0.2438020	0.2365980	
49	C	-1.2956410	-0.2494770	-0.0007820	
50	Н	1.1981220	-0.2971060	1.3346710	
51	0	1.2224710	-1.5620190	-0.3071070	
52	0	-1.4205870	-1.2122340	0.7220080	
52	Н	0.5050680	-2.0484850	0.1173620	
55 57	0	-2.3426980	0.2900380	-0.6666500	
54	Н	-3.1317400	-0.2263660	-0.4407460	
55	Н	-0.2479070	1.7503990	1.4255420	
50	С	2.5238650	0.4218880	-0.2028810	
<i>i</i> 0	Н	2.5651170	1.4547350	0.1438520	
י ר	Н	3.3764300	-0.1287220	0.1989890	
50 50	Н	2.5970890	0.4116940	-1.2941580	

Energy: -438.422948728

SLYP/6-311++G** geometry and energy of conformer: aThr-: 0.1469390 1.8441480 -0.2188930 1.0444240 2.2507980 0.0186950 0.0351320 0.4793590 0.3014670 -0.0666100 0.4326210 1.4009690 -1.1978290 -0.2503050 -0.2873520 1.3115900 -0.2963660 0.0005650 -1.0387560 -1.5292520 0.3159630 1.3707050 -1.4626870 -0.3127690 -0.5713950 -2.0479690 0.0936400 2.4222800 0.4552640 0.1637220 3.1873610 -0.1094880 -0.0254090 -0.5749010 2.4347970 0.1768420 -2.489460 0.5163650 -0.4114660 -2.6422690 0.6834710 1.0293620 evergy: -438.422264697 SLYP/6-311++6** geometry and energy of conformer: aThr-: -0.0891570 1.7228900 0.2217640 0.3490020 1.6604070 1.1358180 -0.0683190 0.4272240 -0.4702970 -0.0849100 0.6348470 -1.5664650 1.01644080 -0.468090 -0.1974050 -1.3859740 -0.3326680 -0.2056250 1.0185890 -1.3940950 -0.7617110 2.3541240 0.2023690 -0.6368980 -1.5480790 -1.4878790 -0.532730 2.4512550 0.083850 -1.586230 -2.3423230 0.4190980 0.352350 -1.5480790 -1.342930 1.678260 -2.6422400 -1.4878790 -0.532730 2.4512550 0.083550 -1.294180 1.3607160 -0.8135510 1.2725730 0.4789450 -1.3142930 1.6782660 2.2164130 -1.4819000 1.3784580 1.5732560 0.0787700 1.8691920 hergy: -438.422230945 SLYP/6-311++G** geometry and energy of conformer: aThr-: 0.1158580 1.9111030 0.0026970 1.0805230 2.1701190 -0.18505990 -0.0762030 0.3375390 1.4366790 -1.3369290 -0.1587480 0.152710 -0.9381290 -0.2058440 -1.4221570 -0.3581290 -0.1587480 -0.359390					
<pre>SLYP/6-311++G** geometry and energy of conformer: aThr-3</pre>					
<pre>SLYP/6-311++G** geometry and energy of conformer: aThr-: 0.1469390 1.8441480 -0.2188930 0.0351320 0.4793590 0.3014670 -0.0666100 0.4326210 1.4009690 -1.1978290 -0.2503050 -0.2873520 1.3115900 -0.2963660 0.0005650 -1.0387560 -0.555120 -1.3687040 -1.3557960 -1.5292520 0.3169630 1.3707050 -1.4626870 -0.3127690 -0.5713950 -2.0479690 0.936400 2.4222800 0.4552640 0.1637220 3.1873610 -0.1094880 -0.0254090 -0.5749010 2.4347970 0.1768420 -2.4994680 1.479640 -0.553340 -3.3296370 -0.0738430 -0.4114660 -2.6422690 0.6834710 1.0293620 mergy: -438.422264697</pre>					
<pre>BLYP/6-311++G** geometry and energy of conformer: aThr-3 0.1469390 1.8441480 -0.2188930 1.0444240 2.2507980 0.0186950 0.0351320 0.4793590 0.3014670 -0.0666100 0.4326210 1.4009690 -1.1978290 -0.2963660 0.0005650 1.0387560 -0.3553120 -1.3687040 -1.3557960 -1.5292520 0.3166930 1.3707050 -1.4626870 -0.3127690 -0.5713950 -2.0479690 0.0936400 2.4222800 0.4552640 0.1637220 3.1873610 -0.1094880 -0.0254090 -0.5749010 2.4347970 0.1768420 -2.4894680 0.5163650 -0.415330 -2.4908480 1.4749640 -0.5638340 -3.3296370 -0.0738430 -0.4114660 -2.6422690 0.6834710 1.0293620 hergy: -438.422264697 BLYP/6-311++G** geometry and energy of conformer: aThr-3 -0.0891570 1.7228900 0.2217640 0.3490020 1.6604070 1.1358180 -0.0683190 0.4272240 -0.4702970 -0.0849100 0.6348470 -1.5646500 1.1644080 -0.4688090 -0.1974050 -1.355740 -0.3326680 -0.256250 1.0185890 -1.3940950 -0.6368980 -1.5480790 -1.487290 -0.5332350 -1.9349630 1.3055260 0.4333250 -1.9349630 1.3055260 0.433322 0.4217430 2.4252430 -0.2994180 1.3607160 -0.8135110 1.2725730 0.4789450 -1.3142930 1.5782660 2.2164130 -1.4819000 1.3784580 1.5732560 0.0787700 1.8691920 hergy: -438.422230945 BLYP/6-311++G** geometry and energy of conformer: aThr-3 0.115880 1.911103 0.0026970 -0.0782309-2.342330 0.4190980 0.335099 -0.0762030 0.3375390 1.4366790 -1.134750 -0.1856550 -0.3450390 -1.134750 -0.1856550 -0.3450390 -1.134750 -0.1856550 -0.3450390 -1.134750 -0.1856550 -0.3450390 -1.134750 -0.185650 -0.3450390 -1.134750 -0.185650 -0.3450390 -1.134750 -0.1857480 0.0152710 -0.9381290 -0.2058440 -1.4241570 -1.1342760 -0.157480 0.0152710 -0.9381290 -0.2058440 -0.152710 -0.9381290 -0.2058440 -1.4241570 -1.1456400 -0.157480 0.0152710 -0.3381290 -0.2058440 -1.4241570 -1.136760 -0.157480 0.0152710 -0.3381290 -0.2058440 -1.4241570 -1.136760 -0.157480 0.0152710 -0.3381290 -0.2058440 -1.4241570 -1.136760 -0.1567480 0.0152710 -0.3381290 -0.2058440 -0.157400 -0.345930 -1.134750 -0.1567480 0.0152710 -0.3381290 -0.2058440 -0.157400 -0.345930 -1.4224510 -0.1567480 0.0152710 -0.3381290 -0.2058440 -0.157400 -0.345930</pre>					
<pre>BLYP/6-311++G** geometry and energy of conformer: aThr-:</pre>					
0.1469390 1.8441480 -0.2188930 1.0444240 2.2507980 0.0186950 0.0351320 0.4793590 0.3014670 -0.0666100 0.4326210 1.4009690 -1.1978290 -0.2503050 -0.2873520 1.3115900 -0.2963660 0.0005650 -1.0387560 -0.3553120 -1.3687040 -1.3557960 -1.5292520 0.3169630 1.3707050 -1.4626870 -0.3127690 -0.5713950 -2.0479690 0.0936400 2.4222800 0.4552640 0.1637220 3.1873610 -0.1094880 -0.0254090 -0.5749010 2.4347970 0.1768420 -2.4994680 0.5163650 -0.0415430 -2.4994680 0.5163650 -0.4114660 -2.6422690 0.6834710 1.0293620 hergy: -438.422264697 3LYP/6-311++G** geometry and energy of conformer: aThr-3 -0.0891570 1.7228900 0.2217640 0.3490020 1.6604070 1.1358180 -0.0683190 0.4272240 -0.4702970 -0.0849100 0.6348470 -1.5464650 1.1644080 -0.4688090 -0.1974050 -1.3859740 -0.3326680 -0.2056250 1.0185890 -1.3940950 -0.7617110 2.3541240 0.2023690 -0.6638800 -1.5480790 -1.4878790 -0.5032730 2.4512550 0.0833850 -1.5868230 -2.3423230 0.4190980 0.3532350 -1.9349630 1.3055260 0.4803420 0.4217430 2.4252430 -0.2994180 1.3607160 -0.813510 1.2725733 0.4789450 -1.3142930 1.6782660 2.2164130 -1.4819000 1.3784580 1.5732560 0.0787700 1.8691920 hergy: -438.422230945 3LYP/6-311++G** geometry and energy of conformer: aThr-3 0.1158580 -1.9111030 0.0026970 1.0805230 2.1701190 -0.1850590 0.0641450 0.4990990 0.3560990 -0.0762030 0.3375390 1.4366790 -1.134750 -0.185750 -0.3450930 1.422810 -0.158740 0.0152710 -0.9381290 -0.2058440 -1.4241570 -1.1626500 -1.5464070 -1.157160 -0.9381290 -0.2058440 -1.4241570 -1.1626500 -1.5460790	B3LYP/6-	-311++G** geome	try and energy	of conformer:	aThr-XI
<pre>1.0444240 2.2507980 0.0186950 0.0351320 0.4793590 0.3014670 -0.0666100 0.4326210 1.4009690 -1.1978290 -0.2503050 -0.2873520 1.3115900 -0.2963660 0.0005650 -1.0387560 -1.5292520 0.3169630 1.3707050 -1.4626870 -0.3127690 -0.5713950 -2.0479690 0.0936400 2.4222800 0.4552640 0.1637220 3.1873610 -0.1094880 -0.0254090 -0.5749010 2.4347970 0.1768420 -2.4894680 0.5163650 -0.0415430 -2.4908480 1.4749640 -0.5663340 -3.3296370 -0.0738430 -0.4114660 -2.6422690 0.6834710 1.0293620 hergy: -438.422264697</pre>	N	0.1469390	1.8441480	-0.2188930	
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1.5732560 0.0787700 1.8691920 hergy: -438.422230945 BLYP/6-311++G** geometry and energy of conformer: aThr-2 0.1158580 1.9111030 0.0026970 1.0805230 2.1701190 -0.1850590 0.0641450 0.4990990 0.3560990 -0.0762030 0.3375390 1.4366790 -1.1334750 -0.1856550 -0.3450930 1.4228810 -0.1587480 0.0152710 -0.9381290 -0.2058440 -1.4241570 -1 1676360 -1 5454070 0 1603980	С Н С Н О Н О Н Н С Н Н	-0.0683190 -0.0849100 1.1644080 -1.3859740 1.0185890 2.3541240 -1.5480790 2.4512550 -2.3423230 -1.9349630 0.4217430 1.3607160 0.4789450	$\begin{array}{c} 0.4272240\\ 0.6348470\\ -0.4688090\\ -0.3326680\\ -1.3940950\\ 0.2023690\\ -1.4878790\\ 0.0833850\\ 0.4190980\\ 1.3055260\\ 2.4252430\\ -0.8135510\\ -1.3142930 \end{array}$	-0.4702970 -1.5464650 -0.1974050 -0.2056250 -0.7617110 -0.6368980 -0.5032730 -1.5868230 0.3532350 0.4803420 -0.2994180 1.2725730 1.6782660	
hergy: -438.422230945 BLYP/6-311++G** geometry and energy of conformer: aThr-3 0.1158580 1.9111030 0.0026970 1.0805230 2.1701190 -0.1850590 0.0641450 0.4990990 0.3560990 -0.0762030 0.3375390 1.4366790 -1.1334750 -0.1856550 -0.3450930 1.4228810 -0.1587480 0.0152710 -0.9381290 -0.2058440 -1.4241570 -1 1676360 -1 5454070 0 1603980	С Н С С Н О О Н О О Н Н С Н Н С Н Н О О Н Н О О Н Н О О Н Н О О Н Н О О Н Н О О Н Н О О Н Н О О О Н Н О О О Н Н О О Н Н О О Н Н Н О О Н Н О Н Н О Н Н О Н Н О Н Н О Н Н О Н Н О Н Н О Н Н О Н Н О Н Н О Н Н О Н Н О С Н О О Н О Н	-0.0683190 -0.0849100 1.1644080 -1.3859740 1.0185890 2.3541240 -1.5480790 2.4512550 -2.3423230 -1.9349630 0.4217430 1.3607160 0.4789450 2.2164130	$\begin{array}{c} 0.4272240\\ 0.6348470\\ -0.4688090\\ -0.3326680\\ -1.3940950\\ 0.2023690\\ -1.4878790\\ 0.0833850\\ 0.4190980\\ 1.3055260\\ 2.4252430\\ -0.8135510\\ -1.3142930\\ -1.4819000 \end{array}$	-0.4702970 -1.5464650 -0.1974050 -0.2056250 -0.7617110 -0.6368980 -0.5032730 -1.5868230 0.3532350 0.4803420 -0.2994180 1.2725730 1.6782660 1.3784580	
BLYP/6-311++G** geometry and energy of conformer: aThr-3 0.1158580 1.9111030 0.0026970 1.0805230 2.1701190 -0.1850590 0.0641450 0.4990990 0.3560990 -0.0762030 0.3375390 1.4366790 -1.1334750 -0.1856550 -0.3450930 1.4228810 -0.1587480 0.0152710 -0.9381290 -0.2058440 -1.4241570 -1 1676360 -1 5454070 0 1603980	С Н С Н О О Н О Н О Н Н Н Н Н Н Н Н Н Н	-0.0683190 -0.0849100 1.1644080 -1.3859740 1.0185890 2.3541240 -1.5480790 2.4512550 -2.3423230 -1.9349630 0.4217430 1.3607160 0.4789450 2.2164130 1.5732560	$\begin{array}{c} 0.4272240\\ 0.6348470\\ -0.4688090\\ -0.3326680\\ -1.3940950\\ 0.2023690\\ -1.4878790\\ 0.0833850\\ 0.4190980\\ 1.3055260\\ 2.4252430\\ -0.8135510\\ -1.3142930\\ -1.4819000\\ 0.0787700 \end{array}$	-0.4702970 -1.5464650 -0.1974050 -0.2056250 -0.7617110 -0.6368980 -0.5032730 -1.5868230 0.3532350 0.4803420 -0.2994180 1.2725730 1.6782660 1.3784580 1.8691920	
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0.11585801.91110300.00269701.08052302.1701190-0.18505900.06414500.49909900.3560990-0.07620300.33753901.4366790-1.1334750-0.1856550-0.34509301.4228810-0.15874800.0152710-0.9381290-0.2058440-1.4241570-11676360-1<5454070	C H C C H O O H H H C H H H Energy:	-0.0683190 -0.0849100 1.1644080 -1.3859740 1.0185890 2.3541240 -1.5480790 2.4512550 -2.3423230 -1.9349630 0.4217430 1.3607160 0.4789450 2.2164130 1.5732560 -438.42223094	0.4272240 0.6348470 -0.4688090 -0.3326680 -1.3940950 0.2023690 -1.4878790 0.0833850 0.4190980 1.3055260 2.4252430 -0.8135510 -1.3142930 -1.4819000 0.0787700 5	-0.4702970 -1.5464650 -0.1974050 -0.2056250 -0.7617110 -0.6368980 -0.5032730 -1.5868230 0.3532350 0.4803420 -0.2994180 1.2725730 1.6782660 1.3784580 1.8691920	0
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-0.07620300.33753901.4366790-1.1334750-0.1856550-0.34509301.4228810-0.15874800.0152710-0.9381290-0.2058440-1.4241570-1.1676360-1.54540700.1603980	C H C C H O H H C H H H Energy: B3LYP/6- N H	-0.0683190 -0.0849100 1.1644080 -1.3859740 1.0185890 2.3541240 -1.5480790 2.4512550 -2.3423230 -1.9349630 0.4217430 1.3607160 0.4789450 2.2164130 1.5732560 -438.42223094 -311++G** geome 0.1158580 1.0805230	0.4272240 0.6348470 -0.4688090 -0.3326680 -1.3940950 0.2023690 -1.4878790 0.0833850 0.4190980 1.3055260 2.4252430 -0.8135510 -1.3142930 -1.4819000 0.0787700 5 try and energy 1.9111030 2.1701190	-0.4702970 -1.5464650 -0.1974050 -0.2056250 -0.7617110 -0.6368980 -0.5032730 -1.5868230 0.3532350 0.4803420 -0.2994180 1.2725730 1.6782660 1.3784580 1.8691920 of conformer: 0.0026970 -0.1850590	aThr-XI
-1.1334750-0.1856550-0.34509301.4228810-0.15874800.0152710-0.9381290-0.2058440-1.4241570-1.1676360-1.54540700.1603980	C H C C H O H H C H H H Energy: B3LYP/6- N H C	-0.0683190 -0.0849100 1.1644080 -1.3859740 1.0185890 2.3541240 -1.5480790 2.4512550 -2.3423230 -1.9349630 0.4217430 1.3607160 0.4789450 2.2164130 1.5732560 -438.42223094 -311++G** geome 0.1158580 1.0805230 0.0641450	0.4272240 0.6348470 -0.4688090 -0.3326680 -1.3940950 0.2023690 -1.4878790 0.0833850 0.4190980 1.3055260 2.4252430 -0.8135510 -1.3142930 -1.4819000 0.0787700 5 try and energy 1.9111030 2.1701190 0.4990990	-0.4702970 -1.5464650 -0.1974050 -0.2056250 -0.7617110 -0.6368980 -0.5032730 -1.5868230 0.3532350 0.4803420 -0.2994180 1.2725730 1.6782660 1.3784580 1.8691920 of conformer: 0.0026970 -0.1850590 0.3560990	aThr-XI
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T • T • 1 • 1 • 1 • 1 • 1 • 1 • 1 • 1 •	C H C C H O O H H C H H B 3 L Y P / 6- N H C H C H H C H H C H H C H H H H H H	-0.0683190 -0.0849100 1.1644080 -1.3859740 1.0185890 2.3541240 -1.5480790 2.4512550 -2.3423230 -1.9349630 0.4217430 1.3607160 0.4789450 2.2164130 1.5732560 -438.42223094 -311++G** geome 0.1158580 1.0805230 0.0641450 -0.0762030 -1.1334750 1.4228810 -0.9381290	0.4272240 0.6348470 -0.4688090 -0.3326680 -1.3940950 0.2023690 -1.4878790 0.0833850 0.4190980 1.3055260 2.4252430 -0.8135510 -1.3142930 -1.4819000 0.0787700 5 try and energy 1.9111030 2.1701190 0.4990990 0.3375390 -0.1856550 -0.1587480 -0.2058440	-0.4702970 -1.5464650 -0.1974050 -0.2056250 -0.7617110 -0.6368980 -0.5032730 -1.5868230 0.3532350 0.4803420 -0.2994180 1.2725730 1.6782660 1.3784580 1.8691920 of conformer: 0.0026970 -0.1850590 0.3560990 1.4366790 -0.3450930 0.0152710 -1.4241570	aThr-XI:

1					
2					
3	0	2.4008870	0.4959440	-0.2412560	
4	н	-1 8436190	-2 0486490	-0 3050580	
5	0	1 4683700	_1 /957880	0.0562940	
6	U	0 5635150	_1 8470890	0.1931630	
7	11	0.0000100	-1.0470090	0.1931030	
0	H	-0.2344520	2.4998300	0.7473510	
0	C	-2.4552460	0.5147660	-0.0/0/120	
9	Н	-2.4264030	1.5341060	-0.45/25/0	
10	Н	-3.2774300	-0.0122920	-0.5647450	
11	H	-2.6615990	0.5397900	1.0033220	
12					
13	Energy:	-438.422218686)		
14					
15					
16					
17					
17	B3LYP/6-	311++G** geomet	ry and energy	of conformer.	aThr-XIV
18	DOUIL/0	JIIIIO geomee	ing and energy	or conformer.	
19	NT	0 7751260	1 72/0100	0 1750070	
20	IN	0.7751200	-1.7240190	-0.4736970	
21	H	0.3038300	-2.2180650	0.2770570	
22	С	0.1/19150	-0.3943200	-0.6706380	
23	Н	0.1789760	-0.1529840	-1.7376480	
24	С	-1.2909930	-0.3575850	-0.1876570	
25	С	1.0742560	0.6783180	-0.0042650	
26	Н	-1.2372330	-0.7751200	1.1853570	
20	0	0.8024680	1.8510420	0.0140900	
27	0	-2.1070570	-0.6731630	1.5834840	
28	Н	2.2102410	0.1884310	0.4995500	
29	0	2.1805470	-0.7773710	0.3073910	
30	Н	0.7408280	-2.2929180	-1.3129930	
31	Н	-2.0291190	0.9633640	-0.3637190	
32	С	-1.5644350	1.7582940	0.2168870	
33	H	-2.0313080	1,2653700	-1 4147540	
34	ч	-3 0729760	0 8/33870	-0.0537440	
35	11 U	_1 8144520		-0.7687000	
36	п	-1.0144520	-1.1323040	-0.7007000	
37		420 40010000)		
20	Energy:	-438.422129382			
30					
39					
40					
41	B3LYP/6-	311++G** geomet	ry and energy	of conformer:	aThr-XV
42					
43	Ν	-0.3833390	1.9501280	-0.2376000	
44	Н	0.0990310	2.1654390	0.6307180	
45	С	-0.1203530	0.5557770	-0.6070070	
46	Н	-0.3389180	0.4368510	-1.6703970	
47	С	1.3293600	0.0862610	-0.3259530	
48	С	-1.1302340	-0.2856700	0.1698980	
49	Н	1.9831030	0.7405290	-0.9123140	
50	0	1.6866600	0.3380700	1.0309350	
50	0	-0.9880250	-0.6435880	1.3188490	
51	H	1.0558260	-0.1410600	1,5883970	
52 50	0	-2.2269680	-0.5845690	-0.5492320	
53	ч	-2 8373550	-1 0631780	0 0338380	
54	и П	-0 0366060 2.03/3330	2 5001060	_0 0520200	
55	11 C	-U.UJUUJUU 1 5000770	2.JOUI30U 1 2652600	-U.JJZUIIU	
56		1.002//U	-1.505209U	-U./SIUUOU	
57	H	1.3/13220	-1.5223/60	-1./923260	
58	H	2.6363210	-1.6146280	-0.5545420	
59	Н	0.9/50950	-2.0585680	-0.1481520	
60					
	Energy:	-438.422021799)		

1 2 3					
4 5 6	B3LYP/6-	311++G** geome	trv and energy	of conformer:	aThr-XVI
7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24	N H C H C C H O O H O H H C H H H H	-0.4278870 -0.0323130 -0.1849850 -0.3578330 1.2850930 -1.2172610 1.9082510 1.5089420 -2.2611460 1.2070720 -0.9146800 -0.0204370 -1.4222640 1.7123820 1.5809770 2.7658190 1.1296390	1.9034380 2.6176180 0.5620140 0.5204760 0.2017140 -0.4082460 0.9677570 0.2606320 -0.6424840 1.1403910 -0.9439810 -0.6463270 2.0964830 -1.1684240 -1.2343430 -1.3357760 -1.9660320	-0.0420630 -0.6469940 -0.6134030 -1.6948000 -0.3222380 0.0015880 -0.8042200 1.0997010 -0.5497270 1.3766870 1.1935370 1.4688160 0.0275360 -0.8211510 -1.9041250 -0.5906460 -0.3546830	
25 26 27 28	Energy:	-438.42153588	5		
29 30	B3LYP/6-	311++G** geome	try and energy	of conformer:	aThr-XVII
31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 40	N H C H C C H O O H O H H C H H H H H	-0.2297340 -1.1646910 -0.1088510 -0.2467870 1.3174410 -1.2106510 1.6468340 -2.1376670 1.0524110 -1.0722580 -1.8286000 0.0360520 1.5644250 0.9216780 1.3760510 2.6023200 1.9902490	1.9470650 2.2910160 0.5104460 0.3173010 0.0555880 -0.2979920 0.4338870 -0.8320280 -0.3295370 -0.8212050 2.1838420 -1.4303980 -2.0586030 -1.6899050 -1.6734370 0.6499230	-0.4745560 -0.6614080 -0.7039720 -1.7706480 -0.3161510 -0.0140570 1.0201920 -0.5668760 1.6211000 1.3460660 1.7019970 0.4755720 -0.5677110 0.0574810 -1.6134420 -0.3333070 -0.9391650	
49 50 51	Energy:	-438.42143177	4		
52 53 54 55	B3LYP/6-	311++G** geome [.]	try and energy	of conformer:	aThr-XVIII
56 57 58 59 60	N H C H C C	0.1367420 1.1092390 0.0685810 -0.0690430 -1.1321920 1.4246690	1.9111710 2.1729220 0.5042900 0.3585950 -0.1829680 -0.1664190	-0.0195110 -0.1564180 0.3503230 1.4360650 -0.3512630 0.0236070	

Н	-0.9404890	-0.2019300	-1.4268040	
0	-1.2010840	-1.5780670	0.0407520	
0	2.4198160	0.4811200	-0.1788630	
Н	-1.7302420	-1.6579050	0.8426370	
0	1.4462850	-1.5042150	0.0141820	
Н	0.5319020	-1.8473900	0.1104770	
Н	-0.2606610	2.5112030	0.6918150	
С	-2.4541690	0.5153590	-0.0788160	
Н	-2.4182110	1.5435650	-0.4396280	
Н	-3.2678850	-0.0044110	-0.5895460	
Н	-2.6732730	0.5348780	0.9963060	
Energy:	-438.42136433	1		
B3LYP/6-	-311++G** geome	try and energy	of conformer:	aThr-XIX
N	0.1671450	1.9561490	-0.1718390	
Н	-0.3723320	2.4885980	-0.8459240	
С	0.0342680	0.5218640	-0.4094280	
H	0.1674140	0.3279530	-1.4779020	
C	1.1390660	-0.2372620	0.3747630	
C	-1 3327830	-0.0205040	0 0104540	
ч	1 0692050	0.0203040	1 /19/270	
0	1.0092030	1 6204220	1.4194270	
0	1 0222610	-1.0394320	1 0050460	
0	-1.9223010	0.3109000	1.0039460	
H	1.0153240	-2.0108990	-0.4642360	
0	-1.8300440	-0.9182520	-0.8702630	
H	-2.6680760	-1.2460920	-0.50/9580	
H	-0.1966740	2.1851100	0.7495690	
С	2.5301180	0.0657240	-0.1669890	
Н	2.7120540	1.1411190	-0.1758400	
Н	3.2861900	-0.4228710	0.4511410	
Н	2.6330140	-0.3057310	-1.1937160	
Energy:	-438.42120484	5		
B3LYP/6-	-311++G** geome	try and energy	of conformer:	aThr-XX
N	-0.4951630	1.8015490	-0.5771520	
Н	-1.5005070	1.9208360	-0.5652420	
С	-0.0938610	0.3975930	-0.7380120	
Н	-0.0341500	0.0748980	-1.7856670	
С	1.3288430	0.2623880	-0.1160000	
С	-1.0782190	-0.5614060	-0.0851940	
Н	1.9502370	0.9697670	-0.6898680	
0	1.2897060	0.6617970	1.2443070	
0	-1.0718660	-1.7535550	-0.2596650	
Н	0.7689090	1.4788490	1.2666600	
0	-1.9855560	0.0526560	0.7102510	
H	-2.5499500	-0.6417760	1.0831530	
н	-0.1096510	2,3741530	-1.3195130	
C	1 960390	_1 1157170	_0 2012190	
ч	1.JUUJJZU 2 0137860	_1 /552020	_1 2300610	
ц	2.013/000 2 97/2960	-1 06708/0	1 2000010	
11	2.7/42700 1 2010620	-1.00/904U	0.2013200	
11	エ・フヺエヺやてい	-1.040/140	0.3/14000	

1					
3	Energy:	-438.421165644			
4 5					
6					
7 8	B3LYP/6-	311++G** geomet	ry and energy	of conformer:	aThr-XXI
9 10	Ν	0.1550590	1.9403860	-0.1050090	
11	Н	-0.1862400	2.1358790	0.8323630	
12	С	0.0300920	0.5121720	-0.3937590	
13	H	0.1395260	0.3546680	-1.4686200	
14 15	C	-1 3260100	-0.2640180	0.3308230	
15 16	H	1.0597460	-0.0335880	1.4019900	
17	0	0.8543870	-1.6499770	0.1152550	
18	0	-1.7922750	0.1196250	1.1517150	
19	H	1.4723300	-2.1816090	0.6258860	
20	0	-1.9773990	-0.6946550	-0.9352320	
21	л Н	-0.3995170	2 4908820	-0.7513510	
22	С	2.5351150	0.1079310	-0.1713640	
23	H	2.7059130	1.1797390	-0.0606470	
24 25	Н	3.3028570	-0.4255870	0.3979590	
25	Н	2.6410210	-0.1620040	-1.2258180	
27	_				
28	Energy:	-438.421106779			
29					
30					
31	B3LYP/6-	311++G** geomet	ry and energy	of conformer:	aThr-XXII
32					
33 34	N	-0.1124730	1.9266840	0.2569850	
35	H	0.28/1330	2.2110180	-0.6328570	
36	н	-0.1516610	0.4037490	1 4761780	
37	C	-1.1208590	-0.2676600	-0.3698590	
38	С	1.3827810	-0.0286220	0.0087170	
39	Н	-0.8929340	-0.1798850	-1.4443190	
40	0	-1.1885150	-1.6423510	-0.0013230	
41	0	2.2193330	0.6104530	-0.5747550	
4Z 42	H	-0.3046750	-2.02/2800	-0.0214280	
43 44	Н	2.4655530	-1.5860110	0.0292480	
45	Н	0.4189510	2.4093410	0.9731870	
46	С	-2.4987920	0.3171920	-0.1027020	
47	Н	-2.5527210	1.3587760	-0.4145730	
48	Н	-3.2416440	-0.2685830	-0.6482270	
49	Н	-2.7312760	0.2588410	0.9640520	
50 51 52	Energy:	-438.420944975			
53 54	B3LYP/6-	311++G** apompt	rv and energy	of conformer.	aThr-XXTTT
55 56	, -				
57	Ν	0.2097500	1.8057310	-0.1676450	
58	Н	-0.1877190	1.9895030	0.7473180	
59	С	-0.0217050	0.4297000	-0.5665910	
60	п С	-U.U423/5U 1 071/630	U.J/IJUJU _0 59121/0	-1.002/93U -0 1048360	
	C	-1.3885330	-0.0185340	-0.0863530	
		UR	L: http://mc.manu	uscriptcentral.com	/tandf/tmph

Ν	0.2097500	1.8057310	-0.1676450
Н	-0.1877190	1.9895030	0.7473180
С	-0.0217050	0.4297000	-0.5665910
Н	-0.0423750	0.3713030	-1.6627930
С	1.0714630	-0.5912140	-0.1048360
С	-1.3885330	-0.0185340	-0.0863530

2					
3	Н	0.8179830	-1.5692990	-0.5311040	
4	0	2.3414320	-0.1580460	-0.6080570	
5	0	-2 0218220	0 4941680	0 8010970	
6	о ц	2 3556710	-0 269//90	-1 56/7710	
7	0	1 0102040	1 11/0000	0 7564050	
0	0	-1.0192040	-1.1140000	-0.7564950	
0	H	-2.6/5/500	-1.365/910	-0.3/80900	
9	Н	1.2041230	2.0049380	-0.1519620	
10	С	1.2175380	-0.7105330	1.4035170	
11	Н	0.2901000	-1.0572990	1.8651450	
12	Н	2.0103750	-1.4227020	1.6383170	
13	Н	1.4841610	0.2522940	1.8446700	
14					
15	Energy:	-438.42092109	6		
16	21				
17					
17					
18	B3LYP/6-	311++G** geome	try and energy	of conformer.	aThr-XXIV
19	DOLII,0	SIIIIG GCOME	ery and energy	or conformer.	
20	N	0 1000200	1 0121770	0 1004000	
21	IN	0.1990200	1.0121770	-0.1094000	
22	П	-0.0969370	1.9402520	0.6520420	
23	C	-0.0254920	0.4496320	-0.5552190	
24	Н	-0.0384/80	0.4320180	-1.6496890	
25	С	1.0619570	-0.5854300	-0.1404790	
26	С	-1.3873510	-0.0188260	-0.0773540	
20	Н	0.7965950	-1.5458740	-0.5997710	
21	0	2.2631170	-0.0846300	-0.7432940	
28	0	-1.9996800	0.4452380	0.8507490	
29	Н	3.0049420	-0.6274440	-0.4584330	
30	0	-1.8409650	-1.0700160	-0.8016230	
31	Н	-2.6942080	-1.3324490	-0.4236850	
32	Н	1,1788750	2.0541600	-0.2034550	
33	C	1 2265880	-0 7611090	1 3655920	
34	U U	0 3140480	_1 1509200	1 8243920	
35	11 U	2 0202000	1 4722070	1 5770270	
36	п	2.0303000	-1.4/320/0	1.9445600	
37	п	1.4///290	0.10/0000	1.8443600	
20	-	400 40061004			
30	Energy:	-438.42061084	4		
39					
40					
41					
42	B3LYP/6-	311++G** geome	try and energy	of conformer:	aThr-XXV
43					
44	Ν	-0.4745510	1.8888600	-0.6668210	
45	Н	-1.4168640	2.0321000	-1.0150590	
46	С	-0.1301400	0.4754950	-0.6909840	
47	Н	-0.0994220	0.1369900	-1.7320910	
48	С	1.2921290	0.3057560	-0.1151160	
49	С	-1.1695020	-0.4010630	0.0256040	
50	Н	1.8751290	1.1052930	-0.5880990	
50	0	1.1728320	0.5732660	1.2899320	
บ 50	0	-2.0872870	0.0115050	0.6851070	
52	ч	2.0072070	0 6200000	1 6756220	
53		2.UJZ442U 0.0006770	U.UZJUOJU 1 7051040	1.0/JUJZU	
54	U	-0.9020//0	-1./251040	-0.2103640	
55	н	-1.6814210	-2.1990930	0.2661420	
56	Н	-0.4/26320	2.2125680	U.2965460	
57	С	1.9707380	-1.0336830	-0.3836690	
58	Η	2.0305040	-1.2273890	-1.4585670	
59	Н	2.9942500	-1.0100430	0.0035800	
60	Н	1.4375730	-1.8579010	0.0888570	
00					

Energy: -438.420378965
B3LYP/6-	-311++G** geome	try and energy	of conformer:	aThr-XX
N	0.0887170	1.9404360	-0.0629900	
H	-0.2379260	2.0886900	0.8869430	
С	0.0336140	0.5214450	-0.4163080	
п С	1 1372430	-0 2562770	-1.4915170	
C	-1.3295100	-0.1267800	-0.1737220	
Н	1.0236740	-0.0437440	1.4074880	
0	0.9161160	-1.6640930	0.2365470	
0	-2.0014580	-0.6751930	-1.0101430	
H	1.1071550	-1.9473310	-0.6650710	
н	-2.5901200	-0.4245240	1.2001590	
н	-0.4926990	2.4971170	-0.6798450	
С	2.5341780	0.1403610	-0.1199130	
Н	2.6788990	1.2173480	-0.0225360	
Н	3.2868710	-0.3791250	0.4766970	
H	2.6836240	-0.1281460	-1.1723670	
Energy:	-438.42030151	5		
B3LYP/6-	-311++G** geome	try and energy	of conformer:	aThr-XX
N	-0.4172310	1.9407700	-0.3528340	
Н	-1.3701950	2.2039770	-0.5807030	
С	-0.1808790	0.5244910	-0.6504790	
п С	-0.3368820	0.3808760	-1.7214120	
C	-1.2141740	-0.3997820	0.0365090	
Н	1.4519820	0.3756870	1.0808940	
0	-2.1888990	-0.8069270	-0.5405590	
0	2.3609360	0.1864730	1.3342520	
H	-1.0161220	-0.6692430	1.3442660	
	-0.1426900	-0.3276460	0 6291120	
н	0.2070200	1 00000040	0.0271120	
H H	1.6835560	-1.2282340	-0.7682420	
H H C	1.0835560	-1.2282340 -1.9874950	-0.7682420 -0.2602630	
H H C H	1.6835560 1.0838090 1.5568450	-1.2282340 -1.9874950 -1.3519850	-0.7682420 -0.2602630 -1.8469030	
H H C H H	1.6835560 1.0838090 1.5568450 2.7369220	-1.2282340 -1.9874950 -1.3519850 -1.4126970	-0.7682420 -0.2602630 -1.8469030 -0.5373430	
н Н С Н Н Н	1.6835560 1.0838090 1.5568450 2.7369220 1.8914410	-1.2282340 -1.9874950 -1.3519850 -1.4126970 0.9247320	-0.7682420 -0.2602630 -1.8469030 -0.5373430 -0.8693310	
H H C H H H Energy:	1.6835560 1.0838090 1.5568450 2.7369220 1.8914410 -438.42012634	-1.2282340 -1.9874950 -1.3519850 -1.4126970 0.9247320	-0.7682420 -0.2602630 -1.8469030 -0.5373430 -0.8693310	
H H C H H Energy:	1.6835560 1.0838090 1.5568450 2.7369220 1.8914410 -438.42012634	-1.2282340 -1.9874950 -1.3519850 -1.4126970 0.9247320	-0.7682420 -0.2602630 -1.8469030 -0.5373430 -0.8693310	
H H C H H Energy:	1.6835560 1.0838090 1.5568450 2.7369220 1.8914410 -438.42012634	-1.2282340 -1.9874950 -1.3519850 -1.4126970 0.9247320	-0.7682420 -0.2602630 -1.8469030 -0.5373430 -0.8693310	
H H C H H Energy: B3LYP/6-	1.6835560 1.0838090 1.5568450 2.7369220 1.8914410 -438.42012634 -311++G** geome	-1.2282340 -1.9874950 -1.3519850 -1.4126970 0.9247320 8	-0.7682420 -0.2602630 -1.8469030 -0.5373430 -0.8693310	aThr-XX
H H C H H Energy: B3LYP/6-	-311++G** geome	-1.2282340 -1.9874950 -1.3519850 -1.4126970 0.9247320 8 try and energy	-0.7682420 -0.2602630 -1.8469030 -0.5373430 -0.8693310	aThr-XX
H H C H H Energy: B3LYP/6- N H	1.6835560 1.0838090 1.5568450 2.7369220 1.8914410 -438.42012634 -311++G** geome -0.5144560 -1.4408890	-1.2282340 -1.9874950 -1.3519850 -1.4126970 0.9247320 8 try and energy 1.8248030 1.9395570	-0.7682420 -0.2602630 -1.8469030 -0.5373430 -0.8693310 v of conformer: -0.7228020 -1.1185240	aThr-XX
H H C H H Energy: B3LYP/6- N H C	1.6835560 1.0838090 1.5568450 2.7369220 1.8914410 -438.42012634 -311++G** geome -0.5144560 -1.4408890 -0.1054560	-1.2282340 -1.9874950 -1.3519850 -1.4126970 0.9247320 8 try and energy 1.8248030 1.9395570 0.4275490	-0.7682420 -0.2602630 -1.8469030 -0.5373430 -0.8693310 y of conformer: -0.7228020 -1.1185240 -0.7351730	aThr-XX
H H C H H Energy: B3LYP/6- N H C H	1.6835560 1.0838090 1.5568450 2.7369220 1.8914410 -438.42012634 -311++G** geome -0.5144560 -1.4408890 -0.1054560 -0.0198210	-1.2282340 -1.9874950 -1.3519850 -1.4126970 0.9247320 8 try and energy 1.8248030 1.9395570 0.4275490 0.0957020	-0.7682420 -0.2602630 -1.8469030 -0.5373430 -0.8693310 y of conformer: -0.7228020 -1.1185240 -0.7351730 -1.7742600	aThr-XX
H H C H H Energy: B3LYP/6- N H C H C	1.6835560 1.0838090 1.5568450 2.7369220 1.8914410 -438.42012634 -311++G** geome -0.5144560 -1.4408890 -0.1054560 -0.0198210 1.3022030	-1.2282340 -1.9874950 -1.3519850 -1.4126970 0.9247320 8 try and energy 1.8248030 1.9395570 0.4275490 0.0957020 0.3183490	-0.7682420 -0.2602630 -1.8469030 -0.5373430 -0.8693310 y of conformer: -0.7228020 -1.1185240 -0.7351730 -1.7742600 -0.1116580	aThr-XX

О О Н О Н Н С О Н	1.1318040 -1.0225550 1.9964390 -1.9973410 -2.5336540 -0.5510850 2.0019510 2.1223060	0.6382860 -1.7682450 0.6806790 0.0164320 -0.6951690 2.1618520 -1.0219300 -1.2434640	1.2780800 -0.2405790 1.6977850 0.7073200 1.0888480 0.2341760 -0.3051960 -1.3693650	
Н Э н	3.0017860	-0.9830390	0.1391880	
2 II 3 7	1.4434070	-1.0372300	0.1330320	
t Energy 5	: -438.42001814	10		
5				
3				
B3LYP/	6-311++G** geome	etry and energy	of conformer:	aThr-XXIX
N N	-0.1258460	1.8768710	0.4103310	
3 ^H	0.0314360	1.8188730	1.4113610	
C	-0.0035910	0.5654980	-0.2310840	
H C	0.0665930	0.7241820	-1.3105750	
i C	1.1991030	-0.2900310	0.2319350	
, C	-1.3136530	-0.1751890	-0.3085740	
	-1 4808860	-1.0060490	0 8933250	
	-1.4000000	-2.0716860	1513400	
) U	-2 2973900	-2.0710000	-0.8056690	
0	-3 1038680	-0.2611650	-0.5448450	
. н	0 5214780	2 5489040	0.0186760	
н	2 5281470	0 2965230	-0.2208460	
· C	2 5798800	0.3181260	-1 3132690	
н	2.6695400	1,3107310	0.1597720	
й Н	3,3488580	-0.3230060	0.1447600	
Н	1.1716070	-0.3389880	1.3296390	
Energy	: −438.41998422	25		
)				
2				
B3LYP/	6-311++G** geome	etry and energy	of conformer:	aThr-XXX
S N	0.0477930	1.5981070	0.5746330	
7 H	0.8722460	2.1447190	0.3490730	
3 С	-0.0617450	0.4958820	-0.3780540	
) H	-0.1086820	0.8409760	-1.4271680	
) C	1.1718400	-0.4194810	-0.2993050	
С	-1.3509030	-0.2878550	-0.1895800	
2 H	1.0273360	-1.2291190	-1.0223220	
3 0	2.2548640	0.4228160	-0.7334320	
4 <u>0</u>	-1.4893290	-1.4708730	-0.3761380	
; н	3.0831680	-0.0481420	-0.6010470	
3	-2.3840620	0.51/5210	0.1551120	
, H	-3.1/35050	-0.0406490	0.2218220	
H	-0./642060	2.2023480	U.528448U	
C	1.4352580	-1.UUXUU/U	1,U82585U	
п	U.UZJOJZU 2 3572020	-1.5026010	1 0677000	
п	2.JJ/2720 1 570/000	-1.J90094U _0 9105590	1 2720000	
п	1.JZ9400U	-0.2100020	T.0703300	

Energy:	-438.41994161	5		
B3L15/0-	-311++G** geome	try and energy	of conformer:	alhr-XXXI
Ν	-0.3052320	1.9290640	-0.5005250	
Н	0.1379480	2.2130500	0.3683950	
С	-0.0947260	0.4972240	-0.7206240	
Н	-0.2339910	0.2850160	-1.7821520	
C	1 3133770	-0 0116770	-0 3003430	
C	_1 219/190	-0 2614730	_0 0213480	
	1 (520240	0.2014/30	1 0120540	
п	1.6559540	0.42/0000	1.0130340	
0	-2.0771670	-0.9103930	-0.55/5160	
0	1.0160210	0.0513170	1.6339930	
Н	-1.1475590	-0.1346010	1.3363190	
0	-1.9092500	-0.6022540	1.7124760	
Н	0.1098300	2.4682540	-1.2519740	
н	1.4903940	-1.5200550	-0.4659720	
C	Δ 2127/60	-2 078/120	0 10309720 0 1030050	
C	1 2020000	-2.0784130	1 4044110	
H	1.2839880	-1.8306120	-1.4944110	
Н	2.5157040	-1.8011390	-0.2182450	
Н	2.0262000	0.5062990	-0.9498330	
Energy:	-438.41990423	0		
21				
	C 011 011			
B3LYP/6	⊳-311++G** geom	etry and energ	y of conformer:	aThr-XXXII
Ν	-0.1348270	1.8943190	-0.3262450	
Н	-0.3958050	2.1844250	0.6095700	
С	-0.0198280	0.4499580	-0.4489730	
Н	0.1762220	0.2069170	-1.4994800	
С	1.1238500	-0.2519510	0.3686660	
C	-1 3260640	-0 2462220	-0 0989990	
	1 2007520	1 5000110	0.0102790	
п	1.2907520	-1.3990110	-0.0492700	
U	-1.5120590	-1.4352860	-0.2515410	
0	0.4167930	-2.0117900	-0.1108110	
Н	-2.2485220	0.5532210	0.4654220	
0	-3.0121870	-0.0033860	0.6841060	
Н	0.7305920	2.3530170	-0.5817000	
 H	2 4702210	0 4329770	0 1215250	
11	2.7202010 2.7202020	0.4004700	0.0707040	
C			6 / 4 / 5 / 1 1	
С	2.7303930	0.4884/20	-0.8797340	
C H	2.4790300	1.4371630	0.6096270	
С Н Н	2.4790300 3.2379760	1.4371630 -0.1572890	0.6096270	
C H H H	2.7303930 2.4790300 3.2379760 0.8499770	0.4884720 1.4371630 -0.1572890 -0.2177290	0.6096270 0.6853330 1.4363040	
C H H H	2.7303930 2.4790300 3.2379760 0.8499770	0.4884720 1.4371630 -0.1572890 -0.2177290	0.6096270 0.6853330 1.4363040	
C H H H	2.7303930 2.4790300 3.2379760 0.8499770	0.4884720 1.4371630 -0.1572890 -0.2177290	0.6096270 0.6853330 1.4363040	
C H H H Energy:	2.7303930 2.4790300 3.2379760 0.8499770 -438.41986492	0.4884720 1.4371630 -0.1572890 -0.2177290	0.6096270 0.6853330 1.4363040	
C H H Energy:	2.7303930 2.4790300 3.2379760 0.8499770 -438.41986492	0.4884720 1.4371630 -0.1572890 -0.2177290 7	0.6096270 0.6853330 1.4363040	
C H H Energy:	2.7303930 2.4790300 3.2379760 0.8499770 -438.41986492	0.4884720 1.4371630 -0.1572890 -0.2177290 7	0.6096270 0.6853330 1.4363040	
C H H Energy:	2.7303930 2.4790300 3.2379760 0.8499770 -438.41986492	0.4884720 1.4371630 -0.1572890 -0.2177290 7	0.6096270 0.6853330 1.4363040	
C H H Energy: B3LYP/6-	2.7303930 2.4790300 3.2379760 0.8499770 -438.41986492	0.4884720 1.4371630 -0.1572890 -0.2177290 7 try and energy	0.6096270 0.6853330 1.4363040	aThr-XXXIII
C H H Energy: B3LYP/6-	-311++G** geome	0.4884720 1.4371630 -0.1572890 -0.2177290 7 try and energy	0.6096270 0.6853330 1.4363040	aThr-XXXIII
C H H Energy: B3LYP/6-N	-311++G** geome	0.4884720 1.4371630 -0.1572890 -0.2177290 7 try and energy 1.9199590	<pre>0.6797340 0.6096270 0.6853330 1.4363040 7 of conformer: 0.0596680</pre>	aThr-XXXIII
C H H Energy: B3LYP/6- N	-311++G** geome 0.0612960	0.4884720 1.4371630 -0.1572890 -0.2177290 7 try and energy 1.9199590 2.5057250	0.6096270 0.6853330 1.4363040 v of conformer: 0.0596680	aThr-XXXIII
C H H Energy: B3LYP/6- N H	-311++G** geome 0.0612960 -0.5237330	0.4884720 1.4371630 -0.1572890 -0.2177290 7 try and energy 1.9199590 2.5057250	<pre>0.0797340 0.6096270 0.6853330 1.4363040 v of conformer: 0.0596680 -0.5257170 0.02000000</pre>	aThr-XXXIII
C H H Energy: B3LYP/6- N H C	2.7303930 2.4790300 3.2379760 0.8499770 -438.41986492 -311++G** geome 0.0612960 -0.5237330 0.0230810	0.4884720 1.4371630 -0.1572890 -0.2177290 7 try and energy 1.9199590 2.5057250 0.5245530	0.6096270 0.6853330 1.4363040 v of conformer: 0.0596680 -0.5257170 -0.3868390	aThr-XXXIII
C H H Energy: B3LYP/6- N H C H	2.7303930 2.4790300 3.2379760 0.8499770 -438.41986492 -311++G** geome 0.0612960 -0.5237330 0.0230810 0.1846600	0.4884720 1.4371630 -0.1572890 -0.2177290 7 try and energy 1.9199590 2.5057250 0.5245530 0.5018460	0.6096270 0.6853330 1.4363040 v of conformer: 0.0596680 -0.5257170 -0.3868390 -1.4663370	aThr-XXXIII

C -1.3435420 -0.1215370 -0.1573620

2					
3	ц	1 016/070	0 1044400	1 270/100	
4	11	1.0104970	1 (204050	1.3794190	
5	0	0.9230030	-1.0304030	-0.0987170	
5	0	-2.1223130	-0.4405040	-1.0181120	
0	Н	1.5735750	-2.1986630	0.3364330	
1	0	-1.6338280	-0.2267200	1.1674310	
8	Н	-2.5189140	-0.6144210	1.2359780	
9	Н	-0.2699320	2.0056060	1.0156980	
10	С	2.5309680	0.2096420	-0.1093870	
11	Н	2 6493000	1 2665930	0.1343580	
12	н	3 3043430	-0.3556000	0 4203630	
12	и П	2 6020020	0.0340670	1 1020/70	
13	п	2.0030920	0.0/490/0	-1.1030470	
14	-	400 41001100	-		
15	Energy:	-438.41981168	5		
16					
17					
18					
19	B3LYP/6-	311++G** geome	try and energy	of conformer:	aThr-XXXIV
20					
20	Ν	-0.6448760	1.9569030	-0.2472940	
21	Н	-0.5704360	2,1156960	0.7545320	
22	C	-0.1743860	0 6129430	-0 5547100	
23	U U	_0 1209950	0.5096420	-1 6/68550	
24	II C	1 2506240	0.1221600	-1.0400550	
25	C	1.2396240	0.4331690	0.0096010	
26	C	-1.168/240	-0.4652200	-0.09/4/80	
27	H	1.7203470	1.4180010	-0.0918210	
28	0	1.2216850	0.2025040	1.4228810	
20	0	-2.3225770	-0.2591350	0.1752450	
29	Н	1.0162370	-0.7280950	1.5705310	
30	0	-0.6356100	-1.7167280	-0.0589770	
31	Н	-1.3510490	-2.3221640	0.1918660	
32	Н	-1.6287320	2.0486750	-0.4805640	
33	С	2.1288870	-0.5878960	-0.7192000	
34	ч	2 2131930	-0 3334940	-1 7796160	
35	и П	3 132/820	-0 5795700	-0.2882040	
36	11	1 7227020	1 5001100	-0.2002040	
37	п	1.7227020	-1.5961190	-0.0420300	
20	_		<u>_</u>		
30	Energy:	-438.41969599	0		
39					
40					
41					
42					
43	B3LYP/6-	311++G** geome	try and energy	of conformer:	aThr-XXXV
44					
45	Ν	0.2133880	1.7984030	-0.3404260	
46	Н	-0.6538950	2.3132400	-0.2297770	
47	С	0.0565040	0.4767580	0.2802730	
19 / 9	- H	-0.0212200	0.5235880	1.3792060	
40	C	_1 21/2/00	_0 1001100	-0 2500/20	
49	C	1 212E000	_0 2010E10	_0 0505070	
50		1 10400C0	-0.3212310		
51	н	-1.1040960	-U.3228410	-1.3331430	
52	0	-2.2628370	0./503/90	0.0208560	
53	0	1.3903590	-1.3095740	-0.7336400	
54	Н	-3.0729330	0.4417280	-0.3956850	
55	0	2.3978170	0.2487970	0.5305000	
56	Н	3.1752800	-0.2585800	0.2519930	
50	Н	0.9595990	2.3170680	0.1091730	
57 F0	С	-1.5165090	-1.5392990	0.4107240	
58	H	-0.7351570	-2.2682510	0.1928850	
59	H	-1.6126560	-1.4207290	1.4936500	
60	11	1.0120300	1 0 0 0 4 5 0 0	1.1990000	

-2.4613990 -1.9394590 0.0304180

Η

Energy: -438.419617424

	211			
BOLIF/0-	-SII++G^^ geome	erry and energy	of conformer:	allir-XXX
Ν	0.0060310	1.9204190	-0.3972340	
Н	-0.3972190	2.2598230	0.4691130	
С	-0.0043250	0.4697090	-0.4622250	
Н	0.1367670	0.1495630	-1.5006730	
С	1.0886270	-0.2882070	0.3760060	
C	-1.3772290	0.0039820	-0.0057660	
н	1 1615230	-1 6620820	0 0040770	
0	-2 1460760	0 6382080	0.6669170	
0	0 2711930	-2 0314760	-0.035/510	
U	1 6200220	1 2702110	0.2005070	
п	-1.0300220	-1.2/02110	-0.3903070	
0	-2.5032850	-1.5190060	-0.0238140	
H	0.9343880	2.3023950	-0.51/86/0	
Н	2.4838910	0.2797370	0.1560930	
С	2.7351940	0.2861890	-0.9085530	
Н	2.5813390	1.2900190	0.5580100	
Н	3.2066110	-0.3572820	0.6693910	
Н	0.8276130	-0.1978110	1.4419290	
Energy:	-438.41957325	59		
B3LYP/6-	-311++G** geome	etry and energy	of conformer:	aThr-XXX
N	0.1817750	1.7319630	0.2297290	
Н	0.9841720	2.2181860	-0.1500650	
С	-0.0361020	0.4763910	-0.4628620	
Н	-0.0680270	0.5775130	-1.5652790	
C	1.1139560	-0.5229720	-0.1627380	
C	-1 4121240	-0.0648180	-0 1094900	
с u	2 3//5800	0.0380510	-0 6/89190	
0	2.2443030	0.5525140	0.0400100	
0	-2.2024070	0.0000000	1 (02(050	
0	2.3840390	-0.0/////20	-1.6036950	
н	-1.586//90	-1.335/460	-0.5504920	
0	-2.4943410	-1.5926570	-0.3275180	
Н	-0.6376870	2.3262340	0.1978920	
Н	1.3023010	-0.8084660	1.3182760	
С	1.5112110	0.1144630	1.8591870	
Н	0.4025380	-1.2619310	1.7424290	
Н	2.1352430	-1.5007960	1.4536870	
Н	0.8994980	-1.4543410	-0.6958870	
Energy:	-438.41938688	35		
LHELGY.	430.41930000			
B3LYP/6-	-311++G** geome	etry and energy	of conformer:	aThr-XXX
N	0 1017000	1 700/270	-0 0965260	
T T T T T T T T T T T T T T T T T T T	U.IZI/ZOU 1 0007040	1./0943/U 2.0025120	-0.0900000	
п	L.U89/940	2.0825130	-U.18446UU	
C .	-0.0137230	0.4224880	-0.5/52420	
H	0.0346880	0.4389510	-1.6702090	
2	1.1079810	-0.5690870	-0.1167500	

С	-1.3696230	-0.1852730	-0.2634130	
Н	0.9047870	-1.5375830	-0.5885290	
0	2.3731940	-0.0642630	-0.5614340	
0	-1.8262880	-1.1420120	-0.8392560	
Н	2.4433800	-0.1874710	-1.5140110	
0	-2.0050560	0.4161360	0.7684730	
Н	-2.8430940	-0.0525380	0.9016740	
H	-0.1513670	1.8747930	0.8758690	
С	1.2096440	-0.7435270	1.3898780	
H	0.2820100	-1.1456050	1.8041870	
H	2.0206390	-1.4350610	1.6241060	
Н	1.4265890	0.2094520	1.8/80310	
Energy	: -438.41920694	16		
B3LYP/	6-311++G** geome	etry and energy	of conformer:	aThr-XXXI
N	0.6360290	-1.7147460	-0.6782690	
Н	1.4463640	-1.8474740	-1.2763470	
С	0.1260780	-0.3333750	-0.7607010	
Н	0.0483420	0.0412720	-1.7873440	
С	-1.2941420	-0.2942860	-0.1382370	
С	1.0890680	0.6146040	-0.0253170	
Н	-1.8892340	-1.0277730	-0.7077490	
0	-1.2724610	-0.6689130	1.2366920	
0	1.1258660	1.7964580	-0.2380460	
Н	-0.8513700	-1.5317270	1.3203570	
0	1.8895720	0.0227330	0.8783280	
H	1.6793740	-0.9296760	0.8684910	
H	-0.0663670	-2.3808020	-0.9872310	
С	-1.9738470	1.0612120	-0.2317380	
H	-2.0510870	1.3850840	-1.2722620	
H H	-2.9788360 -1.4161520	0.9866720 1.8164850	0.1874840 0.3226510	
Energy	: -438.41919713	38		
B3LYP/	6-311++G** geome	etry and energy	of conformer:	aThr-XL
Ν	0.1168490	1.7942960	0.0305650	
Н	-0.1079050	1.8038380	1.0187390	
С	-0.0144460	0.4664790	-0.5483330	
H	0.0381530	0.5659550	-1.6365240	
С	1.1046640	-0.5515510	-0.1812790	
С	-1.3662090	-0.1692940	-0.2703360	
H	0.9100480	-1.4657550	-0.7549530	
0	2.3070470	0.0692350	-0.6551790	
0	-1.8177810	-1.0967290	-0.8952930	
Н	3.0578080	-0.4868000	-0.4249410	
0	-2.0079600	0.3747400	0./895210	
H	-2.84619/0	-U.LUL38/0	0.8906260	
п С	1 1072000	2.12UJZIU _0 8052020	-U.UYIZ6UU 1 3042570	
с ц	U 2884530 T.T.A./7.A.A.A	-U.000383U _1 3005060	1 6571000	
11	U.ZO0403U 2 0212600	-1.5000000 -1.5700060	1 /Q75000	
-				

Н	1.3623510	0.0146320	1.9014630	
Energy:	-438.41889118	7		
	211 211			
B3LYP/6-	311++G** geome	try and energy	of conformer:	aThr-XLI
N	0.0599990	1.6321440	0.4792430	
H C	0.9234720	2.1254/10	0.2/85/40	
Н	-0.0900630	0.7569020	-1.4755980	
С	1.1745770	-0.4496830	-0.2451280	
С	-1.3555570	-0.2821510	-0.1975960	
Н	1.0260490	-1.3100550	-0.9041150	
0	2.3498320	0.2770920	-0.6461600	
0	-1.5193740	-1.4517870	-0.4420200	
H	2.3899740	0.2997880	-1.6076230	
0	-2.3600550	0.5185600	0.2276090	
H	-3.1559630	-0.030/380	0.2945600	
С	-0.7192330	-0 9328440	1 1778130	
Н	0.5521680	-1.5134410	1.5296060	
Н	2.2928790	-1.5708260	1.2032070	
Н	1.5583990	-0.0890520	1.8515290	
Energy:	-438.41862488	0		
B3LYP/6-	311++G** geome	try and energy	of conformer:	aThr-XLII
Ν	0.0268110	1.9494890	-0.2850380	
Н	-0.2374930	2.2114810	0.6597180	
С	0.0267550	0.4973090	-0.4321480	
H	0.1437040	0.2536750	-1.4934780	
C	1.1205680	-0.2629990	0.3724790	
U U	-1.3393300	0.0003810	0.0239950	
п 0	-1 8727140	-1.0729030	1 0484700	
0	0.9854550	-1.9875030	-0.5674330	
H	-1.8924150	-0.8746120	-0.8413710	
0	-2.7314450	-1.1706370	-0.4549520	
Н	0.9310490	2.3511810	-0.5002150	
Н	2.5329310	0.0747600	-0.0974310	
С	2.6678520	-0.1911870	-1.1522650	
H	2.7585780	1.1382450	0.0163480	
Н н	3.2597610	-0.4868530	U.4926240 1 4256370	
11	T.00273T0	0.0000470	1.4230370	
Energy:	-438.41848618	4		
B3LYP/6-	-311++G** geome	try and energy	of conformer:	aThr-XLIII
, - N	0.0000000	1 0240000	0 1002510	
IN Ц	U.UU3833U _0 1052730	1,9340960 2 1/21130	-U.169351U 0 8183050	
С	0.0164960	2.142113U 0.4920620	-0.4034210	
Ч Н	0.1032880	0.3117130	-1.4771620	
C	1.1320070	-0.2967860	0.3174960	

С	-1 3357000	-0 0332250	0 0705410	
H	0.8920210	-1.6714830	-0.0092250	
0	-1.7271390	0.0617790	1.2081790	
0	1.4432230	-2.2300600	0.5473130	
Н	-2.0625820	-0.5888090	-0.9163210	
0	-2.8983930	-0.8871390	-0.5249990	
Н	0.8461640	2.3795070	-0.5120130	
Н	2.5341250	0.1330920	-0.1030470	
С	2.6693560	0.0023930	-1.1804340	
Н	2.7294670	1.1766100	0.1577870	
Н	3.2865490	-0.4737720	0.4092930	
Н	0.9988180	-0.1427950	1.3968810	
Energy:	-438.41845256	6		
B3LYP/6-	-311++G** geome	try and energy	of conformer:	aThr-XL
N	-0.0455280	1.9367630	-0.2061400	
н	-0.188/880	2.1425040	0.///1550	
с u	U.UZ/9/2U 0.2040410	0.495/6/0	-U.444929U _1 5125040	
11 C	U.ZU404IU 1 110/150	-0 2660210	-I.JIJJJ940 0 3558/20	
C	_1 3398130	-0.2009840 -0.1187500	-0 1701290	
н	0.9247230	-1.6792590	0.2607830	
0	-1.9807270	-0.7765840	-0.9468330	
0	1.0125110	-1.9529650	-0.6598550	
H	-1.7642920	0.1654240	1.0848540	
0	-2.6297530	-0.2544270	1.2012160	
Н	0.7927250	2.4100440	-0.5211210	
Н	2.5318920	0.1310990	-0.0642680	
С	2.6996560	-0.0866540	-1.1251800	
Н	2.7172770	1.1962070	0.0980560	
Н	3.2627540	-0.4312410	0.5199490	
Н	0.9730420	-0.0451220	1.4168360	
Energy:	-438.41753852	5		
B3LYP/6-	-311++G** aeome	try and energy	of conformer.	aThr-XI
	0.000070	1 2000000	0.7401000	
IN LI	-U.63829/U _0 7409920	L./88696U 2 1275400	-U./43198U	
п	-U./4U&&ZU _0 1061070	2.12/34UU	U.ZU&U36U _0 7/15000	
ч	-0.13/3/0	U.431249U 0 0967950	-U./413U8U _1 7783520	
C	-0.0134340 1 3005580	0.0904030	-1.1103320 -0 0976160	
C	-1.0849280	-0.5438160	-0.0922730	
H	1.9208620	1.0546230	-0.5880870	
0	1.1418100	0.6256430	1.2843090	
0	-1.1027660	-1.7297610	-0.3195450	
H	1.9968640	0.5695110	1.7218240	
0	-1.9215600	0.0416350	0.7856700	
Н	-2.4746650	-0.6596180	1.1615800	
Н	-0.0023670	2.4133430	-1.2283760	
С	1.9619610	-1.0732440	-0.2838870	
Н	2.0671760	-1.3097660	-1.3464370	
Н	2.9656270	-1.0643190	0.1539500	
TT	1 3801280	-1.8665770	0.1864610	

Energy: -438.417432710

		orly and onorgy	or conformer.	aini Anv
Ν	0.3558960	1.7481230	0.0362010	
Н	-0.0559220	1.8589370	0.9588270	
С	-0.0207130	0.4567710	-0.5268660	
Н	-0.0252070	0.5493140	-1.6183380	
С	1.0893950	-0.5881020	-0.1870610	
С	-1.4060030	-0.0177110	-0.0714990	
Н	0.9037100	-1.5047740	-0.7576010	
0	2.3221510	-0.0845930	-0.6723440	
0	-2.0295290	0.4930570	0.8171010	
Н	2.3587660	0.8394380	-0.3793170	
0	-1.9064660	-1.1004470	-0.7217200	
Н	-1.3048720	-1.3941080	-1.4177220	
Н	0.0037790	2.5097580	-0.5319310	
С	1.1636080	-0.9330210	1.2999660	
Н	0.2425560	-1.4046050	1.6544690	
Н	1.9917210	-1.6242730	1.4657910	
Н	1.3472270	-0.0383170	1.9008780	
Energy:	-438.41718576	3		
B3LYP/6-	-311++G** geome	try and energy	of conformer:	aThr-XLV
Ν	-0.5905490	1.8438300	-0.7329650	
Н	-0.8834180	2.1235550	0.1980120	
С	-0.1223480	0.4652020	-0.7113660	
Н	-0.0746820	0.0882300	-1.7383740	
С	1.2938100	0.2717370	-0.1001210	
C	-1.1690060	-0.3646570	0 0264360	
0			0.0204300	
H	1.1808860	0.5692470	1.2926410	
H O	1.1808860 -1.9747600	0.5692470 0.0660140	1.2926410 0.8067460	
н О О	1.1808860 -1.9747600 2.0513210	0.5692470 0.0660140 0.5128730	1.2926410 0.8067460 1.6987630	
н О О Н	1.1808860 -1.9747600 2.0513210 -1.0983430	0.5692470 0.0660140 0.5128730 -1.6800000	1.2926410 0.8067460 1.6987630 -0.3012260	
н О О Н	1.1808860 -1.9747600 2.0513210 -1.0983430 -1.7768140	0.5692470 0.0660140 0.5128730 -1.6800000 -2.1359900	1.2926410 0.8067460 1.6987630 -0.3012260 0.2200050	
н О О Н О Н	1.1808860 -1.9747600 2.0513210 -1.0983430 -1.7768140 0.1469160	0.5692470 0.0660140 0.5128730 -1.6800000 -2.1359900 2.4699440	1.2926410 0.8067460 1.6987630 -0.3012260 0.2200050 -1.0370480	
н О О Н О Н Н	1.1808860 -1.9747600 2.0513210 -1.0983430 -1.7768140 0.1469160 1.9292480	0.5692470 0.0660140 0.5128730 -1.6800000 -2.1359900 2.4699440 -1.0949150	1.2926410 0.8067460 1.6987630 -0.3012260 0.2200050 -1.0370480 -0.3447810	
н О О Н О Н Н С	1.1808860 -1.9747600 2.0513210 -1.0983430 -1.7768140 0.1469160 1.9292480 1.3617000	$\begin{array}{c} 0.5692470\\ 0.0660140\\ 0.5128730\\ -1.6800000\\ -2.1359900\\ 2.4699440\\ -1.0949150\\ -1.8910660\end{array}$	1.2926410 0.8067460 1.6987630 -0.3012260 0.2200050 -1.0370480 -0.3447810 0.1372870	
н О О Н О Н Н С Н	1.1808860 -1.9747600 2.0513210 -1.0983430 -1.7768140 0.1469160 1.9292480 1.3617000 1.9860430	$\begin{array}{c} 0.5692470\\ 0.0660140\\ 0.5128730\\ -1.6800000\\ -2.1359900\\ 2.4699440\\ -1.0949150\\ -1.8910660\\ -1.3103150 \end{array}$	1.2926410 0.8067460 1.6987630 -0.3012260 0.2200050 -1.0370480 -0.3447810 0.1372870 -1.4156160	
н О О Н О Н Н Н С Н Н Н	1.1808860 -1.9747600 2.0513210 -1.0983430 -1.7768140 0.1469160 1.9292480 1.3617000 1.9860430 2.9509190	$\begin{array}{c} 0.5692470\\ 0.0660140\\ 0.5128730\\ -1.6800000\\ -2.1359900\\ 2.4699440\\ -1.0949150\\ -1.8910660\\ -1.3103150\\ -1.1062770\end{array}$	1.2926410 0.8067460 1.6987630 -0.3012260 0.2200050 -1.0370480 -0.3447810 0.1372870 -1.4156160 0.0483960	
н О О Н О Н Н Н С Н Н Н Н Н Н	1.1808860 -1.9747600 2.0513210 -1.0983430 -1.7768140 0.1469160 1.9292480 1.3617000 1.9860430 2.9509190 1.9193640	$\begin{array}{c} 0.5692470\\ 0.0660140\\ 0.5128730\\ -1.6800000\\ -2.1359900\\ 2.4699440\\ -1.0949150\\ -1.8910660\\ -1.3103150\\ -1.1062770\\ 1.0359460 \end{array}$	$\begin{array}{c} 1.2926410\\ 0.8067460\\ 1.6987630\\ -0.3012260\\ 0.2200050\\ -1.0370480\\ -0.3447810\\ 0.1372870\\ -1.4156160\\ 0.0483960\\ -0.5869620 \end{array}$	
H O O H H H C H H H H Energy:	1.1808860 -1.9747600 2.0513210 -1.0983430 -1.7768140 0.1469160 1.9292480 1.3617000 1.9860430 2.9509190 1.9193640 -438.41717749	0.5692470 0.0660140 0.5128730 -1.6800000 -2.1359900 2.4699440 -1.0949150 -1.8910660 -1.3103150 -1.1062770 1.0359460	1.2926410 0.8067460 1.6987630 -0.3012260 0.2200050 -1.0370480 -0.3447810 0.1372870 -1.4156160 0.0483960 -0.5869620	
H O O H O H H H H Energy:	1.1808860 -1.9747600 2.0513210 -1.0983430 -1.7768140 0.1469160 1.9292480 1.3617000 1.9860430 2.9509190 1.9193640 -438.41717749	0.5692470 0.0660140 0.5128730 -1.6800000 -2.1359900 2.4699440 -1.0949150 -1.8910660 -1.3103150 -1.1062770 1.0359460	1.2926410 0.8067460 1.6987630 -0.3012260 0.2200050 -1.0370480 -0.3447810 0.1372870 -1.4156160 0.0483960 -0.5869620	
H O O H H H H Energy: B3LYP/6-	1.1808860 -1.9747600 2.0513210 -1.0983430 -1.7768140 0.1469160 1.9292480 1.3617000 1.9860430 2.9509190 1.9193640 -438.41717749	0.5692470 0.0660140 0.5128730 -1.6800000 -2.1359900 2.4699440 -1.0949150 -1.8910660 -1.3103150 -1.1062770 1.0359460 5	1.2926410 0.8067460 1.6987630 -0.3012260 0.2200050 -1.0370480 -0.3447810 0.1372870 -1.4156160 0.0483960 -0.5869620 of conformer:	aThr-XLV

С	0.0275030	0.5807890	-0.3372480	
H	0.1865160	0.6668680	-1.4138140	
C	1.1458060	-0.3054290	0.2715670	
C	-1.3512130	-0.0559220	-0.1865640	
н	0.9984870	-1.6694720	-0.1353060	
0	-2.1636270	-0.2075310	-1.0569210	
0	0.2961250	-2.0745960	0.3840540	
H	-1.5844570	-0.4332680	1.1053300	
0	-2.4959840	-0.7607670	1.1480070	
H	0.6713660	2.5330950	-0.1284930	
Н	2.5295940	0.1412120	-0.1763030	
С	2.6314650	0.0208920	-1.2584160	
H	2.7122450	1.1871550	0.0812380	
H	3.2942640	-0.4689350	0.3075700	
Н	1.0712010	-0.2356560	1.3651460	
Energy:	-438.41707120	1		
B3LYP/6-	311++G** geome	try and energy	of conformer:	aThr-XLI
N	-0.0573360	1.9225070	-0.1069100	
Н	-0.1259560	2.0790760	0.8931060	
С	0.0163750	0.4972920	-0.4275210	
Н	0.1735790	0.3930810	-1.5028890	
С	1.1212660	-0.2918920	0.3096250	
С	-1.3570770	-0.1096890	-0.1534670	
H	0.9221590	-1.6610010	-0.0564140	
0	-2.1050290	-0.5680630	-0.9733170	
0	1.5250330	-2.2151420	0.4488010	
H	-1.6675240	-0.0366070	1.1687650	
0	-2.5577230	-0.4040030	1.2742000	
H	0.7406910	2.4308070	-0.4674840	
H	2.5251150	0.1819250	-0.0562920	
С	2.6978170	0.0751120	-1.1309000	
H	2.6827040	1.2255780	0.2283650	
H	3.2776150	-0.4132740	0.4698370	
H	0.9566620	-0.1692270	1.3889920	
Energy:	-438.41679296	1		
B3LYP/6-	311++G** geome	try and energy	of conformer:	aThr-L
N	0.1681890	1.7389080	-0.4087770	
н С	-0.46/0/30	2.2836560	-U.98U1/UU	
	-0.0183250	U.J100690	-0.6232220	
п	U.UZ3Z43U	U.12/8/60	-1./U14860	
	1.1238950	-0.5400840	0.0105050	
C	-1.3612990	-0.2869570	-0.1916390	
Н	2.3/54000	-U.2/92130	-0.61310/0	
0	-1.//94660	-1.3524310	-0.5/26170	
U	2.30/1610	-0.4628690	-1.5555890	
н	-2.0420/30	U.4891/80	U.6869/LU	
U	-2.8582770	U.U158620	0.9101380	
н	U.UUJII6U	1.9980240	U.556885U	
п	1.3212950	-U.2806/20	1.49/3230	
C	1.6503850	0.7473300	1.6645180	
Н	0.4017900	-0.4605400	2.0601140	

Н н	2.0955880	-0.9464180	1.8822380	
11	0.0121020	T.JUJ2030	0.112/200	
Energy:	-438.41600276	6		
B3LYP/6-	-311++G** geome	try and energy	of conformer:	aThr-I
Ν	-0.4560830	1.9232240	-0.4195430	
H	-0.0743350	2.5146910	-1.1486670	
С	-0.1693930	0.5109420	-0.6809320	
H	-0.3422960	0.3238/40	-1./4149/0	
C	1.2783350	0.08/0220	-0.3536270	
U U	-1.2305370	-0.3431150	0.0478840	
П	1.9435510	0.7268180	-0.94/8900	
0	-2 1378670		-0 52/9900	
н	2 3408970	0 1030740	1 3346580	
0	-1.0965050	-0.4355490	1.3889240	
H	-0.2345730	-0.0674850	1.6562560	
 Н	-0.0666300	2.2230240	0.4678870	
С	1.5766320	-1.3796060	-0.6436350	
Н	1.4160620	-1.5979870	-1.7027930	
Н	2.6199920	-1.6165270	-0.4133000	
Н	0.9361220	-2.0416730	-0.0559820	
Energy:	-438.41569721	7		
B3LYP/6-	-311++G** geome	try and energy	of conformer:	aThr-I
N	-0.2979340	1.9441450	-0.3811970	
Н	0.0942490	2.1728720	0.5277890	
С	-0.1508270	0.5101330	-0.6290640	
Н	-0.3525630	0.3234100	-1.6918950	
С	1.3162650	0.1055450	-0.3531960	
С	-1.1205130	-0.3235350	0.2277120	
H	1.9279550	0.7585170	-0.9814000	
U	1.6861590	0.4300130	0.9827340	
U	-0.9345540	-0.5919700	1.3879190	
Н	1.0864580	-0.0488240	1.5743480	
U U	-2.2/25120	-U./198690	-U.J/L/610	
п u	-2.200022U	-0.4/42800	-1.3031620	
п	-1.204252U	2.2512050	-U.4U6U16U	
с u	1 3870720	-1.5660010	-U.093241U _1 7453540	
11 H	1.30/U/ZU 2 6702320	-1.5009010 -1.55866/0	-1.1400040 -0 5259/20	
H	2.0/02320 1 0325060	-1.JJ00040 -2 A4AA250	-0.JZJ94ZU -0 0703890	
11	T.0323000	2.0400230	0.0703090	
Energy:	-438.41440982	5		
B3LYP/6-				
	-311++G** geome	try and energy	of conformer:	aThr-I
NT	-311++G** geome	try and energy	of conformer:	aThr-I

Н	0.4118430	-2.3605190	-1.3680470	
C	0.1611350	-0.4202560	-0.6876790	
H	0.1784950	-0.1003080	-1.7412270	
С	-1.3059190	-0.2835430	-0.1720660	
С	1.1936210	0.4484110	0.0494620	
Н	-1.8875840	-0.9407390	-0.8379870	
0	-1.3868380	-0.7562970	1.1572120	
0	2.1188490	-0.0057680	0.6638590	
Н	-0.8840930	-1.5861340	1.1705140	
0	1.0537080	1.7886960	-0.0702220	
Н	0.2583350	2.0123770	-0.5684950	
Н	1.5029830	-1.8991330	-0.2092090	
С	-1.9329870	1.1031540	-0.2153180	
Н	-1.8497330	1.5512310	-1.2123310	
Н	-2.9963540	1.0247820	0.0174550	
Н	-1.4909690	1.7644020	0.5339260	
Energy:	-438.41428142	9		
B3LYP/6-	-311++G** geome	try and energy	y of conformer:	aThr-LIV
N	-0.0934140	1 8185110	0.2926450	
Н	0.6845720	2.3803730	-0.0353470	
C	-0.0316840	0.4675200	-0.2871040	
Н	0.0127810	0.4783690	-1.3887170	
С	1.1790620	-0.3289850	0.2294800	
C	-1.3327980	-0.2359620	0.1019890	
Н	1.2319270	-1.5877900	-0.4488490	
0	-1.4953010	-0.9951190	1.0165000	
0	1.5452990	-1.4406870	-1.3484610	
Н	-2.3468760	0.1597710	-0.7149890	
0	-3.1552870	-0.2728330	-0.3998630	
Н	-0.9433590	2.2895320	-0.0009310	
Н	2.4979840	0.4264400	0.0950950	
С	2.6826290	0.7297590	-0.9433290	
Н	2.5158020	1.3183490	0.7256610	
Н	3.3190670	-0.2211660	0.4088390	
Н	0.9990120	-0.5802510	1.2755700	
Energy:	-438.41421133	0		
B3LYP/6-	311++G** geome	try and energy	y of conformer:	aThr-LV
N	-0.0923170	1.8388530	-0.2240380	
Н	0.8207470	2.2769010	-0.2565260	
С	-0.0218520	0.3933800	-0.4971070	
H	0.1557640	0.1408860	-1.5480230	
С	1.1102880	-0.2356270	0.3467480	
С	-1.3810100	-0.2270470	-0.1137440	
Н	0.9043260	-0.0126470	1.4031930	
0	1.0351990	-1.6385910	0.1179510	
0	-1.8921470	-1.1424330	-0.6924800	
Н	1.6033460	-2.0901710	0.7493330	
0	-1.9577400	0.3666120	0.9554630	
H	-1.4366080	1.1719080	1.1410890	
Н	-0.6724690	2.3090970	-0.9120520	

С	2.4955590	0.2991870	-0.0238290	
H	2.6161300	1.3599430	0.2147990	
H U	3.2610040	-0.23/1380	U.544317U 1 0977450	
п	2.0933770	0.1451640	-1.0877450	
Energy:	-438.41390997	4		
B3LYP/6-	311++G** geome	try and energy	of conformer:	aThr-L
N	0.1729360	1.7808940	-0.3190110	
Н	-0.1492230	2.0212350	0.6123840	
С	-0.0473200	0.3758020	-0.5961410	
Н	-0.0604460	0.2377720	-1.6856410	
С	1.0541530	-0.5936370	-0.0716840	
С	-1.4054020	-0.0412950	-0.0324290	
Н	0.7876970	-1.6145550	-0.3836120	
0	2.2361770	-0.1855790	-0.7714420	
0	-1.9178260	0.4719350	0.9223430	
Н	2.9960320	-0.6414570	-0.3955780	
0	-2.0036750	-1.0956010	-0.6453870	
H	-1.5187030	-1.3450850	-1.4419360	
Н	1.1538670	2.0152080	-0.4209140	
C	1.2539400	-0.5679710	1.4391650	
Н	0.3533960	-0.8935370	1.9648400	
н	2 0656970	-1 2453640	1 7228090	
H	1.5114930	0.4361020	1.7831400	
Enora	120 11010000	0		
muerdy:	-400.41212089	2		
B3LYP/6-	311++G** geome	try and energy	of conformer:	aThr-L
N	0.3187900	1.8028530	0.0479700	
Н	0.2347370	2.0148230	-0.9421430	
С	0.0863860	0.3767240	0.3284250	
Н	0.0081170	0.2881340	1.4198600	
С	-1.1840750	-0.2861280	-0.2709520	
С	1.3763100	-0.3932440	-0.0498570	
Н	-1.4879220	-1.4850970	0.4383800	
0	1.4049640	-1.5229490	-0.4474460	
0	-1.8601000	-1.2515310	1.2965290	
Н	2.4967130	0.3364110	0.1289710	
0	2.2022850	1.2482470	0.3237080	
Н	-0.3268040	2.4008250	0.5494660	
Н	-2.3957220	0.6454340	-0.2982260	
С	-2.6382200	1.0142000	0.7063690	
Н	-2.2422650	1.5106050	-0.9474620	
Н	-3.2603660	0.0938760	-0.6722290	
Н	-0.9563540	-0.6227880	-1.2854760	
Energy:	-438.41187260	1		
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	. 1.6.0.0.0	1 5000500		
N	0.1622800	1.7398730	0.1035560	
H	0.8193760	2.2900240	-0.4335420	
С	-0.0540160	0.4392940	-0.5003720	
Н	-0.0736930	0.4729250	-1.6041720	
С	1.1037230	-0.5236600	-0.1359360	
С	-1.4291930	-0.0925400	-0.0858390	
Н	0.9084890	-1.5088040	-0.5911920	
0	2.2508610	0.0400490	-0.7792000	
0	-2.2322270	0.5438120	0.5362560	
Н	3.0457870	-0.3302960	-0.3830050	
0	-1.7368060	-1.3475970	-0.5053510	
Н	-1.0086010	-1.7303140	-1.0106480	
Н	-0.7114600	2.2396760	0.2188030	
С	1.3065140	-0.6989760	1.3636670	
Н	0.4368250	-1.1783430	1.8219340	
Н	2.1728230	-1.3399780	1.5571890	
Н	1.4577120	0.2711820	1.8369870	
D		<i>c</i>		
Energy	-438.41138294	.6		
B3LYP/	'6-311++G** geome	try and energy	of conformer:	aThr-LIX
N	0.1973060	1.7887000	-0.2515890	
Н	1.1914510	1.9822820	-0.1999410	
С	-0.0368080	0.3990620	-0.5867150	
Н	-0.0593550	0.2998290	-1.6846470	
С	1.0682930	-0.5915500	-0.0867830	
C	-1.4052840	-0.0297820	-0.0568320	
Н	0.8413830	-1.5927830	-0.4816400	
0	2.3363210	-0.1588570	-0.5915340	
0	-1.9621120	0.4999990	0.8629960	
H	2.3523150	-0.2609410	-1.5494010	
0	-1.9620990	-1.1124610	-0.6601480	
Н	-1.4422440	-1.3824920	-1.4272010	
Н	-0.2448420	2.0204360	0.6319530	
С	1.2003810	-0.6689530	1.4251930	
H	0.2825670	-1.0420120	1.8838310	
H	2.0197630	-1.3417300	1.6834780	
H	1.4214510	0.3144000	1.8449920	
_		<u>_</u>		
Energy	-438.41120413	0		
ВЗГЛБ\	b-JII++G** geome	try and energy	of conformer:	ainr-LX
N	0.4476980	-1.8422390	-0.7662680	
Н	0.4102800	-2.2193410	0.1767970	
С	0.1474640	-0.4219790	-0.7118200	
Н	0.1492820	-0.0324680	-1.7381650	
С	-1.2908200	-0.2531880	-0.1713180	
С	1.1956130	0.3852110	0.0929830	
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0	-1.2598720	-0.7201940	1.1801800	

2.0018680 -0.1101330 0.8252640

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(С	-1.8785310	1.1552450	-0.2574070	
8	Н	-1.8406980	1.5406040	-1.2824830	
9	Н	-2.9321750	1.1360300	0.0345710	
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21	Ν	0.5523640	-1.8025000	-0.8192360	
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23	С	0.1388480	-0.4117870	-0.7332690	
2 4 25	Н	0.1348320	0.0165200	-1.7454910	
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20	0	1.8658200	-0.1818210	0.9430890	
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32	0	1.3289090	1.6643680	-0.1620710	
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Conformers of gaseous threonine

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Conformers of Gaseous Threonine

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Abstract

Following an extensive search on the potential energy surfaces (PES) of the natural amino acid L-threonine (Thr) and its allotropic form L-allo-threonine (aThr), 56 and 61 conformers of Thr and aThr, respectively, have been located with the help of density functional theory (DFT). Accurate structures, relative energies, rotational as well as quartic and sextic centrifugal distortion constants, dipole moments, ¹⁴N nuclear quadrupole coupling constants, anharmonic vibrational frequencies and double-harmonic infrared intensities have been determined from ab initio electronic structure calculations for the five most stable Thr and aThr conformers. The global minimum, **Thr-I**, has a cyclic triple H-bond motif with strong OH^{...}N, C=O^{...}HO, and a weaker NH^{...}OH H-bond, where the latter two involves the side chain OH, and an energetically unfavorable trans -COOH arrangement. The best relative energies of the conformers, accurate within $\pm 1 \text{ kJ mol}^{-1}$, have been determined through the first-principles composite focal-point analysis (FPA) approach. There are four and three conformers of Thr and aThr, respectively, within a relative energy of 5 kJ mol⁻¹. Similarly to other amino acids investigated, lower levels of electronic structure theory, especially the Hartree-Fock level, are unable to determine the correct relative energies of the conformers. The rotational, the quartic and sextic centrifugal distortion, and the ¹⁴N nuclear quadrupole coupling constants as well as the anharmonic vibrational fundamentals and double-harmonic infrared intensities, all determined using DFT, should aid identification and characterization of the conformers of threonine and allo-threonine by rotational and vibrational spectroscopies, respectively.

Keywords: neutral L-threonine • neutral L-allo-threonine • amino acids • *ab initio* calculations • conformational analysis • structure elucidation

This paper is dedicated to Professor Fritz Schaefer on the occasion of his 65th birthday.

I. INTRODUCTION

During the last decades, determination and characterization of the structures of biomolecules, in particular those of proteins and peptides, have been in the focal point of experimental and theoretical research. Since amino acids (AA) are the building blocks of these biopolymers, the structural investigation of AAs, extending from solids to the gas phase, also received considerable attention. Experimental and theoretical structural investigations related to AAs, executed prior to 1999, have been reviewed in ref. 1. During the last decade a considerable number of novel experimental and first-principles computational investigations have been performed on different aspects of the structures of amino acids [2-4], peptides [5,6], and their various complexes [7]. The review of all these studies is out of the scope of the present study and thus only a small number of high-level computational studies originating from our own group are mentioned.

There is only a limited number of natural amino acids and the relatively small size of these molecules allows the application of highly sophisticated experimental and computational techniques during studies related to their equilibrium and dynamical structures usually investigated through their rotational-vibrational spectra. Consequently, we have a detailed understanding of the basics of the structural characteristics of AAs. AAs are chiral, with the sole exception of glycine. In solution and in the solid state, AAs are found in different zwitterionic forms. In the gas phase, however, AAs exist in their neutral form. Furthermore, as AAs are very flexible molecules, all of them exhibit a large number of low-energy conformers and a complex, highly structured potential energy surface (PES). Due partially to the low volatility of AAs and their tendency to decomposition when heated, most of these conformers are not amenable to experimental scrutiny but they can be subjected to detailed quantum chemical investigations. Characterization of the complex PESs of amino acids should precede and supplement related experimental structural studies.

Chiral AAs can play a role in chirally selective organocatalysis, the most important amino acid in this respect appears to be proline (Pro) [8]. As to other applicatons of AAs in chemistry, one may mention functionalization of fullerenes, carbon nanotubes and semiconductor quantum dots with amino acids [9]. Search for signs of life in the universe is also based principally on structural and spectroscopic characterization of Aas [10]. As of today, it seems that none of the AAs have been found outside of our own planet. Threonine, being an essential amino acid is involved in many studies with biochemical importance, for which the present conformational results could prove useful. As examples, we mention the

Molecular Physics

studies of metallic complexes of threonine [11-13] and the possible use of Thr and its derivatives in organocatalysis [14].

The number of local minima on the respective PESs and the structural properties of the related conformers, including accurate relative energy estimates, are available for a number of amino acids [1]. The most accurate relative energies, mostly obtained within the focal-point analysis (FPA) approach [15,16], are available for the amino acids glycine (Gly) [4,17-19], alanine (Ala) [18,20], and proline (Pro) [1-3]. The present computational study expands the list of structurally particularly well characterized amino acids by establishing all of the lowerenergy and almost all of the higher-energy conformers of L-threonine (see Figure 1), one of the two amino acids, the other one being isoleucine, exhibiting two chirality centers. This feature of threonine was one of the reasons for performing this study. The two diastereomers need to be examined separately during conformational and spectroscopic studies as for all practical purposes they appear as two distinct molecules. Obviously, both L-threonine and Lallo-threonine has an enantiomer pair, D-threonine and D-allo-threonine, respectively. In what follows, L-threonine and L-allo-threonine will be abbreviated as Thr and aThr, respectively. In the biosphere only Thr is abundant. Detailed structural characterization of the lowest-energy conformers of these diastereomers was another important aim of the present study. The present study yielded, as primary information, equilibrium structures, relative energies, and a large number of spectroscopic molecular parameters related to the vibrational and rotational spectra of the most important conformers of the two forms of threonine, Thr and aThr. The computational results obtained should help identification of at least some of the conformers of threonine by means of rotational and vibrational spectroscopies.





Figure 1. Pictorial representation of the five lowest-energy conformers of L-threonine (Thr) and L-allo-threonine (aThr)

URL: http://mc.manuscriptcentral.com/tandf/tmph

II. COMPUTATIONAL DETAILS

Most of the atom-centered Gaussian basis sets selected for the electronic structure computations of this study contain both polarization and diffuse functions, as they are both needed for the determination of accurate structures and relative energies for H-bonded systems [21]. The subcompact 3-21G basis [22] lacks these functions and thus it has been used only for pre-screening the conformers at the Hartree-Fock [23] level of electronic structure theory. The 6-31G* [24] and 6-311++G** [25] bases, used in this study extensively for geometry optimizations and subsequent force field determinations, contain 260 and 369 contracted Gaussian functions (CGFs), respectively, for threonine. The correlation-consistent, polarized-valence (aug)-cc-p(C)VnZ, n = 2 (D), 3 (T), 4 (Q) basis sets of Dunning and coworkers [26,27] have been employed extensively for single-point energy calculations within the FPA approach. (Note that only the augmented (aug) basis set contains diffuse functions, while tight functions, necessary for calculation of core correlation [28] and relativistic effects [29] are only part of core-polarized (C) basis sets.) For Thr, the aug-cc-pVDZ, ccpVTZ, cc-pCVTZ, aug-cc-pVTZ, and aug-cc-pVQZ basis sets contain 265, 366, 470, 575, and 1054 CGFs, respectively. Only the pure spherical harmonics have been employed in the cc basis sets used in this study.

Electronic wave functions have been determined in this study by the singleconfiguration, self-consistent-field, restricted Hartree–Fock (RHF) method [23,30,31], by second-order Møller–Plesset perturbation theory, *i.e.*, MP2 [32], by coupled cluster (CC) methods [33] including all single and double excitations (CCSD) [34] and in cases, additionally, a perturbative correction for contributions from connected triple excitations [CCSD(T)] [35], and by a hybrid density functional theory (DFT) approach usually abbreviated as B3LYP [36]. The T_1 diagnostic values of coupled cluster theory [37] are around 0.013 for the different conformers of Thr, suggesting that they can adequately be described by single-reference-based electron correlation methods. The eight lowest 1s-like core orbitals were kept frozen in all post-Hartree–Fock treatments unless otherwise noted.

Rotation barriers corresponding to the methyl group were computed via restricted optimizations [38-40], fixing the methyl torsional coordinate, at the MP2/cc-pVDZ level.

The electronic structure program packages Gaussian03 [41] and MOLPRO [42] have been used extensively during this study. The package MAB-ACESII [43] was employed for the methyl rotational barrier computations.

II.1. Geometry optimizations

Similarly to a scheme first employed for glycine [17], the conformers of Thr and aThr determined in this study are numbered by Roman numerals (see Figure 1) and reflect the energy order of the conformers determined at the B3LYP/6-311++G** level.

Initial structures for the geometry optimizations of the conformers of Thr and aThr were generated by replacing the appropriate H atom of the global minimum of serine with a CH₃ group followed by an optimization at the HF/3-21G level. Then, 5 of the 6 torsional angles characterizing threonine, CCOH (carboxyl), CCC=O, CCNH, CCC-O, and CCOH (side chain), were modified systematically by 60 degrees. This resulted in 6⁵ = 7776 initial structures for one diastereomer. Initial geometry optimizations on the 7776 structures were performed for each diastereomer at the inexpensive RHF/3-21G level. This simple level of electronic structure theory was chosen for the prescreening of the conformers as it was widely assumed [1] that the RHF/3-21G PESs of amino acids and peptides are more structured than their counterparts determined at more sophisticated, and thus computationally more demanding levels of electronic structure theory. Further optimizations were executed at the more reliable B3LYP/6-31G*, B3LYP/6-311++G**, and MP2/aug-cc-pVTZ levels. Initial structures for the latter optimizations were the local minima found on the RHF/3-21G PES of Thr and aThr.

Relative energies of the lowest-energy conformers of Thr and aThr, obtained by geometry optimizations at the HF/3-21G, DFT(B3LYP)/6-31G*, DFT(B3LYP)/6-311++G**, and MP2/aug-cc-pVTZ levels, are given in Table 1. Cartesian coordinates of the optimized structures and energies of all the conformers found in this study are provided as Supplementary Material.



Molecular Physics

Table 1. Relative energies $(kJ mol^{-1})$ of the most stable L-threonine and L-allo-threonine
conformers obtained from geometry optimizations performed at the MP2/aug-cc-pVTZ,
DFT(B3LYP)/6-311++G**, DFT(B3LYP)/6-31G*, and RHF/3-21G levels ^[a]

Conformer	MP2/	DFT(B3LYP)/	DFT(B3LYP)/	RHF/
	aug-cc-pVTZ	6-311++G**	6-31G*	3-21G
Thr-I	0.00	0.00	0.00	0.00
Thr-II	2.54	1.34	3.18	4.24
Thr-III	4.29	4.33	7.15	-0.96
Thr-IV	4.41	4.80	1.38	3.54
Thr-V	6.77	5.34	9.07	7.69
Thr-VI		7.30		2.68
Thr-VII		7.86		9.95
Thr-VIII		8.06		11.16
Thr-IX		10.82		24.21
Thr-X		11.34		-0.71
Thr-XI		11.47		4.49
Thr-XII		11.91		14.07
aThr-I	0.00	0.00	0.00	0.00
aThr-II	-1.13	0.64	5.48	-0.30
aThr-III	3.18	4.13	4.27	1.39
aThr-IV	5.79	6.43	8.77	1.87
aThr-V	3.50	7.08	13.65	12.53
aThr-VI		7.23		13.02
aThr-VII		7.30		8.32
aThr-VIII		7.42		14.56
aThr-IX		8.11		7.36
aThr-X		8.21		5.62
aThr-XI		10.01		7.81
aThr-XII		10.10		19.49
aThr-XIII		10.13		0.34

^[a] The relative energies of conformer **aThr-I** with respect to conformer **Thr-I** at the MP2, B3LYP/6-311++G**, B3LYP/6-31G*, and RHF levels is 3.67, 2.20, -1.06, and 2.37 kJ mol⁻¹, respectively.

II.2. Focal-point analysis (FPA)

In order to obtain accurate estimates of the relative energies of the conformers of Thr and aThr with corresponding uncertainties, the FPA approach [15,16] was utilized for both diastereomers. The five lowest-energy structures of Thr and aThr (Figure 1), obtained at the B3LYP/6-311++G** level, were included in this investigation.

Extrapolation of the energies to the complete basis set (CBS) limit at the RHF and MP2 levels was performed, as part of the FPA approach, using the formulas $E_n = E_{\text{CBS}} + A(n+1)\exp(-9\sqrt{n})$ [44] and $\varepsilon_n = \varepsilon_{\text{CBS}} + Bn^{-3}$ [45], respectively. In these formulas *n* is the cardinal number of the augmented, correlation-consistent basis sets aug-cc-pVnZ ($n \in \{3,4\}$), *A* and *B* are parameters, E_n is the RHF energy, and ε_n is the MP2 correlation energy increment, and CBS refers to the complete basis set limit. Energy corrections were treated additively, taking advantage of the fact that the contribution of higher-level electron correlation to the requested relative energies does not change significantly with the size of the basis set. CCSD and CCSD(T) correlation energy increments were calculated using the cc-pVTZ basis set.

From the auxiliary corrections needed to be determined within the FPA approach, the core correction was obtained at the MP2/cc-pCVTZ level as the difference between explicit frozen-core (fc) and all-electron (ae) energy computations. The relativistic contributions to the relative energies were estimated within the Douglas-Kroll (DK) formalism [46], as implemented in MOLPRO, at the MP2(ae)/cc-pCVTZ level. After deemed to be unimportant even at the level of precision of this study, the diagonal Born–Oppenheimer corrections (DBOC) [47] were not computed and thus were completely neglected. Zero-point vibrational energies (ZPVE) were obtained as harmonic and anharmonic correction values at the B3LYP/6-311++G** and B3LYP/6-31G* levels, respectively.

The resulting composite single-point relative energies are shown in Tables 2 and 3 for Thr and aThr, respectively.

Molecular Physics

Table 2. FPA relative energies and energy increments (δ), all in kJ mol ⁻¹ , for the 5 lowest-energy	gy
conformers of L-threonine ^[a]	

Energy term	Basis	Thr-I	Thr-II	Thr-III	Thr-IV	Thr-V
RHF	aug-cc-pVDZ	0.00	-3.14	-2.01	7.52	0.42
	aug-cc-pVTZ	0.00	-3.01	-2.11	7.80	0.72
	aug-cc-pVQZ	0.00	-2.99	-2.20	7.80	0.77
	CBS	0.00	-2.99	-2.21	7.79	0.78
δ[MP2]	aug-cc-pVDZ	0.00	4.60	6.25	-2.48	5.05
	aug-cc-pVTZ	0.00	5.36	6.47	-3.43	5.90
	aug-cc-pVQZ	0.00	5.36	6.43	-3.47	5.94
	CBS	0.00	5.36	6.39	-3.49	5.98
δ[CCSD]	cc-pVTZ	0.00	-0.74	-1.38	0.66	-0.93
δ [CCSD(T)]	cc-pVTZ	0.00	0.93	1.35	-1.08	1.19
MP2(ae) – MP2(fc)	cc-pCVTZ	0.00	0.08	0.00	0.04	0.08
Relativistic	cc-pCVTZ	0.00	-0.05	0.00	0.03	-0.04
ZPVE(harm)		0.00	-0.41	-1.05	0.68	-0.72
ZPVE(anharm) – ZPVE(harm)		0.00	0.14	0.20	-0.21	0.44
FPA relative energies		0.00	2.32	3.30	4.42	6.77

^[a] All the FPA energy computations were performed employing the fully optimized B3LYP/6-311++G** structures as references. Energy increments (δ) refer to the previous level of theory, MP2 to RHF, CCSD to MP2, and CCSD(T) to CCSD. The abbreviations (fc) and (ae) show that the correlated-level electronic structure computations were done with the frozen core approximation or with all electrons, respectively. The ZPVE(harm)s (harmonic zero-point vibrational energies) correspond to B3LYP/6-311++G** harmonic frequencies. The ZPVE(anharm)s (anharmonic zeropoint vibrational energies) were obtained at the B3LYP/6-31G* level based on quartic normal coordinate force fields and second-order vibrational perturbation theory (VPT2).

Energy term	Basis	aThr-I	aThr-II	aThr-III	aThr-IV	aThr-V
RHF	aug-cc-pVDZ	0.00	-8.53	2.19	-3.63	4.70
	aug-cc-pVTZ	0.00	-8.55	2.22	-3.17	4.66
	aug-cc-pVQZ	0.00	-8.42	2.40	-2.98	4.88
	CBS	0.00	-8.41	2.43	-2.95	4.91
δ[MP2]	aug-cc-pVDZ	0.00	6.46	0.47	7.56	-1.77
	aug-cc-pVTZ	0.00	7.94	1.18	9.11	-0.66
	aug-cc-pVQZ	0.00	8.25	1.41	9.39	-0.29
	CBS	0.00	8.48	1.57	9.60	-0.01
δ[CCSD]	cc-pVTZ	0.00	-1.54	-0.68	-2.32	0.26
δ [CCSD(T)]	cc-pVTZ	0.00	2.14	0.53	1.89	0.89
MP2(ae) – MP2(fc)	cc-pCVTZ	0.00	-0.01	0.04	0.08	-0.04
Relativistic	cc-pCVTZ	0.00	-0.05	-0.03	-0.06	-0.02
ZPVE(harm)		0.00	-1.40	-0.53	-0.85	-0.91
ZPVE(anharm) – ZPVE(harm)		0.00	-0.01	0.09	-0.02	0.13
FPA rel. energies		0.00	-0.80	3.42	5.37	5.21

Table 3. FPA relative energies and energy increments (δ), all in kJ mol⁻¹, for the 5 lowest-energy conformers of L-allo-threonine.^[a]

^[a] See footnote [a] to Table 2. The relative energy of conformer **aThr-I** with respect to conformer

Thr-I is 3.07 kJ mol^{-1} .

II.3. Spectroscopic parameters

For all local minima, quadratic force constants were computed at the B3LYP/6-311++G** level using the B3LYP/6-311++G** optimized structures, thus avoiding the nonzero-force dilemma [48]. For the five lowest-energy conformers of Thr and aThr quartic force fields in normal coordinate space have been determined at the B3LYP/6-31G* level, again at the fully optimized B3LYP/6-31G* structure. The related harmonic and anharmonic vibrational fundamentals of Thr and aThr are reported in Tables 4 and 5, respectively. No scaling of the force fields or of the resulting vibrational wavenumbers has been attempted. The anharmonic vibrational fundamentals were obtained through second-order vibrational perturbation theory (VPT2) [49].

The optimized structures determine the equilibrium rotational constants, while the quadratic and cubic force fields yield the equilibrium quartic and sextic centrifugal distortion constants in the *A*-reduced representation. The anharmonic force fields determined also allow the calculation of vibrationally averaged ground-state rotational constants. For the five lowest-energy Thr and aThr conformers these spectrosopic constants are reported in Tables 6 and 7, respectively.

The ¹⁴N nuclear quadruple coupling constants, resulting from the non-spherical distribution of the nuclear charge, have been determined at the B3LYP/6-311++G** level.

Table 4. Harmonic vibrational fundamentals (ω), their VPT2 anharmonic corrections (Δv), and double-harmonic vibrational intensities (*I*) of the 5 lowest energy conformers of L-threonine^[a]

		Thr-I			Thr-II			II Thr-III			Thr-IV				Thr-V		
number	ω	Δv	Ι	ω	Δv	Ι	ω	Δv	Ι	ω	Δv	Ι	ω	∆v	Ι		
1	3819	-177	46.8	3742	-186	64.9	3762	-188	84.1	3705	-195	131.3	3758	-187	78.7		
2	3595	-181	15.3	3708	-199	91.8	3713	-196	60.9	3600	-182	16.1	3718	-198	84.5		
3	3495	-108	11.1	3582	-181	12.1	3612	-183	21.9	3518	-129	1.1	3592	-181	11.8		
4	3455	-262	277.5	3497	-191	6.2	3516	-142	18.8	3467	-259	264.4	3511	-105	4.8		
5	3114	-142	18.4	3115	-142	18.9	3109	-148	23.5	3114	-143	15.6	3113	-143	18.3		
6	3098	-141	28.9	3109	-143	24.4	3095	-135	35.2	3086	-113	26.6	3107	-143	24.9		
7	3055	-131	9.9	3085	-139	8.3	3078	-130	2.0	3055	-138	5.1	3092	-141	5.7		
8	3041	-119	7.7	3040	-133	13.2	3023	-160	23.0	3034	-144	29.1	3038	-134	11.9		
9	3033	-132	13.5	2959	-106	38.3	3000	-137	19.8	3021	-165	21.4	2964	-109	39.5		
10	1824	-31	324.4	1800	-31	296.8	1808	-33	304.2	1808	-31	287.4	1811	-29	321.0		
11	1651	-50	32.9	1662	-31	39.5	1642	-58	77.4	1658	-48	38.1	1659	-57	36.8		
12	1503	-42	4.4	1502	-36	3.2	1501	-73	4.8	1502	-51	9.7	1502	-39	4.0		
13	1484	-9	6.7	1484	-20	6.0	1489	-39	6.0	1491	-48	5.5	1483	-19	3.6		
14	1430	-34	6.3	1441	-46	54.3	1431	-30	55.5	1445	-39	16.5	1439	-47	44.4		
15	1418	-40	427.2	1425	-32	4.4	1416	-44	23.4	1419	-45	232.8	1409	-32	29.7		
16	1409	-34	9.6	1404	-34	23.6	1401	-17	5.6	1409	-33	215.9	1400	-36	0.9		
17	1387	-36	4.9	1375	-5	20.3	1370	-34	11.6	1394	-39	21.4	1377	-5	3.6		
18	1359	-35	8.0	1339	-19	31.8	1337	-4	24.0	1371	-33	41.7	1333	-14	53.6		
19	1280	-32	57.0	1311	-11	81.1	1302	-30	3.1	1311	-30	18.0	1309	-26	59.6		
20	1276	-37	0.4	1265	-39	7.5	1258	-31	21.0	1270	-23	2.5	1289	-29	14.8		
21	1209	-40	21.5	1226	-33	20.0	1221	-35	49.2	1220	-46	23.6	1229	-18	17.5		
22	1197	-37	9.7	1158	-34	75.1	1162	-33	112.9	1192	-36	9.6	1163	-37	213.1		
23	1151	-29	24.6	1136	-31	167.6	1136	-32	154.5	1140	-32	8.9	1138	-31	43.8		
24	1084	-24	14.4	1113	-40	54.7	1104	-28	27.3	1106	-31	50.5	1110	-37	7.7		
25	1052	-18	55.9	1074	-29	12.9	1076	-30	52.8	1090	-31	79.6	1072	-31	14.8		
26	1017	-24	11.5	1052	-21	35.6	1026	-22	25.2	1045	-21	5.2	1050	-19	31.7		
27	984	-35	88.3	958	-41	46.6	937	-28	0.7	968	-32	23.1	932	-41	16.9		
28	909	-24	54.3	925	-22	35.3	892	-45	77.0	903	-41	84.1	921	-23	88.3		
29	878	-47	103.5	872	-29	38.8	869	-24	23.9	872	-40	83.5	868	-20	36.4		
30	854	-26	51.0	854	-14	98.7	830	-27	75.8	837	-52	61.4	831	-21	92.2		
31	822	-18	13.7	742	-19	37.1	728	-14	28.6	799	-18	26.7	752	-16	24.0		
32	751	-15	6.7	666	-16	17.3	659	-3	34.0	754	-10	3.1	643	-20	58.8		
33	650	-11	8.9	610	-41	108.9	630	-31	58.1	609	-29	18.0	595	-46	56.3		
34	559	-12	9.3	601	-18	125.4	575	-41	163.9	575	-19	117.5	586	-19	160.0		
35	532	-23	3.9	543	-11	1.0	545	-12	22.0	549	-11	3.8	548	-11	6.9		
36	453	-50	7.9	469	-1	8.8	476	-10	28.5	491	-5	7.3	467	0	10.6		
37	403	-11	88.0	385	-6	21.8	450	-3	4.6	456	-6	3.1	396	-8	6.7		
38	368	-17	34.8	366	-3	6.3	349	-4	3.3	377	-5	7.8	365	-3	9.4		
39	356	-7	24.7	307	-7	4.1	301	-3	0.5	337	-11	18.2	309	-8	8.3		
40	310	-2	3.7	290	-21	7.4	270	-8	6.0	298	-29	13.0	291	-2	2.3		
41	251	-2	12.6	267	-3	3.2	240	-12	0.9	251	-16	3.5	260	-1	1.5		
42	225	-19	1.2	230	5	0.5	215	-23	11.8	245	-12	3.6	221	-4	0.6		
43	179	-1	5.4	171	-1	1.0	181	-1	0.5	203	-11	8.0	162	-1	0.7		
44	86	-3	3.1	84	0	5.3	81	2	1.2	111	-9	3.0	86	-2	3.5		
45	51	-4	5.7	47	-2	0.9	69	7	2.2	67	-9	1.2	41	-3	1.6		

^[a] Harmonic frequencies and intensities were calculated at the B3LYP/6-311++G^{**} level, while anharmonic corrections correspond to the B3LYP/6-31G^{*} level of theory. Frequencies and intensities are given in cm⁻¹ and in km⁻¹, respectively.

1 2 3 4 5 6 7 8 9 1 1 1 1 . . 1

Table 5. Harmonic vibrational fundamentals (ω), their VPT2 anharmonic corrections (Δv), and double-harmonic vibrational intensities (1) of the 5 lowest energy conformers of L-allothreonine^[a]

9 10		aThr-I			aThr-II			aThr-III				aThr-I	V	aThr-V		
11 12	number	ω	Δv	Ι	ω	Δv	Ι	ω	Δv	Ι	ω	Δv	Ι	ω	Δv	Ι
13	1	3690	-197	191.6	3751	-186	70.1	3789	-182	38.5	3752	-190	56.6	3837	-175	35.5
14	2	3596	-180	12.5	3718	-196	67.3	3586	-182	14.0	3740	-186	85.5	3574	-182	19.3
15	3	3506	-125	1.6	3589	-182	13.4	3493	-103	9.8	3595	-182	12.3	3507	-100	1.4
16	4	3464	-263	268.4	3512	-188	6.8	3455	-265	279.7	3505	-131	4.9	3453	-251	273.3
17	5	3114	-142	16.0	3111	-142	20.3	3128	-141	7.0	3110	-142	20.6	3112	-143	15.5
18	6	3101	-141	27.5	3096	-137	36.5	3095	-137	25.1	3094	-128	32.1	3092	-137	22.6
19	7	3041	-140	7.3	3076	-138	9.1	3043	-106	19.6	3066	-133	7.3	3049	-132	20.6
20	8	3034	-117	15.4	3068	-130	1.6	3035	-116	24.0	3059	-136	13.2	3037	-128	5.6
21	9	2937	-85	50.2	3029	-101	13.8	3032	-128	14.0	3028	-151	13.8	3031	-121	15.2
22	10	1808	-21	307.4	1804	-33	299.0	1821	-28	305.2	1780	-34	279.2	1834	-30	338.2
23	11	1660	-45	32.5	1672	-8	40.7	1653	-45	35.2	1643	-80	39.6	1668	-33	45.6
24	12	1501	-37	5.5	1503	-100	5.0	1507	-69	3.5	1505	-68	5.9	1501	-42	10.3
25	13	1488	-6	4.0	1489	17	5.1	1490	11	13.0	1493	-40	10.4	1497	-43	3.5
26	14	1446	-54	11.0	1429	-30	45.2	1429	-46	174 .6	1444	-39	31.2	1426	-58	128.5
27	15	1416	-52	435.3	1425	-35	26.8	1415	-41	158.8	1412	-14	14.9	1417	-20	232.0
28	16	1405	-30	61.4	1412	-19	13.8	1408	-30	107.8	1395	-54	19.3	1405	-46	30.6
29	17	1385	-38	12.3	1377	-40	7.6	1400	-36	42.5	1394	-41	31.4	1384	-33	5.3
30	18	1369	-5	0.3	1330	-28	36.2	1352	-34	14.5	1343	-32	12.7	1364	-39	14.6
31	19	1315	-1	76.0	1295	-27	16.1	1316	-34	7.6	1317	-34	9.3	1317	-41	1.5
32	20	1269	-32	4.4	1263	-33	9.6	1267	-39	4.5	1285	-35	2.9	1260	-34	11.6
33	21	1216	-42	36.9	1215	-36	31.0	1204	-41	27.4	1212	-34	10.7	1228	-36	14.4
34	22	1189	-28	4.8	11/3	-35	14.3	1194	-32	19.2	114/	-37	243.0	1192	-34	25.8
35	23	1152	-31	15.1	1130	-34	250.5	1141	-30	33.0	1143	-30	129.4	1125	-30	34.9 70.0
36	24 25	1111	-31	20.0 57.0	1111	-28	98.0 19.5	1091	-27	34.9 8.0	1090	-20	11.2	1062	-28	/9.0
37	25	1064	-52	37.0 10.0	1072	-29	10.5	1074	-23	0.9	1045	-54	19.9	1005	-27	4./
38	20	075	-30	10.9 26.3	058	-28	30.0	073	-21	106.0	043	-22	52.0 7.8	064	-29	100.8
39	27	975	-28	20.3	938	-39	30.9 48.2	975	-30	46 6	945	-23	32 5	904	-34	109.8 42.1
40	20	884	-29	63 6	850	-20	131 1	880	-20	110.3	829	-72	136.2	883	-20	72.8
41	30	847	-62	18 9	828	-18	4 7	860	-23	38 2	816	-23	25 2	867	-25	25.9
42	31	840	-14	102.8	723	-21	19.4	813	-17	87	771	-17	34 4	829	-15	89
43	32	736	-12	5.8	650	-13	15.8	754	-14	8.2	709	_9	9.6	731	-10	17.0
44	33	631	-20	126.3	644	-8	78.3	607	-9	0.6	629	-30	99.3	648	-13	16.6
45	34	591	-9	3.9	570	-64	20.4	552	-34	11.0	569	-49	207.7	623	-10	8.5
46	35	571	-8	5.7	549	-21	152.0	524	-27	11.6	531	-9	19.6	495	-7	0.6
47	36	485	-1	15.6	457	-5	25.9	476	-15	20.1	498	-5	6.9	424	-5	11.7
48	37	406	-10	1.6	414	-2	4.0	437	-9	102.2	391	-2	0.9	362	-10	12.1
49 50	38	357	-10	10.2	362	-5	7.2	366	-18	31.0	358	-6	26.1	325	-32	5.6
50	39	347	-32	25.7	302	-10	5.1	349	-6	9.7	324	-3	14.7	306	-7	38.7
51	40	331	-7	3.7	255	-19	1.7	331	-3	8.0	269	-4	3.7	280	3	73.4
52	41	302	-13	10.6	249	-2	3.2	241	-1	3.0	241	-7	0.2	272	1	25.4
53 E4	42	235	-18	6.2	228	-18	8.6	229	-1	5.1	230	-6	3.6	248	-11	0.3
04 55	43	208	-7	6.7	166	0	1.9	199	0	5.5	187	-5	3.6	174	-1	10.5
56	44	94	-2	0.9	82	-1	6.0	86	-2	4.1	120	-6	3.5	86	-7	3.9
57	45	71	-8	2.0	62	1	0.9	47	-4	5.1	45	-5	0.6	80	-4	2.2
58	^[a] See	footnote	e [a] to t	able 4.												

^[a] See footnote [a] to table 4.

III. CONFORMATIONAL ANALYSISIII.1. Preliminary testsThe method described in section II.

The method described in section II.1 for studying the conformational space of Thr and aThr systematically was tested on the neutral amino acids glycine (Gly) and L-alanine (Ala), where the number of conformers are well established as a result of previous high-level first-principles studies [17-20].

At the RHF/3-21G level, only 6 of the 8 and 11 of the 13 conformers were found for Gly and Ala, respectively. The RHF/3-21G optimizations failed to yield the high-energy conformers **Gly-VIIp** and **Gly-VIIIn** for Gly. The most stable conformers **{Gly-Ip,Gly-IIn**} [4] were obtained {28,49} times out of a total of 216 initial structures. Using the same conformational search but this time at the RHF/6-31G** level, all Gly conformers were found. These observations show the possible dangers of using RHF/3-21G optimizations for prescreening the possible conformers of amino acids (and most likely peptides). It is comforting, nevertheless, that RHF/3-21G optimizations always missed only the highest-energy conformers.

The discrepancies obtained for the amino acids Gly and Ala based on the initial prescreening of the conformers at the RHF/3-21G level led us to an extended study of the role of initial geometry optimizations. Taking the Thr conformers determined at the B3LYP/6-311++G** level, preliminary optimizations at the RHF/3-21G, RHF/3-21G**, and RHF/3-21+G** levels were done, continued by B3LYP/6-311++G** level optimizations. It was found that the final B3LYP/6-311++G** structures were often different from the initial B3LYP/6-311++G** structures when using the different basis sets for the preoptimizations at the RHF level. Thus, the conformers found on the PES corresponding to the final optimization level depend somewhat on the level of the initial optimizations. Since the conformers found by only one of the methods were of high relative energy (above 15 kJ mol⁻¹ in all cases), it is safely concluded that this effect is due to the fine structure of the high-energy regions of the different PESs. While this observation is certainly somewhat disturbing, it seems to be not relevant for the low-energy conformers, of highest relevance for practical applications.

III.2. Initial optimizations

Using the inexpensive RHF/3-21G method, 68 and 66 conformers were found for Lthreonine and L-allo-threonine, respectively. When B3LYP/6-311++G** geometry optimizations were performed, using the RHF/3-21G conformers as initial structures, some of the higher-energy RHF/3-21G conformers disappeared, thus finally 56 and 61 conformers were found this way for Thr and aThr, respectively. Of the 7776 initial structures for each diastereomer, {202, 455, 328, 78, 146} and {220, 422, 534, 336, 131} ended up as {**Thr-I**, **Thr-II**, **Thr-III**, **Thr-IV**, **Thr-V**} and {**aThr-I**, **aThr-III**, **aThr-III**, **aThr-IV**, **aThr-V**}, respectively. This clearly shows that these lowest-energy conformers have substantial catchment regions. The smallest region corresponds to **Thr-XV** with only 12 initial structures ending up at that conformer.

III.3. Comparison with the study of Zhang and Lin [50]

The recent investigation of Zhang and Lin [50] is similar to our work in many respect. An important distinction is that in that paper only the L-threonine diastereomer was considered. For L-Thr, Zhang and Lin found 71 conformers at the B3LYP/6-311++G** level, while, as stated above, we found only 56 conformers. This result is the more curious as their grid for the initial optimization was somewhat less systematic, it was based partially on chemical intuition, and they included much less (only 1296) initial points than the grid corresponding to the present study contains (7776). The difference is due to the different theoretical levels used for the initial optimizations, and in this case show that the RHF/3-21G PES is less structured (68 conformers found) than the PES obtained at the B3LYP/6-311++G** level (71 conformers found). Overall, Zhang and Lin obtained 16 conformers which were not found and missed one conformer which was found in the present study. Since the dependence of the results of the conformational search on the method of initial optimization seems to be only relevant for higher-energy conformers, it is important to stress that all conformers of L-Thr up to a relative energy of 19 kJ mol⁻¹ agree in the two studies.

IV. STRUCTURES

The MP2 and DFT(B3LYP) levels of electronic structure theory yield equilibrium structures which may suffer from different problems. It is the intramolecular basis set superposition error (BSSE) that can be quite significant at the MP2 level, especially when smaller basis sets are used, hindering the determination of truly accurate equilibrium structures. By design, this is much less of a problem at the DFT levels. The usual functionals of DFT theory, like B3LYP, suffer, however, from the inability to describe dispersion effects. Therefore, it is comforting to note that the RHF, DFT(B3LYP), and MP2 levels produce the same minima for the five lowest-energy conformers of Thr and aThr. This means that the structures predicted for the lowest-energy conformers are as dependable as can be expected at these levels of electronic structure theory.

It is of fundamental interest to investigate which intramolecular factors (electronic effects including exchange, electrostatic, and hyperconjugative interactions, steric repulsion, H-bonding capabilities, and dispersive interactions) lead to stabilization of the many possible conformers of Thr and aThr. Most of these effects are operative in stabilizing the configurations resulting from rotations around the appropriate single bonds of these molecules.

Threonine is a representative of the three hydroxyamino acids whereby the OH group in the side chain is capable of strong intramolecular H-bonds. The subsequent increase in the number of low-energy conformations has been proved in this study. The presence of NH, carboxylic OH, and side-chain OH H-bond donors and N, C=O, carboxylic OH, and sidechain OH H-bond acceptors allow for the existence of the following types of H-bonds: (a) bifurcated H-bonds between NH₂ and C=O, similar to that found in the most stable conformers of glycine [4,17] and alanine [18,20]; (b) simple H-bonds, like N-H to side-chain OH, carboxylic O–H, and C=O; (c) carboxylic O–H to C=O, side-chain O–H, and NH₂; and (d) side-chain O–H to carbonyl oxygen, nitrogen, and carboxylic OH.

The structure of the global minimum, **Thr-I**, is stabilized by strong OH[…]N, OH[…]O=C and weaker NH[…]O H-bonds, whereby the COOH, NH₂, and the side-chain OH functional groups are interconnected via the three intramolecular H-bonds, while the –COOH group is in an energetically unfavorable trans conformation. In the case of **Thr-II**, although the –COOH group is now in the favorable cis conformation, this substantial energy gain, on the order of 20 kJ mol⁻¹, is not able to compensate for the energy difference between the H-bonds in **Thr-I** and **Thr-II**. **Thr-II** exhibits weaker NH[…]O=C and OH[…]N H-bonds. The H-bond arrangements in the most stable conformers of Thr are completely different from those for

Molecular Physics

glycine and α -alanine, where the global minima have a cis –COOH arrangement with a bifurcated (and thus less strong) NH^{...}O=C H-bonds, while the second lowest energy conformers have a trans –COOH arrangement and strong OH^{...}N H-bonds. This shows, and this conclusion is similar to that obtained in a MW study on the conformers of cysteine [51], that the presence of a polar side chain has a major effect on the conformational preferences of amino acids.

In the case of L-allo-threonine, the global minimum, **aThr-I**, is stabilized, very similarly to **Thr-I**, by strong OH^{...}O=C and OH^{...}N H-bonds, while the –COOH group is again in the less favorable trans conformation. As to **aThr-II**, the –COOH group is in a cis conformation, while OH^{...}N and NH^{...}O=C H-bonds can be found.

A number of different secondary structural effects characterize the other conformers. Among them one can find the OH^{...}NH^{...}O=C structural motif in **Thr-III** whereby the same NH group is included in a H-bond chain. In **Thr-IV**, the stability is due to the OH^{...}O=C and OH^{...}N bonds. While **aThr-III** has the same H-bonds as **Thr-I**, the change in chirality causes the methyl group to be in a highly unfavorable position. Furthermore, **aThr-IV** is stabilized by a sequential NH^{...}OH^{...}O=C H-bond arrangement involving NH^{...}OH and OH^{...}O=C Hbond, including the same side-chain OH group.

In all five low-energy Thr and aThr conformers, the methyl group is found in a staggered position with respect to the β -carbon atom. One can compute straightforwardly the pure (vibrationless) internal rotation barrier of the CH₃ group in Thr and aThr. This was done in the present study at the MP2(fc)/cc-pVDZ level. The rotation barriers determined for the methyl group in Thr and aThr are between 1100 and 1300 cm⁻¹. Furthermore, note that for the three lowest-energy conformers of alanine [20], the methyl rotation barrier is also about 1200 cm⁻¹, computed, as part of this study, at the same level of theory. The characteristic increase of the rotation barrier in these natural amino acids with respect to ethane, where the barrier is 1140 cm⁻¹ at this level [16], originates most probably from increased hyperconjugation, due to the presence of CC and CX (X = O, N) bonds. Note also that the internal rotation barrier of the methyl group can be substantially smaller than the barriers reported; for example, it is only about 400 cm^{-1} in acetaldehyde [40] and much smaller in toluene. Observation of transitions between the energy levels under the slightly different barriers, aimedcompounded by different reduced masses due to the structural differences of the conformers, should help identification of the low-energy conformers of Thr and Ala, as well.

Note, finally, that the only threonine conformer considered by Lakard [52] in a study of the vibrational fundamentals of hydroxyamino acids at the harmonic level, though the figure included in that paper is not particularly instructive, is definitely not the global minimum and it is not even among the five most stable conformers.

V. RELATIVE ENERGIES

As observed repeatedly for amino acids, the introductory Hartree-Fock level of electronic structure theory, independently of the basis set used, is unable to yield the correct relative energies of the conformers of Thr and aThr (see Tables 2 and 3). At the extrapolated RHF/CBS level, **Thr-II** and **Thr-III** both have lower energies than **Thr-I**, while **Thr-IV** has a very high relative energy. These RHF/CBS results clearly show the inadequacy of this level of theory in predicting relative conformational energies for this class of compounds due to its inadequacy in describing fine electrostatic and H-bonding effects. The MP2 level of theory stabilizes Thr-IV substantially, while it destabilizes all the other conformers considered. For Thr, the explicit MP2/aug-cc-pVQZ and the extrapolated MP2/CBS relative energies deviate at most by 0.04 kJ mol⁻¹, an excellent agreement indeed, contributing greatly to the overall accuracy of the FPA relative conformational energies. For aThr, the extrapolation contributions are larger by almost an order of magnitude but they are still surprisingly small on an absolute scale; consequently, the error due to MP2 extrapolation remains a small factor of the overall estimated precision of the FPA relative energies. Compared to δ [MP2], the δ [CCSD] and δ [CCSD(T)] energy increments are relatively small though can affect relative energies by at most 2 kJ mol⁻¹. Overall, it seems safe to attribute about 0.7 kJ mol⁻¹ accuracy to the CCSD(T)/CBS limit FPA relative energies. Based on the CCSD – HF and CCSD(T) – CCSD increments, the relative energy corrections due to electron correlation effects beyond CCSD(T) are estimated to be considerably less than 0.5 kJ mol⁻¹, thus these missing corrections should not affect significantly the CCSD(T)/CBS limit FPA relative energies and their uncertainty estimates.

The DFT(B3LYP) level performs reasonably well, the FPA relative energies, including the ZPVE corrections, are quite similar to the B3LYP/6-311++ G^{**} relative energies. This shows again the utility of the DFT approach for conformational energy studies.

Interestingly, but again in line with our study on the conformers of Pro [2], the relative energies are barely affected by consideration of the core-core and core-valence correlation

Molecular Physics

ZPVE corrections are substantial and can affect relative energies on the order of 2 $kJ mol^{-1}$. It is also of general interest to compare harmonic and anharmonic ZPVE corrections to the relative energies. The anharmonic contributions to relative energies of the Thr conformers are on the order of 0.5 $kJ mol^{-1}$. This is significant but not substantial given the other sources of error in the present computations contributing to the final FPA relative energy estimates.

The above statements nearly stand for aThr, as well. The RHF level of theory gives relative energies with considerable error, underestimating the relative energies of **aThr-II** and **aThr-IV**. The MP2 increment compensates most of this error by destabilizing these conformers. Compared to MP2, δ [CCSD] and δ [CCSD(T)] energy corrections are fairly small yet can affect relative energies by over 2 kJ mol⁻¹. Core correlation and relativistic effects are on the order of 0.01 kJ mol⁻¹, while ZPVE corrections can reach nearly 1.5 kJ mol⁻¹.

In the case of aThr, the B3LYP/6-311++ G^{**} level gives a different relative energy order than the FPA approach. In the cases of **aThr-I** and **aThr-II**, this is due to the ZPVE corrections, which shows the importance of including ZPVE for conformational studies. It is interesting to find that the FPA relative energies give the same relative energy order as the MP2/aug-cc-pVTZ level for the optimized structures.

Since the FPA energy difference between **aThr-I** and **aThr-II** is only 0.8 kJ mol⁻¹ and the assumed uncertainty of the present FPA relative energies is ± 1 kJ mol⁻¹, even the present extensive computations are insufficient to determine the lowest-energy conformer of aThr. Similarly, the small FPA energy difference between **aThr-IV** and **aThr-V** does not allow an unambiguous determination of their energy order.

In order to estimate the uncertainty on the FPA energies resulting from the choice of reference structures, MP2/aug-cc-pVTZ//B3LYP/6-311++G** relative energies were compared to MP2/aug-cc-pVTZ//MP2/aug-cc-pVTZ energies. The average effect is 0.1 and 0.3 kJ mol⁻¹ for Thr and aThr, respectively, suggesting that the DFT reference structures chosen are appropriate for the purposes of the present study.

VI. VIBRATIONAL FUNDAMENTALS

Many vibrational fundamentals are found to be characteristic for some of the conformers of Thr and aThr (*cf.* Tables 4 and 5). One of the most useful fundamentals characterizing the conformers is the intense streching vibrational motion of the carboxyl group, ω_{10} , at about 1 800 cm⁻¹. The spread in ω_{10} is substantial, from 1780 (**aThr-IV**) to 1834 cm⁻¹ (**aThr-V**). The anharmonic corrections alter this picture only slightly as all the VPT2 corrections are between 28 and 34 cm⁻¹. When the C=O group is not involved in H-bonding, *e.g.*, for **Thr-V**, the fundamental is at a high wavenumber, while a strong H-bond between C=O and the side-chain OH results in a substantially lower wavenumber, as for **aThr-IV**. The exact wavenumber of this fundamental should also depend on the cis *vs* trans arrangement of the carboxylic group, though this effect cannot be seen clearly from the data of Tables 4 and 5.

Other simple nuclear motions, such as OH stretching (ω_1 , ω_2) and NH stretching (ω_3 , ω_4), should also be discussed. The OH stretching motion characterizes conformers by intensity ratios (I_1/I_2) varying from 0.7 to 15.3, and by frequency differences ($\omega_1 - \omega_2$) varying between 12 and 263 cm⁻¹, with anharmonic corrections altering only slightly these differences. Correlation between the H-bond structure and the OH band origins cannot be so easily used for identification purposes as ω_{10} . Nearly the same stands for the NH stretching motion. The NH stretches also characterize conformers by their relative intensities (I_3/I_4) and frequency differences ($\omega_3 - \omega_4$). Interestingly, in most cases the $\omega_3 - \omega_4$ frequency differences are considerably modified by the anharmonic corrections.

Various other fundamentals, including ω_{14} , ω_{15} , ω_{18} , ω_{21} , ω_{22} , ω_{24} , and ω_{26} , can also be found where the intensities or the wavenumbers are characteristic of the different conformers. Nevertheless, in these cases the use of this information to identify conformers based on the availability of the infrared spectrum, for example in a matrix isolation study, is not straightforward due to the presence of nearby fundamentals of similar energies.
VII. ROTATIONAL SPECTRA

There are three possible routes to identify conformers via rotational spectroscopy if results from related electronic structure computations are available. The most obvious route is based on the comparison of measured effective rotational constants with equilibrium or vibrationally averaged computed rotational constants. The second route uses the information contained in computed dipole moments and selection rules and thus allows interpretation of measured relative intensities of rotational lines. In the case of amino acids a third route is also open, namely one can use computed ¹⁴N nuclear quadruple coupling constants for the identification of a conformer.

At the B3LYP/6-311+++G^{**} level, the rotational constants corresponding to the optimized equilibrium structures are accurate enough to be useful to deduce the presence of most of the conformers when evaluating experimental data of microwave and millimeterwave spectroscopic studies. Furthermore, some of the conformers (*e.g.*, **Thr-I** and **Thr-IV**, as well as **aThr-I**) have substantial dipole moments thus helping the observation of the related rotational transitions. Nevertheless, given the limited accuracy of the rotational constants obtained at the B3LYP and MP2 levels, in certain cases it might be quite difficult to distinguish the conformers of Thr and aThr based on this information alone. This holds, for example, for **Thr-II** and **Thr-V**. Unfortunately, in this case the ¹⁴N nuclear quadruple coupling constants are also rather similar, hindering further the unequivoval identification of these conformers. In contrast, while the rotational constants of **Thr-II** and **Thr-III** are rather similar, in this case the ¹⁴N nuclear quadruple coupling constants allow for an easy distinction between the measured spectroscopic data of the two conformers.

The relatively accurate rotational and quartic centrifugal distortion (QCD) constants determined should facilitate the observation of the low-energy conformers of L-Thr and L-aThr, especially **Thr-I** and **aThr-I**. The sextic centrifugal distortion constants are so small (they are given in mHz units in Tables 6 and 7) that it is unlikely that they could be determined experimentally with any reasonable certainty. Their smallness also means that the experimental spectrum could straightforwardly be fitted with just the effective rotational and quartic centrifugal distortion constants.

Table 6. Equilibrium rotational constants (A_e , B_e , C_e), their vibrational corrections (ΔA , ΔB , ΔC) leading to ground-state rotational constants A_0 , B_0 , and C_0 , A-reduced quartic (Δ_J , Δ_K , Δ_{JK} , δ_J , δ_J , δ_K) and sextic (Φ_J , Φ_K , Φ_{JK} , Φ_{KJ} , ϕ_j , ϕ_k , ϕ_{jk}) centrifugal distortion constants, ¹⁴N nuclear quadrupole coupling tensor elements (χ_{aa} , χ_{bb} , χ_{cc}), and total dipole moments (μ_{total}) of the five lowest-energy conformers of L-threonine^[a]

	Thr-I	Thr-II	Thr-III	Thr-IV	Thr-V
Ae	3 201.77	2 865.57	3 128.28	2 679.22	2 882.14
ΔA	-32.91	-24.61	-38.07	-27.82	-25.09
Be	1 498.69	1 587.52	1 476.30	1 749.67	1 549.45
ΔB	-25.80	-13.55	-14.75	-17.45	-17.18
$C_{\rm e}$	1 256.81	1 194.30	1 294.91	1 354.93	1 222.85
ΔC	-8.64	-10.49	-9.29	-10.67	-6.24
Δ_J	0.258	0.270	0.172	0.211	0.300
Δ_K	-0.017	-0.142	-0.118	0.192	-0.526
Δ_{JK}	0.404	0.269	0.723	0.006	0.697
δ_J	0.065	0.052	0.020	0.035	0.069
δ_K	0.155	0.620	-1.217	-0.028	-0.727
Φ_J	-0.15	-0.10	0.08	-0.02	-0.15
Φ_{K}	20.45	13.57	-1.49	-0.20	61.88
Φ_{JK}	6.61	4.77	-4.70	0.10	26.28
Φ_{KJ}	-27.18	-18.09	5.05	-0.47	-87.56
ϕ_{j}	-0.08	-0.04	0.02	0.00	-0.04
ϕ_k	70.70	27.48	-59.03	1.89	138.08
ϕ_{jk}	-0.36	-1.23	2.03	-0.06	-1.54
Xaa	-4.08	-4.83	-0.94	-4.51	-4.80
χbb	2.12	2.92	3.24	2.66	2.84
χ_{cc}	1.96	1.90	-2.30	1.85	1.95
$\mu_{ ext{total}}$	4.37	2.36	3.02	5.14	3.00

Table 6. cont.

^[a] The equilibrium rotational and quartic centrifugal distortion constants, given in MHz and kHz, respectively, correspond to the parent isotopologue, and were determined at the B3LYP/6-311++G** level. Vibrational corrections and sextic centrifugal distortion constants, given in MHz and mHz, respectively, were determined from anharmonic force fields obtained at the B3LYP/6-31G* level. The nuclear quadrupole coupling tensor elements given correspond to the ¹⁴N nucleus (in MHz). Dipole moments are given in debye.

Table 7. Equilibrium (A_e , B_e , C_e) rotational constants, their vibrational corrections (ΔA , ΔB , ΔC) leading to ground-state rotational constants A_0 , B_0 , and C_0 , A-reduced quartic (Δ_J , Δ_K , Δ_{JK} , δ_J , δ_K) and sextic (Φ_J , Φ_K , Φ_{JK} , Φ_{KJ} , ϕ_j , ϕ_k , ϕ_{jk}) centrifugal distortion constants, ¹⁴N nuclear quadrupole coupling constants (χ_{aa} , χ_{bb} , χ_{cc}), and total dipole moments (μ_{total}) of the five lowest-energy conformers of L-allo-threonine^[a]

	aThr-I	aThr-II	aThr-III	aThr-IV	aThr-V
$A_{ m e}$	3 076.01	3 019.18	2 773.73	2 738.22	3 059.09
ΔA	-25.24	-29.23	-29.65	-24.31	-28.66
Be	1 639.65	1 464.42	1 702.83	1 627.34	1 483.53
ΔB	-15.83	-9.65	-15.32	-17.21	-14.60
$C_{ m e}$	1 117.74	1 316.22	1 341.31	1 417.04	1 336.00
ΔC	-9.71	-16.16	-13.67	-15.98	-14.96
Δ_J	0.102	0.278	0.250	0.277	0.244
Δ_K	0.248	0.084	0.157	0.909	0.055
Δ_{JK}	0.027	0.170	0.438	0.226	0.190
δ_J	0.032	0.048	0.060	0.016	0.030
δ_{K}	0.170	2.004	-1.337	-0.661	1.386
$arPhi_J$	0.00	-0.13	0.03	-0.11	0.01
Φ_{K}	-0.37	28.67	1.20	7.30	18.87
Φ_{JK}	-0.06	11.43	-0.45	4.46	6.76
Φ_{KJ}	0.10	-40.04	-1.50	-16.01	-25.65
ϕ_{j}	0.00	0.01	0.04	0.03	0.04
ϕ_k	0.00	117.36	-1.27	20.51	89.59
ϕ_{jk}	0.00	-5.55	1.60	-6.23	-1.09
Хаа	-4.64	-5.02	-4.65	-0.34	-0.21
χbb	2.67	3.02	2.75	0.67	2.86
χ_{cc}	1.97	2.00	1.90	-0.33	-2.65
$\mu_{ ext{total}}$	5.31	1.85	4.41	2.75	4.57

^[a] See footnote [a] to Table 6.

VIII. SUMMARY

Following an extensive search utilizing $6^5 = 7776$ initial structures for each diastereomer, 68 and 66 conformers (local minima on their related PESs) were found for L-threonine and L-allo-threonine, respectively, at the RHF/3-21G level of electronic structure theory. After geometry optimizations at the B3LYP/6-311++G** level, 56 and 61 conformers remained for L-threonine and L-allo-threonine, respectively, within an energy range of 51 and 52 kJ mol⁻¹, respectively. The PESs of the Thr and aThr molecules clearly depend on the level of theory used for their determination. Lacking high-level definitive computational studies, only conformers obtained at several medium theoretical levels should be considered as ones whose likely existence is confirmed by theory. Fortunately, the results obtained show that the conformers found in the lower-energy regions of the PESs have the same bonding arrangements at the HF, DFT(B3LYP), and MP2 levels of theory, thus these conformers should in fact exist.

Following the FPA approach, relative energy predictions with an accuracy of ± 1 kJ mol⁻¹ were determined for the five lowest-energy conformers of both diastereomers of Thr. The computations clearly predict the global minimum for Thr, called **Thr-I**. However, for aThr the relative energies of two conformers, aThr-I and aThr-II are the same within the uncertainty of the FPA approach. In contrast to the global minimum of Gly and Ala, Thr-I contains an energetically unfavorable trans carboxylic group, and it is stabilized by strong OH^{...}N, OH^{...}O=C and weaker NH^{...}O H-bonds, whereby the COOH, NH₂, and the side-chain OH functional groups are interconnected via three intramolecular H-bonds. aThr-I is stabilized, very similarly to Thr-I, by strong OH...O=C and OH...N H-bonds, while the COOH group, to allow for these bonds, is again in the less favorable trans conformation. Thr-II and aThr-II also have similar structures, with energetically favorable cis carboxylic groups, but weaker H-bonds, NH^{...}O=C and OH^{...}N for both **Thr-II** and **aThr-II**. The structural differences between the most stable conformers of Gly and Ala and those of Thr and aThr are clearly due to the presence of the polar side chain. The side chain's significant effect on conformer stability was already observed for cysteine [51]. In the notation of Alonso et al., the presence of OH and SH polar side chains favor type-III conformers over type-I conformers known as global minima for Gly and Ala. As expected, the methyl group is in a staggered conformation for all the low-energy conformers of Thr and aThr, with rotational barriers varying between 1100 and 1300 cm^{-1} .

Spectroscopic parameters (harmonic and anharmonic frequencies, double-harmonic vibrational intensities, rotational constants with corresponding vibrational corrections, A-

reduced quartic and sextic centrifugal distortion constants, dipole moments and nuclear quadrupole coupling constants) were calculated for the conformers of Thr and aThr. Several of these parameters show the possibility for the experimental distinction of the conformers. Most important are the characteristic streching C=O (ω_{10}), NH (ω_3 , ω_4) and OH (ω_1 , ω_2) vibrational fundamentals if the vibrational spectra of the conformers were available. Assignment of the conformers based on pure rotational spectra can be based on rotational constant (equilibrium, A_e , B_e , and C_e , as well as vibrationally averaged A_0 , B_0 , and C_0 constants are provided), A-reduced quartic centrifugal distortion constants (Δ_J , Δ_K , Δ_{JK} , δ_J , and δ_K) and nuclear quadrupole coupling constants (χ_{aa} , χ_{bb} , and χ_{cc}) corresponding to the ¹⁴N nucleus. It seems feasible that conformers of Thr (and similarly those of Ala) could be identified if transitions between the energy levels corresponding to internal rotation characterized by slightly different methyl rotation barriers became available.

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Supplementary material to

Conformers of Gaseous Threonine

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Coordinates and energies are given in angstroms and Hartrees, respectively.

B3LYP/6	-311++G** geome	try and energy	of conformer:	Thr-
N	-0.0533470	1.7038990	0.2314590	
н	-0.0442190	1.5838260	-0.4896880	
H	-0.0363780	0.6334110	-1.5655940	
С	1.1430510	-0.5037890	-0.1593510	
С	-1.3815210	-0.3070190	-0.2275860	
H	0.980/530	-1.4445550	-0.6929990	
0	-1.5379430	-1.4843320	-0.4334870	
Н	0.5281650	-1.4335760	1.4592670	
0	-2.3522510	0.4880920	0.2309000	
H H	-1.9233980	1.3640610 2.4261160	0.3658960	
C	2.4888610	0.0865890	-0.5502360	
Н	2.6921460	1.0080080	0.0020550	
H	3.2850080	-0.6229850	-0.3194590	
Н	2.5202000	0.3067220	-1.6209910	
Energy:	-438.42691584	.4		
MP2/aug	-cc-pVTZ geomet	ry and energy	of conformer:	Thr-I
N	-0.0228480	1.6903810	0.2688530	
H C	-0.0325080	1.5014330	-0.4999460	
H	-0.0298410	0.6933330	-1.5652570	
С	1.1266340	-0.5049620	-0.2019770	
С	-1.3566840	-0.2788850	-0.2338380	
П	1.0926700	-0.8586950	1.1824380	
0	-1.5115450	-1.4644300	-0.4282970	
Н	0.3890420	-1.5121760	1.2899200	
0	-2.3254110	0.5169110	0.2285460	
н	-1.8/49420	1.3828820 2.3913320	-0 1672090	
C	2.4747650	0.1241160	-0.4701750	
Н	2.6378010	0.9763930	0.1888130	
H H	3.2640720 2.5423180	-0.6010270 0.4597270	-0.2850380 -1.5052230	
Energy:	-437.56950605	2		

B3LYP/6-	311++G** geome	etry and energy	of conformer:	Thr-I]
Ν	0.1698080	1.9023870	-0.2684410	
Н	-0.2646530	2.2031330	0.6005130	
С	0.0095320	0.4556970	-0.4335040	
Н	0.1436610	0.2014940	-1.4869980	
С	1.1509880	-0.2394760	0.3675790	
С	-1.3579540	-0.0283770	0.0303600	
Н	0.9800490	-0.0154010	1.4325370	
0	2.3843380	0.3221540	-0.0481070	
0	-1.9633040	0.4334080	0.9670390	
Н	2.2258460	1.2762680	-0.1233500	
0	-1.8319130	-1.0523370	-0.7148490	
Н	-2.6858660	-1.3164590	-0.3376500	
Н	-0.2736900	2.4134800	-1.0233540	
С	1.2294720	-1.7442590	0.1711070	
Н	2.0924090	-2.1322730	0.7155260	
Н	0.3336330	-2.2460040	0.5428480	
Н	1.3547640	-1.9882530	-0.8868970	
Energy:	-438.42640584	2		
MP2/aug-	cc-pVTZ geomet	ry and energy	of conformer:	Thr-I
N	0 2150220	1 9005500	0 2575950	
IN LI	0.2130230	1.0995500	-0.2373630	
С	-0.1945080	2.1704510	-0 4423400	
u u	0.0255010	0.2119030	-0.4423400	
C	1 1255050	-0 2468140	0 3655030	
C	-1 3322570	-0.0060160	0.0244210	
н	0 9583930	0.0023120	1 4228040	
0	2.3791580	0.2520800	-0.0617590	
0	-1.9065580	0.4302560	0 9989700	
H	2.2461020	1.2094890	-0.1537030	
0	-1.8337900	-0.9937040	-0.7499910	
Н	-2.6799650	-1.2499270	-0.3476670	
Н	-0.2729080	2.4221520	-0.9748690	
С	1.1348810	-1.7470710	0.1852070	
Н	1.9852550	-2.1657050	0.7198930	
Н	0.2231230	-2.1980880	0.5736040	
Н	1.2312190	-1.9974390	-0.8707660	
Energy:	-437.56853718	3		

B3LYP/	6-311++G** geome	try and energy	of conformer:	Thr-III
N	0.2094330	1.7152330	-0.1760860	
H	-0.6680670	2.1553750	0.0824120	
С н	-0.0118/20	0.3237980	-0.5681810 -1 6565370	
C	1.0858580	-0.5745470	0.0705780	
С	-1.4037190	-0.1054630	-0.1245350	
Н	0.7987080	-1.6203050	-0.0509580	
0	1.1203250	-0.3330130	1.4690640	
О Н	-2.2215460 1 1141340	0.6197410	0.3847900 1 5671760	
0	-1.6434660	-1.4057260	-0.3949310	
Н	-2.5376390	-1.6066530	-0.0800330	
H	0.6467190	2.2569870	-0.9096480	
С н	2.4509340	-0.3415200	-0.5768270	
п Н	2.4364200	-0.6061270	-0.0783840 -1.6392160	
H	2.7584420	0.7036820	-0.4798050	
Energy	: -438.42526722	2		
MP2/au	g-cc-pVTZ geomet.	ry and energy	of conformer:	Thr-III
N	0.2492490	1.7005400	-0.0943430	
H	-0.6354210	2.1587430	0.0954840	
С u	0.0053990	0.3490860	-0.5806540	
п С	1.0622810	-0.5943080	0.0167490	
C	-1.3768040	-0.0776380	-0.1403450	
Н	0.7963960	-1.6228230	-0.2230430	
0	1.0116590	-0.4870430	1.4301680	
O u	-2.1809450	0.6371420	0.4151040	
0	-1.6271430	-1.3628440	-0.4648840	
H	-2.5218930	-1.5520120	-0.1410080	
H	0.7611310	2.2526500	-0.7679740	
С	2.4464370	-0.2736420	-0.5189330	
Н Н	3.1//5120 2.4894600	-0.9316470	-0.0533970	
H	2.7157510	0.7557890	-0.2815170	
_		_		
Energy	: -437.56787161	1		
	UF	RL: http://mc.man	uscriptcentral.con	n/tandf/tmp

B3LYP/6	-311++G** geome	etry and energy	of conformer:	Thr-IV
Ν	-0.8186040	1.7821470	-0.3309400	
Н	-0.4205930	2.2264530	0.4902180	
С	-0.1907550	0.4827140	-0.6154870	
Н	-0.2403160	0.3129490	-1.6958070	
С	1.3049830	0.3558530	-0.2214000	
С	-1.0409900	-0.6447280	0.0052240	
Н	1.8278280	1.1798690	-0.7182750	
0	1.8587050	-0.8277410	-0.7734890	
0	-0.6466930	-1.7830180	0.1086290	
Н	1.2999960	-1.5654680	-0.4817550	
0	-2.2578630	-0.2671330	0.3987980	
Н	-2.2986430	0.7001230	0.2224650	
Н	-0.7310480	2.4259210	-1.1077820	
С	1.5543040	0.4490370	1.2868790	
Н	2.6267670	0.3784660	1.4762780	
Η	1.2076150	1.3994270	1.7078940	
Н	1.0601870	-0.3668810	1.8205460	
Energy:	-438.42508780	16		
MP2/aug	-cc-pVTZ geomet	ry and energy	of conformer:	Thr-IV
	0.0460500		0 0 5 1 5 1 0 0	
N	-0.8469700	1.7575370	-0.3515190	
H	-0.4202520	2.2160600	0.4449560	
	-0.1000000	0.4010100	-0.6407020	
Г	-0.2038270	0.3110200	-1.7109970	
C	-0 9985460	-0 6609140	-0.1900970 -0.0233860	
н	1 8031190	1 2381650	-0 6495230	
0	1.8855410	-0.7690010	-0.7349080	
0	-0.5854010	-1.8013960	0 0445680	
H	1.3019170	-1.5067420	-0.4896980	
0	-2.1993670	-0.3017450	0.4305310	
H	-2.2366340	0.6681460	0.2544960	
Н	-0.7843440	2.3915280	-1.1365740	
С	1.4380670	0.4501610	1.3170880	
Н	2.4963730	0.4107630	1.5663950	
Н	1.0286300	1.3685400	1.7429320	
Н	0.9430750	-0.4017230	1.7837030	
Energy.	-437 56810939	8		
BHELGY.	437.30010333			

B3LYP/6	-311++G** geomet	ry and energy	of conformer:	Thr
Ν	0.0878610	1.8845440	-0.2474540	
Н	-0.3917680	2.3981650	-0.9779090	
С	0.0107380	0.4342910	-0.4629700	
H	0.1992680	0.2340690	-1.5192340	
C	1.1514520	-0.2329730	0.3539300	
	-1.34/1450	-0.1/54040	-0.1421140	
П	0.9439590	-0.0532130	-0.0067480	
0	-1 9674510	-0.9263050	-0.8509510	
н	2.1852190	1.3350420	-0.0707650	
0	-1.8030990	0.2224500	1.0760170	
H	-2.6616110	-0.2041570	1.2184690	
Н	-0.3257800	2.1450650	0.6425700	
С	1.2860290	-1.7265050	0.1067550	
Н	0.3901020	-2.2680380	0.4198280	
Н	1.4616040	-1.9248700	-0.9535260	
Н	2.1362480	-2.1122220	0.6723260	
Energy	120 101000010			
Energy:	-438.424882619			
MP2/aug	-cc-pVTZ geometr	y and energy	of conformer:	Thr-
N	0.1323170	1.8850100	-0.2398030	
Н	-0.3851820	2.4055810	-0.9373440	
С	0.0255380	0.4460660	-0.4714850	
Н	0.2234190	0.2429400	-1.5234790	
С	1.1249650	-0.2390800	0.3539410	
С	-1.3254930	-0.1491490	-0.1490500	
H	0.9202350	-0.0342170	1.4133990	
0	2.3721180	0.3200200	-0.0177380	
0	-1.9554290	-0.905/310	-0.8526960	
П	2.2067270	1.2/29040	-0.0975950	
ч	-2 6155270	-0 1864530	1 212/170	
н	-0 2621800	2 1194620	0 6649800	
C	1 1905960	-1 7306230	0.1205030	
Н	0.2719570	-2.2211660	0.4408860	
Н	1.3476350	-1.9355180	-0.9379430	
Н	2.0231640	-2.1487700	0.6826920	
Fnergy.	-437 566928008			
LIICI GY .	437.300920000			

	-311++C** acomo	try and onergy	of conformor.	ጥነ
DOLIF/0-	-SIIFFG geome	cry and energy	or conformer.	11
N	-0.1205910	-1.3994510	0.9934550	
H	0.6843540	-1.9870540	1.1766820	
С	0.0453620	-0.6034940	-0.2238470	
Н	0.1076370	-1.2881030	-1.0755180	
С	-1.1634380	0.3346920	-0.4254480	
C.	1.3463630	0.2005650	-0.1861960	
ч	-0.9657120	0 9360790	-1 3234400	
0	-1 32283/0	1 1989520	0 7008040	
0	-1.3220340	1 2772040	0.000040	
0	1.4324000	1.77040	0.0002000	
н О	-0.544/420	1.7724370	0./2810/0	
0	2.424/430	-0.5//0420	-0.43/2330	
Н	3.2153660	-0.0241560	-0.3365820	
H	-0.2848060	-0.7932050	1.7912620	
С	-2.4662010	-0.4274630	-0.6119270	
H	-2.4117260	-1.0770210	-1.4898120	
Н	-2.6786830	-1.0439070	0.2621090	
H	-3.2845380	0.2809320	-0.7533560	
Energy:	-438.42413392	2		
B3LYP/6-	-311++G** geome	try and energy	of conformer:	Т
	0 0 1 2 2 2 2 2		0 0 0 0 0 0 0 0	
N	-0.2126490	-1.8206810	0.2695310	
N H	-0.2126490 0.6963680	-1.8206810 -2.2371360	0.2695310 0.0915470	
N H C	-0.2126490 0.6963680 -0.0588590	-1.8206810 -2.2371360 -0.3743060	0.2695310 0.0915470 0.4934350	
N H C H	-0.2126490 0.6963680 -0.0588590 0.1337270	-1.8206810 -2.2371360 -0.3743060 -0.1187090	0.2695310 0.0915470 0.4934350 1.5409580	
N H C H C	-0.2126490 0.6963680 -0.0588590 0.1337270 1.1198260	-1.8206810 -2.2371360 -0.3743060 -0.1187090 0.1563020	0.2695310 0.0915470 0.4934350 1.5409580 -0.3520380	
N C H C C	-0.2126490 0.6963680 -0.0588590 0.1337270 1.1198260 -1.3643260	-1.8206810 -2.2371360 -0.3743060 -0.1187090 0.1563020 0.3376500	0.2695310 0.0915470 0.4934350 1.5409580 -0.3520380 0.0770720	
N H C H C C H	-0.2126490 0.6963680 -0.0588590 0.1337270 1.1198260 -1.3643260 0.8613840	-1.8206810 -2.2371360 -0.3743060 -0.1187090 0.1563020 0.3376500 0.0300670	0.2695310 0.0915470 0.4934350 1.5409580 -0.3520380 0.0770720 -1.4131850	
N H C H C H O	-0.2126490 0.6963680 -0.0588590 0.1337270 1.1198260 -1.3643260 0.8613840 2.2224130	-1.8206810 -2.2371360 -0.3743060 -0.1187090 0.1563020 0.3376500 0.0300670 -0.7126690	$\begin{array}{c} 0.2695310\\ 0.0915470\\ 0.4934350\\ 1.5409580\\ -0.3520380\\ 0.0770720\\ -1.4131850\\ -0.0397190\end{array}$	
N H C H C H O O	-0.2126490 0.6963680 -0.0588590 0.1337270 1.1198260 -1.3643260 0.8613840 2.2224130	-1.8206810 -2.2371360 -0.3743060 -0.1187090 0.1563020 0.3376500 0.0300670 -0.7126690	0.2695310 0.0915470 0.4934350 1.5409580 -0.3520380 0.0770720 -1.4131850 -0.0397190 0.4122000	
N H C H C H O O U	-0.2126490 0.6963680 -0.0588590 0.1337270 1.1198260 -1.3643260 0.8613840 2.2224130 -1.6463270	-1.8206810 -2.2371360 -0.3743060 -0.1187090 0.1563020 0.3376500 0.0300670 -0.7126690 1.4582080	0.2695310 0.0915470 0.4934350 1.5409580 -0.3520380 0.0770720 -1.4131850 -0.0397190 0.4133890	
N H C C H O O H	-0.2126490 0.6963680 -0.0588590 0.1337270 1.1198260 -1.3643260 0.8613840 2.2224130 -1.6463270 2.9926440	-1.8206810 -2.2371360 -0.3743060 -0.1187090 0.1563020 0.3376500 0.0300670 -0.7126690 1.4582080 -0.4272070	$\begin{array}{c} 0.2695310\\ 0.0915470\\ 0.4934350\\ 1.5409580\\ -0.3520380\\ 0.0770720\\ -1.4131850\\ -0.0397190\\ 0.4133890\\ -0.5413650\\ 0.71702000\\ \end{array}$	
N H C C H O O H O O H	-0.2126490 0.6963680 -0.0588590 0.1337270 1.1198260 -1.3643260 0.8613840 2.2224130 -1.6463270 2.9926440 -2.1464320	-1.8206810 -2.2371360 -0.3743060 -0.1187090 0.1563020 0.3376500 0.0300670 -0.7126690 1.4582080 -0.4272070 -0.4043400	$\begin{array}{c} 0.2695310\\ 0.0915470\\ 0.4934350\\ 1.5409580\\ -0.3520380\\ 0.0770720\\ -1.4131850\\ -0.0397190\\ 0.4133890\\ -0.5413650\\ -0.7179290\\ 0.57152000\\ -0.571500\\ -0.5715000\\ -0.5710000\\ -0.5710000\\ -0.5710000\\ -0.5710000\\ -0.5710000\\ -0.5710000\\ -0.57100000\\ -0.57100000\\ -0.5710000\\ -0.57100000\\ -0.57100000\\ -0.57100000\\ -0.57100000\\ -0.57100000\\ -0.57100000\\ -0.57100000\\ -0.571000000\\ -0.571000000\\ -0.571000000\\ -0.57100000000\\ -0.571000000000000000\\ -0.571000000000000000000\\ -0.5710000000000000000000000000000$	
N H C C H O O H O H	-0.2126490 0.6963680 -0.0588590 0.1337270 1.1198260 -1.3643260 0.8613840 2.2224130 -1.6463270 2.9926440 -2.1464320 -1.6964710	-1.8206810 -2.2371360 -0.3743060 -0.1187090 0.1563020 0.3376500 0.0300670 -0.7126690 1.4582080 -0.4272070 -0.4043400 -1.2791270	0.2695310 0.0915470 0.4934350 1.5409580 -0.3520380 0.0770720 -1.4131850 -0.0397190 0.4133890 -0.5413650 -0.7179290 -0.7789300	
N H C C H O O H O H H	-0.2126490 0.6963680 -0.0588590 0.1337270 1.1198260 -1.3643260 0.8613840 2.2224130 -1.6463270 2.9926440 -2.1464320 -1.6964710 -0.6015280	-1.8206810 -2.2371360 -0.3743060 -0.1187090 0.1563020 0.3376500 0.0300670 -0.7126690 1.4582080 -0.4272070 -0.4043400 -1.2791270 -2.2763270	0.2695310 0.0915470 0.4934350 1.5409580 -0.3520380 0.0770720 -1.4131850 -0.0397190 0.4133890 -0.5413650 -0.7179290 -0.7789300 1.0887040	
N H С C H O O H H C C H O C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C C H C C C H C C C H C C C H C C C H C C C H C C С Н С С С Н С С С Н С С С С Н С С С Н С С С Н С	-0.2126490 0.6963680 -0.0588590 0.1337270 1.1198260 -1.3643260 0.8613840 2.2224130 -1.6463270 2.9926440 -2.1464320 -1.6964710 -0.6015280 1.4670790	-1.8206810 -2.2371360 -0.3743060 -0.1187090 0.1563020 0.3376500 0.0300670 -0.7126690 1.4582080 -0.4272070 -0.4043400 -1.2791270 -2.2763270 1.6123580	0.2695310 0.0915470 0.4934350 1.5409580 -0.3520380 0.0770720 -1.4131850 -0.0397190 0.4133890 -0.5413650 -0.7179290 -0.7789300 1.0887040 -0.0711460	
N H С H С С H O O H H C H H C H	-0.2126490 0.6963680 -0.0588590 0.1337270 1.1198260 -1.3643260 0.8613840 2.2224130 -1.6463270 2.9926440 -2.1464320 -1.6964710 -0.6015280 1.4670790 0.6175860	-1.8206810 -2.2371360 -0.3743060 -0.1187090 0.1563020 0.3376500 0.0300670 -0.7126690 1.4582080 -0.4272070 -0.4043400 -1.2791270 -2.2763270 1.6123580 2.2674990	0.2695310 0.0915470 0.4934350 1.5409580 -0.3520380 0.0770720 -1.4131850 -0.0397190 0.4133890 -0.5413650 -0.7179290 -0.7789300 1.0887040 -0.0711460 -0.2664390	
N H С H С С H О O H H C H H	-0.2126490 0.6963680 -0.0588590 0.1337270 1.1198260 -1.3643260 0.8613840 2.2224130 -1.6463270 2.9926440 -2.1464320 -1.6964710 -0.6015280 1.4670790 0.6175860 1.7673000	-1.8206810 -2.2371360 -0.3743060 -0.1187090 0.1563020 0.3376500 0.0300670 -0.7126690 1.4582080 -0.4272070 -0.4043400 -1.2791270 -2.2763270 1.6123580 2.2674990 1.7364090	0.2695310 0.0915470 0.4934350 1.5409580 -0.3520380 0.0770720 -1.4131850 -0.0397190 0.4133890 -0.5413650 -0.7179290 -0.7789300 1.0887040 -0.0711460 -0.2664390 0.9722120	
N Н С Н С С Н О О Н О Н Н Н Н Н	-0.2126490 0.6963680 -0.0588590 0.1337270 1.1198260 -1.3643260 0.8613840 2.2224130 -1.6463270 2.9926440 -2.1464320 -1.6964710 -0.6015280 1.4670790 0.6175860 1.7673000 2.2979840	-1.8206810 -2.2371360 -0.3743060 -0.1187090 0.1563020 0.3376500 0.0300670 -0.7126690 1.4582080 -0.4272070 -0.4043400 -1.2791270 -2.2763270 1.6123580 2.2674990 1.7364090 1.9276830	0.2695310 0.0915470 0.4934350 1.5409580 -0.3520380 0.0770720 -1.4131850 -0.0397190 0.4133890 -0.5413650 -0.7179290 -0.7789300 1.0887040 -0.0711460 -0.2664390 0.9722120 -0.7100800	
I I I I I I I I I I I I I I I I I I I	-0.2126490 0.6963680 -0.0588590 0.1337270 1.1198260 -1.3643260 0.8613840 2.2224130 -1.6463270 2.9926440 -2.1464320 -1.6964710 -0.6015280 1.4670790 0.6175860 1.7673000 2.2979840 -438.42392102	-1.8206810 -2.2371360 -0.3743060 -0.1187090 0.1563020 0.3376500 0.0300670 -0.7126690 1.4582080 -0.4272070 -0.4043400 -1.2791270 -2.2763270 1.6123580 2.2674990 1.7364090 1.9276830	0.2695310 0.0915470 0.4934350 1.5409580 -0.3520380 0.0770720 -1.4131850 -0.0397190 0.4133890 -0.5413650 -0.7179290 -0.7789300 1.0887040 -0.0711460 -0.2664390 0.9722120 -0.7100800	
N H C C H C H O O H H C H H H Energy:	-0.2126490 0.6963680 -0.0588590 0.1337270 1.1198260 -1.3643260 0.8613840 2.2224130 -1.6463270 2.9926440 -2.1464320 -1.6964710 -0.6015280 1.4670790 0.6175860 1.7673000 2.2979840 -438.42392102	-1.8206810 -2.2371360 -0.3743060 -0.1187090 0.1563020 0.3376500 0.0300670 -0.7126690 1.4582080 -0.4272070 -0.4043400 -1.2791270 -2.2763270 1.6123580 2.2674990 1.7364090 1.9276830	0.2695310 0.0915470 0.4934350 1.5409580 -0.3520380 0.0770720 -1.4131850 -0.0397190 0.4133890 -0.5413650 -0.7179290 -0.7789300 1.0887040 -0.2664390 0.9722120 -0.7100800	
N H C C H C H O O H O H H Energy: B3LYP/6-	-0.2126490 0.6963680 -0.0588590 0.1337270 1.1198260 -1.3643260 0.8613840 2.2224130 -1.6463270 2.9926440 -2.1464320 -1.6964710 -0.6015280 1.4670790 0.6175860 1.7673000 2.2979840 -438.42392102	-1.8206810 -2.2371360 -0.3743060 -0.1187090 0.1563020 0.3376500 0.0300670 -0.7126690 1.4582080 -0.4272070 -0.4043400 -1.2791270 -2.2763270 1.6123580 2.2674990 1.7364090 1.9276830 8	0.2695310 0.0915470 0.4934350 1.5409580 -0.3520380 0.0770720 -1.4131850 -0.0397190 0.4133890 -0.5413650 -0.7179290 -0.7789300 1.0887040 -0.2664390 0.9722120 -0.7100800	Т
N H C C H C H O O H O H H H Energy: B3LYP/6- N	-0.2126490 0.6963680 -0.0588590 0.1337270 1.1198260 -1.3643260 0.8613840 2.2224130 -1.6463270 2.9926440 -2.1464320 -1.6964710 -0.6015280 1.4670790 0.6175860 1.7673000 2.2979840 -438.42392102 -311++G** geome -0.2084540	-1.8206810 -2.2371360 -0.3743060 -0.1187090 0.1563020 0.3376500 0.0300670 -0.7126690 1.4582080 -0.4272070 -0.4043400 -1.2791270 -2.2763270 1.6123580 2.2674990 1.7364090 1.9276830 8 **********************************	0.2695310 0.0915470 0.4934350 1.5409580 -0.3520380 0.0770720 -1.4131850 -0.0397190 0.4133890 -0.5413650 -0.7179290 -0.7789300 1.0887040 -0.0711460 -0.2664390 0.9722120 -0.7100800 of conformer: 0.2747170	Т
N H C C H C H O O H O H H H Energy: B3LYP/6- N H	-0.2126490 0.6963680 -0.0588590 0.1337270 1.1198260 -1.3643260 0.8613840 2.2224130 -1.6463270 2.9926440 -2.1464320 -1.6964710 -0.6015280 1.4670790 0.6175860 1.7673000 2.2979840 -438.42392102 -311++G** geome -0.2084540 -0.5884260	-1.8206810 -2.2371360 -0.3743060 -0.1187090 0.1563020 0.3376500 0.0300670 -0.7126690 1.4582080 -0.4272070 -0.4043400 -1.2791270 -2.2763270 1.6123580 2.2674990 1.7364090 1.9276830 8 try and energy -1.8209760 -2.2874110	0.2695310 0.0915470 0.4934350 1.5409580 -0.3520380 0.0770720 -1.4131850 -0.0397190 0.4133890 -0.5413650 -0.7179290 -0.7789300 1.0887040 -0.0711460 -0.2664390 0.9722120 -0.7100800 of conformer: 0.2747170 1.0915720	Т
N H C C H C H O O H O H H H Energy: B3LYP/6- N H C	-0.2126490 0.6963680 -0.0588590 0.1337270 1.1198260 -1.3643260 0.8613840 2.2224130 -1.6463270 2.9926440 -2.1464320 -1.6964710 -0.6015280 1.4670790 0.6175860 1.7673000 2.2979840 -438.42392102 -311++G** geome -0.2084540 -0.5884260 -0.0611780	-1.8206810 -2.2371360 -0.3743060 -0.1187090 0.1563020 0.3376500 0.0300670 -0.7126690 1.4582080 -0.4272070 -0.4043400 -1.2791270 -2.2763270 1.6123580 2.2674990 1.7364090 1.9276830 8 try and energy -1.8209760 -2.2874110 -0.3761680	0.2695310 0.0915470 0.4934350 1.5409580 -0.3520380 0.0770720 -1.4131850 -0.0397190 0.4133890 -0.5413650 -0.7179290 -0.7789300 1.0887040 -0.0711460 -0.2664390 0.9722120 -0.7100800 of conformer: 0.2747170 1.0915720 0.4970470	Т
N H C C H C H O O H O H H E nergy: B3LYP/6- N H C H	-0.2126490 0.6963680 -0.0588590 0.1337270 1.1198260 -1.3643260 0.8613840 2.2224130 -1.6463270 2.9926440 -2.1464320 -1.6964710 -0.6015280 1.4670790 0.6175860 1.7673000 2.2979840 -438.42392102 -311++G** geome -0.2084540 -0.5884260 -0.0611780 0.1300150	-1.8206810 -2.2371360 -0.3743060 -0.1187090 0.1563020 0.3376500 0.0300670 -0.7126690 1.4582080 -0.4272070 -0.4043400 -1.2791270 -2.2763270 1.6123580 2.2674990 1.7364090 1.9276830 8 try and energy -1.8209760 -2.2874110 -0.3761680 -0.1147640	0.2695310 0.0915470 0.4934350 1.5409580 -0.3520380 0.0770720 -1.4131850 -0.0397190 0.4133890 -0.5413650 -0.7179290 -0.7789300 1.0887040 -0.0711460 -0.2664390 0.9722120 -0.7100800 of conformer: 0.2747170 1.0915720 0.4970470 1.5449710	Т
N H C C H C H O O H O H H H Energy: B3LYP/6- N H C H C H C H C H C C H C C H C C H C C H C C C H C C C H C C C C H C C C C C H C C C C H C C C C H C C C C H C C C C H C C C C H C C H C C C H C C C H C C C H C C C H C C C H C C C C C H C C C C H C C C C H C C C C H C C C C H C C C C H C C C H C C H C C C H C C C H C	-0.2126490 0.6963680 -0.0588590 0.1337270 1.1198260 -1.3643260 0.8613840 2.2224130 -1.6463270 2.9926440 -2.1464320 -1.6964710 -0.6015280 1.4670790 0.6175860 1.7673000 2.2979840 -438.42392102 -438.42392102 -311++G** geome -0.2084540 -0.5884260 -0.0611780 0.1300150 1.1216980	-1.8206810 -2.2371360 -0.3743060 -0.1187090 0.1563020 0.3376500 0.0300670 -0.7126690 1.4582080 -0.4272070 -0.4043400 -1.2791270 -2.2763270 1.6123580 2.2674990 1.7364090 1.9276830 8 try and energy -1.8209760 -2.2874110 -0.3761680 -0.1147640 0.1503630	0.2695310 0.0915470 0.4934350 1.5409580 -0.3520380 0.0770720 -1.4131850 -0.0397190 0.4133890 -0.5413650 -0.7179290 -0.7789300 1.0887040 -0.0711460 -0.2664390 0.9722120 -0.7100800 of conformer: 0.2747170 1.0915720 0.4970470 1.5449710 -0.3647410	Т
N H C H C C H C H H C H H Energy: B 3 L Y P / 6- N H C H C H C C C C C C C C C C C C C C	-0.2126490 0.6963680 -0.0588590 0.1337270 1.1198260 -1.3643260 0.8613840 2.2224130 -1.6463270 2.9926440 -2.1464320 -1.6964710 -0.6015280 1.4670790 0.6175860 1.7673000 2.2979840 -438.42392102 -311++G** geome -0.2084540 -0.5884260 -0.0611780 0.1300150 1.1216980 -1.3683130	-1.8206810 -2.2371360 -0.3743060 -0.1187090 0.1563020 0.3376500 0.0300670 -0.7126690 1.4582080 -0.4272070 -0.4043400 -1.2791270 -2.2763270 1.6123580 2.2674990 1.7364090 1.9276830 8 try and energy -1.8209760 -2.2874110 -0.3761680 -0.1147640 0.1503630 0.3333540	0.2695310 0.0915470 0.4934350 1.5409580 -0.3520380 0.0770720 -1.4131850 -0.0397190 0.4133890 -0.5413650 -0.7179290 -0.7789300 1.0887040 -0.0711460 -0.2664390 0.9722120 -0.7100800 of conformer: 0.2747170 1.0915720 0.4970470 1.5449710 -0.3647410 0.0879310	Ŀ

O O H O H H H H Energy:	2.2620890 -1.6539280 2.7424990 -2.1450690 -1.6980480 0.6994060 1.4647860 0.6032420 1.7896870 2.2751070 -438.42384514	-0.6977210 1.4500480 -0.3963070 -0.4006600 -1.2759530 -2.2316040 1.6096880 2.2577260 1.7492970 1.9206650	-0.1707490 0.4350620 0.6088270 -0.7198480 -0.7845350 0.0752000 -0.1035720 -0.2648960 0.9339650 -0.7662380	
B3LYP/6	-311++G** geome	try and energy	of conformer:	Thr-IX
N H C H C C H O O H O H H C H H H H H	-0.0413720 -0.4512880 0.0489910 0.1221530 -1.1244190 1.3669610 -0.8688630 -1.3193560 1.5026810 -0.4926710 2.3929550 3.1961640 -0.6188080 -2.4390040 -3.2299950 -2.3656490 -2.7268480	-1.2438400 -0.5827480 -0.6334050 -1.4314140 0.3107930 0.1376410 0.8061800 1.2905110 1.2866770 1.7887950 -0.5994420 -0.0599000 -2.0753080 -0.4345690 0.2721390 -1.1788380 -0.9367590	$\begin{array}{c} 1.2151860\\ 1.8688640\\ -0.1137760\\ -0.8563140\\ -0.4859690\\ -0.1436700\\ -1.4346770\\ 0.5314350\\ 0.2175540\\ 0.6097410\\ -0.6046390\\ -0.5337760\\ 1.1987160\\ -0.6583710\\ -0.9154470\\ -1.4561210\\ 0.2686250\\ \end{array}$	
Energy:	-438.42279390	7		
B3LYP/6	-311++G** geome	try and energy	of conformer:	Thr-X
N H C H C C H O H H C H	-0.7159900 -1.6256120 -0.2274210 -0.2443500 1.2519180 -1.1431430 1.7960570 1.7132030 -2.2010150 2.5869850 -0.7044020 0.2085550 -0.8149610 1.4653320 2.5324730	1.8667120 1.8132780 0.5196140 0.2711770 0.4003020 -0.5226050 1.1940310 -0.8796130 -0.2314190 -1.0707420 -1.7898210 -1.8088900 2.4009910 0.5363510 0.5170550	-0.3779960 0.0724060 -0.6370400 -1.7078130 -0.1951320 0.0383960 -0.7177100 -0.6972480 0.5339270 -0.3407960 0.0132530 -0.3413880 -1.2315750 1.3051990 1.5479870	

Fnormer	-130 10050607	Q		
Energy:	-430.42239007	5		
B3LYP/6-	-311++G** geome	try and energy	of conformer:	Thr-XI
N	0.2721470	1.7740430	-0.1393730	
Н	-0.4706620	2.3967660	-0.4377880	
С	-0.0160480	0.4107210	-0.5430580	
H	-0.01001/0	0.3536420	-1.6383150	
C	-1 4075120	-0.0760430	-0.0410440 -0.1107240	
Н	0.8021700	-1.5640000	-0.3625790	
0	1.0197440	-0.4778630	1.3906870	
0	-2.2209430	0.5799150	0.4862410	
Н	1.7380740	-0.9988080	1.7621040	
0	-1.6549650	-1.3431230	-0.5296150	
Н	-2.5487490	-1.5733900	-0.2340880	
H	0.3044390	1.8222300	0.8747980	
С	2.4625120	-0.2056670	-0.5753600	
H	3.2066290	-0.9019880	-0.1/46/80	
H	2.7395710	0.8123810	-0.3008560	
-		7		
Energy:	-438.42254554	/		
/ -				
B3LYP/6-	-311++G** geome	try and energy	of conformer:	Thr-XI]
B3LYP/6-	-311++G** geome -0.3918680	try and energy -1.8080200	of conformer: 0.0591660	Thr-XI
B3LYP/6- N H	-311++G** geome -0.3918680 0.2072020	try and energy -1.8080200 -2.4092460	of conformer: 0.0591660 0.6133980	Thr-XII
N H C	-311++G** geome -0.3918680 0.2072020 -0.0940770	try and energy -1.8080200 -2.4092460 -0.3946940	of conformer: 0.0591660 0.6133980 0.3435790	Thr-XII
B3LYP/6- N H C H	-311++G** geome -0.3918680 0.2072020 -0.0940770 0.0322280	try and energy -1.8080200 -2.4092460 -0.3946940 -0.3089030	of conformer: 0.0591660 0.6133980 0.3435790 1.4295700	Thr-XII
B3LYP/6- N H C H	-311++G** geome -0.3918680 0.2072020 -0.0940770 0.0322280 1.1925940	try and energy -1.8080200 -2.4092460 -0.3946940 -0.3089030 0.1328910	of conformer: 0.0591660 0.6133980 0.3435790 1.4295700 -0.3226840	Thr-XII
B3LYP/6- N H C C C	-311++G** geome -0.3918680 0.2072020 -0.0940770 0.0322280 1.1925940 -1.3475190 1.0092600	try and energy -1.8080200 -2.4092460 -0.3946940 -0.3089030 0.1328910 0.4463280 0.2262620	<pre>of conformer: 0.0591660 0.6133980 0.3435790 1.4295700 -0.3226840 0.0038290 -1.4026040</pre>	Thr-XII
B3LYP/6- N H C H C H	-311++G** geome -0.3918680 0.2072020 -0.0940770 0.0322280 1.1925940 -1.3475190 1.0098690 2.1675350	try and energy -1.8080200 -2.4092460 -0.3946940 -0.3089030 0.1328910 0.4463280 0.2263680 -0.9003230	<pre>of conformer: 0.0591660 0.6133980 0.3435790 1.4295700 -0.3226840 0.0038290 -1.4036040 -0.0999060</pre>	Thr-XII
B3LYP/6- N H C H C C H O O	-311++G** geome -0.3918680 0.2072020 -0.0940770 0.0322280 1.1925940 -1.3475190 1.0098690 2.1675350 -1.3404290	try and energy -1.8080200 -2.4092460 -0.3946940 -0.3089030 0.1328910 0.4463280 0.2263680 -0.9003230 1.6372420	<pre> of conformer: 0.0591660 0.6133980 0.3435790 1.4295700 -0.3226840 0.0038290 -1.4036040 -0.0999060 -0.1713370 -0.1713370 -0.00000 -0.00000 -0.00000 -0.00000 -0.000000 -0.000000 -0.000000 -0.000000 -0.000000 -0.000000 -0.0000000 -0.00000000 -0.00000000 -0.00000000 -0.000000000 -0.0000000000</pre>	Thr-XII
B3LYP/6- N H C H C C H O O H	-311++G** geome -0.3918680 0.2072020 -0.0940770 0.0322280 1.1925940 -1.3475190 1.0098690 2.1675350 -1.3404290 3.0300670	try and energy -1.8080200 -2.4092460 -0.3946940 -0.3089030 0.1328910 0.4463280 0.2263680 -0.9003230 1.6372420 -0.5665560	<pre>of conformer: 0.0591660 0.6133980 0.3435790 1.4295700 -0.3226840 0.0038290 -1.4036040 -0.0999060 -0.1713370 -0.3662960</pre>	Thr-XII
B3LYP/6- N H C H C C H O O H O	-311++G** geome -0.3918680 0.2072020 -0.0940770 0.0322280 1.1925940 -1.3475190 1.0098690 2.1675350 -1.3404290 3.0300670 -2.4704220	try and energy -1.8080200 -2.4092460 -0.3946940 -0.3089030 0.1328910 0.4463280 0.2263680 -0.9003230 1.6372420 -0.5665560 -0.2815410	of conformer: 0.0591660 0.6133980 0.3435790 1.4295700 -0.3226840 0.0038290 -1.4036040 -0.0999060 -0.1713370 -0.3662960 -0.0416310	Thr-XII
B3LYP/6- N H C C H O O H O H	-311++G** geome -0.3918680 0.2072020 -0.0940770 0.0322280 1.1925940 -1.3475190 1.0098690 2.1675350 -1.3404290 3.0300670 -2.4704220 -2.1822440	try and energy -1.8080200 -2.4092460 -0.3946940 -0.3089030 0.1328910 0.4463280 0.2263680 -0.9003230 1.6372420 -0.5665560 -0.2815410 -1.2144770	of conformer: 0.0591660 0.6133980 0.3435790 1.4295700 -0.3226840 0.0038290 -1.4036040 -0.0999060 -0.1713370 -0.3662960 -0.0416310 0.0855630	Thr-XII
B3LYP/6- N H C C H O O H O H H	-311++G** geome -0.3918680 0.2072020 -0.0940770 0.0322280 1.1925940 -1.3475190 1.0098690 2.1675350 -1.3404290 3.0300670 -2.4704220 -2.1822440 -0.1835860	try and energy -1.8080200 -2.4092460 -0.3946940 -0.3089030 0.1328910 0.4463280 0.2263680 -0.9003230 1.6372420 -0.5665560 -0.2815410 -1.2144770 -2.0259460	<pre> of conformer: 0.0591660 0.6133980 0.3435790 1.4295700 -0.3226840 0.0038290 -1.4036040 -0.0999060 -0.1713370 -0.3662960 -0.0416310 0.0855630 -0.9124850 </pre>	Thr-XII
B3LYP/6- N H C C H C C H O O H H C	-311++G** geome -0.3918680 0.2072020 -0.0940770 0.0322280 1.1925940 -1.3475190 1.0098690 2.1675350 -1.3404290 3.0300670 -2.4704220 -2.1822440 -0.1835860 1.6762110	try and energy -1.8080200 -2.4092460 -0.3946940 -0.3089030 0.1328910 0.4463280 0.2263680 -0.9003230 1.6372420 -0.5665560 -0.2815410 -1.2144770 -2.0259460 1.4681240	<pre> of conformer: 0.0591660 0.6133980 0.3435790 1.4295700 -0.3226840 0.0038290 -1.4036040 -0.0999060 -0.1713370 -0.3662960 -0.0416310 0.0855630 -0.9124850 0.2313580 </pre>	Thr-XII
B3LYP/6- N H C H C C H O O H C H C H H	-311++G** geome -0.3918680 0.2072020 -0.0940770 0.0322280 1.1925940 -1.3475190 1.0098690 2.1675350 -1.3404290 3.0300670 -2.4704220 -2.1822440 -0.1835860 1.6762110 0.9374760	try and energy -1.8080200 -2.4092460 -0.3946940 -0.3089030 0.1328910 0.4463280 0.2263680 -0.9003230 1.6372420 -0.5665560 -0.2815410 -1.2144770 -2.0259460 1.4681240 2.2493880	<pre> of conformer: 0.0591660 0.6133980 0.3435790 1.4295700 -0.3226840 0.0038290 -1.4036040 -0.0999060 -0.1713370 -0.3662960 -0.0416310 0.0855630 -0.9124850 0.2313580 0.0579500 </pre>	Thr-XII
B3LYP/6- N H C H C C H O O H H C H H H	-311++G** geome -0.3918680 0.2072020 -0.0940770 0.0322280 1.1925940 -1.3475190 1.0098690 2.1675350 -1.3404290 3.0300670 -2.4704220 -2.1822440 -0.1835860 1.6762110 0.9374760 1.8636890	try and energy -1.8080200 -2.4092460 -0.3946940 -0.3089030 0.1328910 0.4463280 0.2263680 -0.9003230 1.6372420 -0.5665560 -0.2815410 -1.2144770 -2.0259460 1.4681240 2.2493880 1.3864030	<pre> of conformer: 0.0591660 0.6133980 0.3435790 1.4295700 -0.3226840 0.0038290 -1.4036040 -0.0999060 -0.1713370 -0.3662960 -0.0416310 0.0855630 -0.9124850 0.2313580 0.0579500 1.3060920 </pre>	Thr-XII
B3LYP/6- N H C C H O O H O H H H H H	-311++G** geome -0.3918680 0.2072020 -0.0940770 0.0322280 1.1925940 -1.3475190 1.0098690 2.1675350 -1.3404290 3.0300670 -2.4704220 -2.1822440 -0.1835860 1.6762110 0.9374760 1.8636890 2.6116440	try and energy -1.8080200 -2.4092460 -0.3946940 -0.3089030 0.1328910 0.4463280 0.2263680 -0.9003230 1.6372420 -0.5665560 -0.2815410 -1.2144770 -2.0259460 1.4681240 2.2493880 1.3864030 1.7601980	<pre> of conformer: 0.0591660 0.6133980 0.3435790 1.4295700 -0.3226840 0.0038290 -1.4036040 -0.0999060 -0.1713370 -0.3662960 -0.0416310 0.0855630 -0.9124850 0.2313580 0.0579500 1.3060920 -0.2578590 </pre>	Thr-XII
B3LYP/6- N H C C H O O H O H H H H Energy:	-311++G** geome -0.3918680 0.2072020 -0.0940770 0.0322280 1.1925940 -1.3475190 1.0098690 2.1675350 -1.3404290 3.0300670 -2.4704220 -2.1822440 -0.1835860 1.6762110 0.9374760 1.8636890 2.6116440 -438.42238139	try and energy -1.8080200 -2.4092460 -0.3946940 -0.3089030 0.1328910 0.4463280 0.2263680 -0.9003230 1.6372420 -0.5665560 -0.2815410 -1.2144770 -2.0259460 1.4681240 2.2493880 1.3864030 1.7601980	<pre>of conformer: 0.0591660 0.6133980 0.3435790 1.4295700 -0.3226840 0.0038290 -1.4036040 -0.0999060 -0.1713370 -0.3662960 -0.0416310 0.0855630 -0.9124850 0.2313580 0.0579500 1.3060920 -0.2578590</pre>	Thr-XII
B3LYP/6- N H C C H C C H O O H H C H H H Energy:	-311++G** geome -0.3918680 0.2072020 -0.0940770 0.0322280 1.1925940 -1.3475190 1.0098690 2.1675350 -1.3404290 3.0300670 -2.4704220 -2.1822440 -0.1835860 1.6762110 0.9374760 1.8636890 2.6116440 -438.42238139	try and energy -1.8080200 -2.4092460 -0.3946940 -0.3089030 0.1328910 0.4463280 0.2263680 -0.9003230 1.6372420 -0.5665560 -0.2815410 -1.2144770 -2.0259460 1.4681240 2.2493880 1.3864030 1.7601980 4	<pre>of conformer: 0.0591660 0.6133980 0.3435790 1.4295700 -0.3226840 0.0038290 -1.4036040 -0.0999060 -0.1713370 -0.3662960 -0.0416310 0.0855630 -0.9124850 0.2313580 0.0579500 1.3060920 -0.2578590</pre>	Thr-XII

Ν	0.1393900	1.6827480	-0.1833630	
H	-0.7556280	2.1431390	-0.0768630	
C	-0.00616/0	0.2798290	-0.585/260	
H	0.0586770	0.1388500	-1.6733230	
С	1.1242110	-0.5572270	0.0774390	
С	-1.3538260	-0.3194580	-0.2039090	
Н	0.8804760	-1.6138220	-0.0470670	
0	1.1221560	-0.3064010	1.4749940	
0	-1.6529560	-1.4685890	-0.4001350	
H	1.0374890	0.6556750	1.5669090	
0	-2.2069690	0.5721520	0.3554310	
Н	-3.0252280	0.0955100	0.5619860	
Н	0.6947530	2.2056200	-0.8488730	
С	2.4892440	-0.2671130	-0.5466740	
Н	3.2540710	-0.8530160	-0.0335630	
Н	2.5046460	-0.5340110	-1.6083410	
Н	2.7563950	0.7893370	-0.4464240	
Enorgy.	120 12210222	2		
LHELGY.	-430.42219332			
B3LYP/6-	311++G** geome	try and energy	of conformer:	Thr-XIV
,				
N	-0.4677310	1.9484360	-0.5428900	
Н	-0.7951780	2.1586770	0.3949690	
С	-0.1411500	0.5362040	-0.6702830	
Н	-0.1310180	0.2699140	-1.7313490	
С	1.3092720	0.2621520	-0.1624140	
С	-1.1642830	-0.3732770	0.0134630	
Н	1.9153790	1.0352330	-0.6370180	
0	1.8202810	-0.9690960	-0.6604630	
0	-2.0967840	-0.0082680	0.6809700	
Н	1.2333110	-1.6835630	-0.3847850	
0	-0.8992500	-1.6951330	-0.1933110	
Н	-1.5737260	-2.2049340	0.2825270	
Н	-1.2235650	2.1996050	-1.1702620	
С	1.4548000	0.3706860	1.3545110	
H	0.8641450	-0.3922640	1.8726270	
 H	2.5015340	0.2302420	1.6303540	
н	1.1374230	1.3534360	1.7139430	
-		4		
Energy:	-438.42167006	4		
Energy:	-438.42167006	4		
Energy:	-438.42167006	4		
Energy:	-438.42167006	4	of conformer.	
Energy: B3LYP/6-	-438.42167006 311++G** geome	4 try and energy	v of conformer:	Thr-XV
Energy: B3LYP/6-	-438.42167006 311++G** geome -0.5212800	4 try and energy 1.9195560	of conformer: -0.3539110	Thr-XV
Energy: B3LYP/6- N H	-438.42167006 311++G** geome -0.5212800 -1.4085510	4 try and energy 1.9195560 2.1468730	<pre>v of conformer: -0.3539110 -0.7876350</pre>	Thr-XV
Energy: B3LYP/6- N H C	-438.42167006 311++G** geome -0.5212800 -1.4085510 -0.1467790	4 try and energy 1.9195560 2.1468730 0.5362390	<pre>v of conformer: -0.3539110 -0.7876350 -0.6136420</pre>	Thr-XV
Energy: B3LYP/6- N H C H	-438.42167006 311++G** geome -0.5212800 -1.4085510 -0.1467790 -0.1970690	4 try and energy 1.9195560 2.1468730 0.5362390 0.3730820	<pre>7 of conformer: -0.3539110 -0.7876350 -0.6136420 -1.6967470</pre>	Thr-XV
Energy: B3LYP/6- N H C H C	-438.42167006 311++G** geome -0.5212800 -1.4085510 -0.1467790 -0.1970690 1.3370160	4 try and energy 1.9195560 2.1468730 0.5362390 0.3730820 0.2839400	<pre>7 of conformer: -0.3539110 -0.7876350 -0.6136420 -1.6967470 -0.2277290</pre>	Thr-XV
Energy: B3LYP/6- N H C H C C C	-438.42167006 311++G** geome -0.5212800 -1.4085510 -0.1467790 -0.1970690 1.3370160 -1.0622550	4 try and energy 1.9195560 2.1468730 0.5362390 0.3730820 0.2839400 -0.5410210	<pre>7 of conformer: -0.3539110 -0.7876350 -0.6136420 -1.6967470 -0.2277290 -0.0179100</pre>	Thr-XV
Energy: B3LYP/6- N H C H C C H	-438.42167006 311++G** geome -0.5212800 -1.4085510 -0.1467790 -0.1970690 1.3370160 -1.0622550 1.9017020	4 try and energy 1.9195560 2.1468730 0.5362390 0.3730820 0.2839400 -0.5410210 1.0668540	<pre> of conformer: -0.3539110 -0.7876350 -0.6136420 -1.6967470 -0.2277290 -0.0179100 -0.7374530 -0.7374530 -0.7374530 -0.017910 -0.7374530 -0.017910 -0.7374530 -0.017910 -0.7374530 -0.017910 -0.7374530 -0.017910 -0.7374530 -0.017910 -0.7374530 -0.017910 -0.7374530 -0.017910 -0.7374530 -0.017910 -0.7374530 -0.017910 -0.7374530 -0.017910 -0.7374530 -0.017910 -0.7374530 -0.017910 -0.7374530 -0.017910 -0.7374530 -0.017910 -0.017910 -0.7374530 -0.017910 -0.017910 -0.7374530 -0.017910 -0.7374530 -0.017910 -0.010 -</pre>	Thr-XV
Energy: B3LYP/6- N H C H C C H O	-438.42167006 311++G** geome -0.5212800 -1.4085510 -0.1467790 -0.1970690 1.3370160 -1.0622550 1.9017020 1.8064530	4 try and energy 1.9195560 2.1468730 0.5362390 0.3730820 0.2839400 -0.5410210 1.0668540 -0.9417070	<pre> of conformer: -0.3539110 -0.7876350 -0.6136420 -1.6967470 -0.2277290 -0.0179100 -0.7374530 -0.7728690 -0.7728690 -0.7728690 -0.0100 -0.7728690 -0.000 -0.7728690 -0.000 -0.0000 -0.0000 -0.0000 -0.0000 -0.0000 -0.0000 -0.0000 -0.0000 -0.0000 -0.0000 -0.0000 -0.0000 -0.0000 -0.0000 -0.000 -0.0000 -0.0000 -0.0000 -0.0000 -0.0000 -0.000 -0.0000 -0.0000 -0.0000 -0.0000 -0.0000 -0.0000 -0.0000 -0.0000 -0.0000 -0.0000 -0.0000 -0.0000 -0.0000 -0.0000 -0.0000 -0.00000 -0.0000 -0.0000 -0.0000 -</pre>	Thr-XV
Energy: B3LYP/6- N H C H C C H O O O	-438.42167006 311++G** geome -0.5212800 -1.4085510 -0.1467790 -0.1970690 1.3370160 -1.0622550 1.9017020 1.8064530 -0.7584980	4 try and energy 1.9195560 2.1468730 0.5362390 0.3730820 0.2839400 -0.5410210 1.0668540 -0.9417070 -1.7042820	<pre>-0.3539110 -0.7876350 -0.6136420 -1.6967470 -0.2277290 -0.0179100 -0.7374530 -0.7728690 0.1308880</pre>	Thr-XV

0 -2.2863880 -0.0781620 0.3159760 4 -2.7965040 -0.8339630 0.6471060 4 -0.6232490 2.0984370 0.632250 2 1.6039220 0.3789600 1.2759790 4 1.0468580 -0.3812500 1.8317710 4 2.6675240 0.2186430 1.46644320 Santa Attache and an energy of conformer: Thr-X 4 -0.5784370 1.9273800 -0.3001630 4 -1.5639310 1.9610530 -0.0624250 5 -0.1618670 0.558300 -0.6153250 4 -0.577770 0.3301220 -1.345260 5 -1.1604060 -0.413220 -0.198620 4 1.8698550 1.1737450 -0.5220660 5 -2.2139900 -0.1214550 -1.3847650 6 -3.302590 -0.5006030 6 -0.4038050 2.5679800 -1.0721420 5 -1.4365850 -2.235080 -1.6673180 6 -0.4038050 2.5679800 -1.0721420 7 1.4435010					
 L. 1900300 C. 0984370 0.6392250 L. 6039220 0.3789600 1.2759790 L. 0466580 - C. 3812500 1.8317710 H. 1.0466580 - C. 3812500 1.8317710 H. 1.3414620 1.3659440 1.6684320 Energy: -438.421541581 B3LYP/6-311++G** geometry and energy of conformer: Thr-X N0.5784370 1.9273800 -0.3001630 H. 1.5639310 1.9610530 -0.6624250 C0.1618670 0.5658300 -0.6153250 H0.1575770 0.3509260 -1.6947020 L. 1.604060 -0.4132230 -0.1345260 L. 1.604060 -0.4132230 -0.1345260 L. 1.8698550 1.737450 -0.5220660 D. 1.8822860 -0.8134290 -0.7654910 C1.1604060 -1.15932590 -0.5006030 D2.213990 -0.1214550 0.485880 H. 1.3800660 -1.5932590 -0.5006030 D2.213990 -0.1214550 1.4347650 H. 435850 2.26579800 -1.6247020 L. 4435010 0.2902270 1.3847650 H. 0.9465270 -0.5871630 1.8114230 L. 4995740 0.2429680 1.6573180 H. 0.9465270 -0.5871630 1.8114230 L. 4995740 0.2429680 1.6573180 H. 0.9465270 -0.5871630 1.8114230 L. 4995740 0.2429680 1.6573180 H. 0.9465270 -0.5871630 1.8114230 L. 4033010 1.3694890 -0.5689890 D0.5504030 2.3440600 -0.4826600 C. 1.0033700 1.1877580 1.8241070 Shergy: -438.421498297 	О н	-2.2863880	-0.0781620	0.3159760	
 1.6039220 0.3789600 1.2759790 1.0468580 -0.3812500 1.8317710 2.6675240 0.2186430 1.4617960 1.3414620 1.3659440 1.6684320 Snergy: -438.421541581 33LYP/6-311++G** geometry and energy of conformer: Thr-X N -0.5784370 1.9273800 -0.3001630 H -1.5633310 1.9610530 -0.0624250 C -0.1618670 0.5658300 -0.6153250 H -0.1575770 0.3309260 -1.6947020 L 3032400 0.3231520 -0.1345260 C -1.1604060 -0.4132230 -0.195820 H .869650 1.1737450 -0.5220660 D 1.8822860 -0.8134290 -0.7654910 D -2.2139900 -0.1214550 0.4850880 L 3800660 -1.5932590 -0.5006030 D -0.7477020 -1.7048750 -0.1311570 H -1.4365850 2.25579800 -1.0721420 C 1.4435010 0.2902270 1.3847650 H 4.09465270 -0.5871630 1.8114230 H 0.9465270 -0.5871630 1.8114230 H 0.9465270 -0.5871630 1.8114230 H 0.9465270 -0.5871630 1.812420 C 1.4435010 0.3902270 1.3847650 H 0.9465270 -0.5871630 1.812420 C 1.4435010 0.3694890 -0.5689890 H 0.0439780 0.3267250 -1.6628590 H 0.0439780 0.3267250 -1.6628590 L 1.174410 -0.5363630 -0.0338600 C -1.3566760 -0.2851970 -0.2228820 H 0.860490 -1.5606770 -0.3458350 D 1.0224870 -0.4406310 1.3969590 L 1.17420 -0.9815570 1.7928540 L 326470 -0.4406310 1.3969590 L 1.152420 -0.9815570 1.7928540 L 2.4967900 -0.1348560 -0.5426870 L 2.5510805 -0.228280 -0.6235180 L 2.4967900 -0.1348560 -0.5426870 <li< td=""><td>Н</td><td>-0.6232490</td><td>2.0984370</td><td>0.6392250</td><td></td></li<>	Н	-0.6232490	2.0984370	0.6392250	
 H. 1.0468580 -0.3812500 1.8317710 H. 2.6675240 0.2186430 1.4617960 H. 3414620 1.3659440 1.6684320 Snergy: -438.421541581 B3LYP/6-311++G** geometry and energy of conformer: Thr-X N0.5784370 1.9273800 -0.3001630 H1.5639310 1.9610530 -0.6624250 C0.1618670 0.558300 -0.6153250 H0.1575770 0.3509260 -1.6947020 C. 1.3032400 0.3231520 -0.1345260 C1.1604060 -0.4132230 -0.0195820 H. 1.8698550 1.1737450 -0.5220660 D. 1.822660 -0.8134290 -0.7654910 D2.2139900 -0.1214550 0.4850880 H. 1.3800660 -1.5932590 -0.5006030 D0.7477020 -1.7048750 -0.1311570 H. 4.365850 2.25579800 -1.0721420 C. 1.4435010 0.2902270 1.3847650 H. 0.4038050 2.5579800 -1.0721420 C. 1.4435010 0.2902270 1.8847650 H. 2.4995740 0.2429680 1.6573180 H. 0.033700 1.1877580 1.8241070 Energy: -438.421498297 B3LYP/6-311++G** geometry and energy of conformer: Thr-X N. 0.1925480 1.7437770 -0.1447390 H. 0.033700 1.1877580 1.8241070 Energy: -438.421498297 B3LYP/6-311++G** geometry and energy of conformer: Thr-X N. 0.1925480 1.7437770 -0.1447390 H. 0.033700 1.1877580 1.8241070 Energy: -438.421498297 	С	1.6039220	0.3789600	1.2759790	
 A. 2.6675240 M. 1.3414620 M. 1.3659440 M. 1.6684320 Chergy: -438.421541581 A. 2.55784370 M. 2.7584370 M. 2.85850 M. 1.737450 M. 2.852860 M. 1.8822860 M. 2.852860 M. 1.8822860 M. 1.8822860 M. 1.8822860 M. 2.850880 M. 1.8822860 M. 2.850880 M. 1.860860 M. 2.850880 M. 3.800660 M. 2.850880 M. 3.800660 M. 2.850880 M. 3.800660 M. 2.850880 M. 3.800660 M. 2.850880 M. 4.435010 M. 2.8508080 M. 4.8435010 M. 2.8995740 M. 2.4995740 M. 2.4995740 M. 4.84241498297 M. 0.1925480 M. 1.7437770 M. 1.8241070 M. 1.0033700 M. 1.877580 M. 4.8241070 M. 4.860430 <	Н	1.0468580	-0.3812500	1.8317710	
4 1.3414620 1.3659440 1.6684320 Snergy: -438.421541581 33LYP/6-311++G** geometry and energy of conformer: Thr-X N -0.5784370 1.9273800 -0.3001630 H -1.5639310 1.9610530 -0.0624250 C -0.1618670 0.3509260 -1.6947020 C 1.3032400 0.3231520 -0.1345260 C 1.3032400 0.3231520 -0.1345260 C 1.3032400 0.3231520 -0.5220660 D 1.8822860 -0.6134290 -0.7654910 D -2.2139900 -0.1214550 0.4850880 H 1.3800660 -1.5932590 -0.5006030 D -0.7477020 1.734760 -0.721420 C 1.4365850 2.2635080 0.2607090 H -0.4038050 2.5579800 -1.0721420 C 1.4365010 0.2902270 1.3847650 H 0.9465270 -0.5871630 1.8114230 H 2.4995740 0.2429680 1.6573180 H 1.0033700 1	Н	2.6675240	0.2186430	1.4617960	
Barergy: -438.421541581 B3LYP/6-311++G** geometry and energy of conformer: Thr-X N -0.5784370 1.9273800 -0.3001630 H -15639310 1.9610530 -0.0624250 C -0.1575770 0.3509260 -1.6947020 C 1.3032400 0.3231520 -0.1345260 C -1.1604060 -0.4132230 -0.195820 C 1.3032400 0.3231520 -0.5220660 D -2.8139900 -0.1214550 0.485080 C -2.4139900 -0.1214550 0.485080 D -2.2139900 -0.1214550 0.485080 D -2.2439900 -0.1214550 0.485080 D -2.439900 -0.2902270 1.3847650 H 1.8806660 2.5579800 1.0721420 C 1.4435510 0.2429680 1.6573180 H 0.9465270 -0.5871630 1.8114230 H 2.4995740 0.2429680 1.6573180 H 1.0033700 1.1877580 1.62841070 C -0.004330 <td>Н</td> <td>1.3414620</td> <td>1.3659440</td> <td>1.6684320</td> <td></td>	Н	1.3414620	1.3659440	1.6684320	
B3LYP/6-311++G** geometry and energy of conformer: Thr-X N -0.5784370 1.9273800 -0.3001630 H -1.5639310 1.9610530 -0.0624250 C -0.1618670 0.5558300 -0.6153250 H -0.1575770 0.3509260 -1.6947020 C 1.3032400 0.3231520 -0.1345260 C -1.1604060 -0.4132230 -0.0195820 H 1.8698550 1.1737450 -0.5220660 D -2.2139900 -0.8134290 -0.7654910 D -2.2139900 -0.8134290 -0.5006030 D -0.7477020 -1.7048750 -0.1311570 H -1.4365850 2.26579800 1.0721420 C 1.4435010 0.2902270 1.3847650 H 0.9465270 -0.5871630 1.8114230 H 2.4995740 0.2429680 1.6573180 H 1.0033700 1.1877580 1.8241070 Energy: -438.421498297 B3LYP/6-311++G** geometry and energy of conformer: Thr-X N 0.1925480 1.7437770 -0.1447390 H 0.0439780 0.3267250 -1.6628590 C 1.1174410 -0.5363630 -0.0338600 C -1.3566760 -0.285170 -0.2228820 H 0.8860490 -1.5606770 -0.3458350 D 1.0254870 -0.4406310 1.3969590 D 2.1.657180 -1.4048070 -0.5485520 H 1.7152420 -0.9816570 1.7928540 D 2.2.1915900 0.5317220 0.458840 H 0.1913940 1.7957730 0.8687470 D 2.2.4967900 -0.1348560 -0.5428520 H 0.1913940 1.7957730 0.8687470 D 2.2.4967900 -0.1348560 -0.5428470 D 2.510850 -0.2423330 -1.628490 H 0.1913940 1.7957730 0.8687470 D 2.2.4967900 -0.1348560 -0.5428470 D 2.510850 -0.2432300 -0.2833100 Energy: -438.421395397	Energy:	-438.42154158	1		
<pre>33LYP/6-311++G** geometry and energy of conformer: Thr-X</pre>					
N -0.5784370 1.9273800 -0.3001630 H -1.5639310 1.9610530 -0.6624250 C -0.1618670 0.5658300 -0.6153250 H -0.1575770 0.3509260 -1.6947020 C 1.3032400 0.3231520 -0.1345260 C -1.1604060 -0.4132230 -0.1395820 H 1.8698550 1.1737450 -0.5220660 D 1.8822860 -0.8134290 -0.7654910 D -2.2139900 -0.1214550 0.4850880 H 1.3800660 -1.5932590 -0.5006030 D -0.7477020 -1.7048750 -0.1311570 H -1.4365850 2.2635080 0.2607090 H -0.4038050 2.5579800 -1.0721420 C 1.4435010 0.2902270 1.3847650 H 0.9465270 -0.5871630 1.8114230 H 2.4995740 0.2429680 1.6573180 H 1.0033700 1.1877580 1.8241070 Energy: -438.421498297 S3LYP/6-311++G** geometry and energy of conformer: Thr-X N 0.1925480 1.7437770 -0.1447390 H 0.0439780 0.3267250 -1.6628590 C 1.1174410 -0.5363630 -0.0338600 C -1.3566760 -0.2851970 -0.2228820 H 0.8860490 -1.5606770 -0.3458350 D 1.0254870 -0.4406310 1.3969590 D 2.21919900 0.5317220 0.4580840 H 3.0037250 0.0282580 0.6235180 H 0.1913940 1.7957730 0.8687470 D 2.21919900 0.531720 0.458050 D 2.21919900 0.531720 0.458050 D 2.21919900 0.531720 0.245870 D 2.21919900 0.531720 0.2458800 D 2.21919900 0.531720 0.2458800 D 2.21919900 0.2547720 0.2458800 D 2.21919900 0.531720 0.2458800 D 2.21919900 0.531720 0.2458800 D 2.21919900 0.2548770 D 2.21919900 0.231720 0.2458800 D 2.21919900 0	B3LYP/6-	311++G** geome	try and energy	of conformer:	Thr-X
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	C	1.3032400	0.3231520	-0.1345260	
<pre>h 1.0030300 1.1/3/400 -0.3220000 D 1.8822860 -0.8134290 -0.7654910 D -2.2139900 -0.1214550 0.4850880 H 1.3800660 -1.5932590 -0.5006030 D -0.7477020 -1.7048750 -0.1311570 H -1.4365850 -2.2635080 0.2607090 H -0.4038050 2.5579800 -1.0721420 D 1.4435010 0.2902270 1.3847650 H 0.9465270 -0.5871630 1.8114230 H 2.4995740 0.2429680 1.6573180 H 1.0033700 1.1877580 1.8241070 Energy: -438.421498297 B3LYP/6-311++G** geometry and energy of conformer: Thr-X N 0.1925480 1.7437770 -0.1447390 H -0.5504030 2.3440600 -0.4826600 D -0.0084330 0.3694890 -0.5689890 H 0.0439780 0.3267250 -1.6628590 D 1.1174410 -0.5363630 -0.038600 D -1.3566760 -0.2851970 -0.2228820 H 0.8860490 -1.5606770 -0.3458350 D 1.0254870 -0.4406310 1.3969590 D 1.6657180 -1.4048070 -0.5485520 H 1.7152420 -0.9816570 1.7928540 D 2.1919900 0.5317220 0.4580840 H 3.2632900 -0.7851120 -0.1088520 H 3.2632900 -0.7851120 -0.1088520 H 3.2632900 -0.7851120 -0.1088520 H 2.7183000 0.9007690 -0.2833100 Energy: -438.421395397</pre>	U U	-1.1004060	-U.413223U	-U.UI95820	
<pre>- 1.0022000 -0.124250 -0.1054910 -2.2139900 -0.1214550 0.4850880 + 1.3800660 -1.5932590 -0.5006030 -0.7477020 -1.7048750 -0.1311570 + -1.4365850 -2.2635080 0.2607090 + 0.4038050 2.5579800 -1.0721420 C 1.4435010 0.2902270 1.3847650 + 0.9465270 -0.5871630 1.8114230 + 2.4995740 0.2429680 1.6573180 + 1.0033700 1.1877580 1.8241070 Energy: -438.421498297</pre> B3LYP/6-311++G** geometry and energy of conformer: Thr-X N 0.1925480 1.7437770 -0.1447390 + 0.0439780 0.3267250 -1.6628590 C 1.1174410 -0.5363630 -0.0338600 C -1.3566760 -0.2851970 -0.2228820 + 0.8860490 -1.5606770 -0.3458350 D 1.0254870 -0.4406310 1.3969590 D 1.0254870 -0.4406310 1.3969590 D 1.0254870 -0.4406310 1.3969590 D 1.0254870 -0.4406310 1.3969590 D -1.6657180 -1.4048070 -0.5485520 H 0.8860490 -1.5606770 1.7928540 D -2.1919900 0.5317220 0.4580840 H 0.1913940 1.7957730 0.8687470 C 2.4967900 -0.1348560 -0.5426870 H 2.5510850 -0.2432930 -1.6298490 H 2.7183000 0.9007690 -0.2833100 Energy: -438.421395397	п О	1,007050U	1.1/3/450	-U.JZZU66U	
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B3LYP/6-311++G** geometry and energy of conformer: Thr-X N 0.1925480 1.7437770 -0.1447390 -0.5504030 2.3440600 -0.4826600 -0.0084330 0.3694890 -0.5689890 0.0439780 0.3267250 -1.6628590 1.1174410 -0.5363630 -0.0338600 -1.3566760 -0.2851970 -0.2228820 0.0.8860490 -1.5606770 -0.3458350 1.0254870 -0.4406310 1.3969590 -1.6657180 -1.4048070 -0.5485520 1.7152420 -0.9816570 1.7928540 0.2.1919900 0.5317220 0.4580840 -2.1919900 0.5317220 0.4580840 -3.0037250 0.0282580 0.6235180 0.1913940 1.7957730 0.8687470 2.4967900 -0.1348560 -0.5426870 -3.2632900 -0.7851120 -0.1088520 -2.5510850 -0.2432930 -1.6298490 -2.7183000 0.9007690 -0.2833100 Energy: -438.421395397					
B3LYP/6-311++G** geometry and energy of conformer: Thr-X N 0.1925480 1.7437770 -0.1447390 H -0.5504030 2.3440600 -0.4826600 C -0.0084330 0.3694890 -0.5689890 H 0.0439780 0.3267250 -1.6628590 C 1.1174410 -0.5363630 -0.0338600 C -1.3566760 -0.2851970 -0.2228820 H 0.8860490 -1.5606770 -0.3458350 D 1.0254870 -0.4406310 1.3969590 D -1.6657180 -1.4048070 -0.5485520 H 1.7152420 -0.9816570 1.7928540 D -2.1919900 0.5317220 0.4580840 H -3.0037250 0.0282580 0.6235180 H 0.1913940 1.7957730 0.8687470 C 2.4967900 -0.1348560 -0.5426870 H 3.2632900 -0.7851120 -0.1088520 H 2.5510850 -0.2432930 -1.6298490 H 2.7183000 0.9007690 -0.2833100 <td></td> <td></td> <td></td> <td></td> <td></td>					
B3LYP/6-311++G** geometry and energy of conformer: Thr-X N 0.1925480 1.7437770 -0.1447390 H -0.5504030 2.3440600 -0.4826600 C -0.0084330 0.3694890 -0.5689890 H 0.0439780 0.3267250 -1.6628590 C 1.1174410 -0.5363630 -0.0338600 C -1.3566760 -0.2851970 -0.2228820 H 0.8860490 -1.5606770 -0.3458350 D 1.0254870 -0.4406310 1.3969590 O -1.6657180 -1.4048070 -0.5485520 H 1.7152420 -0.9816570 1.7928540 O -2.1919900 0.5317220 0.4580840 H -3.0037250 0.0282580 0.6235180 H 0.1913940 1.7957730 0.8687470 C 2.4967900 -0.1348560 -0.5426870 H 3.2632900 -0.7851120 -0.1088520 H 2.5510850 -0.2432930 -1.6298490 H 2.7183000 0.9007690 -0.2833100					
N0.19254801.7437770-0.1447390H-0.55040302.3440600-0.4826600C-0.00843300.3694890-0.5689890H0.04397800.3267250-1.6628590C1.1174410-0.5363630-0.0338600C-1.3566760-0.2851970-0.2228820H0.8860490-1.5606770-0.3458350D1.0254870-0.44063101.3969590O-1.6657180-1.4048070-0.5485520H1.7152420-0.98165701.7928540O-2.19199000.53172200.4580840H0.300372500.02825800.6235180H0.19139401.79577300.8687470C2.4967900-0.1348560-0.5426870H3.2632900-0.7851120-0.1088520H2.5510850-0.2432930-1.6298490H2.71830000.9007690-0.2833100	B3LYP/6-	311++G** geome	try and energy	of conformer:	Thr-X
H -0.5504030 2.3440600 -0.4826600 C -0.0084330 0.3694890 -0.5689890 H 0.0439780 0.3267250 -1.6628590 C 1.1174410 -0.5363630 -0.0338600 C -1.3566760 -0.2851970 -0.2228820 H 0.8860490 -1.5606770 -0.3458350 D 1.0254870 -0.4406310 1.3969590 C -1.6657180 -1.4048070 -0.5485520 H 1.7152420 -0.9816570 1.7928540 D -2.1919900 0.5317220 0.4580840 H -3.0037250 0.0282580 0.6235180 H 0.1913940 1.7957730 0.8687470 C 2.4967900 -0.1348560 -0.5426870 H 3.2632900 -0.7851120 -0.1088520 H 2.5510850 -0.2432930 -1.6298490 H 2.7183000 0.9007690 -0.2833100	N	0.1925480	1.7437770	-0.1447390	
-0.0084330 0.3694890 -0.5689890 H 0.0439780 0.3267250 -1.6628590 1.1174410 -0.5363630 -0.0338600 C -1.3566760 -0.2851970 -0.2228820 H 0.8860490 -1.5606770 -0.3458350 D 1.0254870 -0.4406310 1.3969590 O -1.6657180 -1.4048070 -0.5485520 H 1.7152420 -0.9816570 1.7928540 D -2.1919900 0.5317220 0.4580840 H -3.0037250 0.0282580 0.6235180 H 0.1913940 1.7957730 0.8687470 C 2.4967900 -0.1348560 -0.5426870 H 3.2632900 -0.7851120 -0.1088520 H 2.5510850 -0.2432930 -1.6298490 H 2.7183000 0.9007690 -0.2833100	Н	-0.5504030	2.3440600	-0.4826600	
A0.04397800.3267250-1.66285901.1174410-0.5363630-0.0338600-1.3566760-0.2851970-0.2228820A0.8860490-1.5606770-0.34583501.0254870-0.44063101.3969590-1.6657180-1.4048070-0.5485520-1.7152420-0.98165701.7928540-2.19199000.53172200.4580840-3.00372500.02825800.6235180-4.019139401.79577300.8687470-2.4967900-0.1348560-0.5426870-4.32632900-0.7851120-0.1088520-4.38.421395397-438.421395397	C	-0.0084330	0.3694890	-0.5689890	
1.11/4410 -0.5363630 -0.0338600 -1.3566760 -0.2851970 -0.2228820 H 0.8860490 -1.5606770 -0.3458350 D 1.0254870 -0.4406310 1.3969590 D -1.6657180 -1.4048070 -0.5485520 H 1.7152420 -0.9816570 1.7928540 D -2.1919900 0.5317220 0.4580840 H -3.0037250 0.0282580 0.6235180 H 0.1913940 1.7957730 0.8687470 C 2.4967900 -0.1348560 -0.5426870 H 3.2632900 -0.7851120 -0.1088520 H 2.5510850 -0.2432930 -1.6298490 H 2.7183000 0.9007690 -0.2833100	H	0.0439780	0.3267250	-1.6628590	
-1.3566760 -0.2851970 -0.2228820 H 0.8860490 -1.5606770 -0.3458350 D 1.0254870 -0.4406310 1.3969590 D -1.6657180 -1.4048070 -0.5485520 H 1.7152420 -0.9816570 1.7928540 D -2.1919900 0.5317220 0.4580840 H -3.0037250 0.0282580 0.6235180 H 0.1913940 1.7957730 0.8687470 C 2.4967900 -0.1348560 -0.5426870 H 3.2632900 -0.7851120 -0.1088520 H 2.5510850 -0.2432930 -1.6298490 H 2.7183000 0.9007690 -0.2833100	C C	1.11/4410	-0.5363630	-0.0338600	
10.8860490-1.5606770-0.345835001.0254870-0.44063101.39695900-1.6657180-1.4048070-0.548552041.7152420-0.98165701.79285400-2.19199000.53172200.45808400-3.00372500.02825800.623518040.19139401.79577300.8687470C2.4967900-0.1348560-0.542687043.2632900-0.7851120-0.108852042.5510850-0.2432930-1.629849042.71830000.9007690-0.2833100Energy:-438.421395397	U T	-1.3566/60	-U.28519/U	-0.2228820	
1.0234870 -0.4400310 1.3969590 -1.6657180 -1.4048070 -0.5485520 H 1.7152420 -0.9816570 1.7928540 D -2.1919900 0.5317220 0.4580840 D -3.0037250 0.0282580 0.6235180 H 0.1913940 1.7957730 0.8687470 C 2.4967900 -0.1348560 -0.5426870 H 3.2632900 -0.7851120 -0.1088520 H 2.5510850 -0.2432930 -1.6298490 H 2.7183000 0.9007690 -0.2833100	п	U.886U49U 1 0254070	-1.5606//0	-U.3458350	
-1.0037100 -1.4040070 -0.5405520 H 1.7152420 -0.9816570 1.7928540 D -2.1919900 0.5317220 0.4580840 H -3.0037250 0.0282580 0.6235180 H 0.1913940 1.7957730 0.8687470 C 2.4967900 -0.1348560 -0.5426870 H 3.2632900 -0.7851120 -0.1088520 H 2.5510850 -0.2432930 -1.6298490 H 2.7183000 0.9007690 -0.2833100	0	1.02348/U 1.6657100	-U.44U03IU _1 4049070	1.390939U _0 5/05520	
1.7132420 -0.9816370 1.7928340 0 -2.1919900 0.5317220 0.4580840 H -3.0037250 0.0282580 0.6235180 H 0.1913940 1.7957730 0.8687470 C 2.4967900 -0.1348560 -0.5426870 H 3.2632900 -0.7851120 -0.1088520 H 2.5510850 -0.2432930 -1.6298490 H 2.7183000 0.9007690 -0.2833100	U Ц	-1.003/10U	-1.4048070 _0.9816570	-U.340332U 1 7020570	
-2.1919900 0.031720 0.0430040 H -3.0037250 0.0282580 0.6235180 H 0.1913940 1.7957730 0.8687470 C 2.4967900 -0.1348560 -0.5426870 H 3.2632900 -0.7851120 -0.1088520 H 2.5510850 -0.2432930 -1.6298490 H 2.7183000 0.9007690 -0.2833100	11 0	_2 1919900	-U. YOIUJ/U 0 5317220	1./92034U 0./5808/0	
H 0.1913940 1.7957730 0.8687470 C 2.4967900 -0.1348560 -0.5426870 H 3.2632900 -0.7851120 -0.1088520 H 2.5510850 -0.2432930 -1.6298490 H 2.7183000 0.9007690 -0.2833100	U Ч	-2.1919900	0.0202500	0.400040	
C 2.4967900 -0.1348560 -0.5426870 H 3.2632900 -0.7851120 -0.1088520 H 2.5510850 -0.2432930 -1.6298490 H 2.7183000 0.9007690 -0.2833100	Н	0 1913940	1 7957730	0.0233100	
H 3.2632900 -0.7851120 -0.1088520 H 2.5510850 -0.2432930 -1.6298490 H 2.7183000 0.9007690 -0.2833100 Energy: -438.421395397	C	2,4967900	-0.1348560	-0.5426870	
H 2.5510850 -0.2432930 -1.6298490 H 2.7183000 0.9007690 -0.2833100 Energy: -438.421395397	Ч Н	3.2632900	-0.7851120	-0.1088520	
Energy: -438.421395397	н	2.5510850	-0.2432930	-1.6298490	
Energy: -438.421395397	H	2.7183000	0.9007690	-0.2833100	
	Energy:	-438.42139539	7		

B3LYP/6-	-311++G** geome	etry and energy	of conformer:	Thr-XVI
. , .		1 0 0 0 0 0 0 0 0	1 000000	
N	-0.2129830	-1.0623/70	1.3/29630	
П	0.0100070	-1.6373360	1.7433640	
C	0.0265030	-0.6918630	-0.0182400	
Н	0.0102800	-1.5990650	-0.6270800	
С	-1.0985340	0.2484450	-0.5228210	
С	1.4190500	-0.1000950	-0.2463730	
Н	-0.8162340	0.5952760	-1.5273860	
0	-1.2696890	1.3717290	0.3430670	
0	2.3385430	-0.6609470	-0.7850040	
Н	-0.4479210	1.8772640	0.3501910	
0	1.5504410	1.1615820	0.2656620	
Н	2.4644810	1.4448560	0.1089310	
Н	-0.3111580	-0.2398700	1.9584330	
С	-2.4403560	-0.4649240	-0.6019200	
н	-2.7207720	-0.8558160	0.3767910	
н	-3,2060500	0 2376930	-0.9358340	
н Н	-2 20/0000	-1 20/6220	_1 2112070	
п	-2.3940030	-1.2940200	-1.3110270	
Energy.	-438 42138293	2		
THCT AA .	100.12100292			
B3LYP/6-	-311++G** geome	try and energy	of conformer:	Thr-XI
N	-0.5696310	1.8862950	-0.1508650	
Н	-1.5710780	2.0111070	-0.2426360	
С	-0.1522570	0.5515110	-0.5758770	
Н	-0.2093940	0.4004490	-1.6680100	
С	1.3336840	0.2989270	-0.1978800	
С	-1.0591820	-0.5347480	-0.0200670	
H	1.8968610	1.1266370	-0.6414560	
0	1 8244570	-0 8656270	-0 8487910	
0	-0 7348240	-1 6908140	0.1208040	
U	1 2062000	-1.09U014U	0.1290040	
11	1.2703UZU	-1.011/01U	-0.332/300	
U	-2.3110320	-U.1UZ844U	0.2416540	
Н	-2.8232490	-0.8662890	0.5502290	
Н	-0.1119810	2.5931520	-0.7162030	
С	1.5928720	0.2824840	1.3075740	
Н	1.1042200	-0.5727850	1.7822870	
Н	2.6663120	0.2023140	1.4900590	
Н	1.2199140	1.1983370	1.7707060	
Energy:	-438.42112908	6		
	211.044	±		መሬ ፡፡ ፣፣፣
R3TI5/0-	·311++G** geome	try and energy	oi conformer:	Thr-XX
N	-0.7308580	1.8669150	-0.3601330	
 H	-1 653/570	1 8017010	0 0615/10	
 C	-0 2256/00	1.001/010 0 5201620	_0 6270700	
с ц	-0.2230400	0.3201020	-0.02/3/00	
п	-U.Z41/9UU	0.2921640	-1.1U3009U	
C G	1.2540160	0.4061920	-0.1696320	
С	1 1206760	0 5202060	0 0257520	
	-1.1390400	-0.5302000	0.0254550	

0	1.7894760	-0.8786780	-0.5895420	
0	-2.2222220	-0.2589620	0.4762090	
Н	2.0945190	-0.8200270	-1.5009370	
0	-0.6704930	-1.7866820	0.0312010	
H	0.2600400	-1.7900010	-0.2772600	
H	-0.8053110	2.4195510	-1.2044330	
С	1.4446210	0.5224260	1.3319580	
H	2.50//960	0.51/0690	1.5785010	
H	1.0000950	1.454/610	1.6825500	
Н	0.9686570	-0.3116490	1.8544930	
Energy:	-438.42107530	7		
B3LYP/6-	311++G** geome	try and energy	of conformer:	Thr->
N	-0.1193650	-1.2422280	1.1368790	
Н	-0.7776110	-2.0136960	1.1012910	
С	0.0657780	-0.6525800	-0.2053300	
Н	0.0930950	-1.4052590	-1.0012280	
С	-1.0959750	0.3286130	-0.4698970	
С	1.4563490	0.0192130	-0.2394780	
Н	-0.8754030	0.9044240	-1.3728620	
0	-1.1315500	1.2969050	0.5950170	
0	2.4368950	-0.5963240	-0.5696990	
Н	-1.1403550	0.7782500	1.4164830	
0	1.5240350	1.3032300	0.1397980	
Н	0.6327720	1.6133520	0.4136110	
Н	0.7547210	-1.6216240	1.4865990	
С	-2.4455210	-0.3617540	-0.6339720	
Н	-3.2215390	0.3827010	-0.8204340	
Н	-2.4251390	-1.0579320	-1.4775960	
Н	-2.7238110	-0.9160590	0.2671200	
Energy:	-438.42096752	8		
B3LYP/6-	311++G** geome	trv and energy	of conformer:	Thr->
N	0.1782550	1.7228290	0.2842200	
Н	-0.6668530	2.2807450	0.3206010	
С	-0.0392250	0.4883760	-0.4518520	
Н	-0.0672370	0.6306060	-1.5468320	
С	1.1089650	-0.5127620	-0.2017160	
С	-1.4107930	-0.0678890	-0.1098930	
Н	0.8946880	-1.4207490	-0.7753650	
0	2.2625080	0.1367780	-0.7610310	
0	-2.2905550	0.5491840	0.4347260	
Н	3.0496880	-0.3488870	-0.4963900	
0	-1.5753610	-1.3417690	-0.5425510	
Н	-2.4864820	-1.5973140	-0.3326620	
Н	0.9279740	2.2566180	-0.1373290	
C	1 0101000	0 0 0 2 2 2 2 0	1 2677040	
C	1.3134620	-0.8632360	1.2077040	
н	1.3134620 0.4443980	-1.3956850	1.6643090	
H H	1.3134620 0.4443980 2.1782030	-0.8632360 -1.3956850 -1.5253940	1.6643090 1.3813450	

Energy: -438.420596988

0.0120870 -0.3803690 0.0014210 0.1248570 1.1377810 -1.3554650 1.0035400 2.3872280 -1.9293540 2.6817810 -1.8542620 -2.7049560	1.9356770 2.2146210 0.4814200 0.2008000 -0.2121200 -0.0168880 0.0601490 0.3820180 0.3867380 -0.0087930	-0.3341160 0.5608410 -0.4447510 -1.4964290 0.3696660 0.0213570 1.4204530 0.0007360 1.0022350 -0.8301520	
-0.3803690 0.0014210 0.1248570 1.1377810 -1.3554650 1.0035400 2.3872280 -1.9293540 2.6817810 -1.8542620 -2.7049560	2.2146210 0.4814200 0.2008000 -0.2121200 -0.0168880 0.0601490 0.3820180 0.3867380 -0.0087930	$\begin{array}{c} 0.5608410 \\ -0.4447510 \\ -1.4964290 \\ 0.3696660 \\ 0.0213570 \\ 1.4204530 \\ 0.0007360 \\ 1.0022350 \\ -0.8301520 \end{array}$	
0.0014210 0.1248570 1.1377810 -1.3554650 1.0035400 2.3872280 -1.9293540 2.6817810 -1.8542620 -2.7049560	0.4814200 0.2008000 -0.2121200 -0.0168880 0.0601490 0.3820180 0.3867380 -0.0087930	-0.4447510 -1.4964290 0.3696660 0.0213570 1.4204530 0.0007360 1.0022350 -0.8301520	
0.1248570 1.1377810 -1.3554650 1.0035400 2.3872280 -1.9293540 2.6817810 -1.8542620 -2.7049560	$\begin{array}{c} 0.2008000 \\ -0.2121200 \\ -0.0168880 \\ 0.0601490 \\ 0.3820180 \\ 0.3867380 \\ -0.0087930 \end{array}$	-1.4964290 0.3696660 0.0213570 1.4204530 0.0007360 1.0022350 -0.8301520	
$\begin{array}{c} 1.1377810 \\ -1.3554650 \\ 1.0035400 \\ 2.3872280 \\ -1.9293540 \\ 2.6817810 \\ -1.8542620 \\ -2.7049560 \end{array}$	-0.2121200 -0.0168880 0.0601490 0.3820180 0.3867380 -0.0087930	0.3696660 0.0213570 1.4204530 0.0007360 1.0022350 -0.8301520	
-1.3554650 1.0035400 2.3872280 -1.9293540 2.6817810 -1.8542620 -2.7049560	-0.0168880 0.0601490 0.3820180 0.3867380 -0.0087930	0.0213570 1.4204530 0.0007360 1.0022350 -0.8301520	
1.0035400 2.3872280 -1.9293540 2.6817810 -1.8542620 -2.7049560	0.0601490 0.3820180 0.3867380 -0.0087930	1.4204530 0.0007360 1.0022350 -0.8301520	
2.3872280 -1.9293540 2.6817810 -1.8542620 -2.7049560	0.3820180 0.3867380 -0.0087930	0.0007360 1.0022350 -0.8301520	
-1.9293540 2.6817810 -1.8542620 -2.7049560	0.3867380	1.0022350	
2.6817810 -1.8542620 -2.7049560	-0.0087930	-0 8301520	
-1.8542620		0.0301320	
-2 70/0560	-0.9951490	-0.7680010	
2.1049000	-1.2656010	-0.3882800	
0.9723890	2.2634540	-0.3721110	
1.1824480	-1.7285930	0.2222510	
0.2711830	-2.1973010	0.6001650	
1.2910510	-2.0191660	-0.8287740	
2.0299150	-2.1296730	0.7821950	
-438.42053440	9		
1++C** 00000	try and onorgy	of conformar.	Thr_VV
geome	ery and energy	of conformer.	1111 7373
0.0119250	1.9373550	-0.3075720	
-0.2756370	2.2039380	0.6298530	
0.0074290	0.4839820	-0.4356370	
0.1266720	0.2233540	-1.4904560	
1.1383400	-0.2289210	0.3504060	
-1.3473670	-0.0157720	0.0411010	
1.0170610	0.0255590	1.4123780	
2.3440630	0.3653650	-0.1502420	
-1.8764470	0.3305740	1.0681020	
3.0886180	0.0467400	0.3691960	
-1.9031380	-0.9129260	-0.8025300	
-2.7533580	-1.1802360	-0.4193160	
0.9543590	2.2806180	-0.4612160	
1 1 5 7 7 2 4 0	-1.7445970	0.1751410	
1.13//340	1.110010		
0.2548410	-2.2063460	0.5830840	
1.15//340 0.2548410 1.2380620	-2.2063460 -2.0100760	0.5830840 -0.8819350	
1.15//340 0.2548410 1.2380620 2.0132750	-2.2063460 -2.0100760 -2.1772930	0.5830840 -0.8819350 0.7027090	
	0.2711830 1.2910510 2.0299150 -438.42053440 -438.42053440 -438.42053440 -0.0119250 -0.2756370 0.0074290 0.1266720 1.1383400 -1.3473670 1.0170610 2.3440630 -1.8764470 3.0886180 -1.9031380 -2.7533580	0.2711830 -2.1973010 1.2910510 -2.0191660 2.0299150 -2.1296730 -438.420534409 -438.420534409 -438.420534409 0.0119250 1.9373550 -0.2756370 2.2039380 0.0074290 0.4839820 0.1266720 0.2233540 1.1383400 -0.2289210 -1.3473670 -0.0157720 1.0170610 0.0255590 2.3440630 0.3653650 -1.8764470 0.3305740 3.0886180 0.0467400 -1.9031380 -0.9129260 -2.7533580 -1.1802360	0.2711830-2.19730100.60016501.2910510-2.0191660-0.82877402.0299150-2.12967300.7821950-438.420534409-438.420534409-438.420534409-0.3075720-0.01192501.9373550-0.3075720-0.27563702.20393800.62985300.00742900.4839820-0.43563700.12667200.2233540-1.49045601.1383400-0.22892100.3504060-1.3473670-0.01577200.04110101.01706100.02555901.41237802.34406300.3653650-0.1502420-1.87644700.33057401.06810203.08861800.04674000.3691960-1.9031380-0.9129260-0.8025300-2.7533580-1.1802360-0.4193160

Ν	-0.0982090	-0.9222640	1.5056010
Н	-0.4033540	-0.0727720	1.9712700
С	0.0241960	-0.6964720	0.0660630
Н	-0.0069430	-1.6612420	-0.4428670

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ა ⊿	C	-1.0699750	0.2239260	-0.5571600	
5	U U	1.41/8810	-0.1519/90	-0.22/4/10	
6	П	-0.7621370 -1.2291980	1 4000400	-1.3843370	
7	0	-1.2291900	_0 6897130	-0.8921060	
8	U H	-0 3823340	-0.0897130	-0.8921080	
a	0	1 6133590	1 07/5110	0.2251450	
10	н	2 5212570	1 3481780	0.1375670	
11	Н	-0.7767400	-1.6484490	1.7007460	
12	C	-2.4306990	-0.4553140	-0.5986290	
13	Н	-2.7618690	-0.7198500	0.4087850	
14	Н	-3.1688490	0.2253430	-1.0263690	
15	Н	-2.3959110	-1.3605100	-1.2102240	
16					
17	Energy:	-438.42025585	3		
18					
19					
20					
21	B3IVD/6_	311++C** goome	try and energy	of conformer.	Thr_XXVI
22	DODII/0	JIIIIG Geome	energy	or contormer.	IIII XXVI
23	Ν	0.0633420	1.8760450	-0.8002950	
24	Н	-0.6911350	2.2811890	-1.3437440	
20	С	-0.0618980	0.4246150	-0.7404920	
20	Н	-0.2839710	0.0592170	-1.7473250	
21	С	1.2982590	-0.2071300	-0.3158400	
20	С	-1.1897900	-0.0476620	0.1774590	
29	Н	2.0078960	0.0821460	-1.1011540	
30	0	1.2036510	-1.6294900	-0.2295240	
30	0	-1.5031670	0.4832820	1.2141990	
32	Н	0.8956790	-1.9844830	-1.0702380	
34	0	-1.8235030	-1.1400740	-0.3082810	
35	Н	-2.4854800	-1.4087570	0.3478570	
36	H	0.0023140	2.2/14150	0.1334010	
37	C	1.8210300	0.2769900	1.0274330	
38	п	2.7703770	-0.2090730	1.2322430	
39	п u	1 1286850	1.3339740	1 83/8720	
40	11	1.1200030	0.0300430	1.0340720	
41	Energy:	-438.41993422	4		
42					
43					
44					
45	/ -	0.1.1			
46	B3LYP/6-	-311++G** geome	try and energy	of conformer:	Thr-XXVII
4/	N	_0 1/77/80	_1 2/51090	1 21181/0	
48	N H	0 5851420	-1.9075620	1 4414960	
49	C	0.0718540	-0.6750820	-0.1209180	
50	H	0.0987670	-1.4998220	-0.8359600	
57	С	-1.0995360	0.2391890	-0.5135570	
52	С	1.4566250	0.0029070	-0.2447220	
54	Н	-0.8773570	0.6694560	-1.4987920	
55	0	-1.1125680	1.3122150	0.4627730	
56	0	2.4141490	-0.5827170	-0.6802200	
57	Н	-1.8417980	1.9129960	0.2790870	
58	0	1.5649110	1.2627530	0.2257370	
59	Н	0.6808940	1.5922380	0.4806670	
60	Н	-0.1570900	-0.5225230	1.9244680	
	С	-2.4393920	-0.4807500	-0.5560590	
	Н	-2.6576680	-0.9415590	0.4072180	

H -3.2413630 0.2181820 -0.8141730 H -2.4245310 -1.2612310 -1.3214940

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Energy:	-438.41981170	1		
			с с	
B3LYP/6-	311++G** geome	try and energy	of conformer:	Thr-XXVIII
Ν	-0.6588050	1.8625360	-0.5595770	
Н	-0.8737180	2.1075010	0.4000050	
С	-0.1266380	0.5143400	-0.6877920	
Н	-0.0600670	0.2732550	-1.7542180	
C	1.3184760	0.2840640	-0.1258770	
Ц	-1.0548320	-0.5348160	-0.1000970	
0	1.8753450	-0.9201020	-0.6324910	
0	-0.8413310	-1.7259050	-0.1781570	
H	1.2382390	-1.6322210	-0.4753670	
0	-2.1114040	-0.0377660	0.5676020	
Н	-2.6090450	-0.7930570	0.9182420	
Н	-0.0077870	2.5449210	-0.9316010	
С	1.4101950	0.3578180	1.3984430	
H	0.84/99/0	-0.4538100	1.8/03310	
н н	2.4534480	1 3107010	1.7780340	
11	1.0297100	1.510/010	1.7700340	
Energy:	-438.41961825	9		
B3LYP/6-	311++G** geome	try and energy	of conformer:	Thr-XXIX
N	_0 0871570	1 9085340	-0 3383170	
H	0.8440900	2.3005820	-0.4424250	
C	-0.0019850	0.4566440	-0.4779060	
Н	0.1923090	0.2206870	-1.5288930	
С	1.1339210	-0.1940040	0.3705940	
С	-1.3450910	-0.1778920	-0.1611230	
Н	0.9463610	0.0433070	1.4218420	
0	2.3638060	0.4/30/40	0.0648070	
н	2 7266250	-1.0237130	-0.7443420	
0	-1.8615880	0.2943260	1.0021790	
Н				
	-2.7138580	-0.1457640	1.1410130	
Н	-2.7138580 -0.4192310	-0.1457640 2.1558790	1.1410130 0.5889780	
H C	-2.7138580 -0.4192310 1.2605670	-0.1457640 2.1558790 -1.7019010	1.1410130 0.5889780 0.1872100	
H C H	-2.7138580 -0.4192310 1.2605670 0.3531380	-0.1457640 2.1558790 -1.7019010 -2.2245160	1.1410130 0.5889780 0.1872100 0.4975750	
Н С Н Н	-2.7138580 -0.4192310 1.2605670 0.3531380 1.4391160	-0.1457640 2.1558790 -1.7019010 -2.2245160 -1.9549470	1.1410130 0.5889780 0.1872100 0.4975750 -0.8639970	
Н С Н Н	-2.7138580 -0.4192310 1.2605670 0.3531380 1.4391160 2.0949480	-0.1457640 2.1558790 -1.7019010 -2.2245160 -1.9549470 -2.0799850	1.1410130 0.5889780 0.1872100 0.4975750 -0.8639970 0.7818750	
H C H H Energy:	-2.7138580 -0.4192310 1.2605670 0.3531380 1.4391160 2.0949480 -438.41948404	-0.1457640 2.1558790 -1.7019010 -2.2245160 -1.9549470 -2.0799850	1.1410130 0.5889780 0.1872100 0.4975750 -0.8639970 0.7818750	
H C H H Energy:	-2.7138580 -0.4192310 1.2605670 0.3531380 1.4391160 2.0949480 -438.41948404	-0.1457640 2.1558790 -1.7019010 -2.2245160 -1.9549470 -2.0799850	1.1410130 0.5889780 0.1872100 0.4975750 -0.8639970 0.7818750	
H C H H Energy:	-2.7138580 -0.4192310 1.2605670 0.3531380 1.4391160 2.0949480 -438.41948404	-0.1457640 2.1558790 -1.7019010 -2.2245160 -1.9549470 -2.0799850	1.1410130 0.5889780 0.1872100 0.4975750 -0.8639970 0.7818750	
H C H H Energy:	-2.7138580 -0.4192310 1.2605670 0.3531380 1.4391160 2.0949480 -438.41948404	-0.1457640 2.1558790 -1.7019010 -2.2245160 -1.9549470 -2.0799850	1.1410130 0.5889780 0.1872100 0.4975750 -0.8639970 0.7818750	
H C H H Energy: B3LYP/6-	-2.7138580 -0.4192310 1.2605670 0.3531380 1.4391160 2.0949480 -438.41948404	-0.1457640 2.1558790 -1.7019010 -2.2245160 -1.9549470 -2.0799850	1.1410130 0.5889780 0.1872100 0.4975750 -0.8639970 0.7818750	Thr-XXX

Н	-0.3394860	2.1550230	0.6266150
С	0.0020860	0.4569830	-0.4730680
Н	0.1949150	0.2311420	-1.5244370
С	1.1319070	-0.2085120	0.3550460
С	-1.3445060	-0.1710060	-0.1495830
H	0.9485110	0.0075140	1.4169540
0	2.3226510	0.4689490	-0.0699170
0	-1.9255980	-0.9801220	-0.8250050
H	3.0684270	0.1400290	0.4412950
0	-1.8296330	0.2700200	1.0397620
Н	-2.6914500	-0.1521820	1.1750310
Н	0.8253190	2.3116030	-0.5171120
С	1.2462170	-1.7147260	0.1400390
Н	0.3470720	-2.2376420	0.4754280
Н	1.4024770	-1.9410030	-0.9175840
Н	2.0919340	-2.1172240	0.7062960
Energy:	-438.41944597	3	
B3LYP/6-	-311++G** geome	try and energy	of conformer: Thr-
N	0.0226880	1.8829110	-0.7477320
Н	-0.0475930	2.2518860	0.1961090
С	-0.0780880	0.4250940	-0.7315620
Н	-0.3173430	0.0781800	-1.7377690
С	1.2917580	-0.1916710	-0.3632020
С	-1.1765330	-0.0745510	0.2105690
Н	1.9746650	0.1220520	-1.1627080
0	1.1024600	-1.6101060	-0.4094690
0	-1.3502240	0.3354120	1.3341080
Н	1.9148880	-2.0402240	-0.1257220
0	-1.9709380	-1.0041770	-0.3579820
Н	-2.6198160	-1.2768510	0.3094590
Н	-0.7344130	2.2887150	-1.2864540
С	1.8584040	0.2592780	0.9793800
Н	1.1961620	-0.0108780	1.8036750
Н	2.8334410	-0.2111340	1.1445750
Н	2.0175620	1.3399410	0.9885940
Energy:	-438.41917785	8	
B3LYP/6-	-311++G** geome	try and energy	of conformer: Thr-
N	0.2123150	1.7949590	-0.3540140
Н	-0.6767870	2.2832420	-0.3203950
С	0.0569650	0.4803330	0.2767830
H	-0.0193580	0.5335320	1.3775230
С	-1.2174430	-0.1968910	-0.2613670
C	1.3191750	-0.3137730	-0.0449410
Н	-1.1067690	-0.3137230	-1.3410020
0	-2.3212590	0./096960	-U.U993U3U
U	1.4054250	-1.28//890	-U./4/U46U
п	-2.0000440	0.01159610	U. /95532U
U	2.3952080	0.2415500	0.2002040
н	3 1 / / 4 80		U.Z.&YZU4U

C -0.0141670 0.4038760 -0.5759280 H 0.0054740 0.2835100 -1.6651870 C 1.0553640 -0.5714780 -0.0099780 C -1.3937160 -0.0493330 -0.1107970 H 0.7677450 -1.5828450 -0.3236360 O 0.9793940 -0.4663570 1.4144760 O -2.1132080 0.5439400 0.6462270 H 1.6144900 -1.0712790 1.8097940 O -1.7279690 -1.2479100 -0.6563910 H -2.5939090 -1.4910480 -0.2961730 H 1.0828410 2.1319050 -0.4321430 C 2.4603480 -0.2720870 -0.5254650 H 2.7932880 0.7235320 -0.2209950 H 3.1748030 -0.9969400 -0.1233010 H 2.5001960 -0.3416580 -1.6164960 Energy: -438.418617731 B3LYP/6-311++G** geometry and energy of conformer: Thr-XX N -0.0864220 1.8827520 -0.3881530 H -0.2161500 2.1985570 0.5669810 C -0.0010770 0.4273660 -0.4907660 H 0.1749660 0.1758490 -1.5384330 C 1.1311440 -0.2344060 0.3526040 C -1.3535260 -0.1684670 -0.1313090 H 0.9098310 -0.0636140 1.4151150 O 2.3847960 0.3704120 0.0237010 O -1.9740550 -0.9640620 -0.7870780 H 2.501900 -0.341600 0.1738190
C -0.0141670 0.4038760 -0.5759280 H 0.0054740 0.2835100 -1.6651870 C 1.0553640 -0.5714780 -0.0099780 C -1.3937160 -0.0493330 -0.1107970 H 0.7677450 -1.5828450 -0.3236360 O 0.9793940 -0.4663570 1.4144760 O -2.1132080 0.5439400 0.6462270 H 1.6144900 -1.0712790 1.8097940 O -1.7279690 -1.2479100 -0.6563910 H -2.5939090 -1.4910480 -0.2961730 H 1.0828410 2.1319050 -0.4321430 C 2.4603480 -0.2720870 -0.5254650 H 2.7932880 0.7235320 -0.2209950 H 3.1748030 -0.9969400 -0.1233010 H 2.5001960 -0.3416580 -1.6164960 Energy: -438.418617731 B3LYP/6-311++G** geometry and energy of conformer: Thr-XX N -0.0864220 1.8827520 -0.3881530 H -0.2161500 2.1985570 0.5669810 C -0.0010770 0.4273660 -0.4907660 H 0.1749660 0.1758490 -1.5384330 C 1.1311440 -0.2344060 0.3526040 C -1.3535260 -0.1684670 -0.1313090 H 0.9098310 -0.0636140 1.4151150
C -0.0141670 0.4038760 -0.5759280 H 0.0054740 0.2835100 -1.6651870 C 1.0553640 -0.5714780 -0.0099780 C -1.3937160 -0.0493330 -0.1107970 H 0.7677450 -1.5828450 -0.3236360 O 0.9793940 -0.4663570 1.4144760 O -2.1132080 0.5439400 0.6462270 H 1.6144900 -1.0712790 1.8097940 O -1.7279690 -1.2479100 -0.6563910 H -2.5939090 -1.4910480 -0.2961730 H 1.0828410 2.1319050 -0.4321430 C 2.4603480 -0.2720870 -0.5254650 H 2.7932880 0.7235320 -0.2209950 H 3.1748030 -0.9969400 -0.1233010 H 2.5001960 -0.3416580 -1.6164960 Energy: -438.418617731 B3LYP/6-311++G** geometry and energy of conformer: Thr-XX N -0.0864220 1.8827520 -0.3881530 H -0.2161500 2.1985570 0.5669810 C -0.0010770 0.4273660 -0.4907660 H 0.1749660 0.1758400 1.5254220
C -0.0141670 0.4038760 -0.5759280 H 0.0054740 0.2835100 -1.6651870 C 1.0553640 -0.5714780 -0.0099780 C -1.3937160 -0.0493330 -0.1107970 H 0.7677450 -1.5828450 -0.3236360 O 0.9793940 -0.4663570 1.4144760 O -2.1132080 0.5439400 0.6462270 H 1.6144900 -1.0712790 1.8097940 O -1.7279690 -1.2479100 -0.6563910 H -2.5939090 -1.4910480 -0.2961730 H 1.0828410 2.1319050 -0.4321430 C 2.4603480 -0.2720870 -0.5254650 H 2.7932880 0.7235320 -0.2209950 H 3.1748030 -0.9969400 -0.1233010 H 2.5001960 -0.3416580 -1.6164960 Energy: -438.418617731 B3LYP/6-311++G** geometry and energy of conformer: Thr-XX
$\begin{array}{cccccccccccccccccccccccccccccccccccc$
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C-0.01416700.4038760-0.5759280H0.00547400.2835100-1.6651870C1.0553640-0.5714780-0.0099780C-1.3937160-0.0493330-0.1107970H0.7677450-1.5828450-0.3236360O0.9793940-0.46635701.4144760O-2.11320800.54394000.6462270H1.6144900-1.07127901.8097940O-1.7279690-1.2479100-0.6563910H1.08284102.1319050-0.4321430C2.4603480-0.2720870-0.5254650H2.79328800.7235320-0.2209950
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C-0.01416700.4038760-0.5759280H0.00547400.2835100-1.6651870C1.0553640-0.5714780-0.0099780C-1.3937160-0.0493330-0.1107970H0.7677450-1.5828450-0.3236360O0.9793940-0.46635701.4144760O-2.11320800.54394000.6462270H1.6144900-1.07127901.8097940O-1.7279690-1.2479100-0.6563910H-2.5939090-1.4910480-0.2961730H1.08284102.1319050-0.4321430
$\begin{array}{cccccccccccccccccccccccccccccccccccc$
C -0.0141670 0.4038760 -0.5759280 H 0.0054740 0.2835100 -1.6651870 C 1.0553640 -0.5714780 -0.0099780 C -1.3937160 -0.0493330 -0.1107970 H 0.7677450 -1.5828450 -0.3236360 O 0.9793940 -0.4663570 1.4144760 O -2.1132080 0.5439400 0.6462270 H 1.6144900 -1.0712790 1.8097940 O -1.7279690 -1.2479100 -0.6563910
C -0.0141670 0.4038760 -0.5759280 H 0.0054740 0.2835100 -1.6651870 C 1.0553640 -0.5714780 -0.0099780 C -1.3937160 -0.0493330 -0.1107970 H 0.7677450 -1.5828450 -0.3236360 O 0.9793940 -0.4663570 1.4144760 O -2.1132080 0.5439400 0.6462270 H 1.6144900 -1.0712790 1.8097940
C -0.0141670 0.4038760 -0.5759280 H 0.0054740 0.2835100 -1.6651870 C 1.0553640 -0.5714780 -0.0099780 C -1.3937160 -0.0493330 -0.1107970 H 0.7677450 -1.5828450 -0.3236360 O 0.9793940 -0.4663570 1.4144760 O -2.1132080 0.5439400 0.6462270
C -0.0141670 0.4038760 -0.5759280 H 0.0054740 0.2835100 -1.6651870 C 1.0553640 -0.5714780 -0.0099780 C -1.3937160 -0.0493330 -0.1107970 H 0.7677450 -1.5828450 -0.3236360
C -0.0141670 0.4038760 -0.5759280 H 0.0054740 0.2835100 -1.6651870 C 1.0553640 -0.5714780 -0.0099780 C -1.3937160 -0.0493330 -0.1107970
C -0.0141670 0.4038760 -0.5759280 H 0.0054740 0.2835100 -1.6651870 C 1.0553640 -0.5714780 -0.0099780 C 0.2837160 -0.10092700
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N 0.1397450 1.8101650 -0.2514790

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С	-0.0286220	0.2636940	-0.6443290	
Н	0.0338930	0.0834860	-1.7237960	
С	1.0799940	-0.5797020	0.0323560	
С	-1.4007230	-0.2774530	-0.2038580	
Н	0.8497840	-1.6226300	-0.1935980	
0	1.0101390	-0.4903110	1.4529150	
0	-1.8562380	-1.2992030	-0.6415960	
Н	1.1248270	0.4298200	1.7167150	
0	-2.0433920	0.4716800	0.7065130	
Н	-1.4565220	1.2216190	0.9216580	
Н	1.0504170	2.0097190	-0.3530370	
С	2.4818140	-0.2565940	-0.4865930	
Н	3.2025490	-0.9315590	-0.0218990	
Н	2.5402450	-0.3805410	-1.5715970	
Н	2.7909960	0.7657420	-0.2410720	
Energy:	-438.41854432	5		
B3LYP/6	-311++G** geome	try and energy	of conformer:	Thr-XXX
N	0.0708310	1.7809980	-0.1976800	
Н	0.0381060	1.8727830	0.8122810	
С	-0.0054870	0.3829930	-0.5890670	
Н	0.0662670	0.3254570	-1.6797750	
С	1.0896840	-0.5581780	-0.0195660	
С	-1.3608240	-0.2378110	-0.2528200	
H	0.8456220	-1.5733960	-0.3543720	
0	0.9684250	-0.4745010	1.4062670	
0	-1.7204550	-1.3074780	-0.6828650	
Н	1.5656060	-1.1104280	1.8115760	
0	-2.1098/40	0.501///0	0.5853340	
H	-2.9204380	-0.0015630	0.7557710	
H	0.9318380	2.2026780	-0.5260350	
C	2.4941150	-0.1908/80	-0.48/5280	
H	3.2286470	-0.8853190	-0.068/510	
H	2.5/028/0	-0.2492170	-1.5//4300	
Н	2.7685560	0.8168/90	-0.1655030	
Energy:	-438.41843498	8		
B3LYP/6	-311++G** geome [:]	try and energy	of conformer:	Thr-XXX
N	0.1090110	1.9085680	-0.2778820	
H	-0.3578410	2.1975030	0.5789480	
С	-0.0143240	0.4593990	-0.4314020	
Н	0.1500950	0.2129880	-1.4866650	
С	1.1425100	-0.1986680	0.3784840	
С	-1.3823120	-0.0619370	0.0293890	
Н	0.9671800	0.0404480	1.4388440	
0	2.3633750	0.3772310	-0.0516370	
0	-2.0275380	0.4690960	0.8914280	
Н	2.1914600	1.3290880	-0.1272750	
0	-1.8428990	-1.1886880	-0.5711610	
Н	-1.2186910	-1.4986880	-1.2390940	
Н	-0.3412570	2.4005820	-1.0417190	
С	1.2544310	-1.7061750	0.2142150	

Н	0.3869450	-2.2252250	0.6278000	
н	1.3/19/30 2 1/17200	-1.9/40/50	-0.8411230	
п	2.141/200	-2.0394170	0.7423000	
Energy:	-438.41826893	7		
B3LYP/6-	-311++G** geome	try and energy	of conformer:	Thr-XXXVI
N	-0.0445150	1.8411230	-0.8161040	
Н	-0.0854710	2.2370770	0.1167920	
С	-0.0751130	0.3824500	-0.7732460	
Н	-0.2465950	0.0247420	-1.7923700	
С	1.3084440	-0.1752870	-0.3296780	
С	-1.2177640	-0.2315310	0.0386100	
Н	2.0057670	0.1160630	-1.1257520	
0	1.2658630	-1.5965570	-0.2013670	
0	-1.9137270	-1.1417590	-0.3353580	
H	0.9285230	-1.9878970	-1.0146650	
0	-1.3906670	0.3723350	1.2411960	
H	-2.1212720	-0.0818210	1.6879910	
H	-0.8311320	2.2083060	-1.3400340	
C	1.82/4690	0.3648290	0.9943180	
H U	2 9026100	0.1140490	1.0109030	
и П	1 9537470	1 1/182280	0 9/93130	
Energy:	-438.41821867	7		
Energy: B3LYP/6-	-438.41821867	7 try and energy	of conformer:	Thr-XXXIX
Energy: B3LYP/6-	-438.41821867 -311++G** geome -0.0830810	7 try and energy 1.8518360	<pre>v of conformer: 0.3146390</pre>	Thr-XXXIX
Energy: B3LYP/6- N H	-438.41821867 -311++G** geome -0.0830810 -0.7244710	7 try and energy 1.8518360 2.4595480	<pre>v of conformer:</pre>	Thr-XXXIX
Energy: B3LYP/6- N H C	-438.41821867 -311++G** geome -0.0830810 -0.7244710 -0.0226530	7 try and energy 1.8518360 2.4595480 0.5332950	<pre>v of conformer: 0.3146390 -0.1843000 -0.3298020</pre>	Thr-XXXI)
Energy: B3LYP/6- N H C H	-438.41821867 -311++G** geome -0.0830810 -0.7244710 -0.0226530 0.1033300	1.8518360 2.4595480 0.5332950 0.5918830	<pre>v of conformer: 0.3146390 -0.1843000 -0.3298020 -1.4199590</pre>	Thr-XXXI)
Energy: B3LYP/6- N H C H C	-438.41821867 -311++G** geome -0.0830810 -0.7244710 -0.0226530 0.1033300 1.1584090	1.8518360 2.4595480 0.5332950 0.5918830 -0.2637270	<pre>v of conformer: 0.3146390 -0.1843000 -0.3298020 -1.4199590 0.2390910</pre>	Thr-XXXIX
Energy: B3LYP/6- N H C H C C C	-438.41821867 -438.41821867 -0.0830810 -0.7244710 -0.0226530 0.1033300 1.1584090 -1.3827400	TTY and energy 1.8518360 2.4595480 0.5332950 0.5918830 -0.2637270 -0.1201750	<pre>v of conformer: 0.3146390 -0.1843000 -0.3298020 -1.4199590 0.2390910 -0.1003520</pre>	Thr-XXXIX
Energy: B3LYP/6- N H C H C C H	-438.41821867 -438.41821867 -0.0830810 -0.7244710 -0.0226530 0.1033300 1.1584090 -1.3827400 1.0219930	1.8518360 2.4595480 0.5332950 0.5918830 -0.2637270 -0.1201750 -0.3505930	<pre>v of conformer: 0.3146390 -0.1843000 -0.3298020 -1.4199590 0.2390910 -0.1003520 1.3222030</pre>	Thr-XXXI)
Energy: B3LYP/6- N H C H C C H O O	-438.41821867 -438.41821867 -0.0830810 -0.7244710 -0.0226530 0.1033300 1.1584090 -1.3827400 1.0219930 2.3102310	1.8518360 2.4595480 0.5332950 0.5918830 -0.2637270 -0.1201750 -0.3505930 0.5542040	<pre>v of conformer: 0.3146390 -0.1843000 -0.3298020 -1.4199590 0.2390910 -0.1003520 1.3222030 -0.0344630 0.0344630</pre>	Thr-XXXIX
Energy: B3LYP/6- N H C H C C H O O	-438.41821867 -438.41821867 -0.0830810 -0.7244710 -0.0226530 0.1033300 1.1584090 -1.3827400 1.0219930 2.3102310 -2.3156460	1.8518360 2.4595480 0.5332950 0.5918830 -0.2637270 -0.1201750 -0.3505930 0.5542040 -0.0052540	<pre>v of conformer: 0.3146390 -0.1843000 -0.3298020 -1.4199590 0.2390910 -0.1003520 1.3222030 -0.0344630 -0.8557080 0.4202310</pre>	Thr-XXXIX
Energy: B3LYP/6- N H C H C H O O H	-438.41821867 -438.41821867 -0.0830810 -0.7244710 -0.0226530 0.1033300 1.1584090 -1.3827400 1.0219930 2.3102310 -2.3156460 3.0688680	Try and energy 1.8518360 2.4595480 0.5332950 0.5918830 -0.2637270 -0.1201750 -0.3505930 0.5542040 -0.0052540 0.1872910 0.865750	<pre>v of conformer: 0.3146390 -0.1843000 -0.3298020 -1.4199590 0.2390910 -0.1003520 1.3222030 -0.0344630 -0.8557080 0.4293310 1.06232000</pre>	Thr-XXXIX
Energy: B3LYP/6- N H C H C C H O O H O H O H	-438.41821867 -438.41821867 -0.0830810 -0.7244710 -0.0226530 0.1033300 1.1584090 -1.3827400 1.0219930 2.3102310 -2.3156460 3.0688680 -1.4680440 -2.3826060	Try and energy 1.8518360 2.4595480 0.5332950 0.5918830 -0.2637270 -0.1201750 -0.3505930 0.5542040 -0.0052540 0.1872910 -0.8050750 -1.1161140	<pre>v of conformer: 0.3146390 -0.1843000 -0.3298020 -1.4199590 0.2390910 -0.1003520 1.3222030 -0.0344630 -0.8557080 0.4293310 1.0623800 1.1440460</pre>	Thr-XXXIX
Energy: B3LYP/6- N H C H C C H O O H O H H H	-438.41821867 -438.41821867 -0.0830810 -0.7244710 -0.0226530 0.1033300 1.1584090 -1.3827400 1.0219930 2.3102310 -2.3156460 3.0688680 -1.4680440 -2.3826060 0.8412870	77 try and energy 1.8518360 2.4595480 0.5332950 0.5918830 -0.2637270 -0.1201750 -0.3505930 0.5542040 -0.0052540 0.1872910 -0.8050750 -1.1161140 2.2700580	<pre>v of conformer: 0.3146390 -0.1843000 -0.3298020 -1.4199590 0.2390910 -0.1003520 1.3222030 -0.0344630 -0.8557080 0.4293310 1.0623800 1.1440460 0.2776170</pre>	Thr-XXXIX
Energy: B3LYP/6- N H C H C C H O O H C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C C C C C C C C C C C C	-438.41821867 -438.41821867 -0.0830810 -0.7244710 -0.0226530 0.1033300 1.1584090 -1.3827400 1.0219930 2.3102310 -2.3156460 3.0688680 -1.4680440 -2.3826060 0.8412870 1.3094350	1.8518360 2.4595480 0.5332950 0.5918830 -0.2637270 -0.1201750 -0.3505930 0.5542040 -0.0052540 0.1872910 -0.8050750 -1.1161140 2.2700580 -1.6443720	<pre>v of conformer: 0.3146390 -0.1843000 -0.3298020 -1.4199590 0.2390910 -0.1003520 1.3222030 -0.0344630 -0.8557080 0.4293310 1.0623800 1.1440460 0.2776170 -0.3930080</pre>	Thr-XXXI>
Energy: B3LYP/6- N H C H C H O O H O H H C H H C H H C H H C H H C H C H C H C H C H C H C H C H H H H H H H H H C H H H H H H H H H H H H H	-438.41821867 -438.41821867 -0.0830810 -0.7244710 -0.0226530 0.1033300 1.1584090 -1.3827400 1.0219930 2.3102310 -2.3156460 3.0688680 -1.4680440 -2.3826060 0.8412870 1.3094350 0.4419370	1.8518360 2.4595480 0.5332950 0.5918830 -0.2637270 -0.1201750 -0.3505930 0.5542040 -0.0052540 0.1872910 -0.8050750 -1.1161140 2.2700580 -1.6443720 -2.2737740	<pre>v of conformer: 0.3146390 -0.1843000 -0.3298020 -1.4199590 0.2390910 -0.1003520 1.3222030 -0.0344630 -0.8557080 0.4293310 1.0623800 1.1440460 0.2776170 -0.3930080 -0.1816120</pre>	Thr-XXXIX
Energy: B3LYP/6- N H C H C H O O H O H H C H H H H H H H H H H H H H	-438.41821867 -438.41821867 -0.0830810 -0.7244710 -0.0226530 0.1033300 1.1584090 -1.3827400 1.0219930 2.3102310 -2.3156460 3.0688680 -1.4680440 -2.3826060 0.8412870 1.3094350 0.4419370 1.4348690	1.8518360 2.4595480 0.5332950 0.5918830 -0.2637270 -0.1201750 -0.3505930 0.5542040 -0.0052540 0.1872910 -0.8050750 -1.1161140 2.2700580 -1.6443720 -2.2737740 -1.5600170	<pre>v of conformer: 0.3146390 -0.1843000 -0.3298020 -1.4199590 0.2390910 -0.1003520 1.3222030 -0.0344630 -0.8557080 0.4293310 1.0623800 1.1440460 0.2776170 -0.3930080 -0.1816120 -1.4755450</pre>	Thr-XXXIX
Energy: B3LYP/6- N H C H C C H O O H C H H C H H H H H H	-438.41821867 -438.41821867 -0.0830810 -0.7244710 -0.0226530 0.1033300 1.1584090 -1.3827400 1.0219930 2.3102310 -2.3156460 3.0688680 -1.4680440 -2.3826060 0.8412870 1.3094350 0.4419370 1.4348690 2.1893350	Try and energy 1.8518360 2.4595480 0.5332950 0.5918830 -0.2637270 -0.1201750 -0.3505930 0.5542040 -0.0052540 0.1872910 -0.8050750 -1.1161140 2.2700580 -1.6443720 -2.2737740 -1.5600170 -2.1522550	<pre>v of conformer: 0.3146390 -0.1843000 -0.3298020 -1.4199590 0.2390910 -0.1003520 1.3222030 -0.0344630 -0.8557080 0.4293310 1.0623800 1.1440460 0.2776170 -0.3930080 -0.1816120 -1.4755450 0.0125080</pre>	Thr-XXXIX
Energy: B3LYP/6- N H C H C H O O H O H H C H H Energy:	-438.41821867 -438.41821867 -0.0830810 -0.7244710 -0.0226530 0.1033300 1.1584090 -1.3827400 1.0219930 2.3102310 -2.3156460 3.0688680 -1.4680440 -2.3826060 0.8412870 1.3094350 0.4419370 1.4348690 2.1893350 -438.41802090	1.8518360 2.4595480 0.5332950 0.5918830 -0.2637270 -0.1201750 -0.3505930 0.5542040 -0.0052540 0.1872910 -0.8050750 -1.1161140 2.2700580 -1.6443720 -2.2737740 -1.5600170 -2.1522550	<pre>v of conformer: 0.3146390 -0.1843000 -0.3298020 -1.4199590 0.2390910 -0.1003520 1.3222030 -0.0344630 -0.8557080 0.4293310 1.0623800 1.1440460 0.2776170 -0.3930080 -0.1816120 -1.4755450 0.0125080</pre>	Thr-XXXIX
Energy: B3LYP/6- N H C H C H O O H O H H H Energy: B3LYP/6-	-438.41821867 -438.41821867 -311++G** geome -0.0830810 -0.7244710 -0.0226530 0.1033300 1.1584090 -1.3827400 1.0219930 2.3102310 -2.3156460 3.0688680 -1.4680440 -2.3826060 0.8412870 1.3094350 0.4419370 1.4348690 2.1893350 -438.41802090 -311++G** geome	1.8518360 2.4595480 0.5332950 0.5918830 -0.2637270 -0.1201750 -0.3505930 0.5542040 -0.0052540 0.1872910 -0.8050750 -1.1161140 2.2700580 -1.6443720 -2.2737740 -1.5600170 -2.1522550	<pre>v of conformer: 0.3146390 -0.1843000 -0.3298020 -1.4199590 0.2390910 -0.1003520 1.3222030 -0.0344630 -0.8557080 0.4293310 1.0623800 1.1440460 0.2776170 -0.3930080 -0.1816120 -1.4755450 0.0125080</pre>	Thr-XXXIX
Energy: B3LYP/6- N H C H C H O O H O H H Energy: B3LYP/6- N	-438.41821867 -438.41821867 -0.0830810 -0.7244710 -0.0226530 0.1033300 1.1584090 -1.3827400 1.0219930 2.3102310 -2.3156460 3.0688680 -1.4680440 -2.3826060 0.8412870 1.3094350 0.4419370 1.4348690 2.1893350 -438.41802090 -311++G** geome	1.8518360 2.4595480 0.5332950 0.5918830 -0.2637270 -0.1201750 -0.3505930 0.5542040 -0.0052540 0.1872910 -0.8050750 -1.1161140 2.2700580 -1.6443720 -2.2737740 -1.5600170 -2.1522550 2 2 try and energy 1.8585250	<pre>v of conformer: 0.3146390 -0.1843000 -0.3298020 -1.4199590 0.2390910 -0.1003520 1.3222030 -0.0344630 -0.8557080 0.4293310 1.0623800 1.1440460 0.2776170 -0.3930080 -0.1816120 -1.4755450 0.0125080</pre>	Thr-XXXIX
Energy: B3LYP/6- N H C H C H O H O H H Energy: B3LYP/6- N H	-438.41821867 -438.41821867 -0.0830810 -0.7244710 -0.0226530 0.1033300 1.1584090 -1.3827400 1.0219930 2.3102310 -2.3156460 3.0688680 -1.4680440 -2.3826060 0.8412870 1.3094350 0.4419370 1.4348690 2.1893350 -438.41802090 -311++G** geome -0.1612090 -0.2908270	1.8518360 2.4595480 0.5332950 0.5918830 -0.2637270 -0.1201750 -0.3505930 0.5542040 -0.0052540 0.1872910 -0.8050750 -1.1161140 2.2700580 -1.6443720 -2.2737740 -1.5600170 -2.1522550 2.2675740	<pre>v of conformer: 0.3146390 -0.1843000 -0.3298020 -1.4199590 0.2390910 -0.1003520 1.3222030 -0.0344630 -0.8557080 0.4293310 1.0623800 1.1440460 0.2776170 -0.3930080 -0.1816120 -1.4755450 0.0125080</pre>	Thr-XXXIX
Energy: B3LYP/6- N H C H C H O O H H C H H Energy: B3LYP/6- N H C N H C H C H C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C C H C C H C C H C C H C C H C C H H C C H H C C H H C C H H C C H H C C H H C C H H C C H H C H H C C H H C C H H C C H H C C H H C C H H C C H H C H H H C C H H H C C H H H C C H H H C C H H H H C C H H H H C C H H H C H H H C H H H C H H H C C H H H C C H H H C C H H H C C H H H C C H H H C C N H H C C N H H C C N H C C C C C C C C C C C C C	-438.41821867 -438.41821867 -311++G** geome -0.0830810 -0.7244710 -0.0226530 0.1033300 1.1584090 -1.3827400 1.0219930 2.3102310 -2.3156460 3.0688680 -1.4680440 -2.3826060 0.8412870 1.3094350 0.4419370 1.4348690 2.1893350 -438.41802090 -311++G** geome -0.1612090 -0.2908270 -0.0719470	1.8518360 2.4595480 0.5332950 0.5918830 -0.2637270 -0.1201750 -0.3505930 0.5542040 -0.0052540 0.1872910 -0.8050750 -1.1161140 2.2700580 -1.6443720 -2.2737740 -1.5600170 -2.1522550 22 	<pre>v of conformer: 0.3146390 -0.1843000 -0.3298020 -1.4199590 0.2390910 -0.1003520 1.3222030 -0.0344630 -0.8557080 0.4293310 1.0623800 1.1440460 0.2776170 -0.3930080 -0.1816120 -1.4755450 0.0125080 v of conformer: -0.8496080 0.0700790 -0.7559960</pre>	Thr-XXIX
Energy: B3LYP/6- N H C H C H O O H O H H Energy: B3LYP/6- N H C H H H H H H H H H H H H H	-438.41821867 -438.41821867 -0.0830810 -0.7244710 -0.0226530 0.1033300 1.1584090 -1.3827400 1.0219930 2.3102310 -2.3156460 3.0688680 -1.4680440 -2.3826060 0.8412870 1.3094350 0.4419370 1.4348690 2.1893350 -438.41802090 -311++G** geome -0.1612090 -0.2908270 -0.0719470 -0.2420690	1.8518360 2.4595480 0.5332950 0.5918830 -0.2637270 -0.1201750 -0.3505930 0.5542040 -0.0052540 0.1872910 -0.8050750 -1.1161140 2.2700580 -1.6443720 -2.2737740 -1.5600170 -2.1522550 22 Stry and energy 1.8585250 2.2675740 0.4070660 -0.0169090	<pre>v of conformer: 0.3146390 -0.1843000 -0.3298020 -1.4199590 0.2390910 -0.1003520 1.3222030 -0.0344630 -0.8557080 0.4293310 1.0623800 1.1440460 0.2776170 -0.3930080 -0.1816120 -1.4755450 0.0125080 v of conformer: -0.8496080 0.0700790 -0.7559960 -1.7519930</pre>	Thr-XXXIX

~	1 0000700	0 1000550	0 0045400	
C	1.3092720	-0.1388//0	-0.2645430	
C	-1.1976090	-0.0803980	0.1421810	
H	2.043/980	0.2427830	-0.9914770	
0	1.3369470	-1.5651060	-0.2603410	
0	-1.5/39050	0.4855//0	1.13/9/30	
Н	1.0143320	-1.8980920	-1.1048840	
0	-1.7295370	-1.2433400	-0.2904530	
Н	-2.3948350	-1.5177750	0.3596680	
Н	0.6710300	2.2549010	-1.2724080	
С	1.7203040	0.3100540	1.1293340	
Н	1.0170000	-0.0498200	1.8826770	
Н	2.7078920	-0.0951210	1.3579690	
Н	1.7739890	1.3986790	1.1943340	
Energy:	-438.41786911	.1		
B3LYP/6-	311++G** geome	etry and energy	of conformer:	Thr-XLI
N	_0 022/100	1 0000760	0 01701/0	
11	-0.0324190	1.0009/00	U.ZI/014U	
п	0.91/4830	Z.Z3/1620	0.261/440	
C	-0.0102640	0.5346410	-0.35/2560	
H	0.1228490	0.5293260	-1.4499360	
С	1.1478610	-0.2671260	0.2737380	
С	-1.3777240	-0.1002820	-0.1168230	
Н	1.0090450	-0.2649770	1.3560960	
0	2.3755060	0.4448480	0.0638300	
0	-2.2342510	-0.2074120	-0.9598840	
Н	2.6717170	0.2893440	-0.8405110	
0	-1.5506410	-0.5192870	1.1561710	
Н	-2.4564920	-0.8566440	1.2268390	
Н	-0.5859150	2.5130440	-0.3499110	
C	1,2422390	-1.6966610	-0.2461360	
н	1 3817710	-1 7127060	-1 3331180	
и П	2 0902380	-2 2044780	0 2175360	
H	0.3386540	-2.2655300	-0.0155120	
Enerav:	-438.41773384	6		
Lifer gy .	100.11770001			
	211	true and anarray	of conformer.	The VIT
DOLIF/0-	SIITTG geome	cry and energy	or conformer.	
Ν	-0.1222980	1.8873060	-0.6396680	
Н	-0.9207210	2.2735960	-1.1306130	
С	-0.1057810	0.4266650	-0.7363740	
Н	-0.3007800	0.1536900	-1.7742100	
С	1.2991960	-0.1167110	-0.3963820	
С	-1.2320710	-0.2469870	0.0532940	
Н	1.9536850	0.2695470	-1.1885170	
0	1.1888910	-1.5395840	-0.5044280	
0	-2.1162890	-0.9078920	-0.4258930	
- H	2.0349580	-1.9367710	-0.2766300	
0	-1 1830250	0 0428670	1 3828920	
с ц	_1 0/51560	_0 2011000	1 7052520	
11	-1.94JIJ0U	-U.JJIIJOU	T.120000	
п	-U.I/4UIUU	2.1940600	U.JZJY00U	
	1.0(0/020	0.3069440	U.YJJ661U	
н	1.2004830	-0.05/9250	1.//9868U	
Н	2.8845130	-0.0937390	T.0639980	
Н	1.9501240	1.3950000	1.0166830	

Energy: -438.416965250

B3LYP/6-	311++G** geome	try and energy	of conformer:	Thr-XLIII
N	-0.1884010	1.8592180	-0.8039330	
Н	-0.1763880	2.2626160	0.1269550	
С	-0.0866920	0.4043140	-0.7457610	
Н	-0.2827200	-0.0034590	-1.7391440	
С	1.3024700	-0.1417190	-0.3132850	
С	-1.1871910	-0.0894740	0.1855540	
Н	2.0128020	0.2516140	-1.0572480	
С	1.2184370	-1.5635710	-0.4432620	
C	-1.3958530	0.3624570	1.2860100	
H	2.0395800	-1.9559420	-0.1303880	
C	-1.9183050	-1.0843050	-0.3492670	
H	-2.5748520	-1.3471760	0.3144420	
Н	0.5650520	2.2627820	-1.3494770	
C	1.7707250	0.2713900	1.0785380	
H	1.0997700	-0.1051910	1.8520370	
H	2.7758950	-0.1222930	1.2622740	
H	1.8295590	1.3588160	1.1699600	
Energy:	-438.41679286	7		
B3LYP/6-	-311++G** geome	trv and energy	of conformer:	Thr-XLIV
- , -				
N	-0.2539740	1.8118220	-0.8630330	
H	-0.2459270	2.2387700	0.0565390	
С	-0.0767670	0.3649860	-0.7832200	
H	-0.1973930	-0.0377650	-1.7938440	
С	1.3197120	-0.1199840	-0.2759520	
С	-1.2101560	-0.2684040	0.0115920	
H	2.0404690	0.2451540	-1.0250510	
0	1.3789220	-1.5431340	-0.2061510	
0	-1.7867480	-1.2773090	-0.3034450	
H	0.9824640	-1.9282970	-0.9956810	
0	-1.4976270	0.4183110	1.1431320	
H	-2.2231820	-0.0470650	1.5866210	
Н	0.4770620	2.2372970	-1.4232810	
С	1.7377930	0.3991930	1.0918970	
Н	1.0432690	0.0726830	1.8678610	
Н	2.7288430	0.0087860	1.3312460	
Н	1.7923410	1.4899920	1.1026350	

Energy: -438.416053844

B3LYP/6-311++G** geometry and energy of conformer: Thr-XLV

Ν	0.1630950	1.7075640	-0.0322460
Н	0.6465600	2.2990720	-0.6956160
С	-0.0323770	0.3508990	-0.5364590
Н	-0.0172260	0.2965400	-1.6365640
С	1.1050810	-0.5521540	0.0129250
С	-1.4378860	-0.1215240	-0.1233730
Н	0.9027210	-1.6052370	-0.2222720

0	1.1227050	-0.4729230	1.4261710	
0	-2.2778080	0.6232810	0.3020840	
Н	1.0406050	0.4712750	1.6354030	
0	-1.7249500	-1.4252630	-0.3255160	
Н	-0.9362300	-1.9165780	-0.5858770	
Н	-0.7359660	2.1251710	0.1899360	
C	2 4618020	-0.1940790	-0.5961350	
ч	3 23/5380	_0 8329170	-0 1648700	
11	2.4612040	0.0329170	1 (010050	
п	2.4012040	-0.3342800	-1.0019950	
Н	2.7228330	0.8443880	-0.3/60850	
Energy:	-438.41573763	57		
B3LYP/6-	311++G** geome	etry and energy	of conformer:	Thr-XLVI
N	-0.0508300	-1.1284500	1.3522490	
Н	-0.6861400	-1.9103200	1,4493350	
C	0.0711170	-0 6923310	-0.0389100	
с ц	0.00/111/0	_1 5706100	-0 6729010	
· · · · · · · · · · · · · · · · · · ·	1 0600000	-1.J/9010U	-U.U/20UIU	
	-1.0662360	0.2298520	-0.5392520	
C	1.4626880	-0.0503900	-0.2307850	
Н	-0.7933010	0.6024960	-1.5352830	
0	-1.0968310	1.3452070	0.3845800	
0	2.3657060	-0.6138380	-0.7865340	
Н	-1.7358810	2.0007760	0.0876010	
0	1.6209510	1.1885430	0.2828700	
Н	0.7556060	1.5358060	0 5672710	
u II	-0.3629500	_0 3778700	1 9583500	
П	-0.3029300	-0.3778700	1.9303300	
C	-2.4219130	-0.4597790	-0.6051170	
Н	-3.1953000	0.2378440	-0.9401650	
H	-2.3951920	-1.2888550	-1.3176150	
Н	-2.7136560	-0.8445110	0.3746140	
Energy:	-438.41535560	0		
B3LYP/6-	311++G** geome	try and energy	of conformer:	Thr-XLVII
NT	0 1202770	1 2202060	1 1070000	
T1 T1	-U.IJJJ//U	-I.ZJJZJOU	1 0C00010	
п	-0.3/59920	-0.5238630	1.009Z91U	
C	0.06/3120	-0.6225140	-0.1232850	
Н	0.1245600	-1.4196460	-0.8763400	
С	-1.1396880	0.2800330	-0.4790320	
С	1.3687840	0.1981300	-0.1669470	
Н	-0.9078410	0.7730600	-1.4337810	
0	-1.3412220	1.2622190	0.5326770	
0	1.4511120	1,3587170	0.1476190	
с ц	_0 5372540	1 0011000	0 5600000	
п	-0.00/2040	I.OUIIZOU	0.0000900	
U	2.4918700	-0.4/44940	-0.5292080	
Н	2.2734510	-1.3720590	-0.8091390	
Н	0.6729020	-1.7485960	1.5174310	
С	-2.4327160	-0.5075230	-0.6253210	
Н	-3.2466560	0.1773170	-0.8700350	
Н	-2.3487600	-1.2473270	-1.4261320	
Н	-2.6749960	-1.0252380	0.3033930	
Energy:	-438.41463071	.1		

-0.3093120 1.8173620 -0.7919380 -0.2057330 2.2298510 0.1281830 -0.2361820 -0.0073860 -1.7828960 1.3125220 -0.918840 -0.3201590 -1.2294770 -0.2713500 0.0324150 2.0031750 0.3357620 -1.0639610 1.3047620 -1.5160080 -0.4408370 -1.9866440 -1.1099910 -0.3741840 2.1526800 -1.8621870 -0.1453820 -1.3149460 0.2418950 1.2901770 -2.0754660 -0.16103350 1.7176260 0.3338500 2.2725790 -1.4301000 1.7646010 0.3529890 1.0682660 1.1241500 -0.0610000 1.8476480 2.7923170 0.0187060 1.2443580 1.7646980 1.4425990 1.1567000 nergy: -438.414283769 3LYP/6-311++G** geometry and energy of conformer: Thr-X 0.0188040 1.8879400 -0.6539310 -0.0264390 0.4795030 -0.3705270 0.1084390 0.4689370 -1.4534090 1.736440 -0.2618220 0.2594430 -1.3957570 -0.1640140 -0.1133930 1.0365350 -0.2901230 1.3597310 2.3587350 0.4569650 -0.0276790 -2.2322540 -0.306710 -0.9614520 2.1259980 1.3965790 0.0348010 -1.6689800 -0.453280 1.7293170 0.3321940 2.0166600 1.0051110 1.3369480 -1.6842380 -0.2537480 1.4735680 -0.4457880 1.7293170 0.3321940 2.016600 1.0051110 1.3369480 -1.6842380 -0.2537480 1.4735680 -2.3019710 -0.9614520 2.1259860 -2.3019720 -0.0115240 nergy: -438.413726133 3LYP/6-311++G** geometry and energy of conformer: Thr-I -0.0193390 1.9348650 -0.3129230 0.4680530 -2.3019720 -0.0115240 nergy: -438.413726133	B3LYP/	6-311++G** geome	try and energy	of conformer:	Thr-XLVI
-0.2057330 2.2298510 0.1281830 -0.0999250 0.3707870 -0.7688310 -0.2361820 -0.0079360 -1.7282860 1.3125220 -0.918840 -0.3201590 -1.2294770 -0.2713500 0.0324150 2.0031750 0.3357620 -1.0639610 -1.3866440 -1.1099910 -0.3741840 2.1526800 -1.8621870 -0.1453820 -1.3149460 0.2418950 1.2901770 -2.0754660 -0.1803350 1.7176260 0.3338500 2.2725790 -1.4301000 1.7646010 0.3529890 1.0682660 1.1241500 -0.0610000 1.8476480 2.7923170 0.0187060 1.2443580 1.7646980 1.4425990 1.1567000 nergy: -438.414283769 3LYP/6-311++G** geometry and energy of conformer: Thr-X 0.0188040 1.8879400 -0.5539310 -0.0264390 0.4795030 -0.3705270 0.1084390 0.468370 -1.4534090 1.736440 -0.2618220 0.2594430 -1.3357570 -0.1640140 -0.1133890 1.0365350 -0.2901230 1.3597310 2.3587350 0.4569650 -0.0276790 -2.3222540 -0.3006710 -0.9614520 2.1259980 1.3965790 0.0348010 -1.6698960 -0.5232730 1.1736700 -0.8831860 -0.4457880 1.7293170 0.3381960 -0.5232730 1.1736700 -0.3831960 -0.452780 1.293170 0.336940 -1.6642380 -0.257480 1.4735680 -0.4457880 1.7293170 0.3321940 2.0166600 1.0051110 1.3369480 -1.6642380 -0.257480 1.4735680 -2.3019720 -0.0115240 nergy: -438.413726133 3LYP/6-311++G** geometry and energy of conformer: Thr-I -0.0193390 1.9348650 -0.3129230 0.480530 -2.3019720 -0.0115240 nergy: -438.413726133	N	-0.3093120	1.8173620	-0.7919380	
-0.0999250 0.3707870 -0.7688310 -0.2361820 -0.0079360 -1.7828960 1.3125220 -0.918840 -0.3201590 -1.2294770 0.2713500 0.324150 2.0031750 0.3357620 -1.0639610 1.3047620 -1.5160080 -0.4408370 -1.9866440 -1.1099910 -0.3741840 2.1526800 -1.8621870 -0.1453820 -1.3149460 0.2418950 1.2901770 -2.0754660 -0.1803350 1.7176260 0.3338500 2.2725790 -1.4301000 1.7646910 0.3529890 1.0682660 1.1241500 -0.0610000 1.8476480 2.7923170 0.0187060 1.2443580 1.7646980 1.4425990 1.1567000 nergy: -438.414283769 3LYP/6-311++G** geometry and energy of conformer: Thr-X 0.0188040 1.8879400 -0.5539310 -0.0264390 0.4795030 -0.3705270 0.1084390 0.4689370 -1.4534090 1.1736440 -0.2618220 0.2594430 -1.3957570 -0.1640140 -0.1133930 1.365350 -0.2901230 1.3597310 2.3587350 0.4569550 -0.0276790 -2.2322540 -0.3006710 -0.614520 2.1259980 1.3965790 0.0348010 -1.6698960 -0.5232730 1.1736700 -0.881860 -0.4457880 1.7293170 0.3321940 2.0166600 1.0051110 1.3369480 -1.6842380 -0.2537480 1.4735680 -0.4457880 1.7293170 -0.3821940 2.0166600 1.0051110 1.3369480 -1.6842380 -0.2537480 1.4735680 -2.3019720 -0.0115240 nergy: -438.413726133 3LYP/6-311++G** geometry and energy of conformer: Thr-I -0.0193390 1.9348650 -0.3129230 0.4680530 -2.3019720 -0.0115240 nergy: -438.413726133	Н	-0.2057330	2.2298510	0.1281830	
-0.2361820 -0.007360 -1.7828960 1.312522 -0.0918840 -0.3201590 -1.2294770 -0.2713500 0.0324150 2.0031750 0.3357620 -1.0639610 1.3047620 -1.5160080 -0.4408370 -1.9866440 -1.1099910 -0.3741840 2.1526800 -1.8621870 -0.1453820 -1.3149460 0.2418950 1.2901770 -2.0754660 -0.1803350 1.7176260 0.3338500 2.2725790 -1.4301000 1.7646010 0.3529890 1.0682660 1.1241500 -0.0610000 1.8476480 2.7923170 0.0187060 1.2443580 1.7646980 1.4425990 1.1567000 nergy: -438.414283769 3LYP/6-311++6** geometry and energy of conformer: Thr-> 0.0188040 1.8879400 -0.5539310 -0.0264390 0.4795030 -0.3705270 0.1084390 0.4689370 -1.4534090 1.1736440 -0.2618220 0.2594430 1.3957570 -0.1640140 -0.1133930 1.0365350 -0.2901230 1.3597310 2.3587350 0.4569650 -0.0276790 -2.322540 -0.3006710 -0.9614520 2.1259980 1.3965790 0.0348010 -1.6698960 -0.523730 1.1736700 -0.8831860 -0.4457880 1.7293170 -0.3321940 2.0166600 1.0051110 1.3369480 -1.6842380 -0.2537480 1.4735680 -1.6795700 -1.3377740 2.2195680 -2.1392410 0.1990630 0.4680530 -2.3019720 -0.0115240 nergy: -438.413726133 3LYP/6-311++G** geometry and energy of conformer: Thr-I -0.0193390 1.9348650 -0.3129230 0.4680530 -2.3019720 -0.0115240	С	-0.0999250	0.3707870	-0.7688310	
<pre>1.3125220 -0.0918840 -0.3201590 -1.2294770 -0.2713500 0.0324150 2.0031750 0.3357620 -1.0639610 1.3047620 -1.5160080 -0.4408370 -1.9866440 -1.1099910 -0.3741840 2.1526800 -1.6621870 -0.1453820 -1.3149460 0.2418950 1.2901770 -2.0754660 -0.1803350 1.7176260 0.3338500 2.2725790 -1.4301000 1.7646010 0.3529890 1.0682660 1.1241500 -0.0610000 1.8476480 2.7923170 0.0187060 1.2443580 1.7646980 1.4425990 1.1567000 nergy: -438.414283769</pre>	Н	-0.2361820	-0.0079360	-1.7828960	
-1.2294770 -0.2713500 0.0324150 2.0031750 0.3357620 -1.0639610 1.3047620 -1.5160080 -0.4408370 -1.9866440 -1.1099910 -0.3741840 2.1526800 -1.8621870 -0.1453820 -1.3149460 0.2418950 1.2901770 -2.0754660 -0.1803350 1.7176260 0.3338500 2.2725790 -1.4301000 1.7646010 0.3529890 1.0682660 1.1241500 -0.0610000 1.8476480 2.7923170 0.0187060 1.2443580 1.7646980 1.4425990 1.1567000 nergy: -438.414283769 3LYP/6-311++G** geometry and energy of conformer: Thr-X 0.0188040 1.8879400 0.0602360 -0.5314530 2.4781900 -0.5539310 -0.0264390 0.4795030 -0.3705270 0.1084390 0.4689370 -1.4534090 1.1736440 -0.2618220 0.2594430 -1.3957570 -0.1640140 -0.1133930 1.0365350 -0.2901230 1.3597310 2.3587350 0.4569650 -0.0276790 -2.2322540 -0.3006710 -0.9614520 2.1259980 1.3965790 0.0348010 -1.6698960 -0.5232730 1.1736700 -0.8831860 -0.4457880 1.7293170 -0.3321940 2.0166600 1.0051110 1.3369480 -1.6842380 -0.2537480 1.4735680 -1.6795700 -1.3377740 2.2195680 -2.1392410 0.1990630 0.4680530 -2.3019720 -0.0115240 nergy: -438.413726133 3LYP/6-311++G** geometry and energy of conformer: Thr-I -0.0193390 1.9348650 -0.3129230 -0.3476760 2.2004530 0.6114240 -0.090690 0.4826610 -0.4131910 0.1272900 0.2295700 -1.4911420 1.1328590 -0.2189000 0.3460590	С	1.3125220	-0.0918840	-0.3201590	
<pre>2.0031750 0.3357620 -1.0639610 1.3047620 -1.5160080 -0.4408370 -1.9866440 -1.1099910 -0.3741840 2.1526800 -1.8621870 -0.1453820 -1.3149460 0.2418950 1.2901770 -2.0754660 -0.1803350 1.7176260 0.3338500 2.2725790 -1.4301000 1.7646010 0.3529890 1.0682660 1.1241500 -0.0610000 1.8476480 2.7923170 0.0187060 1.2443580 1.7646980 1.4425990 1.1567000 nergy: -438.414283769 3LYP/6-311++G** geometry and energy of conformer: Thr-X 0.0188040 1.8879400 0.0602360 -0.5539310 -0.5539310 -0.0264390 0.4795030 -0.5539310 -0.0264390 0.4689370 -1.4534090 1.1736440 -0.2618220 0.2594430 -1.3957570 -0.1640140 -0.1133930 1.0365350 -0.2901230 1.3597310 2.3587350 0.4569650 -0.0276790 -2.2322540 -0.3006710 -0.9614520 2.1259980 1.3965790 0.0348010 -1.66698960 -0.4557880 1.7293170 -0.3321940 2.0166600 1.0051110 1.3369480 -1.6795700 -1.3377740 2.2195680 -2.1392410 0.1990630 0.4680530 -2.3019720 -0.0115240 nergy: -438.413726133 3LYP/6-311++G** geometry and energy of conformer: Thr-I -0.0193390 1.9348650 -0.3129230 0.4680530 -2.3019720 -0.0115240</pre>	С	-1.2294770	-0.2713500	0.0324150	
 1.3047620 -1.5160080 -0.4408370 -1.9866440 -1.1099910 -0.3741840 2.1526800 -1.8621870 -0.1453820 -1.3149460 0.2418950 1.2901770 -2.0754660 -0.1803350 1.7176260 0.3338500 2.2725790 -1.4301000 1.7646010 0.3529890 1.0682660 1.1241500 -0.0610000 1.8476480 2.7923170 0.0187060 1.2443580 1.7646980 1.4425990 1.1567000 nergy: -438.414283769 3LYP/6-311++G** geometry and energy of conformer: Thr-X 0.0188040 1.8879400 -0.5539310 -0.0264390 0.4795030 -0.3705270 0.1084390 0.4689370 -1.45340900 1.1736440 -0.2618220 0.2594430 -1.3957570 -0.1640140 -0.1133930 1.0365350 -0.2901230 1.3597310 2.3587350 0.4569650 -0.0276790 -2.2322540 -0.3006710 -0.9614520 2.1259980 1.3965790 0.0348010 -1.669960 -0.523730 1.7736700 -0.8831860 -0.4457880 1.7293170 -0.8831860 -0.4457880 1.7293170 -0.3321940 2.016600 1.0051110 1.3369480 -1.6842380 -0.2537480 1.4735680 -1.6795700 -1.3377740 2.2195680 -2.1392410 0.1990630 0.4680530 -2.3019720 -0.0115240 nergy: -438.413726133 3LYP/6-311++G** geometry and energy of conformer: Thr-I -0.0193390 1.9348650 -0.3129230 -0.3476760 2.2004530 0.6114240 -0.0193390 1.9348650 -0.4315110 0.1272900 0.2295700 -1.4911420 1.1328590 -0.2189090 0.3460590 	Н	2.0031750	0.3357620	-1.0639610	
-1.9866440 -1.1099910 -0.3741840 2.1526800 -1.8621870 -0.1453820 -1.3149460 0.2418950 1.2901770 -2.0754660 -0.1803350 1.7176260 0.3338500 2.2725790 -1.4301000 1.7646010 0.3529890 1.0682660 1.1241500 -0.0610000 1.8476480 2.7923170 0.0187060 1.2443580 1.7646980 1.4425990 1.1567000 nergy: -438.414283769 3LYP/6-311++G** geometry and energy of conformer: Thr-X 0.0188040 1.8879400 -0.5539310 -0.0264390 0.4689370 -1.4534090 1.1736440 -0.2618220 0.2594430 -1.3957570 -0.1640140 -0.1133930 1.0365350 -0.2901230 1.3597310 2.3587350 0.4569650 -0.0276790 -2.2322540 -0.3006710 -0.9614520 2.1259980 1.3965790 0.0348010 -1.6698960 -0.5232730 1.1736700 -0.8831860 -0.4457880 1.7293170 -0.3321940 2.0166600 1.0051110 1.3369480 -1.6842380 -0.2537480 1.4735680 -1.6795700 -1.3377740 2.2195680 -2.1392410 0.1990630 0.4680530 -2.3019720 -0.0115240 nergy: -438.413726133 3LYP/6-311++G** geometry and energy of conformer: Thr-I -0.0193390 1.9348650 -0.3129230 -0.3476760 2.2004530 0.6114240 -0.3470760 -0.282610 -0.415110 0.1272900 0.2295700 -1.4911420 1.1328590 -0.218900 0.3480610 -0.415110 0.1272900 0.2295700 -1.4911420 1.1328590 -0.2189000 0.3460590	0	1.3047620	-1.5160080	-0.4408370	
<pre>2.1526800 -1.8621870 -0.1433820 -1.3149460 0.2418950 1.2901770 -2.0754660 -0.1803350 1.7176260 0.3338500 2.2725790 -1.4301000 1.7646010 0.3529890 1.0682660 1.1241500 -0.0610000 1.8476480 2.7923170 0.0187060 1.2443580 1.7646980 1.4425990 1.1567000 nergy: -438.414283769 3LYP/6-311++G** geometry and energy of conformer: Thr-X 0.0188040 1.8879400 0.0602360 -0.5314530 2.4781900 -0.5533910 -0.0264390 0.4795030 -0.3705270 0.1084390 0.4689370 -1.4534090 1.1736440 -0.2618220 0.2594430 -1.3957570 -0.1640140 -0.1133930 1.0365350 -0.2901230 1.3597310 2.3587350 0.4569650 -0.0276790 -2.2322540 -0.3006710 -0.9614520 2.1259980 1.3965790 0.0348010 -1.6698960 -0.5232730 1.1736700 -0.8831860 -0.4457880 1.7293170 -0.3321940 2.0166600 1.0051110 1.3369480 -1.6842380 -0.2537480 1.4735680 -1.6795700 -1.3377740 2.2195680 -2.1392410 0.1990630 0.4680530 -2.3019720 -0.0115240 nergy: -438.413726133 3LYP/6-311++G** geometry and energy of conformer: Thr-I -0.0193390 1.9348650 -0.3129230 -0.3476760 2.2004530 0.6114240 -0.090690 0.4826610 -0.4315110 0.1272900 0.2295700 -1.4311420 1.1328590 -0.2189090 0.3460590</pre>	0	-1.9866440	-1.1099910	-0.3741840	
-1.3149460 0.2418950 1.2901770 -2.0754660 -0.1803350 1.7176260 0.3338500 2.2725790 -1.4301000 1.7646010 0.3529890 1.0682660 1.1241500 -0.0610000 1.8476480 2.7923170 0.0187060 1.2443580 1.7646980 1.4425990 1.1567000 nergy: -438.414283769 3LYP/6-311++G** geometry and energy of conformer: Thr-X 0.0188040 1.8879400 0.0602360 -0.5314530 2.4781900 -0.5539310 -0.0264390 0.4795030 -0.3705270 0.1084390 0.4689370 -1.4534090 1.1736440 -0.2618220 0.2594430 -1.3957570 -0.1640140 -0.1133930 1.0365350 -0.2901230 1.3597310 2.3587350 0.4569650 -0.0276790 -2.2322540 -0.3006710 -0.9614520 2.1259980 1.3965790 0.0348010 -1.6698960 -0.5232730 1.1736700 -0.8321940 2.0166600 1.0051110 1.3369480 -1.6842380 -0.2537480 1.4735680 -2.1392410 0.1990630 0.4680530 -2.3019720 -0.0115240 nergy: -438.413726133 3LYP/6-311++G** geometry and energy of conformer: Thr-I -0.0193390 1.9348650 -0.3129230 -0.3476760 2.2004530 0.6114240 -0.3476760 2.2004530 0.6114240 -0.3476760 0.2295700 -1.4351110 0.1272900 0.2295700 -1.4911420 1.1326590 -0.2189090 0.3460590	H	2.1526800	-1.8621870	-0.1453820	
 1.1.176280 0.3338500 2.2725790 1.4301000 1.7646010 0.3529890 1.0682660 1.1241500 0.0187060 1.2443580 1.7646980 1.4425990 1.1567000 nergy: -438.414283769 3LYP/6-311++G** geometry and energy of conformer: Thr-X 0.0188040 1.8879400 0.0602360 -0.5314530 2.4781900 -0.5539310 -0.0264390 0.4795030 -0.3705270 0.1084390 0.4689370 -1.4534090 1.1736440 -0.2618220 0.2594430 -1.3957570 -0.1640140 -0.1133930 1.0365350 -0.2901230 1.3597310 2.3587350 0.4569650 -0.0276790 -2.2322540 -0.3006710 -0.9614520 2.1259980 1.3965790 0.0348010 -1.6698960 -0.523730 1.776700 -0.3321940 2.0166600 1.0051110 1.3369480 -1.6795700 -1.3377740 2.2195680 -2.3019720 -0.0115240 nergy: -438.413726133 3LYP/6-311++G** geometry and energy of conformer: Thr-I -0.0193390 1.9348650 -0.3129230 -0.3476760 2.2004530 0.6114240 -0.0909690 4826610 -0.3129230 -0.3476760 2.204530 0.6114240 -0.0909690 4826610 -0.4315110 0.1272900 0.2295700 -1.4911420 1.328590 -0.2189090 0.3460590 	0	-1.3149460	0.2418950	1.2901770	
<pre>0.333500 2.2723790 -1.331000 1.7646010 0.3529890 1.0682660 1.1241500 -0.0610000 1.8476480 2.7923170 0.0187060 1.2443580 1.7646980 1.4425990 1.1567000 nergy: -438.414283769 3LYP/6-311++G** geometry and energy of conformer: Thr-X 0.0188040 1.8879400 0.0602360 -0.5314530 2.4781900 -0.5539310 -0.0264390 0.4795030 -0.3705270 0.1084390 0.4689370 -1.4534090 1.1736440 -0.2618220 0.2594430 -1.3957570 -0.1640140 -0.1133930 1.0365350 -0.2901230 1.3597310 2.3587350 0.4569650 -0.0276790 -2.2322540 -0.3006710 -0.9614520 2.1259980 1.3965790 0.0348010 -1.6698960 -0.5232730 1.7706700 -0.8831860 -0.4457880 1.7293170 -0.3321940 2.0166600 1.0051110 1.3369480 -1.6842380 -0.2537480 1.4735680 -1.6795700 -1.3377740 2.2195680 -2.3392410 0.1990630 0.4680530 -2.3019720 -0.0115240 nergy: -438.413726133 3LYP/6-311++G** geometry and energy of conformer: Thr-I -0.0193390 1.9348650 -0.3129230 -0.3476760 2.2004530 0.6114240 -0.090909 0.4826610 -0.4315110 0.1272900 0.2295700 -1.4911420 1.1328590 -0.2189090 0.3460590</pre>	H U	-2.0754660	-0.1803350	1,7176260	
<pre>1.104001 0.0325050 1.002000 1.1241500 0.0610000 1.2443580 1.7646980 1.4425990 1.1567000 nergy: -438.414283769 3LYP/6-311++G** geometry and energy of conformer: Thr-> 0.0188040 1.8879400 0.0602360 -0.5314530 2.4781900 -0.5539310 -0.0264390 0.4795030 -0.3705270 0.1084390 0.4689370 -1.4534090 1.1736440 -0.2618220 0.2594430 -1.3957570 -0.1640140 -0.1133930 1.0365350 -0.2901230 1.3597310 2.3587350 0.4569650 -0.0276790 -2.2322540 -0.3006710 -0.9614520 2.1259980 1.3965790 0.0348010 -1.6698960 -0.5232730 1.1736700 -0.8831860 -0.4457880 1.7293170 -0.3321940 2.0166600 1.0051110 1.3369480 -1.6842380 -0.2537480 1.4735680 -1.6795700 -1.3377740 2.2195680 -2.1392410 0.1990630 0.4680530 -2.3019720 -0.0115240 nergy: -438.413726133 3LYP/6-311++G** geometry and energy of conformer: Thr-I -0.0193390 1.9348650 -0.3129230 -0.3476760 2.2004530 0.6114240 -0.0090690 0.4826610 -0.4315110 0.1272900 0.2295700 -1.4911420 1.1328590 -0.2189090 0.3460590</pre>	п С	1 7646010	0 3529890	-1.4301000	
2.7923170 0.0187060 1.2443580 1.7646980 1.4425990 1.1567000 nergy: -438.414283769 3LYP/6-311++G** geometry and energy of conformer: Thr-> 0.0188040 1.8879400 0.0602360 -0.5314530 2.4781900 -0.5539310 -0.0264390 0.4795030 -0.3705270 0.1084390 0.4689370 -1.4534090 1.1736440 -0.2618220 0.2594430 -1.3957570 -0.1640140 -0.1133930 1.0365350 -0.2901230 1.3597310 2.3587350 0.4569650 -0.0276790 -2.2322540 -0.3006710 -0.9614520 2.1259980 1.3965790 0.0348010 -1.6698960 -0.5232730 1.1736700 -0.8831860 -0.4457880 1.7293170 -0.3321940 2.0166600 1.0051110 1.3369480 -1.6842380 -0.2537480 1.4735680 -1.6795700 -1.3377740 2.2195680 -2.3019720 -0.0115240 nergy: -438.413726133 3LYP/6-311++G** geometry and energy of conformer: Thr-I -0.0193390 1.9348650 -0.3129230 -0.3476760 2.2004530 0.6114240 -0.0090690 0.4826610 -0.4315110 0.1272900 0.2295700 -1.4911420 1.1328590 -0.2189090 0.3460590	ч	1 12/1500	-0.0610000	1 8476780	
<pre>1.7646980 1.4425990 1.1567000 nergy: -438.414283769 3LYP/6-311++G** geometry and energy of conformer: Thr-> 0.0188040 1.8879400 0.0602360 -0.5314530 2.4781900 -0.5539310 -0.0264390 0.4795030 -0.3705270 0.1084390 0.4689370 -1.4534090 1.1736440 -0.2618220 0.2594430 -1.3957570 -0.1640140 -0.1133930 1.0365350 -0.2901230 1.3597310 2.3587350 0.4569650 -0.0276790 -2.2322540 -0.3006710 -0.9614520 2.1259980 1.3965790 0.0348010 -1.6698960 -0.5232730 1.1736700 -0.8831860 -0.4457880 1.7293170 -0.3321940 2.0166600 1.0051110 1.3369480 -1.6842380 -0.2537480 1.4735680 -1.6795700 -1.3377740 2.2195680 -2.1392410 0.1990630 0.4680530 -2.3019720 -0.0115240 nergy: -438.413726133 3LYP/6-311++G** geometry and energy of conformer: Thr-I -0.0193390 1.9348650 -0.3129230 -0.3476760 2.2004530 0.6114240 -0.0090690 0.4826610 -0.4315110 0.1272900 0.2295700 -1.4911420 1.1328590 -0.2189090 0.3460590</pre>	H	2 7923170	0 0187060	1 2443580	
<pre>nergy: -438.414283769 3LYP/6-311++G** geometry and energy of conformer: Thr-></pre>	H	1.7646980	1.4425990	1.1567000	
<pre>nergy: -438.414283769 3LYP/6-311++G** geometry and energy of conformer: Thr-></pre>	_				
<pre>3LYP/6-311++G** geometry and energy of conformer: Thr-X 0.0188040 1.8879400 0.0602360 -0.5314530 2.4781900 -0.5539310 -0.0264390 0.4795030 -0.3705270 0.1084390 0.4689370 -1.4534090 1.1736440 -0.2618220 0.2594430 -1.3957570 -0.1640140 -0.1133930 1.0365350 -0.2901230 1.3597310 2.3587350 0.4569650 -0.0276790 -2.2322540 -0.3006710 -0.9614520 2.1259980 1.3965790 0.0348010 -1.6698960 -0.5232730 1.1736700 -0.8831860 -0.4457880 1.7293170 -0.3321940 2.0166600 1.0051110 1.3369480 -1.6842380 -0.2537480 1.4735680 -1.6795700 -1.3377740 2.2195680 -2.1392410 0.1990630 0.4680530 -2.3019720 -0.0115240</pre> nergy: -438.413726133 <pre> 3LYP/6-311++G** geometry and energy of conformer: Thr-I -0.0193390 1.9348650 -0.3129230 -0.3476760 2.2004530 0.6114240 -0.0090690 0.4826610 -0.4315110 0.1272900 0.2295700 -1.4911420 1.1328590 -0.2189090 0.3460590</pre>	Energy	-438.41428376	9		
<pre>3LYP/6-311++G** geometry and energy of conformer: Thr-X 0.0188040 1.8879400 0.0602360 -0.5314530 2.4781900 -0.5539310 -0.0264390 0.4795030 -0.3705270 0.1084390 0.4689370 -1.4534090 1.1736440 -0.2618220 0.2594430 -1.3957570 -0.1640140 -0.1133930 1.0365350 -0.2901230 1.3597310 2.3587350 0.4569650 -0.0276790 -2.2322540 -0.3006710 -0.9614520 2.1259980 1.3965790 0.0348010 -1.6698960 -0.5232730 1.1736700 -0.8831860 -0.4457880 1.7293170 -0.3321940 2.0166600 1.0051110 1.3369480 -1.6842380 -0.2537480 1.4735680 -1.6795700 -1.3377740 2.2195680 -2.1392410 0.1990630 0.4680530 -2.3019720 -0.0115240 nergy: -438.413726133</pre>					
<pre>3LYP/6-311++G** geometry and energy of conformer: Thr-> 0.0188040 1.8879400 0.0602360 -0.5314530 2.4781900 -0.5539310 -0.02643990 0.4795030 -0.3705270 0.1084390 0.4689370 -1.4534090 1.1736440 -0.2618220 0.2594430 -1.3957570 -0.1640140 -0.1133930 1.0365350 -0.2901230 1.3597310 2.3587350 0.4569650 -0.0276790 -2.2322540 -0.3006710 -0.9614520 2.1259980 1.3965790 0.0348010 -1.6698960 -0.5232730 1.1736700 -0.8831860 -0.4457880 1.7293170 -0.3321940 2.0166600 1.0051110 1.3369480 -1.6842380 -0.2537480 1.4735680 -1.6795700 -1.3377740 2.2195680 -2.1392410 0.1990630 0.4680530 -2.3019720 -0.0115240 nergy: -438.413726133</pre>					
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-0.5314530 2.4781900 -0.5539310 -0.0264390 0.4795030 -0.3705270 0.1084390 0.4689370 -1.4534090 1.1736440 -0.2618220 0.2594430 -1.3957570 -0.1640140 -0.1133930 1.0365350 -0.2901230 1.3597310 2.3587350 0.4569650 -0.0276790 -2.2322540 -0.3006710 -0.9614520 2.1259980 1.3965790 0.0348010 -1.6698960 -0.5232730 1.1736700 -0.8831860 -0.4457880 1.7293170 -0.3321940 2.0166600 1.0051110 1.3369480 -1.6842380 -0.2537480 1.4735680 -1.6795700 -1.3377740 2.2195680 -2.1392410 0.1990630 0.4680530 -2.3019720 -0.0115240 nergy: -438.413726133 3LYP/6-311++G** geometry and energy of conformer: Thr-I -0.0193390 1.9348650 -0.3129230 -0.3476760 2.2004530 0.6114240 -0.0090690 0.4826610 -0.4315110 0.1272900 0.2295700 -1.4911420 1.1328590 -0.2189090 0.3460590	N	0.0188040	1.8879400	0.0602360	
-0.0264390 0.4795030 -0.3705270 0.1084390 0.4689370 -1.4534090 1.1736440 -0.2618220 0.2594430 -1.3957570 -0.1640140 -0.1133930 1.0365350 -0.2901230 1.3597310 2.3587350 0.4569650 -0.0276790 -2.2322540 -0.3006710 -0.9614520 2.1259980 1.3965790 0.0348010 -1.6698960 -0.5232730 1.1736700 -0.8831860 -0.4457880 1.7293170 -0.3321940 2.0166600 1.0051110 1.3369480 -1.6842380 -0.2537480 1.4735680 -1.6795700 -1.3377740 2.2195680 -2.1392410 0.1990630 0.4680530 -2.3019720 -0.0115240 nergy: -438.413726133 3LYP/6-311++G** geometry and energy of conformer: Thr-I -0.0193390 1.9348650 -0.3129230 -0.3476760 2.2004530 0.6114240 -0.0090690 0.4826610 -0.4315110 0.1272900 0.2295700 -1.4911420 1.1328590 -0.2189090 0.3460590	Н	-0.5314530	2.4781900	-0.5539310	
0.1084390 0.4689370 -1.4534090 1.1736440 -0.2618220 0.2594430 -1.3957570 -0.1640140 -0.1133930 1.0365350 -0.2901230 1.3597310 2.3587350 0.4569650 -0.0276790 -2.2322540 -0.3006710 -0.9614520 2.1259980 1.3965790 0.0348010 -1.6698960 -0.5232730 1.1736700 -0.8831860 -0.4457880 1.7293170 -0.3321940 2.0166600 1.0051110 1.3369480 -1.6842380 -0.2537480 1.4735680 -1.6795700 -1.3377740 2.2195680 -2.1392410 0.1990630 0.4680530 -2.3019720 -0.0115240 nergy: -438.413726133 3LYP/6-311++G** geometry and energy of conformer: Thr-I -0.0193390 1.9348650 -0.3129230 -0.3476760 2.2004530 0.6114240 -0.0090690 0.4826610 -0.4315110 0.1272900 0.2295700 -1.4911420 1.1328590 -0.2189090 0.3460590	С	-0.0264390	0.4795030	-0.3705270	
<pre>1.1736440 -0.2618220 0.2594430 -1.3957570 -0.1640140 -0.1133930 1.0365350 -0.2901230 1.3597310 2.3587350 0.4569650 -0.0276790 -2.2322540 -0.3006710 -0.9614520 2.1259980 1.3965790 0.0348010 -1.6698960 -0.5232730 1.1736700 -0.8831860 -0.4457880 1.7293170 -0.3321940 2.0166600 1.0051110 1.3369480 -1.6842380 -0.2537480 1.4735680 -1.6795700 -1.3377740 2.2195680 -2.1392410 0.1990630 0.4680530 -2.3019720 -0.0115240 nergy: -438.413726133 3LYP/6-311++G** geometry and energy of conformer: Thr-I -0.0193390 1.9348650 -0.3129230 -0.3476760 2.2004530 0.6114240 -0.0090690 0.4826610 -0.4315110 0.1272900 0.2295700 -1.4911420 1.1328590 -0.2189090 0.3460590</pre>	Н	0.1084390	0.4689370	-1.4534090	
-1.3957570 -0.1640140 -0.1133930 1.0365350 -0.2901230 1.3597310 2.3587350 0.4569650 -0.0276790 -2.2322540 -0.3006710 -0.9614520 2.1259980 1.3965790 0.0348010 -1.6698960 -0.5232730 1.1736700 -0.8831860 -0.4457880 1.7293170 -0.3321940 2.0166600 1.0051110 1.3369480 -1.6842380 -0.2537480 1.4735680 -1.6795700 -1.3377740 2.2195680 -2.1392410 0.1990630 0.4680530 -2.3019720 -0.0115240 nergy: -438.413726133 3LYP/6-311++G** geometry and energy of conformer: Thr-I -0.0193390 1.9348650 -0.3129230 -0.3476760 2.2004530 0.6114240 -0.0090690 0.4826610 -0.4315110 0.1272900 0.2295700 -1.4911420 1.1328590 -0.2189090 0.3460590	С	1.1736440	-0.2618220	0.2594430	
1.0365350 -0.2901230 1.3597310 2.3587350 0.4569650 -0.0276790 -2.2322540 -0.3006710 -0.9614520 2.1259980 1.3965790 0.0348010 -1.6698960 -0.5232730 1.1736700 -0.8831860 -0.4457880 1.7293170 -0.3321940 2.0166600 1.0051110 1.3369480 -1.6842380 -0.2537480 1.4735680 -1.6795700 -1.3377740 2.2195680 -2.1392410 0.1990630 0.4680530 -2.3019720 -0.0115240 nergy: -438.413726133 3LYP/6-311++G** geometry and energy of conformer: Thr-I -0.0193390 1.9348650 -0.3129230 -0.3476760 2.2004530 0.6114240 -0.0090690 0.4826610 -0.4315110 0.1272900 0.2295700 -1.4911420 1.1328590 -0.2189090 0.3460590	С	-1.3957570	-0.1640140	-0.1133930	
2.3587350 0.4569650 -0.0276790 -2.2322540 -0.3006710 -0.9614520 2.1259980 1.3965790 0.0348010 -1.6698960 -0.5232730 1.1736700 -0.8831860 -0.4457880 1.7293170 -0.3321940 2.0166600 1.0051110 1.3369480 -1.6842380 -0.2537480 1.4735680 -1.6795700 -1.3377740 2.2195680 -2.1392410 0.1990630 0.4680530 -2.3019720 -0.0115240 nergy: -438.413726133 3LYP/6-311++G** geometry and energy of conformer: Thr-I -0.0193390 1.9348650 -0.3129230 -0.3476760 2.2004530 0.6114240 -0.0090690 0.4826610 -0.4315110 0.1272900 0.2295700 -1.4911420 1.1328590 -0.2189090 0.3460590	H	1.0365350	-0.2901230	1.3597310	
-2.2322540 -0.3006710 -0.9614520 2.1259980 1.3965790 0.0348010 -1.6698960 -0.5232730 1.1736700 -0.8831860 -0.4457880 1.7293170 -0.3321940 2.0166600 1.0051110 1.3369480 -1.6842380 -0.2537480 1.4735680 -1.6795700 -1.3377740 2.2195680 -2.1392410 0.1990630 0.4680530 -2.3019720 -0.0115240 nergy: -438.413726133 3LYP/6-311++G** geometry and energy of conformer: Thr-I -0.0193390 1.9348650 -0.3129230 -0.3476760 2.2004530 0.6114240 -0.0090690 0.4826610 -0.4315110 0.1272900 0.2295700 -1.4911420 1.1328590 -0.2189090 0.3460590	0	2.3587350	0.4569650	-0.0276790	
2.1259980 1.3965790 0.0348010 -1.6698960 -0.5232730 1.1736700 -0.8831860 -0.4457880 1.7293170 -0.3321940 2.0166600 1.0051110 1.3369480 -1.6842380 -0.2537480 1.4735680 -2.1392410 0.1990630 0.4680530 -2.3019720 -0.0115240 nergy: -438.413726133 3LYP/6-311++G** geometry and energy of conformer: Thr-I -0.0193390 1.9348650 -0.3129230 -0.3476760 2.2004530 0.6114240 -0.0090690 0.4826610 -0.4315110 0.1272900 0.2295700 -1.4911420 1.1328590 -0.2189090 0.3460590	0	-2.2322540	-0.3006710	-0.9614520	
-1.6698960 -0.5232730 1.1736700 -0.8831860 -0.4457880 1.7293170 -0.3321940 2.0166600 1.0051110 1.3369480 -1.6842380 -0.2537480 1.4735680 -1.6795700 -1.3377740 2.2195680 -2.1392410 0.1990630 0.4680530 -2.3019720 -0.0115240 nergy: -438.413726133 3LYP/6-311++G** geometry and energy of conformer: Thr-I -0.0193390 1.9348650 -0.3129230 -0.3476760 2.2004530 0.6114240 -0.0090690 0.4826610 -0.4315110 0.1272900 0.2295700 -1.4911420 1.1328590 -0.2189090 0.3460590	H	2.1259980	1.3965790	0.0348010	
-0.8831860 -0.4457880 1.7293170 -0.3321940 2.0166600 1.0051110 1.3369480 -1.6842380 -0.2537480 1.4735680 -1.6795700 -1.3377740 2.2195680 -2.1392410 0.1990630 0.4680530 -2.3019720 -0.0115240 nergy: -438.413726133 3LYP/6-311++G** geometry and energy of conformer: Thr-I -0.0193390 1.9348650 -0.3129230 -0.3476760 2.2004530 0.6114240 -0.0090690 0.4826610 -0.4315110 0.1272900 0.2295700 -1.4911420 1.1328590 -0.2189090 0.3460590	0	-1.6698960	-0.5232730	1.1/36/00	
-0.3321940 2.01066000 1.0031110 1.3369480 -1.6842380 -0.2537480 1.4735680 -1.6795700 -1.3377740 2.2195680 -2.1392410 0.1990630 0.4680530 -2.3019720 -0.0115240 nergy: -438.413726133 3LYP/6-311++G** geometry and energy of conformer: Thr-I -0.0193390 1.9348650 -0.3129230 -0.3476760 2.2004530 0.6114240 -0.0090690 0.4826610 -0.4315110 0.1272900 0.2295700 -1.4911420 1.1328590 -0.2189090 0.3460590	H	-0.8831860	-0.445/880	1.7293170	
1.3309400 -1.0042380 -0.2337480 1.4735680 -1.6795700 -1.3377740 2.2195680 -2.1392410 0.1990630 0.4680530 -2.3019720 -0.0115240 nergy: -438.413726133 3LYP/6-311++G** geometry and energy of conformer: Thr-I -0.0193390 1.9348650 -0.3129230 -0.3476760 2.2004530 0.6114240 -0.0090690 0.4826610 -0.4315110 0.1272900 0.2295700 -1.4911420 1.1328590 -0.2189090 0.3460590	п	-U.JJZI94U	Z.UI666UU 1 6040000	1.UUJIIU 0.2527400	
1.4753660 -1.6753700 -1.3377740 2.2195680 -2.1392410 0.1990630 0.4680530 -2.3019720 -0.0115240 nergy: -438.413726133 3LYP/6-311++G** geometry and energy of conformer: Thr-I -0.0193390 1.9348650 -0.3129230 -0.3476760 2.2004530 0.6114240 -0.0090690 0.4826610 -0.4315110 0.1272900 0.2295700 -1.4911420 1.1328590 -0.2189090 0.3460590	с u	1 1735600	-1.004238U _1.6705700	-U.203/48U _1 3377740	
2.2133000 -2.332410 0.1330030 0.4680530 -2.3019720 -0.0115240 nergy: -438.413726133 3LYP/6-311++G** geometry and energy of conformer: Thr-I -0.0193390 1.9348650 -0.3129230 -0.3476760 2.2004530 0.6114240 -0.0090690 0.4826610 -0.4315110 0.1272900 0.2295700 -1.4911420 1.1328590 -0.2189090 0.3460590	11 Н	1.4/JJ00U 2 2105600	-1.0/90/00 -2 1302/10	-1.33///4U	
nergy: -438.413726133 3LYP/6-311++G** geometry and energy of conformer: Thr-I -0.0193390 1.9348650 -0.3129230 -0.3476760 2.2004530 0.6114240 -0.0090690 0.4826610 -0.4315110 0.1272900 0.2295700 -1.4911420 1.1328590 -0.2189090 0.3460590	H	0.4680530	-2.3019720	-0.0115240	
<pre>Mergy: -438.413720133 3LYP/6-311++G** geometry and energy of conformer: Thr-I</pre>	Enor	100 11000010	2		
3LYP/6-311++G** geometry and energy of conformer: Thr-L -0.0193390 1.9348650 -0.3129230 -0.3476760 2.2004530 0.6114240 -0.0090690 0.4826610 -0.4315110 0.1272900 0.2295700 -1.4911420 1.1328590 -0.2189090 0.3460590	Energy	-438.413/2613	3		
3LYP/6-311++G** geometry and energy of conformer: Thr-I -0.0193390 1.9348650 -0.3129230 -0.3476760 2.2004530 0.6114240 -0.0090690 0.4826610 -0.4315110 0.1272900 0.2295700 -1.4911420 1.1328590 -0.2189090 0.3460590					
-0.01933901.9348650-0.3129230-0.34767602.20045300.6114240-0.00906900.4826610-0.43151100.12729000.2295700-1.49114201.1328590-0.21890900.3460590	B3LYP/	6-311++G** geome	try and energy	of conformer:	Thr-L
-0.3476760 2.2004530 0.6114240 -0.0090690 0.4826610 -0.4315110 0.1272900 0.2295700 -1.4911420 1.1328590 -0.2189090 0.3460590	N	-0.0193390	1.9348650	-0.3129230	
-0.00906900.4826610-0.43151100.12729000.2295700-1.49114201.1328590-0.21890900.3460590	Н	-0.3476760	2.2004530	0.6114240	
0.1272900 0.2295700 -1.4911420 1.1328590 -0.2189090 0.3460590	С	-0.0090690	0.4826610	-0.4315110	
1.1328590 -0.2189090 0.3460590	Н	0.1272900	0.2295700	-1.4911420	
		1 1328590	-0.2189090	0.3460590	
-1.3600240 -0.0349790 0.0716030	С	1.1520550	0.2109090		
1.0153220 0.0412290 1.4059820	C C	-1.3600240	-0.0349790	0.0716030	

1					
2					
3 1	0	-1.8122780	0.2717380	1.1399960	
- 5	Н	3.0/80050	0.09/8320	0.3706940	
6	Ч	-2.0288380	-0.8933130	-0.7341780	
7	и И	0 9246910	2 2878880	_0 /322790	
8	C	1,1505470	-1,7360270	0.1795160	
9	н	0.2485640	-2.1954970	0.5927880	
10	Н	1.2375320	-2.0083120	-0.8766420	
11	Н	2.0063500	-2.1679780	0.7062730	
12					
13	Energy:	-438.412787935			
14					
15					
16					
17	B3LYP/6-	311++G** geomet:	ry and energy	of conformer:	Thr-LI
18					
19	N	-0.5499040	1.8495380	0.1823190	
20	H ~	-0.0445280	2.6264980	-0.2302400	
21	С	-0.1538490	0.5868590	-0.4496230	
22	H	-0.2/20030	0.6103460	-1.5498140	
23	C	1.3446910	0.3140810	-0.1/23850	
24	U U	-1.1011110 1 0557720	-0.5257980	-0.0040250	
25		1 8/86280	-0.7301690	-0.4201020	
26	0	-0.8150630	-1 6338890	0 3571310	
27	н	1 7896270	-0 4590360	-1 9259660	
28	0	-2.3956750	-0.1113140	-0.1141420	
29	H	-2.9562530	-0.8505220	0.1658840	
30	Н	-1.5415740	2.0209590	0.0618960	
31	С	1.6794420	-0.0382060	1.2687200	
32	Н	1.2878900	-1.0241720	1.5170040	
33	Н	2.7633910	-0.0489780	1.3990150	
34	Н	1.2488460	0.7031260	1.9445180	
35					
30	Energy:	-438.412520745			
3/					
20					
<u>70</u>		211 C**	with an an amount	of conformer.	The ITT
40	BSLIP/0-	SII++G"" geomet.	ry and energy	or conformer.	
42	N	0.2369850	1.7669510	-0.1157790	
43	Н	0.2444820	1.8058290	0.8996530	
44	C	-0.0356190	0.4048080	-0.5330590	
45	Н	-0.0339100	0.3710630	-1.6310630	
46	С	1.0887910	-0.5364620	-0.0545660	
47	С	-1.4372410	-0.0943320	-0.0974050	
48	Н	0.8829370	-1.5551740	-0.4236540	
49	0	1.0122230	-0.5341990	1.3717490	
50	0	-2.2380670	0.5957790	0.4653890	
51	Н	1.7946760	-0.9600330	1.7355520	
52	0	-1.7673000	-1.3651360	-0.4534940	
53	Н	-1.0163640	-1.8135060	-0.8609330	
54	H	-0.5136290	2.3/88050	-0.41/9000	
55	U U	2.400400U 2.2206520	-U.122538U	-U.561/240	
56	л Ч	3.23U032U 2 5021720	-U.OUOYOOU _0 1500260	-U.IOZUOOU _1 65/1/20	
57	H	2.7008570	0.8928550	-0.2430900	
58		2.,000070	0.0720000	0.2100000	
59	Energy:	-438.412327313			
00					

-0.0157450 0.9425150 -0.0158390 0.1186900	1.9284530			
0.9425150 -0.0158390 0.1186900	I.JZ0IJJ0	-0 3551070		
-0.0158390 0.1186900	2 2644440	_0 3771390		
0.1186900	0 1717810	-0.3771390		
0.1100,000	0.1948500	-1 5023330		
1 1299630	-0.2047700	-1.3023330		
-1 3684510	-0.2047700	0.5051450		
-1.3004310	-0.0339030	1 /127010		
0.9002930	0.0039390	1.412/010		
2.3744590	0.3973370	-0.0037140		
-1.04/2090	0.3249370	1.0974490		
2.0099430	-0.0091940	-0.8209040		
-2.0023340	-0.9393760	-0.7047700		
-1.5506170	-1.0090370	-1.000050		
-0.4294060	2.2119870	0.5289950		
1.1/82850		U.ZI6819U		
0.26/3/90	-2.1918950	0.5950210		
1.2992960	-2.013/530	-0.8338880		
2.0234900	-2.1236540	0.//89650		
-438.41198888	8			
311++G** geome	try and energy	of conformer:	Thr-LIV	
0.0406680	1.9300640	-0.1267260		
0.8995460	2.3176010	-0.4983940		
-0.0186320	0.5051050	-0.3983340		
0.1265710	0.2537380	-1.4657010		
1.1322660	-0.1816700	0.3724040		
-1.3863840	-0.0457010	0.0328150		
1.0330280	0.1279170	1.4188160		
2.3222680	0.3924520	-0.1922470		
-2.0734610	0.4245080	0.8916290		
3,0523630	0.2677310	0.4216880		
_1 8035300	-1 1529370	-0 6434010		
	1.1529970	0.0454010		
-1.1673720	_1 3880820	-1 3302720		
-1.1673720	-1.3880820	-1.3302720		
-1.1673720 -0.7545930 1.1693010	-1.3880820 2.4290070 -1.7035160	-1.3302720 -0.5067970		
-1.1673720 -0.7545930 1.1693010 0.2937940	-1.3880820 2.4290070 -1.7035160 -2.1644240	-1.3302720 -0.5067970 0.2692830		
-1.1673720 -0.7545930 1.1693010 0.2937940 1.2269210	-1.3880820 2.4290070 -1.7035160 -2.1644340	-1.3302720 -0.5067970 0.2692830 0.7324840		
-1.1673720 -0.7545930 1.1693010 0.2937940 1.2368310 2.0536300	-1.3880820 2.4290070 -1.7035160 -2.1644340 -2.0247000 -2.0867110	-1.3302720 -0.5067970 0.2692830 0.7324840 -0.7749220 0.7853140		
-1.1673720 -0.7545930 1.1693010 0.2937940 1.2368310 2.0536300	-1.3880820 2.4290070 -1.7035160 -2.1644340 -2.0247000 -2.0867110	-1.3302720 -0.5067970 0.2692830 0.7324840 -0.7749220 0.7853140		
	2.6899450 2.6899450 -2.0025540 -1.5308170 -0.4294060 1.1782850 0.2673790 1.2992960 2.0234900 -438.41198888 311++G** geome 0.0406680 0.8995460 -0.0186320 0.1265710 1.1322660 -1.3863840 1.0330280 2.3222680 -2.0734610 2.0522630	2.6899450 -0.0091940 -2.0025540 -0.9595760 -1.5308170 -1.0890570 -0.4294060 2.2119870 1.1782850 -1.7214480 0.2673790 -2.1918950 1.2992960 -2.0137530 2.0234900 -2.1236540 -438.411988888 311++G** geometry and energy 0.0406680 1.9300640 0.8995460 2.3176010 -0.0186320 0.5051050 0.1265710 0.2537380 1.1322660 -0.1816700 -1.3863840 -0.0457010 1.0330280 0.1279170 2.3222680 0.3924520 -2.0734610 0.4245080	2.6899450 -0.0091940 -0.8209040 -2.0025540 -0.9595760 -0.7047700 -1.5308170 -1.0890570 -1.5363530 -0.4294060 2.2119870 0.5289950 1.1782850 -1.7214480 0.2168190 0.2673790 -2.1918950 0.5950210 1.2992960 -2.0137530 -0.8338880 2.0234900 -2.1236540 0.7789650 -438.411988888 0.1267260 -0.4983940 -0.0186320 0.5051050 -0.3983340 0.1265710 0.2537380 -1.4657010 1.1322660 -0.1816700 0.3724040 -1.3863840 -0.0457010 0.0328150 1.0330280 0.1279170 1.4188160 2.3222680 0.3924520 -0.1922470 -2.0734610 0.4245080 0.8916290	
0	-1.8655080	-1.2888320	-0.5103240	
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Н	-1.2568720	-1.6726490	-1.1530050	
Н	1.0706490	2.0700050	-0.4541640	
С	2.4547590	-0.2890290	-0.5180950	
Н	3.1844500	-0.9626690	-0.0587450	
Н	2.4836260	-0.4576530	-1.5985310	
Н	2.7771010	0.7347090	-0.3122020	
Energy:	-438.40798347	9		
				m]
B3L15/0-	-311++G** geome	try and energy	of conformer:	Thr-LV1
Ν	0.0930600	1.9231390	-0.0296460	
Н	1.0479800	2.2371380	-0.1661680	
С	-0.0137050	0.5165040	-0.3755210	
Н	0.0834070	0.3232590	-1.4628520	
С	1.1342270	-0.2502140	0.3279310	
С	-1.3654200	-0.0382280	0.1110090	
Н	1.0294650	-0.0553320	1.3968950	
0	2.3859230	0.3411080	-0.0395730	
0	-1.7407760	0.0029640	1.2455530	
Н	2.6739060	-0.0359060	-0.8786200	
0	-2.1348580	-0.6361750	-0.8438090	
Н	-1.7035400	-0.5759120	-1.7048350	
Н	-0.5335310	2.5085680	-0.5689720	
С	1.1251160	-1.7493860	0.0570910	
Н	1.2180240	-1.9604610	-1.0153740	
Н	1.9642800	-2.2220950	0.5710840	
Н	0.2049640	-2.2164690	0.4159390	
Energy:	-438.40746769	6		
21				

B3LYP/6-	-311++G** geome	try and energy	of conformer:	aTh
N	0.2923440	1.8515520	0.0058230	
H C	0.0289510	2.0580980	-0.953/200	
H	-0.0800310	0.3642720	1.4251160	
С	-1.1837500	-0.2176340	-0.3222290	
С	1.3458670	-0.3568710	0.0329220	
H	-1.0098190	-0.2383200	-1.4117690	
0	-1.3/12230	-1.5348850 -1.5610510	U.1653400 -0 0738490	
H	-0.5259760	-2.0018520	0.0657870	
0	2.4389950	0.3972740	-0.0854610	
Н	2.1233100	1.3260630	-0.0065920	
H	-0.2275260	2.4764410	0.6096490	
Н	-2.4693600 -2.6399370	0.6192240	-0.0373330	
Н	-2.4542010	1.5531140	-0.4640690	
Н	-3.3096980	0.0054080	-0.4747620	
Energy:	-438.42607609	6		
MP2/aug-	-cc-pVTZ geomet	ry and energy o	of conformer:	aThr
N	0.2779100	1.8412290	0.0116870	
H	0.0219000	2.0222540	-0.9537360	
н	-0.0983050	0.4334780	1 4284760	
C	-1.1651990	-0.2188160	-0.3265250	
С	1.3314440	-0.3491660	0.0377150	
H	-0.9799290	-0.2326860	-1.4114700	
0	-1.3534250	-1.5333810 _1.5584090	0.1594/60 -0.0706310	
Н	-0.4906890	-1.9749690	0.0787340	
0	2.4182540	0.4132350	-0.0918330	
Н	2.0755600	1.3332470	-0.0058470	
H	-0.2853630	2.4505600	0.5896710	
н	-2.4433220 -2.5984810	0.5407600	-0.0398110	
H	-2.4271300	1.5425680	-0.4658640	
Н	-3.2817580	-0.0030290	-0.4705160	
Energy:	-435.93324319	6		

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2		211	two and anaway	of conforman.	o The TT
4	DJLIP/0-	SII++G*** geome	try and energy	or contormer:	allii – II
5	Ν	0.3845910	1.7459650	0.1091240	
6	Н	-0.0076120	1.8208290	1.0430750	
7	С	-0.0023820	0.4823340	-0.5098950	
8	H	-0.0121850	0.6105720	-1.5953050	
9	C	1.0913670	-0.5924520	-0.2199330	
10	U U	-1.3845200	1 4690220	-0.0869770	
10		2 3333930	-1.4080330	-0.6746890	
12	0	-2.0387470	0.4683270	0.8134310	
14	H	2.3787120	0.8301190	-0.3403510	
15	0	-1.8044800	-1.0422640	-0.8358020	
16	Н	-2.6737640	-1.3113630	-0.5009800	
17	Н	0.0344840	2.5356120	-0.4203560	
18	С	1.1635060	-1.0059530	1.2505090	
19	Н	1.9840080	-1.7134110	1.3829300	
20	Н	1.3567510	-0.1432830	1.8944120	
21	Н	0.2387730	-1.4864350	1.5842230	
22	Eneray.	-438 42583382	5		
23 24	Luci gy .	100.12000002			
25	MP2/aug-	cc-pVTZ geomet:	ry and energy	of conformer:	aThr-II
26	N	0.4252700	1 7279270	0.0802170	
27	H	0.0052150	1.8007140	1.0015020	
28	С	0.0140320	0.4777880	-0.5389850	
29	Н	0.0133340	0.5931430	-1.6230830	
30 21	С	1.0628600	-0.6080150	-0.2122960	
31 32	С	-1.3582370	0.0215490	-0.1021900	
32 33	Н	0.8484860	-1.4893660	-0.8162380	
34	0	2.3283540	-0.1285860	-0.6299060	
35	U U	-2.0001310	0.5004240	0.8064990	
36	П	-1 7805750	-1 0365590	-0.8313230	
37	H	-2.6448750	-1.2891150	-0.4685780	
38	H	0.0771310	2.5161590	-0.4503700	
39	С	1.0708360	-0.9743800	1.2627500	
40	Н	1.8646780	-1.6953590	1.4465340	
41	Н	1.2658770	-0.0925510	1.8739110	
42	Н	0.1219680	-1.4134730	1.5741970	
43 44	Energy:	-437.56854060	4		
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46 47					
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B3LYP/6-	311++G** geome	try and energy	y of conformer:	aThr-II:
	-	1 - 4010-00	0 0100110	
N	-0.9006290	1.7481870	-0.2100110	
Н	-0.613/430	2.0552030	0./168340	
С	-0.1875900	0.5111930	-0.5698130	
H	-0.1835870	0.4335630	-1.6630430	
С	1.2722380	0.4666440	-0.0591800	
С	-1.0282340	-0.6883160	-0.0699370	
Н	1.7022080	1.4472520	-0.2879700	
0	1.2802490	0.4061520	1.3696180	
0	-0.5803840	-1.7937070	0.1077570	
Н	1.0651210	-0.4986610	1.6300760	
0	-2.3148780	-0.3914370	0.1338070	
Н	-2.3802580	0.5818950	0.0004750	
H	-0.7090630	2.4992030	-0.8627630	
С	2.1481710	-0.6083830	-0.6969090	
Н	3.1679950	-0.5168610	-0.3163470	
Н	1.7698160	-1.6072410	-0.4775380	
Н	2.1785030	-0.4865580	-1.7840710	
Enerav:	-438.42450199	6		
- 51				_,
MP2/aug-	cc-pVTZ geomet:	ry and energy	of conformer:	aThr-III
Ν	-0.9211890	1.7352070	-0.1692450	
Н	-0.6547970	1.9815240	0.7804080	
С	-0.1861370	0.5300810	-0.5660090	
Н	-0.1727840	0.4844290	-1.6583880	
С	1.2509350	0.4858440	-0.0337820	
С	-0.9952070	-0.6850570	-0.0925070	
Н	1.6698990	1.4823170	-0.1922880	
0	1.2223290	0.3330430	1.3840800	
0	-0.5186200	-1.7837330	0.0919080	
Н	0.9784000	-0.5877200	1.5545360	
0	-2.2918140	-0.4223490	0.0948870	
Н	-2.3581610	0.5531170	-0.0294690	
Н	-0.6841900	2.5181670	-0.7647840	
С	2.1425890	-0.5374470	-0.7122100	
Н	3.1506690	-0.4583060	-0.3087350	
Н	1.7656160	-1.5444030	-0.5502960	
Н	2.1854330	-0.3517910	-1.7862180	
Enerav:	-437.56689807	0		
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2 3	B3LYP/6-	311++G** geomet	ry and energy	of conformer:	aThr-IV
4		-			
5	N	-0.3892980	1.9484780	-0.1407350	
0	H	-1.3630650	2.2121010	-0.240/0/0	
7	С	-0.1382820	0.5713100	-0.5719860	
8	H	-0.3208970	0.5120350	-1.6485280	
9	C	1.3359430	0.2164080	-0.2936370	
10	C	-1.09/1610	-0.3984880	0.1209660	
11	H	1.9254210	1.0006590	-0.//514/0	
12	0	1.6341190	0.3370720	1.096/300	
13	0	-0.8841980	-1.0018660	1.1498550	
14	н	1.0848210	-0.3093910	1.3626310	
15	0	-2.2073330	-0.4/10000	-0.51/9610	
16	п	-2.8675950	-1.0442020	0.0082530	
1/	п	-0.1034020	2.0091190	0.0202300	
18	U U	1 1007200	-1.1443130	-0.0342200	
19	п	1.5907290	-1.9500570	-0.3027020	
20	11 U	2 8100860	-1.3083240	-0.6658000	
21	11	2.0100000	-1.5005240	-0.0050000	
22	Energy:	-438.423629378	3		
23	2.1.02 97 •	100,120023070			
24 25	MP2/aug-	cc-pVTZ geometr	ry and energy o	of conformer:	aThr-IV
26	Ν	-0.3790920	1.9401160	-0.1350980	
27	Н	-1.3619210	2.1786020	-0.1948500	
28	С	-0.1361750	0.5698900	-0.5795430	
29	Н	-0.3283600	0.5140030	-1.6518560	
30	С	1.3248370	0.2154370	-0.3096790	
31	С	-1.0760710	-0.3933950	0.1202200	
32	Н	1.9206620	0.9816240	-0.8071580	
33	0	1.6271250	0.3510920	1.0752350	
34	0	-0.8475650	-1.0032430	1.1478020	
35	Н	1.0600390	-0.2873130	1.5333150	
36	0	-2.2743230	-0.4559280	-0.5027490	
37	Н	-2.8354310	-1.0309440	0.0432130	
38	Н	-0.0834380	2.0268120	0.8320320	
39	С	1.6964820	-1.1580140	-0.8407310	
40	Н	1.1271970	-1.9375410	-0.3339980	
41	H	1.5036750	-1.2242780	-1.9123370	
42	Н	2.7548810	-1.3406460	-0.6665720	
43	Enorau.	_/37 565002301			
44	Eller gy.	457.505502501	-		
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B3LYP/6-3 N H C H	11++G** geomet 0.1053490 1.0854160	cry and energy		
B3LYP/6-3 N H C H	11++G** geomet 0.1053490 1.0854160	try and energy		
N H C H	0.1053490 1.0854160		of conformer: a	aThr-V
H C H	1.0854160	1 7111100	0 1581730	
C H		1.8783950	0.3668560	
H	-0.0393510	0.4423970	-0.5739110	
C	-0.0127820	0.5804690	-1.6593570	
0	1.0977130	-0.5395250	-0.2258400	
3	-1.3942710	-0.2099300	-0.2411520	
H	0.9531240	-1.4190970	-0.8614810	
0	2.3017990	0.1453140	-0.6037880	
Ч	-1.8242730	-1.1010300	-0.3967810	
	-2.0341380	0.3603780	0.7885420	
H	-1.4518760	1.1001040	1.0774480	
H	-0.2076160	2.4909730	-0.4107310	
2	1.1397260	-0.9718500	1.2393900	
H	0.2342920	-1.5187110	1.5132360	
H	1.9877770	-1.6432220	1.4051720	
Н	1.2477870	-0.1151550	1.9084820	
Energy:	-438.423380829			
MP2/aug-c	c-pVTZ geometı	ry and energy	of conformer: al	Thr-V
N	0.1575090	1.6961910	0.1338620	
ł	1.1507150	1.8483260	0.2787810	
2	-0.0267150	0.4433150	-0.6005700	
-	0.0049130	0.5677780	-1.6845700	
C	1.0655250	-0.5594850	-0.2244650	
с Н	-1.3/3363U 0 9077530	-U.I&Z3ZIU -1 4438650	-0.24/3020	
	2.2921070	0.0872120	-0.5783160	
0	-1.8372570	-1.1236860	-0.8481290	
- H	3.0186070	-0.4872490	-0.3119620	
С	-1.9674870	0.3778160	0.8156470	
H	-1.3507070	1.1005680	1.0784340	
H	-0.1774380	2.4784930	-0.4160750	
2	1.0498910	-0.9506280	1.2428630	
d U	0.1217560	-1.4618460	1.4974000	
л Н	1.8/3426U 1.1586800	-1.6350450 _0 0753150	1 8813740	
.1	T.T200000	-0.0/33130	1.0013/40	
Energy:	-437.566777895	ō		
	UR	L: http://mc.man	uscriptcentral.com/ta	ndf/tmph
		-	-	-

<pre>B3LYP/6-311++G** geometry and energy of conformer: aThr N</pre>					
N -0.0955450 1.7052140 0.3193320 H 0.4774690 2.4074860 -0.1340140 C -0.0726050 0.4494920 -0.4424550 H -0.0935300 0.7230100 -1.5029350 C 1.1660500 -0.4430630 -0.2519370 C -1.3814260 -0.3300020 -0.2062950 H 1.0391450 -1.3050670 -0.9143420 O 2.2670620 0.3635170 -0.6976100 O -1.5236910 -1.4897210 -0.4952410 H 3.0725230 -0.1617450 -0.6601850 O -2.3635310 0.4165420 0.3158280 H 0.2796840 1.5796930 1.2549450 C 1.3732850 -0.9397380 1.1771510 H 0.5289080 -1.5519480 1.5021080 H 2.2705950 -1.5630170 1.2320000 H 0.3060560 1.7244680 0.1537380 H 0.1197550 2.5140820 -0.3165110 C 0.042770 0.4681200 -0.5281790	B3LYP/6-	-311++G** geome	try and energy	of conformer:	aThr-\
$\begin{array}{llllllllllllllllllllllllllllllllllll$	Ν	-0.0955450	1.7052140	0.3193320	
CC -0.0726050 0.4494920 -0.4424550 H -0.0935300 0.7230100 -1.5029350 CC 1.1660500 -0.4430630 -0.2519370 CC -1.3814260 -0.3300020 -0.2062950 H 1.0391450 -1.3050670 -0.9143420 O 2.2670620 0.3635170 -0.6976100 O -1.5236910 -1.4897210 -0.4952410 H 3.0725230 -0.1617450 -0.6601850 O -2.3635310 0.4165420 0.3158280 H -1.9670610 1.3036330 0.4661020 H 0.2796840 1.5796930 1.2549450 CC 1.3732850 -0.9397380 1.1771510 H 0.5289080 -1.5519480 1.5021080 H 2.2705950 -1.5630170 1.2320000 H 1.5105320 -0.1113850 1.8784040 Energy: -438.423320511 B3LYP/6-311++G** geometry and energy of conformer: aThr N 0.3060560 1.7244680 0.1537380 H -0.1197550 2.5140820 -0.3165110 CC 1.338870 -0.5646780 -0.2303070 CC 1.1338870 -0.5646780 -0.2303070 CC -1.3627410 -0.1561850 -0.2693680 H 0.9785260 -1.4255290 -0.8836850 O 2.3685730 0.0158680 -0.6187760 O -1.823390 -1.0663460 -0.9112650 H 2.3554670 0.9213590 -0.2726940 O -1.823390 -1.0663460 -0.9112650 H 2.3554670 0.9213590 -0.2726940 O -2.0152340 0.3964180 0.7843780 H -2.8531700 -0.883610 0.7843780 H -2.8531700 -0.883630 1.2269030 H 0.9785260 -1.4255290 1.261870 O -2.8531700 -0.812000 0.8831160 H 2.3554670 0.9213590 -0.2726940 O -2.0152340 0.3964180 0.7843780 H 0.2530000 -1.5574210 1.5061570 H 2.0108700 -1.7094250 1.3645110 H 0.2530000 -1.5574210 1.5061570 H 2.0108700 -1.7094250 1.3645110 H 0.2530000 -1.5574210 1.5061570 H 2.0108700 -0.1850180 1.9096770 Energy: -438.423294504	Н	0.4774690	2.4074860	-0.1340140	
H -0.0935300 0.7230100 -1.5029350 C 1.1660500 -0.4430630 -0.2519370 C -1.3814260 -0.3300020 -0.2062950 H 1.0391450 -1.3050670 -0.9143420 O 2.2670620 0.3635170 -0.6976100 O -1.5236910 -1.4897210 -0.4952410 H 3.0725230 -0.1617450 -0.6601850 O -2.3635310 0.4165420 0.3158280 H -1.9670610 1.3036330 0.4661020 H 0.2796840 1.5796930 1.2549450 C 1.3732850 -0.9397380 1.1771510 H 0.5289080 -1.5519480 1.5021080 H 2.2705950 -1.5630170 1.2320000 H 1.5105320 -0.1113850 1.8784040 Energy: -438.423320511 B3LYP/6-311++G** geometry and energy of conformer: aThr N 0.3060560 1.7244680 0.1537380 H -0.1197550 2.5140820 -0.3165110 C 0.0042770 0.4681200 -0.5281790 H 0.0490430 0.6474130 -1.6051200 C 1.1338870 -0.5646780 -0.2303070 C 1.3627410 -0.1561850 +0.2693680 H 0.9785260 -1.4255290 -0.8836850 O 2.3685730 0.0158680 -0.6187760 O -1.823390 -1.0663460 -0.9112650 H 2.3554670 0.9213590 -0.2726940 O -2.0152340 0.3964180 0.7843780 H -2.0152700 -0.0812000 0.8831160 H 2.3554670 0.9213590 -0.2726940 O -2.0152340 0.3964180 0.7843780 H -2.8531700 -0.0812000 0.8831160 H 0.233000 -1.5574210 1.5061570 H 2.0108700 -1.7094250 1.3645110 H 0.2530000 -1.5574210 1.5061570 H 2.0108700 -1.7094250 1.3645110 H 0.2530000 -1.5574210 1.9096770 Energy: -438.423294504	С	-0.0726050	0.4494920	-0.4424550	
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	Energy:	-438.42329450	4		
	B3LYP/6-	-311++G** geome	try and energy	of conformer:	aThr-
B3LYP/6-311++G** geometry and energy of conformer: aThr	Ν	0.1061950	1.7130560	0.1089890	
B3LYP/6-311++G** geometry and energy of conformer: aThr N 0.1061950 1.7130560 0.1089890	Η	-0.1991930	2.4812620	-0.4789130	
B3LYP/6-311++G** geometry and energy of conformer: aThr N 0.1061950 1.7130560 0.1089890 H -0.1991930 2.4812620 -0.4789130	С	-0.0383150	0.4234250	-0.5794570	
B3LYP/6-311++G** geometry and energy of conformer: aThr N 0.1061950 1.7130560 0.1089890 H -0.1991930 2.4812620 -0.4789130 C -0.0383150 0.4234250 -0.5794570	Н	-0.0144500	0.5241650	-1.6712780	
B3LYP/6-311++G** geometry and energy of conformer: aThr N 0.1061950 1.7130560 0.1089890 H -0.1991930 2.4812620 -0.4789130 C -0.0383150 0.4234250 -0.5794570 H -0.0144500 0.5241650 -1.6712780	С	1.1022820	-0.5531840	-0.1850540	
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B3LYP/6-311++G** geometry and energy of conformer: aThr N 0.1061950 1.7130560 0.1089890 H -0.1991930 2.4812620 -0.4789130 C -0.0383150 0.4234250 -0.5794570 H -0.0144500 0.5241650 -1.6712780 C 1.1022820 -0.5531840 -0.1850540 C -1.3976000 -0.2148360 -0.2416990	Н	0.9465960	-1.4692210	-0.7630410	
B3LYP/6-311++G** geometry and energy of conformer: aThr N 0.1061950 1.7130560 0.1089890 H -0.1991930 2.4812620 -0.4789130 C -0.0383150 0.4234250 -0.5794570 H -0.0144500 0.5241650 -1.6712780 C 1.1022820 -0.5531840 -0.1850540 C -1.3976000 -0.2148360 -0.2416990 H 0.9465960 -1.4692210 -0.7630410	0	2.3680850	0.0337640	-0.5154930	
B3LYP/6-311++G** geometry and energy of conformer: aThr N 0.1061950 1.7130560 0.1089890 H -0.1991930 2.4812620 -0.4789130 C -0.0383150 0.4234250 -0.5794570 H -0.0144500 0.5241650 -1.6712780 C 1.1022820 -0.5531840 -0.1850540 C -1.3976000 -0.2148360 -0.2416990 H 0.9465960 -1.4692210 -0.7630410 C 2 3680850 0.0337640 -0.5154930	- -	_1 \$2\$1620	_1 1720000	_0 8201010	
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H -0.8015610 2.4343720 0.0385110 C -0.0101110 0.5454640 -0.2349080 H 0.0760400 0.7191310 -1.3115900 C 1.2292760 -0.2438020 0.2365980 C -1.2956410 -0.2494770 -0.0007820 H 1.1981220 -0.2971060 1.3346710 D 1.2224710 -1.5620190 -0.3071070 D -1.4205870 -1.2122340 0.7220080 H 0.5050680 -2.0484850 0.1173620 D -2.3426980 0.2900380 -0.6666500 H -3.1317400 -0.2263660 -0.4407460 H -0.2479070 1.7503990 1.4255420 C 2.5238650 0.4218880 -0.2028810 H 2.5651170 1.4547350 0.1438520 H 3.3764300 -0.1287220 0.1989890 C 2.5970890 0.4116940 1.2941520	N	-0.0706400	1.8513750	0.4304850	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	H	-0.8015610	2.4343720	0.0385110	
H 0.0760400 0.7191310 -1.3115900 C 1.2292760 -0.2438020 0.2365980 C -1.2956410 -0.2494770 -0.0007820 H 1.1981220 -0.2971060 1.3346710 D 1.2224710 -1.5620190 -0.3071070 D -1.4205870 -1.2122340 0.7220080 H 0.5050680 -2.0484850 0.1173620 D -2.3426980 0.2900380 -0.6666500 H -3.1317400 -0.2263660 -0.4407460 H -0.2479070 1.7503990 1.4255420 C 2.5238650 0.4218880 -0.2028810 H 2.5651170 1.4547350 0.1438520 H 3.3764300 -0.1287220 0.1989890 A 2.5970890 0.4116240 1.2941520	С	-0.0101110	0.5454640	-0.2349080	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Н	0.0760400	0.7191310	-1.3115900	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C	1.2292760	-0.2438020	0.2365980	
H 1.1981220 -0.2971060 1.3346710 D 1.2224710 -1.5620190 -0.3071070 D -1.4205870 -1.2122340 0.7220080 H 0.5050680 -2.0484850 0.1173620 D -2.3426980 0.2900380 -0.6666500 H -3.1317400 -0.2263660 -0.4407460 H -0.2479070 1.7503990 1.4255420 C 2.5238650 0.4218880 -0.2028810 H 2.5651170 1.4547350 0.1438520 H 3.3764300 -0.1287220 0.1989890	C	-1.2956410	-0.2494770	-0.0007820	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Н	1.1981220	-0.2971060	1.3346710	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	0	1.2224710	-1.5620190	-0.3071070	
H 0.5050680 -2.0484850 0.1173620 O -2.3426980 0.2900380 -0.6666500 H -3.1317400 -0.2263660 -0.4407460 H -0.2479070 1.7503990 1.4255420 C 2.5238650 0.4218880 -0.2028810 H 2.5651170 1.4547350 0.1438520 H 3.3764300 -0.1287220 0.1989890	U	-1.4205870	-1.2122340	0./220080	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Н	0.5050680	-2.0484850	0.1173620	
H -3.1317400 -0.2263660 -0.4407460 H -0.2479070 1.7503990 1.4255420 C 2.5238650 0.4218880 -0.2028810 H 2.5651170 1.4547350 0.1438520 H 3.3764300 -0.1287220 0.1989890 L 2.5970890 0.4116940 1.2941520	U	-2.3426980	0.2900380	-0.6666500	
-0.2479070 1.7503990 1.4255420 C 2.5238650 0.4218880 -0.2028810 H 2.5651170 1.4547350 0.1438520 H 3.3764300 -0.1287220 0.1989890 2 5970890 0.4116940 1.2041520	н u	-3.131/400	-U.ZZ6366U	-0.440/460	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	п	-0.24/90/0	T. 1203880	1.4200420	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C) EJJOCEN	0 /010000		
= 25070800 - 0.1207220 0.1202000	С н	2.5238650	0.4218880	-0.2028810	
	С Н Н	2.5238650 2.5651170 3.3764300	0.4218880 1.4547350 -0.1287220	-0.2028810 0.1438520 0.1989890	

	-311++C** goomo	try and onorg	of conformar.	oTbr_V⊺
000000000000000000000000000000000000000	SIIIIG Geome	cry and energy	of conformer.	aini Ai
N	0.1469390	1.8441480	-0.2188930	
H	1.0444240	2.2507980	0.0186950	
U U	0.0351320	0.4/93590	1 4009690	
С	-0.0000100	-0.2503050	_0 2873520	
C	1 3115900	-0.2303030	0.0005650	
н	-1 0387560	-0 3553120	-1 3687040	
0	-1 3557960	-1 5292520	0 3169630	
0	1 3707050	-1.4626870	-0.3127690	
H	-0.5713950	-2.0479690	0.0936400	
0	2.4222800	0.4552640	0.1637220	
Н	3.1873610	-0.1094880	-0.0254090	
Н	-0.5749010	2.4347970	0.1768420	
С	-2.4894680	0.5163650	-0.0415430	
Н	-2.4908480	1.4749640	-0.5638340	
Н	-3.3296370	-0.0738430	-0.4114660	
Н	-2.6422690	0.6834710	1.0293620	
-				
Energy:	-438.42226469			
B3LYP/6-	-311++G** geome	try and energy	of conformer:	aThr-XI
B3LYP/6-	-311++G** geome	try and energy	of conformer:	aThr-XI
B3LYP/6- N	-311++G** geome -0.0891570	try and energy 1.7228900	of conformer: 0.2217640	aThr-XI
B3LYP/6- N H	-311++G** geome -0.0891570 0.3490020	try and energy 1.7228900 1.6604070	of conformer: 0.2217640 1.1358180	aThr-XI.
B3LYP/6- N H C	-311++G** geome -0.0891570 0.3490020 -0.0683190	try and energy 1.7228900 1.6604070 0.4272240	of conformer: 0.2217640 1.1358180 -0.4702970	aThr-XI
B3LYP/6- N H C H	-311++G** geome -0.0891570 0.3490020 -0.0683190 -0.0849100	try and energy 1.7228900 1.6604070 0.4272240 0.6348470	<pre>of conformer: 0.2217640 1.1358180 -0.4702970 -1.5464650</pre>	aThr-XI
B3LYP/6- N H C H C	-311++G** geome -0.0891570 0.3490020 -0.0683190 -0.0849100 1.1644080	try and energy 1.7228900 1.6604070 0.4272240 0.6348470 -0.4688090	<pre>of conformer: 0.2217640 1.1358180 -0.4702970 -1.5464650 -0.1974050</pre>	aThr-XI
B3LYP/6- N H C H C C C	-311++G** geome -0.0891570 0.3490020 -0.0683190 -0.0849100 1.1644080 -1.3859740	try and energy 1.7228900 1.6604070 0.4272240 0.6348470 -0.4688090 -0.3326680	<pre>7 of conformer: 0.2217640 1.1358180 -0.4702970 -1.5464650 -0.1974050 -0.2056250</pre>	aThr-XI
B3LYP/6- N H C H C C H	-311++G** geome -0.0891570 0.3490020 -0.0683190 -0.0849100 1.1644080 -1.3859740 1.0185890	try and energy 1.7228900 1.6604070 0.4272240 0.6348470 -0.4688090 -0.3326680 -1.3940950	<pre>7 of conformer: 0.2217640 1.1358180 -0.4702970 -1.5464650 -0.1974050 -0.2056250 -0.7617110</pre>	aThr-XI
B3LYP/6- N H C H C C H O	-311++G** geome -0.0891570 0.3490020 -0.0683190 -0.0849100 1.1644080 -1.3859740 1.0185890 2.3541240	try and energy 1.7228900 1.6604070 0.4272240 0.6348470 -0.4688090 -0.3326680 -1.3940950 0.2023690	<pre>7 of conformer: 0.2217640 1.1358180 -0.4702970 -1.5464650 -0.1974050 -0.2056250 -0.7617110 -0.6368980</pre>	aThr-XI
B3LYP/6- N H C H C C H O O	-311++G** geome -0.0891570 0.3490020 -0.0683190 -0.0849100 1.1644080 -1.3859740 1.0185890 2.3541240 -1.5480790	try and energy 1.7228900 1.6604070 0.4272240 0.6348470 -0.4688090 -0.3326680 -1.3940950 0.2023690 -1.4878790	<pre>7 of conformer: 0.2217640 1.1358180 -0.4702970 -1.5464650 -0.1974050 -0.2056250 -0.7617110 -0.6368980 -0.5032730</pre>	aThr-XI
B3LYP/6- N H C H C C H O O H	-311++G** geome -0.0891570 0.3490020 -0.0683190 -0.0849100 1.1644080 -1.3859740 1.0185890 2.3541240 -1.5480790 2.4512550	try and energy 1.7228900 1.6604070 0.4272240 0.6348470 -0.4688090 -0.3326680 -1.3940950 0.2023690 -1.4878790 0.0833850	<pre>7 of conformer: 0.2217640 1.1358180 -0.4702970 -1.5464650 -0.1974050 -0.2056250 -0.7617110 -0.6368980 -0.5032730 -1.5868230</pre>	aThr-XI
B3LYP/6- N H C H C C H O O H O	-311++G** geome -0.0891570 0.3490020 -0.0683190 -0.0849100 1.1644080 -1.3859740 1.0185890 2.3541240 -1.5480790 2.4512550 -2.3423230	try and energy 1.7228900 1.6604070 0.4272240 0.6348470 -0.4688090 -0.3326680 -1.3940950 0.2023690 -1.4878790 0.0833850 0.4190980	<pre>7 of conformer: 0.2217640 1.1358180 -0.4702970 -1.5464650 -0.1974050 -0.2056250 -0.7617110 -0.6368980 -0.5032730 -1.5868230 0.3532350</pre>	aThr-XI
B3LYP/6- N H C H C C H O O H O H	-311++G** geome -0.0891570 0.3490020 -0.0683190 -0.0849100 1.1644080 -1.3859740 1.0185890 2.3541240 -1.5480790 2.4512550 -2.3423230 -1.9349630	try and energy 1.7228900 1.6604070 0.4272240 0.6348470 -0.4688090 -0.3326680 -1.3940950 0.2023690 -1.4878790 0.0833850 0.4190980 1.3055260	<pre>7 of conformer: 0.2217640 1.1358180 -0.4702970 -1.5464650 -0.1974050 -0.2056250 -0.7617110 -0.6368980 -0.5032730 -1.5868230 0.3532350 0.4803420</pre>	aThr-XI
B3LYP/6- N H C H C C H O O H H O H	-311++G** geome -0.0891570 0.3490020 -0.0683190 -0.0849100 1.1644080 -1.3859740 1.0185890 2.3541240 -1.5480790 2.4512550 -2.3423230 -1.9349630 0.4217430	try and energy 1.7228900 1.6604070 0.4272240 0.6348470 -0.4688090 -0.3326680 -1.3940950 0.2023690 -1.4878790 0.0833850 0.4190980 1.3055260 2.4252430	<pre>7 of conformer: 0.2217640 1.1358180 -0.4702970 -1.5464650 -0.1974050 -0.2056250 -0.7617110 -0.6368980 -0.5032730 -1.5868230 0.3532350 0.4803420 -0.2994180</pre>	aThr-XI
B3LYP/6- N H C H C C H O O H O H H C C	-311++G** geome -0.0891570 0.3490020 -0.0683190 -0.0849100 1.1644080 -1.3859740 1.0185890 2.3541240 -1.5480790 2.4512550 -2.3423230 -1.9349630 0.4217430 1.3607160	try and energy 1.7228900 1.6604070 0.4272240 0.6348470 -0.4688090 -0.3326680 -1.3940950 0.2023690 -1.4878790 0.0833850 0.4190980 1.3055260 2.4252430 -0.8135510	<pre>7 of conformer: 0.2217640 1.1358180 -0.4702970 -1.5464650 -0.1974050 -0.2056250 -0.7617110 -0.6368980 -0.5032730 -1.5868230 0.3532350 0.4803420 -0.2994180 1.2725730</pre>	aThr-XI
B3LYP/6- N H C H C C H O O H H C H H	-311++G** geome -0.0891570 0.3490020 -0.0683190 -0.0849100 1.1644080 -1.3859740 1.0185890 2.3541240 -1.5480790 2.4512550 -2.3423230 -1.9349630 0.4217430 1.3607160 0.4789450	try and energy 1.7228900 1.6604070 0.4272240 0.6348470 -0.4688090 -0.3326680 -1.3940950 0.2023690 -1.4878790 0.0833850 0.4190980 1.3055260 2.4252430 -0.8135510 -1.3142930	<pre>7 of conformer: 0.2217640 1.1358180 -0.4702970 -1.5464650 -0.1974050 -0.2056250 -0.7617110 -0.6368980 -0.5032730 -1.5868230 0.3532350 0.4803420 -0.2994180 1.2725730 1.6782660 1.2725720</pre>	aThr-XI
B3LYP/6- N H C H C C H O O H H C H H H C H	-311++G** geome -0.0891570 0.3490020 -0.0683190 -0.0849100 1.1644080 -1.3859740 1.0185890 2.3541240 -1.5480790 2.4512550 -2.3423230 -1.9349630 0.4217430 1.3607160 0.4789450 2.2164130	try and energy 1.7228900 1.6604070 0.4272240 0.6348470 -0.4688090 -0.3326680 -1.3940950 0.2023690 -1.4878790 0.0833850 0.4190980 1.3055260 2.4252430 -0.8135510 -1.3142930 -1.4819000	<pre>7 of conformer: 0.2217640 1.1358180 -0.4702970 -1.5464650 -0.1974050 -0.2056250 -0.7617110 -0.6368980 -0.5032730 -1.5868230 0.3532350 0.4803420 -0.2994180 1.2725730 1.6782660 1.3784580 1.6782660</pre>	aThr-XI
B3LYP/6- N H C C C H O O H H C H H H H H	-311++G** geome -0.0891570 0.3490020 -0.0683190 -0.0849100 1.1644080 -1.3859740 1.0185890 2.3541240 -1.5480790 2.4512550 -2.3423230 -1.9349630 0.4217430 1.3607160 0.4789450 2.2164130 1.5732560	try and energy 1.7228900 1.6604070 0.4272240 0.6348470 -0.4688090 -0.3326680 -1.3940950 0.2023690 -1.4878790 0.0833850 0.4190980 1.3055260 2.4252430 -0.8135510 -1.3142930 -1.4819000 0.0787700	<pre>7 of conformer: 0.2217640 1.1358180 -0.4702970 -1.5464650 -0.1974050 -0.2056250 -0.7617110 -0.6368980 -0.5032730 -1.5868230 0.3532350 0.4803420 -0.2994180 1.2725730 1.6782660 1.3784580 1.8691920</pre>	aThr-XI
B3LYP/6- N H C H C C H O O O H O O H H H H H Energy:	-311++G** geome -0.0891570 0.3490020 -0.0683190 -0.0849100 1.1644080 -1.3859740 1.0185890 2.3541240 -1.5480790 2.4512550 -2.3423230 -1.9349630 0.4217430 1.3607160 0.4789450 2.2164130 1.5732560 -438.42223094	try and energy 1.7228900 1.6604070 0.4272240 0.6348470 -0.4688090 -0.3326680 -1.3940950 0.2023690 -1.4878790 0.0833850 0.4190980 1.3055260 2.4252430 -0.8135510 -1.3142930 -1.4819000 0.0787700	<pre>7 of conformer: 0.2217640 1.1358180 -0.4702970 -1.5464650 -0.1974050 -0.2056250 -0.7617110 -0.6368980 -0.5032730 -1.5868230 0.3532350 0.4803420 -0.2994180 1.2725730 1.6782660 1.3784580 1.8691920</pre>	aThr-XI
B3LYP/6- N H C H C C H O O O H O O H H C H H H Energy:	-311++G** geome -0.0891570 0.3490020 -0.0683190 -0.0849100 1.1644080 -1.3859740 1.0185890 2.3541240 -1.5480790 2.4512550 -2.3423230 -1.9349630 0.4217430 1.3607160 0.4789450 2.2164130 1.5732560 -438.42223094	try and energy 1.7228900 1.6604070 0.4272240 0.6348470 -0.4688090 -0.3326680 -1.3940950 0.2023690 -1.4878790 0.0833850 0.4190980 1.3055260 2.4252430 -0.8135510 -1.3142930 -1.4819000 0.0787700	<pre>7 of conformer: 0.2217640 1.1358180 -0.4702970 -1.5464650 -0.1974050 -0.2056250 -0.7617110 -0.6368980 -0.5032730 -1.5868230 0.3532350 0.4803420 -0.2994180 1.2725730 1.6782660 1.3784580 1.8691920</pre>	aThr-XI
B3LYP/6- N H C C H C C H O O H H C H H H Energy:	-311++G** geome -0.0891570 0.3490020 -0.0683190 -0.0849100 1.1644080 -1.3859740 1.0185890 2.3541240 -1.5480790 2.4512550 -2.3423230 -1.9349630 0.4217430 1.3607160 0.4789450 2.2164130 1.5732560 -438.42223094	try and energy 1.7228900 1.6604070 0.4272240 0.6348470 -0.4688090 -0.3326680 -1.3940950 0.2023690 -1.4878790 0.0833850 0.4190980 1.3055260 2.4252430 -0.8135510 -1.3142930 -1.4819000 0.0787700	<pre>7 of conformer: 0.2217640 1.1358180 -0.4702970 -1.5464650 -0.1974050 -0.2056250 -0.7617110 -0.6368980 -0.5032730 -1.5868230 0.3532350 0.4803420 -0.2994180 1.2725730 1.6782660 1.3784580 1.8691920</pre>	aThr-XI
B3LYP/6- N H C C C H O O H H C H H H Energy: B3LYP/6-	-311++G** geome -0.0891570 0.3490020 -0.0683190 -0.0849100 1.1644080 -1.3859740 1.0185890 2.3541240 -1.5480790 2.4512550 -2.3423230 -1.9349630 0.4217430 1.3607160 0.4789450 2.2164130 1.5732560 -438.42223094 -311++G** geome	try and energy 1.7228900 1.6604070 0.4272240 0.6348470 -0.4688090 -0.3326680 -1.3940950 0.2023690 -1.4878790 0.0833850 0.4190980 1.3055260 2.4252430 -0.8135510 -1.3142930 -1.4819000 0.0787700 5 try and energy	<pre>7 of conformer: 0.2217640 1.1358180 -0.4702970 -1.5464650 -0.1974050 -0.2056250 -0.7617110 -0.6368980 -0.5032730 -1.5868230 0.3532350 0.4803420 -0.2994180 1.2725730 1.6782660 1.3784580 1.8691920 7 of conformer:</pre>	aThr-XI
B3LYP/6- N H C C H C C H O O O H O O H O O H C H H H H	-311++G** geome -0.0891570 0.3490020 -0.0683190 -0.0849100 1.1644080 -1.3859740 1.0185890 2.3541240 -1.5480790 2.4512550 -2.3423230 -1.9349630 0.4217430 1.3607160 0.4789450 2.2164130 1.5732560 -438.42223094 -311++G** geome 0.1158580	try and energy 1.7228900 1.6604070 0.4272240 0.6348470 -0.4688090 -0.3326680 -1.3940950 0.2023690 -1.4878790 0.0833850 0.4190980 1.3055260 2.4252430 -0.8135510 -1.3142930 -1.4819000 0.0787700 5 try and energy 1.9111030	<pre>7 of conformer: 0.2217640 1.1358180 -0.4702970 -1.5464650 -0.1974050 -0.2056250 -0.7617110 -0.6368980 -0.5032730 -1.5868230 0.3532350 0.4803420 -0.2994180 1.2725730 1.6782660 1.3784580 1.8691920 7 of conformer: 0.0026970</pre>	aThr-XI
B3LYP/6- N H C C H C C H O O H O O H O H H Energy: B3LYP/6- N H	-311++G** geome -0.0891570 0.3490020 -0.0683190 -0.0849100 1.1644080 -1.3859740 1.0185890 2.3541240 -1.5480790 2.4512550 -2.3423230 -1.9349630 0.4217430 1.3607160 0.4789450 2.2164130 1.5732560 -438.42223094 -311++G** geome 0.1158580 1.0805230	try and energy 1.7228900 1.6604070 0.4272240 0.6348470 -0.4688090 -0.3326680 -1.3940950 0.2023690 -1.4878790 0.0833850 0.4190980 1.3055260 2.4252430 -0.8135510 -1.3142930 -1.4819000 0.0787700 5 try and energy 1.9111030 2.1701190	<pre>7 of conformer: 0.2217640 1.1358180 -0.4702970 -1.5464650 -0.1974050 -0.2056250 -0.7617110 -0.6368980 -0.5032730 -1.5868230 0.3532350 0.4803420 -0.2994180 1.2725730 1.6782660 1.3784580 1.8691920 7 of conformer: 0.0026970 -0.1850590</pre>	aThr-XI
B3LYP/6- N H C C H C C H O O H O O H C H H H Energy: B3LYP/6- N H C	-311++G** geome -0.0891570 0.3490020 -0.0683190 -0.0849100 1.1644080 -1.3859740 1.0185890 2.3541240 -1.5480790 2.4512550 -2.3423230 -1.9349630 0.4217430 1.3607160 0.4789450 2.2164130 1.5732560 -438.42223094 -311++G** geome 0.1158580 1.0805230 0.0641450	try and energy 1.7228900 1.6604070 0.4272240 0.6348470 -0.4688090 -0.3326680 -1.3940950 0.2023690 -1.4878790 0.0833850 0.4190980 1.3055260 2.4252430 -0.8135510 -1.3142930 -1.4819000 0.0787700 5 try and energy 1.9111030 2.1701190 0.4990990	<pre>7 of conformer: 0.2217640 1.1358180 -0.4702970 -1.5464650 -0.1974050 -0.2056250 -0.7617110 -0.6368980 -0.5032730 -1.5868230 0.3532350 0.4803420 -0.2994180 1.2725730 1.6782660 1.3784580 1.8691920 7 of conformer: 0.0026970 -0.1850590 0.3560990</pre>	aThr-XI
B3LYP/6- N H C C H C C H O O H O O H C H H Energy: B3LYP/6- N H C H	-311++G** geome -0.0891570 0.3490020 -0.0683190 -0.0849100 1.1644080 -1.3859740 1.0185890 2.3541240 -1.5480790 2.4512550 -2.3423230 -1.9349630 0.4217430 1.3607160 0.4789450 2.2164130 1.5732560 -438.42223094 -311++G** geome 0.1158580 1.0805230 0.0641450 -0.0762030	try and energy 1.7228900 1.6604070 0.4272240 0.6348470 -0.4688090 -0.3326680 -1.3940950 0.2023690 -1.4878790 0.0833850 0.4190980 1.3055260 2.4252430 -0.8135510 -1.3142930 -1.4819000 0.0787700 5 try and energy 1.9111030 2.1701190 0.4990990 0.3375390	<pre>v of conformer: 0.2217640 1.1358180 -0.4702970 -1.5464650 -0.1974050 -0.2056250 -0.7617110 -0.6368980 -0.5032730 -1.5868230 0.3532350 0.4803420 -0.2994180 1.2725730 1.6782660 1.3784580 1.8691920</pre> v of conformer: 0.0026970 -0.1850590 0.3560990 1.4366790	aThr-XI
B3LYP/6- N H C C H C C H O O H H C H H Energy: B3LYP/6- N H C H C H C H C H C H C C H C C H C C H C C C H C C C H C C C C H C C C C H C C C C C H C C C C C H C C C C C H C C C C C H C C C C C H C C C C H C C C C H C C C C H C C C C C H C C C C C H C C C C C H C C C C C H C C C C C H C C C C C H C C C C C H C	-311++G** geome -0.0891570 0.3490020 -0.0683190 -0.0849100 1.1644080 -1.3859740 1.0185890 2.3541240 -1.5480790 2.4512550 -2.3423230 -1.9349630 0.4217430 1.3607160 0.4789450 2.2164130 1.5732560 -438.42223094 -311++G** geome 0.1158580 1.0805230 0.0641450 -0.0762030 -1.1334750	try and energy 1.7228900 1.6604070 0.4272240 0.6348470 -0.4688090 -0.3326680 -1.3940950 0.2023690 -1.4878790 0.0833850 0.4190980 1.3055260 2.4252430 -0.8135510 -1.3142930 -1.4819000 0.0787700 5 try and energy 1.9111030 2.1701190 0.4990990 0.3375390 -0.1856550	<pre>/ of conformer: 0.2217640 1.1358180 -0.4702970 -1.5464650 -0.1974050 -0.2056250 -0.7617110 -0.6368980 -0.5032730 -1.5868230 0.3532350 0.4803420 -0.2994180 1.2725730 1.6782660 1.3784580 1.8691920</pre> ///	aThr-XI
B3LYP/6- N H C C H C C H O O H H C H H H Energy: B3LYP/6- N H C H C C C C C C C C C C C C C C C C	-311++G** geome -0.0891570 0.3490020 -0.0683190 -0.0849100 1.1644080 -1.3859740 1.0185890 2.3541240 -1.5480790 2.4512550 -2.3423230 -1.9349630 0.4217430 1.3607160 0.4789450 2.2164130 1.5732560 -438.42223094 -311++G** geome 0.1158580 1.0805230 0.0641450 -0.0762030 -1.1334750 1.4228810	try and energy 1.7228900 1.6604070 0.4272240 0.6348470 -0.4688090 -0.3326680 -1.3940950 0.2023690 -1.4878790 0.0833850 0.4190980 1.3055260 2.4252430 -0.8135510 -1.3142930 -1.4819000 0.0787700 5 try and energy 1.9111030 2.1701190 0.4990990 0.3375390 -0.1856550 -0.1587480	<pre>/ of conformer: 0.2217640 1.1358180 -0.4702970 -1.5464650 -0.1974050 -0.2056250 -0.7617110 -0.6368980 -0.5032730 -1.5868230 0.3532350 0.4803420 -0.2994180 1.2725730 1.6782660 1.3784580 1.8691920</pre> ///	aThr-XI
B3LYP/6- N H C C H C C H O O H H C H H Energy: B3LYP/6- N H C H C H C H C H C H	-311++G** geome -0.0891570 0.3490020 -0.0683190 -0.0849100 1.1644080 -1.3859740 1.0185890 2.3541240 -1.5480790 2.4512550 -2.3423230 -1.9349630 0.4217430 1.3607160 0.4789450 2.2164130 1.5732560 -438.42223094 -311++G** geome 0.1158580 1.0805230 0.0641450 -0.0762030 -1.1334750 1.4228810 -0.9381290	try and energy 1.7228900 1.6604070 0.4272240 0.6348470 -0.4688090 -0.3326680 -1.3940950 0.2023690 -1.4878790 0.0833850 0.4190980 1.3055260 2.4252430 -0.8135510 -1.3142930 -1.4819000 0.0787700 5 try and energy 1.9111030 2.1701190 0.4990990 0.3375390 -0.1856550 -0.1587480 -0.2058440	<pre>7 of conformer: 0.2217640 1.1358180 -0.4702970 -1.5464650 -0.1974050 -0.2056250 -0.7617110 -0.6368980 -0.5032730 -1.5868230 0.3532350 0.4803420 -0.2994180 1.2725730 1.6782660 1.3784580 1.8691920 7 of conformer: 0.0026970 -0.1850590 0.3560990 1.4366790 -0.3450930 0.0152710 -1.4241570</pre>	aThr-XI

0 -1.1676360 -1.5454070 0.1603980

0	2 4008870	0 4959440	-0 2412560	
Н	-1.8436190	-2.0486490	-0.3050580	
0	1.4683700	-1.4957880	0.0562940	
Н	0.5635150	-1.8470890	0.1931630	
Н	-0.2344520	2.4998300	0.7473510	
С	-2.4552460	0.5147660	-0.0707120	
H	-2.4264030	1.5341060	-0.45/25/0	
п	-2 6615990	-0.0122920	1 0033220	
11	2.0010000	0.3337300	1.0033220	
Energy:	-438.42221868	6		
B3LYP/6-	-311++G** geome	try and energy	y of conformer:	aThr-XIV
N	0.7751260	-1.7248190	-0.4758970	
Н	0.3038300	-2.2180650	0.2770570	
C	0.1719150	-0.3943200	-0.6706380	
H C	U.1/89/60 1 2000020	-0.1529840	-1./3/6480	
C C	-1.2909930	-0.3373830	-0.1070570	
н	-1 2372330	-0.7751200	1 1853570	
0	0.8024680	1.8510420	0.0140900	
0	-2.1070570	-0.6731630	1.5834840	
H	2.2102410	0.1884310	0.4995500	
0	2.1805470	-0.7773710	0.3073910	
H	0.7408280	-2.2929180	-1.3129930	
H	-2.0291190	0.9633640	-0.3637190	
С	-1.5644350	1.7582940	0.2168870	
H	-2.0313080	1.2653700	-1.4147540	
H U	-3.0/29/60	0.8433870	-0.0537440	
п	-1.0144520	-1.1323040	-0.7887000	
Energy:	-438.42212938	2		
B3LYP/6-	-311++G** geome	try and energy	y of conformer:	aThr-XV
N	-0.3833390	1.9501280	-0.2376000	
Н	0.0990310	2.1654390	0.6307180	
С	-0.1203530	0.5557770	-0.6070070	
H	-0.3389180	0.4368510	-1.6703970	
C	1.3293600	0.0862610	-0.3259530	
С u	-1.1302340	-0.2856/00	0.1698980	
п О	1.9851030	0.7405290	1 0309350	
0	-0.9880250	-0.6435880	1.3188490	
H	1.0558260	-0.1410600	1.5883970	
0	-2.2269680	-0.5845690	-0.5492320	
Н	-2.8373550	-1.0631780	0.0338280	
Н	-0.0366960	2.5801960	-0.9520110	
С	1.5882770	-1.3652690	-0.7310060	
Н	1.3713220	-1.5223760	-1.7923260	
H	2.6363210	-1.6146280	-0.5545420	
н	0.9/50950	-2.0585680	-0.1481520	
_	400 400001 50	2		

1 2					
3 4					
5 6 7	B3LYP/6-	-311++G** geomet	cry and energy	of conformer:	aThr-XVI
7 8 9 10 11 12 13 14 15 16 17 18 19 20	N H C H C H O H H H H	-0.4278870 -0.0323130 -0.1849850 -0.3578330 1.2850930 -1.2172610 1.9082510 1.5089420 -2.2611460 1.2070720 -0.9146800 -0.0204370 -1.4222640	1.9034380 2.6176180 0.5620140 0.5204760 0.2017140 -0.4082460 0.9677570 0.2606320 -0.6424840 1.1403910 -0.9439810 -0.6463270 2.0964830	-0.0420630 -0.6469940 -0.6134030 -1.6948000 -0.3222380 0.0015880 -0.8042200 1.0997010 -0.5497270 1.3766870 1.1935370 1.4688160 0.0275360 0.8211510	
21 22 23	С Н Н	1.7123820 1.5809770 2.7658190	-1.1684240 -1.2343430 -1.3357760	-0.8211510 -1.9041250 -0.5906460	
24 25 26 27 28	п Energy:	-438.421535885	5	-U.JJ4683U	
29 30	B3LYP/6-	-311++G** geomet	try and energy	of conformer:	aThr-XVII
31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49	N H C C H C H O H H C H H H H H H H H H H	-0.2297340 -1.1646910 -0.1088510 -0.2467870 1.3174410 -1.2106510 1.6468340 -2.1376670 1.0524110 -1.0722580 -1.8286000 0.0360520 1.5644250 0.9216780 1.3760510 2.6023200 1.9902490 -438.421431774	1.9470650 2.2910160 0.5104460 0.3173010 0.0555880 -0.2979920 0.4338870 -0.8320280 -0.3295370 -0.8212050 2.1838420 -1.4303980 -2.0586030 -1.6899050 -1.6734370 0.6499230	$\begin{array}{c} -0.4745560\\ -0.6614080\\ -0.7039720\\ -1.7706480\\ -0.3161510\\ -0.0140570\\ 1.0201920\\ -0.5668760\\ 1.6211000\\ 1.3460660\\ 1.7019970\\ 0.4755720\\ -0.5677110\\ 0.0574810\\ -1.6134420\\ -0.3333070\\ -0.9391650\\ \end{array}$	
50 51 52 53 54	9 <i>y</i> •		-		
55 56	B3LYP/6-	-311++G** geomet	cry and energy	of conformer:	aThr-XVIII
57 58 59 60	N H C H C C	0.1367420 1.1092390 0.0685810 -0.0690430 -1.1321920 1.4246690	1.9111710 2.1729220 0.5042900 0.3585950 -0.1829680 -0.1664190	-0.0195110 -0.1564180 0.3503230 1.4360650 -0.3512630 0.0236070	

Н	-0.9404890	-0.2019300	-1.4268040	
0	-1.2010840	-1.5780670	0.0407520	
0	2.4198160	0.4811200	-0.1788630	
H	-1.7302420	-1.6579050	0.8426370	
0	1.4462850	-1.5042150	0.0141820	
H	0.5319020	-1.84/3900	0.1104//0	
H C	-0.2606610	2.5112030	0.6918150	
L L	-2.4341090	1 5435650	-0.0788180	
н Н	-3 2678850	-0 0044110	-0.5895460	
H	-2.6732730	0.5348780	0.9963060	
Energy:	-438.42136433	1		
51				
B31.YP/6-	-311++G** geome	try and energy	of conformer.	aThr-XI
20211,0	geome		01 00111011101	
Ν	0.1671450	1.9561490	-0.1718390	
H	-0.3723320	2.4885980	-0.8459240	
C	0.0342680	0.5218640	-0.4094280	
H	0.16/4140	0.3279530	-1.4//9020	
C	1.1390660	-0.2372620	0.3/4/630	
C	-1.332/830	-0.0205040	0.0104540	
П	1.0692030	-1 6394320	1.4194270	
0	-1 9223610	0 3189850	1 0059460	
Н	1.0153240	-2.0108990	-0.4642360	
0	-1.8300440	-0.9182520	-0.8702630	
H	-2.6680760	-1.2460920	-0.5079580	
Н	-0.1966740	2.1851100	0.7495690	
С	2.5301180	0.0657240	-0.1669890	
Н	2.7120540	1.1411190	-0.1758400	
Н	3.2861900	-0.4228710	0.4511410	
Н	2.6330140	-0.3057310	-1.1937160	
Energy:	-438.42120484	5		
	211	true and anonau	of conformer.	oThe Vi
DOUTE/0-	JIII Gam Geome	ery and energy	or contormet:	alli -AZ
Ν	-0.4951630	1.8015490	-0.5771520	
H	-1.5005070	1.9208360	-0.5652420	
С	-0.0938610	0.3975930	-0.7380120	
H	-0.0341500	0.0748980	-1./856670	
C	1.328843U	U.262388U	-U.1160000	
с ц	-I.U/8219U 1 0500070	-U.J014U6U 0 0607670	-U.U83194U -D 6888600	
0	1 2897060	0.9097070	-0.0090000 1 24/3070	
0	-1 0718660	_1 7525550	-0 2596650	
н	1.07689090 0.7689090	1.4788490	1.2666600	
0	-1.9855560	0.0526560	0.7102510	
H	-2.5499500	-0.6417760	1.0831530	
H	-0.1096510	2.3741530	-1.3195130	
С	1.9603920	-1.1157170	-0.2012190	
Н	2.0137860	-1.4552020	-1.2388610	
Н	2.9742960	-1.0679840	0.2013200	
Н	1.3919620	-1.8487140	0.3714800	

B3LYP/6	-311++G** geome	etry and energy	of conformer:	aThr-
N	0.1550590	1.9403860	-0.1050090	
Н	-0.1862400	2.1358790	0.8323630	
С	0.0300920	0.5121720	-0.3937590	
Н	0.1395260	0.3546680	-1.4686200	
С	1.1462050	-0.2640180	0.3308230	
С	-1.3260100	-0.0425950	0.0496940	
Н	1.0597460	-0.0335880	1.4019900	
0	0.8543870	-1.6499770	0.1152550	
0	-1.7922750	0.1196250	1.1517150	
Н	1.4723300	-2.1816090	0.6258860	
0	-1.9773990	-0.6946550	-0.9352320	
Н	-2.8111690	-1.0219750	-0.5629610	
Н	-0.3995170	2.4908820	-0.7513510	
С	2.5351150	0.1079310	-0.1713640	
Н	2.7059130	1.1797390	-0.0606470	
Н	3.3028570	-0.4255870	0.3979590	
TT	2 6/10210	-0 1620040	-1 2258180	
H Energy:	-438.42110677	79	1.2250100	
H Energy: B3LYP/6	-438.42110677 -311++G** geome	etry and energy	of conformer:	aThr-
H Energy: B3LYP/6 N	-438.42110677 -311++G** geome -0.1124730	29 etry and energy 1.9266840	of conformer: 0.2569850	aThr-
H Energy: B3LYP/6 N H	-438.42110677 -311++G** geome -0.1124730 0.2871330	29 etry and energy 1.9266840 2.2110180	of conformer: 0.2569850 -0.6328570	aThr-
H Energy: B3LYP/6 N H C	-438.42110677 -311++G** geome -0.1124730 0.2871330 -0.0008280	29 etry and energy 1.9266840 2.2110180 0.4857490	of conformer: 0.2569850 -0.6328570 0.4222260	aThr-
H Energy: B3LYP/6 N H C H	-438.42110677 -311++G** geome -0.1124730 0.2871330 -0.0008280 -0.1516610	etry and energy 1.9266840 2.2110180 0.4857490 0.2316800	of conformer: 0.2569850 -0.6328570 0.4222260 1.4761780	aThr-
H Energy: B3LYP/6 N H C H C	-438.42110677 -311++G** geome -0.1124730 0.2871330 -0.0008280 -0.1516610 -1.1208590	29 etry and energy 1.9266840 2.2110180 0.4857490 0.2316800 -0.2676600	of conformer: 0.2569850 -0.6328570 0.4222260 1.4761780 -0.3698590	aThr-
H Energy: B3LYP/6 N H C H C C C	-438.42110677 -311++G** geome -0.1124730 0.2871330 -0.0008280 -0.1516610 -1.1208590 1.3827810	29 etry and energy 1.9266840 2.2110180 0.4857490 0.2316800 -0.2676600 -0.0286220	of conformer: 0.2569850 -0.6328570 0.422260 1.4761780 -0.3698590 0.0087170	aThr-
H Energy: B3LYP/6 N H C H C C H	-438.42110677 -311++G** geome -0.1124730 0.2871330 -0.0008280 -0.1516610 -1.1208590 1.3827810 -0.8929340	29 29 29 1.9266840 2.2110180 0.4857490 0.2316800 -0.2676600 -0.0286220 -0.1798850	of conformer: 0.2569850 -0.6328570 0.422260 1.4761780 -0.3698590 0.0087170 -1.4443190	aThr-
H Energy: B3LYP/6 N H C H C C H C C H O	-438.42110677 -311++G** geome -0.1124730 0.2871330 -0.0008280 -0.1516610 -1.1208590 1.3827810 -0.8929340 -1.1885150	etry and energy 1.9266840 2.2110180 0.4857490 0.2316800 -0.2676600 -0.0286220 -0.1798850 -1.6423510	of conformer: 0.2569850 -0.6328570 0.422260 1.4761780 -0.3698590 0.0087170 -1.4443190 -0.0013230	aThr-
H Energy: B3LYP/6 N H C C H C C H O O	-438.42110677 -438.42110677 -0.1124730 0.2871330 -0.0008280 -0.1516610 -1.1208590 1.3827810 -0.8929340 -1.1885150 2.2193330	29 29 29 1.9266840 2.2110180 0.4857490 0.2316800 -0.2676600 -0.0286220 -0.1798850 -1.6423510 0.6104530	of conformer: 0.2569850 -0.6328570 0.422260 1.4761780 -0.3698590 0.0087170 -1.4443190 -0.0013230 -0.5747550	aThr-
H Energy: B3LYP/6 N H C H C C H O O H	-438.42110677 -438.42110677 -0.1124730 0.2871330 -0.0008280 -0.1516610 -1.1208590 1.3827810 -0.8929340 -1.1885150 2.2193330 -0.3046750	29 29 29 1.9266840 2.2110180 0.4857490 0.2316800 -0.2676600 -0.0286220 -0.1798850 -1.6423510 0.6104530 -2.0272800	of conformer: 0.2569850 -0.6328570 0.4222260 1.4761780 -0.3698590 0.0087170 -1.4443190 -0.0013230 -0.5747550 -0.0214280	aThr
H Energy: B3LYP/6 N H C C H C C H O O H O O	-438.42110677 -438.42110677 -0.1124730 0.2871330 -0.0008280 -0.1516610 -1.1208590 1.3827810 -0.8929340 -1.1885150 2.2193330 -0.3046750 1.5837780	29 29 29 1.9266840 2.2110180 0.4857490 0.2316800 -0.2676600 -0.0286220 -0.1798850 -1.6423510 0.6104530 -2.0272800 -1.3349320	of conformer: 0.2569850 -0.6328570 0.4222260 1.4761780 -0.3698590 0.0087170 -1.4443190 -0.0013230 -0.5747550 -0.0214280 0.3472720	aThr
H Energy: B3LYP/6 N H C H C C H O O H O H	-438.42110677 -438.42110677 -311++G** geome -0.1124730 0.2871330 -0.0008280 -0.1516610 -1.1208590 1.3827810 -0.8929340 -1.1885150 2.2193330 -0.3046750 1.5837780 2.4655530	29 29 29 1.9266840 2.2110180 0.4857490 0.2316800 -0.2676600 -0.0286220 -0.1798850 -1.6423510 0.6104530 -2.0272800 -1.3349320 -1.5860110	of conformer: 0.2569850 -0.6328570 0.4222260 1.4761780 -0.3698590 0.0087170 -1.4443190 -0.0013230 -0.5747550 -0.0214280 0.3472720 0.0292480	aThr-
H Energy: B3LYP/6 N H C H C C H O O H O H H H	-438.42110677 -438.42110677 -311++G** geome -0.1124730 0.2871330 -0.0008280 -0.1516610 -1.1208590 1.3827810 -0.8929340 -1.1885150 2.2193330 -0.3046750 1.5837780 2.4655530 0.4189510	29 29 29 201020040 201020040 2010200 201028620 201798850 -0.0286220 -0.1798850 -1.6423510 0.6104530 -2.0272800 -1.3349320 -1.5860110 2.4093410	of conformer: 0.2569850 -0.6328570 0.4222260 1.4761780 -0.3698590 0.0087170 -1.4443190 -0.0013230 -0.5747550 -0.0214280 0.3472720 0.0292480 0.9731870	aThr-
H Energy: B3LYP/6 N H C H C C H O O H H C C	-438.42110677 -311++G** geome -0.1124730 0.2871330 -0.0008280 -0.1516610 -1.1208590 1.3827810 -0.8929340 -1.1885150 2.2193330 -0.3046750 1.5837780 2.4655530 0.4189510 -2.4987920	29 279 21.9266840 2.2110180 0.4857490 0.2316800 -0.2676600 -0.0286220 -0.1798850 -1.6423510 0.6104530 -2.0272800 -1.3349320 -1.5860110 2.4093410 0.3171920	of conformer: 0.2569850 -0.6328570 0.4222260 1.4761780 -0.3698590 0.0087170 -1.4443190 -0.0013230 -0.5747550 -0.0214280 0.3472720 0.0292480 0.9731870 -0.1027020	aThr-
H Energy: B3LYP/6 N H C H C C H O O H H C H H C H H	-438.42110677 -438.42110677 -0.1124730 0.2871330 -0.0008280 -0.1516610 -1.1208590 1.3827810 -0.8929340 -1.1885150 2.2193330 -0.3046750 1.5837780 2.4655530 0.4189510 -2.4987920 -2.5527210	etry and energy 1.9266840 2.2110180 0.4857490 0.2316800 -0.2676600 -0.0286220 -0.1798850 -1.6423510 0.6104530 -2.0272800 -1.3349320 -1.5860110 2.4093410 0.3171920 1.3587760	of conformer: 0.2569850 -0.6328570 0.4222260 1.4761780 -0.3698590 0.0087170 -1.4443190 -0.0013230 -0.5747550 -0.0214280 0.3472720 0.0292480 0.9731870 -0.1027020 -0.4145730	aThr
H Energy: B3LYP/6 N H C H C C H O O H O C H C H H C H H H	-438.42110677 -438.42110677 -311++G** geome -0.1124730 0.2871330 -0.0008280 -0.1516610 -1.1208590 1.3827810 -0.8929340 -1.1885150 2.2193330 -0.3046750 1.5837780 2.4655530 0.4189510 -2.4987920 -2.5527210 -3.2416440	etry and energy 1.9266840 2.2110180 0.4857490 0.2316800 -0.2676600 -0.0286220 -0.1798850 -1.6423510 0.6104530 -2.0272800 -1.3349320 -1.5860110 2.4093410 0.3171920 1.3587760 -0.2685830	of conformer: 0.2569850 -0.6328570 0.4222260 1.4761780 -0.3698590 0.0087170 -1.4443190 -0.0013230 -0.5747550 -0.0214280 0.3472720 0.0292480 0.9731870 -0.1027020 -0.4145730 -0.6482270	aThr-

B3LYP/0	6-311++G** geomet	ery and energy	of conformer:	aThr-XXIII
Ν	0.2097500	1.8057310	-0.1676450	
Н	-0.1877190	1.9895030	0.7473180	
С	-0.0217050	0.4297000	-0.5665910	
Н	-0.0423750	0.3713030	-1.6627930	
С	1.0714630	-0.5912140	-0.1048360	
С	-1.3885330	-0.0185340	-0.0863530	

	0.0150000	1 5 6 9 9 9 9 9	0 5011040	
H	0.81/9830	-1.5692990	-0.5311040	
0	2.3414320	-0.1580460	-0.6080570	
0	-2.0218220	0.4941680	0.8010970	
H	2.3556710	-0.2694490	-1.5647710	
0	-1.8192840	-1.1148880	-0.7564950	
Н	-2.6757500	-1.3657910	-0.3780900	
Н	1.2041230	2.0049380	-0.1519620	
С	1.2175380	-0.7105330	1.4035170	
Н	0.2901000	-1.0572990	1.8651450	
Н	2.0103750	-1.4227020	1.6383170	
Н	1.4841610	0.2522940	1.8446700	
Energy:	-438.42092109	6		
B3LYP/6-	-311++G** geome	try and energy	of conformer:	aThr-XXIV
N	0.1990200	1.8121770	-0.1094000	
Н	-0.0969370	1.9402520	0.8520420	
С	-0.0254920	0.4496320	-0.5552190	
H	-0.0384780	0.4320180	-1.6496890	
2	1.0619570	-0.5854300	-0.1404790	
C C	-1 3873510			
с u	1.30/3310 0.7065050	-1 5/597/0	_0 5007710	
л О	U. 130333U	-1.3438740	-U.JYY//IU	
	2.26311/0	-0.0846300	-U./432940	
J	-1.9996800	0.4452380	0.850/490	
H	3.0049420	-0.6274440	-0.4584330	
0	-1.8409650	-1.0700160	-0.8016230	
H	-2.6942080	-1.3324490	-0.4236850	
H	1.1788750	2.0541600	-0.2034550	
С	1.2265880	-0.7611090	1.3655920	
H	0.3140480	-1.1509200	1.8243920	
Н	2.0303000	-1.4732070	1.5779370	
Н	1.4777290	0.1878860	1.8445600	
Energy:	-438.42061084	. 4		
B3LYP/6-	-311++G** geome	try and energy	of conformer:	aThr-XXV
N	-0.4745510	1.8888600	-0.6668210	
H ~	-1.4168640	2.0321000	-1.0150590	
С	-0.1301400	0.4754950	-0.6909840	
H	-0.0994220	0.1369900	-1.7320910	
С	1.2921290	0.3057560	-0.1151160	
С	-1.1695020	-0.4010630	0.0256040	
H	1.8751290	1.1052930	-0.5880990	
0	1.1728320	0.5732660	1.2899320	
0	-2.0872870	0.0115050	0.6851070	
- H	2 0524420	0 6290890	1 6756320	
··· 0	_0 9826770	_1 7251040	_0 2105610	
с ц	-0.3020//0	-1.12J1040 -2.1000020	-0.2103040 0.2661420	
п	-1.0014210	-Z.IAAAAAA	0.2001420	
п	-0.4/26320	2.2125680	U.296546U	
C	1.9707380	-1.0336830	-0.3836690	
H	2.0305040	-1.2273890	-1.4585670	
H	2.9942500	-1.0100430	0.0035800	
Н	1.4375730	-1.8579010	0.0888570	

		_		_
B3LYP/6-	-311++G** geome	try and energy	of conformer:	aThr-XX
Ν	0.0887170	1.9404360	-0.0629900	
Н	-0.2379260	2.0886900	0.8869430	
С	0.0336140	0.5214450	-0.4163080	
Н	0.2125200	0.4306330	-1.4915170	
С	1.1372430	-0.2562770	0.3405290	
С	-1.3295100	-0.1267800	-0.1737220	
H	1.0236/40	-0.043/440	1.40/4880	
0	0.9161160	-1.6640930	0.2365470	
0	-2.0014580	-0.6/51930	-1.0101430	
H	1.1071550	-1.94/3310	-0.6650/10	
U U	-2 5901200	-0 4245240	1 2001590	
Н	-2.3301200	2 4971170	-0 6798/50	
 C	2 5341780	0 1403610	-0 1199120	
н	2.6788990	1 2173480	-0.0225360	
H	3.2868710	-0.3791250	0.4766970	
Н	2.6836240	-0.1281460	-1.1723670	
	2.0000210		1.1720070	
Energy:	-438.42030151	.5		
B3LYP/6-	-311++G** geome	try and energy	of conformer:	aThr-XX
N	-0.4172310	1.9407700	-0.3528340	
Н	-1.3701950	2.2039770	-0.5807030	
С	-0.1808790	0.5244910	-0.6504790	
Н	-0.3368820	0.3808760	-1.7214120	
С	1.2818920	0.1802810	-0.3464240	
С	-1.2141740	-0.3997820	0.0365090	
Н	1.4519820	0.3756870	1.0808940	
0	-2.1888990	-0.8069270	-0.5405590	
0	2.3609360	0.1864730	1.3342520	
Н	-1.0161220	-0.6692430	1.3442660	
0	-0.1426900	-0.3276460	1.6174500	
Н	-0.2576260	2.1417040	0.6291120	
Н	1.6835560	-1.2282340	-0.7682420	
C	1.0838090	-1.9874950	-0.2602630	
H	1.5568450	-1.3519850	-1.8469030	
H	2.7369220	-1.4126970	-0.5373430	
Н	1.8914410	0.924/320	-0.8693310	
Energy:	-438.42012634	8		
	211++********	try and anon-	of conformant	5Th~ VV
ΔΟΓΙΚ/ Ρ-	->ıı++G^^ geome	erry and energy	or conformer:	aint-XX
Ν	-0.5144560	1.8248030	-0.7228020	
H	-1.4408890	1.9395570	-1.1185240	
(1	0 10 - 1 - 6 0	0 1275190	-0 7351730	
<u> </u>	-0.1054560	0.42/5490	1 7740600	
H	-0.1054560	0.0957020	-1.7742600	
H C	-0.1054560 -0.0198210 1.3022030	0.0957020 0.3183490	-1.7742600 -0.1116580	
H C C	-0.1054560 -0.0198210 1.3022030 -1.0649660	0.4273490 0.0957020 0.3183490 -0.5732320	-1.7742600 -0.1116580 -0.0738850	

0	1 1010040			
О Н О Н Н С Н Н Н Н Н	$\begin{array}{c} 1.1318040 \\ -1.0225550 \\ 1.9964390 \\ -1.9973410 \\ -2.5336540 \\ -0.5510850 \\ 2.0019510 \\ 2.1223060 \\ 3.0017860 \\ 1.4434870 \end{array}$	$\begin{array}{c} 0.6382860\\ -1.7682450\\ 0.6806790\\ 0.0164320\\ -0.6951690\\ 2.1618520\\ -1.0219300\\ -1.2434640\\ -0.9830390\\ -1.8372360\end{array}$	1.2780800 -0.2405790 1.6977850 0.7073200 1.0888480 0.2341760 -0.3051960 -1.3693650 0.1391880 0.1550320	
Energy:	-438.42001814	0		
B3LYP/6-	-311++G** geome	try and energy	of conformer:	aThr-XXI
N H C H C C H O O H O H H C H H H H Epergy:	-0.1258460 0.0314360 -0.0035910 0.0665930 1.1991630 -1.3158530 1.1205820 -1.4808860 0.4097550 -2.2973900 -3.1038680 0.5214780 2.5281470 2.5281470 2.5798800 2.6695400 3.3488580 1.1716070 -438.41998422	1.8768710 1.8188730 0.5654980 0.7241820 -0.2900310 -0.1751890 -1.6094120 -1.0060490 -2.0716860 0.2098530 -0.2611650 2.5489040 0.2965230 0.3181260 1.3107310 -0.3230060 -0.3389880	0.4103310 1.4113610 -0.2310840 -1.3105750 0.2319350 0.0280230 -0.3085740 0.8933250 0.1513400 -0.8056690 -0.5448450 0.0186760 -0.2208460 -1.3132690 0.1597720 0.1447600 1.3296390	
Energy:	-438.41998422	5		
	-311++G** geome	try and energy	of conformer:	aThr-XXX
B3LYP/6-				

Energy:	-438.41994161	15		
B3LYP/6-	-311++G** geome	etry and energy	of conformer:	aThr-XXXI
N	-0.3052320	1.9290640	-0.5005250	
H	0.1379480	2.2130500	0.3683950	
С	-0.0947260	0.4972240	-0.7206240	
Н	-0.2339910	0.2850160	-1.7821520	
С	1.3133770	-0.0116770	-0.3003430	
С	-1.2194190	-0.2614730	-0.0213480	
Н	1.6539340	0.4276080	1.0138540	
0	-2.0771670	-0.9103930	-0.5575160	
0	1.0160210	0.0513170	1.6339930	
Н	-1.1475590	-0.1346010	1.3363190	
0	-1.9092500	-0.6022540	1.7124760	
Н	0.1098300	2.4682540	-1.2519740	
Н	1.4903940	-1.5200550	-0.4659720	
С	0.8187460	-2.0784130	0.1938850	
Н	1.2839880	-1.8306120	-1.4944110	
Н	2.5157040	-1.8011390	-0.2182450	
Н	2.0262000	0.5062990	-0.9498330	
Energy:	-438.41990423	30		
B3LYP/6	5-311++G** geom	netry and energ	y of conformer:	aThr-XXXII
Ν	-0.1348270	1.8943190	-0.3262450	
Н	-0.3958050	2.1844250	0.6095700	
С	-0.0198280	0.4499580	-0.4489730	
H	0.1762220	0.2069170	-1.4994800	
С	1.1238500	-0.2519510	0.3686660	
С	-1.3260640	-0.2462220	-0.0989990	
Н	1.2907520	-1.5990110	-0.0492780	
0	-1.5120590	-1.4352860	-0.2515410	
U	0.416/930	-2.011/900	-0.1108110	
н	-2.2485220	0.5532210	0.4654220	
U	-3.01218/0	-0.0033860	0.6841060	
н	0./305920	2.35301/0	-U.581/000	
п	2.4/02810	0.4329//0	0.1815850	
	2./303930	U.4884/2U	-0.8/9/340	
п	2.4/90300	1.43/1630	0.0096270	
Н	3.23/9/60	-0.15/2890	0.6853330	
Н	0.8499770	-0.21//290	1.4363040	
Description	100 11000100			
Energy:	-438.41986492	<u> </u>		
	011 011			
ВЗГЛБ\0-	-311++G** geome	erry and energy	of conformer:	aInr-XXXIII
	0 0010000	1 0100500	0 0506600	
N	0.0612960	1.9199590	0.0596680	
Н	-0.5237330	2.5057250	-0.5257170	
C	0.0230810	0.5245530	-0.3868390	
Н	0.1846600	0.5018460	-1.4663370	
C	1.1445070	-0.2785990	0.2921160	
3	-1.3435420	-0.1215370	-0.1573620	

	1 01 0 4 0 7 0	0 1044400	1 2704100	
н	1.0164970	-0.1844400	1.3/94190	
0	0.9230030	-1.0304030	-0.090/1/0	
0	-2.1223130	-0.4405040	-1.0101120	
н	1.5735750	-2.1986630	0.3364330	
0	-1.6338280	-0.226/200	1.16/4310	
H	-2.5189140	-0.6144210	1.2359780	
H	-0.2699320	2.0056060	1.0156980	
C	2.5309680	0.2096420	-0.1093870	
H	2.6493000	1.2665930	0.1343580	
H	3.3043430	-0.3556000	0.4203630	
п	2.0030920	0.0749870	-1.1030470	
Energy:	-438.41981168	5		
B3LYP/6	-311++G** geome	try and energy	y of conformer:	aThr-XXXIV
N	-0.6448760	1.9569030	-0.2472940	
н	-0.5704360	2.1156960	0.7545320	
C	-0.1743860	0.6129430	-0.5547100	
H	-0.1209950	0.5096420	-1.6468550	
C	1.2596240	0.4331690	0.0098610	
С	-1.1687240	-0.4652200	-0.0974780	
H	1.7203470	1.4180010	-0.0918210	
)	1.2216850	0.2025040	1.4228810	
)	-2.3225770	-0.2591350	0.1752450	
H	1.0162370	-0.7280950	1.5705310	
0	-0.6356100	-1.7167280	-0.0589770	
H	-1.3510490	-2.3221640	0.1918660	
Н	-1.6287320	2.0486750	-0.4805640	
C	2.1288870	-0.5878960	-0.7192000	
- H	2,2131930	-0.3334940	-1.7796160	
 H	3.1324820	-0.5795700	-0.2882040	
H	1.7227020	-1.5981190	-0.6428360	
_				
Energy:	-438.41969599	0		
	211	+		
R3F15/0.	-311++G^^ geome	etry and energy	oi conformer:	alnr-XXXV
N	0.2133880	1.7984030	-0.3404260	
H	-0.6538950	2.3132400	-0.2297770	
С	0.0565040	0.4767580	0.2802730	
H	-0.0212200	0.5235880	1.3792060	
С	-1.2142400	-0.1981100	-0.2500480	
С	1.3125890	-0.3212510	-0.0505270	
H	-1.1040960	-0.3228410	-1.3331430	
0	-2.2628370	0.7503790	0.0208560	
0	1.3903590	-1.3095740	-0.7336400	
H	-3.0729330	0.4417280	-0.3956850	
0	2.3978170	0.2487970	0.5305000	
Н	3.1752800	-0.2585800	0.2519930	
Н	0.9595990	2.3170680	0.1091730	
С	-1.5165090	-1.5392990	0.4107240	
Н	-0.7351570	-2.2682510	0.1928850	
Н	-1.6126560	-1.4207290	1.4936500	
H	-2.4613990	-1.9394590	0.0304180	

0.0060310 -0.3972190 -0.0043250 0.1367670 1.0886270 -1.3772290 1.1615230 -2.1460760 0.2711930 -1.6380220 -2.5032850 0.9343880 2.4838910 2.7351940	etry and energy 1.9204190 2.2598230 0.4697090 0.1495630 -0.2882070 0.0039820 -1.6620820 0.6382080 -2.0314760 -1.2782110 -1.5190060 2.3023950	<pre> of conformer: -0.3972340 0.4691130 -0.4622250 -1.5006730 0.3760060 -0.0057660 0.0040770 0.6669170 -0.0354510 -0.3905070 -0.0238140 0.51226720 -0.10000000000000000000000000000</pre>	aThr-XX
$\begin{array}{c} 0.0060310\\ -0.3972190\\ -0.0043250\\ 0.1367670\\ 1.0886270\\ -1.3772290\\ 1.1615230\\ -2.1460760\\ 0.2711930\\ -1.6380220\\ -2.5032850\\ 0.9343880\\ 2.4838910\\ 2.7351940 \end{array}$	$\begin{array}{c} 1.9204190\\ 2.2598230\\ 0.4697090\\ 0.1495630\\ -0.2882070\\ 0.0039820\\ -1.6620820\\ 0.6382080\\ -2.0314760\\ -1.2782110\\ -1.5190060\\ 2.3023950\end{array}$	-0.3972340 0.4691130 -0.4622250 -1.5006730 0.3760060 -0.0057660 0.0040770 0.6669170 -0.0354510 -0.3905070 -0.0238140	
$\begin{array}{c} -0.3972190\\ -0.0043250\\ 0.1367670\\ 1.0886270\\ -1.3772290\\ 1.1615230\\ -2.1460760\\ 0.2711930\\ -1.6380220\\ -2.5032850\\ 0.9343880\\ 2.4838910\\ 2.7351940 \end{array}$	2.2598230 0.4697090 0.1495630 -0.2882070 0.0039820 -1.6620820 0.6382080 -2.0314760 -1.2782110 -1.5190060 2.3023950	$\begin{array}{c} 0.4691130 \\ -0.4622250 \\ -1.5006730 \\ 0.3760060 \\ -0.0057660 \\ 0.0040770 \\ 0.6669170 \\ -0.0354510 \\ -0.3905070 \\ -0.0238140 \\ 0.5122670 \end{array}$	
-0.0043250 0.1367670 1.0886270 -1.3772290 1.1615230 -2.1460760 0.2711930 -1.6380220 -2.5032850 0.9343880 2.4838910 2.7351940	0.4697090 0.1495630 -0.2882070 0.0039820 -1.6620820 0.6382080 -2.0314760 -1.2782110 -1.5190060 2.3023950	$\begin{array}{c} -0.4622250\\ -1.5006730\\ 0.3760060\\ -0.0057660\\ 0.0040770\\ 0.6669170\\ -0.0354510\\ -0.3905070\\ -0.0238140\\ 0.5122670\end{array}$	
$\begin{array}{c} 0.1367670\\ 1.0886270\\ -1.3772290\\ 1.1615230\\ -2.1460760\\ 0.2711930\\ -1.6380220\\ -2.5032850\\ 0.9343880\\ 2.4838910\\ 2.7351940 \end{array}$	0.1495630 -0.2882070 0.0039820 -1.6620820 0.6382080 -2.0314760 -1.2782110 -1.5190060 2.3023950	$\begin{array}{c} -1.5006730\\ 0.3760060\\ -0.0057660\\ 0.0040770\\ 0.6669170\\ -0.0354510\\ -0.3905070\\ -0.0238140\\ 0.5122670\end{array}$	
1.0886270 -1.3772290 1.1615230 -2.1460760 0.2711930 -1.6380220 -2.5032850 0.9343880 2.4838910 2.7351940	-0.2882070 0.0039820 -1.6620820 0.6382080 -2.0314760 -1.2782110 -1.5190060 2.3023950	0.3760060 -0.0057660 0.0040770 0.6669170 -0.0354510 -0.3905070 -0.0238140	
-1.3772290 1.1615230 -2.1460760 0.2711930 -1.6380220 -2.5032850 0.9343880 2.4838910 2.7351940	0.0039820 -1.6620820 0.6382080 -2.0314760 -1.2782110 -1.5190060 2.3023950	-0.0057660 0.0040770 0.6669170 -0.0354510 -0.3905070 -0.0238140	
1.1615230 -2.1460760 0.2711930 -1.6380220 -2.5032850 0.9343880 2.4838910 2.7351940	-1.6620820 0.6382080 -2.0314760 -1.2782110 -1.5190060 2.3023950	0.0040770 0.6669170 -0.0354510 -0.3905070 -0.0238140	
-2.1460760 0.2711930 -1.6380220 -2.5032850 0.9343880 2.4838910 2.7351940	-1.0020820 0.6382080 -2.0314760 -1.2782110 -1.5190060 2.3023950	$\begin{array}{c} 0.0040770\\ 0.6669170\\ -0.0354510\\ -0.3905070\\ -0.0238140\\ 0.5170670\end{array}$	
-2.1460760 0.2711930 -1.6380220 -2.5032850 0.9343880 2.4838910 2.7351940	-2.0314760 -1.2782110 -1.5190060 2.3023950	-0.0354510 -0.3905070 -0.0238140	
0.2711930 -1.6380220 -2.5032850 0.9343880 2.4838910 2.7351940	-2.0314760 -1.2782110 -1.5190060 2.3023950	-0.0354510 -0.3905070 -0.0238140	
-1.6380220 -2.5032850 0.9343880 2.4838910 2.7351940	-1.2782110 -1.5190060 2.3023950	-0.0238140	
-2.5032850 0.9343880 2.4838910 2.7351940	-1.5190060 2.3023950	-0.0238140	
0.9343880 2.4838910 2.7351940	2.3023950	$\Lambda E1 \neg \alpha C \neg \alpha$	
2.4838910 2.7351940	0 0 0 0 0 0 0 0 0 0	-U.31/80/U	
2.7351940	0.2797370	0.1560930	
	0.2861890	-0.9085530	
2.5813390	1.2900190	0.5580100	
3.2066110	-0.3572820	0.6693910	
0.8276130	-0.1978110	1.4419290	
-438.41957325	59		
			o Theory MAX
SII++G geome	icry and energy	or conformer:	allii - AA
0.1817750	1.7319630	0.2297290	
0.9841720	2.2181860	-0.1500650	
-0.0361020	0.4763910	-0.4628620	
-0.0680270	0.5775130	-1.5652790	
1.1139560	-0.5229720	-0.1627380	
-1.4121240	-0.0648180	-0.1094900	
2 3445890	0 0380510	-0 6489190	
-2 2824670	0.55351/0	0.4471650	
2 20/0200	0.0000000	1 6026050	
2.3040390	-0.0777720	-1.0030930	
-1.386//90	-1.335/460	-0.3504920	
-2.4943410	-1.59265/0	-0.32/5180	
-0.6376870	2.3262340	0.1978920	
1.3023010	-0.8084660	1.3182760	
1.5112110	0.1144630	1.8591870	
0.4025380	-1.2619310	1.7424290	
2.1352430	-1.5007960	1.4536870	
0.8994980	-1.4543410	-0.6958870	
		0.000000	
	-438.41957325 311++G** geome 0.1817750 0.9841720 -0.0361020 -0.0680270 1.1139560 -1.4121240 2.3445890 -2.2824670 2.3840390 -1.5867790 -2.4943410 -0.6376870 1.3023010 1.5112110 0.4025380 2.1352430 0.8994980	-438.419573259 311++G** geometry and energy 0.1817750 1.7319630 0.9841720 2.2181860 -0.0361020 0.4763910 -0.0680270 0.5775130 1.1139560 -0.5229720 -1.4121240 -0.0648180 2.3445890 0.0380510 -2.2824670 0.5535140 2.3840390 -0.0777720 -1.5867790 -1.3357460 -2.4943410 -1.5926570 -0.6376870 2.3262340 1.3023010 -0.8084660 1.5112110 0.1144630 0.4025380 -1.2619310 2.1352430 -1.5007960 0.8994980 -1.4543410	-438.419573259 -438.419573259 -438.419573259 -438.419573259 -438.419573259 -438.419573259 -438.419573259 -0.1817750 1.7319630 0.2297290 0.9841720 2.2181860 -0.1500650 -0.0361020 0.4763910 -0.4628620 -0.0680270 0.5775130 -1.5652790 1.1139560 -0.5229720 -0.1627380 -1.4121240 -0.0648180 -0.1094900 2.3445890 0.0380510 -0.6489190 -2.2824670 0.5535140 0.4471650 2.3840390 -0.0777720 -1.6036950 -1.5867790 -1.3357460 -0.5504920 -2.4943410 -1.5926570 -0.3275180 -0.6376870 2.3262340 0.1978920 1.3023010 -0.8084660 1.3182760 1.5112110 0.1144630 1.8591870 0.4025380 -1.2619310 1.7424290 2.1352430 -1.5007960 1.4536870

C	-1 3696230	-0 1852730	-0 2634130	
Н	0.9047870	-1.5375830	-0.5885290	
0	2.3731940	-0.0642630	-0.5614340	
0	-1.8262880	-1.1420120	-0.8392560	
Н	2.4433800	-0.1874710	-1.5140110	
0	-2.0050560	0.4161360	0.7684730	
Н	-2.8430940	-0.0525380	0.9016740	
Н	-0.1513670	1.8747930	0.8758690	
С	1.2096440	-0.7435270	1.3898780	
Н	0.2820100	-1.1456050	1.8041870	
Н	2.0206390	-1.4350610	1.6241060	
H	1.4265890	0.2094520	1.8780310	
Energy	r: −438.41920694	6		
B3LYP/	'6-311++G** geome	etry and energy	y of conformer:	aThr-XXXII
N	0.6360290	-1,7147460	-0.6782690	
Н	1.4463640	-1.8474740	-1.2763470	
С	0.1260780	-0.3333750	-0.7607010	
Н	0.0483420	0.0412720	-1.7873440	
С	-1.2941420	-0.2942860	-0.1382370	
С	1.0890680	0.6146040	-0.0253170	
Н	-1.8892340	-1.0277730	-0.7077490	
0	-1.2724610	-0.6689130	1.2366920	
0	1.1258660	1.7964580	-0.2380460	
Н	-0.8513700	-1.5317270	1.3203570	
0	1.8895720	0.0227330	0.8783280	
H	1.6/93/40	-0.9296760	0.8684910	
H	-0.0663670	-2.3808020	-0.98/2310	
C	-1.9/384/0	1.0612120	-0.2317380	
п u	-2.0310870	1.3030040	-1.2722620	
H	-1.4161520	1.8164850	0.3226510	
Energy	r: −438.41919713	8		
B3LYP/	'6-311++G** geome	etry and energy	y of conformer:	aThr-XL
N	0 1160/00	1 7012060	0 0305650	
П 11	U.II0049U _0 1070050	1 8038380 1 8038380	0.0303630 1 0197390	
C	-0 0144460	1.0030300 0.4664790	-0.5483330	
Н	0.0381530	0.5659550	-1.6365240	
C	1.1046640	-0.5515510	-0.1812790	
C	-1.3662090	-0.1692940	-0.2703360	
H	0.9100480	-1.4657550	-0.7549530	
0	2.3070470	0.0692350	-0.6551790	
0	-1.8177810	-1.0967290	-0.8952930	
Н	3.0578080	-0.4868000	-0.4249410	
0	-2.0079600	0.3747400	0.7895210	
Н	-2.8461970	-0.1013870	0.8906260	
Н	1.0697760	2.1205210	-0.0912600	
С	1.1972990	-0.8853830	1.3042570	
Н	0.2884630	-1.3805060	1.6571220	
Н	2.0312690	-1.5700360	1.4875330	

Н	1.3623510	0.0146320	1.9014630	
Energy.	-438,41889118	7		
<u> </u>	100.11009110	,		
B3LYP/6-	-311++G** geome	try and energy	of conformer:	aThr-XLI
N	0.0599990	1.6321440	0.4792430	
Н	0.9234720	2.1254710	0.2785740	
С	-0.0533750	0.4791110	-0.4031710	
Н	-0.0900630	0.7569020	-1.4755980	
С	1.1745770	-0.4496830	-0.2451280	
С	-1.3555570	-0.2821510	-0.1975960	
H	1.0260490	-1.3100550	-0.9041150	
0	2.3498320	0.2770920	-0.6461600	
0	-1.5193740	-1.4517870	-0.4420200	
Н	2.3899740	0.2997880	-1.6076230	
0	-2.3600550	0.5185600	0.2276090	
Н	-3.1559630	-0.0307380	0.2945600	
H	-0.7192330	2.2694230	0.3682110	
C	1.4075370	-0.9328440	1.1778130	
H	0.5521680	-1.5134410	1.5296060	
H	2.2928790	-1.5708260	1.2032070	
Н	1.5583990	-0.0890520	1.8515290	
Energy:	-438.418624880	0		
N	0 0268110	1 9/9/890	-0.2850380	
Н	-0 2374930	2 2114810	0.6597180	
C	0.0267550	2.2111010	0.00071100	
0		0.49/3090	-0.4321480	
Н	0.1437040	0.4973090	-0.4321480 -1.4934780	
H C	0.1437040	0.4973090 0.2536750 -0.2629990	-0.4321480 -1.4934780 0.3724790	
H C C	0.1437040 1.1205680 -1.3393300	0.4973090 0.2536750 -0.2629990 0.0003810	-0.4321480 -1.4934780 0.3724790 0.0239950	
H C C H	0.1437040 1.1205680 -1.3393300 0.8883830	0.4973090 0.2536750 -0.2629990 0.0003810 -1.6729650	-0.4321480 -1.4934780 0.3724790 0.0239950 0.3388900	
Н С С Н О	0.1437040 1.1205680 -1.3393300 0.8883830 -1.8727140	0.4973090 0.2536750 -0.2629990 0.0003810 -1.6729650 0.3438790	-0.4321480 -1.4934780 0.3724790 0.0239950 0.3388900 1.0484700	
H C C H O O	0.1437040 1.1205680 -1.3393300 0.8883830 -1.8727140 0.9854550	0.4973090 0.2536750 -0.2629990 0.0003810 -1.6729650 0.3438790 -1.9875030	$\begin{array}{c} -0.4321480\\ -1.4934780\\ 0.3724790\\ 0.0239950\\ 0.3388900\\ 1.0484700\\ -0.5674330\end{array}$	
Н С Н О О Н	0.1437040 1.1205680 -1.3393300 0.8883830 -1.8727140 0.9854550 -1.8924150	0.4973090 0.2536750 -0.2629990 0.0003810 -1.6729650 0.3438790 -1.9875030 -0.8746120	-0.4321480 -1.4934780 0.3724790 0.0239950 0.3388900 1.0484700 -0.5674330 -0.8413710	
Н С Н О Н О	0.1437040 1.1205680 -1.3393300 0.8883830 -1.8727140 0.9854550 -1.8924150 -2.7314450	0.4973090 0.2536750 -0.2629990 0.0003810 -1.6729650 0.3438790 -1.9875030 -0.8746120 -1.1706370	$\begin{array}{c} -0.4321480\\ -1.4934780\\ 0.3724790\\ 0.0239950\\ 0.3388900\\ 1.0484700\\ -0.5674330\\ -0.8413710\\ -0.4549520\end{array}$	
H C H O H O H	$\begin{array}{c} 0.1437040\\ 1.1205680\\ -1.3393300\\ 0.8883830\\ -1.8727140\\ 0.9854550\\ -1.8924150\\ -2.7314450\\ 0.9310490 \end{array}$	0.4973090 0.2536750 -0.2629990 0.0003810 -1.6729650 0.3438790 -1.9875030 -0.8746120 -1.1706370 2.3511810	$\begin{array}{c} -0.4321480\\ -1.4934780\\ 0.3724790\\ 0.0239950\\ 0.3388900\\ 1.0484700\\ -0.5674330\\ -0.8413710\\ -0.4549520\\ -0.5002150\end{array}$	
Н С Н О О Н Н Н	0.1437040 1.1205680 -1.3393300 0.8883830 -1.8727140 0.9854550 -1.8924150 -2.7314450 0.9310490 2.5329310	0.4973090 0.2536750 -0.2629990 0.0003810 -1.6729650 0.3438790 -1.9875030 -0.8746120 -1.1706370 2.3511810 0.0747600	$\begin{array}{c} -0.4321480\\ -1.4934780\\ 0.3724790\\ 0.0239950\\ 0.3388900\\ 1.0484700\\ -0.5674330\\ -0.8413710\\ -0.4549520\\ -0.5002150\\ -0.0974310\end{array}$	
Н С Н О О Н О Н Н С	0.1437040 1.1205680 -1.3393300 0.8883830 -1.8727140 0.9854550 -1.8924150 -2.7314450 0.9310490 2.5329310 2.6678520	0.4973090 0.2536750 -0.2629990 0.0003810 -1.6729650 0.3438790 -1.9875030 -0.8746120 -1.1706370 2.3511810 0.0747600 -0.1911870	$\begin{array}{c} -0.4321480\\ -1.4934780\\ 0.3724790\\ 0.0239950\\ 0.3388900\\ 1.0484700\\ -0.5674330\\ -0.8413710\\ -0.4549520\\ -0.5002150\\ -0.9974310\\ -1.1522650\end{array}$	
н С С Н О О Н О Н Н С Н	0.1437040 1.1205680 -1.3393300 0.8883830 -1.8727140 0.9854550 -1.8924150 -2.7314450 0.9310490 2.5329310 2.6678520 2.7585780	0.4973090 0.2536750 -0.2629990 0.0003810 -1.6729650 0.3438790 -1.9875030 -0.8746120 -1.1706370 2.3511810 0.0747600 -0.1911870 1.1382450	$\begin{array}{c} -0.4321480\\ -1.4934780\\ 0.3724790\\ 0.0239950\\ 0.3388900\\ 1.0484700\\ -0.5674330\\ -0.8413710\\ -0.4549520\\ -0.5002150\\ -0.5002150\\ -0.0974310\\ -1.1522650\\ 0.0163480\\ 0.4624511\end{array}$	
H C C H O O H O H H C H H H	0.1437040 1.1205680 -1.3393300 0.8883830 -1.8727140 0.9854550 -1.8924150 -2.7314450 0.9310490 2.5329310 2.6678520 2.7585780 3.2597610 1.0000000000000000000000000000000000	0.4973090 0.2536750 -0.2629990 0.0003810 -1.6729650 0.3438790 -1.9875030 -0.8746120 -1.1706370 2.3511810 0.0747600 -0.1911870 1.1382450 -0.4868530	$\begin{array}{c} -0.4321480\\ -1.4934780\\ 0.3724790\\ 0.0239950\\ 0.3388900\\ 1.0484700\\ -0.5674330\\ -0.8413710\\ -0.4549520\\ -0.5002150\\ -0.5002150\\ -0.0974310\\ -1.1522650\\ 0.0163480\\ 0.4926240\\ 1.4026240\\ \end{array}$	
н С С н О О Н О Н Н Н Н Н Н Н Н Н	0.1437040 1.1205680 -1.3393300 0.8883830 -1.8727140 0.9854550 -1.8924150 -2.7314450 0.9310490 2.5329310 2.6678520 2.7585780 3.2597610 1.0032910	$\begin{array}{c} 0.4973090\\ 0.2536750\\ -0.2629990\\ 0.0003810\\ -1.6729650\\ 0.3438790\\ -1.9875030\\ -0.8746120\\ -1.1706370\\ 2.3511810\\ 0.0747600\\ -0.1911870\\ 1.1382450\\ -0.4868530\\ 0.0080470 \end{array}$	$\begin{array}{c} -0.4321480\\ -1.4934780\\ 0.3724790\\ 0.0239950\\ 0.3388900\\ 1.0484700\\ -0.5674330\\ -0.8413710\\ -0.4549520\\ -0.5002150\\ -0.974310\\ -1.1522650\\ 0.0163480\\ 0.4926240\\ 1.4256370\end{array}$	
H C C H O O H H C H H H Energy:	0.1437040 1.1205680 -1.3393300 0.8883830 -1.8727140 0.9854550 -1.8924150 -2.7314450 0.9310490 2.5329310 2.6678520 2.7585780 3.2597610 1.0032910 -438.418486184	0.4973090 0.2536750 -0.2629990 0.0003810 -1.6729650 0.3438790 -1.9875030 -0.8746120 -1.1706370 2.3511810 0.0747600 -0.1911870 1.1382450 -0.4868530 0.0080470	$\begin{array}{c} -0.4321480\\ -1.4934780\\ 0.3724790\\ 0.0239950\\ 0.3388900\\ 1.0484700\\ -0.5674330\\ -0.8413710\\ -0.4549520\\ -0.5002150\\ -0.0974310\\ -1.1522650\\ 0.0163480\\ 0.4926240\\ 1.4256370\end{array}$	
H C C H O O H O H H H Energy:	0.1437040 1.1205680 -1.3393300 0.8883830 -1.8727140 0.9854550 -1.8924150 -2.7314450 0.9310490 2.5329310 2.6678520 2.7585780 3.2597610 1.0032910 -438.418486184	0.4973090 0.2536750 -0.2629990 0.0003810 -1.6729650 0.3438790 -1.9875030 -0.8746120 -1.1706370 2.3511810 0.0747600 -0.1911870 1.1382450 -0.4868530 0.0080470	$\begin{array}{c} -0.4321480\\ -1.4934780\\ 0.3724790\\ 0.0239950\\ 0.3388900\\ 1.0484700\\ -0.5674330\\ -0.8413710\\ -0.4549520\\ -0.5002150\\ -0.5002150\\ -0.0974310\\ -1.1522650\\ 0.0163480\\ 0.4926240\\ 1.4256370\end{array}$	
H C C H O O H H H Energy: B3LYP/6-	0.1437040 1.1205680 -1.3393300 0.8883830 -1.8727140 0.9854550 -1.8924150 -2.7314450 0.9310490 2.5329310 2.6678520 2.7585780 3.2597610 1.0032910 -438.418486184	0.4973090 0.2536750 -0.2629990 0.0003810 -1.6729650 0.3438790 -1.9875030 -0.8746120 -1.1706370 2.3511810 0.0747600 -0.1911870 1.1382450 -0.4868530 0.0080470 4	-0.4321480 -1.4934780 0.3724790 0.0239950 0.3388900 1.0484700 -0.5674330 -0.8413710 -0.4549520 -0.5002150 -0.0974310 -1.1522650 0.0163480 0.4926240 1.4256370	aThr-XLI
H C C H O O H H H H Energy: B3LYP/6- N	0.1437040 1.1205680 -1.3393300 0.8883830 -1.8727140 0.9854550 -1.8924150 -2.7314450 0.9310490 2.5329310 2.6678520 2.7585780 3.2597610 1.0032910 -438.418486184 -311++G** geometric 0.0038330 0.1058330	0.4973090 0.2536750 -0.2629990 0.0003810 -1.6729650 0.3438790 -1.9875030 -0.8746120 -1.1706370 2.3511810 0.0747600 -0.1911870 1.1382450 -0.4868530 0.0080470 4 try and energy 1.9340960	-0.4321480 -1.4934780 0.3724790 0.0239950 0.3388900 1.0484700 -0.5674330 -0.8413710 -0.4549520 -0.5002150 -0.0974310 -1.1522650 0.0163480 0.4926240 1.4256370 of conformer: -0.1693510	aThr-XLI:
H C C H O O H H H Energy: B3LYP/6- N H C	0.1437040 1.1205680 -1.3393300 0.8883830 -1.8727140 0.9854550 -1.8924150 -2.7314450 0.9310490 2.5329310 2.6678520 2.7585780 3.2597610 1.0032910 -438.418486184 -311++G** geometry 0.0038330 -0.1052730 0.01652730	0.4973090 0.2536750 -0.2629990 0.0003810 -1.6729650 0.3438790 -1.9875030 -0.8746120 -1.1706370 2.3511810 0.0747600 -0.1911870 1.1382450 -0.4868530 0.0080470 4 try and energy 1.9340960 2.1421130 0.022000	-0.4321480 -1.4934780 0.3724790 0.0239950 0.3388900 1.0484700 -0.5674330 -0.8413710 -0.4549520 -0.5002150 -0.0974310 -1.1522650 0.0163480 0.4926240 1.4256370 of conformer: -0.1693510 0.8183050 0.4024010	aThr-XLI
H C C H O O H O H H Energy: B3LYP/6- N H C U	 0.1437040 1.1205680 -1.3393300 0.8883830 -1.8727140 0.9854550 -1.8924150 -2.7314450 0.9310490 2.5329310 2.6678520 2.7585780 3.2597610 1.0032910 -438.418486184 -311++G** geometric structure 0.0038330 -0.1052730 0.0164960 0.022020 	0.4973090 0.2536750 -0.2629990 0.0003810 -1.6729650 0.3438790 -1.9875030 -0.8746120 -1.1706370 2.3511810 0.0747600 -0.1911870 1.1382450 -0.4868530 0.0080470 4 try and energy 1.9340960 2.1421130 0.4920620 0.21171220	-0.4321480 -1.4934780 0.3724790 0.0239950 0.3388900 1.0484700 -0.5674330 -0.8413710 -0.4549520 -0.5002150 -0.0974310 -1.1522650 0.0163480 0.4926240 1.4256370 of conformer: -0.1693510 0.8183050 -0.4034210 1.4771600	aThr-XLI:
H C C H O O H D H H C H H H Energy: 33LYP/6- N H C H S S LYP/6-	 0.1437040 1.1205680 -1.3393300 0.8883830 -1.8727140 0.9854550 -1.8924150 -2.7314450 0.9310490 2.5329310 2.6678520 2.7585780 3.2597610 1.0032910 -438.418486184 -311++G** geometee 0.0038330 -0.1052730 0.0164960 0.1032880 1.202022 	0.4973090 0.2536750 -0.2629990 0.0003810 -1.6729650 0.3438790 -1.9875030 -0.8746120 -1.1706370 2.3511810 0.0747600 -0.1911870 1.1382450 -0.4868530 0.0080470 4 try and energy 1.9340960 2.1421130 0.4920620 0.3117130	-0.4321480 -1.4934780 0.3724790 0.0239950 0.3388900 1.0484700 -0.5674330 -0.8413710 -0.4549520 -0.5002150 -0.0974310 -1.1522650 0.0163480 0.4926240 1.4256370 of conformer: -0.1693510 0.8183050 -0.4034210 -1.4771620 0.2174620	aThr-XLI:

С	-1.3357000	-0.0332250	0.0705410	
Н	0.8920210	-1.6714830	-0.0092250	
0	-1.7271390	0.0617790	1.2081790	
0	1.4432230	-2.2300600	0.5473130	
Н	-2.0625820	-0.5888090	-0.9163210	
0	-2.8983930	-0.8871390	-0.5249990	
Н	0.8461640	2.3795070	-0.5120130	
Н	2.5341250	0.1330920	-0.1030470	
С	2.6693560	0.0023930	-1.1804340	
H	2.7294670	1.1766100	0.1577870	
Н	3,2865490	-0.4737720	0.4092930	
Н	0.9988180	-0.1427950	1.3968810	
Energy:	-438.41845256	6		
B3LYP/6-	311++G** geome	try and energy	of conformer:	aThr-X
N	-0.0455280	1.9367630	-0.2061400	
Н	-0.1887880	2.1425040	0.7771550	
С	0.0279720	0.4957670	-0.4449290	
Н	0.2048410	0.3408670	-1.5135940	
С	1.1194150	-0.2669840	0.3558420	
С	-1.3398130	-0.1187500	-0.1701290	
Н	0.9247230	-1.6792590	0.2607830	
0	-1.9807270	-0.7765840	-0.9468330	
0	1.0125110	-1.9529650	-0.6598550	
Н	-1.7642920	0.1654240	1.0848540	
0	-2.6297530	-0.2544270	1.2012160	
Н	0.7927250	2.4100440	-0.5211210	
Н	2.5318920	0.1310990	-0.0642680	
C	2 6996560	-0 0866540	-1 1251800	
ч	2 7172770	1 1962070	0.0980560	
и П	2.7172770	_0 4312410	0.5199490	
H	0.9730420	-0.04512410	1.4168360	
	0.9700120	0.0101220	1.1100500	
Energy:	-438.41753852	5		
B3LYP/6-	311++G** geome	try and energy	y of conformer:	aThr-X
N	-0.6382970	1.7886960	-0.7431980	
Н	-0.7408820	2.1275400	0.2080560	
С	-0.1061070	0.4312490	-0.7415080	
Н	-0.0134340	0.0964850	-1.7783520	
С	1.3005580	0.2887740	-0.0976160	
С	-1.0849280	-0.5438160	-0.0922730	
Н	1.9208620	1.0546230	-0.5880870	
0	1.1418100	0.6256430	1.2843090	
0	-1.1027660	-1.7297610	-0.3195450	
- H	1,9968640	0.5695110	1.7218240	
	_1 0215600	0 0/16350	1 7856700	
ц	-2 ATAGGEO	_0 6506100	1 1615000	
11 LI		-U.UJUUUU	1 00007C0	
п	-0.0023670	2.413343U	-1.2203/0U	
	T.A0TA0TO	-1.0/32440	-U.28388/U	
н	2.06/1/60	-1.309/660	-1.34643/0	
H	2.9656270	-1.0643190	0.1539500	
Н	1.3801280	-1.8665770	0.1864610	

NT.	0 2550060	1 7401000	0 0060010	
IN II	0.3558960	1.7481230	0.0362010	
H	-0.0559220	1.8589370	0.9588270	
C	-0.0207130	0.4567710	-0.5268660	
H	-0.0252070	0.5493140	-1.6183380	
C	1.0893950	-0.5881020	-0.18/0610	
C	-1.4060030	-0.01//110	-0.0/14990	
H	0.903/100	-1.504//40	-0./5/6010	
0	2.3221510	-0.0845930	-0.6/23440	
0	-2.0295290	0.4930570	0.81/1010	
H	2.3587660	0.8394380	-0.3/931/0	
0	-1.9064660	-1.1004470	-0./21/200	
H	-1.3048/20	-1.3941080	-1.41//220	
H	0.0037790	2.5097580	-0.5319310	
C II	1.1636080	-0.9330210	1.299966U	
H	U.2425560	-1.4046050	1.6544690	
Н	1.991/210	-1.6242730	1.465/910	
н	1.34/22/0	-0.0383170	T.9008/80	
Energy:	-438.41718576	3		
B3LYP/6-	311++G** geome	try and energy	of conformer:	aThr-XLVI
N	-0.5905490	1.8438300	-0.7329650	
Н	-0.8834180	2.1235550	0.1980120	
С	-0.1223480	0.4652020	-0.7113660	
Н	-0.0746820	0.0882300	-1.7383740	
С	1.2938100	0.2717370	-0.1001210	
С	-1.1690060	-0.3646570	0.0264360 🤇	
Н	1.1808860	0.5692470	1.2926410	
0	-1.9747600	0.0660140	0.8067460	
0	2.0513210	0.5128730	1.6987630	
Н	-1.0983430	-1.6800000	-0.3012260	
0	-1.7768140	-2.1359900	0.2200050	
Н	0.1469160	2.4699440	-1.0370480	
Н	1.9292480	-1.0949150	-0.3447810	
С	1.3617000	-1.8910660	0.1372870	
н	1.9860430	-1.3103150	-1.4156160	
11	2,9509190	-1.1062770	0.0483960	
Н	2.0001100	T • T 0 0 D / / 0		
H H	1.9193640	1.0359460	-0.5869620	
H H Energy:	-438.41717749	1.0359460	-0.5869620	
H H Energy:	-438.41717749	1.0359460	-0.5869620	
H H Energy: B3LYP/6-	1.9193640 -438.41717749 311++G** geome	1.0359460 5 try and energy	-0.5869620	aThr-XLVI
H H Energy: B3LYP/6- N	-438.41717749 311++G** geome -0.0648050	1.0359460 5 try and energy 1.9323990	-0.5869620 of conformer: 0.2208920	aThr-XLVI

C 0.0275030 0.5807890 -0.3372480 H 0.1865160 0.6668680 -1.4138140 C 1.3512130 -0.0559220 -0.1865640 H 0.9984870 -1.6694720 -0.1353060 O -2.1636270 -0.2075310 -1.0559210 O 0.2261250 -2.0745960 0.3840540 H -1.5844570 -0.4332680 1.1053300 D -2.4959840 -0.7607670 1.1480070 H 0.6713660 2.5330950 -0.1284930 C 2.6314650 0.0208920 -1.2584160 H 2.7122450 1.1871550 0.0812380 H 3.2942640 -0.4639350 0.3075700 H 1.0712010 -0.2356560 1.3651460 Energy: -438.417071201 B3LYP/6-311++G** geometry and energy of conformer: aThr-XL N -0.0573360 1.9225070 -0.1069100 H 0.1259560 2.0790760 0.8931060 C 0.0163750 0.4972920 -0.4275210 H 0.1735790 0.390810 -1.5028890 C 1.1212660 -0.2918920 0.3096250 C 1.1212600 -0.5680630 -0.9733170 D 1.5250300 -2.2151420 0.4488010 H 0.9221570 -1.610010 -0.46674840 H 2.5251150 0.1819250 -0.4656290 H 3.2776150 -0.4132740 0.4698370 H 2.6827040 1.2255780 0.2283650 H 3.2776150 -0.11692770 1.3889920 Energy: -438.416792961 B3LYP/6-311++G** geometry and energy of conformer: aThr-L N 0.1681890 1.7389080 -0.4087770 H 2.0420730 0.2283650 -0.9801700 C -0.0183250 0.3166590 -0.6332220 H 3.2776150 -0.1692270 1.3889920 Energy: -438.416792961 B3LYP/6-311++G** geometry and energy of conformer: aThr-L N 0.1681890 1.738950 -0.540580 D .1238950 -0.540680 0.0105050 C 1.7354000 -0.2792130 -0.6669710 D -2.8552770 0.0158620 0.9101380 H 0.0031160 -0.4628690 -1.555880 H 2.0420730 0.4891780 0.6669710 D -2.8552770 0.0158620 0.9101380 H 0.0031160 -94628430 0.5					
 H. 0.1865160 0.666880 -1.4138140 L.1438060 -0.3054290 0.2715670 L.3512130 -0.0559220 -0.1865640 H. 0.9984870 -1.6659720 -0.1353060 C.2.1636270 -0.2075310 -1.0569210 D. 0.2861250 -2.0745860 1.1053300 C.2.4959840 -0.7607670 1.1480770 H. 0.6713660 2.5330950 -0.1284930 H. 2.525940 0.1412120 -0.1763030 C.2.6314650 0.0208920 -1.2584460 H. 3.2942640 -0.469350 0.3075700 H. 3.2942640 -0.469350 0.3075700 H. 1.0712010 -0.2356560 1.3651460 Energy: -438.417071201 B3LYP/6-311++G** geometry and energy of conformer: aThr-XL N -0.0573360 1.9225070 -0.1069100 H. 0.1735790 0.390810 -1.5028890 C. 1.1212660 -0.218920 0.3096250 C. 1.1212660 -0.218920 0.3096250 C. 1.3570770 -0.1096890 -0.1534670 H. 0.9221590 -1.610010 -0.0564140 D.9221590 -1.610010 -0.0564140 D.9221590 -1.610010 -0.056420 C. 2.6978170 0.0751120 -1.1309000 H. 2.5251150 0.1819250 -0.4662830 H. 3.2776150 -0.4132740 0.4698370 H. 3.2776150 -0.4132740 0.4698370 H. 3.2776150 -0.4132740 0.4698370 H. 3.2776150 -0.4132740 0.4698370 H. 0.9566620 -0.1692270 1.388920 Energy: -438.416792961 B3LYP/6-311++G** geometry and energy of conformer: aThr-L N 0.1681890 1.738908 -0.4087770 H. 0.2682700 0.22836560 -0.9801700 L.6675240 -0.269570 -0.1916330 H. 2.5754000 -0.2792130 -0.16310770 H. 0.9566620 -0.1692270 1.3889920 Energy: -438.416792961 B3LYP/6-311++G** geometry and energy of conformer: aThr-L N 0.1681890 1.738908 -0.4087770 H. 0.2682700 -0.2792130 -0.46689710 D.2.852770 0.0158620 0.19161330 H. 2.692700 -0.2806720 -0.1916330	С	0.0275030	0.5807890	-0.3372480	
<pre>c 1.1458060 - 0.3054290 0.2715670 C -1.3512130 - 0.0559220 - 0.1865640 H 0.9984870 - 1.6594720 - 0.1353060 D -2.1636270 - 0.2075310 - 1.0569210 D 0.2961250 - 2.0745960 0.3840540 H -1.5844570 - 0.4332680 1.1053300 D -2.4959840 - 0.7607670 1.1480070 D -2.4959840 - 0.7607670 1.1480070 H 0.6713660 2.530950 - 0.128430 H 2.5295940 0.1412120 - 0.1763030 C 2.6314650 0.0208920 - 1.2584160 H 2.7122450 1.1871550 0.0812380 H 3.2942640 - 0.4689350 0.3075700 H 1.0712010 - 0.2356560 1.3651460 Energy: -438.417071201 B3LYP/6-311++G** geometry and energy of conformer: aThr-XL N -0.0573360 1.9225070 - 0.1069100 H -0.1259560 2.0790760 0.8931060 C 0.0163750 0.4972920 - 0.4275210 H 0.1735790 0.3330810 - 1.5028890 C 1.1212660 - 0.2918920 0.3096250 C 1.1212660 - 0.2918920 0.3096250 C 1.121260 - 0.2918920 0.3096250 C 1.121260 - 0.2918920 0.3096250 C 1.557070 - 0.1066930 - 0.9733170 D 1.525030 - 2.2151420 0.4488010 H -1.6675240 - 0.366070 1.1687650 H 0.9221590 - 1.6610010 - 0.0564140 D -2.1050290 - 2.2151420 0.4488010 H -1.6675240 - 0.0366770 1.1687650 H 0.7406910 2.4308070 - 0.4674840 H 2.5251150 0.1819250 - 0.0562920 C 2.6978170 0.0751120 - 1.1309000 H 2.6878170 0.0751120 - 1.1309000 H 2.6878170 0.0751120 - 1.1309000 H 2.687640 1.2255780 0.2283650 H 3.2776150 - 0.4132740 0.4698370 H 0.9566620 - 0.169270 1.3889920 Energy: -438.416792961 Energy: -0.5568850 - 0.9801700 D -1.7794660 - 1.7292430 - 0.5568850 Energy: -438.416792961 Energy: -0.2869570 - 0.1916390 Energy: -438.416792961 Energy: -0.2869570 - 0.1916390 Energy: -2.852770 0.04891780 - 0.5568850 Energy: -2.852770 0.04889780 - 0.5568850 Energy: -2.852770 0.04889780 - 0.5568850 Energy: -2.8562770 0.04688770 Energy: -2.8562770 0.0458620 - 0.191330 Energy: -2.856</pre>	Н	0.1865160	0.6668680	-1.4138140	
 -1.3512130 -0.0559220 -0.1865640 H 0.9994870 -1.6654720 -0.1333060 2.1636270 -0.275310 -1.0559210 0.2961250 -2.0745960 0.3840540 H 1.5844570 -0.4332680 1.1053300 D2.4959940 -0.7607670 1.1480070 H 0.6713660 2.5330950 -0.1284930 C.2.6314650 0.0208920 -1.2584160 H 2.7122450 1.1871550 0.0812380 H 3.2942640 -0.469350 0.3075700 H 1.0712010 -0.2356560 1.3651460 Energy: -438.417071201 B3LYP/6-311++G** geometry and energy of conformer: aThr-XL N -0.0573360 1.9225070 -0.1069100 H 0.1735790 0.3930810 -1.5028890 C.11212660 -0.2918920 -0.4275210 H 0.1735700 0.3930810 -1.5028890 C.11212660 -0.2918920 0.3096250 C.1.3570770 -0.1096990 -0.1534670 H 0.9221590 -1.6610010 -0.0564140 D.2.2150290 -0.22151420 0.4488010 E.2520330 -2.2151420 0.4488010 H 0.7406910 2.4308070 -0.4674840 D.72557320 -0.4040030 1.2742000 H 0.7406910 2.4308070 -0.4674840 H 2.6827040 1.2255780 0.2283500 H 3.2776150 -0.11692270 1.3889920 Energy: -438.416792961 Energy: -438.416792961 Energy: -438.416792961 Energy: -438.416792961 Energy: -438.416792961 Energy: -438.416792961 	С	1.1458060	-0.3054290	0.2715670	
 B. 0.994870 - 1.6694720 - 0.1353060 -2.1636270 - 0.2075310 - 1.0569210 0.2961250 - 2.0745960 0.3840540 H1.5844570 - 0.4332680 1.1053300 -2.4959840 - 0.7607670 1.1480070 H. 0.6713660 2.5330950 - 0.1284930 E. 2.5295940 0.1412120 - 0.1763030 C. 2.6314650 0.0208920 - 1.2584160 H. 2.7122450 1.1871550 0.0812380 H. 3.2942640 - 0.4689350 0.3075700 H. 1.0712010 - 0.2356560 1.3651460 Energy: -438.417071201 B3LYP/6-311++G** geometry and energy of conformer: aThr-XL N - 0.0573360 1.9225070 - 0.1069100 H. 0.1259560 2.0790760 0.8931060 C. 0.0163750 0.4972920 - 0.4275210 H. 0.1735790 0.3930810 - 1.5028890 C. 1.1212660 - 0.2918920 0.3096250 C. 1.1212660 - 0.2918920 0.3096250 C. 1.1212600 - 0.25680630 - 0.9733170 D. 2.20507720 - 0.1069100 H. 0.9221590 - 1.6610010 - 0.0564140 D2.1050720 - 0.1096890 - 0.1534670 H. 0.9221590 - 1.6610010 - 0.0564140 D2.1057230 - 0.4040303 1.2742000 H. 0.7406910 2.4308070 - 0.4674840 H. 0.7406910 2.4308070 - 0.4674840 H. 0.7406910 2.4308070 - 0.467840 H. 2.6827040 1.2255780 0.2283650 H. 3.2775150 - 0.1639270 1.3889920 Energy: -438.416792961 	C	-1.3512130	-0.0559220	-0.1865640	
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D -2.1050290 -0.5680630 -0.9733170 D 1.5250330 -2.2151420 0.4488010 H -1.6675240 -0.0366070 1.1687650 D -2.5577230 -0.4040030 1.2742000 H 0.7406910 2.4308070 -0.4674840 H 2.5251150 0.1819250 -0.0562920 C 2.6978170 0.0751120 -1.1309000 H 2.6827040 1.2255780 0.2283650 H 3.2776150 -0.4132740 0.4698370 H 0.9566620 -0.1692270 1.3889920 Energy: -438.416792961 B3LYP/6-311++G** geometry and energy of conformer: aThr-L N 0.1681890 1.7389080 -0.4087770 H -0.4670730 2.2836560 -0.9801700 C -0.0183250 0.3166690 -0.6232220 H 0.0232430 0.1278760 -1.7014860 C 1.1238950 -0.5400840 0.0105050 C -1.3612990 -0.2869570 -0.1916390 H 2.3754000 -0.2792130 -0.6131070 D -1.7794660 -1.3524310 -0.5726170 D 2.3071610 -0.4628690 -1.5555890 H -2.0420730 0.4891780 0.6869710 D -2.852770 0.0158620 0.9101380 H 0.0031160 1.9980240 0.5568850 H 1.3212950 -0.2806720 1.4973230 C 1.6503850 0.7473300 1.6645180	Н	0.9221590	-1.6610010	-0.0564140	
D 1.5250330 -2.2151420 0.4488010 H -1.6675240 -0.0366070 1.1687650 D 2.5577230 -0.4040030 1.2742000 H 0.7406910 2.4308070 -0.4674840 H 2.5251150 0.1819250 -0.0562920 C 2.6978170 0.0751120 -1.1309000 H 2.6827040 1.2255780 0.2283650 H 3.2776150 -0.4132740 0.4698370 H 0.9566620 -0.1692270 1.3889920 Energy: -438.416792961 B3LYP/6-311++G** geometry and energy of conformer: aThr-L N 0.1681890 1.7389080 -0.4087770 H -0.4670730 2.2836560 -0.9801700 C -0.0183250 0.3166690 -0.6232220 H 0.0232430 0.1278760 -1.7014860 C 1.1238950 -0.5400840 0.0105050 C -1.3612990 -0.2869570 -0.1916390 H 2.3754000 -0.2792130 -0.6131070 D -1.7794660 -1.3524310 -0.5726170 D 2.3071610 -0.4628690 -1.5555890 H -2.0420730 0.4891780 0.6869710 D -1.779460 1.980240 0.5568850 H -2.0420730 0.4891780 0.6869710 D -1.755890 H -2.0420730 0.4891780 0.6869710 D -2.8582770 0.0158620 0.9101380 H 0.0031160 1.9980240 0.5568850 H 1.3212950 -0.2806720 1.4973230 C 1.6503850 0.7473300 1.6645180	0	-2.1050290	-0.5680630	-0.9733170	
H -1.6675240 -0.0366070 1.1687650 -2.5577230 -0.4040030 1.2742000 H 0.7406910 2.4308070 -0.4674840 H 2.5251150 0.1819250 -0.0562920 C 2.6978170 0.0751120 -1.1309000 H 2.6827040 1.2255780 0.2283650 H 3.2776150 -0.4132740 0.4698370 H 0.9566620 -0.1692270 1.3889920 Energy: -438.416792961 B3LYP/6-311++G** geometry and energy of conformer: aThr-L N 0.1681890 1.7389080 -0.4087770 H -0.4670730 2.2836560 -0.9801700 C -0.0183250 0.3166690 -0.6232220 H 0.0232430 0.1278760 -1.7014860 C 1.1238950 -0.5400840 0.0105050 C -1.3612990 -0.2869570 -0.1916390 H 2.3754000 -0.2792130 -0.6131070 D -1.7794660 -1.3524310 -0.5726170 D 2.3071610 -0.4628690 -1.5555890 H -2.0420730 0.4891780 0.6869710 D -2.8582770 0.0158620 0.9101380 H 0.0031160 1.9980240 0.5568850 H 1.3212950 -0.2806720 1.4973230 C 1.6503850 0.7473300 1.6645180	0	1.5250330	-2.2151420	0.4488010	
D -2.5577230 -0.4040030 1.2742000 H 0.7406910 2.4308070 -0.4674840 H 2.5251150 0.1819250 -0.0562920 C 2.6978170 0.0751120 -1.1309000 H 2.6827040 1.2255780 0.2283650 H 3.2776150 -0.4132740 0.4698370 H 0.9566620 -0.1692270 1.3889920 Energy: -438.416792961 B3LYP/6-311++G** geometry and energy of conformer: aThr-L N 0.1681890 1.7389080 -0.4087770 H -0.4670730 2.2836560 -0.9801700 C -0.0183250 0.3166690 -0.6232220 H 0.0232430 0.1278760 -1.7014860 C 1.1238950 -0.5400840 0.0105050 C -1.3612990 -0.280570 -0.1916390 H 2.3754000 -0.2792130 -0.6131070 D -1.7794660 -1.3524310 -0.5726170 D 2.3071610 -0.4628690 -1.5555890 H -2.0420730	Н	-1.6675240	-0.0366070	1.1687650	
H 0.7406910 2.4308070 -0.4674840 H 2.5251150 0.1819250 -0.0562920 C 2.6978170 0.0751120 -1.1309000 H 2.6827040 1.2255780 0.2283650 H 3.2776150 -0.4132740 0.4698370 H 0.9566620 -0.1692270 1.3889920 Energy: -438.416792961 B3LYP/6-311++G** geometry and energy of conformer: aThr-L N 0.1681890 1.7389080 -0.4087770 H -0.4670730 2.2836560 -0.9801700 C -0.0183250 0.3166690 -0.6232220 H 0.0232430 0.1278760 -1.7014860 C 1.1238950 -0.5400840 0.0105050 C -1.3612990 -0.2869570 -0.1916390 H 2.3754000 -0.2792130 -0.6131070 D -1.7794660 -1.3524310 -0.5726170 D 2.3071610 -0.4628690 -1.5555890 H -2.0420730 0.4891780 0.6869710 D -2.8582770 0.0158620 0.9101380 H 0.0031160 1.9980240 0.5568850 H 1.3212950 -0.2806720 1.4973230 C 1.6503850 0.7473300 1.6645180	0	-2.5577230	-0.4040030	1.2742000	
H 2.5251150 0.1819250 -0.0562920 C 2.6978170 0.0751120 -1.1309000 H 2.6827040 1.2255780 0.2283650 H 3.2776150 -0.4132740 0.4698370 H 0.9566620 -0.1692270 1.3889920 Energy: -438.416792961 B3LYP/6-311++G** geometry and energy of conformer: aThr-L N 0.1681890 1.7389080 -0.4087770 H -0.4670730 2.2836560 -0.9801700 C -0.0183250 0.3166690 -0.6232220 H 0.0232430 0.1278760 -1.7014860 C 1.1238950 -0.5400840 0.0105050 C -1.3612990 -0.2869570 -0.1916390 H 2.3754000 -0.2792130 -0.6131070 D -1.7794660 -1.3524310 -0.5726170 D 2.3071610 -0.4628690 -1.5555890 H -2.0420730 0.4891780 0.6869710 D -2.8582770 0.0158620 0.9101380 H 0.0031160	Н	0.7406910	2.4308070	-0.4674840	
C 2.6978170 0.0751120 -1.1309000 H 2.6827040 1.2255780 0.2283650 H 3.2776150 -0.4132740 0.4698370 H 0.9566620 -0.1692270 1.3889920 Energy: -438.416792961 B3LYP/6-311++G** geometry and energy of conformer: aThr-L N 0.1681890 1.7389080 -0.4087770 H -0.4670730 2.2836560 -0.9801700 C -0.0183250 0.3166690 -0.6232220 H 0.0232430 0.1278760 -1.7014860 C 1.1238950 -0.5400840 0.0105050 C -1.3612990 -0.2869570 -0.1916390 H 2.3754000 -0.2792130 -0.6131070 O -1.7794660 -1.3524310 -0.5726170 O 2.3071610 -0.4628690 -1.5555890 H -2.0420730 0.4891780 0.6869710 O -2.8582770 0.0158620 0.9101380 H 0.0031160 1.9980240 0.5568850 H 1.3212950 -0.2806720 1.4973230 C 1.6503850 0.7473300 1.6645180	Н	2.5251150	0.1819250	-0.0562920	
H 2.6827040 1.2255780 0.2283650 H 3.2776150 -0.4132740 0.4698370 H 0.9566620 -0.1692270 1.3889920 Energy: -438.416792961 B3LYP/6-311++G** geometry and energy of conformer: aThr-L N 0.1681890 1.7389080 -0.4087770 H -0.4670730 2.2836560 -0.9801700 C -0.0183250 0.3166690 -0.6232220 H 0.0232430 0.1278760 -1.7014860 C 1.1238950 -0.5400840 0.0105050 C -1.3612990 -0.2869570 -0.1916390 H 2.3754000 -0.2792130 -0.6131070 O -1.7794660 -1.3524310 -0.5726170 O 2.3071610 -0.4628690 -1.5555890 H -2.0420730 0.4891780 0.6869710 O -2.8582770 0.0158620 0.9101380 H 0.0031160 1.9980240 0.5568850 H 1.3212950 -0.2806720 1.4973230 C 1.6503850	С	2.6978170	0.0751120	-1.1309000	
H 3.2776150 -0.4132740 0.4698370 H 0.9566620 -0.1692270 1.3889920 Energy: -438.416792961 B3LYP/6-311++G** geometry and energy of conformer: aThr-L N 0.1681890 1.7389080 -0.4087770 H -0.4670730 2.2836560 -0.9801700 C -0.0183250 0.3166690 -0.6232220 H 0.0232430 0.1278760 -1.7014860 C 1.1238950 -0.5400840 0.0105050 C -1.3612990 -0.2869570 -0.1916390 H 2.3754000 -0.2792130 -0.6131070 O -1.7794660 -1.3524310 -0.5726170 O 2.3071610 -0.4628690 -1.5555890 H -2.0420730 0.4891780 0.6869710 O -2.8582770 0.0158620 0.9101380 H 0.0031160 1.9980240 0.5568850 H 1.3212950 -0.2806720 1.4973230 C 1.6503850 0.7473300 1.6645180	Н	2.6827040	1.2255780	0.2283650	
H 0.9566620 -0.1692270 1.3889920 Energy: -438.416792961 B3LYP/6-311++G** geometry and energy of conformer: aThr-L N 0.1681890 1.7389080 -0.4087770 H -0.4670730 2.2836560 -0.9801700 C -0.0183250 0.3166690 -0.6232220 H 0.0232430 0.1278760 -1.7014860 C 1.1238950 -0.5400840 0.0105050 C -1.3612990 -0.2869570 -0.1916390 H 2.3754000 -0.2792130 -0.6131070 D -1.7794660 -1.3524310 -0.5726170 D 2.3071610 -0.4628690 -1.5555890 H -2.0420730 0.4891780 0.6869710 D -2.8582770 0.0158620 0.9101380 H 0.0031160 1.9980240 0.5568850 H 1.3212950 -0.2806720 1.4973230 C 1.6503850 0.7473300 1.6645180	Н	3.2776150	-0.4132740	0.4698370	
Energy: -438.416792961 B3LYP/6-311++G** geometry and energy of conformer: aThr-L N 0.1681890 1.7389080 -0.4087770 H -0.4670730 2.2836560 -0.9801700 C -0.0183250 0.3166690 -0.6232220 H 0.0232430 0.1278760 -1.7014860 C 1.1238950 -0.5400840 0.0105050 C -1.3612990 -0.2869570 -0.1916390 H 2.3754000 -0.2792130 -0.6131070 D -1.7794660 -1.3524310 -0.5726170 D 2.3071610 -0.4628690 -1.5555890 H -2.0420730 0.4891780 0.6869710 D -2.8582770 0.0158620 0.9101380 H 0.0031160 1.9980240 0.5568850 H 1.3212950 -0.2806720 1.4973230 C 1.6503850 0.7473300 1.6645180	Н	0.9566620	-0.1692270	1.3889920	
B3LYP/6-311++G** geometry and energy of conformer: aThr-L N 0.1681890 1.7389080 -0.4087770 H -0.4670730 2.2836560 -0.9801700 C -0.0183250 0.3166690 -0.6232220 H 0.0232430 0.1278760 -1.7014860 C 1.1238950 -0.5400840 0.0105050 C -1.3612990 -0.2869570 -0.1916390 H 2.3754000 -0.2792130 -0.6131070 D -1.7794660 -1.3524310 -0.5726170 D 2.3071610 -0.4628690 -1.5555890 H -2.0420730 0.4891780 0.6869710 D -2.8582770 0.0158620 0.9101380 H 0.0031160 1.9980240 0.5568850 H 1.3212950 -0.2806720 1.4973230 C 1.6503850 0.7473300 1.6645180	Energy:	-438.41679296	1		
B3LYP/6-311++G** geometry and energy of conformer: aThr-L N 0.1681890 1.7389080 -0.4087770 H -0.4670730 2.2836560 -0.9801700 C -0.0183250 0.3166690 -0.6232220 H 0.0232430 0.1278760 -1.7014860 C 1.1238950 -0.5400840 0.0105050 C -1.3612990 -0.2869570 -0.1916390 H 2.3754000 -0.2792130 -0.6131070 D -1.7794660 -1.3524310 -0.5726170 D 2.3071610 -0.4628690 -1.5555890 H -2.0420730 0.4891780 0.6869710 D -2.8582770 0.0158620 0.9101380 H 0.0031160 1.9980240 0.5568850 H 1.3212950 -0.2806720 1.4973230 C 1.6503850 0.7473300 1.6645180					
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	B3LYP/6-	-311++G** geome	try and energy	of conformer:	aThr-L
H -0.4670730 2.2836560 -0.9801700 C -0.0183250 0.3166690 -0.6232220 H 0.0232430 0.1278760 -1.7014860 C 1.1238950 -0.5400840 0.0105050 C -1.3612990 -0.2869570 -0.1916390 H 2.3754000 -0.2792130 -0.6131070 D -1.7794660 -1.3524310 -0.5726170 D 2.3071610 -0.4628690 -1.5555890 H -2.0420730 0.4891780 0.6869710 D -2.8582770 0.0158620 0.9101380 H 0.0031160 1.9980240 0.5568850 H 1.3212950 -0.2806720 1.4973230 C 1.6503850 0.7473300 1.6645180	N	0.1681890	1.7389080	-0.4087770	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Н	-0.4670730	2.2836560	-0.9801700	
H 0.0232430 0.1278760 -1.7014860 C 1.1238950 -0.5400840 0.0105050 C -1.3612990 -0.2869570 -0.1916390 H 2.3754000 -0.2792130 -0.6131070 D -1.7794660 -1.3524310 -0.5726170 D 2.3071610 -0.4628690 -1.5555890 H -2.0420730 0.4891780 0.6869710 D -2.8582770 0.0158620 0.9101380 H 0.0031160 1.9980240 0.5568850 H 1.3212950 -0.2806720 1.4973230 C 1.6503850 0.7473300 1.6645180	С	-0.0183250	0.3166690	-0.6232220	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Н	0.0232430	0.1278760	-1.7014860	
C -1.3612990 -0.2869570 -0.1916390 H 2.3754000 -0.2792130 -0.6131070 O -1.7794660 -1.3524310 -0.5726170 O 2.3071610 -0.4628690 -1.5555890 H -2.0420730 0.4891780 0.6869710 O -2.8582770 0.0158620 0.9101380 H 0.0031160 1.9980240 0.5568850 H 1.3212950 -0.2806720 1.4973230 C 1.6503850 0.7473300 1.6645180	С	1.1238950	-0.5400840	0.0105050	
H 2.3754000 -0.2792130 -0.6131070 O -1.7794660 -1.3524310 -0.5726170 O 2.3071610 -0.4628690 -1.5555890 H -2.0420730 0.4891780 0.6869710 O -2.8582770 0.0158620 0.9101380 H 0.0031160 1.9980240 0.5568850 H 1.3212950 -0.2806720 1.4973230 C 1.6503850 0.7473300 1.6645180	С	-1.3612990	-0.2869570	-0.1916390	
D -1.7794660 -1.3524310 -0.5726170 D 2.3071610 -0.4628690 -1.5555890 H -2.0420730 0.4891780 0.6869710 D -2.8582770 0.0158620 0.9101380 H 0.0031160 1.9980240 0.5568850 H 1.3212950 -0.2806720 1.4973230 C 1.6503850 0.7473300 1.6645180	Н	2.3754000	-0.2792130	-0.6131070	
D 2.3071610 -0.4628690 -1.5555890 H -2.0420730 0.4891780 0.6869710 D -2.8582770 0.0158620 0.9101380 H 0.0031160 1.9980240 0.5568850 H 1.3212950 -0.2806720 1.4973230 C 1.6503850 0.7473300 1.6645180	0	-1.7794660	-1.3524310	-0.5726170	
H -2.0420730 0.4891780 0.6869710 O -2.8582770 0.0158620 0.9101380 H 0.0031160 1.9980240 0.5568850 H 1.3212950 -0.2806720 1.4973230 C 1.6503850 0.7473300 1.6645180	0	2.3071610	-0.4628690	-1.5555890	
D -2.8582770 0.0158620 0.9101380 H 0.0031160 1.9980240 0.5568850 H 1.3212950 -0.2806720 1.4973230 C 1.6503850 0.7473300 1.6645180	Н	-2.0420730	0.4891780	0.6869710	
H 0.0031160 1.9980240 0.5568850 H 1.3212950 -0.2806720 1.4973230 C 1.6503850 0.7473300 1.6645180	0	-2.8582770	0.0158620	0.9101380	
H 1.3212950 -0.2806720 1.4973230 C 1.6503850 0.7473300 1.6645180	Н	0.0031160	1.9980240	0.5568850	
C 1.6503850 0.7473300 1.6645180	Н	1.3212950	-0.2806720	1.4973230	
	С	1.6503850	0.7473300	1.6645180	
H = 0.401/900 = 0.4605400 = 2.0601140	ч Н	0.4017900	-0.4605400	2.0601140	

Н	2.0955880	-0.9464180	1.8822380	
п	0.0424020	-1.3092030	-0.1429900	
Energy:	-438.41600276	6		
21				
B3LYP/6-	-311++G** geome	try and energy	of conformer:	aThr-L
	2	1 51		
N	-0.4560830	1.9232240	-0.4195430	
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C	-0.1693930	0.5109420	-0.6809320	
H	-0.3422960	0.3238740	-1./4149/0	
С	1.2783350	0.0870220	-0.3536270	
С	-1.2305370	-0.3431150	0.0476840	
H	1.9435510	0.7268180	-0.9478900	
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0	-2.1378670	-0.8814370	-0.5249900	
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Н	-0.2345730	-0.0674850	1.6562560	
Н	-0.0666300	2.2230240	0.4678870	
С	1.5766320	-1.3796060	-0.6436350	
Н	1.4160620	-1.5979870	-1.7027930	
Н	2.6199920	-1.6165270	-0.4133000	
Н	0.9361220	-2.0416730	-0.0559820	
Enor	100 1150001	7		
ruerdy:	-430.41309/21	1		
B3LYP/6-	-311++G** qeome	try and energy	of conformer:	aThr-I
Ν	-0.2979340	1.9441450	-0.3811970	
Н	0.0942490	2.1728720	0.5277890	
С	-0.1508270	0.5101330	-0.6290640	
Н	-0.3525630	0.3234100	-1.6918950	
С	1.3162650	0.1055450	-0.3531960	
С	-1.1205130	-0.3235350	0.2277120	
Н	1.9279550	0.7585170	-0.9814000	
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0	-0.9345540	-0.5919700	1.3879190	
Н	1.0864580	-0.0488240	1.5743480	
0	-2.2725120	-0.7198690	-0.3717610	
Н	-2.2686220	-0.4742800	-1.3051620	
Н	-1.2642520	2.2512050	-0.4060160	
С	1.6117010	-1.3540960	-0.6952410	
Н	1.3870720	-1.5669010	-1.7453540	
Н	2.6702320	-1.5586640	-0.5259420	
Н	1.0325060	-2.0400250	-0.0703890	
-	400 41 4 400	-		
Energy:	-438.41440982	5		
B3LYP/6-	-311++G** apomp	try and energy	of conformer.	aThr-⊺
DODII/0-	JIII G GEOINE	ery and chergy	OF CONTOTINCE.	arnt T
N	0.5394600	-1.8236570	-0.5196840	

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<pre>1 1.5028830 -1.8991330 -0.202090 2 -1.9329870 1.1031540 -0.2153180 4 -1.8497330 1.5512310 -1.2123310 4 -2.9963540 1.0247820 0.0174550 4 -1.4900690 1.7644020 0.5339260 Energy: -438.414281429 33LYP/6-311++G** geometry and energy of conformer: aThr-LIV 4 -0.0934140 1.8185110 0.2926450 4 0.6845720 2.3803730 -0.0353470 5 -0.0316840 0.4675200 -0.2871040 4 0.0127810 0.4783690 -1.3887170 5 1.1790620 -0.3289850 0.2294800 5 -1.3327980 -0.2359620 0.1019890 4 1.2319270 -1.5877900 -0.4488490 5 -1.4953010 -0.9951190 1.0165000 6 -1.4952900 -1.4406870 -1.3484610 6 -2.3468760 0.1597710 -0.7149890 9 -3.1552870 -0.2728330 -0.3998630 4 -0.9433590 2.2895520 -0.009310 4 2.4979840 0.4264400 0.0950950 5 2.6826290 0.7297590 -0.9433290 4 0.990120 -0.5802510 1.2755700 33LYP/6-311++G** geometry and energy of conformer: aThr-LV 4 0.0923170 1.8388530 -0.2240380 4 0.9990120 -0.5802510 1.2755700 33LYP/6-311++G** geometry and energy of conformer: aThr-LV 4 0.0923170 1.8388530 -0.2240380 4 0.33190670 -0.2211660 0.4088390 5 -1.3810100 -0.2270470 -0.1137440 5 -0.0218520 0.3933800 -0.4971070 5 -1.3310100 -0.2270470 -0.1137440 5 -1.3310100 -0.2270470 -0.1137440 5 -1.3310100 -0.2270470 -0.1137440 5 -1.331907 -1.424330 -0.4924800 5 -1.3810100 -0.2270470 0.3467480 5 -1.310100 -0.2270470 0.03467480 5 -1.3466080 1.1719080 1.1410890</pre>	Н	0.2583350	2.0123770	-0.5684950
 -1.9329870 1.1031540 -0.2153180 -1.8497330 1.5512310 -1.2123310 -2.9963540 1.0247820 0.0174550 -1.4909690 1.7644020 0.5339260 Snergy: -438.414281429 33LYP/6-311++G** geometry and energy of conformer: aThr-LIV -0.0934140 1.8185110 0.2926450 0.6845720 2.3803730 -0.0353470 -0.0316840 0.4675200 -0.2871040 0.0127810 0.4783690 -1.3887170 1.1790620 -0.3289850 0.2294800 -1.3327980 -0.2359620 0.1019890 1.2319270 -1.5877900 -0.4488490 -1.4953010 -0.9951190 1.0165000 1.5452990 -1.4406870 -1.3484610 -2.3468760 0.1597710 -0.7149890 -3.1552870 -0.2728330 -0.3998630 -0.9433590 2.289520 -0.0009310 2.4979840 0.4264400 0.0950950 2.6826290 0.7297590 -0.9433290 3.310670 -0.2211660 0.4088390 3.310670 -0.2211660 0.4088390 3.310670 -0.2211660 0.4088390 0.9990120 -0.5802510 1.2755700 SalLYP/6-311++G** geometry and energy of conformer: aThr-LV -0.0923170 1.8388530 -0.2240380 0.9990120 -0.5802510 1.2755700 SalLYP/6-311++G** geometry and energy of conformer: aThr-LV -1.032820 -0.333800 -0.4971070 A.3100670 -0.221660 0.4088390 0.9990120 -0.5802510 1.2755700 SalLYP/6-311++G** geometry and energy of conformer: aThr-LV -0.0923170 1.8389530 -0.2240380 0.9990120 -0.5802510 1.2755700 A.310100 -0.2270470 -0.1137440 0.1557640 0.1408860 -1.5480230 1.1102880 -0.2356270 0.3467480 -1.3810100 -0.2270470 -0.1137440 0.9043260 -0.0126470 1.4031930 -1.3810100 -0.220710 0.7493330 -1.8921470 -1.1424330 -0.6924800 -1.8921470 -1.1424330 -0.6924800 -1.4366080 1.17191080 1.11401890 	Н	1.5029830	-1.8991330	-0.2092090
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 -1.4909690 1.7644020 0.5339260 Energy: -438.414281429 33LYP/6-311++G** geometry and energy of conformer: aThr-LIV -0.0934140 1.8185110 0.2926450 0.6845720 2.3803730 -0.0353470 -0.0316840 0.4675200 -0.2871040 1.1790620 -0.3289850 0.2294800 -1.3327980 -0.2359620 0.1019890 1.2319270 -1.5877900 -0.4488490 -2.3468760 0.1597710 0.7149890 -3.458290 -1.3484610 -2.3468760 0.1597710 0.7149890 -3.1552870 -0.228330 -0.9933590 2.2895320 -0.0009310 -3.1552870 -0.2211660 0.4088390 -0.9990120 -0.5802510 1.2755700 Energy: -438.414211330 SalLYP/6-311++G** geometry and energy of conformer: aThr-LV -0.0923170 1.8388530 -0.2240380 0.9990120 -0.5802510 1.2755700 Snergy: -438.414211330 	Н	-2.9963540	1.0247820	0.0174550
Energy: -438.414281429 33LYP/6-311++G** geometry and energy of conformer: aThr-LIV 4 -0.0934140 1.8185110 0.2926450 5 -0.0316840 0.4675200 -0.2871040 6 0.0127810 0.4783690 -1.3887170 5 1.1790620 -0.3289850 0.2294800 6 1.2319270 -1.5877900 -0.4488490 6 1.2319270 -1.5877900 -0.4488490 9 -1.4953010 -0.9951190 1.0165000 1.6452990 -1.4406870 -1.3484610 8 -2.3468760 0.1597710 -0.7149890 9 -3.1552870 -0.2728330 -0.3998630 9 -3.1552870 -0.2728320 -0.0009310 1 2.4979840 0.4264400 0.0950950 2 2.6826290 0.7297590 -0.9433290 14 2.6158020 1.3183490 0.7256610 13 3.3190670 -0.2211660 0.4088390 14 2.5158020 1.3183490 0.7256610 13 3.3190670 -0.2211660 0.4088390 14 0.9990120 -0.5802510 1.2755700 Energy: -438.414211330 33LYP/6-311++G** geometry and energy of conformer: aThr-LV 4 -0.0923170 1.8388530 -0.2240380 1 0.557640 0.1408860 -1.5480230 2 -1.3810100 -0.2270470 -0.1137440 4 0.9043260 -0.0126470 1.4031930 2 -1.3810100 -0.2270470 -0.1137440 4 0.9043260 -0.0126470 1.4031930 0 1.0351990 -1.6385910 0.1179510 0 1.0351990 -1.6385910 0.1179510 0 1.033460 -2.0901710 0.7493330 0 -1.8921470 1.1424330 -0.6924800 1 0.6924800 1 0.6924800 1 0.727740 0.3666120 0.9554630 1 0.40890	Н	-1.4909690	1.7644020	0.5339260
A3LYP/6-311++G** geometry and energy of conformer: aThr-LIV - 0.0934140 1.8185110 0.2926450 - 0.0316840 0.4675200 -0.2871040 - 0.0127810 0.4783690 -1.3887170 - 1.1790620 -0.3289850 0.2294800 - 1.3327980 -0.2359620 0.1019890 - 1.4953010 -0.9951190 1.0165000 - 1.4953010 -0.9951190 1.0165000 - 1.5452990 -1.4406870 -1.3484610 - 2.3468760 0.1597710 -0.7149890 - 3.1552870 -0.2728330 -0.3998630 - 0.9433590 2.2895320 -0.0009310 - 2.6826290 0.7297590 -0.9433290 - 2.6826290 0.7297590 -0.9433290 - 2.5158020 1.3183490 0.7256610 - 3.3190670 -0.2211660 0.4088390 - 0.9990120 -0.5802510 1.2755700 Energy: -438.414211330 0.0218520 0.393800 -0.4971070 - 0.1557640 0.1408860 -1.5480230 - 1.102880 -0.2356270 0.3467480 - 1.3810100 -0.2270470 -0.1137440 - 0.9043260 -0.0126470 1.4031930 - 1.3810100 -0.2270470 1.4031930 - 1.6351990 -1.6385910 0.1179510 - 1.8921470 -1.1424330 -0.6924800 - 1.633460 -2.0901710 0.7493330 - 1.9577400 0.3666120 0.9554630 - 1.436080 1.1713080 1.1410890	Energy:	-438.414281429)	
<pre>33LYP/6-311++G** geometry and energy of conformer: aThr-LIV</pre>				
A -0.0934140 1.8185110 0.2926450 A 0.6845720 2.3803730 -0.0353470 C -0.0316840 0.4675200 -0.2871040 A 0.0127810 0.4783690 -1.3887170 C -1.3327980 -0.2359620 0.1019890 A 1.2319270 -1.5877900 -0.4488490 O -1.4953010 -0.9951190 1.0165000 D -1.5452990 -1.4406870 -1.3484610 A -2.3468760 0.1597710 -0.7149890 D -3.1552870 -0.2728330 -0.3998630 A -0.9433590 2.2895320 -0.009310 A 2.4979840 0.4264400 0.0950950 C 2.6826290 0.7297590 -0.9433290 A 2.5158020 1.3183490 0.7256510 A 3.190670 -0.2211660 0.4088390 A 0.8207470 2.2769010 -0.2565260 C -0.0218520 0.3933800 -0.4971070 A 0.1557640 0.1408860 -1.5480230	B3LYP/6-	311++G** geomet	ry and energy	of conformer: aThr-LIV
<pre>H 0.6845720 2.3803730 -0.0353470 C -0.0316840 0.4675200 -0.2871040 D 0.0127810 0.478690 -1.3887170 D 1.1790620 -0.3289850 0.2294800 D -1.3327980 -0.2359620 0.1019890 H 1.2319270 -1.5877900 -0.4488490 D -1.4953010 -0.9951190 1.0165000 D 1.5452990 -1.4406870 -1.3484610 H -2.3468760 0.1597710 -0.7149890 D -3.1552870 -0.2728330 -0.3998630 H -0.9433590 2.2895320 -0.0009310 H 2.4979840 0.4264400 0.0950950 D 2.6826290 0.7297590 -0.9433290 H 2.5158020 1.3183490 0.7256610 H 3.3190670 -0.2211660 0.4088390 H 0.9990120 -0.5802510 1.2755700 Energy: -438.414211330 B3LYP/6-311++G** geometry and energy of conformer: aThr-LV H -0.0923170 1.8388530 -0.2240380 H 0.8207470 2.2769010 -0.2565260 D -0.0218520 0.3933800 -0.4971070 H 0.1557640 0.1408860 -1.5480230 D -1.5480230 D -1.3810100 -0.2256270 0.3467480 D -1.436080 -0.0126470 1.4031930 D -1.0351990 -1.6385910 0.1179510 D -1.8921470 -1.1424330 -0.6924800 H 1.6033460 -2.0901710 0.7493330 D -1.9577400 0.3666120 0.9554630 H -1.4366080 1.1719080 1.1410890 </pre>	Ν	-0.0934140	1.8185110	0.2926450
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Н	0.6845720	2.3803730	-0.0353470
<pre>H 0.0127810 0.4783690 -1.3887170 1.1790620 -0.3289850 0.2294800 1.13327980 -0.2359620 0.1019890 1.2319270 -1.5877900 -0.4488490 0.1.5452990 -1.4406870 -1.3484610 1.5452990 -1.4406870 -1.3484610 1.2.3468760 0.1597710 -0.7149890 0.3.1552870 -0.2728330 -0.3998630 1.0.9433590 2.2895320 -0.0009310 2.4979840 0.4264400 0.0950950 2.2.6826290 0.7297590 -0.9433290 1.2.5158020 1.3183490 0.7256610 3.3190670 -0.2211660 0.4088390 1.0.9990120 -0.5802510 1.2755700 Chergy: -438.414211330 H 0.9990120 -0.5802510 1.2755700 Chergy: -438.414211330 H 0.1557640 0.1408860 -1.5480230 0.1557640 0.1408860 -1.5480230 0.11102880 -0.2356270 0.3467480 0.1557640 0.1408860 -1.5480230 0.11102880 -0.2356270 1.3467480 0.1557640 0.1408860 -1.5480230 0.11102880 -0.2356270 1.3467480 0.1557640 0.1408860 -1.5480230 0.1.1102880 -0.2356270 0.3467480 0.19943260 -0.0126470 1.4031930 0.10351990 -1.6385910 0.1179510 0.1633460 -2.0901710 0.7493330 0.1.0351990 -1.6385910 0.1179510 1.6033460 -2.0901710 0.7493330 0.1.9577400 0.3666120 0.9554630 1.140880 1.1719080 1.1410890</pre>	С	-0.0316840	0.4675200	-0.2871040
1.1790620 -0.3289850 0.2294800 2.1.3327980 -0.2359620 0.1019890 4.1.2319270 -1.5877900 -0.4488490 50 -1.4953010 -0.9951190 1.0165000 51 -2.3468760 0.1597710 -0.7149890 52 -3.468760 0.1597710 -0.7149890 54 -2.3468760 0.4284400 0.0950950 52 2.6826290 0.7297590 -0.9433290 52 2.6826290 0.7297590 -0.9433290 52 2.6826290 0.7297590 -0.9433290 53 1.3190670 -0.2211660 0.4088390 6 0.9990120 -0.5802510 1.2755700 50 -0.0213170 1.8388530 -0.2240380 6 0.8207470 2.2769010 -0.2565260 7 -0.0218520 0.3933800 -0.4971070 51 1.110280 -0.2356270 0.3467480 52 1.1102880 -0.2270470 -0.1137440 52 1.3810100 -0.2270470 1.1137440 52 1.3810100 </td <td>Н</td> <td>0.0127810</td> <td>0.4783690</td> <td>-1.3887170</td>	Н	0.0127810	0.4783690	-1.3887170
-1.3327980 -0.2359620 0.1019890 1.2319270 -1.5877900 -0.4488490 0 -1.4953010 -0.9951190 1.0165000 0 1.5452990 -1.4406870 -1.3484610 1.5452990 -1.4406870 -0.7149890 0 -3.1552870 -0.2728330 -0.3998630 1.24979840 0.4264400 0.0950950 2.6826290 0.7297590 -0.9433290 1.25158020 1.3183490 0.7256610 1.33190670 -0.2211660 0.4088390 1.09990120 -0.5802510 1.2755700 Energy: -438.414211330 Backgroup -2.2769010 -0.22565260 2.00213170 1.8388530 -0.2240380 4 0.8207470 2.2769010 -0.2565260 2.00218520 0.3933800 -0.4971070 4 0.1557640 0.1408860 -1.5480230 2.1102880 -0.2356270 0.3467480 2.11102880 -0.2356270 0.3467480 2.11102880 -0.2270470 -0.1137440 4 0.9043260	С	1.1790620	-0.3289850	0.2294800
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$\begin{array}{cccccccccccccccccccccccccccccccccccc$	0	1.5452990	-1.4406870	-1.3484610
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Energy: -438.414211330 B3LYP/6-311++G** geometry and energy of conformer: aThr-LV -0.0923170 1.8388530 -0.2240380 0.8207470 2.2769010 -0.2565260 -0.0218520 0.3933800 -0.4971070 0.1557640 0.1408860 -1.5480230 1.1102880 -0.2356270 0.3467480 -1.3810100 -0.2270470 -0.1137440 0.9043260 -0.0126470 1.4031930 1.0351990 -1.6385910 0.1179510 -1.8921470 -1.1424330 -0.6924800 1.6033460 -2.0901710 0.7493330 0.1.9577400 0.3666120 0.9554630 1.1410890	 H	0.9990120	-0.5802510	1.2755700
Energy: -438.414211330 B3LYP/6-311++G** geometry and energy of conformer: aThr-LV -0.0923170 1.8388530 -0.2240380 0.8207470 2.2769010 -0.2565260 -0.0218520 0.3933800 -0.4971070 0.1557640 0.1408860 -1.5480230 1.1102880 -0.2356270 0.3467480 -1.3810100 -0.2270470 -0.1137440 0.9043260 -0.0126470 1.4031930 0.1.0351990 -1.6385910 0.1179510 -1.8921470 -1.1424330 -0.6924800 1.6033460 -2.0901710 0.7493330 0.1.9577400 0.3666120 0.9554630 -1.4366080 1.1719080 1.1410890	11	0.9990120	0.0002010	1.2700700
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$\begin{array}{cccccccccccccccccccccccccccccccccccc$	B3LYP/6-	311++G** geomet	cry and energy	of conformer: aThr-LV
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$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Н	0.8207470	2.2769010	-0.2565260
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D1.0351990-1.63859100.1179510D-1.8921470-1.1424330-0.6924800H1.6033460-2.09017100.7493330D-1.95774000.36661200.9554630H-1.43660801.17190801.1410890	Н	0.9043260	-0.0126470	1.4031930
D-1.8921470-1.1424330-0.6924800H1.6033460-2.09017100.7493330D-1.95774000.36661200.9554630H-1.43660801.17190801.1410890	0	1.0351990	-1.6385910	0.1179510
H1.6033460-2.09017100.7493330D-1.95774000.36661200.9554630H-1.43660801.17190801.1410890	0	-1.8921470	-1.1424330	-0.6924800
-1.95774000.36661200.9554630I-1.43660801.17190801.1410890	Н	1.6033460	-2.0901710	0.7493330
H -1.4366080 1.1719080 1.1410890	0	-1.9577400	0.3666120	0.9554630
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-0.6724690 2.3090970 -0.9120520

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	B3LYP/6- N H C H C C H O O H H C H H H Energy:	-311++G** geome 0.3187900 0.2347370 0.0863860 0.0081170 -1.1840750 1.3763100 -1.4879220 1.4049640 -1.8601000 2.4967130 2.2022850 -0.3268040 -2.3957220 -2.6382200 -2.2422650 -3.2603660 -0.9563540 -438.41187260	etry and energy 1.8028530 2.0148230 0.3767240 0.2881340 -0.2861280 -0.3932440 -1.4850970 -1.5229490 -1.2515310 0.3364110 1.2482470 2.4008250 0.6454340 1.0142000 1.5106050 0.0938760 -0.6227880	of conformer: 0.0479700 -0.9421430 0.3284250 1.4198600 -0.2709520 -0.0498570 0.4383800 -0.4474460 1.2965290 0.1289710 0.3237080 0.5494660 -0.2982260 0.7063690 -0.9474620 -0.6722290 -1.2854760	aThr-L'
SCHIT'S CITI'S ACOMOCTA WING CUCTAA OT CONTOFINCT. UTILL II	B3LYP/6- N H C H C H C H C H H C H H C H H C H H C H H C H C H C C C H C C C H C C C H C C C H C C C H C	-311++G** geome 0.3187900 0.2347370 0.0863860 0.0081170 -1.1840750 1.3763100 -1.4879220 1.4049640 -1.8601000 2.4967130 2.2022850 -0.3268040 -2.3957220 -2.6382200 -2.2422650 -3.2603660 -0.9563540 -438.41187260	etry and energy 1.8028530 2.0148230 0.3767240 0.2881340 -0.2861280 -0.3932440 -1.4850970 -1.5229490 -1.2515310 0.3364110 1.2482470 2.4008250 0.6454340 1.0142000 1.5106050 0.0938760 -0.6227880	of conformer: 0.0479700 -0.9421430 0.3284250 1.4198600 -0.2709520 -0.0498570 0.4383800 -0.4474460 1.2965290 0.1289710 0.3237080 0.5494660 -0.2982260 0.7063690 -0.9474620 -0.6722290 -1.2854760	aThr-L

2					
3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20	N H C H C C H O O H O H H H H H H	$\begin{array}{c} 0.1622800\\ 0.8193760\\ -0.0540160\\ -0.0736930\\ 1.1037230\\ -1.4291930\\ 0.9084890\\ 2.2508610\\ -2.2322270\\ 3.0457870\\ -1.7368060\\ -1.0086010\\ -0.7114600\\ 1.3065140\\ 0.4368250\\ 2.1728230\\ 1.4577120\\ \end{array}$	$\begin{array}{c} 1.7398730\\ 2.2900240\\ 0.4392940\\ 0.4729250\\ -0.5236600\\ -0.0925400\\ -1.5088040\\ 0.0400490\\ 0.5438120\\ -0.3302960\\ -1.3475970\\ -1.7303140\\ 2.2396760\\ -0.6989760\\ -1.1783430\\ -1.3399780\\ 0.2711820\\ \end{array}$	0.1035560 - 0.4335420 - 0.5003720 - 1.6041720 - 0.1359360 - 0.0858390 - 0.5911920 - 0.7792000 0.5362560 - 0.3830050 - 0.5053510 - 1.0106480 0.2188030 1.3636670 1.8219340 1.5571890 1.8369870	
21 22	Energy:	-438.411382946	5		
22 23 24 25	inci gy .	190.111902910			
26 27	B3LYP/6-	311++G** geomet	ry and energy	of conformer:	aThr-LIX
28		0 10 00 00	1 5005000	0 0515000	
29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44	N Н С Н С С Н О О Н О Н Н С Н Н Н Н	$\begin{array}{c} 0.1973060\\ 1.1914510\\ -0.0368080\\ -0.0593550\\ 1.0682930\\ -1.4052840\\ 0.8413830\\ 2.3363210\\ -1.9621120\\ 2.3523150\\ -1.9620990\\ -1.4422440\\ -0.2448420\\ 1.2003810\\ 0.2825670\\ 2.0197630\\ 1.4214510 \end{array}$	$\begin{array}{c} 1.7887000\\ 1.9822820\\ 0.3990620\\ 0.2998290\\ -0.5915500\\ -0.0297820\\ -1.5927830\\ -0.1588570\\ 0.4999990\\ -0.2609410\\ -1.1124610\\ -1.3824920\\ 2.0204360\\ -0.6689530\\ -1.0420120\\ -1.3417300\\ 0.3144000\end{array}$	-0.2515890 -0.1999410 -0.5867150 -1.6846470 -0.0867830 -0.0568320 -0.4816400 -0.5915340 0.8629960 -1.5494010 -0.6601480 -1.4272010 0.6319530 1.4251930 1.8838310 1.6834780 1.8449920	
45 46 47 48 49 50	Energy:	-438.411204130)		
51 52	B3LYP/6-	311++G** geomet	ry and energy	of conformer:	aThr-LX
53 54 55 56 57 58 59 60	N H C H C H O O	$\begin{array}{c} 0.4476980\\ 0.4102800\\ 0.1474640\\ 0.1492820\\ -1.2908200\\ 1.1956130\\ -1.8953740\\ -1.2598720\\ 2.0018680 \end{array}$	-1.8422390 -2.2193410 -0.4219790 -0.0324680 -0.2531880 0.3852110 -0.9336160 -0.7201940 -0.1101330	-0.7662680 0.1767970 -0.7118200 -1.7381650 -0.1713180 0.0929830 -0.7828860 1.1801800 0.8252640	

Н О Н Н С Н Н	-2.1598880 1.2010270 0.5199690 1.3947240 -1.8785310 -1.8406980 -2.9321750	-0.8630190 1.7343570 1.9896720 -1.9923400 1.1552450 1.5406040 1.1360300	1.4884840 -0.1082910 -0.7417690 -1.0985030 -0.2574070 -1.2824830 0.0345710	
Н	-1.3665430	1.8461750	0.4159890	
Energy:	-438.41038629	8		
- /-	0			
B3LYP/6	-311++G** geome	try and energy	of conformer:	aThr-LX
N H C H C	0.5523640 0.8770620 0.1388480 0.1348320 -1.2959780	-1.8025000 -2.1110980 -0.4117870 0.0165200 -0.2029840	-0.8192360 0.0925610 -0.7332690 -1.7454910 -0.1695720	
Н	-1.9453450	-0.8242550	-0.8063220	
0	-1.2955280 1.8658200	-0.7162050 -0.1818210	1.1586600 0.9430890	
Н	-2.1850160	-0.6604060	1.5213530	
H	0.7757050	1.9216400	-0.9089900	
H C	-0.2219160 -1.8086660	-2.3958690 1.2366410	-1.0968940 -0.2205050	
H	-1.7638380	1.6379600	-1.2389030	
H	-1.2402100	1.8852450	0.4494140	
Energy:	-438.40717105	3		
21				