Norine, Florine, s2m: powerful bioinformatics resource and tools for the discovery of novel nonribosomal peptides, natural metabolites with versatile activities
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Norine, Florine, s2m: powerful bioinformatics resource and tools for the discovery of novel nonribosomal peptides, natural metabolites with versatile activities

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NonRibosomal peptides (NRPs) are a huge untapped resource of natural products displaying activities with applications in health (i.e. antibiotics) or in biocontrol (especially siderophores and lipopeptides with antifungal activity). NRPs are microbial secondary metabolites produced by enzymatic complexes, so-called non-ribosomal peptide synthetases (NRPSs). These modular assembly lines work step by step to build the peptides, each module adding one monomer to the peptidic chain. Considering the modular organization of NRPSs, and the structural specific features of the NRPs, dedicated bioinformatics tools have been developed with the aim of accelerating the screening for new active metabolites.

NORINE  http://bioinfo.cristal.univ-lille.fr/norine/
- A unique database containing more than 1200 annotated NRPs
- Now open to crowdsourcing (Flissi et al., 2016)

Florine workflow: from genomic data to the discovery of new NRPs (Caradec et al. 2014)

Genomic data → Gene clusters → NRPS genes → NRPS proteins → Monomer prediction → Isomery prediction → Structure comparison

Smiles2Monomers  http://bioinfo.cristal.univ-lille.fr/norine/smiles2monomers.jsp
- A software to infer monomeric structure of polymers from their atomic structure (Dufresne et al. 2015)

Burkholderia genome mining: a user case

Burkholderia mallei/pseudomallei

Clade 1

Chromosome → 3 clusters

Plasmide → 8 clusters

Clade 2

Mainly Bcc (cepacia complex)

Phymabactin (siderophore)

Malleobactin (siderophore)

Ornibactin (siderophore)

Pb. rhizoxinica

High potential for lipopeptide synthesis

Clade 3

Mainly Bcc (cepacia complex)

Cepaciachelin (siderophore)

Plant beneficial

Paraburkholderia