Norine: computational platform dedicated to nonribosomal peptides

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Nonribosomal peptides (NRPs) are specific peptides synthesized by huge enzymatic complexes. Bacteria and fungi use this pathway to synthesize peptides with specific structures: they are composed of more than 500 different building blocks, called monomers, that can be proteinogenic amino acids, their derivatives, fatty acids and also glucids; they are not only linear but can also contain cycles and/or branches. This variety of structures gives them a variety of functions from antibiotics to bio-pesticides through siderophores.

We will present Norine [1] (http://bioinfo.cristal.univ-lille.fr/norine/), the unique computational platform dedicated to nonribosomal peptides. It is composed of a database containing valuable annotations on those compounds, including chemical structures and monomer graphs. The data comes from manual annotations entered by our team or by external experts throw MyNorine tool; and from automatic extraction form other databases. In both manual and automatic processes, verification ensures the high quality of the annotations. It also provides tools to analyze those compounds. A monomer graph can be drawn and searched against all graphs of the database [2]. The monomer graph can be inferred from the chemical structure of a peptide represented by a SMILES either by our tools rBAN [3] or s2m [4]. Last, the *Kendrick Formula Predictor* predicts the molecular formula of a NRP from its mass-to-charge ratio. Those tools may be extended to analyze other types of secondary metabolites, if they are composed of monomers.

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