Bioinformatics Tools for the Discovery of New Nonribosomal Peptides - DTU Orbit (08/11/2017)

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This chapter helps in the use of bioinformatics tools relevant to the discovery of new nonribosomal peptides (NRPs) produced by microorganisms. The strategy described can be applied to draft or fully assembled genome sequences. It relies on the identification of the synthetase genes and the deciphering of the domain architecture of the nonribosomal peptide synthetases (NRPSs). In the next step, candidate peptides synthesized by these NRPSs are predicted in silico, considering the specificity of incorporated monomers together with their isomery. To assess their novelty, the two-dimensional structure of the peptides can be compared with the structural patterns of all known NRPs. The presented workflow leads to an efficient and rapid screening of genomic data generated by high throughput technologies. The exploration of such sequenced genomes may lead to the discovery of new drugs (i.e., antibiotics against multi-resistant pathogens or anti-tumors).

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