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A chemoinformatics approach to the discovery of lead-like molecules from marine natural products

Florbela Pereira

New University of Lisbon, Portugal

Nowadays, the presumably high productivity, in terms of compounds numbers, has not yet led to a corresponding increase in the number of new drug candidates. Instead, after more than two decades of combinatorial chemistry research, a declining of the number new chemical entities in drug development pipelines was observed. Therefore, one of the most important questions in drug discovery still remains unanswered: Where in chemical structural space are biologically relevant compounds to be found? The answer to that question is not easy, however as Stockwell stated “The mapping of biological-activity space using small molecules is akin to mapping the stars - uncharted territory is explored using a system of coordinates that describes where each new feature lies”. From these coordinates is possible to identify some of the central criteria in designing compound libraries to modulating the functions of proteins: 1) diversity; 2) drug-likeness; and 3) biological relevance. The last criterion is fulfilled by the natural products (NPs) which have been optimized in a very long natural selection process for optimal interaction with biological macromolecules. NPs or synthetic products inspired by NPs have been the single most productive source leads for the development of drugs, i.e. more than half of the approved drugs are based on NPs. A new branch of NPs chemistry had been fully established-marine natural products. Various chemoinformatics approaches can provide useful help in analyzing NPs and the results of such studies may be used with advantage in the drug discovery process.

Biography

Florbela Pereira obtained her PhD degree in Organic Chemistry from the University of Aveiro (UA, Portugal) in 1997. She undertook postdoctoral research on development of pharmaceutical products at the Instituto de Biologia Experimental e Tecnológica (IBET, Portugal). From 2000-05, she worked in industry as a synthetic chemist in organic synthesis of agrochemicals active substances and formulations, before returning to Academia to take part of Chemoinformatic and Marine Natural Product groups at New University of Lisbon, where she is currently a PhD Researcher. She has published 10 papers in international peer review journals and 12 patents of which 3 are international patents.

florbela.pereira@fct.unl.pt