Cheminformatics in Natural Product-based Drug Discovery

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Natural products (NPs) remain the most prolific resource of inspiration for small-molecule drug discovery. Computational methods can make a substantial contribution to NP research and the design of NP-inspired drugs. This lecture aims to provide an overview of the scope and limitations of modern cheminformatics methods for NP research, such as approaches for virtual screening, target prediction, ADME/T prediction and many other applications. Further to that, we will present our latest works on the (i) assessment of the NP chemical space and its relevance to drug discovery, (ii) analysis of NP ring systems and their representation by synthetic compounds, and (iii) target prediction for structurally complex NPs.