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CHEMICAL SPACE PARADIGM IN CHEMOINFORMATICS

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Although the expression “Chemical Space” (CS) is widely used in the literature, it is not still well defined. Generally speaking, the notion of “space” stands for a set of objects with some particular properties and some relationships between them (metric). Generally, chemoinformatics considers two main types of chemical objects: graphs and descriptor vectors. Graphs-based CS is traditionally described in terms of scaffolds/R-groups concept which is exploited in popular Scaffold Tree and Scaffold Net approaches. Different sets of molecular descriptors can be generated from one same molecular graph and, therefore, one same graphs-based CS may correspond to several different descriptors-based CS. In this presentation, we discuss different methods of analysis and visualization of graphs-based and descriptors-based CS. Particular attention is paid to Generative Topographic Mapping (GTM) approach which could efficiently be used to visualize chemical data, to predict activity profiles, to conduct virtual screening and to compare chemical databases.

1. Varnek A., Baskin I. I. *Mol. Informatics*, 2011, **30:** 20 – 32