

ACS Symposium Series 2016 vol.1222, pages 211-241

Generative topographic mapping approach to chemical space analysis

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Abstract

© 2016 American Chemical Society. This chapter describes Generative Topographic Mapping (GTM) -A dimensionality reduction method which can be used both to data visualization, clustering and modeling. GTM is a probabilistic extension of Kohonen maps. Its probabilistic nature can be exploited in order to build regression or classification models, to define their applicability domain, to predict activity profiles of compounds, to compare large datasets, to screen for compounds of interest, and even to identify new molecules possessing desirable properties. Thus, GTM can be seen as a sort of a multi-purpose Swiss knife, each of its blades being able to shape an answer to a specific chemoinformatics question, based on a unique map.
