

Chemography concept in chemical space analysis

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Explosive raise of chemical data causes a need in the development of new chemoinformatics tools able to analyse, to visualize and to models these data. Generative Topographic Mapping (GTM) is a promising method of Big Data handling. It allows one not only to visualize chemical structures as data points on 2-dimensional space but also to models a data probability distribution function. The latter can efficiently be used in various chemoinformatics tasks including structure-activity modelling, chemical databases analysis, virtual screening and automatized generation of molecules possessing desirable properties/activities profile. Several cases studies describing application of GTM to computer-aided molecular design will be considered.

References

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