Chirotope Generation - A step
towards multi-conformational 3d-QSA

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When in QSAR studies the 3D-structure of a molecule is considered, then in most cases only a single conformer is taken into account (often theoretically calculated only, e.g. by CORINNA). The mutability of structures and the diversity of possibly occurring different stereo isomers is not taken into consideration at all. We need to expect, that this will affect the quality of the results.

Thus, a better approach would be to consider a set of conformations for each structure, and to calculate structural descriptors based on all this information. But how to get a reasonably sized set of conformations, well distributed over the conformation space?

This talk gives part of an answer to this question. Following an approach of A. Dreiding and A. Dress, we use oriented matroids (also known as chirotopes) as a descriptive tool for conformations. This leads to the strategy to generate first a set of (feasable) chirotopes, and secondly to try to find a (feasable) conformation for each of these chirotopes. The chirotopes itself give enough information in order to reject many unfeasible conformations at an early stage, making the generation process efficient.

Examples will be shown and the corresponding software will be demonstrated.