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Statistical Contribution to the Virtual Multicriteria Optimization of Combinatorial Molecules Libraries and to the Validation and Application of QSAR Models

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Abstract.
The development and statistical validation of QSAR models and the techniques to select compounds in a combinatorial library that optimise predicted characteristics are the two major concerns of our research. Quantitative Structure-Activity Relationship models and desirability indexes can be integrated in a screening algorithm to virtually explore a combinatorial molecules library and select the most promising compounds.An integrated methodology is presented and illustrated on a real combinatorial library provided by Eli Lilly and Company.