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Quantitative structure-activity relationship study of COX-2 inhibitors

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ABSTRACT. Quantitative Structure-Activity Relationship (QSAR) is a tool used with success to model biological activity of series of compounds. There is a serious limitation in the use of this method - it works well only on series of highly homogenous compounds. To furnish such sets of structures, several similarity classification schemes have been proposed: Nave Bayesian classifier, artificial neural networks, molecular fingerprints, and maximum overlapping structures method, MOS. The most accurate classifier MOS is the most computationally demanding as well, and until recently its use was limited. Recent development of the algorithm introduced a series of heuristics and a new rapid clique detection procedure led to significant improvements in the speed of MOS, thus making it suitable for virtual screening of large databases of molecules. In the present study we make use of the MOS method to classify unknowns according to their structural features into classes of structurally homogeneous compounds suitable for further analysis by classical QSAR approaches.

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