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QSAR of anti-inflammatory drugs

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The computer analysis of relations between molecular structures and their biological activity using fragment-based methods is very useful to draw conclusions for the understanding of drug action and for the development of more efficient non-toxic drug candidates.

We used the computer system SARD-21 (Structure Activity Relationship & Design) to investigate common structural features (fragments and substituents) typical for high- and low-effective non-steroid anti-inflammatory drugs (NSAIDs) succesfully.

This derived information has been used for the model for prediction of anti-inflammatory effectiveness of medicines with 76% and 81% level of recognition by two methods. This information could be used for creating new highly effective NSAIDs, and for increasing effectiveness of already known components.

In a second part of this paper the interrelation between structure and efficacy for anti-inflammatory drug action is carried out using traditional QSAR with descriptors from topology and from quantum-mechanical calculations followed by regression models from modelling.

The aim of this paper is to compare both molecular approaches of molecular design of drugs.

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Reference

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