

POSTER PRESENTATION

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QSAR of anti-inflammatory drugs

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From 5th German Conference on Cheminformatics: 23. CIC-Workshop
Goslar, Germany. 8-10 November 2009

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) successfully.

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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Published: 4 May 2010

Reference

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doi:10.1186/1758-2946-2-S1-P45

Cite this article as: Khayrullina and Bögel: QSAR of anti-inflammatory drugs. *Journal of Cheminformatics* 2010 **2**(Suppl 1):P45.

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