

WAY2DRUG – REVEALING HIDDEN POTENTIAL IN TRADITIONAL INDIAN MEDICINE AYURVEDA

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Natural products are used in folk medicine since many thousands year. They represent a significant, though often underappreciated resource for the development of new drugs. A lot of empirical knowledge about pharmacotherapeutic properties of Natural products is accumulated in Traditional Indian Medicine (TIM) Ayurveda, which is known earlier than 1000 years BC. This empirical knowledge can be currently analyzed using modern computer and experimental approaches. Such studies could give information about the underlying mechanisms of TIM actions, providing the basis for rational design of new medicinal plant combinations, and identification of new lead compounds for future pharmaceuticals.

In this work, we used Way2Drug platform [1], which contains PASS Online application able to predict over 4000 kinds of biological activity by structure-activity relationships established for more than 250,000 biologically active compounds. PASS Online predictions were analyzed with computer program PharmaExpert, which provides the means for analysis of PASS predictions and, in particular, integration of biological action of phytoconstituents mixtures based on analysis of drug-drug interaction. To input, storage and processing of information about the structure and biological activity of the studied phytoconstituents, a unique web resource [2] was created.

In silico analysis revealed that 50 medicinal plants from traditional Indian medicine possessed the desired pleiotropic effects, i.e., anticonvulsant, antidepressant, and nootropic activities. In the course of experiments the predicted effects for some phytoconstituents (PhC) were confirmed: anticonvulsant effect and its mechanisms have been elucidated in PhC from *Ficus religiosa* L. (Moraceae) [2]; behavioural and neurochemical evaluations confirmed the ameliorative role of *Passiflora incarnata* in epilepsy and the associated depression and memory deficit [3]; Curcumin has the ameliorative effect on seizure severity, depression-like behavior and memory impairment in pentylenetetrazole-kindled mice [4].

Way2Drug 3.0 provides a new way for dynamically estimating of activities/properties of existing and virtual organic molecules. Freely available platform delivers several tools for in silico drug discovery, including GUSAR - to create QSAR/QSPR models on the basis of the appropriate training sets represented as SDfile contained data about chemical structures and endpoint in quantitative terms; DIGEP-Pred - for prediction of drug-induced changes in gene expression profiles based on structural formula; Meta-Pred - for prediction of site of metabolism; CLC-Pred - for prediction of cytotoxicity for tumor and normal cell lines; RA - a web-service for prediction of reacting atoms in drug metabolism; etc.

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References

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2. <http://ayurveda.pharmaexpert.ru>
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