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Experimental confirmation of drug-target interactions predicted by drug profile matching

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Polypharmacology generally states that many drugs exert their effects by multitarget interactions and these multiple actions seem to be essential to obtain efficacy in complex diseases. Accordingly, bioactive molecules possess characteristic interaction patterns to the human proteome that are responsible for their clinical effect profiles and getting acquainted with this typical profile is increasingly desired to promote pharmaceutical research.

We developed a method that approaches polypharmacology by taking into account the interaction of molecules to a set of proteins that are not the true biological targets of the compounds. Drug Profile Matching (DPM) exploits the information content of so-called virtual affinity fingerprints that were generated by molecular docking of all FDA approved drug molecules to the binding site of 149 non-target proteins. Binding affinities were extracted to form a 149-dimensional vector that is characteristic for each drug. This interaction focused molecular descriptor was correlated with the currently known part of pharmacological effect profiles of drugs by multidimensional statistics. As an output, we could calculate the probability of each drug-effect pair, which quantitatively describes the likelihood of possessing a given effect for all drugs in human use. Top predictions were thoroughly checked by literature survey and experimental testing in three selected effect categories. *In vitro* tests confirmed 33% and 23% of the DPM predictions in the case of angiotensin-converting enzyme inhibitor and cyclooxygenase inhibitor categories, respectively. 72% of the newly predicted and tested dopaminergic compounds were confirmed by tests on D1 and D2 expressing cell cultures.

Biography

Agnes Peragovics has completed her M.Sc. degree in 2009 as a chemical engineer majored in pharmaceutical industry from Budapest University of Technology and Economics. She pursued her Ph.D. studies under the supervision of András Málnási-Csizmadia at Eotvos Lorand University of Sciences in Budapest. Currently, she works in the same group as a predoctoral fellow and expects to obtain her Ph.D. this year. She has published 5 papers in reputed journals.

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