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In silico approach to predict ADME-Tox properties of small organic molecules: Challenges and opportunities for drug discovery

Maria Miteva
University Paris Diderot, France

The progress in computational techniques throughout the past decade enables the use of *in silico* approaches to predict several ADME-Tox properties of small organic molecules or drug candidates in parallel or prior to experimental investigations. In particular, the availability of three-dimensional structures of some proteins that are key for ADME-Tox events makes possible to perform protein structure-based computations to complement or to go beyond traditional QSAR modeling. We will briefly discuss current *in silico* methods for ADME-Tox prediction with a focus on drug metabolizing enzymes. Applying structure-based approach to drug metabolizing enzymes is a challenging process because they usually have flexible binding sites. We developed *in silico* structure-based protocol to gain mechanistic insights from probing small molecules binding to two metabolizing enzymes: the phase I, cytochrome P450 2D6 (CYP2D6), and the phase II, sulfotransferase. We used molecular dynamics to generate suitable diverse protein conformations and protein-ligand docking to discriminate binders and non-binders in large chemical compound collections for CYP2D6 and sulfotransferase. Our results suggest that structure-based *in silico* approach is useful for prioritizing compounds interacting with drug metabolizing enzymes and may be used to go 'beyond QSAR profiling' of drug candidates to assist decision-making in drug discovery.

Biography

Maria Miteva has completed her PhD in 2000 from the Bulgarian Academy of Science, the Institute of Organic Chemistry. She has been working on bioinformatics and drug design in Bulgaria, Sweden and France. She is a Research Director at Inserm (the French institute of health research) and the leader of the team"Virtual screening, PPI & ADMET in silico" belonging to mixed Inserm - University of Paris Diderot, UnitMTi. She has published more than 75 papers in reputed journals and she edited ane-book "In silico lead discovery". She is a member of the editorial boards of 5reputed journals and an Associated Editor for *BMC Toxicology & Pharmacology.*

maria.miteva@univ-paris-diderot.fr