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Maria Grishina

South Ural State University, Russia

Chemosophia online computations for drug discovery and design

The web page www.ChemoSophia.com was designed for various on-line computations for in silico drug discovery, design, virtual screening and data mining procedures. The services are based on the software packages such as MERA elastic model, AlteQ quantum approach, multi-conformational MultiGen algorithm, different algorithms of molecular modelling, 3D/4D QSAR molecular exterior-based algorithms (BiS, Cinderella's Shoe), 3D/4D QSAR molecular interior-based algorithms (ConGO, CoMIn), high-quality molecular restricted docking (ReDock) and subsequent analysis of receptor-ligand complexes (CoCon) all of which are authored by Dr Maria Grishina and Dr Vladimir Potemkin. A researcher can perform online automatic computations of bioactivities (46 types), probabilities of metabolism at different isoforms of P450 cytochrome, high-quality (HI-QU) descriptors, physical-chemical properties (logP, thermodynamics, water solubility, melting and boiling points, critical parameters (volume, density, pressure, temperature), virial coefficients, density, etc.), ecotoxicities, thermodynamics and electron properties. The computations are available for single molecules, molecular databases and complex (many-particle) molecular systems with up to 10, 000 atoms. A researcher can perform online automatic computations combined with geometry optimization tools of structures, including conformational analysis.

Biography

Maria Grishina has completed her PhD from Institute of Organic Synthesis (Ekaterinburg, Russia). She is a Principal Scientist of Laboratory of Computational Modeling of Drugs. She has published more than 35 papers in reputed journals.

marialgri29@gmail.com