Slovenian NMR Centre

@ National Institute of Chemistry

vabi na **PREDAVANJE**:

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z naslovom:

QSAR on Biomolecular Interactions

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v Veliki predavalnici na Kemijskem inštitutu, Hajdrihova 19, Ljubljana

Kratek povzetek:

Being able to quantitatively predict the risk of drug resistance and drug selectivity at molecular level will greatly benefit our understanding on biomolecular interactions, such as drug-protein interaction, substrate-enzyme interaction, signal effector-receptor interaction, protein-protein interaction (PPI) and protein-nucleic acid interaction, etc. Many efforts have been dedicated towards these issues. Recently, a new method, called MB-QSAR (Mutation-dependent Biomacromolecular Quantitative Structure-Activity Relationship) was developed in our group, which extended Comparative Molecular Field Analysis (CoMFA) and Comparative Molecular Similarity Indices Analysis (CoMSIA).

Our recent progress on MB-QSAR for biomolecular interactions will be discussed, with several examples that MB-QSAR can give accurate prediction on drug resistance, drug selectivity and enzyme activity. Also, we will discuss the issue of prediction of enzyme activity, specifically the catalytic activity of PPO enzyme, which related to human Variegate Porphyria disease by its mutation.

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