Univerza
v Ljubljani

Fakulteta *za kemijo*
in kemijsko tehnologijo

p.p. 537, Večna pot 113
1001 Ljubljana
telefon: 01 479 80 00
faks: 01 241 91 44
dekanat@fkkt.uni-lj.si

VABILO NA PREDAVANJE
V OKVIRU DOKTORSKEGA ŠTUDIJA
KEMIJSKE ZNANOSTI

Prof. Dr. Alexandre Varnek

Laboratory of Chemoinformatics,
University of Strasbourg, France

z naslovom:

Chemoinformatics – achievements and perspectives

v sredo, 11. maja 2016 ob 15:00 uri
v predavalnici 1 v 1. nadstropju Fakultete
za kemijo in kemijsko tehnologijo, Večna pot 113

Vljudno vabljeni!

Povzetek

Chemoinformatics is a branch of theoretical chemistry based on its specific molecular model, basic concepts, learning approach and areas of application. Unlike quantum chemistry considering molecules as ensemble of electrons and nuclei, or force field molecular mechanics or dynamics simulations based on classical molecular model (“atoms” and “bonds”), chemoinformatics represents molecules as objects in a chemical space defined by either molecular graphs or some numerical parameters called molecular descriptors. Chemoinformatics uses available experimental data in order to establish quantitative relationships linking chemical structure of molecules with their biological activities or physico-chemical properties. These models, in turn, could efficiently be employed in virtual screening for computer-aided design of new molecules possessing desirable properties. Typical chemoinformatics workflow will be illustrated on several examples of successful in silico design of novel biologically active compounds (anti-thrombotic, antimalarial, antiviral), ionic liquids and metal binders. Particular attention will be paid to recently developed approach able to predict conditions (catalyst, solvent, temperature) needed for some selective chemical transformations.