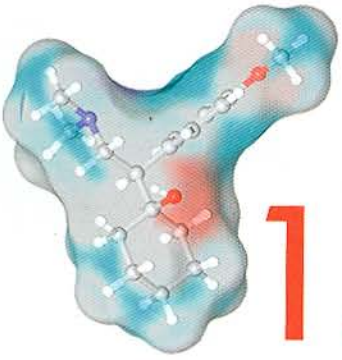

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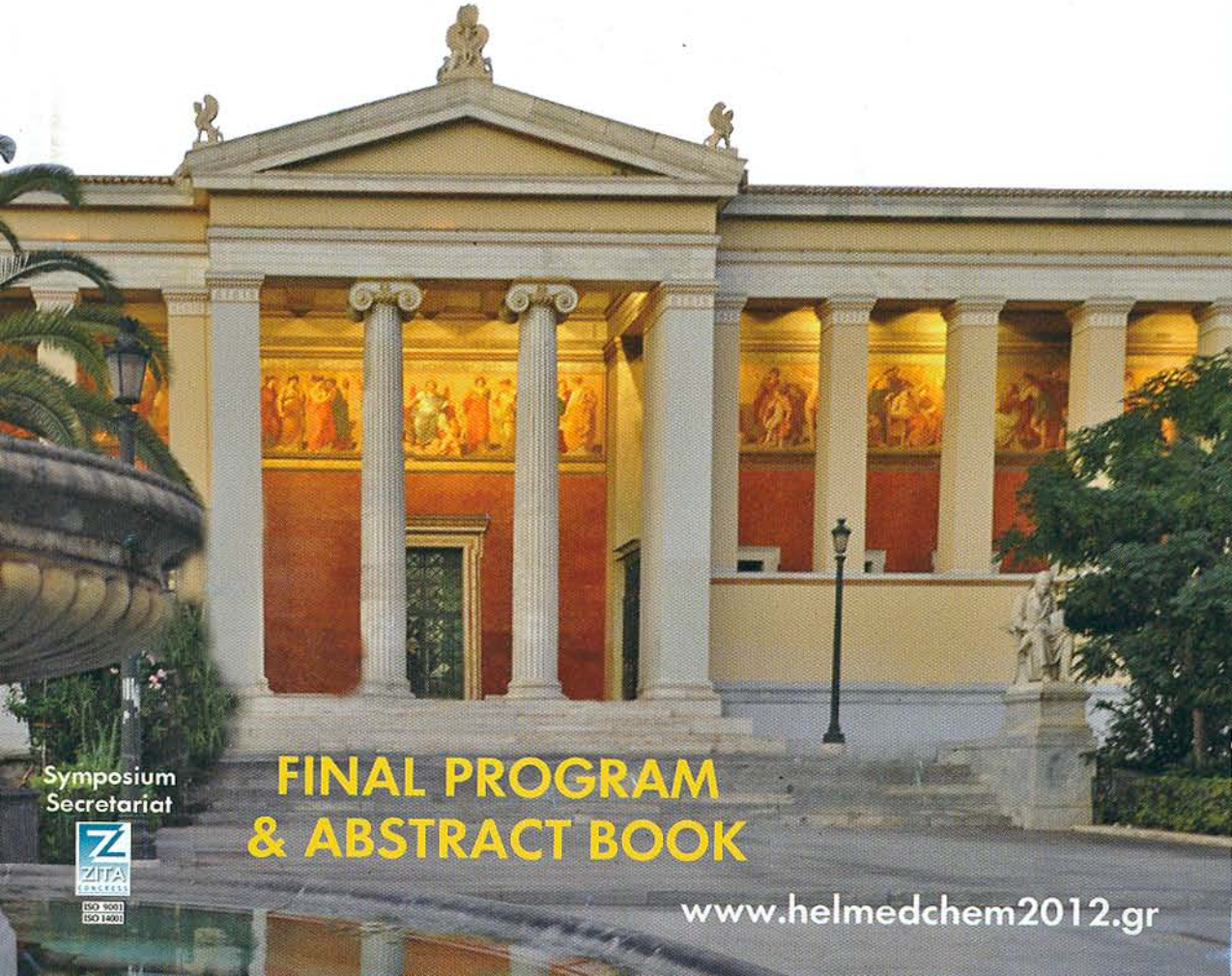

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SUNDAY May 27, 2012

PHARMACOPHORE SEARCHING AND VIRTUAL SCREENING

Chairs: Mavromoustakos Th., Vasileiou S.

09:15-09:55 Plenary Lecture - 6

A COMPUTATIONAL STRATEGY TO INVESTIGATE SUBSTRATE PROMISCUITY IN THE HUMAN CYTOCHROME P450 SYSTEM

Kontoyianni M.

School of Pharmacy, Southern Illinois University, USA

09:55-10:20 Main lecture - 8

EFFECTIVE INHIBITORS FOR ASPARTIC PROTEASES

Leonis G.

National Hellenic Research Foundation, Athens, Greece

10:20-10:45 Main Lecture - 9

TARGETING PROMISING INHIBITORS FOR RHEUMATOID ARTHRITIS: A MULTI STEP CHEMOINFORMATICS APPROACH

Melagraki G.

National Technical University of Athens, Greece

10:45-11:00 Oral Presentation - 10

FREE ENERGY PERTURBATION CALCULATIONS AS A PREDICTIVE TOOL IN STRUCTURE – BASED DRUG DESIGN

Cournia Z.

Biomedical Research Foundation of the Academy of Athens, Athens, Greece

11:00-11:15 Oral Presentation - 11

GAUSSIAN ENSEMBLE SCREENING: A NOVEL WAY TO ANALYSE VIRTUAL SCREENING IN A SYSTEMS PHARMACOLOGY CONTEXT

Perez – Nueno V.

INRIA Nancy – Grand Est, Loria, Vandoeuvre-les Nancy, France

11:15-11:30 Oral Presentation - 12

THE MEDICINAL CHEMISTRY – RELATED APPLICATIONS IN HP-SEE PROJECT. AN END – USER VIEW

Drakulic B. J.

University of Belgrade, Belgrade, Serbia

11:30-12:00 **Coffee**

SUNDAY May 27, 2012

Oral Presentation - 12

THE MEDICINAL CHEMISTRY-RELATED APPLICATIONS IN HP-SEE PROJECT. AN END-USER VIEW

Drakulić Branko J.*, Dragos Ciobanu-Zabet, Ionut Vasile**, Ivanov Petko***,$, Dodoff Nicolay***,&, Karaivanova Aneta***,#, Juranić Ivan O.***

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#Institute of Information and Communication Technologies

*** Bulgarian Academy of Science (BAS), Sofia, Bulgaria

100 years after Alan Turing was born [1], this communication deals with the high-performance computing (HPC) applied to medicinal chemistry in South East Europe. HP-SEE project (the High-Performance Computing Infrastructure for South East Europe's Research Communities) links existing and upcoming HPC facilities in South East Europe in a common infrastructure, and provides operational solutions for it. Partners span area from Hungary to Azerbaijan. The project includes virtual research communities (VRC): Computational Physics, Computational Chemistry, and Computational Life Sciences. The computational chemistry (including material science) is one of the highlighted research areas in computational science, and a typical heavy user of HPC resources. Considering the size of the problems to be studied, the required calculations are often extremely computationally intensive. Ported software in production phase covers the methods spanning from quantum-mechanics to molecular mechanics level of theory (including hybrid methods, molecular dynamics and molecular docking), as well as cheminformatics applications, and are available mainly from HPC centers in Bulgaria, Romania, and Serbia. In the frame of VRC Computational chemistry, following applications are related to medicinal chemistry: a) CompChem (RS) - QM calculations and molecular dynamics (MD) simulation, for the examination of ligands interaction with proteins, as well as for conformational sampling of small drug-like molecules in explicit solvents; b) IsyMAB (RO) - Provide an efficient, interactive tool for the input preparation and data analysis, obtained by MD simulation in NAMD on large biomolecular systems. The main focus is in the modeling of the G Protein-coupled receptors; c) MD Cisplatin (BG) - QM calculations of Pt(II) type complexes with sulfur-containing ligands, as well as organic molecules of biological interest - peptides, comprising non-natural amino acids; d) PCACIC (BG) - MD of the conformational interconversions in large-ring cyclodextrins, typically during 100 ns, in explicit solvent. Trajectories are analyzed by principal component analysis. Usage examples are given, emphasizing need for the HPC resources to cover size of systems under simulation, and/or the complexity of problem solved.

[1] T. Chouard, Nature 482 (2012) 455

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