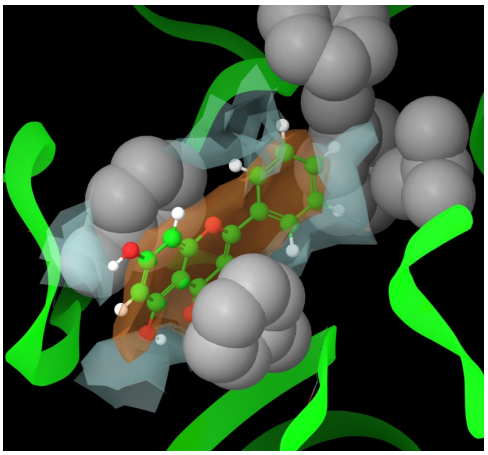
50 ΧΡΟΝΙΑ ΕΘΝΙΚΟ ΙΔΡΥΜΑ ΕΡΕΥΝΩΝ

Marie Curie Actions
Human Resources and Mobility Activity



"Workshop on Molecular Modelling: Approaches to Computational Biophysics"

Marie Curie ToK programme "DRUGDESI"

"Dedicated to the memory of coordinator,

Dr. Nikos G. Oikonomakos"

Athens, 5 – 6 December 2008

Friday 5th December 2008

9.30 – 10.00	***Registration***
Chairpersons	Elias Eliopoulos, Demetres Leonidas
10.00 – 10.15	**Dimitrios Kyriakidis** (Chairman of the National Hellenic Research Foundation and acting Director of the Institute of Organic and Pharmaceutical Chemistry) *"Opening remarks"*
10.15 – 10.50	**Joseph M. Hayes** (DRUGDESI ToK fellow; Institute of Organic and Pharmaceutical Chemistry, National Hellenic Research Foundation, Athens) *"Glycogenolysis control in type 2 diabetes: the role of computation in structure based drug design"*
10.50 – 11.25	**Salvatore Guccione** (Department of Pharmaceutical Science, University of Catania, Italy) "*Computational fishing in protein interactions and neurodegeneration hypotheses*"
11.25 – 11.55	***Coffee break***
Chairpersons	Joseph Hayes, Spyros Zographos
11.55 – 12.30	**Nicholas Glykos** (Department of Molecular Biology and Genetics, Democritus University of Thrace, Alexandroupolis.) "*Molecular dynamics simulations come of age: crystallographically verifiable predictions for the case of a small protein*"
12.30 – 13.05	**Georgios Archontis** (DRUGDESI participant; Department of Physics, University of Cyprus) "*Thermodynamic stability of protein-ligand complexes: Insights from free-energy simulations*"
13.05 – 14.15	***Lunch break***
Chairpersons	Georgios Archontis, Manthos Papadopoulos
14.15 – 14.50	**Thomas Mavromoustakos** (Department of Chemistry, University of Athens) *"Strategies in the application of rational drug design"*
14.50 – 15.25	**Doros Theodorou** (School of Chemical Engineering, National Technical University of Athens) *"Multiscale modelling of synthetic polymers"*
15.25 – 15.55	***Coffee break***
Chairpersons	Nikos Glykos, Evangelia Chrysina
15.55 – 16.30	**Elias Eliopoulos** (Laboratory of Genetics, Department of Biotechnology, Agricultural University of Athens) *"Application of molecular modelling to medical genetics"*
16.30 – 17.00	**Costas Potamitis** (Institute of Organic and Pharmaceutical Chemistry, National Hellenic Research Foundation, Athens) *"Antihypertensive drug Valsartan: conformational analysis, dynamic NMR spectroscopy, in silico docking and membrane associated AT1 receptor molecular dynamics simulations"*

Saturday 6th December 2008

Chairpersons	Elias Eliopoulos, Joe Hayes
10.00 – 10.35	**Nikolaos A. Papandreou** (Laboratory of Genetics, Dept. of Biotechnology, Agricultural University of Athens) *"Protein structure and engineering: from description to prediction"*
10.35 – 11.05	**Marios Zouridakis** (Hellenic Pasteur Institute) *"Molecular modelling-based expressed mutants of the extracellular domain of human α7 nicotinic acetylcholine receptor with enhanced solubility and ligand-binding properties"*
11.05 – 11.40	**Marianna A. Charavgi** (Institute of Organic and Pharmaceutical Chemistry, National Hellenic Research Foundation, Athens) *"Virtual database screening and experimental validation of new classes of glycogen phosphorylase inhibitors"*
	Software demonstration
11.40 – 12.00	**Michail Mamais** (Institute of Organic and Pharmaceutical Chemistry, NHRF, Athens) *"Docking calculations using Glide"*
12.00 – 12.20	**Georgios Archontis** (Department of Physics, University of Cyprus) "*Molecular dynamics analysis*"
12.20 – 12.40	**Nikos Papandreou & Elias Eliopoulos** *(*Dept. of Biotechnology, Agricultural Univ. of Athens) "*Protein folding and modelling*"
12.40 – 13.00	**Discussion, concluding remarks**

The workshop is funded by the ToK Marie Curie Program, **DRUGDESI,** contract No**. MTKD-CT-2006-042776**.

***Organizing committee*: Evangelia D. Chrysina, Joseph M. Hayes, Elias Eliopoulos, Georgios Archontis, Demetres D. Leonidas, Spyros E. Zographos.**