

Haralambos Tzoupis

Curriculum Vitae

PERSONAL INFORMATION

Date of Birth : January 8, 1981
Place of Birth : Agrinion, Greece
Nationality : Hellenic
Email : haralambostz@gmail.com

EDUCATION

September 2009 – April 2014:

PhD: Department of Chemistry, National Kapodistrian University of Athens

Title: Design of Novel inhibitors of renin and HIV-1 protease

Supervisor: Prof. Thomas Mavromoustakos

September 2001- Septembe 2013:

MSc: Infectious Diseases, Imperial College of Science, Medicine and Technology, University of London.

Master Thesis: HIV T-Cell responses in a treatment interruption cohort

Supervisor: Dr. Nesrina Imami

1998-2001:

BSc. Biochemistry, School of Biological Sciences, Queen Mary, University of London
(**Grade:** First Class, Honours)

Diploma thesis: Characterization of a protein (GCAP1) involved in eye disease

Supervisor: Prof. Martin Warren

WORK EXPERIENCE

February 2015- now

Post-doctoral fellow, Department of Chemistry, Laboratory of Organic Chemistry, University of Patras, Greece

Prof. Theodore Tselios

February 2015-October 2015

Post-doctoral fellow, National Centre for Scientific Research "DEMOKRITOS", Institute of Biosciences and Applications, Laboratory of Conformational Analysis and Molecular Modelling, Athens, Greece

Director: Dr. Metaxia Vlassi

2005-2007

Regulatory Assistant Officer, ANTAEA Ltd, Athens, Greece

2003-2004

Compulsory military Service

PUBLICATIONS

1. H. Tzoupis, G. Leonis, A. Avramopoulos, H. Reis, Z. Czyznikowska, S. Zerva, N. Vergadou, L.D. Peristeras, K.D. Papavasileiou, M.N. Alexis T. Mavromoustakos, and M. G. Papadopoulos. "Elucidation of the binding mechanism of renin using a wide array of computational techniques and biological assays" *J. of Molecular Graphics and Modelling* 62, (2015), 138
2. H. Tzoupis, G. Leonis, A. Avramopoulos, T. Mavromoustakos, and M. G. Papadopoulos. "Systematic Molecular Dynamics, MM–PBSA and Ab Initio Approaches to the Saquinavir Resistance Mechanism in HIV-1 PR Due to 11 Double and Multiple Mutations" *J. Phys.Chem B.* 118 (32), (2014), 9538
3. H. Tzoupis, G. Leonis, T. Mavromoustakos, and M. G. Papadopoulos. "A Comparative Molecular Dynamics, MM–PBSA and Thermodynamic Integration Study of Saquinavir Complexes with Wild-Type HIV-1 PR and G48V, L10I, L63P, A71V, G73S, V82A and I84V Single Mutants" *J. Chem. Theory Comput.* 9 (2013) 1754
4. H. Tzoupis, G. Leonis, G. Megariotis, C. T. Supuran, T. Mavromoustakos and M. G. Papadopoulos. "Dual Inhibitors for Aspartic Proteases HIV-1 PR and rennin: Advancements on AIDS-Hypertension-Diabetes Linkage via Molecular Dynamics, Inhibition Assays and Binding Free Energy Calculations" *J. Med. Chem.* 55 (2012) 5784
5. A. Politi, G. Leonis, H. Tzoupis, D. Ntountaniotis, M. G. Papadopoulos, S. G. Grdadolnik, T. Mavromoustakos "Conformational Properties and Energetic Analysis of Aliskiren in Solution and Receptor Site". *Molecular Informatics.* 30 (2011) 973
6. H. Tzoupis, G. Leonis, S. Durdagi, V. Mouchlis, T. Mavromoustakos, M.G. Papadopoulos. "Binding of novel fullerene inhibitors to HIV-1 protease: insight through molecular dynamics and molecular mechanics Poisson–Boltzmann surface area calculations" *J. Comput. Aided Mol. Des.* 25 (2011) 959
7. H. Tzoupis, A. Avramopoulos, H. Reis, G. Leonis, S. Durdagi, T. Mavromoustakos G. Megariotis, and M. G. Papadopoulos. Chapter 8 "Theoretical studies of interactions in nanomaterials and biological systems" p. 148-186

Book Title: Towards Efficient Designing of Safe Nanomaterials,

ATTENDANCE AT CONFERENCES

1. 66th National Conference of the Hellenic Society of Biochemistry and Molecular Biology, 11-13 December 2015, Athens (Poster presentation)
Title: «Molecular Dynamics (MD) simulations of the human Glutamate Dehydrogenase» (P107)
URL: <http://www.eebmb2015.gr/program.pdf>
2. Network Tools and Applications in Biology (NETTAB) workshop 2014, University of Torino, Italy (Oral Presentation)

Title: «Effect of mutations to HIV-1 PR. Insights into Drug Resistance and Drug Design: A Molecular Dynamics Approach»

URL: <http://www.igst.it/nettab/2014/programme/oral-communications/>

3. Participation in the 2nd educational cycle of the National Hellenic Research Foundation (18,25/2 and 4/3/2014) (Oral presentation)

Title: «Computational methods in tackling various infectious diseases».

URL: http://www.eie.gr/epistimiskoinonia/2014/2014_ME_CYCLE_B.pdf

4. 32nd European Peptide Symposium, 2-7 September 2012, Athens (poster presentation)

Title: «Conformational Properties and Energetic Analysis of aliskiren in solution and receptor site»

5. Structure & Computer-aided Design Workshop: Bioactive Molecules & Materials, 7-11 November 2011 National Hellenic Research Foundation, Athens (oral presentation)

Title: «Binding of novel fullerene inhibitors to HIV-1 protease: insight through molecular dynamics and molecular mechanics Poisson–Boltzmann surface area calculations»

MEMBER OF PROFESSIONAL ASSOCIATIONS OR UNIONS

- Member of the Hellenic Society of Biochemistry and Molecular Biology

COMPUTER SKILLS

- Microsoft Office (Word, Power Point, Excel)
- Experience in LINUX environment
- Experience in AMBER, GROMACS (Molecular Dynamics software)