# Lykourgos Chiniadis

Work Address

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## **EDUCATION**

Ph.D candidate in Protein Crystallography and Molecular Dynamics,

Agricultural University of Athens, GR, NCRS Demokritos

Sep2010-now

THESIS - Structural analysis and study of the dynamics of proteins and protein-ligand complexes with anti-cancer drugs, Studentship by Greek Ministry of Education.

Master of Science, M.Sc., Research and Development of Natural Products Agricultural University of Athens, GR

Sep2005-June2007

Bachelor of Science, Chemistry National and Kapodistrian University of Athens, GR

Jan2002

## PROFESSIONAL EXPERIENCE

NCRS "Demokritos" September 2017 – now

Institute of Biosciences and Applications, Athens, GR

- Performed crystallization of proteins, crystal structure refinement and validation using crystallographic tools.
- Performed biomolecular simulations using molecular dynamics and other bioinformatic tools.
- Participated in educational activities with academia and industry (e.g. BASF).
- Participated in several conferences.
- Participated in writing research proposals and articles in journals.

Agricultural University of Athens, GR

September 2009 – September 2012

Research Assistant at Department of Biotechnology, Lab. of Physics

- Prepared solutions and crystallized several protein-ligand complexes.
- Completed refinement and validation of crystal structures.
- Performed molecular dynamics calculations and trajectory analysis with AMBER suite.
- Participated in educational activities of the lab of Chemistry (2009) and lab of Physics (2009-2012) at Agricultural University of Athens (both undergraduate and postgraduate students).

Barcelona Supercomputing Center, SP

May 2010 - June 2010

• Conducted research in protein-protein interactions using High Performance Computing.

Research Assistant, University of Firenze, CERM, IT

September 2007 – June 2008

- Trained in expression and purification of proteins in bacteria.
- Trained in acquiring and analyzing 2D and 3D NMR spectra towards the determination of protein 3D-structures.

Research Assistant, University of Reims, Champagne-Ardennes, FR

January 2007 - July 2008

- Trained in FT-IR and 2D-FTIR spectral acquisition and analysis with Origin software suite.
- Prepared samples for the determination of secondary structure of proteins and protein-ligand complexes.

• Participated in academic (educational) activities at Department of Pharmacy, lab MEDIAN.

Research Assistant, National Hellenic Research Foundation, GR September 2000 – January 2002

- Trained in FT-IR and FT-Raman spectral acquisition and analysis with Origin software suite.
- Prepared samples for the determination of photoinduced coatings using UV-vis chamber.
- Participated in academic (educational) activities at Theoretical Physical Chemistry Institute.

#### COMPUTER SKILLS

Experienced in Linux. Experienced in Molecular Dynamics suites and in Bioinformatic Tools. Experienced in all Crystallographic Tools. Knowledge of Python (certification) and Bash.

## EXPERIMENTAL SKILLS

X-ray crystallography, protein expression and purification, NMR, PCR, FT-IR, FT-Raman, XRD, HPLC, GC-MS, analytical techniques.

## **PUBLICATIONS**

- Lykourgos Chiniadis, Kostas Bethanis, Irene Axarli, Katholiki Skopelitou, Nikos Labrou, Michael Karpusas,
  - "Structural characterization of human glutathione S-transferase A1-1 in complex with the anti-cancer drug chlorambucil,"
  - Acta Crystallographica A, Vol. 65, s151 (2009).
- Michael Karpusas, Irine Axarli, Lykourgos Chiniadis, Athanasios Papakyriakou, Kostas Bethanis, Katholiki Scopelitou, Yannis D. Clonis, Nikolaos E. Labrou,
  - "The Interaction of the Chemotherapeutic Drug Chlorambucil with human Glutathione S-transferase A1-1: Kinetic and Structural Analysis,"
  - PLoS ONE, (2013), 8(2):e563375.

## CONFERENCES

1) Unbound docking studies of Aflatoxin B1 (AFB1) binding to human Glutathione S-transferase A1-1 (oral presentation),

Lykourgos Chiniadis, Athanassios Hountas, Kostas Bethanis, 4th conference of the Hellenic Society for Computational Biology and Bioinformatics HSCBB 2009, Athens, 18-20 December 2009

2) Determination of protein-protein interactions between Glutathione S-transferase P1-1 and C-Jun N-terminal kinase-1 (JNK-1),

Lykourgos Chiniadis, Juan Fernandez-Recio,

- 5th Conference of the Hellenic Crystallographic Association, Larissa, 25-26 September 2010
- 3) Crystal structures of ruthenium anti-cancer compounds bound to hen egg white lysozyme, Lykourgos Chiniadis, Petros Giastas, Ioannis Bratsos, Michael Karpusas, Kostas Bethanis, 6th International Conference of the Hellenic Crystallographic Association, Athens (GREECE), 28–29 September, 2012.

4) Structural insights into the interactions of Collagen type I and tannic acid as revealed by FT-IR spectroscopy and molecular dynamics,

Lykourgos Chiniadis, Anastasia Katsidima, Stamatis C. Boyatzis Proceedings of the Conference of the Hellenic Society for Computational Biology and Bioinformatics (HSCBB17),

Hellenic Pasteur Institute, Athens, Greece, 11–13 October 2017.

- 5) International School of Biological Magnetic Resonance, 9th Course Biophysics and Structure to Counter Threats and Challenges, Erice Italy 22 June–2 July 2009 (NATO ASI, Stanford University, USA and Myotrophic Lateral Sclerosis Foundation).
- 6) PHARE WORKSHOP: Macromolecular crystal structure solution via ABINITO, SIRMIR, SADMAD and Molecular Replacement techniques,

  Bari, Italy, April 2009.
- 7) European Crystallographic Meeting (ECM 25) (poster presentation), Structural characterization of human glutathione S-transferase A1-1/anti-cancer drug chlorambucil complex,

Lykourgos Chiniadis, Kostas Bethanis, Irene Axarli, Katholiki Skopelitou, Nikos Labrou, Michael Karpusas Istanbul, Turkey, 16–21 August 2009.

## **SEMINARS**

- 1) Introduction to Biomolecular modelling and Molecular dynamics in HPC (Classical and Quantum), Greek Research and Technology Network – Networking Reserach and Education, 23 April 2018, Athens, Greece (PRACE training)
- 2) VI-SEEM National dissemination event: Hands on workshop on MD biomolecular simulations and modeling,

Greek Research and Technology Network – Networking Research and Education, 24 April 2018, Athens, Greece (VI-SEEM training)

## **LANGUAGES**

English (excellent), French (very good)

## REFERENCES

Professor Elias Eliopoulos, Professor in Biochemistry, Department of Biotechnology, Agricultural University of Athens, GRe-mail: eliop@aua.gr

Dr. Athanasios Papakyriakou, NCSR Demokritos, Institute of Biosciences and Applications, Athens, Aghia Paraskevi, GR thpap@bio.demokritos.gr

> Dr. Juan Fernandez-Recio, Researcher, Barcelona Supercomputing Center, SP e-mail: juan.fernandez@bsc.es

# Professor Claudio Luchinat, CERM, University of Florence, IT e-mail: luchinat@cerm.unifi.it

Professor Ganesh Sockalingum, University of Reims Champagne-Ardennes, FR e-mail: ganesh.sockalinum@univ-reims.fr

