



Assistant Professor

Laboratory of Organic Chemistry, National and Kapodistrian University of Athens

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EDUCATION

2000 B.Sc. in Chemistry

University of Ioannina, Department of Chemistry, Ioannina (Greece).

2002 M.Sc. in Bioinorganic Chemistry

University of Ioannina, Department of Chemistry, Ioannina (Greece).

2005 Ph.D. in Chemistry

CERM, NMR center of University of Florence, Italy and University of Ioannina, Department of Chemistry, Ioannina, Greece. Research Advisor: Prof. Ivano Bertini.

APPOINTMENTS

2025-today Assistant Professor, Laboratory of Organic Chemistry, Department of Chemistry, National and Kapodistrian University of Athens, Greece

2023-2025 Research Assistant Professor, Group Leader, Institute of Chemical Biology, National Hellenic Research Foundation, Athens, Greece

2019-2022 > NMR Facility Manager, NMR Facility, Instrumental Analysis Laboratory, School of Natural Sciences, University of Patras, Greece

Appointed Assosiate Professor @ School of Agricultural Sciences, University of Patras, Greece

2017-2019 Visiting Researcher @ NRM center, Department of Chemistry and Pharmacy, University of Sassari Italy

2015-2019 Post Doc Researcher, Foundation for Research and Technology – Hellas (FORTH), Institute of Chemical Engineering Sciences (ICEHT)

2008-2015 Visiting Researcher @ CRMN, Very High Field NMR Center of Lyon, Lyon, France

Visiting Researcher @ NMR center of University of Freiburg, Freiburg, Germany

Visiting Researcher @ Faculty of Medicine Imperial College, Hammersmith Hospital Campus, London, UK

2008-2015 Post Doc Researcher, Department of Pharmacy, University of Patras

Appointed Assistant Professor @ Department of Pharmacy, University of Patras

2005-2006 Post Doc Researcher @CERM, NMR center of University of Florence, Italy

2002-2005 Marie Curie Fellow @CERM, NMR center of University of Florence, Italy

RESEARCH FIELDS

- NMR spectroscopy of bioactive organic compounds and drugs, with a focus on their interactions with peptides and proteins
- Computational chemistry, including molecular docking, molecular dynamics simulations, and structure-based prediction of protein–protein and protein–drug interactions
- Drug repurposing and rational design of pharmacological agents

EDUCATION EXPERIENCE

UNDERGRADUATE COURSES

- > 2019-2022 Appointed Associate Professor / Organic Chemistry/ Required course /School of Agricultural Sciences, University of Patras
- > **2018-2019** Appointed Assistant Professor / Instrumental Chemical Analysis/ Required course / Department of Chemistry, University of Patras
- **2011-2015** Appointed Assistant Professor / Molecular simulation/ Required course / Department of Pharmacy, University of Patras

POSTGRADUATE COURSES

2018 TRANSLATIONAL RESEARCH IN BIOMEDICINE / Department of Molecular Biology and Genetic, Democritus University of Thrace

AWARDS AND SCHOLARSHIPS

- 2023 Invited Editorial Board Member of the Journal: Outbreak Management and Response, by Taylor and Francis.
- **2021** Guest Editor of Special issue "Metal Intoxication: General Aspects and Chelating Agents", Molecules, MDPI, impact factor: 4.927
- 2016-2017 Post Doc fellowship, "Structural Systems Biology for Metabolic Engineering Applications" by ARCHERS project Stavros Niarchos Foundation, Foundation for Research and Technology – Hellas (FORTH), Institute of Chemical Engineering Sciences (ICEHT), Greece
- ➤ 2014 The publication: Zinc and human health: an update, Chasapis, C.T., Loutsidou, A.C., Spiliopoulou, C.A, Stefanidou ME., Arch Toxicol 86, 521–534, 2012, https://doi.org/10.1007/s00204-011-0775-1, was characterized as "Review on cutting- edge topics in toxicology" and most cited and downloaded in Archives of Toxicology in 2012: https://doi.org/10.1007/s00204-014-1418-0
- **2003-2004** Marie Curie PhD fellow funded by EU- FP6-CITIZENS project: "Improving the Human Research Potential and Socio-Economic Knowledge Base" ID: HPMT-CT-2000-00137 CERM, University of Florence, Italy
- 2000-2001 Postgraduate Scholarship (12 months) by Greek State Fellowship Foundation (IKY), Dept. of Chemistry, U. of Ioannina
- > 1999-2000 Undergraduate Scholarship (12 months) by EU INTERREG II, Dept. of Chemistry, U. of Ioannina

RESEARCH GRANDS

- **2024-2025** C02BIO/16103 (ΕΛΙΔΕΚ_5): Main researcher of the WP (12 months): Structural Computational Analysis of the Proteome of Extremophilic Bacteria and Anaerobic Carbon Dioxide Assimilation
- 2023-2024 Horizon 2020, JOINTPROMISE, Grant agreement ID: 874837, "JOINTPROMISE", https://www.jointpromise.eu (Participation 12 months)
- ➤ 2021 T2EDK 01332, MIS 5072532, "TOMATOMICS Quantification of Metabolic Profiles in Tomato Tissues Using Spectroscopic Techniques and Participation in Data Analysis within the Context of Biomolecular Networks (Participation 6 months)
- 2018-2019 ELIXIR-GR: Managing and Analysing Life Sciences Data, (Participation 12 months)
- 2015-2017 FP7/2007-2013 KBBE, 2013-17, ContractN° 613877: "STREPSYNTH" http://www.strepsynth.eu/ (Participation 24 months)
- ➤ 2012-2015 EU FP7-REGPOT Establishment of a Centre of Excellence for Structure-based drug target characterization (SEE-DRUG), (Participation 36 months)
- ➤ **2008-2012** EU FP7-HEALTH Neurotransmitter Cys-loop receptors: structure, function and disease (NEUROCYPRES), (Participation 48 months)

ADDITIONAL INFORMATION

- >85 publications in peer reviewed journals (> 3200 citations, h-index: 23; Scopus (09/25)
- >18 invited lectures in Greece and abroad
- Supervision of doctoral theses: 1
- Supervision of graduate students: 3
- Supervision of undergraduate students: >10
- 5 research monographs
- Invited Editorial Board Member of the Journal: Outbreak Management and Response, by Taylor and Francis
- >15 invited reviewer for research articles in peer reviewed journals
- Member of Hellenic Society for Computational Biology and Bioinformatics
- Member of European Peptide Society, EPS
- Member of the Union of Greek Chemists
- Member of the National Research Infrastructures ELIXIR-GR and INSTRUCT-ERIC

Selected Publications

- D.P. Kiouri, G.C. Batsis, C.T. Chasapis*, Structure-Based Deep Learning Framework for Modeling Human–Gut Bacterial Protein Interaction, Proteomes, 13, 10, 2025 https://doi.org/10.3390/proteomes13010010
- ➤ D.P. Kiouri, G.C. Batsis, T. Mavromoustakos, A. Giuliani, C.T. Chasapis*, *Structure-Based Modeling of the Gut Bacteria*—Host Interactome Through Statistical Analysis of Domain—Domain Associations Using Machine Learning. **BioTech**, 14, 13, **2025**. https://doi.org/10.3390/biotech14010013
- V. Apostolopoulos*, N. Georgiou, D. Tzeli*, T. Mavromoustakos*, G. J. Moore, K. Kelaidonis, M.-T. Matsoukas, S. Tsiodras, J. Swiderski, L. K. Gadanec, A. Zulli, C. T. Chasapis*, J. M. Matsoukas*, Density functional theory and enzyme studies support interactions between angiotensin receptor blockers and angiotensin converting enzyme-2: Relevance to coronavirus 2019, Bioorganic Chemistry, Volume 150,107602, ISSN 0045-2068, 2024, https://doi.org/10.1016/j.bioorg.2024.107602
- ➤ K. Kelaidonis, I. Ligielli, S. Letsios, V.P. Vidali, T. Mavromoustakos, N. Vassilaki, G.J. Moore, W. Hoffmann, K. Węgrzyn, H. Ridgway, C.T. Chasapis*, J.M.Matsoukas*, Computational and Enzymatic Studies of Sartans in SARS-CoV-2 Spike RBD-ACE2 Binding: The Role of Tetrazole and Perspectives as Antihypertensive and COVID-19 Therapeutics, Int J Mol Sci. ;24(9):8454, 2023, https://doi.org/10.3390/ijms24098454
- Ridgway H, Orbell JD, Matsoukas MT, Kelaidonis K, Moore GJ, Tsiodras S, Gorgoulis VG, Chasapis CT*, Apostolopoulos V, Matsoukas JM*. W254 in furin functions as a molecular gate promoting anti-viral drug binding: Elucidation of putative drug tunneling and docking by non- equilibrium molecular dynamics, Comput Struct Biotechnol J.;21:4589-4612, 2023, https://doi.org/10.1016/j.csbj.2023.09.003
- M. Spiliopoulou, A. Valmas, D. Triandafillidis, S. Fili, M. Christopoulou, A. J. Filopoulou, A. Piskopou, P. Papadea, A. N. Fitch, D. Beckers, T. Degen, F. Gozzo, M. Morin, M. L.ReinleSchmitt, F. Karavassili, E. Rosmaraki, C. T. Chasapis and I. Margiolaki* High throughput macromolecular polymorph screening via NMR and X-ray powder diffraction synergistic approach: The case of human insulin co-crystallized with resorcinol derivatives J. Appl. Cryst. 54, 963-975, 2021 https://doi.org/10.1107/S160057672100426X
- C.T.Chasapis*, and A. Vlamis-Gardikas Probing conformational dynamics by Protein Contact Networks:comparison with NMR relaxation studies and molecular dynamics simulations, Biophysica, MDPI 1(2), 157-167, 2021, https://doi.org/10.3390/biophysica1020012
- D. G Mintis, A. Chasapi, K.Poulas, G. Lagoumintzis, C. T.Chasapis*, Assessing the Direct Binding of Ark-Like E3 RING Ligases to Ubiquitin and Its Implication on Their Protein Interaction Network,

- Molecules, MDPI, 25(20):4787, 2022, https://doi.org/10.3390/molecules25204787
- C. T. Chasapis*, Hierarchical core decomposition of RING structures as a method to capture novel functional residues within RING-type E3 ligases: a structural systems biology approach, Comput Biol Med., Volume 100, Pages 86–91, 2018, https://doi.org/10.1016/j.compbiomed.2018.06.033
- C.T. Chasapis, A.I. Argyriou, M. Apostolidi, P.Konstantinidou, C.Stathopoulos, D. Bentrop, G.A. Spyroulias*, ¹H, ¹³C and ¹⁵N Backbone and side-chain resonance assignment of theLAM-RRM1 N-terminal module of La protein from Dictyostelium discoideum, Biomol NMR Assign. 9(2):303-7, 2015, https://doi.org/10.1007/s12104-015-9597-z
- C.T. Chasapis, N.G. Kandias ,V. Episkopou, D. Bentrop, G.A. Spyroulias*, NMR-based insights into the Conformational & Interaction properties of Arkadia RING-H2 E3 Ub Ligase, PROTEINS: Structure Notes, 80(5):1484-9, 2012 https://doi.org/10.1002/prot.24048
- L. Banci, I. Bertini, S.C. Bafoni, C.T. Chasapis, N.Hadjiliadis, A. Rosato, *An NMR study of the interaction between the human copper(I) chaperone and the second and fifth metal-binding domains of the Menkes protein.* **FEBS Journal** Vol 272, Issue 3, 865-871, **2005**, https://doi.org/10.1111/j.1742-4658.2004.04526.x
- L. Banci, I. Bertini, F. Cantini, C.T. Chasapis, N. Hadjiliadis, A. Rosato, A NMR study of the interaction of a three-domain construct of ATP7a with copper(I) and copper(I)-HAH1: the interplay of domains, Journal of Biological Chemistry. vol. 280, no.46, pp. 38259–38263, 2005, https://doi.org/10.1074/jbc. M506219200