Michail Papadourakis

Research and Work Experience

April 2024 – present **Hellenic Mediterranean University, Department of Nursing**,
Heraklion, Greece,
Head of the Laboratory: Prof. Evridiki Patelarou.

***1st project*: Computer-aided drug design of small molecules for the inhibition of Glutamate receptors** .

- Identification and analysis of the full free energy landscapes of GluK3 unbound and bound to known inhibitors using naïve and adaptive MD sampling.
- Design and in vitro evaluation of novel GluK3 small-molecule inhibitors.

October 2023 – present **Hellenic Mediterranean University, Department of Nursing**,
Heraklion, Greece.

***Adjunct Instructor*: Fundamental Principles of Pharmacology in Nursing**.

- Preparation and demonstration of teaching materials.
- Marking students' exams and providing feedback on student performance.

March 2023 – Present **Cloudpharm PC**, *Athens, Greece.*

***1st project*: ENVIROMED: Next generation toolbox for greener pharmaceuticals design and manufacturing towards reduced environmental impact** .

- Development of novel in-silico tools for "green-by-design" pharmaceuticals, along with predicting the ecotoxicity impact of pharmaceuticals using Machine Learning models.

***2nd project*: OSTEOME: Design and development of a novel food supplement for osteoporosis based on gut microbiome mechanisms** .

- Design and development a novel dietary supplement for osteoporosis, activating the intestinal microbiome.

November 2020 – present **Molecular Modelling and Drug Design Group, Biomedical Research Foundation Academy of Athens**, *Athens, Greece*,
Head of the Laboratory: Dr. Zoe Cournia.

***1st project*: FEPrepare: A Web-Based Tool for Automating the Setup of Relative Binding Free Energy Calculations**.

- Creation of a web-based server that automates the FEP/MD dual-topology procedure using the OPLS-AA force-field to enable fast and automated input of NAMD FEP/MD files ready for production runs.

***2nd project*: The effect of S427F mutation on RXR activity depends on its dimeric partner**.

- Elucidation of the effect of the S427F mutation on the structure and dynamics of RXR in its homodimeric and heterodimeric form with RAR and PPARg using a combination of biochemical experiments and Molecular Dynamics simulations.

***3rd project*: Investigation of BMAA and its carbamate adducts as potential inhibitors of the GluR2 using MD/FEP calculations**.

- Investigation of the binding affinity of BMAA and its carbamate adducts to glutamate receptors in comparison to the natural agonist, glutamate using MD and relative FEP calculations.

***4th project*: Design of novel synthetic analogs for the inhibition of the oncoprotein c-Myc**.

- Identification and analysis of the full free energy landscapes of c-Myc bioactive peptides unbound and bound to known inhibitors using naïve and adaptive MD sampling.
- Design and in vitro evaluation of novel c-Myc small-molecule inhibitors.

October 2021 – February 2022 **University of Athens, Department of Informatics and Telecommunications**,
Athens, Greece.

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***Teaching Assistant*: Molecular Modeling of Biomolecules**.

- Demonstration of teaching materials and assistance to students on hands-on exercises as and when required.
- Marking students' presentations on a final project set by the course organiser and providing feedback on student performance.

September 2017 – October 2020 **Julien Michel Research Group, University of Edinburgh, Department of Chemistry**, *Edinburgh, United Kingdom*,
Head of the Laboratory: Dr. Julien Michel.

***1st project*: Blinded Predictions of Standard Binding Free Energies: Lesson Learned from the SAMPL6 Challenge**.

- Participation in SAMPL6 challenge and ranking amongst the top groups in terms of results.
- Calculation of protein-ligand binding free energies using alchemical free energy calculations.

***2nd project*: Selective CypA/D inhibition via targeting of the 3 o'clock pocket**.

- Design of novel three-vector ligands with strong dissociation constant and >100 fold selectivity for CypD over CypA and vice versa.

***3rd project*: Prediction of absolute binding free energies of ligands for the intrinsically disordered protein c-Myc**.

- Absolute Free Energy (AFE) and Markov State Model (MSM) protocols to evaluate the binding free energies of the protein-ligand complexes.
- Establishment of efficient and accurate predictive models for the identification of novel c-Myc inhibitors.

***4th project*: Absolute binding free energy calculations of MDM2 ligands**.

- Establishment of an adaptive sampling AFE protocol to evaluate the binding free energies of the protein-ligand complexes.
- Prediction of the binding trend of five-known inhibitors of the MDM2-p53 interaction using a fraction of the computational time of the original AFE protocol.

September 2017 – August 2020 **University of Edinburgh, Department of Chemistry**,
Edinburgh, United Kingdom.

***Laboratory Demonstrator*: Physical Chemistry 3 and Maths for Chemistry 2**.

- Demonstration of the use of practical equipment and assistance to students as and when required.
- Marking student tests set by the course organiser and providing feedback on student performance.

March 2016 – February 2017 **Biomolecular Spectroscopy & Computational Drug Design Group, University of Athens, Department of Pharmaceutical Chemistry**, *Athens, Greece*,
Head of the Laboratory: Prof. Emmanuel Mikros,
Supervisor: Dr. George Lamprinidis.

***Project Thesis*: In silico and in vivo study of the UapA nucleobase transporter and rational design of novel inhibitors**.

- Design of UapA inhibitors through in silico receptor-based drug design.
- Uptake assays to test the biological activity of the potential inhibitors.

July 2016 – September 2016 **Community Pharmacy Intern**, *Michelaki's Pharmacy*, Heraklion, Greece.

- Advised customers on the recommended dosage, warnings, storage and possible side effects of all dispensed medication.
- Assisted with medical performances such as taking blood pressure, temperature and other vitals.
- Administered vaccinations to pharmacy customers.

July 2015 – September 2015 **Intern in Hospital's Pharmacy Intern**, *General University Hospital of Heraklion*, Heraklion, Greece.

- Prepared pediatric suspensions, syrups and other not commercially available formulations and informed patients on their safe and effective use.
- Provided information to patients on the safe and effective use of medicines.
- Managed medicine inventory in the most cost-effective way, resulting in 10% reduced wastage.

Education

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2017 – 2021 **PhD in Chemistry**, University of Edinburgh, United Kingdom.
- Thesis: Molecular Dynamics Based Methods for the Computation of Standard Binding Free Energies and Binding Selectivity of Inhibitors of Proteins of Pharmaceutical Interest

2011 – 2017 **MPharm (5 year degree – 300 ECTS)**, University of Athens, Greece.
- Grade: 8.72/10 - Top 7% of the year.
- 9^{th} highest entrance score between all matriculating students in the Faculty of Pharmacy in 2011.

Publications

Isidora Diakogiannaki, **Papadourakis, Michail**, Vasileia Spyridaki, Zoe Cournia, and Andreas Koutselos. Computational Investigation of BMAA and Its Carbamate Adducts as Potential GluR2 Modulators. *Journal of Chemical Information and Modeling*, 64(13):5140–5150, July 2024. Publisher: American Chemical Society.

Ioannis Galdadas, Vangelis Bonis, Paraskevi Vgenopoulou, **Papadourakis, Michail**, Panos Kakoulidis, Georgia Stergiou, Zoe Cournia, and Apostolos Klinakis. The effect of S427F mutation on RXR activity depends on its dimeric partner. *Chemical Science*, October 2021. Publisher: The Royal Society of Chemistry.

Danai Maria Kotzampasi, **Papadourakis, Michail**, John E. Burke, and Zoe Cournia. Free energy landscape of the PI3K C-terminal activation. *Computational and Structural Biotechnology Journal*, 23:3118–3131, December 2024.

Alexandros-Timotheos Loukas, **Papadourakis, Michail**, Vasilis Panagiotopoulos, Apostolia Zarmpala, Eleni Chontzopoulou, Stephanos Christodoulou, Theodora Katsila, Panagiotis Zoumpoulakis, and Minos-Timotheos Matsoukas. Natural Compounds for Bone Remodeling: A Computational and Experimental Approach Targeting Bone Metabolism-Related Proteins. *International Journal of Molecular Sciences*, 25(9):5047, January 2024. Number: 9 Publisher: Multidisciplinary Digital Publishing Institute.

Minos-Timotheos Matsoukas, Tarryn Radomsky, Vasilis Panagiotopoulos, Robin du Preez, **Papadourakis, Michail**, Konstantinos Tsianakas, Robert P Millar, Ross C Anderson, Georgios A Spyroulias, and Claire L Newton. Identification of Small-Molecule Antagonists Targeting the Growth Hormone Releasing Hormone Receptor (GHRHR). *Journal of Chemical Information and Modeling*, 64(18):7056–7067, September 2024. Publisher: American Chemical Society.

Cesar Mendoza-Martinez, **Papadourakis, Michail**, Salomé Llabrés, Arun Gupta, Paul Barlow, and Julien Michel. Energetics of a protein disorder-order transition in small molecule recognition. *Chemical Science*, April 2022. Publisher: The Royal Society of Chemistry.

Andrea Rizzi, Travis Jensen, David R. Slochower, Matteo Aldeghi, Vytautas Gapsys, Dimitris Ntekoumes, Stefano Bosisio, **Papadourakis, Michail**, Niel M. Henriksen, Bert L. de Groot, Zoe Cournia, Alex Dickson, Julien Michel, Michael K. Gilson, Michael R. Shirts, David L. Mobley, and John D. Chodera. The SAMPL6 SAMPLing challenge: assessing the reliability and efficiency of binding free energy calculations. *Journal of Computer-Aided Molecular Design*, 34(5):601–633, May 2020.

Papadourakis, Michail, Stefano Bosisio, and Julien Michel. Blinded predictions of standard binding free energies: lessons learned from the SAMPL6 challenge. *Journal of Computer-Aided Molecular Design*, 32(10):1047–1058, October 2018.

Papadourakis, Michail, Zoe Cournia, Antonia S. J. S. Mey, and Julien Michel. Comparison of Methodologies for Absolute Binding Free Energy Calculations of Ligands to Intrinsically Disordered Proteins. *Journal of Chemical Theory and Computation*, 20(21):9699–9707, November 2024. Publisher: American Chemical Society.

Papadourakis, Michail, Hryhory Sinenka, Pierre Matricon, Jérôme Hénin, Grace Brannigan, Laura Pérez-Benito, Vineet Pande, Herman van Vlijmen, Chris de Graaf, Francesca Deflorian, Gary Tresadern,

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Marco Cecchini, and Zoe Cournia. Alchemical Free Energy Calculations on Membrane-Associated Proteins. *Journal of Chemical Theory and Computation*, 19(21):7437–7458, November 2023. Publisher: American Chemical Society.

Vasiliki Vakali, **Papadourakis, Michail**, Nikitas Georgiou, Nikoletta Zoupanou, Dimitrios A. Diamantis, Uroš Javornik, Paraskevi Papakyriakopoulou, Janez Plavec, Georgia Valsami, Andreas G. Tzakos, Demeter Tzeli, Zoe Cournia, and Thomas Mauromoustakos. Comparative Interaction Studies of Quercetin with 2-Hydroxyl-propyl--cyclodextrin and 2,6-Methylated--cyclodextrin. *Molecules*, 27(17):5490, January 2022. Number: 17 Publisher: Multidisciplinary Digital Publishing Institute.

Stamatia Zavitsanou, Alexandros Tsengenes, **Papadourakis, Michail**, Giorgio Amendola, Alexios Chatzigoulas, Dimitris Dellis, Sandro Cosconati, and Zoe Cournia. FEPrepare: A Web-Based Tool for Automating the Setup of Relative Binding Free Energy Calculations. *Journal of Chemical Information and Modeling*, 61(9):4131–4138, September 2021.

Computer skills

Molecular Dynamics and Modelling	Homology modelling with Prime, Experience in GROMACS, Desmond, Amber, ACEMD and NAMD simulation packages Markov State Models with PyEMMA software
Free Energy Calculations	Sire/OpenMM (SOMD), FESetup, BioSimSpace, Gromacs, NAMD, AMBER
Structure-based Drug Design	Extensive experience with Schrodinger tools, Virtual Screening: Glide, Induced Fit Docking (IFD), Covalent Docking Spark and Flare programs from Cresset for the creation of virtual libraries and Covalent Docking
Ligand-based Drug Design	Use of ROCS and RDKit for similarity search and filtering of the identification of promiscuous hits
Programming Skills and Operating Systems	Python, Linux, Microsoft Windows, MacOS

Awards

September 2023 **Best poster presentation award**.
Selection of our poster with title "Developing a multimodal platform for in silico design of pharmaceuticals with reduced environmental footprint" for a 500 euro poster award

March 2022 **Access to ARIS supercomputer (12th Call)**.
Selection of our proposal with title "Discovery of new inhibitors of the oncoprotein c-Myc using Molecular Dynamics simulations" for access to ARIS supercomputer to use a total of 200,000 GPUs.

March 2022 **Access to ARIS supercomputer (12th Call)**.
Selection of our proposal with title "Using free energy perturbation calculations to examine BMAA and its carbamate adducts as potential glutamate inhibitors" for access to ARIS supercomputer to use a total of 900,000 CPUs.

November 2021 **Preparatory Access to ARIS supercomputer**.
Selection of our proposal with title "Absolute Free Energy calculations of quercetin with 2-hydroxyl-propyl-cyclodextrin and 2,6 methylated-cyclodextrin" for access to ARIS supercomputer to use a total of 40,000 CPUs and 20,000 GPUs.

October 2021 **Access to Marconi100 supercomputer (23rd Call for PRACE Project Access)** .
Selection of our project n. 2021240075 with title "Understanding how kinase domain mutations of PI3K alter lipid kinase activity using HDX-MS and CryoEM experiments and Molecular Dynamics simulations" for access to Marconi100 supercomputer to use a total of 35.000.000 core hours.

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September 2021 – March 2023 **"Bodosaki" Scholarship**.
The Bodosaki foundation offers scholarships for postdoctoral researchers based on academic excellence of submitted research proposals. Selection of my proposal with title "Design of novel synthetic analogs for the inhibition of the oncoprotein c-Myc" for covering a stipend of £18,000 per annum..

April 2021 **Access to Juelich Supercomputing Centre**.
Selection of our proposal with title "Investigating the effect of the S427F mutation on RXR activity depending on its dimeric partner" for access to JURECA supercomputer to use a total of 1,000,000 CPUs.

March 2021 **Access to ARIS supercomputer (10th Call)**.
Selection of our proposal with title "Investigation of the binding mechanism of monomeric c-Myc/ligand complexes using equilibrium and adaptive MD methods" for access to ARIS supercomputer to use a total of 37,000 GPUs.

December 2020 **Prace Preparatory Access project n. 2010PA5633 to Marconi100 supercomputer**.
Selection of our proposal with title "Investigation of the dimer stability of the membrane-associated KRAS-4B protein with Raf effectors using equilibrium and adaptive MD methods" for access to Marconi100 supercomputer to use a total of 13200 core hours.

November 2020 **Preparatory Access to ARIS supercomputer**.
Selection of our proposal with title "FEPrepare: A web-based tool for automating the setup of relative binding free energy calculations" for access to ARIS supercomputer to use a total of 40,000 CPUs and 20,000 GPUs.

January 2019 – March 2019 **HPC Europa 3**.
Scientific collaboration with Zoe Cournia's lab in BRFAA in order to access world-class HPC systems. Each scholarship covers the travel bursaries as well as a stipend of £4,200.

2017 – 2020 **Principal's Career Development PhD Scholarship**.
The University of Edinburgh offers scholarships for students starting their research at the University. Each scholarship covers the UK/EU rate of tuition fee as well as a stipend of £15,000 per annum.

2013 – 2016 **"Antonios Papadakis" Scholarship**.
Earned €3,500 per annum scholarship based on academic excellence and competitive university-wide written examinations.

Conferences

1 – 3 June 2017 **17th Hellenic Symposium on Medicinal Chemistry**.
Poster with title: *In silico and in vivo study of the UapA nucleobase transporter and rational design of novel inhibitors*

22 – 23 February 2018 **D3R 2018 Workshop at San Francisco, California**.
Talk with title: *SOMD - lesson learned from SAMPL6*

6 – 17 July 2018 **CCP5 Summer School 2018 at Lancaster University**.
Poster with title: *Blinded Predictions of Standard Binding Free Energies: Lesson Learned from the SAMPL6 Challenge*

5 – 7 September 2018 **CCP5BioSim meeting in Oxford**.
Poster with title: *Blinded Predictions of Standard Binding Free Energies: Lesson Learned from the SAMPL6 Challenge*

26 June 2019 **Scotchem Computational Chemistry Symposium, Heriot Watt** .
Poster with title: *A Computational Workflow for the Discovery of Selective Cyclophilin D Inhibitors*

4 – 6 September 2019 **7th annual CCPBioSim conference, Bristol** .
Poster with title: *A Computational Workflow for the Discovery of Selective Cyclophilin D Inhibitors*

22 November 2019 **Young Modellers' Forum 2019, Greenwich** .
Talk with title: *A Computational Workflow for the Discovery of Selective Cyclophilin D Inhibitors*

19 – 24 June 2022 **International HPC Summer School, Athens (Greece)** .
Poster with title: *FEPrepare: A Web-Based Tool for Automating the Setup of Relative Binding Free Energy Calculations*

17 – 22 July 2022 **Computational Chemistry Gordon Research Conference, Barcelona (Spain)** .
Poster with title: *FEPrepare: A Web-Based Tool for Automating the Setup of Relative Binding Free Energy Calculations*

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15 – 16 June 2023 **2nd Plenary Meeting of the Enviromed EU Project, Athens (Greece)** .
Talk with title: *A multimodal platform for in silico development of green-by-design compounds*

16 – 18 July 2023 **Paul Erlich Euro-PhD Network, Thessaloniki (Greece)** .
Poster with title: *A multimodal platform for in silico development of green-by-design compounds*

15 – 17 September 2023 **Bio3 - Biomedicine, Bioinformatics and Biotechnology forum, Athens (Greece)** .
Poster with title: *Developing a multimodal platform for in silico design of pharmaceuticals with reduced environmental footprint*

22 – 23 September 2023 **Innohealth forum, Larissa (Greece)** .
Talk with title: *Cloudpharm: a bio-pharmaceutical RnD Company*

1 – 3 December 2023 **73rd National Conference of the Hellenic Society of Biochemistry and Molecular Biology (HSBMB), Athens (Greece)** .
Poster with title: *Phytochemicals as bone remodelers for the development of nutraceutical for osteoporosis*

8 December 2023 **Medicinal Chemistry 2.0: Emerging Trends Enabling Drug Discovery of the Future, Brussels (Belgium)** .
Poster with title: *A multimodal platform for the in silico design of pharmaceuticals with reduced environmental footprint*

12 – 13 December 2023 **3rd Plenary Meeting of the Enviromed EU Project, Nicosia (Cyprus)** .
Talk with title: *A multimodal platform for in silico development of green-by-design compounds*

13 – 14 May 2024 **AI Approaches in Structural Biology and Drug Discovery workshop, Grenoble (France)** .
Talk with title: *Leveraging Chemoinformatics and ML Methods towards Drug Repurposing and Future Pharmaceuticals*

27 – 28 May 2024 **4th Plenary Meeting of the Enviromed EU Project, Napoli (Italy)** .
Talk with title: *A multimodal platform for in silico development of green-by-design compounds*

25 – 28 September 2024 **23rd Panhellenic Chemistry Conference, Athens (Greece)** .
Talk with title: *Using Free Energy Perturbation Calculations to Predict Binding Affinities in Drug Design*

Languages

Greek	Native	
English	Fluent	*Certificate of Proficiency in English*
German	Basic	*Goethe-Zertifikat B1*

Personal Interests

Debate: Member of University of Athens Debate Club

Chess: Member of S.O. Heraklion chess team, 1^{st} league

Basketball

Tennis

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