ANTONIOS KOLOCOURIS

Current Position
Professor
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Personal details
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Birth: 05/12/1966

Education

10/1997-10/2000: **Post-doctoral researcher**, Laboratory of Molecular Biophysics, Institute of Chemical Biology, National Hellenic Research Foundation (NMR, ssNMR, Differential Scanning Calorimetry, MD simulations).

- 10/1997-10/2000: Conformation in solution of Angiotensin II, peptidic and non-peptidic agonists and antagonists using NMR spectroscopy and MD simulations with CHARMM force field
  Conformation of conjugates of drugs-lipid conjugates, like AZT with long alkyl chain lipids and glycerolipids in micelles and interactions with model membranes using biophysical methods
- 10/1999-10/2000: Conformation and structure elucidation of natural products

01/1997-07/1997: **Post-doctoral researcher**, Laboratory of Medicinal Chemistry, Department of Pharmacy, NKUA, Synthetic medicinal chemistry
03/1990-03/1995, PhD thesis in Medicinal Chemistry, Laboratory of Medicinal Chemistry, Department of Pharmacy, NKUA.
10/1984-10/1989, Degree in Chemistry (MSc equivalent, 8.6/10), Department of Chemistry, NKUA.

Academic Positions

05/2020: **Professor,** Laboratory of Medicinal Chemistry, Department of Pharmaceutical Chemistry, Faculty of Pharmacy, NKUA
05/2011: **Associate Professor,** Laboratory of Medicinal Chemistry, Department of Pharmaceutical Chemistry, Faculty of Pharmacy, NKUA
03/2010: **Assistant Professor (tenure),** Laboratory of Medicinal Chemistry, Department of Pharmaceutical Chemistry, Faculty of Pharmacy, NKUA
04/2006: **Assistant Professor,** Laboratory of Medicinal Chemistry, Department of Pharmaceutical Chemistry, Faculty of Pharmacy, NKUA
10/2000: **Lecturer, Assistant Professor,** Laboratory of Medicinal Chemistry, Department of Pharmaceutical Chemistry, Faculty of Pharmacy, National and Kapodistrian University of Athens (NKUA)

Research Visits

10/2012: **University of Düsseldorf, Department of Pharmacy**
MM-PBSA calculations (AMBER); interactions of aminoadamantanes with influenza A M2 protein

11/2010: **University of Zurich, Department of Biochemistry**
MM-PBSA and LIE calculations (CHARMM)

10/2008, 10/2009: **University of Pisa, Department of Pharmacy**
Docking calculations, and MD simulations (AMBER); interactions of aminoadamantanes with influenza A M2 protein

02/2004: **University of Cambridge, Department of Biochemistry**
^{19}F NMR; interaction study of aminoadamantanes with influenza A M2 protein in micelles using a fluorinated M2TM protein and fluorinated ligand derivatives

07/2002: **University of Cambridge, Department of Biochemistry**
NMR; interaction study of aminoadamantanes with influenza A M2 protein in liposomes

09/1999: **University College London, Department of Chemistry**
Dynamic NMR; study of hindered ring inversion, nitrogen inversion and bond rotation in model-compounds

Awards and Fellowships

1991-1995: State post graduate scholarship, NKUA
07/2002: Research fellowship Royal Society of Chemistry for
02/2004: Research fellowship Royal Society of Chemistry

Other Distinctions

Artwork from study on M2 protein reaches the cover of Journal of American Chemical Society (JACS; issue 45, 14-Nov 2018)
Artwork from study on M2 protein reaches the cover of ACS Biochemistry (issue 4, 2-Jan 2020)
Artwork from study in M2 protein reaches the cover of ChemMedChem (2023)

Research activity

1. Medicinal Chemistry / Computational biochemistry

- Study of membrane protein – ligand interactions, using computational-aided drug design (CADD): all-atom MD (AA MD) simulations, free energy calculations (MM-PBSA, FEP/MD, TI/MD); and biophysical methods (e.g., NMR spectroscopy, DSC).
- Virtual screening of chemical libraries using structure- and ligand-based methods.
- Structure-activity relationships and 3D QSAR.
- Chemical synthesis of bioactive ligands.

Research Areas

- **Influenza A M2 protein:** Studies of the interactions of aminoadamantanes with influenza A M2 constructs, M2(22-46) or M2(22-62) using (a) NMR spectroscopy, ITC, electrophysiology, antiviral assays in amantadine resistant viruses, and (b) MD simulations, binding free energy calculations using FEP/MD, TI/MD **(2002-today)**.
- Application of CADD methods and synthesis of aminoadamantanes and conjugates with polar head heterocyles against influenza A wild type and amantadine-resistant strains S31N, V27A, L27F, G34E, A30T **(2010-today)**.
- **Adenosine receptors (ARs):** Virtual screening of chemical libraries; optimization of hits to leads using TI/MD calculations, synthesis of new selective antagonist derivatives based on chemical probes identified from virtual screening against ARs; ML-based models for prediction of ligands potency.
- CADD and development of antagonists against A_1R, A_3R using MD simulations and TI/MD calculations as well as mutagenesis experiments **(2019-today)**.
- **Mmpl3:** This protein is a transporter of trehalose monomycolate (TMM) of Mtb, and we have designed computationally and developed new analogs of the drug **SQ109**, which is in phase II clinical trials against Mtb, using structure-based drug design. Strikingly, we found SQ109 analogs that are active against other pathogens including malaria, M. Abscessus, and gram-negative bacteria **(2018-today)**.
- **CB2R**: We are developing ligands (CADD, synthesis) against CB2R (**2021-today**).
- **P2X7R**: For P2X7 purinergic receptors we are running CADD for synthesis of antagonists using in the first cryo-EM structure of human P2X7 and orthologs.
- **sEH**: We design and develop new inhibitors of soluble epoxide hydrolase enzyme; ML-based models for prediction of ligands potency (**2021-today**).
- **AT1R**: Design and development of fluorescent probes (**2024-today**).
- **Viral Mpro/PLpro**: We are working with inhibition of Mpro or PLpro from SARS-COV-2 or enteroviruses (**2020-today**).
- **Theranostics**: Design and development of new bioconjugate ligands against PSMA and GRPR (**2020-today**).
- **Conformational analysis of hydrophobic peptides:** MD simulations and DFT calculations are performed to examine the stabilization factors, e.g., N-H/O and C-H/O hydrogen bonds (**2012-today**).
- **Conformational analysis of AngII and AT1 antagonists:** MD simulations and NOE experiments were applied **(1997-2000**).

2. Biophysics

Experimental biophysics (ssNMR, SAXS, DSC), AA MD and coarse-grained MD simulations to investigate lipophilic drugs and membrane proteins interacting with membranes.

Research Areas:

- We are running several biophysics experiments in combination with ssNMR experiments and we are exploring the effect of lipids in M2 contribution in viral budding using coarse-grained (CG MD) MD simulations (**2017-today)**.
- We are exploring the effect of SQ109 in membranes with experimental and computational methods (AA and CG MD simulations) and the transport mechanism of TMM by MmpL3 and its inhibition by SQ109 using CG MD simulations (**2023-today)**.
- We are running CG MD simulations to study interactions between GPCRs and lipids (**2021-today**).

3. Physical - Organic Chemistry

- Dynamic NMR
- Computational organic chemistry

Research Areas:

- Conformational analysis of organic molecules in solution using Dynamic NMR and molecular mechanics or quantum mechanical calculations **(1995-2015)**.
- Weak intramolecular interactions: non-conventional hydrogen bonding C-H---X (X=O, N, F, S) in organic molecules using NMR chemical shift changes, and QM calculations of interactions and chemical shift changes (**2005-today**).
- Non-conventional hydrogen bonding in lipophilic peptides and its effect on the folding using MD simulations, QM calculations and experimental studies of folding (**2010-today**).
- Mechanisms of Au-catalyzed organic reactions using DFT calculations (**2014-today**).
- Evaluation of the accuracy of force fields and quantum mechanical methods and generation of databases for the conformational analysis of organic molecules (**2017-today)**.

Editorial Board in International Journals

Editorial advisory board of *ACS Pharmacology & Translational Science*, **2021-today**
Editorial advisory board of Frontiers in Chemical Biology, **2023-today**

Teaching

05/1997: Seminar (six hours) on high school chemistry professors with title: Personal computers and molecular models. Application for the design of drug molecules, Department of Chemistry, University of Patras.

10/1998-02/1999: One semester teaching of Inorganic Chemistry to first year students of the Hellenic Air Force University.

2000-today: Undergraduate teaching of Organic Chemistry II module at the department of Pharmacy, NKUA.

2000-today: Teaching at Pharmaceutical Chemistry undergraduate labs at the department of Pharmacy, NKUA.

1991-1995: Lab assistant as a PhD student at Pharmaceutical Chemistry undergraduate labs at the department of Pharmacy, NKUA.

2002-2019: Teaching at *Design and synthesis of drugs* Masters courses in *Advanced Topics of Synthetic Medicinal Chemistry* module, the *medicinal chemistry of benzodiazepines* (2002-2017) and *protective groups* (2017-today).

2022: Teaching "*Structure and Fundtion of GPCRs*" for Bioinformatics – Computational Biology MRes cycle in Department of Biology, NKUA

Supervision of undergraduate, Master and PhD thesis work

Supervision of undergraduate final year project theses (few selected):

2007-2008: Nikolaos Zervos, Validation of nine molecular mechanics force fields for their ability to anticipate conformational preferences of a large number of organic molecules. The work resulted in two publications in Tetr. Letters and J. Org. Chem.

2009-2010: Maria Karelou, Synthesis of thiourea derivatives of amantadine and rimantadine, with anti-cancer properties.

2018: Marianna Stampolaki, Synthesis of guanidine derivatives of amantadine acting as inhibitors of influenza A and mutated amantadine-resistant strains. The work included in a publication in Chem. Med. Chem.
2019: Iris Kalenderoglou, Effects of lipid bilayers, chlorine anions and cholesterol on the conformation and pore structure of the influenza A M2 protein in complex with Amt or Rim studied by atomistic and coarse-grained MD simulations. The work was published in J. Chem. Info. Model.

2023: Georgiou Kyriakos, Molecular dynamics study of the transmembrane domain and conductance domain of influenza A M2 proton channel. Part of The work was published in BBA Biomembr.

2023: Nicoletta Fourla, Synthesis of new adamantane-based compounds targeting CB2 receptor

Supervision of master students:

2000-2002: Ioannis Stylianakis (chemist): Synthesis and conformational analysis of C,N-substituted spiro[pyrrolidino-2,2′-adamantanes] with antiviral activity. Part of master thesis was published in Bioorg. Med. Chem. Letters.

2010-2011: Nikolaos Zervos (Pharmacist): Study of the non-conventional hydrogen bond in

axial cyclohexane derivatives using quantum mechanical calculations and NMR spectroscopy of synthetic conformational model compounds.

2010-2011: Stylianos Eleftheratos (Chemist), Study of the interactions between aminoamantadines and transmembrane domain of the M2 M2TM) protein using (a) measurements of binding constant using ITC and (b) molecular docking calculations. The work resulted in two publications in Bioorg. Med. Chem. Letters and ACS J. Chem. Theory Comput.

2011-2013: Ioannidis Charalampos (Chemist), Synthesis of M2TM peptides and study of the interactions of aminoamantadines with the M2TM tetramer using (a) binding constant measurements with ITC, and (b) FEP/MD calculations. This work resulted in publication of two articles in ACS J.Chem.Inf. Model. and one article in J. Phys. Chem. B.

2011-2013: Christina Tzitzoglaki (Chemist), Synthesis of new amino derivatives of amantadine and study of anti-viral effect against the influenza A virus wt and M2 S31N-mutated stain. This work resulted in one publication in J. Med. Chem.

2011-2013: Antonios Drakopoulos (Pharmacist), Study of the interacions between aminoamantadines and A/M2TM using: (a) new synthetic aminoamantadine derivatives, (b) ITC measurements of binding constants to M2TM, and (c) FEP/MD calculations. This work resulted in one publication in ACS J. Chem. Inf. Model., two publications in ACS Med. Chem. Letters, and one publication in Tetrahedron.

2017-2019: Marianna Stampolaki (Pharmacist), Synthetic analogues of SQ109 with potent activity against trypanosoma and tuberculosis. Part of the work was published in ACS Inf. Diseases.

2017-2019: Dimitrios Stamatis (Pharmacist), Mapping the orthosteric binding area of the A_3AR with the agonists IB-MECA and NECA using mutagenesis and functional assays results, MD simulations and MM-GBSA calculations. This work resulted was published in J. Med. Chem.

2020-2023: Vaggelis Machairas (Pharmacist), Design and synthesis of new PSMA pharmacophores for diagnosis and treatment of prostate cancer

2021-2024: Christoforos Kousioris (Chemist), Design and synthesis of new analogs of SQ109 drug against pathogens.

2021-2024: Marina Christofidi (Biologist): Coarse-grained MD simulations ον AT1 receptor.

2022-2024: Evaggelia Vlachou (Chemist): DFT calculation on Au-catalyzed reactions.

Supervision of PhD theses and post-docs:

2012-2017: Irene Tzouma (Chemist), Cassan-furane-diterpenes of pharmaceutical interest: Development of a convergent and enantio-selective synthetic route – Total synthesis of (±)-Soucoutourane C (scientific advisor: Dr. E. Pitsinos - Researcher A at NCSR Demokritos).

2013-2018: Christina Tzitzoglaki (Chemist), Molecular basis of inhibition and resistance of the influenza M2 ion channel by aminoadamantane drugs and discovery of novel resistance-breaking inhibitors targeting the mutant M2 proton channel. The thesis included: (a) The synthesis of M2TM peptide and the study of the interactions between rimantadine enantiomers and M2TM protein using FEP/MD and variety of biophysical methods such as ITC, ssNMR, electrophysiology and anti-viral assays. (b) Binding and Proton Blockage by Amantadine Variants of the Influenza M2WT and M2S31N Explained based on kinetics of synthetic rimantadine derivatives using electrophysiology, MD simulations, ITC and anti-viral assays. (c) Unraveling the Binding, Proton Blockage and Inhibition of influenza M2 WT and S31N by Rimantadine variants using ssNMR, MD simulations, electrophysiology, ITC and anti-viral assays. (d) Synthetic approaches of primary *tert*-alkyl amines as medicinal chemistry building blocks. (e) Synthesis of resistance-breaking inhibitors targeting the M2 proton channel of influenza A viruses. SAR explained using MD simulations. This doctoral thesis resulted in ACS JMedChem, in ACS MedChemLetters, in ACS JChemInfModel, in Tetrahedron etc.

2015-2020: Panagiotis Lagarias (biochemist/molecular biologist), Computational ligand- and structure-based drug design of molecules targeting adenosine receptor. Mapping the orthosteric binding area of the A_3R with the antagonists using mutagenesis and functional assays results, MD simulations and MM-GBSA calculations. This doctoral thesis has resulted in 8 publications in ACS JChemInfModel, ACS JMedChem, ScRep, Mol. Pharmac.

2016-2021: Athina Konstantinidi (chemist), Combination of Computational and Biophysical methods to study the interactions of aminoadamantanes with influenza A M2 protein. The thesis included: (a) Accurate calculations of M2TM pore structure in complex with aminoadamantanes, based on x-ray crystal structures. (b) Calculations of the relative binding free energy using alchemical calculations and FEP/MD, TI/MD methods. (c) Application of biophysical methods such as ssNMR, SAXS, WAXS, and DSC for studying the effects of aminoadamantane derivatives and influenza A M2 protein and excess aminoadamantanes to membrane bilayers. This doctoral thesis resulted in 10 publications in ACS JPhysChemB in ACS JAmChemSoc, BBA etc.
Athina is a post-doc in the lab for 3 years 2023-205.

2018-2023: Efpraxia Tzortzini (biochemist/molecular biologist), (a) Binding free energies for P2X7 antagonists, (b) Coarse-grained MD simulations of lipid-protein interactions for ARs. We have published with Eva in ACS JChemInfoModel, in Biology Communications and ACS Mol. Pharmaceutics and her first author paper in ACS JChemInfoModel. Eva is a post-doc in the lab for 3 years 2023-205.

2019-2023: Margarita Stampelou (biochemist/molecular biologist), Structure-based drug design of adenosine receptor antagonists. We have published with Margarita in ACS JChemInfoModel, ACS JMedChem, ACS MedChemLett, ACS JPhysChemB.

2019-2023: Marianna Stampolaki (Pharmacist), SBDD and synthesis of SQ109 with potent activity against pathogens and biophysical studies; ssNMR studies of M2CD WT and S31N bound with ligands (Max-Planck Institute). We have published with Marianna from her PhD thesis in SynOpen, ACS ID, JCAMD.

2019-2023: Ioannis Stylianakis (chemist), DFT Calculations to Study the Mechanism of Gold-Catalyzed Organic Reactions. His PhD work was in RSC Organic Chemistry Frontiers, JPhysOrgChem and Catalysts. He is currently research associate in my lab.

2017-2019: Dr Eleni Vrontaki was a post-doctoral researcher (chemist) in my lab using Computational ligand- and structure-based drug design of molecules targeting adenosine receptor. Mapping the orthosteric binding area of the A_3AR with the antagonists using mutagenesis and functional assays results, MD simulations and MM-GBSA calculations. Testing the accuracy of MM-PBSA calculations and 3D QSAR models for antagonistic activity in A_1, A_{2A} and A_3 adenosine receptors. She has been a co-author in three publications two in JChemInfoModel and in ScRep.

2019-2022: Dr Christos Liolios, chemical biology; theranostics, molecular imaging; Design and synthesis of targeted carrier-small molecules therapeutics for simultaneous delivery of small molecules cancer therapeutics and imaging (theranostics). We have published with Christos during 3 years stay in my lab as a post-doc in MDPI Molecules, ACS Mol. Pharmaceutics and Eur. J. Med Chem Rep during his stay in my lab.

2019-2022: Dr Iraklis Litinas (chemist) was a post-doctoral researcher in my lab using Density Functional Calculations to Study the Mechanism of Gold-Catalyzed Organic Reactions. We have published with Iraklis in JPhysOrgChem, Catalysts, RSC OrgChemAdv.

Participation in PhD Committees

Participation as examiner or advisor in committees of degree project, master and PhD theses in the areas of computational drug design and development of drugs, computational biophysics.

Selected are listed below:

- 7-member committee in the PhD thesis of K. Moschovou (Supervisor T. Mavromoustakos)
- 7-member committee in the PhD thesis of L. Zorba (Supervisor G. Vougioukalakis)
- 7-member committee in the PhD thesis of N. Lesgidou (Supervisor N. Glykos)
- 7-member committee in the PhD thesis of A. Foscolou (Supervisor I. Papanastasiou)
- 7-member committee in the PhD thesis of N. Athinaios (Supervisor E. Pitsinos)
- 7-member committee in the PhD thesis of S. Riganas (Supervisor G. Foskolos)
- 7-member committee in the PhD thesis of C. Fytas (Supervisor G. Fytas)
- 7-member committee in the PhD thesis of A. Foscolou (Supervisor I. Papanastasiou)
- 3-member committee in MSc thesis of A. Papageorgiou (Supervisor I. Papanastasiou)

- 3-member committee in MSc thesis of K. Mosxovou (Supervisor T. Mavromoustakos)
- 3-member committee in MSc thesis of A. Konstantinidi (Supervisor T. Mavromoustakos)
- 3-member committee in MSc thesis of Z. Vergou (Supervisor T. Tselios)
- 3-member committee in degree thesis of M. Papadourakis (Supervisor E. Mikros)
- 3-member committee in degree project thesis of D. Xasapis (Supervisor E. Mikros)
- 3-member committee in degree project thesis of P. Kalkounou (Supervisor N. Lougiakis)
- 8-member committee in PhD thesis of Morganne Mannes (Prof Steven Ballet, Vrije Universiteit Brussel, Belgium
- 7-member committee in the PhD thesis of N.L. Lesgidou (Supervisor N. Glykos, Department of Biology and Genetics, School of Health Sciences, Democritus University of Thrace)

Books

Co-author of high-school (Lyceum) textbook, laboratory exercise guide, tutor book and supervisory material for the Chemistry courses that were taught in the period **1999-2001** (T. Mavromoustakos, A. Kolocouris, K. Papakonstantinou, P. Sinigalias, K. Lappas).

- *Lyceum Chemistry textbook (and exercise solutions) – specialization: Science;*

Pages: 262, Publisher: ΟΕΔΒ, **1999**
Chapters: Structure of atoms and molecules – Periodic Table • Chemical Thermodynamics • Ionic Equilibrium • Electrochemistry • Organic Chemistry

- *Lyceum Chemistry textbook (and exercise solutinos) – specialization: Technology;*

Pages 128, Publisher: ΟΕΔΒ, **1999**
Chapters: Ionic Equilibrium • Electrochemistry • Organic Chemistry

- *Laboratory exercise guide*, ΟΕΔΒ, **1999**

Author of the book *Computational Chemistry of Molecular Systems – Basic standards and Laboratory Exercises*
Pages: 436, Publisher: Συμμετρία, **2010**

Author of the book *Computational Chemistry and Molecular Simulations – Theory and Methods*
Pages: 1200, In Greek, Publisher: Παρισιάνος, **2020,** processed for publication.
Chapters: Molecular Mechanics • Potential Energy Surface • Molecular orbitals – Hartree-Fock method • Semi-empirical approaches of molecular orbital theory • Implementation of the HF method – Basis sets • Beyond the HF limit: Calculation of the electronic correlation • Calculation of electronic correlation in large molecules • Density Functional Theory • Calculations of Charge distribution, vibrational, rotational and NMR spectroscopy properties • Thermodynamic properties • Simulations methods of molecular systems • Improved simulation algorithms • Advances in the methodology and applications of atomistic molecular dynamics simulations in biomolecular systems • Mesoscopic scale MD simulations – Coarse-grained models • Solvation models • Accurate free energy calculation methods in biomolecular systems • Approximate binding free energy calculation methods in biomolecular systems and quantum mechanical methods • Calculations of reaction kinetics – Transition state theory • Hybrid quantum mechanical / molecular mechanics methods.

Co-author of the book *Nuclear Magnetic Resonance* (T. Mavromoustakos, A. Tzakos, G. Spyroulias, E. Mikros, A. Kolocouris, C. Papakonstantinou, I. Gerothanasis, I. Matsoukas), Publisher: Συμμετρία, **2018**

Teaching material

Educational material (slides, exercises) for the instruction of the Organic Chemistry II undergraduate course (deposited online at e-class platform of NKUA).

Educational material for the instruction of the *Advanced Topics of Synthetic Medicinal Chemistry* module in masters courses (Notes on *medicinal chemistry of benzodiazepines*: **2002-2017**; Notes on *protective groups in organic synthesis*: **2018**; Notes on *modern organic reactions for drugs synthesis*: **2021**).

Military Service

Chemist, Navy - Fuel Department, Laboratory of fuel and lubricant testing (**06/1995-12/1996**)

Research programs - Funding

Summary

State Scholarships Foundation Fellowships on one PhD student and one post-doc from computational chemistry projects (IKY) (44,400 €).

Two competitive CERIC programs for the performance of biophysical experiments.

One competitive program for access to the ssNMR facilities at the National High Magnetic Lab Laboratory, Florida, USA.

One competitive DAAD program for the collaboration with the professor H. Gohlke Dusseldorf, Germany (5,000 €).

Seven competitive programs for access to supercomputers (~3,800,000 CPU core-hours).

Full list

Special Account for Research Grants (SARG) 70/4/5857, Scientific coordinator, program title: Synthesis and study of the conformation of pharmaceutical molecules using NMR spectroscopy and computational chemistry; **20/06/2001-20/06/2002**

SARG 70/4/5857, Scientific coordinator, program title: Pharmaceutical chemistry - Study of the conformation of pharmaceutical molecules using NMR Spectroscopy and computational chemistry. **04/12/2002-04/12/2003**

SARG 70/4/5857, Scientific coordinator, program title: Use of NMR spectroscopy for the study of 2-alkyl-2-X-adamantane derivatives with potent antiviral activity as part of the research to

understand how the derivatives interact with the influenza A M2TM protein; **24/01/2005-24/01/2006**

SARG 70/4/5857, Scientific coordinator, program title: Use of NMR spectroscopy for the study of 2-alkyl-2-X-derivatives of adamantane with strong antiviral activity as part of the research to understand how the derivatives interact with the influenza A M2TM protein; **01/01/2008-31/12/2008**

SARG 70/4/5857, Scientific coordinator, Program title: Pharmaceutical chemistry against the influenza A virus: in silico study of the molecular basis of the antiviral action of amantadine analogues; **02/02/2009-02/02/2010**

03/2009: Funding for the development of new pharmacophore probes (CHIESI: 5,000 €).

03/2010: Funding for the development of new pharmacophore probes (CHIESI: 6,000 €).

12/2011: Funding for lab reconstruction (CHIESI: 32,000 €).

2012: Funding for the development of new pharmacophore probes (OKAPI: 15,000 €).

2012: Funding from Brigham Young University for the development of new pharmacophore probes against influenza virus, Prof. D. Busath (17,000 $).

2012: Funding for the development of new pharmacophore probes (CHIESI: 3,000 €).

2012: Funding for the Greek-German collaboration with a group of computational medicinal chemistry, Dept. Pharmacy, Prof. H. Gohlke, Univ. Dusseldorf (IKYDA: 5,000 €).

2013: Funding for the development of new pharmacophore probes (CHIESI: 13,000 €).

2013: Funding from the Florida State University for the study of interactions between S31N M2TM and aminoamantadine derivatives using computational chemistry and ssNMR using d-labeled peptides, Prof. T. Cross (11,600 $).

2014: Funding for the development of new pharmacophore probes (CHIESI: 6,000 €).

2014-2017: Funding for ssNMR experiments at the National High Magnetic Laboratory (Florida). PI: Professor Tim Cross, Collaborator: Antonios Kolocouris (Research Proposal P08383: ssNMR characterization of S31N M2 bound state with novel aminoadamane derivatives.

2015: Funding for the development of new pharmacophore probes (CHIESI: 14,230 €).

2015: Funding for the 7-step synthesis of a new synthetic analogue (ARATANA: 4,000 €).

2015-2016: Access to the ARIS supercomputer (GrNET) for the Virtual Screening on Adenosine Receptors (1st Production Call – pr001004: 100,000 CPU core-hours).

2015-2016: Access to the Cy-Tera supercomputer (The Cyprus Institute) for the Virtual Screening on Adenosine Receptors (preparatory access: 12,800 CPU and 2,000 GPU core-hours, production access - pro15b105s1: 140,000 CPU and 7,200 GPU core-hours).

2016: Funding of a PhD student (A. Konstantinidi) for the travel, accommodation and use of instruments in Ljubljana (600 MHz NMR) and Trieste (X-rays) under the CERIC Program.

2016-2017: Access to the ARIS supercomputer (GrNET) for the structure-based drug design on adenosine Receptors (2nd Call for Production Access – pr002021: 162,000 CPU core-hours).

2016: Funding for the development of new pharmacophore probes (CHIESI: 17,230 €).

2016: Funding of a PhD student (P. Lagarias) for the project "In silico drug design of molecules targeting Adenosine Receptors" from the State Scholarships Foundation (IKY) (total amount: 22,400 €).

2017: Funding of a PhD student (A. Konstantinidi) for the travel, accommodation and use of instruments in Ljubljana (600 MHz NMR) and Trieste (X-rays) under the CERIC Program.

2017: Funding of a post-doctoral researcher (E. Vrontaki) for the project "In silico drug design of molecules acting as selective inhibitors of Adenosine Receptors" from the State Scholarships Foundation (IKY) (total amount: 22,000 €).

2017: Funding for the development of new pharmacophore probes (CHIESI: 14,000 €).

2017-2018: Access to the ARIS supercomputer (GrNET) for the project "IOSIS: Development of new drugs to combat amantadine-resistant influenza viruses" (4th Call for Production Access – pr004022: 760,000 CPU core-hours).

2017-2018: Access to the ARIS supercomputer (GrNET) for the project "CADD_AKPL: CADD for Adenosine GPCRs" (4th Call for Production Access – pr004008: 300,000 CPU core-hours).

2018: Access to the ARIS supercomputer (GrNET) for the project "CADD_AKPL: CADD for Adenosine GPCRs" (5th Call for Production Access – pr005010: 540,000 CPU core-hours).

2018: Funding for the development of new pharmacophore probes (CHIESI:12,000 €).

2019: Access to the ARIS supercomputer for three projects including CADDfor Class A GPCRs and TI free energy calculations for M2TM-aminoadamanes complexes (6th Call for Production Access – pr006008, pr006031, pr006052: 1,750,000 CPU core-hours).

2019: Funding for the development of new pharmacophore probes (CHIESI: 11,000 €).

2019: Funding of a PhD student (E. Tzortzini) for the project "Binding free energy models for drug - GPCR complexes of family A. In silico drug design of compounds targeting adenosine receptors" from the Hellenic Foundation for Research and Innovation (total amount: ca 32,000 €).

2019: Funding for the computational design of allosteric antagonists against P2X7R (University of Barcelona: 12,000 €).

09/2020: Funding for the development of new pharmacophore probes (CHIESI: 10,000 €).

2020: Access to the ARIS supercomputer for proposal 'CADD-AK': three projects including the MD simulations and TI/MD binding free energy calculations for CADD against (a) adenosine A_1R and A_3R receptors and (b) Mtb MmpL3 transporther. Also for coarse-grained MD simulations to investigate the effect of cholesterol to ARs. ((7th Call for Production Access – pr006008, pr006031, pr006052: 1,750,000 CPU core-hours).

2020: Funding for the development of new pharmacophore probes (CHIESI: 10,000 €).

2021: Access to the ARIS supercomputer for the proposal 'CADD-AK'; three projects including the CADD for Class A GPCRs and TI free energy calculations for M2TM-aminoadamanes complexes pr?? (8th Call for Production Projects Access: pr010007, 1300000 cpu core hours, 2,000 gpu core hours).

2021: Funding for the development of new pharmacophore probes (CHIESI: 10,000 €).

2022: Access to the ARIS supercomputer for the proposal 'CADD-Kolocouris 2.0'; three projects including the CADD for Class A GPCRs and TI free energy calculations for M2TM-aminoadamanes complexes pr?? (12th Call for Production Projects Access: pr??, 100,000 cpu core hours 400,000 gpu core hours).

2022: Funding for the development of new pharmacophore probes (CHIESI: 10,000 €).

2023: Access to the ARIS supercomputer for the proposal 'CADD-Kolocouris_??'; three projects including the CADD for Class A GPCRs and TI free energy calculations for M2TM-aminoadamanes complexes pr?? (??th Call for Production Projects Access: pr??, 400,000 gpu core hours).

2023: Funding for the development of new pharmacophore probes (CHIESI: 10,000 €).

2024: Access to the ARIS supercomputer for the proposal 'CADD-Kolocouris_5.0'; three projects including the Computer-Aided Drug Design for Class A GPCRs and TI free energy calculations for M2TM-aminoadamanes complexes pr?? (16th Call for Production Projects Access: 400,000 gpu core hours).

Administrative Committees

Member of the Senate of the NKUA **(2004-2005**).

Member of the entry examiners committee in Organic Chemistry for graduate applicants at the Department of Pharmacy, NKUA (**2006-today**).

Examiner in Organic Chemistry for bequest scholarships at the Department of Pharmacy, NKUA (**2006-today**).

Member of academic staff evaluation committees of the NKUA and other Research Institutes.

Member of the Quality Assurance committee of the department of Pharmacy, NKUA (**2017, 2018, 2019**).

Member of the two members-committee for writing the Internal Affairs Formulation of the Department of Pharmacy, NKUA (**2019**).

Organization of the postgraduate seminars at the Department of Pharmacy, NKUA (**2017, 2018**).

Committee for website (I wrote text description of postgraduate, doctoral studies, project thesis procedure etc)

Departmental contributions

- Having arranged the development of a post-graduate meeting room (supported by Prof. T. Sfikopoulos)
- Office office-rooms for colleagues from Pharmaceutical Analysis (supported by Prof. N. Thomaidis), section secretariat room.
- Having arranged the donation from pharmaceutical companies of office and computers labs furniture (3 times fully loaded trucks), monitors, 15 poster-stands from ELTA for internal conferences, the polishing of passageways of the Department (from damaged refrigerators, PCs and other damaged equipment)
- Departmental gardens with species useful as teaching material for botanics
- Detailed description of the specifications for benches and hoods for more than 1000 m2 of undergraduate and research labs. Having arranged to obtain these benches and hoods during 2023.
- Contribution in obtaining a new NMR 400 MHz in the Department from Universities programs.
- Contribution in hiring PhD students by pharmaceutical companies
- Looking for possibilities to bring staff in the Department

Reviewer for scientific journals and research proposals

ACS Industrial & Engineering Chemistry Research (1)
ACS J. Am. Chem. Soc. (4)
ACS J. Am. Chem. Soc. Au (2)
ACS Bioconjugates (2)
ACS Biomaterials Science & Engineering (1)
ACS Central Science (3)
ACS Chemical Neuroscience (3

ACS ID (3)
ACS J. Chem. Info. Model. (24)
ACS J. Chem. Theory Comp. (1)
ACS J. Med. Chem. (49)
ACS Med Chem Lett (7)
ACS J. Org. Chem. (12)
ACS J. Phys. Chem. B (4)
ACS J. Phys. Chem. Lett (3)
ACS Pharmacol Trans Sc (9)
ACS Mol Pharmaceutics (1)
ACS Omega (2)
ARKIVOC(1)
BBA-Biomembranes (1)
Bioorg. Chem. (4)
Bioorg. Med. Chem. (6)
Bioorg. Med. Chem. Lett. (8)
Biophysics Colab (2)
Brain Injury (1)
BJP (1)
ChemJournal (2) Cell Series
Chem. Med. Chem. (3)
Chem. Phys. (1)
Computational and Structural Biotechnology Journal (3)
Current Opinion in Investigational Drugs (1)
Drugs in R&D (1)
Eur. J. Med. Chem. (16)
Expert Opinion on Drug Discovery (1)
Expert Opinion on Investigational Drugs (1)
Frontiers Mol. Biosciences (2)
Frontiers in Pharmacology (1)
International Journal of Antimicrobial Agents (1)
Journal of Chemistry (2)
Journal of Computational Chemistry (2)
Journal of Chemistry (2)
Journal of Enzyme Inhibition and Medicinal Chemistry (2)
Journal of Liposome Research (1)
Journal of Molecular Graphics and Modeling (8)
Journal of Molecular Recognition (3)
Journal of the Servian Chemical Society (1)
Magnetic Resonance in Chemistry (1)
Med. Chem. Commun. (3)
Molecules (5)
PLOS Computational Biology (2)
PLOS One (2)
Phytochemistry (2)
RSC Chem. Commun. (1)
RSC Chemical Science (2)

RSC Medicinal Chemistry (4)
RSC PCCP(3)
Structure (2), Cell series
Tetrahedron Letters (3)

Welcome Trust: Research proposal grant 1,000,000 € (8/2009)

Partnership Agreement programs (PA 2014-2020) for the support of new scientists

Selected Collaborations

Recent – current co-operation

Medicinal Chemistry

Professor Günter Gauglitz, Department of Chemistry, Section of Physical Chemistry, University of Tubingen, Germany; Measurements of thermodynamic binding data of aminoadamantane derivatives in complex with the M2TM membrane protein using ITC.

Professor Michaela Schmidtke, Jena hospital, Germany; In vitro antiviral assays for molecules against influenza A and mutant strains generated using inverse genetics.

Professor Holger Gohlke and Dr Nadine Homeyer (computational pharmaceutical chemistry), Department of Pharmacy, University of Dusseldorf; Application of free energy calculation methods with Amber software to study the binding of ligands against protein targets.

Professor David Busath, Biophysics, BYU, Utah, USA; Electrophysiology experiments, measurement of K_{on}/K_{off} binding constants of aminoadamantane derivatives in complex with the M2TM membrane protein.

Associate Professor Jun Wang, Department of Pharmacy, University of Arizona, Electrophysiology experiments, measurement of K_{on}/K_{off} binding constants of aminoadamantane derivatives with the M2TM membrane protein, in vitro antiviral assays for molecules against influenza A

Professor Tim Cross, Department of Chemistry, University of Florida and Head of National High Magnetic Field Laboratory (MagLab), ssNMR experiments to study the interactions of aminoadamantane drugs in complex with the membrane protein M2TM and S31N M2TM mutant.

Professor Bill DeGrado, Department of Pharmacy, UCSF; First, high-resolution x-ray structures of aminoadamantane derivatives in complex with the membrane protein M2TM and MD simulations of the complex and water cluster inside the pore.

Professor Mei Hong, Department of Pharmacy, UCSF; Measurement of long-distance interactions using ssNMR experiments to study the interactions of a ^{19}F-labeled aminoadamantane derivative in complex with ^{19}F-labeled full M2 protein.

Professor Isaiah Arkin, Department of Biochemistry, Hebrew University of Jerusalem; Study of the activity of aminoadamantane derivatives on the M2 protein using bacterial assays; Study of the folding of lipophilic peptides using Circular Dichroism (CD).

Assist. Professor, Ian Tietjen, Faculty of Health Sciences, Simon Fraser University, Burnaby, Canada; Electrophysiology experiments to study the interactions of aminoadamantane derivatives with the M2 protein.

Professor Karl-Norbert Klotz, Department of Biochemistry, University of Wurzburg; Measurement of binding kinetics of novel Adenosine receptor antagonists.

Reader Graham Ladds, Department of Pharmacology, Cambridge; pharmacology, mutagenesis studies, activity determination using functional assays and kinetics measurements using BRET of agonists and antagonists against the adenosine receptors.

Professor Santiago Vazquez, Department of Chemistry, Organic Chemistry, Barcelona; Drug design on P2X7 receptors.

Professor Rebecca Wade and Dr Daria Koch, Biophysics, Heidelberg Institute for Theoretical Studies; Molecular dynamics simulation algorithms for the prediction of receptor-ligand K_{on}/K_{off} binding constants.

Professor Jonathan Essex, Department of Chemistry Southampton, Simulation of tightly-bound water molecules in mediating protein-ligand interactions in the X-ray structures of M2TM with ligands, and calculations of their their binding affinities and which is the sequence on their displacement for drug design purposes.

Professor Mark Sansom, University of Oxford, UK; Coarse-grained MD simulations of M2 protein aggregation.

Professor John Kelly, Molecular Biology, Department of Pathogen Molecular Biology, London School of Hygiene and Tropical Medicine; testing of new SQ109 derivatives against trypanosome.

Professor Eric Oldfield, Kelly, Molecular Biology, Department of Chemistry, Illinois; chemical biology and testing of new SQ109 derivatives against tuberculsosis.

Professor Peter Schreiner, Department of Chemistry, Section of Organic Chemistry, Justus-Liebig University of Giessen; using of diamondoids as substituents in compounds of anti-viral interest.

Professor Edward Wu, Case Western University, USA; Crystal structures of MmpL3 with our structure-based drug designed and synthetic SQ109 analogues.

Professor Thomas Mavromoustakos, Department of Chemistry, NKUA; ssNMR and small angle x-ray experiments to study the interactions between aminoadamantane derivatives and the membrane bilayers including the M2TM membrane protein.

Professor Constantinos Demetzos, Department of Pharmacy, NKUA; DSC experiments to study the interactions between aminoadamantane and M2TM protein and other membrane perturbing molecules with model membrane bilayers.

Associate Professor Nikolaos Glykos, Department of Biochemistry and Genetics, University of Thrace; folding dynamics of lipophilic peptides.

Associate Professor Ioannis Papanastasiou, Department of Pharmacy, NKUA; Use of structure-based drug design methods to study the interaction of ligands with M2TM protein.

Professor Constantinos Demetzos, Department of Pharmacy, NKUA; DSC experiments to study the interactions between aminoadamantane and M2TM protein and other membrane perturbing molecules with model membrane bilayers.

Associate Professor Grigoris Zoidis, Department of Pharmacy, NKUA; Department of Pharmacy, NKUA; Use of structure-based drug design methods to study ligands of the M2TM protein.

Assistant Professor Nikolaos Lougiakis, Department of Pharmacy, NKUA; Use of structure-based drug design methods to design and synthesis of antagonists against adenosine receptors.

Professor Nikoleta Pouli, Department of Pharmacy, NKUA; Use of structure-based drug design methods to design and synthesis of antagonists against adenosine receptors.

Professor Panagiotis Marakos, Department of Pharmacy, NKUA; Use of structure-based drug design methods to design and synthesis of antagonists against adenosine receptors.

Professor Johan Neyts, Department of Chemistry, Rega Institute for Medical Research, Leuven, Belgium.

Dr Anna Duncan, Department of Chemistry, Aarhus University, CG MD simulations.

Dr Robin Corey, Department of Chemistry, Aarhus University, CG MD simulations.

Prof Mette Roskenklide, Dept of Pharmacology, Univ of Copenhagen, SARS-CoV-2 E protein drug discovery.

Professor Johan Neyts, Catholic University of Leuven, Belgium

Professor Steve deJongue, Catholic University of Leuven, Belgium

<u>Physical Organic Chemistry</u>

Carlos Silvia Lopez, Organic Chemistry, Department of Chemistry, Vigo; Study of organic reaction mechanisms using DFT calculations.

Professor David Scheiner, Department of Chemistry, Utah; Study of non-conventional hydrogen bonds.

Professor Andreas Mazzanti, Department of Chemistry, Bologna; Dynamic NMR.

Selected past collaborations

Medicinal Chemistry

Professor David Fedida, Canada; Electrophysiology experiments to study the interactions between aminoadamantane derivatives and the M2TM membrane protein.

Professor Alan Hay, Francis Crick Institute; Biological evaluation of influenza A virus inhibitors.

Professor Eric De Clercq, Catholic University of Leuven, Belgium

Professor Rolland Zell; Development of influenza A virus M2-mutated strains.

Professor Brent Johnson; Antiviral effect of molecules against influenza A virus, M2 protein.

Dr T. Calogeropoulou, Research Director; Biophysics of synthetic lipid-drug conjugates, Institute of Biology, Medicinal Chemistry and Biotechnology, Athens.

Professor A. Makriyannis, Biophysics of synthetic lipid-drug conjugates, College of Science, Department of Pharmaceutical Sciences, School of Pharmacy, Institute of Biology, Medicinal Chemistry and Biotechnology, Northeastern University, USA.

Associate Professor, R. W. Broadhurst; NMR spectroscopy of M2 protein constructs, Biochemistry, Cambridge

Organic Chemistry-Physical Organic Chemistry-NMR spectroscopy

Professor Frank De Proft; Application of new DFT standards to study the C-H···O non-conventional hydrogen bond, Chemistry, Brussels, Belgium.

Professor Edgar J. Anderson; Dynamic NMR, Chemistry, UCL.

Professor G. Varvounis; Structure evaluation with 2D NMR and computational structure prediction of heterocyclic drug-like molecules, Department of Chemistry, Organic Chemistry, Ioannina.

Professor Konstantinos Demetzos; Structure evaluation with 2D NMR and computational structure prediction of terpenoid natural products, Department of Pharmaceutical Technology, NKUA.

Professor Benoit Rigo; Synthesis of derivatives of pyroglutamic acid, French School of High Studies in Engineering, Department of Chemistry, Lille, France.

Patents

Antiviral compounds (US9840465B2): **A Kolocouris,** DD Busath, B Johnson
Patent No.: US Patent 9,840,465 B2; 2017

Conferences

1. 6th Hellenic Symposium on Medicinal Chemistry (Athens, May 1993).
A. Kolocouris, N. Kolocouris, G. B. Foscolos, P.Marakos, G. Fytas N. Pouli
New spiranic aminoadamantanes with antiviral activity.

2. 7th Hellenic Pharmaceutical Conference (Athens, June 1994).
A. Kolocouris, N. Kolocouris and G. B. Foscolos
Synthesis and pharmacological evaluation of aminoadamantane derivatives with putative antiviral activity.

3. 4th Advance Medicinal Chemistry conference (Thessaloniki, May 1995).
N. Kolocouris, **A. Kolocouris**, G. B. Foscolos, G. Fytas and E. De Clercq
Synthesis and antiviral activity evaluation of some aminoadamantane derivatives.

4. 7th Hellenic Symposium on Medicinal Chemistry (Athens, November 1995)
G. D. Stamatiou, G. Fytas, N. Kolocouris, G. B. Foscolos & **A. Kolocouris**.
Synthesis of 2-(1-adamantyl)-piperidines and 2-(1-adamantyl)-hexahydro-1H-azepines derivatives with putative antiviral activity.

5. 5th Advanced Medicinal Chemistry conference (Thessaloniki, May 1997).
G. Stamatiou, G. Fytas, G. B. Foscolos, **A. Kolocouris**, N. Kolocouris & E. DeClercq
Synthesis and anti-HIV activity of new aminoadamantane heterocycles.

6. 8th Hellenic Symposium on Medicinal Chemistry (Athens, December 1997).
D. Tataridis, G. Fytas, G. B. Foscolos, **A. Kolocouris** & N. Kolocouris
Synthesis of 2-(2-adamantyl)piperidines and 3-(2-adamantyl)pyrrolidines with putative antiviral activity.

7. 8th Hellenic *Symposium* on Medicinal Chemistry (Αθήνα, Δεκέμβριος 1997).
M. Zervou, **A. Kolocouris**, T. Mavromoustakos, C. Skrettas& I. Matsoukas.
Conformational analysis of the reactive EXP-3174 metabolite of the anti-hypertensive drug Losartan.

8. EENC 98, 14th European Experimental Conference, May 10-15, 1998 Bled, Slovenia.
T. Mavromoustakos, **A. Kolocouris**, M. Zervou and I. Matsoukas
The molecular basis of hypertension.

9. XVth EFMC International Symposium of Medicinal Chemistry, Edimburgh, Scotland, 6-10 September 1998.
A. Kolocouris, T. Mavromoustakos, M. Zervou, I. Matsoukas, E. Humpher
An effort to understand the molecular Basis of Hypertension through the conformational analysis of Losartan and Sarmesin using a combination of NMR spectroscopy and theoretical calculations.

10. 9th Hellenic Pharmaceutical Conference (Athens, November 1998).
A. Kolocouris, T. Mavromoustakos & I. Matsoukas
Molecular basis behind anti-hypertensive action of Losartan.

11. Workshop: Peptides and Peptide Mimetics, Drug Discovery and Design (Patra, December 1998).
T. Mavromoustakos, **A. Kolocouris**, M. Zervou, I. Daliani
The combination of NMR spectroscopy and molecular modelling in Drug Design: Implications in the synthesis of non-peptide mimetics of ANG II, TRAP, MBP and GnRH.

12,13. The 8th Cyprus Conference on New Methods in Drug Research (Limassol, 25-30 April 1999, Cyprus - Conference Chairman: A. Makriyannis (USA).
i) T. Mavromoustakos, **A. Kolocouris**, J. Matsoukas and M. Zervou
Study of the Molecular Basis of Hypertension using NMR Spectroscopy and Computational Analysis studies.
ii) T. Mavromoustakos, I. Daliani, **A. Kolocouris** and M. Zervou
Study of the effects of cannabinoids in lipid bilayers using ssNMR Spectroscopy and DSC.

14. 9th Hellenic *Symposium* on Medicinal Chemistry (Athens, January 2000).
P. Karagiannis, G. Foscolos, N. Kolocouris, G. Fytas & **A. Kolocouris**
Synthesis of new aminoadamantanes with as analogues of rimantadine.

15. 9th Hellenic Pharmaceutical Conference (Athens, January 2000).
A. Kolocouris, T. Mavromoustakos, T. Kalogeropoulos, M. Koufaki, I. Daliani, A. Makrigiannis, C. Demetzos, J. Balzarini & E. DeClercq
Conformational analysis and study of the effect on membranes of a novel synthetic glycerolipid derivative of AZT with anti-cancer and anti-HIV activities using NMR and MD simulations.

16. 9th Hellenic Pharmaceutical Conference (Athens, January 2000).
M. Zervou, **A. Kolocouris,** T. Mavromoustakos & I. Matsoukas
Analysis of peptidomimetic and peptide antagonists of Angiotensin II using a combination of NMR Spectroscopy and Computational Chemistry. Prospects in the design of new antihypertensive molecules.

17. 9th Hellenic Pharmaceutical Conference (Athens, January 2000).
H. Maswadeh, C. Demetzos, M. Rallis, T. Mavromoustakos, I. Daliani ,**A. Kolocouris,** P. Dallas, G. Papaioannou
Insertion of viblastion into liposomes. Study of thermotropic changes using model membranes using a combination of DSC and ^{13}C-ssNMR.

18. Proceedings of 16th Conference on Peptides (Saint Louis, USA, 1999).
P. Roumelioti, L. Polevaya, D. V. Vlahakos, T. Mavromoustakos, **A. Kolocouris,** T. Tselios, J. M. Matsoukas
Design and synthesis of two potent amide-linked cyclic analogues of the hormone angiotensin II confirm the importance of ring cluster and relay system in its possible bioactive conformation.

19. 10th Hellenic Symposium on Medicinal Chemistry (Athens, 2002).

N. Kolocouris, G. Zoidis, G. B. Foscolos, G. Fytas, **A. Kolocouris**
Synthesis of aminoadamantane derivatives with significant activity against the influenza A virus.

As Lecturer:

20. 10th Hellinic Symposium on Medicinal Chemistry (Athens, 2002).
A. Kolocouris, I. Stylianakis, N. Kolocouris, G. B. Foscolos, G. Fytas, J. Neyts E. Padalko, E. DeClercq
Investigation for new drugs against the influenza A virus: Conformational analysis and structure-activity relationships of the 2-substituted aminoadamantane heterocyclic and carbocyclic derivatives.

21. 10th Hellinic Symposium on Medicinal Chemistry (Athens, 2002).
A. Kolocouris, I. Stylianakis, N. Kolocouris, G. B. Foscolos, G. Fytas, J. Neyts E. Padalko, E. DeClercq
Design and synthesis of C- and N-substituted spiro[pyrrolidino-2,2'-adamantanes] with putative antiviral activity.

22. 10th Hellinic Symposium on Medicinal Chemistry (Athens, 2002).
N. Kolocouris, **A. Kolocouris**, G. B. Foscolos, G. Stamatiou, G. Fytas, G. Zoidis
New thiosemicarbazones and thiocarbohydrazones: Synthesis, Synthesis, conformational study and in vitro evaluation of their antineoplastic, antiviral and antimicrobial activity.

23. 8th Advanced medicinal chemistry conference (Thessaloniki, 2003).
I. Stylianakis, **A. Kolocouris,** N. Kolocouris, G. Fytas, G. B. Foscolos, E. Padalko, J. Neyts, E. De Clercq
Spiro[pyrrolidine-2,2´-adamantanes]: Synthesis, Anti-Influenza Virus Activity and Conformational Properties Study Using Dynamic NMR Spectroscopy and Molecular Mechanics Calculations.

24. Liposome Advances: Progress in Drug and Vaccine Delivery (London 2003).
E. Kaourma, S. Hatziantoniou, A. Georgopoulos, **A. Kolocouris**, C. Demetzos
A Fast and Simple Approach for Preparing and Incorporating Lipoamine Conjugates into Liposomes and Studies on their Physicochemical Properties.

25. 11th Hellenic Symposium on Medicinal Chemistry (Patras, 2004).
E. Kaourma, S. Hatziantoniou, A. Georgopoulos, **A. Kolocouris**, C. Demetzos
Synthesis of 3-maleimidopropanoic-N-succinimidyl derivatives, and incorporation into physicochemically characterized liposomes for the preparation of immunoliposomes.

26. 11th Hellenic Symposium on Medicinal Chemistry (Patras, 2004).
C. Fytas, G. Fytas, **A. Kolocouris**, G. B. Foskolos, N. Kolocouris
Synthesis of new spiropiperazine derivatives of adamantane and cyclooctane with putative antiviral activity.

27. 11th Hellenic Symposium on Medicinal Chemistry (Patras, 2004).
I. Papanastasiou, G. Foskolos, N. Kolocouris, G. Fytas, **A. Kolocouris**

Synthesis of new heterocyclic adamantane derivatives with putative antiviral activity.

28. 11th Hellenic Symposium on Medicinal Chemistry (Patras, 2004).
G. Zoidis, N. Kolocouris, G. B. Foskolos, G. Fytas, **A. Kolocouris**
New amine derivatives of adamantane with pharmacological activity.

29. 5th European Workshop in Drug Design (Siena, 2005).
A. Kolocouris, R. W. Broadhurst, R. Hansen, C. Zikos
Interaction Between Amantadine Analogues and the Transmembrane Portion of the Influenza A M2 Ion Channel Protein in Lipid Environments Probed by means of ^{1}H NMR and ^{19}F NMR Spectroscopy.

As Assistant Professor:

30. Option for the Control of Influenza VI, (Toronto, Canada, June 2007).
T. Betakova, **A. Kolocouris**, P. Gronesova, D. Svetlikova
Quest for new anti-viral drugs against influenza A virus.

31. 13th Hellinic Symposium on Medicinal Chemistry (Athens, 2008).
N. Zervos, **A. Kolocouris**
The Performance of Nine Molecular Mechanics Force Field Methods on Predicting the Conformational Preferences in a Large Set of Small Organic Molecules and Drugs.

32. 13th Hellenic Symposium on Medicinal Chemistry (Athens, 2008).
A. Kolocouris, R. W. Broadhurst, C. Zikos
^{19}F NMR Detection of the Complex Between Amantadine and the Receptor Portion of the Influenza A M2 Ion Channel in Dodecylphosphocholine Micelles: A Candidate System for SAR studies.

33. 18th European Symposium on Quantitative Structure-Activity Relationships (Rhodes, 2010).
S. Eleftheratos, **A. Kolocouris**
Interaction of Aminoadamantane Derivatives with the Influenza A Virus M2 Channel – Role of Water in Molecular Docking Simulations Using a Pore Blocking Model.

As Associate Professor:

34. Ion Channel Workshop, Vancouver, BC, Canada (23/6/2011).
A. Kolocouris, D. Busath
Influenza A M2 is a Drug Target.

35. Biophysical Society 57th Annual Meeting: February 2-6, 2013, Philadelphia.
A. Kolocouris, B. Johnson, C. Tzitzoglaki, N. C. Gay, D. D. Busath
Amantadine analogues that inhibit MDCK cell infection by influenza A with M2(S31N).
Biophys. J. **104** (2), S1, 277a.

36. CECAM Workshop
Coupling between protein, water, and lipid dynamics in complex biological systems: Theory and Experiments, 24-27 September 2013.

P. Gkeka, S. Eleftheratos, **A. Kolocouris**, Z. Cournia
Free Energy Calculations of Aminoadamantane Blockers of Influenza A/M2TM Pore.

37. International Conference on Antiviral Research, San Francisco, CA **(**11/5/2013).
A. Kolocouris, D. Busath
Amantadine Analogues That Inhibit MDCK Cell Infection By Influenza A With M2 (S31N).

38. Ion Channel Workshop, Vancouver, BC, Canada (6/26/2013).
A. Kolocouris, D. Busath
Persistent in vitro inhibition of influenza A by amantadine analogues.

39. 58th Annual Meeting, Biophysical Society, San Francisco, DA (2/2013).
A. Kolocouris, D. Busath
Influenza A Blockers with Reduced Resistance Formation.
Biophys. J. **106** (2), S1, 432a-433a.

40. Biophysical Society 58th Annual Meeting. San Francisco, CA. 2014.
ssNMR Characterization of S31N M2 Transmembrane Domain Bound to Novel Adamantanes with Persistent In Vitro Efficacy.
Wright, A.; Hung, I.; Tzitzoglaki, C.; Busath, D. D.; **Kolocouris, A.;** Cross, T. A. *Biophys. J.* **106** (2), S1, 659a.

41. Biophysical Society 59th Annual Meeting. Baltimore, MD. 2015.
Mitchell L. Gleed, Harris Ioannidis, **A. Kolocouris**, David D. Busath
Molecular Dynamics of Amantadine Block in M2 of Influenza A: WT vs S31N.
Biophys. J. **108** (22), 19a.

42. European Medicinal Chemistry, Athens 2015.
H. Ioannidis, F. Kolarov, P. Gkeka, C. Liolios, C. Zikos, G. Gauglitz, Z. Cournia, **A. Kolocouris**
Investigation of aminoadamantane derivatives binding to the closed state of Influenza A/M2TM pore.

43. European Medicinal Chemistry, Athens 2015.
M. L. Gleed, H. Ioannidis, C. Tzitzoglaki, **A. Kolocouris**, D. D. Busath
Why Bound Amantadine Fails to Inhibit Proton Conductance According to Simulations of the Drug-Resistant Influenza A M2TM (S31N).

44. European Medicinal Chemistry, Athens 2015
C. Tzitzoglaki, A. Hoffmann, F. B. Johnson, R. Zell, I. Tietjen, A. K. Wright, F. Kolarov, K. Freudenberger, C. Zikos, G. Gauglitz, D. Fedida, T. A. Cross, D. D. Busath, M. Schmidtke, **A.** Kolocouris.
The development of old and new class of aminoadamantane derivatives against S31N H1N1 Influenza A viruses.

45. European Medicinal Chemistry, Athens 2015
A. Drakopoulos, F. Kolarov, K. Freudenberger, C. Liolios, A. Hoffmann, M. Schmidtke, G. Gauglitz, **A. Kolocouris**

The development of old and new class of aminoadamantane derivatives against S31N H1N1 Influenza A viruses.

46. European Medicinal Chemistry, Athens 2015
S. Kiriakidi, C. -S. Lopez, **A. Kolocouris**
A DFT study of gold-catalyzed cycloisomerization of functionalized allenes.

47. ACS meeting in Computational Chemistry, August 2016
N. Homeyer, H. Ioannidis, F. Kolarov, G. Gauglitz, C. Zikos, **A. Kolocouris**, H. Gohlke
Interpreting Thermodynamic Profiles of Aminoadamantane Compounds Inhibiting the M2 Proton Channel of Influenza A by Free Energy Calculations.

48. European Federation for Medicinal Chemistry EFMC-ISMC 2016 (Manchester, August 2016).
H. Ioannidis, A. Drakopoulos, C. Tzitzoglaki, F. Kolarov, K. Freudenberger, P. Gkeka, G. Gauglitz, Z. Cournia, **A. Kolocouris**
Alchemical Free Energy calculations and Isothermal Titration Calorimetry measurements of aminoadamantanes bound to the closed state of Influenza A/M2TM.

49. European Federation for Medicinal Chemistry EFMC-ISMC 2016 (Manchester, August 2016).
C. Tzitzoglaki, A. Wright, F. Kolarov, I. Tejen, K.-M. Freudenberger, C. Zikos, D. Fedida, G. Gauglitz, T. Cross, **A. Kolocouris**
Binding and Proton Blockage by Amantadine Variants of the Influenza $M2TM_{WT}$ and $M2TM_{S31N}$ Explained.

50. Schrödinger workshop (London, 2016)
P. Lagarias, K.-N. Klotz, **A. Kolocouris**
Structure-based drug design of Novel Adenosine Receptor Ligands with Subtype A3 Selectivity.

51. 17th Hellenic Symposium on Medicinal Chemistry (HSMC-17), June 2017
A. Konstantinidi, G. Mali, H.-W. Amenitsch, T. Mavromoustakos, **A. Kolocouris**
ssNMR, X-rays and Molecular Dynamics Study of the Interactions between Aminoadamantane Ligands and their Complexes with the Influenza A M2TM in DMPC lipid bilayers.

52. ACSMEDI-EFMC: Medicinal Chemistry Frontiers 2017, June 25-28, 2017 Philadelphia, USA
C. Tzitzoglaki, A. Wright, K. Freudenberger, A. Hoffmann, I. Tietjen, I. Stylianakis, F. Kolarov, D. Fedida, M. Schmidtke, G. Gauglitz, T. A. Cross, A**. Kolocouris**
Binding and Proton Blockage by Amantadine Variants of the Influenza $M2_{WT}$ and $M2_{S31N}$ Explained.

53. ACSMEDI-EFMC: Medicinal Chemistry Frontiers 2017, June 25-28, 2017, Philadelphia, USA
A. Drakopoulos, C. Tzitzoglaki, C. Ma, K. Freudenberger, A. Hoffmann, Y. Hu, G. Gauglitz, M. Schmidtke, J. Wang, **A. Kolocouris**
Affinity of rimantadine enantiomers against influenza A/M2 protein revisited.

54. 8th Hellenic Conference on Calorimetry and Thermal Analysis, HECTA 2018, Athens.
Athina Konstantinidi, Maria Chountoulesi, Nikolaos Naziris, Dimitris Kolokouris, Costas Demetzos, Thomas Mavromoustakos, **A. Kolocouris**

Kinetic study of the thermodynamic behavior of lipid bilayers in the presence of small drug molecules.

55. EuroQSAR Thessaloniki 2018
C. Tzitzoglaki, A. Wright, A. Drakopoulos, K. McGuire, A. Hoffmann, K. Freudenberger, A. Konstantinidi, D. Kolokouris, G. Glauglitz, M. Schmidtke, D. D. Busath, T. Cross, **A. Kolocouris**
Binding, Proton Blockage, Inhibition and Resistance of the Influenza M2 WT and S31N by Amantadine Variants Explained.

56. EuroQSAR Thessaloniki 2018
A. Konstantinidi, N. Naziris, S. Kiriakidi, M. Chountoulesi, H. W. Amenitsch, B. Sartori, G. Mali, D. Kolokouris, C. Demetzos, T. Mavromoustakos, **A. Kolocouris**.
Application of a Combined Methodology Including Computational Chemistry, Biophysics and Synthetic Organic Chemistry to Optimize the Structure of Aminoadamantane Drugs Acting at Influenza A/M2 Protein.

57. EuroQSAR Thessaloniki 2018
P. Lagarias, E. Vrontaki, D. Stamatis, **A. Kolocouris**.
Discovery of Novel Adenosine Receptor Antagonists through a Combined Structure- and Ligand-Based Approach.

58. EuroQSAR Thessaloniki 2018
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