

## Personal Information

Family name, first name	Papakyriakou Athanasios (Thanos)
Place, date of birth	Athens, 7 October 1975
Marital status	Married with two children
Home address	Kanari 3, GR-15562, Cholargos, Greece
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## EDUCATION

**Ph.D. (2001 – 2004)** National and Kapodistrian University of Athens, Department of Chemistry, Inorganic Chemistry Section, thesis title: *“Structure and interaction of complexes of the anticancer drug Bleomycin with DNA using Nuclear Magnetic Resonance Spectroscopy and Molecular Dynamics Simulations”* carried out at the Bioinorganic Laboratory of Dr. Nikos Katsaros, Institute of Physical Chemistry, NCSR “Demokritos”

**M.Sc. (1999 – 2001)** National and Kapodistrian University of Athens, Department of Chemistry, Inorganic Chemistry Section, thesis title: *“Study on the complexation of uranyl ions with the anticancer drugs Daunorubicin, Adriamycin and their interaction with natural DNA”* carried out at the Bioinorganic Laboratory of Dr. Nikos Katsaros, Institute of Physical Chemistry, NCSR “Demokritos”

**B.Sc. (1994 – 1999)** National and Kapodistrian University of Athens, Department of Chemistry. Dissertation carried out at the Inorganic Chemistry Section under the supervision of Prof. K. Mertis.

## CURRENT EMPLOYMENT

**Sep 2018 – present** Senior Researcher at the Institute of Biosciences and Applications, National Centre for Scientific Research “Demokritos”.

## RESEARCH EXPERIENCE

**Sep 2016 – Sep 2018** Individual Marie-Curie Research Fellow at the Faculty of Medicine (Prof. Tim Elliott) and Biological Sciences (Dr. Jörn Werner), University of Southampton, UK.

**Feb 2014 – Sep 2016** Research associate, Protein Chemistry Laboratory, NCSR “Demokritos”, research grant in collaboration with Dr. E. Stratikos.

**Mar – Jul 2015** Research associate, Chemical Biology Group, INN, NCSR “Demokritos”, research grant “Kripis” in collaboration with Dr. Emmanouel Pitsinos and Dr. Konstantina Yannakopoulou.

**Mar 2012 – Feb 2014** Visiting research scholar at Prof. Emmanuel Theodorakis Lab, Department of Chemistry and Biochemistry, University of California, San Diego, US.

**Sep 2009 – Feb 2012** Research associate, Laboratory of Chemical Biology of Dr. D. Vourloumis, NCSR “Demokritos”, Athens, Greece. Marie-Curie grant “*ExploRNA*” for the design of spirocyclic aminoglycoside-analogues that target the ribosomal RNA.

**Mar 2010 – Feb 2012** Research collaborator at the Laboratory of Prof. E. Eliopoulos, Department of Biochemistry and Biotechnology, Agricultural University of Athens hit-to-lead optimization of ligands that target validated molecules involved in the pathogenesis of Rheumatoid Arthritis

**Mar – Aug 2009** Research collaborator at the Laboratory of Prof. G.A. Spyroulias University of Patras, Department of Pharmacy for the simulation of acetylcholine receptor–toxin interactions and the design of novel small-molecule inhibitors.

**Mar 2007 – Feb 2009** Research fellow at the Laboratory of Chemical Biology, National Center for Scientific Research “Demokritos”, Athens, Greece with a postdoctoral grant for the “*Design and Synthesis of Selective Inhibitors of Vascular Endothelial Growth Factor Receptor-2 (VEGF-R2) Using Structural Methods for the Treatment of Cancer*”.

**Sep 2006 – Feb 2007** Adjunct lecturer at the Department of Pharmacy, University of Patras, and research collaborator of the research group of Prof. G.A. Spyroulias for the simulation of metalloprotease–substrate interactions.

**Mar 2005 – Aug 2006** Adjunct lecturer at the Department of Chemistry, University of Ioannina, and postdoctoral researcher at the program PYTHAGORAS II “*Development of Combinatorial Library of Selective Chemical Nucleases based on Ruthenium(II) complexes with bound peptides*”.

**[May 2004 – Feb 2005** *Compulsory nine-month military service]*

**Oct 2002 – Apr 2004** Research fellow at the Laboratory of Dr. N. Katsaros, National Center for Scientific Research “Demokritos”, Athens, Greece, for the synthesis of anticancer drug complexes and structural studies on DNA interactions.

**Apr – Oct 2003** Marie-Curie Fellow at the Center of Nuclear Magnetic Resonance, CERM, University of Florence, Italy, under the supervision of Prof. Claudio Luchinat for the study of small-molecule binding to protein targets using Nuclear Magnetic Resonance NMR screening techniques in combination with docking simulations and molecular dynamics calculations.

**Nov – Dec 2001** “Platon” exchange program fellow at the Laboratory of Prof. Arlette Garnier-Suillerot, University XII of North Paris, France, for studying the cytotoxic effect of anticancer drug complexes using flow cytometry and atomic absorption techniques.

**Nov 2000 – Jun 2001** Greek-Italian Ministry of Education fellow at the Center of Nuclear Magnetic Resonance, University of Florence. Graduate student under the supervision of Prof. Ivano Bertini for studying bioinorganic systems using Nuclear Magnetic Resonance (NMR) in combination with molecular dynamics simulations and quantum mechanics calculations.

**Oct 1998 – Sep 2002** PhD scholar at the Institute of Physical Chemistry, National Center for Scientific Research “Demokritos” under the supervision of Dr. Nikos Katsaros.

## FELLOWSHIPS – AWARDS

**ELIDEK Grant (10/2018)** Individual research 3-year grant of €180,000 for research: “ARIA: Atomic Resolution Insight into the Antigen processing machinery”

**Marie-Curie IEF (9/2016)** 2-year individual Marie Curie fellowship “Dynamis: Dynamic Origins of MHC class I Selector function” Prof. Tim Elliott, Faculty of Medicine, University of Southampton (Total score: 97.4%, granted €195,455)

**GSRT Grant (2/2012)** 3-year research grant from the General Secretariat of Research and Technology of Greece, comprising a 2-year research scholarship at the University of California, Sand Diego, US, and a 1-year return phase at the NCSR “Demokritos” (€150,000)

**SYNERGASIA (3/2010)** 2-year research grant in collaboration with the Lab of Prof. E. Eliopoulos, Department of Biochemistry, Agricultural University of Athens.

**EXPRORNA (9/2009)** 18-month Marie-Curie Fellowship for postdoctoral research at the Chemical Biology Laboratory of Dr. D. Vourloumis, Institute of Physical Chemistry, NCSR “Demokritos”.

**NEUROCYPRES (3/2009)** 6-month European funding (Cooperation) research fellowship at the University of Patras, Department of Pharmacy.

**ENTER2004 (3/2007)** 18-month research funding at the Chemical Biology Laboratory of D. Vourloumis, Institute of Physical Chemistry NCSR “Demokritos”

**IKY Postdoctoral (2/2007)** 12-month fellowship for postdoctoral research.

**PYTHOGORAS II (3 / 2005)** 18-month funding at the Bioinorganic Laboratory, Department of Chemistry, University of Ioannina.

**Marie-Curie (4/2003)** 6-month fellowship at the Center of Nuclear Magnetic Resonance, CERM, University of Florence, Italy.

**IKY Honors (3/2002)** Distinction prize for the M.Sc. diploma during the academic year 2000 – 2001.

**M. of Education (11/2000)** 7-month fellowship from the Ministry of Education at the Center of Nuclear Magnetic Resonance, CERM, University of Florence, Italy.

**DEMOKRITOS** (10/1999) 4-year scholarship at the Institute of Physical Chemistry, National Center for Scientific Research “Demokritos” for obtaining a PhD from the Department of Chemistry, University of Athens, Greece.

## SCIENTIFIC SKILLS

**Laboratory skills.** Experience on the synthesis, isolation and characterization of organic compounds of pharmacological interest (enzyme inhibitors) and inorganic complexes with anticancer drug ligands, isolation and structural characterization using a series of spectroscopic techniques. Expertise on Nuclear Magnetic Resonance (NMR) techniques for structural characterization and small-molecule binding to protein and DNA/RNA screening. Skilled on acquiring and analyzing spectroscopic data from UV-Vis, IR, circular dichroism, fluorescence, electrospray mass spectroscopy, atomic absorption and electron spin resonance spectroscopy. Experienced in studying the binding equilibrium between protein/nucleotide-ligand complexes using optical spectroscopy, fluorescence and isothermal titration calorimetry.

**Computational Chemistry.** Excellent skill on Linux/Unix operating systems and knowledge of script programming, employing molecular dynamics calculations and force field parameter development using quantum chemical calculations. Skilled on chemoinformatics and molecular database analyses, bioinformatics and protein homology modeling. Expertise in docking-based methods for the prediction of nucleotide/protein–protein/substrate/ligand interactions; homology modelling and quality assessment; performing and analysing conventional, accelerated, essential and targeted molecular dynamics simulations; free energy calculations with MM-GBSA/PBSA, FEP and TI methods; quantum mechanics calculations for optimization and ESP fit. Skilled in cheminformatics tools and model visualization.

**Languages:** Greek (native speaker), English (Proficiency in English) and spoken Italian.

## TEACHING EXPERIENCE

**Mar 2019 – now** Lecture series at the Postgraduate Program Molecular Pharmacology, Department of Chemistry, University of Patras

**Sep 2006 – Feb 2007** Adjunct Lecturer, Department of Pharmacy, University of Patras  
1 semester for the course of “General and Analytical Chemistry”.

**Mar 2005 – Feb 2006** Adjunct Lecturer, Department of Chemistry, University of Ioannina  
2 semesters for the course of “General and Inorganic Chemistry”.

## STUDENTS SUPERVISED

Sep 2018–now Lykourgos Chiniadis PhD Student, Department of Biotechnology, Agricultural University of Athens

- Feb 2019–now Kleanthis Xanthopoulos, PhD Student, Department of Biomedical Sciences, University of West Attica
- July – Sep 2019 Agoritsa Kalabaliki, Undergraduate student, Department of Biotechnology, Agricultural University of Athens

## PEER-REVIEWED PUBLICATIONS

Dr. Papakyriakou is the co-author in **68 peer-reviewed research articles** in addition to **4 reviews**. According to Scopus (Author ID: 7801330433), these articles have received **1200 citations** and the author's ***h-index* is 18** (May 2020):

72. Chiniadis L, Bratsos I, Bethanis K, Karpusas M, Giastas P, **Papakyriakou A.** \* High-resolution crystal structures of a "half sandwich"-type Ru(II) coordination compound bound to hen egg-white lysozyme and proteinase K. **(2020)** *J Biol Inorg Chem.* 202, 25, 635-645 \**corresponding author*
71. **Papakyriakou A**, Cencetti F, Puliti E, Morelli L, Tricomi J, Bruni P, Compostella F, Richichi B. Glycans Meet Sphingolipids: Structure-Based Design of Glycan Containing Analogues of a Sphingosine Kinase Inhibitor **(2020)** *ACS Med Chem Lett.* 11, 913-920.
70. Mavridis G, Arya R, Domnick A, Zoidakis J, Makridakis M, Vlahou A, Mpakali A, Lelis A, Georgiadis D, Tampé R, Papakyriakou A, Stern LJ, Stratikos E. A systematic re-examination of processing of MHCI-bound antigenic peptide precursors by endoplasmic reticulum aminopeptidase 1. **(2020)** *J Biol Chem.* 295, 7193-7210
69. Giastas P, Mpakali A, **Papakyriakou A**, et al. Mechanism for antigenic peptide selection by endoplasmic reticulum aminopeptidase 1 **(2019)** *Proc Natl Acad Sci USA.* 116, 26709–26716. doi:10.1073/pnas.1912070116
68. Tsoukalidou S, Kakou M, Mavridis I, Koumantou D, Calderone V, Fragai M, Stratikos E, **Papakyriakou A\*** and Vourloumis D\* Exploration of zinc-binding groups for the design of inhibitors for the oxytocinase subfamily of M1 aminopeptidases **(2019)** *Bioorg Med Chem.* 27, 115177. doi:10.1016/j.bmc.2019.115177 \**corresponding author*
67. MacLachlan BJ, Dolton G, **Papakyriakou A**, et al. Human leukocyte antigen (HLA) class II peptide flanking residues tune the immunogenicity of a human tumor-derived epitope **(2019)** *Journal of Biological Chemistry*, 294, 20246–20258. doi:10.1074/jbc.RA119.009437
66. Koumantou D, Barnea E, Martin-Esteban A, Maben Z, **Papakyriakou A** et al. Editing the immunopeptidome of melanoma cells using a potent inhibitor of endoplasmic reticulum aminopeptidase 1 (ERAP1). **(2019)** *Cancer Immunology & Immunotherapy*, 68, 1245–1261. doi:10.1007/s00262-019-02358-0
65. Zouridakis M, **Papakyriakou A**, Ivanov IA, et al. Crystal Structure of the Monomeric Extracellular Domain of  $\alpha 9$  Nicotinic Receptor Subunit in Complex With  $\alpha$ -Conotoxin RgIA:

Molecular Dynamics Insights Into RglA Binding to  $\alpha 9\alpha 10$  Nicotinic Receptors (2019) Front Pharmacol. 10, 474. doi:10.3389/fphar.2019.00474

64. **Papakyriakou, A.**, Reeves, E., Beton, M., Mikolajek, H., Douglas, L., Cooper, G., Elliott, T., Werner, J.M., James, E. The partial dissociation of MHC class I– bound peptides exposes their N terminus to trimming by endoplasmic reticulum aminopeptidase 1. (2018) Journal of Biological Chemistry, 293 (20), pp. 7538-7548. DOI: 10.1074/jbc.RA117.000313

63. Giastas, P., Andreou, A., **Papakyriakou, A.**, Koutsioulis, D., Balomenou, S., Tzartos, S.J., Bouriotis, V., Eliopoulos, E.E. Structures of the Peptidoglycan N-Acetylglucosamine Deacetylase Bc1974 and Its Complexes with Zinc Metalloenzyme Inhibitors (2018) Biochemistry, 57 (5), pp. 753-763. DOI: 10.1021/acs.biochem.7b00919

62. Agalou, A., Thrapsianiotis, M., Angelis, A., **Papakyriakou, A.**, Skaltsounis, A.-L., Aligiannis, N., Beis, D. Identification of novel melanin synthesis inhibitors from *Crataegus pycnoloba* using an in vivo zebrafish phenotypic assay. (2018) Frontiers in Pharmacology, 9 (MAR), art. no. 265, DOI: 10.3389/fphar.2018.00265

61. Mettou, A., Papaneophytou, C., Melagraki, G., Maranti, A., Liepouri, F., Alexiou, P., **Papakyriakou, A.**, Couladouros, E., Eliopoulos, E., Afantitis, A., Kontopidis, G. Aqueous Solubility Enhancement for Bioassays of Insoluble Inhibitors and QSPR Analysis: A TNF- $\alpha$  Study (2018) SLAS Discovery, 23 (1), pp. 84-93. DOI: 10.1177/2472555217712507

60. Stamatopoulou, V., Apostolidi, M., Li, S., Lamprinou, K., **Papakyriakou, A.**, Zhang, J., Stathopoulos, C. Direct modulation of T-box riboswitch-controlled transcription by protein synthesis inhibitors. (2017) Nucleic Acids Research, 45 (17), pp. 10242-10258. DOI: 10.1093/nar/gkx663

59. Chatziefthimiou, S.D., Inclán, M., Giastas, P., **Papakyriakou, A.**, Yannakopoulou, K., Mavridis, I.M. Molecular recognition of N-acetyltryptophan enantiomers by  $\beta$ -cyclodextrin (2017) Beilstein Journal of Organic Chemistry, 13, pp. 1572-1582. DOI: 10.3762/bjoc.13.157

58. **Papakyriakou, A.**, Stratikos, E. The role of conformational dynamics in antigen trimming by intracellular aminopeptidases (2017) Frontiers in Immunology, 8 (AUG), art. no. 946, DOI: 10.3389/fimmu.2017.00946 *\*corresponding author*

57. Mpakali A., Saridakis E., Harlos K., Zhao Y., Kokkala P., Georgiadis D., Giastas P., **Papakyriakou A.** and Stratikos E. “Ligand-induced conformational change of Insulin-regulated aminopeptidase: insights on catalytic mechanism and active site plasticity” J. Med. Chem. 2017, 60, 2963-2972.

56. Argyros O., Karampelas T., Varela A., Asvos X., **Papakyriakou A.**, Agalou A., Beis D., Davos C.H., Fokas D., Tamvakopoulos C., “Targeting of the Breast Cancer Microenvironment with A Potent And Linkable Oxindole Based Antiangiogenic Small Molecule” Oncotarget 2017, doi: 10.18632/oncotarget.16763

55. Vlastaridis P., **Papakyriakou A.**, Chaliotis A., Stratikos E., Oliver S.G. and Amoutzias G.D. "The pivotal role of protein phosphorylation in the control of yeast central metabolism" *G3: Genes Genomes Genetics* **2017**, 7, 1239-1249.
54. Stamogiannos A., Maben Z., **Papakyriakou A.**, Mpakali A., Kokkala P., Georgiadis D., Stern L.J. and Stratikos E. "Critical role of inter-domain interactions on the conformational change and catalytic mechanism of Endoplasmic Reticulum Aminopeptidase 1" *Biochemistry* **2017**, 56, 1546-1558.
53. Mpakali A., Giastas P., Deprez-Poulain R., **Papakyriakou A.**, Koumantou D., Tsoukalidou S., Vourloumis D., Mavridis I.M., Stratikos E. and Saridakis E. "Crystal Structures of ER Aminopeptidase 2 in Complex with Ligands Reveal Protein Sites Important for Binding" *ACS Med. Chem. Lett.* **2017**, 8, 333-337.
52. Kokkala P., Mpakali A., Mauvais F.X, **Papakyriakou A.**, Daskalaki I., Petropoulou I., Kavvalou S., Papathanasopoulou M., Agrotis S., Fonsou T.M., van Endert P., Stratikos E., Georgiadis D. "Optimization and Structure-Activity Relationships of Phosphinic Pseudotriptide Inhibitors of Aminopeptidases that Generate Antigenic Peptides." *J. Med. Chem.* **2016**, 59, 9107-9123.
51. Anastasakis D., Skeparnias I., Shaukat A.N., Grafanaki K., Kanellou A., Taraviras S., Papachristou D.J., **Papakyriakou A.**, Stathopoulos C. "Mammalian PNLDC1 is a novel poly(A) specific exonuclease with discrete expression during early development" *Nucleic Acids Res.* **2016**, 44, 8908-8920.
- 50.** Stamogiannos A.\*, **Papakyriakou A.\***, Mauvais F.X., van Endert P., Stratikos E. "Screening Identifies Thimerosal as a Selective Inhibitor of Endoplasmic Reticulum Aminopeptidase 1", *ACS Med Chem Lett* **2016**, 7, 681-685. *\*Equal contribution*
49. Eleftheriou K., Sideratou Z., Thanassoulas A., **Papakyriakou A.**, Tsiourvas D. "Comparative Experimental and Computational Study of Monoalkyl Chain Phosphatidylcholine-Containing Thermoresponsive Liposomes" *J Phys Chem B* **2016**, 120, 5417-5428.
48. Argyros O., Karampelas T., Asvos X., Varela A., Sayyad N., **Papakyriakou A.**, Davos C.H., Tzakos A.G., Fokas D., Tamvakopoulos C., "Peptide-drug conjugate GnRH-sunitinib targets angiogenesis selectively at the site of action to inhibit tumor growth", *Cancer Research*, **2016**, 76, 1181-1192.
47. Nicolaou K.C., Vourloumis D., Totokotsopoulos S., **Papakyriakou A.**, Karsunky H., Fernando H., Gavrilyuk J., Webb D., Stepan A.F., "Synthesis and Biopharmaceutical Evaluation of Imatinib Analogues Featuring Unusual Structural Motifs", *ChemMedChem* **2016**, 11, 31-37.
- 46.** **Papakyriakou A.**, Zervoudi E., Tsoukalidou S., Mauvais F. X., Sfyroera G., Mastellos D. C., van Endert P., Theodorakis E. A., Vourloumis D., Stratikos E., "3, 4-diaminobenzoic acid derivatives as inhibitors of the oxytocinase subfamily of M1 aminopeptidases with immune regulating properties", *J. Med. Chem.* **2015**, 58, 1524-1543.

45. Stamogiannos A., Koumantou D., **Papakyriakou A.\*** and Stratikos E.\* “Effects of polymorphic variation on the mechanism of Endoplasmic Reticulum Aminopeptidase 1”, *Mol. Immunol.* **2015**, 67, 426-435. *\*corresponding authors*
44. Mpakali A., Saridakis E., Harlos K., Zhao Y., **Papakyriakou A.**, Kokkala P., Georgiadis D., Stratikos E., “Crystal Structure of Insulin-Regulated Aminopeptidase with Bound Substrate Analogue Provides Insight on Antigenic Epitope Precursor Recognition and Processing”, *J. Immunol.* **2015**, 195, 2842-2851.
43. Azam L., **Papakyriakou A.**, Marios Zouridakis M., Giastas P., Tzartos S. J., McIntosh M. J., “Molecular Interaction of  $\alpha$ -Conotoxin Rg1A with the Rat  $\alpha 9\alpha 10$  Nicotinic Acetylcholine Receptor”, *Mol. Pharmacol.* **2015**, 87, 855–864.
42. Sharina I.G., Sobolevsky M., **Papakyriakou A.**, Rukoyatkina N., Spyroulias G.A., Gambaryan S., Martin E., “The fibrate gemfibrozil is an NO–and heme-independent activator of soluble guanylyl cyclase: in vitro studies”, *Brit. J. Pharm.* **2015**, 172, 2316–2329.
41. Kalyva M., Zografos A.L., Kapourani E., Giambazolias E., Devel L., **Papakyriakou A.**, Dive V., Lazarou Y. G., Georgiadis D., “Probing the Mechanism of Allylic Substitution of Morita–Baylis–Hillman Acetates (MBHAs) by using the Silyl Phosphonite Paradigm: Scope and Applications of a Versatile Transformation”, *Chemistry Eur. J.* **2015**, 21, 3278–3289.
40. Papaneophytou C., Alexiou P., **Papakyriakou A.**, Ntougkos E., Tsiliouka K., Maranti A., Liepouri F., Strongilos A., Mettou A., Couladouros E., Eliopoulos E., Douni E., Kollias G., Kontopidis G. “Synthesis and biological evaluation of potential small molecule inhibitors of Tumor Necrosis Factor”, *MedChemComm* **2015**, 6, 1196–1209.
- 39.** **Papakyriakou A.**, Kefalos P., Sarantis P., Tsiamantas, C., Xanthopoulos K., Vourloumis D., Beis D., “A Zebrafish In Vivo Phenotypic Assay to Identify 3-Aminothiophene-2-Carboxylic Acid-Based Angiogenesis Inhibitors”, *Assay and Drug Dev. Tech.* **2014**, 9-10, 527–535.
38. Alexiou P., **Papakyriakou A.**, Ntougkos E., Papaneophytou C. P., Liepouri F., Mettou A., Katsoulis I., Maranti A., Tsiliouka K., Strongilos A., Chaitidou S., Douni E., Kontopidis G., Kollias G., Couladouros E., Eliopoulos E., “Rationally designed less toxic SPD-304 analogs and preliminary evaluation of their TNF inhibitory effects”. *Arch. Pharm. Chem. Life Sci.* **2014**, 11, 798–805.
- 37.** **Papakyriakou A.**, Stamatakis G. M., Demopoulos C. A. “Computational Investigation of Darapladib and Rilapladib Binding to Platelet Activating Factor Receptor. A Possible Mechanism of Their Involvement in Atherosclerosis”. *Int. J. Chem.* **2014**, 6, 50–60.
36. **Papakyriakou A.**, Zervoudi E., Theodorakis E. A., Saveanu L., Stratikos E., Vourloumis D. “Novel selective inhibitors of aminopeptidases that generate antigenic peptides” *Bioorg. Med. Chem. Lett.* **2013**, 23, 4832-4836.
35. Karpusas M., Axarli I., Chiniadis L., **Papakyriakou A.**, Bethanis K., Scopelitou K., Clonis Y. D., Labrou N. E. “The Interaction of the Chemotherapeutic Drug Chlorambucil with Human Glutathione Transferase A1-1: Kinetic and Structural Analysis”. *PLoS One*, **2013**, e56337.



34. Tsoupras A.B., **Papakyriakou A.**, Demopoulos C.A., Philippopoulos A.I. "Synthesis, biochemical evaluation and molecular modeling studies of novel rhodium complexes with nanomolar activity against platelet activating factor". *J. Inorg. Biochem.* **2013**, 120, 63–73.
33. Richichi B., Lunghi C., **Papakyriakou A.**, Francesconi O., Nativi C. "Sialyloxoenoitols as precursors for new analogues of sialidase inhibitors". *Pure & Appl. Chem.* **2013**, 85, 1803–1811.
32. Karidi K., Ypsilantis K., **Papakyriakou A.**, Garoufis A. "Synthesis and characterization of ruthenium(II)-oligopyridine-peptide conjugates. Interactions of the diastereomers  $\Delta$ - And  $\Lambda$ ". *J. Inorg. Biochem.* **2013**, 127, 13–23.
31. Evnouchidou I., Birtley J., Seregin S., **Papakyriakou A.**, Zervoudi E., Samiotaki M., Panayotou G., Giastas P., Petrakis O., Georgiadis D., Amalfitano A., Saridakis E., Mavridis I. M., Stratikos, E. "A common single nucleotide polymorphism in endoplasmic reticulum aminopeptidase 2 induces a specificity switch that leads to altered antigen processing". *J. Immunol.* **2012**, 189, 2383-2392.
30. Zervoudi E.\*, **Papakyriakou A.\***, Georgiadou D., Evnouchidou I., Gajda A., Poreba M., Salvesen G.S., Drag M., Hattori A., Swevers L., Vourloumis D., Stratikos E. "Probing the S1 specificity pocket of the aminopeptidases that generate antigenic peptides". *Biochem J.* **2011**, 435, 411-420. *\*equal contribution*
29. Katsoulis I.A., Kythreoti G., **Papakyriakou A.**, Koltsida K., Anastasopoulou P., Stathakis C.I., Mavridis I., Cottin T., Saridakis E., Vourloumis D. "Synthesis of 5,6-spiroethers and evaluation of their affinity for the bacterial A-site". *ChemBioChem* **2011**, 12, 1188-1192.
28. Androutsopoulos V., Ruparelia K. C, **Papakyriakou A.**, Filippakis C., Tsatsakis A. M., Spandidos D. A. "Anticancer effects of the metabolic products of the resveratrol analogue, DMU-212: Structural requirements for potency". *Eur. J. Med. Chem.* **2011**, 46, 2586-2595.
27. Androutsopoulos V., **Papakyriakou A.**, Vourloumis D., Spandidos D.A. "Comparative CYP1A1 and CYP1B1 Substrate and Inhibitor Profile of Dietary Flavonoids". *Bioorg. Med. Chem.* **2011**, 19, 2842-2849.
26. Cottin T., Pyrkotis C., Stathakis C.I., Mavridis I., Katsoulis I.A., Anastasopoulou P., Kythreoti G., Zografos A.L., Nahmias V.R., **Papakyriakou A.**, Vourloumis D. "Designed spiro-bicyclic analogues targeting the ribosomal decoding center". *ChemBioChem.* **2011**, 12, 71–87.
25. Dimitropoulos N., **Papakyriakou A.**, Dalkas G.A., Chasapis C.T., Poulas K., Spyroulias G.A. "A computational investigation on the role of glycosylation in the binding of alpha1 nicotinic acetylcholine receptor with two alpha-neurotoxins". *Proteins* **2011**, 79, 142–152.
24. Stathakis C.I., Mavridis I., Kythreoti G., **Papakyriakou A.**, Katsoulis I.A., Cottin T., Anastasopoulou P., Vourloumis D. "Second generation analogs of rigid 6,7-spiro scaffolds targeting the bacterial ribosome". *Bioorg Med Chem Lett.* **2010**, 20, 7488–7492.

23. Kokkinou A., Tsorteki F., Karpusas M., **Papakyriakou A.**, Bethanis K. and Mentzafos D. "Study of the inclusion of the (R)- and (S)-camphor enantiomers in  $\alpha$ -cyclodextrin by X-ray crystallography and molecular dynamics" *Carbohydrate Res.* **2010**, 345, 1034–1040.
22. Dimitropoulos N., **Papakyriakou A.**, Dalkas G.A., Sturrock E.D. and Spyroulias G.A. "A Computational Approach to the Study of the Binding Mode of Dual ACE/NEP Inhibitors" *J. Chem. Inf. Model.* **2010**, 50, 388–396.
21. Androutsopoulos V.P., **Papakyriakou A.**, Vourloumis D., Tsatsakis A.M. and Spandidos D.A. "Dietary flavonoids in cancer therapy and prevention: Substrates and inhibitors of cytochrome P450 CYP1 enzymes" *Pharmacol. Ther.* **2010**, 126, 9–20.
- 20. Papakyriakou A.**, Katsarou M.E., Belimezi M., Karpusas M. and Vourloumis D. "Discovery of potent vascular endothelial growth factor receptor-2 inhibitors" *ChemMedChem* **2010**, 5, 118–129.
19. Evnouchidou I., **Papakyriakou A.**, Stratikos E. "A new role for Zn(II) aminopeptidases: Antigenic peptide generation and destruction" *Curr. Pharm. Design* **2009**, 15, 3656-3670.
18. Katsoulis I., Pyrkotis C., **Papakyriakou A.**, Kythreoti G., Zografos A., Mavridis I., Nahmias V., Anastasopoulou P. and Vourloumis D. "Unnatural Rigid Scaffolds Targeting the Bacterial Ribosome" *ChemBioChem.* **2009**, 10, 1969–1972.
17. Dalkas G. A., **Papakyriakou A.**, Vlamis-Gardikas A. and Spyroulias G.A. "Insight into the Anthrax Lethal Factor substrate interaction and selectivity using docking and molecular dynamics simulations" *Protein Sci.* **2009**, 18, 1774–1785.
- 16. Papakyriakou A.**, Vourloumis D., Tzortzatou-Stathopoulou F. and Karpouzas M. "Conformational dynamics of the EGFR kinase domain reveals structural features involved in activation" *Proteins* **2009**, 76, 375–386.
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9. **Papakyriakou A.**, Malandrinos, G., Garoufis, A., "Interaction of  $\Lambda$ - and  $\Delta$ -[Ru(bpy)<sub>2</sub>(pbmz)](PF<sub>6</sub>)<sub>2</sub> with the oligonucleotide duplex d(CGCGAATTCGCG)<sub>2</sub>" *J. Inorg. Biochem.* **2006**, 100, 1842-1848.
8. Antoniadis C., Hadjikakou S., Hadjiliadis N., **Papakyriakou A.**, Baril M., Butler I. S., "Synthesis and Structure of Se analogues of the antithyroid drug 6-n-propyl-2-thiouracil and its alkyl derivatives. Formation of dimeric Se-Se compounds and deselenation reactions of charge-transfer adducts of diiodine." *Chemistry Eur. J.* **2006**, 12, 6888-6897.
7. Christofis P., Katsarou M., **Papakyriakou A.**, Sanakis Y., Katsaros N., Psomas G., "Mononuclear metal complexes with Piroxicam: Synthesis, structure and biological activity." *J. Inorg Biochem.* **2005**, 99, 2197-2200.
6. Katsarou M.E., **Papakyriakou A.**, Katsaros N., and Scorilas A. "Expression of the C-terminal domain of novel human SR-A1 protein: Interaction with the CTD domain of RNA polymerase II." *Biochem. Biophys. Res. Comm.* **2005**, 334, 61-68.
5. **Papakyriakou A.**, Bratsos I., Katsarou M., Katsaros N. "Preparation, structure determination and cytotoxicity of the Pd(II)-bleomycin A2 complex." *Eur. J. Inorg. Chem.* **2004**, 15, 3118-3126.
4. **Papakyriakou A.**, Katsaros N. "NMR and molecular modelling studies on the solution structure of the In(III)-bleomycin A2 complex." *Eur. J. Inorg. Chem.* **2003**, 16, 3001-3006.
3. **Papakyriakou A.**, Mouzopoulou B., Katsaros N. "The solution structure of the Ga(III)-bleomycin A2 complex resolved by NMR and molecular modeling; interaction with d(CCAGGCCTGG)." *J. Biol. Inorg. Chem.* **2003**, 8, 549-559.
2. **Papakyriakou A.**, Bratsos I., Katsaros N. "Structural studies on metallobleomycins: The interaction of Pt(II) and Pd(II) with bleomycin." *J. Serb. Chem. Soc.* **2003**, 68, 339-348.
1. **Papakyriakou A.**, Anagnostopoulou A., Garnier-Suillerot A., Katsaros N. "Interaction of uranyl ions with daunorubicin and adriamycin." *Eur. J. Inorg. Chem.* **2002**, 5, 1146-1154.

## PROCEEDINGS – BOOK CHAPTERS

1. Karidi K., Triantafillidi K., Lekkas N., **Papakyriakou A.**, Garoufis A. Synthesis, characterization and DNA binding properties of Ruthenium peptide conjugates. *Drugs of the Future* **2007**, 32, 110.
2. Dalkas G.A., **Papakyriakou A.**, Vlamis-Gardikas A., Spyroulias G.A., Cordopatis P. Anthrax lethal factor (ALF)-MEK peptide interaction through molecular dynamics simulations. *Amino Acids* **2007**, 33, 9.
3. **Papakyriakou A.**, Spyroulias G.A., Manessi-Zoupa E., Cordopatis P. Angiotensin-I converting enzyme (ACE)-peptide interaction through molecular dynamics simulations. *Amino Acids* **2007**, 33, 10.
4. **Papakyriakou A.**, Vlachopoulos G.F., Spyroulias G.A., Manessi-Zoupa E., Cordopatis P. "Angiotensin-I Converting Enzyme (ACE); Substrate Interaction through Molecular Dynamics Simulations" in *Peptides* (K. Rolka, P. Rekowski, J. Silberring, Eds.) *J. Peptide Science* **2006**, Suppl. Vol. 12, 189.
5. Dalkas G.A., **Papakyriakou A.**, Vlamis-Gardikas A., Spyroulias G.A., Pairas G., Cordopatis P. "Anthrax Lethal Factor (ALF) : Substrate Interaction through Molecular Dynamics Simulations" in *Peptides* (K. Rolka, P. Rekowski, J. Silberring, Eds.) *J. Peptide Science* **2006** Suppl. Vol. 12, 189.
6. **Papakyriakou A.**, Galanakis P., Gkazonis P., Spyroulias G.A. "Structure Variation in E3 Ligases Ubiquitination Platform" in *Peptides* (K. Rolka, P. Rekowski, J. Silberring, Eds.) *J. Peptide Science* **2006**, Suppl. Vol. 12, 191.
7. Vlachopoulos G., **Papakyriakou A.**, Dalkas G., Spyroulias G.A., Cordopatis P., "In silico evaluation of bioactive compounds: Docking Simulations based Enzyme-Inhibitor Interaction compared with X-ray models." *Lecture Series on Computer and Computational Science*, **2005**, 4, 1379-1382. (Book chapter)
8. **Papakyriakou A.**, Mouzopoulou B., Katsaros N. "The detailed structural characterization of the Ga(III)-bleomycin A2 complex by NMR and molecular modelling" *J Inorg. Biochem.* **2001**, 86 (1), 371.

## PATENTS GRANTED

**A. Papakyriakou**, E. Zervoudi, E. Stratikos, D. Vourloumis, "3,4-diaminobenzoic acid derivatives as inhibitors of Endoplasmic Reticulum Aminopeptidase 1, 2 (ERAP1, ERAP2) and Insulin-regulated Aminopeptidase (IRAP) and uses thereof" Appl. No. 20130100419 /12-7-2013, Greece.

## ORAL PRESENTATIONS

15. "Structure-based design and virtual screening of small-molecule databases", *OpeenscreenGR* **2019**, 4 October, Aristotle University of Thessaloniki, Greece.
14. "Structure-based virtual screening for drug-like allosteric inhibitors of IRAP", *IRAP meeting* **2019**, 27–30 August, Nafplio, Greece.

13. “Computer-aided drug discovery”, CHARME Training School, COST ACTION, **2019**, March Agricultural University of Athens, Greece.
12. “Interactions at the Amino Terminus Binding Pocket of a Single-Chain MHC Class I Molecule Can Affect the Function of Endoplasmic Reticulum Aminopeptidase”, South West Structural Biology Consortium meeting **2017**, 3-4 July, Cardiff, UK.
11. “The role of conformational dynamics in antigen presentation”, 68<sup>th</sup> Congress of the Hellenic Society of Biochemistry and Molecular Biology, 10-12 November **2017**, Athens, Greece.
10. “Identifying Molecular Mechanisms of Antigen Processing in silico” CompBioMed Workshop, Barcelona Supercomputer Center, 11–12 April **2017**
9. “Practical Considerations in Structure-Based Virtual Screening”, Dilemmas in structural biology: selection and integration of methods Workshop, NHRF Athens 14 – 17 February **2016**
8. “Docking Calculations Using AutoDock 4 With AutoDockTools”, 2<sup>nd</sup> Workshop: NMR Basics and Applications in Life Sciences, University of Patras, 13–15 May **2013**
7. “Computational Inorganic Chemistry: Molecular modeling of DNA–drug and metalloprotein–substrate interactions”, Seminar at the Chemistry Department, University of Athens, 23 September **2010**, Greece.
6. “A Computational Study on the Role of Glycosylation in the Binding of alpha1 Nicotinic Acetylcholine Receptor with two alpha Neurotoxins”, 2<sup>nd</sup> Neurocyprus Meeting, May 7-9 **2010**, Marseille, France
5. “Applications of Bioinformatics and Computational Biology in Drug Design”, Seminar at the Medical School of Patras, March 24 **2010**, University of Patras.
4. “Targeted Molecular Dynamics of the EGFR Kinase Domain Reveals Structural Features Involved in Activation”, 4<sup>th</sup> Conference of the Hellenic Society for Computational Biology and Bioinformatics, December 18-20 **2009**, NHRF, Athens, Greece.
3. “Biomolecular Simulations and Structure-Based Inhibitor Design” Seminar at the Biomedical Research Foundation, April 1 **2009**, Academy of Athens.
2. “Insights into Angiotensin-I Converting Enzyme (ACE) – Angiotensin/ Bradykinin/LHRH Interaction through Docking Methods and Molecular Dynamics Simulations”, 5<sup>th</sup> Hellenic Forum on Bioactive Peptides, May 14-16 **2006**, University of Patras.
1. “The Detailed Structural Characterization of the Ga(III)-Bleomycin A2 Complex by NMR and Molecular Modelling”, Biophysics of the Genome and Its Interactions, 15-17 October **2001**, Hlohovez, Czech Republic.

**POSTER PRESENTATIONS**

- 5–7 Oct 2018** 19<sup>th</sup> International Conference of the Hellenic Crystallographic Association.  
Patras, Greece
- 11-13 July 2018** British Biophysical Society biennial meeting, Southampton, UK
- 19-24 August 2018** 28<sup>th</sup> International Conference on Magnetic Resonance in Biological Systems, Dublin, UK
- 28–31 May 2017** EMBO workshop, Salamanca, Spain
- September 2014** 20<sup>th</sup> EuroQSAR, St. Petersburg, Russia
- June 2012** 13<sup>th</sup> Tetrahedron Symposium, Amsterdam
- March 2010** 239<sup>th</sup> American Chemical Society National Meeting, San Francisco, USA
- September 2010** Training School and MC Meeting ANGIOKEM, COST, Rhodes Island, Greece.
- December 2009** 4<sup>th</sup> Conference of the Hellenic Society for Computational Biology and Bioinformatics, Athens
- August 2009** 3<sup>rd</sup> International Symposium on Advances in Synthetic and Medicinal Chemistry, Kiev, Ukraine
- June 2009** 10<sup>th</sup> Tetrahedron Symposium, Paris, France
- July 2008** 11<sup>th</sup> Belgian Organic Synthesis Symposium BOSS XI, Ghent, Belgium
- March 2008** 13<sup>th</sup> Hellenic Congress of Pharmaceutical Chemistry, Athens, Greece.
- February 2008** 1<sup>st</sup> International Conference on Drug Design & Discovery, Dubai, UAE.
- August 2007** 10<sup>th</sup> International Conference on Aminoacids and Proteins (ICAAP), Kallithea, Chalkidiki, Greece.
- November 2006** 58<sup>th</sup> Meeting of EEBMB, Patras, Greece.
- September 2006** 26<sup>th</sup> European Peptide Symposium, Gdansk, Poland
- March 2006** 7<sup>th</sup> Conference on Medicinal Chemistry: “Drug Discovery and Design”, Patras, Greece
- June 2005** 8<sup>th</sup> FIGIPAS Meeting in Inorganic Chemistry, University of Athens, Greece
- March 2005** 6<sup>th</sup> Conference on Medicinal Chemistry: “Drug Discovery and Design”, Patra, Greece
- March 2004** 1<sup>st</sup> International Meeting: Genome-Based Drug Discovery, Florence, Italy
- April 2003** 10<sup>th</sup> Chianti Meeting on NMR, Montecatini, Italy.
- October 2002** 6<sup>th</sup> European LSF Meeting, Montecatini, Italy.
- August 2002** 6<sup>th</sup> European Conference on Bioinorganic Chemistry, Lund, Sweden and Copenhagen, Denmark.

- July 2002** 11<sup>th</sup> International Conference on Biological Inorganic Chemistry, Heidelberg, Germany.
- October 2001** 5<sup>th</sup> European LSF Meeting, Frankfurt, Germany.
- October 2001** Conference on Biophysics of the Genome and Its Interactions, Hlohovec, Czech Republic.
- August 2001** 10<sup>th</sup> International Conference on Bioinorganic Chemistry, Florence, Italy.
- July 2000** 5<sup>th</sup> European Biological Inorganic Chemistry Conference, Toulouse, France.
- July 2000** 34<sup>th</sup> International Conference on Coordination Chemistry, Edinburgh, United Kingdom.

**JOURNAL REVIEWER:** Molecules, Pharmaceuticals, International Journal of Molecular Sciences, ACS Medicinal Chemistry Letters, Journal of Chemical Information & Modeling, Journal of Coordination Chemistry, Bioinorganic Chemistry & Applications, Bioorganic & Medicinal Chemistry, Bioorganic & Medicinal Chemistry Letters, European Journal of Medicinal Chemistry.

#### **MEMBERSHIP IN SCIENTIFIC SOCIETIES**

- 2014 – Present** Member, ESP, European Peptide Society
- 2012 – 2014** Member, ACS, American Chemical Society
- 2002 – Present** Member, Association of Greek Chemists