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
Telephone, mobile	+30 2106503526, +30 6936290344
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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, Andriamicin 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. Konstantinos 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 "Dynomis: 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 (10/1998) 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 Lectures at the MSc Program Molecular Pharmacology, Department of Chemistry, University of Patras and Institute of Biosciences & Applications

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

Jun 2020 – now Alexandros Athanasoulis, **PhD student**, Department of Chemistry, National and Kapodistrian University of Athens

Sep 2018–Nov 2021 Lykourgos Chiniadis **PhD student**, Department of Biotechnology, Agricultural University of Athens

Nov 2023 – Aug 2024 Batoul Khalil, **MSc student**, MSc student, Department of Informatics & Telecommunications, National & Kapodistrian University of Athens

Jun – Sep 2021 Luca Landini, **MSc student**, Erasmus+ from the University of Florence, Italy

Jun 2021 – now	Evangelos Tsoukas, **MSc student**, Department of Pharmacy, University of Patras
Aug – Sep 2023	Stella Anastasiou, **Undergraduate student**, Department of Biotechnology, Agricultural University of Athens
Nov 2021 – July 2022	Soultana Kechagia, **Undergraduate student**, Department of Biotechnology, Agricultural University of Athens
Mar – May 2022	Constantinos Constantinidis, **Undergraduate student**, Department of Biotechnology, Agricultural University of Athens
Mar – May 2021	Maria-Angeliki Sioundri, **Undergraduate student**, Department of Biotechnology, Agricultural University of Athens
July – Sep 2019	Agoritsa Kalabaliki, **Undergraduate student**, Department of Biotechnology, Agricultural University of Athens

MEMBERSHIP IN SCIENTIFIC SOCIETIES

2020 – Present	Board Member (Treasurer) of the Hellenic Crystallographic Association
2014 – Present	Member, ESP, European Peptide Society
2012 – 2014	Member, ACS, American Chemical Society
2002 – Present	Member, Association of Greek Chemists

SCIENTIFIC PROJECT EVALUATOR

2018 – Present European Union Horizon 2020 PATHFINDER program evaluator and Marie-Curie fellowships evaluator

2020 – Present Latvian Council of Science evaluator and rapporteur in Basic & Applied Research in Health projects

2019 – Present Hellenic Foundation for Research & Innovation evaluator and rapporteur in Basic Research programs and PhD fellowships

SCIENTIFIC 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.

PEER-REVIEWED PUBLICATIONS

Dr. Papakyriakou is the co-author in **87 peer-reviewed scientific research articles** in addition to **5 review articles** (Scopus Author ID: 7801330433), which have received **2,819 citations** and author's ***h*-index** is **31** (Google Scholar, Aug. 2024):

93. Rinotas, V., Liepouri, F., Ouzouni, M.-D., Chalkidi, N., Papaneophytou, C., Lampropoulou, M., Vidali, V.P., Kontopidis, G., Couladouros, E., Eliopoulos, E., **Papakyriakou, A.***, Douni, E.* Structure-Based Discovery of Receptor Activator of Nuclear Factor-κB Ligand (RANKL)-Induced Osteoclastogenesis Inhibitors (**2023**) International Journal of Molecular Sciences, 24 (14), art. no. 11290. doi: 10.3390/ijms241411290. **corresponding author*

92. Andreou, A., **Papakyriakou, A.**, Zervou, M.I., Goulielmos, G.N., Eliopoulos, E.E. Is the Association of the Rare rs35667974 IFIH1 Gene Polymorphism With Autoimmune Diseases a Case of RNA Epigenetics? (**2023**) Journal of Molecular Evolution, 91 (2), pp. 204-213. DOI: 10.1007/s00239-022-10090-0

91. Tricomi, J., Landini, L., Nieddu, V., Cavallaro, U., Baker, J.G., **Papakyriakou, A.***, Richichi, B.* Rational design, synthesis, and pharmacological evaluation of a cohort of novel beta-adrenergic receptors ligands enables an assessment of structure-activity relationships (**2023**) European Journal of Medicinal Chemistry, 246, art. no. 114961. DOI: 10.1016/j.ejmech.2022.114961. **corresponding authors*

90. Agnarelli, A., Lauer Betrán, A., **Papakyriakou, A.**, Vella, V., Samuels, M., Papanastasopoulos, P., Giamas, C., Mancini, E.J., Stebbing, J., Spencer, J., Cilibrasi, C., Ditsiou, A., Giamas, G. The Inhibitory Properties of a Novel, Selective LMTK3 Kinase Inhibitor (**2023**) International Journal of Molecular Sciences, 24 (1), art. no. 865. DOI: 10.3390/ijms24010865

89. Georgiadis, D., Skoulikas, N., **Papakyriakou, A.**, Stratikos, E. Phosphinic Peptides as Tool Compounds for the Study of Pharmacologically Relevant Zn-Metalloproteases (**2022**) ACS Pharmacology and Translational Science, 5 (12), pp. 1228-1253. DOI: 10.1021/acsptsci.2c00183

88. da Silva, R.L., **Papakyriakou, A.**, Carmona, A.K., Spyroulias, G.A., Sturrock, E.D., Bersanetti, P.A., Nakaie, C.R. Peptide inhibitors of angiotensin-I converting enzyme based on angiotensin (1–7) with selectivity for the C-terminal domain (**2022**) Bioorganic Chemistry, 129, art. no. 106204. DOI: 10.1016/j.bioorg.2022.106204

87. Kintos, D.-P., Salagiannis, K., Vazoura, V., Wittrien, T., **Papakyriakou, A.**, Nikolaropoulos, S.S., Behrends, S., Topouzis, S., Fousteris, M.A. Design, synthesis and biological evaluation of new 3,4-dihydroquinoxalin-2(1H)-one derivatives as soluble guanylyl cyclase (sGC) activators (**2022**) Heliyon, 8 (11), art. no. e11438. DOI: 10.1016/j.heliyon.2022.e11438

86. Giarimoglou, N., Kouvela, A., Maniatis, A., **Papakyriakou, A.**, Zhang, J., Stamatopoulou, V., Stathopoulos, C. A Riboswitch-Driven Era of New Antibacterials (**2022**) Antibiotics, 11 (9), art. no. 1243. DOI: 10.3390/antibiotics11091243

85. Grigalavicius, M., Ezzatpanah, S., **Papakyriakou, A.**, Raabe, T.T.H., Yannakopoulou, K., Theodossiou, T.A. 5-ALA Is a Potent Lactate Dehydrogenase Inhibitor but Not a Substrate:

Implications for Cell Glycolysis and New Avenues in 5-ALA-Mediated Anticancer Action (**2022**) Cancers, 14 (16), art. no. 4003. doi: 10.3390/cancers14164003

84. Vourloumis, D., Mavridis, I., Athanasoulis, A., Temponeras, I., Koumantou, D., Giastas, P., Mpakali, A., Magrioti, V., Leib, J., Van Endert, P., Stratikos, E.*, **Papakyriakou, A.*** Discovery of Selective Nanomolar Inhibitors for Insulin-Regulated Aminopeptidase Based on α-Hydroxy-β-amino Acid Derivatives of Bestatin (**2022**) Journal of Medicinal Chemistry, 65 (14), pp. 10098-10117. doi: 10.1021/acs.jmedchem.2c00904. **corresponding authors*

83. Giastas, P., **Papakyriakou, A.**, Tsafaras, G., Tzartos, S.J., Zouridakis, M. Structural Insights into the Role of β3 nAChR Subunit in the Activation of Nicotinic Receptors (**2022**) Molecules, 27 (14), art. no. 4642. doi: 10.3390/molecules27144642

82. **Papakyriakou A***, Mpakali A, Stratikos E.* Can ERAP1 and ERAP2 Form Functional Heterodimers? A Structural Dynamics Investigation (**2022**) *Frontiers in Immunology* 13, 863529. doi: 10.3389/fimmu.2022.863529. **corresponding authors*

81. Nikolaidis M, **Papakyriakou A**, Chlichlia K, Marcoulatos P, Oliver SG, Amoutzias GD. Comparative Analysis of SARS-CoV-2 Variants of Concern, Including Omicron, Highlights Their Common and Distinctive Amino Acid Substitution Patterns, Especially at the Spike ORF (**2022**) *Viruses* 14(4), 707. doi: 10.3390/v14040707

80. Chiniadis L, Giastas P, Bratsos I, **Papakyriakou A.*** Insights into the Protein Ruthenation Mechanism by Antimetastatic Metallodrugs: High-Resolution X-ray Structures of the Adduct Formed between Hen Egg-White Lysozyme and NAMI-A at Various Time Points. (**2021**) *Inorganic Chemistry* 60(14), 10729-10737. doi: 10.1021/acs.inorgchem.1c01441. **corresponding author*

79. Mavridis G, Mpakali A, Zoidakis J, Makridakis M, Vlahou A, Kaloumenou E, Ziotopoulou A, Georgiadis D, **Papakyriakou A,** Stratikos E. The ERAP1 active site cannot productively access the N-terminus of antigenic peptide precursors stably bound onto MHC class I. (**2021**) *Scientific Reports* 11(1), 16475. doi: 10.1038/s41598-021-95786-x.

78. Temponeras I, Chiniadis L, **Papakyriakou A,*** Stratikos E.* Discovery of Selective Inhibitor Leads by Targeting an Allosteric Site in Insulin-Regulated Aminopeptidase. (**2021**) *Pharmaceuticals* 14(6), 584. doi: 10.3390/ph14060584. **corresponding authors*

77. Kalampalidis A, Peppas A, Schnakenburg G, **Papakyriakou A**, Tsoupras A, Zabetakis I, Philippopoulos A.I. Antithrombotic and antiplatelet activity of an organometallic rhodium(I) complex incorporating a substituted thieno-[2,3-d]-pyrimidine ligand: Synthesis, structural characterization, and molecular docking calculations. (2021) *Applied Organometallic Chemistry* 35(6), e6210. doi: 10.1002/aoc.6210

76. Lepore A, Choy PM, Lee NCW, Carella MA, Favicchio R, Briones-Orta MA, Glaser SS, Alpini G, D'Santos C, Tooze RM, Lorger M, Syn WK, **Papakyriakou A,** Giamas G, Bubici C, Papa S. Phosphorylation and Stabilization of PIN1 by JNK Promote Intrahepatic Cholangiocarcinoma Growth. (**2021**) *Hepatology* First published: 28 May. doi: 10.1002/hep.31983

75. Cilibrasi C, Ditsiou A, **Papakyriakou A**, Mavridis G, Eravci M, Stebbing J, Gagliano T, Giamas G. LMTK3 inhibition affects microtubule stability. (**2021**) *Molecular Cancer* 20(1), 53. doi: 10.1186/s12943-021-01345-3.

74. Ditsiou A, Cilibrasi C, Simigdala N, **Papakyriakou A,** Milton-Harris L, Vella V, Nettleship JE, Lo JH, Soni S, Smbatyan G, Ntavelou P, Gagliano T, Iachini MC, Khurshid S, Simon T, Zhou L, Hassell-Hart S, Carter P, Pearl LH, Owen RL, Owens RJ, Roe SM, Chayen NE, Lenz HJ, Spencer J, Prodromou C, Klinakis A, Stebbing J, Giamas G. The structure-function relationship of oncogenic LMTK3. (**2020**) *Science Advances* 6(46), eabc3099. doi: 10.1126/sciadv.abc3099

73. Rinotas V, **Papakyriakou A,** Violitzi F, Papaneophytou C, Ouzouni MD, Alexiou P, Strongilos A, Couladouros E, Kontopidis G, Eliopoulos E, Douni E. Discovery of Small-Molecule Inhibitors of Receptor Activator of Nuclear Factor-κB Ligand with a Superior Therapeutic Index. (**2020**) *J Med Chem.* 63(20), 12043-12059. doi: 10.1021/acs.jmedchem.0c01316

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. doi: 10.1007/s00775-020-01786-z **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. doi: 10.1021/acsmedchemlett.9b00665

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. doi: 10.1074/jbc.RA120.012976

69. Giastas P, Mpakali A, **Papakyriakou A,** Lelis A, Kokkala P, Neu M, Rowland P, Liddle J, Georgiadis D, Stratikos E. 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 authors*

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**) J*ournal 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, Kasheverov IE, Tsetlin V, Tzartos S, Giastas P. Crystal Structure of the Monomeric Extracellular Domain of α9 Nicotinic Receptor Subunit in Complex With α-Conotoxin RgIA: Molecular Dynamics Insights Into RgIA Binding to α9α10 Nicotinic Receptors (**2019**) *Frontiers in Pharmacology* 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-α 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 β-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 Pseudotripeptide 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*

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19. "The drug development roadmap: from bench to clinic", EMBL–IBA seminar, **2021**, September 12, Athens, Greece

18. "Computational study of protein dynamics and free energy calculations in drug design", **2021**, May 20, ELIXIR-GR, University of Patras, Greece.

17. "Structure-based discovery of bioactive molecules and computational studies of protein dynamics", **2020**, July 13–17, 53rd Demokritos Summer School, Athens, Greece.

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13. "An Introduction to Computer-aided drug discovery", CHARME Training School, COST ACTION, **2019,** March 14, 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**, July 3–4, Cardiff, UK.

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8. "Docking Calculations Using AutoDock 4 With AutoDockTools", 2nd Workshop: NMR Basics and Applications in Life Sciences, University of Patras, 13–15 May **2013**

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