

## CURRICULUM VITAE

**Name :** **Georgios A. SPYROULIAS**

**Date of Birth :** 16 October 1965, Thessaloniki

**Marital Status :** Married (1 child)

**Nationality :** Greek

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### Academic Background :

- September 1989 **B.Sc. In Chemistry**, Aristotle University of Thessaloniki, **Thessaloniki, Greece.**
- February 1992 **M.Sc. In Chemistry, (Supervisor Prof. Athanassios Coutsolelos)** « *Bioinorganic Chemistry of Coordination Compounds* », Department of Chemistry, University of Crete, **Greece.**
- June 1995 **Ph.D. In Chemistry, (Supervisor Prof. Athanassios Coutsolelos)**, Department of Chemistry, University of Crete, **Heraklion, Greece.**

### Current Professional Status :

- September 2014 **Professor** University of Patras, Department of Pharmacy, **Patras, GREECE.**  
*Design/Simulation of bioactive molecules with pharmacological interest.*
- November 2015 **Head of the Pharmacy Department,** University of Patras (2015-2017 & 2017-2020)

### Professional Appointments :

- July-August 1987 «**EKO**» **Chemicals, Co.** Department of Chemical Processes, **Thessaloniki, GREECE.**
- June 1995 **Short-term Post-Doctoral Research (in Prof. I. Bertini's lab,** Università degli Studi di Firenze, **Firenze, ITALY)**
- July 1995 **Short-term Post-Doctoral Research (in Prof. R. Poilblanc's lab,** Laboratoire de Chimie de Coordination, C.N.R.S, **Toulouse, FRANCE.)**
- October 1995 **Post-Doctoral Fellow (in Dr. D. Mansuy's lab,** René Descartes, Paris V, Laboratoire De Chimie et Biochimie, C.N.R.S. URA 400, **Paris, FRANCE.)**
- January 1997 **Post-Doctoral Fellow (in Prof. I. Bertini's lab,** Università degli Studi di Firenze, Laboratorio di Chimica Inorganica e Bioinorganica, **Firenze, ITALY)**
- May 2000 **Post-Doctoral Fellow (in Prof P. Kordopatis' lab,** University of Patras, Department of Pharmacy, **Patras, GREECE).**
- Nov 2001 **Post-Doctoral Researcher, 2001-2003,** Department of Pharmacy, U of Patras, **GREECE.**
- May 2001 **Research Associate,** University of Patras, Department of Pharmacy, **Patras, GREECE.**
- August 2003 **Assistant Professor** University of Patras, Department of Pharmacy, **Patras, GREECE.**
- December 2009 **Associate Professor** University of Patras, Department of Pharmacy, **Patras, GREECE.**

### Current Research Activities and Interests:

- ⊙ **Design/Simulation and Engineering of Bioactive Molecules**, such as bioactive peptides and modified proteins.
- ⊙ **Structural Bioinformatics**, such as homology modeling, docking and molecular dynamics, *in silico* design and development of combinatorial libraries of compounds and virtual screening process towards the quest of lead-molecules with biological activity towards protein/enzyme targets, etc.
- ⊙ **Protein preparation for NMR structural studies**: polypeptide overexpression/purification and uniform or selective labeling (<sup>15</sup>N, <sup>13</sup>C, <sup>2</sup>H, residue specific labeling, segmental labeling, etc.).
- ⊙ **Structure-Activity Relationship by NMR and Solution Conformational Analysis & 3D Structure determination of Biomolecules**, such as metalloproteins/metalloenzymes (implicated in electron transfer, proteolysis, ubiquitination pathway and NO signaling, viral protein domains implicated in viral replication or suppression of human Innate Immune Response, RNA and nucleotide binding proteins, Protein-protein/RNA/small molecule interaction and complexes, (poly)peptides, etc. (<https://research.upatras.gr/idrymatikes-ypodomes/>)
- ⊙ **Biophysical Characterization of protein and their complexes** through a number of techniques, such as: (a) UV-visible (**UV-vis**)& Circular Dichroism (**CD**) Spectroscopy for structure and thermal stability analysis, (b) Size Exclusion Chromatography coupled with Multiple Angle Laser Light Scattering (**SEC-MALLS**) to determine protein concentration, shape and oligomerization state, (c) Isothermal Titration Calorimetry (**ITC**) to determine the physicochemical properties and binding kinetics of the association of protein with other molecules.
- ⊙ **NMR metabolomics**: analysis of biological fluids (urine, blood serum & plasma, tissues/cell extracts, etc.) for the identification of biomarkers, metabolic fingerprint and disorders.

### Fellowships & Awards:

- « **EMY** » Fellowship for PhD research, Ministry of Education (U of Crete, **GREECE**; 11/1989-10/1994).
- « **ERASMUS** » Grant (Contract N° : ICP-92-G-2002/13. University Paul Sabatier, CNRS, **Toulouse, FRANCE** ; 11/1992-4/1993).
- « **DIGITAL CORPORATION AWARD** » for Achievements in PhD Research (U of Crete, **GREECE**; 1993).
- « **CLAUDE BERNARD Fondation** » Grant (U René Descartes, **Paris, FRANCE** ; 11/1996-12/1996).
- « **Platon** » **Bilateral Cooperation Scientifique Franco-Hellenique**, REF. PAI/GRC 9508. **1994-1995**, University of Crete, Department of Chemistry, **GREECE** & Laboratoire de Chimie de Coordination, C.N.R.S, Toulouse, **FRANCE**.

### Participation in Research Programs During Post-Doctoral Research Activities:

1. **Human Capital & Mobility**, Université René Descartes, Paris V, Laboratoire De Chimie et Biochimie, C.N.R.S. URA 400, Paris, **FRANCE** :
  - Contract N° : ERBCHRXCT 9460492, “*Transition Metals In Supramolecular Catalysis*”, **1995-1996**.
2. **Training & Mobility of Researchers**, Università degli Studi di Firenze, Laboratorio di Chimica Inorganica e Bioinorganica, Florence, **ITALY**:
  - Contract N° : CHRX-CT 940540, “*Structure –Function Relationships in Haemoproteins*”, **1997**.
  - Contract N° : FMGE-CT98-0107, “*Development of NMR Instrumentation and Software to Achieve Excitation and Detection of Large Bandwidths and Dipolar Couplings in High Resolution Spectra at High-Field*”, **2000**.

### Approved Proposal for Access/Use of Large Scale Facilities/Infrastructures :

1. **FLORMARPARM Large Scale Facility** - Contract N° : ERBCHGECT 940060. **1995**, Università degli Studi di Firenze, Laboratorio di Chimica Inorganica e Bioinorganica, Florence, **ITALY**.
2. **NMRPARABIO Large Scale Facility** - Contract N° : ERBFMGECT 950033. **1997**, Università degli Studi di Firenze, Laboratorio di Chimica Inorganica e Bioinorganica, Florence, **ITALY**.
3. **NMRPARABIO Large Scale Facility** - Contract N° : HPRI-CT-1999-00009. **2000-2003**, Center of Magnetic Resonance (CERM), Florence, **ITALY**.
4. **EU-NMR Large Scale Infrastructure** - Contract N° : RII3-026145. **2006-2010**, Center of Magnetic Resonance (CERM), Florence, **ITALY** & RALF-NMR Large-Scale Facility, Lyon, **FRANCE**.

### Competitive Research Grants Awarded :

1. **Marie Curie Research Training Grant (European Union)** - Contract N° : ERBFMBICT 972477. "NMR Spectroscopy to study the factors controlling the folding/unfolding process in Paramagnetic Metalloproteins", **1997-1999**, Department of Chemistry, University of Florence, **ITALY**. Grant Holder
2. **Marie Curie Research Grant (European Union)** - Contract N° : HPMF-CT-1999-00344. "NMR Structural Studies of Chemically Modified c-Cytochromes as a probe of Protein Folding Pathways", **2000-2001**, Department of Pharmacy, University of Patras, **GREECE**. Grant Holder
3. **"C. Carathéodory" Research Grant** – Program No 2790, 'Structure-Function Relationship of the blood pressure regulating factors through NMR conformational studies of molecular complexes of Angiotensin Converting Enzyme catalytic sites with vasoactive peptides', **2001-2003**, University of Patras, **GREECE**. Principal Investigator.
4. **EMBO Short-term Research Grant**, Center of Magnetic Resonance, Florence, **ITALY**. Principal Investigator.  
- Contract N° : ASTF 53-2003, "NMR Structure Elucidation of Angiotensin-I Converting Enzyme (ACE) Catalytic Sites and Their Complexes With Angiotensin-I", **2003**.  
- Contract N° : ASTF 99-2004, "Mapping the Contact Interface of HIV gp120 V3 and CD4+ T-Cell CCR5 N-terminal Peptides through NMR Spectroscopy : Implications for HIV Inhibitors Design", **2004**.
5. **IKYDA Bilateral Cooperation Greece-Germany**, "Interaction between Calmodulin and a Calmodulin Binding Peptide of SK2 Potassium Channels by NMR", **2003-2005**, University of Patras, **GREECE** & University of Freiburg, **GERMANY**. Principal Investigator.
6. **"PYTHAGORAS" Research Program** (Ministry of Education, GREECE) "Structural Study of recombinant extracellular domains of Acetylcholine Receptor" **2004-2005**, University of Patras. Co-Investigator.
7. **EQUAL/εΠΙΜΕΝΩ Program** (Ministry of Occupation, GREECE) «Enhancement of the capabilities of individuals suffering from Neuromascular diseases through an e-learning program» **2005-2007**, University of Patras, Co-Investigator.
8. **"PENED 2003" Research Program** (GSRT, Ministry of Development, GREECE) 'Study of Structure-Function Relationship of the growth factor Pleiotropin for the identification of protein fragments with anticancer activity' **2005-2008**, University of Patras. Co-Investigator.
9. **Spanish Ministry of Education and Science Research Grant** - CTQ2005-00360/BQU, "Caracterizacion Mediante Resonancia Magnetica Nuclear del Extremo C-terminal del Receptor Vaniloide Y de Proteinas Helice-Lazo-Helice Implicadas en el Crecimiento del Sistema Neuronal", **2006-2008**, University of Patras, **GREECE** & Universidad Miguel Hernández, Alicante, **SPAIN**. Collaborating Researcher.
10. **"INNO-FARM – Joint Research & Technological development Programm of West Greece"** (GSRT, Ministry of Development, GREECE) 'Design, Evolution and Therapeutic Development of New Biomolecules' University of Patras (Total budget: 500 K€; Team budget 70 K€), **2006-2008**. Co-Investigator.
11. **"Greek-Spanish Joint R+T Collaboration Program – ΕΠΑν Μ.4.3.6.1.ε"** (GSRT, Ministry of Development, GREECE) 'Determination of the Key Residues Implicated in the Stability of the Blue Copper Protein Rusticyanin and in the Electron Transfer' - University of Patras (Total budget: 11 K€), **2005-2007**. Principal Investigator.
12. **"FP6-2005-LIFESHEALTH. Life Sciences, genomics & biotechnology for health" (European Union)** "Applied Venomics of the Cone Snail Species Conus Consors for the Accelerated, Cheaper, Safer and More Ethical Production of Innovative Biomedical Drugs (CONCO)". ContractN° 037592, [www.conco.eu](http://www.conco.eu), **2005-2010**. University of Patras, Partner #9, Co-Investigator
13. **"C. Carathéodory" Research Grant**, 'NMR Structural Study of HDM2 & HDMX Ring Finger Domains, regulators of tumor-suppressor protein p53' Program C.181, **2007-2010**, University of Patras (Total budget: 28 K€). Principal Investigator.
14. **"FP7-HEALTH-2007-2.1.1-5. Structure-function analysis of membrane-transporters and channels for the identification of potential drug target sites." (European Union)** 'NEUROCYPRES: Neurotransmitter Cys-loop receptors: structure, function and disease (I)', CP-Collaborative Project, Contract N° HEALTH-F4-2008-202088, [www.neurocypres.eu](http://www.neurocypres.eu), **2008-2012**. University of Patras (Total budget: 589 K€), Partner #15, Principal Investigator

15. **“FP7-INFRA-2008-1.1.1. Capacities – Research Infrastructures” (European Union)**, *“EAST-NMR: Enhancing Access and Services To East European users towards an efficient and coordinated pan-European pool of NMR capacities to enable global collaborative research and boost technological advancements”*, Integrated Activities, Contract N° CP-CSA-Infra-228461, [www.east-nmr.eu](http://www.east-nmr.eu), **2009-2013**. University of Patras (Total budget: 91 K€), Partner #12, Principal Investigator
16. **Internal Networks of University of Patras**, Collaborating Researcher in three networks
- Program No C.766, *“METSNET: A network for the study of the molecular mechanisms implicated in various factors of Metabolic Syndrome”*, **2009-2012**.
  - Program No C.787, *“Network for the development and biological Evaluation of potent anti-inflammatory and anti-microbial pharmaceutical products”*, [www.multipotentdrugs.upatras.gr](http://www.multipotentdrugs.upatras.gr), **2009-2012**.
  - Program No C.851, *“PHARMANET: Network of Structural and Functional Studies of Molecules with Pharmaceutical value”*, [www.pharmanet.upatras.gr](http://www.pharmanet.upatras.gr), **2009-2012**.
17. **“Greek-Turkish (GSRT-TUBITAK) Joint R+T Collaboration Program”** (GSRT, Ministry of Development, GREECE), *“Structure-Function Relationship of a new RING finger E3 ubiquitin ligase, a dominant regulator of TGF- $\beta$  signaling pathway and TGF- $\beta$ -dependent tumor suppression”* **2010-2012**, University of Patras (Total budget: 15 K€). Principal Investigator.
18. **«HERACLITUS II: Reinforcing the Human Research Potential through Graduate Research »** (Greek Ministry of Education, GREECE), *“Expression, Characterization and Structural Investigation through Nuclear Magnetic Resonance (NMR) of the Bacillus anthracis Anthrax Lethal Factor Zn-protease Catalytic Site”*, **2011-2014**. University of Patras (Total budget: 45 K€), Principal Investigator.
19. **“GSRT- THALIS: Reinforcing the Human Research Potential through Graduate Research”** (GSRT, Greek Ministry of Education, GREECE), *“Hydrogen sulfide, a new endogenous regulator of angiogenesis: signaling, physiology/pathophysiology and development of pharmacological inhibitors”*, **2011-2015**. (Coordinator: Lab. of Mol. Pharmacology, Dept. of Pharmacy), Co-Investigator.
20. **“FP7-REGPOT-2011-1. Capacities – Research Potential” (European Union)**, *“SEE-DRUG: Establishment of Centre of Excellence for Structure-Based Drug Target Characterization: Strengthening the Research Capacity of South-Eastern Europe”*, Coordination & Support Actions, Contract N° CT-2011-285950, [www.seedrug.upatras.gr](http://www.seedrug.upatras.gr), **2012-2015**. University of Patras (Total budget: 3.2 M€), Coordinator.
21. **“K. Caratheodory 2013” Research Program for Post-Doctoral Research**, Program No 2013-6661, *«Urine Metabolite analysis through high-resolution homo-/hetero-nuclear NMR-based metabolomics»*, **2014-2016**. University of Patras, Budget 51,5 K€ Principal Investigator.
22. **“GSRT - ARISTEIA II”**, Program No 4659, *«Biophysics-DRUGS: Diffraction and NMR experimental platform for drug screening»*, **2014-2015**. University of Patras (PI Dr. Irene Margiolaki), Team Budget ~45 K€, Co-Investigator.
23. **National Greek Roadmap of Research Infrastructure – GSRT**, Greek Ministry of Education
- **Research Infrastructure “INSPIRED” MIS 5002550** – Coordinator of “UPAT-RISF” core facility of INSIPRED RI (Budget 1,57 M€)
  - **Research Infrastructure “OMIC-ENGINE” MIS 5002636** – PI of UPAT Team & Research Coordinator (Budget 600 K€)
24. **H2020-BG-2014-2**, BG-03-2014 - Novel marine derived biomolecules and industrial biomaterials (**European Union**), *“MARISURF: Novel, Sustainable marine Bio-surfactant / Bio-emulsifiers for commercial exploitation”*, Contract No 635340, <http://www.marisurf.eu/project-partners/university-of-patras/>, **2015-2020**. University of Patras (Total budget: 571 K€), Partner #11. Principal Investigator
25. **H2020-INFRAIA-2014-2015** - Integrating and opening existing national and regional research infrastructures of European interest (**European Union**), *“iNEXT: Infrastructure for NMR, EM and X-ray crystallography for translational research”*, Contract No 653706, <http://www.inext-eu.org/department/22-upat/>, **2015-2020**. University of Patras (Total budget: 31.5 K€), Partner #22. Principal Investigator.
26. **COST Action – CA15133 – FesBioNET, 2014-2015 - (European Union)**, *“The Biogenesis of Iron-sulfur Proteins: from Cellular Biology to Molecular Aspects”*, Contract No 653706, **2015-2020**. University of Patras (<http://www.fesbionet.eu/index.php>). UPAT Team Leader & Vice-Chair of the action.

27. **EDMB34 - «Supporting Research teams with emphasis in the support of Young Investigators », ESPA 2014-2020:** *“The role of the catalytic domain of the E3 Ubiquitin Ligase Arkadia in enzyme’s function regulation and in diagnosis”*, 2018-2019, University of Patras, (Total Budget: 56.5 K€), Principal Investigator.
28. **HFRI (ELIDEK) Program «Supporting Post-Doctoral Researchers», «ECHNO: Enlightening the Conformational Changes of HNOX domain of soluble guanylate cyclase (sGC) by discrimination of diatomic gases», 2018-2021,** (Grant Holder: Dr. Aikaterini Zompra, Total Budget: 180 K€), PI of the Coordinating Organization.
29. **H2020-MSCA-IF-2017 - MARIE SKŁODOWSKA-CURIE ACTIONS (European Union), “NMRSIGN: NMR insights on the soluble Guanylyl Cyclase conformational dynamics to illuminate the SIGNALING pathway”** Contract No 795175, 2018-2020, (Grant Holder: Dr. George Dalkas, Total Budget: 165 K€), PI of the Coordinating Organization.
30. **Region of Western Greece – “Supporting the Greek National Research Infrastructures of Western Greece”, Total Budget 1.78 M€, Coordinator Prof. G. Angelopoulos, Dept of Chemical Engineering; Scientific Responsible for the Dept of Pharmacy: Prof. G.A. Spyroulias, Budget 550 K€.**
31. **RESEARCH–CREATE-INNOVATE, MIS 5067545 (GSRT), “POLYPEPPHARM: Improved generic polypeptide drugs with innovative pharmaceutical forms - Τ2ΕΔΚ-00996”, 2020-2023,** (Total Budget: 130 K€), Co-Investigator.

**Supervisor on Independent Competitive Research Grants (fellowships, training grants) Awarded to group members :**

1. **HFRI - Hellenic Foundation for Research and Innovation, PhD Fellowship** Awarded to
  - **Aikaterini Tsika** (BSc. Pharmacy, MSc, PhD Candidate), *“Structural framework study of the function of protein domains belonging to alphaviruses’ replication complex via NMR spectroscopy”*, (no 2430) **2017-2019**.
  - **Styliani Chasapi** (BSc. Chemistry, MSc, PhD Candidate), *“Analysis and study of biomolecules and biomarkers in biofluids through NMR Spectroscopy”* (no. 1019) **2019-2021**
  - **Maria Politi** (BSc. Biology, MSc, PhD Candidate), *“Expression, isolation and physicochemical characterization and Structure-Activity study of recombinant polypeptides of the transcription complex of Hepatitis 1 virus (HEV1)”*, (no. 663) **2019-2022**.
2. **IKY PhD-Research Scholarships “MIS 5000432”,** awarded to:
  - **Garyfallia Makrynitsa** *“Conformational study and dynamics of HNOX proteins and their complexes with signaling molecules”* **2018-2021**.
3. **“IKY Post-Doctoral Research Grants, 2019”,** awarded to:
  - **Dr. Aikaterini Argyriou** *“Study of the structural and physicochemical determinants for the recognition and binding Hepatitis C RNA molecules by La protein, through NMR Spectroscopy”*, (no. 18646) **2020-2022**.
  - **Dr. Maria Birkou** *“Study of the mechanism of action of Arkadia RING Domain E3 Ubiquitin Ligase in ubiquitination pathway”* (no 16984) **2020-2022**.
  - **Dr. Minos-Timotheos Matsoukas** *“Allosteric targeting, structural studies and molecular basis of activation of the type 1 corticotropin-releasing factor receptor (CRF1R)”*, (no 17071) **2020-2022**.

**Facilities & Institutional Infrastructures:**

- **Protein Production:** (a) a Cold room equipped with AKTA START GO FPLC system, (b) INFORS Bioreactor (bacteria and yeast), 3x Refrigerated Incubation Shakers & autoclave (c) 3x UV-Visible Spectrometers (Jasco V-630iRM Quawell Q5000 // Q9000), (d) AKTApurifier 10, AKTA PURE M25 & AKTA START FPLC systems, (e) Millipore Direct Q3-UV, (f) 2xPCR, (g) 5 refrigerated centrifuges/supercentrifuge (10-45.000rpm) & 7 rotors, (h) Electrophoresis systems, Analytical Balances, incubators, powerful sonicator system, water baths, -86°C and -20°C refrigerators, peristaltic pumps etc.
- **Imaging facility:** imager with visible light (RGB) and far red/near infrared (FR/NIR) fluorescence and chemiluminescence detection and all general gel documentation applications for stain-free imaging.
- **Structural Biology & Biophysics :** (i) High-field & high-definition **Bruker 700MHz NMR**, equipped with a cryogenically cooled probe for enhanced sensitivity and 4-channels (<sup>1</sup>H/<sup>2</sup>H/<sup>13</sup>C/<sup>15</sup>N), (ii) **Circular Dichroism qChirascan** Spectrometer (iii) **SEC-MALS:** Size Exclusion Chromatography coupled with Multiple Angle Light Scattering system, (iv) **micro-ITC:** Micro Isothermal Titration Calorimetry.

<https://research.upatras.gr/idrymatikes-ypodomes/>

### **Teaching Experience & Educational Activities in post-Graduate Programs :**

- November 1989 - February 1994: **Department of Chemistry – University of Crete**
  - General Chemistry - Course & Lab training
  - Organic Chemistry - Laboratory training
  - Inorganic Chemistry - Course & Lab training
- June 2000 - July 2004: **Greek Open University**
  - Principles of General & Inorganic Chemistry - Course
- August 2003 - **Department of Pharmacy – University of Patras**
  - 2003 - General & Analytical Chemistry - Laboratory Training
  - 2003 -2006 Isolation/Purification of Natural Products - Laboratory Training
  - 2003 - Instrumental Analysis (NMR Spectroscopy) - Course
  - 2003 - Biochemistry - Course
  - 2006 - Informatics - Course
  - 2008 - Bioinorganic Chemistry – Molecular Simulations - Course & Lab Training
  - 2003 -2012 Chemistry of Aminoacids, Peptides and Proteins – **Graduate** Course
  - 2003 Drug Design – **Graduate** Course
  - 2003 -2018 Conformational Analysis of Biomacromolecules – **Graduate** Course
  - 2003 -2012 Protein Biochemistry – **Graduate** Course
  - 2012 - Biomolecular NMR – **Graduate** Course

Teaching activities to various Inter-departmental or Inter-University Graduate Studies Programs since 2003.

### **Training activities in Graduate Research Programs & Supervision of Experienced Researchers (since 2003)**

Supervised 6 Post-Docs, 4 PhDs, 20 Masters and 45 Degree Thesis.

Advisory Committee in 15 Masters, 9 Ph.D. and Examination Committee in 21 Ph.D.

**Currently:** Supervision of 5 Doctoral, 7 Masters and 15 Diploma Theses. Member in Advisory Committee of 2 PhD Thesis

### **Professional Memberships:**

- Greek Chemists Association,
- Marie-Curie Fellowship Association (Hellenic MCFA, Vice-Chair, 2006- 2008),
- European Peptide Society (Greek Effective Member in EPS, 2014- ),
- Ampere Committee Member (2016- )
- Hellenic Society for Biochemistry & Molecular Biology
- Hellenic Society for Computational Biology and Bioinformatics
- Hellenic Crystallographic Association

### **Languages:**

Greek (Native), English, French, Italian.

### Oral Presentations & Seminars :

- (1) **05/09/1991** - «*Synthesis and Physicochemical Characterization of porphyrinic dimers with light Lanthanide ions*». **13<sup>th</sup> Greek Chemistry Conference**, Athens, GREECE.
- (2) **10/07/1995** - «*Synthesis and Spectroscopy of Lanthanide Mono- and Bis- Porphyrinates*». **Invited by Prof. René Poilblanc**. Laboratoire de Chimie de Coordination, C.N.R.S, Toulouse, FRANCE.
- (3) **23/04/1996** - «*Lanthanide Sandwich-like Porphyrin Complexes with Strong  $\pi$ - $\pi$  Interactions. Synthesis, Structure and Properties*». **Invited by Prof. Jean-Claude Marchon**. Laboratoire de Chimie de Coordination. CNRS N°1194, CEA/Grenoble-DRFMC/SCIB, 17, Grenoble, France.
- (4) **12/11/1999** - «*Solution Structure of Horse Heart Cytochrome c. Monitoring the Redox State-dependent Structural changes*». Department of Chemistry, University of Crete, GREECE.
- (5) **23/12/1999** - «*3-D Solution Structure of Fe(III) and Fe(II) Cytochrome c through NMR Spectroscopy*». Department of Chemistry, National Kapodistrian University. Athens, GREECE.
- (6) **02/03/2001** - «*Conformational Analysis of Biomolecules in Solution: NMR - 3D Structures - Biological Implications*» **2<sup>nd</sup> Conference in Medicinal Chemistry**, Patras, GREECE.
- (7) **16/05/2001** – «*3D Solution Structure Of CRH Synthetic Analogues through NMR Spectroscopy*» **4<sup>th</sup> Chemistry Congress**, University of Ioannina, May 16<sup>th</sup> **2001**, Ioannina, GREECE.
- (8) **05/12/2001** - «*Experimental Studies of Biomolecular Systems*» Department of Material Science, University of Patras, December 5<sup>th</sup> **2001**, Patras, GREECE.
- (9) **8/03/2002** - «*Folding and Redox-State Dependent Structural Changes of Electron Transfer Haem Proteins*» **3<sup>rd</sup> Conference in Medicinal Chemistry: Drug Design & Development**, Patras, GREECE.
- (10) **12/04/2002** - «*Conformational Analysis of Synthetic Peptides as Models of Angiotensin Converting Enzyme Active Sites*» **3<sup>rd</sup> Hellenic Forum on Bioactive Peptides.**, Patras, GREECE.
- (11) **08/11/2002** - «*Structural Features Analysis of Angiotensin-I Converting Enzyme Catalytic Sites*» **19<sup>th</sup> Hellenic Chemistry Conference**, Heraklion Crete, GREECE.
- (12) **14/03/2003** - «*NMR Models of Angiotensin-I Converting Enzyme Catalytic Sites*» **4<sup>th</sup> Conference in Medicinal Chemistry : Drug Design & Development**. Patras, GREECE.
- (13) **11/02/2003** - «*Design/Simulation of Bioactive Compounds of Pharmaceutical Interest*» Department of Pharmacy, University of Patras, Patras, GREECE.
- (14) **12/06/2003** - «*NMR Models of the Angiotensin-I Converting Enzyme Zn(II) Catalytic Sites : The basis for a structural study on the enzyme-substrate interaction*» **7<sup>th</sup> FIGIPS (Invited Lecture)**, Lisbon, PORTUGAL.
- (15) **11/03/2004** - «*Monitoring the interaction between the HIV-1 gp120 V3-loop and the N-terminal CCR5 peptide constructs through NMR Spectroscopy*» **5<sup>th</sup> Conference in Medicinal Chemistry**, Patras, GREECE.
- (16) **10/05/2004** - «*Solid-phase synthesis and Conformational Properties of peptide models that represents the active sites of Angiotensin-I Converting Enzyme*» **9<sup>th</sup> Naples Workshop – Peptides as therapeutics diagnostics & vaccines**, Anacapri, ITALY.
- (17) **10/03/2005** - «*Molecular Modeling & NMR conformational Analysis applied in the study of Zn(II) binding sites of Biomolecules*» **6<sup>th</sup> Conference in Medicinal Chemistry**, Patras, GREECE.
- (18) **09/03/2006** - «*Structure and Dynamics of E3 Ubiquitin Ligases Hdm2 & Hdmx tumor-suppressor protein p53 regulators* » **7<sup>th</sup> Conference in Medicinal Chemistry: Drug Design & Development**, Patras, GREECE.
- (19) **16/05/2006** - «*NMR Study of Angiotensin-I Converting Enzyme (ACE) Synthetic Peptide-based Catalytic Site Maquettes (CSM) and CSM–Substrate/Inhibitor Interaction*» **5<sup>th</sup> Hellenic Forum on Bioactive Peptides**, Patras, GREECE.
- (20) **25/10/2006** – «*Laptop Molecular Modelling – In silico polypeptide folding into three-dimensional and functional structure*» **Welcome Ceremony for the 1<sup>st</sup> year Undergraduate Pharmacy Students**, Patras, GREECE.
- (21) **16/03/2007** - «*Study of Anthrax Lethal Factor – peptide substrate Interaction: Implications for Structure-Guided Design of Bioactive Molecules*» **8<sup>th</sup> Conference in Medicinal Chemistry**, Patras, GREECE.

- (22) **26/06/2007** - «*Anthrax Lethal Factor catalytic domain: A Platform for Structure-Guided Design of Bioactive Molecules*» Invited by **Dr. Nikos Oikonomakos**, National Hellenic Research Foundation Institute of Organic & Pharmaceutical Chemistry, Athens, GREECE.
- (23) **20/10/2007** - «*Protein Data Bank and Structure Quality Assessment*» **Workshop on “Bioinformatics - “Computational Methods in Biological Data Mining”, 5th General Meeting of the International Proteolysis Society (IPS2007)**, Patras, GREECE.
- (24) **15/11/2007** - «*A residue specific view of Anthrax Lethal Factor – peptide substrate Interaction: Implications for Structure-Guided Design of Bioactive Molecules*» Invited by **Prof. Morten Grötl**, University of Göteborg, Department of Chemistry, Medicinal Chemistry, Göteborg, SWEDEN.
- (25) **14/03/2008** - «*An Atomic Level Insight into Anthrax Lethal Factor (LF) Substrate Selectivity* » Invited by **Organizing Committee, 13th Hellenic Symposium on Medicinal Chemistry (HSMC-13)**, Athens, GREECE.
- (26) **21/05/2008** «*Conformational properties of Proteins & Biomolecular Simulations*», **Workshop - 4<sup>th</sup> CONCO Consortium Meeting**, Patras, GREECE.
- (27) **04/06/2008** - «*NMR-based structure determination of biomolecules – Part I & II* » & «*Practical session: Analysis of 2D Homonuclear NMR Data*» Invited by **Organizing Committee, 1<sup>st</sup> Workshop on Structure-Based Drug Design**, Athens, GREECE.
- (28) **26/09/2008** - «*NMR insights into the concerted action of a Sco1 and a putative copper chaperone to the CuA assembly mechanism*» Invited by **Organizing Committee, 4th Conference of the Hellenic Crystallographic Association**, Athens, GREECE.
- (29) **30/10/2008** - «*Docking and Molecular Dynamics Simulations to gain an atomic level insight into Anthrax Lethal Factor (LF) Substrate interaction*» **3rd Conference of the Hellenic Society for Computational Biology and Bioinformatics HSCBB08**, EKETA, Thassaloniki, GREECE.
- (30) **30/10/2008** - «*Conformational Plasticity of Ring finger E3 Ubiquitin ligases of p53 tumor suppressor protein*» **3rd Conference of the Hellenic Society for Computational Biology and Bioinformatics HSCBB08**, EKETA, Thassaloniki, GREECE.
- (31) **30/01/2009** – «*Computational Insights into the conformational dynamics of nAChR 5mer and  $\alpha$ 1-toxin complexes – Preliminary NMR studies of nAChR subunits*» **1<sup>st</sup> Annual meeting - EU FP7 Neurocypres**. Hellenic Pasteur Institute, Athens, GREECE.
- (32) **31/01/2009** - «*Preliminary NMR studies of a Cys-loop family prokaryotic homologue*» **1<sup>st</sup> Annual meeting - EU FP7 Neurocypres**. Hellenic Pasteur Institute, Athens, GREECE.
- (33) **01/02/2009** - «*1. NMR Screening of ligand-AChR interaction, first results; 2. Virtual screening of 400 di-peptides on nAChR*» **1<sup>st</sup> Annual meeting - EU FP7 Neurocypres**. Hellenic Pasteur Institute, Athens, GREECE.
- (34) **18/03/2009** – «*Structure-Activity Relationship in Biomolecules through NMR*» Invited by **Prof. K. Kypraios**, Department of Medicine, University of Patras, GREECE.
- (35) **30/03/2009** – «*Structural bioinformatics at University of Patras. Biomolecular simulations & NMR applications to study protein architecture and socialization*» **HSCBB – GSRT – ELIXIR meeting**, National Hellenic Research Foundation Institute, Athens, GREECE.
- (36) **08/05/2010** – «*NMR Studies of GLIC prokaryotic AChR homologue and Current Progress in Labeling Strategies towards a Complete Resonance Assignment and Structure Determination* » **2<sup>nd</sup> Annual meeting - EU FP7 Neurocypres**. Marseille, FRANCE.
- (37) **17/06/2010** – «*Bioinorganic Chemistry of Zinc(II): NMR study of the Structure-Activity Relationship of oncoproteins and tumor suppressors*» **Department of Chemistry, University of Patras**, 17 June 2010, Patras, GREECE.
- (38) **24/09/2010** – «*Structure-Activity Relationship of Arkadia Ring finger E3 ubiquitin ligase through NMR spectroscopy*» **18<sup>th</sup> Euro QSAR**, 19-24 September 2010, Rhodes, GREECE.
- (39) **01/10/2010** – «*NMR-Based Residue Specific Insights into the Structure-Function Correlation of Arkadia E3 Ubiquitin Ligase Ring Finger Domain*» **EAST-NMR 1st Young Investigators Meeting**, 29 September to 1 October 2010, Istanbul, TURKEY.
- (40) **02/11/2010** – «*NMR insights into the conformational dynamics of native and engineered forms of Arkadia E3 Ubiquitin ligase C-terminal Domain*» **"NMR in Life Sciences" – 3<sup>rd</sup> International Symposium on Organic Chemistry**,



30<sup>th</sup> October to 2<sup>nd</sup> November, Sofia, BULGARY.

(41) **17/01/2011** – «*Conformation, Dynamics and Interaction of peptides and proteins observed through NMR Spectroscopy*» **Department of Pharmacy, University of Patras**, 17 January 2011, Patras, GREECE.

(42) **19/09/2011** – «*NMR Structural Biology at University of Patras*» **GREEK NMR Users Meeting** organized by BRUKER Biospin & FP7 EAST-NMR, 19-20 September 2011, Athens, GREECE.

(43) **8/10/2011** – «*NMR-driven docking of protein partners involved in ubiquitination pathway*», **6th Conference of the Hellenic Society for Computational Biology and Bioinformatics - HSCBB11**, University of Patras, 08 October 2011, Patras, GREECE.

(44) **17/10/2011** – «*Expression, characterization and NMR studies of RING domain of Arkadia tumor suppressor*», Invited by **Prof. C. Kalofonos**, Department of Medicine, Oncology Sector, University of Patras, GREECE.

(45) **04/11/2011** – «*Structural Biology Through Biomolecular NMR*» Invited by **Dr. E Tsilibary**, Director of Institute of Biology, N.C.S.R. "Demokritos", 04 November 2011, Athens, GREECE.

(46) **07/11/2011** – «*NMR Structural Biology at University of Patras – The SEE-DRUG project*» **Structure– & Computer– Aided Design Workshop: Bioactive Molecules & Materials & INSTRUCT-EL Meeting**, National Hellenic Research Foundation, 07-11 November 2011, Athens, GREECE.

(47) **11/12/2011** – «*Solution NMR study of the monomeric extracellular domain of a nAChR prokaryotic homologue*» **62<sup>nd</sup> EEBMB Conference**, 9-11 December 2011, Athens, GREECE.

(48) **11/01/2012** – «*Conformational plasticity of polypeptides through Biomolecular NMR Spectroscopy*» Invited by **Prof. T. Mavromoustakos**, Department of Chemistry, University of Athens, Athens, GREECE.

(49) **17/04/2012** – «*NMR study of Arkadia E3 ubiquitin ligase domain to correlate Zn(II) coordination with protein architecture, dynamics and function*» **12<sup>th</sup> EURASIA Conference in Chemical Sciences**, 17-21 April 2012, Corfu GREECE.

(50) **19/05/2012** – «*Conformational Dynamics and Drug Design Approaches through NMR - Basics and Applications* » **2nd Summer School of Proteins**, Invited by **Prof. C. Vorgias**, Department of Biology, University of Athens, 18-20 May 2012, Athens, GREECE.

(51) **26/05/2012** – «*Identifying functionally important residues of Arkadia E3 Ubiquitin Ligase RING Domain in E2 Recruitment and E3-E2 Interaction* » **15th Symposium on Medicinal Chemistry**, 25-27 May 2012, Athens, GREECE.

(52) **28/05/2012** – «*NMR Conformational Dynamics and SAR studies of biologically relevant macromolecules*» **3<sup>rd</sup> ARCADE Workshop**, National Hellenic Research Foundation, 28-30 May 2012, Athens GREECE.

(53) **04/06/2012** – «*The SEE DRUG Project at University of Patras*» **WIRE2012 – Week of Innovative Regions in Europe**, Invited by the **WIRE2012 Organizing Committee & REGPOT Program Officer**, 03-05 June 2012, Krakow, POLLAND.

(54) **09/06/2012** – «*Insights on the conformational exchange properties of GLIC ECD by solution NMR - Implications on 5/6mer subunit socialization*». **4<sup>th</sup> Annual meeting - EU FP7 Neurocypres**, 07-10 June 2012, Vienna, AUSTRIA.

(55) **22/06/2012** – «*Elucidating the intrinsic plasticity of the extracellular domain of a prokaryotic nAChR homologue by solution NMR - implications on 5/6mer subunit socialization*», Invited by **Prof. Anna-Maria Papini**, Department of Chemistry, University of Florence, ITALY.

(56) **04/09/2012** – «*Selective amino acid isotope labeling strategies for solution NMR studies of high-molecular-weight protein drug-targets*» **32<sup>nd</sup> European Peptide Symposium**, 04 September 2012, Athens, GREECE.

(57) **29/09/2012** – «*NMR-driven Structure Function Correlation studies of Arkadia E3 Ubiquitin Ligase RING domain*», **6<sup>th</sup> Conference of the Hellenic Crystallographic Association**, 28-29 September, Athens, GREECE.

(58) **09/11/2012** – «*Conformational Dynamics & Function of Proteins by Solution NMR*», Invited by **Prof. Michael Orfanopoulos**, Department of Chemistry, University of Crete, GREECE.

(59) **10/11/2012** – «*NMR Insights on the functional modulation of the RING domain of Arkadia tumor suppressor*», **63<sup>rd</sup> EEBMB Conference**, 9-11 November 2012, Heraklion Crete, GREECE.

(60) **15/11/2012** – «*NMR Structural Biology at University of Patras & the SEEDRUG Project* », **3<sup>rd</sup> EAST-NMR Annual User Meeting**, 13-16 November 2012, Lasko, SLOVENIA.

(61) **08/12/2012** – «*Solution NMR Studies of E3 Ub Ligase RING and Alphaviruses MACRO Domains*», **Turkish NMR Meeting**, 07-09 December 2012, Istanbul, TURKEY.

- (62) **19/03/2013** – «*Conformational Dynamics of Proteins, Biomolecular Interactions and Drug Design Efforts using NMR*», Invited by Assoc Prof. S. Taraviras, **Department of Medicine, University of Patras**, GREECE.
- (63) **12/04/2013** – «*State-of-the-art NMR instrumentation & modern NMR applications in the service of Life Sciences*», **1<sup>st</sup> Forum of Health**, Patras, GREECE.
- (64) **31/05/2013** – «*High-resolution analysis of protein structure, dynamics and interaction through Biomolecular NMR* », «**NANOTHEO**» **Workshop, University of Patras**, GREECE.
- (65) **24/09/2013** – «*NMR conformational dynamics of proteins & protein complexes* », IAEA Meeting, **University of Patras**, GREECE.
- (66) **26/09/2013** – «*Conformational Dynamics and Drug Design Approaches through NMR*», **5th BBBB International Conference 2013, 26-28 September, Athens**, GREECE.
- (67) **11/10/2013** – «*SEEDRUG Biomolecular 700MHz NMR Facility*», **Inauguration of the SEEDRUG Biomolecular NMR Facility**, Rion, GREECE.
- (68) **06/04/2014** - «*Structural Biology by NMR: Knowledge transfer form EU RIs to Greece*», **ICRI-2014 – Strategic pipeline planning: from sample preparation to 3D structure determination with bio SAXS and other biophysical techniques**, National Hellenic Research Foundation, Athens, GREECE.
- (69) **20/05/2014** - «*Insights on the conformational plasticity of drug-target proteins*» **32<sup>nd</sup> Cyprus – Noordwijkerhout – Camerino Symposium – Trends in Drug Research**, May 18-23, 2014, Limassol, CYPRUS.
- (70) **28/05/2014** - «*Atomic-level investigation of Structure, Dynamics & Interactions of proteins, through Biomolecular NMR*», Invited by Assoc Prof. D. Leonidas, **Department of Biochemistry & Biotechnology, University of Thessaly**, Larissa, GREECE.
- (71) **21/09/2014** - «*NMR Conformational Dynamics of La and RRM1 Motifs of La Protein*», **CTSB & HeCrA7**, FORTH-IMBB, Heraklion Crete, GREECE.
- (72) **10/10/2014** - «*Application of NMR Spectroscopy to the study of biomolecules and pharmaceutical targets*», **2<sup>nd</sup> Conference of Pharmaceutical Sciences**, University of Patras, GREECE.
- (73) **13/10/2014** - «*Atomic-level investigation of Structure, Dynamics & Interactions of proteins, through Biomolecular NMR*», **Greek NMR Users Meeting**, Athens, GREECE.
- (74) **13/02/2015** - «*Conformation, Plasticity and Socialization of biomolecules through NMR* » invited by Dr. Iro Georgoussi, **NCSR Demokritos**, Institute of Biosciences & Applications, Athens, GREECE.
- (75) **26/04/2015** – «*Biomolecular NMR methods for the study of biologically relevant macromolecules and their complexes*» University of Thrace, Alexandroupoli, GREECE.
- (76) **27/05/2015** – «*NMR insights into the Conformational Dynamics and interaction of biomolecules with therapeutic interest*» invited by the Organizing Committee of the **1<sup>st</sup> International Conference of Controlled Release Society**, Athens, GREECE.
- (77) **26/06/2015** – «*High Resolution solution NMR studies of Biomacromolecules*» In Memorial Event for the Late Prof Giannis Elemen (1962-2014), Department of Chemistry, University of Ioannina. GREECE
- (78) **09/10/2015** – «*NMR Spectroscopy Applications to study biomolecules and biomolecular drug targets*», **17<sup>th</sup> Greek National Pharmaceutical Conference**, Athens.
- (79) **21/04/2016** – «*NMR Insights on the conformational plasticity and interaction of biomolecules*», **REGPOT-InnovCrete Seminars**, FORTH-IMBB, University of Crete, Heraklion, Crete, Greece
- (80) **14/05/2016** – «*NMR Applications on the study of the biomolecules as potential drug target*», **2<sup>nd</sup> Greek Conference of Applied Pharmacy**, Thessaloniki, Greece
- (81) **21/05/2016** – «*Biomolecular NMR methods for the study of biologically relevant macromolecules and their complexes*» University of Thrace, Alexandroupoli, GREECE.
- (82) **08/06/2016** – «*NMR conformational dynamics & RNA recognition properties of La protein domains La, RRM1 and RRM2*», **Chianti Workshop 2016**, June 5-10, 2016, Grosseto, Italy
- (83) **23/06/2016** – «*NMR insights into the Conformational Dynamics and interaction of biomolecules with therapeutic interest*» invited by the Organizing Committee of the **2<sup>nd</sup> International Conference of Controlled Release Society**, Athens, GREECE.

- (84) **02/12/2016** – “*Solution NMR Spectroscopy to study the conformation, the dynamics and the interaction of biomolecules*”, invited by Assoc. Prof. Leufkothea Papadopoulou, **Department of Pharmacy, Aristotle University of Thessaloniki**, December 2, GREECE.
- (85) **03/12/2016** – “*NMR in Chemistry, Biology, Drug Design & Diagnostics*”, **22<sup>nd</sup> PanHellenic Conference of Chemistry**, December 2-4, Thessaloniki, GREECE.
- (86) **18/02/2017** – “*The role of Biomolecular NMR on Health Sciences*”, **3<sup>rd</sup> Conference of Pharmaceutical Sciences**, 18-19 February, Thessaloniki.
- (87) **12/03/2017** – «*Applications of NMR Spectroscopy in the study of biomolecules and pharmaceutical targets*», **U of Thrace Graduate Studies Program “Translational Research in Biomedicine”**, Department of Molecular Biology & Genetics, **University of Thrace**, Alexandroupoli, Greece.
- (88) **27/04/2017** – “*Targeting the architecture, the plasticity and the socialization determinants of biomolecules with pharmaceutical interest by NMR*”, Invited by Prof. Steve Euston, **Heriot-Watt University, Edinburgh, UK**.
- (89) **05/05/2017** – “*NMR Approaches in Structural Biology & Drug Design*”, **Meeting on “Biochemistry & Health: From the cell to the therapy”**, University of Thessaly, Larissa, Greece.
- (90) **6/05/2017** – “*Modern NMR methods in Drug Design and Metabolomics*”, **3<sup>rd</sup> Greek Conference of Applied Pharmacy**, Thessaloniki, Greece.
- (91) **20/05/2017** – «*NMR Application in Biomedicine*», **5<sup>th</sup> Forum of Health**, Patras, Greece.
- (92) **26/06/2017** – “*NMR studies of RNA and ADP-ribose binding proteins*”, Invited by Prof. Michael Sattler, Chair for Biomolecular NMR Spectroscopy, **Technical University of Munich, STB Institute of Structural Biology**, Bavarian NMR Center (BNMRZ), Munich, Germany.
- (93) **02/10/2017** – “*Gas sensing in a heme protein monitored through NMR*”, **2<sup>nd</sup> COST “FesBioNet” Meeting**, Trest 1-4 October 2017, Czech Republic.
- (94) **04/05/2018** – “*NMR Applications in Metabolomic Analysis of Bio-fluids/tissues and Diagnostics*”, **4<sup>th</sup> Greek Conference of Applied Pharmacy**, Thessaloniki, Greece.
- (95) **21/05/2018** – “*NMR Studies of Heme Proteins*”, **2<sup>nd</sup> Synthetic & Medicinal Chemistry Symposium**, Department of Pharmacy, U of Patras, Greece
- (96) **30/05/2018** – «*Gas-inflow triggered stimulation of a heme enzyme monitored by NMR*», **EMBO Workshop - Challenges for magnetic resonance in life sciences**, 27-31 May 2018, Grosseto, Italy.
- (97) **22/09/2018** – “*Studies of Heme Proteins*” Invited Lecture, “**Chemistry at the interface of Biology and Medicine**”, 21-25 September 2018, Heraklion - Crete, Greece
- (98) **06/10/2018** – “*NMR conformational Dynamics of RNA- and nucleotide- binding proteins*”, Invited Lecture **HeCrA9**, 6-8 October, Patras, Greece
- (99) **25/11/2018** – “*The structural and dynamic basis for the function of biological molecules through solution NMR spectroscopy*”, Invited Lecture, **69<sup>th</sup> Conference of the Hellenic Society of Biochemistry & Molecular Biology** November 23-25, 2018 Hotel Imperial, Larissa, Greece
- (100) **14/12/2018** – «*NMR Conformational Dynamics of soluble Guanylate Cyclase (sGC) bacterial homologues – Implication for enzyme activation*», Invited by Assoc. Prof. Lefkothea Papadopoulou, Department of Pharmacy, Aristotle University of Thessaloniki, Greece.
- (101) **13/02/2019** – «*Modern research Approaches in Biosciences*», **Diakideios School of Patras**, Patras, Greece.
- (102) **15/03/2019** - «*NMR Conformational Dynamics of soluble Guanylate Cyclase (sGC) bacterial homologues – Implication for enzyme activation*», Invited by Assoc. Prof. Aglaia Pappa, Department of Molecular Biology & Genetics, **Democritus University of Thrace**, Alexandroupoli, Greece.
- (103) **04/09/2019** – “*NMR insights on the activation mechanism of a heme enzyme*” Invited Lecture, **Central European NMR Symposium & Bruker users meeting**, University of Belgrade, Faculty of Chemistry, 04-05 September 2019, Serbia
- (104) **17/09/2019** – “*NMR studies of RNA- and nucleotide- binding proteins*”, **4<sup>nd</sup> COST “FesBioNet” Meeting**, Gdansk 16-19 September 2019, Poland.
- (105) **12/10/2019** – “*NMR studies of RNA- and nucleotide-binding proteins*”, **Hellenic Bioinformatic Conference 2019**, Heraklion Crete, 10-13 October, Greece.

- (106) 24/09/2020** - «*The structural and dynamic basis for the function of biological molecules through solution NMR spectroscopy*» **Adriatic NMR Conference 2020**, May 26-28, Peroj, Croatia, 2020
- (107) 25/02/2021** – “*NMR Structural biology of SARS-CoV-2 nsP3 proteins; new targets for viral replication inhibition*”, **18<sup>th</sup> Hellenic Symposium on Medicinal Chemistry, On-line Symposium**, 25-27 February, 2021.
- (108) 23/05/2021** – “*New SARS-CoV-2 protein targets for Remdesivir – A potential new approach against COVID-19*”, **7<sup>th</sup> Greek Conference of Applied Pharmacy**, Thessaloniki, Greece

***Journal Publications in peer-reviewed scientific journals (as corresponding author: underlined) :***

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1. A.G. Coutsolelos, **G.A. Spyroulias**. *Dysprosium Metallation to Substituted Tetraaryl-porphyrin Complexes; Synthesis and Spectroscopic Characterization*. ***Polyhedron*, 13, 647-653 (1994).**
2. E.M. Davoras, **G.A. Spyroulias**, E. Mikros, A.G. Coutsolelos. *<sup>1</sup>H NMR Spectroscopic Elucidation of Stereochemical Effects of Substituted Cerium Porphyrin Double-Deckers*. ***Inorganic Chemistry*, 33, 3430-3434 (1994).**
3. **G.A. Spyroulias**, A.G. Coutsolelos. *Synthesis and Spectroscopic studies of Lanthanide monoporphyrinates with meso-tetra-aryl porphyrinate Bearing Bromides on β -Pyrrole Positions or Fluorides on phenyl groups*. ***Polyhedron*, 14, 2483-2490 (1995).**
4. **G.A. Spyroulias**, A.G. Coutsolelos, C.P. Raptopoulou, A. Terzis. *Synthesis, Characterization, and X-ray Study of Sm(III) Heteroleptic Porphyrin Double-Decker*. ***Inorganic Chemistry*, 34, 2476-2479 (1995).**
5. **G.A. Spyroulias**, M.P. Sioubara, A.G. Coutsolelos. *Cationic Lanthanide Monoporphyrinates with Sm, Eu, Gd and Tb. Synthesis and Spectroscopic Properties in Aqueous and Non Aqueous Media*. ***Polyhedron*, 14, 3563-3571 (1995).**
6. **G.A. Spyroulias**, A.G. Coutsolelos. *Evidence of Protonated and Deprotonated Forms of Symmetrical and Asymmetrical Lutetium(III) Porphyrin Double-Deckers by <sup>1</sup>H NMR Spectroscopy*. ***Inorganic Chemistry*, 35, 1382-1385 (1996).**
7. **G. A. Spyroulias**, A.G. Coutsolelos, D. de Montauzon, R. Poilblanc. *Electrochemical Studies of Protonated and Deprotonated Forms of Heteroleptic and Homoleptic Europium and Dysprosium Porphyrin Double-Deckers*. ***Journal of Coordination Chemistry*, 39, 89-96 (1996).**
8. I. Bertini, A.G. Coutsolelos, A. Dikiy, C. Luchinat, **G.A. Spyroulias**, A. Troganis. *Structural and Dynamic Information on Double-Decker Yb<sup>3+</sup> and Dy<sup>3+</sup> Porphyrin Complexes in Solution through <sup>1</sup>H NMR*. ***Inorganic Chemistry*, 35, 6308-6315 (1996).**
9. P. Battioni, E. Cardin, M. Louloudi, B. Schöllhorn, **G.A. Spyroulias**, D. Mansuy, T.G. Traylor. «Metalloporphyrinosilicas»: A New Class of Hybrid Organic-Inorganic Materials Acting as Selective Biomimetic Oxidation Catalysts. ***J. Chem. Soc., Chemical Communication*, 2037-2038 (1996).**
10. **G.A. Spyroulias**, A.P. Despotopoulos, C.P. Raptopoulou, A. Terzis, A.G. Coutsolelos. *First X-ray Crystal Structure of a Non-Planar Lanthanide(III) Monoporphyrinate*. ***J. Chem. Soc., Chemical Communication*, 783-784 (1997).**
11. **G.A. Spyroulias**, D. de Montauzon, A. Maisonnat, R. Poilblanc, A.G. Coutsolelos. *Synthesis, UV-visible and electrochemical studies of Lipophilic and Hydrophilic Lanthanide(III), (Ln=La, Sm, Eu, Gd), Porphyrinic Double-Deckers*. ***Inorganica Chimica Acta*, (Issue in Honor of Prof. Ivano Bertini), 275-6, 182-191 (1998). Invited Article Contribution**
12. L. Banci, I. Bertini, **G.A. Spyroulias**, P. Turano. *The Conformational flexibility of Oxidized cytochrome c, studied through its interaction with NH<sub>3</sub> and at High Temperature*. ***European Journal of Inorganic Chemistry*, 583-591 (1998).**
13. D. Deniaud, **G.A. Spyroulias**, J.-F. Bartolli, P. Battioni, D. Mansuy, C. Pinel, F. Odobel, B. Bujoli. *Shape selectivity for alkane hydroxylation in heterogenised manganese porphyrins*. ***New Journal of Chemistry*, 901-906 (1998).**
14. L. Banci, S. Berners-Price, I. Bertini, V. Clementi, C. Luchinat, **G.A. Spyroulias**, P. Turano. *Water-Protein Interactions in native and partially unfolded equine Cytochrome c*. ***Molecular Physics*, (Issue in Honor of Prof. R.R. Ernst, Nobel Prize in Chemistry 1991), 95, 797-808 (1998). Invited Article Contribution**
15. **G.A. Spyroulias**, C.P. Raptopoulou, D. de Montauzon, A. Mari, R. Poilblanc, A. Terzis, A.G. Coutsolelos. *Synthesis and Physicochemical Characterization of Protonated and Deprotonated Forms in Heteroleptic Ln(III), Porphyrinate Double-Deckers. X-Ray Structure of Gd<sup>III</sup>H(OEP)(TPP) at 298 and 21K*.

- Inorganic Chemistry*, 38, 1683-1696 (1999).
16. L. Banci, I. Bertini, G. Huber, **G.A. Spyroulias**, P. Turano. *Solution Structure of reduced horse heart cytochrome c*. *Journal of Biological Inorganic Chemistry*, 4, 21-31 (1999).
17. V. Tangoulis, D. Malamataris, **G.A. Spyroulias**, C.P. Raptopoulou, A. Terzis, D.P. Kessissoglou. *An EPR and  $^1\text{H}$  NMR Active Mixed Valence Manganese(III/II/III) Trinuclear Compound*. *Inorganic Chemistry*, 39, 2621-2630 (2000).
18. L. Banci, I. Bertini, B. Bianchini, P. Hajieva, **G.A. Spyroulias**, P. Turano. *DME-substituted cytochrome  $b_5$ : Structure and Stability*. *Journal of Biological Inorganic Chemistry*, 6, 490-503 (2001).
19. S. Babajilov, A.G. Coutsolelos, A. Dikiy, **G.A. Spyroulias**. *Intramolecular Dynamics of Lanthanide Bis(porphyrinates) through  $^1\text{H}$  NMR Spectroscopy*. *European Journal of Inorganic Chemistry*, 303-306 (2001).
20. A.K. Boudalis, N. Lalioti, **G.A. Spyroulias**, C.P. Raptopoulou, A. Terzis, V. Tangoulis, S.P. Perlepes. *Tetranuclear iron(III) carboxylate clusters with 1,10-phenanthroline, and 2,2'-bipyridine: a new  $[\text{Fe}_4(\mu_4\text{-OHO})(\mu\text{-OH})_2]^{7+}$  core*. *J. Chem. Soc., Dalton Transaction*, 955-957 (2001).
21. J.-H. Agondanou, **G.A. Spyroulias**, S. Benazeth, J. Purans, C. Souleau, A. Coutsolelos. *XAFS Study of Symmetrical and Asymmetrical Gadolinium Bisporphyrinate Complexes*. *Inorganic Chemistry*, 40, 6088-6096 (2001).
22. **G.A. Spyroulias**, A.P. Despotopoulos, C.P. Raptopoulou, A. Terzis, D. de Montauzon, R. Poilblanc, A.G. Coutsolelos. *Comparative Study of Structure-Properties relationship for Novel  $\beta$ -Halogenated Lanthanide Porphyrins and their Nickel and Free Bases Precursors, as a function of number & nature of Halogens atoms*. *Inorganic Chemistry*, 41, 2648-2659 (2002).
23. **G.A. Spyroulias**, S. Papazacharias, G. Pairas, P. Cordopatis. *Monitoring the Structural Consequences of Phe12DPhe12 and Leu15Aib15 substitution in h/r Corticotropin Releasing Hormone: Implications for Design of CRH antagonists*. *Eur. J. Biochemistry* 269, 6009-6019 (2002).
24. A. K. Boudalis, N. Lalioti, **G. A. Spyroulias**, C. P. Raptopoulou, A. Terzis, V. Tangoulis, A. Bousseksou, J.-P. Tuchagues, S. P. Perlepes. *New tetranuclear iron(III) carboxylate clusters exhibiting different core topologies: the case of the novel  $[\text{Fe}_4(\mu_4\text{-OHO})(\mu\text{-OH})_2]^{7+}$  versus the butterfly  $[\text{Fe}_4(\mu_3\text{-O})_2]^{8+}$  core in the  $\text{Fe}^{\text{II}}/\text{RCO}_2^-/1,10\text{-phenanthroline}$  systems ( $R=\text{Me}, \text{Ph}$ )*. *Inorganic Chemistry*, 41, 6474-6487 (2002).
25. **G.A. Spyroulias**, P. Nikolakopoulou, A. Tzakos, I. Gerothanassis, V. Magafa, E. Manesi-Zoupa, P. Cordopatis. *Comparison of the Solution Structures of Angiotensin I & II: Implication for Structure-Function Relationship*. *Eur. J. Biochemistry* 270, 2163-2173 (2003).
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**Corresponding Author (since 2003) : 54 @129**

**Citations : >2900 & h-index 28, h10-index 68**

**PDB – Protein Data Bank (<http://www.rcsb.org/pdb/> )**

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- (5) **1MNY** Dimethyl propionate ester heme-containing cytochrome b5 (**2002**)
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- (13) **2K6W** Solution structures of apo PCuA (*trans* conformation of the peptide bond involving the nitrogen of P14) (**2008**)
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- (21) **5IQ5** NMR solution structure of Mayaro virus macro domain, 21 models (**2016**)
- (22) **5ISN** NMR solution structure of macro domain from Venezuelan equine encephalitis virus, 21 models (**2016**)
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- (24) **5LG7** Solution NMR structure of Tryptophan to Arginine mutant of Arkadia RING domain, 31 models (**2016**)
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- (27) **7P27** NMR solution structure of from Chikungunya virus macro domain (**2021**)
- (28) **7P2K** Solution NMR Structure of Arginine to Cysteine mutant of Arkadia RING domain (**2021**)
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**BMRB – Biological Magnetic Resonance Bank (<http://www.bmrwisc.edu/> )**

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- (2) **20015** NMR evidence of charge-dependent interaction between various PND V3 and CCR5 N-terminal peptides, SF2, NMR 21 structures (2008)
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- (5) **20062** 3D Solution Structure of MBP83-99 peptide in DMSO, NMR 21 structures (2008)
- (6) **15948**  $^1\text{H}$ ,  $^{13}\text{C}$ , and  $^{15}\text{N}$  Chemical Shift Assignments for the RING finger of the E3 ubiquitin ligase *Arkadia* (RNF111) (2008)
- (7) **16735** NMR resonance assignment of the apo C-terminal polypeptide of the *Anthrax Lethal Factor* catalytic domain (2010)
- (8) **17695** Backbone Chemical Shift Assignments of the Extracellular domain of *GLIC*, a prokaryotic nAChR homologue (2011)
- (9) **18620** NMR Chemical Shift Assignments of N terminal RRM domain of La protein from *Dictyostelium Discoedium* (2012)
- (10) **18621** NMR Chemical Shift Assignments of N terminal La motif domain of La protein from *Dictyostelium Discoedium* (2012)
- (11) **19803** NMR resonance assignment of the N-terminal polypeptide of the *Anthrax Lethal Factor* (2014)
- (12) **19927** NMR study of non-structural proteins – Part I.  $^1\text{H}$ ,  $^{13}\text{C}$ ,  $^{15}\text{N}$  backbone and side-chain resonance assignment of macro domain from *Mayaro virus* (MAYV) (2014)
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- (14) **25132** NMR study of non-structural proteins – Part II.  $^1\text{H}$ ,  $^{13}\text{C}$ ,  $^{15}\text{N}$  backbone and side-chain resonance assignment of macro domain from *Venezuelean Equine Encephalitis virus* (VEEV) (2014)
- (15) **25239** NMR Chemical Shift Assignments of LAM-RRM1 of La protein from *Dictyostelium Discoedium* (2014)
- (16) **25248**  $^1\text{H}$ ,  $^{13}\text{C}$ , and  $^{15}\text{N}$  Chemical Shift Assignments for the W972R mutant of *Arkadia* (RNF111) E3 RING domain (2014)
- (17) **25249**  $^1\text{H}$ ,  $^{13}\text{C}$ , and  $^{15}\text{N}$  Chemical Shift Assignments for the W972A mutant of *Arkadia* (RNF111) E3 RING domain (2014)
- (18) **25351**  $^1\text{H}$ ,  $^{13}\text{C}$  and  $^{15}\text{N}$  Chemical Shift Assignments for the H962C mutant of *Arkadia* (RNF111) E3 RING domain (2014)
- (19) **25392**  $^1\text{H}$ ,  $^{13}\text{C}$  and  $^{15}\text{N}$  Chemical Shift Assignments for the H965C mutant of *Arkadia* (RNF111) E3 RING domain (2014)
- (20) **26748** NMR study of Met-1 *Human* Angiogenin -  $^1\text{H}$ ,  $^{13}\text{C}$ ,  $^{15}\text{N}$  backbone and side chain resonance assignment (2016)
- (21) **26753** NMR study of non-structural proteins -  $^1\text{H}$ ,  $^{13}\text{C}$ ,  $^{15}\text{N}$  resonance assignment of macro domain from *Venezuelean Equine Encephalitis virus* (VEEV) in complex with ADP-ribose (2016)
- (22) **26048**  $^1\text{H}$ ,  $^{13}\text{C}$ ,  $^{15}\text{N}$  backbone and side-chain resonance assignment of *Nostoc sp.* C139A variant of the heme-nitric oxide/oxygen binding (H-NOX) domain (2016)
- (23) **27158** NMR study of non-structural proteins – Part III.  $^1\text{H}$ ,  $^{13}\text{C}$ ,  $^{15}\text{N}$  resonance assignment of macro domain from *Chikungunya virus* (CHIKV) (2017)
- (24) **27612** NMR study of non-structural proteins -  $^1\text{H}$ ,  $^{13}\text{C}$ ,  $^{15}\text{N}$  resonance assignment of macro domain from *Mayaro virus* (MAYV) in complex with ADP-ribose (2018)
- (25) **28028**  $^1\text{H}$ ,  $^{13}\text{C}$ ,  $^{15}\text{N}$  backbone and side-chain assignment of the native form of Ubch7 (UBE3L2) (2019)
- (26) **28118**  $^1\text{H}$ ,  $^{13}\text{C}$ ,  $^{15}\text{N}$  backbone and side-chain resonance assignment of *Nostoc sp.* C139A variant of the heme nitric oxide/oxygen binding (H-NOX) domain in complex with cinaciguat (2020)



- (27) **50448**  $^1\text{H}$ - $^{13}\text{C}$ - $^{15}\text{N}$  SARS Unique Domain CoV-2 (nsp3c) N-terminal domain **(2020)**
- (28) **50516**  $^1\text{H}$ - $^{13}\text{C}$ - $^{15}\text{N}$  SARS Unique Domain CoV-2 (nsp3c) M (middle) domain **(2020)**
- (29) **50517**  $^1\text{H}$ - $^{13}\text{C}$ - $^{15}\text{N}$  SARS Unique Domain CoV-2 (nsp3c) C-terminal domain **(2020)**
- (30) **50969**  $^1\text{H}$ ,  $^{13}\text{C}$ ,  $^{15}\text{N}$  resonance assignment of macro domain from *SARS-CoV* in complex with ADP-ribose **(2021)**
- (31) **50970**  $^1\text{H}$ ,  $^{13}\text{C}$ ,  $^{15}\text{N}$  resonance assignment of macro domain from *MERS-CoV* **(2021)**
- (32) **50971**  $^1\text{H}$ ,  $^{13}\text{C}$ ,  $^{15}\text{N}$  resonance assignment of macro domain from *MERS-CoV* in complex with ADP-ribose **(2021)**
- (33) **50993**  $^1\text{H}$ ,  $^{13}\text{C}$ ,  $^{15}\text{N}$  resonance assignment of macro domain from *SARS-CoV* in the free state **(2021)**
- (34) **50985**  $^1\text{H}$ ,  $^{13}\text{C}$  and  $^{15}\text{N}$  Chemical Shift Assignments of the R957C mutant from Arkadia (RNF111) E3 RING domain in solution **(2021)**

### **Other Publications : (A) Book Chapters**

**A1.** A. Coutsolelos, **G.A. Spyroulias**. “**Chapter 4: NMR of Organozinc compounds -  $^{67}\text{Zn}$  NMR, a tool for coordination chemistry problems.**”

In “**The Chemistry of Organic Zinc Compounds**”, Zvi Rappoport (Editor), Ilan Marek (Editor), John Wiley & Sons, Ltd., 2006.

**A2.** T. Mavromoustakos, S. Golic Grdadolnik, M. Zervou, P. Zoumpoulakis, C. Potamitis, A. Politi, E. Mantzourani, J. A. Platts, C. Koukoulitsa, P. Minakakis, G. Kokotos, T. Tselios, J. Matsoukas, S. Durdagi, M.G. Papadopoulos, D.P. Papahatjis, Z.S. Spyranti, G.A. Dalkas, **G.A. Spyroulias**. **Chapter 7: Putative Bioactive Conformers of Small Molecules: A Concerted Approach Using NMR Spectroscopy and Computational Chemistry.**

In “**Medicinal Chemistry Research progress**”, Editors: Giulia P. Colombo and Sofia Ricci, Nova Science Publishers, Inc., **2008**.

**A3.** **G.A. Spyroulias**. *Peptide substrate selectivity and Dual Inhibitors of ACE and NEP vasopeptidases*

In “**Essays on Contemporary Peptide Science**”: 75-94 ISBN: 978-81-308-0428-6. Editor: Paul Cordopatis, **2011**.

**A4.** Makrynitsa, Garyfallia I; Lykouras, Michail; Spyroulias, Georgios A; and Matsoukas, Minos-Timotheos (August 2018), *In silico Drug Design*. In: **eLS**. John Wiley & Sons, Ltd: Chichester. DOI: 10.1002/9780470015902.a0028112

**A5.** Chasapi, Styliani; Mantzarapi, Konstantina; Karagkouni, Evdokia; Varvarigou, Natassa; Spyroulias Georgios A. *NMR and Metabollomics*. In **eLS** John Wiley & Sons, Ltd: Chichester.

### **Workshops and Training Courses:**

- **7<sup>th</sup> Chianti Workshop on Magnetic Resonance – Nuclear and Electron Relaxation** May 25-31, **1997**, San Miniato, Pisa, **Italy**.
- **Advanced Computing in NMR Spectroscopy** September 20-27, **1997**, University of Florence, **Italy**.
- **Advanced Computing in NMR Spectroscopy** September 24-28, **1999**, University of Florence, **Italy**.
- **8<sup>th</sup> Chianti Workshop on Magnetic Resonance** May 30- June 5, **1999**, San Miniato, Pisa, **Italy**.

### **Participation in Congresses and Conferences :**

Participation to ~**100** Scientific Congresses and Conferences (**60** International and **40** National – Greek) with a total number of ~**300** Communications, Abstracts and Short papers