Logo/names of your institution

University of Patras – Department of Pharmacy Group

Description of the group

The BioNMR group of the UPAT's Department of Pharmacy is led by Prof. Georgios A. Spyroulias and is recognized as National Research Infrastructure entity in two Greek RI project, in the field of Life Sciences (namely ISPIRED & OMIC-ENGINE). The group hosts unique research facilities, such as 700MHz NMR equipped with 4 channels and a cryoprobe for biomolecular studies; with applications for proteins conformational dynamics and metabolomics. The group is well equipped for the high-yield protein production, purification and characterization using a wide array of spectroscopies in addition to NMR, such as UV-visible, fluorescence, Circular Dichroism, along with other biophysical methods, such as, Size Exclusion Chromatography coupled with Multiple Angle Light/Laser Scattering, Isothermal Titration Calorimetry and Microscale Thermopheresis (anticipated by the end of 2025). Also, the group exhibit a long-term experience in the conformational dynamics of proteins involved in several signaling pathways that are related with human diseases and studies the metabolism of individuals in a number of pathological states, like Chronic Kidney Diseases, premature adrenarche, infants metabolism, etc. The group is involved in several EU and National projects and exhibits a wide network of international collaborations

The personnel involved (or to be involved) in the project

Title/Name/Surname	Email	Role	Reference Identifier	Type of Identifier
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Infrastructure available

https://bionmr.upatras.gr/research/lab-equipment/

Available research equipment at the Department of Pharmacy:

Protein Production:

- Cold room equipped with AKTA GO FPLC system,
- INFORS Bioreactor, 3x Refrigerated Incubation Shakers & autoclave
- **3x** UV-Visible Spectrometers (Jasco V-630iRM 190-1100nm & Quawell Q5000 // Q9000 micro volume & cuvette spectrometers) and 1 Fluroscence spectrometer (thermos Scientific),
- AKTApurifier 10 & AKTA PURE M25 & AKTA START FPLC systems, **(e)** Millipore Direct Q3-UV, **(f)** 2x thermal cyclers (PCR),
- 5 refrigerated centrifuges/supercentrifuge (10-45.000rpm) & 7 rotors, for small (1ml) and large volumes (100-250ml),
- Classic electrophoresis systems and Experion (patented Lab-On-Chip technology) automated gel electrophoresis systems,
- Analytical Balances, incubators, powerful sonicator system for cell lysis, water baths, -86^{o}C and -20^{o}C refrigerators, peristaltic pumps etc.
- Glove Box/Chamber with oxygen-free working environment

Structural Biology:

- High-field & high-definition Bruker 700MHz NMR, equipped with a cryogenically cooled probe for enhanced sensitivity and 4-channels ($^{1}H/^{2}H/^{13}C/^{15}N$),
- Circular Dichroism qChirascan Spectrometer by Applied Photophysics.
- Workstations for (a) Processing and analysis of NMR data (assignment of homo/hetero-nuclear multidimensional spectra, (b) Conformational analysis and structure calculation/determination (c) Alphafold2 calculations

Biophysics & Imaging:

- Size Exclusion Chromatography coupled with Multiple Angle Light Scattering (SEC-MALS)
- Micro Isothermal Titration Calorimetry (ITC)
- Imager/Gel Documentation
- Microscale Thermophoresis (anticipated at the end of 2024 – beginning of 2025)

Representative publications

1. M. Birkou, V. Raptis, K.D. Marousis, A. Tsevis, K. Bourikas, D. Bentrop, V. Episkopou, G.A. Spyroulias. *Impact of a single nucleotide polymorphism on the 3D protein structure and ubiquitination activity of E3 ubiquitin ligase Arkadia*. *Special Issue: "Insights in Structural Biology"*.
   Front. Mol. Biosci. *9,* 844129 **(2022).** 10.3389/fmolb.2022.844129
2. G. I. Makrynitsa, A.I. Argyriou, A. Zompra, K. Salagiannis, V. Vazoura, A. Papapetropoulos, S.Topouzis, G.A. Spyroulias. *Structural perspectives on sGC stimulators' binding to H-NOX domain regulated by the redox state of the heme.*
   Front. Cell Develop. Biol., Special Issue: "*Bioinorganic Chemistry of Metals in Cell Function and Disease*", *10*, 925457, **(2022)**. https://doi.org/10.3389/fcell.2022.925457
3. A.C. Tsika, A. Gallo, N.K. Fourkiotis, A.I. Argyriou, S. Sreeramulu, F. Löhr, V.V. Rogov, C. Richter, V. Linhard, S.L. Gande, N. Altincekic, R. Krishnathas, I. Elamri, H. Schwalbe, J. Wollenhaupt, M.S. Weiss, G.A. Spyroulias. *Binding adaption of GS-441524 diversifies macro domains and downregulate SARS-CoV-2 de-MARylation capacity.*
   J. Mol. Biol. *434,* 167720 **(2022).** https://doi.org/10.1016/j.jmb.2022.167720
4. COVID19-NMR Consortium, and A.C. Tsika, N.K. Fourkiotis, A. Gallo, G.A. Spyroulias. *Comprehensive fragment screening of the SARS-CoV-2 proteome explores novel chemical space for drug development.*
   Angewandte Chemie Int Ed Engl *61,* e202205858 **(2022)**. https://doi.org/10.1002/anie.202205858
5. A.I. Argyriou, G. Mahaliotis, G. I. Makrynitsa, E. Kaliatsi, C. Stathopoulos, G.A.Spyroulias. *NMR analysis suggests synergy between the RRM2 and carboxy-terminus segment of human La protein in the recognition and interaction with HCV IRES.*
   International Journal of Molecular Sciences, *Special Issue: "Research Progress in RNA-Binding Proteins,. 24,* 2572 **(2023)**. https://doi.org/10.3390/ijms24032572
6. G.N. Delegkou, M. Birkou, N. Fragkaki, T.I. Munoz Toro, K.D. Marousis, V. Episkopou, G.A. Spyroulias. *E2 partner tunes ubiquitination specificity of Arkadia E3 Ubiquitin Ligase*
   Cancers, *Special Issue on "Protein Structure and Cancer" 15*, 1040 **(2023).** https://doi.org/10.3390/cancers15041040.