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Current Focus of Research

- Design/Simulation of bioactive molecules of pharmaceutical interest and Conformational Analysis of biomolecules through Nuclear Magnetic Resonance Spectroscopy (NMR).
- Structural Bioinformatics applied in homology modeling of unknown structures of biomolecules, protein-protein/peptide/substrate interaction through molecular dynamics simulation, docking simulation protocols.
- 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.

SELECTED PUBLICATIONS

1. G.I. Makrynitsa, D. Ntonti, K.D. Marousis, M. Birkou, M.-T. Matsoukas, S. Asami, D. Bentrop, N. Papageorgiou, B. Canard, B. Coutard, G.A. Spyroulias. Conformational plasticity of the VEEV macro domain is important for binding of ADP-ribose. *Journal of Structural Biology*, 206, 119-127, (2019).
2. M.S. Twigg, L. Tripathi, A. Zompra, K. Salek, V.U. Irorere, T. Gutierrez, G.A. Spyroulias, R. Marchant, I.M. Banat. Identification and Characterisation of Short Chain Rhamnolipid Production in a Previously Uninvestigated, Non-Pathogenic Marine Pseudomonad. *Applied Microbiology and Biotechnology* 102, 8537–8549, (2018).
3. K.D. Marousis, A.C. Tsika, M. Mbirkou, M.-T. Matsoukas, G.A. Spyroulias. Lead Identification through the synergistic action of Biomolecular NMR and in silico methodologies. *Methods in Molecular Biology* 1824, 299-316, (2018).
4. D.S.M. Chatzileontiadou, A.C. Tsika, Z. Diamantopoulou, J. Delbé, J. Badet, J. Courty, V. Parmenopoulou, D. Komiotis, J.M. Hayes, G.A. Spyroulias, D.D. Leonidas. Triazole pyrimidine nucleosides are potent inhibitors of human Angiogenin in vivo. Evidence for novel action at the cell binding site revealed by heteronuclear NMR spectroscopy and modelling studies. *ChemMedChem* 13, 259-269, (2018).
5. M. Lykouras, A.C. Tsika, J. Lichièrre, N. Papageorgiou, B. Coutard, G.A. Spyroulias. NMR study of non-structural proteins - Part III. ¹H, ¹³C, ¹⁵N backbone and side-chain resonance assignment of macro domain from Chikungunya virus (VEEV). *Biomol NMR Assignments* 12, 31-35, (2018).
6. E. Zvintzou, M. Lhomme, S.A. Chasapi, S. Filou, V. Theodoropoulos, E. Xapapadaki, A. Kontush, G.A. Spyroulias, K.E. Kypreos. Pleiotropic Effects of Apolipoprotein C3 on HDL Functionality and Adipose Tissue Metabolic Activity. *Journal of Lipid Research* 58, 1869-1883, (2017).
7. M. Birkou, C.T. Chasapis, K.D. Marousis, A.K. Loutsidou, D. Bentrop, M. Leli, T.

Herrmann, Carthy JM, V. Episkopou, G.A. Spyroulias. A residue-specific insight into the Arkadia E3 ubiquitin ligase activity and conformational plasticity. *Journal of Molecular Biology* 429, 2373-2386 (2017).

8. M. Suarez-Diez, J. Adam, J. Adamski, S.A. Chasapi, C. Luchinat, A. Peters, C. Prehn, C. Santucci, A. Spyridonidis, G.A. Spyroulias, L. Tenori, R. Wang-Sattler, E. Saccenti. Plasma and serum metabolite association networks: comparability within and between studies using NMR and MS profiling. *Journal of Proteome Research* 16, 2547-2559, (2017).

9. D. Liourdi, P. Kallidonis, I. Kyriazis, A. Tsamandas, D. Karnabatidis, P. Kitrou, G.A. Spyroulias, O.N. Kostopoulou, K. Marousis, D.L. Kalpaxis, D.S. Goumenos, E. Liatsikos. Evaluation of the distribution of Paclitaxel by Immunohistochemistry and Nuclear Magnetic Resonance Spectroscopy after the application of Drug-eluting balloon in porcine ureter. *Journal of Endourology* 29, 580-589 (2015).

10. T. Katsila, G.A. Spyroulias, G.P. Patrinos, M.-T. Matsoukas. Computational approaches in target identification and drug discovery. *Computational and Structural Biotechnology Journal* 14, 177-84, (2016).

11. I. Sharina, M. Sobolevsky, A. Papakyriakou, N. Rukoyatkina, G.A. Spyroulias, S. Gambaryan, E. Martin. The fibrate gemfibrozil is an NO- and heme-independent activator of soluble guanylyl cyclase: in vitro studies. *British Journal of Pharmacology* 172, 2316-2329 (2015).

12. M. von Wantoch Rekowski, V. Kumar, Z. Zhou,; M. Bantzi, A. Marazioti, J. Moschner, G.A. Spyroulias, F. van den Akker, A. Giannis, A. Papapetropoulos. Insights into soluble guanylyl cyclase activation derived from improved heme-mimetics. *Journal of Medicinal Chemistry* 56, 8948–8952 (2013).

13. Abriata LA, Banci L, Bertini I, Ciofi-Baffoni S, Gkazonis P, Spyroulias GA, Vila AJ, Wang S. Mechanism of Cu(A) assembly. *Nat Chem Biol.* 4, 599-601 (2008).

14. A. Papakyriakou, G.A. Spyroulias, E. Sturrock, E. Manessi-Zoupa, P. Cordopatis. Simulated Interactions between Angiotensin-Converting Enzyme and Substrate Gonadotropin-Releasing Hormone: Novel Insights into Domain-Selectivity. *Biochemistry* 46, 8753-8765 (2007).

15. L. Banci, I. Bertini, S. Ciofi-Baffoni, N.G. Kandias, G.A. Spyroulias, N.J. Robinson, M. Vanarotti, X.-C. Su. The delivery of copper for thylakoid import observed by NMR. *Proc. Natl Acad Sci. USA* 103, 8320-8325 (2006).

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Tuesday 11:00-14:00 Thursday 11:00-14:00 Wednesday 11:00-14:00

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