

## Scientific production ensuing from the theses defended on the PhD programme in Theoretical Chemistry and Computational Modelling (RD99/2011)

### UIB Doctorands

| Year of viva | Doctorand           | Thesis title                                                                                                                            |
|--------------|---------------------|-----------------------------------------------------------------------------------------------------------------------------------------|
| 2021         | Rafael Ramis Cortés | On the structural and conformational effects of glycation and metal binding on the intrinsically disordered protein $\alpha$ -synuclein |

#### Ensuing scientific contributions:

Copper (II) Binding Sites in N-Terminally Acetylated  $\alpha$ -Synuclein: A Theoretical Rationalization

Ramis, R.; Ortega-Castro, J.; Vilanova, B.; Adrover, M.; Frau, J.  
Journal of Physical Chemistry A (2017), 121, 5711-5719

A Systematic DFT Study of Some Plausible Zn (II) and Al (III) Interaction Sites in N-Terminally Acetylated  $\alpha$ -Synuclein

Ramis, R.; Ortega-Castro, J.; Vilanova, B.; Adrover, M.; Frau, J.  
Journal of Physical Chemistry A (2018), 122, 690-699

Does Glycation Really Distort the Peptide  $\alpha$ -helicity?

Marino, L.; Casasnovas, R.; Ramis, R.; Vilanova, B.; Ortega-Castro, J.; Frau, J.; Adrover, M.

International Journal of Biological Macromolecules (2019), 129, 254-266

A Coarse-Grained Molecular Dynamics Approach to the Study of the Intrinsically Disordered Protein  $\alpha$ -Synuclein

Ramis, R.; Ortega-Castro, J.; Casasnovas, R.; Marino, L.; Vilanova, B.; Adrover, M.; Frau, J.

Journal of Chemical Information and Modelling (2019), 59, 1458-1471

Unravelling the Effect of N( $\epsilon$ )-(carboxyethyl)lysine on the Conformation, Dynamics and Aggregation Propensity of  $\alpha$ -Synuclein  
Marino, L.; Ramis, R.; Casanovas, R.; Ortega-Castro, J.; Vilanova, B.; Frau, J.; Adrover, M.  
Chemical Science (2020), 11, 3332-3344

Unravelling the NaCl Concentration Effect on the First Stages of  $\alpha$ -Synuclein Aggregation  
Ramis, R.; Ortega-Castro, J.; Vilanova, B.; Adrover, M.; Frau, J.  
Biomacromolecules (2020), 21, 5200-5212

Cu<sup>2+</sup>, Ca<sup>2+</sup>, and Methionine Oxidation Expose the Hydrophobic  $\alpha$ -synuclein NAC Domain  
Ramis, R.; Ortega-Castro, J.; Vilanova, B.; Adrover, M.; Frau, J.  
International Journal of Biological Macromolecules (2021), 169, 251-263.

## Scientific production ensuing from the theses defended on the PhD programme in Theoretical Chemistry and Computational Modelling (RD1393/2007))

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| Year of viva | Doctorand               | Thesis title                                                                                                                                                                                                                                        |
|--------------|-------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 2017         | David Fernández Payeras | Deciphering the molecular descriptors that modulate the therapeutic applications of bisphosphonates as pathological deposition inhibitors and antiresorptive bone drugs for further rational design of new drugs based on crystal growth inhibitors |

### Ensuing scientific contributions:

Human Farnesyl Pyrophosphate Synthase Inhibition by Nitrogen Bisphosphonates: A 3D-QSAR Study  
Fernández, D.; Ortega-Castro, J.; Frau, J.  
Journal of Computer-Aided Molecular Design (2013), 27, 739-754

Mechanistic Insights into Protonation State as a Critical Factor in hFPPS Enzyme Inhibition

Fernández, D.; Ortega-Castro, J.; Mariño, L.; Perelló, J.; Frau, J.

Journal of Computer-Aided Molecular Design (2015), 29, 667-680

Theoretical Study of the Deposition and Adsorption Bisphosphonates on the 001 Hydroxyapatite Surface: Implications in the Pathological Crystallization Inhibition and the Bone Antiresorptive Action

Fernández, D.; Ortega-Castro J.; Frau, J.

Applied Surface Science (2017), 392. 204-214

Theoretical Study of the HAP Crystal Growth Inhibition Potency of Pyrophosphate, Etidronate, Citrate and Phytate. Deciphered the Adsorbed Conformation of Phytate on the HAP (001) Surface

Fernández, D.; Ortega-Castro, J.; Frau, J.

Applied Surface Science (2017), 408, 110-116

New Insights into Human Farnesyl Pyrophosphate Synthase Inhibition by Second-generation Bisphosphonate Drugs

Fernández, D.; Ramis, R.; Ortega-Castro, J.; Casanovas, R.; Vilanova, B.; Frau, J.

Journal of Computer-Aided Molecular Design (2017), 31, 675-688

| Year of viva | Doctorand              | Thesis title                                                                                                                                                          |
|--------------|------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 2014         | Christian Solis Calero | Estudio DFT de la reactividad sobre superficies aminofosfolipidicas. Mecanismo de reacciones relacionadas con la generación de productos de glicación avanzada (AGEs) |

#### Ensuing scientific contributions:

Reactivity of a Phospholipid Monolayer Model under Periodic Boundary Conditions: A Density Functional Theory Study of the Schiff Base Formation between Phosphatidylethanolamine and Acetaldehyde

Solis-Calero, C., Ortega-Castro, J., Muñoz, F.

J. Phys Chem. (2010), 114, 15879-15885

DFT Study on Amino-Phospholipids Surface-Mediated Decomposition of Hydrogen Peroxide

Solis-Calero, C.; Ortega-Castro, J.; Munoz, F.

Journal of Physical Chemistry C (2011), 115, 22945-22953

A Comparative DFT Study of the Schiff Base Formation from Acetaldehyde and Butylamines, Glycine and Phosphatidylethanolamine

Solis-Calero, C., Ortega-Castro, J., Hernández-Laguna, A., Muñoz, F.

Theor. Chem. Acc. (2012), 131, 1263-1275

A DFT Study of the Amadori Rearrangement above a Phosphatidylethanolamine Surface: Comparison to Reactions in Aqueous Environment

Solis-Calero, C., Ortega-Castro, J., Hernández-Laguna, A., Muñoz, F.

J. Phys. Chem. C (2013), 117, 8299-8309

DFT Study of the Mechanism of the Reaction of Aminoguanidine with Methylglyoxal

Solis-Calero, C.; Ortega-Castro, J.; Hernandez-Laguna, A.; Munoz, F.

Journal of Molecular Modelling (2014), 20, 1

A DFT Study of the Carboxymethyl-phosphatidylethanolamine Formation from Glyoxal and Phosphatidylethanolamine Surface. Comparison with the Formation of N(e)-(carboxymethyl)lysine from Glyoxal and l-lysine

Solis-Calero C.; Ortega-Castro J.; Hernández-Laguna A.; Frau J.; Muñoz, F.

Physical Chemistry Chemical Physics (2015), 17, 8210-8222

Scavenger Mechanism of Methylglyoxal by Metformin. A DFT Study

Solis-Calero, C.; Ortega-Castro, J.; Frau, J.; Muñoz, F.

Theoretical Chemistry Accounts (2015), 134, 48

Nonenzymatic Reactions above Phospholipid Surfaces of Biological Membranes.

Reactivity of Phospholipids and their Oxidation Derivatives

Solis Calero, C.; Ortega Castro, J.; Frau, J.; Muñoz, F.

Oxidative Medicine and Cellular Longevity (2015), 2015, 319505

| Year of viva | Doctorand                 | Thesis title                                                                              |
|--------------|---------------------------|-------------------------------------------------------------------------------------------|
| 2014         | Rodrigo Casasnovas Perera | Theoretical studies on pyridoxal 5'-phosphate catalyzed reactions of biological relevance |

#### Ensuing scientific contributions:

Theoretical Study on the Distribution of Atomic Charges in the Schiff Bases of 3-hydroxypyridine-4-aldehyde and Alanine. The Effect of the Protonation State of the Pyridine and Imine Nitrogen Atoms

Casasnovas, R.; Salvà, A.; Frau, J.; Donoso, J.; Muñoz, F.  
Chemical Physics (2009), 355, 149-156

Absolute and Relative pKa Calculations of Mono and Diprotic Pyridines by Quantum Methods

Casasnovas, R.; Frau, J.; Ortega-Castro, J.; Salvà, A.; Donoso, J.; Muñoz, F.  
Journal of Molecular Structure-Theochem (2009), 912, 5-12

Simplification of the CBS-QB3 Method for Predicting Gas-Phase Deprotonation Free Energies

Casasnovas, R.; Frau, J.; Ortega-Castro, J.; Salvà, A.; Donoso, J.; Muñoz, F.  
International Journal of Quantum Chemistry (2010), 110, 323-330

Avoiding Gas-phase Calculations in Theoretical pKa Predictions

Casasnovas, R.; Fernández, D.; Ortega-Castro, J.; Frau, J.; Donoso, J.; Muñoz, F.  
Theoretical Chemistry Accounts (2011), 130, 1-13

C-H Activation in Pyridoxal-5'-phosphate Schiff Bases: The Role of the Imine Nitrogen. A Combined Experimental and Computational Study

Casasnovas, R.; Adrover, M.; Ortega-Castro, J.; Frau, J.; Donoso, J.; Muñoz, F.  
Journal of Physical Chemistry B (2012), 116, 10665-10675

C-H Activation in Pyridoxal-5'-phosphate and Pyridoxamine-5'-Phosphate Schiff Bases: Effect of Metal Chelation. A Computational Study

Casasnovas, R.; Frau, J.; Ortega-Castro, J.; Donoso, J.; Muñoz, F.  
Journal of Physical Chemistry B (2013), 117, 2339-2347



Theoretical Calculations of Stability Constants and pKa Values of Metal Complexes in Solution: Application to Pyridoxamine Copper(II) Complexes and their Biological Implications in AGE Inhibition

Casasnovas, R.; Ortega-Castro, J.; Donoso, J.; Frau, J.; Muñoz, F.  
Physical Chemistry Chemical Physics (2013), 15, 16303-16313

Theoretical pKa Calculations with Continuum Model Solvents, Alternative Protocols to Thermodynamic Cycles

Casasnovas, R.; Ortega-Castro, J.; Frau, J.; Donoso, J.; Muñoz, F.  
International Journal of Quantum Chemistry (2014), 114, 1350-1363