Producción científica derivada de las tesis defendidas en el programa de Doctorado en Química Teórica y Modelización Computacional / Theoretical Chemistry and Computational Modelling (RD 99/2011)

Doctorandos de la UIB

Año de defensa	Doctorando/a	Título de la tesis
2021	Rafael Ramis Cortés	On the structural and conformational effects of glycation and metal binding on the intrinsically disordered protein α-synuclein

Contribuciones científicas derivadas:

Copper (II) Binding Sites in N-Terminally Acetylated α-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 α-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 α-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 α-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(ε)-(carboxyethyl)lysine on the conformation, dynamics and aggregation propensity of α-synuclein
Marino, L.; Ramis, R.; Casasnovas, 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 α-Synuclein Aggregation
Ramis, R.; Ortega-Castro, J.; Vilanova, B.; Adrover, M.; Frau, J.
Biomacromolecules (2020), 21, 5200-5212

Cu2+, Ca2+, and methionine oxidation expose the hydrophobic α-synuclein NAC domain
Ramis, R.; Ortega-Castro, J.; Vilanova, B.; Adrover, M.; Frau, J.
International Journal of Biological Macromolecules (2021), 169, 251-263.

Producción científica derivada de las tesis defendidas en el programa de Doctorado en Química Teórica y Modelización Computacional (RD 1393/2007)

Año de defensa	Doctorando/a	Título de la tesis
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

Contribuciones científicas derivadas:

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.; Casasnovas, R.; Vilanova, B.; Frau, J.
Journal of Computer-Aided Molecular Design (2017), 31, 675-688

Año de defensa	Doctorando/a	Título de la tesis
2014	Christian Solis Calero	Estudio DFT de la reactividad sobre superficies aminofosfolipídicas. Mecanismo de reacciones relacionadas con la generación de productos de glicación avanzada (AGE)

Contribuciones científicas derivadas:

Reactivity of a Phospholipid Monolayer model under periodic boundary conditions: a density functional theory study of the Schiff Base Formation between Phophatidylethanoamine 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.; Muñoz, 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.; Hernández-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

Año de defensa	Doctorando/a	Título de la tesis
2014	Rodrigo Casasnovas Perera	Theoretical studies on pyridoxal 5'-phosphatecatalyzed reactions of biological relevance

Contribuciones científicas derivadas:

Theoretical study on the distribution of atomic charges in the Schiff bases of 3-hydroxypyrine-4-aldehyde and alanine. The effect of the protonation state of the pyridine and imine nitrogen atoms.
Casanovas, 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 p*K*a 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