

Date of the CVA

07/10/2021

Section A. PERSONAL DATA

Name and Surname	JOAQUÍN ORTEGA CASTRO		
DNI	44292759A	Age	45
Researcher's identification number	Researcher ID	L-4956-2014	
	Scopus Author ID		
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* Obligatorio

A.1. Current professional situation

Institution	Universidad de las Islas Baleares		
Dpt. / Centre	Faculty of Sciences / Department of Chemistry		
Address	Edifici Mateu Orfila i Rotger, Campus universitari. Cra. de Valldemossa, km 7.5, Palma, (Illes Balears)., 07122, Palma		
Phone	971259833 - 9833	Email	joaquin.castro@uib.es
Professional category	Senior university lecturer	Start date	2017
Keywords			

A.2. Academic education (Degrees, institutions, dates)

Bachelor/Master/PhD	University	Year
Doctor en Ciencias Químicas	Universidad de Granada	2007
Licenciatura de Ciencias Químicas	Universidad de Granada	2002

Section C. MOST RELEVANT MERITS (ordered by typology)

C.1. Publications

AC: Autor de correspondencia; (nº x / nº y): posición firma solicitante / total autores

- Scientific paper.** Ahmed, F.; Ortega-Castro, J.; Frontera, A.; Mir, M.H.(0/4). 2021. Semiconducting properties of pyridyl appended linear dicarboxylate based coordination polymers: Theoretical prediction: Via DFT study 912705 - Dalton Transactions. 50-1, pp.270-278. ISSN 1477-9226.
- Scientific paper.** Hossain, A.; Dey, A.; Seth, S.K.; Ray, P.P.; Ortega-Castro, J.; Frontera, A.; Mukhopadhyay, S.(0/7). 2021. Anion-dependent structural variations and charge transport property analysis of 4-(3-pyridyl)-4,2:6,4-terpyridinium salts 912697 - Crystengcomm. 23-19, pp.3569-3581. ISSN 1466-8033.
- Scientific paper.** Ramis, R.; Ortega-Castro, J.; Vilanova, B.; Adrover, M.; Frau, J.(0/5). 2021. Cu²⁺, Ca²⁺, and methionine oxidation expose the hydrophobic -synuclein NAC domain 900293 - International Journal of Biological Macromolecules. 169, pp.251-263. ISSN 0141-8130.
- Scientific paper.** Dbuleanu, D.; Bauzá, A.; Ortega-Castro, J.; Escudero-Adán, E.C.; Ballester, P.; Frontera, A.(0/6). 2020. Synthesis, X-ray Characterization and Density Functional Theory (DFT) Studies of Two Polymorphs of the ,,, Isomer of Tetra-p-Iodophenyl Tetramethyl Calix[4]pyrrole: On the Importance of Halogen Bonds 910462 - Molecules. MDPI. 25-2. ISSN 1420-3049.
- Scientific paper.** Martínez, D.; Pérez, A.; Cañellas, S.; et al; Frontera, A.(0/12). 2020. Synthesis, reactivity, X-ray characterization and docking studies of N7/N9- (2-pyrimidyl)-adenine derivatives 900757 - Journal of Inorganic Biochemistry. 203, pp.110879. ISSN 0162-0134.
- Scientific paper.** García-Raso, A.; Terrón, A.; Ortega-Castro, J.; et al; Fiol, J.J.(0/10). 2020. Iridium(III) coordination of N(6)modified adenine derivatives with aminoacidchains 900757 - Journal of Inorganic Biochemistry. 205, pp.111000. ISSN 0162-0134.

- 7 **Scientific paper.** Marino, L.; Ramis, R.; Casanovas, R.; Ortega-Castro, J.; Casanovas, R.; Vilanova, B.; Frau, J.; Adrover, M.(4/8). 2020. Unravelling the effect of N(ϵ)-(carboxyethyl)lysine on the conformation, dynamics and aggregation propensity of α -synuclein 915573 - Chemical Science. Royal Society of Chemistry. 11, pp.3332-3344. ISSN 2041-6520.
- 8 **Scientific paper.** Miquel Oliver; Miquel Adrover; Antonio Frontera; Joaquin Ortega-Castro; Manuel Miró*. (0/5). 2020. In-vitro prediction of the membranotropic action of emerging organic contaminants using a liposome-based multidisciplinary approach 901502 - Science of the Total Environment. Elsevier B.V.. 738, pp.140096. ISSN 0048-9697.
- 9 **Scientific paper.** Saha, D.; Gayen, S.; Maity, T.; et al; Koner, S.(0/10). 2020. Combined experimental and computational studies on preferential CO₂ adsorption over a zinc-based porous framework solid 900672 - New Journal of Chemistry. 44-5, pp.1806-1816. ISSN 1144-0546.
- 10 **Scientific paper.** Rafael Ramis; Joaquín Ortega-Castro; Bartolomé Vilanova; Miquel Adrover; Juan Frau. (0/5). 2020. Unraveling the NaCl Concentration Effect on the First Stages of α -Synuclein Aggregation 910816 - Biomacromolecules. 21, pp.5200-5212. ISSN 1525-7797.
- 11 **Scientific paper.** Rafael Ramis; Joaquín Ortega-Castro; Bartolomé Vilanova; Miquel Adrover; Juan Frau. (0/). 2020. Cu²⁺, Ca²⁺, and methionine oxidation expose the hydrophobic α -synuclein NAC domain 900293 - International Journal of Biological Macromolecules. 169, pp.251-263. ISSN 0141-8130.
- 12 **Scientific paper.** Ramis, R.; Casanovas R.; Ortega-Castro, J.; Frau J.; Alvarez-Idaboy J.R.; Mora-Diez N.(0/6). 2019. Modelling the repair of carbon-centred protein radicals by the antioxidants glutathione and Trolox 900672 - New Journal of Chemistry. 43, pp.2085-2097. ISSN 1144-0546.
- 13 **Scientific paper.** Ramis, R.; Casanovas, R.; Marino, L.; Frau, J.; Adrover, M.; Vilanova, B.; Mora-Diez, N.; Ortega-Castro, J.(0/8). 2019. A density functional theory study of the free-radical scavenging activity of aminoguanidine. Comparison with its reactive carbonyl compound and metal scavenging activities 900829 - International Journal of Quantum Chemistry. 119. ISSN 0020-7608.
- 14 **Scientific paper.** Laura Mariño; Rodrigo Casanovas; Rafael Ramis; Bartolomé Vilanova; Joaquín Ortega-Castro; Juan Frau; Miquel Adrover. (0/7). 2019. Does glycation really distort the peptide α -helicity? 900293 - International Journal of Biological Macromolecules. 129, pp.254-266. ISSN 0141-8130.
- 15 **Scientific paper.** Rafael Ramis; Joaquín Ortega-Castro; Rodrigo Casanovas; Laura Mariño; Bartolomé Vilanova; Miquel Adrover; Juan Frau. (0/7). 2019. A Coarse-grained molecular dynamics approach to the study of the intrinsically disordered protein α -synuclein 913199 - Journal Of Chemical Information And Modeling. 59-4, pp.1458-1471. ISSN 1549-9596.
- 16 **Scientific paper.** T. Mandal; S. Pathak; A. Dey; et al; S. Mukhopadhyay.(0/). 2019. Structure, Photo Response Properties and Biological Activity of Dicyano-substituted 4-Aryl-2-Pyridone Derivatives.919226 - Acs Omega. 4-4, pp.7200-7212. ISSN 2470-1343.
- 17 **Scientific paper.** Mandal, T.; Dey, A.; Pathak, S.; et al; Mukhopadhyay, S.(0/). 2019. Structures, photoresponse properties and DNA binding abilities of 4-(4-pyridinyl)-2-pyridone salts 917082 - Rsc Advances. 9, pp.9663-9677. ISSN 2046-2069.
- 18 **Scientific paper.** Mandal, T.; Pathak, S.; Dey, A.; et al; Mukhopadhyay, S. (0/). 2019. Structures, Photoresponse Properties, and Biological Activity of Dicyano-Substituted 4-Aryl-2-pyridone Derivatives 919226 - Acs Omega. 4, pp.7200-7212. ISSN 2470-1343.
- 19 **Scientific paper.** Ramis, R.; Ortega-Castro, J.; Caballero, C.; Casanovas, R.; Cerrillo, A.; Vilanova, B.; Adrover, M.; Frau, J. (0/8). 2019. How does pyridoxamine inhibit the formation of advanced glycation end products? the role of its primary antioxidant activity 919088 - Antioxidants. 8, pp.344. ISSN 2076-3921.

- 20 **Scientific paper.** Humberto Martínez-Orozco; Laura Mariño; Ana Belén Uceda; Joaquín Ortega-Castro; Bartolomé Vilanova; Juan Frau; Miquel Adrover. (0/). 2019. Nitration and Glycation Diminish the α -Synuclein Role in the Formation and Scavenging of Cu^{2+} -Catalyzed Reactive Oxygen Species 915369 - Acs Chemical Neuroscience. 10-6, pp.2919-2930. ISSN 1948-7193.
- 21 **Scientific paper.** N. Hernandez-Haro; J. Ortega-Castro; Y.B. Martynov; R. G. Nazmitdinov; A. Frontera. (2/5). 2019. DFT prediction of band gap in organic-inorganic metal halide perovskites: An exchange-correlation functional benchmark study.903310 - Chemical Physics. 516, pp.225-231. ISSN 0301-0104.
- 22 **Scientific paper.** Ghosh, K.; Sil, S.; Ray, P.P.; Ortega-Castro, J.; Frontera, A.; Chattopadhyay, S.(4/6). 2019. Photosensitive Schottky barrier diode behavior of a semiconducting Co(III)-Na complex with a compartmental Schiff base ligand 917082 - Rsc Advances. 9-60, pp.34710-34719. ISSN 2046-2069.
- 23 **Scientific paper.** Rafael Ramis; Rodrigo Casasnovas; Laura Mariño; Juan Frau; Miquel Adrover; Bartolomé Vilanova; Nelaine Mora-Diez; Joaquín Ortega-Castro. (0/8). 2019. A Density functional theory study of the free-radical scavenging activity of aminoguanidine. Comparison with its reactive carbonyl compound and metal scavenging activities.900829 - International Journal of Quantum Chemistry. 119, pp.1-8. ISSN 0020-7608.
- 24 **Scientific paper.** R. Ramis; J. Ortega-Castro; C. Caballero; R. Casasnovas; A. Cerrillo; B. Vilanova; M. Adrover; J. Frau.(0/8). 2019. How does pyridoxamine inhibit the formation of advanced glycation end products? The role of its primary antioxidant activity 919088 - Antioxidants. 8, pp.344. ISSN 2076-3921.
- 25 **Scientific paper.** Martinez-Orozco, H.; Marino, L.; Uceda, A.B.; Ortega-Castro, J.; Vilanova, B.; Frau, J.; Adrover, M.(0/7). 2019. Nitration and Glycation Diminish the α -Synuclein Role in the Formation and Scavenging of Cu^{2+} -Catalyzed Reactive Oxygen Species 915369 - Acs Chemical Neuroscience. 10, pp.2919-2930. ISSN 1948-7193.
- 26 **Scientific paper.** Ramis, R.; Ortega-Castro, J.; Casasnovas, R.; Marino, L.; Vilanova, B.; Adrover, M.; Frau, J.(0/7). 2019. A Coarse-Grained Molecular Dynamics Approach to the Study of the Intrinsically Disordered Protein α -Synuclein 913199 - Journal Of Chemical Information And Modeling. 59, pp.1458-1471. ISSN 1549-9596.
- 27 **Scientific paper.** Ramis, R.; Ortega-Castro, J.; Vilanova, B.; Adrover, M.; Frau, J.(0/ 5). 2018. A Systematic DFT study of some plausible Zn(II) and Al(III) interaction sites in N-terminally acetylated α -synuclein 909612 - Journal of Physical Chemistry A. 122-2, pp.690-699. ISSN 1089-5639.
- 28 **Scientific paper.** Konar, S.; Dey, A.; Ray, S.; et al; Mukhopadhyay, S.(0/). 2018. Two Zinc(II)-Based Metal Complexes of New Pyrimidine Derived Ligand: Anion-Dependent Structural Variations and Charge Transport Property Analysis 914198 - Journal Of Physical Chemistry C. 122, pp.8724-8734. ISSN 1932-7447.
- 29 **Scientific paper.** Hossain, A.; Dey, A.; Seth, S. K.; et al; Mukhopadhyay, S.(0/). 2018. Enhanced Photosensitive Schottky Diode Behavior of Pyrazine over 2-Aminopyrimidine Ligand in Copper(II)-Phthalate MOFs: Experimental and Theoretical Rationalization 919226 - Acs Omega. 3, pp.9160-9171. ISSN 2470-1343.
- 30 **Scientific paper.** David Fernández; Joaquín Ortega-Castro; Juan Frau. (0/ 3). 2017. Theoretical study of the deposition and adsorption of bisphosphonates on the 001 hydroxyapatite surface: Implications in the pathological crystallization inhibition and the bone antiresorptive action 903326 - Applied Surface Science. 392, pp.204-214. ISSN 0169-4332.
- 31 **Scientific paper.** Halder, S.; Mondal, J.; Ortega-Castro, J.; Frontera, A.; Roy, P.(0/). 2017. A Ni-based MOF for selective detection and removal of Hg^{2+} in aqueous medium: a facile strategy 912705 - Dalton Transactions. 46, pp.1943. ISSN 1477-9226.
- 32 **Scientific paper.** D. Fernández; J. Ortega-Castro; J. Frau. (0/). 2017. 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 903326 - Applied Surface Science. 408, pp.110-116. ISSN 0169-4332.
- 33 **Scientific paper.** D. Fernández; R. Ramis; J. Ortega-Castro; R. Casasnovas; B. Vilanova; J. Frau. (0/6). 2017. New insights into human farnesyl pyrophosphate synthase inhibition by second-generation bisphosphonate drugs 904209 - Journal of Computer-Aided Molecular Design. 31, pp.675-688. ISSN 0920-654X.

- 34 Scientific paper.** Laura Mariño; Carlos Andrés Maya- Aguirre; Kris Pauwels; Bartolomé Vilanova; Joaquín Ortega-Castro; Juan Frau; Josefa Donodo; Miquel Adrover. (0/8). 2017. Glycation of Lysozyme by Glycolaldehyde Provides New Mechanistic Insights in Diabetes-Related Protein Aggregation 913322 - Acs Chemical Biology. 12-6, pp.1152-2017. ISSN 1554-8929.
- 35 Scientific paper.** B. Vilanova; D. Fernández; R. Casasnovas; et al; J. Ortega-Castro. (12/12). 2017. Formation mechanism of glyoxal-DNA adduct, a DNA cross-link precursor 900293 - International Journal of Biological Macromolecules. 98, pp.664-675. ISSN 0141-8130.
- 36 Scientific paper.** Ramis, R.; Ortega-Castro, J.; Vilanova, B.; Adrover, M.; Frau, J.(0/). 2017. Copper(II) binding sites in N-terminally acetylated α -synuclein: a theoretical rationalization 909612 - Journal of Physical Chemistry A. 121, pp.5711-5719. ISSN 1089-5639.
- 37 Scientific paper.** Halder, S.; Dey, A.; Bhattacharjee, A.; Ortega-Castro, J.; Frontera, A.; Ray, P. P.; Roy, P.(0/). 2017. A Cd(II)-based MOF as a photosensitive Schottky diode: experimental and theoretical studies 912705 - Dalton Transactions. 46, pp.11239-11249. ISSN 1477-9226.
- 38 Scientific paper.** N. Hernández-Haro; D. Muñoz-Santiburcio; C. Pérez del Valle; J. Ortega-Castro; C. I. Sainz-Díaz; C. J. Garrido; A. Hernández-Laguna.(4/7). 2016. Compressibility of 2M1 muscovite-paragonite series minerals: A computational study to 6GPa.901670 - American Mineralogist. 101-5, pp.1207-1216. ISSN 0003-004X.
- 39 Scientific paper.** Halder, S.; Dey, A.; Ortega-Castro, J.; Frontera, A.; Ray, P. P.; Roy, P.(3/6). 2016. Irradiation Specified Conformational Change in a Small Organic Compound and Its Effect on Electrical Properties 914198 - Journal Of Physical Chemistry C. 120-44, pp.25557-25563. ISSN 1932-7447.
- 40 Scientific paper.** Roy, S.; Dey, A.; Ray, P.P.; Ortega-Castro, J.; Frontera, A.; Chattopadhyay, S.(4/6). 2015. Application of a novel 2D cadmium(II)-MOF in the formation of a photo-switch with substantial on off ratio 909184 - Chemical Communications. Royal Society of Chemistry. pp.12974-12976. ISSN 1359-7345.

C.2. Participation in R&D and Innovation projects

- 1** CTQ2014-55835-R, Relación entre la diabetes mellitus y la enfermedad del Parkinson: estudio de los mecanismos moleculares que inducen la glicación y agregación de la alfa-sinucleína. Acrónimo: DIMEPARK Ministerio de Economía y Competitividad (MINECO). Juan Frau Munar; Bartolomé Vilanova Canet. (Universidad de las Islas Baleares). 01/01/2015-31/12/2018. 76.230 €.
- 2** CTQ2008 02207, Estudio de la inhibición de la Formación de ALE Ministerio de Educación y Ciencia. Francisco Muñoz Izquierdo. (Universidad de las Islas Baleares). 01/01/2009-31/12/2011. 114.950 €.
- 3** PROGEICB 28 A, Estudio de los mecanismo de inhibición de la formación de los AGEs asociados a los estados de hiperglucemia Conselleria d'Economia, Hisenda i Innovació. Govern de les Illes Balears. Juan Frau Munar. (Universidad de las Islas Baleares). 01/01/2007-31/12/2008. 32.500 €.
- 4** CGL2005-02681/BTE, "Investigación teórica de la influencia de la sustitución isomórfica de cationes sobre los mecanismos de las reacciones de deshidroxilación de silicatos laminares" Plan Nacional de Investigación y Desarrollo. Alfonso Hernández Laguna. (Universidad de las Islas Baleares). 2005-2008. 65.000 €.
- 5** BTE2002-03838, Efecto de la sustitución isomórfica de cationes y su distribución sobre las propiedades cristalográficas y las reacciones de deshidroxilación en silicatos laminares DGI. Alfonso Hernández Laguna. (Universidad de las Islas Baleares). 2002-2006. 103.155 €.