Dr. José Pedro Cerón-Carrasco

Contact Information

Reconocimiento y Encapsulación Molecular
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Research Experience

Modeling complex problems with computational approaches

- My main line of research is the study of the interactions of biosystems (DNA and targeted proteins) with external agents, e.g., drugs, free radicals and electric fields.
- Additionally, I have developed theoretical strategies to characterize the antioxidant properties of natural products, to simulate the electronic properties of organic molecules used in optical materials, and to assess novel encapsulation technologies.
- In the framework of drug, I adapted a computational strategy to design a novel drug against Zika Virus through an international collaboration between my current group and the University of Hong Kong. The results were patented and licensed by the American biopharma company.
- I have also experienced in modeling metallodrugs based on platinum with experimental groups, including a collaboration with Prof. Maria Contel at the City University of New York.
- My experience includes but is not limited to:

  (i) DNA: mutation, adiation damaged, metal-DNA interactions, antitumoural agents, carrier molecules, antibody-drug interactions

  (ii) Natural products: free radical reactivity, absorption and emission spectra, antioxidant power, protein binding pocket, hydrogen-bonds

  (iii) Reactivity: heterogeneous catalysis, organometallic compounds, new materials, optoelectronic properties

  (iv) Levels of theory: molecular dynamics, density functional theory (DFT), hybrid QM:MM methods, explicit/implicit solution models

Academic Appointments

I am currently working as a Scientist at UCAM while teaching Organic Chemistry in Pharmacy Degree and in other PhD and Master courses.

Full Scientist, July 2015 to present
Reconocimiento y Encapsulación Molecular (REM)
Universidad Católica San Antonio de Murcia,Spain
– "Searching new drugs by using Quantum Chemistry"

Postdoctoral Researcher, July 2013 to June 2015
Quantum Chemistry, Molecular Spectroscopy and Laser Group,
Universidad de Murcia, Spain
– Founded by Marie Curie Actions, FP7-UIMPACT Program
– "Antitumoral Drugs and Theoretical Simulations"
– Supervisors: Prof. Alberto Requena and Prof. José Zúñiga

Postdoctoral Researcher, January 2011 to June 2013
CEISAM laboratory: Interdisciplinary Chemistry: Synthesis, Analysis and Modeling, Université de Nantes, France
- Funded by Fundación Séneca and Université de Nantes
- "Modeling Biological Environments: Antitumoral Drugs"
- Supervisor: Prof. Denis Jacquemin

Postdoctoral Researcher, May 2009 to December 2010
Laboratoire de Chimie Théorique Apliquée, Université de Namur, Belgium
- Researcher Grant (2010)
- Funded by Fundación Esteban Romero
- "Computational Study of the Spontaneous Mutation Processes in RNA/DNA"
- Host: Prof. Jean-Marie André Group

Education

Universidad de Murcia, Murcia, Spain

Ph.D., Computational and Theoretical Chemistry, May 2009

- Thesis Topic: *Theoretical Modeling in Biological Environments: Study of the Interactions Between DNA Base Pairs and the Antioxidant Character of Carotenoids*
- Mark: *Summa cum Laude*, With Honors in Chemistry
- European Mention
- Quanlity distinction: Doctorate Extraordinary Award, best PhD Thesis
- Doctoral Supervisors: Prof. Alberto Requena and Prof. José Zúñiga
- Area of Study: Computational Chemistry

M.S., Chemistry, October 2006

- Thesis Topic: *DFT Study and Vibrational Spectroscopic Analysis of β-Carotene, Capsanthin and Capsorubin*
- Supervisor: Professor Alberto Requena
- Area of Study: Computational Chemistry, Vibrational Spectroscopy

B.S., Chemistry, September 2004

- Advanced Fundamental Chemistry Specialization
- Intern in the Department of Physical Chemistry, 2004
- Intern in the Department of Inorganic Chemistry, 1999–2003

Language skills

Language	Speaking	Reading	Writing
Spanish	G	G	G
English	G	G	G
French	F	F	F

(S=sufficient, F=fair ,G=good)

Experience in Science and Technology: Participation in I+D Projects

Title: Molecular Astrophysics: The Herschel and Alma Era
- Funding Institution: Consejo Superior de Investigaciones CientÃficas
- Project leader: José Cernicharo Quintanilla
- Number of participating researchers: 90
- From: 01/01/2010 to: 31/12/2014
- Funding amount: 400000 euros

Title: Redistribution of intramolecular vibrational energy in molecules with peptide bonds
- Funding Institution: Ministerio de Educación y Ciencia
- Project leader: Alberto Requena Rodríguez
- Number of participating researchers: 6
- From: 01/10/2007 to: 30/09/2010
- Funding amount: 60500 euros

Title: Enhancing the Therapeutical Properties of Antitumoural Drugs with Computational Chemistry
- Funding Institution: FP7 Marie Curie Actions
- Project leader: José PedroCerón-Carrasco
- Number of participating researchers: 3
- From: 01/07/2013 to: 30/06/2015
- Funding amount: 88300 euros

Title: Discovery of Novel Blood Anticoagulants using Hybrid Artificial Intelligence Techniques
- Funding Institution: EEAA GRANTS
- Project leader: Horacio Pérez
- Number of participating researchers: 5
- From: 01/10/2014 to: 31/12/2015
- Funding amount: 36190 euros

Title: Molecular Design of novel Anti-inflammatories
- Funding Institution: Dirección General de Deportes, Región de Murcia
- Project leader: José PedroCerón-Carrasco
- Number of participating researchers: 5
- From: 01/10/2015 to: 30/09/2016
- Funding amount: 5000 euros

Title: Assembling carrier molecules, active ligands and transition metal in a novel antitumoural drug
- Funding Institution: Fundacón Séneca–Agencia de Ciencia y Tecnología de Murcia
- Project leader: José Pedro Cerón-Carrasco
- Number of participating researchers: 5
- From: 01/07/2015 to: 30/06/2017
- Funding amount: 19000 euros

Title: Blind Docking Transfer Technology
- Funding Institution: EuroLab-4-HPC Business Prototyping: Call 2017
- Entrepreneurial leader: José PedroCerón-Carrasco
- Number of participating researchers: 3
- From: 01/05/2017 to: 31/07/2017
- Funding amount: 25000 euros

Title: Design of novel online computational tools and web server whiting the framework of drug design
- Funding Institution: Ministerio de Ciencia, Innovación y Universidades
- Project leader: Horacio Sánchez-Pérez
- Number of participating researchers: 12
- From: 01/07/2018 to: 30/06/2021
- Funding amount: 71000 euros

Title: Potential Metal-based cancer chemotherapeutics
- Funding Institution: Fundacón Séneca–Agencia de Ciencia y Tecnología de Murcia
- Project leader: José PedroCerón-Carrasco
- Number of participating researchers: 4
- From: 01/05/2019 to: 31/07/2019
- Funding amount: 7950 euros

Refereed Journal Publications

I am the main author in most of my works, including the eight papers highlighted as covers. My last collaborations with experimental colleges have lead to papers in Nature Chemical Biology and Angewandte International.

[1] A. Requena*, J. P.Cerón-Carrasco, A. Bastida, J. Zúñiga* and J. B. Miguel. A Density Functional Theory Study of the Structure and Vibrational Spectra of $\beta-$carotene, capsanthin and capsorubin. *Journal of Physical Chemistry A*, 112, 4815 (2008) IF=2.775

[2] J. P.Cerón-Carrasco*, A. Requena, C. Michaux, E. A. Perpète and D. Jacquemin. Effects of Hydration on the Proton Transfer Mechanism in the Adenine-Thymine Base Pair. *Journal of Physical Chemistry A*, 113, 7892 (2009) IF=2.775

[3] J. P.Cerón-Carrasco*, A. Bastida, J. Zúñiga*, A. Requena* and B. Miguel. Density Functional Theory Study of the Stability and Vibrational Spectra of the β-Carotene Isomers. *Journal of Physical Chemistry A*, 113, 9899 (2009) IF=2.775

[4] J. P.Cerón-Carrasco*, A. Requena, J. Zúñiga, C. Michaux, E. A. Perpète and D. Jacquemin. Intermolecular Proton Transfer in Microhydrated Guanine-Cytosine Base Pair: a New Mechanism for Spontaneous Mutation in DNA. *Journal of Physical Chemistry A*, 113, 10549 (2009) IF=2.775

[5] J. P.Cerón-Carrasco*, A. Requena, E. A. Perpète C. Michaux and D. Jacquemin. Double Proton Transfer Mechanism in the Adenine−Uracil Base Pair and Spontaneous Mutation in RNA Duplex. *Chemical Physics Letters*, 484, 64 (2009) IF=1.991

[6] J. P.Cerón-Carrasco, A. Bastida, A. Requena, J. Zúñiga* and B. Miguel. A Theoretical Study of the Mechanism of Reaction of β-Carotene with the Nitrogen Dioxide Radical in Solution. *Journal of Physical Chemistry B*, 114, 4366 (2010) IF=3.377

[7] J. P.Cerón-Carrasco, A. Requena and C. M. Marian*. Theoretical Study of the Low-Lying Excited States of Beta-Carotene Isomers. *Chemical Physics*, 373, 98 (2010) IF=2.028

[8] J. P.Cerón-Carrasco*, A. Requena, E. A. Perpète C. Michaux and D. Jacquemin. Theoretical Study of the Tautomerism in One-Electron Oxidized Guanine-Cytosine Base Pair. *Journal of Physical Chemistry B*, 114, 13439 (2010) IF=3.377

[9] J. P.Cerón-Carrasco*, J. Zúñiga, A. Requena, E. A. Perpète C. Michaux and D. Jacquemin. Combined Effect of Stacking and Solvation on the Spontaneous Mutation in DNA. *Physical Chemistry Chemical Physics*, 13, 14584 (2011) IF=4.198 [Issue Cover and Editor's Choice]

[10] J. Cerezo*, J. Zúñiga*, A. Bastida, A. Requena* and J. P.Cerón-Carrasco. Atomistic Molecular Dynamics Simulations of the Interactions of Oleic and 2-Hydroxyoleic Acids with Phosphatidylcholine Bilayers. *Journal of Physical Chemistry B*, 115, 11727 (2011) IF=3.377

[11] J. P.Cerón-Carrasco* and D. Jacquemin*. Influence of Mg^{2+} on the Guanine-Cytosine Tautomeric Equilibrium: Simulations of the Induced Intermolecular Proton Transfer. *ChemPhysChem*, 12, 2615 (2011) IF=3.360

[12] J.-Y. Le Questel*, J. Graton, J. P.Cerón-Carrasco, D. Jacquemin, A. Planchat and S. H. Thany*. New Insights on the Molecular Features and Electrophysiological Properties of Dinotefuran Imidacloprid and Acetamiprid Neonicotinoid Insecticides. *Bioorganic & Medicinal Chemistry*, 19, 7623 (2011) IF=2.951

[13] J. P.Cerón-Carrasco, A. Ripoche, F. Odobel and D. Jacquemin*. Excited-state Nature in Benzodifuranone Dyes: Insights From *Ab Initio* Simulations. *Dyes and Pigments*, 92, 1144 (2012) IF=4.055

[14] J. Cerezo*, J. Zúñiga*, A. Bastida, A. Requena*, J. P.Cerón-Carrasco and L. A. Eriksson. Antioxidant Properties of β-Carotene Isomers and Their Role in Photosystems: Insights from *Ab Initio* Simulations. *Journal of Physical Chemistry B*, 116, 3498 (2012) IF=3.377

[15] J. P.Cerón-Carrasco*, A. Requena and D. Jacquemin*. Impact of DFT Functionals on the Predicted Magnesium-DNA Interaction: An ONIOM Study. *Theoretical Chemistry Accounts*, 131, 1188 (2012) IF=2.143

[16] J. P.Cerón-Carrasco*, D. Jacquemin, J. Zúñiga and A. Requena. Claves Teóricas de la Mutación Espontánea en el ADN. *Anales de QuÃmica de la RSEQ*, 108, 197 (2012) IF= N/A [Issue Cover]

[17] J. P.Cerón-Carrasco, D. Jacquemin* and E. CaÃ$\frac{1}{4}$et. Cisplatin Cytotoxicity: A Theoretical Study of Induced Mutations. *Physical Chemistry Chemical Physics*, 14, 12457 (2012) IF=4.198

[18] J. P.Cerón-Carrasco and D. Jacquemin*. Interplay between Hydroxyl Radical Attack and H-bond Stability in Guanine–Cytosine. *RCS Advance*, 2, 11867 (2012) IF=3.708

[19] J. P.Cerón-Carrasco*, M. Fanuel, A. Charaf-Eddin and D. Jacquemin*. Interplay Between Solvent Models and Predicted Optical Spectra: a TD-DFT Study of 7-OH-Coumarin *Chemical Physics Letters*, 556, 122 (2013) IF=1.991

[20] J. P.Cerón-Carrasco* and D. Jacquemin. Electric-field Induced Mutation on DNA: A Theoretical Investigation of the GC Nase Pair *Physical Chemistry Chemical Physics*, 15, 4548 (2013) IF=4.198 [Issue Cover and Hot Paper]

[21] B. Yassine, X. Leray, C. Falaise, S. Quinchard, J. P.Cerón-Carrasco, D. Jacquemin, J. Graton, J.-Y. Le Questel and S. Thany*. Pretreatment of the Cockroach Cercal Afferent/Giant Interneuron Synapses with Nicotinoids and Neonicotinoids Differently Affects Acetylcholine and Nicotine-induced Ganglionic Depolarizations. *Invertebrate Neuroscience*, 13, 91 (2013) IF=2.055

[22] J. P.Cerón-Carrasco*, D. Jacquemin, J. Graton, S. Thany and J.-Y. Le Questel*. New Insights on the Molecular Recognition of Imidacloprid with *Aplysia Californica* AChBP: A Computational Study. *Journal of Physical Chemistry B*, 117, 3944 (2013) IF=3.377

[23] J. Cerezo*, J. Zúñiga*, A. Bastida, A. Requena* and J. P.Cerón-Carrasco. Conformational changes of f β-carotene and zeaxanthin immersed in a model membrane through atomistic molecular dynamics simulations. *Physical Chemistry Chemical Physics*, 15, 6527 (2013) IF=4.198

[24] J. P.Cerón-Carrasco* and D. Jacquemin*. Electric Field Induced DNA Damage: An Open Door for Selective Mutations. *Chemical Communications*, 49, 7578 (2013) IF=6.718 [Issue Cover]

[25] J. P.Cerón-Carrasco, A. Siard and D. Jacquemin*. Spectral Signatures of Thieno[3,4-b]pyrazines: Theoretical Interpretations and Design of Improved Structures. *Dyes and Pigments*, 99, 972 (2013) IF=4.055

[26] J. P.Cerón-Carrasco*, D. Jacquemin and E. Dumont* Impact of DNA Environment on the Intrastrand Cross-Link Lesions: Hydrogen Atom Release as the Last Step of Formation of G[8-5m]T *Journal of Physical Chemistry B*, 117, 16397 (2013) IF=3.377

[27] J. P.Cerón-Carrasco*, J. Cerezo and D. Jacquemin*. How DNA is Damaged by External Electric Fields: Selective Mutation *vs.* Random Degradation. *Physical Chemistry Chemical Physics*, 16, 8243 (2014) IF=4.198 [Issue Cover]

[28] J. P.Cerón-Carrasco, D. Jacquemin, C. Laurence*, A. Planchat, C. Reichardt and K. Sraïdi Solvent Polarity Scales: Determination of New ET(30) Values for 84 Organic Solvents. *Journal of Physical Organic Chemistry*, 27, 512 (2014) IF=1.245

[29] J. P.Cerón-Carrasco, H. Roy, J. Cerezo, D. Jacquemin and A. D. Laurent* Theoretical insights on the antioxidant activity of edaravone free radical scavengers derivatives. *Chemical Physics Letters*, 599, 73 (2014) IF=1.991

[30] J. P.Cerón-Carrasco, D. Jacquemin, C. Laurence*, A. Planchat, C. Reichardt and K. Sraïdi Determination of a Solvent Hydrogen-Bond Acidity Scale by Means of the Solvatochromism of Pyridinium-N-Phenolate Betaine Dye 30 and PCM-TD-DFT Calculations. *Journal of Physical Chemistry B*, 118, 4605 (2014) IF=3.377

[31] D. Jacqueminm, J. Zúñiga, A. Requena and J. P.Cerón-Carrasco* Assessing the Importance of Proton Transfer Reactions in DNA. *Account of Chemical Research*, 47, 2467 (2014) IF=24.348

[32] J. P.Cerón-Carrasco*, J. Cerezo, J. Zúñiga, A. Requena, J. Contreras-García, S. Chavan, M. Manrubia-Cobo and H. E. Pérez-Sánchez. Labeling Herceptin with Platinum(II): Towards the Selective Delivery of Anticancer Drugs. *Journal of Molecular Modeling*, 20, 2401 (2014) IF=1.867

[33] J. P.Cerón-Carrasco*, A. Requena, J. Zúñiga and D. Jacquemin*. Mutagenic Effects Induced by the Attack of NO_2 Radical to the Guanine-Cytosine Base Pair. *Frontiers in Chemistry*, 3 (2015) IF=4.155

[34] J. P.Cerón-Carrasco* and D. Jacquemin*. DNA spontaneous mutation and evolution of GC-content. *Physical Chemistry Chemical Physics*, 17, 7754-7760 (2015) IF=4.198 [Selected paper in the World Chemistry Journal]

[35] J. P.Cerón-Carrasco* and D. Jacquemin*. Photoactivatable platinum(II) compounds: in search of novel anticancer drugs. *Theoretical Chemistry Accounts*, 134, 146-153 (2015) IF=2.143

[36] J. P.Cerón-Carrasco*, T. Coronado-Parra, B. Ibernón, A. J. Banegas, F. Ghasemi, J. M. Vegara, I. Luque, S. S. Azam, S. Traedal-Henden and H. Pérez-Sánchez. Application of Computational Drug Discovery Techniques for Designing New Drugs against Zika Virus. *Drug Design*,526, e131 (2016)

[37] J. P.Cerón-Carrasco*, D. Jacquemin, A. D. Laurent*. First computational step towards the understanding of the antioxidant activity of the Phycocyanobilin:Ferredoxin Oxidoreductase in complex with biliverdin IXa *Computational and Theoretical Chemistry*, 11077, 58-64 (2016) IF=1.403

[38] J. P.Cerón-Carrasco*, H. den-Haan, J. Peña-García, J. Contreras-García and H. Pérez-Sánchez*. Exploiting the cyclodextrins ability for antioxidants encapsulation: A computational approach to carnosol and carnosic acid embedding *Computational and Theoretical Chemistry*, 1077, 65-73 (2016) IF=1.403

[39] R. Q. Paulpandi, S. Ramasamy, M. S. Paulraj, F. G. Díaz Baños, G. Villora, J. P.Cerón-Carrasco, H. Pérez-Sánchez* and I. V. M Enoch* Enhanced Zn^{2+} ion-sensing behavior of a benzothiazole derivative on encapsulation by β-cyclodextrin. *RCS Advance*, 26, 15670-15677 (2016) IF=3.708

[40] Z. Alamiddine, B. Selvam, J. P.Cerón-Carrasco, M. Mathé-Allainmat, J. Lebreton, S. H. Thany, A. D. Laurent, J. Graton and J.-Y. Le Questel* Molecular recognition properties of thiaclopride: from the isolated state to the binding site of *Aplysia californica* AChBP. *Journal of Computer-Aided Molecular Design*, 29, 1151-1167 (2016) IF=3.199

[41] A. Rauf, T. Ben Hadda, G. Uddin, J.P. Cerón-Carrasco, J. Peñ-García, H. Pérez, H. Khan, S. Bawazer, S. Patel, M.S. Mubarak, T. Abu-Izneid, Y.N. Mabkhot*. Sedative-hypnotic-like effect and molecular docking of di-naphthodiospyrol from Diospyros lotus in an animal model *Biomedicine & Pharmacotherapy*, 88, 109 (2017) IF=2.779

[42] B. Naskar, A. Dhara, R. Modak, D.K. Maiti, C. Prodhan, K. Chaudhuri, A. Requena, J. P.Cerón-Carrasco and S. Goswami*. A Pyrene-Pyrazole-Based Rotamer Senses Hg^{2+} on the Nanomolar Scale. *Chemistry Select*, 2, 2512 (2017) IF=1.505.

[43] F.S. Senol, S. Slusarczyk, A. Matkowski, A. Pérez-Garrido, F. Giron-Rodriguez, J. P.Cerón-Carrasco, H. den-Haan, J. Peñ-García, H. Pérez-Sánchez, K. Domaradzki and I. E. Orhan. Selective in vitro and in silico butyrylcholinesterase inhibitory activity of diterpenes and rosmarinic acid isolated from Perovskia atriplicifolia Benth. and Salvia glutinosa L. *Phytochemistry*, 133, 33 (2017) IF=2.779

[44] M. Yar, L. Shahzadi, A. Farroq, S. J. Imran, J. P. Cerón-Carrasco, H. den-Haan, S. Kumar, J. Peñ-García, H. Pérez-Sánchez, A. Grycova, Z. Dvorak and R. Virzal *In vitro* modulatory effects of functionalized pyrimidines and piperidine derivatives on Aryl hydrocarbon receptor (AhR) and glucocorticoid receptor (GR) activities *Bioorganic chemistry*, 71, 285 (2017) IF=2.252

[45] E. Orhan, N. Kucukboyaci, I Calis, J. P. Cerón-Carrasco, H. den-Haan, J. Peñ-García, H. Pérez-Sánchez. Acetylcholinesterase inhibitory assessment of isolated constituents from Salsola grandis Freitag, Vural & Adiguzel and molecular modeling studies on N-acetyltryptophan *Phytochemistry Letters*, 20, 373 (2017) IF=1.575

[46] J. P. Cerón-Carrasco* and D. Jacquemin. Exposing the G-quadruplex to electric fields: the role played by telomeres in the propagation of DNA errors. *Physical Chemistry Chemical Physics*, 19, 9358 (2017) IF=4.198 [Issue Cover]

[47] J. P. Cerón-Carrasco*. Photooxidation of DNA as a key step in the cytotoxicity of photochromic diarylethenes. *Dyes and Pigments*, 142, 530 (2017) IF=4.055

[48] T. Suzuki*, J.P. Cerón-Carrasco, H. Tamaoki, Y. Ishigaki, R. Katoono, T. Fukushima, H. Pérez. Stereoselective encapsulation for a triarylmethylium o,o-dimer by natural gamma-cyclodextrin: origin of chiral recognition for the axially chiral dicationic guest *Heterocycles*, 94, 1123 (2017) IF=1.036

[49] J. P.Cerón-Carrasco*, J. Ruiz, C. Vicente, C. de Haro, C Bautista, J. Zúñiga, A. Requena. DFT Simulation of Structural and Optical Properties of 9-Aminoacridine Half-Sandwich Ru(II), Rh(III), and Ir(III) Antitumoral Complexes and Their Interaction with DNA. *Journal of Chemical Theory and Computation*, 13, 3898 (2017) IF=5.399

[50] S. Yuan, J.F.W. Chan*, H. den-Haan, K.K.H. Chik, A.J. Zhang, C.C.S. Chan, V.K.M. Poon, C.C.Y. Yip, W.W.N. Mak, Z. Zhu, Z. Zou, K.M. Tee, J.P. Cai, K.H. Chan, J. Peñ-García, H. Pérez*, J. P.Cerón-Carrasco*, K.Y. Yuen *. Structure-based discovery of clinically approved drugs as Zika virus NS2B- NS3 protease inhibitors that potently inhibit Zika virus infection in vitro and in vivo *Antiviral Research*, 145, 33 (2017) IF=4.307

[51] J. P. Cerón-Carrasco* and D. Jacquemin. Tuning the Optical Properties of Phenanthriplatin: Towards New Photoactivatable Analogues. *ChemPhotoChem*, 1, 504 (2017) IF=(new journal, still not available) [Issue Cover]

[52] P. Gómez, M. Más-Montoy, I. da Silva, J. P. Cerón-Carrasco, A. Tárraga, D. Curiel*. Hydrogen Bond-Directed Cruciform and Stacked Packing of a Pyrrole-Based Azaphenacene. *Crystal Growth & Design*, 17, 3371 (2017) IF=3.972

[53] M. Más-Montoya, J. P. Cerón-Carrasco, S. Hamao, R. Eguchi, Y. Kubozono, A. Tárraga, D. Curiel*. Synthesis and characterization of carbazolo[2,1-a]carbazole in thin film and single crystal field-effect transistors. *Journal of Materials Chemistry C*, 5, 7020 (2018) IF=4.484

[54] M. Pérez-Abril, C. Lucas-Abellán, J. Castillo-Sánchez, H. Pérez-Sánchez, J. P. Cerón-Carrasco, I. Fortea, J.A. Gabaldón, E. Núñez-Delicadol*. Systematic investigation and molecular modelling of complexation between several groups of flavonoids and HP-β-cyclodextrins. *Journal of Functional Foods*, 36, 122 (2017) IF=3.470

[55] A. Rauf*, U. Farooq A. Khan, T.B. Hadda, S. Naz, A. Ibrar, N. Jehan, J. P. Cerón-Carrasco, H. den Haan, J. Peña-García, H. Pérez-Sánchez, H. Khan, M.F. Ramadan, T. Abu-Izneid, S. Bawazeer* Sedative and muscle relaxant activities of diterpenoids from Phlomidoschema parviflorum. *Brazilian Journal of Pharmacongnosy*, 27, 636 (2017) IF=1.596

[56] J. Jerbi*, M. Springborg, H. de Haan, J. P. Cerón-Carrasco*. S-adenosyl-L-methionine analogs as enhanced methyl donors: Towards novel epigenetic regulators. *Chemical Physics Letters*, 690, 74 (2017) IF=1.991

[57] B. Naskar, K. Das, R.R. Mondal, D.K. Maiti, A. Requena, J. P. Cerón-Carrasco, C. Prodhan, K. Chaudhuri, S. Goswami*. A new fluorescence turn-on chemosensor for nanomolar detection of Al3+ constructed from a pyridine-pyrazole system. *New Journal of Chemistry*, 42, 2933 (2018) IF=3.201

[58] G. Budryn*, I. Galazka-Czarnecka, E. Brzozowska, J. Grzelczyk, R. Mostowski, D. Zyzelewicz, J. P. Cerón-Carrasco, H. Pérez-Sánchez. Evaluation of estrogenic activity of red clover (Trifolium pratense L.) sprouts cultivated under different conditions by content of isoflavones, calorimetric study and molecular modelling. *Food Chemistry*, 245, 324 (2018) IF=4.946

[59] P. Gómez, S. Georgakopoulos, J. P. Cerón-Carrasco, I. da Silva, M. Más-Montoya, J. Pérez, A. Tárraga, D. Curiel*. Hydrogen-bonded azaphenacene: A strategy for the organization of π-conjugated materials. *Journal of Materials Chemistry C*, 6, 3968 (2018) IF=5.976

[60] G. Budryn*, J. Grzelczyk, A. Jaskiewicz, D. Zyzelewicz, H. Pérez-Sánchez, J. P. Cerón-Carrasco. Evaluation of butyrylcholinesterase inhibitory activity by chlorogenic acids and coffee extracts assed in ITC and docking simulation models. *Food Research International*, 109, 268 (2018) IF=3.520

[61] M. Más-Montoya, S. Georgakopoulos, J. P. Cerón-Carrasco, J. Pérez, A. Tárraga, D. Curiel*. Structure-Property Correlation behind the High Mobility of Carbazolocarbazole. *Journal of Physical Chemistry C*, 122, 11736 (2018) IF=4.484

[62] J. P.Cerón-Carrasco*, H. Pérez-Sánchez J. Zúñiga and A. Requena. Antibodies as Carrier Molecules: Encapsulating Anti-Inflammatory Drugs inside Herceptine. *Journal of Physical Chemistry B*, 122, 2064 (2018) IF=3.377

[63] D. Veclani, A. Melchior,* M. Tolazzi and J. P.Cerón-Carrasco*. Using Theory To Reinterpret the Kinetics of Monofunctional Platinum Anticancer Drugs: Stacking Matters *Journal of American Chemical Society*, 140, 14024 (2018) IF=14.357 [Issue Cover]

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