

Dr. José Pedro Cerón-Carrasco

CONTACT INFORMATION

Bioinformatics and High Performance Computing
Research Group (BIO-HPC)
Universidad Católica San Antonio de Murcia
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RESEARCH EXPERIENCE

Modeling biological environments by employing state-of-the-art computational approaches:

- (i) DNA: spontaneous mutation, rare tautomers, proton transfer reactions, ionizing radiation damaged, metal-DNA interactions, antitumoural activity, cisplatin, carrier molecules, antibody-drug interactions
- (ii) Natural products: free radical reactivity, absorption and emission spectra, antioxidant power, neonicotinoids, protein binding pocket, hydrogen-bonds
- (iii) Levels of theory: density functional theory (DFT and TD-DFT), hybrid QMMM methods, MP2, explicit/implicit solution models...

ACADEMIC APPOINTMENTS

Researcher, July 2015 to present

Bioinformatics and High Performance Computing Research Group (BIO-HPC)
Universidad Católica San Antonio de Murcia, España
– Plan Propio de Investigación UCAM
– “Searching new drugs by using Quantum Chemistry”
– Dr. Horacio E. Pérez-Sánchez

Postdoctoral Researcher, July 2013 to June 2015

Quantum Chemistry, Molecular Spectroscopy and Laser Group,
Universidad de Murcia, Spain
– Marie Curie Actions, FP7-UIMPACT Program
– “Antitumoral Drugs and Theoretical Simulations”
– 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
– Fundación Séneca, Postdoctoral Research Staff Training Program
– “Modeling Biological Environments: Antitumoral Drugs”
– Prof. Denis Jacquemin Group

Postdoctoral Researcher, May 2009 to December 2010

Laboratoire de Chimie Théorique Appliquée, Université de Namur, Belgium
– Researcher Grant (2010)
– Fundación Esteban Romero, Researcher Mobility Fellowship (2009)
– “Computational Study of the Spontaneous Mutation Processes in RNA/DNA”
– 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
- Quality 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 of the Project:** Molecular Astrophysics: The Herschel and Alma Era
- Funding Institution: Consejo Superior de Investigaciones Científicas
 - Project leader: José Cernicharo Quintanilla
 - Number of participating researchers: 90
 - From: 01/01/2010 to: 31/12/2014
 - Funding amount: 400000 euros

Title of the Project: 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

Título: Enhancing the Therapeutical Properties of Antitumoural Drugs with Computational Chemistry

- Funding Institution: FP7 Marie Curie Actions
- Project leader: José Pedro Cerón-Carrasco
- Number of participating researchers: 3
- From: 01/07/2013 to: 30/06/2015
- Funding amount: 88300 euros

Título: Molecular Design of novel Anti-inflammatories

- Funding Institution: Dirección General de Deportes, Región de Murcia
- Project leader: José Pedro Cerón-Carrasco
- Number of participating researchers: 5

- From: 01/10/2015 to: 30/09/2016
- Funding amount: 5000 euros

Título: Assembling carrier molecules, active ligands and transition metal in a novel antitumoural drug

- Funding Institution: Fundación 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

REFEREED
JOURNAL
PUBLICATIONS



I am both first and corresponding author of most of my works, including the five paper highlighted as cover of their corresponding issues, which clearly stands for my independence as researcher. Please, see below the complete list of my contributions.

- [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 β -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 Mg²⁺ 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=3.468
- [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 Química de la RSEQ*, 108, 197 (2012) IF= N/A [Issue Cover]
- [17] J. P. Cerón-Carrasco, D. Jacquemin* and E. Caiet. 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 Base 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 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=3.468
- [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. Jacquemin, 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 NO₂ Radical to the Guanine-Cytosine Base Pair. *Frontiers in Chemistry*, 3 (2015) IF=N/A (new journal of Nature group)
- [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*, 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
- [37] 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
- [38] 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 Zn²⁺ ion-sensing behavior of a benzothiazole derivative on encapsulation by β -cyclodextrin. *RCS Advance*, 26, 15670-15677 (2016) IF=3.708

- [39] 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

CONFERENCE
BOOKS OF
ABSTRACTS

- [1] J. P. Cerón-Carrasco, J. Zúñiga, B. Miguel and A. Requena. Theoretical Determination of Potential Energy Surface for β -Carotene. In: *Gaussian Workshop*, Barcelona, Spain, June 6–9, 2006. Poster
- [2] J. P. Cerón-Carrasco, J. Zúñiga, B. Miguel and A. Requena. Density Functional Theory Study and Vibrational Spectroscopic Analysis for β -Carotene, Capsanthin and Capsorubin. In: *5th Congress on Electronic Structure: Principles and Applications*, Santiago de Compostela, Spain, July 18–21, 2006. Poster
- [3] B. Miguel, G. León and J. P. Cerón-Carrasco. Resonance Theory and Molecular Orbitals in the Molecular Stabilization and Electronic Delocalization for Engineer. In: *II National Meeting about Chemistry Education*, Murcia, Spain, October 4–7, 2007. Poster
- [4] J. P. Cerón-Carrasco, J. Zúñiga, B. Miguel and A. Requena. Effects of Hydration on the Hydrogen Transfer Mechanism in the Adenine-Thymine DNA Base Pair. In: *IV Symposium of Young Spanish Researchers RSEQ-Aldrich*, Burgos, Spain, November 20–22, 2007. Poster
- [5] B. Miguel, J. P. Cerón-Carrasco, J. Zúñiga and A. Requena. Reactivity between β -Carotene and NO₂ Radical: Theoretical Interpretation of Vis-UV Spectra. In: *XXI National Meeting of Spectroscopy*, Murcia, Spain, September 9–11, 2008. Talk
- [6] J. P. Cerón-Carrasco. Interaction between cigarette smoke and β -carotene: a theoretical point of view. In: *V Congrès International des Chimistes d'Orientation Théorique Actifs en Wallonie*, Namur, Belgium, September 17–20, 2008. Talk
- [7] J. P. Cerón-Carrasco, J. Zúñiga, B. Miguel and A. Requena. Theoretical Study of the Reactions of β -Carotene with NO₂ Radical. In: *Novel Methods in Exploring Carotenoid Excited State Dynamics*, Nove Hradý, Czech Republic, September 21–25, 2008. Poster
- [8] J. P. Cerón-Carrasco. Spontaneous Mutation in DNA and RNA. In: *V Congrès International des Chimistes d'Orientation Théorique Actifs en Wallonie*, Namur, Belgium, September 16–19, 2009. Talk
- [9] J. P. Cerón-Carrasco, A. Requena, E.A. Perpète, C. Michaux and D. Jacquemin. Effects of Stacking and Hydration on the Proton Transfer in the Guanine-Cytosine Base Pair. In: *7th Congress on Electronic Structure: Principles and Applications*, Oviedo, Spain, June 29– July 2, 2010. Poster
- [10] J. P. Cerón-Carrasco, A. Requena, E.A. Perpète, C. Michaux and D. Jacquemin. Molecular Mechanisms of DNA Damage. In: *12ème Rencontre des Chimistes Théoriciens Francophones*, Namur, Belgium, July 4–8, 2010. Poster
- [11] J. P. Cerón-Carrasco. Effects of Stacking and Hydration on the Proton Transfer in the Guanine-Cytosine Base Pair. In: *Journée du Pôle Ouest de Réseau Français de Chimie Théorique*, Nantes, France, June 6–7, 2011. Poster

- [12] J. P. Cerón-Carrasco, A. Requena, E.A. Perpète, C. Michaux and D. Jacquemin. Effects of Stacking and Hydration on the Proton Transfer in the Guanine-Cytosine Base Pair. In: *5th Theoretical Biophysics International Symposium*, Madeira, Portugal, June 8–12, 2011. Talk
- [13] J. Cerezo, J. Zúñiga, A. Requena and J. P. Cerón-Carrasco. Molecular Dynamics Study of the Influence of Oleic Acid and 2-Hydroxyoleic Acids on Model Membranes. In: *9th World Association of Theoretical and Computational Chemists*, Santiago de Compostela, Spain, July 17-22, 2011. Poster
- [14] J. P. Cerón-Carrasco, J. Zúñiga, A. Requena and D. Jacquemin. Effects of Stacking and Hydration on the Proton Transfer in the Guanine-Cytosine Base Pair. In: *VIII Symposium of Young Spanish Researchers RSEQ-Aldrich*, Málaga, Spain, October 25–28, 2011. Talk
- [15] J. Cerezo, J. Zúñiga, A. Bastida, J. P. Cerón-Carrasco, and A. Requena. β -Carotene as Dietary Supplement: Tenability of its Antioxidant Activity. In: *International Congress of Chemical Engineering*, Sevilla, Spain, June 24–27, 2012. Talk
- [16] J. Cerezo, J. Zúñiga, A. Bastida, J. P. Cerón-Carrasco, and A. Requena. Conformational Study of Carotenoids within Biological Systems. In: *Theoretical and Computational Chemistry for the Modeling of Biochemical Systems*, Girona, Spain, July 2–5, 2012. Talk
- [17] J. P. Cerón-Carrasco and D. Jacquemin. Interplay between Tautomeric Equilibria and Mutations in DNA. In: *IMAMPC2012, International Meeting on Atomic and Molecular Physics and Chemistry*, Pisa, Italy, September 12–14, 2012. Talk
- [18] J. P. Cerón-Carrasco A. Charaf-Eddin and D. Jacquemin. Optical Spectra of Coumarins in Solution: Comparison of the LR and SS Approaches. In: *TD-DFT Conference in Nantes*, Nantes, France, April 23–26, 2013. Poster
- [19] J. P. Cerón-Carrasco and D. Jacquemin. Spontaneous vs. Induced Mutations in DNA: A QMMM Approach. In: *6th Theoretical Biophysics Symposium*, Göteborg, Sweden, June 24–26, 2013. Talk
- [20] J. P. Cerón-Carrasco and D. Jacquemin. Electric Fields: A Potent Tool to Induce Genetic Errors. In: *Modeling Interactions in Biomolecules VI*, Mariánské Lázně, Czech Republic, September 16–19, 2013. Talk
- [21] J. P. Cerón-Carrasco J. Cerezo, J. Zúñiga, A. Requena and D. Jacquemin. Assessing the Antioxidant Activity by Means of Theoretical Calculations. In: *14th World Congress on Antioxidants*, Paris, France June 12–13, 2014. Poster
- [22] J. P. Cerón-Carrasco J. Zúñiga and A. Requena. Targeted Drug Delivery for Cancer Therapy: Labeling Herceptin with Platinum(II). In: *9th Congress on Electronic Structure: Principles and Applications*, Badajoz, Spain, July 2-4, 2014. **Invited speaker**
- [23] J. P. Cerón-Carrasco, J. Zúñiga and A. Requena, and D. Jacquemin. Proton Transfer Reactions in DNA: From Spontaneous to Induced Genetic Mutations. In: *10th Congress of the World Association of Theoretical and Computational Chemists*, Santiago de Chile, Chile, October 5-10, 2014. Poster
- [24] J. P. Cerón-Carrasco. Assessing the Importance of Proton Transfer Reaction in DNA. In: *Spain-Japan Joint Symposium on Theoretical and Computational Chemistry*, Tarragona, Spain, November 25–27, 2015. Poster

- [25] J. P. Cerón-Carrasco Revisiting Rare Tautomeric Forms in DNA. In: CECAM Workshop: DNA Damage, Modeling and Rationalize Structure and Reactivity, Lyon, France, November 3–6, 2015. **Invited speaker**
- [26] J. P. Cerón-Carrasco H. den-Haan, J. Peña-García, H. Thapa, and H. Pérez-Sánchez. Oleocanthal in Extra-Virgin Olive Oil: The Chemistry Behind its Beneficial Effects In: *1st International Congress in Current Trends and New Challenges in Olive Sector*, Murcia, Spain, September 24–26, 2015. Talk
- [27] R. Rodríguez-Schmidt, J. Peña-García, A. Pérez-Garrido, H. den-Haan, A. Bueno-Crespo, J. P. Cerón-Carrasco, A. Thapa, J. Atli-Benediktsson, J. Soto, and H. Pérez-Sánchez. A hybrid machine learning and molecular modeling methodology for the prediction of novel blood anticoagulants In: *4th International Work-Conference on Bioinformatics and Biomedical Engineering*, Granada, Spain, April 24–26, 2016. Poster
- [28] J. P. Cerón-Carrasco, J. Peña-García, H. Tapa, and H. Pérez-Sánchez. Non-steroidal anti-inflammatory drugs as inhibitors of cyclooxygenases: what we have learned and what is next In: *4th International Work-Conference on Bioinformatics and Biomedical Engineering*, Granada, Spain, April 24–26, 2016. Talk
- [29] J. P. Cerón-Carrasco. Photochromic Diarylethenes as Photoactivatable Drugs In: *EMN Meeting on Computational and Theory*, Las Vegas, NV USA. October 10–14, 2016. **Invited speaker**

GRANTS AND
CONTRACTS
OBTAINED

Marie Curie Postdoctoral Contract, July 1, 2013 to present
European FP7-People program and Universidad de Murcia, Spain

Research Contract, March 1, 2013 to June 30, 2013
Région Pays de la Loire and Université de Nantes, France

Postdoctoral Training Program, March 1, 2011 to February 28, 2013
Fundación Séneca, Agencia de Ciencia y Tecnología de la Región de Murcia, Spain

Researcher Contract, January 1, 2010 to December 31, 2010
Université Notre-Dame de la Paix, Namur, Belgium

International Mobility Fellowship, August 1, 2009 to December 31, 2009
Fundación Esteban Romero, CajaMurcia, Spain

Continuity Grant for PhD, April 1, 2009 to July 31, 2009
Universidad de Murcia, Spain

FPU Mobility, August 15, 2008 to November 15, 2008
National Ministry of Science and Innovation, Spain

FPU Fellowship-Contract PhD Program, April 1, 2005 to March 31, 2009
National Ministry of Science and Innovation, Spain

STUDENTS
SUPERVISOR

Alexis Ripoche

- Université de Nantes
- L3 Student in Chemistry
- Excited-state nature in benzodifuranone dyes
- 2 months. 2011

Mathieu Fanel

- Université de Nantes
- Master I in Chemistry
- Simulations of the solvatochromic effects in coumarins
- 4 months. 2012

Hélène Roy

- Université de Nantes
- L3 Student I in Chemistry
- Quantifying the antioxidant properties of natural products.
- 2 months. 2013

Aymeric Siard

- Université de Nantes
- Magister student
- Computing the properties of charge-transfer organic dyes
- 2 months. 2013

TEACHING
EXPERIENCE

Universidad de Murcia, Murcia, Spain

March 2006 to April 2009

- Code 00W3: Laboratory of Advanced Physical Chemistry
 - Responsible for lectures and supervision of laboratory
 - Students designed simple experiments with LASER
 - Time commitment: 60 hours/year

September 2013 to June 2015

- Code 1615: Basic operations in the Laboratory
- Code 1629: Principles of Physical Chemistry
- Code 1756: Biological Physical Chemistry
 - Responsible for lectures and supervision of laboratory
 - Students acquired basic chemical knowledge
 - Time commitment: 80 hours/year

September 2015 to present

- Code 15401: Molecular Biology
- Code 15SEC2S: Computer Methods
- Code 15SEC2S: Scientific Methodolgy
- Code 15831: Biochemistry
- Code 15401: Biochemistry and Molecular Biology in Medicine
 - Responsible for lectures
 - Students acquired basic knowledge in biochemical sciences
 - Time commitment: 80 hours/year

PEER-REVIEW
ACTIVITIES
(~30 PAPERS/YEAR)

- Account of Chemical Research
- Journal of American Chemical Society
- Journal of Physical Chemistry A
- Journal of Physical Chemistry B
- Journal of Molecular Modeling

- Journal of Molecular Structure
- Journal of Biomolecular Structure and Dynamics
- Chemistry Central Journal
- ChemPhysChem
- Wiley-VCH Books
- Comptes Rendus Chimie
- Molecules
- Dyes & Pigments
- Physical Chemistry Chemical Physics
- New Journal of Chemistry
- International Nano Letters
- Journal of Theoretical and Computational Chemistry.
- Journal of Biochemistry & Pharmacology
- Cell Proliferation
- Biochemistry
- Environmental Toxicology and Pharmacology
- Chemical Research in Toxicology
- Review Editor for Theoretical and Computational Chemistry. Frontiers in Chemistry