PERSONAL DATA

Family Name: MARÉCHAL
Forenames: Jean-Didier Pierre
Spanish Foreigner ID (NIE): X2549503-E
Gender: Male
Birth date and place: 05 de maig 1974, Colombes (France)
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PRESENT POSITION

Professor Agregat (Associate Professor) in **Physical Chemistry**
Departament de Química, Facultat de Ciències, Universitat Autònoma de Barcelona
08193 Bellaterra, Cerdanyola del Vallès (Barcelona)

RESEARCH INTERESTS:

Computational Chemistry – Molecular Modeling – Software development – Computational Bioinorganics – Drug Design – Enzyme Design

Publications

H index: 26 (source: Web of Science Core Collection on 01/09/2019 and 29 from google scholar)
Number of international peer reviewed manuscripts: 98 publication with 66 in 1st Quart
(no not account for abstracts at conference – full entry in web of Science 105 publications)
Book Chapters: 4 book chapters, **Book Editor**: 1 book
Citations 1633 (ca. 1300 without self-Cit.)
Average Citations per article: ca. 15,6. Average Citations per year: ca. 82.

Projects:

3 individual grants including 1 Marie Curie Fellowship
15 Research projects, 2 as Principal Investigator

Technology Transfer and outreaching

Involved in three private projects. Two spin-off. Co-funder of the Spin-off BioEclosion of the Eureka technological Park of the Universitat Autònoma de Barcelona.

ACADEMIC BACKGROUND

- 2002 Double doctorate in Chemistry and Bioinorganic Chemistry, Universitat Autònoma de Barcelona and Université Paris-Sud, France

- 1997 DEA in Bioinorganic Systems, Université Paris-Sud and École Normale Supérieure de Paris (ENS), France
- 1997 "MAGISTÈRE" in Chemistry ENS
- 1995 M. Sc. in Molecular Chemical-Physics, ENS Paris
- 1995 B. Sc. in Molecular Chemical-Physics, ENS Paris

PAST POSITIONS AND SCIENTIFIC EXPERIENCE

- 2013-2019 *Professor Agregat Interí* in Physical Chemistry, Department of Chemistry, Universitat Autònoma de Barcelona (Spain)
- 2011-2013: Post Doctoral (Bridge contract between + amb dedicació docent, Unitat de Química Física, Departament de Química, Universitat Autònoma de Barcelona (Spain)
- 2006-2011: Professor Lector Unitat de Química Física, Departament de Química, UAB
- 2005-2006: Individual Post Doctoral fellow, SIDACTION ENSEMBLE CONTRE LE SIDA, Institut de Biochimie et Biophysique Moléculaire et Cellulaire Université Paris Sud (France)
- 2005: Research Assistant (Post-Doc), University of Manchester (UK)
- 2004-2005: Molecular Modeller at DeCypher (spin-off), regional individual fellowship, University of Leicester (UK)
- 2002-2004: Research Assistant of the DMC pharmaceutical consortium (Post-Doc), consortium of private (Astra-Zeneca, Pfizer, Aventis, Boehringer Ingelheim, CellTech Chiroscience, GlaxoSmithKline, Hoffmann-La Roche, Johnson and Johnson Pharmaceuticals, Merck Sharp and Dohme, Novartis, NovoNordisk, Pharmacia, Wyeth) and public entities (Universities of Dundee and Leicester), Department of Chemistry and Biochemistry, Leicester (UK)
- 2000-2002: Teaching Assistant in Physical Chemistry, Unitat de Química Física, Departament de Química, UAB
- 1997-2000 Pre-Doctorate Marie Curie Fellow (individual grantee) Unitat de Química Física, Departament de Química, UAB

PUBLICATIONS

2019

99. Alonso-Cotchico L., Rodríguez-Guerra J., Lledós A., Maréchal J.-D.* Molecular Modeling for Artificial Metalloenzyme Design and Optimization Acc. Chem. Res. 2020, https://doi.org/10.1021/acs.accounts.0c00031

98. Norjmaa G.; Maréchal J.-D.*; Ujaque G.*; Microsolvation and Encapsulation Effects on Supramolecular Catalysis: C–C Reductive Elimination inside [Ga4L6]12– Metallocage *J. Am. Chem. Soc.* **2019**, 141,13114-13123 IF: 14.695, 1st Quart.; Cit.: 0

97. Sciortino G.; Sanna D.; Ugone V.; Maréchal J.-D.; Alemany_Chavaria; Garribba E. Secondary interactions, steric hindrance and electric charge effect on the interaction of V IV O species with proteins *New J. Chem.* **2019**, accepted IF: 3.069, 2nd Quart.; Cit.: 0

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95. Sanchez-Aparicio J.E.; Sciortino G.; Herrmannsdoerfer D.V.; Chueca P.O.; Pedregal J.R.G.; Maréchal J.-D.* GPathFinder: Identification of Ligand-Binding Pathways by a Multi-Objective Genetic Algorithm *Int. J. Mol. Sci.* **2019**, 20, 3155 IF: 4.183, 2nd Quart.; Cit.: 0

94. Ugone V.; Sanna D.; Sciortino G.; Maréchal J.-D.; Garribba E. Interaction of Vanadium(IV) Species with Ubiquitin: A Combined Instrumental and Computational Approach *Inorg. Chem.* **2019**, 58, 8064-8078 IF: 4.850, 1st Quart.; Cit.: 0

923. Sciortino G.; Sanna D.; Ugone V.; Maréchal J.-D.*; Garribba E.* Integrated ESI-MS/EPR/computational characterization of the binding of metal species to proteins: vanadium drug-myoglobin application *Inorg. Chem. Front.* **2019**, 6, 1561-1578 IF: 5.934, 1st Quart.; Cit.: 0

92. Pena Q.; Lorenzo J.; Sciortino G.; Rodriguez-Calado S.; Maréchal J.-D.; Bayon P.; Simaan A.J.; Iranzo O.; Capdevila M.; Palacios O. Studying the reactivity of "old" Cu(II) complexes for "novel" anticancer purposes *J. Inorg. Biochem.* **2019**, 195, 51-60 IF: 3.348, 1st Quart.; Cit.: 0

91. Streltsov V.A.; Luang S.; Peisley A.; Varghese J.N.; Cairns J.R.K.; Fort S.; Hijnen M.; Tvaroska I.; Arda A.; Jimenez-Barbero J.; Alfonso-Prieto M.; Rovira C.; Mendoza F.; Tiessler-Sala L.; Sanchez-Aparicio J.E.; Rodriguez-Guerra J. ; Lluch J.M.; Maréchal J.-D.; Masgrau L.; Hrmova M. Discovery of processive catalysis by an exo-hydrolase with a pocket-shaped active site *Nat. Commun.* **2019**, 10, 2222 IF: 11.880, 1st Quart.; Cit.: 1

90. Alonso-Cotchico L.; Sciortino G.; Vidossich P.; Pedregal J.R.G.; Drienovska I.; Roelfes G.; Lledós A.; Maréchal J.-D.* Integrated Computational Study of the Cu-Catalyzed Hydration of Alkenes in Water Solvent and into the Context of an Artificial Metallohydratase *ACS Catal.* **2019**, 9, 4616-4626 IF: 12.221, 1st Quart.; Cit.: 0

89. Alonso-Cotchico L.; Pedregal J.R.G.; Lledós A.; Maréchal J.-D.* The Effect of Cofactor Binding on the Conformational Plasticity of the Biological Receptors in Artificial Metalloenzymes: The Case Study of LmrR *Front. Chem.* **2019**, 7, 211 IF: 4.155, 2nd Quart.; Cit.: 0

88. Sciortino G.; Sanchez-Aparicio J.E.; Pedregal J.R.G.; Garribba E.; Maréchal J.-D.* Computational insight into the interaction of oxaliplatin with insulin *Metallomics* **2019** 11, 765-773 IF: 3.571, 2nd Quart.; Cit.: 0

87. Sciortino G.; Garriba E.; Pedregal J.R.G.; Maréchal J.-D.* Simple Coordination Geometry Descriptors Allow to Accurately Predict Metal-Binding Sites in Proteins *ACS Omega* **2019** 4, 3726-3731 IF: 2.584, 2nd Quart.; Cit.: 2

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85. Schmielau L.; Dvorak M.; Niederwanger M.; Dobieszewski, N.; Pedrini-Martha, V.; Ladurner, P.; Ródriguez-Guerra Pedregal J.; Maréchal J.-D.; Dallinger, R.; Differential response to Cadmium exposure by expression of a two and a three-domain metallothionein isoform in the land winkle Pomatias elegans: Valuating the marine heritage of a land snail *Science of the Total Environment* **2019** 648, 561-571 IF: 5.589, 1st Quart.; Cit.: 3

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2018

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82. Rodriguez-Guerra Pedregal, J.; Maréchal, J.-D. * PyChimera: use UCSF Chimera modules in any Python 2.7 project *Bioinformatics* **2018**, 34, 1784-1785, IF: 5,481; 1st Quart.; Cit.: 2

81. Sciortino, G; Sanna, D.; Ugone, V; Lledós, A; Maréchal, J.-D.*; Garribba, E.* Decoding Surface Interaction of (VO)-O-IV Metallodrug Candidates with Lysozyme 2018, *Inorganic Chemistry* **2018**, 57, 4456-4469 IF:4.7, 1st Quart., citation:4

80. Rodriguez-Guerra Pedregal, J.; Gomez-Orellana, P; Maréchal, J.-D.* ESIgen: Electronic Supporting Information Generator for Computational Chemistry Publications *Journal of Chemical Information and Modeling* **2018**, 58, 561-564 IF:3.8, 1st Quart., Cit.:3

79. Sciortino G.; Lubinu G.; Maréchal J.-D.; Garribba E. DFT Protocol for EPR Prediction of Paramagnetic Cu (II) Complexes and Application to Protein Binding Sites *Magnetochemistry* **2018** 4, 55

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74. Gómez-González J.; Peña D.G.; Barka G.; Sciortino G.; Maréchal J.-D.; Vázquez López M.; Vázquez M.E. Directed self-assembly of trimeric DNA-binding chiral miniprotein helicates *Frontiers in Chemistry* **2018**, 6, 520

2017

73. Sciortino, G.; Sanna, D.; Ugone, V.; Micera, G.; Lledós, A.; Maréchal, J.-D.*; Garribba, E.* Elucidation of Binding Site and Chiral Specificity of Oxidovanadium Drugs with Lysozyme through Theoretical Calculations *Inorganic Chemistry* **2017**, 56, 12938-12951, IF: 4.7, 1st Quart., Cit.:9

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71. Rodriguez-Guerra Pedregal, J.; Sciortino, G; Guasp, J; Municoy, M.; Maréchal, J.-D. * GaudiMM: A modular multi-objective platform for molecular modeling. *Journal of computational chemistry* **2017**, 38, 2118-2126 IF: 3.221, 2nd Quart., Cit.: 10

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2016

68. de Cozar A., Larranaga O., Bickelhaupt F. M., Sebastian E.S., Ortega-Carrasco E., Maréchal, J.-D., Lledós A and Cossió F. P. New Insights into the Reactivity of Cisplatin with Free and Restrained Nucleophiles: Energetic Costs of the Three Nucleophilic Substitution Reactions Involved in Cisplatin Activation *ChemPhysChem* **2016**, 17, 3932-3947 FI: 3.138, 1st Quart., Cit.:4

2015

67. Saura P., Maréchal J.-D.*, Masgrau L., Lluch, J.M. and González-Lafont A. Computational insight into the catalytic implication of head/tail-first orientation of arachidonic acid in human 5-lipoxygenase: consequences for the positional specificity of oxygenation *Physical Chemistry Chemical Physics* **2015**, 18, 33, 23017-23035 FI: 4,449, 1st Quart., Cit.: 5

66. Ghattas W., Cotchico-Alonso L., Maréchal J.-D., Urvoas A., Rousseau M. and Mahy J.-P., Ricoux R. Artificial Metalloenzymes with the Neocarzinostatin Scaffold: Toward a Biocatalyst for the Diels-Alder Reaction *ChemBioChem* **2015**, 17, 433-440 FI: 2,85, 2nd Quart., Cit.: 13

65. Gamba I., Rama G., Ortega-Carrasco E., Berardozzi R., Sanchez-Pedregal V.M., Di Bari L., Maréchal J.-D.*, Vazquez M. E. and Vazquez Lopez, M. V. The folding of a metallopeptide *Dalton Transactions* **2015**, 45, 3 881-885 FI: 4,177, 1st Quart., Cit.: 3

64. Dominguez-Perez B., Ferrer E., Figueredo M., Maréchal J.-D. Balzarini J., Alibes R. and Busqué F. Synthesis of Novel Nucleoside Analogues Built on a Bicyclo[4.1.0]heptane Scaffold *Journal of Organic Chemistry* **2015**, 80, 19, 9495-9505 FI: 4,785, 1st Quart., Cit.: 4

63. Ali-Torres J., Mirats A., Maréchal J.-D., Rodríguez-Santiago L. and Sodupe M. Modeling Cu2+-A beta complexes from computational approaches *AIP Advances* **2015** 5, 092402 IF: 1,444, 3rd Quart., Cit.: 11

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61. Mahy J.-P., Maréchal J.-D. and Ricoux R. From "hemoabzymes" to "hemozymes": towards new biocatalysts for selective oxidations *Chemical Communications* **2015**, 51, 2476-2494 IF: 6,657, 1st Quart., Cit.: 25

2014

60. Muñoz Robles V., Dürrenberger M., Heinisch T., Lledós A., Schirmer T., Ward T. R. and Maréchal J.-D.* Structural-, Kinetic- and Docking Studies of Artificial Imine Reductases Based on the Biotin-Streptavidin Technology: An Induced Lock-and-Key Hypothesis *The Journal of the American Chemical Society* 2014, 136, 15676-15683 IF: 12.113, 1st Quart., Cit.: 38

59. Mahy J.-P., Maréchal J.-D. and Ricoux R. From “hemobazymes” to “hemozymes”: towards new biocatalysts for selective oxidations *Journal of Porphyrins and Phtalocyanines* **2014**, 18, 1063-1092. IF: 2,285, 2nd Quart., Cit.: 0

58. Samper K. G., Rodríguez V., Ortega-Carrasco E., Atrian S., Maréchal J.-D., Cutillas N., Zamora A., de Haro C., Capdevila M., Ruiz J. and Palacios O Understanding the interaction of an antitumoral platinum(II) 7-azaindolate complex with proteins and DNA *Biometals* **2014** doi: 10.1007/s10534-014-9780-1 IF: 3,578, 2nd Quart., Cit.: 7

57. Gamba I., Rama G., Ortega-Carrasco E., Maréchal J.-D., Martinez Costas J., Vázquez M. E. and Vázquez López M. V. Programmed stereoselective assembly of DNA-binding helical metallopeptides *Chemical Communications* **2014**, 50, 11097-11100 (cover) IF: 6.718, 1st Quart., Cit.: 6

56. Urvoas A., Ghattasa W., Maréchal J.-D., Aveniera F., Bellande F., Mao W., Ricoux R. and Mahy J.-P. Neocarzinostatin-based hybrid biocatalysts with a RNase like activity, *Bioorganic & Medicinal Chemistry* **2014**, 22, 5678-5686 IF: 2,903, 2nd Quart., Cit.:5

55. Sansiaume-Dagousset E., Urvoas A., Chelly K., Ghattas W., Maréchal J.-D., Mahy J.-P. and Ricoux R. Neocarzinostatin-based hybrid biocatalysts for oxidation reactions, *Dalton Transactions* **2014**, 43, 8344-8354 IF: 4,197, 1st Quart., Cit.: 18

54. Ortega-Carrasco E., Lledós A. and Maréchal J.-D.* Unravelling novel synergies between organometallic and biological partners: a QM/MM study of an artificial metalloenzyme The *Journal of the Royal Society Interface* **2014**, 11, 96, 20140090 IF: 4,875, 1st Quart., Cit.:7

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51. Muñoz Robles V., Lledós A., Ward T. R. and Maréchal J.-D.* Application of an integrative computational protocol in the study of an artificial transfer hydrogenase *Journal of Biological Inorganic Chemistry* **2014**, 19 S241-S241 (book of Abstracts)

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2012

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38. Muñoz-Robles V., Ortega-Carrasco E., González Fuentes E., Lledós A.and Maréchal J.-D.* What can Molecular Modeling bring into the design of artificial inorganic cofactors? *Faraday Discussions* **2011**, 148, 137-159 IF: 4,538, 1st Quart., Cit.: 21

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23. Huang W., Westlake A., Maréchal J.-D., Joyce G., Moody P. and Roberts G. Filling a Hole in Cytochrome P450 BM3 Improves Substrate Binding and Catalytic Efficiency *Journal of Molecular Biology* **2007**, 373, 3, 633-651 IF:4,89, 1st Quart., Cit. 51

22. Champouret Y. D. M., Maréchal J.-D., Chaggar R. K., Fawcett J., Singha K., Maseras F. and Solan G. A. Factors affecting imine coordination in [{Imino-terpyridine}MX2] (M = Fe, Co, Ni, Zn): Synthesis, structures, DFT calculations and ethylene oligomerisation studies *New Journal of Chemistry* **2007**, 31, 1, 75-85 IF: 2,647, 1st Quart., Cit.: 26

21. Floquet N., Maréchal J.-D., Badet-Denisot M.-A., Robert C. H., Dauchez M. and David Perahia, Normal mode analysis as a prerequisite for drug design: Application to matrix metalloproteinases inhibitors *FEBS Letters* **2006**, 580, 22, 5130– 5136 IF:3,37, 1st Quart., Cit.: 52

20. Maréchal J.-D. and Sutcliffe M. J. Insights into drug metabolism from modelling studies of cytochrome P450-drug interactions *Current Topics in Medicinal Chemistry* **2006**, 6, 15, 1619-1626 IF: 4,17, 1st Quart., Cit.: 26

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Study of Metoclopramide metabolism by Cytochrome P450 2D6 *Drug Metabolism and Disposition* **2006**, 34, 8, 1386-1392, IF: 3,638, 1st Quart., Cit.: 28

18. Maréchal J.-D., Yu J., Brown S., Kapelioukh Y., Rankin E. M., Wolf R. C., Roberts C. K. R., Paine M. J. and Sutcliffe M. J. In silico and in vitro screening for inhibition of cytochrome P450CYP3A4 by comedications commonly used by patients with cancer *Drug Metabolism and Disposition* **2006**, 34, 4, 534-538 IF: 3,826, 1st Quart., Cit.: 41

17. Mahale S., Aubry C., Jenkins P. R., Maréchal J.-D., Sutcliffe M. J. and Chaudhuri B. Inhibition of cancer cell growth by cyclin dependent kinase 4 inhibitors synthesized based on the structure of fascaplysin *Bioorganic Chemistry* **2006**, 34, 5, 287-297 IF: 2,05, 2nd Quart., Cit.:18

16. Mahale S., Aubry C., Jenkins P. R., Maréchal J.-D., Sutcliffe M. J. and Chaudhuri B. CA224, a non-planar analogue of fascaplysin, inhibits Cdk4 but not Cdk2 and arrests cells at G0/G1 inhibiting pRB phosphorylation *Bioorganic and Medicinal Chemistry Letters* **2006**, 16, 4272-4278, IF: 2,54, 1st Quart., Cit.: 21

15. Aubry C., Wilson J., Jenkins P. R., Mahale S., Chaudhuri B., Maréchal J.-D. and Sutcliffe M. J. Design, synthesis and biological activity of new CDK4-specific inhibitors, based on fascaplysin *Organic and Biomolecular Chemistry* **2006**, 4, 787-801 IF: 2,19, 2nd Quart., Cit.: 34

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13. Champouret Y. D. M., Maréchal J.-D., Dadhiwala I., Fawcett J., Palmer D., Singha K. and Solan G. A., Mono- versus Bi-metallic Assembly on a Bulky Bis(imino)terpyridine Framework: A Combined Experimental and Theoretical Study *Dalton Transactions* **2006**, 21, 19, 2350-236 IF: 2,926, 1st Quart., Cit.: 27

12. Aubry C., Jenkins P. R., Mahale S., Chaudhuri B., Maréchal J.-D. and Sutcliffe M. J. The Design and Synthesis of Novel 3-[2-indol-1-yl-ethyl]-1H-indole Derivatives as Inhibitors of CDK4 *Tetrahedron Letters* **2005**, 9, 1423-1425 IF: 2,484, 1st Quart., Cit.: 44

11. Mouawad L., Maréchal J.-D. and David Perahia Internal cavities and ligand passageways in human hemoglobin characterized by molecular dynamics simulation *Biochimica et Biophysica Acta* **2005**, 1724, 385-393, IF: 3,369, 1st Quart., Cit.: 20

10. McLaughlin L.A, Paine M. J., Kemp C. A., Maréchal J.-D., Flanagan J. U., Ward C. J., Sutcliffe M. J., Roberts G. C. K. and Wolf C. R. Why Is Quinidine an Inhibitor of Cytochrome P450 2D6?: The role of key active-site residues in quinidine binding *Journal of Biological Chemistry* **2005**, 280, 38617-38624, IF: 6.355, 1st Quart., Cit.: 55

9. Kemp C. A., Maréchal J.-D. and Sutcliffe M. J. Progress in cytochrome P450 active site modelling *Archives of Biochemistry and Biophysics* **2005**, 433, 361-368, IF: 2.657, 2nd Quart., Cit.: 22

8. Flanagan J.-U., Maréchal J.-D., Ward R., Kemp C. A., McLaughlin L. A., Sutcliffe M. J., Roberts G. C. K., Paine M. J. I. and Wolf R. C. Phe120 contributes to the regiospecificity of cytochrome P450 2D6: mutation leads to the formation of a novel dextromethorphan metabolite *Biochemical Journal* **2004**, 380, 353-360, IF: 4.278, 1st Quart., Cit.: 59

7. Kemp C. A., Flanagan J. U., van Eldik A. J., Maréchal J.-D., Wolf C. R., Roberts G. C. K., Paine M. J. I. and Sutcliffe M. J. Validation of Model of Cytochrome P450 2D6: An In Silico Tool for Predicting Metabolism and Inhibition *Journal of Medicinal Chemistry* **2004**, 47, 5340-5346, IF: 5.076, 1st Quart., Cit.: 64

6. Aubry C., Jenkins P. R., Mahale S., Chaudhuri B., Maréchal J.-D. and Sutcliffe M. J. New fascaplysin-based CDK4-specific inhibitors: design, synthesis and biological activity *Chemical Communications* **2004**, 15, 1696-1697, IF: 3,997, 1st Quart., Cit.: 26

5. Cowdell R., Davies C. J., Hilton S. J., Maréchal J.-D., Solan G. A., Thomas O. and Fawcett J. Flexible N,N,N-Chelates as Supports for Iron and Cobalt Chloride Complexes; Synthesis, Structures, DFT calculations and Ethylene Oligomerisation Studies *Dalton Transactions* **2004** 3231-3240, IF: 2.926, 1st Quart. , Cit.: 37

4. van Eldik A. J., Maréchal J.-D., Kemp C., Flanagan J. U., Sutcliffe M. J., Paine M. J., Roberts G: C. K. and Wolf R. C. Theoretical and experimental validation of cytochrome 2D6 structural model Drug Metabolism Reviews, 2003, 35, 330 Suppl. 2, Proceedings, IF: 4,537, 1st Quart.

3. Maréchal J.-D., Maseras F., Lledós A., Perahia D. and Mouawad L. Ab initio calculations predict a very low barrier for the rotation of the axial ligand in Fe(P)(Im) *Chemical Physics Letters* **2002** 353, 379-382 IF: 4,537, 2nd Quart., Cit.: 8

2. Maréchal J.-D., Barea G., Maseras F., Lledós A., Mouawad L. and Perahia D. Theoretical Modeling of the heme group with a Hybrid QM/MM Method *Journal of Computational Chemistry* **2000** 21, 4, 282-294, IF: 2,990, 1st Quart., Cit.: 33

1. Morgenstern-Badarau I., Lambert F., Renault J.-P., Cesario M., Maréchal J.-D. and Maseras F. Amine conformational change and spin conversion induced by Metal-assisted ligand oxidation: from the seven-coordinate iron(II)-TPAA complex to the oxidized iron(II)-(py)3tren isomers, Characterization, crystal structures, and density functional study *Inorganica Quimica Acta* **2000** 297, 338-350, IF: 2,990, 1st Quart., Cit.:56

Book Chapters

Rodríguez-Guerra J., Alonso-Cotchico L., Sciortino G., Lledós A.andMaréchal J.-D. Computational studies of Artificial Metalloenzymes: From methods and models to design and optimization en Artificial metalloenzymes and metalloDNAzymes in catalysis. From design to applications. Editorial Wiley, Editors: Dieguez M., Pamies O., Bäckvall J. E. 2017

Muñoz-Robles V., Ortega-Carrasco E., Alonso-Cotchico L., Rodríguez-Guerra J., Lledós A. and Maréchal J.-D. Enzyme Design en Simulating Enzyme Reactivity: Computational Methods in Enzyme Catalysis, Editors: Vicenç Moliner and Iñaki Tuñón, Editorial Royal Society of Chemistry, 2016, 481 DOI:10.1039/9781782626831-00481

Miteva M., Robert C., Maréchal J.-D. and Perahia A. Receptor Flexibility in Ligand Docking and Virtual Screening in In silico Lead Discovery Ed. Bentham, 2011, eISBN 978-1-60805-142-7

Book Editor

I am working with the Wiley editorial company as Editor for a new book entitled “Computational Bioinorganics: From Description to Prediction” with the contribution of more than 17 leading groups in the field. Publication is expected on may 2020.

Other Publications:

More than 30 note presses based on the publication of New Advances on the Study of Alzheimer Disease”, related to article 37, 4 disseminative works on metal in Alzheimer and drug metabolism.

RESEARCH PROJECTS

Individual grants

- **2004-2005: Post-Doctoral grantee** - *computer assisted rational drug design of genotype independent hiv protease inhibitors* – Funding: Ensemble contre le SIDA - Institut de Biophysique et Biochimie Moleculaire et Cellulaire (D. Perahia Group), Université Paris XI, France (19.200,00 €)

- **2002-2004 Post-Doctoral grantee** - *predicting drug metabolism for safe and efficient drugs* - Funding: Higher Education Funding Council for England - Spin-off Initiative University of Leicester – (13.454,00 £)

- **1997-2000 Pre-Doctoral Individual Fellowship** - THEORETICAL STUDY OF THE HEMOGLOBIN CO-OPERATIVE BINDING MECHANISM BY QUANTUM MECHANICAL AND MOLECULAR DYNAMICS CALCULATIONS - Funding: EU, Marie Curie project ERBFMICT-972056 (88.316,00 €)

Research projects

- **01/01/2018-31/12/2020**: *De la catalisis molecular a la supra-bio-catalisis, un enfoque computacional* - CTQ2017-87889-P, MINECO (DGI) - 91000,00 € PIs: J.D. Maréchal & G. Ujaque

- **2017-2020**: Computational BioNanoCat, Generalitat de Catalunya, 2017_SGR_1323, 19000€ - Princ. Invest.: M. Sodupe

- **2015-2017**: *hacia el diseño de nuevas rutas catalíticas* - MINECO (DGI) CTQ2014-54071-P - 137.940,00 € - Princ. Invest.: G. Ujaque, Jean-Didier Maréchal

- **2014 – 2017**: *grupo de síntesis y modelización de sistemas con metales de transición* - Generalitat de Catalunya (ref: 2014 SGR 989) - 12.000,00 € - Princ. Invest.: A. Lledós

- **2015 – 2018**: *GDRI heteroelements and coordination chemistry: from concepts to applications* (HTTP://GDRI-HC3A.CNRS.FR/) - CNRS (France) French-Spanish Network GDRI-HC3A - 100.00,00 € (first year) - PRINC. INVEST.: Montserrat Gómez (Paul Sabatier University, Toulouse, coordinator)

- **2014 – 2016**: Red orfeo-cinqa, centro de innovación en química avanzada - MINECO (DGI) CTQ2014-51912-REDC (Red CONSOLIDER) -Univ. Zaragoza, Univ. Valencia, Univ. Oviedo, UAB, Univ. Santiago, Univ. Castilla-La Mancha, Univ. Sevilla-IIQ, Univ. Complutense Madrid, Univ. Alicante, Univ. York - 41.000,00 € PRINC. INVEST.: M. A. Esteruelas (Univ. Zaragoza-CSIC)

- **2012 – 2014**: Descripción a nivel atómico de la catálisis: moléculas, superficies y enzimas - MICINN (DGI) CTQ2011-23336 – 192.390,00 € - PRINC. INVEST.: A. Lledós

- **2012 – 2016**: reference network in theoretical and computational chemistry (HTTP://WWW.XRQTC.COM/EN/) - Generalitat de Catalunya - CSIC, ICIQ, UAB, UB, UdG, UPC, URV - 600.000 € - F. Illas (UB)

- **2009 – 2011**: Interpretació molecular de los mecanismes de la catàlisis homogènia, catàlisis asimètrica y catalizadores bioinspiraDOS – MEC CTQ2011-23336 - 154.396,00 euros € - PRINC. INVEST.: A. Lledós

- **2009 – 2013**: Grupo de síntesis y modelización de sistemas con metales de transición – Generalitat de Catalunya (ref: 2009 SGR 00896) - 43.680,00 €- PI: A. Lledós

- **2008-2013** Desarrollo de entidades organometálicas para reacciones de funcionalización selectiva de moléculas orgánicas - MEC/Consolider Ingenio 2010 CSD2007-00006 – Partners: Univ. Zaragoza, Univ. Valencia, Univ. Oviedo, UAB, Univ. Santiago, Univ. Castilla-La Mancha, Univ. Sevilla-IIQ, Univ. Complutense Madrid, Univ. Alicante, Univ. York - 5.000.000 €, Grup Lledós: 300.000 euros € - Coordinator: PRINC. INVEST.: M.A.

- **2007 – 2012**: Una visión molecular de la química organometálica y su aplicación en catálisis – MEC ref: CTQ2005-0900-CO2-01 –91.630,00€ - PRINC. INVEST.: A. Lledós

- **2002 – 2005**: Modelización molecular de sistemas con metales de transición: aplicaciones en química organometálica y bioinorgánica, compuestos de alta nuclearidad y catálisis homogénea – MCYT BQU2002-04110-CO2-01 - 11.1050,00 € - PI: A. Lledós

- **2001 – 2004**: Grupo de síntesis y modelización de sistemas con metales de transición – Generalitat de Catalunya2001SGR 00179 – 43.874,00€ - A. Lledós

- **1999 – 2001:** Grupo de síntesis y modelización de sistemas con metales de transición – Generalitat de Catalunya 1999SGR 0089 – 15.663,00€ - A. Lledós.

RESEARCH SUPERVISION

Ph.D.

- **2019**-present **Lorena Roldán**, Doctoral school in Bioinformatics
- **2019**-present **Iker Zapirain Gysling**, De la Catálisis Molecular a la Supra-Bio-Catálisis, un enfoque computacional, Doctoral school in Chemistry
- **2019-present**: **Laura Tiessler Sala**, Estrategias computacionales para el diseño de metaloenzimas artificiales, Doctoral school in Bioinformatics
- **2017-present**: **José Emilio Sánchez Aparició**, *Bringing Chemical Space Explorations in the GaudiMM Framework*, Doctoral school in Bioinformatics
- **2017-present**: **Gantulga Norjmaa**, Computational Insights on the Utilization of Metallocages as Nanovessels for Catalysis, Doctoral school in Chemistry
- **2016-2019**: **Giuseppe Sciortino**, *Estudio de las interacciones de metalo-fármacos con sus dianas proteicas*, Doctoral school in Chemistry – Excellent Cum Laude
- **2015-2018: Lur Alonso-Cotchico** *Computational Design of Chemobiological Hybrids for Biocatalytic Platforms*, Dr. in Biotechnology, UAB – Excelent Cum Laude (27/07/2018)

- **2015-2018 Jaime Rodríguez-Guerra Pedregal** *Development and Applications of a novel computational plateform for complex molecular design*, Dr. in Biotechnology, Excellent Cum Laude. (20/09/2018)
- **2010 – 2015**: **Elisabeth Ortega-Carrasco** *Development and applications of new computational approaches for the accurate prediction of the interaction of metal containing species with biological macromolecules*, Theoretical and Computational Chemistry, UAB, Excellent Cum Laude (15/07/2015)
- **2011 – 2015: Beatriz Domínguez Pérez** *rational design and synthesis of new nucleoside analogues bearing a cyclohexane core*, Dr. Chemistry, UAB, Spain, Excellent Cum Laude (06/07/2015)
- **2009 – 2013: Rosa Miralles Lluma** síntesis estereoselectiva de análogos ciclobuténicos de nucleósidos y estudio teórico de su mecanismo de acción, Chemistry, Dr. in Chemistry, UAB, Spain, Excellent
- **2011 – 2014: Victor Muñoz Robles** *application of molecular modeling techniques for the design of artificial metalloenzymes*, Dr. In Biotechnology, UAB, Excellent Cum Laude
- **2005 – 2009: Safwat Abdel-Azeim** *prediction of protein-ligand interactions by computational means: from qm/mm to molecular dockings,* Dr. in Physical-Chemistry, Université Paris-Sud, France

Others

- 13 Master Thesis (8 bioinformatics, 1 biotechnology, 1 Theoretical and Computational Chemistry)
- 13 Grade Thesis (4 Chemistry, 4 biosciences, 4 double grade in Physics and Chemistry, 2 double grade in Physics and Mathematics, 2 Mathematics)
- 3 Incoming guests: 1 Erasmus Student (2017), three Ph. Student formation (from Groningen 2016, 2019 and Hamburg 2017)

Technological Transfer

- Post-Doctoral in the "Predicting drug metabolism for safe and efficient drugs" consortium (2002-2004)
- Molecular Modeler of the Spin-off Initiative DECIPHER, University of Leicester
- Co-Founder of the BioEclosion company (EBT - *Empresa a Base tecnologica*) with Pr. PividoriandIlla and Dr. Ferrer Dalmau BioEclosion based on the development of novel biosensors. This lead to more than four different fund raising (richi foundation – one start, empenta, llavor (AGAUR) valortec (ACCIÓ),) in between 2014 and 2018 which raises from 5000 to 15000 euros by calls
- Opening a Technological service at the UAB for structural bioinformatics

TALKS IN CONFERENCES, SYMPOSIA, WORKSHOPS:

I only mention in this section talks for which I have been the presenter. Added to 30 poster presentations, I have performed 43 talks; 21 in congresses (8 as invited plenary) and 22 invited in Research institutes

My most significant contributions since 2014 are:

- **19-21/02/2020** - GaudiMM: Opening New Horizons in Molecular Modeling of Chemobiological Systems, V meeting of the Chemical Biology group of the Spanish Royal Society of Chemistry, Granada, Spain, Oral Communication

- **28-29/11/2019** - What about cofactor and substrate binding in metalloenzyme design? TrenCa Meeting, Benicassim, Spain, Invited Lecture.

- **07/2019** - Understanding, Modeling and Analysing Protein-Ligand Interactions Taller Computacional Avanzado para resolver problemas de Investigación, Indicasat (Instituto de Investigaciones Científicas y Servicios de Alta Tecnología de Panamá), Panama city, Panama, Invited teacher
- **05/2018** - Computational chemistry : a usefultool for enzymatic processes, 1st Summer School "Catalysis: from understanding to applications" (Albi, France, June 18-21, 2019), Albi, France, Invited Speaker
- **03/2018** – Modeling Biometallic Systems with Integrative Approaches: Applications and Platform Development 2019 AMBER's Developers meeting, Tampa, Florida, USA, Invited speaker
- **09/2018** - Challenges in Computer-Assisted Design of Artificial Metalloenzymes, congress: The Future of Enzyme Modeling, Stockholm, Sweden
- **06/2018** - *New Computational Developments for the Design of Chemobiological Architectures*, CIQUS, Universidad de Santiago de Compostela, Invited Seminar
- **04/2018** - *Modeling Modeling of Biohybrids* – University of Groningen, The Netherlands, Invited Seminar
- **05/2018** - *Modeling of Bioinorganic Interactions*, Bioinformatics Unit, University of Basel, Swisserland, Invited Seminar
- **01/2017** - *Pushing the limits of protein-ligand dockings: integration, advances and challenges for bioinorganics* - DESY research centre, Hamburgh, Germany
- **09/2016** - *Advances in computational bioinorganics: predicting interactions of coordination complexes with biomolecular scaffolds* - XXXIV GECO Congress on Organometallic Group, GECO, Girona, Spain, Oral Communication
- **06/2016** - *On the role of molecular modeling in the development of artificial metalloenzymes* - CECAM on Enzyme Engineering: Bright Strategies from Theory and Experiments - CECAM, Lausanne, Suissa, Invited speaker
- **04/2016** *Genetic algorithms for unified design inference*, International Work-Conference on Bioinformatics and Biomedical Engineering, Universidad de Granada, Espanya, Oral Communication
- **07/2015**: *on the role of molecular modeling in the development of artificial metalloenzymes*; EuCheMS – 2015 – Inorganic Chemistry Conference, EuChemS, Worclaw, Polonia, Oral Communication
- **01/2016**: *multi-scale modeling of the hydration of alkene by copper containing artificial metalloenzymes*, VII French-Catalan Meeting, Toulouse, France, Invited Speaker
- **04/2015** *on the role of molecular modeling in building artificial metalloenzymes*, Institut de Chimie Moléculaire et de Materiaux d'Orsay Université Paris Sud, Orsay, France

- **06/2014**: *computational strategies for non-natural chemobiological architectures* COST CM 1306 Annual Meeting Budapest, hongria Invited
- **06/2014**: *integrative molecular modeling study of artificial metalloenzymes*, XRQTC Annual Meeting Barcelona, Spain Invited Speaker

OUTREACHING

- **05/2019:** *Artificial Metalloenzymes and Protein Design: Applications in Catalysis.* Symposium of the Bienal of the Real Sociedad Española de Química, Co-organizer with M. Dieguez, San Sebastian, Spain
- **10/2011**: *chemistry, computing and society*, one day meeting, Organizer, Cesca, Barcelona, SPain
- **02/2011**: MOLECULAR MODELING AND MOLECULAR VISUALIZATION; a training course for colleges teachers, head teacher and co-organizer, UAB, Barcelona, Spain
- **06/2010**: *Python Applied To Molecular Modeling And Computational Chemistry*, XRQTC Annual Meeting Barcelona, Spain, Organizer (+60 participants, 10 speakers)

AWARDS

- Habilitation from the french "Ministère de l'Education" for "Maître de conférence" and "Professeur d'Université"
- Escollit com a un dels 20 investigadors per excel•ència de la seva investigació pel parc de recerca de la Universitat Autònoma de Barcelona (2014)
- Best poster price of the "14th european congress on biotechnology"

REFEREE ACTIVITIES

Scientific Publications

Proceedings of the National American of Sciences, Physical Chemistry Chemical Physics
Journal of Physical Chemistry B, Cristalografica Acta B, Plos One, International Journal of Biological Macromolecules, Expert Opinion on Drug Metabolism and Toxicology, Molecular Biosystems, Catalysis Letters, Journal of Molecular Modeling, Inorganic Chemistry, Medicinal Chemistry Communications, The Journal of American Chemical Society, Computational and Structural Biotechnology Journal, RSC Advances

National Agencies

Agencia Nacional de Evaluación y Prospectiva, Spain
Agence Nationale pour la Recherche Scientifique, France
Agencia nacional de Promoción Científica y tecnológica, Argentina.

Scientific Society Memberships

Royal Society of Chemistry (UK), Sociedad Española de Bioinorgánica(ES), Real Sociedad Española de Química(ES), Club Metaloprotéines (Fr), European Biotechnological Association

(UE), Xarxa de Referència de Química Teórica i Computacional (CAT), NIH contributor through collaboration with the University of California San Francisco (US)