CURRICULUM VITAE

Carme Rovira Virgili

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PRESENT POSITION

ICREA Research Professor

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ACADEMIC BACKGROUND

- Bachelor's degree in Chemistry. University of Barcelona. 1991.
- M.Sc. in Chemistry. University of Barcelona. 1993.
- Ph.D. in Chemistry. University of Barcelona. 1995. Title: *Theoretical study of intermolecular interactions in small-sized systems and molecular organic crystals*. Qualification: Excellent Cum Laude. Thesis director: Prof. Juan J. Novoa

AWARDS

- ***Premi Extraordinari de Llicenciatura*** (Price for excellence as undergraduate student). University of Barcelona. 1994.
- ***Premi Extraordinari de Doctorat*** (Price for excellence in the PhD work). University of Barcelona. 1997.
- ***Distinció de la Generalitat de Catalunya per a la Promoció de la Recerca Universitaria*** (Award for excellence in research). Young scientist category. Generalitat de Catalunya. 2003.
- ***Premi Ciutat de Barcelona*** (City of Barcelona Award). Experimental Sciences and Technology. 2016.
- ***Emil Fisher Award***. European Carbohydrate Organisation. 2019.
- ***ERC Synergy Grant***. European Research Council. 2020.

LANGUAGES

Catalan, Spanish, English (fluent), French (average) and some German (DAF certificate).

FELLOWSHIP APPOINTMENTS

1992-1995 PhD fellowship (FPI). Generalitat de Catalunya.

1992-1994 Three fellowships for a stay in USA. Generalitat de Catalunya.

1996 Postdoctoral fellowship. Generalitat de Catalunya.

1997 – 1998 *Marie Curie* postdoctoral fellowship. European Commission.

1998 –2001 Programa de Incorporación de doctores y tecnólogos. Spanish Ministry of Science and Technology.

1999 – 2000 Two fellowships for short collaborative visits (MPI-Stuttgart and MPI-Göttingen). European Science Foundation.

2002 - 2006 *Ramón y Cajal* fellowship. Spanish Ministry of Science and Technology.

2019 *Salvador de Madariaga* fellowship for a visit to the University of York (UK). Spanish Ministry of Sport and Culture.

EMPLOYMENT

1992-1995 PhD student at the Chemistry Department of the University of Barcelona, UB (4 years).

1996-1998 Postdoctoral fellow. Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany (2 years, 9 months).

1998 – 2001 Postdoctoral fellow. Chemistry Department, UB (3 years).

2001 Teaching assistant. Chemistry Department, UB (2 months).

2002 - 2006 *Ramón y Cajal* researcher. Parc Científic de Barcelona, PCB (5 years).

2007 - 2012 ICREA Research Professor. Parc Científic de Barcelona (6 years, 8 months).

2013 - ICREA Research Professor. University of Barcelona (since Sept 2013).

STAYS IN FOREIGN RESEARCH CENTERS

1992 *North Carolina State University* (USA). With Prof. M.-H. Whangbo. 6 months. PhD research stay.

1993 *North Carolina State University* (USA). With Prof. M.-H. Whangbo. 3 months. PhD research stay.

1994 *Southern Illinois University* (USA). With Prof. S. Scheiner. 3 months. PhD research stay.

1996-1998 *Max-Planck-Institut für Festkörperforschung* (Stuttgart, Germany). With Prof. M. Parrinello. 2 years + 9 months. Postdoc.

2019 *University of York*. York Structural Biology Laboratory (York, UK). Invited by Prof. G. J. Davies. Six months. Visiting Professor.

SHORT VISITS TO FOREIGN RESEARCH CENTERS

- Université Pierre et Marie Curie (Paris, France). Invited by Prof. K. Kunc. Dec. 1996 (3 weeks).
- Université Pierre et Marie Curie (Paris, France). Invited by Prof. K. Kunc. Apr. 1997 (2 weeks).
- MPI für Festkörperforschung (Stuttgart, Germany). Invited by Prof. M. Parrinello. Jan. 1999 (2 weeks) and Apr. 1999 (2 weeks).
- MPI für Biophysicalische Chemie (Göttingen, Germany). Invited by Prof. H. Grubmüller. Nov. 1999 (1 week).

- MPI für Festkörperforschung (Stuttgart, Germany). Invited by Prof. M. Parrinello. Nov. 1999 (1 week).
- MPI für Festkörperforschung (Stuttgart, Germany). Invited by Prof. M. Parrinello. Aug.-Sept. 2000 (2 weeks).
- National Institute for Advanced Interdisciplinary research (NAIR). Tsukuba (Japan). Invited by Prof. Terakura. Nov. 2000 (2 weeks).
- MPI für Festkörperforschung (Stuttgart, Germany). Invited by Prof. M. Parrinello. Jan. 2001 (1 week).
- Eidgenössiche Technishe Hohschule Zürich (ETH). Zürich (Switzerland). Invited by Prof. U. Röthlisberger. Mar. 2001 (1 week) and Jul. 2001 (1 week).
- Swiss Center for Scientific Computing (CSCS). Manno (Switzerland). Invited by Prof. M. Parrinello. Mar. 2002 (1 week).
- Helsinki University of Technology. Finland. Invited by Prof. R. Nieminen. May 2002 (1 week).

CITATIONS SUMMARY (updated Sept 2024. Source: WoS / Google Scholar)

Number of ISI publications: 197 (excluding book chapters)

Number of citations: 7400 / 10105

h index: 47 / 56

Five most cited papers:

1) Rovira, Kunc, Hutter, Ballone, Parrinello. *J. Phys. Chem. A* 1997, 101, 8914-8925 (*356/449* citations)

2) Alfonso-Prieto, Biarnés, Vidossich, Rovira. *J. Am. Chem. Soc.* 2009, 131, 11751-11761 (*326/532* citations)

3) Agirre, Iglesias-Fernández, Rovira, Davies, Wilson, Cowtan. Nat. Struct. Mol. Biol. 2015, 22, 833-34 (*265/355* citations)

4) Davies, Planas, Rovira. *Acc. Chem. Res. 2012*, 45, 308-316 (*197/293* citations)

5) Ardèvol, Rovira. *J. Am. Chem. Soc.* 2015, 137, 7528-7528 (*184/273* citations).

ISI PUBLICATIONS

(*corresponding author. #Equal contribution)

1. **C. Rovira**, M.-H. Whangbo*. "On the nature of the metal-insulator transition in ß-(BEDT-TTF)4Pt(CN)4". Synthetic Metals, 60, 145-147, (1993).

2. **C. Rovira**, M.-H. Whangbo*. "Factors governing the charge density wave patterns of layered transition-metal compounds of octahedral coordination with d2 and d3 electron counts. Inorganic Chemistry, 32, 4094-4097, (1993).

3. L. K. Montgomery, T. Burgin, J. C. Huffman, K. D. Carlson, J. D. Dudek, G. A. Yaconi, L. A. Megna, P. R. Mobley, W. K. Kwok, J. M. Williams, J. E. Schirber, D. L. Overmyer, J. Ren, **C. Rovira**, M.-H.

Whangbo*. "The synthesis and characterization of radical cation salts of BEDT-TSF." Synthetic Metals, 55-57, 2990, (1993).

4. **C. Rovira**, P. Constants, M.-H. Whangbo, J. J. Novoa*. "Theoretical study of the structure and vibrational spectra of the (H2O)2···HF and H2O···(HF)2 molecular complexes." International Journal of Quantum Chemistry, 52, 177-189 (1994).

5. S. Kahlich, D. Schweitzer, **C. Rovira**, J. A. Paradis, M.-H. Whangbo, I. Heinen, H. J. Keller, B. Nuber, P. Bele, H. Brunner, R. P. Shibaeva*. "Characterization of the Fermi surface and phase transitions of (BEDO-TTF)2ReO4.(H2O) by physical property measurements and electronic band structure calculations." Zeitschrift für Physik B, Condensed Matter, 94, 39-47 (1994).

6. A. J. Schultz, H. H. Whang, J. M. Williams, L. W. Finger, R. M. Hazen, **C. Rovira**, M.-H. Whangbo*. "X-Ray diffraction and electronic band structure study of the organic superconductor κ-(BEDT-TTF)2Cu[N(CN)2]Cl at pressures up to 28 kbar." Physica C, 234, 300-306, (1994).

7. J. J. Novoa*, **M. C. Rovira**, C. Rovira*, J. Veciana, J. Tarrés. "C-H···S and S···S as two major forces explaining the packing of organic conducting and superconducting crystals." Advanced Materials, 7, 233-237 (1995).

8. S. Sportouch, C. Belin, M. Tillard-Charbonnel, **C. Rovira**, E. Canadell*. "Crystal and electronic structure of the ternary phase LiZnGe." New Journal of Chemistry, 19, 243-251 (1995).

9. S. Kahlich, W. Sommer, D. Schweitzer, I. Heinen, H. J. Keller, **C. Rovira**, J. A. Paradis, M.-H. Whangbo*. "Electronic properties of the organic superconductor (BEDO-TTF)2ReO4.(H2O)." Synthetic Metals, 70, 865-866 (1995).

10. **M. C. Rovira**, S. Scheiner*. "Ground and excited state proton transfers in a NCCCN ring." The Journal of Physical Chemistry, 99, 9854-9861 (1995).

11. **C. Rovira**, J. J. Novoa*, M.-H. Whangbo, J. M. Williams. "Ab initio computation of the potential energy surfaces of the water···hydrocarbon complexes H2O···C2H2, H2O···C2H4 and H2O···CH4: minimum-energy structures, vibrational frequencies and hydrogen bond energies." Chemical Physics, 200, 319-335 (1995).

12. T. Burgin, T. Miebach, J. C. Huffman, L. K. Montgomery, J. A. Paradis, **C. Rovira**, M.-H. Whangbo*,

S. N. Magonov. S. I. Khan, C. E. Strouse, D. L. Overmyer, J. E. Schirber. "20 K crystal structure, electrical transport origin of the different electrical behaviour of the isostructural organic conductors κ-(BEDT-TSF)2Cu[N(CN)2]Br". Journal of Materials Chemistry, 5, 1659-1669 (1995).

13. **C. Rovira**, J. J. Novoa, J. Tarrés, C. Rovira, J. Veciana, S. Yang, D. O. Cowan, E. Canadell*. "Bis(ethylenethio)tetrathiofulvalene, an organic metal with hight electrical conductivity". Advanced Materials, 7, 1023-1027 (1995).

14. J. J. Novoa*, M. Planas, **C. Rovira**. "On the usefulness of the Counterpoise method on hydrogen bonded complexes. A numerical test using near complete basis sets on H2O···HF, (H2O)2 and CH4···H2O". Chemical Physics Letters, 251, 33-36 (1996).

15. L. A. Kushch, S. V. Konovalikhin, L. I. Buravov, A. G. Khomenko, G. V. Shilov, K. Van, O. A. Dyachenko, E. B. Yagubskii, **C. Rovira**, E. Canadell*. "Stable molecular metal [Pd(dddt)2]. Ag1.54Br3.50: Synthesis, crystal structure, transport properties and electronic band structure". Journal de Physique I, 6, 1555 (1996).

16. C. Faulmann, A. Errami, B. Donnadieu, I. Malfant, J.-P. Legros, P. Cassoux, **C. Rovira**, E. Canadell*. "Metal Complexes of 1,2-Dithiolate Ligands, 5,6-dihydro-1,4-dithiin-2,3- dithiolato (dddt2-), 5,7-dihydro-1,4,6-trithiin-2,3-dithiolato (dtdt2-) and 2-thioxo-1,3-dithia-4,5-dithiolato (dmit2-). Synthesis, Electrochemical Studies, Crystal and Electronic Structures, and Conducting Properties". Inorganic Chemistry, 35, 3856 (1996).

17. **C. Rovira**, J. J. Novoa*. "Strength and direccionality of the C(sp3)-H···S(sp3) interaction. An ab initio study using the H2S···CH4 model complex". Chemical Physics Letters, 279, 247-250 (1997).

18. **C. Rovira**, P. Ballone, M. Parrinello*. "A density functional study of iron-porphyrin complexes". Chemical Physics Letters, 271, 140-150 (1997).

19. **C. Rovira**, K. Kunc, J. Hutter, P. Ballone, M. Parrinello*. "Equilibrium structures and energy of iron-porphyrin complexes. A density functional study". The Journal of Physical Chemistry A, 101, 8914-8925 (1997).

20. **C. Rovira**, M. Parrinello*. "Oxygen binding to iron-porphyrin. A density functionalstudy using both LSD and LSD+GC schemes". International Journal of Quantum Chemistry, 70, 387-394 (1998).

21. **C. Rovira**, K. Kunc, J. Hutter, P. Ballone, M. Parrinello*. "A comparative study of O2, CO and NO binding to iron-porphyrin". International Journal of Quantum Chemistry, 69, 31-35 (1998).

22. R. P. Shibaeva, S. S. Khasanov, B. Z. Narymbetov, L. V. Zorina, L. P. Rozenberg, A. V. Bazhenov, N. D. Kushch, E. B. Yagubskii, **C. Rovira**, E. Canadell*. "Low temperature crystal and electronic structures of the (BEDO-TTF)2Cl1.28(H3O)0.28. 2.44H2O stable molecular metal". Journal of Materials Chemistry, 8, 1151-1156 (1998).

23. **C. Rovira**, M. Parrinello*. "Factors influencing ligand binding properties of heme models. A first principles study of picket fence and protoheme complexes". Chemistry-A European Journal, 5, 250-262 (1999).

24. **C. Rovira**, J. J. Novoa*. "Strength and direccionality of the S···S intermolecular interactions present in TTF - based molecular crystals. A combined statistical and *ab initio* study". Chemistry-A European Journal, 5, 3689-3697 (1999).

25. **C. Rovira**, P. Carloni*, M. Parrinello. "The iron-sulfur bond in cytochrome *c*". The Journal of Physical Chemistry B, 103, 7031-7035 (1999).

26. C. Massobrio*, P. Rabu, M. Drillon, **C. Rovira**. "Structural Properties, Electron Localization and Magnetic Behavior of Copper Hydroxonitrate: A Density Functional Study". The Journal of Physical Chemistry B, 103, 9387-9391 (1999). *Issue cover*.

27. **C. Rovira**, M. Parrinello*. "Harmonic and anharmonic dynamics of Fe-CO and Fe-O2 in heme models". Biophysical Journal, 78, 93-100 (2000).

28. M. Kaupp*, **C. Rovira**, M. Parrinello. "Density functional study of 17O NMR chemical shift and nuclear quadrupole coupling tensors in oxyheme model complexes". The Journal of Physical Chemistry B, 104, 5200-5208 (2000).

29. **C. Rovira**, M. Parrinello*. "First principles molecular dynamics simulations of models for the myoglobin active center". International Journal of Quantum Chemistry, 80, 1172-1180 (2000).

30. D. Braga, F. Grepioni, F. Mota, **C. Rovira**, J. J. Novoa*. "Inter-anionic O-H···O interactions: a solid state and computational study of the ring and chain motifs". Chemistry - A European Journal, 6, 4536-4551 (2000).

31. **C. Rovira***, J. J. Novoa*. "A density functional study of crystalline acetic acid and its proton transfer polymorphic forms". The Journal of Chemical Physics, 113, 9208-9216 (2000).

32. I. Garzón, **C. Rovira**, K. Michaelian, M. R. Beltrán, P. Ordejón, J. Junquera, D. Sánchez-Portal, E. Artacho, J. M. Soler*. "Do thiols merely passivate gold nanoclusters?". Physical Review Letters, 85, 5250-5251 (2000).

33. I. Garzón, E. Artacho, M. R. Beltrán, A. García, J. Junquera, K. Michaelian, P. Ordejón, **C. Rovira**, D. Sánchez-Portal, J. M. Soler*. "Hybrid DNA-gold nanostructured materials: an *ab initio* approach?". Nanotechnology, 12, 126-131 (2001).

34. **C. Rovira**, K. Kunc, J. Hutter, M. Parrinello*. "Structural and Electronic Properties of Cobalt-corrole, Cobalt-corrin and Cobalt-porphyrin". Inorganic Chemistry, 40, 11-17 (2001).

35. **C. Rovira***, J. J. Novoa*. "A first principles computation of the low-energy polymorphic forms of the acetic acid crystal. A test of the atom-atom force field predictions". The Journal of Physical Chemistry B, 105, 1710-1719 (2001).

36. **C. Rovira***, B. Schulze, M. Eichinger, J. D. Evanseck and M. Parrinello. "Influence of the heme pocket conformation on the structure and vibrations of the Fe-CO bond in myoglobin". A QM/MM density functional study. Biophysical Journal, 81, 435-445 (2001).

37. **C. Rovira***, J. J. Novoa, P. Ballone. Hydrogen bonding and collective proton modes in clusters and periodic layers of squaric acid: a density functional study. The Journal of Chemical Physics. 115, 6406-6417 (2001).

38. **C. Rovira**, J. J. Novoa, J.-L. Mozos, P. Ordejón, E. Canadell*. "First principles study of the neutral molecular metal Ni(tmdt)2". Physical Review B, 65, 81104-81108 (2002).

39. **C. Rovira***, K. Kunc, M. Parrinello. "Protonation state of the equatorial ligands and dynamics of the OH...O units in a cobaloxime biomimetic". Inorganic Chemistry. 41, 4810-4814 (2002).

40. **C. Rovira**. "The structure and dynamics of the Fe-CO bond in myoglobin". Journal of Physics: Condensed Matter. 15, 1809-1822 (2003).

41. **C. Rovira***, I. Fita. "The proximal hydrogen bonded residue controls the stability of the compound II intermediate in peroxidases and catalases". Journal of Physical Chemistry B. 107, 5300-5305 (2003).

42. **C. Rovira.** "Role of the His64 residue on the properties of the Fe-CO and Fe-O2 bonds in myoglobin. A CHARMM/DFT study". Theochem: Journal of Molecular Structure. 632, 309-321 (2003). *Invited article.*

43. S. A. Baudron, P. Batail*, **C. Rovira**, E. Canadell, R. Clérac. "Interdependence of redox state, hydrogen bonding, anion recognition and charge partition in crystals of (EDT-TTF-CONHMe)6 [Re6Se8(CN)6] (CH3CN)2(CH2Cl2)2 ". Chemical Communications. 1820-1821 (2003).

44. D. A. Scherlis, Y. J. Lee, **C. Rovira**, S. Adams, R. M. Nieminen, P. Ordejón, E. Canadell*. "Concerning the origin of superstructures in hydrogen molybdenum bronzes HxMoO3". Solid State Ionics. 168, 291-298 (2004).

45. P. C. Loewen*, X. Carpena, R. Perez-Luque, **C. Rovira**, R. Haas, S. Odenbreit, P. Nichols, I. Fita. "Structure of Helicobacter pylori catalase, with and without formic acid bound, at 1.6 Å resolution". Biochemistry. 43, 3089-3103 (2004).

46. **C. Rovira***, X. Biarnés, K. Kunc. "Structure-energy relations in methylcobalamin with and without bound axial base". Inorganic Chemistry. 43, 6628-6632 (2004).

47. M. Ø. Jensen*, U. Röthlisberger, **C. Rovira**. "Hydroxide and proton migration in aquaporins". Biophysical Journal. 89, 1744-1759 (2005).

48. **C. Rovira**. "Structure, protonation state and dynamics of the compound II intermediate of catalase. ChemPhysChem. 6, 1-8 (2005).

49. **C. Rovira***, M. Alfonso-Prieto, X. Biarnés, I. Fita, P. Loewen. "A first principles study of the binding of formic acid in catalase complementing high resolution X-ray structures". Chemical Physics. 323, 129-137 (2006). *Invited article*.

50. X. Biarnés, J. Nieto, A. Planas, **C. Rovira***. "Substrate distortion in the Michaelis complex of *Bacillus* 1,3-1,4-β-glucanase. Insight from first principles molecular dynamics simulations". Journal of Biological Chemistry. 281, 1432-1441 (2006).

51. I. Degtyarenko, R. M. Nieminen, **C. Rovira***. "Structure and dynamics of dioxygen bound to cobalt and iron heme". Biophysical Journal. 91, 2024-2034 (2006).

52. T. P. Nygaard, **C. Rovira**, G. H. Peters, M. Ø. Jensen*. "Ammonium recruitment and ammonia transport by E.coli ammonia channel AmtB". Biophysical Journal. 91, 4401-4412 (2006).

53. A. Rodríguez-Fortea, **C. Rovira**, P. Ordejón, C. Hérold, P. Lagrange, E. Canadell*. "Electronic structure and charge transfer in the ternary intercalated graphite β-KS0.25C3". Inorganic Chemistry. 45, 9387-9393 (2006).

54. B. Chiavarino, M. E. Crestoni, S. Fornarini*, **C. Rovira***. "Protonated heme". Chemistry-A European Journal. 13, 776-785 (2007).

55. **C. Rovira***, P. M. Kozlowski*. "First principles study of coenzyme B12. Crystal packing forces effect on axial bond lengths". Journal of Physical Chemistry B. 111, 3251-3257 (2007).

56. M. Alfonso-Prieto, A. Borovik, X. Carpena, G. Murshudov, W. Melik-Adamyan, I. Fita, **C. Rovira***, P. C. Loewen*. "The structures and electronic configuration of compound I intermediates of *Helicobacter pylori* and *Penicillium vitale* catalases determined by X-Ray crystallography and QM/MM DFT calculations". Journal of the American Chemical Society. 129, 4193-4205 (2007).

57. E. Derat, S. Shaik*, **C. Rovira**, P. Vidossich, M. Alfonso-Prieto. "The effect of a water molecule on the mechanism of formation of Compound 0 in HRP". Journal of the American Chemical Society. 129, 6346-6347 (2007).

58. X. Biarnés, A. Ardèvol, A. Planas, **C. Rovira***, A. Laio, M. Parrinello. "The conformational free energy landscape of β-D-glucopyranose. Implications for substrate preactivation in β-glucoside hydrolases". Journal of the American Chemical Society. 129, 10686-10693 (2007).

59. P. Vidossich, M. Alfonso-Prieto, X. Carpena, P. C. Loewen, I. Fita, **C. Rovira***. "Versatility of the electronic structure of compound I in catalase-peroxidases (KatGs)". Journal of the American Chemical Society. 129, 13436-13446 (2007).

60. O. Gallego, F. X.Ruiz, A. Ardèvol, M. Domínguez, R. Àlvarez, A. R. de Lera, **C. Rovira**, J. Farrés, I. Fita, X. Parés*. "Structural basis for the high all-*trans*-retinaldehyde reductase activity of the tumor marker AKR1B10". Proceedings of the National Academy of Sciences USA. 104, 20764-20769 (2007).

61. I. Degtyarenko, X. Biarnés, R. M. Nieminen, **C. Rovira***. "Density-functional molecular dynamics studies of biologically relevant iron and cobalt complexes with macrocyclic ligands". Coordination Chemistry Reviews. 252, 1497–1513 (2008). *Invited article.*

62. B. Chiavarino, M. E. Crestoni, S. Fornarini*, **C. Rovira***. "Unravelling the intrinsic features of NO binding to iron(II)- and iron(III)-hemes". Inorganic Chemistry. 47, 7792-7801 (2008).

63. M. Alfonso-Prieto, P. Vidossich, A. Rodríguez-Fortea, X. Carpena, I. Fita, P. C. Loewen, **C. Rovira***. "Electronic state of the molecular oxygen released by catalase". Journal of Physical Chemistry A. 112, 12842–12848 (2008). *Invited article***.**

64. F. Xavier Ruiz, O. Gallego, A. Ardèvol, A. Moro, M. Domínguez, R. Alvarez, A. R. de Lera, **C. Rovira**, I. Fita, X. Parés, J. Farrés*. "Aldo-keto reductases from the AKR1B subfamily: retinoid specificity and control of cellular retinoic acid levels". Chemico-Biological Interactions. 178, 171-177 (2009).

65. L. Petersen, A. Ardèvol, **C. Rovira**, P. Reilly*. "Mechanism of cellulose hydrolysis by inverting GH8 endoglucanases: A QM/MM metadynamics study". Journal of Physical Chemistry B. 113, 7331–7339 (2009).

66. M. Alfonso-Prieto, X. Biarnés, P. Vidossich, **C. Rovira***. "The molecular mechanism of the catalase reaction". Journal of the American Chemical Society. 131, 11751–11761 (2009).

67. X. Carpena, P. Vidossich, K. Schroettner, B. M. Calisto, S. Banerjee, J. Stampler, M. Soudi, P. G. Furtmüller, **C. Rovira**, I. Fita, C. Obinger*. "Essential role of proximal histidine-asparagine interaction in mammalian peroxidases". Journal of Biological Chemistry. 284, 25929-25937 (2009).

68. A. El-Ghayoury, C. Mézière, S. Simonov, L. Zorina, M. Cobián, E. Canadell, **C. Rovira**, B. Náfrádi, B. Sipos, L. Forró, P. Batail*. "A neutral-zwitterionic molecular solid". Chemistry-A European Journal. 16, 14051-14059 (2010).

69. X. Biarnés, A. Ardèvol, A. Planas, **C. Rovira***. "Substrate conformational changes in glycoside hydrolase catalysis. A first principles molecular dynamics study". Biocatalysis and Biotransformation. 28, 33-40 (2010). *Invited article.*

70. A. Lammerts van Bueren, A. Ardèvol, J. Fayers-Kerr, B. Luo, Y. Zhang, M. Sollogoub, Y. Blériot, **C. Rovira**, G. J. Davies*. "Analysis of the reaction coordinate of α–L-fucosidases: a combined structural and quantum mechanical approach". Journal of the American Chemical Society. 132, 1804-1806 (2010).

71. P. Vidossich, G. Fiorin, M. Alfonso-Prieto, E. Derat, S. Shaik*, **C. Rovira***. "On the role of water in peroxidase catalysis: A theoretical investigation of HRP compound I formation". Journal of Physical Chemistry B. 114, 5161-5169 (2010). Highlighted by the Editor (*Editor's choice*).

72. L. Petersen, A. Ardèvol, **C. Rovira**, P. Reilly*. "Molecular Mechanism of the Glycosylation Step Catalyzed by Golgi α-Mannosidase II. A QM/MM Metadynamics Investigation". Journal of the American Chemical Society. 132, 8291-8300 (2010).

73. P. Vidossich, M. Alfonso-Prieto, X. Carpena, I. Fita, P. C. Loewen, **C. Rovira***. "The dynamic role of distal side residues in heme hydroperoxidase catalysis. Interplay between X-ray crystallography and *ab initio* MD simulations". Archives of Biochemistry and Biophysics. 500, 37-44 (2010). *Invited article.*

74. M. Alfonso-Prieto, X. Biarnés, M. Kumar, **C. Rovira**, P. M. Kozlowski*. "Reductive cleavage mechanism of Co−C Bond in cobalamin-dependent methionine synthase". Journal of Physical Chemistry B. 114, 12965-12971 (2010).

75. T. P. Nygaard, M. Alfonso-Prieto, G. H. Peters, M. Ø. Jensen, **C. Rovira***. "Substrate Recognition in the *Escherichia coli* Ammonia Channel AmtB: A QM/MM Investigation". Journal of Physical Chemistry B. 114, 11859-11865 (2010).

76. J. J. Valle-Delgado, M. Alfonso-Prieto, N. S. de Groot, S. Ventura, J. Samitier, **C. Rovira**, X. Fernández-Busquets*. "Modulation of Aβ42 fibrillogenesis by glycosaminoglycan structure". The FASEB Journal. 24, 4250-4261 (2010).

77. A. Ardèvol, X. Biarnés, A. Planas, **C. Rovira***. "The conformational free energy landscape of β-D-mannopyranose. Evidence for a 1S5 – B2,5 – OS2 catalytic itinerary in β-mannosidases". Journal of the American Chemical Society. 132, 16058-16065 (2010).

78. T. Addington, B. Calisto, M. Alfonso-Prieto, **C. Rovira**, I. Fita, A. Planas*. "Reengineering specificity in 1,3-1,4-β-glucanase to accept branched xyloglucan substrates". Proteins. 79, 365–375 (2011).

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Note: A. Nin-Hill received two awards for this work: the 2021 Prize to the best chemistry paper published in 2020 by a PhD student from the Computational Chemistry Group of the Spanish Royal Chemical Society (GEQC-RSEQ), as well as the 2021 Award of the Spanish Supercomputing Network (RES).

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M. I. Giannotti*, A. Lagunas*. "Phosphorylation disrupts long-distance electron transport in cytochrome c". Nature Communications, 13, 7100 (2022).

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INVITED BOOK CHAPTERS

1. **C. Rovira**. "Applications of Car-Parrinello molecular dynamics in biochemistry: binding of ligands in myoglobin" in *Medicinal Quantum Chemistry*. Eds: P. Carloni and F. Alber (Book series: Methods and Principles in Medicinal Chemistry. Editors: R. Mannhold, H. Kubinyi, G. Folkers). Wiley-VCH. pp. 73-102, 2003.
2. **C. Rovira**. "The Study of ligand-protein interactions by means of Density Functional Theory and first-principles molecular dynamics" in *Methods in Molecular Biology*, Vol 305, Protein-Ligand Interactions: Methods and Applications, ed.: G. U. Nienhaus, Humana Press, Totowa NJ, *pp.* 527-566, 2005.
3. **C. Rovira**. "Car-Parrinello simulations of chemical reactions in proteins" in *Protein Modelling*, ed.: G. Náray-Szabó, Springer international publishing, Switzerland, *pp.* 51-70, 2014.

4. M. Alfonso-Prieto*, **C. Rovira***. "Modeling reactivity in metalloproteins: hydrogen peroxide decomposition by heme enzymes" in *Simulating Enzyme Reactivity*, ed: I. Tuñón and V. Moliner, Royal Society of Chemistry, Cambridge (UK). Chapter 14. *pp.* 453-480*,* 2016.

POPULAR SCIENCE ARTICLES

1. **C. Rovira***, A. Ardèvol. "Dulces misterios de la naturaleza". *Investigación y Ciencia* (Spanish edition of *Scientific American*) 423, 12-14 (2011).
2. L. Raich, **C. Rovira***. "Unraveling enzymatic mechanisms by means of computational tools: biotechnological implications in the study of glycosidases". Revista de la Societat Catalana de Química, núm 15, p. 9-20 (2016).

PROCEEDINGS

1. V. Rojas-Cervellera, **C. Rovira**, J. Akola*. "QM/MM simulations of Au nanoclusters and glutathione ligands in water solvent". Proceedings of the 16th International Conference on Computational and Mathematical Methods in Science and Engineering, CMMSE. 2016. Pags. 1474-1484.
2. **C. Rovira***, M. Parrinello. "First principles simulations of hemeproteins: From the active center to the full protein". *Ψ_k-newsletter* (Scientific Highlight of the Month). August issue, 2001.
3. **C. Rovira**. "Electronic structure and reaction mechanisms of heme peroxidases". Proceedings of the 9th European Biological Inorganic Chemistry Conference (EUROBIC 9). Editor: H. Kozlowski. MEDIMONT International Proceedings. 2008. Pags 21-23.
4. L. Guidoni*, **C. Rovira**, M. Sulpizi. "Ab initio methods for biological systems: state of the art and perspectives". *Ψ_k-newsletter* (Scientific Highlight of the Month). August issue, 2009.

ORGANISATION OF I+D ACTIVITIES

1. School *"Applications of Car-Parrinello molecular dynamics to the study of biological problems"* (Organizers: P. Alemany, R. Rousseau and **C. Rovira**). Centre de Recerca en Química Teòrica. PCB. November 23-26, 2004.
2. School "Hybrid Quantum Mechanics / Molecular Mechanics (QM/MM) Approaches to Biochemistry (and beyond)". Centre Européen de Calcul Atomique et Moléculaire (CECAM). EPFL Lausanne. 14-18 February 2011. Organizers: M. Boero, I. Tavernelli, **C. Rovira**.
3. Conference "CPMD2011: Extending the limits of ab initio molecular dynamics for materials science and biophysics". Organizers: M. Parrinello, R. Car, P. Carloni, **C. Rovira** (Chair). Parc Científic de Barcelona. September 4-9, 2011. 190 participants.

4. School “Hybrid Quantum Mechanics / Molecular Mechanics (QM/MM) Approaches to Biochemistry (and beyond)”. Centre Européen de Calcul Atomique et Moléculaire (CECAM). EPFL Lausanne. 11-15 February 2013. Organizers: M. Boero, A. Seitsonen, **C. Rovira**.
5. School “Hybrid Quantum Mechanics / Molecular Mechanics (QM/MM) Approaches to Biochemistry and beyond”. Centre Européen de Calcul Atomique et Moléculaire (CECAM). EPFL Lausanne. 9-13 February 2015. Organizers: M. Boero, A. Seitsonen, U. Röthlisberger, **C. Rovira**.
6. Member of the International Scientific Organizing Committee of the conference “CPMD2016: Ab initio Molecular Dynamics Simulations: State-of-the-Art and Milestones for the Future”. University of Chicago (USA). May 18-20, 2016. Organizers: G. Galli, G. Voth, J. de Pablo, M. Chan.
7. School “Hybrid Quantum Mechanics / Molecular Mechanics (QM/MM) Approaches to Biochemistry and beyond”. Centre Européen de Calcul Atomique et Moléculaire (CECAM). EPFL Lausanne. 14-19 May 2017. Organizers: M. Boero, A. Seitsonen, U. Röthlisberger, **C. Rovira**.
8. School “Hybrid Quantum Mechanics / Molecular Mechanics (QM/MM) Approaches to Biochemistry and beyond”. Centre Européen de Calcul Atomique et Moléculaire (CECAM). EPFL Lausanne. 8-12 April 2019. Organizers: M. Boero, A. Seitsonen, P. Campomanes, **C. Rovira**.
9. School “Hybrid Quantum Mechanics / Molecular Mechanics (QM/MM) Approaches to Biochemistry and beyond”. Centre Européen de Calcul Atomique et Moléculaire (CECAM). EPFL Lausanne. 16-20 May 2022. Organizers: M. Boero, A. Seitsonen, P. Campomanes, **C. Rovira**.
10. Symposium “Molecules, Macromolecules and Biomolecules” within the Psik 2022 conference. EPFL Lausanne. Aug 22, 2022. Organizers: C. Molteni, **C. Rovira**.
11. Symposium *"Chemical Reactivity: Computational Methods and Applications"*, within the XXXIX Biennial meeting of the Spanish Royal Chemical Society. Zaragoza, June 25-29, 2023. Organizers: M. Swart and **C. Rovira**.

SUPERVISION OF POSTDOCTORATE FELLOWS

1. Dr. Pietro Vidossich (2008-2011)
2. Dr. Mercedes Alfonso-Prieto (2015-2016)
3. Dr. Binju Wang (2027-2018)
4. Dr. Kshatrech D. Dubey (2018)
5. Dr. Mariana B. Morais (2019)
6. Dr. Thomas Hansen (2021)
7. Dr. Alba Nin-Hill (2021-2022)
8. Dr. Qinghua Liao (2021-current)
9. Dr. Martín Calvelo (2021-2023)
10. Dr. Marina Corbella (2023-current)
11. Samanta Romanowska (2024)

SUPERVISION OF PhD & GRADUATE THESES

PhD theses

1. **PhD thesis** of Xevi Biarnés. “Substrate Preactivation mechanisms in 1,3-1,4-β-glucanase”. University of Barcelona. 07 Nov 2007. Qualification: excellent with honors & *Extraordinary Chemistry Award*. European doctorate title. Thesis director: C. Rovira.
2. **PhD thesis** of Mercedes Alfonso-Prieto. "*Ab initio* molecular dynamics study of catalase reaction mechanisms". Universidad Autònoma de Barcelona. Dec 17th 2009. Qualification: excellent with honors. Thesis director: C. Rovira.
3. **PhD thesis** of Albert Ardèvol. "Study of molecular mechanisms in glycoside hydrolases and transferases by *ab initio* molecular dynamics". Universitat Autònoma de Barcelona. Jan 20 2012. Qualification: excellent with honors. Thesis director: C. Rovira.
4. **PhD thesis** of Javier Iglesias Fernández. "Elucidating catalytic mechanisms in carbohydrate-active enzymes by means of *ab initio* molecular dynamics simulations". Universitat de Barcelona. Sept 19 2014. Qualification: excellent with honors. Thesis director: C. Rovira.
5. **PhD thesis** of Víctor Rojas Cervellera. “*Ab initio* molecular dynamics study of thiolate-protected gold clusters and their interaction with biomolecules”. Universitat Politècnica de Catalunya. July 17 2015. Qualification: excellent with honors. European doctorate title. Thesis director: C. Rovira.
6. **PhD thesis** of Santiago Alonso Gil. “Conformational and mechanistic analyses of α- and β-glycosidase substrates by ab initio QM/MM methods”. Universitat de Barcelona. July 12 2017. Qualification: excellent. Thesis director: C. Rovira.
7. **PhD thesis** of Lluís Raich Armendáriz. “Unveiling protein-substrate interactions and conformations that influence catalysis in carbohydrate-active enzymes”. Universitat de Barcelona. June 14 2018. Qualification: excellent with honors & *Extraordinary Chemistry Award*. European doctorate title. Thesis director: C. Rovira.
8. **PhD thesis** of Alba Nin Hill. “Conformational catalytic itineraries of five- and six-membered sugar rings in enzymatic and superacid media”. Universitat de Barcelona. Oct 26 2020. Qualification: excellent with honors. European doctorate title. Thesis director: C. Rovira.
9. **PhD thesis** of Joan Coines López-Nieto. “Mechanistic insights into substrate-assisted catalysis in glycosidases by means of QM/MM molecular dynamics”. Universitat de Barcelona. Jan 20, 2021. Qualification: excellent with honors. European doctorate title. Thesis director: C. Rovira.
10. **PhD thesis** of Oriol Esquivias Bautista de Lisbona. “Computational insights into carbohydrate epimerase mechanisms”. Universitat de Barcelona. Nov 17, 2023. Qualification: excellent with honors. European doctorate title. Thesis director: C. Rovira.
11. **PhD thesis** of Irene Cuxart Sánchez. “Simulations of glycoside hydrolase and phosphorylase reaction mechanism: families GH20, GH29, GH129 and GH130”. Universitat de Barcelona. Defense date: Dec 4th, 2024. Qualification: excellent. European doctorate title. Thesis director: C. Rovira.

12. **PhD thesis** of Beatriz Piniello Castillo. “Computational modeling of inverting glycosyltransferase reaction mechanisms”. Universitat de Barcelona. Defense date: Dec 12, 2024. Qualification: excellent with honors. European doctorate title. Thesis director: C. Rovira.

Msc theses

1. **Msc thesis** (Treball Fi de Carrera de l’Institut Químic de Sarrià) of Xevi Biarnés Fontal. “First principles simulations of substrate distortion in 1,3-1,4–β-glucanase. June 2005. Institut Químic de Sarrià-Universitat Ramon Llull (IQS-URL). Qualification: Excellent with honours (10/10). Thesis directors: A. Planas (IQS-URL) and C. Rovira (PCB).
2. **Msc thesis** (Diploma de Estudis avançats) of Mercedes Alfonso Prieto. “The reaction mechanisms of catalase enzymes”. Universitat Autònoma de Barcelona (UAB). 2006. Qualification: Excellent (10/10). Thesis director: C. Rovira.
3. **Msc thesis** of Albert Ardèvol Grau “Enzyme-retinoid interactions in aldo-keto reductases”. Universitat Autònoma de Barcelona (UAB). June 2007. Qualification: Excellent (9/10). Thesis director: C. Rovira.
4. **Msc thesis** of Javier Iglesias Fernández. "Substrate Distortion in the Michaelis Complex of enzyme Cel5A from Bacillus agaradhaerens ". July 2010. Universitat Ramon Llull. Qualification: Excellent (10/10). Thesis directors: A. Planas (IQS) and C. Rovira (PCB).
5. **Msc thesis** of Víctor Rojas Cervellera. “Thiol-protected gold clusters: Searching for the formation mechanism”. February 4th 2011. Universitat Politècnica de Catalunya. Qualification: Excellent (9.5/10). Thesis director: C. Rovira.
6. **Msc thesis** of Lluís Raich Armendáriz. “La substitució nucleòfila interna: estudi computacional de la descomposició d’alquil clorosulfits per mitjà de càlculs estàtics i dinàmics”. Universitat de Barcelona. September 2013. Qualification: Excellent (9.3/10). Thesis director: C. Rovira.
7. **Msc thesis** of Alba Nin Hill. “Catalytic reaction of β-galactocerebrosidase investigated by QM/MM ab initio metadynamics”. Universitat de Barcelona. July 2016. Qualification: Excellent (9.4/10). Thesis director: C. Rovira.
8. **Msc thesis** of Joan Coines López-Nieto. “Modelització de l’intermedi de reacció en quitinases”. Institut Químic de Sarrià-Universitat Ramon Llull. July 2016. Qualification: Excellent (9.5/10). Thesis directors: X. Biarnés (IQS-URL) and C. Rovira (UB).
9. **Msc thesis** of David Almacellas Salillas. “Computational study of enzyme-substrate interactions in α-1,3-galactosyltranferase”. Universitat de Barcelona. 13 July 2017. Qualification: Notable (7.9/10). Thesis director: C. Rovira.
10. **Msc thesis** of Albert Pla Mas. “Modelling the Michaelis complex of CtCel124 glycosyl hydrolase”. Universitat de Barcelona. 20 July 2017. Qualification: Notable (8/10). Thesis director: C. Rovira.
11. **Msc thesis** of Charlotte Madill. “A Molecular Dynamics investigation of Lipooligosaccharide α-galactosyltransferase C (LgtC)”. Imperial College London. July 2018. Qualification: A. Thesis director: C. Rovira.

12. **Msc thesis** of Iker Zapiráin Gysling. "Study of the transglycosylation complex of β-galactosidase using molecular dynamics". Universitat de Barcelona. 4 July 2019. Qualification: Notable (7/10). Thesis director: C. Rovira.
13. **Msc thesis** of Beatriz Piniello Castillo. "Theoretical insight into the active site dynamics of O-fucosyltransferase 1". Universitat de Barcelona. 22 July 2019. Qualification: Excellent (9.7/10). Thesis director: C. Rovira.
14. **Msc thesis** of Irene Cuxart Sánchez. "Modelling lacto-n-biosidase from *Bifidobacterium bifidum* by means of molecular dynamics". Institut Químic de Sarrià-Universitat Ramon Llull. 27 September 2019. Qualification: M. H. (10/10). Thesis directors: X. Biarnés (IQS-URL) and C. Rovira (UB).
15. **Msc thesis** of Daniel Conde Torres. "Exploring innate immune system peptides and their cell membrane interactions: a computational study". University of Barcelona. July 2022. Qualification : Excellent (10/10). Thesis directors: R. García Fandiño and C. Rovira.
16. **Msc thesis** of Oscar Vidal Gironès. "Use of AlphaFold and other computational methods in glycosyltransferase research". July 8, 2022. Qualification : Excellent (9.1/10). Thesis directors: C. Rovira and Q. Liao.
17. **Msc thesis** of David John Eliezar de Lima. "Insights into the Catalytic Mechanism of Maltodextrin Phosphorylase using QM/MM MD: Assessment of a Long-Lived Oxocarbenium Ion Intermediate". July 5, 2023. Qualification : Excellent (9.3/10). Thesis directors: C. Rovira and A. Magistrato.
18. **Msc thesis** of Laura Meiya Mazo Porras. "Structure determination and computer simulations of the genetically-modified MGAT5 enzyme for biorthogonal chemistry". *Erasmus Mundus* TCCM Program. July 5, 2024. Qualification : Excellent (9.8/10). Thesis directors: C. Rovira and G. J. Davies.
19. **Msc thesis** of Pridhi Balhara. "Computational investigation of sugar donor substrate selectivity of N-glycosyltransferases". July 12, 2024. *Erasmus Mundus* TCCM Program. July 2024 (defense at the University of Groningen). Thesis director : C. Rovira.

Undergraduate research works (TFG). Those with score ≥ 9/10 are marked with an asterisk.

1. **TFG work** of Víctor José Gallardo López (Biotechnology, UB). "Modeling of the *Burkholderia pseudomallei* catalase-peroxidase enzyme". June 2013. Supervisor: C. Rovira.
2. **TFG work** of Alba Nin Hill (Chemistry, UB). "Computational study of carbohydrate-active enzymes: glycoside hydrolases". June 2014. Supervisorr: C. Rovira.
3. **TFG work** of Iago Méndez Sobrado (Chemistry, UB). "Structural and computational study of carbohydrate-active enzymes: glycosyltransferases". June 2014. Supervisor: C. Rovira.
4. **TFG work** of Raquel Herrero Bueno (Chemistry, UB). "Protonation state of the active site residues in peroxidases". February 2015. Supervisor: C. Rovira.
5. **TFG work*** of Marta Escalé Fité (Chemistry, UB). "Influence of hydrogen bond interactions in the cleavage of sugar-phosphate bonds". June 2015. Supervisor: C. Rovira.

6. **TFG work** of Víctor Arredondo Ávila (Chemistry, UB). "Computational study of the influence of a nearby carboxylate group in the mechanism of glycosidic bond formation with retention of configuration". June 2016. Supervisor: C. Rovira.
7. **TFG work**[*] of Beatriz Piniello Castillo (Chemistry, UB). "Computational study of the Michaelis Complex of a bacterial β-glucosidase". Jan 2018. Supervisor: C. Rovira.
8. **TFG work**[*] of Ricard Silvestre Barceló (Chemistry, UB). "Computational study of the active center of an endo-β-1,4-mannosidase". June 2020. Supervisor: C. Rovira.
9. **TFG work** of Marc Muñoz Ferras (Chemistry, UB). "Computational analysis of the active center of carbohydrate-degrading enzymes: retaining glucosidases". Jan 2021. Supervisor: C. Rovira.
10. **TFG work**[*] of Adrià Olives Salmerón (Chemistry, UB). "Computational study of the conformational free energy landscape of β-D-glucopyranose". 29 June 2021. Supervisors: C. Rovira, A. Nin-Hill.
11. **TFG work**[*] of Alba Recio Sierra (Chemistry, UB). "Neuraminidase superfamily compendium". 27 Jan 2022. Supervisor: C. Rovira.

MANAGERIAL ACTIVITIES

- Member of the evaluation panel of the Spanish Ministry of Science and Innovation (MICINN-ANEP) for the the *Ramón y Cajal* and *Juan de la Cierva* programmes 2010.
- Chair of the *User's Committee of the Red Nacional de Supercomputación* (CURES). 2014-2016
- Vice-chair of the *User's Committee of the Red Nacional de Supercomputación* (CURES). 2011-2013
- Member of the direction board of the Institute of Theoretical and Computational Chemistry of the University of Barcelona (IQTCUB). 01/2014 – 01/2018.
- Member of the Editorial Advisory Board of the journal *ACS Catalysis* (01/2016 – 12/2019)
- Member of the access committee of the *Partnership for Advanced Computing in Europe*, PRACE (10/2016 – 09/2018).
- Member of the scientific committee for the Barcelona City Prize in Experimental Sciences and Technology. 02/2018 – 02/2020.
- Vice-president of the Computational Chemistry Group of the Spanish Royal Chemical Society (GEQC-RSEQ). Jun 2018 – Oct 2023
- Member of the evaluation panel of the Spanish Ministry of Science, Innovation and Universities (MICINN-ANEP) for national research projects (I+D+i PGC-RTI 2019). 03/02/2020 – 07/02/2020.
- Member of the Editorial Advisory Board of the journal *ACS Omega* (01/2021 – current)
- Member of the evaluation panel of the "Juan de la Cierva Formación 2020" programme in the área of Chemical and Sciences and Technologies. Agencia Estatal de Investigación (AEI) from the Ministerio de Ciencia e Innovación (MICINN). 15-06-2021.
- Member of the working group "Molecules, Macromolecules and Biomolecules" of the Psik European Network. Jan 2021 - current.

- Chair of the Life Sciences Panel of the European High Performance Computing Joint Undertaking (EuroHPC JU). European Union. Jan 2022-current.
- Evaluation of research projects from several research agencies in Spain and worldwide (AEI-Spain, VIDI-Netherlands, NSF-USA, MSCA-EU, NRF-South Africa).
- Secretary of the Academic Commission of the Doctorate Program in Organic Chemistry of the UB. Jan 2022 – current.
- Member of the Scientific Commission of the Organic Chemistry section of the UB Department of Inorganic and Organic Chemistry. Jan 2022 – current
- President of the Computational Chemistry Group of the Spanish Royal Chemical Society (GEQC-RSEQ). Oct 2023 – current.
- Member of the Scientific Advisory Commiteee of the *Hylleraas Centre for Quantum Molecular Sciences* (Norway). Nov 2023 - current.

PARTICIPATION IN PHD THESES COMMITTEES

In chronological order:

1. Jean Didier Maréchal (Universitat Autònoma de Barcelona, May 2003)
2. Fernando Ortega (Universitat de Barcelona, November 2004),
3. Cristina Horcajada (Universitat de Barcelona, 2005),
4. Cristian Obiol Pardo (Universitat de Barcelona, 2008),
5. Mireia Abel (Instititut Químic de Sarrià- Universitat Ramon Llull, June 2009),
6. Ophélie Kwasnieski (Université Pierre et Marie Curie, Paris, France, December 2010).
7. Varomylan Tipmanee (University of Cambridge, Cambridge, UK, January 2012).
8. Rachel Helbling (University of Bern, Bern, Switzerland, May 2013).
9. Melchor Sánchez Martínez (Universitat de Barcelona, Spain, December 2014. Committee Chair).
10. Juan Aranda (University of Valencia, Spain, June 2015. President).
11. Joan Jiménez Dejoz (Universitat Autònoma de Barcelona, Spain, July 2016).
12. María Fernanda Mendoza Muñoz (Universitat Autònoma de Barcelona, Spain, November 2016).
13. Lorenzo Casalino (International School for Advanced Studies, SISSA, Trieste, Italy, October 2017).
14. Marina Corbella Morató (Universitat de Barcelona, July 2018. Committee Chair).
15. Albert Solé Daura (Universitat Rovira Virgili, January 2020).
16. Miguel Àngel María Solano (Universitat de Girona, 12 February 2021. Committee Chair).
17. Martín Calvelo Souto (Universidad de Santiago de Compostela, 9 April 2021. Committee Chair).
18. Alberto Pérez de Alba Ortiz (University of Amsterdam, The Netherlands, Sept 22, 2021).
19. Myriam Torres Rico (Universidad de Sevilla, Spain, Dec 3rd, 2021).
20. Susana Barreda (Universitat de Barcelona, Spain, March 15, 2022. Committee Chair)
21. Sergi Rodà Llordés (Universitat de Barcelona, Spain, January 10, 2023. Committee Chair)

22. Carl Fogarty (Maynooth University, Ireland, April 10, 2024. Committee Chair)
23. Daniel Tianhou Zhang (Norwegian University of Science and Technology, Trondheim, May 20, 2024. Opponent).

INVITED TALKS IN INTERNATIONAL CONFERENCES

1. *"Ab initio molecular dynamics simulations of heme models".* Computer simulation of systems of biological interest. FORUM/INFM-SNS Workshop. Pisa (Italy). May 1997.
2. *"Density functional-based molecular dynamics: principles and applications in biology".* Workshop on the structure and function of biological macromolecules. Trieste (Italy). March 16-17th, 1998.
3. *"CPMD applied to heme protein modeling"* 1st Car-Parrinello molecular dynamics workshop (CPMD 1999). Schloss Ringberg - München (Germany). January 18-22nd, 1999.
4. *"Structure and dynamics of the myoglobin active site. QM/MM calculations".* Workshop on advances in first-principles computational condensed-matter physics. Madrid. January 13-15th, 2000.
5. *"First principles simulations of the binding of ligands in myoglobin".* 40th SANIBEL Symposium. St. Agustine - Florida (USA). February 26th - March 3rd, 2000.
6. *"First principles simulations of the binding of ligands in myoglobin".* Ab initio (from electronic structure) calculation of complex processes in materials. Schwabish Gmünd (Germany). August 21-26th, 2000.
7. *"Ab initio MD imulations of CO, NO and O_2 binding to myoglobin".* CECAM tutorial: Car-Parrinello molecular dynamics. Lyon (France). September 11-15th, 2000.
8. *"Structure and dynamics of the myoglobin active site." QM/MM calculations"* 2nd Car-Parrinello molecular dynamics workshop (CPMD 2001). Schloss Ringberg - München (Germany). January 29th - February 2nd, 2001.
9. *"First principles QM/MM simulations of ligand binding to myoglobin".* CECAM workshop: Ab initio modeling in biology. Lyon (France). June 11-13th, 2001.
10. *"First principles QM/MM simulations of ligand binding to myoglobin".* CECAM workshop: Mixed or hybrid quantum/classical methods. Lyon (France). June 14-15th, 2001.
11. *"First principles calculations of ligand binding in hemeproteins".* Workshop on advances in first-principles computational condensed-matter physics. Tenerife (Spain). January 10-12th, 2002.
12. Symposium on Nano-physics of life systems. Carlsberg Academy. Copenhagen (Denmark). June 21-22nd, 2002.
13. *"Ligand binding properties of hemeproteins modeled by first principles molecular dynamics".* Second conference on quantum bioinorganic chemistry (QBIC-2). Örenas castle, Lünd (Sweden). July 27-29th, 2002.
14. *"First principles calculations of the binding of ligands in heme proteins: myoglobin, cytochrome c and catalases".* EURESCO conference: Computational Biophysics: Integrating Theoretical Physics and Biology. San Feliu de Guixols, Spain. September 10,12th, 2002.

15. *"Binding of ligands in catalase".* Ab initio of Modeling of Biological Systems. Workshop of the Ψ_k-network. Trieste, Italy. May 15-16th, 2004.

16. *"Binding of substrates to glycoside hydrolases. Insights from Car-Parrinello simulations".* New developments for first principles molecular dynamics simulations in condensed matter and molecular physics. Workshop. CECAM (Lyon, France). May 15-18th, 2006.

17. *"First principles simulations of biochemical processes".* Annual project meeting of the Pan-European Research Infrastructure on High Performance Computing (TAM2006). Barcelona Supercomputing Center /Centro Nacional de Supercomputación. Barcelona, Spain. June 14-16th, 2006. **Plenary** (50').

18. *"Substrate distortion in the Michaelis complex of glycoside hydrolases".* Progress in ab initio modeling of biomolecules: methods and applications. Workshop. Leiden (Holland). July 3-7th, 2006.

19. *"First-principles MD simulations of the reaction intermediates of catalase. Electronic consequences of heme modifications".* Peroxidase2006 (Satellite of EUROBIC 2006). Aveiro (Portugal). July 7-9th 2006.

20. *"Identification of reaction intermediates of bifunctional catalase-peroxidase enzymes by means of QM/MM calculations*". BSC-IRB Barcelona Conference on Computational Biology. Barcelona, May 24th, 2007.

21. *"The reaction mechanisms of heme peroxidases. A QM/MM investigation".* 2nd CMM Workshop on QM/MM Simulations. Philadelphia (USA). Aug. 24– 27th, 2007.

22. *"First principles simulations of substrate distortion in β-glycoside hydrolases".* 235th National Meeting of the American Chemical Society. Symposium on Bioenergy and Carbohydrate Structure: Modeling and Experiment (New Orleans, USA, April 6-10th, 2008).

23. *"The reaction mechanisms of heme peroxidases. A QM/MM investigation".* CPMD2008 Conference on modeling and computation of structure and dynamics condensed phase systems. Trieste (Italy), June 23-27th, 2008.

24. *"The reaction mechanisms of heme peroxidases by first-principles simulations".* 9th European Biological Inorganic Chemistry Conference (EUROBIC9). Wroclaw (Poland), September 2-6th, 2008.

25. *"Substrate conformational changes in carbohydrate-binding enzymes. Insights from ab initio simulations".* Morphology and dynamics of nanostructures and disordered materials via atomic-scale modelling (EMRS Symposium). Warsaw (Poland), September 15-19th, 2008.

26. *"Substrate conformational changes in carbohydrate-binding enzymes: glycoside hydrolases".* Ab Initio Modelling in Applied Biosciences: Structure, Dynamics and Function. Uppsala (Sweden), December 11-12th, 2008.

27. *"Substrate conformational changes in glycoside hydrolase catalysis"*, and *"The reaction mechanisms of heme peroxidases by first-principles simulations"* (2 lectures). Summer School on Simulation Approaches to Problems in Molecular and Cellular Biology (CECAM/Psi_k school). San Sebastian (Spain). August 31th – September 5th 2009.

28. *"Substrate conformational changes in glycoside hydrolase catalysis. Insight from QM/MM molecular*

dynamics simulations". 12th Bratislava Symposium on Saccharides. Smolenice castle (Bratislava, Slovakia). June 19-23, 2011.

29. Advances in Quantum Chemistry: Interfacing electronic structure with dynamics (satellite symposium of the 14th International Congress of Quantum Chemistry). *"How does nature break and form glycosidic bonds: QM/MM metadynamics investigations"*. University of Minnesota, Minneapolis. USA. June 20-22, 2012.

30. "*How does nature break and form glycosidic bonds"*. X Girona Seminar on Theoretical and Computational Chemistry for the Modeling of Biochemical Systems: From Theory to Applications. Girona (Spain). 2nd -5th July 2012.

31. "*Using CPMD QM/MM metadynamics to study enzyme mechanisms"*. pDYNAMO (program library designed for the simulation of molecular systems using quantum chemical, QC, molecular mechanical, MM, and hybrid QC/MM potential energy functions) workshop. Barcelona (Spain). 12th to 14th September 2012.

32. *"How does nature break and make glycosidic bonds. QM/MM metadynamics investigations"*. 53rd SANIBEL Symposium. St. Simons Island (Georgia), USA. February 17-22, 2013.

33. *"Why using a QM/MM approach and how to set up a QM/MM simulation"*. Summer School on ab initio Molecular Dynamics for Biomolecules. S. Stefano di Sessanio (L'Aquila), Italy. June 9th-14th 2013.

34. *"An atomistic view to glucan hydrolysis by quantum mechanics/molecular dynamics"*. Gordon Resarch Conference: Cellulosomes, Cellulases & Other Carbohydrate Modifying Enzymes. Proctor Academy, Andover, NH, USA. August 4-9, 2013.

35. *"Sweet mysteries of nature: conformational changes and reactive processes in carbohydrate-active enzymes"*. CPMD2013. Matter, life, light from ab initio molecular dynamics simulations. Leipzig, Germany. September 2-6, 2013. **Keynote** (50').

36. *"Molecular mechanisms of retaining glycosyltransferases. QM/MM metadynamics investigations"*. XI Carbohydrate Symposium. Logroño, Spain. May 28-30, 2014.

37. *"The catalytic mechanism of catalase-peroxidases (KatGs)"*. Minisymposium on Structural Biology. Oslo, Sweden. September 8, 2014.

38. *"An ionizable triptophan residue imparts catalase activity to a peroxidase core. Insights from QM/MM simulations"*. Explicit control over spin states in technology and biochemistry (ECOSTBIO) workshop. Marseille, France. January 12-13, 2015.

39. *"Sugar conformational changes and reactivity of carbohydrate-active enzymes. Ab initio QM/MM metadynamics investigations"*. Carbohydrate active enzymes in medicine and biotechnology. Biochemical Society conference. St. Andrews (UK). 19-21 August 2015.

40. **"***How does nature make glycosidic bonds. Ab initio QM/MM Metadynamics Investigations*". ICIQ-FIFC Spain-Japan joint symposium on theoretical and Computational chemistry of complex systems. Tarragona (Spain). November 25-27, 2015.
41. *"How does nature make glycosidic Bonds"*. Future trends in protein science. 13th workshop in Protein.DTU. Lyngby (Denmark). Dec. 1st, 2015.
42. *"Sugar conformational changes and reactivity of carbohydrate-active enzymes. Insight from QM/MM metadynamics"*. Glycosyl cation day. Potiers (France). December 14, 2015.
43. *"Computer simulation to understand how enzymes work"*. Partnership for advanced computing in Europe (PRACEdays16). Prague (Check Republic). 10-12 May 2016. **Keynote** (50').
44. *"How carbohydrate-active enzymes work"*. 10th congress on electronic structure: principles and applications (ESPA). Castellón de la Plana (Spain). June 28-July 2, 2016.
45. *"How carbohydrate active enzymes work. Insights from QM/MM simulations"*. 252th National ACS Meeting. Symposium: Advanced Potential Energy Surfaces. Philadelphia (USA). Aug 21-25, 2016.
46. *"Sugar conformational changes and reactivity of carbohydrate-active enzymes. Insight from QM/MM metadynamics simulations"*. 19th European Carbohydrate Symposium (EUROCARB). Barcelona (Spain). July 2-6 2017. **Keynote** (30')**.**
47. *"Catalysis by natural and engineered glycosidases. An atomistic view from QM/MM simulations"*. 254th National ACS Meeting. Symposium: New Paradigm for Catalyst Design: From Enzymatic Function to Functional Mimics. Washington DC (USA). Aug 20-24, 2017.
48. *"Sugar conformational changes and catalytic mechanisms of carbohydrate-active enzymes"*. MGMS international meeting: QM/MM Methods and Applications. Manchester (UK). Sept 4-6, 2017.
49. *"Sugar conformational changes and catalytic mechanisms of carbohydrate-active enzymes"*. Conference: Computational Advances in Drug Discovery - SBDD2017. Lausanne (Switzerland). Sept 5-8, 2017.
50. *"Carbohydrate-active enzymes: sugar conformations and reactivity"*. Sissa Mini-Workshop on Statistical and Molecular Biophysics. Trieste (Italy). Oct 18, 2017.
51. *"Catalysis by natural and engineered glycosidases"*. 16th Iberian Meeting/ 4th ChemBio Group Meeting of the *Real Sociedad de Química Española*. Barcelona (Spain). Feb 5-7, 2018.
52. *"Computer simulation of biological processes*: enzyme catalysis". HPC for next generation nanomaterials & nanodevices engineering. Catalan Institute of Nanoscience and Nanotechnology (ICN2). Bellaterra (Spain). May 30-31, 2018. **Keynote**.
53. *"The Fita-Rossmann catalytic mechanism"*. 25th Years of Macromolecular Crystallography in Barcelona. Residència d'investigadors, Barcelona (Spain). June 18-19, 2018.
54. *"Catalysis by natural and engineered carbohydrate-active enzymes"*. International Society of Quantum Biology and Pharmacology (ISQBP) President's Meeting 2018. Institut d'Estudis Catalans, Barcelona (Spain). June 19-21, 2018.
55. *"The reaction mechanism of catalase-peroxidases*. CECAM workshop: Frontiers and challenges of

computing metals for biochemical, medical and technological applications. Paris (France). July 11-13, 2018.

56. *"How carbohydrate-active enzymes work. Insight from computer simulation"*. II Jornadas Españolas de Biocatálisis 2018. Oviedo (Spain). July 25-16, 2018.

57. *"An atomistic view to glycan hydrolysis by quantum mechanics/molecular dynamics"*. 2nd Carbohydrate and Fluorine Symposium. Poitiers (France). 18-19th October 2018.

58. *"An atomistic view to glycan hydrolysis by quantum mechanics/molecular dynamics".* Trends in Enzyme Catalysis. Merging Theory and Experiment. Benicàssim (Spain). Nov 29-30, 2018.

59. *"Modeling catalytic mechanisms in carbohydrate-active enzymes".* An introductory workshop in biomedical glycoscience. CIC bioGUNE. San Sebastian (Spain), June 3-5, 2019.

60. *"How does nature make glycosidic bonds. Insight from enhanced-sampling QM/MM simulations".* Exploring Complex Free Energy Landscapes: Structure/Function Formation, Multiscales, and Long-timescales. Max Planck Institut for Polymer Research. Mainz (Germany), June 5-7, 2019.

61. *"How carbohydrate-active enzymes work. Insight from enhanced-sampling QM/MM simulations"*. Milestones in Molecular Simulations. London (UK). June 21, 2019.

62. *"How carbohydrate-active enzymes work. Insight from computer simulation"*. 20th European Carbohydrate Symposium (EUROCARB). Leiden (The Netherlands). June 30-July 4, 2019. **Opening plenary** (50').

63. "Modeling catalytic mechanisms in carbohydrate-active enzymes with QM/MM MD methods". BioExcel Virtual Workshop on Best Practices in QM/MM Simulation of Biomolecular Systems (7th Bioexcel webinar). 12 Jan 2021. Invited talk + round table participation.

64. "QM/MM metadynamics simulations of novel chemical reaction in glycoprocessing enzymes". Recent Advances in Modelling Rare Events (RARE2021). 15-17 December 2021.

65. "Computer simulation of unusual reaction mechanisms in glycosidases". 1st Network Meeting on Glycan Structural Biology, Analytics & Computational Studies. Naples (Italy). April 4-6, 2022.

66. "Computer simulation of new reaction mechanisms in glycosidases". Girona Seminar 2022. May 31st - June 3rd, 2022. **Keynote.**

67. "Computer simulation of new reaction mechanisms in carbohydrate-active enzymes (CAZymes)". Molecular Simulation 2022: Present, Past and Future. 25-29 June 2022, Erice (Italy).

68. "Modeling mechanisms of glycosylation reactions in CAZymes hand-in-hand with experiments". 30th International Carbohydrate Symposium. Brazil (virtual symposium). July 10-15, 2022. **Plenary address** (45 min).

69. "QM/MM metadynamics simulations of new reaction mechanisms". Twenty years of metadynamics. Lausanne (Switzerland). September 5-8, 2022.

70. "Computer simulation of mechanisms in glycoprocessing enzymes using QM/MM approaches". Modeling and design of molecular materials 2022 (MDMM 2022). Gdansk (Poland). September 19-22, 2022.

71. "How enzymes work. Insight from computer simulation". ZCAM and CECAM. Present and future. Zaragoza (Spain), June 8-9, 2023.

72. "Simulation of glycosyltransferase catalytic mechanisms". Gordon Research Conference (GRC) on Carbohydrate-Active Enzymes for Glycan Conversions. Proctor Academy, Andover (USA), July 23-28, 2023.

73. "Fundamental aspects of enzyme catalysis to inform biotechnology approaches". Digitally Driven Biotechnology Symposium. Danish Technical University. Copenhagen (DK). 26 Oct 2023. **Keynote**.

74. "QM/MM studies of protein glycosylation reactions". Trends in Enzyme Catalysis. Merging Theory and Experiments. TrEnCa 2023". Benicàssim (Spain). Nov 30 – Dec 1st, 2023.

75. "QM/MM MD simulations of protein glycosylation reactions". JNCASR - CECAM Conference MD@60. Bangalore (India). Feb 26-29, 2024.

76. "QM/MM studies of protein glycosylation reactions". Electronic Structure, Principles and Applications (ESPA). Tarragona, 3-7 June, 2024.

77. "Non-classical glycosylation mechanisms: a modelling approach". 16th Bratislava Symposium on Saccharides. Smolenice Cabstle (Slovakia). Sept 23-27, 2024. **Plenary address**.

78. "Discovering glycosylation mechanisms". Computational chemistry across scales and disciplines: celebrating the 60th birthday of Ursula Röthlisberger. CECAM (Lausanne). Oct 1-3, 2024.

79. "QM/MM simulation of protein glycosylation mechanisms". Innovative high-performance computing approaches for molecular neuromedicine. Institute of Neurosciences and Medicine (INM). Forchungszentrum Julich. Germany. Nov 5-8, 2024. Virtual symposium.

80. "Protein glycosylation mechanisms". Highlighting Organic Chemistry in Catalonia. Joint virtual symposium of the European Chemical Society (EuChemS) and the Catalan Society of Chemistry (SCQ). Nov. 8, 2024.

81. "Fundamental aspects of enzyme catalysis to inform biotechnology approaches". VII RSEQ Chemical Biology Group Meeting - ChemBioVII. **Plenary address**. Sevilla. 18-20 Nov 2024.

SELECTED CONTRIBUTED TALKS AT INTERNATIONAL CONFERENCES

1. Ab initio calculation of complex processes on materials. *"Binding of CO, O2 and NO to myoglobin. A first principles study".* Schwabish Gmund (Germany). 16-18 September 1996. Oral communication.

2. 8th Carbohydrate Bioengineering Meeting. *"Substrate conformational changes in glycoside hydrolase catalysis".* Naples (Ischia, Italy), May 10-13th, 2009. Oral communication.

3. International Symposium on Applied Bioinorganic Chemistry (11 ISABC). *"The molecular mechanism of catalase by QM/MM metadynamics"*. Barcelona. 2-5 December 2011. Oral communication.

4. 26th International Carbohydrate Symposium. *"The molecular mechanism of enzymatic glycosyl transfer with retention of configuration: evidence for a short-lived oxocarbenium ion-like species".* Madrid (Spain). 22nd to 27th July 2012. Oral communication.

5. 10th Carbohydrate Bioengineering Meeting. ***"****The molecular mechanism of enzymatic glycosyl transfer with retention of configuration. QM/MM metadynamics investigations"*. Prague (Czech Republic), April 21-24, 2013. Oral communication.
6. Barcelona Biomed Conference: Frontiers in Dynamics Simulations of Biological Molecules. *"Atomistic simulations of glycosidic bond formation".* Barcelona. November 4-6, 2013. Oral communication.
7. 12th Carbohydrate Bioengineering Meeting (CBM12). "A Front-Face Mechanism 'Synthase' Engineered from a Retaining Hydrolase. Mechanistic insight from QM/MM metadynamics". Vienna**.** April 23-26, 2017. Oral communication.
8. 29th International Carbohydrate Symposium (ICS 2018). *"Unusual catalytic itineraries of glycosidases unveiled from QM/MM metadynamics simulations"*. Lisboa (Portugal), July 15-19, 2018. Oral communication.
9. 13th Carbohydrate Bioengineering Meeting (CBM13). *"Early stages of glycogen biosynthesis: mechanism of action of glycogenin"*. Tolouse (France), May 19-22 2019. Oral communication.
10. "Using computers to understand how carbohydrates are processed in Nature". 7th European Chemical Biology Symposium (7ECBS). 26-28 May, 2021. Oral communication.
11. 14th Carbohydrate Bioengineering Meeting (CBM14). *"Uncovering novel catalytic mechanisms in glycosidases with the help of computer simulation"*. Oslo/ Norefjell (Norway), Sept 25-28, 2022. Oral communication.
12. 21st European Carbohydrate Symposium (Eurocarb21). "How glycosidases operate: combining crystallography and quantum mechanics to uncover new mechanisms". Duo oral communication, together with Mariana Morais (CNPEM, Brazil). Paris, 9-13 July 2023.
13. 7th Iberian Carbohydrate Meeting. "Novel mechanisms of glycosyltransferases involved in protein glycosylation". Oral communication. Sitges (Spain), 15-17 January 2024. Oral communication.
14. 15th Carbohydrate Bioengineering Meeting (CBM15). *"*QM/MM simulations of GT-mediated protein glycosylation reactions*"*. Ghent (Belgium), May 5-8, 2024. Oral communication.

INVITED TALKS IN NATIONAL CONFERENCES

1. Reunión de la red nacional de materiales moleculares. Barcelona. 6-7 July 2000.
2. Primera reunión de la red nacional de modelización molecular. Barcelona. 22-23 March 2002.
3. Reunión de la red temática de aleaciones moleculares. Vilanova (Barcelona). 14-16 June 2002.
4. XX Reunió de la Xarxa de Química Teòrica. Barcelona. 12-13 July 2004. **Plenary address**.
5. "Molecular modeling of enzyme-substrate interactions and reaction mechansims in peroxidases and aldo-keto reductases". Reunión de usuarios de la Red Española de Supercomputación (RES). Santander. 23 September 2009.
6. 1st Symposium of the Institut de Química Teòrica of the UB. Barcelona. 14 May 2010.
7. "Substrate preactivation mechanisms in glycoside hydrolase catalysis". XXVI Reunió Anual de la Xarxa de Referència de Química Teòrica i Computacional. UAB, Barcelona, 12-13 July 2010. Plenary lecture.

8. "Mecanismos moleculares de la oxidación celular". XXVI congreso nacional de la Sociedad Española de Nutrición Parenteral y Enteral (SENPE). Girona, 24-27 May 2011. Invited talk and round table.
9. "First principles simulation of biomolecular processes". XVII Congreso de Física Estadística. Barcelona, 2-4 June 2011. Plenary lecture.
10. "How does nature form glycosidic bonds? Reunión de usuarios de la Red Española de Supercomputación (RES). Málaga. 14 September 2012.
11. "How does nature break and make glycosidic bonds". Theoretical Chemistry in Spain told by women. A Symposium in Honour of Rosa Caballol. Tarragona (Spain). January 30-31, 2013.
12. "Simulacions computacionals per a entendre com funcionen els enzims". Jornada catalana de supercomputació (JOCS). Barcelona, 25 May 2016. Plenary lecture.
13. "How carbohydrate-active enzymes work". Annual symposium and scientific advisory board meeting of the Institute of Theoretical and Computational Chemistry of the UB. 20-Nov-2019. Plenary lecture.
14. "New mechanisms of carbohydrate-active enzymes unveiled by computational methods". 2021 Webinar Biocatalysis Cycle. Spanish Network of Biocatalysis (RTBIOCAT). Oct 28, 2021.

INVITED SEMINARS AT UNIVERSITIES AND RESEARCH CENTERS

1. University of Barcelona. Department of Physical Chemistry. 18-12-1996. Invited by Prof. J. J. Novoa.
2. International School for Advanced Studies (SISSA), Trieste (Italy), 18-3-1997. Invited by Prof. E. Tosatti.
3. Max-Planck Institut für Biophysicalische Chemie, Göttingen (Germany), 9-11-1999. Invited by Prof. H. Grubmüller.
4. Ulm Universität. Biophysics Department, Ulm (Germany), 18-11-1999. Invited by Prof. U. Nienhaus.
5. Institut municipal d'investigació mèdica (IMIM). Barcelona, 14-2-2000. Invited by Prof. F. Sanz.
6. University of Barcelona. Department of Physical Chemistry. 4-5-2000. Series of conferences organized by Prof. P. Alemany.
7. National Institute for Advanced Interdisciplinary research (NAIR). Tsukuba (Japan). 2 seminars: 6-11-2000 and 13-11-2000 Invited by Prof. K. Terakura.
8. Barcelona Science Park. 9-1-2001. Series of conferences organized by the Research Center on Theoretical Chemistry (CeRQT). Director: Prof. S. Olivella.
9. Eidgenössiche Technishe Hohschule Zürich (ETH). Zürich (Switzerland). 28-3-2001. Invited by Prof. U. Röthlisberger.
10. Centro di Calcolo Scientifico de la Switzera (CSCS). Lugano (Switzerland). 27-7-2001. Invited by Prof. M. Parrinello.
11. Centro di Calcolo Scientifico de la Switzera (CSCS). Lugano (Switzerland). 6-3-2002. Invited by Prof. M. Parrinello.
12. Helsinki University of Technology. Helsinki (Finland). Invited by Prof. R. Nieminen. 21-5-2002.
13. Technical University of Denmark. Copenhagen (Denmark). Invited by Prof. H. Bohr. 24-6-2002.

14. Institut municipal d'investigació mèdica (IMIM). Barcelona, 25-11-2003. Invited by Dr. J. Villà.

15. Parc Científic de Barcelona (PCB). Barcelona, 3-06-2004. Invited by the PCB Scientific Director.

16. Universitat Autònoma de Barcelona (UAB). Barcelona, 2-03-2005. Invited by Prof. A. Lledós.

17. University of Cambridge (Chemistry Department). Cambridge (UK), 14-05-2008. Invited by Prof. Michiel Sprik and Dr. Jochen Blumberger.

18. Centre de Recerca en Salut Internacional de Barcelona (CRESIB). Hospital Clínic – IDIBAPS. Barcelona, 8-10-2008. Invited by Prof. Pedro L. Alonso.

19. Centro de Investigaciones Biológicas (CIB-CSIC). Madrid, 20-07-2010. Invited by Prof. Jesús Jiménez Barbero.

20. University of Porto, Department of Chemistry and Biochemistry. Portugal, 19-11-2010. Invited by Prof. Maria Joao Ramos.

21. Université Pierre et Marie Curie, Institut Parisien de Chimie Moléculaire. 17-12-2010. Invited by Prof. Max Malacria and Dr. Etienne Derat.

22. Universitat de Girona - Parc Científic de Girona. April 20, 2012. Invited by Prof. Miquel Costas.

23. Barcelona Supercomputing Center (BSC). Barcelona. April 27, 2012. Invited by Prof. Modesto Orozco.

24. University of Bern. Bern, Switzerland. May 8, 2013. Invited by Prof. Michele Cascella.

25. National Center for Biomolecular Research (NCBR). Brno, Czech Republic. May 30, 2013. Invited by Prof. Jarek Koca.

26. University of Barcelona. Departament of Chemistry. Barcelona. Invited by Prof. Pere Romea, coordinator of the Master program on Organic Chemistry. 22 October 2013.

27. University of Barcelona. Departament of Chemistry. Barcelona. Invited by the head of the Chemistry Department to talk about the Nobel Prize in Chemistry. December 2013.

28. Institute of Biomedical Research. Barcelona Biomed Seminars. Barcelona. March 12, 2014. Invited by the structural biology research groups of IRB and IBMB-CSIC.

29. University of York. Department of Chemistry. June 26, 2014. Invited by Prof. Gideon J. Davies.

30. Institut National des Sciences Appliquées de Toulouse. December 23, 2015. Invited by Prof. Isabelle André.

31. CIC bioGUNE, Center for Cooperative Research in Biosciences. Bilbao. May 26, 2017. Invited by Prof. Jesús Jiménez Barbero and Prof. Marcelo Guerin.

32. Oxford University. Chemistry Research Laboratory. Oxford (UK). Oct 4, 2019. Invited by Prof. Benjamin G. Davis.

33. Aix Marseille Université – CNRS. Marseille (France). Nov 18, 2019. Invited by Prof. Gerlind Sulzenbacher.

34. St. Jude Children's Research Hospital. Chemical Biology and Therapeutics Department. Memphis, Tennessee (USA). Aug 5th 2021, invited by the Dept. Director Prof. Aseem Ansari.

35. Barcelona Supercomputing Center. Life Sciences Department and *Bio4InfoWomen* seminar series. Barcelona, Spain. Sept 2nd 2021, invited by the Life Sci. director Alfonso Valencia and Life Sci. group

leader Victor Guallar.

36. Kings College London. Biological Physics Across Scales (BiPAS) seminar series. Apr 12th, 2022. Invited by Profs. S. Garcia-Manyes, I. Diez-Pérez and C. Molteni.
37. Sorbonne Université, Campus Pierre & Marie Curie, Paris. Institute of Mineralogy, Materials Physics and Cosmochemistry (IMPMC). July 12th, 2023. Invited by Prof. Fabio Pietrucci.
38. Universitat de Barcelona. Departament de Química Inorgànica i Orgànica. Oct 6th, 2023. Conference series of the Doctorate program in organic chemistry of UB (PDQO).

OUTREACH

1. Public exhibition about the life and work of Rosalind Franklin. Library of the Chemistry and Physics Departments. University of Barcelona. Title: "*Rosalind Franklin: 100 + 1 years after her birth"* (Rosalind Franklin: 100 + 1 anys del seu naixement). Curators: C. Rovira and A. Guash. November 19, 2021.

2. Public talk "The marvelous world of enzymes and sugars" (El meravellós món dels enzims i els sucres). La Nou de Gaià Castle (Castell de la Nou de Gaià). "Territori i Pensament" conferences series Tarragona. Spain. 26 Nov. 2021.

3. Colloquium "From Women Eye's". Centre Européen de Calcul Atomique et Moléculaire (CECAM). February 10, 2023. Virtual event.

4. Talk for 2nd-course high school students "The marvelous world of enzymes and sugars" (El meravellós món dels enzims i els sucres). Institut public Mercè Rodoreda (L'Hospitalet de Llobregat). Spain. 4 Nov. 2024.

SELECTED POSTER PRESENTATIONS AT INTERNATIONAL MEETINGS

Note: Posters presented by members of my group are also listed. The person presenting the poster is indicated.

5. First Congress of the International Society for Theoretical Chemistry. Girona (Spain). 1993 (poster presented by C. Rovira).
6. Eigth international workshop on computational condensed matter physics: total energy and force methods. Trieste (Italy). January 9-11th, 1997 (poster presented by C. Rovira).
7. Theoretical chemistry in biology: from molecular structures to functional mechanisms. Savannah (GA, USA). June 3-7th, 1997 (poster presented by C. Rovira).
8. 9th International Congress of Quantum Chemistry. Atlanta (GA, USA). June 9-14th, 1997 (poster presented by C. Rovira).
9. 6th Carbohydrate Bioengineering Meeting (CBM6). Barcelona, April 3-6th, 2005 (poster presented by X. Biarnés).

10. Ab-initio Molecular Dynamics Simulations - from Solid State Physics to Chemistry and Biology (CPMD2005). Ascona (Switzerland), September 3-8th, 2005 (poster presented by X. Biarnés).
11. 7th Carbohydrate Bioengineering Meeting (CBM7). Braunschweig (Germany), April 22-25th, 2007 (2 posters were presented by X. Biarnés and A. Ardèvol, respectively).
12. Workshop on ab initio modelling of biomolecules. Univ. of Rome "La Sapienza". April 2-4th, 2007 (2 posters were presented by M. Alfonso-Prieto and P. Vidossich, respectively).
13. Conference on modeling and computation of structure and dynamics of condensed phase systems. (CPMD2008). Trieste (Italy), June 23-27th, 2008 (3 posters were presented by M. Alfonso-Prieto, X. Biarnés and A. Ardèvol, respectively).
14. 8th Carbohydrate Bioengineering Meeting. Naples (Ischia, Italy), May 10-13th, 2009 (poster presented by A. Ardèvol).
15. Theoretical Chemistry: Modeling reactivity from gas phase to biomolecules and solids *(Celebrating 25 years of the Theoretical Chemistry Network in Catalonia. Dedicated to Prof. S. Olivella).* June 29th - July 3rd 2009. Barcelona (3 posters presented by M. Alfonso-Prieto, P. Vidossich and A. Ardèvol, respectively).
16. CPMD2013. Matter, life, light from ab initio molecular dynamics simulations. Leipzig, Germany. September 2-6, 2013. 2 posters presented by Javier Iglesias-Fernández and Víctor Rojas-Cervellera, respectively.

I stopped keeping track of the group posters in 2013.

RESEARCH GRANTS AS PI

(Amounts given as direct costs, unless specified)

1. I+D project of the Spanish Ministry of Science, Innovation and Universities (MICIU). Proyectos de Generación de Conocimiento. Title: "Computer simulation of the molecular basis of substrate recognition and catalysis in glycoprocessing enzymes" (acronym SimMolGly). PI: C. Rovira. Reference: PID2023-147939NB-I00 (from 01/09/2024 to 31/08/2027). 150.000,00 € (187.500,00 €, indirect).
2. HORIZON-MSCA-2022-DN-01-01. "GLYCOprotein N-glycosylation from non-life to eukaryotes: a Doctoral Network to expand the knowledge on a ubiquitous posttranslational modification of proteins (GLYCO-N)". Proposal ID 101119499. From 01/02/2024 to 30/01/2027. Co-PI: C. Rovira. Coordinator: A. Molinaro (U. Naples). 2.724.364,80 € (full consortium), 251.971,20 € (UB-C. Rovira).
3. Spanish Structures of Excellence María de Maeztu awarded to the Institute of Theoretical and Computational Chemistry (IQTCUB, https://www.iqtc.ub.edu). Reference: CEX2021-001202-M (from 01/01/2023 to 31/12/2027). 2.000.000,00 € (whole Institute). C. Rovira is one of the six project guarantees. One PhD student of the group was covered with the grant.

4. Grup de recerca consolidat (GRC): Estructura i funció en macromolècules. PI-Coordinator: C. Rovira (UB). Co-PI: I. Fita (CSIC). Funding agency: AGAUR (Generalitat de Catalunya). Reference: 2021SGR-00680. From 01/01/2022 to 31/12/2024. Amount awarded: 60.000 €
5. I+D project of the Spanish Ministry of Science and Innovation (MICINN). Programa estatal de generación de conocimiento. Title: "Computer simulation of catalytic mechanisms in glycoprocessing enzymes by means of QM/MM molecular dynamics techniques" (acronym COMPGLYCO). PI: C. Rovira. Reference: PID2020-118893GB-100 (from 01/09/2021 to 31/08/2024). 120.000,00 € (145.200,00 €, indirect).
6. ERC-2020-SyG-951231 "Activity-Based Profiling of Glycoprocessing Enzymes for Human Health and a Sustainable Society". European Research Council. Grant agreement No 951231. Acronym: CARBOCENTRE. Together with G. J. Davies (U. York, UK) and H. S. Overkleeft (U. Leiden, NL). Total grant 9,057,250 €. Amount corresponding to UB (C. Rovira): 1.984,750 € (indirect costs). https://cordis.europa.eu/project/id/951231. From 01/06/2021 to 31/05/2027.
7. IRP GLYCOMIMIC. French National Research Agency (ANR). "Mimicking the reaction transition state of carbohydrate-active enzymes with superacids". Collaborative research project between IC2MP (CNRS-Université de Poitiers, Prof. S. Thibadeau), University of Barcelona (Prof. C. Rovira) and CICbioGUNE, Bilbao (Prof. J. Jiménez Barbero). From 01/02/2022 to 31/12/2027.
8. Spanish Structures of Excellence María de Maeztu awarded to the Institute of Theoretical and Computational Chemistry (IQTCUB, https://www.iqtc.ub.edu). Reference: MDM-2017-0767 (from 01/07/2018 to 31/06/2022). 2.000.000,00 € (whole Institute). C. Rovira is one of the six project guarantees.
9. H2020-MSCA-ITN-2018. "Training interdisciplinary glycoscientists to get a molecular-level grip on glycocodes at the human mucosa–microbiota interface (SWEET CROSSTALK)". Proposal ID 814102. https://cordis.europa.eu/project/id/814102. From 01/01/2019 to 31/12/2022. Coordinator: T. Weenekes (U. Utrecht). Co-PI: C. Rovira. 4,117,674.96 € (full consortium), 250.904,88 € (UB-C. Rovira).
10. COST Action CA18132 - Functional Glyconanomaterials for the Development of Diagnostics and Targeted Therapeutic Probes. https://www.cost.eu/actions/CA181. From 14/03/2019 to 13/03/2023. Coordinator: M. C. Galan (University of Bristol). C. Rovira is PI and member of the management committee.
11. Grup de recerca consolidat: Estructura i funció en macromolècules. Coordinator: C. Rovira (UB). Co-PI: I. Fita (CSIC). Funding agency: AGAUR (Generalitat de Catalunya). Reference: 2017SGR-1189. From 01/01/2017 to 31/12/2020. Amount awarded: 40.950 Euros.
12. I+D project of the Spanish Ministry of Economy, Industry and Competitiveness (MINECO). Programa estatal de fomento de la investigación científica y técnica de excelencia. Title: "Modeling and simulation of reactive processes in enzymes by means of ab initio molecular dynamics and QM/MM methods." PI: C. Rovira. Reference: CTQ2017-85496-P (from 01/01/2018 to 30/09/2021). 75.000,00 € (90.750,00 €, indirect).
13. I+D project of the Spanish Ministry of Economy, Industry and Competitiveness (MINECO). Programa Estatal de I+D+I Orientada a los Retos de la Sociedad. Subprograma de Actuaciones de Programación Conjunta Internacional. Title: "Synthetic photoswitchable modulators to harness endogenous proteins: in vivo

remote control of pentameric ligand-gated ion channels with light (MODULIGHTOR)". PI: C. Rovira. Coordinator: Pau Gorostiza (IBEC). Reference: PCIN-2015-163-C02-01 (from 09/01/2015 to 08/31/2018). 81.000,00 €.

14. I+D project of the Spanish Ministry of Economy, Industry and Competitiveness (MINECO). Programa estatal de fomento de la investigación científica y técnica de excelencia. Title: "Simulation of reactive processes in proteins and enzymes by means of *ab initio* molecular dynamics and QM/MM techniques." PI: C. Rovira. Reference: CTQ2014-55174-P (from 01/01/2015 to 31/12/2017). 87.000,00 € (105.270,00 €, indirect).

15. Grup de Recerca Consolidat (Estructura i funció en macromolècules). AGAUR (Generalitat de Catalunya). Coordinator: C. Rovira. Reference: 2014SGR-987 (years 2014-2016). 15.000 €.

16. COST Action CM1305. 'Explicit control over spin states in technology and biochemistry" (ECOSTBIO). April 24, 2014 – April 27, 2018. Coordinator: M. Swart (Universiy of Girona). C. Rovira is PI and member of the management committee.

17. Partnership for advanced computing in Europe (PRACE). "First principles design of a biocatalyst for water oxidation (BioWatOx)". Proposal number: 2011040558 (year 2012) 37.500.000,00 supercomputer hours. PI: C. Rovira.

18. I+D project of the Spanish Ministry of Economy, Industry and Competitiveness (MINECO). Title: "Simulation of reactive processes in heme enzymes, glycoside hydrolases/transferases and peptide-bound nanoparticles by means of ab initio molecular dynamics-based methods." PI: C. Rovira. Reference: CTQ2011-25871 (years 2012-2014). 85.000,00 € (102.850,00 €, indirect)

19. Acción Complementaria. MINECO. Ref: CTQ2011-13832-E. CPMD2011: Simulaciones de dinámica molecular ab initio en Química, Ciencia de Materiales y Biofísica. 5000 €. 2011.

20. Centre Européen de Calcul Atomique et Moléculaire (CECAM). Conference support (year 2011). 10.000 €.

21. I+D project of the Spanish Ministry of Science and Innovation (MICINN). Title: "Simulación de procesos reactivos en proteínas y enzimas mediante métodos de dinámica molecular ab initio". PI: C. Rovira (Parc Científic de Barcelona, Spain). Reference: FIS2008-03845 (years 2009-2011). 75.000 €.

22. I+D project of the Spanish Ministry of Science and Education (MEC). Title: "Modelización de procesos reactivos en proteínas y de interacción biomolécula-superfície mediante métodos de primeros principios". PI: C. Rovira (Parc Científic de Barcelona, Spain). Reference: FIS2005-00655 (years 2006-2008). 24.000 €.

23. "Distinció de la Generalitat de Catalunya per a la promoció de la recerca Universitaria" (2003-2007). Young Scientists category. PI: C. Rovira. 150.000 €.

MAIN SCIENTIFIC COLLABORATIONS

- Prof. Gideon J. Davies (University of York, UK)
- Prof. Antoni Planas (IQS-Universitat Ramon Llull, Barcelona).

- Prof. Benjamin G. Davis (University of Oxford, UK)
- Prof. Spencer Williams (University of Melbourne, Australia)
- Prof. Herman S. Overkleeft (University of Leiden)
- Prof. Ramón Hurtado-Guerrero (BIFI-ARAID, Zaragoza)
- Prof. Birte Svensson, Dr. Ditte Welner, DTU, Denmark.
- Prof. Pau Gorostiza (ICREA-IBEC, Barcelona)
- Prof. Ignacio Fita (Molecular Biology Institute of Barcelona, IBMAB-CSIC).

TEACHING EXPERIENCE

Teaching at Universitat de Barcelona, Department of Chemistry

- Undergratuate lectures: "The protein data bank (PDB)", included in the course "Chemistry documentation" (3rd year, Chemistry degree). 4h /year. 2022-2023
- Master in Organic Chemistry. "Molecular Modeling course". 26 hours/year (**2015-2020** and **2022-**current)
- Master in Atomistic and Multiscale Computational Modelling in Physics, Chemistry and Biochemistry. Lectures on "QM/MM methods and applications". 4h/year (**2018-current**)
- Master in Theoretical Chemistry and Computational Modelling. Research lecturer. 1h/year, biennially (**2015-current).**
- Computer programming (Recursos Informàtics). 14 hours (**2015**)
- Master in Organic Chemistry. "Molecular Modeling course". 16 hours (**2014**)
- General Chemistry Laboratory (QAII): 20 hours (**2014**)
- Computer programming: 21 hours/year (**1993-1994; 2001-2002; 2004-2007**).
- Master in Biophysics. "Molecular modeling of biological processes". 2h/year (**2006** and **2008)**.
- Physical Chemistry laboratory. 60 hours (**2001**).
- Introduction to Quantum Chemistry (practices). 90 hours (**1998 - 2001**).
- Spectroscopy Fundamentals (practices). 120 hours (**1998 - 2001**).
- Statistical Thermodynamics (practices). 90 hours (**1994 - 1995**).
- Quantum Chemistry (practices). 60 hours (**1993 - 1994**).

Teaching at other Universities and research centers

- *Universitat Ramon Llull (Institut Químic de Sarrià, Barcelona).* Master in Bioengineering. "Modeling and Simulation". 14 hours/year (**2009-2023**). 6h/year (**2024-current**)
- Université Grenoble Alpes, France. École Doctorale Chimie et Science du Vivant. Three lectures (6h) on QM/MM methods and its applications to decipher enzyme catalytic mechanisms. November **2019**.

- Institut National des Sciences Appliquées de Toulouse (INSA), France. Lecture (4h) "Quantum mechanics/molecular mechanics methods for computational biology", within the course *Biologie Computationnelle pour les Biotechnologies.* November **2015**.