

CURRICULUM VITAE

MARIA JOÃO ROMÃO

PERSONAL DATA

Place and date of birth: Lisbon, 11th January 1955

Nationality: Portuguese

ADDRESS

Departamento de Química / Faculdade de Ciências e Tecnologia

Universidade Nova de Lisboa; 2829-516 Caparica PORTUGAL

Tel: +351-212948345

e-mail : mjr@fct.unl.pt

url: <http://sites.fct.unl.pt/xtal>

<http://www.researcherid.com/rid/A-4115-2013>

<http://orcid.org/0000-0002-3004-0543>

EDUCATION

2001 Habilitation in Biochemistry, Faculdade de Ciências e Tecnologia/ Universidade Nova de Lisboa (FCT-UNL)

1988 PhD in Chemistry, Instituto Superior Técnico (IST)

1978 Degree in Chemical Engineering, IST

ACADEMIC CAREER

1977/1978 Junior Demonstrator at IST

1978/1979 Assistant at FCT-UNL

1979/1989 Assistant at IST

1989/1998 Assistant Professor at IST

1992/1998 Responsible for an independent research group at ITQB

1998/2012 Associate Professor at IST (position declined)

since 1998 Associate Professor of Biochemistry at FCT-UNL

since 1998 Responsible for an independent research group of Structural Biology at FCT-UNL: <http://sites.fct.unl.pt/xtal>

2012 Full Professor of Biochemistry at FCT-UNL

CURRENT POSITION

Head of the Chemistry Department of FCT-UNL (2013-) (www.dq.fct.unl.pt/en)

Director of the Research Unit on Applied Biomolecular Sciences (www.ucibio.pt)

MAIN RESEARCH INTERESTS

Structural and Functional Biology focused on the following main topics: (1) Metalloproteins and/or proteins involved in electron transfer processes, in particular (2) Molybdopterine-containing enzymes (Mo active site, associated to other redox centers involved in electron transfer) in particular aldehyde oxidases and relation to drug metabolism; (3) Enzymatic and molecular recognition components of the Cellulosome assembly; (4) Novel methods for protein crystallization.

AWARDS AND HONORS

Prizes:

1995 Prize Fundação Marquês de Pombal 1995-"Oeiras, Ciência e o Desenvolvimento" ("Oeiras, Science and Development).

1993 "Crystal Award" - Max-Planck-Institut für Biochemie, Martinsried, Germany.

1978 "Hylleraas Prize"- Uppsala University, Sweden.

Refereeing activities:

International

- Evaluator at International Funding Agencies:
 - Evaluation Panel of Research Units and Doctoral Programs of the German Science Foundation (DFG) (2009-...).
 - Evaluator of research projects from the national research council of the Netherlands (NWO) (2014-...)
 - Evaluator of research projects from BSF - The U.S.-Israel Binational Science Foundation (BSF) <http://www.bsf.org.il> USA- IL (2016)
- Evaluator at other Entities:
 - Member of the Beam Time Allocation Panel for Structural Biology of the ESRF (2016-...)
 - Member of the European Science Foundation (ESF) College of Expert Reviewers (2016-...)
 -
 - NATO, Scientific Exchange Programs (1996-99)
 - The Wellcome Trust (UK) (1996-98)
 - The Leverhulme Trust (UK) (1996-99)
- Evaluation of EU proposals (1995-98):
 - Expert Evaluators Panel for Marie Curie Individual Fellowships;
 - Life Sciences Evaluation Panel for Research Training Networks
- Regular Reviewer of several International Journals.

National

- Member of the Evaluation Panel of grant proposals at FCT-MCTES (2002-11)
- EU-India Networking Pilot Program (Indigo) (since 2010)
- Bilateral agreements - FCT-MCTES (since 2010)
- Final Reports evaluation & Co-coordination – FCT-MCTES (since 2014)

Other Distinctions:

- Member of the national committee for the preparatory phase of the European program INSTRUCT: An Integrated Structural Biology Infrastructure for Europe (Biomedical Sciences Infrastructure) <http://www.structuralbiology.eu/>
- Member of the Scientific Council of INSTRUCT
- Elected for the Executive Committee of the European Synchrotron User Organization (ESUO) <http://www.esuo.org/> (until 2012)
- 2006-2012: Editorial Advisory Board of the Journal of Biological Inorganic Chemistry
- 2012-... Portuguese Observer to the Council of the European Synchrotron Radiation Facility (ERSF), Grenoble (Nomination by the Portuguese Secretary of State for Science, Sept 2012).

ACADEMIC AND SCIENCE MANAGEMENT ACTIVITIES

2001-2007	Executive Committee of the Chemistry Department of FCT-UNL.
2002-2004	Installation Committee of the Conservation and Restoration Degree (FCT-UNL).
2003-2005	President of the Pedagogical Committee of the Conservation and Restoration Degree (FCT-UNL).
2007-2009	Coordinator of the Degree in Applied Chemistry, FCT-UNL.
2008-2009	Coordinator of the Biochemistry section, Chemistry Department, FCT-UNL.
2009-2013	Coordinator of the Doctoral Program in Biochemistry, FCT-UNL
2011-2012	Executive Coordinator of the Scientific Council for Exact Sciences and Engineering (Fundação para a Ciência e a Tecnologia, MCTES)

- 2013- Member of the Directive Board and Executive Board of the Doctoral Program on Molecular Biosciences (ITQB- UNL)
 2012- Head of the Chemistry Department at FCT-UNL
 2014- Director of the Research Unit UCIBIO (www.ucibio.pt)

ORGANIZATION OF CONGRESSES AND WORKSHOPS

- 1997 Workshop “Pteridines: Regulation, Biosynthesis and Pharmacology” (ERB-FMRX-CT98-0204), ITQB, Oeiras.
 1997 ECM 17- 17th European Crystallographic Meeting, IST, Lisboa.
 1998 Summer School I “Structure And Function Of Metalloproteins”, ITQB, Oeiras.
 1998 Summer School II “Structure And Function Of Metalloproteins”, ITQB, Oeiras.
 2000 Workshop within the European Network “XONET” (HPRN-CT-1999-00084), FCT-UNL.
 2006 EUROBIC 2006 8th European Biological Chemistry Conference, Aveiro (Organizing & Scientific Committee).
 2006 6th Ibero-American Congress Of Biophysics, Madrid (Scientific Committee).
 2009 6th GORDON RESEARCH CONFERENCE on “Molybdenum & Tungsten Enzymes”, Il Ciocco, Italy (**Chair**).
 2010 Zaragoza Biophysics Congress (7-10 July 2010) (Session chair).
 2011 Carbohydrate Biotechnology Meeting (CBM9), (Organizing Committee), Lisbon.
 2012 1st National Meeting of Portuguese Synchrotron Radiation Users (ENURS), FCT-UNL, Lisbon. ((Co-organizer))
 2012 Joint Research Center JRC-Info Days: (a) Conference on Cooperation between JRC and Portugal and (b) Seminar for Young Researchers: JRC activities, Cooperation and Job Opportunities. Lisbon, 28 & 29 November 2012 (Co-organizer)
 2013 2nd National Meeting of Synchrotron Radiation Users and ESRF day (2nd ENURS & ESRF Day), Feb 2013, Lisbon (Main organizer)
 2014 3rd National Meeting of Synchrotron Radiation Users and ESRF day (3rd ENURS & ESRF Day), March 2014, Leiria (co-organizer)

RESEARCH SUPERVISION

10 PhD Students supervised (3 of which co-supervised)
 3 PhD Students, on-going
 4 MSc Students
 12 Post-doctoral fellows

SCIENTIFIC PRODUCTIVITY AND IMPACT

RID: <http://www.researcherid.com/rid/A-4115-2013>

Scientific Productivity:

Publications: **139**

Book Chapters: **6**

Conference Proceedings: **17**

Invited Talks at Congresses and Workshops: **49**

Invited Talks at Research Institutions: **16**

Impact:

Number of Publications (WoK ISI): **137**

Sum of Times Cited without self-citations : **3825**

Average Citations per Item: **30.3**

H-index: **35**

FULL LIST OF INTERNATIONAL PUBLICATIONS

1. H.-W. Frühauf, F. Seils, M.J. Romão, R. Goddard. "Zur Aktivität koordiniert 1,4-diaza-1,3-diene(dad) bei C-C-Verknüpfungsreaktionen: 3-Pyrrolin-2-one aus (dad)Fe(CO)₃ und Dimethyl-acetylendicarboxylat" ANGEW. CHEMIE SUPPL., 22, 992-993 (1983).
2. H. Hoberg, D. Schaefer, G. Burkhart, C. Krüger, M.J. Romão. "Nickel(0)-induzierte C-C-Verknüpfung zwischen Kohlendioxid und Alkinen sowie Alkenen". J. ORGANOMET. CHEM., 226, 203-224 (1984).
3. P.W. Jolly, C. Krüger, C.C. Romão, M.J. Romão. " η^3 -Allyl Complexes of Molybdenum. The Preparation and structure of [Mo(η^3 -C₃H₅)₂(η^5 -C₅H₅)]". ORGANOMETALLICS, 3, 936-937 (1984).
4. K.R. Pörschke, R. Mynott, C. Krüger, M.J. Romão. "Tris(phosphan)-Nickel(0)-Ethen-Komplexe (dmpe)(PR₃)Ni(C₂H₄). Molekülstruktur des (dmpe)(PPh₃)Ni(C₂H₄)". Z. NATURFORSCHUNG, 39b, 1076-1081 (1984).
5. H. Hoberg, F.J. Fañanás, K. Angermund, C. Krüger, M.J. Romão. "Strukturen und Eigenschaften Neuartiger Carbamoylnickel-Komplexe". J. ORGANOMET. CHEM., 281, 379-388 (1985).
6. A. Döhring, P.W. Jolly, C. Krüger, M.J. Romão. "The Ni(0)-CO₂ System: Structure and Reactions of [Ni(PCy₃)₂(η^2 -CO₂)]". Z. NATURFORSCHUNG, 40b, 484-488 (1985).
7. H. Hoberg, K. Radine, C. Krüger, M.J. Romão. "Synthese neuer Phosphan-Nickel(I)-Komplexe und Kristallstruktur von η^3 -Iodo-tris(η^5 -iodocyclotris(triphenylphosphan-nickel)),(TPP)₃Ni₃I₄". Z. NATURFORSCHUNG, 40b, 607-614 (1985).
8. J.J. Eisch, A.M. Piotrowski, A.A. Aradi, C. Krüger, M.J. Romão. "Die oxidative Addition von Nickel(0)-Komplexen an Kohlenstoff-Kohlenstoff-Bindungen in Cyclobutadien. Zur Frage der Überführbarkeit von Cyclobutadien-Nickel (0)-Komplexen in Nickelringe" Z. NATURFORSCHUNG, 40b, 624-635 (1985).
9. H.-W. Frühauf, F. Seils, R.J. Goddard, M.J. Romão. "1,5-Dihydropyrrol-2-ones from (1,4-Diaza-1,3-diene)tricarbonyliron and Alkyne. 2. Structure of a [2.2.2] Bicyclic Intermediate with Iron at the Bridgehead Position" ORGANOMETALLICS, 4, 948-949 (1985).
10. J. Barluenga, J. Joglar, S. Fustero, V. Gotor, C. Krüger, M.J. Romão. "Preparation and Reactivity of 2-Aza-1,3-butadienes: A Diels-Alder Route to 5,6-Dihydro-2-H-1,3-oxazine Derivatives". CHEM. BER., 118, 3652-3663 (1985).
11. D.J. Bauer, S. Hietkamp, H. Sommer, O. Stelzer, G. Müller, M.J. Romão, C. Krüger. "Lineare Oligophosphaalkane-XIII-Triphosphaalkane mit dem P-C-P-C-P-Donor-skelett; Liganden für den Aufbau von Mehrkernkomplexen" J. ORGANOMET. CHEM., 296, 411-433 (1985).
12. R. Benn, S. Holle, P.W. Jolly, C. Krüger, C.C. Romão, M.J. Romão, A. Rufinska, G. Schroth. " η^3 -Allyl Complexes of Molybdenum: reactions of [MoCl(η^3 -C₃H₅)₃]₂ and the Crystal Structure of [MoOAc(η^3 -C₃H₅)₃]" POLYHEDRON, 5, 461-471 (1986).
13. B.J. Herold, M.J. Romão, J.M.A. Empis, J.C. Evans, C.C. Rowlands. "The Use of Electron Spin Resonance and ENDOR and TRIPLE Resonance Methods for Structural Elucidation". J. CHEM. SOC., FARADAY TRANS. I, 83, 43-49 (1987). (DOI=F19878300043)
14. C. Krüger, M.J. Romão. "Structure of 6-Fluoro-10,10-diphenyl-9-phenanthrene(1), 7-Chloro-10,10-diphenyl-9-phenanthrene(2) and 3-Methoxy-10,10-diphenyl-9-phenanthrene(3)". ACTA CRYSTALLOGR, C42, 1404-1408 (1986).
15. H. Angermund, F.-W. Grevels, R. Moser, R. Behn, C. Krüger, M.J. Romão. " η^2 -trans-Cyclooctene)₂Fe(CO)₃ and Related Complexes: Structure and Dynamic Behavior". ORGANOMETALLICS, 7, 1994-2004 (1988).
16. R. Mynott, M.J. Romão, B.J. Herold. "A ¹³C NMR Study of Substituted 10,10-Diphenyl-9-Phenanthrenes. Structure Determination and Signal Assignment using 2D-NMR

- Techniques". MAGNETIC RESONANCE IN CHEM. **27**, 1130-1133 (1989).
17. M.J. Romão, D. Turk, F.X. Gomis-Rüth, R. Huber, G. Schumacher, H. Möllering, L. Rüssmann. "Crystal Structure Analysis, Refinement and Enzymatic Reaction Mechanism of N-Carbamoylsarcosine Amidohydrolase from *Arthrobacter* sp. at 2.0 Å Resolution". J. MOL. BIOL., **226**, 1111-1130 (1992).
 18. B. Laber, F.X. Gomis-Rüth, M.J. Romão, R. Huber. "*Escherichia coli* Dihdropicolinate Synthase. Crystallization and Identificaton of the Active Site." BIOCHEM. J., **288**, 691-695 (1992).
 19. M.A.A.F.C.T. Carrondo, J. Morais, C.C. Romão, M.J. Romão, L.F. Veiros. "Cationic derivatives of Niobocene (IV). Crystal structures of $[Cp_2NbL_2][BF_4]_2$ (L=CNMe, NCMe)." POLYHEDRON , **12**, 7, 765-770 (1993).
 20. M.J. Romão, B.A.S. Barata, K. Lobeck, I. Moura, M.A. Carrondo, J. LeGall, F. Lottspeich, R. Huber, J.J.G. Moura. "Subunit Composition, Crystallization and Preliminary Crystallographic Studies of the *Desulfovibrio gigas* Aldehyde Oxido-reductase Containing Molybdenum and [2Fe-2S] Centers". EUR. J. BIOCHEM., **215**, 729-732 (1993).
 21. U. Thoenes, O.L. Flores, A. Neves, B. Devreese, J.J.V. Beeumen, R. Huber, M.J. Romão, J. LeGall, J.J.G. Moura e C. Rodrigues-Pousada.. "Molecular Cloning and Sequence Analysis of the Gene of the Molybdenum-Containing Aldehyde Oxido-Reductase of *Desulfovibrio gigas*. The Deduced Amino Acid Sequence Shows Similarity to Xanthine Dehydrogenase". EUR. J. BIOCHEM., **220**, 901-910 (1994).
 22. C. Frazão, J.M .Dias, P.M. Matias, M.J. Romão, M.A. Carrondo, M. Hervás, J.A. Navarro, M.A. de la Rosa e G. M. Sheldrick, "Cytochrome c_6 from the green alga *Monoraphidium braunii*. Crystallization and Preliminary Diffraction Studies" ACTA CRYSTALLOGR. **D51**, 232-234 (1995).
 23. M. Archer, R. Huber, P. Tavares, I. Moura, J.J.G. Moura, M.A. Carrondo, L.C. Sieker, J. LeGall, M.J. Romão. "Crystal Structure of Desulforedoxin from *Desulfovibrio gigas* Determined at 1.8 Å Resolution: A Novel Non-Heme Iron Protein Structure". J. MOL. BIOL., **251**, 690-702 (1995)
 24. M. J. Romão, M. Archer, I. Moura, J. J. G. Moura, J. LeGall, R. Engh, M. Schneider, P. Hof, R. Huber. "Structure Of The Aldehyde Oxido-Reductase From *Desulfovibrio gigas* At 2.25 Å Resolution : A Member Of The Xanthine Oxidase Protein Family". SCIENCE, **270**, 1170-1176 (1995).
 25. R. Huber, P. Hof, R.O. Duarte, J.J.G. Moura, I. Moura, M-Y. Liu, J. LeGall, R. Hille, M. Archer, M.J. Romão. "A Structure-Based Catalytic Mechanism For The Xanthine Oxidase Family Of Molybdenum Enzymes" PROC. NATL. ACAD. SCI. USA , **93**, 8846-8851 (1996).
 26. B.J. Goodfellow, P. Tavares, M.J. Romão, C. Czaja, F. Rusnak, J. LeGall, I. Moura, J.J.G. Moura. "The Solution Structure of Desulforedoxin, a Simple Iron-Sulfur Protein: an NMR Study of the Zinc Derivative". J. BIOL. INORG. CHEM., **1**, 341-354 (1996).
 27. A. Romero, J. Caldeira, I. Moura, J. LeGall, J. J. G. Moura, M.J. Romão. "Crystal Structure of Flavodoxin from *Desulfovibrio Desulfuricans* ATCC 27774 in two Oxidation States". EUR. J. BIOCHEM., **239**, 190-196 (1996).
 28. R. Kiefersauer, J. Stetefeld, F. Gomis-Rüth, M. J. Romão, F. Lottspeich, R. Huber. "Protein-Crystal Density by Volume Measurement and Amino-Acid Analysis". J. APPL. CRYSTALLOGR., **29**, 311-317 (1996).
 29. A. Zajc, M. J. Romão, B. Turk, R. Huber. "Crystallographic and Fluorescence Studies of ligand binding to N-Carbamoylsarcosine Amidohydrolase from *Arthrobacter* sp." J. MOL. BIOL., **263**, 269-283 (1996).
 30. J.J.G. Moura, B.J. Goodfellow, M.J. Romão, F. Rusnak, I. Moura. "Analysis, design and engineering of simple iron-sulfur proteins: tales from rubredoxin and desulforedoxin." COMMENTS ON INORG. CHEM., **19**, 47-66 (1996)

31. J. M. Dias, A. L. Carvalho, I. Kölln, J. J. Calvete, E. Töpfer-Petersen, P. F. Varela, A. Romero, C. Urbanke, M. J. Romão. "Crystallization and preliminary X-ray diffraction studies of aSFP, a bovine seminal plasma protein with a single CUB domain architecture" *PROTEIN SCIENCE*, **6**, 725-727 (1997).
32. A. Voityuk, K. Albert, S. Köstlmeier, V. A. Nasluzov, K. M. Neyman, P. Hof, R. Huber, M. J. Romão, N. Rösch. "Prediction of Alternative Structures of the Molybdenum Site in the Xanthine Oxidase-Related Aldehyde Oxido-Reductase" *J. AMER. CHEM. SOC.*, **119**, 3159-3160 (1997).
33. M. Archer, L. Banci, E. Dikaya, M. J. Romão "Crystal structure of cytochrome c' from *Rhodocyclus gelatinosus* and comparison with other cytochromes c" *J. BIOL. INORG. CHEM.*, **2**, 611-622 (1997).
34. A. Romero, M. J. Romão, P. F. Varela, I. Kölln, J. M. Dias, A. L. Carvalho, L. Sanz, E. T. Petersen, J. J. Calvete "The crystal structure of two members of the spermadhesin family, porcine PSP-I/PSP-II and bovine aSFP, reveals the folding of the CUB domain" *NATURE STRUCTURAL BIOLOGY*, **4**, 783-788 (1997).
35. M. J. Romão, I. Kölln, J. M. Dias, A. L. Carvalho, A. Romero, P. F. Varela, L. Sanz, E. T. Petersen, J. J. Calvete "Crystal Structure of acidic seminal fluid protein (aSFP) at 1.9 Å resolution: a bovine polypeptide from the spermadhesin family" *J. MOL. BIOL*, **274**, 650-660 (1997).
36. P. F. Varela, A. Romero, L. Sanz, M. J. Romão, E. T. Petersen, J. J. Calvete. "The 2.4 Å resolution crystal structure of boar seminal plasma PSP-I/PSP-II: a zona pellucida-binding glycoprotein heterodimer of the spermadhesin family built by a CUB domain architecture" *J. MOL. BIOL.*, **274**, 635-649 (1997).
37. M. J. Romão e R. Huber "Crystal Structure and Mechanism of action of the Xanthine-Oxidase Related Aldehyde Oxido-Reductase from *D. gigas*" *BIOCHEM. SOC. TRANS.* **25**, 755-757 (1997).
38. M. J. Romão, J. Knäblein, R. Huber, J.J.G. Moura. "Structure and function of Molybdopterin containing enzymes". *PROG. IN BIOPH. MOL. BIOL.*, **68**, 121-144 (1997)
39. M. J. Romão, N. Rösch, R. Huber "The Molybdenum Site in the Xanthine Oxidase related Aldehyde Oxidoreductase from *D. gigas* and a catalytic mechanism for this class of enzymes" *J. BIOL. INORG. CHEM.*, **2**, 782-785 (1997)
40. A.A. Voityuk, K. Albert, M. J. Romão, R. Huber, N. Rösch "Substrate Oxidation in the Active Site of Xanthine Oxidase and Related Enzymes" *INORG. CHEM.* **37**, 176-180 (1998).
41. M. J. Romão, R. Huber. "Structure and function of the xanthine-oxidase family of molybdenum enzymes", *METAL SITES IN PROTEINS AND MODELS, STRUCTURE & BONDING VOL. 90*, 69-96, (1998)
42. A. Glatigny, P. Hof, M. J. Romão, R. Huber, C. Scazzocchio "Altered specificity mutations define residues essential for substrate positioning in xanthine dehydrogenase" *J. MOL. BIOL*, **278**, 431-438 (1998).
43. J. M. Dias, S. Bursakov, C. Carneiro, J. J. G. Moura, I. Moura, M. J. Romão. "Crystallization and Preliminary X-Ray Analysis of a Nitrate Reductase from *Desulfovibrio desulfuricans* ATCC 27774" *ACTA CRYSTALLOGR. D* **55**, 877-879 (1999).
44. J. M. Dias, M. E. Than, A. Humm, R. Huber, G. P. Bourenkov, H. D. Bartunik, S. Bursakov, J. Calvete, J. Caldeira, J. J.G. Moura, I. Moura and M. J. Romão. "Crystal structure of the first dissimilatory nitrate reductase at 1.9 Å solved by MAD methods" *STRUCTURE*, **7**, 65-79 (1999).
45. C. A. Cunha, M. J. Romão, S.J. Sadeghi, F. Valetti, G. Gilardi, C.M. Soares. "Effects of protein-protein interactions on electron transfer: docking and electron transfer calculations for complexes between flavodoxin and c-type cytochromes" *J. BIOL. INORG. CHEM.*, **4**, 360-374 (1999).

46. M. Archer, A. L. Carvalho, S. Teixeira, I. Moura, J. J. G Moura, F. Rusnak, M. J. Romão "Structural studies by X-ray diffraction on metal substituted desulforedoxin, a rubredoxin type protein" PROTEIN SCIENCE, 8, 1536-1545 (1999).
47. J. M. Dias, C. A. Cunha, S. Teixeira, G. Almeida, C. Costa, J. Lampreia, J. J. G. Moura, I. Moura, M. J. Romão "Crystallisation and Preliminary X-Ray Analysis of a Membrane Bound Nitrite Reductase from Desulfovibrio desulfuricans ATCC 27774" ACTA CRYSTALLOGR. D56, 215-217 (2000).
48. J. Rebelo, S. Macieira, J. M. Dias, R. Huber, C. S. Ascenso, F. Rusnak, J. J.G. Moura, I. Moura, M. J. Romão "Gene Sequence and Crystal Structure of the Aldehyde Oxidoreductase from Desulfovibrio desulfuricans ATCC 27774" J. MOL. BIOL., 297, 135-146 (2000).
49. R. O. Duarte, M. Archer, J. M. Dias, S. Bursakov, R. Huber, I. Moura, M. J. Romão, J.G. Moura "Biochemical/spectroscopic characterization and preliminary X-ray analysis of a new aldehyde oxido-reductase isolated from Desulfovibrio desulfuricans ATCC2774" BIOCHEM. BIOL. RESEARCH. COMM, 24, 745-749 (2000).
50. S. J. Sadeghi, F. Valetti, C. A. Cunha, M. J. Romão, C. M. Soares, G. Gilardi. "Ionic strength dependence of the non-physiological electron transfer between flavodoxin and cytochrome c₅₅₃ from D. vulgaris" J. BIOL. INORG. CHEM., 5, 730-737 (2000)
51. H. Raaijmakers, S. Teixeira, J. M. Dias, M. J. Almendra, C. Brondino, I. Moura, J. J. G. Moura, M. J. Romão. "Tungsten-containing Formate Dehydrogenase from Desulfovibrio gigas: Metal Identification and Preliminary Structural data by Multi-Wavelength Crystallography" J. BIOL. INORG. CHEM., 6, 398-404 (2001).
52. J.M. Rebelo, J.M. Dias, R. Huber, J.J.G. Moura, M.J. Romão. "Refinement of the Aldehyde Oxidoreductase from Desulfovibrio gigas (Mop) at 1.28 Å." J. BIOL. INORG. CHEM., 6, 791-800 (2001)
53. Carvalho AL, Dias JM, Sanz L, Romero A, Calvete JJ, Romão MJ : "Purification, Crystallization And Identification By X-Ray Analysis Of A Prostate KalliKrein From Horse Seminal Plasma",ACTA CRYSTALLOGR. D BIOL. CRYSTALLOGR. 57,1180-1183 (2001)
54. M.J. Romão, C.A. Cunha, C.D. Brondino, J.J.G. Moura "Molybdenum enzymes in reactions involving aldehydes and acids", METAL IONS IN BIOLOGICAL SYSTEMS, Vol. 39,539-570 (2002)
55. JM. Dias, C Bonifácio, T Alves, JJ.G. Moura, I Moura and M J. Romão ." Crystallization And Preliminary X-Ray Analysis Of Two PH-Dependent Forms Of Cytocrome C Peroxidase From Pseudomonas Nautica " ACTA CRYSTALLOGR. D BIOL. CRYSTALLOGR., 58, 697-699 (2002)
56. Carvalho AL, Sanz L, Baretino D., Romero A, Calvete JJ, Romão MJ . "Crystal structure of a prostate kallikrein isolated from stallion seminal plasma: a putative PSA" J. MOL. BIOL., 2002 322(2):325-337.
57. H. Raaijmakers, S. Macieira, J. M. Dias, S. Teixeira, S. Bursakov, R. Huber, J. J. G. Moura, I. Moura, M. J. Romão. "Gene Sequence and the 1.8 Å Crystal Structure of the Tungsten-containing Formate Dehydrogenase from Desulfovibrio gigas" STRUCTURE, 10, 1261-1272 (2002)
58. C. A. Cunha, S. Macieira, J. M. Dias G. Almeida, L. L. Gonçalves, C. Costa, J. Lampreia, R. Huber, J. J. G. Moura, I. Moura, M. J. Romão "Cytochrome c nitrite reductase from Desulfovibrio desulfuricans ATCC 27774. Part I: the relevance of the two calcium sites in the structure of the catalytic subunit (NrfA)." J. BIOL. CHEM., 278, 17455-17465 (2003)
59. Enrico Garattini, Ralf Mendel, Maria João Romão, Richard Wright and Mineko Terao. "Mammalian molybdo-flavoenzymes, an expanding family of proteins: structure, genetics, regulation, function and patho-physiology" BIOCHEM.J. 372, 15-32 (2003)
60. C. Bonifácio, C.A. Cunha, A. Müller, C.G. Timóteo, João M. Dias, I. Moura & M.J. Romão "Crystallization and preliminary X-ray diffraction analysis of the di-haem cytochrome c peroxidase from Pseudomonas stutzeri", ACTA CRYSTALLOGR. D BIOL. CRYSTALLOGR, 59,

345-347 (2003)

61. M. G. Almeida, S. Macieira, L. L. Gonçalves, R. Huber, C. A. Cunha, M. J. Romão, J. Lampreia, J. J. G. Moura and I. Moura, "The isolation and characterization of Cytochrome c nitrite reductase subunits (NrfA and NrfH) from Desulfovibrio desulfuricans ATCC 27774. Re-evaluation of the spectroscopic data and redox properties", EUR. J. BIOCHEM., 270, 3904-3915 (2003)
62. Thomas Hettmann, Roman A. Siddiqui, Johannes von Langen, Christa Frey, Maria J. Romão and Stephan Diekmann. "Mutagenesis study on the role of a lysine residue highly conserved in formate dehydrogenases and periplasmic nitrate reductases", BIOCHEM BIOPHYS RES COMMUN. 310, 40-47 (2003)
63. Ana L. Carvalho, Fernando M.V. Dias, José A.M. Prates, Luís M.A. Ferreira, Harry J. Gilbert, Gideon J. Davies, Maria J. Romão* and Carlos M.G.A. Fontes*. "Cellulosome assembly revealed by the crystal structure of the cohesin-dockerin complex: a template for the construction of nanosomal catalytical machines", PROC NATL ACAD SCI USA, 100, 13809-13814 (2003)
64. M. M. Correia dos Santos, P. M. Paes de Sousa, M. L. Simoes Goncalves, M. J. Romão, I. Moura, J. J. G. Moura. "Direct electrochemistry of the Desulfovibrio gigas aldehyde oxidoreductase" EUR. J. BIOCHEM., 270, 1329-1338 (2004).
65. João M. Dias, Cecília Bonifácio, Teresa Alves, Alice Pereira, D. Bourgeois, Isabel Moura and Maria João Romão. "Structural basis for the mechanism of Ca²⁺ activation of the di-haem Cytochrome c Peroxidase from Pseudomonas nautica 617" STRUCTURE, 12, 961-973 (2004)
66. D. Roeland Boer, Athapper, C D. Brondino, M J. Romão and J. G. Moura. "X-ray crystal structure and EPR-spectra of "arsenite-inhibited" Desulfovibrio gigas aldehyde dehydrogenase; a member of the xanthine oxidase family", J. AM. CHEM. SOC, 126, 8614-8615 (2004)
67. Carvalho AL, Goyal A, Prates JA, Bolam DN, Gilbert HJ, Pires VM, Ferreira LM, Planas A, Romao MJ, Fontes CM. "The family 11 carbohydrate-binding module of Clostridium thermocellum Lic26A-Cel5E accommodates beta -1,4 and beta -1,3-1,4-mixed linked glucans at a single binding site." J. BIOL: CHEM 279, 34785-34793 (2004).
68. Santos-Silva T, Dias J JM, Bourenkov G, Bartunik H, Moura I, Romao MJ "Crystallization and preliminary X-ray diffraction analysis of the 16-haem cytochrome of Desulfovibrio gigas." ACTA CRYSTALLOGR D BIOL CRYSTALLOGR. 60, 968-970 (2004).
69. T. Hettmann, R. A. Siddiqui, C. Frey, T. Santos-Silva, M. J. Romão and S. Diekmann. "Mutagenesis study on amino acids around the molybdenum centre of the periplasmic nitrate reductase from Ralstonia eutropha", BIOCHEM BIOPHYS RES COMMUN. 320, 1211-1219 (2004).
70. J. J. G. Moura, C. D. Brondino, J. Trincão and M. J. Romão. "Mo and W bis-MGD Enzymes: Nitrate Reductases and Formate Dehydrogenases" J. BIOL. INORG. CHEM 9, 791-799 (2004)
71. D. Roeland Boer, Axel Müller, Susanne Fetzner, David J. Lowe and Maria João Romão. "On the purification and preliminary crystallographic analysis of isoquinoline 1-oxidoreductase from Brevundimonas diminuta 7 ACTA CRYST. F, STRUCTURE BIOLOGY & CRYST. COMM. 61, 137-140 (2005).
72. A.L. Carvalho, V.M.R. Pires, T.M. Gloster, J.P. Turkenburg, J.A.M. Prates, L.M.A. Ferreira, M.J. Romao, G.J. Davies, C.M.G.A. Fontes, H.J. Gilbert Insights into the Structural Determinants of Cohesin-Dockerin Specificity Revealed by the Crystal Structure of the Type II Cohesin from Clostridium thermocellum SdbA J. MOL. BIOL., 349 pp 909-915 (2005)
73. Teresa Santos-Silva, José Trincão, Ana L. Carvalho, Cecília Bonifácio, Françoise Auchère, Isabel Moura, José J.G. Moura and Maria J. Romão, "Superoxide reductase from the syphilis spirochete Treponema pallidum: Crystallization and structure determination using soft X-rays", ACTA CRYST. F, STRUCTURE BIOLOGY & CRYST. COMM. 61, 967-970 (2005)

74. S. Najmudin C.P. D. Guerreiro, L.M. A. Ferreira, M. J. Romão C. M. G. A. Fontes and J. A. M. Prates, Overexpression, purification and crystallization of the two C-terminal domains of the bi-functional cellulase CtCel9D-Cel44A from *Clostridium thermocellum*, ACTA CRYST., F61, 1043-1045. (2005)
75. Najmudin S, Guerreiro CI, Carvalho AL, Prates JA, Correia MA, Alves VD, Ferreira LM, Romao MJ, Gilbert HJ, Bolam DN, Fontes CM. Xyloglucan is recognised by carbohydrate-binding modules that bind to beta -glucan chains. J BIOL CHEM. 281(13):8815-28 (2006)
76. Teresa Santos-Silva, José Trincão, Ana L. Carvalho, Cecília Bonifácio, Françoise Auchère, Patrícia Raleiras, Isabel Moura, José J.G. Moura and Maria J. Romão, "The first crystal structure of class III superoxide reductase from *Treponema pallidum*", J BIOL INORG CHEM., 11(5):548-58. (2006)
77. Carlos Brondino, Maria J. Romão, Isabel Moura, and José J.G. Moura. "Molybdenum and tungsten enzymes: the xanthine oxidase family". CURR OPIN CHEM BIOL. 10(2):109-14. (2006)
78. Hans CA Raaijmakers and M. João Romão, "Formate-reduced E. coli formate dehydrogenase H: The reinterpretation of the crystal structure suggests a new reaction mechanism" J BIOL INORG CHEM. 2006 Oct;11(7):849-54. Epub 2006 Jul 8.
79. José Trincão, MS Silva, L Barata, C Bonifácio, A M Tomás, C Cordeiro, AP Freire and M. J Romão "Purification, crystallization and preliminary X-ray diffraction analysis of the glyoxalase II from *Leishmania infantum*" ACTA CRYSTALLOGR SECT F STRUCT BIOL COMMUN, 62 805-807 (2006)
80. Carlos Brondino, Maria G. Rivas, Maria J. Romão, José J.G. Moura, and Isabel Moura."Structural and EPR Studies of Mononuclear Molybdenum Enzymes from Sulfate Reducing Bacteria", ACCOUNTS OF CHEMICAL RESEARCH, 2006 Oct;39(10):788-96.
81. Thapper A, Boer DR, Brondino CD, Moura JJ, Romao MJ. Correlating EPR and X-ray structural analysis of arsenite-inhibited forms of aldehyde oxidoreductase., J BIOL INORG CHEM. 2007 12(3) 353-366.
82. Carvalho AL, Dias FM, Nagy T, Prates JA, Proctor MR, Smith N, Bayer EA, Davies GJ, Ferreira LM, Romao MJ*, Fontes CM*, Gilbert HJ. "Evidence for a dual binding mode of dockerin modules to cohesins". PROC NATL ACAD SCI U S A. 2007 Feb 27;104(9):3089-94.
83. Coelho C, Gonzalez PJ, Trincão J, Carvalho AL, Najmudin S, Hettman T, Dieckman S, Moura JJ, Moura I, Romao MJ. Heterodimeric nitrate reductase (NapAB) from *Cupriavidus necator* H16: purification, crystallization and preliminary X-ray analysis. ACTA CRYSTALLOGR SECT F STRUCT BIOL Jun 1;63(Pt 6):516-9. 2007.
84. Santos-Silva T, Dias JM, Dolla A, Durand MC, Gonçalves LL, Lampreia J, Moura I, Romao MJ. Crystal structure of the 16 heme cytochrome from *Desulfovibrio gigas*: a glycosylated protein in a sulphate-reducing bacterium. J MOL BIOL. 2007 Jul 20;370(4):659-73. Epub 2007 May 4.
85. S. Chaves, M. Gil, S. Canário., R.Jelic, M. J. Romão, J. Trincão, E. Herdtweck, J. Sousa, C. Diniz, P. Fresco and M. A. Santos. Biologically Relevant O,S-Donor Compounds. Synthesis, Molybdenum Complexation and Xanthine Oxidase Inhibition J. CHEM. SOC., DALTON TRANSACTIONS, (2008) Apr 7;(13) 1773-1782.
86. S. Najmudin, P. J. González, J. Trincão, C. Coelho, A. Mukhopadhyay, N. Cerqueira, C. C. Romão, I. Moura, José J. Moura, C. D. Brondino and M. J. Romão. Periplasmic Nitrate Reductase Revisited: A Sulfur Atom completes the Sixth Coordination of the Catalytic Mo, J BIOL INORG CHEM. 2008 Jun;13(5):737-53.
87. A. Viegas, N. F. Brás, N. M. F. S. A. Cerqueira, P. A. Fernandes, J. A. M. Prates, Carlos M. G. A. Fontes, M. Bruix, M. J. Romão, A. L. Carvalho, M. J. Ramos, A. L. Macedo, E. J. Cabrita. CBM11 c NMR Molecular Determinants of Ligand Specificity in Family 11 Carbohydrate Binding

- Modules (CBM11): an NMR, X-Ray Crystallography and Computational Chemistry Approach, FEBS J. May;275(10):2524-35. Epub 2008 Apr 15.
88. O. Y. Gavel, A.V. Kladova, S. A. Bursakov, J. M. Dias, S. Texeira, V. L. Shnyrov, J.J.G. Moura, I. Moura, M. J. Romão and J. Trincão. Purification, crystallization and preliminary X-ray diffraction analysis of the Adenosine Triphosphate Sulfurylase (ATPS) from the sulfate-reducing bacterium *Desulfovibrio desulfuricans* ATCC 27774. ACTA CRYSTALLOGR SECT F STRUCT BIOL CRYST COMMUN. (2008), 64(Pt 7):593-5. Epub 2008.
 89. Najmudin S, Pinheiro BA, Romão MJ, Prates JA, Fontes CM. Purification, crystallization and crystallographic analysis of *Clostridium thermocellum* endo-1,4-beta-D-xylanase 10B in complex with xylohexase. ACTA CRYSTALLOGR SECT F STRUCT BIOL CRYST COMMUN. 2008 Aug 1;64(Pt 8):715-8. Epub 2008 Jul 5.
 90. Vidinha P, Lourenço NM, Pinheiro C, Brás AR, Carvalho T, Santos-Silva T, Mukhopadhyay A, Romão MJ, Parola J, Dionisio M, Cabral JM, Afonso CA, Barreiros S. Ion jelly: a tailor-made conducting material for smart electrochemical devices. CHEM COMMUN (CAMB). 2008 Nov 30;(44):5842-4. Epub 2008 Oct 3
 91. Jan Honzík, Abhik Mukhopadhyay, Teresa S. Silva, Maria J. Romão, Carlos C. Romão. Ring-functionalized molybdenocene complexes, ORGANOMETALICS, 2009, 28 (9), pp 2871–2879
 92. Santos-Silva, T.; Ferroni, F.; Thapper, A.; Marangon, J.; González, P.; Rizzi, A.; Moura, I.; Moura, J.; Romão, J. M.; Brondino, C. Kinetic, Structural, and EPR Studies Reveal that Aldehyde Oxidoreductase from *Desulfovibrio gigas* Does Not Need a Sulfido Ligand for Catalysis and Give Evidence for a Direct Mo-C Interaction in a Biological System" J. AM. CHEM. SOC. 2009 Jun 17;131(23):7990-8.
 93. Maria J. Romão, Molybdenum and tungsten enzymes: a crystallographic and mechanistic overview, DALTON TRANS., 2009, Jun 7;(21):4053-68.
 94. Freire F, Romão MJ, Macedo AL, Aveiro SS, Goodfellow BJ, Carvalho AL. Preliminary structural characterization of human SOUL, a haem-binding protein. ACTA CRYSTALLOGR SECT F STRUCT BIOL CRYST COMMUN. 2009;65(Pt 7):723-6.
 95. Najmudin S, Bonifácio C, Duarte AG, Pauleta SR, Moura I, Moura JJ, Romão MJ. Crystallization and crystallographic analysis of the apo form of the orange protein (ORP) from *Desulfovibrio gigas*. ACTA CRYSTALLOGR SECT F STRUCT BIOL CRYST COMMUN. 2009 Jul 1;65(Pt 7):730-2. Epub 2009
 96. Kladova AV, Gavel OY, Mukhopadhyay A, Boer DR, Teixeira S, Shnyrov VL, Moura I, Moura JJ, Romão MJ, Trincão J, Bursakov SA. Cobalt-, zinc- and iron-bound forms of adenylate kinase (AK) from the sulfate-reducing bacterium *Desulfovibrio gigas*: purification, crystallization and preliminary X-ray diffraction analysis. ACTA CRYSTALLOGR SECT F STRUCT BIOL CRYST COMMUN. 2009 Sep 1;65(Pt 9):926-9
 97. Viciosa MT, Correia NT, Sanchez MS, Carvalho AL, Romão MJ, Gómez Ribelles JL, Dionísio M. Real-Time Monitoring of Molecular Dynamics of Ethylene Glycol Dimethacrylate Glass Former. J PHYS CHEM B. 2009 Oct 5
 98. Cerqueira, NMFS; Gonzalez, PJ; Brondino, CD, M. J. Romão, C. C. Romão, I. Moura, M. J. Ramos, J. J.G. Moura The Effect of the Sixth Sulfur Ligand in the Catalytic Mechanism of Periplasmic Nitrate Reductase JOURNAL OF COMPUTATIONAL CHEMISTRY Volume: 30 Issue: 15 Pages: 2466-2484, 2009
 99. C.Coelho, J. Trincão and M. J. Romão "The use of ionic liquids as crystallization additives allowed to overcome nanodrop scaling up problems: A success case for producing diffraction-quality crystals of a nitrate reductase" JOURNAL OF CRYSTAL GROWTH, Volume 312, Issue 5, 714-719.
 100. Najmudin, S., Pauleta S. R, Moura I. and Romão MJ "The 1.4 angstrom resolution structure of *Paracoccus pantotrophus* pseudoazurin" ACTA CRYSTALLOGR SECT F STRUCT BIOL CRYST COMMUN. Volume: 66 Pages: 627-635 JUN 2010

101. Shabir Najmudin, Benedita A. Pinheiro, José A.M. Prates, Harry J. Gilbert, Maria J. Romão and Carlos M.G.A. Fontes. "Putting an N-terminal end to the Clostridium thermocellum xylanase Xyn10B story: Crystal structure of the CBM22-1-GH10 modules complexed with xylohexaose". JOURNAL OF STRUCTURAL BIOLOGY, Volume: 172 Issue: 3 Pages: 353-362 , 2010
102. Teresa Ribeiro, Teresa Santos-Silva, Victor D. Alves, Fernando M.V. Dias, Ana S. Luís , José A.M. Prates, Luís M.A. Ferreira, Maria J. Romão, Carlos M.G.A Fontes, "Family 42 carbohydrate-binding modules display multiple arabinoxylan-binding interfaces presenting different ligand affinities" BIOCHIMICA ET BIOPHYSICA ACTA Volume: 1804 Issue: 10 Pages: 2054-2062
103. A. Mukhopadhyay, A.V. Kladova, S.A. Bursakov , O. Yu. Gavel, J.J. Calvete, V.L. Shnyrov, I. Moura, J.J.G. Moura, M.J. Romão, J. Trincão. "Crystal structure of the zinc, cobalt and iron containing adenylate kinase from Desulfovibrio gigas: a novel metal containing adenylate kinase from Gram-negative bacteria" J BIOL INORG CHEM Volume: 16 Issue: 1 Pages: 51-61
104. Santos-Silva T, Mukhopadhyay A, Seixas JD, Bernardes, GJL, Romao, CC, Romao, MJ. "CORM-3 Reactivity toward Proteins: The Crystal Structure of a Ru(II) Dicarbonyl-Lysozyme Complex" JOURNAL OF THE AMERICAN CHEMICAL SOCIETY Volume: 133 Issue: 5 Pages: 1192-1195
105. C. Coelho, P.J. González, J.J.G. Moura, I. Moura, J. Trincão and M.J. Romão, (2011) "The crystal structure of Cupriavidus necator Nitrate Reductase in oxidized and partially reduced states" JOURNAL OF MOLECULAR BIOLOGY, 408, 932-948.
106. Bras, JLA; Cartmell, A; Carvalho, ALM; Verze, G; Bayer, EA; Vazana, Y; Correia, MAS; Prates, JAM; Ratnaparkhe, S; Boraston, AB; Romao, MJ; Fontes, CMGA; Gilbert, HJ. Structural insights into a unique cellulase fold and mechanism of cellulose hydrolysis. PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA Volume: 108 Issue: 13 Pages: 5237-5242 Published: 2011
107. Garcia-Alvarez, B; Melero, R; Dias, FMV; Prates, JAM; Fontes, CMGA; Smith, SP; Romao, MJ; Carvalho, AL; Llorca, O. "Molecular Architecture and Structural Transitions of a Clostridium thermocellum Mini-Cellulosome". JOURNAL OF MOLECULAR BIOLOGY Volume: 407 Issue: 4 Pages: 571-580 2011
108. Luis, AS; Alves, VD; Romao, MJ, Prates, JAM; Fontes CMG; Najmudin S. "Overproduction, purification, crystallization and preliminary X-ray characterization of a novel carbohydrate-binding module of endoglucanase Cel5A from Eubacterium cellulosolvens" ACTA CRYSTALLOGRAPHICA SECTION F-STRUCTURAL BIOLOGY AND CRYSTALLIZATION COMMUNICATIONS Volume: 67 Pages: 491-493 Published: 2011.
109. M. Mahro, C. Coelho, J. Trincão, D. Rodrigues, M. Terao, E. Garattini, M. Saggi, F. Lenzian, P. Hildebrandt, M.J. Romão and S. Leimkühler (2011) "Characterization and crystallization of mouse Aldehyde Oxidase 3 (mAox3): from mouse liver to E.coli heterologous protein expression", DRUG METABOLISM AND DISPOSITION, 2011 Volume: 39 Issue: 10 Pages: 1939-1945.
110. T Santos-Silva, A Mukhopadhyay, J D Seixas, G J L Bernardes, C C Romão, M J Romão "Towards Improved Therapeutic CORMs: Understanding the Reactivity of CORM-3 with Proteins" CURRENT MEDICINAL CHEMISTRY Volume: 18 Issue: 22 Pages: 3361-3366 Published: AUG 2011
111. Joana L A Brás, Márcia A S Correia, Maria J Romão, José A M Prates, Carlos M G A Fontes, Shabir Najmudin. "Purification, crystallization and preliminary X-ray characterization of the pentamodular arabinoxylanase CtXyl5A from Clostridium thermocellum." ACTA CRYSTALLOGRAPHICA. SECTION F, STRUCTURAL BIOLOGY AND CRYSTALLIZATION COMMUNICATIONS. 07/2011; 67(Pt 7):833-6. ·
112. Magdalena Kowacz , Abhik Mukhopadhyay , Ana Luísa Carvalho , José M. S. S. Esperança, Maria J. Romão and Luís Paulo N. Rebelo. "Hofmeister effects of ionic liquids in

- protein crystallization: Direct and water-mediated interactions” CRYSTENGCOMM Volume: 14 Issue: 15 Pages: 4912-4921 DOI: 10.1039/c2ce25129a Published: 2012
113. Brás JL, Carvalho AL, Viegas A, Najmudin S, Alves VD, Prates JA, Ferreira LM, Romão MJ, Gilbert HJ, Fontes CM. “Escherichia coli expression, purification, crystallization, and structure determination of bacterial cohesin-dockerin complexes.” METHODS ENZYMOL. 2012; 510:395-415
114. Coelho C, Mahro M, Trincão J, Carvalho AT, Ramos MJ, Terao M, Garattini E, Leimkühler S, Romão MJ. “The First Mammalian Aldehyde Oxidase Crystal Structure: Insights Into Substrate specificity.” J BIOL CHEM. 23;287(48):40690-702. doi: 10.1074/jbc.M112.390419. Epub 2012 Sep 27.
115. Santos MF, Seixas JD, Coelho AC, Mukhopadhyay A, Reis PM, Romão MJ, Romão CC, Santos-Silva T. “New insights into the chemistry of fac-[Ru(CO)(3)](2+) fragments in biologically relevant conditions: The CO releasing activity of [Ru(CO)(3)Cl(2)(1,3-thiazole)], and the X-ray crystal structure of its adduct with lysozyme.” J INORG BIOCHEM. 117 (2012) 285–291
116. Joana L A Brás, Victor D Alves, Ana Luísa Carvalho, Shabir Najmudin, José A M Prates, Luis M A Ferreira, David N Bolam, Maria João Romão, Harry J Gilbert, Carlos M G A Fontes. “Novel Clostridium thermocellum type I cohesin-dockerin complexes reveal a single binding mode.” J BIOL CHEM. 2012; DOI:10.1074/jbc.M112.407700
117. João D. Seixas, Abhik Mukhopadhyay, Teresa Santos-Silva, Leo E. Otterbein, David J. Gallo, Sandra S. Rodrigues, Bruno H. Guerreiro, Ana M. L. Gonçalves, Nuno Penacho, Ana R. Marques, Ana C. Coelho, Patrícia M. Reis, Maria J. Romão and Carlos C. Romão. “Characterization of a versatile organometallic pro-drug (CORM) for experimental CO based therapeutics” DALTON TRANSACTIONS Volume: 42 Issue: 17 Pages: 5985-5998 DOI: 10.1039/c2dt32174b Published: 2013 DOI: 10.1039/C2DT32174B
118. Aldino Viegas, João Sardinha, Filipe Freire, Daniel F Duarte, Ana Luísa Carvalho, Carlos Mga Fontes, Maria João Romão, Anjos L Macedo, Eurico J Cabrita. “Solution Structure, Dynamics and Binding Studies of a Family 11 Carbohydrate-Binding Module from Clostridium thermocellum (CtCBM11)”. BIOCHEMICAL JOURNAL 01/2013; DOI:10.1042/BJ20120627
119. Coelho C, Marangon J, Rodrigues D, Moura JG, Romão MJ, Paes de Sousa PM, Correia dos Santos MM “Induced peroxidase activity of haem containing nitrate reductases revealed by protein film electrochemistry” JOURNAL OF ELECTROANALYTICAL CHEMISTRY. 2013 Feb 9;693:105-113. doi: 10.1016/j.jelechem.2013.01.030
120. Mehtab S, Gonçalves G, Roy S, Tomaz AI, Santos-Silva T, Santos MF, Romão MJ, Jakusch T, Kiss T, Pessoa JC. “Interaction of vanadium(IV) with human serum apo-transferrin.” J INORG BIOCHEM. 2013 Apr;121:187-95. doi: 10.1016/j.jinorgbio.2012.12.020.
121. Verma AK, Goyal A, Freire F, Bule P, Venditto I, Brás JLA, Santos H, Cardoso V, Bonifacio C, Thompson A, Romao MJ, Prates JAM, Ferreira LMA, Fontes CMGA and Najmudin S. “Overexpression, crystallization and preliminary X-ray crystallographic analysis of glucuronoxylan xylanohydrolase (Xyn30A) from Clostridium thermocellum.” ACTA CRYST. (2013). F69, 1440–1442
122. M Mahro; NF Brás; NMFS Cerqueira; C Teutloff; C Coelho; MJ Romão; S Leimkühler, “Identification of crucial amino acids in mouse aldehyde oxidase 3 that determine substrate specificity.” PLOS ONE, December 2013 | Volume 8 | Issue 12 | e82285
123. J Marangon, HD Correia, CD Brondino, JG Moura, MJ Romao, PJ Gonzalez, T Santos-Silva. “Kinetic and Structural Studies of Aldehyde Oxidoreductase from Desulfovibrio gigas reveal a Dithiolene-Based Chemistry for Enzyme Activation and Inhibition by H₂O₂.” PLOS ONE, Volume: 8 Issue: 12 Published: DEC 31 2013
124. Ribeiro, D.; Kulakova, A.; Quaresma, P.; Pereira, E.; Bonifácio, C.; Romão, M. J.; Franco, R; Carvalho, A L, The use of Gold Nanoparticles as Additives in Protein Crystallization,

- CRYSTAL GROWTH & DESIGN., Volume: 14 Issue: 1 Pages: 222-227 Published: JAN 2014
125. A.R. Otrelo-Cardoso, V. Schwuchow, D. Rodrigues, E.J. Cabrita, S. Leimkühler, M. J. Romão, T. Santos-Silva "Biochemical, Stabilization and Crystallization Studies on a Molecular Chaperone (PaoD) Involved in the Maturation of Molybdoenzymes" PLOS ONE, Research Article | published 31 Jan 2014
 126. Otrelo-Cardoso, A.R.; da Silva Correia, M.A.; Schwuchow, V.; Svergun, D.I.; Romão, M.J.; Leimkühler, S.; Santos-Silva, T. "Structural Data on the Periplasmic Aldehyde Oxidoreductase PaoABC from *Escherichia coli*: SAXS and Preliminary X-ray Crystallography Analysis." INT. J. MOL. SCI. 2014, 15, 2223-2236
 127. Cerqueira N, Coelho N, Bras N, Fernandes P, Garattini E, Terao M, Romão MJ, Ramos MJ, Insights Into The Structural Determinants Of Substrate Specificity And Activity In Mouse Aldehyde Oxidase. J BIOL INORG CHEM, 2014, 20, 2 Pages: 209-217 doi: 10.1007/s00775-014-1198-2
 128. Correia, H.D.; Marangon, J.; Brondino, C.D.; Moura, J.J.G.; Romão, M.J.; González, P.J.; Santos-Silva, T., Aromatic aldehydes at the active site of aldehyde oxidoreductase from *Desulfovibrio gigas*: reactivity and molecular details of the enzyme-substrate and enzyme-product interaction. J BIOL INORG CHEM, 20, 2, 219-229. DOI:10.1007/s00775-014-1196-4.
 129. Seixas JD, Santos MF, Mukhopadhyay A, Coelho AC, Reis PM, Veiros LF, Marques AR, Penacho N, Gonçalves AM, Romão MJ, Bernardes GJ, Santos-Silva T, Romão CC. A contribution to the rational design of Ru(CO)3Cl2L complexes for in vivo delivery of CO. DALTON TRANSACTIONS 2014 Nov 27. [Epub ahead of print]. DOI: 10.1039/C4DT02966F
 130. Kowacz, M; Marchel, M; Juknaite, L; Esperança, J; Romão, MJ; Carvalho, AL; Rebelo, LP, "Ionic liquid-functionalized mineral particles for protein crystallization" CRYSTAL GROWTH & DESIGN, 15, 6, 2994-3003 , 2015 DOI: 10.1021/acs.cgd.5b00403
 131. C Coelho, A Foti, T Santos-Silva, T Hartmann, S Leimkühler and MJ Romão, Human Aldehyde Oxidase: crystal structure and inhibition studies for the understanding of xenobiotics metabolism, NATURE CHEMICAL BIOLOGY 11, 779-783 (2015) doi:10.1038/nchembio.1895
 132. Coelho and Maria J Romão, Structural and mechanistic insights on nitrate reductases, PROTEIN SCIENCE, 2015 Dec;24(12):1901-11 DOI: 10.1002/pro.2801
 133. Terao, Mineko; Romao, Maria Joao; Leimkuehler, S; Bolis, M; Fratelli, M; Coelho, C; Santos-Silva, T; Garattini, E. Structure and function of mammalian aldehyde oxidases, ARCHIVES OF TOXICOLOGY, 90, 4, 753-780, : APR 2016 DOI: 10.1007/s00204-016-1683-1
 134. Foti, A; Hartmann, T; Coelho, C; Santos-Silva, T; Romao, MJ; Leimkuhler Optimization of the Expression of Human Aldehyde Oxidase for Investigations of Single-Nucleotide Polymorphisms, S. DRUG METABOLISM AND DISPOSITION Volume: 44 Issue: 8 Pages: 1277-1285 Published: AUG 2016
 135. Correia, M. A.; Otrelo-Cardoso, A. R.; Schwuchow, V.; Sigfridsson Clauss, K. G.; Haumann, M.; Romao, M. J.; Leimkühler, S.; Santos-Silva, T. The *Escherichia coli* Periplasmic Aldehyde Oxidoreductase Is an Exceptional Member of the Xanthine oxidase family of molybdoenzymes. ACS CHEM. BIOL. 2016, 11, 2923-2935.
 136. Kowacz, M, Marchel M, Juknaitė L, Esperança JMSS, Romão MJ, Carvalho AL, Rebelo LPN. 2017. Infrared light-induced protein crystallization. Structuring of protein interfacial water and periodic self-assembly, JOURNAL OF CRYSTAL GROWTH, 457, Special Issue: SI Pages: 362-368
 137. Brás, JLA, Pinheiro BA, Cameron K, Cuskin F, Viegas A, Najmudin S, Bule P, Pires VMR, Romão MJ, Bayer EA, Spencer HL, Smith S, Gilbert HJ, Alves VD, Carvalho AL, Fontes CMGA. 2016. Diverse specificity of cellulosome attachment to the bacterial cell surface, dec. SCIENTIFIC REPORTS. 6:38292.:

138. Romão, MJ, Coelho C, Santos-Silva T, Foti A, Terao M, Garattini E, Leimkühler S. 2017. Structural basis for the role of mammalian aldehyde oxidases in the metabolism of drugs and xenobiotics, *CURR OPIN CHEM BIOL*. 2017 Apr;37:39-47.
139. Pires, VMR, Pereira PMM, Brás JLA, Correia M, Cardoso V, Bule P, Alves VD, Najmudin S, Venditto I, Ferreira LMA, Romão MJ, Carvalho AL, Fontes CMGA, Prazeres DM. 2017. Stability and ligand promiscuity of type A carbohydrate-binding modules are illustrated by the structure of *Spirochaeta thermophila* StCBM64C. 2017, *THE JOURNAL OF BIOLOGICAL CHEMISTRY*, 292, 12, 4847-4860