

Curriculum Vitae

Dr Rocco Caliendo got the degree in Physics from the University of Bari (Italy) in 1993. After a year of mandatory military service, in 1995 he worked as post-degree fellowship at the Institute for the Research and Development of Crystallographic Methodologies of the National Research Council (CNR). In 1996 he joined the PhD program of the Department of Physics at the University of Bari. During his PhD he carried out researches in high-energy physics, participating to several heavy-ion collisions experiments at the European Organization for Nuclear Research (CERN) of Geneva. In 1999 he got the PhD in Physics. He prosecuted his research in high-energy physics during his permanence at CERN from February to May 1999, during a two years post-doctoral fellowship for experimental physicists from the National Institute of Nuclear Physics (INFN), and during a fixed-term contract from the University of Bari for the research project "Search for the Quark-Gluon Plasma". In December 2001 he became permanent employee as researcher of the Institute of Crystallography of CNR. In 2014 he got the national academic qualification to associate professor in Molecular Biology (05/E2).

He taught Physics (as course holder) at several degree courses of the Polytechnic of Bari from 2012 to 2015, and at the course of Natural Sciences of the Department of Biology of the University of Bari in 2016. He was teaching assistant in Physics of the Polytechnic of Bari in 1995/96, 1996/97 and 2000/01. He also teaches Protein Crystallography at the degree course of Medical Biotechnology of the University of Bari, starting from 2013 (few hours per year). He taught Crystallography at the European School of Medicinal Chemistry in 2012, at the school "Crystallography beyond diffraction", organized by the Italian Crystallographic Association in 2013 and at the 4th European Crystallography School in 2017. He will be lecturer at the Crystallographic School "From Gene to Protein Crystal Structure", to be held in Trieste from 3 to 6 March 2020.

He was advisor of two PhD students: Benny Danilo Belviso (PhD in Chemical and Molecular Sciences, XXIV cycle), and Valentina Mirabelli (PhD in Healthy Foods: Innovation and Management, XXX cycle) and of two degree students of the Polytechnic of Bari: Loris Vagali, course in Engineering of Industrial and Electronic Systems and Antonella Galati, course of Environmental and territorial engineering of the Polytechnic of Bari. He was trainee tutor of three students: Maurizio Colizzi, course of Management Engineering of the Polytechnic of Bari (January-June 2016); Paolo Pastorelli, course of Pharmacy of the University of Bari (April-July 2014); Isabella Ventura, course of Pharmacy of the University of Bari (October 2011- March 2012). He was tutor of the post-graduate internship of Dr. Valentina Mirabelli funded by Italia lavoro S.p.A. (January-July 2014).

He won a selective procedure for a salary upgrade for CNR researchers (call CNR n.364.174 in 2019); a prize for researchers and technologists of the CNR in 2005 for having achieved excellence and innovation performance of particular strategic importance, recognized by the President of CNR; two poster prizes at the Conference of the Department of Chemical Sciences and Materials Technologies of CNR, held in Bressanone (28-30 October 2019), and at the "2011 Meeting of the Swiss Crystallographic Association, held in Bern (16 September 2012).

He is the contact author of the CNR press release n. 8914 of 11/09/2019 entitled: "Scoperto il meccanismo di inibizione del trasporto del rame da parte di farmaci antitumorali a base di platino", also reported in the journal "Nuove Direzioni" 57 (2020), at pag 73.

He was editor of the article "A new resolution limit has been established by crystallography", included in the volume "Highlights CNR 2008-2009" at pag.66.

He spent several periods of study and research abroad:

- visiting scientist at the California University of San Francisco, USA, February 3-24 2020, to carry out protein structural investigations by Bragg and diffuse X-ray scattering, guest of Prof. James Fraser.
- visiting scientist at the Kyungpook National University, Daegu, South Korea, October 16-November 4 2016 and November 19-December 7 2017, to carry out crystal structure determination of epigenetic targets, guest of Prof. Eric di Luccio.
- visiting scientist at the Medical Research Centre of the Polish Academy of Sciences, Warsaw, Poland, November 28-December 11 and November 2-9 2014, to develop algorithms for structural characterization of protein dynamics from simulated data, guest of Prof. Bogdan Lesyng.

- visiting scientist at the National Synchrotron Light Source II of the Brookhaven National Laboratory (Brookhaven, New York state, USA), July 17-August 8 2014 and July 5-25 2016, to carry out experiments and data analysis on modulated enhanced diffraction, guest of Dr. Eric Dorhyee.
- visiting scientist at German Research School for Simulation Sciences of Julich, carried out 28 August-4 September 2012, to carry out research activities on Computational Biophysics, guest of Prof. Paolo Carloni.
- Short Visit Grant founded by the European Science Foundation to carry out research activities entitled "Investigation on mutations in prion protein", conducted at the "German Research School for Simulations" of Julich, Germany, 16-30 October 2010, collaborating with Prof. Paolo Carloni.
- Training course "Experimental Aspects of X-ray powder diffraction using Synchrotron Radiation", held at the Paul Scherrer Institute, Villigen, Switzerland, 20-31 January 2008, within the individual training program in 2004 CNR. Supervisor Dr. Fabia Gozzo.
- Training course "Development of crystallographic methods for structural biology", conducted at the Structural Biology Laboratory at the University of York, England, February 15-March 2 2005, as part of individual training program in 2007 CNR. Supervisor Dr. Garib Murshudov.
- Research activity at the European Centre for Nuclear Research (CERN) in Geneva, conducted from 1997 to 1999, to participate to high-energy Physics experiments.

He is member of the Board of the Institute of Crystallography and member of the board of the Biological Macromolecular Section of the Italian Crystallographic Association.

He is member of the Italian Crystallographic Association from 2001, of the Centro Dipartimentale Magna Grecia of the Polytechnic of Bari, from 2012, of the Accademia Pugliese delle Science from 2018, and of the Italian Chemistry Association from 2019.

He is editor-in-chief of the journal Applied Physics Research and member of the editorial board of the following journals: Crystals, Sci, Annals of nanoscience and Nanotechnology, Open journal of Materials Science, Innovations in Pharmacy and Pharmaceutical Technology.

He edited two special issue of Crystals, entitled "Multivariate Analysis Applications to Crystallography" and "Development of Computational Methods for Structural Determination of Biological Macromolecules".

He reviewed four articles for the Italian Scientific Evaluation ANVUR for the call VQR 2011-2014.

He reviewed manuscripts submitted to: *Scientific Reports*, *Physical Chemistry Chemical Physics*, *Acta Crystallographica A and D*, *Crystals*, *Applied Physics Research*, *Bioinorganic Chemistry and Applications*, *Chemical Engineering Research and Design*, *Journal of Genetics Syndromes & Gene Therapy*, *Journal of Materials Science Research*, *Journal of Molecular Structure*, *Journal of Pharmaceutical and Biomedical Analysis*, *Molecules*, *Pharmacology Research & Perspectives*, *Phytomedicine*, *Molecules*, *Materials letters*, *Microgravity*, *International Journal of Molecular Sciences*.

He reviewed the following research projects:

"Structural studies on proteins from Helicobacter pylori relevant for Bacterial host colonization and survival" presented for the programme PISCOPIA of the University of Padua, cofounded by the Marie Curie COFUND Programme.

"New methods to solve macromolecular structures from limited data" presented for the call HTSM2017 of the Netherlands Organization for Scientific Research (NOW).

"Optimization of GEMMA methodology by design of experiment for detection of nanoparticles occurred during enzymatic reactions" presented for the call JESH of the Austrian Academy of Sciences (ÖAW).

"Molecular basis of the 14-3-3 protein-dependent regulation of protein kinase activity" presented for the Czech Science Foundation (GAČR).

"Dynamic behaviour of nanoalloys during CO₂ activation: modulation excitation spectroscopy", presented for the Research Foundation – Flanders (FWO).

"Molecular modeling of RNA molecules and their complexes: the role of structural dynamics", presented for the the Czech Science Foundation (GAČR).

"Nanocrystallography of molecular crystals", presented for the Czech Science Foundation (GAČR).

"Amyloid fibrils unravelled by neutron scattering & molecular dynamics simulations", presented for the call "Beyond Borders" of the University of Rome Tor Vergata.

He is scientific evaluator appointed by the CNR for the following projects in the context of the call MISE Horizon 2020 - PON 2014/2020 (starting from 2016):

- “Nuova generazione di prodotti alimentari salutistica base carne: Antibiotic Free – Allergenic Free” by Martini S.p.A. (Pos. n.30);
- “Sviluppo di una nuova piattaforma polimerica basata su idrogeli superassorbenti per il controllo glicemico” by Gelesis S.r.l. (Pos. n.174);
- “Micro/nanofornulati innovativi per la valorizzazione dei molecole bioattive, utili per la salute e il benessere della popolazione, ottenute da prodotti di scarto della filiera ittica” by Avantech Group S.r.l. (Pos. n.347).

He organized:

- the XLVII National Congress of the Inorganic Chemistry Division of the Italian Chemical Society, held in Bari (9-12 September 2019);
- the “EXPO&more International Workshop”, held in Bari (30 September-3 October 2019);
- the “3rd International Conference on Applied Mineralogy & Advanced Materials”, held in Bari (24-26 July 2018);
- the “3rd International Conference on Food & Beverage Packaging”, held in Rome (16-18 July 2018);
- the workshop “Analisi quantitative di fasi cristalline: metodi tradizionali e chemiometria a confronto”, held in Bologna (6 February 2018);
- the workshop “Multivariate DOE and PCA Methods in Materials Science and Crystallography”, held in Vercelli (14 September 2015);
- the session “Crystal structure solution by single crystal data” of the “International EXPO/SIR workshop”, held in Bari (10-13 June 2014);
- the meeting “La Biologia Strutturale in Puglia: stato dell’arte e prospettive future”, held in Bari (9 July 2010);
- the session “Macromolecular crystal structure solution via AB-INITIO, SIR-MIR, SAD-MAD and MOLECULAR REPLACEMENT techniques” of the “PHARE 2009: A modular workshop on global PHASE RETRIVAL”, held in Martina Franca (20-22 April 2009).
- the course “Computational Structural Biology” held from 27 to 30 September 2009 for the doctorate course in Physics of the University of Bari.

He was chair of:

- the session devoted to the RootProf program of the EXPO&more International workshop, held in Bari (30 September-3 October 2019);
- the microsimsposia “The Universe of Materials & Minerals”, “Hybrid materials for efficient enzymatic catalysis” and “In situ and in operando structural characterization of nano and micro materials” of the “3rd International Conference on Applied Mineralogy & Advanced Materials,” held in Bari (24-26 July 2018);
- the microsimsposium “From APIs to nanocarriers to target macromolecules: a multiscale and multitechnique approach to modern medicine”; of the XLVI Meeting of Italian Crystallographic Association, held in Perugia (26-29 June 2017);
- the session “Theory and modeling of soft materials” of the workshop “Probing Dynamic Processes in Soft Materials Using Advanced Light Sources”, held in Santa Fe (USA) (25-27 July 2016);
- the session "Automated Data Processing and Structural Solution for High Throughput Crystallography" of the XXII International Congress and General Assembly of the International Union of Crystallography held in Madrid (22-30 August 2011);
- the session on computational structural biology of the national conference "Modeling Winter 2008", held in Pisa (18 December 2008).

He leads the research line entitled “Application of crystallographic techniques and computational modelling to structural studies of biomolecules” of the Department of Chemical sciences and materials technology of CNR, starting in 2011.

He is author of the computer programs SIR and RootProf, devoted to Crystallographic calculations.

He is responsible for the code on the Molecular Replacement and Patterson-based algorithms included in the open source software package IL MILIONE.

Research sectors: Protein Crystallography, Crystallographic Methods and Techniques, Computational Biophysics, Chemometrics.

Recent Scientific Activities: Structural characterization of protein by using X-rays, development of new phasing methods, study of protein flexibility, application of the Modulated Enhanced Diffraction technique.

Grants Awarded

- 2019-2022 Project “The inorganic side of lysosome cell biology: the network of metal-protein interactions” research project of National Relevance (PRIN) of the Italian Ministry of Education, Universities and Research (Prot. 2017WBZFHL). Responsible for the CNR unit (116,000€).
- 2016-2020 Project “Revolutionising Downstream Processing of Monoclonal Antibodies by Continuous Template-Assisted Membrane Crystallization — AMECRYS” of the HORIZON 2020-FETOPEN-2014-2015-RIA programme (grant agreement n. 712965). Responsible for the CNR unit (200,674€), and coordinator of activities of work task 5.3, entitled “Structural, morphological & biological characterizations”.
- 2015-2017 Collaborative project “Static and dynamic crystallographic investigations for developing specific and selective inhibitors for the epigenetic therapy of cancers”, funded within the scientific cooperation agreement between the CNR and the National Research Foundation of Korea. Responsible for the Italian activities (20,000€).
- 2013-2015 Project “Promozione di Processi ECO_sostenibili per la valorizzazione delle Produzioni agroalimentari Pugliesi - ECO_P4” of the Programma Operativo Nazionale per la Ricerca e la Competitività 2007-2013 (n. 713/Ric. of the 29/10/2010). Responsible for the CNR unit (41,000€).
- 2014-2016 Collaborative project “New algorithms for protein dynamics studies and their applications to protein crystallography”, funded within the scientific cooperation agreement between the CNR and the Polish Academy of Sciences. Responsible for the Italian activities.
- 2014-2014 XRD analysis on wine leaves samples, conducted within a sub-contract between the Department of Civil, Environmental, Territorial, Architectural and Chemical Engineering of the Polytechnic of Bari and the Institute of Crystallography of CNR, prot.5059 del 27/11/2013. Responsible for the activities (5,500€).
- 2010-2010 Scientific activity "Structural characterization of luminescent molecular markers" conducted within the research project presented by Meditekology Srl, entitled "New diagnostic system for the detection of biomaterials", funded by Regione Puglia, call "POR Puglia 2007-2013: Aiuti agli Investimenti in Ricerca per le PMI ". Responsible for the activities (20,000€).
- 2009-2009 Project "Crystal structure solution by iterative modeling, approved by CASPUR - Inter-University Consortium for Supercomputing Applications for Universities and Research, call Standard HPC Grant 2009. Project manager.
- 2008-2008 Project "Crystallographic Computing", approved by CASPUR - Inter-University Consortium for Supercomputing Applications for Universities and Research, call DMP @ CASPUR 2008. Project manager.

Participation to Research projects:

- 2017-2021 Horizon 2020– PON 2014/2020 project MISE D.M. 1/06/2016 entitled "Study, design and development of an innovative kit for the early and non-invasive diagnosis of celiac disease using genetic markers ".
- 2012-2015 High Qualification Human Capital Development Call 2011 project entitled "Towards Personalized Medicine: Development of new selective molecules for the treatment of Neuroblastoma, approved by the CON IL SUD Foundation".
- 2013-2014 Project “Collezione di Composti Chimici ed attività di Screening (CCCSN), coordinated by CNR.

- 2008-2010 project PRIN 2007 prot. n. 200755ZKR3_005 entitled “Applicazioni delle tecniche MAD e Sviluppo di nuovi algoritmi di calcolo per migliorare il processo di risoluzione delle strutture cristalline attraverso i dati di diffrazione da polveri”.
- 2004-2008 project MIUR rif. N.97, D.M. 1105 9/10/2002 entitled “Global Phasing: dalle polveri alle Macromolecole”

Keynote speaker at the:

Fifth Meeting of the Italian (AIC) and Spanish Crystallographic (GE3C) Associations (MISCA V), held in Naples (4-7 September 2019).

3rd Joint AIC-SILS Conference, held in Rome (25-28 June 2018).

29th European Crystallographic Meeting, held in Rovinj, Croazia (23-28 August 2015).

Invited talks:

“Enzymes and advanced materials for active food packaging” at the 3rd International Conference on Food & Beverage Packaging, Roma. (16-18 July 2018).

“Structural Dynamics by Modulated Enhanced Diffraction” at the Matter-Radiation Interactions in Extremes (MaRIE) workshop, Santa Fe, USA (25-27 July 2016).

“Modulation enhanced diffraction: theory and applications” at the Annual meeting of the American Crystallographic Association, held in Honolulu, Hawaii, (20-24 July 2013).

“Data Analysis by Modulation Enhanced Diffraction (MED)” at the workshop on advanced analysis of X-ray and neutron scattering data: getting from data to science, held at the Brookhaven National Laboratory (14-15 August 2013).

“Selective structural investigation by MED” at the NSLS-II First-Experiments Workshop, held at the Brookhaven National Laboratory (12-13 August 2013).

“Modulated Enhanced Diffraction: la nuova sfida” at the workshop “Davide Viterbo: una vita per la cristallografia...ma non solo” held in Alessandria, (19 December 2012).

“New tools for flexibility assessment of protein structures” at the congress “Computationally Driven Drug Discovery” organized by Dompè S.p.A., held at L’Aquila (21-23 November 2011).

“Molecular replacement in IL MILIONE” at the workshop “Recent Advances in Macromolecular Crystallography”, held at Copanello di Stalettì (CZ), (23-24 September 2007).

Invited seminars in the last 6 years:

“Multivariate analysis for structural characterization of materials by situ X-ray diffraction” held at the Los Alamos National Laboratory, USA (20 February 2020).

“Multivariate analysis for in situ characterization of structural dynamics”, held at the Nanochemistry Department of IIT, Genoa (18 October 2019).

“La cristallografia come metodo di indagine strutturale di macromolecole biologiche e materiali avanzati”, held at the Accademia Pugliese delle Scienze and the Accademia dei Georgofili, Sezione del Sud-Est, Bari (30 maggio 2018).

“Structural investigation of macromolecules by x-ray: theoretical background and applications”, held at the Creative BioResearch Group & Advanced Bio-resource Research Center of the Kyungpook National University, Daegu, South Korea (30 November 2017).

“Structural dynamics by Modulated Enhanced Diffraction”, held at the Photon Science Division of the Brookhaven National Laboratory (20 July 2016)

“New tools and techniques for investigating protein structural dynamics” held at the Department of genetic engineering of the Kyungpook National University (27 October 2016).

“New tools and techniques for investigating protein structural dynamics”, held at the Institute of Biophysics and Biochemistry of the Polish Academy of Sciences (30 November 2016).

“Advances in methods for macromolecular crystal structure solution”, held at the Faculty of Physics, University of Warsaw (7 November 2016).

“New algorithms for protein dynamics studies and their applications to protein crystallography”, held at the Institute of Biophysics and Biochemistry of the Polish Academy of Sciences (5 novembre 2014).

Publications:

Dr. Caliendo is co-author of >170 scientific publications [H-index 34 (Google Scholar), 26 (WoS), number of citations=6013, average citations per article=34.9 (WoS)] in international journals with high impact factor.

List of papers of the last 5 years:

R Caliendo, D Altamura, BD Belviso, A Rizzo, S Masi, C Giannini “Investigating temperature-induced structural changes of lead halide perovskites by in situ X-ray powder diffraction” *J. Appl. Cryst.* 52, 2019. *Note: corresponding author*

A Lasorsa, MI Nardella, A Rosato, V Mirabelli, R Caliendo, R Caliendo, G Natile, F Arnesano “Mechanistic and structural basis for inhibition of copper trafficking by platinum anticancer drugs” *J. Am. Chem. Soc.*, 141, 12109-12120, 2019. *Note: article awarded by the front cover of the journal issue and mentioned in the CNR press release n. 8914 of 11/09/2019 entitled “Scoperto il meccanismo di inibizione del trasporto del rame da parte di farmaci antitumorali a base di platino”.*

R Caliendo, V Toson, L Palin, E Conterosito, M Aceto, V. Giannotti, E Boccaleri, E Dooryhee, M Milaneseo “New hints on Maya Blue formation process by PCA-assisted in situ XRPD/PDF and optical spectroscopy” *Chemistry–A European Journal*, 25, 1-10, 2019.

BD Belviso, R Caliendo, SM Salehi, G Di Profio, R Caliendo “Protein Crystallization in Ionic-Liquid Hydrogel Composite Membranes” *Crystals*, 9, 253, 2019. *Note: corresponding author.*

H Yang, BD Belviso, X Li, W Chen, TF Mastropietro, G Di Profio, R Caliendo, J.Y.Y. Heng ”Optimization of Vapor Diffusion Conditions for Anti-CD20 Crystallization and Scale-Up to Meso Batch”, *Crystals*, 9, 230, 2019. *Note: corresponding author.*

A Zappi, L Maini, G Galimberti, R Caliendo, D Melucci “Quantifying API polymorphs in formulations using X-ray powder diffraction and multivariate standard addition method combined with net analyte signal analysis” *European Journal of Pharmaceutical Sciences*, 130, 36-43, 2019.

E Conterosito, L Palin, R Caliendo, W van Beek, D Chernyshov, M. Milaneseo “CO₂ adsorption in Y zeolite: a structural and dynamic view by a novel principal-component-analysis-assisted in situ single-crystal X-ray diffraction experiment” *Acta Cryst. A. Advances*, 75, 214-222, 2019.

Y Shen, DEHF Mevius, R Caliendo, B Carrozzini, Y Roh, J Kim, S Kim, S.C. Ha, M. Morishita, E. di Luccio “Set7 Is a H3K37 Methyltransferase in *Schizosaccharomyces pombe* and Is Required for Proper Gametogenesis” *Structure* 27, 631-639, 2019. *Note: article mentioned in the CNR news of 28/02/2019 entitled “Scoperta una nuova proteina coinvolta nei meccanismi epigenetici alla base della infertilità maschile”.*

B Carrozzini, BD Belviso, C Bruno, MM Cavalluzzi, A Lovece, G Lentini, R Caliendo “The Crystal Structure of N-[(2E)-3-(4-Chlorophenyl)prop-2-en-1-yl]-4-methoxy-N-methylbenzenesulfonamide” *Journal of Chemical Crystallography*, 49, 87-91, 2019. *Note: corresponding author.*

F Italiano, A Agostiano, BD Belviso, R Caliendo, B Carrozzini, R. Comparelli, M.T. Melillo, E. Mesto, G. Tempesta, M. Trotta “Interaction between the photosynthetic anoxygenic microorganism *Rhodobacter sphaeroides* and soluble gold compounds. From toxicity to gold nanoparticle synthesis”, *Colloids and Surfaces B: Biointerfaces* 172, 362-371, 2018.

- M Loi, F Fanelli, MT Cimmarusti, V Mirabelli, M Haidukowski, AF Logrieco, R. Caliandro, G. Mulè “In vitro single and combined mycotoxins degradation by Ery4 laccase from *Pleurotus eryngii* and redox mediators” *Food control* 90, 401-406, 2018.
- S Colella, M Todaro, S Masi, A Listorti, D Altamura, R Caliandro, C Giannini, E Carignani, M Geppi, D Meggiolaro, G Buscarino, F De Angelis, A Rizzo “Light-Induced Formation of Pb³⁺ Paramagnetic Species in Lead Halide Perovskites” *ACS Energy Letters*, 3, 1840-1847, 2018. *Note: corresponding author.*
- P Guccione, L Palin, BD Belviso, M Milanesio, R Caliandro “Principal component analysis for automatic extraction of solid-state kinetics from combined in situ experiments” *Phys. Chem. Chem. Phys.*, 20, 19560 - 19571, 2018. *Notes: corresponding author, article selected for 2018 PCCP HOT Articles.*
- S Masi, F Aiello, A Listorti, F Balzano, D Altamura, C Giannini, R Caliandro, G Uccello-Barretta, A Rizzo, S Colella “Connecting the solution chemistry of PbI₂ and MAI: a cyclodextrin-based supramolecular approach to the formation of hybrid halide perovskites” *Chemical Science* 9, 3200-3208, 2018.
- SM Salehi, AC Manju, BD Belviso, CAM Portugal, IM Coelho, V Mirabelli, E Fontananova, R Caliandro, JG Crespo, E Curcio, G Di Profio “Hydrogel Composite Membranes Incorporating Iron Oxide Nanoparticles as Topographical Designers for Controlled Heteronucleation of Proteins” *Cryst. Growth Des.*, 18, 3317-3327, 2018.
- P Guccione, L Palin, M Milanesio, BD Belviso, R Caliandro “Improved multivariate analysis for fast and selective monitoring of structural dynamics by in situ X-ray powder diffraction” *Phys. Chem. Chem. Phys.* 20, 2175-2187, 2018. *Notes: corresponding author, article awarded by the back cover of the journal issue.*
- V Mirabelli, SM Salehi, L Angiolillo, BD Belviso, A Conte, MA Del Nobile, G Di Profio, R Caliandro “Enzyme Crystals and Hydrogel Composite Membranes as New Active Food Packaging Material” *Global Challenges*, 2, n.1700089, 2018. *Note: corresponding author.*
- R Caliandro, BD Belviso, C Cuocci, S Fuertes, V Sicilia, JC Hanson, G Tutuncu, E Doorhyee, A Altomare “Dynamic characterization of structural changes in vapochromic compounds by pair distribution function” *Powder Diffraction* 32, S118-S122, 2017. *Note: corresponding author.*
- L Padalino, R Caliandro, G Chita, A Conte, MA Del Nobile “Study of drying process on starch structural properties and their effect on semolina pasta sensory quality” *Carbohydr. Polym.* 153, 229-235, 2016.
- MM Dell'Anna, V Censi, B Carrozzini, R Caliandro, N Denora, M Franco, D Veclani, A Melchior, M Tolazzi, P Mastroianni “Triphenylphosphane Pt(II) complexes containing biologically active natural polyphenols: Synthesis, crystal structure, molecular modeling and cytotoxic studies” *J. Inorg. Biochem.* 163, 356-361, 2016.
- BD Belviso, A Galliani, A Lasorsa, V Mirabelli, R Caliandro, F Arnesano, G Natile “Oxaliplatin Binding to Human Copper Chaperone Atox1 and Protein Dimerization” *Inorg. Chem.* 55, 6563-6573, 2016. *Note: corresponding author.*
- R Caliandro, T Sibillano, BD Belviso, R Scarfiello, JC Hanson, E Doorhyee, M Manca, PD Cozzoli, C Giannini “Static and Dynamical Structural Investigations of Metal-Oxide Nanocrystals by Powder X-ray Diffraction: Colloidal Tungsten Oxide as a Case Study” *ChemPhysChem* 17, 699-709, 2016. *Note: corresponding author.*
- G Di Profio, SM Salehi, R Caliandro, P Guccione, G Nico, E Curcio, E Fontananova “Bioinspired Synthesis of CaCO₃ Superstructures through a Novel Hydrogel Composite Membranes Mineralization Platform: A Comprehensive View” *Adv. Mat.*, 28, 610-616, 2016.
- R Caliandro, P Guccione, G Nico, G Tutuncu, JC Hanson “Tailored multivariate analysis for modulated enhanced diffraction” *J. Appl. Cryst.* 48, 1679-1691, 2015. *Note: corresponding author.*
- MC Burla, R Caliandro, B Carrozzini, GL Cascarano, C Cuocci, C Giacobozzo, M Mallamo, A Mazzone, G Polidori “Crystal structure determination and refinement via SIR2014” *J. Appl. Cryst.* 48 306-309, 2015.

L Palin, R Caliandro, D Viterbo, M Milanesio “Chemical selectivity in structure determination by the time dependent analysis of in situ XRPD data: a clear view of Xe thermal behavior inside a MFI zeolite” *Phys. Chem. Chem. Phys.* 17, 17480-17493, 2015.

New protein crystal structures determined:

6Y3C: Human COX-1 Crystal Structure.

6QUF: Protein crystallization by ionic liquid hydrogel support: reference crystal of glucose isomerase grown on standard silanized glass.

6QUK: Protein crystallization by ionic liquid hydrogel support: glucose isomerase grown by using ionic liquid hydrogel.

6TOV: Crystal Structure of Teicoplanin Aglycone.

6EO8: Crystal structure of thrombin in complex with a novel glucose-conjugated potent inhibitor.

6EO9: Crystal structure of thrombin in complex with a novel glucose-conjugated potent inhibitor.

5T7L: Pt(II)-mediated copper-dependent interactions between ATOX1 and MNK1.

5H6Z: Crystal structure of Set7, a novel histone methyltransferase in *Schizosacharomyces pombe*.

5WW0: Crystal structure of Set7, a novel histone methyltransferase in *Schizosacharomyces pombe*.

4DPE: Structure of MMP3 complexed with a platinum-based inhibitor.

4G9L: Structure of MMP3 complexed with NNGH inhibitor.

4JA1: Structure of MMP3 complexed with a platinum-based inhibitor.

4QOT: Crystal structure of human copper chaperone bound to the platinum ion.

3N30: Crystal Structure of cubic Zn₃-hUb (human ubiquitin) adduct.

3N32: The crystal structure of human Ubiquitin adduct with Zeise's salt.