

CURRICULUM VITAE

FORMATO EUROPEO/EUROPEAN FORMAT

INFORMAZIONI PERSONALI/ PERSONAL INFORMATION

Nome, Cognome/Name, Surname Rocco Caliandro
Indirizzo/Address Via, numero civico, c.a.p., città, nazione/ House number, street name, postcode, city, country Via Robert Schuman n.15/3 70126 Bari, Italy
Telefono/Telephone +39 - 080 – 5929150
Fax +39 - 080 – 5929170
E-mail rocco.caliandro@ic.cnr.it
Sito web/Website <http://users.ba.cnr.it/crisrc25>
Nazionalità/Nationality Italian
Luogo e data di nascita/ Place and Date of birth Bari, Italy, 11.11.1967

SPERIENZA PROFESSIONALE /WORK EXPERIENCE

Se dipendente CNR indicare:

N. MATRICOLA 009282; QUALIFICA RICERCATORE; LIVELLO II

In ordine di data /Dates (from – to)

12/2001 – today

Nome e indirizzo del datore di lavoro / Name and address of employer

Italian Council of Researches – Institute of Crystallography

Tipo o settore di attività / Type of business or sector

Funzione o posto occupato / Occupation or position held

Researcher

In July 2018 he was eligible in the public competition based on qualifications and interview call 367.171 - strategic area "Biomolecules and Biomaterials for health" and, following the provision issued on August 13, 2020, in execution of resolution 65/2020, will be hired by the CNR with a Senior Researcher II professional level profile during 2020.

Principali mansioni e responsabilità / Main activities and responsibilities

Responsible for 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.

Head of the research unit of the CNR (46,000€) of the Industrial Research Project of National Interest (ARS01_00783) entitled "Sviluppo di alimenti funzionali per l'innovazione dei prodotti alimentari di tradizione italiana - ALIFUN", starting from 2021.

Head of the research unit of the CNR (116,000€) of the PRIN project entitled "The inorganic side of lysosome cell biology: the network of metal-protein interactions", Prot. 2017WBZFHL, starting from 2019.

Head of research unit of the Institute of Crystallography (200,674€) and coordinator of activities of work task 5.3, entitled "Structural, morphological & biological characterizations" of the HORIZON 2020- FETOPEN-2014-2015-RIA project entitled "Revolutionizing Downstream Processing of Monoclonal Antibodies by Continuous Template-Assisted Membrane Crystallization - AMECRY", Gant agreement n.712965, starting from 2016

Responsible for the Italian activities (20,000€) of the collaborative project "Static and dynamic crystallographic investigations for developing new inhibitors for the epigenetic therapy of cancers" funded within the scientific cooperation agreement between the CNR and the National Research Foundation (NRF) of South Korea, from 2016 to 2017.

Responsible for the Italian activities of the 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 (PAS) of Poland, from 2014 to 2016.

Responsible for the CNR unit (41,000€) of the PON project "Recovery of BIOCHAR for the competitive strengthening of a local agro-energy supply chain" presented by the Agro-Food District of the Puglia Region (DARe) (Art.13, DD prot. 713 / Ric of 29 October 2010), from 2013 to 2015.

Responsible for the activities on XRD analysis on wine leaves samples (5,500€), 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. Activities carried out in 2014.

Responsible for the activities "Structural characterization of luminescent molecular markers" (20,000€) conducted within the research project presented by Mediteknology 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". Activities carried out in 2010.

Project manager of the 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. Activities carried out in 2009.

Project manager of the project "Crystallographic Computing", approved by CASPUR - Inter-University Consortium for Supercomputing Applications for Universities and Research, call DMP @ CASPUR 2008. Activities carried out in 2008.

Participant in the Horizon 2020– PON 2014/2020 project ", MISE, DM 1 June 2016 entitled" Study, design and development of an innovative kit for the early and non-invasive diagnosis of celiac disease using genetic markers ". Activities carried out from 2017 to 2021.

Participant in the 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". Activities carried out from 2012 to 2015.

Participant in the project entitled ""Collezione di Composti Chimici ed attività di Screening (CCCSN), coordinated by CNR. Activities carried out from 2013 to 2014.

Participant in the 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". Activities carried out from 2008 to 2010.

Participant in the project MIUR rif. N.97, D.M. 1105 9/10/2002 entitled "Global Phasing: dalle polveri alle Macromolecole". Activities carried out from 2004 to 2008.

Co-inventor in the Italian patent appl. n. 102022000001577, entitled "Process for the production of nanocrystals of metal chalcogenides".

Author of the computer programs ILMILIONE, SIR and RootProf, devoted to Crystallographic calculations.

Responsible for the code on the Molecular Replacement and Patterson-based algorithms included in the open source software package IL MILIONE. Activity carried out from 2006.

Coordinator of the CNR for the management of the reports relating to the activities provided for in the training and orientation internship agreement between the Institute of Crystallography of the CNR and the Polytechnic of Bari. Assignment conferred by Dr. M. Saviano (prot. CNR- IC n.32 of 13/01/2015) and carried out starting from 2015.

Disabled Personnel Officer in the management of an emergency. Appointment conferred by Dr. M. Saviano (prot. CNR-IC n.163 of 03/02/2014) and carried out since 2014.

Editor-in-chief of the journal Applied Physics Research

Editor-in-chief of Applied Physics Research, section board member of Crystals, Advisory board member of Sci, Editorial board Member of Solids and PhysChem.

Editor of three special issues of Crystals, entitled "Development of Computational Methods for Structural Determination of Biological Macromolecules", "Multivariate Analysis Applications to Crystallography" and "Selected Papers from the 2nd International Online Conference on Crystals".

Member of the Board of the Institute of Crystallography from 2019.

Member of the board of the Biological Macromolecular Section of the Italian Crystallographic Association, from 2018.

Member of the Italian Crystallographic Association from 2002.

Member of the Centro Dipartimentale Magna Grecia of the Polytechnic of Bari, from 2012.

Member of the Accademia Pugliese delle Science from 2018.

Member of the Italian Chemistry Association from 2019.

Reviewer for the Italian Scientific Evaluation ANVUR, member of GEV 5 (Biological Sciences) board for the call VQR 2015-2019.

Reviewer of four articles for the Italian Scientific Evaluation ANVUR for the call VQR 2011-2014:
Product n. 142636, published in Physical Review E - Statistical, Nonlinear and Soft Matter Physics, GEV 2 – Scienze Fisiche, review submitted on 31/12/2016;
Product n. 185415, published in Nucleic Acids Research, 3 - Scienze Chimiche, review submitted on 28/12/2016;
Product n. 273621, published in La Rivista del Nuovo Cimento della Società Italiana di Fisica, 6 – Scienze Mediche, review submitted on 07/07/2016;
Product n. 446828, published in CELL, GEV 5 – Scienze Biologiche, review submitted on 27/12/2016;

Reviewer of manuscripts submitted to: Acta Crystallographica A (2), Acta Crystallographica B (2), Applied Physics Research (14), Bioinorganic Chemistry and Applications (1), Cellular and Molecular Life Sciences (1), Chemical Engineering Research and Design (3), Crystals (3), Drug Designing (2), Future Medicinal Chemistry (1), International journal of Drug Development and Research (1), International journal of Molecular Biology and Medicine (1), International Journal of Molecular Sciences (1), International journal of Pharmaceutics (1), Journal of Applied Crystallography (2), Journal of Genetics Syndromes & Gene Therapy (1), Journal of Materials Science Research (1), Journal of Molecular Structure (1), Journal of Molecular Liquids (1), Journal of Pharmaceutical and Biomedical Analysis (2), Materials Letters (1), Medicinal Chemistry (1), Microgravity (1), Molecules (2), Minerals (1), Physical Chemistry Chemical Physics (1), Pharmacology Research & Perspectives (1), Phytomedicine (1), Scientific Reports (2), The Journal of Chemical Physics (1).

Editor of 10 publications for the journal Crystals.

Scientific evaluator of 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). Extra-institutional assignment n.898 authorized by the CNR carried out in October 2018.

“Dynamic behaviour of nanoalloys during CO₂ activation: modulation excitation spectroscopy”, presented for the Research Foundation – Flanders (FWO). Extra-institutional assignment n.3091 authorized by the CNR carried out in July 2019.

“Molecular modeling of RNA molecules and their complexes: the role of structural dynamics”, presented for the Czech Science Foundation (GAČR). Extra-institutional assignment n.3069 authorized by the CNR carried out in July 2019.

“Nanocrystallography of molecular crystals”, presented for the Czech Science Foundation (GAČR). Extra-institutional assignment n.3266 authorized by the CNR carried out in August 2019.

“Amyloid fibrils unravelled by neutron scattering & molecular dynamics simulations”, presented for the call “Beyond Borders” of the University of Rome Tor Vergata. Extra-institutional assignment n.3326 authorized by the CNR carried out in August 2019.

“The fascinating physical chemistry of DNA studied by advanced computations”, presented for the Czech Science Foundation (GAČR). Extra-institutional assignment n.5520 authorized by the CNR carried out in July 2020.

“Protein and peptide nanocrystal growth and delivery for crystallography at continuous and femtosecond X-ray sources” presented for the Czech Science Foundation (GAČR). Extra-institutional assignment n.5630 authorized by the CNR carried out in July 2020.

“Development of method for polymorph control in case of concomitant polymorphs using crystallization additives” presented for the Central Finance Contracting Agency (CFCA) of Latvia. Extra-institutional assignment n. 2020/1829 authorized by the CNR carried out in October 2020.

Reviewer and rapporteur of two projects: “Development of method for polymorph control in case of unselective formation of polymorphs using crystallization additives” and “Carrier-supported antioxidants – a novel concept for enhanced activity” presented for the Latvian Council of Science (LCS). Extra-institutional assignment n.2021/2809 authorized by the CNR carried out in November 2021.

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/nanoformulati 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).

In ordine di data /Dates (from – to)	06/2001 – 12/2001
Nome e indirizzo del datore di lavoro / Name and address of employer	Department of Physics of the University of Bari
Tipo o settore di attività / Type of business or sector	Research fellowship (D.R. n.11042 del 20/12/2000)
Funzione o posto occupato / Occupation or position held	Researcher
Principali mansioni e responsabilità / Main activities and responsibilities	Research on quark-gluon plasma
In ordine di data /Dates (from – to)	06/1999 – 05/2001
Nome e indirizzo del datore di lavoro / Name and address of employer	Italian Institute of Nuclear Physics (INFN), seat of Bari
Tipo o settore di attività / Type of business or sector	Post-doctoral fellowship for experimental physicists (call n.7197 of14/6/1998)
Funzione o posto occupato / Occupation or position held	Researcher
Principali mansioni e responsabilità / Main activities and responsibilities	Study on strangeness production in heavy-ion collisions
In ordine di data /Dates (from – to)	03/1995 – 01/1996
Nome e indirizzo del datore di lavoro / Name and address of employer	CNR – Institute of Research for the Development of Crystallographic Methods
Tipo o settore di attività / Type of business or sector	Research fellowship (call n. 201.19.1 del 30/11/94)
Funzione o posto occupato / Occupation or position held	Researcher
Principali mansioni e responsabilità / Main activities and responsibilities	Development of Crystallographic methods
ISTRUZIONE E FORMAZIONE / EDUCATION AND TRAINING	
In ordine di data /Dates (from – to)	02/1996 – 07/1999
Nome e tipo d’istituto di istruzione o formazione / Name and type of organisation providing education and training	University of Bari – Department of Physics
Principali materie e competenze professionali apprese / Principal subjects occupational skills covered	High-Energy Physics
Certificato o diploma ottenuto /Title of qualification awarded	Ph.D in Physics
Livello nella classificazione nazionale o internazionale / Level in National classification	PhD
In ordine di data /Dates (from – to)	11/1987 – 12/1993
Nome e tipo d’istituto di istruzione o formazione / Name and type of organisation providing education and training	University of Bari – Department of Physics
Principali materie e competenze professionali apprese / Principal subjects occupational skills covered	High-Energy Physics
Certificato o diploma ottenuto /Title of qualification awarded	Degree in Physics
Livello nella classificazione nazionale o internazionale / Level in National classification	Degree

ATTIVITA' DI RICERCA / RESEARCH ACTIVITIES

Attuali campi di ricerca / Research sectors

Recenti attività scientifiche/ Recent Scientific Activities.

Pubblicazioni/ Books and Articles

Protein Crystallography, Phasing Methods, Computational Biophysics, Chemometrics.

Structural characterization of protein by X-ray, development of new phasing methods, study of protein flexibility, application of the Modulated Enhanced Diffraction technique.

Total number of publications in peer-review journals 155 (Scopus)

Total number of citations: 6889 (Scopus)

H index: 28 (Scopus)

List of papers of the last 5 years:

- BD Belviso, GF Mangiatordi, D Alberga, V Mangini, B Carrozzini, R Caliandro "Structural Characterization of the Full-Length Anti-CD20 Antibody Rituximab" 2022 *Frontiers in Molecular Biosciences* 9,823174. *Note: corresponding author.*
- B Zhang, D Altamura, R Caliandro, C Giannini, L Peng, L De Trizio, L Manna "Stable CsPbBr₃ Nanoclusters Feature a Disk-like Shape and a Distorted Orthorhombic Structure" 2022, *Journal of the American Chemical Society* 144, 5059-5066.
- D Quarta, S Toso, R Giannuzzi, R Caliandro, A Moliterni, G Saleh, A-L Capodilupo, D Debellis, M Prato, C Nobile, V Maiorano, I Infante, G Gigli, C Giannini, L Manna, C Giansante "Colloidal Bismuth Chalcohalide Nanocrystals" 2022 *Angewandte Chemie - International Edition*. *Note: corresponding author.*
- I Bolognino, A Carrieri, R Purgatorio, M. Catto, R Caliandro, B Carrozzini, BD Belviso, M Majellaro, E Sotelo, S Cellamare, CD Altomare "Enantiomeric Separation and Molecular Modelling of Bioactive 4-Aryl-3,4-dihydropyrimidin-2(1H)-one Ester Derivatives on Teicoplanin-Based Chiral Stationary Phase" 2022 *Separations* 9, 7.
- BD Belviso, F Marin, S Fuertes, V Sicilia, R Rizzi, F Ciriaco, C Cappuccino, E Dooryhee, A Falcicchio, L Maini, A Altomare, R Caliandro "Structural Insights into the Vapochromic Behavior of Pt- And Pd-Based Compounds" 2021 *Inorganic Chemistry* 60, 6349-6366. *Note: corresponding author.*
- R Caliandro, M Milanesio "Multivariate analysis applications to crystallography" 2021 *Crystals* 11,166, 1-2. *Note: corresponding author.*
- P Guccione, M Lopresti, M Milanesio, R Caliandro "Multivariate analysis applications in x-ray diffraction" 2021 *Crystals* 11,12, 1-21. *Note: corresponding author.*
- M Miciaccia, BD Belviso, M Iaselli, G Cingolani, S Ferorelli, M Cappellari, PL Polosa, MG Perrone, R Caliandro, A Scilimati "Three-dimensional structure of human cyclooxygenase (hCOX)-1" *Scientific Reports*, 11, 4312, 2021. *Note: corresponding author.*
- BD Belviso, FM Perna, B Carrozzini, M Trotta*, V Capriati, R Caliandro "Introducing Protein Crystallization in Hydrated Deep Eutectic Solvents" *ACS Sustainable Chem. Eng.* 9, 25, 8435-8449, 2021. *Note: corresponding author.*
- M Catto, L Pisani, E de la Mora, BD Belviso, GF Mangiatordi, A Pinto, A De Palma, N Denora, R Caliandro, J-P Colletier, I Silman, O Nicolotti, CD Altomare "Chiral Separation, X-ray Structure, and Biological Evaluation of a Potent and Reversible Dual Binding Site AChE Inhibitor" *Medicinal Chemistry Letters*, 5, 869-876, 2020.
- R Caliandro, 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, 1104-1118, 2019. *Note: corresponding author*
- A Lasorsa, MI Nardella, A Rosato, V Mirabelli, R Caliandro, R Caliandro, 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". The press release is also reported in the journal "Nuove Direzioni" 57 (2020), at pag 73.*
- MI Nardella, A Rosato, BD Belviso, R Caliandro, G Natile, F Arnesano "Oxidation of Human Copper Chaperone Atox1 and Disulfide Bond Cleavage by Cisplatin and Glutathione" *Int. J. Mol. Sciences* 20, 4390, 2019.
- R Caliandro, V Toson, L Palin, E Conterposito, M Aceto, V. Giannotti, E Boccaleri, E Dooryhee, M Milanesio "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 Caliandro, SM Salehi, G Di Profio, R Caliandro "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 Caliandro, 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 Caliandro, 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 Conterposito, L Palin, R Caliandro, W van Beek, D Chernyshov, M. Milanese “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 Caliandro, 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 Caliandro “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 Caliandro, 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 Milanese, 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 Milanese, 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.*
- GL Tiscia, G Favuzzi, MR Lupone, F Cappucci, M Schiavulli, V Mirabelli, G D’Andrea, E Chinni, N Giuliani, R Caliandro, E Grandone “Factor XI gene variants in factor XI-deficient patients of Southern Italy: identification of a novel mutation and genotype-phenotype relationship” *Human Genome Variation* 4, UNSP 17043, 2017.
- A Carrieri, E Lacivita, BD Belviso, R Caliandro, P Mastroianni, V Gallo, M Niso, M Leopoldo, “Structural Determinants in the Binding of BB2 Receptor Ligands: In Silico, X-Ray and NMR Studies in PD176252 Analogues” *Current Topics Med. Chem.* 17, 1599-1610, 2017.

Awards won:

- national academic qualification to associate professor in Applied Physics (02/D1), got in 2020.
- appointed in the triad of suitable candidates for the direction of the Institute of Crystallography of the CNR (prot. n 0074743 of 23/11/2020- call n.390.365).
- selective procedure for a salary upgrade for CNR researchers (call CNR n.364.174 in 2019);
- national academic qualification to associate professor in Molecular Biology (05/E2), got in 2014.
- 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;
- poster prize for the session "advanced materials" of the Conference of the Department of Chemical Sciences and Materials Technologies of CNR, held in Bressanone (28-30 October 2019),
- certificate of appreciation from ACS Publications in February 2013, awarded for the success of the book Powder Diffraction Theory and Practice, edited by R.E. Dinnebier and S.J.L. Billinge, RSC Publishing (2008), to which he contributed with the chapter Crystal Structure Determination p.227-261, and for the refereeing activity carried out for newspapers published by ACS Publications.
- poster prize at the "2011 Meeting of the Swiss Crystallographic Association", held in Bern (16 September 2012).

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 Novembre 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.

New protein crystal structures determined:

- 7ZC3: Crystal structure of human copper chaperone Atox1 bound to zinc ion by CxxC motif
- 7BB1: Lysozyme crystallized in the presence of the hydrated deep eutectic solvent Choline chloride-Glutamic acid 2:1.
- 7BAZ: Lysozyme crystallized in the presence of the hydrated deep eutectic solvent Choline chloride-Glycerol 1:2.
- 7B9J: Lysozyme crystallized in the presence of the hydrated deep eutectic solvent Choline chloride-Urea 1:2.
- 7OBF: Crystal structure of the human VH antibody domain HEL4.
- 6TT0: Crystal structure of a potent and reversible dual binding site Acetylcholinesterase chiral inhibitor.

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.

Keynote speeches:

"Protein crystallization in hydrogel composite membranes and deep eutectic solvents "Fifth Meeting of the Italian and Spanish Crystallographic Associations", Naples (4-7 September 2019).
 "New methods and applications for in situ characterization of structural dynamics", 3rd Joint AIC-SILS Conference, Rome (25-28 June 2018).
 "Methods for extracting and combining information from different datasets" 29th European Crystallographic Meeting, Rovinj, Croatia (23-28 August 2015).

Invited talks:

"Structural basis of metal ion trafficking in lysosome" at the 3rd International Online Conference on Crystals (15-30 January 2022).
 "Multivariate analysis of X-ray diffraction and XAFS data" at the XXV General Assembly and Congress of the International Union of Crystallography, Prague (14-22 August 2021).
 "Enzymes and advanced materials for active food packaging" at the 3rd International Conference on Food & Beverage Packaging, Rome (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 Staletti (CZ), (23-24 September 2007).

Invited seminars in the last 5 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).

Chaired sessions:

- the session devoted to the Cool & hot structures- Difficult Cases – Disordered Proteins of the 2nd meeting of the Biological Macromolecules Section of the Italian Crystallographic Association, held online (7-9 June 2021);
- 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).

Organized congresses:

- the 3rd meeting of the Biological Macromolecules Section of the Italian Crystallographic Association, held in Fiesole (FI) (23-24 May 2022);
- the 2nd meeting of the Biological Macromolecules Section of the Italian Crystallographic Association, held online (7-9 June 2021);
- the 1st meeting of the Biological Macromolecules Section of the Italian Crystallographic Association, held in Fiesole (FI) (20-21 February 2020);
- 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 REtrivial”, 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.

Teaching activities:

Protein Crystallography at the degree course of Medical Biotechnology of the University of Bari, starting from 2013 (few hours per year).

Crystallography at the European School of Medicinal Chemistry in 2012, at the school "Crystallography beyond diffraction", organized by the Italian Crystallographic Association in 2013, at the 4th European Crystallography School in 2017, at the school "From Gene to Protein Crystal Structure" in 2020.

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.

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)

Advisor 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.

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).

Tutor of the post-graduate internship of Dr.Valentina Mirabelli funded by Italia lavoro S.p.A. (January-July 2014).

**TRATTAMENTO DEI DATI PERSONALI,
INFORMATIVA E CONSENSO**

Il D.Lgs. 30/6/2003, n. 196 "*Codice in materia di protezione dei dati personali*" regola il trattamento dei dati personali, con particolare riferimento alla riservatezza, all'identità personale e al diritto di protezione dei dati personali; l'interessato deve essere previamente informato del trattamento. La norma in considerazione intende come "trattamento" qualunque operazione o complesso di operazioni concernenti la raccolta, la registrazione, l'organizzazione, la conservazione, la consultazione, l'elaborazione, la modifica, la selezione, l'estrazione, il raffronto, l'utilizzo, l'interconnessione, il blocco, la comunicazione, la diffusione, la cancellazione e la distruzione di dati, anche se non registrati in una banca dati. In relazione a quanto riportato, autorizzo il CNR al trattamento dei dati contenuti nel presente *curriculum vitae* e nella documentazione della quale fa parte integrante

(*barrare la casella*) Sì, acconsento