BENEDETTA CARROZZINI

PROFESSIONAL PROFILE

Researcher (full time / permanent position) at

Institute of Crystallography (IC) - National Research Council (CNR)

WORK EXPERIENCE

Research Unit Leader, **01/2009 - current**
Institute of Crystallography - CNR - Bari, Ba
Development and application of crystallographic methodologies on single crystal diffraction data (X-ray and electrons), for the structure solution of compounds of different nature and complexity (from small molecules up to proteins).
(2009-2014: PM.P01.024.002 ; 2015- : DCM.AD003.082.001)

Researcher, **02/2001 - current**
Institute of Crystallography - CNR - Bari, Ba
Development and implementation in crystallographic automatic software of innovative methodologies (theories and computing algorithms) for the characterization of crystalline materials of different composition and structural complexity, *via* single crystal (or powder) diffraction data.

EDUCATION AND TRAINING

Visiting Scientist, Crystallography
Kyungpook National University (KNU) - Daegu, South Korea
Research activity: Development of new inhibitors for epigenetic cancer therapy. Supervisor: Prof. E. di Luccio;
activity period: Oct. 2016

Advanced Training Course, Crystallography
Fondazione E. Majorana & IUCR - Erice
International School of Crystallography: "Electron Crystallography: New Methods to Explore Structure and Properties of the Nano World"; activity period: 2-12/6/2011.

Advanced Training Course (CNR Projet), Crystallography
IBB-CNR - Napoli
Course: "Use of Ab-Initio, Molecular Replacement and SAD / MAD techniques for the resolution of protein structures: study of new algorithms"; Teachers: M.Saviano, R. Berisio, L. Vitaliano;
activity period: 7-11/3/2005; 26-29/6/2006.

Visiting Scientist, Crystallography
IRMEC- CNR - Bari
Research activity: Development of crystallographic methodologies and implementation of new algorithms in software for automatic calculation Supervisor: Prof. C. Giacovazzo;
activity period: Jun. 1997 - Feb. 2001

CONTACTS

Address: Istituto di Cristallografia - Via G. Amendola 122/o, 70126, Bari, Ba

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Birth date: 01/05/1965

PERSONAL SKILLS

- Development of innovative methodologies aimed at improving the solution process of materials with chemical composition and structural complexity (from small organic or inorganic molecules up to nucleic acids and proteins).
- Implementation of the new theories and related algorithms in modern software for crystallographic computing, devoted to the automatic structure solution *via* diffraction data (X-rays or electrons) from single crystal.
- Analysis of experimental data aimed at the structure determination of small compounds and macromolecules.

The results of the research activity are reported in more than 85 publications in international

CNR Fellowship, Crystallography
IRMEC-CNR - Bari
Training and research activities: “Crystallographic Methodologies applied to Earth Sciences”. Supervisor: Prof. C. Giacovazzo; activity period: Jun. 1996 - June 1997

CNR Fellowship, Crystallography
IRMEC-CNR - Bari
Training and research activities: “Diffraction Techniques and Crystallographic Methodologies applied to Earth Sciences”. Supervisor: Prof. C. Giacovazzo; activity period: Mar. 1995 - Feb. 1996

Post-Doc Fellowship, **Earth Sciences**
Bari University - Geology and Geophysics Dept.
Research activity: “Mineralogical study of carbonate phases of the Montalbano Jonico section”. Supervisor: Prof. N. Ciaranfi; activity period: May. 1993 - dec. 1994

PhD Diploma, **Earth Sciences**
Bari University - Geominaralogical Dept.
Thesis: “Crystal chemistry and experimental alteration of ilvaites”. Supervisor: Prof. C.L. Garavelli; activity period: Nov. 1988 - Oct. 1991
National Qualification: 27/7/1992

Degree, **Geological Sciences**
Bari University - Geominaralogical Dept.
Thesis: “Metallic minerals from Frigido (Apuan Alps)”. Supervisors: Proff. C.L. Garavelli and F. Vurro; activity period: Nov. 1982 - Jul. 1987 Thesis defense: 16/7/1987; score: 110/110 with honors

LANGUAGES

Italian: Native Language

English: B2
Advanced intermediate

RESEARCH PROJECTS

Research Project: MUR – PNR 2015-2020
“*Development of functional foods for the innovation of traditional Italian food products (ALIFUN)”.*
IC-CNR Leader: R. Caliandro; activity period: Gen. 2022 - Dec. 2023.

Bilateral Research Project: CNR – Royal Society (UK)
“*Bioremediation of aflatoxins by DypB: towards a full understanding of the reaction mechanism by time-resolved structural investigations*”.
IC-CNR Leader: B.D. Belviso; activity period: Gen. 2021 - Dec. 2022

Research Project: PON "R&I" 2014-2020
“*Innovative Devices For SHAping the RIsk of Diabetes (IDF SHARID)”.* Project Leader: M. Saviano; activity period: Apr. 2018 - Oct. 2022.

scientific journals (Scopus H-index = 21) and attested by various communications at conferences and meetings (national and international) and by participation, as a teacher, in training schools and workshops (often being a member of the respective scientific and organizing committees).

Research Project: H2020 – PON2014/2020 "*Study, design and development of an innovative kit for the early and non-invasive diagnosis of celiac disease using genetic markers*".
Project Leader: M. Saviano; activity period: Gen. 2017- Dec. 2020.

European Research Project H2020-FET Open-RIA.

"*Revolutionizing Downstream Processing of Monoclonal Antibodies by Continuous Template-Assisted Membrane Crystallization (AMECRYS)*",
Grant no. 712965. IC-CNR Leader: R. Caliandro - Communication & dissemination WorkTask Leader: B. Carrozzini; activity period: Oct. 2016 - Mar. 2021.

Bilateral Research Project: CNR - National Research Foundation of Korea (NRF) *"Static and dynamic crystallographic investigations for developing new inhibitors for the epigenetic therapy of cancers"*.
IC-CNR Leader: R. Caliandro. activity period: Gen. 2016 – Dec. 2017.

Bilateral Research Project: CNR - Polish Academy of Sciences (PAS) "*New algorithms for protein dynamic studies and their application to protein crystallography*".
IC-CNR Leader: R. Caliandro. activity period: Gen. 2014 - Dec. 2016.

Research Project: Fondazione CON IL SUD (2011-PDR-20)
"*Towards Personalized Medicine: development of new selective molecules for the treatment of Neuroblastoma*". Project Leader: M. Saviano; activity period: Oct. 2012 - Sept. 2015.

Research Project: MIUR "*Global Phasing: from powders to macromolecules*". Project Leader: C. Giacovazzo. activity period: May 2004 - Jul. 2007.

ASSOCIATIONS, COMMISSIONS AND COMMITTEES

Crystallographic Computing Commission dell'International Union of Crystallography (IUCr): Effective Member (2008-2011); Consultant (2011-2018)

Member of the International Union of Crystallography (IUCr)

Member of the European Crystallographic Association (ECA)

Member of the Italian Crystallographic Association (AIC)

Chair of the MS6: "*Frontiers in Methods and Techniques for crystal structure characterization" at the XLIX AIC National Conference*, 6-9/9/2021, Parma, Italy.

Member of the Scientific and Organizing Committees: *International EXPO/SIR workshop 2014*.10-13/6/2014, Bari, Italy

Member of the Scientific and Organizing Committees: *PHARE2009: a modular workshop on global PHAse Retrivial.* 15–24/4/2009, Martina Franca (Ta), Italy

Member of the Organizing Committee: *1st Precession Electron Diffraction User Meeting*. 8-9/5/2008, Martina Franca (Ta), Italy

Member of the Organizing Committee: *PHABIO: PHAsing BIOlogical macromolecules*. 23-27/6/2001, Martina Franca (Ta), Italy

Member of the Organizing Committee: *XXX AIC National Conference*. 19-22/9/2000, Martina Franca (Ta), Italy.

Member of the Organizing Committee: *The fifth SIR Workshop: SIRWARE.96 – Single Crystal and Powder Data; X-Rays, Neutrons and Electrons*. 17-20/12/1996, Bari, Italy

TEACHING AND LECTURES

TEACHING:

PCTO Course Teacher (12h): *Crystallography: the secrets of thr powerful microscope* (Liceo Scientifico IISS Marconi-Hack, 3rd class), Bari, Italy. activity period: March-June 2022.

Workshop Teacher (30h): *1st Brazilian Hands-on Workshop: SIR/EXPO 2014*. 3-7/11/2014, Sao Carlos, Brazil.

Workshop Teacher (20h): *International EXPO/SIR workshop 2014.* 10-13/6/2014, Bari, Italy

Workshop Teacher (20h): *PHARE2009: a modular workshop on global PHAse Retrivial.* 15–24/4/2009, Martina Franca (Ta), Italy

Practical Session Teacher (80h): Mineralogy and Crystallography courses (Chemistry Degree and Material Sciences Degree), Bari University. Course Holder: Prof. C. Giacovazzo; activity period: 1996-2009.

AIC2002 School Teacher (2h): *The Phase Problem in Crystallography: Theory and Applications*. 23-24/9/2002, Bressanone, Italy

Euroconference Teacher (20h): *PHABIO: PHAsing BIOlogical macromolecules*. 23-27/6/2001, Martina Franca (Ta), Italy.

AIC1998 School Teacher (4h): *Diffractomety from polycrystalline materials: recent developments in structure solution and refimente techniquies*. 8-12/9/1998, Perugia, Italy.

Workshop Teacher (20h): *The fifth SIR Workshop: SIRWARE.96 – Single Crystal and Powder Data; X-Rays, Neutrons and Electrons*. 17-20/12/1996, Bari, Italy

Course Teacher (10h): *Training for Specialists in Historic Settlements Recovery* (promoted by Basilicata Regione), Matera, Italy. Course Director: Prof. S. Lorenzoni; activity period: March-June 1995.

SCIENTIFIC COMMUNICATIONS (since 2015 -) :

Invited Lecture: Structural characterization of crystalline materials (with different complexity) by Single-Crystal Diffraction Analysis - *IC-ICB Workshop* (Webinar, 10/3/2022)

Invited Lecture: The Sir Program - *XLVI Congresso Nazionale AIC* (software fayre) – Perugia (Italy), 26-29/6/2017.

Invited Lecture: Advances in Methods for Macromolecular Structure Solution: Ab Initio and MR Approaches - International

Joint Seminar: *KNU Creative BioResearch Group & Advanced Bio-resource Research Center* – Daegu (S. Korea), 27/10/2016.

Invited Lecture (Key Note): Advances in Methods for Macromolecular Structure Solution:Ab Initio and MR Approaches - *XLIV Congresso Nazionale AIC* – Vercelli (Italy), 14-17/9/2015.

DEPOSITATED STRUCTURES

Protein Data Bank (PDB)

7OBF: Crystal structure of the human VH antibody domain HEL4 - Belviso, B.D., Caliandro, R., Carrozzini, B. - DOI: 10.2210/pdb7OBF/pdb - Deposited: 22/04/2021; Released: 05/05/2021

7B9J: Lysozyme crystallized in the presence of the hydrated deep eutectic solvent Choline chloride-Urea 2:1 - Belviso, B.D., Caliandro, R., Carrozzini, B. - DOI: 10.2210/pdb7B9J/pdb - Deposited: 16/12/2020; Released: 20/10/2021

7BAZ: Lysozyme crystallized in the presence of the hydrated deep eutectic solvent Choline chloride-Glicerol 1:2 - Belviso, B.D., Caliandro, R., Carrozzini, B. - DOI: 10.2210/pdb7BAZ/pdb - Deposited: 16/12/2020; Released: 20/10/2021

7BB1: Lysozyme crystallized in the presence of the hydrated deep eutectic solvent Choline chloride-Glutamic acid 2:1 - Belviso, B.D., Caliandro, R., Carrozzini, B. - DOI: 10.2210/pdb7BB1/pdb - Deposited: 16/12/2020; Released: 20/10/2021

5H6Z: Crystal structure of Set7, a novel histone methyltransferase in Schizossacharomycespombe - Mevius, D.E.H.F., Shen, Y., Morishita, M., Carrozzini, B., Caliandro, R., Luccio, E.D. - DOI: 10.2210/pdb5H6Z/pdb - Deposited: 15/11/2016; Released: 22/11/2017

5WW0: Crystal structure of Set7, a novelhistonemethyltransferase in Schizossacharomycespombe - Mevius, D.E.H.F., Shen, Y., Morishita, M., Carrozzini, B., Caliandro, R., Luccio, E.D. - DOI: 10.2210/pdb5WWO/pdb - Deposited: 30/12/2016; Released: 06/12/2017

6TOV: Crystal structure of Teicoplanin Aglycone - Belviso, B.D., Carrozzini, B., Caliandro, R., Altomare, C.D., Bolognino, I., Cellamare, S. - DOI: 10.2210/pdb6TOV/pdb – Deposited: 12/12/2019; Released: 15/01/2020

Cambridge Crystallographic Data Centre (CCDC)

EFISIY: CCDC 1468879: Experimental Crystal Structure Determination, Deposited 02/08/2018, DOI: 10.5517/ccdc.csd.cc1l9h6l – Carrozzini B., Belviso B.D., Bruno C., Cavalluzzi M.M., Lovece A., Lentini G., Caliandro R., Journal of Chemical Crystallography, 2019, 49, 87, DOI: 10.1007/s10870-018-0739-x

ATOGAT: CCDC 1430059: Experimental Crystal Structure Determination, Deposited 09/03/2016, DOI:

10.5517/ccdc.csd.cc1k02yl - Dell'Anna M.M., Censi V., Carrozzini B., Caliandro R., Denora N., Franco M., Veclani D., Melchior A., Tolazzi M., Mastrorilli P., Journal of Inorganic Biochemistry, 2016, 163, 346, DOI: 10.1016/j.jinorgbio.2016.08.006

ATOGEX: CCDC 1430058: Experimental Crystal Structure Determination, Deposited 09/03/2016, DOI: 10.5517/ccdc.csd.cc1k02xk - Dell'Anna M.M., Censi V., Carrozzini B., Caliandro R., Denora N., Franco M., Veclani D., Melchior A., Tolazzi M., Mastrorilli P., Journal of Inorganic Biochemistry, 2016, 163, 346, DOI: 10.1016/j.jinorgbio.2016.08.006

IYUKAQ: CCDC 1430050: Experimental Crystal Structure Determination, Deposited 07/10/2015, DOI: 10.5517/ccdc.csd.cc1k02xk1430050 - Dell'Anna M.M., Censi V., Carrozzini B., Caliandro R., Denora N., Franco M., Veclani D., Melchior A., Tolazzi M., Mastrorilli P., Journal of Inorganic Biochemistry, 2016, 163, 346, DOI: 10.1016/j.jinorgbio.2016.08.006

CRYSTALLOGRAPHIC SOFTWARE

Dr. Carrozzini is co-author (and main developer) of crystallographic software for the automatic solution of small, medium and large structures (proteins or nucleic acids), using single crystal (o powder) diffraction data (X-rays or electrons) form cristallo singolo.
The software is widely and profitably used by the international scientific community in thousands of laboratories in around the world. (Number of Citations from SCOPUS, as of 20/9/2022)

Sir2014/19: Burla M.C., Caliandro R., Carrozzini B., Cascarano G.L., Cuocci C., Giacovazzo C., Mallamo M., Mazzone A. & Polidori G. (2015) – Crystal structure determination and refinement *via* SIR2014- *Jour. Appl. Cryst.*, 48, 306-309. N. Cit. 578

Sir2011: Burla M.C., Caliandro R., Camalli M., Carrozzini B., Cascarano G.L., Giacovazzo C., Mazzone A., Polidori G., Siliqi D. & Spagna R. (2012) – SIR2011: a new package for crystal structure determination and refinement - *Jour. Appl. Cryst.*, 45, 357-361. N. Cit. 499

Software and Know-How License Agreement between DPM-CNR and RIGAKU Corporation for royalties' payment (by RIGAKU to CNR) for each non-exclusive license per each SIR2011 sale (validity period: March 2012- March 2016)

Il Milione: Burla M.C., Caliandro R., Camalli M., Carrozzini B., Cascarano G.L., De Caro L., Giacovazzo C., Polidori G., Siliqi D. & Spagna R. (2007) – *Il Milione*: a suite of computer programs for crystal structure solution of proteins - *Jour. Appl. Cryst.*, 40, 609-613. N. Cit. 605

Sir2004: Burla M.C., Caliandro R., Camalli M., Carrozzini B., Cascarano G.L., De Caro L., Giacovazzo C., Polidori G. & Spagna R. (2005) – SIR2004: an improved tool for crystal structure determination and refinement - *Jour. Appl. Cryst.*, 38, 381-388. n. Cit. 2489

Sir2002: Burla M.C., Carrozzini B., Cascarano G.L., Giacovazzo C. & Polidori G. (2002) – More power for Direct Methods: *SIR2002 – Zeit. Kristall.*, 217, 629-635. (Special Issue on *Direct Methods for Macromolecular Crystallography*). N. Cit. 62

Expo: Altomare A., Burla M.C., Camalli M., Carrozzini B., Cascarano G.L., Giacovazzo C., Guagliardi a., Moliterni A.G.G., Polidori G. & Rizzi R. (1999) - *EXPO*: a program for full powder pattern decomposition and crystal structure solution - *Jour. Appl. Cryst.,* 32, 339-340. N. Cit. 449

PUBBLICAZIONI

ARTICLES (since 2015 -):

1. Belviso B.D., Mangiatordi G.F., Alberga D., Mangini V., Carrozzini B. & Caliandro R. (2022) - Structural Characterization of the Full-Length Anti-CD20 Antibody Rituximab, *Front. Mol. Biosci.*, 9, 823174.

2. Bolognino I., Carrieri A., Purgatorio R., Catto M., Caliandro R., Carrozzini B., Belviso B.D., Majellaro M., Sotelo E., Cellamare S. & Altomare C.D. (2022) - Enantiomeric Separation and Molecular Modelling of Bioactive 4-Aryl-3,4-dihydropyrimidin-2(1H)-one Ester Derivatives on Teicoplanin-Based Chiral Stationary Phase, *Separations*, 9, 7.

3. Belviso, B.D., Perna, F.M., Carrozzini, B., Trotta, M., Capriati, V. & Caliandro, R. (2021) - Introducing Protein Crystallization in Hydrated Deep Eutectic Solvents, *ACS Sustain. Chem. Eng.* 9, 8435-8449.

4. Burla M.C., Carrozzini B., Cascarano G.L., Giacovazzo C. & Polidori G. (2020) – Properties of fourier syntheses and new syntheses - *Crystals*, 10, 538.

5. Burla M.C., Carrozzini B., Cascarano G.L., Giacovazzo C. & Polidori G. (2020) – Cyclic automated model building (CAB) applied to nucleic acids - *Crystals*, 10, 280.

6. Burla M.C., Carrozzini B., Cascarano G.L., Giacovazzo C. & Polidori G. (2020) – How far are we from automatic crystal structure solution via molecular-replacement techniques? - *Acta Cryst.,* D76, 9-18.

7. Shen Y., Mevius D., Caliandro R., Carrozzini B., Roh Y., Kim J., Kim S., Ha S.C., Morishita M. & Eric di Luccio (2019) - Set7 is a Novel H3k37 Methyltransferase in Schizosaccharomyces Pombe and Required for Proper Gametogenesis – *Structure* 27, 631-638.

8. Carrozzini B., Belviso B.D., Bruno C., Cavalluzzi M.M., Lovece A., Lentini G. & Caliandro R. (2019) - The crystal structure of *N*-[(2*E*)-3-(4-chlorophenyl)prop-2-en-1-yl]-4-methoxy-*N*-methylbenzenesulfonamide – *J. Chem. Crystallogr.* 49, 87-91.

9. Burla M.C., Carrozzini B., Cascarano G.L., Giacovazzo C. & Polidori G. (2018) – CAB, a cyclic automatic model building procedure - *Acta Cryst.* D74, 1096-1104.

10. Italiano F., Agostiano A., Belviso B.D., Caliandro R., Carrozzini B., Comparelli R., Melillo M.T., Mesto E. Tempesta G. & Trotta M. (2018) - Interaction between the photosynthetic anoxygenic microorganism Rhodobacter sphaeroides and soluble gold compounds. From toxicity to gold nanoparticle synthesis – *Colloids Surf. B*, 172, 362-371.

11. Giacovazzo C., Carrozzini B. & Cascarano G.L. (2018) - Probabilistic Estimate of |Foa| from FEL Data - *Crystals*, 8, 175-185.

12. Burla M.C., Carrozzini B., Cascarano G.L., Giacovazzo C. & Polidori G. (2018) - Phasing *via* pure crystallographic least squares: an unexpected feature - *Acta Cryst.*, A74, 123-130.

13. Burla M.C., Carrozzini B., Cascarano G.L., Giacovazzo C. & Polidori G. (2017) - About difference electron densities and their properties - *Acta Cryst.*, A73, 460-473.

14. Burla M.C., Carrozzini B., Cascarano G.L., Giacovazzo C. & Polidori G. (2017) - Solving proteins at non-atomic resolution by Direct Methods: update - *Jour. Appl. Cryst.*, 50, 1048-1055.

15. Burla M.C., Carrozzini B., Cascarano G.L., Giacovazzo C. & Polidori G. (2017) – MPF, a multipurpose FOM for phasing procedures - *Acta Cryst.*, A73, 69-76.

16. Dell'Anna M.M., Censi V., Carrozzini B., Caliandro R., Denora N., Franco M., Veclani D., Melchior A., Tolazzi M. & Mastrorilli P. (2016) – Triphenylphosphane Pt(II) complexes containing biologically active natural polyphenols: Synthesis, crystal structure, molecular modeling and cytotoxic studies – *J. Inorg. Biochem.,* 163, 346-361.

17. Carrozzini B., Cascarano G.L. & Giacovazzo C. (2016) – Phase improvement *via* the *Phantom Derivative* technique: ancils that are related to the target structure - *Acta Cryst.*, D72, 551-557.

18. Burla M.C., Carrozzini B., Cascarano G.L., Giacovazzo C. & Polidori G. (2015) – Solving protein at non-atomic resolution by Direct Methods- *Jour. Appl. Cryst.*, 48, 1692-1698.

19. Burla M.C., Carrozzini B., Cascarano G.L., Giacovazzo C. & Polidori G. (2015) – Refining a model electron-density map *via* the *Phantom Derivative* method - *Acta Cryst.*, D71, 1864-1871.

20. Carrozzini B., Cascarano G.L., Giacovazzo C. & Mazzone A. (2015) – Advances in molecular-replacement procedures: the REVAN pipeline - *Acta Cryst.*, D71, 1856-1863.

21. Burla M.C., Caliandro R., Carrozzini B., Cascarano G.L., Cuocci C., Giacovazzo C., Mallamo M., Mazzone A. & Polidori G. (2015) – Crystal structure determination and refinement *via* SIR2014- *Jour. Appl. Cryst.*, 48, 306-309.

BOOK CHAPTERS:

1. Caliandro R., Carrozzini B. & Mazzone A. (2012) – Phasing Methods in Crystallography: Theory and Applications – in: *Crystallography: Research, Technology and Applications* (Ed. by

Hokkaido & Nagano), Nova Science Publishers, NY (USA) pp. 1-30. ISBN 978-1-62081-574-8

2. Giacovazzo C., Altomare A., Burla M.C., Carrozzini B., Cascarano G.L., Guagliardi A., Moliterni A.G.G., Polidori G. & Rizzi R. (2002) - Direct Methods in powder diffraction – applications – In: *Structure Determination from Powder Diffraction Data*, Edited by David W.I.F., Shankland K.. McCusker L.B., Baerlocher C., IUCr Monographs in Crystallography n.13, Oxford University Press ISBN 0-19-850091-2

For the complete list of publications, please see:
https://scholar.google.com/citations?hl=it&user=fXFl3dIAAAAJ