

# Benedetta Carrozzini

## List of Publications by Year in descending order

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85

papers

6,915

citations

304743

22

h-index

76900

74

g-index

86

all docs

86

docs citations

86

times ranked

6940

citing authors

#	ARTICLE	IF	CITATIONS
1	Enantiomeric Separation and Molecular Modelling of Bioactive 4-Aryl-3,4-dihydropyrimidin-2(1H)-one Ester Derivatives on Teicoplanin-Based Chiral Stationary Phase. <i>Separations</i> , 2022, 9, 7.	2.4	3
2	Introducing Protein Crystallization in Hydrated Deep Eutectic Solvents. <i>ACS Sustainable Chemistry and Engineering</i> , 2021, 9, 8435-8449.	6.7	26
3	Properties of Fourier Syntheses and New Syntheses. <i>Crystals</i> , 2020, 10, 538.	2.2	1
4	Cyclic Automated Model Building (CAB) Applied to Nucleic Acids. <i>Crystals</i> , 2020, 10, 280.	2.2	3
5	How far are we from automatic crystal structure solution via molecular-replacement techniques?. <i>Acta Crystallographica Section D: Structural Biology</i> , 2020, 76, 9-18.	2.3	3
6	Set7 Is a H3K37 Methyltransferase in <i>Schizosaccharomyces pombe</i> and Is Required for Proper Gametogenesis. <i>Structure</i> , 2019, 27, 631-638.e8.	3.3	8
7	The Crystal Structure of N-[(2E)-3-(4-Chlorophenyl)prop-2-en-1-yl]-4-methoxy-N-methylbenzenesulfonamide. <i>Journal of Chemical Crystallography</i> , 2019, 49, 87-91.	1.1	2
8	Phasingviapure crystallographic least squares: an unexpected feature. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2018, 74, 123-130.	0.1	0
9	CAB: a cyclic automatic model-building procedure. <i>Acta Crystallographica Section D: Structural Biology</i> , 2018, 74, 1096-1104.	2.3	5
10	Probabilistic Estimate of  F <sub>oa</sub>   from FEL Data. <i>Crystals</i> , 2018, 8, 175.	2.2	0
11	Interaction between the photosynthetic anoxygenic microorganism Rhodobacter sphaeroides and soluble gold compounds. From toxicity to gold nanoparticle synthesis. <i>Colloids and Surfaces B: Biointerfaces</i> , 2018, 172, 362-371.	5.0	18
12	About difference electron densities and their properties. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2017, 73, 460-473.	0.1	3
13	Solving proteins at non-atomic resolution by direct methods: update. <i>Journal of Applied Crystallography</i> , 2017, 50, 1048-1055.	4.5	6
14	MPF, a multipurpose figure of merit for phasing procedures. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2017, 73, 69-76.	0.1	1
15	Phase improvementviathePhantom Derivative technique: ancils that are related to the target structure. <i>Acta Crystallographica Section D: Structural Biology</i> , 2016, 72, 551-557.	2.3	9
16	Triphenylphosphane Pt(II) complexes containing biologically active natural polyphenols: Synthesis, crystal structure, molecular modeling and cytotoxic studies. <i>Journal of Inorganic Biochemistry</i> , 2016, 163, 346-361.	3.5	24
17	Crystal structure determination and refinement <i>&lt; i&gt;via&lt;/i&gt;&lt; i&gt;SIR2014&lt;/i&gt;</i> . <i>Journal of Applied Crystallography</i> , 2015, 48, 306-309.	4.5	729
18	Refining a model electron-density mapviathePhantom Derivative method. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2015, 71, 1864-1871.	2.5	5

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19	Advances in molecular-replacement procedures: theREVANpipeline. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2015, 71, 1856-1863.	2.5	8
20	Solving proteins at non-atomic resolution by direct methods. <i>Journal of Applied Crystallography</i> , 2015, 48, 1692-1698.	4.5	9
21	Protein phasing at non-atomic resolution by combining Patterson and <i>VLD</i> techniques. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2014, 70, 1994-2006.	2.5	9
22	On the use of the <i>C</i> map in Patterson deconvolution procedures. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2013, 69, 98-107.	0.3	6
23	The use of <i>VLD</i> (vive la difference) in the molecular-replacement approach: a pipeline. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013, 69, 1038-1044.	2.5	8
24	Cobalt binding in the photosynthetic bacterium <i>R. sphaeroides</i> by X-ray absorption spectroscopy. <i>BioMetals</i> , 2013, 26, 693-703.	4.1	9
25	A new interpretation of the $\text{f}_{\text{i}}$ parameter. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2013, 69, 408-412.	0.3	4
26	About the first <i>VLD</i> (Vive La Difference) applications. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2013, 69, s182-s183.	0.3	0
27	New features inSIR2011. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2013, 69, s267-s267.	0.3	0
28	VLD algorithm and hybrid Fourier syntheses. <i>Journal of Applied Crystallography</i> , 2012, 45, 1287-1294.	4.5	19
29	<i>SIR2011</i> : a new package for crystal structure determination and refinement. <i>Journal of Applied Crystallography</i> , 2012, 45, 357-361.	4.5	538
30	Automated determination of the extinction symbol via electron diffraction data. <i>Journal of Applied Crystallography</i> , 2012, 45, 351-356.	4.5	48
31	Estimates of triplet invariants given a model structure. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2012, 68, 513-520.	0.3	7
32	Advances in the VLD algorithm. <i>Journal of Applied Crystallography</i> , 2011, 44, 1143-1151.	4.5	23
33	About the hybrid Fourier syntheses: a probabilistic approach. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2011, 67, 447-455.	0.3	3
34	From <i>Sir2008</i> to <i>Sir2011</i> : the role of electron diffraction. <i>Crystal Research and Technology</i> , 2011, 46, 555-560.	1.3	6
35	Crystal structure solution via precession electron diffraction data: The BEA algorithm. <i>Ultramicroscopy</i> , 2010, 111, 56-61.	1.9	11
36	The cross-correlation function: main properties and first applications. <i>Journal of Applied Crystallography</i> , 2010, 43, 221-226.	4.5	5

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37	New computational tools for H/D determination in macromolecular structures from neutron data. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2010, 66, 1164-1171.	2.5	0
38	Crystal structure solution via precession electron diffraction data: the BEA algorithm. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2010, 66, s65-s66.	0.3	0
39	Molecular replacement: the probabilistic approach of the program <i>REMO09</i> and its applications. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2009, 65, 512-527.	0.3	26
40	Advances in the EDMâ€“DEDM procedure. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2009, 65, 249-256.	2.5	7
41	EDMâ€“DEDM and protein crystal structure solution. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2009, 65, 477-484.	2.5	9
42	Crystal structure solution of small-to-medium-sized molecules at non-atomic resolution. <i>Journal of Applied Crystallography</i> , 2009, 42, 302-307.	4.5	9
43	DEA: the combination of the DEDM-EDM procedure with automatic model-building packages to solve difficult protein phasing cases. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2009, 65, s38-s39.	0.3	0
44	Molecular replacement: a new probabilistic approach. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2009, 65, s33-s33.	0.3	0
45	The ( <i>i</i> F <sub>o</sub> - <i>i</i> F <sub>c</sub> ) Fourier synthesis: a probabilistic study. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2008, 64, 519-528.	0.3	10
46	<i>Ab initio</i> phasing of proteins with heavy atoms at non-atomic resolution: pushing the size limit of solvable structures up to 7890 non-H atoms in the asymmetric unit. <i>Journal of Applied Crystallography</i> , 2008, 41, 548-553.	4.5	28
47	The revenge of the Patterson methods. II. Substructure applications. <i>Journal of Applied Crystallography</i> , 2007, 40, 211-217.	4.5	10
48	IL MILIONE: a suite of computer programs for crystal structure solution of proteins. <i>Journal of Applied Crystallography</i> , 2007, 40, 609-613.	4.5	679
49	The revenge of the Patterson methods. III. <i>Ab initio</i> phasing from powder diffraction data. <i>Journal of Applied Crystallography</i> , 2007, 40, 834-840.	4.5	8
50	Advances in the free lunch method. <i>Journal of Applied Crystallography</i> , 2007, 40, 931-937.	4.5	24
51	Advances in <i>ab initio</i> protein phasing by Patterson deconvolution techniques. <i>Journal of Applied Crystallography</i> , 2007, 40, 883-890.	4.5	22
52	Molecular replacement: the approach of the program REMO. <i>Journal of Applied Crystallography</i> , 2006, 39, 185-193.	4.5	21
53	The revenge of the Patterson methods. I. Protein <i>ab initio</i> phasing. <i>Journal of Applied Crystallography</i> , 2006, 39, 527-535.	4.5	25
54	Use of Patterson-based methods automatically to determine the structures of heavy-atom-containing proteins with up to 6000 non-hydrogen atoms in the asymmetric unit. <i>Journal of Applied Crystallography</i> , 2006, 39, 728-734.	4.5	17

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55	Direct methods in powder diffraction—“applications. , 2006, , 190-201.	0	
56	The partial structure with errors: a probabilistic treatment. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2005, 61, 343-349.	0.3	26
57	Phasing at resolution higher than the experimental resolution. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2005, 61, 556-565.	2.5	40
58	Ab initio phasing at resolution higher than experimental resolution. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2005, 61, 1080-1087.	2.5	26
59	SIR2004: an improved tool for crystal structure determination and refinement. <i>Journal of Applied Crystallography</i> , 2005, 38, 381-388.	4.5	2,564
60	Phasing diffuse scattering. Application of the SIR2002 algorithm to the non-crystallographic phase problem. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2004, 60, 331-338.	0.3	6
61	MAD phasing: choosing the most informative wavelength combination. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2004, 60, 1683-1686.	2.5	1
62	Ab initio protein phasing: the Patterson deconvolution method in SIR2002. <i>Journal of Applied Crystallography</i> , 2004, 37, 258-264.	4.5	19
63	About the efficiency of the early FOMs in ab initio protein phasing. <i>Journal of Applied Crystallography</i> , 2004, 37, 791-801.	4.5	2
64	Benzophenone Photophore Flexibility and Proximity: Molecular and Crystal-State Structure of a Bpa-Containing Trichogin Dodecapeptide Analogue. <i>ChemBioChem</i> , 2004, 5, 541-544.	2.6	18
65	Separated and Aligned Molecular Fibres in Solid State Self-Assemblies of Cyclodextrin[2]Rotaxanes. <i>Chemistry - A European Journal</i> , 2003, 9, 5971-5977.	3.3	28
66	SIR2002: the program. <i>Journal of Applied Crystallography</i> , 2003, 36, 1103-1103.	4.5	914
67	Ab initio protein phasing at 1.4– Å resolution. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2003, 59, 245-249.	0.3	10
68	Solving non-periodic structures using direct methods: phasing diffuse scattering. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2003, 59, 255-261.	0.3	12
69	Ab initio protein phasing at 1.4– Å resolution: the new phasing approach of SIR2003-N. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2003, 59, 560-568.	0.3	9
70	SAD or MAD phasing: location of the anomalous scatterers. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2003, 59, 662-669.	2.5	8
71	More power for direct methods: SIR2002. <i>Zeitschrift Fur Kristallographie - Crystalline Materials</i> , 2002, 217, 629-635.	0.8	53
72	Phase extension to weaker reflections of proteins via a partial structure based tangent formula. <i>Zeitschrift Fur Kristallographie - Crystalline Materials</i> , 2002, 217, 139-142.	0.8	0

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73	MAD phasing: probabilistic estimate of $ F_{\alpha} $ . <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2002, 58, 928-935.	2.5	6
74	SIR2000-N, a program for large and small crystal structures. <i>Journal of Applied Crystallography</i> , 2001, 34, 523-526.	4.5	19
75	Mechanistic and stereochemical aspects of the Lewis acid mediated cleavage of $\pm$ -aminoacetals. <i>Tetrahedron Letters</i> , 2001, 42, 2865-2868.	1.4	5
76	Solving crystal structures in P1: an automated procedure for finding an allowed origin in the correct space group. <i>Journal of Applied Crystallography</i> , 2000, 33, 307-311.	4.5	27
77	SIR2000, a program for the automatical initio crystal structure solution of proteins. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2000, 56, 451-457.	0.3	38
78	EXPO: a program for full powder pattern decomposition and crystal structure solution. <i>Journal of Applied Crystallography</i> , 1999, 32, 339-340.	4.5	445
79	The probability distribution of structure factors with non-integral indices. II. The $P1\bar{A}$ case. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 1999, 55, 314-321.	0.3	4
80	The joint probability distribution function of structure factors with rational indices. VI. Cases with reduced dimensionality. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 1999, 55, 984-990.	0.3	1
81	SIR99, a program for the automatic solution of small and large crystal structures. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 1999, 55, 991-999.	0.3	24
82	Preparation, Characterization, and Activity of Cu/TiO <sub>2</sub> Catalysts. I. Influence of the Preparation Method on the Dispersion of Copper in Cu/TiO <sub>2</sub> . <i>Journal of Catalysis</i> , 1997, 165, 129-139.	6.2	138
83	Solving Crystal Structures from Powder Data. III. The Use of the Probability Distributions for Estimating the $ F $ 's. <i>Journal of Applied Crystallography</i> , 1997, 30, 92-97.	4.5	11
84	Solving Crystal Structures from Powder Data. I. The Role of the Prior Information in the Two-Stage Method. <i>Journal of Applied Crystallography</i> , 1996, 29, 667-673.	4.5	7
85	Set7 is a Novel H3k37 Methyltransferase in <i>Schizosaccharomyces Pombe</i> and Required for Proper Gametogenesis. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0