List of Publications by Year in descending order

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Hedredt Nad

#	Article	IF	CITATIONS
1	Crystal structure analysis of oxidized Pseudomonas aeruginosa azurin at pH 5·5 and pH 9·0. Journal of Molecular Biology, 1991, 221, 765-772.	4.2	571
2	A specific antidote for dabigatran: functional and structural characterization. Blood, 2013, 121, 3554-3562.	1.4	541
3	Structure-Based Design of Novel Potent Nonpeptide Thrombin Inhibitors. Journal of Medicinal Chemistry, 2002, 45, 1757-1766.	6.4	425
4	Biophysics in drug discovery: impact, challenges and opportunities. Nature Reviews Drug Discovery, 2016, 15, 679-698.	46.4	285
5	8-(3-(<i>R</i>)-Aminopiperidin-1-yl)-7-but-2-ynyl-3-methyl-1-(4-methyl-quinazolin-2-ylmethyl)-3,7-dihydropurine-2,6 (BI 1356), a Highly Potent, Selective, Long-Acting, and Orally Bioavailable DPP-4 Inhibitor for the Treatment of Type 2 Diabetes. Journal of Medicinal Chemistry, 2007, 50, 6450-6453.	-dione 6.4	254
6	X-ray Analysis and Spectroscopic Characterization of M121Q Azurin. Journal of Molecular Biology, 1993, 229, 1007-1021.	4.2	186
7	Structural basis for photo-induced protein cleavage and green-to-red conversion of fluorescent protein EosFP. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 9156-9159.	7.1	184
8	Structure-Based Design of an in Vivo Active Selective BRD9 Inhibitor. Journal of Medicinal Chemistry, 2016, 59, 4462-4475.	6.4	172
9	X-ray crystal structure of the two site-specific mutants His35Cln and His35Leu of azurin from Pseudomonas aeruginosa. Journal of Molecular Biology, 1991, 218, 427-447.	4.2	170
10	Macrocyclic Inhibitors of the NS3 Protease as Potential Therapeutic Agents of Hepatitis C Virus Infection. Angewandte Chemie - International Edition, 2003, 42, 1356-1360.	13.8	166
11	Atomic structure of GTP cyclohydrolase I. Structure, 1995, 3, 459-466.	3.3	131
12	Characterization and crystal structure of zinc azurin, a by-product of heterologous expression in Escherichia coli of Pseudomonas aeruginosa copper azurin. FEBS Journal, 1992, 205, 1123-1129.	0.2	126
13	Crystal structure ofPseudomonas aeruginosaapo-azurin at 1.85 Ã resolution. FEBS Letters, 1992, 306, 119-124.	2.8	122
14	Photoconvertible Fluorescent Protein EosFP: Biophysical Properties and Cell Biology Applications. Photochemistry and Photobiology, 2006, 82, 351.	2.5	118
15	Plasminogen activator inhibitor 1. Structure of the native serpin, comparison to its other conformers and implications for serpin inactivation. Journal of Molecular Biology, 2000, 297, 683-695.	4.2	94
16	Crystal structure analysis and refinement at 2·15à resolution of amicyanin, a type I blue copper protein, from Thiobacillus versutus. Journal of Molecular Biology, 1994, 236, 1196-1211.	4.2	83
17	Structural Basis for Inhibition Promiscuity of Dual Specific Thrombin and Factor Xa Blood Coagulation Inhibitors. Structure, 2001, 9, 29-37.	3.3	82
18	Crystal Structure of Bisphosphorylated IGF-1 Receptor Kinase. Structure, 2001, 9, 955-965.	3.3	82

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19	Crystal structure of human macrophage elastase (MMP-12) in complex with a hydroxamic acid inhibitor 1 1Edited by I. Wilson. Journal of Molecular Biology, 2001, 312, 743-751.	4.2	78
20	Structure of a CBS-domain pair from the regulatory Î ³ 1 subunit of human AMPK in complex with AMP and ZMP. Acta Crystallographica Section D: Biological Crystallography, 2007, 63, 587-596.	2.5	75
21	Crystal Structure of the Human Liver X Receptor β Ligand-binding Domain in Complex with a Synthetic Agonist. Journal of Molecular Biology, 2003, 334, 853-861.	4.2	74
22	One Target—Two Different Binding Modes: Structural Insights into Gevokizumab and Canakinumab Interactions to Interleukin-1β. Journal of Molecular Biology, 2013, 425, 94-111.	4.2	73
23	Biosynthesis of Pteridines. Reaction Mechanism of GTP Cyclohydrolase I. Journal of Molecular Biology, 2003, 326, 503-516.	4.2	70
24	6-Pyruvoyl Tetrahydropterin Synthase, An Enzyme With a Novel Type of Active Site Involving Both Zinc Binding and an Intersubunit Catalytic Triad Motif; Site-directed Mutagenesis of the Proposed Active Center, Characterization of the Metal Binding Site and Modelling of substrate Binding. Journal of Molecular Biology, 1995, 253, 358-369.	4.2	67
25	Complete sequential proton and nitrogen-15 nuclear magnetic resonance assignments and solution secondary structure of the blue copper protein azurin from Pseudomonas aeruginosa. Biochemistry, 1992, 31, 10194-10207.	2.5	65
26	Heterocyclic thrombin inhibitors. Part 2: quinoxalinone derivatives as novel, potent antithrombotic agents. Bioorganic and Medicinal Chemistry Letters, 2003, 13, 2297-2302.	2.2	65
27	X-ray Structure Determination and Characterization of the Pseudomonas aeruginosa Azurin Mutant Met121Glu,. Biochemistry, 1997, 36, 4089-4095.	2.5	63
28	Crystallographic and kinetic investigations on the mechanism of 6-pyruvoyl tetrahydropterin synthase 1 1Edited by K. Nagai. Journal of Molecular Biology, 1999, 286, 851-860.	4.2	62
29	Structural basis of inhibition of the human SGLT2–MAP17 glucose transporter. Nature, 2022, 601, 280-284.	27.8	58
30	A study of asymmetric induction during the addition of enolate nucleophiles, having sulfoximine chiral auxiliaries, to diene-molybdenum and dienyliron complexes. Journal of the American Chemical Society, 1989, 111, 134-144.	13.7	55
31	Structural Characterization of Three Crystalline Modifications of Telmisartan by Single Crystal and Highâ€Resolution Xâ€ray Powder Diffraction. Journal of Pharmaceutical Sciences, 2000, 89, 1465-1479.	3.3	55
32	The Discovery of Dabigatran Etexilate. Frontiers in Pharmacology, 2013, 4, 12.	3.5	52
33	Transâ^'Cis Isomerization is Responsible for the Red-Shifted Fluorescence in Variants of the Red Fluorescent Protein eqFP611. Journal of the American Chemical Society, 2008, 130, 12578-12579.	13.7	50
34	Comparative Analysis of Binding Kinetics and Thermodynamics of Dipeptidyl Peptidase-4 Inhibitors and Their Relationship to Structure. Journal of Medicinal Chemistry, 2016, 59, 7466-7477.	6.4	49
35	The metal site of Pseudomonas aeruginosa azurin, revealed by a crystal structure determination of the co(II) derivative and co-EPR spectroscopy. , 1997, 27, 385-394.		47
36	Histidine 179 Mutants of GTP Cyclohydrolase I Catalyze the Formation of 2-Amino-5-formylamino-6-ribofuranosylamino-4(3H)-pyrimidinone Triphosphate. Journal of Biological Chemistry, 1999, 274, 16727-16735.	3.4	46

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37	The role of structural information in the discovery of direct thrombin and factor Xa inhibitors. Trends in Pharmacological Sciences, 2012, 33, 279-288.	8.7	43
38	Ligand Bioactive Conformation Plays a Critical Role in the Design of Drugs That Target the Hepatitis C Virus NS3 Protease. Journal of Medicinal Chemistry, 2014, 57, 1777-1789.	6.4	43
39	3,5-Dihydro-imidazo[4,5-d]pyridazin-4-ones: A class of potent DPP-4 inhibitors. Bioorganic and Medicinal Chemistry Letters, 2008, 18, 3158-3162.	2.2	39
40	Crystal Structure of Glucokinase Regulatory Protein. Biochemistry, 2013, 52, 3523-3531.	2.5	39
41	Structural and Functional Consequences of Mutations in 6-Pyruvoyltetrahydropterin Synthase Causing Hyperphenylalaninemia in Humans. Journal of Biological Chemistry, 1995, 270, 29498-29506.	3.4	37
42	Crystal Structure of CC Chemokine Receptor 2A in Complex with an Orthosteric Antagonist Provides Insights for the Design of Selective Antagonists. Structure, 2019, 27, 427-438.e5.	3.3	37
43	X-ray Crystal Structure of the Two Site-specific Mutants Ile7Ser and Phe110Ser of Azurin fromPseudomonas aeruginosa. Journal of Molecular Biology, 1996, 255, 362-366.	4.2	34
44	Highâ€Resolution Crystal Structure of a Lasso Peptide. ChemMedChem, 2010, 5, 1689-1692.	3.2	34
45	An Antibody against the C-Terminal Domain of PCSK9 Lowers LDL Cholesterol Levels In Vivo. Journal of Molecular Biology, 2014, 426, 843-852.	4.2	31
46	Reaction mechanism of GTP cyclohydrolase I: single turnover experiments using a kinetically competent reaction intermediate. Journal of Molecular Biology, 2002, 316, 829-837.	4.2	29
47	Locking mixed-lineage kinase domain-like protein in its auto-inhibited state prevents necroptosis. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 33272-33281.	7.1	29
48	Pharmacological characterization of the selective 11β-hydroxysteroid dehydrogenase 1 inhibitor, BI 135585, a clinical candidate for the treatment of type 2 diabetes. European Journal of Pharmacology, 2015, 746, 50-55.	3.5	27
49	Crystal-contact engineering to obtain a crystal form of the Kelch domain of human Keap1 suitable for ligand-soaking experiments. Acta Crystallographica Section F: Structural Biology Communications, 2013, 69, 592-596.	0.7	25
50	Potent Cholesteryl Ester Transfer Protein Inhibitors of Reduced Lipophilicity: 1,1′-Spiro-Substituted Hexahydrofuroquinoline Derivatives. Journal of Medicinal Chemistry, 2014, 57, 8766-8776.	6.4	23
51	Crystal structures of modified apo-His117Gly and apo-His46Gly mutants of Pseudomonas aeruginosa azurin a aEdited by I. A. Wilson. Journal of Molecular Biology, 1997, 266, 357-365.	4.2	22
52	Elucidation of Crystal Packing by X-ray Diffraction and Freeze-etching Electron Microscopy. Studies on GTP Cyclohydrolase I ofEscherichia coli. Journal of Molecular Biology, 1995, 253, 208-218.	4.2	21
53	Crystal structure and receptor-interacting residues of MYDGF — a protein mediating ischemic tissue repair. Nature Communications, 2019, 10, 5379.	12.8	19
54	Molecular structure of human GM-CSF in complex with a disease-associated anti-human GM-CSF autoantibody and its potential biological implications. Biochemical Journal, 2012, 447, 205-215.	3.7	15

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55	Synthesis and Structureâ^'Activity Relationships of 6,7-Benzomorphan Derivatives as Use-Dependent Sodium Channel Blockers for the Treatment of Stroke. Journal of Medicinal Chemistry, 2002, 45, 3755-3764.	6.4	14
56	Heterocyclic thrombin inhibitors. Part 1: design and synthesis of amidino-phenoxy quinoline derivatives. Bioorganic and Medicinal Chemistry Letters, 2003, 13, 2291-2295.	2.2	14
57	Discovery and optimization of adamantyl carbamate inhibitors of 11β-HSD1. Bioorganic and Medicinal Chemistry Letters, 2010, 20, 6725-6729.	2.2	12
58	Development and Characterization of a Cocrystal as a Viable Solid Form for an Active Pharmaceutical Ingredient. Organic Process Research and Development, 2013, 17, 540-548.	2.7	12
59	Structure-guided residence time optimization of a dabigatran reversal agent. MAbs, 2015, 7, 871-880.	5.2	11
60	A small-molecule inhibitor of lectin-like oxidized LDL receptor-1 acts by stabilizing an inactive receptor tetramer state. Communications Chemistry, 2020, 3, .	4.5	11
61	Hybrid Screening Approach for Very Small Fragments: X-ray and Computational Screening on FKBP51. Journal of Medicinal Chemistry, 2020, 63, 5856-5864.	6.4	11
62	Discovery and Structure-Based Optimization of Fragments Binding the Mixed Lineage Kinase Domain-like Protein Executioner Domain. Journal of Medicinal Chemistry, 2021, 64, 15629-15638.	6.4	10
63	Structure and mechanism of GTP cyclohydrolase I of <i>Escherichia coli</i> . Biochemical Society Transactions, 1996, 24, 37S-37S.	3.4	9
64	Action of Dipeptidyl Peptidaseâ€4 Inhibitors on SARS oVâ€2 Main Protease. ChemMedChem, 2021, 16, 1425-1426.	3.2	9
65	Studies on GTP Cyclohydrolase I of Escherichia Coli. Advances in Experimental Medicine and Biology, 1993, 338, 157-162.	1.6	9
66	Synthesis of cyclic dipeptide templates, their incorporation into peptides and studies on their conformational and biological properties. Chemical Biology and Drug Design, 1998, 51, 323-336.	1.1	8
67	A hybrid approach reveals the allosteric regulation of GTP cyclohydrolase I. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 31838-31849.	7.1	7
68	InÂsitu crystallography as an emerging method for structure solution of membrane proteins: the case of CCR2A. FEBS Journal, 2020, 287, 866-873.	4.7	5
69	Synthesis and characterization of phosphinimine-substituted trifluoro- or trichloro-p-benzoquinones and their cationic Rh(I) complexes. The crystal and molecular structure of 3,5,6-trichloro-2-(triphenylphosphinimino)-p-benzoquinone. Canadian Journal of Chemistry, 1996, 74, 2378-2385.	1.1	4
70	A Single Second Shell Amino Acid Determines Affinity and Kinetics of Linagliptin Binding to Type 4 Dipeptidyl Peptidase and Fibroblast Activation Protein. ChemMedChem, 2021, 16, 630-639.	3.2	4
71	Sequential Backbone Assignment of Peroxisome Proliferator-Activated Receptor-Î ³ Ligand Binding Domain. Journal of Biomolecular NMR, 2005, 32, 259-259.	2.8	3

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73	Biophysical and structural investigation of the regulation of human GTP cyclohydrolase I by its regulatory protein GFRP. Journal of Structural Biology, 2021, 213, 107691.	2.8	1
74	Heterocyclic Thrombin Inhibitors. Part 1. Design and Synthesis of Amidino-Phenoxy Quinoline Derivatives ChemInform, 2003, 34, no.	0.0	0
75	Heterocyclic Thrombin Inhibitors. Part 2. Quinoxalinone Derivatives as Novel, Potent Antithrombotic Agents ChemInform, 2003, 34, no.	0.0	0