

Andrey Kovalevsky

List of Publications by Year in descending order

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127
papers

5,061
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85707

38
h-index

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65
g-index

232
all docs

232
docs citations

232
times ranked

6755
citing authors

#	ARTICLE	IF	CITATIONS
1	Photoinduced Linkage Isomers of Transition-Metal Nitrosyl Compounds and Related Complexes. <i>Chemical Reviews</i> , 2002, 102, 861-884.	51.4	412
2	Structural plasticity of SARS-CoV-2 3CL Mpro active site cavity revealed by room temperature X-ray crystallography. <i>Nature Communications</i> , 2020, 11, 3202.	13.2	368
3	Physical and Kinetic Analysis of the Cooperative Role of Metal Ions in Catalysis of Phosphodiester Cleavage by a Dinuclear Zn(II) Complex. <i>Journal of the American Chemical Society</i> , 2003, 125, 1988-1993.	14.6	224
4	Creating nanocavities of tunable sizes: Hollow helices. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2002, 99, 11583-11588.	7.6	153
5	Supercomputer-Based Ensemble Docking Drug Discovery Pipeline with Application to Covid-19. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 5832-5852.	5.7	144
6	Metal Ion Roles and the Movement of Hydrogen during Reaction Catalyzed by D-Xylose Isomerase: A Joint X-Ray and Neutron Diffraction Study. <i>Structure</i> , 2010, 18, 688-699.	3.4	143
7	Ultra-high Resolution Crystal Structure of HIV-1 Protease Mutant Reveals Two Binding Sites for Clinical Inhibitor TMC114. <i>Journal of Molecular Biology</i> , 2006, 363, 161-173.	4.3	137
8	Malleability of the SARS-CoV-2 3CL Mpro Active-Site Cavity Facilitates Binding of Clinical Antivirals. <i>Structure</i> , 2020, 28, 1313-1320.e3.	3.4	115
9	The Catalytic Mechanism of an Aspartic Proteinase Explored with Neutron and X-ray Diffraction. <i>Journal of the American Chemical Society</i> , 2008, 130, 7235-7237.	14.6	108
10	Unusual zwitterionic catalytic site of SARS-CoV-2 main protease revealed by neutron crystallography. <i>Journal of Biological Chemistry</i> , 2020, 295, 17365-17373.	3.5	104
11	Neutron Diffraction of Acetazolamide-Bound Human Carbonic Anhydrase II Reveals Atomic Details of Drug Binding. <i>Journal of the American Chemical Society</i> , 2012, 134, 14726-14729.	14.6	100
12	A new crystal form of human acetylcholinesterase for exploratory room-temperature crystallography studies. <i>Chemico-Biological Interactions</i> , 2019, 309, 108698.	4.2	97
13	Atomic resolution crystal structures of HIV-1 protease and mutants V82A and I84V with saquinavir. <i>Proteins: Structure, Function and Bioinformatics</i> , 2007, 67, 232-242.	3.2	86
14	Neutron Structure of Human Carbonic Anhydrase II: Implications for Proton Transfer. <i>Biochemistry</i> , 2010, 49, 415-421.	2.6	82
15	Effect of Flap Mutations on Structure of HIV-1 Protease and Inhibition by Saquinavir and Darunavir. <i>Journal of Molecular Biology</i> , 2008, 381, 102-115.	4.3	81
16	Covalent narpaprevir- and boceprevir-derived hybrid inhibitors of SARS-CoV-2 main protease. <i>Nature Communications</i> , 2022, 13, 2268.	13.2	77
17	First Observation of Photoinduced Nitrosyl Linkage Isomers of Iron Nitrosyl Porphyrins. <i>Journal of the American Chemical Society</i> , 2000, 122, 7142-7143.	14.6	76
18	The IMAGINE instrument: first neutron protein structure and new capabilities for neutron macromolecular crystallography. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013, 69, 2157-2160.	2.4	76

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19	Toward resolving the catalytic mechanism of dihydrofolate reductase using neutron and ultrahigh-resolution X-ray crystallography. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014, 111, 18225-18230.	7.6	76
20	High-Throughput Virtual Screening and Validation of a SARS-CoV-2 Main Protease Noncovalent Inhibitor. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 116-128.	5.7	64
21	Identification of the Elusive Hydronium Ion Exchanging Roles with a Proton in an Enzyme at Lower pH Values. <i>Angewandte Chemie - International Edition</i> , 2011, 50, 7520-7523.	14.8	62
22	Joint X-ray/Neutron Crystallographic Study of HIV-1 Protease with Clinical Inhibitor Amprenavir: Insights for Drug Design. <i>Journal of Medicinal Chemistry</i> , 2013, 56, 5631-5635.	6.6	62
23	Direct visualization of critical hydrogen atoms in a pyridoxal 5'-phosphate enzyme. <i>Nature Communications</i> , 2017, 8, 955.	13.2	59
24	Neutron and Atomic Resolution X-ray Structures of a Lytic Polysaccharide Monooxygenase Reveal Copper-Mediated Dioxygen Binding and Evidence for N-Terminal Deprotonation. <i>Biochemistry</i> , 2017, 56, 2529-2532.	2.6	55
25	Room-temperature X-ray crystallography reveals the oxidation and reactivity of cysteine residues in SARS-CoV-2 3CL M ^{pro} : insights into enzyme mechanism and drug design. <i>IUCr</i> , 2020, 7, 1028-1035.	2.3	54
26	Neutron Structure of Human Carbonic Anhydrase II: A Hydrogen-Bonded Water Network "Switch" Observed between pH 7.8 and 10.0. <i>Biochemistry</i> , 2011, 50, 9421-9423.	2.6	53
27	Direct observation of hydrogen atom dynamics and interactions by ultrahigh resolution neutron protein crystallography. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2012, 109, 15301-15306.	7.6	52
28	Inhibitor binding influences the protonation states of histidines in SARS-CoV-2 main protease. <i>Chemical Science</i> , 2021, 12, 1513-1527.	7.8	51
29	Neutron scattering in the biological sciences: progress and prospects. <i>Acta Crystallographica Section D: Structural Biology</i> , 2018, 74, 1129-1168.	2.4	49
30	Mechanism of Drug Resistance Revealed by the Crystal Structure of the Unliganded HIV-1 Protease with F53L Mutation. <i>Journal of Molecular Biology</i> , 2006, 358, 1191-1199.	4.3	48
31	Synthesis, Crystal Structures, Magnetic Properties and Photoconductivity of C60 and C70 Complexes with Metal Dialkyldithiocarbamates M(R ₂ dtc) _x , where M = CuI, CuI, AgI, ZnII, CdII, HgII, MnII, NiII, and PtII; R = Me, Et, and nPr. <i>European Journal of Inorganic Chemistry</i> , 2006, 2006, 1881-1895.	2.2	44
32	Caught in the Act: The 1.5 Å Resolution Crystal Structures of the HIV-1 Protease and the I54V Mutant Reveal a Tetrahedral Reaction Intermediate. <i>Biochemistry</i> , 2007, 46, 14854-14864.	2.6	44
33	Structural Evidence for Effectiveness of Darunavir and Two Related Antiviral Inhibitors against HIV-2 Protease. <i>Journal of Molecular Biology</i> , 2008, 384, 178-192.	4.3	44
34	Hydrogen Location in Stages of an Enzyme-Catalyzed Reaction: Time-of-Flight Neutron Structure of Xylose Isomerase with Bound Xylulose. <i>Biochemistry</i> , 2008, 47, 7595-7597.	2.6	44
35	Long-Range Electrostatics-Induced Two-Proton Transfer Captured by Neutron Crystallography in an Enzyme Catalytic Site. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 4924-4927.	14.8	43
36	Direct evidence that an extended hydrogen-bonding network influences activation of pyridoxal 5'-phosphate in aspartate aminotransferase. <i>Journal of Biological Chemistry</i> , 2017, 292, 5970-5980.	3.5	42

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37	Design, Synthesis, Protein-Ligand X-ray Structure, and Biological Evaluation of a Series of Novel Macrocyclic Human Immunodeficiency Virus-1 Protease Inhibitors to Combat Drug Resistance. <i>Journal of Medicinal Chemistry</i> , 2009, 52, 7689-7705.	6.6	41
38	"To Be or Not to Be" Protonated: Atomic Details of Human Carbonic Anhydrase-Clinical Drug Complexes by Neutron Crystallography and Simulation. <i>Structure</i> , 2018, 26, 383-390.e3.	3.4	41
39	Direct Observation of Protonation State Modulation in SARS-CoV-2 Main Protease upon Inhibitor Binding with Neutron Crystallography. <i>Journal of Medicinal Chemistry</i> , 2021, 64, 4991-5000.	6.6	41
40	Joint neutron crystallographic and NMR solution studies of Tyr residue ionization and hydrogen bonding: Implications for enzyme-mediated proton transfer. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015, 112, 5673-5678.	7.6	39
41	X-ray crystallographic studies of family 11 xylanase Michaelis and product complexes: implications for the catalytic mechanism. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2014, 70, 11-23.	2.4	38
42	Structural aspects of two-stage dimerization in an ionic C60 complex with bis(benzene)chromium: Cr(C6H6)2·C60·C6H4Cl2. <i>Dalton Transactions</i> , 2006, , 3716-3720.	3.4	37
43	Direct Determination of Protonation States of Histidine Residues in a 2.2 Å Neutron Structure of Deoxy-Human Normal Adult Hemoglobin and Implications for the Bohr Effect. <i>Journal of Molecular Biology</i> , 2010, 398, 276-291.	4.3	37
44	Direct determination of protonation states and visualization of hydrogen bonding in a glycoside hydrolase with neutron crystallography. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015, 112, 12384-12389.	7.6	37
45	Structural, Electronic, and Electrostatic Determinants for Inhibitor Binding to Subsites S1 and S2 in SARS-CoV-2 Main Protease. <i>Journal of Medicinal Chemistry</i> , 2021, 64, 17366-17383.	6.6	35
46	Neutron Diffraction Reveals Hydrogen Bonds Critical for cGMP-Selective Activation: Insights for cGMP-Dependent Protein Kinase Agonist Design. <i>Biochemistry</i> , 2014, 53, 6725-6727.	2.6	34
47	Zooming in on protons: Neutron structure of protein kinase A trapped in a product complex. <i>Science Advances</i> , 2019, 5, eaav0482.	10.9	33
48	Neutron structures of the <i>Helicobacter pylori</i> 5-methylthioadenosine nucleosidase highlight proton sharing and protonation states. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2016, 113, 13756-13761.	7.6	31
49	Solution Kinetics Measurements Suggest HIV-1 Protease Has Two Binding Sites for Darunavir and Amprenavir. <i>Journal of Medicinal Chemistry</i> , 2008, 51, 6599-6603.	6.6	30
50	High-resolution neutron crystallographic studies of the hydration of the coenzyme cob(II)alamin. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2011, 67, 584-591.	2.4	30
51	The mechanisms of catalysis and ligand binding for the SARS-CoV-2 NSP3 macrodomain from neutron and x-ray diffraction at room temperature. <i>Science Advances</i> , 2022, 8, .	10.9	30
52	Neutron structure of human carbonic anhydrase II in complex with methazolamide: mapping the solvent and hydrogen-bonding patterns of an effective clinical drug. <i>IUCr</i> , 2016, 3, 319-325.	2.3	29
53	Michaelis-like complex of SARS-CoV-2 main protease visualized by room-temperature X-ray crystallography. <i>IUCr</i> , 2021, 8, 973-979.	2.3	28
54	Rational design, synthesis, and evaluation of uncharged, bis-oxime antidotes of organophosphate-inhibited human acetylcholinesterase. <i>Journal of Biological Chemistry</i> , 2020, 295, 4079-4092.	3.5	27

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55	Low- and room-temperature X-ray structures of protein kinase A ternary complexes shed new light on its activity. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012, 68, 854-860.	2.4	26
56	The Neutron Macromolecular Crystallography Instruments at Oak Ridge National Laboratory: Advances, Challenges, and Opportunities. <i>Crystals</i> , 2018, 8, 388.	2.3	26
57	L-Arabinose Binding, Isomerization, and Epimerization by D-Xylose Isomerase: X-Ray/Neutron Crystallographic and Molecular Simulation Study. <i>Structure</i> , 2014, 22, 1287-1300.	3.4	25
58	Phosphoryl Transfer Reaction Snapshots in Crystals. <i>Journal of Biological Chemistry</i> , 2015, 290, 15538-15548.	3.5	25
59	Room Temperature Neutron Crystallography of Drug Resistant HIV-1 Protease Uncovers Limitations of X-ray Structural Analysis at 100 K. <i>Journal of Medicinal Chemistry</i> , 2017, 60, 2018-2025.	6.6	25
60	Mannobiose Binding Induces Changes in Hydrogen Bonding and Protonation States of Acidic Residues in Concanavalin A As Revealed by Neutron Crystallography. <i>Biochemistry</i> , 2017, 56, 4747-4750.	2.6	25
61	IMAGINE: neutrons reveal enzyme chemistry. <i>Acta Crystallographica Section D: Structural Biology</i> , 2018, 74, 778-786.	2.4	25
62	Insights into the Phosphoryl Transfer Catalyzed by cAMP-Dependent Protein Kinase: An X-ray Crystallographic Study of Complexes with Various Metals and Peptide Substrate SP20. <i>Biochemistry</i> , 2013, 52, 3721-3727.	2.6	24
63	Protein Kinase A Catalytic Subunit Primed for Action: Time-Lapse Crystallography of Michaelis Complex Formation. <i>Structure</i> , 2015, 23, 2331-2340.	3.4	22
64	Inorganic pyrophosphatase crystals from <i>Thermococcus thio-reducens</i> for X-ray and neutron diffraction. <i>Acta Crystallographica Section F: Structural Biology Communications</i> , 2012, 68, 1482-1487.	0.7	21
65	IMAGINE: The neutron protein crystallography beamline at the high flux isotope reactor. <i>Methods in Enzymology</i> , 2020, 634, 69-85.	1.7	21
66	Room-temperature neutron and X-ray data collection of 3CL M ^{pro} from SARS-CoV-2. <i>Acta Crystallographica Section F, Structural Biology Communications</i> , 2020, 76, 483-487.	0.9	21
67	Synthesis, crystal structure and photoconductivity of the first [60]fullerene complex with metal diethyldithiocarbamate: {Cull(dedtc) ₂ } ₂ ·C ₆₀ . <i>Dalton Transactions</i> , 2005, , 1821.	3.4	20
68	Evolution and characterization of a new reversibly photoswitching chromogenic protein, Dathail. <i>Journal of Molecular Biology</i> , 2016, 428, 1776-1789.	4.3	20
69	Engineering acidic <i>Streptomyces rubiginosus</i> D-xylose isomerase by rational enzyme design. <i>Protein Engineering, Design and Selection</i> , 2014, 27, 59-64.	2.4	19
70	Inhibition of D-xylose isomerase by polyols: atomic details by joint X-ray/neutron crystallography. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012, 68, 1201-1206.	2.4	18
71	Metal-Free cAMP-Dependent Protein Kinase Can Catalyze Phosphoryl Transfer. <i>Biochemistry</i> , 2014, 53, 3179-3186.	2.6	18
72	Hit Expansion of a Noncovalent SARS-CoV-2 Main Protease Inhibitor. <i>ACS Pharmacology and Translational Science</i> , 2022, 5, 255-265.	4.7	18

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73	Potent HIV-1 protease inhibitors incorporating meso-bicyclic urethanes as P2-ligands: structure-based design, synthesis, biological evaluation and protein-ligand X-ray studies. <i>Organic and Biomolecular Chemistry</i> , 2008, 6, 3703.	2.9	17
74	Novel complex MAD phasing and RNase H structural insights using selenium oligonucleotides. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2014, 70, 354-361.	2.4	17
75	Understanding the pH-Dependent Reaction Mechanism of a Glycoside Hydrolase Using High-Resolution X-ray and Neutron Crystallography. <i>ACS Catalysis</i> , 2018, 8, 8058-8069.	11.7	17
76	Structural and functional characterization of NEMO cleavage by SARS-CoV-2 3CLpro. <i>Nature Communications</i> , 2022, 13, .	13.2	17
77	Hyperconjugation Promotes Catalysis in a Pyridoxal 5'-Phosphate-Dependent Enzyme. <i>ACS Catalysis</i> , 2018, 8, 6733-6737.	11.7	16
78	Capturing the Reaction Pathway in Near-Atomic-Resolution Crystal Structures of HIV-1 Protease. <i>Biochemistry</i> , 2012, 51, 7726-7732.	2.6	14
79	Autoprocessing and oxyanion loop reorganization upon GC373 and nirmatrelvir binding of monomeric SARS-CoV-2 main protease catalytic domain. <i>Communications Biology</i> , 2022, 5, .	4.5	14
80	Productive reorientation of a bound oxime reactivator revealed in room temperature X-ray structures of native and VX-inhibited human acetylcholinesterase. <i>Journal of Biological Chemistry</i> , 2019, 294, 10607-10618.	3.5	13
81	Pyridoxal 5'-phosphate dependent reactions: Analyzing the mechanism of aspartate aminotransferase. <i>Methods in Enzymology</i> , 2020, 634, 333-359.	1.7	13
82	Macromolecular neutron crystallography at the Protein Crystallography Station (PCS). <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2010, 66, 1206-1212.	2.4	11
83	Biological Structures. <i>Experimental Methods in the Physical Sciences</i> , 2017, 49, 1-75.	0.1	10
84	Characterization and structural analysis of a thermophilic GH11 xylanase from compost metatranscriptome. <i>Applied Microbiology and Biotechnology</i> , 2021, 105, 7757-7767.	3.7	10
85	Room-temperature ultrahigh-resolution time-of-flight neutron and X-ray diffraction studies of H/D-exchanged crambin. <i>Acta Crystallographica Section F: Structural Biology Communications</i> , 2012, 68, 119-123.	0.7	9
86	Protonation states of histidine and other key residues in deoxy normal human adult hemoglobin by neutron protein crystallography. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2010, 66, 1144-1152.	2.4	8
87	Identification of the Elusive Hydronium Ion Exchanging Roles with a Proton in an Enzyme at Lower pH-Values. <i>Angewandte Chemie</i> , 2011, 123, 7662-7665.	2.1	8
88	Neutron and high-resolution room-temperature X-ray data collection from crystallized lytic polysaccharide monoxygenase. <i>Acta Crystallographica Section F, Structural Biology Communications</i> , 2015, 71, 1448-1452.	0.9	8
89	Visualizing the Bohr effect in hemoglobin: neutron structure of equine cyanomethemoglobin in the R state and comparison with human deoxyhemoglobin in the T state. <i>Acta Crystallographica Section D: Structural Biology</i> , 2016, 72, 892-903.	2.4	8
90	Pressure and Temperature Effects on the Formation of Aminoacrylate Intermediates of Tyrosine Phenol-lyase Demonstrate Reaction Dynamics. <i>ACS Catalysis</i> , 2020, 10, 1692-1703.	11.7	8

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91	Room temperature crystallography of human acetylcholinesterase bound to a substrate analogue 4K-TMA: Towards a neutron structure. <i>Current Research in Structural Biology</i> , 2021, 3, 206-215.	2.3	8
92	Capturing the Catalytic Proton of Dihydrofolate Reductase: Implications for General Acid-Base Catalysis. <i>ACS Catalysis</i> , 2021, 11, 5873-5884.	11.7	8
93	Covalent inhibition of hAChE by organophosphates causes homodimer dissociation through long-range allosteric effects. <i>Journal of Biological Chemistry</i> , 2021, 297, 101007.	3.5	8
94	Anion Chain Structure Controlled Behavior of Phase Transition in Quasi-Two-Dimensional Organic Metal (EDT-TTF) ₄ [Hg ₃ I ₈]·x. <i>Crystal Growth and Design</i> , 2007, 7, 2768-2773.	3.2	7
95	Preliminary joint X-ray and neutron protein crystallographic studies of ecDHFR complexed with folate and NADP ⁺ . <i>Acta Crystallographica Section F, Structural Biology Communications</i> , 2014, 70, 814-818.	0.9	7
96	Visualizing Tetrahedral Oxanion Bound in HIV-1 Protease Using Neutrons: Implications for the Catalytic Mechanism and Drug Design. <i>ACS Omega</i> , 2020, 5, 11605-11617.	3.6	7
97	Substrate Binding Stiffens Aspartate Aminotransferase by Altering the Enzyme Picosecond Vibrational Dynamics. <i>ACS Omega</i> , 2020, 5, 18787-18797.	3.6	7
98	AI-Accelerated Design of Targeted Covalent Inhibitors for SARS-CoV-2. <i>Journal of Chemical Information and Modeling</i> , 2023, 63, 1438-1453.	5.7	7
99	Preliminary joint X-ray and neutron protein crystallographic studies of endoxylanase II from the fungus <i>Trichoderma longibrachiatum</i> . <i>Acta Crystallographica Section F: Structural Biology Communications</i> , 2011, 67, 283-286.	0.7	6
100	Long-Range Electrostatics-Induced Two-Proton Transfer Captured by Neutron Crystallography in an Enzyme Catalytic Site. <i>Angewandte Chemie</i> , 2016, 128, 5008-5011.	2.1	6
101	Microgravity crystallization of perdeuterated tryptophan synthase for neutron diffraction. <i>Npj Microgravity</i> , 2022, 8, 13.	3.8	6
102	An N-H...N low-barrier hydrogen bond preorganizes the catalytic site of aspartate aminotransferase to facilitate the second half-reaction. <i>Chemical Science</i> , 2022, 13, 10057-10065.	7.8	6
103	Discovering and Designing a Chimeric Hyperthermophilic Chitinase for Crystalline Chitin Degradation. <i>ACS Sustainable Chemistry and Engineering</i> , 2023, 11, 4690-4698.	6.9	6
104	Insights into the mechanism of SARS-CoV-2 main protease autocatalytic maturation from model precursors. <i>Communications Biology</i> , 2023, 6, .	4.5	6
105	Using neutron protein crystallography to understand enzyme mechanisms. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2010, 66, 1257-1261.	2.4	5
106	Preliminary joint neutron time-of-flight and X-ray crystallographic study of human ABO(H) blood group A glycosyltransferase. <i>Acta Crystallographica Section F: Structural Biology Communications</i> , 2011, 67, 258-262.	0.7	4
107	Temperature-Induced Replacement of Phosphate Proton with Metal Ion Captured in Neutron Structures of A-DNA. <i>Structure</i> , 2018, 26, 1645-1650.e3.	3.4	4
108	Proton transfer and drug binding details revealed in neutron diffraction studies of wild-type and drug resistant HIV-1 protease. <i>Methods in Enzymology</i> , 2020, 634, 257-279.	1.7	4

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109	EWALD: A macromolecular diffractometer for the second target station. Review of Scientific Instruments, 2022, 93, .	1.4	4
110	Studying the Role of a Single Mutation of a Family 11 Glycoside Hydrolase Using High-Resolution X-ray Crystallography. Protein Journal, 2020, 39, 671-680.	1.6	3
111	Joint neutron/molecular dynamics vibrational spectroscopy reveals softening of HIV-1 protease upon binding of a tight inhibitor. Physical Chemistry Chemical Physics, 2022, 24, 3586-3597.	2.9	3
112	Heterologous expression, purification, crystallization and preliminary X-ray analysis of Trichoderma reesei xylanase II and four variants. Acta Crystallographica Section F: Structural Biology Communications, 2013, 69, 320-323.	0.7	2
113	Room-temperature photo-induced martensitic transformation in a protein crystal. IUCr, 2019, 6, 619-629.	2.3	2
114	Hemoglobin redux: combining neutron and X-ray diffraction with mass spectrometry to analyse the quaternary state of oxidized hemoglobins. Acta Crystallographica Section D: Biological Crystallography, 2010, 66, 1249-1256.	2.4	1
115	Time-of-flight neutron diffraction study of bovine \hat{I}^3 -chymotrypsin at the Protein Crystallography Station. Acta Crystallographica Section F: Structural Biology Communications, 2011, 67, 587-590.	0.7	1
116	Neutron Crystallography Detects Differences in Protein Dynamics: Structure of the PKG II Cyclic Nucleotide Binding Domain in Complex with an Activator. Biochemistry, 2018, 57, 1833-1837.	2.6	1
117	Revertant mutation V48G alters conformational dynamics of highly drug resistant HIV protease PRS17. Journal of Molecular Graphics and Modelling, 2021, 108, 108005.	2.5	1
118	Direct observation of protonation states in a PLP-dependent enzyme by neutron crystallography. Acta Crystallographica Section A: Foundations and Advances, 2017, 73, a26-a26.	0.1	1
119	Revealing protonation states and tracking substrate in serine hydroxymethyltransferase with room-temperature X-ray and neutron crystallography. Communications Chemistry, 2023, 6, .	4.9	1
120	Discovery of Novel <i>Rhizoctonia solani</i> DHFR Inhibitors as Fungicides Using Virtual Screening. Journal of Agricultural and Food Chemistry, 2023, 71, 19385-19395.	5.3	1
121	Visualizing the Active Site Oxyanion Loop Transition Upon Ensitrelvir Binding and Transient Dimerization of SARS-CoV-2 Main Protease. Journal of Molecular Biology, 2024, 436, 168616.	4.3	1
122	Bis[bis(3-phenylpyrazol-1-yl)(pyrazol-1-yl)methane]copper(II) bis(perchlorate) acetonitrile disolvate. Acta Crystallographica Section C: Crystal Structure Communications, 2006, 62, m30-m32.	0.4	0
123	Neutron protein crystallography reveals unique details of clinical drug binding to a human target enzyme. Neutron News, 2013, 24, 20-23.	0.2	0
124	Protein kinase A in the neutron beam: Insights for catalysis from directly observing protons. Methods in Enzymology, 2020, 634, 311-331.	1.7	0
125	Universality of critical active site glutamate as an acid-base catalyst in serine hydroxymethyltransferase function. Chemical Science, 0, , .	7.8	0
126	Dual Enhancement of Thermostability and Activity of Xylanase through Computer-Aided Rational Design. ACS Sustainable Chemistry and Engineering, 0, , .	6.9	0

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127	Effects of SARS-CoV-2 Main Protease Mutations at Positions L50, E166, and L167 Rendering Resistance to Covalent and Noncovalent Inhibitors. <i>Journal of Medicinal Chemistry</i> , 0, , .	6.6	0