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Citation Report

#	ARTICLE	IF	CITATIONS
1	Structure-Based Drug Design and Optimization of Mannoside Bacterial FimH Antagonists. <i>Journal of Medicinal Chemistry</i> , 2010, 53, 4779-4792.	2.9	220
2	QM methods in structure based design: Utility in probing protein-ligand interactions. <i>Journal of Molecular Graphics and Modelling</i> , 2010, 29, 507-517.	1.3	5
3	Acyldepsipeptide Antibiotics Induce the Formation of a Structured Axial Channel in ClpP: A Model for the ClpX/ClpA-Bound State of ClpP. <i>Chemistry and Biology</i> , 2010, 17, 959-969.	6.2	168
4	<i>phenix.model_vs_data</i> : a high-level tool for the calculation of crystallographic model and data statistics. <i>Journal of Applied Crystallography</i> , 2010, 43, 669-676.	1.9	112
5	<i>PHENIX</i> : a comprehensive Python-based system for macromolecular structure solution. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2010, 66, 213-221.	2.5	20,564
6	Joint X-ray and neutron refinement with <i>phenix.refine</i> . <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2010, 66, 1153-1163.	2.5	259
7	Structural basis for selective activation of ABA receptors. <i>Nature Structural and Molecular Biology</i> , 2010, 17, 1109-1113.	3.6	104
8	Toxoflavin Lyase Requires a Novel 1-His-2-Carboxylate Facial Triad. <i>Biochemistry</i> , 2011, 50, 1091-1100.	1.2	13
9	Mechanism of the Intramolecular Claisen Condensation Reaction Catalyzed by MenB, a Crotonase Superfamily Member. <i>Biochemistry</i> , 2011, 50, 9532-9544.	1.2	62
10	Structure of Estradiol Metal Chelate and Estrogen Receptor Complex: The Basis for Designing a New Class of Selective Estrogen Receptor Modulators. <i>Journal of Medicinal Chemistry</i> , 2011, 54, 3575-3580.	2.9	28
11	Synthesis, Crystal Structure, and in Vitro Biological Evaluation of C-6 Pyrimidine Derivatives: New Lead Structures for Monitoring Gene Expression in Vivo. <i>Nucleosides, Nucleotides and Nucleic Acids</i> , 2011, 30, 293-315.	0.4	9
12	Riboneogenesis in Yeast. <i>Cell</i> , 2011, 145, 969-980.	13.5	105
13	X-ray crystallography: assessment and validation of protein-small molecule complexes for drug discovery. <i>Expert Opinion on Drug Discovery</i> , 2011, 6, 771-782.	2.5	53
14	A reversibly photoswitchable GFP-like protein with fluorescence excitation decoupled from switching. <i>Nature Biotechnology</i> , 2011, 29, 942-947.	9.4	254
15	A Small-Molecule Probe Induces a Conformation in HIV TAR RNA Capable of Binding Drug-Like Fragments. <i>Journal of Molecular Biology</i> , 2011, 410, 984-996.	2.0	50
16	The Phenix software for automated determination of macromolecular structures. <i>Methods</i> , 2011, 55, 94-106.	1.9	764
17	A New Generation of Crystallographic Validation Tools for the Protein Data Bank. <i>Structure</i> , 2011, 19, 1395-1412.	1.6	405
18	Atomic resolution structure of EhpR: phenazine resistance in <i>Enterobacter agglomerans</i> Eh1087 follows principles of bleomycin/mitomycin C resistance in other bacteria. <i>BMC Structural Biology</i> , 2011, 11, 33.	2.3	4

#	ARTICLE	IF	CITATIONS
19	An Automated Force Field Topology Builder (ATB) and Repository: Version 1.0. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 4026-4037.	2.3	1,425
20	Structural Basis for Antiviral Inhibition of the Main Protease, 3C, from Human Enterovirus 93. <i>Journal of Virology</i> , 2011, 85, 10764-10773.	1.5	20
21	The Gal3p transducer of the <i>GAL</i> regulon interacts with the Gal80p repressor in its ligand-induced closed conformation. <i>Genes and Development</i> , 2012, 26, 294-303.	2.7	42
22	Simple Pseudo-dipeptides with a P2 ⁺ Glutamate. <i>Journal of Biological Chemistry</i> , 2012, 287, 26647-26656.	1.6	35
23	The Molecular Mechanism of Thermostable β -Galactosidases AgaA and AgaB Explained by X-ray Crystallography and Mutational Studies. <i>Journal of Biological Chemistry</i> , 2012, 287, 39642-39652.	1.6	41
24	Detection of alternative conformations by unrestrained refinement. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012, 68, 1118-1127.	2.5	5
25	Determinants of substrate specificity and biochemical properties of the <i>sn</i> glycerol 3-phosphate <i>ATP</i> binding cassette transporter (<i>UgpB</i>) of <i>E. coli</i> . <i>Molecular Microbiology</i> , 2012, 86, 908-920.	1.2	30
26	Pharmacological and structural characterization of conformationally restricted (S)-glutamate analogues at ionotropic glutamate receptors. <i>Journal of Structural Biology</i> , 2012, 180, 39-46.	1.3	14
27	Structure of Mandelate Racemase with Bound Intermediate Analogues Benzohydroxamate and Cupferron. <i>Biochemistry</i> , 2012, 51, 1160-1170.	1.2	28
28	Kainate induces various domain closures in AMPA and kainate receptors. <i>Neurochemistry International</i> , 2012, 61, 536-545.	1.9	17
29	Structural basis for the influence of a single mutation K145N on the oligomerization and photoswitching rate of Dronpa. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012, 68, 1653-1659.	2.5	8
30	Automation of AMOEBA polarizable force field parameterization for small molecules. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1138.	0.5	134
31	Improving the Accuracy of Macromolecular Structure Refinement at 7 \AA Resolution. <i>Structure</i> , 2012, 20, 957-966.	1.6	37
32	Graphical tools for macromolecular crystallography in <i>PHENIX</i> . <i>Journal of Applied Crystallography</i> , 2012, 45, 581-586.	1.9	139
33	Handling ligands with <i>Coot</i> . <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012, 68, 425-430.	2.5	105
34	Towards automated crystallographic structure refinement with <i>phenix.refine</i> . <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012, 68, 352-367.	2.5	4,573
35	<i>Ligand</i> : a graphical tool for the <i>CCP4</i> template-restraint library. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012, 68, 431-440.	2.5	373
36	Sparkle/RM1 parameters for the semiempirical quantum chemical calculation of lanthanide complexes. <i>RSC Advances</i> , 2013, 3, 16747.	1.7	58

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37	Synthesis, Pharmacological and Structural Characterization, and Thermodynamic Aspects of GluA2-Positive Allosteric Modulators with a 3,4-Dihydro-2 <i>H</i> -1,2,4-benzothiadiazine 1,1-Dioxide Scaffold. <i>Journal of Medicinal Chemistry</i> , 2013, 56, 8736-8745.	2.9	38
38	HCF-1 Is Cleaved in the Active Site of O-GlcNAc Transferase. <i>Science</i> , 2013, 342, 1235-1239.	6.0	162
39	Crystal Structure and Pharmacological Characterization of a Novel N-Methyl-d-aspartate (NMDA) Receptor Antagonist at the GluN1 Glycine Binding Site. <i>Journal of Biological Chemistry</i> , 2013, 288, 33124-33135.	1.6	22
40	Electron microscopy analysis of a disaccharide analog complex reveals receptor interactions of adeno-associated virus. <i>Journal of Structural Biology</i> , 2013, 184, 129-135.	1.3	15
41	Synthesis, Pharmacology, and Biostructural Characterization of Novel $\hat{\pm}4^2$ Nicotinic Acetylcholine Receptor Agonists. <i>Journal of Medicinal Chemistry</i> , 2013, 56, 940-951.	2.9	15
42	Structural insights into cofactor recognition of yeast mitochondria 3-oxoacyl-ACP reductase OAR1. <i>IUBMB Life</i> , 2013, 65, 154-162.	1.5	7
43	Crystallization of bi-functional ligand protein complexes. <i>Journal of Structural Biology</i> , 2013, 182, 246-254.	1.3	45
44	Cysteine Dioxygenase Structures from pH4 to 9: Consistent Cys-Persulfenate Formation at Intermediate pH and a Cys-Bound Enzyme at Higher pH. <i>Journal of Molecular Biology</i> , 2013, 425, 3121-3136.	2.0	59
45	Structural basis of substrate selectivity of \hat{P}^1 -pyrroline-5-carboxylate dehydrogenase (ALDH4A1): Semialdehyde chain length. <i>Archives of Biochemistry and Biophysics</i> , 2013, 538, 34-40.	1.4	24
46	Structure-guided studies of the SHP-1/JAK1 interaction provide new insights into phosphatase catalytic domain substrate recognition. <i>Journal of Structural Biology</i> , 2013, 181, 243-251.	1.3	13
47	Techniques, tools and best practices for ligand electron-density analysis and results from their application to deposited crystal structures. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013, 69, 150-167.	2.5	94
48	Studies on an (<i>S</i>)-2-Amino-3-(3-hydroxy-5-methyl-4-isoxazolyl)propionic Acid (AMPA) Receptor Antagonist IKM-159: Asymmetric Synthesis, Neuroactivity, and Structural Characterization. <i>Journal of Medicinal Chemistry</i> , 2013, 56, 2283-2293.	2.9	23
49	Molecular Determinants of a Selective Matrix Metalloprotease-12 Inhibitor: Insights from Crystallography and Thermodynamic Studies. <i>Journal of Medicinal Chemistry</i> , 2013, 56, 1149-1159.	2.9	37
50	Chemoenzymatic Synthesis of New 2,4-syn-Functionalized (<i>S</i>)-Glutamate Analogues and Structure-Activity Relationship Studies at Ionotropic Glutamate Receptors and Excitatory Amino Acid Transporters. <i>Journal of Medicinal Chemistry</i> , 2013, 56, 1614-1628.	2.9	42
51	Structural and Functional Characterization of MppR, an Enduracididine Biosynthetic Enzyme from <i>Streptomyces hygroscopicus</i> : Functional Diversity in the Acetoacetate Decarboxylase-like Superfamily. <i>Biochemistry</i> , 2013, 52, 4492-4506.	1.2	31
52	Converting NAD-Specific Inositol Dehydrogenase to an Efficient NADP-Selective Catalyst, with a Surprising Twist. <i>Biochemistry</i> , 2013, 52, 5876-5883.	1.2	18
53	Conformational Plasticity and Ligand Binding of Bacterial Monoacylglycerol Lipase. <i>Journal of Biological Chemistry</i> , 2013, 288, 31093-31104.	1.6	44
54	<i>Mycobacterium tuberculosis</i> DNA gyrase ATPase domain structures suggest a dissociative mechanism that explains how ATP hydrolysis is coupled to domain motion. <i>Biochemical Journal</i> , 2013, 456, 263-273.	1.7	38

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55	Structures of enzymeâ€™s intermediate complexes of yeast Nit2: insights into its catalytic mechanism and different substrate specificity compared with mammalian Nit2. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013, 69, 1470-1481.	2.5	16
56	Mutations inducing an active-site aperture in <i>Rhizobium</i> sp. sucrose isomerase confer hydrolytic activity. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013, 69, 298-307.	2.5	11
57	The landscape of cytokinin binding by a plant nodulin. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013, 69, 2365-2380.	2.5	16
58	Structural basis of L-phosphoserine binding to <i>Bacillus alcalophilus</i> phosphoserine aminotransferase. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013, 69, 804-811.	2.5	12
59	On the propagation of errors. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013, 69, 1865-1866.	2.5	15
60	Expanded use of sense codons is regulated by modified cytidines in tRNA. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2013, 110, 10964-10969.	3.3	67
61	Identification of NAD(P)H Quinone Oxidoreductase Activity in Azoreductases from <i>P. aeruginosa</i> : Azoreductases and NAD(P)H Quinone Oxidoreductases Belong to the Same FMN-Dependent Superfamily of Enzymes. <i>PLoS ONE</i> , 2014, 9, e98551.	1.1	55
62	Structures of PI4KIII ² complexes show simultaneous recruitment of Rab11 and its effectors. <i>Science</i> , 2014, 344, 1035-1038.	6.0	131
63	Specific binding of gibberellic acid by Cytokinin-Specific Binding Proteins: a new aspect of plant hormone-binding proteins with the PR-10 fold. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2014, 70, 2032-2041.	2.5	27
64	Crystallographic Analysis of TPP Riboswitch Binding by Small-Molecule Ligands Discovered Through Fragment-Based Drug Discovery Approaches. <i>Methods in Enzymology</i> , 2014, 549, 221-233.	0.4	3
65	Characterization of Selective Exosite-Binding Inhibitors of Matrix Metalloproteinase 13 That Prevent Articular Cartilage Degradation in Vitro. <i>Journal of Medicinal Chemistry</i> , 2014, 57, 9598-9611.	2.9	29
66	Conformationâ€‘dependent backbone geometry restraints set a new standard for protein crystallographic refinement. <i>FEBS Journal</i> , 2014, 281, 4061-4071.	2.2	36
67	Timeâ€‘Dependent Diaryl Ether Inhibitors of InhA: Structureâ€‘Activity Relationship Studies of Enzyme Inhibition, Antibacterial Activity, and inâ€‘vivo Efficacy. <i>ChemMedChem</i> , 2014, 9, 776-791.	1.6	48
68	Molecular Recognition of Two 2,4â€‘synâ€‘Functionalized (<i>S</i>)â€‘Glutamate Analogues by the Kainate Receptor GluK3 Ligand Binding Domain. <i>ChemMedChem</i> , 2014, 9, 2254-2259.	1.6	12
69	Molecular Basis of the General Base Catalysis of an Î±/Î²-Hydrolase Catalytic Triad. <i>Journal of Biological Chemistry</i> , 2014, 289, 15867-15879.	1.6	21
70	Ligand-dependent active-site closure revealed in the crystal structure of <i>Mycobacterium tuberculosis</i> MenB complexed with product analogues. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2014, 70, 2959-2969.	2.5	3
71	A Conserved Hydrogen-Bonding Network of P2 <i>bis</i> -Tetrahydrofuran-Containing HIV-1 Protease Inhibitors (PIs) with a Protease Active-Site Amino Acid Backbone Aids in Their Activity against PI-Resistant HIV. <i>Antimicrobial Agents and Chemotherapy</i> , 2014, 58, 3679-3688.	1.4	17
72	Structure of tomato wound-induced leucine aminopeptidase sheds light on substrate specificity. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2014, 70, 1649-1658.	2.5	13

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73	Structural Basis for Substrate Specificity in ArnB. A Key Enzyme in the Polymyxin Resistance Pathway of Gram-Negative Bacteria. <i>Biochemistry</i> , 2014, 53, 796-805.	1.2	25
74	Native-like Photosystem II Superstructure at 2.44 Å... Resolution through Detergent Extraction from the Protein Crystal. <i>Structure</i> , 2014, 22, 1607-1615.	1.6	67
75	Positive Allosteric Modulators of 2-Amino-3-(3-hydroxy-5-methylisoxazol-4-yl)propionic Acid Receptors Belonging to 4-Cyclopropyl-3,4-dihydro-2 <i>H</i> -1,2,4-pyridothiadiazine Dioxides and Diversely Chloro-Substituted 4-Cyclopropyl-3,4-dihydro-2 <i>H</i> -1,2,4-benzothiadiazine 1,1-Dioxides. <i>Journal of Medicinal Chemistry</i> , 2014, 57, 9539-9553.	2.9	25
76	Covalent docking of large libraries for the discovery of chemical probes. <i>Nature Chemical Biology</i> , 2014, 10, 1066-1072.	3.9	225
77	Molecular Basis of 1-Deoxygalactonojirimycin Arylthiourea Binding to Human β -Galactosidase A: Pharmacological Chaperoning Efficacy on Fabry Disease Mutants. <i>ACS Chemical Biology</i> , 2014, 9, 1460-1469.	1.6	50
78	Structure and mechanism of action of the hydroxy- α -aldehyde class of IRE1 endoribonuclease inhibitors. <i>Nature Communications</i> , 2014, 5, 4202.	5.8	108
79	Structural basis for organohalide respiration. <i>Science</i> , 2014, 346, 455-458.	6.0	220
80	Structural insights into the role of iron-histidine bond cleavage in nitric oxide-induced activation of H-NOX gas sensor proteins. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014, 111, E4156-64.	3.3	87
81	Crystal structure of the nucleotide-binding domain of mortalin, the mitochondrial Hsp70 chaperone. <i>Protein Science</i> , 2014, 23, 833-842.	3.1	40
82	Unravelling the mechanism of non-ribosomal peptide synthesis by cyclodipeptide synthases. <i>Nature Communications</i> , 2014, 5, 5141.	5.8	54
83	Inactivation of the Mycobacterium tuberculosis Antigen 85 Complex by Covalent, Allosteric Inhibitors. <i>Journal of Biological Chemistry</i> , 2014, 289, 25031-25040.	1.6	35
84	Structural Basis of Furan-Amino Acid Recognition by a Polyspecific Aminoacyl-tRNA-Synthetase and its Genetic Encoding in Human Cells. <i>ChemBioChem</i> , 2014, 15, 1755-1760.	1.3	21
85	Crystallographic Evidence of Drastic Conformational Changes in the Active Site of a Flavin-Dependent <i>N</i> -Hydroxylase. <i>Biochemistry</i> , 2014, 53, 6063-6077.	1.2	31
86	Structure of a Dihydroxycoumarin Active-Site Inhibitor in Complex with the RNase H Domain of HIV-1 Reverse Transcriptase and Structure-Activity Analysis of Inhibitor Analogs. <i>Journal of Molecular Biology</i> , 2014, 426, 2617-2631.	2.0	36
87	An enzyme captured in two conformational states: crystal structure of <i>S</i> -adenosyl-L-homocysteine hydrolase from <i>Bradyrhizobium elkanii</i> . <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2015, 71, 2422-2432.	2.5	9
88	Crystal structures of Mycobacterium tuberculosis GlgE and complexes with non-covalent inhibitors. <i>Scientific Reports</i> , 2015, 5, 12830.	1.6	13
89	Crystallographic characterization of the ribosomal binding site and molecular mechanism of action of Hygromycin A. <i>Nucleic Acids Research</i> , 2015, 43, gkv975.	6.5	15
90	A Newcomer's Guide to Peptide Crystallography. <i>Israel Journal of Chemistry</i> , 2015, 55, 698-710.	1.0	20

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91	An allosteric model for control of pore opening by substrate binding in the <i>E. coli</i> microcompartment shell protein. <i>Protein Science</i> , 2015, 24, 956-975.	3.1	38
92	Structural Determinants of the Selectivity of β -Benzyluracil α -Acetic Acids toward Human Enzymes Aldose Reductase and AKR1B10. <i>ChemMedChem</i> , 2015, 10, 1989-2003.	1.6	13
93	A Novel Small-Molecule Inhibitor Targeting CREB-CBP Complex Possesses Anti-Cancer Effects along with Cell Cycle Regulation, Autophagy Suppression and Endoplasmic Reticulum Stress. <i>PLoS ONE</i> , 2015, 10, e0122628.	1.1	20
94	Structures of potent anticancer compounds bound to tubulin. <i>Protein Science</i> , 2015, 24, 1164-1172.	3.1	20
95	Tandem Benzophenone Amino Pyridines, Potent and Selective Inhibitors of Human Leukotriene C ₄ Synthase. <i>Journal of Pharmacology and Experimental Therapeutics</i> , 2015, 355, 108-116.	1.3	19
96	<i>Streptomyces wadayamensis</i> MppP Is a Pyridoxal 5 ² -Phosphate-Dependent <i>l</i> -Arginine β -Deaminase, β -Hydroxylase in the Enduracididine Biosynthetic Pathway. <i>Biochemistry</i> , 2015, 54, 7029-7040.	1.2	35
97	Carbonic Anhydrase Inhibitors with Dual-Tail Moieties To Match the Hydrophobic and Hydrophilic Halves of the Carbonic Anhydrase Active Site. <i>Journal of Medicinal Chemistry</i> , 2015, 58, 1494-1501.	2.9	83
98	Synthesis of hydrolysis-resistant pyridoxal 5 ² -phosphate analogs and their biochemical and X-ray crystallographic characterization with the pyridoxal phosphatase chronophin. <i>Bioorganic and Medicinal Chemistry</i> , 2015, 23, 2819-2827.	1.4	12
99	Design, synthesis and evaluation of XZH-5 analogues as STAT3 inhibitors. <i>Bioorganic and Medicinal Chemistry</i> , 2015, 23, 1348-1355.	1.4	16
100	The tuberculosis necrotizing toxin kills macrophages by hydrolyzing NAD. <i>Nature Structural and Molecular Biology</i> , 2015, 22, 672-678.	3.6	114
101	Ionic-Liquid-Functionalized Mineral Particles for Protein Crystallization. <i>Crystal Growth and Design</i> , 2015, 15, 2994-3003.	1.4	8
102	Macromolecular Crystallography for Synthetic Abiological Molecules: Combining xMDFF and PHENIX for Structure Determination of Cyanostar Macrocyces. <i>Journal of the American Chemical Society</i> , 2015, 137, 8810-8818.	6.6	29
103	The solvent component of macromolecular crystals. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2015, 71, 1023-1038.	2.5	47
104	CBR antimicrobials inhibit RNA polymerase via at least two bridge-helix cap-mediated effects on nucleotide addition. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015, 112, E4178-87.	3.3	33
105	Structure-Activity Relationship Study of Ionotropic Glutamate Receptor Antagonist (2 <i>S</i> ,3 <i>R</i>)-3-(3-Carboxyphenyl)pyrrolidine-2-carboxylic Acid. <i>Journal of Medicinal Chemistry</i> , 2015, 58, 6131-6150.	2.9	19
106	Structure of β -conglutin: insight into the quaternary structure of 7S basic globulins from legumes. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2015, 71, 224-238.	2.5	31
107	Synthesis of 2-deoxy-2,2-difluoro- β -maltosyl fluoride and its X-ray structure in complex with <i>Streptomyces coelicolor</i> GlgEI-V279S. <i>Organic and Biomolecular Chemistry</i> , 2015, 13, 7542-7550.	1.5	20
108	Structural Studies of Potassium Transport Protein KtrA Regulator of Conductance of K ⁺ (RCK) C Domain in Complex with Cyclic Diadenosine Monophosphate (c-di-AMP). <i>Journal of Biological Chemistry</i> , 2015, 290, 16393-16402.	1.6	74

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109	Formation of a Novel Macrocyclic Alkaloid from the Unnatural Farnesyl Diphosphate Analogue Anilinogeranyl Diphosphate by 5-Epi-Aristolochene Synthase. <i>ACS Chemical Biology</i> , 2015, 10, 1729-1736.	1.6	31
110	Azasugar inhibitors as pharmacological chaperones for Krabbe disease. <i>Chemical Science</i> , 2015, 6, 3075-3086.	3.7	42
111	Calcium ions open a selectivity filter gate during activation of the MthK potassium channel. <i>Nature Communications</i> , 2015, 6, 8342.	5.8	35
112	Cyclic Peptides Incorporating Phosphotyrosine Mimetics as Potent and Specific Inhibitors of the Grb7 Breast Cancer Target. <i>Journal of Medicinal Chemistry</i> , 2015, 58, 7707-7718.	2.9	19
113	Creaserin uses a TOG domain array to regulate microtubules in the primary cilium. <i>Molecular Biology of the Cell</i> , 2015, 26, 4248-4264.	0.9	52
114	Structure of the Ergothioneine Biosynthesis Amidohydrolase EgtC. <i>ChemBioChem</i> , 2015, 16, 1490-1496.	1.3	32
116	Structural Basis for Substrate Specificity in Adenosylcobalamin-dependent Isobutyryl-CoA Mutase and Related Acyl-CoA Mutases. <i>Journal of Biological Chemistry</i> , 2015, 290, 26882-26898.	1.6	24
117	The amylase inhibitor montbretin A reveals a new glycosidase inhibition motif. <i>Nature Chemical Biology</i> , 2015, 11, 691-696.	3.9	113
118	The Substrate-free and -bound Crystal Structures of the Duplicated Taurocyamine Kinase from the Human Parasite <i>Schistosoma mansoni</i> . <i>Journal of Biological Chemistry</i> , 2015, 290, 12951-12963.	1.6	9
119	Structural basis for drug-induced allosteric changes to human β^2 -cardiac myosin motor activity. <i>Nature Communications</i> , 2015, 6, 7974.	5.8	94
120	Isoform-Selective and Stereoselective Inhibition of Hypoxia Inducible Factor-2. <i>Journal of Medicinal Chemistry</i> , 2015, 58, 5930-5941.	2.9	59
121	The non-detergent sulfobetaine-201 acts as a pharmacological chaperone to promote folding and crystallization of the type II TGF- β^2 receptor extracellular domain. <i>Protein Expression and Purification</i> , 2015, 115, 19-25.	0.6	5
122	Discovery and structure of a new inhibitor scaffold of the autophagy initiating kinase ULK1. <i>Bioorganic and Medicinal Chemistry</i> , 2015, 23, 5483-5488.	1.4	58
123	Newton's cradle-proton relay with amide-imidic acid tautomerization in inverting cellulase visualized by neutron crystallography. <i>Science Advances</i> , 2015, 1, e1500263.	4.7	80
124	Structural Basis for the ATP-dependent Configuration of Adenylation Active Site in <i>Bacillus subtilis</i> o-Succinylbenzoyl-CoA Synthetase. <i>Journal of Biological Chemistry</i> , 2015, 290, 23971-23983.	1.6	13
125	Combining 'dry' co-crystallization and <i>in situ</i> diffraction to facilitate ligand screening by X-ray crystallography. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2015, 71, 1777-1787.	2.5	40
126	Identification and Characterization of a Methionine β -Lyase in the Calicheamicin Biosynthetic Cluster of <i>Micromonospora echinospora</i> . <i>ChemBioChem</i> , 2015, 16, 100-109.	1.3	21
127	Ergothioneine Biosynthetic Methyltransferase EgtD Reveals the Structural Basis of Aromatic Amino Acid Betaine Biosynthesis. <i>ChemBioChem</i> , 2015, 16, 119-125.	1.3	48

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128	Structural basis for small molecule targeting of the programmed death ligand 1 (PD-L1). <i>Oncotarget</i> , 2016, 7, 30323-30335.	0.8	297
129	Relief of autoinhibition by conformational switch explains enzyme activation by a catalytically dead paralog. <i>ELife</i> , 2016, 5, .	2.8	19
130	Structural Investigations of N-carbamoylputrescine Amidohydrolase from <i>Medicago truncatula</i> : Insights into the Ultimate Step of Putrescine Biosynthesis in Plants. <i>Frontiers in Plant Science</i> , 2016, 7, 350.	1.7	23
131	ID388 Polyhalogenated Derivatives as Probes for an Improved Structure-Based Selectivity of AKR1B10 Inhibitors. <i>ACS Chemical Biology</i> , 2016, 11, 2693-2705.	1.6	19
132	Structure of Mammalian Respiratory Supercomplex I 1 III 2 IV 1. <i>Cell</i> , 2016, 167, 1598-1609.e10.	13.5	311
133	Molecular basis of cobalamin-dependent RNA modification. <i>Nucleic Acids Research</i> , 2016, 44, gkw806.	6.5	29
134	Ribosomal 18S rRNA base pairs with mRNA during eukaryotic translation initiation. <i>Nature Communications</i> , 2016, 7, 12622.	5.8	41
135	Using hydrogen deuterium exchange mass spectrometry to engineer optimized constructs for crystallization of protein complexes: Case study of PI4KIII ² with Rab11. <i>Protein Science</i> , 2016, 25, 826-839.	3.1	39
136	Reversible, partial inactivation of plant betaine aldehyde dehydrogenase by betaine aldehyde: mechanism and possible physiological implications. <i>Biochemical Journal</i> , 2016, 473, 873-885.	1.7	8
137	TRPV1 structures in nanodiscs reveal mechanisms of ligand and lipid action. <i>Nature</i> , 2016, 534, 347-351.	13.7	702
138	Influence of cysteine 164 on active site structure in rat cysteine dioxygenase. <i>Journal of Biological Inorganic Chemistry</i> , 2016, 21, 501-510.	1.1	18
139	Structural insights into chaperone-activity enhancement by a K354E mutation in tomato acidic leucine aminopeptidase. <i>Acta Crystallographica Section D: Structural Biology</i> , 2016, 72, 694-702.	1.1	4
140	Chemically Linked Vemurafenib Inhibitors Promote an Inactive BRAF ^{V600E} Conformation. <i>ACS Chemical Biology</i> , 2016, 11, 2876-2888.	1.6	26
141	Enzymatic hydrolysis by transition-metal-dependent nucleophilic aromatic substitution. <i>Nature Chemical Biology</i> , 2016, 12, 1031-1036.	3.9	12
142	A Modified P1 Moiety Enhances <i>In Vitro</i> Antiviral Activity against Various Multidrug-Resistant HIV-1 Variants and <i>In Vitro</i> Central Nervous System Penetration Properties of a Novel Nonpeptidic Protease Inhibitor, GRL-10413. <i>Antimicrobial Agents and Chemotherapy</i> , 2016, 60, 7046-7059.	1.4	14
143	Arginine phosphorylation marks proteins for degradation by a Clp protease. <i>Nature</i> , 2016, 539, 48-53.	13.7	168
144	Discovery of Potent Pantothenamide Inhibitors of <i>Staphylococcus aureus</i> Pantothenate Kinase through a Minimal SAR Study: Inhibition Is Due to Trapping of the Product. <i>ACS Infectious Diseases</i> , 2016, 2, 627-641.	1.8	13
145	Structural basis of HIV inhibition by translocation-defective RT inhibitor 4 ϵ -ethynyl-2-fluoro-2'-deoxyadenosine (EFdA). <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2016, 113, 9274-9279.	3.3	73

#	ARTICLE	IF	CITATIONS
146	The Structure of the Antibiotic Deactivating, N-hydroxylating Rifampicin Monooxygenase. <i>Journal of Biological Chemistry</i> , 2016, 291, 21553-21562.	1.6	36
147	Drug design from the cryptic inhibitor envelope. <i>Nature Communications</i> , 2016, 7, 10638.	5.8	50
148	Structure-Activity Relationship for Sulfonamide Inhibition of <i>Helicobacter pylori</i> β -Carbonic Anhydrase. <i>Journal of Medicinal Chemistry</i> , 2016, 59, 11098-11109.	2.9	48
149	Mechanistic Insights from the Crystal Structure of <i>Bacillus subtilis</i> α -Succinylbenzoyl-CoA Synthetase Complexed with the Adenylate Intermediate. <i>Biochemistry</i> , 2016, 55, 6685-6695.	1.2	8
150	An HD domain phosphohydrolase active site tailored for oxetanocin-A biosynthesis. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2016, 113, 13750-13755.	3.3	27
151	Vinylogous Dehydration by a Polyketide Dehydratase Domain in Curacin Biosynthesis. <i>Journal of the American Chemical Society</i> , 2016, 138, 16024-16036.	6.6	36
152	Rational Design of Thermodynamic and Kinetic Binding Profiles by Optimizing Surface Water Networks Coating Protein-Bound Ligands. <i>Journal of Medicinal Chemistry</i> , 2016, 59, 10530-10548.	2.9	64
153	Highly selective inhibition of myosin motors provides the basis of potential therapeutic application. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2016, 113, E7448-E7455.	3.3	34
154	Unexpected involvement of staple leads to redesign of selective bicyclic peptide inhibitor of Grb7. <i>Scientific Reports</i> , 2016, 6, 27060.	1.6	20
155	Crystal structure of the cyan fluorescent protein Cerulean-S175G. <i>Acta Crystallographica Section F, Structural Biology Communications</i> , 2016, 72, 516-522.	0.4	2
156	Cross-class metallo- β -lactamase inhibition by bithiazolidines reveals multiple binding modes. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2016, 113, E3745-54.	3.3	122
157	Direct-methods structure determination of a trypanosome RNA-editing substrate fragment with translational pseudosymmetry. <i>Acta Crystallographica Section D: Structural Biology</i> , 2016, 72, 477-487.	1.1	5
158	Glucosyl epigallocatechin gallate allows mechanism-based inactivation and structural analysis of human pancreatic α -amylase. <i>FEBS Letters</i> , 2016, 590, 1143-1151.	1.3	19
159	Studies on Aryl-Substituted Phenylalanines: Synthesis, Activity, and Different Binding Modes at AMPA Receptors. <i>Journal of Medicinal Chemistry</i> , 2016, 59, 448-461.	2.9	8
160	The <i>Ascaris suum</i> nicotinic receptor, ACR-16, as a drug target: Four novel negative allosteric modulators from virtual screening. <i>International Journal for Parasitology: Drugs and Drug Resistance</i> , 2016, 6, 60-73.	1.4	16
161	Tweaking Subtype Selectivity and Agonist Efficacy at (S)-2-Amino-3-(3-hydroxy-5-methyl-isoxazol-4-yl)propionic acid (AMPA) Receptors in a Small Series of BnTetAMPA Analogues. <i>Journal of Medicinal Chemistry</i> , 2016, 59, 2244-2254.	2.9	4
162	Design and Structural Characterization of Potent and Selective Inhibitors of Phosphatidylinositol 4 Kinase III β . <i>Journal of Medicinal Chemistry</i> , 2016, 59, 1830-1839.	2.9	52
163	Hepatitis B Virus Capsids Have Diverse Structural Responses to Small-Molecule Ligands Bound to the Heteroaryldihydropyrimidine Pocket. <i>Journal of Virology</i> , 2016, 90, 3994-4004.	1.5	65

#	ARTICLE	IF	CITATIONS
164	Synthesis and Pharmacology of Mono-, Di-, and Trialkyl-Substituted 7-Chloro-3,4-dihydro-2 <i>H</i> -1,2,4-benzothiadiazine 1,1-Dioxides Combined with X-ray Structure Analysis to Understand the Unexpected Structure-Activity Relationship at AMPA Receptors. <i>ACS Chemical Neuroscience</i> , 2016, 7, 378-390.	1.7	29
165	Crystal structure of the <i>Saccharomyces cerevisiae</i> monoglyceride lipase Yju3p. <i>Biochimica Et Biophysica Acta - Molecular and Cell Biology of Lipids</i> , 2016, 1861, 462-470.	1.2	25
166	The Structure of the Transcriptional Repressor KstR in Complex with CoA Thioester Cholesterol Metabolites Sheds Light on the Regulation of Cholesterol Catabolism in <i>Mycobacterium tuberculosis</i> . <i>Journal of Biological Chemistry</i> , 2016, 291, 7256-7266.	1.6	32
167	Structural and Mechanistic Insights into the Regulation of the Fundamental Rho Regulator RhoGDI± by Lysine Acetylation. <i>Journal of Biological Chemistry</i> , 2016, 291, 5484-5499.	1.6	45
168	Structure of an Actinobacterial-Type [NiFe]-Hydrogenase Reveals Insight into O ₂ -Tolerant H ₂ Oxidation. <i>Structure</i> , 2016, 24, 285-292.	1.6	43
169	C-5-Modified Tetrahydropyrano-Tetrahydrofuran-Derived Protease Inhibitors (PIs) Exert Potent Inhibition of the Replication of HIV-1 Variants Highly Resistant to Various PIs, including Darunavir. <i>Journal of Virology</i> , 2016, 90, 2180-2194.	1.5	15
170	Structural Insights into Anthranilate Priming during Type II Polyketide Biosynthesis. <i>ACS Chemical Biology</i> , 2016, 11, 95-103.	1.6	25
171	Conformational energy range of ligands in protein crystal structures: The difficult quest for accurate understanding. <i>Journal of Molecular Recognition</i> , 2017, 30, e2618.	1.1	23
172	Structural Basis of Substrate Recognition by the Multidrug Resistance Protein MRP1. <i>Cell</i> , 2017, 168, 1075-1085.e9.	13.5	309
173	Mechanism-Based Inhibition of the <i>Mycobacterium tuberculosis</i> Branched-Chain Aminotransferase by <i>d</i> - and <i>l</i> -Cycloserine. <i>ACS Chemical Biology</i> , 2017, 12, 1235-1244.	1.6	33
174	Development of 1,2,4-Oxadiazoles as Potent and Selective Inhibitors of the Human Deacetylase Sirtuin 2: Structure-Activity Relationship, X-ray Crystal Structure, and Anticancer Activity. <i>Journal of Medicinal Chemistry</i> , 2017, 60, 2344-2360.	2.9	82
175	Structure of human IFIT1 with capped RNA reveals adaptable mRNA binding and mechanisms for sensing N1 and N2 ribose 2'-O methylations. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, E2106-E2115.	3.3	86
176	Rapid Discovery of Potent and Selective Glycosidase-Inhibiting De Novo Peptides. <i>Cell Chemical Biology</i> , 2017, 24, 381-390.	2.5	46
177	Keep it together: restraints in crystallographic refinement of macromolecule-ligand complexes. <i>Acta Crystallographica Section D: Structural Biology</i> , 2017, 73, 93-102.	1.1	19
178	Crystallographic structure of recombinant <i>Lactococcus lactis</i> prolidase to support proposed structure-function relationships. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2017, 1865, 473-480.	1.1	8
179	Elucidating the Origin of Long Residence Time Binding for Inhibitors of the Metalloprotease Thermolysin. <i>ACS Chemical Biology</i> , 2017, 12, 225-233.	1.6	14
180	Probing the influence of non-covalent contact networks identified by charge density analysis on the oxidoreductase BacC. <i>Protein Engineering, Design and Selection</i> , 2017, 30, 265-272.	1.0	5
181	Efficient switching of mCherry fluorescence using chemical caging. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, 7013-7018.	3.3	19

#	ARTICLE	IF	CITATIONS
182	Structure of human Fe ⁴ S assembly subcomplex reveals unexpected cysteine desulfurase architecture and acyl-ACP ⁴ ISD11 interactions. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E5325-E5334.	3.3	132
183	Paying the Price of Desolvation in Solvent-Exposed Protein Pockets: Impact of Distal Solubilizing Groups on Affinity and Binding Thermodynamics in a Series of Thermolysin Inhibitors. Journal of Medicinal Chemistry, 2017, 60, 5791-5799.	2.9	35
184	<sc>l</sc>-Arginine intercedes bio-crosslinking of a collagen ⁴ chitosan 3D-hybrid scaffold for tissue engineering and regeneration: in silico, in vitro, and in vivo studies. RSC Advances, 2017, 7, 25070-25088.	1.7	44
185	Assessing therapeutic potential of molecules: molecular property diagnostic suite for tuberculosis $\mathbf{MPDS}^{\mathbf{TB}}$ (MPDS TB). Journal of Chemical Sciences, 2017, 129, 515-531.	0.7	20
186	Insights into Hunter syndrome from the structure of iduronate-2-sulfatase. Nature Communications, 2017, 8, 15786.	5.8	68
187	Crystal structure of the thioesterification conformation of Bacillus subtilis o-succinylbenzoyl-CoA synthetase reveals a distinct substrate-binding mode. Journal of Biological Chemistry, 2017, 292, 12296-12310.	1.6	6
188	Conformational Control of UDP-Galactopyranose Mutase Inhibition. Biochemistry, 2017, 56, 3983-3992.	1.2	2
189	Structural basis for the inhibition of AKR1B10 by the C3 brominated TTNPB derivative UVI2008. Chemico-Biological Interactions, 2017, 276, 174-181.	1.7	3
190	Inositol phosphates and phosphoinositides activate insulin-degrading enzyme, while phosphoinositides also mediate binding to endosomes. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E2826-E2835.	3.3	17
191	A new class of inhibitors of the AraC family virulence regulator Vibrio cholerae ToxT. Scientific Reports, 2017, 7, 45011.	1.6	16
192	A B12-dependent radical SAM enzyme involved in oxetanocin A biosynthesis. Nature, 2017, 544, 322-326.	13.7	91
193	Investigation of the mycobacterial enzyme HsaD as a potential novel target for anti ⁴ tubercular agents using a fragment ⁴ based drug design approach. British Journal of Pharmacology, 2017, 174, 2209-2224.	2.7	19
194	Inducer exclusion in Firmicutes: insights into the regulation of a carbohydrate ATP binding cassette transporter from <i>Lactobacillus casei</i> BL23 by the signal transducing protein ⁴ Ser46 ⁴ HP. Molecular Microbiology, 2017, 105, 25-45.	1.2	20
195	Identification and Structure-Function Study of Positive Allosteric Modulators of Kainate Receptors. Molecular Pharmacology, 2017, 91, 576-585.	1.0	21
196	Exploring Covalent Allosteric Inhibition of Antigen 85C from Mycobacterium tuberculosis by Ebselen Derivatives. ACS Infectious Diseases, 2017, 3, 378-387.	1.8	26
197	Price for Opening the Transient Specificity Pocket in Human Aldose Reductase upon Ligand Binding: Structural, Thermodynamic, Kinetic, and Computational Analysis. ACS Chemical Biology, 2017, 12, 1397-1415.	1.6	23
198	Structural and Molecular Mechanisms of Cytokine-Mediated Endocrine Resistance in Human Breast Cancer Cells. Molecular Cell, 2017, 65, 1122-1135.e5.	4.5	99
199	Design and Synthesis of a Series of <i>trans</i> -4-Substituted Prolines as Selective Antagonists for the Ionotropic Glutamate Receptors Including Functional and X-ray Crystallographic Studies of New Subtype Selective Kainic Acid Receptor Subtype 1 (GluK1) Antagonist (2 <i>S</i> ,4 <i>R</i>)-4-(2-Carboxyphenoxy)pyrrolidine-2-carboxylic Acid. Journal of Medicinal Chemistry, 2017, 60, 441-457.	2.9	6

#	ARTICLE	IF	CITATIONS
200	Pyocyanin degradation by a tautomerizing demethylase inhibits <i>Pseudomonas aeruginosa</i> biofilms. <i>Science</i> , 2017, 355, 170-173.	6.0	53
201	Identification of mouse cathepsin K structural elements that regulate the potency of odanacatib. <i>Biochemical Journal</i> , 2017, 474, 851-864.	1.7	24
202	Discovery, Development, and Cellular Delivery of Potent and Selective Bicyclic Peptide Inhibitors of Grb7 Cancer Target. <i>Journal of Medicinal Chemistry</i> , 2017, 60, 9349-9359.	2.9	24
203	GRL-09510, a Unique P2-Crown-Tetrahydrofuranylurethane -Containing HIV-1 Protease Inhibitor, Maintains Its Favorable Antiviral Activity against Highly-Drug-Resistant HIV-1 Variants in vitro. <i>Scientific Reports</i> , 2017, 7, 12235.	1.6	16
204	Isomer activation controls stereospecificity of class I fructose-1,6-bisphosphate aldolases. <i>Journal of Biological Chemistry</i> , 2017, 292, 19849-19860.	1.6	5
205	Structural basis for maintenance of bacterial outer membrane lipid asymmetry. <i>Nature Microbiology</i> , 2017, 2, 1616-1623.	5.9	118
206	Ras Binder Induces a Modified Switch-II Pocket in GTP and GDP States. <i>Cell Chemical Biology</i> , 2017, 24, 1455-1466.e14.	2.5	78
207	Architecture of Human Mitochondrial Respiratory Megacomplex I2III2IV2. <i>Cell</i> , 2017, 170, 1247-1257.e12.	13.5	362
208	5-(4,6-Dimorpholino-1,3,5-triazin-2-yl)-4-(trifluoromethyl)pyridin-2-amine (PQR309), a Potent, Brain-Penetrant, Orally Bioavailable, Pan-Class I PI3K/mTOR Inhibitor as Clinical Candidate in Oncology. <i>Journal of Medicinal Chemistry</i> , 2017, 60, 7524-7538.	2.9	109
209	Structural/mechanistic insights into the efficacy of nonclassical β -lactamase inhibitors against extensively drug resistant <i>Stenotrophomonas maltophilia</i> clinical isolates. <i>Molecular Microbiology</i> , 2017, 106, 492-504.	1.2	39
210	An Activator-Blocker Pair Provides a Controllable On-Off Switch for a Ketosteroid Isomerase Active Site Mutant. <i>Journal of the American Chemical Society</i> , 2017, 139, 11089-11095.	6.6	3
211	How Nothing Boosts Affinity: Hydrophobic Ligand Binding to the Virtually Vacated S ₁ Pocket of Thermolysin. <i>Journal of the American Chemical Society</i> , 2017, 139, 10419-10431.	6.6	23
212	Curative Treatment of Severe Gram-Negative Bacterial Infections by a New Class of Antibiotics Targeting LpxC. <i>MBio</i> , 2017, 8, .	1.8	24
213	TubZ filament assembly dynamics requires the flexible C-terminal tail. <i>Scientific Reports</i> , 2017, 7, 43342.	1.6	3
214	Identification of a New Zinc Binding Chemotype by Fragment Screening. <i>Journal of Medicinal Chemistry</i> , 2017, 60, 7333-7349.	2.9	18
215	Mechanistic and structural basis for activation of cardiac myosin force production by omecamtiv mecarbil. <i>Nature Communications</i> , 2017, 8, 190.	5.8	153
216	Structural insight into a CE15 esterase from the marine bacterial metagenome. <i>Scientific Reports</i> , 2017, 7, 17278.	1.6	17
217	Architecture of the human PI4KIII β lipid kinase complex. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, 13720-13725.	3.3	54

#	ARTICLE	IF	CITATIONS
218	Eudicot plant-specific sphingolipids determine host selectivity of microbial NLP cytolysins. <i>Science</i> , 2017, 358, 1431-1434.	6.0	167
219	Structural insights into enzymatic [4+2] <i>cycloaddition</i> in thiopeptide antibiotic biosynthesis. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, 12928-12933.	3.3	70
220	Pink-beam serial crystallography. <i>Nature Communications</i> , 2017, 8, 1281.	5.8	101
221	Structure and Affinity of Two Bicyclic Glutamate Analogues at AMPA and Kainate Receptors. <i>ACS Chemical Neuroscience</i> , 2017, 8, 2056-2064.	1.7	15
222	Structural analyses of human thymidylate synthase reveal a site that may control conformational switching between active and inactive states. <i>Journal of Biological Chemistry</i> , 2017, 292, 13449-13458.	1.6	44
223	Caught before Released: Structural Mapping of the Reaction Trajectory for the Sofosbuvir Activating Enzyme, Human Histidine Triad Nucleotide Binding Protein 1 (hHint1). <i>Biochemistry</i> , 2017, 56, 3559-3570.	1.2	22
224	Cobamide-mediated enzymatic reductive dehalogenation via long-range electron transfer. <i>Nature Communications</i> , 2017, 8, 15858.	5.8	68
225	Development of a Novel Lead that Targets M. <i>tuberculosis</i> Polyketide Synthase 13. <i>Cell</i> , 2017, 170, 249-259.e25.	13.5	124
226	Optimized 4,5-Diarylimidazoles as Potent/Selective Inhibitors of Protein Kinase CK1 α and Their Structural Relation to p38 β MAPK. <i>Molecules</i> , 2017, 22, 522.	1.7	35
227	A novel central nervous system-penetrating protease inhibitor overcomes human immunodeficiency virus 1 resistance with unprecedented aM to pM potency. <i>ELife</i> , 2017, 6, .	2.8	44
228	Crystallographic and SAXS studies of <i>S</i> -adenosyl-L-homocysteine hydrolase from <i>Bradyrhizobium elkanii</i> . <i>IUCr</i> , 2017, 4, 271-282.	1.0	11
229	La-related protein 1 (LARP1) binds the mRNA cap, blocking eIF4F assembly on TOP mRNAs. <i>ELife</i> , 2017, 6, .	2.8	136
230	Fragment library screening identifies hits that bind to the non-catalytic surface of <i>Pseudomonas aeruginosa</i> DsbA1. <i>PLoS ONE</i> , 2017, 12, e0173436.	1.1	17
231	Metal ion coordination in the <i>E. coli</i> Nudix hydrolase dihydroneopterin triphosphate pyrophosphatase: New clues into catalytic mechanism. <i>PLoS ONE</i> , 2017, 12, e0180241.	1.1	3
232	Crystal structure and functional characterization of an isoaspartyl dipeptidase (CpsladA) from <i>Colwellia psychrerythraea</i> strain 34H. <i>PLoS ONE</i> , 2017, 12, e0181705.	1.1	7
233	<i>AceDRG</i> : a stereochemical description generator for ligands. <i>Acta Crystallographica Section D: Structural Biology</i> , 2017, 73, 112-122.	1.1	254
234	Strategies for carbohydrate model building, refinement and validation. <i>Acta Crystallographica Section D: Structural Biology</i> , 2017, 73, 171-186.	1.1	49
235	The AibR-isovaleryl coenzyme A regulator and its DNA binding site – a model for the regulation of alternative de novo isovaleryl coenzyme A biosynthesis in <i>Mycococcus xanthus</i> . <i>Nucleic Acids Research</i> , 2017, 45, 2166-2178.	6.5	7

#	ARTICLE	IF	CITATIONS
236	<i>Streptomyces wadayamensis</i> MppP is a PLP-Dependent Oxidase, Not an Oxygenase. <i>Biochemistry</i> , 2018, 57, 3252-3264.	1.2	19
237	Snapshots of the Catalytic Cycle of an O ₂ , Pyridoxal Phosphate-Dependent Hydroxylase. <i>ACS Chemical Biology</i> , 2018, 13, 965-974.	1.6	12
238	A family of unconventional deubiquitinases with modular chain specificity determinants. <i>Nature Communications</i> , 2018, 9, 799.	5.8	108
239	Elucidation of Hydrogen Bonding Patterns in Ligand-Free, Lactose- and Glycerol-Bound Galectin-3C by Neutron Crystallography to Guide Drug Design. <i>Journal of Medicinal Chemistry</i> , 2018, 61, 4412-4420.	2.9	32
240	Design, synthesis, structure-activity relationships and X-ray structural studies of novel 1-oxopyrimido[4,5-c]quinoline-2-acetic acid derivatives as selective and potent inhibitors of human aldose reductase. <i>European Journal of Medicinal Chemistry</i> , 2018, 152, 160-174.	2.6	26
241	Potent 3-Hydroxy-2-Pyridine Aldoxime Reactivators of Organophosphate-Inhibited Cholinesterases with Predicted Blood-Brain Barrier Penetration. <i>Chemistry - A European Journal</i> , 2018, 24, 9675-9691.	1.7	50
242	Validating Resolution Revolution. <i>Structure</i> , 2018, 26, 785-795.e4.	1.6	25
243	Discovery of Inhibitor of Wnt Production 2 (IWP-2) and Related Compounds As Selective ATP-Competitive Inhibitors of Casein Kinase 1 (CK1) β . <i>Journal of Medicinal Chemistry</i> , 2018, 61, 4087-4102.	2.9	42
244	Effects of rigidity on the selectivity of protein kinase inhibitors. <i>European Journal of Medicinal Chemistry</i> , 2018, 146, 519-528.	2.6	11
245	Phenylboronic Acid Derivatives as Validated Leads Active in Clinical Strains Overexpressing KPC β : A Step against Bacterial Resistance. <i>ChemMedChem</i> , 2018, 13, 713-724.	1.6	24
246	Mycolytransferase from <i>Mycobacterium tuberculosis</i> in covalent complex with tetrahydrolipstatin provides insights into antigen 85 catalysis. <i>Journal of Biological Chemistry</i> , 2018, 293, 3651-3662.	1.6	16
247	Species-Selective Pyrimidineamine Inhibitors of <i>Trypanosoma brucei</i> S-Adenosylmethionine Decarboxylase. <i>Journal of Medicinal Chemistry</i> , 2018, 61, 1182-1203.	2.9	13
248	Structure of the G119S Mutant Acetylcholinesterase of the Malaria Vector <i>Anopheles gambiae</i> Reveals Basis of Insecticide Resistance. <i>Structure</i> , 2018, 26, 130-136.e2.	1.6	44
249	Systematic Tuning of Fluoro-galectin-3 Interactions Provides Thiodigalactoside Derivatives with Single-Digit nM Affinity and High Selectivity. <i>Journal of Medicinal Chemistry</i> , 2018, 61, 1164-1175.	2.9	76
250	7-Phenoxy-Substituted 3,4-Dihydro-2H-1,2,4-benzothiadiazine 1,1-Dioxides as Positive Allosteric Modulators of β -Amino-3-hydroxy-5-methyl-4-isoxazolepropionic Acid (AMPA) Receptors with Nanomolar Potency. <i>Journal of Medicinal Chemistry</i> , 2018, 61, 251-264.	2.9	41
251	Structures of the Peptidoglycan N-Acetylglucosamine Deacetylase Bc1974 and Its Complexes with Zinc Metalloenzyme Inhibitors. <i>Biochemistry</i> , 2018, 57, 753-763.	1.2	18
252	Design, Synthesis, and Biological Evaluation of 4-Quinoline Carboxylic Acids as Inhibitors of Dihydroorotate Dehydrogenase. <i>Journal of Medicinal Chemistry</i> , 2018, 61, 5162-5186.	2.9	45
253	Development of Thioaryl-Based Matrix Metalloproteinase-12 Inhibitors with Alternative Zinc-Binding Groups: Synthesis, Potentiometric, NMR, and Crystallographic Studies. <i>Journal of Medicinal Chemistry</i> , 2018, 61, 4421-4435.	2.9	34

#	ARTICLE	IF	CITATIONS
254	Improved protein-crystal identification by using 2,2,2-trichloroethanol as a fluorescence enhancer. <i>Acta Crystallographica Section F, Structural Biology Communications</i> , 2018, 74, 307-314.	0.4	2
255	Structure of the nucleotide exchange factor eIF2B reveals mechanism of memory-enhancing molecule. <i>Science</i> , 2018, 359, .	6.0	143
256	Structural basis of small-molecule inhibition of human multidrug transporter ABCG2. <i>Nature Structural and Molecular Biology</i> , 2018, 25, 333-340.	3.6	258
257	Halogenation of Biotin Protein Ligase Inhibitors Improves Whole Cell Activity against <i>Staphylococcus aureus</i> . <i>ACS Infectious Diseases</i> , 2018, 4, 175-184.	1.8	22
258	Structural and Functional Studies of the Daunorubicin Priming Ketosynthase DpsC. <i>ACS Chemical Biology</i> , 2018, 13, 141-151.	1.6	15
259	High-throughput quantum-mechanics/molecular-mechanics (ONIOM) macromolecular crystallographic refinement with <i>PHENIX</i> / <i>DivCon</i> : the impact of mixed Hamiltonian methods on ligand and protein structure. <i>Acta Crystallographica Section D: Structural Biology</i> , 2018, 74, 1063-1077.	1.1	18
260	Bisphosphonate Inhibitors of Mammalian Glycolytic Aldolase. <i>Journal of Medicinal Chemistry</i> , 2018, 61, 10558-10572.	2.9	8
261	Cryo-EM structures of a human ABCG2 mutant trapped in ATP-bound and substrate-bound states. <i>Nature</i> , 2018, 563, 426-430.	13.7	188
263	Widespread bacterial lysine degradation proceeding via glutarate and L-2-hydroxyglutarate. <i>Nature Communications</i> , 2018, 9, 5071.	5.8	65
264	Structures of human cytochrome P450 1A1 with bergamottin and erlotinib reveal active-site modifications for binding of diverse ligands. <i>Journal of Biological Chemistry</i> , 2018, 293, 19201-19210.	1.6	41
265	myo-Inositol dehydrogenase and scyllo-inositol dehydrogenase from <i>Lactobacillus casei</i> BL23 bind their substrates in very different orientations. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2018, 1866, 1115-1124.	1.1	6
266	Refining the macromolecular model “ achieving the best agreement with the data from X-ray diffraction experiment. <i>Crystallography Reviews</i> , 2018, 24, 236-262.	0.4	43
267	Towards a comprehensive understanding of the structural dynamics of a bacterial diterpene synthase during catalysis. <i>Nature Communications</i> , 2018, 9, 3971.	5.8	57
268	Crystal structure of yeast xylose reductase in complex with a novel <i>NADP</i> â€‹ <i>DTT</i> adduct provides insights into substrate recognition and catalysis. <i>FEBS Journal</i> , 2018, 285, 4445-4464.	2.2	9
269	Structural Insight into a Novel Formyltransferase and Evolution to a Nonribosomal Peptide Synthetase Tailoring Domain. <i>ACS Chemical Biology</i> , 2018, 13, 3161-3172.	1.6	8
270	Structural Analysis of Phosphoserine Aminotransferase (Isoform 1) From <i>Arabidopsis thaliana</i> â€‹ the Enzyme Involved in the Phosphorylated Pathway of Serine Biosynthesis. <i>Frontiers in Plant Science</i> , 2018, 9, 876.	1.7	21
271	Molecular mechanism of activation of the immunoregulatory amidase NAAA. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018, 115, E10032-E10040.	3.3	36
272	Two active site arginines are critical determinants of substrate binding and catalysis in MenD: a thiamine-dependent enzyme in menaquinone biosynthesis. <i>Biochemical Journal</i> , 2018, 475, 3651-3667.	1.7	11

#	ARTICLE	IF	CITATIONS
273	Structural basis of the filamin A actin-binding domain interaction with F-actin. <i>Nature Structural and Molecular Biology</i> , 2018, 25, 918-927.	3.6	60
274	Carboxylic Acid Derivatives of Amlexanox Display Enhanced Potency toward TBK1 and IKK μ and Reveal Mechanisms for Selective Inhibition. <i>Molecular Pharmacology</i> , 2018, 94, 1210-1219.	1.0	36
275	Structural basis for potent and broad inhibition of HIV-1 RT by thiophene[3,2-d]pyrimidine non-nucleoside inhibitors. <i>ELife</i> , 2018, 7, .	2.8	57
276	Substrate-assisted enzymatic formation of lysinoalanine in duramycin. <i>Nature Chemical Biology</i> , 2018, 14, 928-933.	3.9	25
277	The synthesis and kinetic evaluation of aryl β -aminophosphonates as novel inhibitors of T. β cruzi trans-sialidase. <i>European Journal of Medicinal Chemistry</i> , 2018, 158, 25-33.	2.6	10
278	Structure of the <i>Cladosporium fulvum</i> Avr4 effector in complex with (GlcNAc) ₆ reveals the ligand-binding mechanism and uncouples its intrinsic function from recognition by the Cf-4 resistance protein. <i>PLoS Pathogens</i> , 2018, 14, e1007263.	2.1	37
279	Enhancing Action of Positive Allosteric Modulators through the Design of Dimeric Compounds. <i>Journal of Medicinal Chemistry</i> , 2018, 61, 5279-5291.	2.9	41
280	Antibacterial Spectrum of a Tetrazole-Based Reversible Inhibitor of Serine β -Lactamases. <i>Antimicrobial Agents and Chemotherapy</i> , 2018, 62, .	1.4	11
281	Deciphering the mechanism of potent peptidomimetic inhibitors targeting plasmepsins – biochemical and structural insights. <i>FEBS Journal</i> , 2018, 285, 3077-3096.	2.2	11
282	Cryo-EM structure of a mitochondrial calcium uniporter. <i>Science</i> , 2018, 361, 506-511.	6.0	116
283	An expanded allosteric network in PTP1B by multitemperature crystallography, fragment screening, and covalent tethering. <i>ELife</i> , 2018, 7, .	2.8	120
284	X-ray Crystal Structures Show DNA Stacking Advantage of Terminal Nitrile Substitution in Ru β ppz Complexes. <i>Chemistry - A European Journal</i> , 2018, 24, 15859-15867.	1.7	16
285	Hepatitis B virus core protein allosteric modulators can distort and disrupt intact capsids. <i>ELife</i> , 2018, 7, .	2.8	76
286	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.	5.5	15
287	Structure of the intact 14-subunit human cytochrome c oxidase. <i>Cell Research</i> , 2018, 28, 1026-1034.	5.7	159
288	The phage T4 MotA transcription factor contains a novel DNA binding motif that specifically recognizes modified DNA. <i>Nucleic Acids Research</i> , 2018, 46, 5308-5318.	6.5	6
289	Overview of refinement procedures within <i>REFMAC</i> 5: utilizing data from different sources. <i>Acta Crystallographica Section D: Structural Biology</i> , 2018, 74, 215-227.	1.1	194
290	The Structural and Functional Basis for Recurring Sulfa Drug Resistance Mutations in <i>Staphylococcus aureus</i> Dihydropteroate Synthase. <i>Frontiers in Microbiology</i> , 2018, 9, 1369.	1.5	58

#	ARTICLE	IF	CITATIONS
291	Crystal structure of highly glycosylated human leukocyte elastase in complex with an S2â€² site binding inhibitor. <i>Acta Crystallographica Section F, Structural Biology Communications</i> , 2018, 74, 480-489.	0.4	15
292	Validation of ligands in macromolecular structures determined by X-ray crystallography. <i>Acta Crystallographica Section D: Structural Biology</i> , 2018, 74, 228-236.	1.1	45
293	Molecular Recognition of a Thomsenâ€™Friedenreich Antigen Mimetic Targeting Human Galectinâ€™3. <i>ChemMedChem</i> , 2018, 13, 2030-2036.	1.6	13
294	Structure-Based Optimization of Nonquaternary Reactivators of Acetylcholinesterase Inhibited by Organophosphorus Nerve Agents. <i>Journal of Medicinal Chemistry</i> , 2018, 61, 7630-7639.	2.9	44
295	Snapshots of an evolved DNA polymerase pre- and post-incorporation of an unnatural nucleotide. <i>Nucleic Acids Research</i> , 2018, 46, 7977-7988.	6.5	18
296	Structural basis of transcriptional regulation by CouR, a repressor of coumarate catabolism, in <i>Rhodospseudomonas palustris</i> . <i>Journal of Biological Chemistry</i> , 2018, 293, 11727-11735.	1.6	10
297	Plasticity in binding confers selectivity in ligand-induced protein degradation. <i>Nature Chemical Biology</i> , 2018, 14, 706-714.	3.9	391
298	An Evolutionarily Conserved Structural Platform for PRC2 Inhibition by a Class of Ezh2 Inhibitors. <i>Scientific Reports</i> , 2018, 8, 9092.	1.6	27
299	HIV-1 Protease Inhibitors Incorporating Stereochemically Defined P2â€™ Ligands To Optimize Hydrogen Bonding in the Substrate Envelope. <i>Journal of Medicinal Chemistry</i> , 2019, 62, 8062-8079.	2.9	21
300	Molecular Determinants of Epistasis in HIV-1 Protease: Elucidating the Interdependence of L89V and L90M Mutations in Resistance. <i>Biochemistry</i> , 2019, 58, 3711-3726.	1.2	15
301	The ligand-mediated affinity of brain-type fatty acid-binding protein for membranes determines the directionality of lipophilic cargo transport. <i>Biochimica Et Biophysica Acta - Molecular and Cell Biology of Lipids</i> , 2019, 1864, 158506.	1.2	6
302	Convergent biosynthetic transformations to a bacterial specialized metabolite. <i>Nature Chemical Biology</i> , 2019, 15, 1043-1048.	3.9	10
303	Picomolar to Micromolar: Elucidating the Role of Distal Mutations in HIV-1 Protease in Conferring Drug Resistance. <i>ACS Chemical Biology</i> , 2019, 14, 2441-2452.	1.6	36
304	Structural insights into the recognition of nucleoside reverse transcriptase inhibitors by HIVâ€™1 reverse transcriptase: First crystal structures with reverse transcriptase and the active triphosphate forms of lamivudine and emtricitabine. <i>Protein Science</i> , 2019, 28, 1664-1675.	3.1	20
305	Mechanistic investigation of mEos4b reveals a strategy to reduce track interruptions in sptPALM. <i>Nature Methods</i> , 2019, 16, 707-710.	9.0	43
306	Structural, Biochemical, and <i>In Vivo</i> Characterization of MtrR-Mediated Resistance to Innate Antimicrobials by the Human Pathogen <i>Neisseria gonorrhoeae</i> . <i>Journal of Bacteriology</i> , 2019, 201, .	1.0	13
307	The structural basis of N-acyl-Î±-amino-Î²-lactone formation catalyzed by a nonribosomal peptide synthetase. <i>Nature Communications</i> , 2019, 10, 3432.	5.8	50
308	Mechanism of Î²₂ AR regulation by an intracellular positive allosteric modulator. <i>Science</i> , 2019, 364, 1283-1287.	6.0	82

#	ARTICLE	IF	CITATIONS
309	Structure and Energetics of Ligand-Fluorine Interactions with Galectin-3 Backbone and Side-Chain Amides: Insight into Solvation Effects and Multipolar Interactions. <i>ChemMedChem</i> , 2019, 14, 1528-1536.	1.6	24
310	Large conformation shifts of <i>Vibrio cholerae</i> VqmA dimer in the absence of target DNA provide insight into DNA-binding mechanisms of LuxR-type receptors. <i>Biochemical and Biophysical Research Communications</i> , 2019, 520, 399-405.	1.0	9
311	Itaconyl-CoA forms a stable biradical in methylmalonyl-CoA mutase and derails its activity and repair. <i>Science</i> , 2019, 366, 589-593.	6.0	71
312	Optimizing Targeted Inhibitors of P-Glycoprotein Using Computational and Structure-Guided Approaches. <i>Journal of Medicinal Chemistry</i> , 2019, 62, 10645-10663.	2.9	17
313	Structures of a dimodular nonribosomal peptide synthetase reveal conformational flexibility. <i>Science</i> , 2019, 366, .	6.0	99
314	New Insight into the Mechanism of Anaerobic Heme Degradation. <i>Biochemistry</i> , 2019, 58, 4641-4654.	1.2	17
315	Structural and biochemical characterization of iminodiacetate oxidase from <i>Chelativorans</i> sp. BNC1. <i>Molecular Microbiology</i> , 2019, 112, 1863-1874.	1.2	1
316	<i>N</i> -(7-(1 <i>H</i> -imidazol-1-yl)-2,3-dioxo-6-(trifluoromethyl)-3,4-dihydroquinoxalin-1(2 <i>H</i>)-yl)benzamide, a New Kainate Receptor Selective Antagonist and Analgesic: Synthesis, X-ray Crystallography, Structure-Affinity Relationships, and in Vitro and in Vivo Pharmacology. <i>ACS Chemical Neuroscience</i> , 2019, 10, 4685-4695.	1.7	8
317	The crystal structure of haemoglobin from Atlantic cod. <i>Acta Crystallographica Section F, Structural Biology Communications</i> , 2019, 75, 537-542.	0.4	0
318	Discovery of the First in Vivo Active Inhibitors of the Soluble Epoxide Hydrolase Phosphatase Domain. <i>Journal of Medicinal Chemistry</i> , 2019, 62, 8443-8460.	2.9	19
319	Visualizing structural transitions of ligand-dependent gating of the TRPM2 channel. <i>Nature Communications</i> , 2019, 10, 3740.	5.8	34
320	Heteroaryl Phosphonates as Noncovalent Inhibitors of Both Serine- and Metalloproteases. <i>Journal of Medicinal Chemistry</i> , 2019, 62, 8480-8496.	2.9	28
321	Structural insights into the G-loop dynamics of <i>E. coli</i> FtsY NG domain. <i>Journal of Structural Biology</i> , 2019, 208, 107387.	1.3	2
322	Mechanistic Studies of the <i>Streptomyces bingchenggensis</i> Aldolase-Dehydratase: Implications for Substrate and Reaction Specificity in the Acetoacetate Decarboxylase-like Superfamily. <i>Biochemistry</i> , 2019, 58, 4136-4147.	1.2	1
323	Phenylboronic Acids Probing Molecular Recognition against Class A and Class C β -lactamases. <i>Antibiotics</i> , 2019, 8, 171.	1.5	9
324	Gut bacteria responding to dietary change encode sialidases that exhibit preference for red meat-associated carbohydrates. <i>Nature Microbiology</i> , 2019, 4, 2082-2089.	5.9	56
325	Substituted polyfluoroaryl interactions with an arginine side chain in galectin-3 are governed by steric-, desolvation and electronic conjugation effects. <i>Organic and Biomolecular Chemistry</i> , 2019, 17, 1081-1089.	1.5	14
326	Predicting protein-ligand binding affinity and correcting crystal structures with quantum mechanical calculations: lactate dehydrogenase A. <i>Chemical Science</i> , 2019, 10, 2218-2227.	3.7	11

#	ARTICLE	IF	CITATIONS
327	PvdF of pyoverdin biosynthesis is a structurally unique N10-formyltetrahydrofolate-dependent formyltransferase. Archives of Biochemistry and Biophysics, 2019, 664, 40-50.	1.4	6
328	Identification of a ligand binding hot spot and structural motifs replicating aspects of tyrosyl-DNA phosphodiesterase I (TDP1) phosphoryl recognition by crystallographic fragment cocktail screening. Nucleic Acids Research, 2019, 47, 10134-10150.	6.5	27
329	Crystal structures of phage NrS-1 N300-dNTPs-Mg ²⁺ complex provide molecular mechanisms for substrate specificity. Biochemical and Biophysical Research Communications, 2019, 515, 551-557.	1.0	6
330	2'- and 6'-functionalized adenosine 5'-diphosphate analogs for the inhibition of mortalin. FEBS Letters, 2019, 593, 2030-2039.	1.3	4
331	Unravelling the covalent binding of zampanolide and taccalonolide A to a minimalist representation of a human microtubule. Journal of Computer-Aided Molecular Design, 2019, 33, 627-644.	1.3	11
332	First crystal structure of an endo-levanase – the BT1760 from a human gut commensal Bacteroides thetaiotaomicron. Scientific Reports, 2019, 9, 8443.	1.6	18
333	Spermidine Synthase (SPDS) Undergoes Concerted Structural Rearrangements Upon Ligand Binding – A Case Study of the Two SPDS Isoforms From Arabidopsis thaliana. Frontiers in Plant Science, 2019, 10, 555.	1.7	8
334	The UbiX flavin prenyltransferase reaction mechanism resembles class I terpene cyclase chemistry. Nature Communications, 2019, 10, 2357.	5.8	28
335	Structural basis of the inhibition of GH1 β -glucosidases by multivalent pyrrolidine iminosugars. Bioorganic Chemistry, 2019, 89, 103026.	2.0	12
336	Novel Central Nervous System (CNS)-Targeting Protease Inhibitors for Drug-Resistant HIV Infection and HIV-Associated CNS Complications. Antimicrobial Agents and Chemotherapy, 2019, 63, .	1.4	9
337	Crystal structure of Maternal Embryonic Leucine Zipper Kinase (MELK) in complex with dorsomorphin (Compound C). Archives of Biochemistry and Biophysics, 2019, 671, 1-7.	1.4	2
338	Structural and pharmacological evaluation of a novel non-nucleoside reverse transcriptase inhibitor as a promising long acting nanoformulation for treating HIV. Antiviral Research, 2019, 167, 110-116.	1.9	15
339	Structural analysis of a plant fatty acid amide hydrolase provides insights into the evolutionary diversity of bioactive acylethanolamides. Journal of Biological Chemistry, 2019, 294, 7419-7432.	1.6	13
340	Discovery of Novel Spiroindoline Derivatives as Selective Tankyrase Inhibitors. Journal of Medicinal Chemistry, 2019, 62, 3407-3427.	2.9	43
341	Putative structural rearrangements associated with the interaction of macrocyclic inhibitors with norovirus 3CL protease. Proteins: Structure, Function and Bioinformatics, 2019, 87, 579-587.	1.5	7
342	Covalent Modification and Regulation of the Nuclear Receptor Nurr1 by a Dopamine Metabolite. Cell Chemical Biology, 2019, 26, 674-685.e6.	2.5	41
343	Crystal structure of a domain-swapped photoactivatable sfGFP variant provides evidence for GFP folding pathway. FEBS Journal, 2019, 286, 2329-2340.	2.2	5
344	High-Resolution Structure of Cas13b and Biochemical Characterization of RNA Targeting and Cleavage. Cell Reports, 2019, 26, 3741-3751.e5.	2.9	102

#	ARTICLE	IF	CITATIONS
345	Design, Synthesis and Biological Evaluation of Isoxazole-Based CK1 Inhibitors Modified with Chiral Pyrrolidine Scaffolds. <i>Molecules</i> , 2019, 24, 873.	1.7	9
346	Crystallographic Analysis of the Catalytic Mechanism of Phosphopantothenoylcysteine Synthetase from <i>Saccharomyces cerevisiae</i> . <i>Journal of Molecular Biology</i> , 2019, 431, 764-776.	2.0	4
347	Prospective discovery of small molecule enhancers of an E3 ligase-substrate interaction. <i>Nature Communications</i> , 2019, 10, 1402.	5.8	110
348	Use of the 4-Hydroxytriazole Moiety as a Bioisosteric Tool in the Development of Ionotropic Glutamate Receptor Ligands. <i>Journal of Medicinal Chemistry</i> , 2019, 62, 4467-4482.	2.9	18
349	Active-Site Druggability of Carbapenemases and Broad-Spectrum Inhibitor Discovery. <i>ACS Infectious Diseases</i> , 2019, 5, 1013-1021.	1.8	18
350	Structural basis of DSF recognition by its receptor RpfR and its regulatory interaction with the DSF synthase RpfF. <i>PLoS Biology</i> , 2019, 17, e3000123.	2.6	23
351	Structural and biochemical studies of the glucuronoyl esterase OtCE15A illuminate its interaction with lignocellulosic components. <i>Journal of Biological Chemistry</i> , 2019, 294, 19978-19987.	1.6	17
352	Evaluation of a crystallographic surrogate for kallikrein 5 in the discovery of novel inhibitors for Netherton syndrome. <i>Acta Crystallographica Section F, Structural Biology Communications</i> , 2019, 75, 385-391.	0.4	2
353	Fragment screening for a protein-protein interaction inhibitor to WDR5. <i>Structural Dynamics</i> , 2019, 6, 064701.	0.9	6
354	Computational design of a modular protein sense-response system. <i>Science</i> , 2019, 366, 1024-1028.	6.0	91
355	Structural basis of denuded glycan recognition by SPOR domains in bacterial cell division. <i>Nature Communications</i> , 2019, 10, 5567.	5.8	29
356	Cryo-electron microscopy structures of human oligosaccharyltransferase complexes OST-A and OST-B. <i>Science</i> , 2019, 366, 1372-1375.	6.0	77
357	Crystal Structure of Aldehyde Dehydrogenase 16 Reveals Trans-Hierarchical Structural Similarity and a New Dimer. <i>Journal of Molecular Biology</i> , 2019, 431, 524-541.	2.0	15
358	Structural Adaptation of Darunavir Analogues against Primary Mutations in HIV-1 Protease. <i>ACS Infectious Diseases</i> , 2019, 5, 316-325.	1.8	27
359	Structural basis of 7SK RNA 5'-phosphate methylation and retention by MePCE. <i>Nature Chemical Biology</i> , 2019, 15, 132-140.	3.9	38
360	Identifying purine nucleoside phosphorylase as the target of quinine using cellular thermal shift assay. <i>Science Translational Medicine</i> , 2019, 11, .	5.8	153
361	Insights into Thiotemplated Pyrrole Biosynthesis Gained from the Crystal Structure of Flavin-Dependent Oxidase in Complex with Carrier Protein. <i>Biochemistry</i> , 2019, 58, 918-929.	1.2	12
362	Structure of a Signaling Cannabinoid Receptor 1-G Protein Complex. <i>Cell</i> , 2019, 176, 448-458.e12.	13.5	323

#	ARTICLE	IF	CITATIONS
363	<i>N</i> -1-Substituted Quinoxaline-2,3-diones as Kainate Receptor Antagonists: X-ray Crystallography, Structure–Affinity Relationships, and in Vitro Pharmacology. <i>ACS Chemical Neuroscience</i> , 2019, 10, 1841-1853.	1.7	13
364	Interplay between Conformational Entropy and Solvation Entropy in Protein–Ligand Binding. <i>Journal of the American Chemical Society</i> , 2019, 141, 2012-2026.	6.6	89
365	Automatically Fixing Errors in Glycoprotein Structures with Rosetta. <i>Structure</i> , 2019, 27, 134-139.e3.	1.6	93
366	Reactions of Cyclometalated Platinum(II) [Pt(N [§] C)(PR ₃)Cl] Complexes with Imidazole and Imidazole-Containing Biomolecules: Fine-Tuning of Reactivity and Photophysical Properties via Ligand Design. <i>Inorganic Chemistry</i> , 2019, 58, 204-217.	1.9	26
367	Two new ene-reductases from photosynthetic extremophiles enlarge the panel of old yellow enzymes: CtOYE and GsOYE. <i>Applied Microbiology and Biotechnology</i> , 2020, 104, 2051-2066.	1.7	14
368	Development of potent reversible selective inhibitors of butyrylcholinesterase as fluorescent probes. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2020, 35, 498-505.	2.5	16
369	Activation of the GLP-1 receptor by a non-peptidic agonist. <i>Nature</i> , 2020, 577, 432-436.	13.7	119
370	Structural glycobiology in the age of electron cryo-microscopy. <i>Current Opinion in Structural Biology</i> , 2020, 62, 70-78.	2.6	17
371	Structural Basis for Substrate Specificity and Carbapenemase Activity of OXA-48 Class D β -Lactamase. <i>ACS Infectious Diseases</i> , 2020, 6, 261-271.	1.8	13
372	Human Cytochrome P450 1A1 Adapts Active Site for Atypical Nonplanar Substrate. <i>Drug Metabolism and Disposition</i> , 2020, 48, 86-92.	1.7	17
373	Synthesis and Biological Investigation of (+)-JD1, an Organometallic BET Bromodomain Inhibitor. <i>Organometallics</i> , 2020, 39, 408-416.	1.1	6
374	Structure and redox properties of the diheme electron carrier cytochrome c4 from <i>Pseudomonas aeruginosa</i> . <i>Journal of Inorganic Biochemistry</i> , 2020, 203, 110889.	1.5	9
375	Design, Synthesis, and Study of Lactam and Ring-Expanded Analogues of Teixobactin. <i>Journal of Organic Chemistry</i> , 2020, 85, 1331-1339.	1.7	10
376	Structural Basis for the Inhibitor and Substrate Specificity of the Unique Fph Serine Hydrolases of <i>Staphylococcus aureus</i> . <i>ACS Infectious Diseases</i> , 2020, 6, 2771-2782.	1.8	14
377	Structure-activity relationship study of tryptophan-based butyrylcholinesterase inhibitors. <i>European Journal of Medicinal Chemistry</i> , 2020, 208, 112766.	2.6	17
378	Structural analysis of full-length SARS-CoV-2 spike protein from an advanced vaccine candidate. <i>Science</i> , 2020, 370, 1089-1094.	6.0	290
379	Cryo-EM structure of the highly atypical cytoplasmic ribosome of <i>Euglena gracilis</i> . <i>Nucleic Acids Research</i> , 2020, 48, 11750-11761.	6.5	19
380	Design, Synthesis, and Structure–Activity Relationship Studies of Dual Inhibitors of Soluble Epoxide Hydrolase and 5-Lipoxygenase. <i>Journal of Medicinal Chemistry</i> , 2020, 63, 11498-11521.	2.9	13

#	ARTICLE	IF	CITATIONS
381	Differential GLP-1R Binding and Activation by Peptide and Non-peptide Agonists. <i>Molecular Cell</i> , 2020, 80, 485-500.e7.	4.5	111
382	Selective inhibition of human translation termination by a drug-like compound. <i>Nature Communications</i> , 2020, 11, 4941.	5.8	31
383	Cryo-EM structures reveal distinct mechanisms of inhibition of the human multidrug transporter ABCB1. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 26245-26253.	3.3	137
384	Structural Analysis of Potent Hybrid HIV-1 Protease Inhibitors Containing Bis-tetrahydrofuran in a Pseudosymmetric Dipeptide Isostere. <i>Journal of Medicinal Chemistry</i> , 2020, 63, 8296-8313.	2.9	6
385	A Radical Exploration of the Cobalamin-Dependent Radical SAM Enzyme CysS. <i>Trends in Chemistry</i> , 2020, 2, 1037-1040.	4.4	1
386	Architecture of the photosynthetic complex from a green sulfur bacterium. <i>Science</i> , 2020, 370, .	6.0	55
387	The nitrosoamphetamine metabolite is accommodated in the active site of human hemoglobin: Spectroscopy and crystal structure. <i>Journal of Inorganic Biochemistry</i> , 2020, 213, 111262.	1.5	3
388	Substrate specificity of 2-deoxy-D-ribose 5-phosphate aldolase (DERA) assessed by different protein engineering and machine learning methods. <i>Applied Microbiology and Biotechnology</i> , 2020, 104, 10515-10529.	1.7	21
389	Cryo-electron microscopy structures of pyrene-labeled ADP-Pi- and ADP-actin filaments. <i>Nature Communications</i> , 2020, 11, 5897.	5.8	16
390	An Aromatic Cluster in the Active Site of <i>ε</i> -Isozizaene Synthase Is an Electrostatic Toggle for Divergent Terpene Cyclization Pathways. <i>Biochemistry</i> , 2020, 59, 4744-4754.	1.2	14
391	A Combined Spectroscopic and Protein Crystallography Study Reveals Protein Interactions of Rh ^I (NHC) Complexes at the Molecular Level. <i>Inorganic Chemistry</i> , 2020, 59, 17191-17199.	1.9	14
392	Structural basis for the action of the drug trametinib at KSR-bound MEK. <i>Nature</i> , 2020, 588, 509-514.	13.7	86
393	Trapping conformational states of a flavin-dependent N-monooxygenase in crystallo reveals protein and flavin dynamics. <i>Journal of Biological Chemistry</i> , 2020, 295, 13239-13249.	1.6	13
394	Functional characterization of a PROTAC directed against BRAF mutant V600E. <i>Nature Chemical Biology</i> , 2020, 16, 1170-1178.	3.9	80
395	Structural Basis and Binding Kinetics of Vaborbactam in Class A β -Lactamase Inhibition. <i>Antimicrobial Agents and Chemotherapy</i> , 2020, 64, .	1.4	9
396	Virtual screening identifies broad-spectrum β -lactamase inhibitors with activity on clinically relevant serine- and metallo-carbapenemases. <i>Scientific Reports</i> , 2020, 10, 12763.	1.6	25
397	Monoaryl derivatives as transthyretin fibril formation inhibitors: Design, synthesis, biological evaluation and structural analysis. <i>Bioorganic and Medicinal Chemistry</i> , 2020, 28, 115673.	1.4	8
398	Potent Inhibition of Mandelate Racemase by Boronic Acids: Boron as a Mimic of a Carbon Acid Center. <i>Biochemistry</i> , 2020, 59, 3026-3037.	1.2	6

#	ARTICLE	IF	CITATIONS
399	Structural basis for polyglutamate chain initiation and elongation by TLL family enzymes. <i>Nature Structural and Molecular Biology</i> , 2020, 27, 802-813.	3.6	35
400	Structural basis for RING-Cys-Relay E3 ligase activity and its role in axon integrity. <i>Nature Chemical Biology</i> , 2020, 16, 1227-1236.	3.9	46
401	Rules for the design of aza-glycine stabilized triple-helical collagen peptides. <i>Chemical Science</i> , 2020, 11, 10638-10646.	3.7	11
402	Post-Catalytic Complexes with Emtricitabine or Stavudine and HIV-1 Reverse Transcriptase Reveal New Mechanistic Insights for Nucleotide Incorporation and Drug Resistance. <i>Molecules</i> , 2020, 25, 4868.	1.7	3
403	Insight into human Miro1/2 domain organization based on the structure of its N-terminal GTPase. <i>Journal of Structural Biology</i> , 2020, 212, 107656.	1.3	17
404	In crystallo screening for proline analog inhibitors of the proline cycle enzyme PYCR1. <i>Journal of Biological Chemistry</i> , 2020, 295, 18316-18327.	1.6	22
405	An Interprotein Co ²⁺ S Coordination Complex in the B ₁₂ -Trafficking Pathway. <i>Journal of the American Chemical Society</i> , 2020, 142, 16334-16345.	6.6	20
406	Synthetic group A streptogramin antibiotics that overcome Vat resistance. <i>Nature</i> , 2020, 586, 145-150.	13.7	63
407	Ensemble-based enzyme design can recapitulate the effects of laboratory directed evolution in silico. <i>Nature Communications</i> , 2020, 11, 4808.	5.8	67
408	Connexin-46/50 in a dynamic lipid environment resolved by CryoEM at 1.9 Å. <i>Nature Communications</i> , 2020, 11, 4331.	5.8	66
409	Structural basis of redox modulation on chloroplast ATP synthase. <i>Communications Biology</i> , 2020, 3, 482.	2.0	25
410	Free fatty acid binding pocket in the locked structure of SARS-CoV-2 spike protein. <i>Science</i> , 2020, 370, 725-730.	6.0	348
411	Expanding the space of protein geometries by computational design of de novo fold families. <i>Science</i> , 2020, 369, 1132-1136.	6.0	57
412	The cryoelectron microscopy structure of the human CDK-activating kinase. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 22849-22857.	3.3	42
413	BAK core dimers bind lipids and can be bridged by them. <i>Nature Structural and Molecular Biology</i> , 2020, 27, 1024-1031.	3.6	49
414	Tuning the Properties of Natural Promiscuous Enzymes by Engineering Their Nano-environment. <i>ACS Nano</i> , 2020, 14, 17652-17664.	7.3	22
415	Functional Characterization of Primordial Protein Repair Enzyme M38 Metallo-Peptidase From <i>Fervidobacterium islandicum</i> AW-1. <i>Frontiers in Molecular Biosciences</i> , 2020, 7, 600634.	1.6	2
416	A Strain-Specific Inhibitor of Receptor-Bound HIV-1 Targets a Pocket near the Fusion Peptide. <i>Cell Reports</i> , 2020, 33, 108428.	2.9	5

#	ARTICLE	IF	CITATIONS
417	Crystal Structure of the Kinase Domain of MerTK in Complex with AZD7762 Provides Clues for Structure-Based Drug Development. <i>International Journal of Molecular Sciences</i> , 2020, 21, 7878.	1.8	3
418	Combining native and ¹⁵ N mass spectrometry to identify endogenous ligands bound to membrane proteins. <i>Nature Methods</i> , 2020, 17, 505-508.	9.0	111
419	Structure-function study of AKR4C14, an aldo-keto reductase from Thai jasmine rice (<i>Oryza</i>). <i>Journal of Biological Chemistry</i> , 2020, 295, 472-483.	1.1	4
420	Practical Considerations for Atomistic Structure Modeling with Cryo-EM Maps. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 2436-2442.	2.5	11
421	Glycan-dependent cell adhesion mechanism of Tc toxins. <i>Nature Communications</i> , 2020, 11, 2694.	5.8	24
422	Biosynthesis, Mechanism of Action, and Inhibition of the Enterotoxin Tilimycin Produced by the Opportunistic Pathogen <i>Klebsiella oxytoca</i> . <i>ACS Infectious Diseases</i> , 2020, 6, 1976-1997.	1.8	18
423	The CDK inhibitor CR8 acts as a molecular glue degrader that depletes cyclin K. <i>Nature</i> , 2020, 585, 293-297.	13.7	219
424	Ionotropic Glutamate Receptor GluA2 in Complex with Bicyclic Pyrimidinedione-Based Compounds: When Small Compound Modifications Have Distinct Effects on Binding Interactions. <i>ACS Chemical Neuroscience</i> , 2020, 11, 1791-1800.	1.7	8
425	Structural basis for membrane insertion by the human ER membrane protein complex. <i>Science</i> , 2020, 369, 433-436.	6.0	127
426	Structural basis for divergent C-H hydroxylation selectivity in two Rieske oxygenases. <i>Nature Communications</i> , 2020, 11, 2991.	5.8	34
427	Distinct binding of cetirizine enantiomers to human serum albumin and the human histamine receptor H1. <i>Journal of Computer-Aided Molecular Design</i> , 2020, 34, 1045-1062.	1.3	8
428	Dynamic RNA acetylation revealed by quantitative cross-evolutionary mapping. <i>Nature</i> , 2020, 583, 638-643.	13.7	175
429	Molecular basis of β -arrestin coupling to formoterol-bound β -1-adrenoceptor. <i>Nature</i> , 2020, 583, 862-866.	13.7	177
430	Substrate Recognition and Catalytic Mechanism of the Phosphate Acyltransferase PlsX from <i>Bacillus subtilis</i> . <i>ChemBioChem</i> , 2020, 21, 2019-2028.	1.3	1
431	Discovery of Cyclic Boronic Acid QPX7728, an Ultrabroad-Spectrum Inhibitor of Serine and Metallo- β -lactamases. <i>Journal of Medicinal Chemistry</i> , 2020, 63, 7491-7507.	2.9	135
432	Covalent Modification of the Flavin in Proline Dehydrogenase by Thiazolidine-2-Carboxylate. <i>ACS Chemical Biology</i> , 2020, 15, 936-944.	1.6	10
433	Structure of an ancestral mammalian family 1B1 cytochrome P450 with increased thermostability. <i>Journal of Biological Chemistry</i> , 2020, 295, 5640-5653.	1.6	14
434	Mechanism of proton transfer in class A β -lactamase catalysis and inhibition by avibactam. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 5818-5825.	3.3	35

#	ARTICLE	IF	CITATIONS
435	Design and Discovery of an Orally Efficacious Spiroindolinone-Based Tankyrase Inhibitor for the Treatment of Colon Cancer. <i>Journal of Medicinal Chemistry</i> , 2020, 63, 4183-4204.	2.9	25
436	Tetracenomycin X inhibits translation by binding within the ribosomal exit tunnel. <i>Nature Chemical Biology</i> , 2020, 16, 1071-1077.	3.9	43
437	The Structural Basis of the Binding of Various Aminopolycarboxylates by the Periplasmic EDTA-Binding Protein EppA from <i>Chelativorans</i> sp. BNC1. <i>International Journal of Molecular Sciences</i> , 2020, 21, 3940.	1.8	3
438	Irritant-evoked activation and calcium modulation of the TRPA1 receptor. <i>Nature</i> , 2020, 585, 141-145.	13.7	93
439	Design, synthesis, and <i>in vitro</i> evaluation of aza-peptide aldehydes and ketones as novel and selective protease inhibitors. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2020, 35, 1387-1402.	2.5	6
440	Synthesis and evaluation of sulfonyl piperazine LpxH inhibitors. <i>Bioorganic Chemistry</i> , 2020, 102, 104055.	2.0	10
441	Chiral Separation, X-ray Structure, and Biological Evaluation of a Potent and Reversible Dual Binding Site AChE Inhibitor. <i>ACS Medicinal Chemistry Letters</i> , 2020, 11, 869-876.	1.3	7
442	Structure and mechanism of the ER-based glucosyltransferase ALG6. <i>Nature</i> , 2020, 579, 443-447.	13.7	52
443	X-ray crystallography of Epacadostat in adduct with Carbonic Anhydrase IX. <i>Bioorganic Chemistry</i> , 2020, 97, 103669.	2.0	6
444	Structural Effects and Functional Implications of Phalloidin and Jasplakinolide Binding to Actin Filaments. <i>Structure</i> , 2020, 28, 437-449.e5.	1.6	83
445	Structural basis of the UDP-diacylglucosamine pyrophosphohydrolase LpxH inhibition by sulfonyl piperazine antibiotics. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 4109-4116.	3.3	17
446	A Structural Basis for Restricted Codon Recognition Mediated by 2-thiocytidine in tRNA Containing a Wobble Position Inosine. <i>Journal of Molecular Biology</i> , 2020, 432, 913-929.	2.0	12
447	Structural basis for strand-transfer inhibitor binding to HIV intasomes. <i>Science</i> , 2020, 367, 810-814.	6.0	74
449	Tuning melatonin receptor subtype selectivity in oxadiazolone-based analogues: Discovery of QR2 ligands and NRF2 activators with neurogenic properties. <i>European Journal of Medicinal Chemistry</i> , 2020, 190, 112090.	2.6	15
450	Synthesis and Biological Validation of a Harmine-Based, Central Nervous System (CNS)-Avoidant, Selective, Human β -Cell Regenerative Dual-Specificity Tyrosine Phosphorylation-Regulated Kinase A (DYRK1A) Inhibitor. <i>Journal of Medicinal Chemistry</i> , 2020, 63, 2986-3003.	2.9	36
451	Selective PP2A Enhancement through Biased Heterotrimer Stabilization. <i>Cell</i> , 2020, 181, 688-701.e16.	13.5	107
452	Conformational plasticity of the ClpAP AAA+ protease couples protein unfolding and proteolysis. <i>Nature Structural and Molecular Biology</i> , 2020, 27, 406-416.	3.6	51
453	Optimizing the refinement of merohedrally twinned P61 HIV-1 protease inhibitor cocrystal structures. <i>Acta Crystallographica Section D: Structural Biology</i> , 2020, 76, 302-310.	1.1	1

#	ARTICLE	IF	CITATIONS
454	N-alkylpiperidine carbamates as potential anti-Alzheimer's agents. <i>European Journal of Medicinal Chemistry</i> , 2020, 197, 112282.	2.6	33
455	Synthesis, biological properties and structural study of new halogenated azolo[4,5-b]pyridines as inhibitors of CK2 kinase. <i>Bioorganic Chemistry</i> , 2021, 106, 104502.	2.0	11
456	Structure of the class D GPCR Ste2 dimer coupled to two G proteins. <i>Nature</i> , 2021, 589, 148-153.	13.7	55
457	Structural basis of carnitine monooxygenase CntA substrate specificity, inhibition, and intersubunit electron transfer. <i>Journal of Biological Chemistry</i> , 2021, 296, 100038.	1.6	15
458	KPC-2 β -lactamase enables carbapenem antibiotic resistance through fast deacylation of the covalent intermediate. <i>Journal of Biological Chemistry</i> , 2021, 296, 100155.	1.6	18
459	Structural analysis of prolines and hydroxyprolines binding to the l-glutamate- β -semialdehyde dehydrogenase active site of bifunctional proline utilization A. <i>Archives of Biochemistry and Biophysics</i> , 2021, 698, 108727.	1.4	6
460	Structural Cues for Understanding eEF1A2 Moonlighting. <i>ChemBioChem</i> , 2021, 22, 374-391.	1.3	8
461	Experimental evaluation of super-resolution imaging and magnification choice in single-particle cryo-EM. <i>Journal of Structural Biology: X</i> , 2021, 5, 100047.	0.7	8
462	A Thermophilic Bacterial Esterase for Scavenging Nerve Agents: A Kinetic, Biophysical and Structural Study. <i>Molecules</i> , 2021, 26, 657.	1.7	1
463	Active site architecture reveals coordination sphere flexibility and specificity determinants in a group of closely related molybdoenzymes. <i>Journal of Biological Chemistry</i> , 2021, 296, 100672.	1.6	7
464	Structures and mechanism of human glycosyltransferase β 1,3-N-acetylglucosaminyltransferase 2 (B3GNT2), an important player in immune homeostasis. <i>Journal of Biological Chemistry</i> , 2021, 296, 100042.	1.6	14
465	Conformational constraints of cyclopentane peptide nucleic acids facilitate tunable binding to DNA. <i>Nucleic Acids Research</i> , 2021, 49, 713-725.	6.5	20
466	Update and Potential Opportunities in CBP [Cyclic Adenosine Monophosphate (cAMP) Response Element-Binding Protein (CREB)-Binding Protein] Research Using Computational Techniques. <i>Protein Journal</i> , 2021, 40, 19-27.	0.7	4
467	Structure and evolutionary trace-assisted screening of a residue swapping the substrate ambiguity and chiral specificity in an esterase. <i>Computational and Structural Biotechnology Journal</i> , 2021, 19, 2307-2317.	1.9	6
468	A polysaccharide utilization locus from the gut bacterium <i>Dysgonomonas mossii</i> encodes functionally distinct carbohydrate esterases. <i>Journal of Biological Chemistry</i> , 2021, 296, 100500.	1.6	21
469	Development of versatile and potent monoquaternary reactivators of acetylcholinesterase. <i>Archives of Toxicology</i> , 2021, 95, 985-1001.	1.9	7
470	Key role of a structural water molecule for the specificity of 14F7 [®] An antitumor antibody targeting the NeuGc GM3 ganglioside. <i>Glycobiology</i> , 2021, 31, 1500-1509.	1.3	3
471	Structural basis of Naa20 activity towards a canonical NatB substrate. <i>Communications Biology</i> , 2021, 4, 2.	2.0	6

#	ARTICLE	IF	CITATIONS
473	Crystal Structure of SARS-CoV-2 Main Protease in Complex with the Non-Covalent Inhibitor ML188. <i>Viruses</i> , 2021, 13, 174.	1.5	80
474	Discovery of an Allosteric Ligand Binding Site in SMYD3 Lysine Methyltransferase. <i>ChemBioChem</i> , 2021, 22, 1597-1608.	1.3	8
475	Metabolic Fate of Human Immunoactive Sterols in <i>Mycobacterium tuberculosis</i> . <i>Journal of Molecular Biology</i> , 2021, 433, 166763.	2.0	15
476	Structural basis of catalysis and substrate recognition by the NAD(H)-dependent β -D-glucuronidase from the glycoside hydrolase family 4. <i>Biochemical Journal</i> , 2021, 478, 943-959.	1.7	2
477	Structural Insight into the Two-Step Mechanism of PAI-1 Inhibition by Small Molecule TM5484. <i>International Journal of Molecular Sciences</i> , 2021, 22, 1482.	1.8	10
478	A Single-Point Mutation in <i>scpA</i> -Arginine Dehydrogenase Unlocks a Transient Conformational State Resulting in Altered Cofactor Reactivity. <i>Biochemistry</i> , 2021, 60, 711-724.	1.2	7
479	Inhibiting HTLV-1 Protease: A Viable Antiviral Target. <i>ACS Chemical Biology</i> , 2021, 16, 529-538.	1.6	12
480	2.5 Å resolution structure of human CDK-activating kinase bound to the clinical inhibitor ICEC0942. <i>Biophysical Journal</i> , 2021, 120, 677-686.	0.2	22
482	Structural Characterization of Diazabicyclooctane β -Lactam Enhancers in Complex with Penicillin-Binding Proteins PBP2 and PBP3 of <i>Pseudomonas aeruginosa</i> . <i>MBio</i> , 2021, 12, .	1.8	19
483	Synthesis and Structure-Activity Relationships of Aristoyagonine Derivatives as Brd4 Bromodomain Inhibitors with X-ray Co-Crystal Research. <i>Molecules</i> , 2021, 26, 1686.	1.7	11
484	Early-stage dynamics of chloride ion-pumping rhodopsin revealed by a femtosecond X-ray laser. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021, 118, .	3.3	41
489	A chemical genetics approach to examine the functions of AAA proteins. <i>Nature Structural and Molecular Biology</i> , 2021, 28, 388-397.	3.6	4
490	Structural basis for human TRPC5 channel inhibition by two distinct inhibitors. <i>ELife</i> , 2021, 10, .	2.8	39
491	Cryo-EM structure of the Rous sarcoma virus octameric cleaved synaptic complex intasome. <i>Communications Biology</i> , 2021, 4, 330.	2.0	12
492	Structural characterization of the microbial enzyme urocanate reductase mediating imidazole propionate production. <i>Nature Communications</i> , 2021, 12, 1347.	5.8	9
493	Parallel molecular mechanisms for enzyme temperature adaptation. <i>Science</i> , 2021, 371, .	6.0	48
494	Characterization of a broadly specific cadaverine N-hydroxylase involved in desferrioxamine B biosynthesis in <i>Streptomyces sviveus</i> . <i>PLoS ONE</i> , 2021, 16, e0248385.	1.1	3
495	Discovery of fungal surface NADases predominantly present in pathogenic species. <i>Nature Communications</i> , 2021, 12, 1631.	5.8	6

#	ARTICLE	IF	CITATIONS
496	Remdesivir is a delayed translocation inhibitor of SARS-CoV-2 replication. <i>Molecular Cell</i> , 2021, 81, 1548-1552.e4.	4.5	90
497	Discovery of AG-270, a First-in-Class Oral MAT2A Inhibitor for the Treatment of Tumors with Homozygous <i>MTAP</i> Deletion. <i>Journal of Medicinal Chemistry</i> , 2021, 64, 4430-4449.	2.9	39
499	Sustainable Drug Discovery of Multi-Target-Directed Ligands for Alzheimer's Disease. <i>Journal of Medicinal Chemistry</i> , 2021, 64, 4972-4990.	2.9	63
501	Structural Insights into the Molecular Recognition Mechanism of the Cancer and Pathogenic Epitope, LacdiNAc by Immune-Related Lectins. <i>Chemistry - A European Journal</i> , 2021, 27, 7951-7958.	1.7	4
502	Fragment binding to the Nsp3 macrodomain of SARS-CoV-2 identified through crystallographic screening and computational docking. <i>Science Advances</i> , 2021, 7, .	4.7	100
503	Structure reveals the activation mechanism of the MC4 receptor to initiate satiation signaling. <i>Science</i> , 2021, 372, 808-814.	6.0	64
504	Entropy-Entropy Compensation between the Protein, Ligand, and Solvent Degrees of Freedom Fine-Tunes Affinity in Ligand Binding to Galectin-3C. <i>Jacs Au</i> , 2021, 1, 484-500.	3.6	17
505	Structure of the far-red light utilizing photosystem I of <i>Acaryochloris marina</i> . <i>Nature Communications</i> , 2021, 12, 2333.	5.8	35
506	Modelling covalent linkages in <i>CCP4</i> . <i>Acta Crystallographica Section D: Structural Biology</i> , 2021, 77, 712-726.	1.1	10
507	The Glitazone Class of Drugs as Carbonic Anhydrase Inhibitors—A Spin-Off Discovery from Fragment Screening. <i>Molecules</i> , 2021, 26, 3010.	1.7	6
508	Context-specific action of macrolide antibiotics on the eukaryotic ribosome. <i>Nature Communications</i> , 2021, 12, 2803.	5.8	18
509	Structural basis of antifolate recognition and transport by PCFT. <i>Nature</i> , 2021, 595, 130-134.	13.7	36
510	<i>FragMAXapp</i> : crystallographic fragment-screening data-analysis and project-management system. <i>Acta Crystallographica Section D: Structural Biology</i> , 2021, 77, 799-808.	1.1	9
512	Discovery of an H3K36me3-Derived Peptidomimetic Ligand with Enhanced Affinity for Plant Homeodomain Finger Protein 1 (PHF1). <i>Journal of Medicinal Chemistry</i> , 2021, 64, 8510-8522.	2.9	12
513	Structural insights on ligand recognition at the human leukotriene B4 receptor 1. <i>Nature Communications</i> , 2021, 12, 2971.	5.8	13
515	The missing link: covalent linkages in structural models. <i>Acta Crystallographica Section D: Structural Biology</i> , 2021, 77, 727-745.	1.1	10
520	Structure-Activity Relationship and Mode of Action Studies Highlight <i>(4-(Biphenylmethyl)imidazole</i> -Derived Small Molecules as Potent CYP121 Inhibitors. <i>ChemMedChem</i> , 2021, 16, 2786-2801.	1.6	9
521	Structural basis of GTPase-mediated mitochondrial ribosome biogenesis and recycling. <i>Nature Communications</i> , 2021, 12, 3672.	5.8	41

#	ARTICLE	IF	CITATIONS
522	Discovery of multifunctional anti-Alzheimer's agents with a unique mechanism of action including inhibition of the enzyme butyrylcholinesterase and l ³ -aminobutyric acid transporters. <i>European Journal of Medicinal Chemistry</i> , 2021, 218, 113397.	2.6	14
526	Structures of the human cholecystokinin 1 (CCK1) receptor bound to G _s and G _q mimetic proteins provide insight into mechanisms of G protein selectivity. <i>PLoS Biology</i> , 2021, 19, e3001295.	2.6	41
527	Structural basis for plazomicin antibiotic action and resistance. <i>Communications Biology</i> , 2021, 4, 729.	2.0	13
528	Structural and phylogenetic analyses of resistance to next-generation aminoglycosides conferred by AAC(2- ϵ) enzymes. <i>Scientific Reports</i> , 2021, 11, 11614.	1.6	9
529	Acyclic nucleoside phosphonates with adenine nucleobase inhibit <i>Trypanosoma brucei</i> adenine phosphoribosyltransferase in vitro. <i>Scientific Reports</i> , 2021, 11, 13317.	1.6	8
531	Structural Basis of Drug Recognition by the Multidrug Transporter ABCG2. <i>Journal of Molecular Biology</i> , 2021, 433, 166980.	2.0	52
533	Structural basis for the stereospecific inhibition of the dual proline/hydroxyproline catabolic enzyme ALDH4A1 by trans-4-hydroxy-L-proline. <i>Protein Science</i> , 2021, 30, 1714-1722.	3.1	4
534	Structures of ABCG2 under turnover conditions reveal a key step in the drug transport mechanism. <i>Nature Communications</i> , 2021, 12, 4376.	5.8	46
535	H-Bonding Networks Dictate the Molecular Mechanism of H ₂ O ₂ Activation by P450. <i>ACS Catalysis</i> , 2021, 11, 8774-8785.	5.5	37
536	Development of Thiochroman Dioxide Analogues of Benzothiadiazine Dioxides as New Positive Allosteric Modulators of α -Amino-3-hydroxy-5-methyl-4-isoxazolepropionic Acid (AMPA) Receptors. <i>ACS Chemical Neuroscience</i> , 2021, 12, 2679-2692.	1.7	11
537	Molecular Plasticity of Crystalline CK2 β Leads to KN2, a Bivalent Inhibitor of Protein Kinase CK2 with Extraordinary Selectivity. <i>Journal of Medicinal Chemistry</i> , 2022, 65, 1302-1312.	2.9	13
538	Enzymatic electrochemical biosensor for glyphosate detection based on acid phosphatase inhibition. <i>Analytical and Bioanalytical Chemistry</i> , 2021, 413, 5859-5869.	1.9	14
539	An on-demand, drop-on-drop method for studying enzyme catalysis by serial crystallography. <i>Nature Communications</i> , 2021, 12, 4461.	5.8	34
541	Structural basis of early translocation events on the ribosome. <i>Nature</i> , 2021, 595, 741-745.	13.7	60
543	2-Mercaptomethyl Thiazolidines (MMTZs) Inhibit All Metallo- β -Lactamase Classes by Maintaining a Conserved Binding Mode. <i>ACS Infectious Diseases</i> , 2021, 7, 2697-2706.	1.8	16
544	Slow-Onset, Potent Inhibition of Mandelate Racemase by 2-Formylphenylboronic Acid. An Unexpected Adduct Clasps the Catalytic Machinery. <i>Biochemistry</i> , 2021, 60, 2508-2518.	1.2	3
545	Targeted Degradation of the Oncogenic Phosphatase SHP2. <i>Biochemistry</i> , 2021, 60, 2593-2609.	1.2	21
546	Targeting SARS-CoV-2 Nsp3 macrodomain structure with insights from human poly(ADP-ribose) glycohydrolase (PARG) structures with inhibitors. <i>Progress in Biophysics and Molecular Biology</i> , 2021, 163, 171-186.	1.4	39

#	ARTICLE	IF	CITATIONS
547	X-ray crystallography reveals molecular recognition mechanism for sugar binding in a melibiose transporter MelB. <i>Communications Biology</i> , 2021, 4, 931.	2.0	19
548	Macromolecular refinement of X-ray and cryoelectron microscopy structures with Phenix/OPLS3e for improved structure and ligand quality. <i>Structure</i> , 2021, 29, 913-921.e4.	1.6	29
549	Mechanism of molnupiravir-induced SARS-CoV-2 mutagenesis. <i>Nature Structural and Molecular Biology</i> , 2021, 28, 740-746.	3.6	450
550	Structure-Based Optimization of ML300-Derived, Noncovalent Inhibitors Targeting the Severe Acute Respiratory Syndrome Coronavirus 3CL Protease (SARS-CoV-2 3CL ^{pro}). <i>Journal of Medicinal Chemistry</i> , 2022, 65, 2880-2904.	2.9	78
551	Inhibition of lytic polysaccharide monoxygenase by natural plant extracts. <i>New Phytologist</i> , 2021, 232, 1337-1349.	3.5	12
552	Dual-mechanism estrogen receptor inhibitors. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021, 118, .	3.3	16
553	Structure of the ancient TRPY1 channel from <i>Saccharomyces cerevisiae</i> reveals mechanisms of modulation by lipids and calcium. <i>Structure</i> , 2022, 30, 139-155.e5.	1.6	12
554	Mechanism of LolCDE as a molecular extruder of bacterial triacylated lipoproteins. <i>Nature Communications</i> , 2021, 12, 4687.	5.8	34
556	DNA interference states of the hypercompact CRISPR-Cas1 effector. <i>Nature Structural and Molecular Biology</i> , 2021, 28, 652-661.	3.6	50
558	Structure of Usutu virus SAAR-1776 displays fusion loop asymmetry. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021, 118, .	3.3	11
559	Structures of ABCB4 provide insight into phosphatidylcholine translocation. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021, 118, .	3.3	24
560	The structural basis of odorant recognition in insect olfactory receptors. <i>Nature</i> , 2021, 597, 126-131.	13.7	141
561	Acquired JAK2 mutations confer resistance to JAK inhibitors in cell models of acute lymphoblastic leukemia. <i>Npj Precision Oncology</i> , 2021, 5, 75.	2.3	10
562	Structural Changes in the Cap of Rv0183/mtbMGL Modulate the Shape of the Binding Pocket. <i>Biomolecules</i> , 2021, 11, 1299.	1.8	2
563	Visualization of hydrogen atoms in a perdeuterated lectin-fucose complex reveals key details of protein-carbohydrate interactions. <i>Structure</i> , 2021, 29, 1003-1013.e4.	1.6	8
565	Distinct allosteric mechanisms of first-generation MsbA inhibitors. <i>Science</i> , 2021, 374, 580-585.	6.0	29
567	Discovery of a first-in-class reversible DNMT1-selective inhibitor with improved tolerability and efficacy in acute myeloid leukemia. <i>Nature Cancer</i> , 2021, 2, 1002-1017.	5.7	99
568	Rational design of a hydrolysis-resistant mycobacterial phosphoglycolipid antigen presented by CD1c to T cells. <i>Journal of Biological Chemistry</i> , 2021, 297, 101197.	1.6	5

#	ARTICLE	IF	CITATIONS
569	Structure and function of aerotolerant, multiple-turnover THI4 thiazole synthases. <i>Biochemical Journal</i> , 2021, 478, 3265-3279.	1.7	6
570	Pan-3C Protease Inhibitor Rupintrivir Binds SARS-CoV-2 Main Protease in a Unique Binding Mode. <i>Biochemistry</i> , 2021, 60, 2925-2931.	1.2	21
571	A selective WDR5 degrader inhibits acute myeloid leukemia in patient-derived mouse models. <i>Science Translational Medicine</i> , 2021, 13, eabj1578.	5.8	67
572	A Crystallographic Snapshot of SARS-CoV-2 Main Protease Maturation Process. <i>Journal of Molecular Biology</i> , 2021, 433, 167118.	2.0	45
573	Mutations in PBP2 from ceftriaxone-resistant <i>Neisseria gonorrhoeae</i> alter the dynamics of the $\hat{I}^{23}\hat{\epsilon}^{\hat{I}24}$ loop to favor a low-affinity drug-binding state. <i>Journal of Biological Chemistry</i> , 2021, 297, 101188.	1.6	7
574	Total Synthesis of Tetrahydrolipstatin, Its Derivatives, and Evaluation of Their Ability to Potentiate Multiple Antibiotic Classes against <i>Mycobacterium</i> Species. <i>ACS Infectious Diseases</i> , 2021, 7, 2876-2888.	1.8	2
575	Indole Chloropyridinyl Ester-Derived SARS-CoV-2 3CLpro Inhibitors: Enzyme Inhibition, Antiviral Efficacy, Structure-Activity Relationship, and X-ray Structural Studies. <i>Journal of Medicinal Chemistry</i> , 2021, 64, 14702-14714.	2.9	55
576	Structural Insights into the Inhibition of Undecaprenyl Pyrophosphate Synthase from Gram-Positive Bacteria. <i>Journal of Medicinal Chemistry</i> , 2021, 64, 13540-13550.	2.9	2
577	Molecular basis of C-S bond cleavage in the glycyl radical enzyme isethionate sulfite-lyase. <i>Cell Chemical Biology</i> , 2021, 28, 1333-1346.e7.	2.5	11
578	Cryo-EM structure of the <i>Rhodospirillum rubrum</i> RC-LH1 complex at 2.5 Å. <i>Biochemical Journal</i> , 2021, 478, 3253-3263.	1.7	23
579	Conformational dynamics linked to domain closure and substrate binding explain the ERAP1 allosteric regulation mechanism. <i>Nature Communications</i> , 2021, 12, 5302.	5.8	22
581	Photoinduced Covalent Irreversible Inactivation of Proline Dehydrogenase by S-Heterocycles. <i>ACS Chemical Biology</i> , 2021, 16, 2268-2279.	1.6	2
582	Towards Consistency in Geometry Restraints for Carbohydrates in the Pyranose form: Modern Dictionary Generators Reviewed. <i>Current Medicinal Chemistry</i> , 2022, 29, 1193-1207.	1.2	7
583	A novel thermostable prokaryotic fucoidan active sulfatase PsFucS1 with an unusual quaternary hexameric structure. <i>Scientific Reports</i> , 2021, 11, 19523.	1.6	8
584	N-acetylmannosamine-6-phosphate 2-epimerase uses a novel substrate-assisted mechanism to catalyze amino sugar epimerization. <i>Journal of Biological Chemistry</i> , 2021, 297, 101113.	1.6	4
585	Development and crystallography-aided SAR studies of multifunctional BuChE inhibitors and 5-HT6R antagonists with \hat{I}^2 -amyloid anti-aggregation properties. <i>European Journal of Medicinal Chemistry</i> , 2021, 225, 113792.	2.6	13
586	Development of [18F]MIPS15692, a radiotracer with <i>in vitro</i> proof-of-concept for the imaging of MER tyrosine kinase (MERTK) in neuroinflammatory disease. <i>European Journal of Medicinal Chemistry</i> , 2021, 226, 113822.	2.6	5
587	Ligand Incorporation into Protein Microcrystals for MicroED by On-Grid Soaking. <i>Structure</i> , 2021, 29, 88-95.e2.	1.6	16

#	ARTICLE	IF	CITATIONS
588	Design and synthesis of a new orthogonally protected glutamic acid analog and its use in the preparation of high affinity polo-like kinase 1 polo-box domain " binding peptide macrocycles. <i>Organic and Biomolecular Chemistry</i> , 2021, 19, 7843-7854.	1.5	5
589	Structural characterization of a PCP"R didomain from an archaeal nonribosomal peptide synthetase reveals novel interdomain interactions. <i>Journal of Biological Chemistry</i> , 2021, 296, 100432.	1.6	8
590	<i>CERES</i>: a cryo-EM re-refinement system for continuous improvement of deposited models. <i>Acta Crystallographica Section D: Structural Biology</i> , 2021, 77, 48-61.	1.1	14
591	Mechanism of SARS-CoV-2 polymerase stalling by remdesivir. <i>Nature Communications</i> , 2021, 12, 279.	5.8	412
592	Small-Angle X-Ray Scattering to Obtain Models of Multivalent Lectin" Glycan Complexes. <i>Methods in Molecular Biology</i> , 2014, 1200, 511-526.	0.4	4
593	Structural and biochemical evaluation of bisubstrate inhibitors of protein arginine N-methyltransferases PRMT1 and CARM1 (PRMT4). <i>Biochemical Journal</i> , 2020, 477, 787-800.	1.7	11
594	Enantioseparation, <i>in vitro</i> testing, and structural characterization of triple-binding reactivators of organophosphate-inhibited cholinesterases. <i>Biochemical Journal</i> , 2020, 477, 2771-2790.	1.7	12
616	Automating crystallographic structure solution and refinement of protein"ligand complexes. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2014, 70, 144-154.	2.5	43
617	Ligand placement based on prior structures: the guided ligand-replacement method. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2014, 70, 134-143.	2.5	11
618	Accurate macromolecular crystallographic refinement: incorporation of the linear scaling, semiempirical quantum-mechanics program <i>DivCon</i> into the <i>PHENIX</i> refinement package. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2014, 70, 1233-1247.	2.5	46
619	Sent packing: protein engineering generates a new crystal form of <i>Pseudomonas aeruginosa</i> DsbA1 with increased catalytic surface accessibility. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2015, 71, 2386-2395.	2.5	5
620	Mix-and-diffuse serial synchrotron crystallography. <i>IUCrJ</i> , 2017, 4, 769-777.	1.0	98
621	Crystal structures of Lymphocytic choriomeningitis virus endonuclease domain complexed with diketo-acid ligands. <i>IUCrJ</i> , 2018, 5, 223-235.	1.0	12
622	A cytosine modification mechanism revealed by the structure of a ternary complex of deoxycytidylate hydroxymethylase from bacteriophage T4 with its cofactor and substrate. <i>IUCrJ</i> , 2019, 6, 206-217.	1.0	4
623	Formation of a highly dense tetra-rhenium cluster in a protein crystal and its implications in medical imaging. <i>IUCrJ</i> , 2019, 6, 695-702.	1.0	11
624	Why is interoperability between the two fields of chemical crystallography and protein crystallography so difficult?. <i>IUCrJ</i> , 2019, 6, 788-793.	1.0	11
625	Structures of soluble rabbit neprilysin complexed with phosphoramidon or thiorphan. <i>Acta Crystallographica Section F, Structural Biology Communications</i> , 2019, 75, 405-411.	0.4	4
626	<i>XModeScore</i>: a novel method for accurate protonation/tautomer-state determination using quantum-mechanically driven macromolecular X-ray crystallographic refinement. <i>Acta Crystallographica Section D: Structural Biology</i> , 2016, 72, 586-598.	1.1	15

#	ARTICLE	IF	CITATIONS
627	Improved ligand geometries in crystallographic refinement using <i>AFITT</i> in <i>PHENIX</i> . <i>Acta Crystallographica Section D: Structural Biology</i> , 2016, 72, 1062-1072.	1.1	29
628	An editor for the generation and customization of geometry restraints. <i>Acta Crystallographica Section D: Structural Biology</i> , 2017, 73, 123-130.	1.1	27
629	Ligand fitting with <i>CCP4</i> . <i>Acta Crystallographica Section D: Structural Biology</i> , 2017, 73, 158-170.	1.1	18
630	Validation and extraction of molecular-geometry information from small-molecule databases. <i>Acta Crystallographica Section D: Structural Biology</i> , 2017, 73, 103-111.	1.1	19
631	Iron–sulfur clusters have no right angles. <i>Acta Crystallographica Section D: Structural Biology</i> , 2019, 75, 16-20.	1.1	16
632	Analysis and validation of macromolecular <i>B</i> values. <i>Acta Crystallographica Section D: Structural Biology</i> , 2019, 75, 505-518.	1.1	14
633	Macromolecular structure determination using X-rays, neutrons and electrons: recent developments in <i>Phenix</i> . <i>Acta Crystallographica Section D: Structural Biology</i> , 2019, 75, 861-877.	1.1	4,060
634	The evolving story of AtzT, a periplasmic binding protein. <i>Acta Crystallographica Section D: Structural Biology</i> , 2019, 75, 995-1002.	1.1	1
635	Improved chemistry restraints for crystallographic refinement by integrating the Amber force field into <i>Phenix</i> . <i>Acta Crystallographica Section D: Structural Biology</i> , 2020, 76, 51-62.	1.1	29
636	FragMAX: the fragment-screening platform at the MAX IV Laboratory. <i>Acta Crystallographica Section D: Structural Biology</i> , 2020, 76, 771-777.	1.1	26
637	Influence of the presence of the heme cofactor on the JK-loop structure in indoleamine 2,3-dioxygenase 1. <i>Acta Crystallographica Section D: Structural Biology</i> , 2020, 76, 1211-1221.	1.1	12
638	Structure of the Lifeact–F-actin complex. <i>PLoS Biology</i> , 2020, 18, e3000925.	2.6	40
639	Structural Basis of the Induced-Fit Mechanism of 1,4-Dihydroxy-2-Naphthoyl Coenzyme A Synthase from the Crotonase Fold Superfamily. <i>PLoS ONE</i> , 2013, 8, e63095.	1.1	5
640	Elucidation of Substrate Specificity in <i>Aspergillus nidulans</i> UDP-Galactose-4-Epimerase. <i>PLoS ONE</i> , 2013, 8, e76803.	1.1	7
641	Probing the ATP Site of GRP78 with Nucleotide Triphosphate Analogs. <i>PLoS ONE</i> , 2016, 11, e0154862.	1.1	21
642	Structural basis for exploring the allosteric inhibition of human kidney type glutaminase. <i>Oncotarget</i> , 2016, 7, 57943-57954.	0.8	39
643	Phytosphingosine exhibits an anti-epithelial–mesenchymal transition function by the inhibition of EGFR signaling in human breast cancer cells. <i>Oncotarget</i> , 2017, 8, 77794-77808.	0.8	10
644	Computational design of environmental sensors for the potent opioid fentanyl. <i>ELife</i> , 2017, 6, .	2.8	78

#	ARTICLE	IF	CITATIONS
645	Molecular mechanism of TRPV2 channel modulation by cannabidiol. <i>ELife</i> , 2019, 8, .	2.8	106
646	Structure-based characterization of novel TRPV5 inhibitors. <i>ELife</i> , 2019, 8, .	2.8	44
647	Molecular basis for catabolism of the abundant metabolite trans-4-hydroxy-L-proline by a microbial glycyl radical enzyme. <i>ELife</i> , 2020, 9, .	2.8	16
648	A Sec14-like phosphatidylinositol transfer protein paralog defines a novel class of heme-binding proteins. <i>ELife</i> , 2020, 9, .	2.8	10
649	Epoxyqueuosine Reductase QueH in the Biosynthetic Pathway to tRNA Queuosine Is a Unique Metalloenzyme. <i>Biochemistry</i> , 2021, 60, 3152-3161.	1.2	7
650	Cytochrome P450 Binding and Bioactivation of Tumor-targeted Duocarmycin Agents. <i>Drug Metabolism and Disposition</i> , 2021, , DMD-AR-2021-000642.	1.7	8
651	Cryo-EM reconstructions of inhibitor-bound SMG1 kinase reveal an autoinhibitory state dependent on SMG8. <i>ELife</i> , 2021, 10, .	2.8	18
652	Efficacy of epetraborole against <i>Mycobacterium abscessus</i> is increased with norvaline. <i>PLoS Pathogens</i> , 2021, 17, e1009965.	2.1	19
653	Optimization of TopoIV Potency, ADMET Properties, and hERG Inhibition of 5-Amino-1,3-dioxane-Linked Novel Bacterial Topoisomerase Inhibitors: Identification of a Lead with <i>In Vivo</i> Efficacy against MRSA. <i>Journal of Medicinal Chemistry</i> , 2021, 64, 15214-15249.	2.9	16
654	Protein Three-Dimensional Structure Validation. , 2013, , .		0
655	Structures of Large RNA Molecules and Their Complexes. <i>Methods in Enzymology</i> , 2015, , .	0.4	0
657	High-Throughput Crystallography and Its Applications in Drug Discovery. , 2017, , 153-179.		0
669	Allosteric Antagonist Modulation of TRPV2 by Piperlongumine Impairs Glioblastoma Progression. <i>SSRN Electronic Journal</i> , 0, , .	0.4	1
682	Cocktailed fragment screening by X-ray crystallography of the antibacterial target undecaprenyl pyrophosphate synthase from <i>Acinetobacter baumannii</i> . <i>Acta Crystallographica Section F, Structural Biology Communications</i> , 2020, 76, 40-46.	0.4	3
690	Crystallographic and biophysical analyses of <i>Pseudomonas aeruginosa</i> ketopantoate reductase: Implications of ligand induced conformational changes in cofactor recognition. <i>Biochimie</i> , 2021, 193, 103-103.	1.3	1
691	Patient mutations in human ATP:cob(I)alamin adenosyltransferase differentially affect its catalytic versus chaperone functions. <i>Journal of Biological Chemistry</i> , 2021, 297, 101373.	1.6	3
692	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.	2.9	32
697	Remdesivir is a Delayed Translocation Inhibitor of SARS CoV-2 Replication. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0

#	ARTICLE	IF	CITATIONS
703	Cryo-EM structures of PI3K β reveal conformational changes during inhibition and activation. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	17
704	Room temperature XFEL crystallography reveals asymmetry in the vicinity of the two phylloquinones in photosystem I. Scientific Reports, 2021, 11, 21787.	1.6	11
707	C-Glycoside metabolism in the gut and in nature: Identification, characterization, structural analyses and distribution of C-C bond-cleaving enzymes. Nature Communications, 2021, 12, 6294.	5.8	25
712	The crystal structure of benzophenone synthase from <i>Garcinia mangostana</i> L. pericarps reveals the basis for substrate specificity and catalysis. Acta Crystallographica Section F, Structural Biology Communications, 2020, 76, 597-603.	0.4	5
713	Arginine off-kilter: guanidinium is not as planar as restraints denote. Acta Crystallographica Section D: Structural Biology, 2020, 76, 1159-1166.	1.1	7
714	Inhibitors of Mycobacterium tuberculosis EgtD target both substrate binding sites to limit hercynine production. Scientific Reports, 2021, 11, 22240.	1.6	1
715	Three-dimensional structure of xylonolactonase from <i>Caulobacter crescentus</i> : A mononuclear iron enzyme of the β -lactamase β -propeller hydrolase family. Protein Science, 2022, 31, 371-383.	3.1	4
716	A new ALK inhibitor overcomes resistance to first- and second-generation inhibitors in NSCLC. EMBO Molecular Medicine, 2022, 14, e14296.	3.3	9
717	Mechanism of actin-dependent activation of nucleotidyl cyclase toxins from bacterial human pathogens. Nature Communications, 2021, 12, 6628.	5.8	13
718	Ten things I 'hate' about refinement. Acta Crystallographica Section D: Structural Biology, 2021, 77, 1497-1515.	1.1	4
720	Structure of the translating <i>Neurospora</i> ribosome arrested by cycloheximide. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	18
721	High-resolution structures of the actomyosin-V complex in three nucleotide states provide insights into the force generation mechanism. ELife, 2021, 10, .	2.8	27
722	Structural basis of reactivation of oncogenic p53 mutants by a small molecule: methylene quinuclidinone (MQ). Nature Communications, 2021, 12, 7057.	5.8	39
723	Temporary Intermediates of L-Trp Along the Reaction Pathway of Human Indoleamine 2,3-Dioxygenase 1 and Identification of an Exo Site. International Journal of Tryptophan Research, 2021, 14, 117864692110529.	1.0	3
724	Structure-affinity relationships of reversible proline analog inhibitors targeting proline dehydrogenase. Organic and Biomolecular Chemistry, 2022, 20, 895-905.	1.5	6
725	Directed evolution of the rRNA methylating enzyme Cfr reveals molecular basis of antibiotic resistance. ELife, 2022, 11, .	2.8	10
726	Neutron crystallography reveals mechanisms used by <i>Pseudomonas aeruginosa</i> for host-cell binding. Nature Communications, 2022, 13, 194.	5.8	13
727	Cryo-electron microscopy reveals how acetogenins inhibit mitochondrial respiratory complex I. Journal of Biological Chemistry, 2022, 298, 101602.	1.6	19

#	ARTICLE	IF	CITATIONS
728	Antivitamins B12: Synthesis and application as inhibitory ligand of the B12-tailoring enzyme CblC. <i>Methods in Enzymology</i> , 2022, 668, 157-178.	0.4	1
729	A radical approach to radicals. <i>Acta Crystallographica Section D: Structural Biology</i> , 2022, 78, 43-51.	1.1	0
730	Rearrangement of a unique Kv1.3 selectivity filter conformation upon binding of a drug. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2022, 119, .	3.3	20
731	Generation of bright monomeric red fluorescent proteins <i>via</i> computational design of enhanced chromophore packing. <i>Chemical Science</i> , 2022, 13, 1408-1418.	3.7	9
732	A structural basis for the diverse linkage specificities within the ZUFSP deubiquitinase family. <i>Nature Communications</i> , 2022, 13, 401.	5.8	10
733	Mechanism of CFTR correction by type I folding correctors. <i>Cell</i> , 2022, 185, 158-168.e11.	13.5	95
734	Structural Characterization of Dicyanopyridine Containing DNMT1-Selective, Non-Nucleoside Inhibitors. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
735	Fluorine Modifications Contribute to Potent Antiviral Activity against Highly Drug-Resistant HIV-1 and Favorable Blood-Brain Barrier Penetration Property of Novel Central Nervous System-Targeting HIV-1 Protease Inhibitors <i>In Vitro</i> . <i>Antimicrobial Agents and Chemotherapy</i> , 2022, 66, AAC0171521.	1.4	5
736	Structural insights in cell-type specific evolution of intra-host diversity by SARS-CoV-2. <i>Nature Communications</i> , 2022, 13, 222.	5.8	23
737	Discovery of a new flavin N5-adduct in a tyrosine to phenylalanine variant of d-Arginine dehydrogenase. <i>Archives of Biochemistry and Biophysics</i> , 2022, 715, 109100.	1.4	1
738	Identification and characterization of two drug-like fragments that bind to the same cryptic binding pocket of <i>Burkholderia pseudomallei</i> DsbA. <i>Acta Crystallographica Section D: Structural Biology</i> , 2022, 78, 75-90.	1.1	2
739	Identification of a diarylpentanoid-producing polyketide synthase revealing an unusual biosynthetic pathway of 2-(2-phenylethyl)chromones in agarwood. <i>Nature Communications</i> , 2022, 13, 348.	5.8	29
740	Juggling with fluorescent proteins: Spectrum and structural changes of the mCardinal2 variants. <i>Biochemical and Biophysical Research Communications</i> , 2022, 593, 79-83.	1.0	3
743	Pore structure controls stability and molecular flux in engineered protein cages. <i>Science Advances</i> , 2022, 8, eabl7346.	4.7	30
744	The coupling mechanism of mammalian mitochondrial complex I. <i>Nature Structural and Molecular Biology</i> , 2022, 29, 172-182.	3.6	45
745	Crystal structure of the adenylation domain from an $\hat{\mu}$ -poly-l-lysine synthetase provides molecular mechanism for substrate specificity. <i>Biochemical and Biophysical Research Communications</i> , 2022, 596, 43-48.	1.0	6
746	Discovery of a first-in-class reversible DNMT1-selective inhibitor with improved tolerability and efficacy in acute myeloid leukemia. <i>Nature Cancer</i> , 2021, 2, 1002-1017.	5.7	23
747	Structural insights into the Venus flytrap mechanosensitive ion channel Flycatcher1. <i>Nature Communications</i> , 2022, 13, 850.	5.8	13

#	ARTICLE	IF	CITATIONS
748	Fast fragment- and compound-screening pipeline at the Swiss Light Source. <i>Acta Crystallographica Section D: Structural Biology</i> , 2022, 78, 328-336.	1.1	11
750	Non-covalent SARS-CoV-2 Mpro inhibitors developed from in silico screen hits. <i>Scientific Reports</i> , 2022, 12, 2505.	1.6	41
751	Structural basis for context-specific inhibition of translation by oxazolidinone antibiotics. <i>Nature Structural and Molecular Biology</i> , 2022, 29, 162-171.	3.6	31
752	Structure and mechanism of the methyltransferase ribozyme MTR1. <i>Nature Chemical Biology</i> , 2022, 18, 547-555.	3.9	16
753	Updated restraint dictionaries for carbohydrates in the pyranose form. <i>Acta Crystallographica Section D: Structural Biology</i> , 2022, 78, 455-465.	1.1	6
754	Accurate positioning of functional residues with robotics-inspired computational protein design. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2022, 119, e2115480119.	3.3	6
755	Comparative structural analysis provides new insights into the function of R2α-like ligand-binding oxidase. <i>FEBS Letters</i> , 2022, 596, 1600-1610.	1.3	2
757	Structural and Biochemical Basis for Development of Diketo Acid Inhibitors Targeting the Cap-Snatching Endonuclease of the Ebinur Lake Virus (Order: <i>Bunyavirales</i>). <i>Journal of Virology</i> , 2022, 96, e0217321.	1.5	1
758	Activation mechanism of the class D fungal GPCR dimer Ste2. <i>Nature</i> , 2022, 603, 743-748.	13.7	13
760	From tryptophan-based amides to tertiary amines: Optimization of a butyrylcholinesterase inhibitor series. <i>European Journal of Medicinal Chemistry</i> , 2022, 234, 114248.	2.6	11
762	Structural characterization of dicyanopyridine containing DNMT1-selective, non-nucleoside inhibitors. <i>Structure</i> , 2022, 30, 793-802.e5.	1.6	11
763	Interplay between DsbA1, DsbA2 and C8J_1298 Periplasmic Oxidoreductases of <i>Campylobacter jejuni</i> and Their Impact on Bacterial Physiology and Pathogenesis. <i>International Journal of Molecular Sciences</i> , 2021, 22, 13451.	1.8	5
764	Mutasynthetic Production and Antimicrobial Characterization of Darobactin Analogs. <i>Microbiology Spectrum</i> , 2021, 9, e0153521.	1.2	26
765	Evolution of a histone variant involved in compartmental regulation of NAD metabolism. <i>Nature Structural and Molecular Biology</i> , 2021, 28, 1009-1019.	3.6	7
766	Cryo-Electron Microscopy and Biochemical Analysis Offer Insights Into the Effects of Acidic pH, Such as Occur During Acidosis, on the Complement Binding Properties of C-Reactive Protein. <i>Frontiers in Immunology</i> , 2021, 12, 757633.	2.2	5
767	Discovery and Characterization of Potent Dual P-Glycoprotein and CYP3A4 Inhibitors: Design, Synthesis, Cryo-EM Analysis, and Biological Evaluations. <i>Journal of Medicinal Chemistry</i> , 2022, 65, 191-216.	2.9	25
768	Conformational changes in the yeast mitochondrial ABC transporter Atm1 during the transport cycle. <i>Science Advances</i> , 2021, 7, eabk2392.	4.7	4
769	Hydrazones and Thiosemicarbazones Targeting Protein-Protein-Interactions of SARS-CoV-2 Papain-like Protease. <i>Frontiers in Chemistry</i> , 2022, 10, 832431.	1.8	5

#	ARTICLE	IF	CITATIONS
770	Structural and molecular determinants for the interaction of ExbB from <i>Serratia marcescens</i> and HasB, a TonB paralogue. <i>Communications Biology</i> , 2022, 5, 355.	2.0	5
776	Structural basis of TRPV5 regulation by physiological and pathophysiological modulators. <i>Cell Reports</i> , 2022, 39, 110737.	2.9	22
777	Structural insights into TRPV2 activation by small molecules. <i>Nature Communications</i> , 2022, 13, 2334.	5.8	25
778	Covalent narpaprevir- and boceprevir-derived hybrid inhibitors of SARS-CoV-2 main protease. <i>Nature Communications</i> , 2022, 13, 2268.	5.8	69
779	Structural mapping of antibody landscapes to human betacoronavirus spike proteins. <i>Science Advances</i> , 2022, 8, eabn2911.	4.7	28
781	Rational inhibitor design for <i>Pseudomonas aeruginosa</i> salicylate adenylation enzyme PchD. <i>Journal of Biological Inorganic Chemistry</i> , 2022, 27, 541-551.	1.1	5
782	Racemic crystal structures of A-DNA duplexes. <i>Acta Crystallographica Section D: Structural Biology</i> , 2022, 78, 709-715.	1.1	0
783	Molecular basis for cooperative binding and synergy of ATP-site and allosteric EGFR inhibitors. <i>Nature Communications</i> , 2022, 13, 2530.	5.8	29
784	Structures of oxysterol sensor EB12/GPR183, a key regulator of the immune response. <i>Structure</i> , 2022, 30, 1016-1024.e5.	1.6	15
785	Structural anatomy of Protein Kinase C C1 domain interactions with diacylglycerol and other agonists. <i>Nature Communications</i> , 2022, 13, 2695.	5.8	17
786	Inhibition mechanism of the chloride channel TMEM16A by the pore blocker 1PBC. <i>Nature Communications</i> , 2022, 13, 2798.	5.8	10
787	Targeting dual-specificity tyrosine phosphorylation-regulated kinase 2 with a highly selective inhibitor for the treatment of prostate cancer. <i>Nature Communications</i> , 2022, 13, .	5.8	6
788	The unconventional activation of the muscarinic acetylcholine receptor M4R by diverse ligands. <i>Nature Communications</i> , 2022, 13, .	5.8	13
790	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, .	4.7	24
791	Reaction hijacking of tyrosine tRNA synthetase as a new whole-of-life-cycle antimalarial strategy. <i>Science</i> , 2022, 376, 1074-1079.	6.0	25
792	Rhodopsin-bestrophin fusion proteins from unicellular algae form gigantic pentameric ion channels. <i>Nature Structural and Molecular Biology</i> , 2022, 29, 592-603.	3.6	23
793	Crystal structure of a family β -lactamase fold hydrolase reveals the molecular mechanism for its broad substrate scope. <i>FEBS Journal</i> , 2022, 289, 6714-6730.	2.2	1
794	Core and rod structures of a thermophilic cyanobacterial light-harvesting phycobilisome. <i>Nature Communications</i> , 2022, 13, .	5.8	20

#	ARTICLE	IF	CITATIONS
795	Structural basis of ligand binding modes of human EAAT2. Nature Communications, 2022, 13, .	5.8	12
796	Structures and mechanism of the plant PIN-FORMED auxin transporter. Nature, 2022, 609, 605-610.	13.7	58
798	Phenylsulfamoyl Benzoic Acid Inhibitor of ERAP2 with a Novel Mode of Inhibition. ACS Chemical Biology, 2022, 17, 1756-1768.	1.6	2
799	Enzymatic formation of a prenyl $\hat{1}^2$ -carboline by a fungal indole prenyltransferase. Journal of Natural Medicines, 2022, 76, 873-879.	1.1	1
802	Evidence for the Chemical Mechanism of RibB (3,4-Dihydroxy-2-butanone 4-phosphate Synthase) of Riboflavin Biosynthesis. Journal of the American Chemical Society, 2022, 144, 12769-12780.	6.6	4
803	Structural and Biochemical Investigation of the Heterodimeric Murine tRNA-Guanine Transglycosylase. ACS Chemical Biology, 2022, 17, 2229-2247.	1.6	7
804	<i>N</i> -Acylamino Saccharin as an Emerging Cysteine-Directed Covalent Warhead and Its Application in the Identification of Novel FBPase Inhibitors toward Glucose Reduction. Journal of Medicinal Chemistry, 2022, 65, 9126-9143.	2.9	3
805	Mechanism of threonine ADP-ribosylation of F-actin by a Tc toxin. Nature Communications, 2022, 13, .	5.8	12
806	Membrane-anchored HDCR nanowires drive hydrogen-powered CO ₂ fixation. Nature, 2022, 607, 823-830.	13.7	36
807	<i>Erwinia tasmaniensis</i> levansucrase shows enantiomer selection for (<i>S</i>)-1,2,4-butanetriol. Acta Crystallographica Section F, Structural Biology Communications, 2022, 78, 289-296.	0.4	1
808	Probing ligand binding of endothiapepsin by 'temperature-resolved' macromolecular crystallography. Acta Crystallographica Section D: Structural Biology, 2022, 78, 964-974.	1.1	9
809	The Crystal Structure of the Defense Conferring Rice Protein OsJAC1 Reveals a Carbohydrate Binding Site on the Dirigent-like Domain. Biomolecules, 2022, 12, 1126.	1.8	3
810	Phosphonic acid-containing inhibitors of tyrosyl-DNA phosphodiesterase 1. Frontiers in Chemistry, 0, 10, .	1.8	3
811	The temperature-dependent conformational ensemble of SARS-CoV-2 main protease (M ^{pro}). IUCr, 2022, 9, 682-694.	1.0	22
812	AvmM catalyses macrocyclization through dehydration/Michael-type addition in alchivemycin A biosynthesis. Nature Communications, 2022, 13, .	5.8	8
813	Structural insights into inhibitory mechanism of human excitatory amino acid transporter EAAT2. Nature Communications, 2022, 13, .	5.8	13
814	The structure and characterization of human cytochrome P450 8B1 supports future drug design for nonalcoholic fatty liver disease and diabetes. Journal of Biological Chemistry, 2022, 298, 102344.	1.6	7
815	Catalytic potential of a fungal indole prenyltransferase toward $\hat{1}^2$ -carbolines, harmine and harman, and their prenylation effects on antibacterial activity. Journal of Bioscience and Bioengineering, 2022, 134, 311-317.	1.1	1

#	ARTICLE	IF	CITATIONS
816	Structures of Streptococcus pyogenes class A sortase in complex with substrate and product mimics provide key details of target recognition. Journal of Biological Chemistry, 2022, 298, 102446.	1.6	8
818	Crystallographic analysis of engineered polymerases synthesizing phosphonomethylthreosyl nucleic acid. Nucleic Acids Research, 2022, 50, 9663-9674.	6.5	2
819	A small molecule antagonist of SMN disrupts the interaction between SMN and RNAP II. Nature Communications, 2022, 13, .	5.8	7
820	Exploring the RNase A scaffold to combine catalytic and antimicrobial activities. Structural characterization of RNase 3/1 chimeras. Frontiers in Molecular Biosciences, 0, 9, .	1.6	0
821	Redox-controlled reorganization and flavin strain within the ribonucleotide reductase R2bâ€“NrdI complex monitored by serial femtosecond crystallography. ELife, 0, 11, .	2.8	4
822	Investigating the Active Oxidants Involved in Cytochrome P450 Catalyzed Sulfoxidation Reactions. Chemistry - A European Journal, 2022, 28, .	1.7	12
823	Uncompetitive, adduct-forming SARM1 inhibitors are neuroprotective in preclinical models of nerve injury and disease. Neuron, 2022, 110, 3711-3726.e16.	3.8	18
824	High-resolution structures of the SARS-CoV-2 N7-methyltransferase inform therapeutic development. Nature Structural and Molecular Biology, 2022, 29, 850-853.	3.6	12
825	Autoprocessing and oxyanion loop reorganization upon GC373 and nirmatrelvir binding of monomeric SARS-CoV-2 main protease catalytic domain. Communications Biology, 2022, 5, .	2.0	8
826	The primary familial brain calcification-associated protein MYORG is an α -galactosidase with restricted substrate specificity. PLoS Biology, 2022, 20, e3001764.	2.6	7
829	Gridâ€“type Quaternary Metallosupramolecular Compounds Inhibit Human Cholinesterases through Dynamic Multivalent Interactions. ChemBioChem, 2022, 23, .	1.3	3
830	Molecular asymmetry of a photosynthetic supercomplex from green sulfur bacteria. Nature Communications, 2022, 13, .	5.8	4
831	Enzymatic Lateâ€“Stage Halogenation of Peptides. ChemBioChem, 2023, 24, .	1.3	8
832	Activation mechanism of the mouse cold-sensing TRPM8 channel by cooling agonist and PIP ₂ . Science, 2022, 378, .	6.0	22
833	Structural basis for HflXr-mediated antibiotic resistance in <i>Listeria monocytogenes</i> . Nucleic Acids Research, 2022, 50, 11285-11300.	6.5	9
834	Small-molecule inhibition of the archetypal UbiB protein COQ8. Nature Chemical Biology, 2023, 19, 230-238.	3.9	4
835	Unmasking the Conformational Stability and Inhibitor Binding to SARS-CoV-2 Main Protease Active Site Mutants and Miniprecursor. Journal of Molecular Biology, 2022, 434, 167876.	2.0	4
837	Discovery and structural characterization of chicoric acid as a SARS-CoV-2 nucleocapsid protein ligand and RNA binding disruptor. Scientific Reports, 2022, 12, .	1.6	4

#	ARTICLE	IF	CITATIONS
840	Combinatorial and antagonistic effects of tubulin glutamylation and glycylation on katanin microtubule severing. <i>Developmental Cell</i> , 2022, 57, 2497-2513.e6.	3.1	15
841	Engineering a Conformationally Switchable Artificial Metalloprotein. <i>Journal of the American Chemical Society</i> , 0, , .	6.6	2
843	Fragment screening libraries for the identification of protein hot spots and their minimal binding pharmacophores. <i>RSC Medicinal Chemistry</i> , 2023, 14, 135-143.	1.7	1
844	Structure-based engineering of minimal Proline dehydrogenase domains for inhibitor discovery. <i>Protein Engineering, Design and Selection</i> , 0, , .	1.0	0
845	Integrating model simulation tools and cryo-electron microscopy. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2023, 13, .	6.2	8
846	The free fatty acid-binding pocket is a conserved hallmark in pathogenic β -coronavirus spike proteins from SARS-CoV to Omicron. <i>Science Advances</i> , 2022, 8, .	4.7	21
847	Conformational changes in mitochondrial complex I of the thermophilic eukaryote <i>Chaetomium thermophilum</i> . <i>Science Advances</i> , 2022, 8, .	4.7	10
848	Uptake mechanism of iron-phytosiderophore from the soil based on the structure of yellow stripe transporter. <i>Nature Communications</i> , 2022, 13, .	5.8	5
849	A broad specificity β -propeller enzyme from <i>Rhodospseudomonas palustris</i> that hydrolyzes many lactones including β -valerolactone. <i>Journal of Biological Chemistry</i> , 2022, , 102782.	1.6	0
851	Pseudo-irreversible butyrylcholinesterase inhibitors: Structure-activity relationships, computational and crystallographic study of the N-dialkyl O-arylcarbamate warhead. <i>European Journal of Medicinal Chemistry</i> , 2023, 247, 115048.	2.6	1
854	Linking medicinal cannabis to autotaxin-lysophosphatidic acid signaling. <i>Life Science Alliance</i> , 2023, 6, e202201595.	1.3	3
855	The Myxobacterial Antibiotic Myxovalargin: Biosynthesis, Structural Revision, Total Synthesis, and Molecular Characterization of Ribosomal Inhibition. <i>Journal of the American Chemical Society</i> , 2023, 145, 851-863.	6.6	4
856	A specific G9a inhibitor unveils BGLT3 lncRNA as a universal mediator of chemically induced fetal globin gene expression. <i>Nature Communications</i> , 2023, 14, .	5.8	7
858	Structural insights into the effects of glycerol on ligand binding to cytochrome P450. <i>Acta Crystallographica Section D: Structural Biology</i> , 2023, 79, 66-77.	1.1	1
859	Structural characterization on a β -agarase Aga86A_Wa from <i>Wenyngzhuangia aestuarii</i> reveals the prevalent methyl-galactose accommodation capacity of GH86 enzymes at subsite β 1. <i>Carbohydrate Polymers</i> , 2023, 306, 120594.	5.1	2
860	Differential dynamics and direct interaction of bound ligands with lipids in multidrug transporter ABCG2. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2023, 120, .	3.3	10
861	Physachenolide C is a Potent, Selective BET Inhibitor. <i>Journal of Medicinal Chemistry</i> , 2023, 66, 913-933.	2.9	3
862	Potent Long-Acting Inhibitors Targeting the HIV-1 Capsid Based on a Versatile Quinazolin-4-one Scaffold. <i>Journal of Medicinal Chemistry</i> , 2023, 66, 1941-1954.	2.9	8

#	ARTICLE	IF	CITATIONS
863	Ligand recognition mechanism of the human relaxin family peptide receptor 4 (RXFP4). <i>Nature Communications</i> , 2023, 14, .	5.8	2
864	Architecture of chloroplast TOC-TIC translocon supercomplex. <i>Nature</i> , 2023, 615, 349-357.	13.7	19
865	Structural insight into the hydrolase and synthase activities of an alkaline Î±-galactosidase from <i>Arabidopsis</i> from complexes with substrate/product. <i>Acta Crystallographica Section D: Structural Biology</i> , 2023, 79, 154-167.	1.1	1
866	8-Hydroxyquinolyl nitrones as multifunctional ligands for the therapy of neurodegenerative diseases. <i>Acta Pharmaceutica Sinica B</i> , 2023, 13, 2152-2175.	5.7	5
867	Screening through Lead Optimization of High Affinity, Allosteric Cyclin-Dependent Kinase 2 (CDK2) Inhibitors as Male Contraceptives That Reduce Sperm Counts in Mice. <i>Journal of Medicinal Chemistry</i> , 2023, 66, 1928-1940.	2.9	8
868	Cryo-EM structure of the whole photosynthetic reaction center apparatus from the green sulfur bacterium <i>Chlorobaculum tepidum</i> . <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2023, 120, .	3.3	6
870	Crystal structure and ligandability of the 14-3-3/pyrin interface. <i>Biochemical and Biophysical Research Communications</i> , 2023, 651, 1-7.	1.0	0
871	Targeting <i>Enterococcus faecalis</i> HMG-CoA reductase with a non-statin inhibitor. <i>Communications Biology</i> , 2023, 6, .	2.0	3
872	Conformation-dependent ligand hot spots in the spliceosomal RNA helicase BRR2. <i>Acta Crystallographica Section D: Structural Biology</i> , 2023, 79, 304-317.	1.1	0
873	Rapid discovery and crystallography study of highly potent and selective butylcholinesterase inhibitors based on oxime-containing libraries and conformational restriction strategies. <i>Bioorganic Chemistry</i> , 2023, 134, 106465.	2.0	1
874	Discovery of new, highly potent and selective inhibitors of BuChE - design, synthesis, in vitro and in vivo evaluation and crystallography studies. <i>European Journal of Medicinal Chemistry</i> , 2023, 249, 115135.	2.6	4
875	<i>In situ</i> ligand restraints from quantum-mechanical methods. <i>Acta Crystallographica Section D: Structural Biology</i> , 2023, 79, 100-110.	1.1	4
877	Diversity in the ligand binding pocket of HapR attributes to its uniqueness towards several inhibitors with respect to other homologues - A structural and molecular perspective. <i>International Journal of Biological Macromolecules</i> , 2023, 233, 123495.	3.6	2
878	Does the presence of ground state complex between a PR-10 protein and a sensitizer affect the mechanism of sensitized photo-oxidation?. <i>Free Radical Biology and Medicine</i> , 2023, 198, 27-43.	1.3	0
880	The Drug-Induced Interface That Drives HIV-1 Integrase Hypermultimerization and Loss of Function. <i>MBio</i> , 2023, 14, .	1.8	2
881	Human cytochrome P450 17A1 structures with metabolites of prostate cancer drug abiraterone reveal substrate-binding plasticity and a second binding site. <i>Journal of Biological Chemistry</i> , 2023, 299, 102999.	1.6	4
882	Small molecule inhibitors of 15-PGDH exploit a physiologic induced-fit closing system. <i>Nature Communications</i> , 2023, 14, .	5.8	2
885	Pyridine-containing substrate analogs are restricted from accessing the human cytochrome P450 8B1 active site by tryptophan 281. <i>Journal of Biological Chemistry</i> , 2023, 299, 103032.	1.6	0

#	ARTICLE	IF	CITATIONS
887	Conformational changes in the human Cx43/GJA1 gap junction channel visualized using cryo-EM. <i>Nature Communications</i> , 2023, 14, .	5.8	13
888	Structural basis of the activation of PPAR α by the plasticizer metabolites MEHP and MINCH. <i>Environment International</i> , 2023, 173, 107822.	4.8	3
889	Discovery of natural-product-derived sequanamycins as potent oral anti-tuberculosis agents. <i>Cell</i> , 2023, 186, 1013-1025.e24.	13.5	11
890	Automatic and accurate ligand structure determination guided by cryo-electron microscopy maps. <i>Nature Communications</i> , 2023, 14, .	5.8	2
891	Room-temperature crystallography reveals altered binding of small-molecule fragments to PTP1B. <i>ELife</i> , 0, 12, .	2.8	16
892	Bivalent molecular mimicry by ADP protects metal redox state and promotes coenzyme B ₁₂ repair. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2023, 120, .	3.3	5
893	Discovery of Novel Substrate-Competitive Lysine Methyltransferase G9a Inhibitors as Anticancer Agents. <i>Journal of Medicinal Chemistry</i> , 2023, 66, 4059-4085.	2.9	5
894	Structural basis of the inhibition of cystathionine β -lyase from <i>Toxoplasma gondii</i> by propargylglycine and cysteine. <i>Protein Science</i> , 2023, 32, .	3.1	1
896	Crystal Structures of Inhibitor-Bound Main Protease from Delta- and Gamma-Coronaviruses. <i>Viruses</i> , 2023, 15, 781.	1.5	2
897	Highly selective butyrylcholinesterase inhibitors related to Amaryllidaceae alkaloids - Design, synthesis, and biological evaluation. <i>European Journal of Medicinal Chemistry</i> , 2023, 252, 115301.	2.6	4
898	Structural basis for CaV β 2 δ 1: gabapentin binding. <i>Nature Structural and Molecular Biology</i> , 2023, 30, 735-739.	3.6	8
899	Cryo-EM reveals an unprecedented binding site for NaV1.7 inhibitors enabling rational design of potent hybrid inhibitors. <i>ELife</i> , 0, 12, .	2.8	5
900	Structural basis of the substrate recognition and inhibition mechanism of Plasmodium falciparum nucleoside transporter PfENT1. <i>Nature Communications</i> , 2023, 14, .	5.8	3
903	ADP enhances the allosteric activation of eukaryotic elongation factor 2 kinase by β -calmodulin. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2023, 120, .	3.3	2
904	Cytochrome P450-catalyzed oxidation of halogen-containing substrates. <i>Journal of Inorganic Biochemistry</i> , 2023, , 112234.	1.5	3
906	Biochemical and structural characterization of a robust and thermostable ascorbate recycling monodehydroascorbate reductase (MDHAR) from stress adapted pearl millet. <i>Biochemical and Biophysical Research Communications</i> , 2023, 662, 135-141.	1.0	3
966	Fast fragment and compound screening pipeline at the Swiss Light Source. <i>Methods in Enzymology</i> , 2023, , 235-284.	0.4	2