

CITATION REPORT

List of articles citing

MolProbity: all-atom structure validation for macromolecular crystallography

DOI: 10.1107/s0907444909042073

Acta Crystallographica Section D: Biological Crystallography, 2010, 66, 12-21.

Source: <https://exaly.com/paper-pdf/48384597/citation-report.pdf>

Version: 2024-04-27

This report has been generated based on the citations recorded by exaly.com for the above article. For the latest version of this publication list, visit the link given above.

The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

#	Paper	IF	Citations
2265	Purification, biochemical characterization, and cloning of phospholipase D from <i>Streptomyces racemochromogenes</i> strain 10-3. 2010 , 29, 598-608		13
2264	Crystal structure of the three FK506 binding protein domains of wheat FKBP73: evidence for a unique wFK73_2 domain. 2010 , 11, 113-23		10
2263	Unmet challenges of structural genomics. 2010 , 20, 587-97		40
2262	phenix.model_vs_data: a high-level tool for the calculation of crystallographic model and data statistics. 2010 , 43, 669-676		91
2261	PHENIX: a comprehensive Python-based system for macromolecular structure solution. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2010 , 66, 213-21		16067
2260	Structure of D-tyrosyl-tRNA ^{Tyr} deacylase using home-source Cu K α and moderate-quality iodide-SAD data: structural polymorphism and HEPES-bound enzyme states. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2010 , 66, 584-92		10
2259	High-resolution X-ray crystal structure of bovine H-protein at 0.88 Å resolution. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2010 , 66, 698-708		9
2258	Near-atomic resolution structures of urate oxidase complexed with its substrate and analogues: the protonation state of the ligand. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2010 , 66, 714-24		23
2257	The high-resolution structure of pig heart succinyl-CoA:3-oxoacid coenzyme A transferase. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2010 , 66, 797-805		6
2256	Structure of the <i>Escherichia coli</i> RNA polymerase alpha subunit C-terminal domain. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2010 , 66, 806-12		7
2255	Structures of apo and GTP-bound molybdenum cofactor biosynthesis protein MoaC from <i>Thermus thermophilus</i> HB8. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2010 , 66, 821-33		22
2254	Structure of <i>Staphylococcus aureus</i> adenylosuccinate lyase (PurB) and assessment of its potential as a target for structure-based inhibitor discovery. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2010 , 66, 881-8		13
2253	Validation of crystallographic models containing TLS or other descriptions of anisotropy. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2010 , 66, 889-900		45
2252	Crystallographic binding studies with an engineered monomeric variant of triosephosphate isomerase. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2010 , 66, 934-44		10
2251	Atomic resolution studies of haloalkane dehalogenases DhaA04, DhaA14 and DhaA15 with engineered access tunnels. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2010 , 66, 962-9		10
2250	Comparison of a nontoxic variant of <i>Clostridium perfringens</i> β -toxin with the toxic wild-type strain. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2010 , 66, 1067-74		4
2249	The 2.7 Å resolution structure of the glycopeptide sulfotransferase Teg14. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2010 , 66, 1278-86		6

2248	The structure of PhaZ7 at atomic (1.2 Å) resolution reveals details of the active site and suggests a substrate-binding mode. 2010 , 66, 648-54	11
2247	Structure of autophagy-related protein Atg8 from the silkworm <i>Bombyx mori</i> . 2010 , 66, 787-90	23
2246	The role of a topologically conserved isoleucine in glutathione transferase structure, stability and function. 2010 , 66, 776-80	3
2245	Structure of Rv1848 (UreA), the <i>Mycobacterium tuberculosis</i> urease gamma subunit. 2010 , 66, 781-6	10
2244	Structures of three members of Pfam PF02663 (FmdE) implicated in microbial methanogenesis reveal a conserved β -core domain and an auxiliary C-terminal treble-clef zinc finger. 2010 , 66, 1335-46	7
2243	Structure of the β -glutamyl-L-diamino acid endopeptidase YkfC from <i>Bacillus cereus</i> in complex with L-Ala- β -Glu: insights into substrate recognition by NlpC/P60 cysteine peptidases. 2010 , 66, 1354-64	45
2242	The structure of <i>Haemophilus influenzae</i> prephenate dehydrogenase suggests unique features of bifunctional TyrA enzymes. 2010 , 66, 1317-25	9
2241	Structure of a fibronectin type III-like module from <i>Clostridium thermocellum</i> . 2010 , 66, 878-80	11
2240	Structure of a membrane-attack complex/perforin (MACPF) family protein from the human gut symbiont <i>Bacteroides thetaiotaomicron</i> . 2010 , 66, 1297-305	26
2239	Structure of a putative NTP pyrophosphohydrolase: YP_001813558.1 from <i>Exiguobacterium sibiricum</i> 255-15. 2010 , 66, 1237-44	2
2238	The structure of a family GH25 lysozyme from <i>Aspergillus fumigatus</i> . 2010 , 66, 973-7	11
2237	Structure of <i>Bacteroides thetaiotaomicron</i> BT2081 at 2.05 Å resolution: the first structural representative of a new protein family that may play a role in carbohydrate metabolism. 2010 , 66, 1287-96	1
2236	Structure of the endonuclease IV homologue from <i>Thermotoga maritima</i> in the presence of active-site divalent metal ions. 2010 , 66, 1003-12	6
2235	High-resolution structure of an alpha-spectrin SH3-domain mutant with a redesigned hydrophobic core. 2010 , 66, 1023-7	3
2234	Structural analysis of <i>Bacillus pumilus</i> phenolic acid decarboxylase, a lipocalin-fold enzyme. 2010 , 66, 1407-14	21
2233	Structure of BT_3984, a member of the SusD/RagB family of nutrient-binding molecules. 2010 , 66, 1274-80	9
2232	Structure of <i>Plasmodium falciparum</i> ADP-ribosylation factor 1. 2010 , 66, 1426-31	6
2231	Structure of dihydroorotase from <i>Bacillus anthracis</i> at 2.6 Å resolution. 2010 , 66, 1432-5	10

2230	Structure of a tryptophanyl-tRNA synthetase containing an iron-sulfur cluster. 2010 , 66, 1326-34	16
2229	Structure of the <i>Francisella tularensis</i> enoyl-acyl carrier protein reductase (FabI) in complex with NAD(+) and triclosan. 2010 , 66, 1436-40	11
2228	Structure of Hsp33/YOR391Cp from the yeast <i>Saccharomyces cerevisiae</i> . 2010 , 66, 1557-61	5
2227	Structure of the iSH2 domain of human phosphatidylinositol 3-kinase p85 α subunit reveals conformational plasticity in the interhelical turn region. 2010 , 66, 1567-71	6
2226	Crystal structure of an archaeal cleavage and polyadenylation specificity factor subunit from <i>Pyrococcus horikoshii</i> . 2010 , 78, 2395-8	19
2225	Modeling single nucleotide polymorphisms in the human AKR1C1 and AKR1C2 genes: implications for functional and genotyping analyses. 2010 , 5, e15604	10
2224	The <i>Trypanosoma brucei</i> life cycle switch TbPPT1 is structurally conserved and dephosphorylates the nucleolar protein NOPP44/46. 2010 , 285, 22075-81	16
2223	Crystallographic structure of porcine adenovirus type 4 fiber head and galectin domains. 2010 , 84, 10558-68	18
2222	Structure of a classical MHC class I molecule that binds "non-classical" ligands. 2010 , 8, e1000557	36
2221	Structure of the bacteriophage T4 long tail fiber receptor-binding tip. 2010 , 107, 20287-92	130
2220	The 1.5 Å crystal structure of human receptor for advanced glycation endproducts (RAGE) ectodomains reveals unique features determining ligand binding. 2010 , 285, 40762-70	100
2219	Structure and biological importance of the Spn1-Spt6 interaction, and its regulatory role in nucleosome binding. 2010 , 40, 725-35	44
2218	A novel mechanism for azoreduction. 2010 , 400, 24-37	41
2217	Structure and engineering of L-arabinitol 4-dehydrogenase from <i>Neurospora crassa</i> . 2010 , 402, 230-40	14
2216	Gradual adaptive changes of a protein facing high salt concentrations. 2010 , 404, 493-505	35
2215	Structural analysis of the receptor binding domain of botulinum neurotoxin serotype D. 2010 , 401, 498-503	14
2214	Insights into egg coat assembly and egg-sperm interaction from the X-ray structure of full-length ZP3. 2010 , 143, 404-15	112
2213	Crystal structure of PG16 and chimeric dissection with somatically related PG9: structure-function analysis of two quaternary-specific antibodies that effectively neutralize HIV-1. 2010 , 84, 8098-110	185

2212	Structural analysis of <i>Saccharomyces cerevisiae</i> alpha-galactosidase and its complexes with natural substrates reveals new insights into substrate specificity of GH27 glycosidases. 2010 , 285, 28020-33	31
2211	Molecular adaptability of nucleoside diphosphate kinase b from trypanosomatid parasites: stability, oligomerization and structural determinants of nucleotide binding. 2011 , 7, 2189-95	30
2210	Conformationally constrained peptides from CD2 to modulate protein-protein interactions between CD2 and CD58. 2011 , 54, 5307-19	32
2209	Structure of the response regulator PhoP from <i>Mycobacterium tuberculosis</i> reveals a dimer through the receiver domain. 2011 , 50, 5948-57	54
2208	Polarizable Atomic Multipole X-Ray Refinement: Particle Mesh Ewald Electrostatics for Macromolecular Crystals. 2011 , 7, 1141-56	31
2207	Cofactor mobility determines reaction outcome in the IMPDH and GMPTG (H ₂ B barrel) enzymes. 2011 , 7, 950-8	27
2206	On the mechanism of dimethylarginine dimethylaminohydrolase inactivation by 4-halopyridines. 2011 , 133, 10951-9	16
2205	Metal-binding loop length is a determinant of the pKa of a histidine ligand at a type 1 copper site. 2011 , 50, 482-8	12
2204	Mechanism of the intramolecular Claisen condensation reaction catalyzed by MenB, a crotonase superfamily member. 2011 , 50, 9532-44	41
2203	Flavin-induced oligomerization in <i>Escherichia coli</i> adaptive response protein AidB. 2011 , 50, 10159-69	6
2202	Structure of the USP15 N-terminal domains: a β -hairpin mediates close association between the DUSP and UBL domains. 2011 , 50, 7995-8004	22
2201	A structural study of norovirus 3C protease specificity: binding of a designed active site-directed peptide inhibitor. 2011 , 50, 240-9	44
2200	Crystal structure and characterization of particulate methane monooxygenase from <i>Methylocystis</i> species strain M. 2011 , 50, 10231-40	101
2199	Structure of estradiol metal chelate and estrogen receptor complex: the basis for designing a new class of selective estrogen receptor modulators. 2011 , 54, 3575-80	24
2198	Improving the physical realism and structural accuracy of protein models by a two-step atomic-level energy minimization. 2011 , 101, 2525-34	600
2197	Structure-based design of short peptide ligands binding onto the <i>E. coli</i> processivity ring. 2011 , 54, 4627-37	21
2196	Effective techniques for protein structure mining. 2012 , 857, 33-54	1
2195	Re(CO)(3)(H(2)O)(3)(+) binding to lysozyme: structure and reactivity. 2011 , 3, 909-16	30

2194	A prodrug approach for improving antituberculosis activity of potent Mycobacterium tuberculosis type II dehydroquinase inhibitors. 2011 , 54, 6063-84	29
2193	Impact of BRCA1 BRCT domain missense substitutions on phosphopeptide recognition. 2011 , 50, 4579-89	35
2192	A Burkholderia pseudomallei toxin inhibits helicase activity of translation factor eIF4A. 2011 , 334, 821-4	81
2191	Insights into noncanonical E1 enzyme activation from the structure of autophagic E1 Atg7 with Atg8. 2011 , 18, 1323-30	70
2190	Molecular mechanism of selectivity among G protein-coupled receptor kinase 2 inhibitors. 2011 , 80, 294-303	82
2189	Host cell invasion by apicomplexan parasites: insights from the co-structure of AMA1 with a RON2 peptide. 2011 , 333, 463-7	145
2188	Pyochelin enantiomers and their outer-membrane siderophore transporters in fluorescent pseudomonads: structural bases for unique enantiospecific recognition. 2011 , 133, 16503-9	25
2187	Fragment screening of infectious disease targets in a structural genomics environment. 2011 , 493, 533-56	5
2186	Fragment screening purely with protein crystallography. 2011 , 493, 321-56	19
2185	Structural basis of the 9-fold symmetry of centrioles. 2011 , 144, 364-75	263
2184	The Min oscillator uses MinD-dependent conformational changes in MinE to spatially regulate cytokinesis. 2011 , 146, 396-407	117
2183	Structural basis for the activation of innate immune pattern-recognition receptor RIG-I by viral RNA. 2011 , 147, 423-35	439
2182	The molecular basis for the endocytosis of small R-SNAREs by the clathrin adaptor CALM. 2011 , 147, 1118-31	140
2181	Structural and functional analysis of a plant resistance protein TIR domain reveals interfaces for self-association, signaling, and autoregulation. 2011 , 9, 200-211	243
2180	Crystal structure of the cysteine protease inhibitor 2 from Entamoeba histolytica: functional convergence of a common protein fold. 2011 , 471, 45-52	14
2179	Expression, purification, electron microscopy, N-glycosylation mutagenesis and molecular modeling of human P2X4 and Dictyostelium discoideum P2XA. 2011 , 1808, 2859-66	4
2178	Characterization of monomeric dihydrodipicolinate synthase variant reveals the importance of substrate binding in optimizing oligomerization. 2011 , 1814, 1900-9	12
2177	Crystal structure of the receptor binding domain of the botulinum C-D mosaic neurotoxin reveals potential roles of lysines 1118 and 1136 in membrane interactions. 2011 , 404, 407-12	19

2176	Insights into role of the hydrogen bond networks in substrate recognition by UDP-GalNAc 4-epimerases. 2011 , 412, 232-7	7
2175	X-ray crystallography: Assessment and validation of protein-small molecule complexes for drug discovery. 2011 , 6, 771-782	46
2174	Structure and activity of the Cas3 HD nuclease MJ0384, an effector enzyme of the CRISPR interference. 2011 , 30, 4616-27	104
2173	Pharmacological validation of <i>Trypanosoma brucei</i> phosphodiesterases B1 and B2 as druggable targets for African sleeping sickness. 2011 , 54, 8188-94	42
2172	Crystal structure of a copper-transporting PIB-type ATPase. 2011 , 475, 59-64	257
2171	Crystal structure of the β_2 adrenergic receptor-Gs protein complex. 2011 , 477, 549-55	2228
2170	Methicillin-resistant <i>Staphylococcus aureus</i> (MRSA) pyruvate kinase as a target for bis-indole alkaloids with antibacterial activities. 2011 , 286, 44716-25	85
2169	Structural insights to how mammalian capping enzyme reads the CTD code. 2011 , 43, 299-310	72
2168	The 1.9Å crystal structure of Prp20p from <i>Saccharomyces cerevisiae</i> and its binding properties to Gsp1p and histones. 2011 , 174, 213-22	4
2167	Crystal structures of <i>Pseudomonas aeruginosa</i> guanidinobutyrase and guanidinopropionase, members of the ureohydrolase superfamily. 2011 , 175, 329-38	10
2166	Crystal structures of YwqE from <i>Bacillus subtilis</i> and CpsB from <i>Streptococcus pneumoniae</i> , unique metal-dependent tyrosine phosphatases. 2011 , 175, 442-50	17
2165	Structure and dynamics of the kinase IKK- α -A key regulator of the NF-kappa B transcription factor. 2011 , 176, 133-42	11
2164	Structural basis for the broad substrate range of the UDP-sugar pyrophosphorylase from <i>Leishmania major</i> . 2011 , 405, 461-78	32
2163	Alternate states of proteins revealed by detailed energy landscape mapping. 2011 , 405, 607-18	207
2162	A conformational switch involved in maturation of <i>Staphylococcus aureus</i> bacteriophage 80 β capsids. 2011 , 405, 863-76	28
2161	A leukotriene A4 hydrolase-related aminopeptidase from yeast undergoes induced fit upon inhibitor binding. 2011 , 406, 120-34	9
2160	Crystal structures exploring the origins of the broader specificity of <i>Escherichia coli</i> heat-labile enterotoxin compared to cholera toxin. 2011 , 406, 387-402	23
2159	Biochemical and structural characterization of lysophosphatidic Acid binding by a humanized monoclonal antibody. 2011 , 408, 462-76	16

2158	Structure of the dimeric autoinhibited conformation of DAPK2, a pro-apoptotic protein kinase. 2011 , 409, 369-83	19
2157	The extra-membranous domains of the competence protein HofQ show DNA binding, flexibility and a shared fold with type I KH domains. 2011 , 409, 642-53	18
2156	Structural insights into the novel diadenosine 5',5'-P ₄ tetraphosphate phosphorylase from <i>Mycobacterium tuberculosis</i> H37Rv. 2011 , 410, 93-104	7
2155	A new apo-caspase-6 crystal form reveals the active conformation of the apoenzyme. 2011 , 410, 307-15	12
2154	Crystallographic snapshots of the complete catalytic cycle of the unregulated aspartate transcarbamoylase from <i>Bacillus subtilis</i> . 2011 , 411, 190-200	9
2153	The overall architecture and receptor binding of pneumococcal carbohydrate-antigen-hydrolyzing enzymes. 2011 , 411, 1017-36	21
2152	Crystal structure of <i>Serratia fonticola</i> Sfh-I: activation of the nucleophile in mono-zinc metallo- β -lactamases. 2011 , 411, 951-9	39
2151	The crystal structure of zebrafish S100Z: implications for calcium-promoted S100 protein oligomerisation. 2011 , 411, 1072-82	7
2150	Structural basis of binding by cyclic nonphosphorylated peptide antagonists of Grb7 implicated in breast cancer progression. 2011 , 412, 397-411	22
2149	Crystal structure of the archaeal asparagine synthetase: interrelation with aspartyl-tRNA and asparaginyl-tRNA synthetases. 2011 , 412, 437-52	9
2148	Construction and crystal structure of recombinant STNV capsids. 2011 , 413, 41-50	37
2147	Structure of the food-poisoning <i>Clostridium perfringens</i> enterotoxin reveals similarity to the aerolysin-like pore-forming toxins. 2011 , 413, 138-49	70
2146	Peptidoglycan remodeling in <i>Mycobacterium tuberculosis</i> : comparison of structures and catalytic activities of RipA and RipB. 2011 , 413, 247-60	41
2145	A new structural form in the SAM/metal-dependent o-methyltransferase family: MycE from the mycinamicin biosynthetic pathway. 2011 , 413, 438-50	19
2144	Cyt1Aa toxin: crystal structure reveals implications for its membrane-perforating function. 2011 , 413, 804-14	53
2143	Structure of the <i>Escherichia coli</i> phosphonate binding protein PhnD and rationally optimized phosphonate biosensors. 2011 , 414, 356-69	46
2142	Disparate degrees of hypervariable loop flexibility control T-cell receptor cross-reactivity, specificity, and binding mechanism. 2011 , 414, 385-400	56
2141	Crystal structure of human prostate-specific antigen in a sandwich antibody complex. 2011 , 414, 530-44	45

2140	Crystal structure of the ligand binding domain of netrin G2. 2011 , 414, 723-34	19
2139	The E3 CR1-gamma gene in human adenoviruses associated with epidemic keratoconjunctivitis. 2011 , 160, 120-7	15
2138	The Phenix software for automated determination of macromolecular structures. 2011 , 55, 94-106	580
2137	Structure of prokaryotic polyamine deacetylase reveals evolutionary functional relationships with eukaryotic histone deacetylases. 2011 , 50, 1808-17	40
2136	Two distinct ferritin-like molecules in <i>Pseudomonas aeruginosa</i> : the product of the bfrA gene is a bacterial ferritin (FtnA) and not a bacterioferritin (Bfr). 2011 , 50, 5236-48	37
2135	Protective effects of <i>Commiphora erythroa</i> resin constituents against cellular oxidative damage. 2011 , 16, 10357-69	12
2134	The N-terminal tail of hERG contains an amphipathic helix that regulates channel deactivation. 2011 , 6, e16191	72
2133	Co-crystal structures of PKG II (92-227) with cGMP and cAMP reveal the molecular details of cyclic-nucleotide binding. 2011 , 6, e18413	44
2132	From isotropic to anisotropic side chain representations: comparison of three models for residue contact estimation. 2011 , 6, e19238	12
2131	L,L-diaminopimelate aminotransferase from <i>Chlamydomonas reinhardtii</i> : a target for algaecide development. 2011 , 6, e20439	19
2130	An inserted α subdomain shapes the catalytic pocket of <i>Lactobacillus johnsonii</i> cinnamoyl esterase. 2011 , 6, e23269	32
2129	The minimal domain of adipose triglyceride lipase (ATGL) ranges until leucine 254 and can be activated and inhibited by CGI-58 and G0S2, respectively. 2011 , 6, e26349	60
2128	Structural and enzymatic characterization of a glycoside hydrolase family 31 xylosidase from <i>Cellvibrio japonicus</i> involved in xyloglucan saccharification. 2011 , 436, 567-80	62
2127	The crystal structure of human GLRX5: iron-sulfur cluster co-ordination, tetrameric assembly and monomer activity. 2011 , 433, 303-11	100
2126	A drug targeting only p110 β can block phosphoinositide 3-kinase signalling and tumour growth in certain cell types. 2011 , 438, 53-62	127
2125	Root hair-specific expansins modulate root hair elongation in rice. 2011 , 66, 725-34	110
2124	Structure of UvrA nucleotide excision repair protein in complex with modified DNA. 2011 , 18, 191-7	62
2123	Genetic selection designed to stabilize proteins uncovers a chaperone called Spy. 2011 , 18, 262-9	115

2122	Molecular design principles underlying β -strand swapping in the adhesive dimerization of cadherins. 2011 , 18, 693-700	80
2121	The DNA-binding domain of the Chd1 chromatin-remodelling enzyme contains SANT and SLIDE domains. 2011 , 30, 2596-609	88
2120	Architecture of the RNA polymerase-Spt4/5 complex and basis of universal transcription processivity. 2011 , 30, 1302-10	184
2119	Atomic-level modelling of the HIV capsid. 2011 , 469, 424-7	282
2118	Streptococcal M1 protein constructs a pathological host fibrinogen network. 2011 , 472, 64-8	80
2117	Principles of activation and permeation in an anion-selective Cys-loop receptor. 2011 , 474, 54-60	787
2116	Structural and mechanistic basis of Parl activity and regulation. 2011 , 18, 1531-9	23
2115	Structural and biochemical insights into MLL1 core complex assembly. 2011 , 19, 101-8	81
2114	Structural characterization of the Boca/Mesd maturation factors for LDL-receptor-type β propeller domains. 2011 , 19, 324-36	6
2113	The crystal structure of the β neurexin-1 extracellular region reveals a hinge point for mediating synaptic adhesion and function. 2011 , 19, 767-78	56
2112	The structure of neurexin 1 β reveals features promoting a role as synaptic organizer. 2011 , 19, 779-89	55
2111	Unusual, dual endo- and exonuclease activity in the degradosome explained by crystal structure analysis of RNase J1. 2011 , 19, 1241-51	43
2110	A new generation of crystallographic validation tools for the protein data bank. 2011 , 19, 1395-412	335
2109	Atomic-level protein structure refinement using fragment-guided molecular dynamics conformation sampling. 2011 , 19, 1784-95	243
2108	Real space refinement of crystal structures with canonical distributions of electrons. 2011 , 19, 1739-43	1
2107	Crystal structure of human germline antibody 3-23/B3. 2011 , 48, 1586-8	8
2106	Structural characterization of a ribose-5-phosphate isomerase B from the pathogenic fungus <i>Coccidioides immitis</i> . 2011 , 11, 39	6
2105	Ultra-high resolution crystal structure of a dimeric defensin SPE10. 2011 , 585, 300-6	23

2104	Crystal structure of E339K mutated human glucokinase reveals changes in the ATP binding site. 2011 , 585, 1175-9	6
2103	Methods of protein structure comparison. 2012 , 857, 231-57	190
2102	Identification of benzoxazin-3-one derivatives as novel, potent, and selective nonsteroidal mineralocorticoid receptor antagonists. 2011 , 54, 8616-31	74
2101	Tricyclic series of heat shock protein 90 (Hsp90) inhibitors part I: discovery of tricyclic imidazo[4,5-c]pyridines as potent inhibitors of the Hsp90 molecular chaperone. 2011 , 54, 7206-19	37
2100	Derlin-1 is a rhomboid pseudoprotease required for the dislocation of mutant β 1 antitrypsin from the endoplasmic reticulum. 2011 , 18, 1147-52	143
2099	Structure of the membrane domain of respiratory complex I. 2011 , 476, 414-20	297
2098	Structure and activity of the <i>Saccharomyces cerevisiae</i> dUTP pyrophosphatase DUT1, an essential housekeeping enzyme. 2011 , 437, 243-53	17
2097	Structural-dynamical investigation of the ZnuA histidine-rich loop: involvement in zinc management and transport. 2011 , 25, 181-94	14
2096	Active site similarity between human and <i>Plasmodium falciparum</i> phosphodiesterases: considerations for antimalarial drug design. 2011 , 25, 753-62	6
2095	Computational investigation of the binding mode of bis(hydroxylphenyl)arenes in 17 β -HSD1: molecular dynamics simulations, MM-PBSA free energy calculations, and molecular electrostatic potential maps. 2011 , 25, 795-811	16
2094	ARABIDILLO proteins have a novel and conserved domain structure important for the regulation of their stability. 2011 , 75, 77-92	13
2093	SAD phasing using iodide ions in a high-throughput structural genomics environment. 2011 , 12, 83-95	61
2092	Leveraging structure determination with fragment screening for infectious disease drug targets: MECP synthase from <i>Burkholderia pseudomallei</i> . 2011 , 12, 63-76	19
2091	Exploring the structure of opioid receptors with homology modeling based on single and multiple templates and subsequent docking: a comparative study. 2011 , 17, 1207-21	12
2090	Fragmental modeling of hPepT2 and analysis of its binding features by docking studies and pharmacophore mapping. 2011 , 19, 4544-51	4
2089	Interdomain compactization in human tyrosyl-tRNA synthetase studied by the hierarchical rotations technique. 2011 , 154, 90-8	11
2088	Biochemical and structural characterization of a α -1,3 β ,4-glucoanase from <i>Bacillus subtilis</i> 168. 2011 , 46, 1202-1206	43
2087	Structural characterization of CalO1: a putative orsellinic acid methyltransferase in the calicheamicin-biosynthetic pathway. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2011 , 67, 197-203	15

2086	Structure of Greyhound hemoglobin: origin of high oxygen affinity. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2011 , 67, 395-402	4
2085	Structure of HLA-A*0301 in complex with a peptide of proteolipid protein: insights into the role of HLA-A alleles in susceptibility to multiple sclerosis. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2011 , 67, 447-54	23
2084	Structure of human dual-specificity phosphatase 27 at 2.38 Å resolution. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2011 , 67, 471-9	16
2083	Structure and biochemical characterization of proliferating cellular nuclear antigen from a parasitic protozoon. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2011 , 67, 497-505	13
2082	Involvement of the distal Arg residue in Cl ⁻ binding of midge larval haemoglobin. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2011 , 67, 488-95	5
2081	Scaffoldin-borne family 3b carbohydrate-binding module from the cellulosome of <i>Bacteroides cellulosolvens</i> : structural diversity and significance of calcium for carbohydrate binding. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2011 , 67, 506-15	16
2080	Crystallographic determination of the disease-associated T1184R variant of complement regulator factor H. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2011 , 67, 593-600	7
2079	Structure analysis of <i>Entamoeba histolytica</i> enolase. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2011 , 67, 619-27	12
2078	Isothiazolidinone (IZD) as a phosphoryl mimetic in inhibitors of the <i>Yersinia pestis</i> protein tyrosine phosphatase YopH. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2011 , 67, 639-45	11
2077	Structure of 2-oxo-3-deoxygalactonate kinase from <i>Klebsiella pneumoniae</i> . <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2011 , 67, 678-89	4
2076	Structural features of peroxisomal catalase from the yeast <i>Hansenula polymorpha</i> . <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2011 , 67, 690-8	10
2075	Sixty years from discovery to solution: crystal structure of bovine liver catalase form III. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2011 , 67, 756-62	4
2074	Streptavidin and its biotin complex at atomic resolution. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2011 , 67, 813-21	62
2073	Structure of a highly NADP ⁺ -specific isocitrate dehydrogenase. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2011 , 67, 856-69	8
2072	Structure of N5-carboxyaminoimidazole ribonucleotide synthase (PurK) from <i>Bacillus anthracis</i> . <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2011 , 67, 870-4	2
2071	Polarizable atomic multipole X-ray refinement: weighting schemes for macromolecular diffraction. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2011 , 67, 957-65	18
2070	A suite of Switch I and Switch II mutant structures from the G-protein domain of FeoB. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2011 , 67, 973-80	13
2069	The structure of <i>Serratia marcescens</i> Lip, a membrane-bound component of the type VI secretion system. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2011 , 67, 1065-72	26

2068	Structure of laccase from <i>Streptomyces coelicolor</i> after soaking with potassium hexacyanoferrate and at an improved resolution of 2.3 Å 2011 , 67, 27-32	9
2067	Pentapeptide-repeat proteins that act as topoisomerase poison resistance factors have a common dimer interface. 2011 , 67, 296-302	24
2066	Structure of CBM4 from <i>Clostridium thermocellum</i> cellulase K. 2011 , 67, 527-30	5
2065	Structures of phosphopantetheine adenylyltransferase from <i>Burkholderia pseudomallei</i> . 2011 , 67, 1032-7	11
2064	The role of Co ²⁺ in the crystallization of human SENP1 and comments on the limitations of automated refinement protocols. 2011 , 67, 442-5	2
2063	Structural analysis of full-length Hfq from <i>Escherichia coli</i> . 2011 , 67, 536-40	23
2062	Structures of a putative ß-class glutathione S-transferase from the pathogenic fungus <i>Coccidioides immitis</i> . 2011 , 67, 1038-43	4
2061	BrabA.11339.a: anomalous diffraction and ligand binding guide towards the elucidation of the function of a 'putative ß-lactamase-like protein' from <i>Brucella melitensis</i> . 2011 , 67, 1106-12	4
2060	Structure of <i>Mycobacterium tuberculosis</i> phosphopantetheine adenylyltransferase in complex with the feedback inhibitor CoA reveals only one active-site conformation. 2011 , 67, 541-5	8
2059	Structure of a Nudix hydrolase (MutT) in the Mg(2+)-bound state from <i>Bartonella henselae</i> , the bacterium responsible for cat scratch fever. 2011 , 67, 1078-83	4
2058	Comparative analysis of glutaredoxin domains from bacterial opportunistic pathogens. 2011 , 67, 1141-7	7
2057	Structure of human R-state aquomethemoglobin at 2.0 Å resolution. 2011 , 67, 647-51	23
2056	Structure of nitrilotriacetate monooxygenase component B from <i>Mycobacterium thermoresistibile</i> . 2011 , 67, 1100-5	13
2055	Probing conformational states of glutaryl-CoA dehydrogenase by fragment screening. 2011 , 67, 1060-9	7
2054	Structure of thymidylate kinase from <i>Ehrlichia chaffeensis</i> . 2011 , 67, 1090-4	1
2053	Structure of the <i>Drosophila melanogaster</i> Rab6 GTPase at 1.4 Å resolution. 2011 , 67, 744-8	3
2052	Structure of a cyclin-dependent kinase from <i>Giardia lamblia</i> . 2011 , 67, 1084-9	1
2051	Structure of fructose bisphosphate aldolase from <i>Bartonella henselae</i> bound to fructose 1,6-bisphosphate. 2011 , 67, 1051-4	2

2050	Structure of triosephosphate isomerase from <i>Cryptosporidium parvum</i> . 2011 , 67, 1095-9	1
2049	Conservation of a crystallographic interface suggests a role for β -sheet augmentation in influenza virus NS1 multifunctionality. 2011 , 67, 858-61	8
2048	Structure of filamin A immunoglobulin-like repeat 10 from <i>Homo sapiens</i> . 2011 , 67, 871-6	11
2047	Structure of fumarate hydratase from <i>Rickettsia prowazekii</i> , the agent of typhus and suspected relative of the mitochondria. 2011 , 67, 1123-8	3
2046	Antigen recognition by antibody C836 through adjustment of V(L)/V(H) packing. 2011 , 67, 1165-7	14
2045	ADP-Mg ²⁺ bound to the ATP-grasp domain of ATP-citrate lyase. 2011 , 67, 1168-72	15
2044	Inhibitor-bound complexes of dihydrofolate reductase-thymidylate synthase from <i>Babesia bovis</i> . 2011 , 67, 1070-7	11
2043	Structures of respiratory syncytial virus nucleocapsid protein from two crystal forms: details of potential packing interactions in the native helical form. 2011 , 67, 1179-83	14
2042	Structure of PA4019, a putative aromatic acid decarboxylase from <i>Pseudomonas aeruginosa</i> . 2011 , 67, 1184-8	20
2041	The 1.75 Å resolution structure of fission protein Fis1 from <i>Saccharomyces cerevisiae</i> reveals elusive interactions of the autoinhibitory domain. 2011 , 67, 1310-5	4
2040	Structure of the cystathionine β -synthase MetB from <i>Mycobacterium ulcerans</i> . 2011 , 67, 1154-8	9
2039	Structure of 3-ketoacyl-(acyl-carrier-protein) reductase from <i>Rickettsia prowazekii</i> at 2.25 Å resolution. 2011 , 67, 1118-22	9
2038	Structure of aldose reductase from <i>Giardia lamblia</i> . 2011 , 67, 1113-7	4
2037	Structure of the catalytic domain of <i>Plasmodium falciparum</i> ARF GTPase-activating protein (ARFGAP). 2011 , 67, 1339-44	0
2036	Structure of cellobiose phosphorylase from <i>Clostridium thermocellum</i> in complex with phosphate. 2011 , 67, 1345-9	20
2035	Structures of engineered <i>Clostridium botulinum</i> neurotoxin derivatives. 2011 , 67, 1466-72	7
2034	Structure of hyperthermophilic α -glucosidase from <i>Pyrococcus furiosus</i> . 2011 , 67, 1473-9	23
2033	The 1.7 Å resolution structure of At2g44920, a pentapeptide-repeat protein in the thylakoid lumen of <i>Arabidopsis thaliana</i> . 2011 , 67, 1480-4	7

2032	A 1.5 Å resolution X-ray structure of the catalytic module of Caldicellulosiruptor bescii family 3 pectate lyase. 2011 , 67, 1498-500	13
2031	The structure of an N11A mutant of the G-protein domain of FeoB. 2011 , 67, 1511-5	8
2030	Crystallization and preliminary X-ray structure analysis of human ribosomal protein L30e. 2011 , 67, 1516-8	0
2029	Structure of the H107R variant of the extracellular domain of mouse NKR-P1A at 2.3 Å resolution. 2011 , 67, 1519-23	6
2028	Structure of the fucose mutarotase from Streptococcus pneumoniae in complex with L-fucose. 2011 , 67, 1524-30	7
2027	Stereochemical errors and their implications for molecular dynamics simulations. 2011 , 12, 190	42
2026	Structural basis for branching-enzyme activity of glycoside hydrolase family 57: structure and stability studies of a novel branching enzyme from the hyperthermophilic archaeon Thermococcus kodakaraensis KOD1. 2011 , 79, 547-57	44
2025	Crystal structure of HP0721, a novel secreted protein from Helicobacter pylori. 2011 , 79, 1678-81	4
2024	Crystal structure of the catalytic domain of cholesterol-β-glucosyltransferase from Helicobacter pylori. 2011 , 79, 2321-6	12
2023	Observing the osmophobic effect in action at the single molecule level. 2011 , 79, 2214-23	12
2022	Automated protein structure modeling in CASP9 by I-TASSER pipeline combined with QUARK-based ab initio folding and FG-MD-based structure refinement. 2011 , 79 Suppl 10, 147-60	111
2021	Structural analysis of CPF_2247, a novel α-amylase from Clostridium perfringens. 2011 , 79, 2771-7	20
2020	Antibody modeling assessment. 2011 , 79, 3050-66	94
2019	Assessment of protein structure refinement in CASP9. 2011 , 79 Suppl 10, 74-90	79
2018	Loss of recognition by cross-reactive T cells and its relation to a C-terminus-induced conformational reorientation of an HLA-B*2705-bound peptide. 2011 , 20, 278-90	4
2017	Altered architecture of substrate binding region defines the unique specificity of UDP-GalNAc 4-epimerases. 2011 , 20, 856-66	12
2016	Structural and functional characterization of Schistosoma mansoni Thioredoxin. 2011 , 20, 1069-76	20
2015	Structural and enzymatic characterization of NanS (YjhS), a 9-O-Acetyl N-acetylneuraminic acid esterase from Escherichia coli O157:H7. 2011 , 20, 1208-19	27

2014	Apo raver1 structure reveals distinct RRM domain orientations. 2011 , 20, 1464-70	3
2013	Intermolecular versus intramolecular interactions of the vinculin binding site 33 of talin. 2011 , 20, 1471-6	9
2012	Structure of a novel thermostable GH51 β -arabinofuranosidase from <i>Thermotoga petrophila</i> RKU-1. 2011 , 20, 1632-7	15
2011	Crystal structure of the read-through domain from bacteriophage Q ϕ A1 protein. 2011 , 20, 1707-12	16
2010	Monitoring and validating active site redox states in protein crystals. 2011 , 1814, 778-84	29
2009	Crystal structure of an enzymatically inactive trans-sialidase-like lectin from <i>Trypanosoma cruzi</i> : the carbohydrate binding mechanism involves residual sialidase activity. 2011 , 1814, 1154-61	18
2008	iMod: multipurpose normal mode analysis in internal coordinates. 2011 , 27, 2843-50	122
2007	Calcium modulates force sensing by the von Willebrand factor A2 domain. 2011 , 2, 385	70
2006	Crystal structure of human antibody 2909 reveals conserved features of quaternary structure-specific antibodies that potently neutralize HIV-1. 2011 , 85, 2524-35	40
2005	Fitting spheres to electron density. 2011 ,	
2004	Activation of nitrofurazone by azoreductases: multiple activities in one enzyme. 2011 , 1, 63	20
2003	<i>Arabidopsis</i> chloroplastic glutaredoxin C5 as a model to explore molecular determinants for iron-sulfur cluster binding into glutaredoxins. 2011 , 286, 27515-27	63
2002	Crystal structures of a cysteine-modified mutant in loop D of acetylcholine-binding protein. 2011 , 286, 4420-8	41
2001	Structural basis of silencing: Sir3 BAH domain in complex with a nucleosome at 3.0 \AA resolution. 2011 , 334, 977-82	196
2000	Kinked β -strands mediate high-affinity recognition of mRNA targets by the germ-cell regulator DAZL. 2011 , 108, 18266-71	46
1999	Novel vinculin binding site of the IpaA invasin of <i>Shigella</i> . 2011 , 286, 23214-21	31
1998	Molecular sensing by the aptamer domain of the FMN riboswitch: a general model for ligand binding by conformational selection. 2011 , 39, 8586-98	73
1997	Structural and functional studies of the <i>Escherichia coli</i> phenylacetyl-CoA monooxygenase complex. 2011 , 286, 10735-43	35

1996	Structural and thermodynamic basis for weak interactions between dihydrolipoamide dehydrogenase and subunit-binding domain of the branched-chain alpha-ketoacid dehydrogenase complex. 2011 , 286, 23476-88	17
1995	Analysis of a new family of widely distributed metal-independent alpha-mannosidases provides unique insight into the processing of N-linked glycans. 2011 , 286, 15586-96	51
1994	The H/ACA RNP assembly factor SHQ1 functions as an RNA mimic. 2011 , 25, 2398-408	33
1993	Snapshots of enzymatic Baeyer-Villiger catalysis: oxygen activation and intermediate stabilization. 2011 , 286, 29284-29291	110
1992	Structure and mechanism of an Arabidopsis medium/long-chain-length prenyl pyrophosphate synthase. 2011 , 155, 1079-90	59
1991	Molecular basis of the recognition of the ap65-1 gene transcription promoter elements by a Myb protein from the protozoan parasite <i>Trichomonas vaginalis</i> . 2011 , 39, 8992-9008	18
1990	The crystal structure of the TetR family transcriptional repressor SimR bound to DNA and the role of a flexible N-terminal extension in minor groove binding. 2011 , 39, 9433-47	49
1989	Fine-tuning the stimulation of MLL1 methyltransferase activity by a histone H3-based peptide mimetic. 2011 , 25, 960-7	16
1988	Structural plasticity of the thioredoxin recognition site of yeast methionine S-sulfoxide reductase Mxr1. 2011 , 286, 13430-7	22
1987	Crystal structure of <i>Toxoplasma gondii</i> porphobilinogen synthase: insights on octameric structure and porphobilinogen formation. 2011 , 286, 15298-307	20
1986	Molecular basis for the unique role of the AAA+ chaperone ClpV in type VI protein secretion. 2011 , 286, 30010-21	79
1985	Crystal structure of <i>Mycobacterium tuberculosis</i> zinc-dependent metalloprotease-1 (Zmp1), a metalloprotease involved in pathogenicity. 2011 , 286, 32475-82	25
1984	β-Galactosidase/sucrose kinase (AgaSK), a novel bifunctional enzyme from the human microbiome coupling galactosidase and kinase activities. 2011 , 286, 40814-23	21
1983	Stabilizing salt-bridge enhances protein thermostability by reducing the heat capacity change of unfolding. 2011 , 6, e21624	79
1982	Structure of a pentavalent G-actin* MRTF-A complex reveals how G-actin controls nucleocytoplasmic shuttling of a transcriptional coactivator. 2011 , 4, ra40	71
1981	Proteomic analyses reveal an acidic prime side specificity for the astacin metalloprotease family reflected by physiological substrates. 2011 , 10, M111.009233	100
1980	3-Keto-5-amino-hexanoate cleavage enzyme: a common fold for an uncommon Claisen-type condensation. 2011 , 286, 27399-405	14
1979	<i>Thermus thermophilus</i> glycoside hydrolase family 57 branching enzyme: crystal structure, mechanism of action, and products formed. 2011 , 286, 3520-30	71

1978	The rickettsia surface cell antigen 4 applies mimicry to bind to and activate vinculin. 2011 , 286, 35096-103	37
1977	Crystal Structure of the cis-Dimer of Nectin-1: implications for the architecture of cell-cell junctions. 2011 , 286, 12659-69	41
1976	Loss of T cell antigen recognition arising from changes in peptide and major histocompatibility complex protein flexibility: implications for vaccine design. 2011 , 286, 40163-73	42
1975	Tyrosine latching of a regulatory gate affords allosteric control of aromatic amino acid biosynthesis. 2011 , 286, 10216-24	43
1974	A conserved non-canonical motif in the pseudoactive site of the ROP5 pseudokinase domain mediates its effect on Toxoplasma virulence. 2011 , 286, 29366-29375	65
1973	Structure and histone binding properties of the Vps75-Rtt109 chaperone-lysine acetyltransferase complex. 2011 , 286, 15625-9	30
1972	TCRs used in cancer gene therapy cross-react with MART-1/Melan-A tumor antigens via distinct mechanisms. 2011 , 187, 2453-63	98
1971	How the biotin-streptavidin interaction was made even stronger: investigation via crystallography and a chimaeric tetramer. 2011 , 435, 55-63	87
1970	Structure and mutagenesis of the parainfluenza virus 5 hemagglutinin-neuraminidase stalk domain reveals a four-helix bundle and the role of the stalk in fusion promotion. 2011 , 85, 12855-66	69
1969	The virulence factor PEB4 (Cj0596) and the periplasmic protein Cj1289 are two structurally related SurA-like chaperones in the human pathogen Campylobacter jejuni. 2011 , 286, 21254-65	27
1968	Structure of collagen receptor integrin $\alpha 1$ domain carrying the activating mutation E317A. 2011 , 286, 43343-51	19
1967	The structure of the kinesin-1 motor-tail complex reveals the mechanism of autoinhibition. 2011 , 333, 883-5	118
1966	Molecular basis of 1,6-anhydro bond cleavage and phosphoryl transfer by Pseudomonas aeruginosa 1,6-anhydro-N-acetylmuramic acid kinase. 2011 , 286, 12283-91	21
1965	Assembly of preactivation complex for urease maturation in Helicobacter pylori: crystal structure of UreF-UreH protein complex. 2011 , 286, 43241-9	36
1964	Structural basis for nonribosomal peptide synthesis by an aminoacyl-tRNA synthetase paralog. 2011 , 108, 3912-7	68
1963	Solution structure of RNase P RNA. 2011 , 17, 1159-71	32
1962	Crystal structure of clustered regularly interspaced short palindromic repeats (CRISPR)-associated Csn2 protein revealed Ca ²⁺ -dependent double-stranded DNA binding activity. 2011 , 286, 30759-30768	44
1961	Recognition of the F&H motif by the Lowe syndrome protein OCRL. 2011 , 18, 789-95	32

1960	Mutant alcohol dehydrogenase leads to improved ethanol tolerance in <i>Clostridium thermocellum</i> . 2011 , 108, 13752-7	147
1959	Crystal structure of Toll-like receptor adaptor MAL/TIRAP reveals the molecular basis for signal transduction and disease protection. 2011 , 108, 14879-84	105
1958	Structural insight into maintenance methylation by mouse DNA methyltransferase 1 (Dnmt1). 2011 , 108, 9055-9	147
1957	Crystal structure of a KSHV-SOX-DNA complex: insights into the molecular mechanisms underlying DNase activity and host shutoff. 2011 , 39, 5744-56	26
1956	Mitotic centromeric targeting of HP1 and its binding to Sgo1 are dispensable for sister-chromatid cohesion in human cells. 2011 , 22, 1181-90	64
1955	Structure-based modification of a <i>Clostridium difficile</i> -targeting endolysin affects activity and host range. 2011 , 193, 5477-86	70
1954	Structural and functional studies on the interaction of GspC and GspD in the type II secretion system. 2011 , 7, e1002228	74
1953	Activities of human RRP6 and structure of the human RRP6 catalytic domain. 2011 , 17, 1566-77	54
1952	Crystal structures of <i>T. b. rhodesiense</i> adenosine kinase complexed with inhibitor and activator: implications for catalysis and hyperactivation. 2011 , 5, e1164	18
1951	Recognition of UbcH5c and the nucleosome by the Bmi1/Ring1b ubiquitin ligase complex. 2011 , 30, 3285-97	105
1950	Blockade of neuronal α -nAChR by α -conotoxin Iml explained by computational scanning and energy calculations. 2011 , 7, e1002011	61
1949	Structural insights into quinolone antibiotic resistance mediated by pentapeptide repeat proteins: conserved surface loops direct the activity of a Qnr protein from a gram-negative bacterium. 2011 , 39, 3917-27	61
1948	The influence of the local sequence environment on RNA loop structures. 2011 , 17, 1247-57	1
1947	Structure-function analyses of a caffeic acid O-methyltransferase from perennial ryegrass reveal the molecular basis for substrate preference. 2010 , 22, 4114-27	64
1946	Exhaustive sampling of docking poses reveals binding hypotheses for propafenone type inhibitors of P-glycoprotein. 2011 , 7, e1002036	65
1945	The binding of triclosan to SmeT, the repressor of the multidrug efflux pump SmeDEF, induces antibiotic resistance in <i>Stenotrophomonas maltophilia</i> . 2011 , 7, e1002103	77
1944	Membrane remodeling by the double-barrel scaffolding protein of poxvirus. 2011 , 7, e1002239	33
1943	Acid stability of the hemagglutinin protein regulates H5N1 influenza virus pathogenicity. 2011 , 7, e1002398	93

1942	Inhibition of apoptosis and NF- κ B activation by vaccinia protein N1 occur via distinct binding surfaces and make different contributions to virulence. 2011 , 7, e1002430	57
1941	Ensemble-based computational approach discriminates functional activity of p53 cancer and rescue mutants. 2011 , 7, e1002238	28
1940	Non-specific protein-DNA interactions control I-Crel target binding and cleavage. 2012 , 40, 6936-45	22
1939	Architecture of the catalytic HPN motif is conserved in all E2 conjugating enzymes. 2012 , 445, 167-74	23
1938	Crystal structures of the tRNA:m2G6 methyltransferase Trm14/TrmN from two domains of life. 2012 , 40, 5149-61	29
1937	Structural analysis of a bacterial exo- β -D-N-acetylglucosaminidase in complex with an unusual disaccharide found in class III mucin. 2012 , 22, 590-5	11
1936	Crystal structures of Physcomitrella patens AOC1 and AOC2: insights into the enzyme mechanism and differences in substrate specificity. 2012 , 160, 1251-66	31
1935	Crystal structure of xenotropic murine leukaemia virus-related virus (XMRV) ribonuclease H. 2012 , 32, 455-63	3
1934	The NC2 domain of type IX collagen determines the chain register of the triple helix. 2012 , 287, 44536-45	15
1933	Biochemical identification and crystal structure of kynurenine formamidase from Drosophila melanogaster. 2012 , 446, 253-60	23
1932	De novo GTP biosynthesis is critical for virulence of the fungal pathogen Cryptococcus neoformans. 2012 , 8, e1002957	45
1931	Insights into ubiquitin-conjugating enzyme/ co-activator interactions from the structure of the Pex4p:Pex22p complex. 2012 , 31, 391-402	46
1930	Csy4 relies on an unusual catalytic dyad to position and cleave CRISPR RNA. 2012 , 31, 2824-32	77
1929	MpaA is a murein-tripeptide-specific zinc carboxypeptidase that functions as part of a catabolic pathway for peptidoglycan-derived peptides in β proteobacteria. 2012 , 448, 329-41	8
1928	Molecular requirements for peroxisomal targeting of alanine-glyoxylate aminotransferase as an essential determinant in primary hyperoxaluria type 1. 2012 , 10, e1001309	52
1927	H1N1 2009 pandemic influenza virus: resistance of the I223R neuraminidase mutant explained by kinetic and structural analysis. 2012 , 8, e1002914	60
1926	Molecular basis for genetic resistance of Anopheles gambiae to Plasmodium: structural analysis of TEP1 susceptible and resistant alleles. 2012 , 8, e1002958	26
1925	Structural conservation of an ancient tRNA sensor in eukaryotic glutaminyl-tRNA synthetase. 2012 , 40, 3723-31	13

1924	Bacterial over-expression and purification of the 3'phosphoadenosine 5'phosphosulfate (PAPS) reductase domain of human FAD synthase: functional characterization and homology modeling. 2012 , 13, 16880-98	19
1923	A volumetric method for representing and comparing regions of electrostatic focusing in molecular structure. 2012 ,	2
1922	Novel Clostridium thermocellum type I cohesin-dockerin complexes reveal a single binding mode. 2012 , 287, 44394-405	25
1921	Structural insight into the unique properties of adeno-associated virus serotype 9. 2012 , 86, 6947-58	123
1920	Sizzled is unique among secreted frizzled-related proteins for its ability to specifically inhibit bone morphogenetic protein-1 (BMP-1)/tolloid-like proteinases. 2012 , 287, 33581-93	25
1919	The crystal structure of <i>S. cerevisiae</i> Ski2, a DExH helicase associated with the cytoplasmic functions of the exosome. 2012 , 18, 124-34	54
1918	Structural and functional insights into (S)-ureidoglycine aminohydrolase, key enzyme of purine catabolism in <i>Arabidopsis thaliana</i> . 2012 , 287, 18796-805	12
1917	Structure and activity of the only human RNase T2. 2012 , 40, 8733-42	25
1916	Molecular basis for phosphospecific recognition of histone H3 tails by Survivin paralogues at inner centromeres. 2012 , 23, 1457-66	43
1915	Multidomain Carbohydrate-binding Proteins Involved in <i>Bacteroides thetaiotaomicron</i> Starch Metabolism. 2012 , 287, 34614-25	72
1914	Functional and structural characterization of the mammalian TREX-2 complex that links transcription with nuclear messenger RNA export. 2012 , 40, 4562-73	91
1913	Functional and structural analysis of the human SLO3 pH- and voltage-gated K ⁺ channel. 2012 , 109, 19274-9	42
1912	Structural evidence of a new catalytic intermediate in the pathway of ATP hydrolysis by F1-ATPase from bovine heart mitochondria. 2012 , 109, 11139-43	67
1911	Characterization of a <i>Phanerochaete chrysosporium</i> glutathione transferase reveals a novel structural and functional class with ligandin properties. 2012 , 287, 39001-11	29
1910	The plasticity of WDR5 peptide-binding cleft enables the binding of the SET1 family of histone methyltransferases. 2012 , 40, 4237-46	80
1909	Small-molecule targeting of proliferating cell nuclear antigen chromatin association inhibits tumor cell growth. 2012 , 81, 811-9	61
1908	Structure of the cytoplasmic region of PelD, a degenerate diguanylate cyclase receptor that regulates exopolysaccharide production in <i>Pseudomonas aeruginosa</i> . 2012 , 287, 23582-93	79
1907	NF45 dimerizes with NF90, Zfr and SPNR via a conserved domain that has a nucleotidyltransferase fold. 2012 , 40, 9356-68	41

1906	Invariant gly residue is important for α -defensin folding, dimerization, and function: a case study of the human neutrophil α -defensin HNP1. 2012 , 287, 18900-12	23
1905	Structural elucidation of the mechanistic basis of degeneracy in the primary humoral response. 2012 , 188, 1819-27	23
1904	Structure of the carboxy-terminal region of a KCNH channel. 2012 , 481, 530-3	94
1903	The dynamic stator stalk of rotary ATPases. 2012 , 3, 687	53
1902	A phosphorylated pseudokinase complex controls cell wall synthesis in mycobacteria. 2012 , 5, ra7	124
1901	Protein molecules in 3D. 2012 ,	
1900	Structure of the Mediator head module. 2012 , 492, 448-51	81
1899	Functional consequence of covalent reaction of phosphoenolpyruvate with UDP-N-acetylglucosamine 1-carboxyvinyltransferase (MurA). 2012 , 287, 12657-67	34
1898	Structures of LeuT in bicelles define conformation and substrate binding in a membrane-like context. 2012 , 19, 212-9	91
1897	Structural basis of fibrillar collagen trimerization and related genetic disorders. 2012 , 19, 1031-6	69
1896	Antidiabetic phospholipid-nuclear receptor complex reveals the mechanism for phospholipid-driven gene regulation. 2012 , 19, 532-S2	61
1895	The binding of Varp to VAMP7 traps VAMP7 in a closed, fusogenically inactive conformation. 2012 , 19, 1300-9	56
1894	Crystal structure of LpxK, the 4'-kinase of lipid A biosynthesis and atypical P-loop kinase functioning at the membrane interface. 2012 , 109, 12956-61	17
1893	Structural snapshots of yeast alkyl hydroperoxide reductase Ahp1 peroxiredoxin reveal a novel two-cysteine mechanism of electron transfer to eliminate reactive oxygen species. 2012 , 287, 17077-17087	33
1892	Structure of RPE65 isomerase in a lipidic matrix reveals roles for phospholipids and iron in catalysis. 2012 , 109, E2747-56	51
1891	Structure of human Mad1 C-terminal domain reveals its involvement in kinetochore targeting. 2012 , 109, 6549-54	74
1890	The molecular mechanism of thermostable β -galactosidases AgaA and AgaB explained by x-ray crystallography and mutational studies. 2012 , 287, 39642-52	34
1889	Structure of Salmonella effector protein SopB N-terminal domain in complex with host Rho GTPase Cdc42. 2012 , 287, 13348-55	16

1888	Structure of factor H-binding protein B (FhbB) of the periopathogen, <i>Treponema denticola</i> : insights into progression of periodontal disease. 2012 , 287, 12715-22	35
1887	Crystal structure of reduced MsAcg, a putative nitroreductase from <i>Mycobacterium smegmatis</i> and a close homologue of <i>Mycobacterium tuberculosis</i> Acg. 2012 , 287, 44372-83	11
1886	The cytoskeletal protein β -catenin unfurls upon binding to vinculin. 2012 , 287, 18492-9	69
1885	Certhrax toxin, an anthrax-related ADP-ribosyltransferase from <i>Bacillus cereus</i> . 2012 , 287, 41089-102	25
1884	Identification and characterization of the <i>Thermus thermophilus</i> 5-methylcytidine (m5C) methyltransferase modifying 23 S ribosomal RNA (rRNA) base C1942. 2012 , 287, 27593-600	6
1883	Substrate specificity of the two mitochondrial ornithine carriers can be swapped by single mutation in substrate binding site. 2012 , 287, 7925-34	38
1882	The extracellular protein factor Epf from <i>Streptococcus pyogenes</i> is a cell surface adhesin that binds to cells through an N-terminal domain containing a carbohydrate-binding module. 2012 , 287, 38178-89	17
1881	P6981, an arylstibonic acid, is a novel low nanomolar inhibitor of cAMP response element-binding protein binding to DNA. 2012 , 82, 814-23	11
1880	Structure of the cleavage-activated prefusion form of the parainfluenza virus 5 fusion protein. 2012 , 109, 16672-7	75
1879	Trimming down a protein structure to its bare foldons: spatial organization of the cooperative unit. 2012 , 287, 2731-8	15
1878	Structure of a bacterial voltage-gated sodium channel pore reveals mechanisms of opening and closing. 2012 , 3, 1102	222
1877	Structure of a calcium-dependent 11R-lipoxygenase suggests a mechanism for Ca ²⁺ regulation. 2012 , 287, 22377-86	40
1876	Structure of the heterodimer of human NONO and paraspeckle protein component 1 and analysis of its role in subnuclear body formation. 2012 , 109, 4846-50	98
1875	Biophysical and bioinformatic analyses implicate the <i>Treponema pallidum</i> Tp34 lipoprotein (Tp0971) in transition metal homeostasis. 2012 , 194, 6771-81	14
1874	Mechanism of elongation factor-G-mediated fusidic acid resistance and fitness compensation in <i>Staphylococcus aureus</i> . 2012 , 287, 30257-67	18
1873	The human transporter associated with antigen processing: molecular models to describe peptide binding competent states. 2012 , 287, 28099-111	22
1872	Crystal structure of the UvrB dimer: insights into the nature and functioning of the UvrAB damage engagement and UvrB-DNA complexes. 2012 , 40, 8743-58	20
1871	The structure- and metal-dependent activity of <i>Escherichia coli</i> PgaB provides insight into the partial de-N-acetylation of poly- β -1,6-N-acetyl-D-glucosamine. 2012 , 287, 31126-37	58

1870	Structural basis for WDR5 interaction (Win) motif recognition in human SET1 family histone methyltransferases. 2012 , 287, 27275-89	69
1869	An amino acid position at crossroads of evolution of protein function: antibiotic sensor domain of BlaR1 protein from <i>Staphylococcus aureus</i> versus clasS D β -lactamases. 2012 , 287, 8232-41	14
1868	Crystal structure of N-glycosylated human glypican-1 core protein: structure of two loops evolutionarily conserved in vertebrate glypican-1. 2012 , 287, 14040-51	40
1867	Diversity in the C3b [corrected] contact residues and tertiary structures of the staphylococcal complement inhibitor (SCIN) protein family. 2012 , 287, 628-640	20
1866	Crystal structures of N-acetylmannosamine kinase provide insights into enzyme activity and inhibition. 2012 , 287, 13656-65	24
1865	Structure and interactions of the cytoplasmic domain of the <i>Yersinia</i> type III secretion protein YscD. 2012 , 194, 5949-58	17
1864	Heterosubtypic antibody recognition of the influenza virus hemagglutinin receptor binding site enhanced by avidity. 2012 , 109, 17040-5	119
1863	Enzymology and structure of the GH13_31 glucan 1,6- β -glucosidase that confers isomaltooligosaccharide utilization in the probiotic <i>Lactobacillus acidophilus</i> NCFM. 2012 , 194, 4249-59	47
1862	Crystal structure of human CDC7 kinase in complex with its activator DBF4. 2012 , 19, 1101-7	48
1861	Highly conserved protective epitopes on influenza B viruses. 2012 , 337, 1343-8	543
1860	Structural basis for the assembly and nucleic acid binding of the TREX-2 transcription-export complex. 2012 , 19, 328-36	69
1859	Sequence, structure, and evolution of cellulases in glycoside hydrolase family 48. 2012 , 287, 41068-77	28
1858	Crystal structure of a minimal eIF4E-Cup complex reveals a general mechanism of eIF4E regulation in translational repression. 2012 , 18, 1624-34	41
1857	Crystal structure of RlmM, the 2'-O-ribose methyltransferase for C2498 of <i>Escherichia coli</i> 23S rRNA. 2012 , 40, 10507-20	8
1856	Crystal structure of a heterodimer of editosome interaction proteins in complex with two copies of a cross-reacting nanobody. 2012 , 40, 1828-40	26
1855	Structure, function, and evolution of the Crimean-Congo hemorrhagic fever virus nucleocapsid protein. 2012 , 86, 10914-23	80
1854	Structure/function relationships of adipose phospholipase A2 containing a cys-his-his catalytic triad. 2012 , 287, 35260-35274	36
1853	The RGD finger of Del-1 is a unique structural feature critical for integrin binding. 2012 , 26, 3412-20	27

1852	Ribosome clearance by FusB-type proteins mediates resistance to the antibiotic fusidic acid. 2012 , 109, 2102-7	31
1851	Crystal structure of the <i>Leishmania major</i> peroxidase-cytochrome c complex. 2012 , 109, 18390-4	14
1850	Determinants of small ubiquitin-like modifier 1 (SUMO1) protein specificity, E3 ligase, and SUMO-RanGAP1 binding activities of nucleoporin RanBP2. 2012 , 287, 4740-51	53
1849	Structural basis for selective vascular endothelial growth factor-A (VEGF-A) binding to neuropilin-1. 2012 , 287, 11082-9	139
1848	Potential state-selective hydrogen bond formation can modulate activation and desensitization of the $\alpha 7$ nicotinic acetylcholine receptor. 2012 , 287, 21957-69	8
1847	Insights into substrate specificity and metal activation of mammalian tetrahedral aspartyl aminopeptidase. 2012 , 287, 13356-70	27
1846	Membrane curvature protein exhibits interdomain flexibility and binds a small GTPase. 2012 , 287, 40996-1006	16
1845	Crystal structures of the scaffolding protein LGN reveal the general mechanism by which GoLoco binding motifs inhibit the release of GDP from G β . 2012 , 287, 36766-76	18
1844	Crystal structures of complexes of the branched-chain aminotransferase from <i>Deinococcus radiodurans</i> with β -ketoisocaproate and L-glutamate suggest the radiation resistance of this enzyme for catalysis. 2012 , 194, 6206-16	19
1843	Structure of an antibody in complex with its mucin domain linear epitope that is protective against Ebola virus. 2012 , 86, 2809-16	40
1842	Genome3D: a UK collaborative project to annotate genomic sequences with predicted 3D structures based on SCOP and CATH domains. 2013 , 41, D499-507	48
1841	Protein-protein interactions in the β -oxidation part of the phenylacetate utilization pathway: crystal structure of the PaaF-PaaG hydratase-isomerase complex. 2012 , 287, 37986-96	9
1840	Structural determinants of the β -selectivity of a bacterial aminotransferase. 2012 , 287, 28495-502	29
1839	Computational insights for the discovery of non-ATP competitive inhibitors of MAP kinases. 2012 , 18, 1173-85	18
1838	Structure and function of cytidine monophosphate kinase from <i>Yersinia pseudotuberculosis</i> , essential for virulence but not for survival. 2012 , 2, 120142	9
1837	Neck-motor interactions trigger rotation of the kinesin stalk. 2012 , 2, 236	9
1836	Triazole pyrimidine nucleosides as inhibitors of Ribonuclease A. Synthesis, biochemical, and structural evaluation. 2012 , 20, 7184-93	20
1835	Crystal structure of the human ecto-5'-nucleotidase (CD73): insights into the regulation of purinergic signaling. 2012 , 20, 2161-73	119

1834	A direct interaction between DCP1 and XRN1 couples mRNA decapping to 5' exonucleolytic degradation. 2012 , 19, 1324-31	111
1833	Nucleic acid binding surface and dimer interface revealed by CRISPR-associated CasB protein structures. 2012 , 586, 3956-61	16
1832	RCrane: semi-automated RNA model building. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012 , 68, 985-95	71
1831	The promiscuous binding of the Fyn SH3 domain to a peptide from the NS5A protein. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012 , 68, 1030-40	19
1830	Structural features of the single-stranded DNA-binding protein MoSub1 from <i>Magnaporthe oryzae</i> . <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012 , 68, 1071-6	8
1829	Structure of <i>Escherichia coli</i> BamB and its interaction with POTRA domains of BamA. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012 , 68, 1134-9	15
1828	Structural analysis of the Asn152Gly mutant of P99 cephalosporinase. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012 , 68, 1189-93	4
1827	Structure of the prolyl-tRNA synthetase from the eukaryotic pathogen <i>Giardia lamblia</i> . <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012 , 68, 1194-200	8
1826	Structure determination of enterovirus 71. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012 , 68, 1217-22	12
1825	The structure of the ternary Eg5-ADP-ispinesib complex. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012 , 68, 1311-9	35
1824	The accessory domain changes the accessibility and molecular topography of the catalytic interface in monomeric GH39 β -xylosidases. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012 , 68, 1339-45	20
1823	Structural characterization and comparison of three acyl-carrier-protein synthases from pathogenic bacteria. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012 , 68, 1359-70	5
1822	Crystallization, dehydration and experimental phasing of WbdD, a bifunctional kinase and methyltransferase from <i>Escherichia coli</i> O9a. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012 , 68, 1371-9	5
1821	CrystalDirect: a new method for automated crystal harvesting based on laser-induced photoablation of thin films. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012 , 68, 1393-9	64
1820	Structure of the autophagic E2 enzyme Atg10. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012 , 68, 1409-17	18
1819	Structure of the CFA/III major pilin subunit CofA from human enterotoxigenic <i>Escherichia coli</i> determined at 0.90 \AA resolution by sulfur-SAD phasing. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012 , 68, 1418-29	10
1818	Structure of the starch-debranching enzyme barley limit dextrinase reveals homology of the N-terminal domain to CBM21. 2012 , 68, 1008-12	14
1817	Structure of anabolic ornithine carbamoyltransferase from <i>Campylobacter jejuni</i> at 2.7 \AA resolution. 2012 , 68, 1018-24	3

1816	High-resolution structures of <i>Thermus thermophilus</i> enoyl-acyl carrier protein reductase in the apo form, in complex with NAD ⁺ and in complex with NAD ⁺ and triclosan. 2012 , 68, 1139-48	2
1815	Structure of the [NiFe]-hydrogenase maturation protein HypF from <i>Thermococcus kodakarensis</i> KOD1. 2012 , 68, 1153-7	11
1814	Structure of WbdD: a bifunctional kinase and methyltransferase that regulates the chain length of the O antigen in <i>Escherichia coli</i> O9a. 2012 , 86, 730-42	25
1813	Crystal structure of the MrkD1P receptor binding domain of <i>Klebsiella pneumoniae</i> and identification of the human collagen V binding interface. 2012 , 86, 882-93	9
1812	Determinants of substrate specificity and biochemical properties of the sn-glycerol-3-phosphate ATP binding cassette transporter (UgpB-AEC2) of <i>Escherichia coli</i> . 2012 , 86, 908-20	26
1811	Crystal structures of two subtype N10 neuraminidase-like proteins from bat influenza A viruses reveal a diverged putative active site. 2012 , 109, 18903-8	101
1810	Structural analysis of a dengue cross-reactive antibody complexed with envelope domain III reveals the molecular basis of cross-reactivity. 2012 , 188, 4971-9	65
1809	Structure of a topoisomerase II-DNA-nucleotide complex reveals a new control mechanism for ATPase activity. 2012 , 19, 1147-54	96
1808	Cross-docking study on InhA inhibitors: a combination of Autodock Vina and PM6-DH2 simulations to retrieve bio-active conformations. 2012 , 10, 6341-9	47
1807	A bipolar spindle of antiparallel ParM filaments drives bacterial plasmid segregation. 2012 , 338, 1334-7	70
1806	The loop lid domain of phosphoenolpyruvate carboxykinase is essential for catalytic function. 2012 , 51, 9547-59	24
1805	Structural basis for the activity of a cytoplasmic RNA terminal uridylyl transferase. 2012 , 19, 782-787	40
1804	Cytochrome P450-catalyzed degradation of nicotine: fundamental parameters determining hydroxylation by cytochrome P450 2A6 at the 5'-carbon or the n-methyl carbon. 2012 , 116, 7827-40	12
1803	Structure of a RING E3 ligase and ubiquitin-loaded E2 primed for catalysis. 2012 , 489, 115-20	339
1802	Structural basis for allosteric regulation of GPCRs by sodium ions. 2012 , 337, 232-6	714
1801	Structural characterization of human cytochrome P450 2C19: active site differences between P450s 2C8, 2C9, and 2C19. 2012 , 287, 44581-91	77
1800	Structural mechanisms of allostery and autoinhibition in JNK family kinases. 2012 , 20, 2174-84	36
1799	Structure of NPP1, an ectonucleotide pyrophosphatase/phosphodiesterase involved in tissue calcification. 2012 , 20, 1948-59	53

1798	The zinc-finger domains of PARP1 cooperate to recognize DNA strand breaks. 2012 , 19, 685-692	157
1797	Visualizing group II intron catalysis through the stages of splicing. 2012 , 151, 497-507	134
1796	Crystal structure of the HLA-DM-HLA-DR1 complex defines mechanisms for rapid peptide selection. 2012 , 151, 1557-68	123
1795	Structure of human POFUT2: insights into thrombospondin type 1 repeat fold and O-fucosylation. 2012 , 31, 3183-97	44
1794	Structure and catalytic mechanism of 3-ketosteroid-Delta4-(5)-dehydrogenase from <i>Rhodococcus jostii</i> RHA1 genome. 2012 , 287, 30975-83	21
1793	Cheminformatics-driven discovery of selective, nanomolar inhibitors for staphylococcal pyruvate kinase. 2012 , 7, 350-9	15
1792	The basis for carbapenem hydrolysis by class A β -lactamases: a combined investigation using crystallography and simulations. 2012 , 134, 18275-85	60
1791	Binding mechanism of metal-NTP substrates and stringent-response alarmones to bacterial DnaG-type primases. 2012 , 20, 1478-89	58
1790	Structural and functional characterization of NikO, an enolpyruvyl transferase essential in nikkomycin biosynthesis. 2012 , 287, 31427-36	12
1789	Crystal structure of <i>Brucella abortus</i> deoxyxylulose-5-phosphate reductoisomerase-like (DRL) enzyme involved in isoprenoid biosynthesis. 2012 , 287, 15803-9	8
1788	Scaffoldin conformation and dynamics revealed by a ternary complex from the <i>Clostridium thermocellum</i> cellulosome. 2012 , 287, 26953-61	26
1787	Crystal structure of the human two-pore domain potassium channel K2P1. 2012 , 335, 432-6	232
1786	Structure of the TatC core of the twin-arginine protein transport system. 2012 , 492, 210-4	126
1785	LpxI structures reveal how a lipid A precursor is synthesized. 2012 , 19, 1132-8	18
1784	Structural basis of mouse cytomegalovirus m152/gp40 interaction with RAE1 β reveals a paradigm for MHC/MHC interaction in immune evasion. 2012 , 109, E3578-87	28
1783	Structural basis for Arf6-MKLP1 complex formation on the Flemming body responsible for cytokinesis. 2012 , 31, 2590-603	42
1782	Structural basis of functional group activation by sulfotransferases in complex metabolic pathways. 2012 , 7, 1994-2003	27
1781	Tet3 CXXC domain and dioxygenase activity cooperatively regulate key genes for <i>Xenopus</i> eye and neural development. 2012 , 151, 1200-13	188

1780	High-resolution crystal structure of human protease-activated receptor 1. 2012 , 492, 387-92	353
1779	Uncoupling intramolecular processing and substrate hydrolysis in the N-terminal nucleophile hydrolase hASRGL1 by circular permutation. 2012 , 7, 1840-7	13
1778	The molecular basis for substrate specificity of the nuclear NIPP1:PP1 holoenzyme. 2012 , 20, 1746-56	51
1777	Structural basis of potent and broad HIV-1 fusion inhibitor CP32M. 2012 , 287, 26618-29	18
1776	Tailoring encodable lanthanide-binding tags as MRI contrast agents. 2012 , 13, 2567-74	20
1775	Investigation of the substrate range of CYP199A4: modification of the partition between hydroxylation and desaturation activities by substrate and protein engineering. 2012 , 18, 16677-88	36
1774	Smooth statistical torsion angle potential derived from a large conformational database via adaptive kernel density estimation improves the quality of NMR protein structures. 2012 , 21, 1824-36	46
1773	Crystal structure of NirD, the small subunit of the nitrite reductase NirbD from <i>Mycobacterium tuberculosis</i> at 2.0 Å resolution. 2012 , 80, 2799-803	7
1772	Resolution-by-proxy: a simple measure for assessing and comparing the overall quality of NMR protein structures. 2012 , 53, 167-80	52
1771	How simple can a model of an empty viral capsid be? Charge distributions in viral capsids. 2012 , 38, 657-71	46
1770	Utility of anion and cation combinations for phasing of protein structures. 2012 , 13, 135-43	7
1769	Site-directed mutagenesis of a tetrameric dandelion polyphenol oxidase (PPO-6) reveals the site of subunit interaction. 2012 , 80, 203-17	22
1768	Active site plasticity within the glycoside hydrolase NagZ underlies a dynamic mechanism of substrate distortion. 2012 , 19, 1471-82	58
1767	Crystal structure of type VI effector Tse1 from <i>Pseudomonas aeruginosa</i> . 2012 , 586, 3193-9	20
1766	Low-resolution structure of <i>Drosophila</i> translin. 2012 , 2, 37-46	6
1765	Biased T cell receptor usage directed against human leukocyte antigen DQ8-restricted gliadin peptides is associated with celiac disease. 2012 , 37, 611-21	101
1764	Explorations of linked editosome domains leading to the discovery of motifs defining conserved pockets in editosome OB-folds. 2012 , 180, 362-73	4
1763	Crystal structure of 1,3Gal43A, an exo-β-1,3-galactanase from <i>Clostridium thermocellum</i> . 2012 , 180, 447-57	23

1762	Ligand binding stepwise disrupts water network in thrombin: enthalpic and entropic changes reveal classical hydrophobic effect. 2012 , 55, 6094-110	74
1761	The dynamic disulphide relay of quiescin sulphydryl oxidase. 2012 , 488, 414-8	62
1760	GABA binding to an insect GABA receptor: a molecular dynamics and mutagenesis study. 2012 , 103, 2071-81	33
1759	Evolution of the receptor binding properties of the influenza A(H3N2) hemagglutinin. 2012 , 109, 21474-9	194
1758	Broad antiviral activity and crystal structure of HIV-1 fusion inhibitor sifuvirtide. 2012 , 287, 6788-96	54
1757	Helical repeat structure of apoptosis inhibitor 5 reveals protein-protein interaction modules. 2012 , 287, 10727-37	15
1756	Exploring the structural basis of substrate preferences in Baeyer-Villiger monooxygenases: insight from steroid monooxygenase. 2012 , 287, 22626-34	39
1755	Structural and functional characterization of the kindlin-1 pleckstrin homology domain. 2012 , 287, 43246-61	27
1754	Inhibition of protein-protein interaction of HER2-EGFR and HER2-HER3 by a rationally designed peptidomimetic. 2012 , 30, 594-606	28
1753	The dimanganese(II) site of <i>Bacillus subtilis</i> class Ib ribonucleotide reductase. 2012 , 51, 3861-71	27
1752	The kinase activity of the <i>Helicobacter pylori</i> Asp-tRNA(Asn)/Glu-tRNA(Gln) amidotransferase is sensitive to distal mutations in its putative ammonia tunnel. 2012 , 51, 273-85	5
1751	Two translation products of <i>Yersinia yscQ</i> assemble to form a complex essential to type III secretion. 2012 , 51, 1669-77	40
1750	Zinc-mediated allosteric inhibition of caspase-6. 2012 , 287, 36000-11	59
1749	Crystal structure of the Marburg virus GP2 core domain in its postfusion conformation. 2012 , 51, 7665-75	36
1748	Domain-swapped dimeric structure of a stable and functional de novo four-helix bundle protein, WA20. 2012 , 116, 6789-97	26
1747	A bimodular mechanism of calcium control in eukaryotes. 2012 , 491, 468-72	89
1746	The structure of the C-terminal domain of the largest editosome interaction protein and its role in promoting RNA binding by RNA-editing ligase L2. 2012 , 40, 6966-77	16
1745	Crystal structure of the human NKX2.5 homeodomain in complex with DNA target. 2012 , 51, 6312-9	30

1744	Discrimination between CO and O(2) in heme oxygenase: comparison of static structures and dynamic conformation changes following CO photolysis. 2012 , 51, 8554-62	13
1743	Elements of nucleotide specificity in the <i>Trypanosoma brucei</i> mitochondrial RNA editing enzyme RET2. 2012 , 52, 1308-18	7
1742	Botulinum neurotoxin is shielded by NTNHA in an interlocked complex. 2012 , 335, 977-81	160
1741	<i>Entamoeba histolytica</i> Rho1 regulates actin polymerization through a divergent, diaphanous-related formin. 2012 , 51, 8791-801	14
1740	Structural insights into the conformation and oligomerization of E2~ubiquitin conjugates. 2012 , 51, 4175-87	58
1739	Crystal structures of <i>Trypanosoma cruzi</i> UDP-galactopyranose mutase implicate flexibility of the histidine loop in enzyme activation. 2012 , 51, 4968-79	23
1738	Crystal structures of <i>Xanthomonas campestris</i> OleA reveal features that promote head-to-head condensation of two long-chain fatty acids. 2012 , 51, 4138-46	23
1737	Structural studies of E73 from a hyperthermophilic archaeal virus identify the "RH3" domain, an elaborated ribbon-helix-helix motif involved in DNA recognition. 2012 , 51, 2899-910	19
1736	Structure and glycolipid binding properties of the nematocidal protein Cry5B. 2012 , 51, 9911-21	48
1735	High-resolution structure of a protein spin-label in a solvent-exposed β -sheet and comparison with DEER spectroscopy. 2012 , 51, 6350-9	22
1734	Fragment screening using capillary electrophoresis (CEfrag) for hit identification of heat shock protein 90 ATPase inhibitors. 2012 , 17, 868-76	41
1733	The structure of the BfrB-Bfd complex reveals protein-protein interactions enabling iron release from bacterioferritin. 2012 , 134, 13470-81	49
1732	Transition state analysis of enolpyruvylshikimate 3-phosphate (EPSP) synthase (AroA)-catalyzed EPSP hydrolysis. 2012 , 134, 12958-69	8
1731	Hidden relationship between conserved residues and locally conserved phosphate-binding structures in NAD(P)-binding proteins. 2012 , 116, 5644-52	9
1730	Evidence in support of lysine 77 and histidine 96 as acid-base catalytic residues in saccharopine dehydrogenase from <i>Saccharomyces cerevisiae</i> . 2012 , 51, 857-66	8
1729	Efficient and versatile one-step affinity purification of in vivo biotinylated proteins: expression, characterization and structure analysis of recombinant human glutamate carboxypeptidase II. 2012 , 82, 106-15	31
1728	An allosteric inhibitor of protein arginine methyltransferase 3. 2012 , 20, 1425-35	72
1727	Crystal structure and functional analysis of JMJD5 indicate an alternate specificity and function. 2012 , 32, 4044-52	47

1726	Structural, functional, and evolutionary analysis of the unusually large stilbene synthase gene family in grapevine. 2012 , 160, 1407-19	101
1725	Triphenylbutanamines: kinesin spindle protein inhibitors with in vivo antitumor activity. 2012 , 55, 1511-25	33
1724	Structural basis for RNA-duplex recognition and unwinding by the DEAD-box helicase Mss116p. 2012 , 490, 121-5	81
1723	pH-dependent structural conformations of B-phycoerythrin from <i>Porphyridium cruentum</i> . 2012 , 279, 3680-3691	23
1722	Structure of a KirBac potassium channel with an open bundle crossing indicates a mechanism of channel gating. 2012 , 19, 158-63	78
1721	Exome sequencing identifies recurrent somatic RAC1 mutations in melanoma. 2012 , 44, 1006-14	887
1720	Influenza virus neuraminidases with reduced enzymatic activity that avidly bind sialic Acid receptors. 2012 , 86, 13371-83	97
1719	Black mamba venom peptides target acid-sensing ion channels to abolish pain. 2012 , 490, 552-5	283
1718	Structural characterization of binding mode of smoking cessation drugs to nicotinic acetylcholine receptors through study of ligand complexes with acetylcholine-binding protein. 2012 , 287, 23283-93	38
1717	Diverse HIV viruses are targeted by a conformationally dynamic antiviral. 2012 , 19, 411-6	21
1716	Ab initio quantum chemistry for protein structures. 2012 , 116, 12501-9	88
1715	Structural and molecular insights into the mechanism of action of human angiogenin-ALS variants in neurons. 2012 , 3, 1121	65
1714	Identification of a ubiquitin-binding structure in the S-locus F-box protein controlling S-RNase-based self-incompatibility. 2012 , 39, 93-102	12
1713	Solution structure of the HIV-1 exon splicing silencer 3. 2012 , 415, 680-98	18
1712	Protein kinase domain of CTR1 from <i>Arabidopsis thaliana</i> promotes ethylene receptor cross talk. 2012 , 415, 768-79	33
1711	Structurally similar but functionally diverse ZU5 domains in human erythrocyte ankyrin. 2012 , 417, 336-50	14
1710	Impact of ligand and protein desolvation on ligand binding to the S1 pocket of thrombin. 2012 , 418, 350-66	34
1709	Structural basis for profilin-mediated actin nucleotide exchange. 2012 , 418, 103-16	18

1708	Improved modeling of side-chain--base interactions and plasticity in protein--DNA interface design. 2012 , 419, 255-74	17
1707	Crystallographically mapped ligand binding differs in high and low IgE binding isoforms of birch pollen allergen bet v 1. 2012 , 422, 109-23	73
1706	Crystal structure of the coat protein of the flexible filamentous papaya mosaic virus. 2012 , 422, 263-73	38
1705	Structure and catalytic mechanism of a cyclic dipeptide prenyltransferase with broad substrate promiscuity. 2012 , 422, 87-99	57
1704	pH-dependent dimerization of spider silk N-terminal domain requires relocation of a wedged tryptophan side chain. 2012 , 422, 477-87	61
1703	X-ray crystal structure and specificity of the Plasmodium falciparum malaria aminopeptidase PfM18AAP. 2012 , 422, 495-507	27
1702	Structure of the sensor domain of Mycobacterium tuberculosis PknH receptor kinase reveals a conserved binding cleft. 2012 , 422, 488-94	15
1701	Identification of a conserved aggregation-prone intermediate state in the folding pathways of Spc-SH3 amyloidogenic variants. 2012 , 422, 705-722	33
1700	Homology models of four Agaricus bisporus tyrosinases. 2012 , 50, 283-93	4
1699	Structures of the HIN domain:DNA complexes reveal ligand binding and activation mechanisms of the AIM2 inflammasome and IFI16 receptor. 2012 , 36, 561-71	352
1698	Structural basis of specificity in tetrameric Kluyveromyces lactis β -galactosidase. 2012 , 177, 392-401	78
1697	Crystal structure of a mono- and diacylglycerol lipase from Malassezia globosa reveals a novel lid conformation and insights into the substrate specificity. 2012 , 178, 363-9	52
1696	The crystal structure of the CRISPR-associated protein Csn2 from Streptococcus agalactiae. 2012 , 178, 350-62	21
1695	The structure of monoacylglycerol lipase from Bacillus sp. H257 reveals unexpected conservation of the cap architecture between bacterial and human enzymes. 2012 , 1821, 1012-21	32
1694	Crystal structures of the Arabidopsis thaliana abscisic acid receptor PYL10 and its complex with abscisic acid. 2012 , 418, 122-7	27
1693	Crystal structure of the Rasputin NTF2-like domain from Drosophila melanogaster. 2012 , 420, 188-92	10
1692	Crystal structure of Plasmodium falciparum thioredoxin reductase, a validated drug target. 2012 , 425, 806-11	19
1691	Crystal structure of a pro-inflammatory lectin from the seeds of Dioclea wilsonii Standl. 2012 , 94, 525-32	18

1690	Crystal structure of dihydroorotate dehydrogenase from <i>Leishmania major</i> . 2012 , 94, 1739-48	27
1689	Comparative biophysical characterization of chicken β_2 -microglobulin. 2012 , 167, 26-35	4
1688	A phage tubulin assembles dynamic filaments by an atypical mechanism to center viral DNA within the host cell. 2012 , 149, 1488-99	69
1687	The peptide-receptive transition state of MHC class I molecules: insight from structure and molecular dynamics. 2012 , 189, 1391-9	45
1686	Structure of a proteasome Pba1-Pba2 complex: implications for proteasome assembly, activation, and biological function. 2012 , 287, 37371-82	43
1685	The 1.2 Å resolution crystal structure of TcpG, the <i>Vibrio cholerae</i> DsbA disulfide-forming protein required for pilus and cholera-toxin production. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012 , 68, 1290-302	18
1684	Crystal structure of a soluble form of human CD73 with ecto-5'-nucleotidase activity. 2012 , 13, 2384-91	50
1683	Engineered variants of InlB with an additional leucine-rich repeat discriminate between physiologically relevant and packing contacts in crystal structures of the InlB:MET complex. 2012 , 21, 1528-39	6
1682	Crystal structure of the <i>Yersinia enterocolitica</i> type III secretion chaperone SycD in complex with a peptide of the minor translocator YopD. 2012 , 12, 13	19
1681	Two structurally discrete GH7-cellobiohydrolases compete for the same cellulosic substrate fiber. 2012 , 5, 21	19
1680	Crystal structures of wild-type and mutated cyclophilin B that causes hyperelastosis cutis in the American quarter horse. 2012 , 5, 626	8
1679	Effects of a buried cysteine-to-serine mutation on yeast triosephosphate isomerase structure and stability. 2012 , 13, 10010-21	6
1678	Role of arginine 29 and glutamic acid 81 interactions in the conformational stability of human chloride intracellular channel 1. 2012 , 51, 7854-62	13
1677	<i>Acinetobacter baumannii</i> F ₀ D ligand complexes –potent inhibitors of folate metabolism and a re-evaluation of the structure of LY374571. 2012 , 279, 4350-60	12
1676	Crystal structure of greglin, a novel non-classical Kazal inhibitor, in complex with subtilisin. 2012 , 279, 4466-78	11
1675	Structural basis for dual inhibitory role of tamarind Kunitz inhibitor (TKI) against factor Xa and trypsin. 2012 , 279, 4547-64	26
1674	Cross-neutralization of influenza A viruses mediated by a single antibody loop. 2012 , 489, 526-32	344
1673	Applications and limitations of in silico models in drug discovery. 2012 , 910, 87-124	28

1672	Restoring methicillin-resistant <i>Staphylococcus aureus</i> susceptibility to β -lactam antibiotics. 2012 , 4, 126ra35	169
1671	Structure and mode of peptide binding of pheromone receptor PrgZ. 2012 , 287, 37165-70	15
1670	Characterisation of the organophosphate hydrolase catalytic activity of SsoPox. 2012 , 2, 779	67
1669	<i>Trypanosoma cruzi</i> trans-sialidase in complex with a neutralizing antibody: structure/function studies towards the rational design of inhibitors. 2012 , 8, e1002474	32
1668	A basis set of de novo coiled-coil peptide oligomers for rational protein design and synthetic biology. 2012 , 1, 240-50	159
1667	Crystal structure of a plectonemic RNA supercoil. 2012 , 3, 901	2
1666	The structural biochemistry of Zucchini implicates it as a nuclease in piRNA biogenesis. 2012 , 491, 279-83	229
1665	Structure of FabH and factors affecting the distribution of branched fatty acids in <i>Micrococcus luteus</i> . <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012 , 68, 1320-8	6
1664	Endo- β -D-1,4-mannanase from <i>Chrysonilia sitophila</i> displays a novel loop arrangement for substrate selectivity. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012 , 68, 1468-78	18
1663	A monomeric TIM-barrel structure from <i>Pyrococcus furiosus</i> is optimized for extreme temperatures. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012 , 68, 1479-87	2
1662	Structure analysis of geranyl pyrophosphate methyltransferase and the proposed reaction mechanism of SAM-dependent C-methylation. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012 , 68, 1558-69	7
1661	Structure of the corrinoid:coenzyme M methyltransferase MtaA from <i>Methanosarcina mazei</i> . <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012 , 68, 1549-57	4
1660	Structural characterization of a modification subunit of a putative type I restriction enzyme from <i>Vibrio vulnificus</i> YJ016. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012 , 68, 1570-7	5
1659	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, 1653-9	6
1658	Structure of the recombinant BPTI/Kunitz-type inhibitor rShPI-1A from the marine invertebrate <i>Stichodactyla helianthus</i> . 2012 , 68, 1289-93	7
1657	Structure of <i>Escherichia coli</i> RutC, a member of the YjgF family and putative aminoacrylate peracid reductase of the rut operon. 2012 , 68, 1294-9	12
1656	Structure of ribose 5-phosphate isomerase from the probiotic bacterium <i>Lactobacillus salivarius</i> UCC118. 2012 , 68, 1427-33	7
1655	Structure of the β ,6/ β ,4-specific glucansucrase GTFA from <i>Lactobacillus reuteri</i> 121. 2012 , 68, 1448-54	47

1654	Recombinant production, crystallization and X-ray crystallographic structure determination of the peptidyl-tRNA hydrolase of <i>Pseudomonas aeruginosa</i> . 2012 , 68, 1472-6	20
1653	<i>Alternaria alternata</i> allergen Alt a 1: a unique β -barrel protein dimer found exclusively in fungi. 2012 , 130, 241-7.e9	71
1652	A nuclear export sequence in GPN-loop GTPase 1, an essential protein for nuclear targeting of RNA polymerase II, is necessary and sufficient for nuclear export. 2012 , 1823, 1756-66	17
1651	Worm-like Ising model for protein mechanical unfolding under the effect of osmolytes. 2012 , 102, 342-50	11
1650	The binding of C5-alkynyl and alkylfurano[2,3-d]pyrimidine glucopyranonucleosides to glycogen phosphorylase b: synthesis, biochemical and biological assessment. 2012 , 54, 740-9	19
1649	Structures of lysenin reveal a shared evolutionary origin for pore-forming proteins and its mode of sphingomyelin recognition. 2012 , 20, 1498-507	75
1648	The crystal structure of the MAP kinase LmaMPK10 from <i>Leishmania major</i> reveals parasite-specific features and regulatory mechanisms. 2012 , 20, 1649-60	12
1647	Distinct states of methionyl-tRNA synthetase indicate inhibitor binding by conformational selection. 2012 , 20, 1681-91	54
1646	Crystal structures of the HypCD complex and the HypCDE ternary complex: transient intermediate complexes during [NiFe] hydrogenase maturation. 2012 , 20, 2124-37	37
1645	Target binding to S100B reduces dynamic properties and increases Ca(2+)-binding affinity for wild type and EF-hand mutant proteins. 2012 , 423, 365-85	13
1644	The structure of DNA-bound human topoisomerase II alpha: conformational mechanisms for coordinating inter-subunit interactions with DNA cleavage. 2012 , 424, 109-24	138
1643	Molecular recognition of canonical and deaminated bases by <i>P. abyssi</i> family B DNA polymerase. 2012 , 423, 315-36	26
1642	Structural basis of substrate specificity and selectivity of murine cytosolic 5'-nucleotidase III. 2012 , 423, 540-54	3
1641	Characterization of transport proteins for aromatic compounds derived from lignin: benzoate derivative binding proteins. 2012 , 423, 555-75	22
1640	Histone recognition by human malignant brain tumor domains. 2012 , 423, 702-18	45
1639	Bacterial and plant ketol-acid reductoisomerases have different mechanisms of induced fit during the catalytic cycle. 2012 , 424, 168-79	26
1638	Structure of PA1221, a nonribosomal peptide synthetase containing adenylation and peptidyl carrier protein domains. 2012 , 51, 3252-63	101
1637	Development of a tetrameric streptavidin mutein with reversible biotin binding capability: engineering a mobile loop as an exit door for biotin. 2012 , 7, e35203	18

1636	Substrate binds in the S1 site of the F253A mutant of LeuT, a neurotransmitter sodium symporter homologue. 2012 , 13, 861-6	36
1635	Structural basis of DNA ligase IV-Artemis interaction in nonhomologous end-joining. 2012 , 2, 1505-12	29
1634	Induced fit and the catalytic mechanism of isocitrate dehydrogenase. 2012 , 51, 7098-115	23
1633	Structure of an As(III) S-adenosylmethionine methyltransferase: insights into the mechanism of arsenic biotransformation. 2012 , 51, 5476-85	85
1632	The SLC10 carrier family: transport functions and molecular structure. 2012 , 70, 105-68	87
1631	Reflection on design and testing of pancreatic alpha-amylase inhibitors: an in silico comparison between rat and rabbit enzyme models. 2012 , 20, 77	3
1630	Structural basis of agrin-LRP4-MuSK signaling. 2012 , 26, 247-58	116
1629	Accelerated disassembly of IgE-receptor complexes by a disruptive macromolecular inhibitor. 2012 , 491, 613-7	76
1628	X-ray structures of LeuT in substrate-free outward-open and apo inward-open states. 2012 , 481, 469-74	394
1627	1.8 Structure Validation and Analysis. 2012 , 116-135	1
1626	Design and synthesis of novel lactate dehydrogenase A inhibitors by fragment-based lead generation. 2012 , 55, 3285-306	125
1625	Solution structure of kurtoxin: a gating modifier selective for Cav3 voltage-gated Ca(2+) channels. 2012 , 51, 1862-73	16
1624	Cyclic AMP regulation of protein lysine acetylation in Mycobacterium tuberculosis. 2012 , 19, 811-8	40
1623	Myelin 2',3'-cyclic nucleotide 3'-phosphodiesterase: active-site ligand binding and molecular conformation. 2012 , 7, e32336	27
1622	Carbohydrate recognition by an architecturally complex N-acetylglucosaminidase from Clostridium perfringens. 2012 , 7, e33524	34
1621	Crystal structures of the tetratricopeptide repeat domains of kinesin light chains: insight into cargo recognition mechanisms. 2012 , 7, e33943	33
1620	Assessment of Pseudomonas aeruginosa N5,N10-methylenetetrahydrofolate dehydrogenase-cyclohydrolase as a potential antibacterial drug target. 2012 , 7, e35973	17
1619	Structure of a murine norovirus NS6 protease-product complex revealed by adventitious crystallisation. 2012 , 7, e38723	21

1618	Structure analysis of <i>Entamoeba histolytica</i> DNMT2 (EhMeth). 2012 , 7, e38728	14
1617	Acetylcholine-binding protein in the hemolymph of the planorbid snail <i>Biomphalaria glabrata</i> is a pentagonal dodecahedron (60 subunits). 2012 , 7, e43685	12
1616	Crystal structures of archaemetzincin reveal a moldable substrate-binding site. 2012 , 7, e43863	4
1615	Crystal structures of three classes of non-steroidal anti-inflammatory drugs in complex with aldo-keto reductase 1C3. 2012 , 7, e43965	43
1614	Insights into phosphate cooperativity and influence of substrate modifications on binding and catalysis of hexameric purine nucleoside phosphorylases. 2012 , 7, e44282	10
1613	N-terminal T4 lysozyme fusion facilitates crystallization of a G protein coupled receptor. 2012 , 7, e46039	99
1612	A green fluorescent protein containing a QFG tri-peptide chromophore: optical properties and X-ray crystal structure. 2012 , 7, e47331	5
1611	Structural insight into the <i>Clostridium difficile</i> ethanolamine utilisation microcompartment. 2012 , 7, e48360	42
1610	Structural analyses of a constitutively active mutant of exchange protein directly activated by cAMP. 2012 , 7, e49932	9
1609	Tolerance of protein folding to a circular permutation in a PDZ domain. 2012 , 7, e50055	10
1608	Structures of the human poly (ADP-ribose) glycohydrolase catalytic domain confirm catalytic mechanism and explain inhibition by ADP-HPD derivatives. 2012 , 7, e50889	38
1607	Bin2 is a membrane sculpting N-BAR protein that influences leucocyte podosomes, motility and phagocytosis. 2012 , 7, e52401	31
1606	DNA binding in high salt: analysing the salt dependence of replication protein A3 from the halophile <i>Haloferax volcanii</i> . 2012 , 2012, 719092	4
1605	The structure of the Bach2 POZ-domain dimer reveals an intersubunit disulfide bond. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012 , 68, 26-34	10
1604	Four complete turns of a curved 3 α helix at atomic resolution: the crystal structure of the peptaibol trichovirin I-4A in a polar environment suggests a transition to α helix for membrane function. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012 , 68, 109-16	15
1603	A corrected space group for <i>Sulfolobus sulfataricus</i> 5'-deoxy-5'-methylthioadenosine phosphorylase II. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012 , 68, 249-52	2
1602	Structure of the effector-binding domain of the arabinose repressor AraR from <i>Bacillus subtilis</i> . <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012 , 68, 176-85	10
1601	Structure of the cytoplasmic domain of <i>Yersinia pestis</i> YscD, an essential component of the type III secretion system. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012 , 68, 201-9	12

1600	Structure and function of CYP108D1 from <i>Novosphingobium aromaticivorans</i> DSM12444: an aromatic hydrocarbon-binding P450 enzyme. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012 , 68, 277-91	20
1599	Structure and function of the <i>Clostridium thermocellum</i> cellobiohydrolase A X1-module repeat: enhancement through stabilization of the CbhA complex. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012 , 68, 292-9	13
1598	Structural insights into RipC, a putative citrate lyase α subunit from a <i>Yersinia pestis</i> virulence operon. 2012 , 68, 2-7	14
1597	Structure of CBM3b of the major cellulosomal scaffoldin subunit ScaA from <i>Acetivibrio cellulolyticus</i> . 2012 , 68, 8-13	8
1596	Structure of a pectin methylesterase from <i>Yersinia enterocolitica</i> . 2012 , 68, 129-33	17
1595	Lysozyme contamination facilitates crystallization of a heterotrimeric cortactin-Arg-lysozyme complex. 2012 , 68, 154-8	8
1594	Protein structure validation by generalized linear model root-mean-square deviation prediction. 2012 , 21, 229-38	38
1593	Structure and activity of DmmA, a marine haloalkane dehalogenase. 2012 , 21, 239-48	29
1592	Environment-dependent long-range structural distortion in a temperature-sensitive point mutant. 2012 , 21, 63-74	2
1591	Protein loop closure using orientational restraints from NMR data. 2012 , 80, 433-53	13
1590	Crystal structure of vinculin in complex with vinculin binding site 50 (VBS50), the integrin binding site 2 (IBS2) of talin. 2012 , 21, 583-8	11
1589	<i>Mycobacterium thermoresistibile</i> as a source of thermostable orthologs of <i>Mycobacterium tuberculosis</i> proteins. 2012 , 21, 1093-6	13
1588	Functional and structural characterization of a thermostable acetyl esterase from <i>Thermotoga maritima</i> . 2012 , 80, 1545-59	36
1587	The ST Pinch: A side chain-to-side chain hydrogen-bonded motif. 2012 , 80, 1259-63	2
1586	Crystal structure of the TLDC domain of oxidation resistance protein 2 from zebrafish. 2012 , 80, 1694-8	23
1585	Crystal structure of agkisacucetin, a Gpib-binding snake C-type lectin that inhibits platelet adhesion and aggregation. 2012 , 80, 1707-11	17
1584	An intersubunit disulfide bridge stabilizes the tetrameric nucleoside diphosphate kinase of <i>Aquifex aeolicus</i> . 2012 , 80, 1658-68	8
1583	Crystal structure of a supercharged variant of the human enteropeptidase light chain. 2012 , 80, 1907-10	10

1582	Structure of the μ -opioid receptor bound to naltrindole. 2012 , 485, 400-4	538
1581	Crystal structure of the μ -opioid receptor bound to a morphinan antagonist. 2012 , 485, 321-6	1003
1580	Contribution of the first K-homology domain of poly(C)-binding protein 1 to its affinity and specificity for C-rich oligonucleotides. 2012 , 40, 5101-14	29
1579	Structural analysis of the STING adaptor protein reveals a hydrophobic dimer interface and mode of cyclic di-GMP binding. 2012 , 36, 1073-86	232
1578	Structure of hepatitis C virus polymerase in complex with primer-template RNA. 2012 , 86, 6503-11	105
1577	Structural and biochemical basis of Yos9 protein dimerization and possible contribution to self-association of 3-hydroxy-3-methylglutaryl-coenzyme A reductase degradation ubiquitin-ligase complex. 2012 , 287, 8633-40	9
1576	Protein camouflage in cytochrome c-calixarene complexes. 2012 , 4, 527-33	164
1575	Ultrahigh and high resolution structures and mutational analysis of monomeric <i>Streptococcus pyogenes</i> SpeB reveal a functional role for the glycine-rich C-terminal loop. 2012 , 287, 24412-26	12
1574	Significant reduction in errors associated with nonbonded contacts in protein crystal structures: automated all-atom refinement with PrimeX. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012 , 68, 935-52	19
1573	Interpreting the structural mechanism of action for MT7 and human muscarinic acetylcholine receptor 1 complex by modeling protein-protein interaction. 2012 , 30, 30-44	6
1572	X-ray structure of <i>Salmonella typhimurium</i> uridine phosphorylase complexed with 5-fluorouracil and molecular modelling of the complex of 5-fluorouracil with uridine phosphorylase from <i>Vibrio cholerae</i> . <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012 , 68, 968-74	6
1571	Structure of the branched-chain aminotransferase from <i>Streptococcus mutans</i> . <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012 , 68, 996-1002	4
1570	Discovery of ligands for ADP-ribosyltransferases via docking-based virtual screening. 2012 , 55, 7706-18	35
1569	Structural insights into electron transfer in <i>caa3</i> -type cytochrome oxidase. 2012 , 487, 514-8	97
1568	Recognition of SUMO-modified PCNA requires tandem receptor motifs in Srs2. 2012 , 483, 59-63	100
1567	G-protein-coupled receptor inactivation by an allosteric inverse-agonist antibody. 2012 , 482, 237-40	240
1566	Optimization of affinity, specificity and function of designed influenza inhibitors using deep sequencing. 2012 , 30, 543-8	279
1565	Structure of the receptor-binding carboxy-terminal domain of bacteriophage T7 tail fibers. 2012 , 109, 9390-5	71

1564	Cheminformatics meets molecular mechanics: a combined application of knowledge-based pose scoring and physical force field-based hit scoring functions improves the accuracy of structure-based virtual screening. 2012 , 52, 16-28	32
1563	Structural basis of Wnt recognition by Frizzled. 2012 , 337, 59-64	563
1562	Improving the accuracy of macromolecular structure refinement at 7 Å resolution. 2012 , 20, 957-66	36
1561	Crystal structure of the heterodimeric CLOCK:BMAL1 transcriptional activator complex. 2012 , 337, 189-94	198
1560	A carrier protein strategy yields the structure of dalbavancin. 2012 , 134, 4637-45	28
1559	Structure and functional interaction of the extracellular domain of human GABA(B) receptor GBR2. 2012 , 15, 970-8	53
1558	Monospecific inhibitors show that both mannan-binding lectin-associated serine protease-1 (MASP-1) and -2 Are essential for lectin pathway activation and reveal structural plasticity of MASP-2. 2012 , 287, 20290-300	58
1557	Dimeric α -obratoxin X-ray structure: localization of intermolecular disulfides and possible mode of binding to nicotinic acetylcholine receptors. 2012 , 287, 6725-34	28
1556	Structural dynamics of the aminoacylation and proofreading functional cycle of bacterial leucyl-tRNA synthetase. 2012 , 19, 677-84	111
1555	The structure of a GH10 xylanase from <i>Fusarium oxysporum</i> reveals the presence of an extended loop on top of the catalytic cleft. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012 , 68, 735-42	12
1554	Biochemical and structural characterization of the GTP-preferring succinyl-CoA synthetase from <i>Thermus aquaticus</i> . <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012 , 68, 751-62	6
1553	Structural plasticity of tubulin assembly probed by vinca-domain ligands. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012 , 68, 927-34	59
1552	An enlarged, adaptable active site in CYP164 family P450 enzymes, the sole P450 in <i>Mycobacterium leprae</i> . 2012 , 56, 391-402	5
1551	Structure and permeation mechanism of a mammalian urea transporter. 2012 , 109, 11194-9	58
1550	Structural and Catalytic Characterization of <i>Pichia stipitis</i> OYE 2.6, a Useful Biocatalyst for Asymmetric Alkene Reductions. 2012 , 354, 1949-1960	27
1549	Real-space refinement with DireX: from global fitting to side-chain improvements. 2012 , 97, 687-97	40
1548	Water makes the difference: rearrangement of water solvation layer triggers non-additivity of functional group contributions in protein-ligand binding. 2012 , 7, 1423-34	60
1547	Phosphorylation-dependent activity of the deubiquitinase DUBA. 2012 , 19, 171-5	81

1546	Structural insights into a human anti-IFN antibody exerting therapeutic potential for systemic lupus erythematosus. 2012 , 90, 837-46	23
1545	Simultaneous single-structure and bundle representation of protein NMR structures in torsion angle space. 2012 , 52, 351-64	19
1544	Solution NMR structures reveal unique homodimer formation by a winged helix-turn-helix motif and provide first structures for protein domain family PF10771. 2012 , 13, 1-7	2
1543	Solution NMR structures reveal a distinct architecture and provide first structures for protein domain family PF04536. 2012 , 13, 9-14	7
1542	3D modeling and molecular dynamics simulation of an immune-regulatory cytokine, interleukin-10, from the Indian major carp, <i>Catla catla</i> . 2012 , 18, 1713-22	4
1541	The conjugation protein TcpC from <i>Clostridium perfringens</i> is structurally related to the type IV secretion system protein VirB8 from Gram-negative bacteria. 2012 , 83, 275-88	63
1540	Redesign of coenzyme B(12) dependent diol dehydratase to be resistant to the mechanism-based inactivation by glycerol and act on longer chain 1,2-diols. 2012 , 279, 793-804	30
1539	Structural and functional investigation of the intermolecular interaction between NRPS adenylation and carrier protein domains. 2012 , 19, 188-98	107
1538	Crystal structures of the Tudor domains of human PHF20 reveal novel structural variations on the Royal Family of proteins. 2012 , 586, 859-65	20
1537	Conformational changes upon ligand binding in the essential class II fumarase Rv1098c from <i>Mycobacterium tuberculosis</i> . 2012 , 586, 1606-11	17
1536	Solution structure of CyanoP from <i>Synechocystis</i> sp. PCC 6803: new insights on the structural basis for functional specialization amongst PsbP family proteins. 2012 , 1817, 1331-8	19
1535	Structural basis of high-affinity nuclear localization signal interactions with importin- β . 2012 , 13, 532-48	70
1534	Contribution of active site glutamine to rate enhancement in ubiquitin C-terminal hydrolases. 2012 , 279, 1106-18	13
1533	3'-axial CH ₂ OH substitution on glucopyranose does not increase glycogen phosphorylase inhibitory potency. QM/MM-PBSA calculations suggest why. 2012 , 79, 663-73	19
1532	Stimulation and clustering of cytochrome b5 reductase in caveolin-rich lipid microdomains is an early event in oxidative stress-mediated apoptosis of cerebellar granule neurons. 2012 , 75, 2934-49	20
1531	The crystal structure of <i>Leishmania major</i> N(5),N(10)-methylene tetrahydrofolate dehydrogenase/cyclohydrolase and assessment of a potential drug target. 2012 , 181, 178-85	8
1530	Structure of the <i>Yersinia pestis</i> FabV enoyl-ACP reductase and its interaction with two 2-pyridone inhibitors. 2012 , 20, 89-100	15
1529	Mechanism of regulation of receptor histidine kinases. 2012 , 20, 56-66	78

1528	Structure of the discoidin domain receptor 1 extracellular region bound to an inhibitory Fab fragment reveals features important for signaling. 2012 , 20, 688-97	67
1527	The structure of dimeric apolipoprotein A-IV and its mechanism of self-association. 2012 , 20, 767-79	34
1526	Graphical tools for macromolecular crystallography in PHENIX. 2012 , 45, 581-586	95
1525	To B or not to B: a question of resolution?. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012 , 68, 468-77	47
1524	Use of knowledge-based restraints in phenix.refine to improve macromolecular refinement at low resolution. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012 , 68, 381-90	156
1523	Application of DEN refinement and automated model building to a difficult case of molecular-replacement phasing: the structure of a putative succinyl-diaminopimelate desuccinylase from <i>Corynebacterium glutamicum</i> . <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012 , 68, 381-400	24
1522	Implementing an X-ray validation pipeline for the Protein Data Bank. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012 , 68, 478-83	73
1521	PDB_REDO: constructive validation, more than just looking for errors. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012 , 68, 484-96	160
1520	Exploiting structure similarity in refinement: automated NCS and target-structure restraints in BUSTER. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012 , 68, 368-80	432
1519	Low-resolution refinement tools in REFMAC5. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012 , 68, 404-17	179
1518	Towards automated crystallographic structure refinement with phenix.refine. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012 , 68, 352-67	3236
1517	S-SAD phasing study of death receptor 6 and its solution conformation revealed by SAXS. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012 , 68, 521-30	22
1516	The mammalian DUF59 protein Fam96a forms two distinct types of domain-swapped dimer. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012 , 68, 637-48	20
1515	Structural and functional characterization of the C-terminal catalytic domain of SSV1 integrase. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012 , 68, 659-70	11
1514	Two high-resolution structures of potato endo-1,3- β -glucanase reveal subdomain flexibility with implications for substrate binding. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012 , 68, 713-23	12
1513	Structures of <i>Helicobacter pylori</i> uridylyate kinase: insight into release of the product UDP. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012 , 68, 773-83	3
1512	Structures of <i>Staphylococcus aureus</i> peptide deformylase in complex with two classes of new inhibitors. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012 , 68, 784-93	4
1511	Structure of a post-translationally processed heterodimeric double-headed Kunitz-type serine protease inhibitor from potato. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012 , 68, 794-9	19

1510	A single mutation reforms the binding activity of an adhesion-deficient family 3 carbohydrate-binding module. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012 , 68, 819-28	11
1509	Structure of a bacterial cytoplasmic cyclophilin A in complex with a tetrapeptide. 2012 , 68, 259-64	5
1508	Structure of AKR1C3 with 3-phenoxybenzoic acid bound. 2012 , 68, 409-13	9
1507	Structure of the regulatory domain of the LysR family regulator NMB2055 (MetR-like protein) from <i>Neisseria meningitidis</i> . 2012 , 68, 730-7	1
1506	The structure of an orthorhombic crystal form of a 'forced reduced' thiol peroxidase reveals lattice formation aided by the presence of the affinity tag. 2012 , 68, 522-6	2
1505	The precursor form of <i>Hansenula polymorpha</i> copper amine oxidase 1 in complex with CuI and Coll. 2012 , 68, 501-10	4
1504	A model for 3-methyladenine recognition by 3-methyladenine DNA glycosylase I (TAG) from <i>Staphylococcus aureus</i> . 2012 , 68, 610-5	3
1503	Structure of a monomeric variant of rhodopsin kinase at 2.5 Å resolution. 2012 , 68, 622-5	9
1502	Structure of a short-chain dehydrogenase/reductase from <i>Bacillus anthracis</i> . 2012 , 68, 632-7	1
1501	Structure of <i>Leishmania major</i> cysteine synthase. 2012 , 68, 738-43	16
1500	A cationic lumen in the Wzx flippase mediates anionic O-antigen subunit translocation in <i>Pseudomonas aeruginosa</i> PAO1. 2012 , 84, 1165-76	34
1499	Enzymatic activity and immunoreactivity of Aca s 4, an alpha-amylase allergen from the storage mite <i>Acarus siro</i> . 2012 , 13, 3	11
1498	A discriminative Ramachandran potential of mean force aimed at minimizing secondary structure bias. 2012 , 33, 791-9	
1497	Synthetic polyamines as potential amine oxidase inhibitors: a preliminary study. 2012 , 42, 913-28	12
1496	Vaspin inhibits kallikrein 7 by serpin mechanism. 2013 , 70, 2569-83	95
1495	Crystal structure and activating effect on RyRs of AhV _{TL} -I, a glycosylated thrombin-like enzyme from <i>Agkistrodon halys</i> snake venom. 2013 , 87, 535-45	17
1494	Structural, kinetic and computational investigation of <i>Vitis vinifera</i> DHDPS reveals new insight into the mechanism of lysine-mediated allosteric inhibition. 2013 , 81, 431-46	26
1493	Sequence divergence in the <i>Treponema denticola</i> FhbB protein and its impact on factor H binding. 2013 , 28, 316-30	8

1492	An in vivo human-plasmablast enrichment technique allows rapid identification of therapeutic influenza A antibodies. 2013 , 14, 93-103	131
1491	Structure of class B GPCR corticotropin-releasing factor receptor 1. 2013 , 499, 438-43	344
1490	Full-length structure of a sensor histidine kinase pinpoints coaxial coiled coils as signal transducers and modulators. 2013 , 21, 1127-36	140
1489	Design of synthetic autonomous VH domain libraries and structural analysis of a VH domain bound to vascular endothelial growth factor. 2013 , 425, 2247-59	21
1488	Structural and thermodynamic insights into the recognition of native proteins by anti-peptide antibodies. 2013 , 425, 2027-2038	5
1487	Structure of the second RRM domain of Nrd1, a fission yeast MAPK target RNA binding protein, and implication for its RNA recognition and regulation. 2013 , 437, 12-7	2
1486	Structure of a kinesin-tubulin complex and implications for kinesin motility. 2013 , 20, 1001-7	107
1485	Crystal structure of Dioclea violacea lectin and a comparative study of vasorelaxant properties with Dioclea rostrata lectin. 2013 , 45, 807-15	25
1484	A dodecameric ring-like structure of the N0 domain of the type II secretin from enterotoxigenic Escherichia coli. 2013 , 183, 354-362	14
1483	Structural basis for assembly of the Mn(IV)/Fe(III) cofactor in the class Ic ribonucleotide reductase from Chlamydia trachomatis. 2013 , 52, 6424-36	32
1482	Molecular assembly of the aerolysin pore reveals a swirling membrane-insertion mechanism. 2013 , 9, 623-9	150
1481	Conservation of protein structure over four billion years. 2013 , 21, 1690-7	84
1480	Trapped intermediates in crystals of the FMN-dependent oxidase PhzG provide insight into the final steps of phenazine biosynthesis. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 1403-13	20
1479	Roles of the A and C sites in the manganese-specific activation of MntR. 2013 , 52, 701-13	27
1478	HASP server: a database and structural visualization platform for comparative models of influenza A hemagglutinin proteins. 2013 , 14, 197	4
1477	The UmuC subunit of the E. coli DNA polymerase V shows a unique interaction with the β -clamp processivity factor. 2013 , 13, 12	16
1476	Structural studies of several clinically important oncology drugs in complex with human serum albumin. 2013 , 1830, 5356-74	87
1475	Structural basis for the nuclear export activity of Importin13. 2013 , 32, 899-913	28

1474	Structural and functional insights on folate receptor (FR) by homology modeling, ligand docking and molecular dynamics. 2013 , 44, 197-207	19
1473	Defining the limits of homology modeling in information-driven protein docking. 2013 , 81, 2119-28	47
1472	The effects of cation adduction upon the conformation of three-helix bundle protein domains. 2013 , 16, 19-27	3
1471	X-Ray Crystallography of Biological Macromolecules: Fundamentals and Applications. 2013 , 1-22	0
1470	Identification of MDP (muramyl dipeptide)-binding key domains in NOD2 (nucleotide-binding and oligomerization domain-2) receptor of <i>Labeo rohita</i> . 2013 , 39, 1007-23	19
1469	Structural rearrangement in an RsmA/CsrA ortholog of <i>Pseudomonas aeruginosa</i> creates a dimeric RNA-binding protein, RsmN. 2013 , 21, 1659-71	54
1468	Structural rearrangement of ebola virus VP40 begets multiple functions in the virus life cycle. 2013 , 154, 763-74	155
1467	The yeast ski complex: crystal structure and RNA channeling to the exosome complex. 2013 , 154, 814-26	126
1466	New molecular interaction of IIA(Ntr) and HPr from <i>Burkholderia pseudomallei</i> identified by X-ray crystallography and docking studies. 2013 , 81, 1499-508	2
1465	Structural biology computing: Lessons for the biomedical research sciences. 2013 , 99, 809-16	6
1464	Concerted proton transfer mechanism of <i>Clostridium thermocellum</i> ribose-5-phosphate isomerase. 2013 , 117, 9354-61	8
1463	Nature-inspired design of motif-specific antibody scaffolds. 2013 , 31, 916-21	56
1462	Expression, purification and molecular modeling of the NIa protease of <i>Cardamom mosaic virus</i> . 2013 , 31, 602-11	3
1461	Improving the affinity and activity of CYP101D2 for hydrophobic substrates. 2013 , 97, 3979-90	13
1460	The human Aurora kinase inhibitor danusertib is a lead compound for anti-trypanosomal drug discovery via target repurposing. 2013 , 62, 777-84	39
1459	Structural basis for recognition of autophagic receptor NDP52 by the sugar receptor galectin-8. 2013 , 4, 1613	64
1458	Structural basis for regulation of human glucokinase by glucokinase regulatory protein. 2013 , 52, 6232-9	36
1457	Crystal-contact engineering to obtain a crystal form of the Kelch domain of human Keap1 suitable for ligand-soaking experiments. 2013 , 69, 592-6	22

1456	The toxicity of anti-prion antibodies is mediated by the flexible tail of the prion protein. 2013 , 501, 102-6	145
1455	A conserved asparagine has a structural role in ubiquitin-conjugating enzymes. 2013 , 9, 154-6	49
1454	Insights into the structure-function relationship of disease resistance protein HCTR in maize (<i>Zea mays</i> L.): a computational structural biology approach. 2013 , 45, 50-64	6
1453	Structural and functional analysis of the regulator of G protein signaling 2-g \bar{q} complex. 2013 , 21, 438-48	47
1452	A proteomic Ramachandran plot (PRplot). 2013 , 44, 781-90	12
1451	In silico discrimination of nsSNPs in hTERT gene by means of local DNA sequence context and regularity. 2013 , 19, 3517-27	6
1450	New pockets in dengue virus 2 surface identified by molecular dynamics simulation. 2013 , 19, 1369-77	8
1449	Vivaldi: visualization and validation of biomacromolecular NMR structures from the PDB. 2013 , 81, 583-91	12
1448	Crystal structure of the S187F variant of human liver alanine: glyoxylate [corrected] aminotransferase associated with primary hyperoxaluria type I and its functional implications. 2013 , 81, 1457-65	20
1447	Branched signal wiring of an essential bacterial cell-cycle phosphotransfer protein. 2013 , 21, 1590-601	17
1446	Structural and mechanistic studies of the orf12 gene product from the clavulanic acid biosynthesis pathway. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 1567-79	6
1445	Structural insight into the giant Ca ²⁺ -binding adhesin SiiE: implications for the adhesion of <i>Salmonella enterica</i> to polarized epithelial cells. 2013 , 21, 741-52	38
1444	Structural bases for a complete myotoxic mechanism: crystal structures of two non-catalytic phospholipases A2-like from <i>Bothrops brazili</i> venom. 2013 , 1834, 2772-81	27
1443	Structural, catalytic and stabilizing consequences of aromatic cluster variants in human carbonic anhydrase II. 2013 , 539, 31-7	6
1442	Structure of an atypical periplasmic adaptor from a multidrug efflux pump of the spirochete <i>Borrelia burgdorferi</i> . 2013 , 587, 2984-8	15
1441	Structural determinants of RGS-RhoGEF signaling critical to <i>Entamoeba histolytica</i> pathogenesis. 2013 , 21, 65-75	5
1440	Identification, characterization, and crystal structure of an aldo-keto reductase (AKR2E4) from the silkworm <i>Bombyx mori</i> . 2013 , 538, 156-63	12
1439	The structure of the neisserial lipooligosaccharide phosphoethanolamine transferase A (LptA) required for resistance to polymyxin. 2013 , 425, 3389-402	83

1438	Structural insights into recognition of MDC1 by TopBP1 in DNA replication checkpoint control. 2013 , 21, 1450-9	19
1437	Structure of a bifunctional alcohol dehydrogenase involved in bioethanol generation in <i>Geobacillus thermoglucosidasius</i> . <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 2104-15	24
1436	Crystal structures of copper-depleted and copper-bound fungal pro-tyrosinase: insights into endogenous cysteine-dependent copper incorporation. 2013 , 288, 22128-40	63
1435	The structure of the Fnl-EGF-like tandem domain of coagulation factor XII solved using SIRAS. 2013 , 69, 94-102	7
1434	Crystal structures of Sirt3 complexes with 4'-bromo-resveratrol reveal binding sites and inhibition mechanism. 2013 , 20, 1375-85	53
1433	Histone deacetylase (HDAC) inhibitor kinetic rate constants correlate with cellular histone acetylation but not transcription and cell viability. 2013 , 288, 26926-43	247
1432	Investigation into the feasibility of thioditaloside as a novel scaffold for galectin-3-specific inhibitors. 2013 , 14, 1331-42	29
1431	Understanding specificity of the mycosin proteases in ESX/type VII secretion by structural and functional analysis. 2013 , 184, 115-28	33
1430	Crystal structure of the effector protein XOO4466 from <i>Xanthomonas oryzae</i> . 2013 , 184, 361-6	4
1429	Crystal structure of apo and copper bound HP0894 toxin from <i>Helicobacter pylori</i> 26695 and insight into mRNase activity. 2013 , 1834, 2579-90	4
1428	New insights into the catalytic mechanism of <i>Bombyx mori</i> prostaglandin E synthase gained from structure-function analysis. 2013 , 440, 762-7	8
1427	Vinylogous chain branching catalysed by a dedicated polyketide synthase module. 2013 , 502, 124-8	93
1426	Structural evidence of a productive active site architecture for an evolved quorum-quenching GKL lactonase. 2013 , 52, 2359-70	11
1425	The c-di-GMP recognition mechanism of the PilZ domain of bacterial cellulose synthase subunit A. 2013 , 431, 802-7	36
1424	The exomer cargo adaptor features a flexible hinge domain. 2013 , 21, 486-92	7
1423	Exploitation of the catalytic site and 150 cavity for design of influenza A neuraminidase inhibitors. 2013 , 78, 10867-77	24
1422	Analysis of the structure of calpain-10 and its interaction with the protease inhibitor SNJ-1715. 2013 , 43, 1334-40	3
1421	Crystal structure of the 14-subunit RNA polymerase β . 2013 , 502, 644-9	140

1420	A report of 2 new cases of MODY2 and review of the literature: implications in the search for type 2 diabetes drugs. 2013 , 62, 1535-42	9
1419	High-resolution structure of TBP with TAF1 reveals anchoring patterns in transcriptional regulation. 2013 , 20, 1008-14	45
1418	New nucleotide-competitive non-nucleoside inhibitors of terminal deoxynucleotidyl transferase: discovery, characterization, and crystal structure in complex with the target. 2013 , 56, 7431-41	16
1417	Cytochrome p450sky interacts directly with the nonribosomal peptide synthetase to generate three amino acid precursors in skylamyacin biosynthesis. 2013 , 8, 2586-96	68
1416	Crystal structure of a soluble cleaved HIV-1 envelope trimer. 2013 , 342, 1477-83	687
1415	Structural basis of preferential binding of fucose-containing saccharide by the <i>Caenorhabditis elegans</i> galectin LEC-6. 2013 , 23, 797-805	11
1414	Isosteric and nonisosteric base pairs in RNA motifs: molecular dynamics and bioinformatics study of the sarcin-ricin internal loop. 2013 , 117, 14302-19	18
1413	Structural basis of ATG3 recognition by the autophagic ubiquitin-like protein ATG12. 2013 , 110, 18844-9	59
1412	Structural and functional studies with mytoxin II from <i>Bothrops moojeni</i> reveal remarkable similarities and differences compared to other catalytically inactive phospholipases A ₂ like. 2013 , 72, 52-63	22
1411	Crystal structure of the human eIF4AIII-CWC22 complex shows how a DEAD-box protein is inhibited by a MIF4G domain. 2013 , 110, E4611-8	31
1410	A unique and conserved neutralization epitope in H5N1 influenza viruses identified by an antibody against the A/Goose/Guangdong/1/96 hemagglutinin. 2013 , 87, 12619-35	40
1409	Diffraction and Scattering by X-Rays and Neutrons. 2013 , 91-112	
1408	Active glutaminase C self-assembles into a supratetrameric oligomer that can be disrupted by an allosteric inhibitor. 2013 , 288, 28009-20	55
1407	Structure of the polycomb group protein PCGF1 in complex with BCOR reveals basis for binding selectivity of PCGF homologs. 2013 , 21, 665-71	71
1406	Structure of the essential diversity-generating retroelement protein bAvd and its functionally important interaction with reverse transcriptase. 2013 , 21, 266-76	19
1405	Discovery of potent Mcl-1/Bcl-xL dual inhibitors by using a hybridization strategy based on structural analysis of target proteins. 2013 , 56, 9635-45	72
1404	Structural studies of the <i>Trypanosoma cruzi</i> Old Yellow Enzyme: insights into enzyme dynamics and specificity. 2013 , 184, 44-53	8
1403	Design, synthesis, biological and structural evaluation of functionalized resveratrol analogues as inhibitors of quinone reductase 2. 2013 , 21, 6022-37	15

1402	The E295K cancer variant of human polymerase β favors the mismatch conformational pathway during nucleotide selection. 2013 , 288, 34850-60	13
1401	Biochemical analysis and structure determination of bacterial acetyltransferases responsible for the biosynthesis of UDP-N,N'-diacetylbaicillosamine. 2013 , 288, 32248-32260	10
1400	Crystal structure of Schmallenberg orthobunyavirus nucleoprotein-RNA complex reveals a novel RNA sequestration mechanism. 2013 , 19, 1129-36	31
1399	The structure of yeast glutaminyl-tRNA synthetase and modeling of its interaction with tRNA. 2013 , 425, 2480-93	10
1398	Structural mechanism of ligand activation in human GABA(B) receptor. 2013 , 504, 254-9	132
1397	Antibody recognition of the pandemic H1N1 Influenza virus hemagglutinin receptor binding site. 2013 , 87, 12471-80	107
1396	Structures of P-glycoprotein reveal its conformational flexibility and an epitope on the nucleotide-binding domain. 2013 , 110, 13386-91	197
1395	Revealing nature's cellulase diversity: the digestion mechanism of <i>Caldicellulosiruptor bescii</i> CelA. 2013 , 342, 1513-6	221
1394	Structural basis for hijacking of cellular LxxLL motifs by papillomavirus E6 oncoproteins. 2013 , 339, 694-8	128
1393	Structural basis for action by diverse antidepressants on biogenic amine transporters. 2013 , 503, 141-5	112
1392	Structure of a photosynthetic reaction centre determined by serial femtosecond crystallography. 2013 , 4, 2911	74
1391	A photo-labile thioether linkage to phycoviolobin provides the foundation for the blue/green photocycles in DXCF-cyanobacteriochromes. 2013 , 21, 88-97	80
1390	Nucleotide and partner-protein control of bacterial replicative helicase structure and function. 2013 , 52, 844-54	37
1389	Architecture of the <i>Lsm1-7-Pat1</i> complex: a conserved assembly in eukaryotic mRNA turnover. 2013 , 5, 283-91	59
1388	Biochemical and structural characterisation of dehydroquinase synthase from the New Zealand kiwifruit <i>Actinidia chinensis</i> . 2013 , 537, 185-91	12
1387	Outer domain of HIV-1 gp120: antigenic optimization, structural malleability, and crystal structure with antibody VRC-PG04. 2013 , 87, 2294-306	32
1386	Structural basis for arabinosylo-oligosaccharide capture by the probiotic <i>Bifidobacterium animalis</i> subsp. <i>lactis</i> BI-04. 2013 , 90, 1100-12	48
1385	PepBind: a comprehensive database and computational tool for analysis of protein-peptide interactions. 2013 , 11, 241-6	43

1384	Enzymatic basis for N-glycan sialylation: structure of rat α 2,6-sialyltransferase (ST6GAL1) reveals conserved and unique features for glycan sialylation. 2013 , 288, 34680-98	85
1383	Crystal structure of the pilotin from the enterohemorrhagic Escherichia coli type II secretion system. 2013 , 182, 186-91	9
1382	Crystal structure of Pseudomonas aeruginosa transcriptional regulator PA2196 bound to its operator DNA. 2013 , 440, 317-21	3
1381	HIV-1 capsid undergoes coupled binding and isomerization by the nuclear pore protein NUP358. 2013 , 10, 81	76
1380	Crystal structure of AcrB complexed with linezolid at 3.5 Å resolution. 2013 , 14, 71-5	32
1379	Improved low-resolution crystallographic refinement with Phenix and Rosetta. 2013 , 10, 1102-4	137
1378	X-ray structure of dopamine transporter elucidates antidepressant mechanism. 2013 , 503, 85-90	448
1377	Molecular structure of β -amyloid fibrils in Alzheimer's disease brain tissue. 2013 , 154, 1257-68	808
1376	Effect of incorporating a thiophene tail in the scaffold of acetazolamide on the inhibition of human carbonic anhydrase isoforms I, II, IX and XII. 2013 , 23, 5646-9	17
1375	Molecular phylogeny, homology modeling, and molecular dynamics simulation of race-specific bacterial blight disease resistance protein (xa5) of rice: a comparative agriproteomics approach. 2013 , 17, 423-38	6
1374	Insights into the mechanism of pyrrole polymerization catalysed by porphobilinogen deaminase: high-resolution X-ray studies of the Arabidopsis thaliana enzyme. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 471-85	19
1373	Scientific benchmarks for guiding macromolecular energy function improvement. 2013 , 523, 109-43	164
1372	Protein structural statistics with PSS. 2013 , 53, 2471-82	10
1371	Protein modeling: what happened to the "protein structure gap"? 2013 , 21, 1531-40	89
1370	Solid-state NMR spectroscopy structure determination of a lipid-embedded heptahelical membrane protein. 2013 , 10, 1007-12	172
1369	Crystal structure of peroxisomal targeting signal-2 bound to its receptor complex Pex7p-Pex21p. 2013 , 20, 987-93	42
1368	Phylogenetic and structural studies of a novel equine papillomavirus identified from aural plaques. 2013 , 162, 85-93	12
1367	The crystal structure of an octapeptide repeat of the prion protein in complex with a Fab fragment of the POM2 antibody. 2013 , 22, 893-903	7

1366	Comparison of complexes formed by a crustacean and a vertebrate trypsin with bovine pancreatic trypsin inhibitor - the key to achieving extreme stability?. 2013 , 280, 5750-63	8
1365	Improved crystallographic structures using extensive combinatorial refinement. 2013 , 21, 1923-30	15
1364	Conservation and functional importance of carbon-oxygen hydrogen bonding in AdoMet-dependent methyltransferases. 2013 , 135, 15536-48	73
1363	Divergent evolution of protein conformational dynamics in dihydrofolate reductase. 2013 , 20, 1243-9	104
1362	Mechanistic insights from the binding of substrate and carbocation intermediate analogues to aristolochene synthase. 2013 , 52, 5441-53	44
1361	Structure-function studies of Escherichia coli RnIA reveal a novel toxin structure involved in bacteriophage resistance. 2013 , 90, 956-65	18
1360	The putative propeptide of MycP1 in mycobacterial type VII secretion system does not inhibit protease activity but improves protein stability. 2013 , 4, 921-31	9
1359	Crystal structure of the N-terminal domains of the surface cell antigen 4 of Rickettsia. 2013 , 22, 1425-31	4
1358	Structure of the uracil complex of Vaccinia virus uracil DNA glycosylase. 2013 , 69, 1328-34	6
1357	Structural analysis of the Rhizoctonia solani agglutinin reveals a domain-swapping dimeric assembly. 2013 , 280, 1750-63	16
1356	The tertiary structure of an i-type lysozyme isolated from the common orient clam (Meretrix lusoria). 2013 , 69, 1202-6	6
1355	Determining protein structures from NOESY distance constraints by semidefinite programming. 2013 , 20, 296-310	19
1354	The structural basis of ZMPSTE24-dependent laminopathies. 2013 , 339, 1604-7	75
1353	Structural characterization and biological properties of human gastrokine 1. 2013 , 9, 412-21	16
1352	Polarized Protein-Specific Charges from Atoms-in-Molecule Electron Density Partitioning. 2013 , 9, 2981-2991	28
1351	Structural and mechanistic characterization of L-histidinol phosphate phosphatase from the polymerase and histidinol phosphatase family of proteins. 2013 , 52, 1101-12	27
1350	Inhibition of the family 20 glycoside hydrolase catalytic modules in the Streptococcus pneumoniae exo-β-D-N-acetylglucosaminidase, StrH. 2013 , 11, 7907-15	9
1349	A novel role for coenzyme A during hydride transfer in 3-hydroxy-3-methylglutaryl-coenzyme A reductase. 2013 , 52, 5195-205	10

1348	A bacterial toxin catalyzing tyrosine glycosylation of Rho and deamidation of Gq and Gi proteins. 2013 , 20, 1273-80	48
1347	Structure and assembly of an inner membrane platform for initiation of type IV pilus biogenesis. 2013 , 110, E4638-47	46
1346	Structural and functional characterization of <i>Pseudomonas aeruginosa</i> AlgX: role of AlgX in alginate acetylation. 2013 , 288, 22299-314	37
1345	Structural basis for dsRNA recognition, filament formation, and antiviral signal activation by MDA5. 2013 , 152, 276-89	347
1344	Structural and functional analysis of JMJD2D reveals molecular basis for site-specific demethylation among JMJD2 demethylases. 2013 , 21, 98-108	55
1343	Synthesis, pharmacology, and biostructural characterization of novel $\alpha 7$ nicotinic acetylcholine receptor agonists. 2013 , 56, 940-51	15
1342	Structure of a VP1-VP3 complex suggests how birnaviruses package the VP1 polymerase. 2013 , 87, 3229-36	13
1341	CDR-H3 diversity is not required for antigen recognition by synthetic antibodies. 2013 , 425, 803-11	118
1340	Efficient firefly chemi/bioluminescence: evidence for chemiexcitation resulting from the decomposition of a neutral firefly dioxetanone molecule. 2013 , 117, 94-100	25
1339	Nonequivalence observed for the 16-meric structure of a small heat shock protein, SpHsp16.0, from <i>Schizosaccharomyces pombe</i> . 2013 , 21, 220-8	49
1338	Identification of a hidden strain switch provides clues to an ancient structural mechanism in protein kinases. 2013 , 110, 924-9	32
1337	Asymmetric structure and domain binding interfaces of human tyrosyl-tRNA synthetase studied by molecular dynamics simulations. 2013 , 26, 113-20	6
1336	Understanding Trends in the Electrocatalytic Activity of Metals and Enzymes for CO ₂ Reduction to CO. 2013 , 4, 388-92	485
1335	Structure of the human ATG12~ATG5 conjugate required for LC3 lipidation in autophagy. 2013 , 20, 59-66	265
1334	Protein Structure Refinement through Structure Selection and Averaging from Molecular Dynamics Ensembles. 2013 , 9, 1294-1303	75
1333	ATP-directed capture of bioactive herbal-based medicine on human tRNA synthetase. 2013 , 494, 121-4	110
1332	Crystal structure of the cowpox virus-encoded NKG2D ligand OMCP. 2013 , 87, 840-50	16
1331	Computational identification of a transiently open L1/S3 pocket for reactivation of mutant p53. 2013 , 4, 1407	148

1330	Crystal structure of the entire respiratory complex I. 2013 , 494, 443-8	571
1329	Point-to-point ligand-receptor interactions across the subunit interface modulate the induction and stabilization of conformational states of alpha7 nAChR by benzylidene anabaseines. 2013 , 85, 817-28	3
1328	Engineering allosteric control to an unregulated enzyme by transfer of a regulatory domain. 2013 , 110, 2111-6	40
1327	Optimized S-trityl-L-cysteine-based inhibitors of kinesin spindle protein with potent in vivo antitumor activity in lung cancer xenograft models. 2013 , 56, 1878-93	28
1326	Discovery of a chemical probe for the L3MBTL3 methyllysine reader domain. 2013 , 9, 184-91	129
1325	Studying and polishing the PDB's macromolecules. 2013 , 99, 170-82	9
1324	Structural insights into cofactor recognition of yeast mitochondria 3-oxoacyl-ACP reductase OAR1. 2013 , 65, 154-62	3
1323	CAD-score: a new contact area difference-based function for evaluation of protein structural models. 2013 , 81, 149-62	90
1322	Crystal structure of human multiple copies in T-cell lymphoma-1 oncoprotein. 2013 , 81, 519-25	9
1321	Crystal structure of 6-guanidinohexanoyl trypsin near the optimum pH reveals the acyl-enzyme intermediate to be deacylated. 2013 , 81, 526-30	4
1320	Structural analysis of the G-box domain of the microcephaly protein CPAP suggests a role in centriole architecture. 2013 , 21, 2069-77	59
1319	Structure and function of palladin's actin binding domain. 2013 , 425, 3325-37	18
1318	The crystal structure of novel chondroitin lyase ODV-E66, a baculovirus envelope protein. 2013 , 587, 3943	13
1317	Structural investigation of a viral ortholog of human NEIL2/3 DNA glycosylases. 2013 , 12, 1062-71	14
1316	Catalytic mechanism of stereospecific formation of cis-configured prenylated pyrroloindoline diketopiperazines by indole prenyltransferases. 2013 , 20, 1492-501	39
1315	Structural basis for recognizing phosphoarginine and evolving residue-specific protein phosphatases in gram-positive bacteria. 2013 , 3, 1832-9	37
1314	Structure of stem cell growth factor R-spondin 1 in complex with the ectodomain of its receptor LGR5. 2013 , 3, 1885-92	60
1313	Structure of a Ca(2+)/CaM:Kv7.4 (KCNQ4) B-helix complex provides insight into M current modulation. 2013 , 425, 378-94	38

1312	Catalytic site conformations in human PNP by 19F-NMR and crystallography. 2013 , 20, 212-22	11
1311	Structural insights into the mechanism and inhibition of the α -hydroxydecanoyl-acyl carrier protein dehydratase from <i>Pseudomonas aeruginosa</i> . 2013 , 425, 365-77	26
1310	Three-dimensional structure of a <i>Bombyx mori</i> Omega-class glutathione transferase. 2013 , 438, 588-93	15
1309	Structural study of the location of the phenyl tail of benzene sulfonamides and the effect on human carbonic anhydrase inhibition. 2013 , 21, 6674-80	12
1308	Crystallographic model validation: from diagnosis to healing. 2013 , 23, 707-14	12
1307	The crystal structure of the luminal domain of Erv41p, a protein involved in transport between the endoplasmic reticulum and Golgi apparatus. 2013 , 425, 2208-18	9
1306	Structural and kinetic characterization of two 4-oxalocrotonate tautomerase in <i>Methylobium petroleiphilum</i> strain PM1. 2013 , 537, 113-24	1
1305	Structural basis for cell-cycle-dependent nuclear import mediated by the karyopherin Kap121p. 2013 , 425, 1852-1868	35
1304	Development of RNA aptamers targeting Ebola virus VP35. 2013 , 52, 8406-19	61
1303	Structures of human sirtuin 3 complexes with ADP-ribose and with carba-NAD ⁺ and SRT1720: binding details and inhibition mechanism. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 1423-32	43
1302	Crystal structure of Na ⁺ , K ⁽⁺⁾ -ATPase in the Na ⁽⁺⁾ -bound state. 2013 , 342, 123-7	135
1301	Structural basis for effector control and redox partner recognition in cytochrome P450. 2013 , 340, 1227-30	138
1300	Structure of the type IVa major pilin from the electrically conductive bacterial nanowires of <i>Geobacter sulfurreducens</i> . 2013 , 288, 29260-6	86
1299	Zinc co-ordination by the DHHC cysteine-rich domain of the palmitoyltransferase Swf1. 2013 , 454, 427-35	25
1298	Structural studies on the forward and reverse binding modes of peptides to the chaperone DnaK. 2013 , 425, 2463-79	84
1297	iMODFIT: efficient and robust flexible fitting based on vibrational analysis in internal coordinates. 2013 , 184, 261-70	127
1296	Structures of intermediates along the catalytic cycle of terminal deoxynucleotidyltransferase: dynamical aspects of the two-metal ion mechanism. 2013 , 425, 4334-52	31
1295	Structural determinants of oligomerization of α (1)-pyrroline-5-carboxylate dehydrogenase: identification of a hexamerization hot spot. 2013 , 425, 3106-20	19

1294	Conformational plasticity at the IgE-binding site of the B-cell receptor CD23. 2013 , 56, 693-7	13
1293	Crystal structure of 2A proteinase from hand, foot and mouth disease virus. 2013 , 425, 4530-43	19
1292	Evolutionary variation and adaptation in a conserved protein kinase allosteric network: implications for inhibitor design. 2013 , 1834, 1322-9	7
1291	Crystal structure of the response regulator spr1814 from <i>Streptococcus pneumoniae</i> reveals unique interdomain contacts among NarL family proteins. 2013 , 434, 65-9	12
1290	CtpB assembles a gated protease tunnel regulating cell-cell signaling during spore formation in <i>Bacillus subtilis</i> . 2013 , 155, 647-58	21
1289	Three sites and you are out: ternary synergistic allostery controls aromatic amino acid biosynthesis in <i>Mycobacterium tuberculosis</i> . 2013 , 425, 1582-92	30
1288	<i>Salmonella enterica</i> MTAN at 1.36 Å resolution: a structure-based design of tailored transition state analogs. 2013 , 21, 963-74	16
1287	Estimating structure quality trends in the Protein Data Bank by equivalent resolution. 2013 , 46, 8-15	11
1286	Quality assessment of protein NMR structures. 2013 , 23, 715-24	20
1285	Crystal structure of human angiogenin with an engineered loop exhibits conformational flexibility at the functional regions of the molecule. 2013 , 3, 65-70	7
1284	Structural insights into the functional role of the Hcn sub-domain of the receptor-binding domain of the botulinum neurotoxin mosaic serotype C/D. 2013 , 95, 1379-85	7
1283	Arranged sevenfold: structural insights into the C-terminal oligomerization domain of human C4b-binding protein. 2013 , 425, 1302-17	54
1282	Crystal structure of a <i>Bombyx mori</i> sigma-class glutathione transferase exhibiting prostaglandin E synthase activity. 2013 , 1830, 3711-8	16
1281	Structure-guided studies of the SHP-1/JAK1 interaction provide new insights into phosphatase catalytic domain substrate recognition. 2013 , 181, 243-51	8
1280	Crystal structure at 1.5 Å resolution of the PsbV2 cytochrome from the cyanobacterium <i>Thermosynechococcus elongatus</i> . 2013 , 587, 3267-72	11
1279	Isolation and characterization of β -conotoxin Ls1A with potent activity at nicotinic acetylcholine receptors. 2013 , 86, 791-9	42
1278	Redox state-dependent changes in the crystal structure of [NiFeSe] hydrogenase from <i>Desulfobivrio vulgaris</i> Hildenborough. 2013 , 38, 8664-8682	31
1277	Nonspecific recognition is achieved in Pot1pC through the use of multiple binding modes. 2013 , 21, 121-132	23

1276	The local dinucleotide preference of APOBEC3G can be altered from 5'-CC to 5'-TC by a single amino acid substitution. 2013 , 425, 4442-54	64
1275	Kinetic mechanism and energetics of binding of phosphoryl group acceptors to Mycobacterium tuberculosis cytidine monophosphate kinase. 2013 , 536, 53-63	1
1274	Recommendations of the wwPDB NMR Validation Task Force. 2013 , 21, 1563-70	117
1273	A 2.1-Å resolution crystal structure of unliganded CRM1 reveals the mechanism of autoinhibition. 2013 , 425, 350-64	25
1272	Key residues at the riboflavin kinase catalytic site of the bifunctional riboflavin kinase/FMN adenylyltransferase from <i>Corynebacterium ammoniagenes</i> . 2013 , 65, 57-68	16
1271	The structure of a novel glucuronoyl esterase from <i>Myceliophthora thermophila</i> gives new insights into its role as a potential biocatalyst. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 63-73	29
1270	Structure and ligand-binding properties of the biogenic amine-binding protein from the saliva of a blood-feeding insect vector of <i>Trypanosoma cruzi</i> . <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 105-13	15
1269	Adenosine kinase from <i>Schistosoma mansoni</i> : structural basis for the differential incorporation of nucleoside analogues. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 126-36	12
1268	The AEROPATH project targeting <i>Pseudomonas aeruginosa</i> : crystallographic studies for assessment of potential targets in early-stage drug discovery. 2013 , 69, 25-34	28
1267	Exploring the cross-reactivity of S25-2: complex with a 5,6-dehydro-Kdo disaccharide. 2013 , 69, 2-5	5
1266	Use of europium ions for SAD phasing of lysozyme at the Cu K α wavelength. 2013 , 69, 20-4	
1265	High-resolution cryo-electron microscopy structure of the <i>Trypanosoma brucei</i> ribosome. 2013 , 494, 385-9	102
1264	Structural and functional analysis of the pro-domain of human cathelicidin, LL-37. 2013 , 52, 1547-58	27
1263	Stereochemical determinants of C-terminal specificity in PDZ peptide-binding domains: a novel contribution of the carboxylate-binding loop. 2013 , 288, 5114-26	22
1262	A unique Oct4 interface is crucial for reprogramming to pluripotency. 2013 , 15, 295-301	109
1261	Molecular basis for manganese sequestration by calprotectin and roles in the innate immune response to invading bacterial pathogens. 2013 , 110, 3841-6	245
1260	Structure, dynamics, evolution, and function of a major scaffold component in the nuclear pore complex. 2013 , 21, 560-71	48
1259	Advances, interactions, and future developments in the CNS, Phenix, and Rosetta structural biology software systems. 2013 , 42, 265-87	76

1258	A structure-based strategy for epitope discovery in Burkholderia pseudomallei OppA antigen. 2013 , 21, 167-175	37
1257	Structural effect of phenyl ring compared to thiazazole based adamantyl-sulfonamides on carbonic anhydrase inhibition. 2013 , 21, 2314-2318	19
1256	Crystal structures of the catalytic domain of human soluble guanylate cyclase. 2013 , 8, e57644	71
1255	Structure of the full-length HCV IRES in solution. 2013 , 4, 1612	63
1254	Structural and functional studies of the 252 kDa nucleoporin ELYS reveal distinct roles for its three tethered domains. 2013 , 21, 572-80	30
1253	One target-two different binding modes: structural insights into gevokizumab and canakinumab interactions to interleukin-1 β 2013 , 425, 94-111	62
1252	Liesegang-like patterns of Toll crystals grown in gel. 2013 , 46, 337-345	2
1251	Conservation and variability in the structure and function of the Cas5d endoribonuclease in the CRISPR-mediated microbial immune system. 2013 , 425, 3799-810	27
1250	The impact of introducing a histidine into an apolar cavity site on docking and ligand recognition. 2013 , 56, 2874-84	7
1249	Doing molecular biophysics: finding, naming, and picturing signal within complexity. 2013 , 42, 1-28	17
1248	Anions mediate ligand binding in Adineta vaga glutamate receptor ion channels. 2013 , 21, 414-25	12
1247	Allosteric inhibition of hypoxia inducible factor-2 with small molecules. 2013 , 9, 271-6	196
1246	Structure of LdtMt2, an L,D-transpeptidase from Mycobacterium tuberculosis. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 432-41	26
1245	Cyclization of the antimicrobial peptide gomesin with native chemical ligation: influences on stability and bioactivity. 2013 , 14, 617-24	47
1244	Structural basis for the inhibition of Mycobacterium tuberculosis L,D-transpeptidase by meropenem, a drug effective against extensively drug-resistant strains. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 420-31	53
1243	Loss-of-function mutations in the IL-21 receptor gene cause a primary immunodeficiency syndrome. 2013 , 210, 433-43	156
1242	Exploiting an allosteric binding site of PRMT3 yields potent and selective inhibitors. 2013 , 56, 2110-24	58
1241	Design of chimeric proteins by combination of subdomain-sized fragments. 2013 , 523, 389-405	7

1240	Single amino acid exchange in bacteriophage HK620 tailspike protein results in thousand-fold increase of its oligosaccharide affinity. 2013 , 23, 59-68	14
1239	Molecular mechanism by which a potent hepatitis C virus NS3-NS4A protease inhibitor overcomes emergence of resistance. 2013 , 288, 5673-81	14
1238	Intrinsic evolutionary constraints on protease structure, enzyme acylation, and the identity of the catalytic triad. 2013 , 110, E653-61	93
1237	Dimer asymmetry defines β -catenin interactions. 2013 , 20, 188-93	84
1236	A homology modeling study toward the understanding of three-dimensional structure and putative pharmacological profile of the G-protein coupled receptor GPR55. 2013 , 39, 50-60	21
1235	Crystal structure analysis of human Sirt2 and its ADP-ribose complex. 2013 , 182, 136-43	77
1234	Crystal structure of Prp8 reveals active site cavity of the spliceosome. 2013 , 493, 638-43	160
1233	Crystal structure and catalytic mechanism of chloromuconolactone dehalogenase ClcF from <i>Rhodococcus opacus</i> 1CP. 2013 , 88, 254-67	3
1232	Structures of protein-protein complexes involved in electron transfer. 2013 , 496, 123-6	54
1231	Solution structure, dynamics and binding studies of a family 11 carbohydrate-binding module from <i>Clostridium thermocellum</i> (CtCBM11). 2013 , 451, 289-300	15
1230	Structure of the <i>Trypanosoma cruzi</i> protein tyrosine phosphatase TcPTP1, a potential therapeutic target for Chagas' disease. 2013 , 187, 1-8	7
1229	A new protein complex promoting the assembly of Rad51 filaments. 2013 , 4, 1676	70
1228	Mutations in WNT1 cause different forms of bone fragility. 2013 , 92, 565-74	197
1227	Structural basis for the drug extrusion mechanism by a MATE multidrug transporter. 2013 , 496, 247-51	193
1226	Structure of <i>Vibrio cholerae</i> ribosome hibernation promoting factor. 2013 , 69, 228-36	8
1225	Structure of the cytoplasmic domain of TcpE, the inner membrane core protein required for assembly of the <i>Vibrio cholerae</i> toxin-coregulated pilus. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 513-9	8
1224	Structure of the NLRP1 caspase recruitment domain suggests potential mechanisms for its association with procaspase-1. 2013 , 81, 1266-70	49
1223	Gating of the TrkH ion channel by its associated RCK protein TrkA. 2013 , 496, 317-22	61

1222	Cryo-EM model validation using independent map reconstructions. 2013 , 22, 865-8	64
1221	The role of structural bioinformatics resources in the era of integrative structural biology. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 710-21	14
1220	A family of macrodomain proteins reverses cellular mono-ADP-ribosylation. 2013 , 20, 508-14	226
1219	Structure of active β -arrestin-1 bound to a G-protein-coupled receptor phosphopeptide. 2013 , 497, 137-41	310
1218	Crystal structure of a eukaryotic phosphate transporter. 2013 , 496, 533-6	170
1217	Staufen1 dimerizes through a conserved motif and a degenerate dsRNA-binding domain to promote mRNA decay. 2013 , 20, 515-24	45
1216	Structural basis of kynurenine 3-monooxygenase inhibition. 2013 , 496, 382-5	90
1215	Nucleotide binding and conformational switching in the hexameric ring of a AAA+ machine. 2013 , 153, 628-39	91
1214	Structures of complexes comprised of Fischerella transcription factor HetR with Anabaena DNA targets. 2013 , 110, E1716-23	20
1213	Structural and biochemical characterisation of a NAD ⁺ -dependent alcohol dehydrogenase from <i>Oenococcus oeni</i> as a new model molecule for industrial biotechnology applications. 2013 , 97, 8963-75	23
1212	Design of a single-chain polypeptide tetrahedron assembled from coiled-coil segments. 2013 , 9, 362-6	224
1211	X-ray Crystallography. 2013 , 217-255	4
1210	Thermodynamic computational approach to capture molecular recognition in the binding of different inhibitors to the DNA gyrase B subunit from <i>Escherichia coli</i> . 2013 , 19, 3187-200	2
1209	Structure of the human smoothed receptor bound to an antitumour agent. 2013 , 497, 338-43	375
1208	Structural and functional characterization of ScsC, a periplasmic thioredoxin-like protein from <i>Salmonella enterica</i> serovar Typhimurium. 2013 , 19, 1494-506	21
1207	Crystal structure analysis of L-fucose-1-phosphate aldolase from <i>Thermus thermophilus</i> HB8 and its catalytic action: as explained through in silico. 2013 , 14, 59-70	2
1206	Structure-function analyses of the human SIX1-EYA2 complex reveal insights into metastasis and BOR syndrome. 2013 , 20, 447-53	68
1205	Structure of mycobacterial β -oxidation trifunctional enzyme reveals its altered assembly and putative substrate channeling pathway. 2013 , 8, 1063-73	24

1204	X-ray crystal structure of ERK5 (MAPK7) in complex with a specific inhibitor. 2013 , 56, 4413-21	27
1203	Structural basis for potentiation by alcohols and anaesthetics in a ligand-gated ion channel. 2013 , 4, 1697	116
1202	Crystal structures of Plasmodium falciparum cytosolic tryptophanyl-tRNA synthetase and its potential as a target for structure-guided drug design. 2013 , 189, 26-32	21
1201	Antigenic switching of hepatitis B virus by alternative dimerization of the capsid protein. 2013 , 21, 133-142	47
1200	Studying protein-ligand interactions using X-ray crystallography. 2013 , 1008, 457-77	7
1199	Stabilization of an unusual salt bridge in ubiquitin by the extra C-terminal domain of the proteasome-associated deubiquitinase UCH37 as a mechanism of its exo specificity. 2013 , 52, 3564-78	19
1198	Structural and functional characterization of MppR, an enduracididine biosynthetic enzyme from streptomyces hygroscopicus: functional diversity in the acetoacetate decarboxylase-like superfamily. 2013 , 52, 4492-506	20
1197	Structure of a human IgA1 Fab fragment at 1.55 Å resolution: potential effect of the constant domains on antigen-affinity modulation. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 388-97	20
1196	Bromo-deaza-SAH: a potent and selective DOT1L inhibitor. 2013 , 21, 1787-1794	54
1195	structural Studies of Wnts and identification of an LRP6 binding site. 2013 , 21, 1235-42	60
1194	Investigating the active centre of the Scytalidium thermophilum catalase. 2013 , 69, 369-75	2
1193	Structure, recombinant expression and mutagenesis studies of the catalase with oxidase activity from Scytalidium thermophilum. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 398-408	7
1192	Structural and thermodynamic basis of (+)- α -pinene binding to human cytochrome P450 2B6. 2013 , 135, 10433-40	30
1191	Allosteric opening of the polypeptide-binding site when an Hsp70 binds ATP. 2013 , 20, 900-7	182
1190	The human ITPA polymorphic variant P32T is destabilized by the unpacking of the hydrophobic core. 2013 , 182, 197-208	12
1189	Computational methods for controlling binding specificity. 2013 , 523, 41-59	18
1188	Protein kinase inhibitor design by targeting the Asp-Phe-Gly (DFG) motif: the role of the DFG motif in the design of epidermal growth factor receptor inhibitors. 2013 , 56, 3889-903	63
1187	Reversal of the substrate specificity of CMP N-glycosidase to dCMP. 2013 , 52, 4037-47	13

1186	Bacteriophage P23-77 capsid protein structures reveal the archetype of an ancient branch from a major virus lineage. 2013 , 21, 718-26	34
1185	Corrected small basis set Hartree-Fock method for large systems. 2013 , 34, 1672-85	276
1184	Structure of a double-stranded DNA (6-4) photoproduct in complex with the 64M-5 antibody Fab. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 504-12	8
1183	Eukaryotic GPN-loop GTPases paralogs use a dimeric assembly reminiscent of archeal GPN. 2013 , 12, 463-72	17
1182	X-ray structure of the mammalian GIRK2- β 1G-protein complex. 2013 , 498, 190-7	218
1181	Rif1 and Rif2 shape telomere function and architecture through multivalent Rap1 interactions. 2013 , 153, 1340-53	77
1180	Crystallization and preliminary structural analysis of dibenzothiophene monooxygenase (DszC) from <i>Rhodococcus erythropolis</i> . 2013 , 69, 597-601	11
1179	Structure of starch synthase I from barley: insight into regulatory mechanisms of starch synthase activity. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 1013-25	33
1178	Reshaping antibody diversity. 2013 , 153, 1379-93	138
1177	Structural mimicry in transcription regulation of human RNA polymerase II by the DNA helicase RECQL5. 2013 , 20, 892-9	25
1176	Assembly of a β 3 stack of ligands in the binding site of an acetylcholine-binding protein. 2013 , 4, 1875	43
1175	novel modifications on C-terminal domain of RNA polymerase II can fine-tune the phosphatase activity of Ssu72. 2013 , 8, 2042-52	23
1174	Structural insights into DNA replication without hydrogen bonds. 2013 , 135, 18637-43	63
1173	Ex-527 inhibits Sirtuins by exploiting their unique NAD ⁺ -dependent deacetylation mechanism. 2013 , 110, E2772-81	202
1172	Crystal and solution studies of the "Plus-C" odorant-binding protein 48 from <i>Anopheles gambiae</i> : control of binding specificity through three-dimensional domain swapping. 2013 , 288, 33427-38	29
1171	Filling out the structural map of the NTF2-like superfamily. 2013 , 14, 327	40
1170	Metal binding properties of <i>Escherichia coli</i> YjiA, a member of the metal homeostasis-associated COG0523 family of GTPases. 2013 , 52, 1788-1801	37
1169	Structures of the class D Carbapenemases OXA-23 and OXA-146: mechanistic basis of activity against carbapenems, extended-spectrum cephalosporins, and aztreonam. 2013 , 57, 4848-55	57

1168	Isolating influential regions of electrostatic focusing in protein and DNA structure. 2013 , 10, 1188-98	2
1167	Converting NAD-specific inositol dehydrogenase to an efficient NADP-selective catalyst, with a surprising twist. 2013 , 52, 5876-83	12
1166	Structural analysis and molecular dynamics simulations of novel β -endotoxin Cry1Id from <i>Bacillus thuringiensis</i> to pave the way for development of novel fusion proteins against insect pests of crops. 2013 , 19, 5301-16	8
1165	Selective detection of caspase-3 versus caspase-7 using activity-based probes with key unnatural amino acids. 2013 , 8, 1558-66	40
1164	Crystal structures of vertebrate dihydropyrimidinase and complexes from <i>Tetraodon nigroviridis</i> with lysine carbamylation: metal and structural requirements for post-translational modification and function. 2013 , 288, 30645-30658	18
1163	Structure and assembly of the NOT module of the human CCR4-NOT complex. 2013 , 20, 1289-97	74
1162	High-resolution structure of an atypical β -phosphoglucomutase related to eukaryotic phosphomannomutases. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 2008-16	4
1161	X-ray Crystallography Reveals How Subtle Changes Control the Orientation of Substrate Binding in an Alkene Reductase. 2013 , 3, 2376-2390	33
1160	Structure of isochorismate synthase Dhbc from <i>Bacillus anthracis</i> . 2013 , 69, 956-61	
1159	Autoinhibition and phosphorylation-induced activation of phospholipase C- β isozymes. 2013 , 52, 4810-9	22
1158	Lipoamide channel-binding sulfonamides selectively inhibit mycobacterial lipoamide dehydrogenase. 2013 , 52, 9375-84	14
1157	Energetic coupling between an oxidizable cysteine and the phosphorylatable N-terminus of human liver pyruvate kinase. 2013 , 52, 466-76	27
1156	Functional insights from the crystal structure of the N-terminal domain of the prototypical toll receptor. 2013 , 21, 143-153	11
1155	Subangstrom resolution X-ray structure details aquaporin-water interactions. 2013 , 340, 1346-1349	147
1154	Simulative and experimental investigation on the cleavage site that generates the soluble human LOX-1. 2013 , 540, 9-18	14
1153	The structure of Rv3717 reveals a novel amidase from <i>Mycobacterium tuberculosis</i> . <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 2543-54	22
1152	Phosphorylation adjacent to the nuclear localization signal of human dUTPase abolishes nuclear import: structural and mechanistic insights. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 2495-505	26
1151	X-ray crystal structure of bovine 3 Glu-osteocalcin. 2013 , 52, 8387-92	19

1150	Specificity of Processing β -glucosidase I is guided by the substrate conformation: crystallographic and in silico studies. 2013 , 288, 13563-74	47
1149	Structure of the homodimeric glycine decarboxylase P-protein from <i>Synechocystis</i> sp. PCC 6803 suggests a mechanism for redox regulation. 2013 , 288, 35333-45	27
1148	Coiled-coil dimerization of the LOV2 domain of the blue-light photoreceptor phototropin 1 from <i>Arabidopsis thaliana</i> . 2013 , 69, 1316-21	29
1147	Structure and enzymatic mechanism of a moonlighting dUTPase. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 2298-308	20
1146	Mechanism of displacement of a catalytically essential loop from the active site of mammalian fructose-1,6-bisphosphatase. 2013 , 52, 5206-16	4
1145	Conformational plasticity and ligand binding of bacterial monoacylglycerol lipase. 2013 , 288, 31093-104	30
1144	Identification, structure, and function of a novel type VI secretion peptidoglycan glycoside hydrolase effector-immunity pair. 2013 , 288, 26616-24	74
1143	The influence of heme ruffling on spin densities in ferricytochromes c probed by heme core 13C NMR. 2013 , 52, 12933-46	20
1142	Plant multifunctional nuclease TBN1 with unexpected phospholipase activity: structural study and reaction-mechanism analysis. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 213-26	11
1141	Structure of a <i>Clostridium botulinum</i> C143S thiaminase I/thiamin complex reveals active site architecture. 2013 , 52, 7830-9	6
1140	Structural analysis of the positive AMPA receptor modulators CX516 and Me-CX516 in complex with the GluA2 ligand-binding domain. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 1645-52	8
1139	Structural insights into the South African HIV-1 subtype C protease: impact of hinge region dynamics and flap flexibility in drug resistance. 2013 , 31, 1370-80	29
1138	Nonconserved active site residues modulate CheY autophosphorylation kinetics and phosphodonor preference. 2013 , 52, 2262-73	23
1137	Mechanistic characterization of the tetraacyldisaccharide-1-phosphate 4'-kinase LpxK involved in lipid A biosynthesis. 2013 , 52, 2280-90	6
1136	3Drefine: consistent protein structure refinement by optimizing hydrogen bonding network and atomic-level energy minimization. 2013 , 81, 119-31	119
1135	Crystal structure of putative CbiT from <i>Methanocaldococcus jannaschii</i> : an intermediate enzyme activity in cobalamin (vitamin B12) biosynthesis. 2013 , 13, 10	
1134	Contactin 4, -5 and -6 differentially regulate neuritogenesis while they display identical PTPRG binding sites. 2013 , 2, 324-34	31
1133	The molecular recognition of kink-turn structure by the L7Ae class of proteins. 2013 , 19, 1703-10	45

1132	An essential serotype recognition pocket on phage P22 tailspike protein forces Salmonella enterica serovar Paratyphi A O-antigen fragments to bind as nonsolution conformers. 2013 , 23, 486-94	12
1131	Evidence for an ABC-type riboflavin transporter system in pathogenic spirochetes. 2013 , 4, e00615-12	33
1130	Crystal structure of 3WJ core revealing divalent ion-promoted thermostability and assembly of the Phi29 hexameric motor pRNA. 2013 , 19, 1226-37	90
1129	Insights into the structure and assembly of the Bacillus subtilis clamp-loader complex and its interaction with the replicative helicase. 2013 , 41, 5115-26	10
1128	Protein Structure Refinement by Iterative Fragment Exchange. 2013 ,	2
1127	Bapineuzumab captures the N-terminus of the Alzheimer's disease amyloid-beta peptide in a helical conformation. 2013 , 3, 1302	78
1126	The Geminin and Idas coiled coils preferentially form a heterodimer that inhibits Geminin function in DNA replication licensing. 2013 , 288, 31624-34	18
1125	Structural characterization of the mechanism through which human glutamic acid decarboxylase auto-activates. 2013 , 33, 137-44	10
1124	Structural insights into the inhibition of typeVI effector Tae3 by its immunity protein Tai3. 2013 , 454, 59-68	23
1123	Functional evolution of scorpion venom peptides with an inhibitor cystine knot fold. 2013 , 33,	38
1122	Assembly of the type II secretion system such as found in Vibrio cholerae depends on the novel Pilotin AspS. 2013 , 9, e1003117	50
1121	Biochemical characterization of Plasmodium falciparum CTP:phosphoethanolamine cytidyltransferase shows that only one of the two cytidyltransferase domains is active. 2013 , 450, 159-67	9
1120	Crystal structure of the gamma-2 herpesvirus LANA DNA binding domain identifies charged surface residues which impact viral latency. 2013 , 9, e1003673	25
1119	A structural basis for IB kinase 2 activation via oligomerization-dependent trans auto-phosphorylation. 2013 , 11, e1001581	73
1118	Elucidation of novel structural scaffold in rohu TLR2 and its binding site analysis with peptidoglycan, lipoteichoic acid and zymosan ligands, and downstream MyD88 adaptor protein. 2013 , 2013, 185282	14
1117	Tubulin tyrosine nitration regulates microtubule organization in plant cells. 2013 , 4, 530	27
1116	Structure of a bimodular botulinum neurotoxin complex provides insights into its oral toxicity. 2013 , 9, e1003690	81
1115	TRAF4 is a novel phosphoinositide-binding protein modulating tight junctions and favoring cell migration. 2013 , 11, e1001726	31

1114	Non-peptidic cruzain inhibitors with trypanocidal activity discovered by virtual screening and in vitro assay. 2013 , 7, e2370	54
1113	In silico identification of a candidate synthetic peptide (Tsgf118-43) to monitor human exposure to tsetse flies in West Africa. 2013 , 7, e2455	15
1112	Peptide-binding dependent conformational changes regulate the transcriptional activity of the quorum-sensor NprR. 2013 , 41, 7920-33	43
1111	Structural basis for the MukB-topoisomerase IV interaction and its functional implications in vivo. 2013 , 32, 2950-62	22
1110	Crystal structures of S6K1 provide insights into the regulation mechanism of S6K1 by the hydrophobic motif. 2013 , 454, 39-47	17
1109	Syntaxin binding mechanism and disease-causing mutations in Munc18-2. 2013 , 110, E4482-91	58
1108	Mimicking of estradiol binding by flame retardants and their metabolites: a crystallographic analysis. 2013 , 121, 1194-9	71
1107	Structure of the parainfluenza virus 5 (PIV5) hemagglutinin-neuraminidase (HN) ectodomain. 2013 , 9, e1003534	55
1106	Cantharidin Impedes Activity of Glutathione S-Transferase in the Midgut of <i>Helicoverpa armigera</i> HBner. 2013 , 14, 5482-500	16
1105	The velvet family of fungal regulators contains a DNA-binding domain structurally similar to NF- κ B. 2013 , 11, e1001750	99
1104	Exploring the <i>Trypanosoma brucei</i> Hsp83 potential as a target for structure guided drug design. 2013 , 7, e2492	25
1103	New world bats harbor diverse influenza A viruses. 2013 , 9, e1003657	825
1102	Small-molecule inhibition of MLL activity by disruption of its interaction with WDR5. 2013 , 449, 151-9	100
1101	Structure of a dimeric crenarchaeal Cas6 enzyme with an atypical active site for CRISPR RNA processing. 2013 , 452, 223-30	29
1100	Gain-of-sensitivity mutations in a Trim5-resistant primary isolate of pathogenic SIV identify two independent conserved determinants of Trim5 specificity. 2013 , 9, e1003352	25
1099	Crystal structure of vaccinia viral A27 protein reveals a novel structure critical for its function and complex formation with A26 protein. 2013 , 9, e1003563	23
1098	Structure of UreG/UreF/UreH complex reveals how urease accessory proteins facilitate maturation of <i>Helicobacter pylori</i> urease. 2013 , 11, e1001678	74
1097	Structural characterization of H-1 parvovirus: comparison of infectious virions to empty capsids. 2013 , 87, 5128-40	23

1096	Heteroresistance to fosfomycin is predominant in <i>Streptococcus pneumoniae</i> and depends on the <i>murA1</i> gene. 2013 , 57, 2801-8	19
1095	Structure of Schmallenberg orthobunyavirus nucleoprotein suggests a novel mechanism of genome encapsidation. 2013 , 87, 5593-601	40
1094	Using stable MutS dimers and tetramers to quantitatively analyze DNA mismatch recognition and sliding clamp formation. 2013 , 41, 8166-81	26
1093	The TP0796 lipoprotein of <i>Treponema pallidum</i> is a bimetal-dependent FAD pyrophosphatase with a potential role in flavin homeostasis. 2013 , 288, 11106-21	21
1092	Structural basis for Cul3 protein assembly with the BTB-Kelch family of E3 ubiquitin ligases. 2013 , 288, 7803-7814	169
1091	1.2 Å resolution crystal structure of <i>Escherichia coli</i> WrbA holoprotein. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 1748-57	5
1090	N-terminal acetylation of the yeast Derlin Der1 is essential for Hrd1 ubiquitin-ligase activity toward luminal ER substrates. 2013 , 24, 890-900	32
1089	A novel family of soluble minimal scaffolds provides structural insight into the catalytic domains of integral membrane metallopeptidases. 2013 , 288, 21279-21294	26
1088	The crystal structure of the protein-disulfide isomerase family member ERp27 provides insights into its substrate binding capabilities. 2013 , 288, 2029-39	17
1087	The sequence and structure of snake gourd (<i>Trichosanthes anguina</i>) seed lectin, a three-chain nontoxic homologue of type II RIPs. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 1493-503	15
1086	GalaxyRefine: Protein structure refinement driven by side-chain repacking. 2013 , 41, W384-8	403
1085	Specificity determinants for lysine incorporation in <i>Staphylococcus aureus</i> peptidoglycan as revealed by the structure of a MurE enzyme ternary complex. 2013 , 288, 33439-48	23
1084	Rv2969c, essential for optimal growth in <i>Mycobacterium tuberculosis</i> , is a DsbA-like enzyme that interacts with VKOR-derived peptides and has atypical features of DsbA-like disulfide oxidases. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 1981-94	26
1083	RNase H2 roles in genome integrity revealed by unlinking its activities. 2013 , 41, 3130-43	103
1082	Structure and properties of the esterase from non-LTR retrotransposons suggest a role for lipids in retrotransposition. 2013 , 41, 10563-72	9
1081	The structure of the CS1 pilus of enterotoxigenic <i>Escherichia coli</i> reveals structural polymorphism. 2013 , 195, 1360-70	15
1080	Structural complexity of Dengue virus untranslated regions: cis-acting RNA motifs and pseudoknot interactions modulating functionality of the viral genome. 2013 , 41, 5075-89	43
1079	The BAH domain of Rsc2 is a histone H3 binding domain. 2013 , 41, 9168-82	22

1078	Structure of formaldehyde dehydrogenase from <i>Pseudomonas aeruginosa</i> : the binary complex with the cofactor NAD ⁺ . 2013 , 69, 967-72	6
1077	Reorganization of an intersubunit bridge induced by disparate 16S ribosomal ambiguity mutations mimics an EF-Tu-bound state. 2013 , 110, 9716-21	24
1076	A mutation of the RNA polymerase β subunit (<i>rpoC</i>) confers cephalosporin resistance in <i>Bacillus subtilis</i> . 2013 , 57, 56-65	22
1075	RNA polymerase III-specific general transcription factor III _C contains a heterodimer resembling TFIIF Rap30/Rap74. 2013 , 41, 9183-96	15
1074	Heavy chain-only IgG2b llama antibody effects near-pan HIV-1 neutralization by recognizing a CD4-induced epitope that includes elements of coreceptor- and CD4-binding sites. 2013 , 87, 10173-81	18
1073	A novel inhibitor-binding site on the HIV-1 capsid N-terminal domain leads to improved crystallization via compound-mediated dimerization. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 1115-23	23
1072	Structural and functional characterization of HP0377, a thioredoxin-fold protein from <i>Helicobacter pylori</i> . <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 735-46	8
1071	The structure of a glycoside hydrolase family 81 endo- β -1,3-glucanase. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 2027-38	11
1070	Structure-informed design of an enzymatically inactive vaccine component for group A <i>Streptococcus</i> . 2013 , 4,	16
1069	lDDT: a local superposition-free score for comparing protein structures and models using distance difference tests. 2013 , 29, 2722-8	193
1068	Structural investigation of a novel N-acetyl glucosamine binding chi-lectin which reveals evolutionary relationship with class III chitinases. 2013 , 8, e63779	18
1067	Structures of enzyme-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, 1470-81	14
1066	Strategies and molecular tools to fight antimicrobial resistance: resistome, transcriptome, and antimicrobial peptides. 2013 , 4, 412	45
1065	Functional convergence of structurally distinct thioesterases from cyanobacteria and plants involved in phylloquinone biosynthesis. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 1876-88	6
1064	Structure of an outer surface lipoprotein BBA64 from the Lyme disease agent <i>Borrelia burgdorferi</i> which is critical to ensure infection after a tick bite. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 1099-107	11
1063	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	9
1062	Atomic resolution structures of the c-Src SH3 domain in complex with two high-affinity peptides from classes I and II. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 756-66	17
1061	The structure and mode of action of <i>Caldicellulosiruptor bescii</i> family 3 pectate lyase in biomass deconstruction. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 534-9	6

1060	The binding of zinc ions to <i>Emergella nidulans</i> endo- β -1,4-galactanase is essential for crystal formation. 2013 , 69, 850-4	5
1059	The landscape of cytokinin binding by a plant nodulin. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 2365-80	11
1058	Structural insights into adeno-associated virus serotype 5. 2013 , 87, 11187-99	51
1057	Structural basis for C-ribosylation in the alnumycin A biosynthetic pathway. 2013 , 110, 1291-6	44
1056	Structures of oncogenic, suppressor and rescued p53 core-domain variants: mechanisms of mutant p53 rescue. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 2146-56	7
1055	Molecular mechanisms for the subversion of MyD88 signaling by TcpC from virulent uropathogenic <i>Escherichia coli</i> . 2013 , 110, 6985-90	63
1054	Diverse specificity and effector function among human antibodies to HIV-1 envelope glycoprotein epitopes exposed by CD4 binding. 2013 , 110, E69-78	119
1053	Chloride binding site of neurotransmitter sodium symporters. 2013 , 110, 8489-94	65
1052	Structure and function of human xylulokinase, an enzyme with important roles in carbohydrate metabolism. 2013 , 288, 1643-52	16
1051	A self-compartmentalizing hexamer serine protease from <i>Pyrococcus horikoshii</i> : substrate selection achieved through multimerization. 2013 , 288, 17884-94	14
1050	Structural basis for a cofactor-dependent oxidation protection and catalysis of cyanobacterial succinic semialdehyde dehydrogenase. 2013 , 288, 15760-70	16
1049	Cloning and structure-function analyses of quinolone- and acridone-producing novel type III polyketide synthases from <i>Citrus microcarpa</i> . 2013 , 288, 28845-58	22
1048	Structure determination through homology modelling and torsion-angle simulated annealing: application to a polysaccharide deacetylase from <i>Bacillus cereus</i> . <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 276-83	16
1047	Dimeric Sfh3 has structural changes in its binding pocket that are associated with a dimer-monomer state transformation induced by substrate binding. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 313-23	9
1046	Novel c-di-GMP recognition modes of the mouse innate immune adaptor protein STING. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 352-66	29
1045	GH1-family 6-P- β -glucosidases from human microbiome lactic acid bacteria. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 451-63	17
1044	Structure of the complex between teicoplanin and a bacterial cell-wall peptide: use of a carrier-protein approach. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 520-33	11
1043	Structural characterization of V57D and V57P mutants of human cystatin C, an amyloidogenic protein. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 577-86	6

1042	Interaction partners of PSD-93 studied by X-ray crystallography and fluorescence polarization spectroscopy. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 587-94	5
1041	Domain-level rocking motion within a polymerase that translocates on single-stranded nucleic acid. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 617-24	1
1040	Robust structural analysis of native biological macromolecules from multi-crystal anomalous diffraction data. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 1314-32	75
1039	The structure of the caspase recruitment domain of BinCARD reveals that all three cysteines can be oxidized. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 774-84	9
1038	Structural basis of L-phosphoserine binding to <i>Bacillus alcalophilus</i> phosphoserine aminotransferase. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 804-11	9
1037	The structure of the SBP-Tag-streptavidin complex reveals a novel helical scaffold bridging binding pockets on separate subunits. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 879-87	21
1036	Structural analysis of coniferyl alcohol 9-O-methyltransferase from <i>Linum nodiflorum</i> reveals a novel active-site environment. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 888-900	4
1035	New model-fitting and model-completion programs for automated iterative nucleic acid refinement. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 1171-9	7
1034	Structural and catalytic characterization of a thermally stable and acid-stable variant of human carbonic anhydrase II containing an engineered disulfide bond. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 1414-22	28
1033	Structural basis for the dephosphorylating activity of PTPRQ towards phosphatidylinositide substrates. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 1522-9	6
1032	Structure of the cobalamin-binding protein of a putative O-demethylase from <i>Desulfitobacterium hafniense</i> DCB-2. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 1609-16	4
1031	Molecular replacement then and now. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 2266-75	38
1030	Fine-tuning of prototype chicken galectins: structure of CG-2 and structure-activity correlations. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 1665-76	10
1029	Structural basis of high-order oligomerization of the cullin-3 adaptor SPOP. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 1677-84	23
1028	Structure of arylamine N-acetyltransferase from <i>Mycobacterium tuberculosis</i> determined by cross-seeding with the homologous protein from <i>M. marinum</i> : triumph over adversity. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 1433-46	19
1027	Structure of the periplasmic copper-binding protein CueP from <i>Salmonella enterica</i> serovar Typhimurium. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 1867-75	13
1026	Complex structure of type VI peptidoglycan muramidase effector and a cognate immunity protein. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 1889-900	16
1025	High-resolution structure of a papaya plant-defense barwin-like protein solved by in-house sulfur-SAD phasing. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 2017-26	10

1024	Conformational changes in human prolyl-tRNA synthetase upon binding of the substrates proline and ATP and the inhibitor halofuginone. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 2136-45	27
1023	Structural insights into the role of the Chl4-Iml3 complex in kinetochore assembly. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 2412-9	6
1022	Structural polymorphism in the L1 loop regions of human H2A.Z.1 and H2A.Z.2. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 2431-9	42
1021	Structural characterization of the ribonuclease H-like type ASKHA superfamily kinase MK0840 from <i>Methanopyrus kandleri</i> . <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 2440-50	4
1020	Protein design by fusion: implications for protein structure prediction and evolution. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 2451-60	3
1019	Structural basis for type VI secreted peptidoglycan DL-endopeptidase function, specificity and neutralization in <i>Serratia marcescens</i> . <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 2468-82	32
1018	Improvements in the order, isotropy and electron density of glypican-1 crystals by controlled dehydration. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 2524-33	10
1017	Structural basis of SUFU-GLI interaction in human Hedgehog signalling regulation. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 2563-79	42
1016	High-resolution crystal structure of <i>Streptococcus pyogenes</i> β -NAD ⁺ glycohydrolase in complex with its endogenous inhibitor IFS reveals a highly water-rich interface. 2013 , 20, 962-7	1
1015	High-resolution X-ray crystal structure of bovine H-protein using the high-pressure cryocooling method. 2013 , 20, 989-93	7
1014	Structure of the hypothetical DUF1811-family protein GK0453 from <i>Geobacillus kaustophilus</i> HTA426. 2013 , 69, 342-5	
1013	Structure of glutaminyl cyclase from <i>Drosophila melanogaster</i> in space group I4. 2013 , 69, 358-61	2
1012	Structure of an atypical FeoB G-domain reveals a putative domain-swapped dimer. 2013 , 69, 399-404	11
1011	Structure of the catalytic domain of the <i>Tannerella forsythia</i> matrix metallopeptidase karilysin in complex with a tetrapeptidic inhibitor. 2013 , 69, 472-6	8
1010	Structure of the <i>Yersinia pestis</i> tip protein LcrV refined to 1.65 Å resolution. 2013 , 69, 477-81	19
1009	The structure of the CARD8 caspase-recruitment domain suggests its association with the FIIND domain and procaspases through adjacent surfaces. 2013 , 69, 482-7	12
1008	Cocrystal structure of the ICAP1 PTB domain in complex with a KRIT1 peptide. 2013 , 69, 494-8	10
1007	Structure of diaminohydroxyphosphoribosylaminopyrimidine deaminase/5-amino-6-(5-phosphoribosylamino)uracil reductase from <i>Acinetobacter baumannii</i> . 2013 , 69, 611-7	0

1006	Structure of PatF from <i>Prochloron didemni</i> . 2013 , 69, 618-23	26
1005	ErpC, a member of the complement regulator-acquiring family of surface proteins from <i>Borrelia burgdorferi</i> , possesses an architecture previously unseen in this protein family. 2013 , 69, 624-8	11
1004	Conformational stability and crystal packing: polymorphism in <i>Neurospora crassa</i> CAT-3. 2013 , 69, 753-8	1
1003	High-resolution structure of the Tiam1 PHn-CC-Ex domain. 2013 , 69, 744-52	4
1002	Three-dimensional structure of RBcel1, a metagenome-derived psychrotolerant family GH5 endoglucanase. 2013 , 69, 828-33	6
1001	Structure of the caspase-recruitment domain from a zebrafish guanylate-binding protein. 2013 , 69, 855-60	13
1000	Structures of <i>Saccharomyces cerevisiae</i> D-arabinose dehydrogenase Ara1 and its complex with NADPH: implications for cofactor-assisted substrate recognition. 2013 , 69, 1190-5	2
999	Structure of CT584 from <i>Chlamydia trachomatis</i> refined to 3.05 Å resolution. 2013 , 69, 1196-201	5
998	Structure of <i>Acidothermus cellulolyticus</i> family 74 glycoside hydrolase at 1.82 Å resolution. 2013 , 69, 1335-8	8
997	Two high-resolution structures of the human E3 ubiquitin ligase Siah1. 2013 , 69, 1339-43	7
996	A conserved mechanism for centromeric nucleosome recognition by centromere protein CENP-C. 2013 , 340, 1110-3	235
995	Structural and functional insights into the molecular mechanism of rRNA m6A methyltransferase RlmJ. 2013 , 41, 9537-48	14
994	Ultratight crystal packing of a 10 kDa protein. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 464-70	9
993	Structure determination of the functional domain interaction of a chimeric nonribosomal peptide synthetase from a challenging crystal with noncrystallographic translational symmetry. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 1482-92	19
992	Structures of purine nucleosidase from <i>Trypanosoma brucei</i> bound to isozyme-specific trypanocidals and a novel metalorganic inhibitor. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 1553-66	9
991	Half a century of Ramachandran plots. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 1333-41	50
990	Novel c-di-GMP recognition modes of the mouse innate immune adaptor protein STING. Corrigendum. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 1191-1191	
989	Putative dioxygen-binding sites and recognition of tigecycline and minocycline in the tetracycline-degrading monooxygenase TetX. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 1758-67	20

988	Analysis of the human cofilin 1 structure reveals conformational changes required for actin binding. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 1780-8	17
987	A functional and structural study of the major metalloprotease secreted by the pathogenic fungus <i>Aspergillus fumigatus</i> . <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 1946-57	15
986	Structure of the prolyl-acyl carrier protein oxidase involved in the biosynthesis of the cyanotoxin anatoxin-a. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 2340-52	8
985	Further structural insights into the binding of complement factor H by complement regulator-acquiring surface protein 1 (CspA) of <i>Borrelia burgdorferi</i> . 2013 , 69, 629-33	12
984	Structure of <i>Escherichia coli</i> AdhP (ethanol-inducible dehydrogenase) with bound NAD. 2013 , 69, 730-2	13
983	Structure of the type VI effector-immunity complex (Tae4-Tai4) provides novel insights into the inhibition mechanism of the effector by its immunity protein. 2013 , 288, 5928-39	46
982	Protein Structure Modeling in a Grid Computing Environment. 2013 ,	
981	Structural and biochemical characterization of an atypical short-chain dehydrogenase/reductase reveals an unusual cofactor preference. 2013 , 280, 1358-70	10
980	Crystal structures of <i>Klebsiella pneumoniae</i> pantothenate kinase in complex with N-substituted pantothenamides. 2013 , 81, 1466-72	12
979	A conserved threonine spring-loads precursor for intein splicing. 2013 , 22, 557-63	23
978	Structural insights into oligomerization and mitochondrial remodelling of dynamin 1-like protein. 2013 , 32, 1280-92	171
977	Structure and activity of the NAD(P) ⁺ -dependent succinate semialdehyde dehydrogenase Ynel from <i>Salmonella typhimurium</i> . 2013 , 81, 1031-41	15
976	On the role of thermal backbone fluctuations in myoglobin ligand gate dynamics. 2013 , 138, 175101	10
975	Structure-function analysis of the LytM domain of EnvC, an activator of cell wall remodelling at the <i>Escherichia coli</i> division site. 2013 , 89, 690-701	37
974	Structural mechanism for the specific assembly and activation of the extracellular signal regulated kinase 5 (ERK5) module. 2013 , 288, 8596-8609	30
973	A homology/ab initio hybrid algorithm for sampling near-native protein conformations. 2013 , 34, 1925-36	14
972	High-quality protein backbone reconstruction from alpha carbons using Gaussian mixture models. 2013 , 34, 1881-9	39
971	The development of selective inhibitors of NagZ: increased susceptibility of Gram-negative bacteria to β -lactams. 2013 , 14, 1973-81	27

970	A gating mechanism of pentameric ligand-gated ion channels. 2013 , 110, E3987-96	103
969	Structure, biochemical characterization and analysis of the pleomorphism of carboxylesterase Cest-2923 from <i>Lactobacillus plantarum</i> WCFS1. 2013 , 280, 6658-71	29
968	Genetic analysis of the biosynthesis of 2-methoxy-3-isobutylpyrazine, a major grape-derived aroma compound impacting wine quality. 2013 , 162, 604-15	59
967	In vitro secretion deficits are common among human coagulation factor XIII subunit B missense mutants: correlations with patient phenotypes and molecular models. 2013 , 34, 1490-500	6
966	<i>Neisseria meningitidis</i> expresses a single 3-deoxy-d-arabino-heptulosonate 7-phosphate synthase that is inhibited primarily by phenylalanine. 2013 , 22, 1087-99	20
965	Mutants of phage bIL67 RuvC with enhanced Holliday junction binding selectivity and resolution symmetry. 2013 , 89, 1240-58	9
964	Structure of an early native-like intermediate of β 2-microglobulin amyloidogenesis. 2013 , 22, 1349-57	12
963	N-[9-(ortho-fluorobenzyl)-2-phenyl-8-azapurin-6-yl]-amides as potent and selective ligands for A β adenosine receptors. 2013 , 82, 22-38	3
962	The Arabidopsis B3 domain protein VERNALIZATION1 (VRN1) is involved in processes essential for development, with structural and mutational studies revealing its DNA-binding surface. 2013 , 288, 3198-207	25
961	Evolution of vitamin B2 biosynthesis: eubacterial RibG and fungal Rib2 deaminases. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 227-36	4
960	Intrinsically disordered protein threads through the bacterial outer-membrane porin OmpF. 2013 , 340, 1570-4	96
959	Solution structure of the recombinant target recognition domain of zoocin A. 2013 , 81, 722-7	3
958	Structural determinants of HIV-1 Vif susceptibility and DNA binding in APOBEC3F. 2013 , 4, 2593	71
957	Preconfiguration of the antigen-binding site during affinity maturation of a broadly neutralizing influenza virus antibody. 2013 , 110, 264-9	170
956	Structural insights into the regulation of foreign genes in <i>Salmonella</i> by the Hha/H-NS complex. 2013 , 288, 13356-69	48
955	Structure-function analysis of ribonucleotide bypass by B family DNA replicases. 2013 , 110, 16802-7	37
954	Hemagglutinin homologue from H17N10 bat influenza virus exhibits divergent receptor-binding and pH-dependent fusion activities. 2013 , 110, 1458-63	125
953	Substrate recognition and hydrolysis by a family 50 exo- β -agarase, Aga50D, from the marine bacterium <i>Saccharophagus degradans</i> . 2013 , 288, 28078-88	44

952	HLA peptide length preferences control CD8+ T cell responses. 2013 , 191, 561-71	45
951	Crystal structure of IL-17 receptor B SEFIR domain. 2013 , 190, 2320-6	26
950	Identification of biochemically distinct properties of the small ubiquitin-related modifier (SUMO) conjugation pathway in Plasmodium falciparum. 2013 , 288, 27724-36	23
949	Enhanced TCR footprint by a novel glycolipid increases NKT-dependent tumor protection. 2013 , 191, 2916-25	32
948	Structural basis of the interaction of MbtH-like proteins, putative regulators of nonribosomal peptide biosynthesis, with adenylating enzymes. 2013 , 288, 1991-2003	69
947	Ca ²⁺ -dependent structural changes in the B-cell receptor CD23 increase its affinity for human immunoglobulin E. 2013 , 288, 21667-77	24
946	Structural and biochemical characterization of an active arylamine N-acetyltransferase possessing a non-canonical Cys-His-Glu catalytic triad. 2013 , 288, 22493-505	13
945	Crystal structure of β -1,4-glucan lyase, a unique glycoside hydrolase family member with a novel catalytic mechanism. 2013 , 288, 26764-74	18
944	Divergent sequence tunes ligand sensitivity in phospholipid-regulated hormone receptors. 2013 , 288, 20702-12	12
943	Tight conformational coupling between the domains of the enterotoxigenic Escherichia coli fimbrial adhesin CfaE regulates binding state transition. 2013 , 288, 9993-10001	7
942	Fusion of dioxygenase and lignin-binding domains in a novel secreted enzyme from cellulolytic Streptomyces sp. SirexAA-E. 2013 , 288, 18574-87	23
941	Dimerization of bacterial diaminopimelate epimerase is essential for catalysis. 2013 , 288, 9238-48	33
940	Structural and biochemical analyses of the eukaryotic heat shock locus V (HslV) from Trypanosoma brucei. 2013 , 288, 23234-43	8
939	Understanding the role of defective invertases in plants: tobacco Nin88 fails to degrade sucrose. 2013 , 161, 1670-81	45
938	The 2.5 Å structure of the enterococcus conjugation protein TraM resembles VirB8 type IV secretion proteins. 2013 , 288, 2018-28	47
937	High-resolution crystal structure of human Dim2/TXNL4B. 2013 , 69, 223-7	3
936	Validated near-atomic resolution structure of bacteriophage epsilon15 derived from cryo-EM and modeling. 2013 , 110, 12301-6	58
935	RAGE is a nucleic acid receptor that promotes inflammatory responses to DNA. 2013 , 210, 2447-63	145

934	Quantitative characterization of the activation steps of mannan-binding lectin (MBL)-associated serine proteases (MASPs) points to the central role of MASP-1 in the initiation of the complement lectin pathway. 2013 , 288, 8922-34	54
933	Structural analysis and insights into the glycon specificity of the rice GH1 Os7BGlu26 α -D-mannosidase. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 2124-35	9
932	Structure of the T6SS lipoprotein TssJ1 from <i>Pseudomonas aeruginosa</i> . 2013 , 69, 607-10	11
931	Correcting pervasive errors in RNA crystallography through enumerative structure prediction. 2013 , 10, 74-6	109
930	Structure of the RecQ C-terminal domain of human Bloom syndrome protein. 2013 , 3, 3294	14
929	Biochemical properties and crystal structure of a α -phenylalanine aminotransferase from <i>Variovorax paradoxus</i> . 2013 , 79, 185-95	24
928	Discovery of novel small-molecule HIV-1 replication inhibitors that stabilize capsid complexes. 2013 , 57, 4622-31	78
927	Novel insights into eukaryotic α -glutamyltranspeptidase 1 from the crystal structure of the glutamate-bound human enzyme. 2013 , 288, 31902-13	50
926	New insights into the assembly of bacterial secretins: structural studies of the periplasmic domain of XcpQ from <i>Pseudomonas aeruginosa</i> . 2013 , 288, 1214-25	24
925	Atomic resolution structure of the orotidine 5'-monophosphate decarboxylase product complex combined with surface plasmon resonance analysis: implications for the catalytic mechanism. 2013 , 288, 9011-6	9
924	Structure of the absent in melanoma 2 (AIM2) pyrin domain provides insights into the mechanisms of AIM2 autoinhibition and inflammasome assembly. 2013 , 288, 13225-35	113
923	The immunoglobulin domain of the sodium channel β subunit contains a surface-localized disulfide bond that is required for homophilic binding. 2013 , 27, 568-80	24
922	Specific interaction of the transcription elongation regulator TCERG1 with RNA polymerase II requires simultaneous phosphorylation at Ser2, Ser5, and Ser7 within the carboxyl-terminal domain repeat. 2013 , 288, 10890-901	20
921	Structural basis for Zn ²⁺ -dependent intercellular adhesion in staphylococcal biofilms. 2013 , 110, E202-11	76
920	<i>Porphyromonas gingivalis</i> virulence factor gingipain RgpB shows a unique zymogenic mechanism for cysteine peptidases. 2013 , 288, 14287-14296	27
919	Structure of a classical broadly neutralizing stem antibody in complex with a pandemic H2 influenza virus hemagglutinin. 2013 , 87, 7149-54	91
918	Three-dimensional structure of <i>Saccharomyces invertase</i> : role of a non-catalytic domain in oligomerization and substrate specificity. 2013 , 288, 9755-9766	62
917	Structure of <i>Pseudomonas aeruginosa</i> inosine 5'-monophosphate dehydrogenase. 2013 , 69, 243-7	11

916	Structure of the archaeal Cascade subunit Csa5: relating the small subunits of CRISPR effector complexes. 2013 , 10, 762-9	20
915	Small molecule Plasmodium FKBP35 inhibitor as a potential antimalaria agent. 2013 , 3, 2501	21
914	The structure of glycerol trinitrate reductase NerA from Agrobacterium radiobacter reveals the molecular reason for nitro- and ene-reductase activity in OYE homologues. 2013 , 14, 836-45	10
913	Structure of the factor VIII C2 domain in a ternary complex with 2 inhibitor antibodies reveals classical and nonclassical epitopes. 2013 , 122, 4270-8	21
912	A disulphide bond in the E2 enzyme Pex4p modulates ubiquitin-conjugating activity. 2013 , 3, 2212	9
911	Crystal structure of Ssfs6, the putative C-glycosyltransferase involved in SF2575 biosynthesis. 2013 , 81, 1277-82	23
910	Adsorption of multimeric T cell antigens on carbon nanotubes: effect on protein structure and antigen-specific T cell stimulation. 2013 , 9, 666-72	34
909	Crystal Structure of Apo- and Metalated Thiolate containing RNase S as Structural Basis for the Design of Artificial Metalloenzymes by Peptide-Protein Complementation. 2013 , 639, 2395-2400	3
908	Protein structure quality assessment based on the distance profiles of consecutive backbone C β atoms. 2013 , 2, 211	9
907	Extended Stokes shift in fluorescent proteins: chromophore-protein interactions in a near-infrared TagRFP675 variant. 2013 , 3, 1847	76
906	Structure and dynamics of the monomer of protein E of dengue virus type 2 with unprotonated histidine residues. 2013 , 12, 348-59	8
905	High-resolution crystal structure of copper amine oxidase from <i>Arthrobacter globiformis</i> : assignment of bound diatomic molecules as O ₂ . <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 2483-94	14
904	Multi-target parallel processing approach for gene-to-structure determination of the influenza polymerase PB2 subunit. 2013 ,	2
903	The 1.6 Å crystal structure of pyranose dehydrogenase from <i>Agaricus meleagris</i> rationalizes substrate specificity and reveals a flavin intermediate. 2013 , 8, e53567	40
902	Solution structures of two homologous venom peptides from <i>Sicarius dolichocephalus</i> . 2013 , 8, e54401	4
901	The structure of the karrikin-insensitive protein (KAI2) in <i>Arabidopsis thaliana</i> . 2013 , 8, e54758	45
900	The N-terminal β -sheet of peroxiredoxin 4 in the large yellow croaker <i>Pseudosciaena crocea</i> is involved in its biological functions. 2013 , 8, e57061	8
899	The <i>E. coli</i> effector protein NleF is a caspase inhibitor. 2013 , 8, e58937	74

898	The CouPSTU and TarPQM transporters in <i>Rhodopseudomonas palustris</i> : redundant, promiscuous uptake systems for lignin-derived aromatic substrates. 2013 , 8, e59844	27
897	Structural insights into the UbiD protein family from the crystal structure of PA0254 from <i>Pseudomonas aeruginosa</i> . 2013 , 8, e63161	28
896	Physicochemical characterization of a thermostable alcohol dehydrogenase from <i>Pyrobaculum aerophilum</i> . 2013 , 8, e63828	3
895	Signal transduction pathways in the pentameric ligand-gated ion channels. 2013 , 8, e64326	19
894	The <i>Pseudomonas aeruginosa</i> catabolite repression control protein Crc is devoid of RNA binding activity. 2013 , 8, e64609	38
893	<i>Mycobacterium tuberculosis</i> Rv3406 is a type II alkyl sulfatase capable of sulfate scavenging. 2013 , 8, e65080	13
892	Structural Insights into <i>Clostridium perfringens</i> Delta Toxin Pore Formation. 2013 , 8, e66673	21
891	Structural studies of a bacterial tRNA(HIS) guanylyltransferase (Thg1)-like protein, with nucleotide in the activation and nucleotidyl transfer sites. 2013 , 8, e67465	15
890	Disruption of hydrogen bonds between major histocompatibility complex class II and the peptide N-terminus is not sufficient to form a human leukocyte antigen-DM receptive state of major histocompatibility complex class II. 2013 , 8, e69228	9
889	i3Drefine software for protein 3D structure refinement and its assessment in CASP10. 2013 , 8, e69648	39
888	An activating mutation reveals a second binding mode of the integrin α I domain to the GFOGER motif in collagens. 2013 , 8, e69833	25
887	Crystal structure of pim1 kinase in complex with a pyrido[4,3-d]pyrimidine derivative suggests a unique binding mode. 2013 , 8, e70358	5
886	Functional identification of close proximity amino acid side chains within the transmembrane-spanning helices of the P2X2 receptor. 2013 , 8, e70629	6
885	Crystal structures of human muscle fructose-1,6-bisphosphatase: novel quaternary states, enhanced AMP affinity, and allosteric signal transmission pathway. 2013 , 8, e71242	10
884	Functional mapping of human dynamin-1-like GTPase domain based on x-ray structure analyses. 2013 , 8, e71835	44
883	Structure of the NheA component of the Nhe toxin from <i>Bacillus cereus</i> : implications for function. 2013 , 8, e74748	47
882	The structural basis of <i>Erwinia rhapontici</i> isomaltulose synthase. 2013 , 8, e74788	12
881	A remote palm domain residue of RB69 DNA polymerase is critical for enzyme activity and influences the conformation of the active site. 2013 , 8, e76700	6

880	Substrate and inhibitor specificity of the type II p21-activated kinase, PAK6. 2013 , 8, e77818	15
879	Comparative sequence, structure and redox analyses of <i>Klebsiella pneumoniae</i> DsbA show that anti-virulence target DsbA enzymes fall into distinct classes. 2013 , 8, e80210	20
878	Diversification of fungal specific class a glutathione transferases in saprotrophic fungi. 2013 , 8, e80298	34
877	Crystal structures of the human G3BP1 NTF2-like domain visualize FxFG Nup repeat specificity. 2013 , 8, e80947	28
876	Structural insights into the mechanism for recognizing substrate of the cytochrome P450 enzyme TxtE. 2013 , 8, e81526	16
875	Crystal structures and molecular dynamics simulations of thermophilic malate dehydrogenase reveal critical loop motion for co-substrate binding. 2013 , 8, e83091	8
874	Structures of Wnt-antagonist ZNRF3 and its complex with R-spondin 1 and implications for signaling. 2013 , 8, e83110	43
873	A monoclinic crystal form of casein kinase 1 α 2013 , 69, 1077-83	4
872	Conserved inhibitory mechanism and competent ATP binding mode for adenylyltransferases with Fic fold. 2013 , 8, e64901	24
871	Atomic resolution view into the structure-function relationships of the human myelin peripheral membrane protein P2. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2014 , 70, 165-76	31
870	Structure of haze forming proteins in white wines: <i>Vitis vinifera</i> thaumatin-like proteins. 2014 , 9, e113757	43
869	Esterase LpEst1 from <i>Lactobacillus plantarum</i> : a novel and atypical member of the β hydrolase superfamily of enzymes. 2014 , 9, e92257	17
868	Crystal structure of yeast DNA polymerase β catalytic domain. 2014 , 9, e94835	30
867	Structural insight into the tetramerization of an iterative ketoreductase siam through aromatic residues in the interfaces. 2014 , 9, e97996	4
866	Structural and mutagenic analysis of the RM controller protein C.Esp1396I. 2014 , 9, e98365	2
865	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. 2014 , 9, e98551	38
864	Structural diversity in the dandelion (<i>Taraxacum officinale</i>) polyphenol oxidase family results in different responses to model substrates. 2014 , 9, e99759	24
863	Discovery of novel GPVI receptor antagonists by structure-based repurposing. 2014 , 9, e101209	20

862	Structural and functional characterization of DUF1471 domains of Salmonella proteins SrfN, YdgH/SssB, and YahO. 2014 , 9, e101787	8
861	Chemically modified peptide scaffolds target the CFTR-associated ligand PDZ domain. 2014 , 9, e103650	11
860	The impact of nitration on the structure and immunogenicity of the major birch pollen allergen Bet v 1.0101. 2014 , 9, e104520	48
859	BdcA, a protein important for Escherichia coli biofilm dispersal, is a short-chain dehydrogenase/reductase that binds specifically to NADPH. 2014 , 9, e105751	11
858	Structure of the N-terminal Gyrase B fragment in complex with ADP?Pi reveals rigid-body motion induced by ATP hydrolysis. 2014 , 9, e107289	28
857	The Eps1p protein disulfide isomerase conserves classic thioredoxin superfamily amino acid motifs but not their functional geometries. 2014 , 9, e113431	5
856	RNA-directed remodeling of the HIV-1 protein Rev orchestrates assembly of the Rev-Rev response element complex. 2014 , 3, e04120	47
855	Identification of Plant Homologues of Dual Specificity Yak1-Related Kinases. 2014 , 2014, 1-14	4
854	Structural analysis of the endogenous glycoallergen Hev b 2 (endo- β -1,3-glucanase) from Hevea brasiliensis and its recognition by human basophils. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2014 , 70, 329-41	9
853	Inhibition and biochemical characterization of methicillin-resistant Staphylococcus aureus shikimate dehydrogenase: an in silico and kinetic study. 2014 , 19, 4491-509	9
852	Identification and characterization of amlexanox as a G protein-coupled receptor kinase 5 inhibitor. 2014 , 19, 16937-49	33
851	Multi-PAS domain-mediated protein oligomerization of PpsR from Rhodobacter sphaeroides. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2014 , 70, 863-76	11
850	Structural characterization of new deoxycytidine kinase inhibitors rationalizes the affinity-determining moieties of the molecules. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2014 , 70, 68-78	6
849	The structure of cytomegalovirus immune modulator UL141 highlights structural Ig-fold versatility for receptor binding. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2014 , 70, 851-62	5
848	A molecular model for the role of SYCP3 in meiotic chromosome organisation. 2014 , 3,	78
847	Structural mechanism of DNA recognition by the p202 HINa domain: insights into the inhibition of Aim2-mediated inflammatory signalling. 2014 , 70, 21-9	16
846	Structure of catalase determined by MicroED. 2014 , 3, e03600	84
845	Vaccine-elicited primate antibodies use a distinct approach to the HIV-1 primary receptor binding site informing vaccine redesign. 2014 , 111, E738-47	63

844	Structural insights into the substrate specificity and transglycosylation activity of a fungal glycoside hydrolase family 5 β -mannosidase. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2014 , 70, 2970-82	22
843	Structure-function analyses of human kallikrein-related peptidase 2 establish the 99-loop as master regulator of activity. 2014 , 289, 34267-83	25
842	Crystal structure of a <i>Schistosoma mansoni</i> septin reveals the phenomenon of strand slippage in septins dependent on the nature of the bound nucleotide. 2014 , 289, 7799-811	26
841	Analysis of carotenoid isomerase activity in a prototypical carotenoid cleavage enzyme, apocarotenoid oxygenase (ACO). 2014 , 289, 12286-99	27
840	E2~Ub conjugates regulate the kinase activity of <i>Shigella</i> effector OspG during pathogenesis. 2014 , 33, 437-49	46
839	Cyclic adenosine 5'-diphosphate ribose analogs without a "southern" ribose inhibit ADP-ribosyl cyclase-hydrolase CD38. 2014 , 57, 8517-29	14
838	Substrate specificities and conformational flexibility of 3-ketosteroid 9 β -hydroxylases. 2014 , 289, 25523-36	24
837	A conserved phenylalanine as a relay between the β helix and the GDP binding region of heterotrimeric Gi protein β subunit. 2014 , 289, 24475-87	35
836	Molecular functions of the TLE tetramerization domain in Wnt target gene repression. 2014 , 33, 719-31	62
835	Adjustable locks and flexible keys: plasticity of epitope-paratope interactions in germline antibodies. 2014 , 192, 5398-405	10
834	A new calmodulin-binding motif for inositol 1,4,5-trisphosphate 3-kinase regulation. 2014 , 463, 319-28	6
833	G-triplex structure and formation propensity. 2014 , 42, 13393-404	51
832	Discovery and characterization of olokizumab: a humanized antibody targeting interleukin-6 and neutralizing gp130-signaling. 2014 , 6, 774-82	47
831	Clathrin adaptors. AP2 controls clathrin polymerization with a membrane-activated switch. 2014 , 345, 459-63	133
830	High thermodynamic stability of parametrically designed helical bundles. 2014 , 346, 481-485	196
829	Molecular Dynamics Simulations of RNA Systems. 2014 , 687-718	1
828	The structure of Rv2372c identifies an RsmE-like methyltransferase from <i>Mycobacterium tuberculosis</i> . <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2014 , 70, 821-32	8
827	Receptor mimicry by antibody F045-092 facilitates universal binding to the H3 subtype of influenza virus. 2014 , 5, 3614	130

826	Crystal structure of the dithiol oxidase DsbA enzyme from proteus mirabilis bound non-covalently to an active site peptide ligand. 2014 , 289, 19810-22	15
825	Crystal structure of EML1 reveals the basis for Hsp90 dependence of oncogenic EML4-ALK by disruption of an atypical α -propeller domain. 2014 , 111, 5195-200	70
824	Structural and spectroscopic insights into BolA-glutaredoxin complexes. 2014 , 289, 24588-98	36
823	Mechanisms of toxin inhibition and transcriptional repression by Escherichia coli DinJ-YafQ. 2014 , 289, 20559-69	34
822	Impact of residues remote from the catalytic centre on enzyme catalysis of copper nitrite reductase. 2014 , 5, 4395	30
821	Structure of the Acinetobacter baumannii dithiol oxidase DsbA bound to elongation factor EF-Tu reveals a novel protein interaction site. 2014 , 289, 19869-80	11
820	Chronophin dimerization is required for proper positioning of its substrate specificity loop. 2014 , 289, 3094-103	12
819	Stabilization of the dimeric birch pollen allergen Bet v 1 impacts its immunological properties. 2014 , 289, 540-51	23
818	Atomic resolution structure of a lysine-specific endoproteinase from Lysobacter enzymogenes suggests a hydroxyl group bound to the oxyanion hole. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2014 , 70, 1832-43	8
817	Evidence that GH115 β -glucuronidase activity, which is required to degrade plant biomass, is dependent on conformational flexibility. 2014 , 289, 53-64	46
816	Human UTY(KDM6C) is a male-specific N ⁷ -methyl lysyl demethylase. 2014 , 289, 18302-13	123
815	Inhibition of plasma kallikrein by a highly specific active site blocking antibody. 2014 , 289, 23596-608	73
814	Structural model for covalent adhesion of the Streptococcus pyogenes pilus through a thioester bond. 2014 , 289, 177-89	37
813	Conformational itinerary of Pseudomonas aeruginosa 1,6-anhydro-N-acetylmuramic acid kinase during its catalytic cycle. 2014 , 289, 4504-14	6
812	Structure and mechanism of cysteine peptidase gingipain K (Kgp), a major virulence factor of Porphyromonas gingivalis in periodontitis. 2014 , 289, 32291-32302	52
811	The X-ray structure of NccX from Cupriavidus metallidurans 31A illustrates potential dangers of detergent solubilization when generating and interpreting crystal structures of membrane proteins. 2014 , 289, 31160-72	9
810	Crystallographic and electron microscopic analyses of a bacterial phytochrome reveal local and global rearrangements during photoconversion. 2014 , 289, 24573-87	76
809	Structural basis for the broad specificity of a new family of amino-acid racemases. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2014 , 70, 79-90	40

808	Binding of Pro-Gly-Pro at the active site of leukotriene A4 hydrolase/aminopeptidase and development of an epoxide hydrolase selective inhibitor. 2014 , 111, 4227-32	41
807	Structure and mechanism of the bifunctional CinA enzyme from <i>Thermus thermophilus</i> . 2014 , 289, 33187-97	8
806	Crystal structures of thermally stable adenylate kinase mutants designed by local structural entropy optimization and structure-guided mutagenesis. 2014 , 57, 661-665	
805	Cancer-relevant splicing factor CAPER engages the essential splicing factor SF3b155 in a specific ternary complex. 2014 , 289, 17325-37	30
804	Electrostatic transition state stabilization rather than reactant destabilization provides the chemical basis for efficient chorismate mutase catalysis. 2014 , 111, 17516-21	23
803	A <i>Plasmodium falciparum</i> PHIST protein binds the virulence factor PfEMP1 and comigrates to knobs on the host cell surface. 2014 , 28, 4420-33	66
802	A critical base pair in k-turns that confers folding characteristics and correlates with biological function. 2014 , 5, 5127	30
801	PconsFold: improved contact predictions improve protein models. 2014 , 30, i482-8	76
800	Potent neutralization of vaccinia virus by divergent murine antibodies targeting a common site of vulnerability in L1 protein. 2014 , 88, 11339-55	22
799	Mechanism of dephosphorylation of glucosyl-3-phosphoglycerate by a histidine phosphatase. 2014 , 289, 21242-51	8
798	Structure-based investigation into the functional roles of the extended loop and substrate-recognition sites in an endo- β -1,4-D-mannanase from the Antarctic springtail, <i>Cryptopygus antarcticus</i> . 2014 , 82, 3217-23	14
797	RPRD1A and RPRD1B are human RNA polymerase II C-terminal domain scaffolds for Ser5 dephosphorylation. 2014 , 21, 686-695	54
796	Architecture of a single membrane spanning cytochrome P450 suggests constraints that orient the catalytic domain relative to a bilayer. 2014 , 111, 3865-70	193
795	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, 2032-41	17
794	Molecular insights into the membrane-associated phosphatidylinositol 4-kinase II β . 2014 , 5, 3552	38
793	Structural basis for the recognition of peptide RJPXD33 by acyltransferases in lipid A biosynthesis. 2014 , 289, 15527-35	17
792	Atomic resolution crystal structure of glutaredoxin 1 from <i>Plasmodium falciparum</i> and comparison with other glutaredoxins. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2014 , 70, 91-100	11
791	Crystal structure of the sodium-proton antiporter NhaA dimer and new mechanistic insights. 2014 , 144, 529-44	60

790	Structural basis of recognition of interferon- β receptor by tyrosine kinase 2. 2014 , 21, 443-8	98
789	Insights into the evolution of divergent nucleotide-binding mechanisms among pseudokinases revealed by crystal structures of human and mouse MLKL. 2014 , 457, 369-77	79
788	Regulation of S-adenosylhomocysteine hydrolase by lysine acetylation. 2014 , 289, 31361-72	22
787	Disarming <i>Burkholderia pseudomallei</i> : structural and functional characterization of a disulfide oxidoreductase (DsbA) required for virulence in vivo. 2014 , 20, 606-17	43
786	Structural analysis of substrate-mimicking inhibitors in complex with <i>Neisseria meningitidis</i> 3-deoxy-d-arabino-heptulosonate 7-phosphate synthase - The importance of accommodating the active site water. 2014 , 57, 242-250	5
785	Structural differences explain diverse functions of <i>Plasmodium</i> actins. 2014 , 10, e1004091	50
784	Structure of the trehalose-6-phosphate phosphatase from <i>Brugia malayi</i> reveals key design principles for anthelmintic drugs. 2014 , 10, e1004245	29
783	Distinct structural features of Rex-family repressors to sense redox levels in anaerobes and aerobes. 2014 , 188, 195-204	8
782	Structures of <i>Trypanosoma brucei</i> methionyl-tRNA synthetase with urea-based inhibitors provide guidance for drug design against sleeping sickness. 2014 , 8, e2775	29
781	The CD27L and CTP1L endolysins targeting <i>Clostridia</i> contain a built-in trigger and release factor. 2014 , 10, e1004228	34
780	Computational design of the affinity and specificity of a therapeutic T cell receptor. 2014 , 10, e1003478	57
779	Structure-based characterization and antifreeze properties of a hyperactive ice-binding protein from the Antarctic bacterium <i>Flavobacterium frigidis</i> PS1. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2014 , 70, 1061-73	45
778	Apo, Zn ²⁺ -bound and Mn ²⁺ -bound structures reveal ligand-binding properties of SitA from the pathogen <i>Staphylococcus pseudintermedius</i> . 2014 , 34, e00154	26
777	The crystal structure of the RhoA-AKAP-Lbc DH-PH domain complex. 2014 , 464, 231-9	20
776	Crystal structure of <i>Deinococcus radiodurans</i> RecQ helicase catalytic core domain: the interdomain flexibility. 2014 , 2014, 342725	6
775	Structural and biochemical characterization of the KLHL3-WNK kinase interaction important in blood pressure regulation. 2014 , 460, 237-46	49
774	Structural basis for the molecular recognition of polyadenosine RNA by Nab2 Zn fingers. 2014 , 42, 672-80	15
773	<i>P. aeruginosa</i> SGNH hydrolase-like proteins AlgJ and AlgX have similar topology but separate and distinct roles in alginate acetylation. 2014 , 10, e1004334	37

772	Lectin-like bacteriocins from <i>Pseudomonas</i> spp. utilise D-rhamnose containing lipopolysaccharide as a cellular receptor. 2014 , 10, e1003898	46
771	A new model for pore formation by cholesterol-dependent cytolysins. 2014 , 10, e1003791	27
770	Cell fate regulation governed by a repurposed bacterial histidine kinase. 2014 , 12, e1001979	47
769	Thermodynamic system drift in protein evolution. 2014 , 12, e1001994	53
768	VASP-E: specificity annotation with a volumetric analysis of electrostatic isopotentials. 2014 , 10, e1003792	11
767	Structure of CfaA suggests a new family of chaperones essential for assembly of class 5 fimbriae. 2014 , 10, e1004316	8
766	How the structure of the large subunit controls function in an oxygen-tolerant [NiFe]-hydrogenase. 2014 , 458, 449-58	32
765	Cryo-EM structure of the HIV-1 Pol polyprotein provides insights into virion maturation. 2022 , 8,	1
764	Mebendazole Conformational Space and Its Predicted Binding to Human Heat-Shock Protein 90.	
763	Structural basis of human TREX1 DNA degradation and autoimmune disease. 2022 , 13,	2
762	Modulating co-translational protein folding by rational design and ribosome engineering. 2022 , 13,	0
761	Divergent evolution of extreme production of variant plant monounsaturated fatty acids. 2022 , 119,	0
760	Cryo-EM structures of Na ⁺ -pumping NADH-ubiquinone oxidoreductase from <i>Vibrio cholerae</i> . 2022 , 13,	
759	Archaic chaperone-usher pili self-secrete into superelastic zigzag springs.	0
758	Potent and Broad Neutralization of SARS-CoV-2 Variants of Concern (VOCs) including Omicron Sub-lineages BA.1 and BA.2 by Biparatopic Human VH Domains. 2022 , 104798	
757	H ₂ S biogenesis by cystathionine beta-synthase: mechanism of inhibition by aminooxyacetic acid and unexpected role of serine. 2022 , 79,	2
756	Hijacking of the Enterobactin Pathway by a Synthetic Catechol Vector Designed for Oxazolidinone Antibiotic Delivery in <i>Pseudomonas aeruginosa</i> .	0
755	Mechanisms of circadian clock timing and entrainment revealed by the structure of Cryptochrome bound to Timeless.	

- 754 Data collection from crystals grown in microfluidic droplets. **2022**, 78, 0
- 753 Membrane-anchored HDCR nanowires drive hydrogen-powered CO₂ fixation. **2022**, 607, 823-830 0
- 752 Mnt1, an α (1 \rightarrow 2)-mannosyltransferase responsible for the elongation of N-glycans and O-glycans in *aspergillus fumigatus*. 2
- 751 Molecular Docking Study of IPBCC.08.610 Glucose Oxidase Mutant for Increasing Gluconic Acid Production. **2022**, 25, 169-178
- 750 Serum-Stable and Selective Backbone-N-Methylated Cyclic Peptides That Inhibit Prokaryotic Glycolytic Mutases. **2022**, 17, 2284-2295 0
- 749 Structural assembly of the nucleic-acid-binding Thp3Usn12Bem1 complex functioning in mRNA splicing. **2022**, 50, 8882-8897 1
- 748 CryoEM of endogenous mammalian V-ATPase interacting with the TLDc protein mEAK-7. **2022**, 5, e202201527 0
- 747 Cryo-EM structure of an active bacterial TIRSTING filament complex. **2022**, 608, 803-807 3
- 746 PTPAMP: prediction tool for plant-derived antimicrobial peptides.
- 745 Structural Insights into Porphyrin Recognition by the Human ATP-Binding Cassette Transporter ABCB6. **2022**, 45, 575-587 0
- 744 Structures of Atm1 provide insight into [2Fe-2S] cluster export from mitochondria. **2022**, 13, 0
- 743 Pathogenic bacteria remodel central metabolic enzyme to build a cyclopropanol warhead. **2022**, 14, 884-890 2
- 742 Room-temperature serial synchrotron crystallography of apo PTP1B.
- 741 Tip60 acetylation of histone H3K4 temporally controls chromosome passenger complex localization. **2022**, 33, 0
- 740 The L,d-Transpeptidase LdtAb from *Acinetobacter baumannii* Is Poorly Inhibited by Carbapenems and Has a Unique Structural Architecture. 0
- 739 Revving an Engine of Human Metabolism: Activity Enhancement of Triosephosphate Isomerase via Hemi-Phosphorylation. 0
- 738 Structure and engineering of the minimal type VI CRISPR-Cas13bt3. **2022**, 0
- 737 The acyclotide ribe 31 from *Rinorea bengalensis* has selective cytotoxicity and potent insecticidal properties in *Drosophila*. **2022**, 102413

- 736 Mechanistic insight into the RNA stimulated-ATPase activity of tick-borne encephalitis virus helicase. **2022**, 102383
- 735 Characterization of a novel GH10 alkali-thermostable xylanase from a termite microbiome. **2022**, 9,
- 734 Residue-wise local quality estimation for protein models from cryo-EM maps. 1
- 733 Structural basis for proton coupled cystine transport by cystinosin. **2022**, 13, 1
- 732 Crystal structure of ChbG from *Klebsiella pneumoniae* reveals the molecular basis of diacetylchitobiose deacetylation. **2022**, 5,
- 731 Mechanistic insights into intramembrane proteolysis by *E. coli* site-2 protease homolog RseP. **2022**, 8, 1
- 730 The four Rs and crystal structure analysis: reliability, reproducibility, replicability and reusability. **2022**, 55,
- 729 Rotavirus VP4 Epitope of a Broadly Neutralizing Human Antibody Defined by Its Structure Bound with an Attenuated-Strain Virion. **2022**, 96, 0
- 728 Delineating the activity of the potent nicotinic acetylcholine receptor agonists (+)-anatoxin-a and (+)-phosieine-A. **2022**, 78,
- 727 Structure of the Monkeypox profilin-like protein A42R reveals potential function differences from cellular profilins. 0
- 726 Megahertz pulse trains enable multi-hit serial femtosecond crystallography experiments at X-ray free electron lasers. **2022**, 13, 0
- 725 Quaternary organization of the human eEF1B complex reveals unique multi-GEF domain assembly. 0
- 724 Structural and dynamic mechanisms of GABAA receptor modulators with opposing activities. **2022**, 13, 0
- 723 Structure of the catalytically active APOBEC3G bound to a DNA oligonucleotide inhibitor reveals tetrahedral geometry of the transition state. 0
- 722 The β -Grasp Domain of Proteasomal ATPase Mpa Makes Critical Contacts with the Mycobacterium tuberculosis 20S Core Particle to Facilitate Degradation.
- 721 Structure of trimeric pre-fusion rabies virus glycoprotein in complex with two protective antibodies. **2022**,
- 720 Sustainable isomaltulose production in *Corynebacterium glutamicum* by engineering the thermostability of sucrose isomerase coupled with one-step simplified cell immobilization. 13,
- 719 The mechanism of RNA capping by SARS-CoV-2. 0

718	Mechanism of client selection by the protein quality-control factor UBE2O. 2022 , 29, 774-780	0
717	Phosphonic acid-containing inhibitors of tyrosyl-DNA phosphodiesterase 1. 10,	0
716	Metabolic and Structural Insights into Hydrogen Sulfide Mis-Regulation in <i>Enterococcus faecalis</i> . 2022 , 11, 1607	
715	Molecular Basis of Mink ACE2 Binding to SARS-CoV-2 and Its Mink-Derived Variants.	2
714	Extensive substrate recognition by the streptococcal antibody-degrading enzymes IdeS and EndoS.	0
713	ModelCraft: an advanced automated model-building pipeline using Buccaneer. 2022 , 78,	2
712	Structural basis for the synergistic neutralization of coxsackievirus B1 by a triple-antibody cocktail. 2022 ,	0
711	Andrographolide and Deoxyandrographolide Inhibit Protease and IFN-Antagonist Activities of Foot-and-Mouth Disease Virus 3Cpro. 2022 , 12, 1995	0
710	Structural analysis of cholesterol binding and sterol selectivity by ABCG5/G8. 2022 , 167795	0
709	Cryo-EM structures of two human B cell receptor isotypes. 2022 , 377, 880-885	2
708	Analysis of protein structures containing HEPES and MES molecules. 2022 , 31,	
707	Cell-surface protein YwFG of <i>Lactococcus lactis</i> binds to β 1,2-linked mannose.	
706	Human anti-ACE2 monoclonal antibodies as pan-sarbecovirus prophylactic agents.	1
705	Structures of human Malic Enzyme 3.	
704	An Immunoinformatic Study on Exploration of Membrane Proteins to Develop Epitope Based Vaccine Against <i>Streptococcus pneumoniae</i> . 2022 , 28,	
703	Engineering an autonomous VH domain to modulate intracellular pathways and to interrogate the eIF4F complex. 2022 , 13,	1
702	The temperature-dependent conformational ensemble of SARS-CoV-2 main protease (Mpro). 2022 , 9,	1
701	FOX L2 and FOX A1 cooperatively assemble on the TP53 promoter in alternative dimer configurations. 2022 , 50, 8929-8946	0

- 700 Endogenous ligand recognition and structural transition of a human PTH receptor. **2022,** 1
- 699 Autoantibody mimicry of hormone action at the thyrotropin receptor. 0
- 698 Virtual screening for the discovery of novel urease inhibitors of rumen bacterial urease.
- 697 Structure of a monomeric photosystem I core associated with iron-stress-induced-A proteins from *Anabaena* sp. PCC 7120. 1
- 696 Structural basis for the dual catalytic activity of the *Legionella pneumophila* ovarian-tumor (OTU) domain deubiquitinase LotA. **2022,** 102414 0
- 695 A common mechanism of Sec61 translocon inhibition by small molecules. 1
- 694 Protein Model Refinement for Cryo-EM Maps Using DAQ score.
- 693 Molecular Basis of Inhibitory Mechanism of Naltrexone and Its Metabolites through Structural and Energetic Analyses. **2022,** 27, 4919 1
- 692 Functional and structural characteristics of HLA-B*13:01-mediated specific T cells reaction in dapsone-induced drug hypersensitivity. **2022,** 29, 0
- 691 The first crystal structure of a xylobiose-bound xylobiohydrolase with high functional specificity from the bacterial glycoside hydrolase family 30, subfamily 10. 0
- 690 Structural identification of lysophosphatidylcholines as activating ligands for orphan receptor GPR119. 0
- 689 The neutralizing breadth of antibodies targeting diverse conserved epitopes between SARS-CoV and SARS-CoV-2. **2022,** 119, 1
- 688 Structure of *Mycobacterium tuberculosis* Cya, an evolutionary ancestor of the mammalian membrane adenylyl cyclases. 11, 0
- 687 Metabolism of Cysteine Conjugates and Production of Flavor Sulfur Compounds by a Carbon Sulfur Lyase from the Oral Anaerobe *Fusobacterium nucleatum*. **2022,** 70, 9969-9979 1
- 686 Immunoinformatics-Based Proteome Mining to Develop a Next-Generation Vaccine Design against *Borrelia burgdorferi*: The Cause of Lyme Borreliosis. **2022,** 10, 1239 1
- 685 Structure of Human Enterovirus 70 and Its Inhibition by Capsid-Binding Compounds. 1
- 684 Universal mechanism of hormone and allosteric agonist mediated activation of glycoprotein hormone receptors as revealed by structures of follicle stimulating hormone receptor. 1
- 683 1,4-Dihydropyridinebutyrolactone-derived ring-opened ester and amide analogs targeting BET bromodomains. 1

- 682 Development of Enzymatic Variants for the Synthesis of Bioresorbable Polyesters. **2022**, 26, 2351-2363
- 681 Harmonin homology domains of human RTEL1 interact with replication protein A and DNA.
- 680 Design and Immunoinformatic Assessment of Candidate Multivariant mRNA Vaccine Construct against Immune Escape Variants of SARS-CoV-2. **2022**, 14, 3263 1
- 679 ERK2-topoisomerase II regulatory axis is important for gene activation in immediate early genes.
- 678 SARS-CoV-2 variants of concern: spike protein mutational analysis and epitope for broad neutralization. **2022**, 13, 1
- 677 Structural analysis of Red1 as a conserved scaffold of the RNA-targeting MTREC/PAXT complex. **2022**, 13, 0
- 676 Coupling to short linear motifs creates versatile PME-1 activities in PP2A holoenzyme demethylation and inhibition. 11, 0
- 675 Structural Comparison of hMDH2 Complexed with Natural Substrates and Cofactors: The Importance of Phosphate Binding for Active Conformation and Catalysis. **2022**, 12, 1175 0
- 674 CD8 coreceptor engagement of MR1 enhances antigen responsiveness by human MAIT and other MR1-reactive T cells. **2022**, 219, 0
- 673 Structural basis for cannabinoid-induced potentiation of alpha1-glycine receptors in lipid nanodiscs. **2022**, 13, 0
- 672 Molecular basis of anti-CRISPR operon repression by Aca10. **2022**, 50, 8919-8928 0
- 671 Robust total X-ray scattering workflow to study correlated motion of proteins in crystals.
- 670 Hormone- and antibody-mediated activation of the thyrotropin receptor. 1
- 669 Structures and mechanisms of the Arabidopsis auxin transporter PIN3. 0
- 668 Visualizing molecular interactions that determine assembly of a bullet-shaped vesicular stomatitis virus particle. **2022**, 13, 1
- 667 Molecular mechanism for strengthening E-cadherin adhesion using a monoclonal antibody. **2022**, 119, 0
- 666 Crystal structure of the Escherichia coli CusS kinase core. **2022**, 214, 107883 1
- 665 Structural characterization of the novel stress response facilitator (SrfA) from Pseudomonas aeruginosa. **2022**, 625, 147-153

664	Atomic resolution Cryo-EM structure of human proteasome activator PA28	2022, 219, 500-507	
663	High-resolution crystal structure of the anti-CRISPR protein AcrIC5.	2022, 625, 102-108	0
662	Exploiting reverse vaccinology approach for the design of a multiepitope subunit vaccine against the major SARS-CoV-2 variants.	2022, 101, 107754	0
661	Plant N -glycan breakdown by human gut Bacteroides.	2022, 119,	2
660	Calcium-induced environmental adaptability of the blood protein Vitronectin.	2022,	0
659	Structures reveal a key mechanism of WAVE regulatory complex activation by Rac1 GTPase.	2022, 13,	3
658	Molecular Characterization of Transesterification Activity of Novel Lipase Family I.1.		0
657	Cryo-EM structure of the type III-E CRISPR-Cas effector gRAMP in complex with TPR-CHAT.		0
656	Conserved intramolecular networks in GDAP1 are closely connected to CMT-linked mutations and protein stability.		0
655	Neuronal RNA granules are ribosome complexes stalled at the pre-translocation state.	2022, 434, 167801	0
654	Structures of Streptococcus pyogenes class A sortase in complex with substrate and product mimics provide key details of target recognition.	2022, 298, 102446	0
653	Characterisation of a Seneca Valley virus thermostable mutant.	2022, 575, 74-82	0
652	Expression, purification and structure determination of the chlorinase CIA2.	2022, 628, 64-67	0
651	Crystal structure of aldehyde dehydrogenase 1A1 from mouse.	2022, 628, 141-146	0
650	Structural basis for the substrate specificity of an S-formylglutathione hydrolase derived from Variovorax sp. PAMC 28711.	2022, 629, 159-164	1
649	Defining the structure-activity relationship for a novel class of allosteric MKP5 inhibitors.	2022, 243, 114712	0
648	Discovery of the 4-aminopiperidine-based compound EM127 for the site-specific covalent inhibition of SMYD3.	2022, 243, 114683	1
647	Overview and applications of map and model validation tools in the CCP-EM software suite.		0

646	Unveiling molecular details behind improved activity at neutral to alkaline pH of an engineered DyP-type peroxidase. 2022 , 20, 3899-3910	0
645	Virus-host interaction analysis in colorectal cancer identifies core virus network signature and small molecules. 2022 , 20, 4025-4039	0
644	Analysis of a novel class A β -lactamase OKP-B-6 of <i>Klebsiella quasipneumoniae</i> : structural characterisation and interaction with commercially available drugs. 117,	0
643	Structural and Dynamic Effects of Paraoxon Binding to Human Acetylcholinesterase by X-Ray Crystallography and Inelastic Neutron Scattering.	0
642	Druggable sites/pockets of the p53-DNAJA1 protein-protein interaction: In silico modeling and in vitro/in vivo validation. 2022 ,	0
641	Molecular mechanism of a large conformational change of the quinone cofactor in the semiquinone intermediate of bacterial copper amine oxidase. 2022 , 13, 10923-10938	2
640	Structural bases for aspartate recognition and polymerization efficiency of cyanobacterial cyanophycin synthetase. 2022 , 13,	0
639	Cryo-EM structures of the Mycobacterium 50S subunit reveal an intrinsic conformational dynamics of 23S rRNA helices.	0
638	Improved methodology for protein NMR structure calculation using hydrogen bond restraints and ANSURR validation: the SH2 domain of SH2B1.	0
637	Structure-Kinetic Relationship Studies for the Development of Long Residence Time LpxC Inhibitors. 2022 , 65, 11854-11875	0
636	Structural and biochemical evidence for the emergence of a calcium-regulated actin cytoskeleton prior to eukaryogenesis. 2022 , 5,	1
635	<i>Staphylococcus aureus</i> Exfoliative Toxin E, Oligomeric State and Flip of P186: Implications for Its Action Mechanism. 2022 , 23, 9857	1
634	CCP4 Cloud for structure determination and project management in macromolecular crystallography. 2022 , 78, 1079-1089	1
633	Biocomputational characterisation of MBO_200107 protein of <i>Mycobacterium tuberculosis</i> variant <i>caprae</i> : a molecular docking and simulation study. 1-20	0
632	Structural basis of substrate recognition by human tRNA splicing endonuclease TSEN.	0
631	Structural basis for directional chitin biosynthesis.	4
630	Structural characterization of human tryptophan hydroxylase 2 reveals L-Phe as the superior regulatory domain ligand relevant for serotonin biosynthesis.	0
629	Coiled-coil structure of meiosis protein TEX12 and conformational regulation by its C-terminal tip. 2022 , 5,	0

628	The structure, catalytic mechanism, and inhibitor identification of phosphatidylinositol remodeling MBOAT7.	1
627	Structural basis for breadth development in a HIV-1 neutralizing antibody.	0
626	Extended N-Terminal Acetyltransferase Naa50 in Filamentous Fungi Adds to Naa50 Diversity. 2022 , 23, 10805	0
625	Potential of Epidermal Growth Factor-like Peptide from the Sea Cucumber <i>Stichopus horrens</i> to Increase the Growth of Human Cells: In Silico Molecular Docking Approach. 2022 , 20, 596	0
624	Structure of the Monkeypox virus profilin-like protein A42R reveals potential functional differences from cellular profilins. 2022 , 78, 371-377	3
623	Structure-based prediction of Ras-effector binding affinities and design of Branchegetic Interface mutations.	0
622	Topological crossing in the misfolded <i>Tetrahymena</i> ribozyme resolved by cryo-EM. 2022 , 119,	0
621	Hybrid in vitro/in silico analysis of low-affinity protein-protein interactions that regulate signal transduction by Sema6D.	1
620	Crystallographic analysis of engineered polymerases synthesizing phosphonomethylthreosyl nucleic acid. 2022 , 50, 9663-9674	0
619	Crystallographic and X-ray scattering study of RdfS, a recombination directionality factor from an integrative and conjugative element. 2022 , 78, 1210-1220	0
618	Identification of a cross-neutralizing antibody that targets the receptor binding site of H1N1 and H5N1 influenza viruses. 2022 , 13,	1
617	Microsecond MD Simulations to Explore the Structural and Energetic Differences between the Human RXR β vs. RXR β DNA. 2022 , 27, 5778	0
616	Development and Characterization of Type I, Type II, and Type III LIM-Kinase Chemical Probes.	1
615	Molecular interactions of FG nucleoporin repeats at high resolution.	0
614	A small molecule antagonist of SMN disrupts the interaction between SMN and RNAP II. 2022 , 13,	0
613	Plant-specific HDT family histone deacetylases are nucleoplasmins.	0
612	Computational identification of a systemic antibiotic for Gram-negative bacteria. 2022 , 7, 1661-1672	1
611	Structural and large-scale analysis unveil the intertwined paths promoting NMT-catalyzed lysine and glycine myristoylation. 2022 , 167843	2

610	Embiggin facilitates monocarboxylate transporter 1 localization to the plasma membrane and transition to a decoupling state. 2022 , 40, 111343	0
609	Membrane-bound mRNA immunogens lower the threshold to activate HIV Env V2 apex-directed broadly neutralizing B cell precursors in humanized mice. 2022 ,	0
608	Viruses inhibit TIR gcADPR signaling to overcome bacterial defense.	2
607	Combined Structural Analysis and Molecular Dynamics Reveal Penicillin-Binding Protein Inhibition Mode with β -Lactones.	1
606	Methotrexate recognition by the human reduced folate carrier SLC19A1. 2022 , 609, 1056-1062	1
605	The hemolysin A secretion system is a multi-engine pump containing three ABC transporters. 2022 , 185, 3329-3340.e13	1
604	In silico identification of potential inhibitors of vital monkeypox virus proteins from FDA approved drugs.	0
603	Structural insights into cyanobacterial RuBisCO assembly coordinated by two chaperones Raf1 and RbcX. 2022 , 8,	0
602	Structural studies reveal that endosomal cations promote formation of infectious CVA9 A particles, facilitating RNA and VP4 release.	0
601	NMR Structures of Calmodulin Bound to Two Separate Regulatory Sites in the Retinal Cyclic Nucleotide-Gated Channel. 2022 , 61, 1955-1965	0
600	Structural insights into human CCAN complex assembled onto DNA. 2022 , 8,	0
599	Hierarchical sequence-affinity landscapes shape the evolution of breadth in an anti-influenza receptor binding site antibody.	0
598	Cryo-EM structures of human m6A writer complexes.	1
597	Comprehensive analysis predicting effects of deleterious SNPs of human progesterone receptor gene on its structure and functions: a computational approach. 1-16	0
596	Unique Structural Fold of LonBA Protease from <i>Bacillus subtilis</i> , a Member of a Newly Identified Subfamily of Lon Proteases. 2022 , 23, 11425	0
595	Allosteric regulation and crystallographic fragment screening of SARS-CoV-2 NSP15 endoribonuclease.	0
594	Investigating the active oxidants involved in cytochrome P450 catalyzed sulfoxidation reactions.	0
593	A monoclonal antibody targeting the Nipah virus fusion glycoprotein apex imparts protection from disease.	0

592	Human immunoglobulin repertoire analysis guides design of vaccine priming immunogens targeting HIV V2-apex broadly neutralizing antibody precursors. 2022,	1
591	Structural insights into the formation of repulsive Netrin guidance complexes.	0
590	Mechanism by which T7 bacteriophage protein Gp1.2 inhibits Escherichia coli dGTPase. 2022, 119,	0
589	X-ray crystallographic characterization of the SARS-CoV-2 main protease polyprotein cleavage sites essential for viral processing and maturation. 2022, 13,	4
588	Functional and Structural Characterization of OXA-935, a Novel OXA-10-Family β -Lactamase from <i>Pseudomonas aeruginosa</i> .	0
587	Structures of β -synuclein filaments from human brains with Lewy pathology.	5
586	Putative SET-domain methyltransferases in <i>Cryptosporidium parvum</i> and histone methylation during infection. 2022, 13, 1632-1650	1
585	Cryo-EM of prion strains from the same genotype of host identifies conformational determinants.	0
584	Structural basis of adhesion GPCR GPR110 activation by stalk peptide and G-proteins coupling. 2022, 13,	0
583	Cytomotive actins and tubulins share a polymerisation switch mechanism conferring robust dynamics.	0
582	ADMET study, spectroscopic characterization and effect of synthetic nitro chalcone in combination with norfloxacin, ciprofloxacin, and ethidium bromide against <i>Staphylococcus aureus</i> efflux pumps.	0
581	Modulation of Drug Resistance by Furanochromones in NorA Overexpressing <i>Staphylococcus Aureus</i> . 2022, 2022, 1-7	1
580	Structure-Function analysis of <i>Lactiplantibacillus plantarum</i> DltE reveals D-alanylated lipoteichoic acids as direct symbiotic cues supporting <i>Drosophila</i> juvenile growth.	0
579	Autoprocessing and oxyanion loop reorganization upon GC373 and nirmatrelvir binding of monomeric SARS-CoV-2 main protease catalytic domain. 2022, 5,	0
578	When two β a crowd - Structural mapping of PEAK pseudokinase interactions identifies 14-3-3 as a molecular switch for PEAK3/Crk signaling.	0
577	A possible mechanism of Cry7Ab4 protein in delaying pupation of <i>Plutella xylostella</i> larvae. 13,	0
576	Atomic resolution studies of S1 nuclease complexes reveal details of RNA interaction with the enzyme despite multiple lattice-translocation defects. 2022, 78, 1194-1209	0
575	Commercial influenza vaccines vary in both the structural arrangements of HA complexes and in induction of antibodies to cross-reactive HA epitopes.	0

574	Assessing the effects of β -triketone herbicides on HPPD from environmental bacteria using a combination of in silico and microbiological approaches.	0
573	Structural basis for APE1 processing DNA damage in the nucleosome. 2022 , 13,	1
572	Design of the SARS-CoV-2 RBD vaccine antigen improves neutralizing antibody response. 2022 , 8,	1
571	Dynamics of the secreted frizzled related protein Sizzled and potential implications for binding to bone morphogenetic protein-1 (BMP-1). 2022 , 12,	0
570	Top-down design of protein nanomaterials with reinforcement learning.	0
569	Structural basis for the transformation of the traditional medicine berberine by bacterial nitroreductase. 2022 , 78, 1273-1282	0
568	A fungal tolerance trait and selective inhibitors proffer HMG-CoA reductase as a herbicide mode-of-action. 2022 , 13,	0
567	Crystal structure of Arabidopsis DWARF14-LIKE2 (DLK2) reveals a distinct substrate binding pocket architecture. 2022 , 6,	0
566	Structure of the Ebola virus polymerase complex.	1
565	Cyclic ADP ribose isomers: Production, chemical structures, and immune signaling. 2022 , 377,	1
564	Structure and Specificity of an Anti-Chloramphenicol Single Domain Antibody for Detection of Amphenicol Residues.	0
563	Structural basis of nirmatrelvir and ensitrelvir resistance profiles against SARS-CoV-2 Main Protease naturally occurring polymorphisms.	1
562	Cryo-electron microscopy and image classification reveal the existence and structure of the coxsackievirus A6 virion. 2022 , 5,	0
561	Structural conservation of Lassa virus glycoproteins and recognition by neutralizing antibodies.	0
560	Aromatic Ring Fluorination Patterns Modulate Inhibitory Potency of Fluorophenylhydroxamates Complexed with Histone Deacetylase 6. 2022 , 61, 1945-1954	0
559	Structural Basis of Substrate Promiscuity and Catalysis by the Reverse Prenyltransferase N-Dimethylallyl-L-tryptophan Synthase from <i>Fusarium fujikuroi</i> . 2022 , 61, 2025-2035	0
558	Structural Basis of Peptide-Based Antimicrobial Inhibition of a Resistance-Nodulation-Cell Division Multidrug Efflux Pump.	0
557	Structural and functional characterization of Cas2 of CRISPR-Cas subtype I-C lacking the CRISPR component. 9,	0

556	Homology Modeling Epitopes of Kirsten Rat Sarcoma (KRAS) G12D, G12V and G12R as Pancreatic Ductal Adenocarcinoma Vaccine Candidates.	0
555	Structural basis for strychnine activation of human bitter taste receptor TAS2R46. 2022 , 377, 1298-1304	1
554	Structural insights into cardiolipin stabilization of yeast respiratory supercomplexes revealed byCryo-EM.	0
553	Structural basis of microRNA biogenesis by Dicer-1 and its partner protein Loqs-PB. 2022 ,	0
552	Improved mammalian retromer cryo-EM structures reveal a new assembly interface. 2022 , 102523	1
551	A potent synthetic nanobody with broad-spectrum activity neutralizes SARS-CoV-2 virus and the Omicron variant BA.1 through a unique binding mode. 2022 , 20,	0
550	Crystal structure and sugar-binding ability of the C-terminal domain of N-acetylglucosaminyltransferase IV establish a new carbohydrate-binding module family.	0
549	Structure of an iminosugar complex of a glycoside hydrolase family 5 lichenase provides insights into the active site. 2022 ,	0
548	Structure and mechanism of human cystine exporter cystinosin. 2022 , 185, 3739-3752.e18	1
547	Structural basis for the allosteric inhibition of hypoxia-inducible factor (HIF)-2 by belzutifan. MOLPHARM-AR-2022-000	0
546	Structural basis for the activity regulation of a potassium channel AKT1 from Arabidopsis. 2022 , 13,	0
545	Structural studies of cilia and flagella associated protein 410 (CFAP410) reveal its bimodular organization with an N-terminal LRR motif and a C-terminal tetrameric helical bundle.	0
544	Slow protein dynamics probed by time-resolved oscillation crystallography at room temperature. 2022 , 9,	0
543	Robust residue-level error detection in cryo-electron microscopy models.	0
542	Molecular insights into antibody-mediated protection against the prototypic simian immunodeficiency virus. 2022 , 13,	0
541	Molecular Determinants for Differential Activation of the Vibrio parahaemolyticus Bile Acid Receptor.	0
540	Structural characterization of SARS-CoV-2 dimeric ORF9b reveals potential fold-switching trigger mechanism.	0
539	A grappling hook interaction balances self-assembly and chaperone activity of Nucleophosmin 1.	0

538	The lysosomal transporter TAPL has a dual role as peptide translocator and phosphatidylserine floppase. 2022 , 13,	0
537	High-resolution structure of a microtubule-like tube composed of FtsZ fibronobody complexes.	0
536	Structures of +1 nucleosome-bound PIC-Mediator complex. 2022 , 378, 62-68	2
535	Signaling snapshots of a serotonin receptor activated by the prototypical psychedelic LSD. 2022 , 110, 3154-3167.e7	1
534	Structure of the two-component S-layer of the archaeon <i>Sulfolobus acidocaldarius</i> .	0
533	NMR-guided directed evolution.	1
532	A review of MMP-2 structures and binding mode analysis of its inhibitors to strategize structure-based drug design. 2022 , 117044	1
531	Mechanistic insights into allosteric regulation of methylated DNA and histone H3 recognition by SRA and SET domains of SUVH5 and the basis for di-methylation of lysine residue.	1
530	The crystal structure of a simian Foamy Virus receptor binding domain provides clues about entry into host cells.	0
529	Prion-like low complexity regions enable avid virus-host interactions during HIV-1 infection. 2022 , 13,	0
528	High-resolution structures of a siderophore-producing cyclization domain from <i>Yersinia pestis</i> offer a refined proposal of substrate binding. 2022 , 298, 102454	0
527	SPACA9 is a luminal protein of human ciliary singlet and doublet microtubules. 2022 , 119,	2
526	Structural and Mechanistic Bases of Viral Resistance to HIV-1 Capsid Inhibitor Lenacapavir.	1
525	The dimeric form of bacterial L-asparaginase YpAI is fully active.	0
524	DNA-delivered antibody cocktail exhibits improved pharmacokinetics and confers prophylactic protection against SARS-CoV-2. 2022 , 13,	1
523	Identifying well-folded de novo proteins in the new era of accurate structure prediction. 9,	0
522	Crystal structure of the Phospholipase A and acyltransferase 4 (PLAAT4) catalytic domain. 2022 , 107903	0
521	Oxidation of bisphenol A (BPA) and related compounds by the multifunctional catalytic globin dehaloperoxidase. 2022 , 112020	0

520	Structural and inhibitor sensitivity analysis of influenza B-like viral neuraminidases derived from Asiatic toad and spiny eel. 2022 , 119,	0
519	Metal ion interactions with nucleic acids. 2022 ,	0
518	A Novel Missense Mutation in ERCC8 Co-Segregates with Cerebellar Ataxia in a Consanguineous Pakistani Family. 2022 , 11, 3090	0
517	Molecular structures reveal synergistic rescue of B08 CFTR by Trikafta modulators. 2022 , 378, 284-290	2
516	Computationally restoring the potency of a clinical antibody against SARS-CoV-2 Omicron subvariants.	0
515	Molecular basis of dual anti-CRISPR and auto-regulatory functions of AcrIF24.	0
514	Structural foundation for the role of enterococcal PrgB in conjugation, biofilm formation and virulence.	0
513	Three-dimensional structure of a mycobacterial oligoribonuclease reveals a unique C-terminal tail that stabilizes the homodimer. 2022 , 102595	0
512	High Efficacy and Drug Synergy of HDAC6-Selective Inhibitor NN-429 in Natural Killer (NK)/T-Cell Lymphoma. 2022 , 15, 1321	0
511	Rapid and efficient room-temperature serial synchrotron crystallography using the CFEL TapeDrive. 2022 , 9, 778-791	0
510	Characterization of two rice GH18 chitinases belonging to family 8 of plant pathogenesis-related proteins. 2022 , 111524	1
509	Structural and functional investigation of the human snRNP assembly factor AAR2 in complex with the RNase H-like domain of PRPF8. 2022 , 78, 1373-1383	0
508	CYP153A71 from <i>Alcanivorax dieselolei</i> : Oxidation beyond Monoterminal Hydroxylation of n-Alkanes. 2022 , 12, 1213	0
507	Novel chimeric proteins mimicking SARS-CoV-2 spike epitopes with broad inhibitory activity. 2022 ,	1
506	Ligand recognition and allosteric modulation of the human MRGPRX1 receptor.	0
505	Structure-function studies can improve binding affinity of cohesin-dockerin interactions for multi-protein assemblies. 2022 ,	0
504	Functional selectivity of insulin receptor revealed by aptamer-trapped receptor structures. 2022 , 13,	0
503	Broad SARS-CoV-2 Neutralization by Monoclonal and Bispecific Antibodies Derived from a Gamma-infected Individual.	0

502	Stochastic chain termination in bacterial pilus assembly.	0
501	Structural journey of an insecticidal pore-forming protein targeting western corn rootworm.	0
500	Ensemble-function relationships to dissect mechanisms of enzyme catalysis. 2022 , 8,	1
499	Structural analysis of human papillomavirus E6 interactions with Scribble PDZ domains.	0
498	Structural Genomics of the Human Dopamine Receptor System.	0
497	Structural Insights into the Chaperone-Assisted Assembly of a Simplified Tail Fiber of the Myocyanophage Pam3. 2022 , 14, 2260	0
496	Helical ultrastructure of the metalloprotease meprin Bn complex with a small molecule inhibitor. 2022 , 13,	2
495	Allelic compatibility in plant immune receptors facilitates engineering of new effector recognition specificities.	1
494	Structural basis for the toxin-coregulated pilus-dependent secretion of Vibrio cholerae colonization factor. 2022 , 8,	0
493	How a methanogen assimilates sulfate: Structural and functional elucidation of the complete sulfate-reduction pathway.	0
492	Bestrophin-2 and glutamine synthetase form a complex for glutamate release. 2022 , 611, 180-187	0
491	Structural and functional analyses of a GPCR-inhibited ion channel TRPM3. 2022 ,	2
490	Evasion of cGAS and TRIM5 defines pandemic HIV. 2022 , 7, 1762-1776	0
489	YcaO-mediated ATP-dependent peptidase activity in ribosomal peptide biosynthesis.	0
488	Molecular basis for isoform-selective inhibition of presenilin-1 by MRK-560. 2022 , 13,	0
487	Relief of CoA sequestration and restoration of mitochondrial function in a mouse model of propionic acidemia.	1
486	Structure and flexibility of the yeast NuA4 histone acetyltransferase complex. 11,	0
485	Mechanism of the Initial Tubulin Nucleation Phase. 2022 , 13, 9725-9735	0

- 484 A dynamic rRNA ribomethylome drives stemness in acute myeloid leukemia. 0
- 483 Activation mechanism of the mouse cold-sensing TRPM8 channel by cooling agonist and PIP 2. **2022**, 378, 0
- 482 The unifying catalytic mechanism of the RING-between-RING E3 ligase family. 0
- 481 Substrate selectivity of the PRDM9 lysine methyltransferase domain. 0
- 480 Structural insights into adhesion GPCR ADGRL3 activation and Gq, Gs, Gi, and G12 coupling. **2022**, 0
- 479 Inhibition mechanism of NKCC1 involves the carboxyl terminus and long-range conformational coupling. **2022**, 8, 0
- 478 Prevalence and mechanisms of evolutionary contingency in human influenza H3N2 neuraminidase. **2022**, 13, 0
- 477 Structural Basis for the Immunogenicity of the C-Terminus of VP1 of Echovirus 3 Revealed by the Binding of a Neutralizing Antibody. **2022**, 14, 2322 0
- 476 Structural basis for HflXr-mediated antibiotic resistance in *Listeria monocytogenes*. 1
- 475 Lineage-mosaic and mutation-patched spike proteins for broad-spectrum COVID-19 vaccine. **2022**, 0
- 474 HBcompare: Classifying Ligand Binding Preferences with Hydrogen Bond Topology. **2022**, 12, 1589 0
- 473 Structure and Dynamics of Human Chemokine CCL16 Implications for Biological Activity. **2022**, 12, 1588 0
- 472 Structural basis for ion selectivity in potassium-selective channelrhodopsins. 0
- 471 Molecular recognition of two endogenous hormones by the human parathyroid hormone receptor-1. 0
- 470 In silico characterization of cysteine-stabilized β defensins from neglected unicellular microeukaryotes. 0
- 469 A selective and orally bioavailable VHL-recruiting PROTAC achieves SMARCA2 degradation in vivo. **2022**, 13, 5
- 468 Atomic model of vesicular stomatitis virus and mechanism of assembly. **2022**, 13, 1
- 467 A second type of N7-guanine RNA cap methyltransferase in an unusual locus of a large RNA virus genome. 0

466	In vitro structural maturation of an early stage pre-40S particle coupled with U3 snoRNA release and central pseudoknot formation.	0
465	Improved NMR-data-compliant protein structure modeling captures context-dependent variations and expands the scope of functional inference.	0
464	Broadly neutralizing SARS-CoV-2 antibodies through epitope-based selection from convalescent patients.	0
463	Synthesis, Characterization, Optical Properties, Molecular Modeling and Urease Inhibition Analysis of Organic Ligands and Their Metal Complexes.	0
462	In Silico Methods for Identification of Potential Active Sites of Therapeutic Targets. 2022 , 27, 7103	0
461	Cryo-EM Structure of Gokushovirus β C6098 Reveals a Novel Capsid Architecture for a Single-Scaffolding Protein, Microvirus Assembly System.	0
460	Neutralizing monoclonal antibodies elicited by mosaic RBD nanoparticles bind conserved sarbecovirus epitopes. 2022 ,	2
459	A multiscale modeling method for therapeutic antibodies in ion exchange chromatography.	0
458	Evolution of increased complexity and specificity at the dawn of form I Rubiscos. 2022 , 378, 155-160	2
457	Binding of Glycerol to Human Galectin-7 Expands Stability and Modulates Its Functions. 2022 , 23, 12318	0
456	Purification and structural characterization of the Na ⁺ -translocating ferredoxin: NAD ⁺ reductase (Rnf) complex of Clostridium tetanomorphum. 2022 , 13,	2
455	Structural basis for Cas9 off-target activity. 2022 , 185, 4067-4081.e21	1
454	Isoform-specific inhibition of FGFR signaling achieved by a de-novo-designed mini-protein. 2022 , 41, 111545	0
453	Prospecting in silico antibacterial activity of a peptide from trypsin inhibitor isolated from tamarind seed. 2023 , 38, 67-83	0
452	Cryo-EM structures of the translocational binary toxin complex CDTa-bound CDTb-pore from Clostridioides difficile. 2022 , 13,	0
451	Bio-Computational Evaluation of Compounds of Bacopa Monnieri as a Potential Treatment for Schizophrenia. 2022 , 27, 7050	0
450	Rab7 Investigation Insights into the Existence of White Spot Syndrome Virus in Crustaceans: An In Silico Approach. 2022 , 2022, 1-16	0
449	Polyelectrolyte coating of cryo-EM grids improves lateral distribution and prevents aggregation of macromolecules. 2022 , 78, 1337-1346	0

448	Discovering cell-active BCL6 inhibitors: effectively combining biochemical HTS with multiple biophysical techniques, X-ray crystallography and cell-based assays. 2022 , 12,	0
447	Unmasking the conformational stability and inhibitor binding to SARS-CoV-2 main protease active site mutants and miniprecursor. 2022 , 167876	0
446	Structural and dynamic effects of paraoxon binding to human acetylcholinesterase by X-ray crystallography and inelastic neutron scattering. 2022 , 30, 1538-1549.e3	1
445	Structure and inhibition of SARS-CoV-1 and SARS-CoV-2 main proteases by oral antiviral compound AG7404. 2022 , 105458	0
444	Cryo-EM structures of mitochondrial respiratory complex I from <i>Drosophila melanogaster</i> .	0
443	Functional E3 ligase hotspots and resistance mechanisms to small-molecule degraders.	2
442	The nucleoplasmic phase of pre-40S formation prior to nuclear export.	1
441	Structural Basis for Rabbit Hemorrhagic Disease Virus Antibody Specificity.	0
440	Crystal structure of a nucleotide-binding domain of fatty acid kinase FakA from <i>Thermus thermophilus</i> HB8. 2022 , 214, 107904	0
439	Theoretical evaluation of the malathion and its chemical derivatives interaction with cytosolic phospholipase A2 from zebrafish. 2023 , 311, 136984	0
438	An intermolecular hydrogen bonded network in the PRELID-TRIAP protein family plays a role in lipid sensing. 2023 , 1871, 140867	0
437	In silico identification of potential inhibitors of vital monkeypox virus proteins from FDA approved drugs.	1
436	The 3D structure of lipidic fibrils of β -synuclein. 2022 , 13,	1
435	Structural insights at acidic pH of Dye-decolorizing peroxidase from <i>Bacillus subtilis</i> .	0
434	Half-calcified calmodulin promotes basal activity and inactivation of the L-type calcium channel CaV1.2. 2022 , 102701	2
433	SARS-CoV-2 spike conformation determines plasma neutralizing activity elicited by a wide panel of human vaccines.	4
432	Cross-linking mass spectrometry discovers, evaluates, and validates the experimental and predicted structural proteome.	0
431	Mechanochemical tuning of a kinesin motor essential for malaria parasite transmission. 2022 , 13,	0

430	An LH1RC photocomplex from an extremophilic phototroph provides insight into origins of two photosynthesis proteins. 2022 , 5,	2
429	Antigenic mapping reveals sites of vulnerability on HCoV spike protein. 2022 , 5,	0
428	Structure insights into selective coupling of G protein subtypes by a class B G protein-coupled receptor. 2022 , 13,	1
427	Data on structural analysis of cholesterol binding and sterol selectivity by ABCG5/G8. 2022 , 108754	0
426	Cryo-EM reveals the conformational epitope of human monoclonal antibody PAM1.4 broadly reacting with polymorphic malarial protein VAR2CSA. 2022 , 18, e1010924	0
425	Rare, convergent antibodies targeting the stem helix broadly neutralize diverse betacoronaviruses. 2022 ,	0
424	A microbial transporter of the dietary antioxidant ergothioneine. 2022 ,	2
423	Common structural attributes of Tyrosinase variants are unlikely to determine differential retentions within Endoplasmic Reticulum: A modelling study with 45 variants.	0
422	Structures of the Ndc80 complex and its interactions at the yeast kinetochore-microtubule interface.	1
421	Structural dynamics of AAA + ATPase Drg1 and mechanism of benzo-diazaborine inhibition. 2022 , 13,	0
420	Molecular recognition of morphine and fentanyl by the human μ opioid receptor. 2022 , 185, 4361-4375.e19	3
419	Cryo-EM of prion strains from the same genotype of host identifies conformational determinants. 2022 , 18, e1010947	0
418	The Nse5/6-like SIMC1-SLF2 complex localizes SMC5/6 to viral replication centers. 11,	0
417	Mutation-Guided Vaccine Design: A Strategy for Developing Boosting Immunogens for HIV Broadly Neutralizing Antibody Induction.	0
416	Development of Fluorinated Peptoid-Based Histone Deacetylase (HDAC) Inhibitors for Therapy-Resistant Acute Leukemia.	2
415	An epitope-enriched immunogen expands responses to a conserved viral site. 2022 , 41, 111628	0
414	Ion selectivity mechanism of the MgtE channel for Mg ²⁺ over Ca ²⁺ . 2022 , 105565	0
413	Gold-Based Metal Drugs as Inhibitors of Coronavirus Proteins: The Inhibition of SARS-CoV-2 Main Protease by Auranofin and Its Analogs. 2022 , 12, 1675	0

412	Structural Basis for (2R,3R)-Taxifolin Binding and Reaction Products to the Bacterial Chalcone Isomerase of <i>Eubacterium ramulus</i> . 2022 , 27, 7909	0
411	Engineering a Conformationally Switchable Artificial Metalloprotein.	0
410	Structural basis of sRNA RsmZ regulation of <i>Pseudomonas aeruginosa</i> virulence.	0
409	Understanding VPAC receptor family peptide binding and selectivity. 2022 , 13,	0
408	Neutralizing epitopes on <i>Clostridioides difficile</i> toxin A revealed by the structures of two camelid VHH antibodies. 13,	0
407	Structural basis for mechanotransduction in a potassium-dependent mechanosensitive ion channel. 2022 , 13,	1
406	Glycolytic flux control by drugging phosphoglycolate phosphatase. 2022 , 13,	0
405	Structure of <i>Escherichia coli</i> heat shock protein Hsp15 in complex with the ribosomal 50S subunit bearing peptidyl-tRNA.	0
404	Regulation of ATAD2B bromodomain binding activity by the histone code.	0
403	Dynamic and thermodynamic impact of L94A, W100A, and W100L mutations on the D2 dopamine receptor bound to risperidone.	0
402	Cryo-EM structures reveal the activation and substrate recognition mechanism of human enteropeptidase. 2022 , 13,	0
401	Aim18p and Aim46p are CHI-domain-containing mitochondrial hemoproteins in <i>Saccharomyces cerevisiae</i> ..	0
400	Microtubule binding-induced allostery promotes LIS1 dissociation from dynein prior to cargo transport.	0
399	The in silico and in vitro analysis of donepezil derivatives for <i>Anopheles</i> acetylcholinesterase inhibition. 2022 , 17, e0277363	0
398	Cryo-EM structure of the human sodium-chloride cotransporter NCC. 2022 , 8,	0
397	Pea and Lentil 7S Globulin Crystal Structures with Comparative Immunoglobulin Epitope Mapping. 2022 , 100146	0
396	TOPOVIBL-REC114 interaction regulates meiotic DNA double-strand breaks. 2022 , 13,	1
395	Structure of the catalytically active APOBEC3G bound to a DNA oligonucleotide inhibitor reveals tetrahedral geometry of the transition state. 2022 , 13,	0

- 394 BtuB TonB-dependent transporters and BtuG surface lipoproteins form stable complexes for vitamin B12 uptake in gut Bacteroides. ○
- 393 Accelerating crystal structure determination with iterative AlphaFold prediction. ○
- 392 Crystal structure of the OrfX1-OrfX3 complex from the PMP1 neurotoxin gene cluster. ○
- 391 Dynamic and thermodynamic impact of L94A, W100A, and W100L mutations on the D2 dopamine receptor bound to risperidone. **2022**, 12, 34359-34368 ○
- 390 A mutagenic analysis of NahE, a hydratase-aldolase in the naphthalene degradative pathway. **2023**, 733, 109471 ○
- 389 Protein model refinement for cryo-EM maps using AlphaFold2 and the DAQ score. **2023**, 79, 1
- 388 A dimer-monomer transition captured by the crystal structures of cyanobacterial apo flavodoxin. **2023**, 639, 134-141 ○
- 387 Structure of fish TRAF4 and its implication in TRAF4-mediated immune cell and platelet signaling. **2023**, 132, 108462 ○
- 386 Room-temperature serial synchrotron crystallography of the human phosphatase PTP1B. **2023**, 79, 23-30 1
- 385 In Vitro and in Silico Insights on the Biological Activities, Phenolic Compounds Composition of Hypericum perforatum L. Hairy Root Cultures. **2023**, 92, 921-941 ○
- 384 The structure of a tautomerase superfamily member linked to the type VI secretion system of Acinetobacter baumannii. **2023**, 79, 8-16 ○
- 383 Structural and biochemical characterization of Leptospira interrogans Lsa45 reveals a penicillin-binding protein with esterase activity. **2023**, 125, 141-153 ○
- 382 Cyclization strategy leads to highly potent Bromodomain and extra-terminal (BET) Bromodomain inhibitors for the treatment of acute liver injury. **2023**, 247, 115023 ○
- 381 Structural Insight Into hnRNP A2/B1 Homodimerization and DNA Recognition. **2023**, 435, 167920 ○
- 380 X-ray structure of human aldo-keto reductase 1C3 in complex with a bile acid fused tetrazole inhibitor: experimental validation, molecular docking and structural analysis. ○
- 379 Structures of transcription preinitiation complex engaged with the +1 nucleosome. 1
- 378 Human neutralizing antibodies to cold linear epitopes and to subdomain 1 of SARS-CoV-2. ○
- 377 Simultaneous solving high-resolution structures of various enzymes from human kidney microsomes. **2023**, 6, e202201580 ○

376	Structure-based engineering of minimal Proline dehydrogenase domains for inhibitor discovery.	0
375	Mechanism of high-mannose N-glycan breakdown and metabolism by <i>Bifidobacterium longum</i> .	1
374	Comparative study of binding pocket structure and dynamics in cardiac and skeletal myosin. 2022 ,	0
373	Crystal structure of <i>Sphingobacterium multivorum</i> serine palmitoyltransferase complexed with tris(hydroxymethyl)aminomethane. 2022 , 78, 408-415	0
372	Inhibition and Mechanism of <i>Plasmodium falciparum</i> Hypoxanthine-Guanine-Xanthine Phosphoribosyltransferase. 2022 , 17, 3407-3419	0
371	Integrating model simulation tools and cryo-electron microscopy.	0
370	High-density binding to <i>Plasmodium falciparum</i> circumsporozoite protein repeats by inhibitory antibody elicited in mouse with human immunoglobulin repertoire. 2022 , 18, e1010999	0
369	Multi-Epitope Vaccine Design against Monkeypox Virus via Reverse Vaccinology Method Exploiting Immunoinformatic and Bioinformatic Approaches. 2022 , 10, 2010	1
368	A class-mismatched TCR bypasses MHC restriction via an unorthodox but fully functional binding geometry. 2022 , 13,	0
367	Antiviral signaling by a cyclic nucleotide activated CRISPR protease.	0
366	A cryo-electron microscopic approach to elucidate protein structures from human brain microsomes. 2023 , 6, e202201724	0
365	The free fatty acid-binding pocket is a conserved hallmark in pathogenic β -coronavirus spike proteins from SARS-CoV to Omicron. 2022 , 8,	0
364	Structural insights into the rational design of a nanobody that binds with high affinity to the SARS-CoV-2 spike variant.	0
363	Molecular basis for selective activation of DREADD-based chemogenetics. 2022 , 612, 354-362	3
362	Conformational changes in mitochondrial complex I of the thermophilic eukaryote <i>Chaetomium thermophilum</i> . 2022 , 8,	2
361	Structure of monkeypox virus DNA polymerase holoenzyme.	3
360	Structural transitions during the cooperative assembly of baculovirus single-stranded DNA-binding protein on ssDNA.	0
359	Structural basis for a human broadly neutralizing influenza A hemagglutinin stem-specific antibody including H17/18 subtypes. 2022 , 13,	0

- 358 Two structural switches in HIV-1 capsid regulate capsid curvature and host factor binding. 0
- 357 VASH1 β VBP and VASH2 β VBP generate different detyrosination profiles on microtubules. **2023**, 222, 0
- 356 Electron microscopy holdings of the Protein Data Bank: the impact of the resolution revolution, new validation tools, and implications for the future. 0
- 355 Multiple sub-state structures of SERCA2b reveal conformational overlap at transition steps during the catalytic cycle. **2022**, 41, 111760 1
- 354 Structural Studies Reveal that Endosomal Cations Promote Formation of Infectious Coxsackievirus A9 A-Particles, Facilitating RNA and VP4 Release. **2022**, 96, 0
- 353 Molecular mechanism of antibody neutralization of coxsackievirus A16. **2022**, 13, 0
- 352 Mechanism of ATP hydrolysis dependent rotation of ATP synthases. 0
- 351 X-ray structure and mechanism of ZgHAD , a l -2-haloacid dehalogenase from the marine Flavobacterium Zobellia galactanivorans. **2023**, 32, 0
- 350 Mechanism of IFT-A polymerization into trains for ciliary transport. **2022**, 185, 4986-4998.e12 0
- 349 Structural basis for translation inhibition by the glycosylated antimicrobial peptide Drosocin from *Drosophila melanogaster*. 0
- 348 An epitope-enriched immunogen increases site targeting in germinal centers. 0
- 347 CryoEM structures of anion exchanger 1 capture multiple states of inward- and outward-facing conformations. **2022**, 5, 3
- 346 IL-2 is inactivated by the acidic pH environment of tumors enabling engineering of a pH-selective mutein. **2022**, 7, 1
- 345 High relatedness of bioinformatic data and realistic experimental works on the potentials of *Fasciola hepatica* and *F. gigantica* cathepsin L1 as a diagnostic and vaccine antigen. 10, 0
- 344 Structural basis for the assembly of the type V CRISPR-associated transposon complex. **2022**, 185, 4999-5010.e17 0
- 343 Molecular Basis for Non-Covalent, Non-Competitive FAAH Inhibition. **2022**, 23, 15502 0
- 342 Calmodulin variant E140G associated with long QT syndrome impairs CaMKII β autophosphorylation and L-type calcium channel (Cav1.2) inactivation. **2022**, 102777 0
- 341 Structural and Mechanistic Basis of Substrate Transport by the Multidrug Transporter MRP4. 0

- 340 Cryo-EM structure of the plant nitrate transporter AtCLCa reveals characteristics of the anion binding site and the ATP binding pocket. **2022**, 102833 ○
- 339 Cannabinoid non-cannabidiol site modulation of TRPV2 structure and function. **2022**, 13, ○
- 338 G1A Activates PIP2 Hydrolysis by Recruiting and Orienting PLCβ on the Membrane Surface. ○
- 337 Molecular recognition of two endogenous hormones by the human parathyroid hormone receptor-1. 1
- 336 Structure of the AlgKX modification and secretion complex required for alginate production and biofilm attachment in *Pseudomonas aeruginosa*. **2022**, 13, ○
- 335 A new polymorphism of human amylin fibrils with similar protofilaments and a conserved core. **2022**, 25, 105705 ○
- 334 Integrative structural and functional analysis of human malic enzyme 3: A potential therapeutic target for pancreatic cancer. **2022**, 8, e12392 ○
- 333 Improvement of protein tertiary and quaternary structure predictions using the ReFOLD4 refinement method and the AlphaFold2 recycling process. ○
- 332 A central helical fulcrum in eIF2B coordinates allosteric regulation of Integrated Stress Response signaling. ○
- 331 Crystal structure and solution state of the C-terminal head region of the narxovirus receptor binding protein. ○
- 330 The structure of caseinolytic protease subunit ClpP2 reveals a functional model of the caseinolytic protease system from *Chlamydia trachomatis*. **2022**, 102762 ○
- 329 Structural basis of the acyl-transfer mechanism of human GPAT1. ○
- 328 Extensive substrate recognition by the streptococcal antibody-degrading enzymes IdeS and EndoS. **2022**, 13, ○
- 327 Characterization of the high-affinity anti-CTLA-4 monoclonal antibody JS007 for immune checkpoint therapy of cancer. **2023**, 15, ○
- 326 Cryo-EM structures of chronic traumatic encephalopathy tau filaments with PET ligand flortaucipir. ○
- 325 Structure and host specificity of *Staphylococcus epidermidis* bacteriophage Andhra. **2022**, 8, 1
- 324 Potential inhibitors of FemC to combat *Staphylococcus aureus*: virtual screening, molecular docking, dynamics simulation, and MM-PBSA analysis. 1-12 ○
- 323 Designing Selective Drug-like Molecular Glues for the Glucocorticoid Receptor/14-3-3 Protein-Protein Interaction. **2022**, 65, 16818-16828 ○

- 322 CHILL & DisCO to discover competitive, connective and allosteric Nanobodies that modulate the SOS1BAS protein-protein interactions and tune the nucleotide exchange rate. 0
- 321 Molecular mechanisms regulating the pH-dependent pr/E interaction in yellow fever virus. 0
- 320 Ligand recognition and activation of neuromedin U receptor 2. **2022**, 13, 0
- 319 Oxygen-insensitive nitroreductase E. coli NfsA , but not NfsB , is inhibited by fumarate. 0
- 318 Identification of an $\alpha(1-16)$ -Mannosyltransferase Contributing To Biosynthesis of the Fungal-Type Galactomannan Core-Mannan Structure in *Aspergillus fumigatus*. **2022**, 7, 1
- 317 Active site architecture of coproporphyrin ferrochelatase with its physiological substrate coproporphyrin III : Propionate interactions and porphyrin core deformation. **2023**, 32, 1
- 316 Can de-phosphorylation of serine-5 in the C-terminal domain of human polymerase II affect its interaction with the PA C-terminal domain of bat Flu A polymerase?. 1-10 0
- 315 An electrostatic cluster guides A β 40 fibril formation in cerebral amyloid angiopathy. 0
- 314 Crystal Structure of Allantoinase from *Escherichia coli* BL21: A Molecular Insight into a Role of the Active Site Loops in Catalysis. **2023**, 28, 827 0
- 313 Structures of the entire human opioid receptor family. **2023**, 0
- 312 Cryo-EM structures of mitochondrial respiratory complex I from *Drosophila melanogaster*. 12, 0
- 311 Bioinformatic Approaches for Characterizing Molecular Structure and Function of Food Proteins. **2023**, 14, 0
- 310 Cryo-EM Structures of AcrD Illuminate a Mechanism for Capturing Aminoglycosides from Its Central Cavity. 0
- 309 Conformational Search for the Building Block of Proteins Based on the Gradient Gravitational Search Algorithm (ConfGGS) Using Force Fields: CHARMM, AMBER, and OPLS-AA. 0
- 308 SHP-1 tyrosine phosphatase binding to c-Src kinase phosphor-dependent conformations: A comparative structural framework. **2023**, 18, e0278448 0
- 307 Hierarchical sequence-affinity landscapes shape the evolution of breadth in an anti-influenza receptor binding site antibody. 12, 0
- 306 Determinants of substrate specificity in a catalytically diverse family of acyl-ACP thioesterases from plants. **2023**, 23, 2
- 305 The Myxobacterial Antibiotic Myxovalargin: Biosynthesis, Structural Revision, Total Synthesis, and Molecular Characterization of Ribosomal Inhibition. **2023**, 145, 851-863 0

- 304 In silico design of a promiscuous chimeric multi-epitope vaccine against Mycobacterium tuberculosis. **2023**,
- 303 The human pre-replication complex is an open complex. **2023**, 186, 98-111.e21
- 302 Disease-associated patterns of acetylation stabilize tau fibril formation.
- 301 An NmrA-like enzyme-catalysed redox-mediated Diels-Alder cycloaddition with anti-selectivity.
- 300 Sterol derivative binding to the orthosteric site causes conformational changes in an invertebrate Cys-loop receptor.
- 299 Alteration of Chain-Length Selectivity and Thermostability of Rhizopus oryzae Lipase via Virtual Saturation Mutagenesis Coupled with Disulfide Bond Design.
- 298 Emergence of an Auxin Sensing Domain in Plant-Associated Bacteria.
- 297 Oxygen-induced chromophore degradation in the photoswitchable red fluorescent protein rsCherry.
- 296 Structural and Biochemical Features of OXA-517: a Carbapenem and Expanded-Spectrum Cephalosporin Hydrolyzing OXA-48 Variant.
- 295 Structural mechanisms of calmodulin activation of Shigella effector OspC3 to ADP-ribosylate caspase-4/11 and block pyroptosis.
- 294 Structure of SALL4 zinc finger domain reveals link between AT-rich DNA binding and Okinawa syndrome. **2023**, 6, e202201588
- 293 Cell-surface protein YwfG of Lactococcus lactis binds to α 1,2-linked mannose. **2023**, 18, e0273955
- 292 A Putative New Role of Tv-PSP1 Recognizes IRE and ERE Hairpin Structures from Trichomonas vaginalis. **2023**, 12, 79
- 291 Design of Diverse Asymmetric Pockets in De Novo Homo-oligomeric Proteins. **2023**, 62, 358-368
- 290 The unifying catalytic mechanism of the RING-between-RING E3 ubiquitin ligase family. **2023**, 14,
- 289 Complexed Crystal Structure of the Dihydroorotase Domain of Human CAD Protein with the Anticancer Drug 5-Fluorouracil. **2023**, 13, 149
- 288 The complex inhibitory mechanism of glycomimetics with human heparanase.
- 287 Mutational fitness landscape of human influenza H3N2 neuraminidase. **2023**, 42, 111951

- 286 Structural Investigation of Diclofenac Binding to Ovine, Caprine, and Leporine Serum Albumins. **2023**, 24, 1534 ○
- 285 Structural analysis of human papillomavirus E6 interactions with Scribble PDZ domains. ○
- 284 LongBondEliminator: A Molecular Simulation Tool to Remove Ring Penetrations in Biomolecular Simulation Systems. **2023**, 13, 107 ○
- 283 Direct Expression of Fluorinated Proteins in Human Cells for ¹⁹F In-Cell NMR Spectroscopy. **2023**, 145, 1389-1399 ○
- 282 An engineered ACE2 decoy broadly neutralizes Omicron subvariants and shows therapeutic effect in SARS-CoV-2-infected cynomolgus macaques. ○
- 281 Structure, Mutagenesis, and QM:MM Modeling of 3-Ketosteroid Δ -Dehydrogenase from *Sterolibacterium denitrificans*-The Role of a New Putative Membrane-Associated Domain and Proton-Relay System in Catalysis. ○
- 280 Functional Impact of a Cancer-Related Variant in Human Δ -Pyrroline-5-Carboxylate Reductase 1. ○
- 279 Enolpyruvate Transferase MurAAA149E, Identified During Adaptation of *Enterococcus faecium* to Daptomycin, Increases Stability of MurAA-MurG Interaction. **2023**, 102912 ○
- 278 Crystal Structure of the SH3 Domain of ASAP1 in Complex with the Proline Rich Motif (PRM) of MICAL1 Reveals a Unique SH3/PRM Interaction Mode. **2023**, 24, 1414 ○
- 277 Structural basis of regulated m7G tRNA modification by METTL1 Δ WDR4. **2023**, 613, 391-397 ○
- 276 Molecular Dynamics Simulations Reveal Novel Interacting Regions of Human Prion Protein to *Brucella abortus* Hsp60 Protein. ○
- 275 Autotaxin facilitates selective LPA receptor signaling. **2023**, ○
- 274 Crystal structure of adenosine 5'-phosphosulfate kinase isolated from *Archaeoglobus fulgidus*. **2023**, 643, 105-110 ○
- 273 Molecular and Structural Basis of Receptor Binding and Signaling of a Fish Type I IFN with Three Disulfide Bonds. **2022**, 209, 806-819 ○
- 272 Toward structural-omics of the bovine retinal pigment epithelium. **2022**, 41, 111876 ○
- 271 Broad-Spectrum Cyclopropane-Based Inhibitors of Coronavirus 3C-like Proteases: Biochemical, Structural, and Virological Studies. **2023**, 6, 181-194 ○
- 270 *Trypanosoma brucei* RRP44: a versatile enzyme for processing structured and non-structured RNA substrates. **2023**, 51, 380-395 ○
- 269 The interaction between transport-segment DNA and topoisomerase I Δ crystal structure of MtbTOP1 in complex with both G- and T-segments. **2023**, 51, 349-364 1

- 268 5-Formyltetrahydrofolate Promotes Conformational Remodeling in a Methylenetetrahydrofolate Reductase Active Site and Inhibits Its Activity. **2022**, 102855 ○
- 267 A Guide to In Silico Drug Design. **2023**, 15, 49 ○
- 266 Identification of potential death-associated protein kinase-1 (DAPK1) inhibitors by an integrated ligand-based and structure-based computational drug design approach. 1-13 ○
- 265 Non-Nucleoside Inhibitors Decrease Foot-and-Mouth Disease Virus Replication by Blocking the Viral 3Dpol. **2023**, 15, 124 ○
- 264 Higher-order SPOP assembly reveals a basis for cancer mutant dysregulation. **2023**, ○
- 263 A structure-function analysis of chlorophyllase reveals a mechanism for activity regulation dependent on disulfide bonds. **2023**, 102958 ○
- 262 Blind Assessment of Monomeric AlphaFold2 Protein Structure Models with Experimental NMR Data. ○
- 261 The *Mythimna separata* general odorant binding protein 2 (MsepGOBP2) is involved in the larval detection of the sex pheromone (Z)-11-hexadecenal. ○
- 260 Illumination of the complement receptors C3aR and C5aR signaling by anaphylatoxins. ○
- 259 A new robust classifier to detect hot-spots and null-spots in protein-protein interface: validation of binding pocket and identification of inhibitors in in vitro and in vivo models. **2023**, 247-263 ○
- 258 B π - π and C π - π Interactions in protein-ligand complexes: carbonic anhydrase II inhibition by carborane sulfonamides. **2023**, 25, 1728-1733 ○
- 257 Characterization of the Native Disulfide Isomers of the Novel β -Conotoxin PnID: Implications for Further Increasing Conotoxin Diversity. **2023**, 21, 61 ○
- 256 Lhcb9-dependent photosystem I structure in moss reveals evolutionary adaptation to changing light conditions during aquatic-terrestrial transition. ○
- 255 KARS mediates intra-translational deposition of N ϵ -acetyl-L-lysine in nascent proteins to contribute the acetylome in cells. ○
- 254 An allosteric switch ensures efficient unidirectional information transmission by the histidine kinase DesK from *Bacillus subtilis*. **2023**, 16, ○
- 253 Discovery, Characterization, and Engineering of LvIC, an β /4-Conotoxin That Selectively Blocks Rat α / β 4 Nicotinic Acetylcholine Receptors. **2023**, 66, 2020-2031 ○
- 252 Structural and dynamic insights into supra-physiological activation and allosteric modulation of a muscarinic acetylcholine receptor. **2023**, 14, ○
- 251 Application of Molecular Simulation Methods in Food Science: Status and Prospects. ○

- 250 Decoupling peptide binding from T cell receptor recognition with engineered chimeric MHC-I molecules. 14, ○
- 249 VelcroVax: a Bolt-On Vaccine Platform for Glycoprotein Display. ○
- 248 A Structural Systems Biology Approach to High-Risk CG23 *Klebsiella pneumoniae*. ○
- 247 Crystal structures of OrfX1 , OrfX2 and the OrfX1 DrfX3 complex from the orfX gene cluster of botulinum neurotoxin E1. ○
- 246 Mechanistic basis of staphylococcal interspecies competition for skin colonization. ○
- 245 Structures of *Arabidopsis thaliana* MDL Proteins and Synergistic Effects with the Cytokine MIF on Human Receptors. ○
- 244 The molecular mechanism of sialic acid transport mediated by Sialin. **2023**, 9, ○
- 243 Caltubin regulates microtubule stability via Ca²⁺-dependent mechanisms favouring neurite regrowth. ○
- 242 Gold drugs as colistin adjuvants in the fight against MCR-1 producing bacteria. ○
- 241 Human neutralizing antibodies to cold linear epitopes and subdomain 1 of the SARS-CoV-2 spike glycoprotein. 2
- 240 Mechanisms of Sugar Aminotransferase-like Enzymes to Synthesize Stereoisomers of Non-proteinogenic Amino Acids in Natural Product Biosynthesis. ○
- 239 Snapshots of the first-step self-splicing of *Tetrahymena* ribozyme revealed by cryo-EM. ○
- 238 The *Mycobacterium tuberculosis* mycothiol S-transferase is divalent metal-dependent for mycothiol binding and transfer. ○
- 237 Mechanism of hormone and allosteric agonist mediated activation of follicle stimulating hormone receptor. **2023**, 14, ○
- 236 Staphylococcal Periscope Proteins Aap, SasG and Pls project non-canonical legume-like lectin adhesin domains from the bacterial surface. **2023**, 102936 ○
- 235 Structure of the Commander endosomal trafficking complex linked to X-linked intellectual disability/Ritscher-Schinzel syndrome. ○
- 234 Production of antigenically stable enterovirus A71 virus-like particles in *Pichia pastoris* as a vaccine candidate. ○
- 233 An unusual disulfide-linked dimerization in the fluorescent protein rsCherryRev1.4. **2023**, 79, 38-44 ○

- 232 Structural basis for inactivation of PRC2 by G-quadruplex RNA. ○
- 231 Interaction Mechanism of Inhibition of Palmitic Acid and Selinene Targeting FabH and FabI Enzymes in Escherichia coli: In Silico Study. **2022**, 25, 427-435 ○
- 230 Structure of the human CLC-7/Ostm1 complex reveals a novel state. **2023**, 53, 0306 ○
- 229 The porphyrin degradation system of the human gut microbiota is complete, phylogenetically diverse and geographically structured across Asian populations. ○
- 228 A novel pan-selective bromodomain inhibitor for epigenetic drug design. **2023**, 249, 115139 ○
- 227 Structural basis for GSDMB pore formation and its targeting by IpaH7.8. ○
- 226 Structural basis of Janus kinase trans-activation. **2023**, 42, 112201 ○
- 225 Structural and mechanistic insights into fungal β -1,3-glucan synthase FKS1. **2023**, 616, 190-198 ○
- 224 Basis of the H2AK119ub specificity of the Polycomb repressive deubiquitinase. **2023**, 616, 176-182 ○
- 223 Structure and interactions of the phloem lectin (phloem protein 2) Cus17 from Cucumis sativus. **2023**, 31, 464-479.e5 ○
- 222 Improving thermostability of Bacillus amyloliquefaciens alpha-amylase by multipoint mutations. **2023**, 653, 69-75 ○
- 221 Targeting Enterococcus faecalis HMG-CoA reductase with a non-statin inhibitor. **2023**, 6, ○
- 220 Engineering the Active Site Lid Dynamics to Improve the Catalytic Efficiency of Yeast Cytosine Deaminase. **2023**, 24, 6592 ○
- 219 Constrained catecholamines gain β 2AR selectivity through allosteric effects on pocket dynamics. **2023**, 14, ○
- 218 Molecular determinants for differential activation of the bile acid receptor from the pathogen Vibrio parahaemolyticus. **2023**, 299, 104591 ○
- 217 Conformation-dependent ligand hot spots in the spliceosomal RNA helicase BRR2. **2023**, 79, 304-317 ○
- 216 Cryo-EM structure of the transposon-associated TnpB enzyme. **2023**, 616, 390-397 ○
- 215 Structural and functional insights of the catalytic GH5 and Calx- β domains from the metagenome-derived endoglucanase CelE2. **2023**, 165, 110206 ○

- 214 Structural basis of membrane skeleton organization in red blood cells. **2023**, ○
- 213 Germline-targeting HIV-1 Env vaccination induces VRC01-class antibodies with rare insertions. **2023**, 101003 ○
- 212 The structure of AgamOBP5 in complex with the natural insect repellents Carvacrol and Thymol: Crystallographic, fluorescence and thermodynamic binding studies. **2023**, 237, 124009 1
- 211 Characterization of new highly selective pyrazolo[4,3-d]pyrimidine inhibitor of CDK7. **2023**, 161, 114492 ○
- 210 Structural basis of main proteases of HCoV-229E bound to inhibitor PF-07304814 and PF-07321332. **2023**, 657, 16-23 ○
- 209 In silico-chemogenomic repurposing of new chemical scaffolds for histoplasmosis treatment. **2023**, 33, 101363 ○
- 208 Oxygen-induced chromophore degradation in the photoswitchable red fluorescent protein rsCherry. **2023**, 239, 124179 ○
- 207 Structural insight into the intraflagellar transport complex IFT-A and its assembly in the anterograde IFT train. **2023**, 14, ○
- 206 A novel single sensor hemoglobin domain from the thermophilic cyanobacteria *Thermosynechococcus elongatus* BP-1 exhibits higher pH but lower thermal stability compared to globins from mesophilic organisms. **2023**, 124471 ○
- 205 Reaction Mechanism of Glycoside Hydrolase Family 116 Utilizes Perpendicular Protonation. 5850-5863 ○
- 204 Structure-guided design of direct-acting antivirals that exploit the gem-dimethyl effect and potently inhibit 3CL proteases of severe acute respiratory syndrome Coronavirus-2 (SARS-CoV-2) and middle east respiratory syndrome coronavirus (MERS-CoV). **2023**, 254, 115376 ○
- 203 Synthesis of deuterated S-217622 (Emsitrelvir) with antiviral activity against coronaviruses including SARS-CoV-2. **2023**, 213, 105586 ○
- 202 Structures of the sulfite detoxifying F420-dependent enzyme from Methanococcales. ○
- 201 Comprehensive in-silico analysis of deleterious SNPs in APOC2 and APOA5 and their differential expression in cancer and cardiovascular diseases conditions. **2023**, 115, 110567 ○
- 200 Distant sequence regions of JBP1 contribute to J-DNA binding. ○
- 199 pH-Driven Polymorphic Behaviour of the Third PDZ Domain of PSD95: The Role of Electrostatic Interactions. **2023**, 13, 218 ○
- 198 Plasmodium sporozoites require the protein B9 to invade hepatocytes. **2023**, 26, 106056 ○
- 197 Identification of potent and selective N-myristoyltransferase inhibitors of Plasmodium vivax liver stage hypnozoites and schizonts. ○

- 196 The cryo-EM structure of full-length RAD52 protein contains an undecameric ring. **2023**, 13, 408-418 1
- 195 Evaluation of the Antioxidant Properties of Carvacrol as a Prospective Replacement for Crude Essential Oils and Synthetic Antioxidants in Food Storage. **2023**, 28, 1315 0
- 194 Mechanism of regulation of the Helicobacter pylori Cag β ATPase by CagZ. **2023**, 14, 0
- 193 Recognition of the CCT5 di-Glu degron by CRL4 DCAF12 is dependent on TRiC assembly. **2023**, 42, 0
- 192 Structural basis for substrate selection by the SARS-CoV-2 replicase. **2023**, 614, 781-787 0
- 191 Structural insights into the interactions of glutathione transferases with a nitric oxide carrier and sodium nitroprusside. **2023**, 649, 79-86 0
- 190 Assessing Variants of Uncertain Significance Implicated in Hearing Loss Using a Comprehensive Deafness Proteome. 0
- 189 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. **2023**, 233, 123495 0
- 188 The uncharacterized Pseudomonas aeruginosa PA4189 is a novel and efficient aminoacetaldehyde dehydrogenase. **2023**, 480, 259-281 0
- 187 Purification and structure of luminal domain C of human Niemann-Pick C1 protein. **2023**, 79, 45-50 0
- 186 Toxicological impacts and likely protein targets of bisphenol a in Paramecium caudatum. **2023**, 88, 125958 0
- 185 Crystal structure of the catalytic ATP-binding domain of the PhoR sensor histidine kinase. 0
- 184 Structural and Biochemical Analyses of the Butanol Dehydrogenase from Fusobacterium nucleatum. **2023**, 24, 2994 0
- 183 Aim18p and Aim46p are chalcone isomerase domain-containing mitochondrial hemoproteins in Saccharomyces cerevisiae. **2023**, 299, 102981 0
- 182 A riboswitch separated from its ribosome-binding site still regulates translation. **2023**, 51, 2464-2484 1
- 181 Atomic crystal structure and sugar specificity of a β -trefoil lectin domain from the ectomycorrhizal basidiomycete Laccaria bicolor. **2023**, 233, 123507 0
- 180 Archaeal DNA-import apparatus is homologous to bacterial conjugation machinery. **2023**, 14, 0
- 179 The binding mode of orphan glycyl-tRNA synthetase with tRNA supports the synthetase classification and reveals large domain movements. **2023**, 9, 0

- 178 Structural and Functional Analysis of a Highly Active Designed Phosphotriesterase for the Detoxification of Organophosphate Nerve Agents Reveals an Unpredicted Conformation of the Active Site Loop. **2023**, 62, 942-955 ○
- 177 Comparison of the structure and activity of thioredoxin 2 and thioredoxin 1 from *Acinetobacter baumannii*. **2023**, 10, 147-155 ○
- 176 The structural basis for HIV-1 Vif antagonism of human APOBEC3G. **2023**, 615, 728-733 ○
- 175 Broadly neutralizing SARS-CoV-2 antibodies through epitope-based selection from convalescent patients. **2023**, 14, ○
- 174 Structural basis of nirmatrelvir and ensitrelvir activity against naturally occurring polymorphisms of the SARS-CoV-2 main protease. **2023**, 299, 103004 ○
- 173 Human IFT-A complex structures provide molecular insights into ciliary transport. **2023**, 33, 288-298 ○
- 172 Selectively Modified Lactose and N-Acetyllactosamine Analogs at Three Key Positions to Afford Effective Galectin-3 Ligands. **2023**, 24, 3718 ○
- 171 Structural insight into guanylyl cyclase receptor hijacking of the kinase Hsp90 regulatory mechanism. ○
- 170 Cyclopia intermedia (Honeybush) Induces Uncoupling Protein 1 and Peroxisome Proliferator-Activated Receptor Alpha Expression in Obese Diabetic Female db/db Mice. **2023**, 24, 3868 ○
- 169 A Brighter picALuc Generated Through the Loss of a Salt Bridge Interaction. ○
- 168 Structure and thiazide inhibition mechanism of the human NaCl cotransporter. **2023**, 614, 788-793 ○
- 167 Structures of importin- β bound to the wild-type and an internal deletion mutant of the bipartite nuclear localization signal of HIF-1 β . **2023**, 652, 1-5 ○
- 166 Structural basis of paralog-specific KDM2A/B nucleosome recognition. ○
- 165 Inhibition of 3-Hydroxykynurenine Transaminase from *Aedes aegypti* and *Anopheles gambiae*: A Mosquito-Specific Target to Combat the Transmission of Arboviruses. **2023**, 3, 211-222 ○
- 164 Crystallographic data of an importin- β dimer in which the two protomers are bridged by a bipartite nuclear localization signal. **2023**, 47, 108988 ○
- 163 Monobody Inhibitor Selective to the Phosphatase Domain of SHP2 and its Use as a Probe for Quantifying SHP2 Allosteric Regulation. **2023**, 435, 168010 ○
- 162 Structure of the *Caenorhabditis elegans* 6A methyltransferase METT10 that regulates SAM homeostasis. **2023**, 51, 2434-2446 ○
- 161 Menin Recruits H3K79me2 mark in a nucleosomal context. **2023**, 379, 717-723 ○

- 160 Architecture and regulation of filamentous human cystathionine beta-synthase. ○
- 159 Structural and biochemical characterization establishes a detailed understanding of KEAP1-CUL3 complex assembly. ○
- 158 Structure of a monomeric photosystem I core associated with iron-stress-induced-A proteins from *Anabaena* sp. PCC 7120. **2023**, 14, ○
- 157 Native structure of mosquito salivary protein uncovers domains relevant to pathogen transmission. **2023**, 14, ○
- 156 Structure of *Dunaliella* photosystem II reveals conformational flexibility of stacked and unstacked supercomplexes. 12, ○
- 155 Detailed analysis of distorted retinal and its interaction with surrounding residues in the K intermediate of bacteriorhodopsin. **2023**, 6, ○
- 154 Avidity engineering of human heavy-chain-only antibodies mitigates neutralization resistance of SARS-CoV-2 variants. 14, ○
- 153 The chemosensory protein 1 contributes to indoxacarb resistance in *Plutella xylostella* (L.). ○
- 152 Repurposing anthocyanins into potential inhibitors of the SARS-CoV-2 main protease (Mpro): An in silico approach. **2023**, ○
- 151 *Rhodobacter capsulatus* forms a compact crescent-shaped LH1BC photocomplex. **2023**, 14, ○
- 150 AI-Accelerated Design of Targeted Covalent Inhibitors for SARS-CoV-2. **2023**, 63, 1438-1453 1
- 149 Structure of the N-terminal coiled-coil domains of the ciliary protein Rpgrip1l. **2023**, 26, 106249 ○
- 148 Prospect of acromegaly therapy: molecular mechanism of clinical drugs octreotide and paltusotine. **2023**, 14, ○
- 147 Two peptides derivate from *Acinetobacter baumannii* outer membrane protein K as vaccine candidates: A comprehensive in silico study. ○
- 146 Equilibrium Dynamics of a Biomolecular Complex Analyzed at Single-amino Acid Resolution by Cryo-electron Microscopy. **2023**, 435, 168024 ○
- 145 Structural basis of lysophosphatidylserine receptor GPR174 ligand recognition and activation. **2023**, 14, ○
- 144 Structural Elucidation of Ivermectin Binding to α 7nAChR and the Induced Channel Desensitization. **2023**, 14, 1156-1165 ○
- 143 Crystal structure of the motor domain of centromere-associated protein E in complex with a non-hydrolysable ATP analogue. ○

- 142 Three-dimensional models of antigens with serodiagnostic potential for leprosy: An in silico study. 13, 1-10 ○
- 141 Design, synthesis and characterisation of a novel type II B-RAF paradox breaker inhibitor. **2023**, 250, 115231 ○
- 140 Design, synthesis, and mechanism of action of novel Ecenotoxin KIIIA analogues for inhibition of the voltage-gated sodium channel Nav1.7. **2023**, 299, 103068 1
- 139 Mycobacterium tuberculosis methyltransferase perturbs host epigenetic programming to promote bacterial survival. ○
- 138 Accelerating crystal structure determination with iterative AlphaFold prediction. **2023**, 79, 234-244 ○
- 137 Crystal structure of adenosine A2A receptor in complex with clinical candidate Etrumadenant reveals novel antagonist interaction. ○
- 136 Structural homology screens reveal poxvirus-encoded proteins impacting inflammasome-mediated defenses. ○
- 135 Characterization of new highly selective pyrazolo[4,3-d]pyrimidine inhibitor of CDK7. ○
- 134 Benchmarking applicability of medium-resolution cryo-EM protein structures for structure-based drug design. ○
- 133 Errors in structural biology are not the exception. **2023**, 79, 206-211 ○
- 132 Pseudomonas aeruginosa Dps (PA0962) Functions in H₂O₂ Mediated Oxidative Stress Defense and Exhibits In Vitro DNA Cleaving Activity. **2023**, 24, 4669 ○
- 131 Structural and Antibacterial Characterization of a New Benzamide FtsZ Inhibitor with Superior Bactericidal Activity and In Vivo Efficacy Against Multidrug-Resistant Staphylococcus aureus. **2023**, 18, 629-642 ○
- 130 In silico molecular docking and molecular dynamic simulation of agarwood compounds with molecular targets of Alzheimer's disease . 12, 230 ○
- 129 Designing antimicrobial peptides using deep learning and molecular dynamic simulations. **2023**, 24, ○
- 128 Molecular determinants of acrylamide neurotoxicity through covalent docking. 14, ○
- 127 Robust total X-ray scattering workflow to study correlated motion of proteins in crystals. **2023**, 14, ○
- 126 Cryo-EM structure of human heptameric pannexin 2 channel. **2023**, 14, ○
- 125 Cryo-EM-guided engineering of T-box-tRNA modules with enhanced selectivity and sensitivity in translational regulation. ○

- 124 Molecular architecture and dynamics of SARS-CoV-2 envelope by integrative modeling. **2023**, 31, 492-503.e7 ○
- 123 Cryo-EM structure of amyloid fibril formed by β -synuclein hereditary A53E mutation reveals a distinct protofilament interface. **2023**, 299, 104566 ○
- 122 The crystal structure of a simian Foamy Virus receptor binding domain provides clues about entry into host cells. **2023**, 14, ○
- 121 Structural and Biochemical Characterization of Silver/Copper Binding by *Dendrorhynchus zhejiangensis* Ferritin. **2023**, 15, 1297 ○
- 120 Monomer and dimer structures of cytochrome bo 3 ubiquinol oxidase from *Escherichia coli*. **2023**, 32, ○
- 119 Structure of the Ndc80 complex and its interactions at the yeast kinetochore-microtubule interface. **2023**, 13, ○
- 118 Investigating In Situ Expression of c-MYC and Candidate Ubiquitin-Specific Proteases in DLBCL and Assessment for Peptidyl Disruptor Molecule against c-MYC-USP37 Complex. **2023**, 28, 2441 ○
- 117 Lipid nanodiscs as a template for high-resolution cryo-EM structures of peripheral membrane proteins. ○
- 116 Structures of calmodulin-helittin complexes show multiple binding modes lacking classical anchoring interactions. **2023**, 299, 104596 ○
- 115 AT-752 targets multiple sites and activities on the Dengue virus replication enzyme NS5. **2023**, 212, 105574 ○
- 114 Decrypting the programming of β -methylation in virginiamycin M biosynthesis. **2023**, 14, ○
- 113 Structures of wild-type and selected CMT1X mutant connexin 32 gap junction channels and hemichannels. ○
- 112 Dynamic Association of ESCRT-II Proteins with ESCRT-I and ESCRT-III Complexes during Phagocytosis of *Entamoeba histolytica*. **2023**, 24, 5267 ○
- 111 Cryo-EM structures of human arachidonate 12S-Lipoxygenase (12-LOX) bound to endogenous and exogenous inhibitors. ○
- 110 Structural insight into TIPE1 functioning as a lipid transfer protein. 1-14 ○
- 109 Structural basis of vitamin C recognition and transport by mammalian SVCT1 transporter. **2023**, 14, ○
- 108 The Chemokine, CCL20, and Its Receptor, CCR6, in the Pathogenesis and Treatment of Psoriasis and Psoriatic Arthritis. 247553032311591 ○
- 107 Extended regulation interface coupled to the allosteric network and disease mutations in the PP2A-B56 holoenzyme. ○

- 106 Finding epitopes of *Klebsiella pneumoniae* outer membrane protein-K17 (OMP_{K17}) and introducing a 25-mer peptide of it as a vaccine candidate. ○
- 105 Structures of apo Cas12a and its complex with crRNA and DNA reveal the dynamics of ternary complex formation and target DNA cleavage. **2023**, 21, e3002023 ○
- 104 Interactions of hydrolyzed β -lactams with the L1 metallo- β -lactamase: Crystallography supports stereoselective binding of cephem/carbapenem products. **2023**, 299, 104606 ○
- 103 Structural basis of selective cannabinoid CB₂ receptor activation. **2023**, 14, ○
- 102 In silico screening of potential compounds from begonia genus as 3CL protease (3CL pro) SARS-CoV-2 inhibitors. ○
- 101 Structure of Photosystem I Supercomplex Isolated from a *Chlamydomonas reinhardtii* Cytochrome b6f Temperature-Sensitive Mutant. **2023**, 13, 537 ○
- 100 Cryo-EM reveals dynamics of *Tetrahymena* group I intron self-splicing. ○
- 99 Structural insights into TRPV4-Rho GTPase signaling complex function and disease. ○
- 98 Antibodies generated *in vitro* and *in vivo* elucidate design of a thermostable ADDomer COVID-19 nasal nanoparticle vaccine. ○
- 97 A general computational design strategy for stabilizing viral class I fusion proteins. ○
- 96 Crystal Structure of the Commercial Herbicide, Amidosulfuron, in Complex with *Arabidopsis thaliana* Acetohydroxyacid Synthase. **2023**, 71, 5117-5126 ○
- 95 Cryo-EM structure of the RuvAB-Holliday junction intermediate complex from *Pseudomonas aeruginosa*. 14, ○
- 94 Structure of a fungal 1,3- β -glucan synthase. ○
- 93 An updated atlas of antibody evasion by SARS-CoV-2 Omicron sub-variants including BQ.1.1 and XBB. **2023**, 4, 100991 ○
- 92 Glutathione disrupts galectin-10 Charcot-Leyden crystal formation to possibly ameliorate eosinophil-based diseases such as asthma. **2023**, ○
- 91 Dynamic lid domain of *Chloroflexus aurantiacus* Malonyl-CoA Reductase controls the reaction. ○
- 90 Structure and Dynamics of Three *Escherichia coli* NfsB Nitro-Reductase Mutants Selected for Enhanced Activity with the Cancer Prodrug CB1954. **2023**, 24, 5987 ○
- 89 Discovery of Nanomolar DCAF1 Small Molecule Ligands. **2023**, 66, 5041-5060 ○

- 70 Direct Blockade of the Norovirus Histo-Blood Group Antigen Binding Pocket by Nanobodies. ○
- 69 Contribution of calcium ligands in substrate binding and product release in the *Acetovibrio thermocellus* glycoside hydrolase family 9 cellulase CelR. **2023**, 299, 104655 ○
- 68 Structural basis of the substrate recognition and inhibition mechanism of *Plasmodium falciparum* nucleoside transporter PfENT1. **2023**, 14, ○
- 67 Biochemical and structural analysis of N-myristoyltransferase mediated protein tagging. **2023**, 1 ○
- 66 P450-mediated dehydrotyrosine formation during WS9326 biosynthesis proceeds via dehydrogenation of a specific acylated dipeptide substrate. **2023**, ○
- 65 KIFKey Interactions Finder: A program to identify the key molecular interactions that regulate protein conformational changes. **2023**, 158, 144114 ○
- 64 PRC domain-containing proteins modulate FtsZ-based archaeal cell division. ○
- 63 Stable mammalian serum albumins designed for bacterial expression. ○
- 62 Identification of potential inhibitor against CTX-M-3 and CTX-M-15 proteins: an in silico and in vitro study. 1-17 ○
- 61 In silico exploration and molecular dynamics of deleterious SNPs on the human TERF1 protein triggering male infertility. 1-24 ○
- 60 Commercial influenza vaccines vary in HA-complex structure and in induction of cross-reactive HA antibodies. **2023**, 14, ○
- 59 A partially open conformation of an androgen receptor ligand-binding domain with drug-resistance mutations. **2023**, 79, 95-104 ○
- 58 The structure of the complex between the arsenite oxidase from *Pseudorhizobium banfieldiae* sp. strain NT-26 and its native electron acceptor cytochrome c 552. **2023**, 79, 345-352 ○
- 57 Structural and enzymatic characterization of the sialidase SiaPG from *Porphyromonas gingivalis*. **2023**, 79, 87-94 ○
- 56 Structural and mechanistic insights into activation of the human RNA ligase RTCB by Arcease. ○
- 55 Alteration of Substrate Specificity and Transglucosylation Activity of GH13_31 β -Glucosidase from *Bacillus* sp. AHU2216 through Site-Directed Mutagenesis of Asn258 on β -Loop 5. **2023**, 28, 3109 ○
- 54 Alloreactivity and autoreactivity converge to support B cell epitope targeting in transplant rejection. ○
- 53 Insights into Nitrosoalkane Binding to Myoglobin Provided by Crystallography of Wild-Type and Distal Pocket Mutant Derivatives. **2023**, 62, 1406-1419 ○

- 52 Biochemical Characterization of *Caenorhabditis elegans* Ferritins. ○
- 51 RAS gene mutations and histomorphometric measurements in oral squamous cell carcinoma. 1-9 ○
- 50 Structure and epitope of a neutralizing monoclonal antibody that targets the stem helix of β coronaviruses. ○
- 49 A class of antibodies that overcome a steric barrier to cross-group neutralization of influenza viruses. ○
- 48 Inhibition of FAM46/TENT5 activity by BCCIP adopting a unique fold. **2023**, 9, ○
- 47 Crystal Structure and Functional Characterization of an S-Formylglutathione Hydrolase (BuSFGH) from Burkholderiaceae sp.. **2023**, 13, 621 ○
- 46 Cryo-EM-based structural insights into supramolecular assemblies of hemolysin from *S. aureus* reveal the pore formation mechanism. **2023**, ○
- 45 Functional tailoring of a PET hydrolytic enzyme expressed in *Pichia pastoris*. **2023**, 10, ○
- 44 Methionine aminopeptidase 2 and its autoproteolysis product have different binding sites on the ribosome. ○
- 43 Uncovering and engineering the mechanical properties of the adhesion GPCR ADGRG1 GAIN domain. ○
- 42 Environmentally Ultrasensitive Fluorine Probe to Resolve Protein Conformational Ensembles by ^{19}F NMR and Cryo-EM. ○
- 41 Differences in the regulation mechanisms of the glutamine synthetase from methanogenic archaea unveiled by structural investigations. ○
- 40 Structural insights into the substrate recognition of serine palmitoyltransferase from *Sphingobacterium multivorum*. **2023**, 104684 ○
- 39 The intestinal MUC2 mucin C-terminus is stabilized by an extra disulfide bond in comparison to von Willebrand factor and other gel-forming mucins. **2023**, 14, ○
- 38 Riparin-B as a Potential Inhibitor of AdeABC Efflux System from *Acinetobacter baumannii*. **2023**, 2023, 1-10 ○
- 37 Mechanistic basis for oxidative stress protection of the human tRNA ligase complex by the oxidoreductase PYROXD1. ○
- 36 Potent Omicron-neutralizing antibodies isolated from a patient vaccinated 6 months before Omicron emergence. **2023**, 42, 112421 ○
- 35 Diverse cytomotive actins and tubulins share a polymerization switch mechanism conferring robust dynamics. **2023**, 9, ○

- 34 AMPK targets a proto-oncogene TPD52 (isoform 3) expression and its interaction with LKB1 suppress AMPK-GSK3 β signaling axis in prostate cancer. ○
- 33 Near-atomic architecture of Singapore grouper iridovirus and implications for giant virus assembly. **2023**, 14, ○
- 32 Crystal Structures of Diaryl Hydrazone and Sulfone Stabilizers in Complex with an Amyloidogenic Light Chain Reveal an Alternate Ligand-Binding Cavity. ○
- 31 Unravelling the allosteric binding mode of β -VxXXB at nicotinic acetylcholine receptors. 14, ○
- 30 Activation and substrate specificity of the human P4-ATPase ATP8B1. ○
- 29 Conserved intramolecular networks in GDAP1 are closely connected to CMT-linked mutations and protein stability. **2023**, 18, e0284532 ○
- 28 Cryo-EM Structures of the *Klebsiella pneumoniae* AcrB Multidrug Efflux Pump. ○
- 27 Structure of anhydrotetracycline-bound Tet(X6) reveals the mechanism for inhibition of type 1 tetracycline destructases. **2023**, 6, ○
- 26 Cytochrome P450-catalyzed oxidation of halogen-containing substrates. **2023**, 112234 ○
- 25 Cryo-EM structure of the folded-back state of human β -cardiac myosin*. ○
- 24 Structure-function Analyses Reveal Key Molecular Determinants of HIV-1 CRF01_AE Resistance to the Entry Inhibitor Temsavir. ○
- 23 Histone divergence in *Trypanosoma brucei* results in unique alterations to nucleosome structure. ○
- 22 Structures of the human Wilson disease copper transporter ATP7B. **2023**, 42, 112417 ○
- 21 Dephosphocholination by *Legionella* effector Lem3 functions through remodelling of the switch II region of Rab1b. **2023**, 14, ○
- 20 Lesion recognition by XPC, TFIIH and XPA in DNA excision repair. ○
- 19 Genetic drift and genome reduction in the plant pathogen *Candidatus Liberibacter solanacearum* shapes a new enzyme in lysine biosynthesis. ○
- 18 In Silico Design of a Chimeric Humanized L-asparaginase. **2023**, 24, 7550 ○
- 17 Top-down design of protein architectures with reinforcement learning. **2023**, 380, 266-273 ○

- 16 Structural basis of centromeric cohesion protection. ○
- 15 Structure guided mimicry of an essential *P. falciparum* receptor-ligand complex enhances cross neutralizing antibodies. ○
- 14 The structure of a 12-segmented dsRNA reovirus: New insights into capsid stabilization and organization. **2023**, 19, e1011341 ○
- 13 Assessing variants of uncertain significance implicated in hearing loss using a comprehensive deafness proteome. ○
- 12 Crystallographic and biophysical analysis of the fusion core from SARS-CoV-2 spike protein. ○
- 11 Structure of YdjH from *Acinetobacter baumannii* revealed an active site of YdjH family sugar kinase. **2023**, ○
- 10 Marine picocyanobacterial PhnD1 shows specificity for various phosphorus sources but likely represents a constitutive inorganic phosphate transporter. ○
- 9 De novo design of protein interactions with learned surface fingerprints. **2023**, 617, 176-184 ○
- 8 Large-scale phage-based screening reveals extensive pan-viral mimicry of host short linear motifs. **2023**, 14, ○
- 7 Assembly and Cation-selectivity Mechanisms of Neuronal Gap Junction Channel Connexin 36 Elucidated by Cryo-EM. ○
- 6 Cryptochrome timeless structure reveals circadian clock timing mechanisms. **2023**, 617, 194-199 ○
- 5 The nucleotide excision repair proteins through the lens of molecular dynamics simulations. **2023**, 127, 103510 ○
- 4 Mutagenic incorporation of inosine into DNA via T:I mismatch formation by human DNA polymerase eta (pol η). **2023**, 480, 649-664 ○
- 3 Atomic Models of All Major Trans-Envelope Complexes Involved in Lipid Trafficking in *Escherichia Coli* Constructed Using a Combination of AlphaFold2, AF2Complex, and Membrane Morphing Simulations. ○
- 2 Structural and biochemical characterization establishes a detailed understanding of KEAP1-CUL3 complex assembly. **2023**, 204, 215-225 ○
- 1 Streptothricin F is a bactericidal antibiotic effective against highly drug-resistant gram-negative bacteria that interacts with the 30S subunit of the 70S ribosome. **2023**, 21, e3002091 ○