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2061	Bovine thrombin complexed with an uncleavable analog of residues 7-19 of fibrinogen A alpha: geometry of the catalytic triad and interactions of the P1', P2', and P3' substrate residues. <b>1996</b> , 35, 13030-9	32
2060	Determinants of enzyme thermostability observed in the molecular structure of <i>Thermus aquaticus</i> D-glyceraldehyde-3-phosphate dehydrogenase at 25 Angstroms Resolution. <b>1996</b> , 35, 2597-609	190
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2058	Three-dimensional structure of meso-diaminopimelic acid dehydrogenase from <i>Corynebacterium glutamicum</i> . <b>1996</b> , 35, 13540-51	49
2057	NMR solution structure of a synthetic troponin C heterodimeric domain. <b>1996</b> , 35, 7429-38	16
2056	Refined crystal structure of adenylosuccinate synthetase from <i>Escherichia coli</i> complexed with hydantocidin 5'-phosphate, GDP, HPO <sub>4</sub> ( <sup>2-</sup> ), Mg <sup>2+</sup> , and hadacidin. <b>1996</b> , 35, 15753-9	38
2055	Molecular model of the solution structure for the paramagnetic four-iron ferredoxin from the hyperthermophilic archaeon <i>Thermococcus litoralis</i> . <b>1996</b> , 35, 11319-28	32
2054	Hormone-sensitive lipase is structurally related to acetylcholinesterase, bile salt-stimulated lipase, and several fungal lipases. Building of a three-dimensional model for the catalytic domain of hormone-sensitive lipase. <b>1996</b> , 271, 31426-30	81
2053	Crystal structure of glycine N-methyltransferase from rat liver. <b>1996</b> , 35, 11985-93	98
2052	Three-dimensional structure of the inosine-uridine nucleoside N-ribohydrolase from <i>Crithidia fasciculata</i> . <b>1996</b> , 35, 5971-81	77
2051	Crystal structures of three misacylating mutants of <i>Escherichia coli</i> glutaminyl-tRNA synthetase complexed with tRNA(Gln) and ATP. <b>1996</b> , 35, 14725-33	31
2050	Structure of the N-terminal cellulose-binding domain of <i>Cellulomonas fimi</i> CenC determined by nuclear magnetic resonance spectroscopy. <b>1996</b> , 35, 14381-94	122
2049	Solution structure of bovine angiogenin by 1H nuclear magnetic resonance spectroscopy. <b>1996</b> , 35, 8870-80	20
2048	Solution structure of rat apo-S100B(beta beta) as determined by NMR spectroscopy. <b>1996</b> , 35, 11577-88	127
2047	Crystal structure of the rat liver fructose-2,6-bisphosphatase based on selenomethionine multiwavelength anomalous dispersion phases. <b>1996</b> , 35, 6010-9	56

2046	Phospholipase A2 engineering. Deletion of the C-terminus segment changes substrate specificity and uncouples calcium and substrate binding at the zwitterionic interface. <b>1996</b> , 35, 12164-74	33
2045	Mutation of arginine 121 in lactoferrin destabilizes iron binding by disruption of anion binding: crystal structures of R121S and R121E mutants. <b>1996</b> , 35, 14473-9	26
2044	Structure and function of the epidermal growth factor domain of P-selectin. <b>1996</b> , 35, 13733-44	16
2043	Origin of carbohydrate recognition specificity of human lysozyme revealed by affinity labeling. <b>1996</b> , 35, 13562-7	34
2042	Crystal structures of complexes of a peptidic inhibitor with wild-type and two mutant HIV-1 proteases. <b>1996</b> , 35, 10627-33	51
2041	Crystal structures of the binary and ternary complexes of 7 alpha-hydroxysteroid dehydrogenase from <i>Escherichia coli</i> . <b>1996</b> , 35, 7715-30	212
2040	High-resolution structure of an engineered Cro monomer shows changes in conformation relative to the native dimer. <b>1996</b> , 35, 735-42	51
2039	Structure of chymopapain at 1.7 Å resolution. <b>1996</b> , 35, 16292-8	46
2038	High-resolution structure of the diphtheria toxin repressor complexed with cobalt and manganese reveals an SH3-like third domain and suggests a possible role of phosphate as co-corepressor. <b>1996</b> , 35, 12292-302	79
2037	(E)-enolbutyryl-UDP-N-acetylglucosamine as a mechanistic probe of UDP-N-acetylenolpyruvylglucosamine reductase (MurB). <b>1996</b> , 35, 1342-51	18
2036	Crystal structure of the hypoxanthine-guanine-xanthine phosphoribosyltransferase from the protozoan parasite <i>Tritrichomonas foetus</i> . <b>1996</b> , 35, 7032-40	97
2035	Structure and dynamics of a CheY-binding domain of the chemotaxis kinase CheA determined by nuclear magnetic resonance spectroscopy. <b>1996</b> , 35, 5633-40	44
2034	Self-Assembling Peptide Nanotubes. <b>1996</b> , 118, 43-50	536
2033	Crystallographic studies of the catalytic and a second site in fumarase C from <i>Escherichia coli</i> . <b>1996</b> , 35, 13955-65	87
2032	Structure of cyclodextrin glycosyltransferase complexed with a maltonaose inhibitor at 2.6 angstrom resolution. Implications for product specificity. <b>1996</b> , 35, 4241-9	139
2031	A model for the photosystem II reaction center core including the structure of the primary donor P680. <b>1996</b> , 35, 14486-502	201
2030	Molecular structure, conformational analysis, and structure-activity studies of Dendrotoxin and its homologues using molecular mechanics and molecular dynamics techniques. <b>1996</b> , 39, 2141-55	17
2029	Structures of the <i>Klebsiella aerogenes</i> urease apoenzyme and two active-site mutants. <b>1996</b> , 35, 10616-26	90

2028	Crystallographic complexes of glucoamylase with maltooligosaccharide analogs: relationship of stereochemical distortions at the nonreducing end to the catalytic mechanism. <b>1996</b> , 35, 8319-28	94
2027	A pseudo-michaelis quaternary complex in the reverse reaction of a ligase: structure of Escherichia coli B glutathione synthetase complexed with ADP, glutathione, and sulfate at 2.0 Å resolution. <b>1996</b> , 35, 11967-74	63
2026	Heteronuclear (1H, 13C, 15N) NMR assignments and solution structure of the monocyte chemoattractant protein-1 (MCP-1) dimer. <b>1996</b> , 35, 6569-84	155
2025	The three-dimensional solution structure of the SH2 domain from p55blk kinase. <b>1996</b> , 35, 6201-11	26
2024	A flexible loop at the dimer interface is a part of the active site of the adjacent monomer of Escherichia coli orotate phosphoribosyltransferase. <b>1996</b> , 35, 3803-9	72
2023	Structure of the Fusarium oxysporum endoglucanase I with a nonhydrolyzable substrate analogue: substrate distortion gives rise to the preferred axial orientation for the leaving group. <b>1996</b> , 35, 15280-7	227
2022	A Weak Calcium Binding Site in Subtilisin BPN <sub>I</sub> Has a Dramatic Effect on Protein Stability. <b>1996</b> , 118, 1645-1650	32
2021	Solution structure of the immunodominant region of protein G of bovine respiratory syncytial virus. <b>1996</b> , 35, 14684-8	29
2020	Crystallographic identification of metal-binding sites in Escherichia coli inorganic pyrophosphatase. <b>1996</b> , 35, 4670-7	58
2019	Secondary structure of an armadillo single repeat from the APC protein. <b>1996</b> , 383, 31-6	12
2018	X-ray structure analysis of an engineered Fe-superoxide dismutase Gly-Ala mutant with significantly reduced stability to denaturant. <b>1996</b> , 387, 105-8	6
2017	Crystal structure of macrophage migration inhibitory factor from human lymphocyte at 2.1 Å resolution. <b>1996</b> , 389, 145-8	47
2016	The protein fold of the hyaluronate-binding proteoglycan tandem repeat domain of link protein, aggrecan and CD44 is similar to that of the C-type lectin superfamily. <b>1996</b> , 388, 211-6	32
2015	The three-dimensional structure of capsule-specific CMP: 2-keto-3-deoxy-manno-octonic acid synthetase from Escherichia coli. <b>1996</b> , 391, 157-61	23
2014	Modified, cyclic dodecapeptide analog of neuropeptide Y is the smallest full agonist at the human Y2 receptor. <b>1996</b> , 394, 169-73	37
2013	A molecular model for human Big-Endothelin-1 (Big ET-1). <b>1996</b> , 394, 191-5	14
2012	Three-dimensional structure of glutathione S-transferase from Arabidopsis thaliana at 2.2 Å resolution: structural characterization of herbicide-conjugating plant glutathione S-transferases and a novel active site architecture. <b>1996</b> , 255, 289-309	189
2011	Crystal structures of adenylosuccinate synthetase from Escherichia coli complexed with GDP, IMP hadacidin, NO <sub>3</sub> <sup>-</sup> , and Mg <sup>2+</sup> . <b>1996</b> , 264, 1013-27	43

2010	Deviations from planarity of the peptide bond in peptides and proteins. <b>1996</b> , 264, 1180-95	148
2009	Complexes of HIV-1 reverse transcriptase with inhibitors of the HEPT series reveal conformational changes relevant to the design of potent non-nucleoside inhibitors. <b>1996</b> , 39, 1589-600	326
2008	Homology modeling of human methylmalonyl-CoA mutase: a structural basis for point mutations causing methylmalonic aciduria. <b>1996</b> , 5, 1922-7	29
2007	Crystal structures of guinea-pig, goat and bovine alpha-lactalbumin highlight the enhanced conformational flexibility of regions that are significant for its action in lactose synthase. <b>1996</b> , 4, 691-703	186
2006	The crystal structure of human cyclin H. <b>1996</b> , 397, 65-9	27
2005	Structure of the FGF receptor tyrosine kinase domain reveals a novel autoinhibitory mechanism. <b>1996</b> , 86, 577-87	347
2004	Structure of the human cytomegalovirus protease catalytic domain reveals a novel serine protease fold and catalytic triad. <b>1996</b> , 86, 835-43	149
2003	2.0 A crystal structure of a four-domain segment of human fibronectin encompassing the RGD loop and synergy region. <b>1996</b> , 84, 155-64	576
2002	Crystal structure and mutational analysis of the human CDK2 kinase complex with cell cycle-regulatory protein CksHs1. <b>1996</b> , 84, 863-74	216
2001	The crystal structure of hepatitis C virus NS3 proteinase reveals a trypsin-like fold and a structural zinc binding site. <b>1996</b> , 87, 331-42	466
2000	Crystal structure of human cyclophilin A bound to the amino-terminal domain of HIV-1 capsid. <b>1996</b> , 87, 1285-94	598
1999	Crystal structure of an IHF-DNA complex: a protein-induced DNA U-turn. <b>1996</b> , 87, 1295-306	688
1998	The C-terminal (haemopexin-like) domain structure of human gelatinase A (MMP2): structural implications for its function. <b>1996</b> , 378, 126-30	76
1997	Computer modeling of 3D structures of cytochrome P450s. <b>1996</b> , 78, 771-9	24
1996	Structure of the [NiFe] Hydrogenase Active Site: Evidence for Biologically Uncommon Fe Ligands?. <b>1996</b> , 118, 12989-12996	579
1995	An altered position of the alpha 2 helix of MHC class I is revealed by the crystal structure of HLA-B*3501. <b>1996</b> , 4, 203-13	154
1994	Bound water structure and polymorphic amino acids act together to allow the binding of different peptides to MHC class I HLA-B53. <b>1996</b> , 4, 215-28	142
1993	High-resolution solution structure of the EGF-like domain of heregulin-alpha. <b>1996</b> , 35, 3402-17	61

1992	Crystal structure of soybean lipoxygenase L-1 at 1.4 Å resolution. <b>1996</b> , 35, 10687-701	390
1991	Anion binding by transferrins: importance of second-shell effects revealed by the crystal structure of oxalate-substituted diferric lactoferrin. <b>1996</b> , 35, 9007-13	41
1990	The 1.5-Å resolution crystal structure of bacterial luciferase in low salt conditions. <b>1996</b> , 271, 21956-68	99
1989	Crystal structure of thermostable family 5 endocellulase E1 from <i>Acidothermus cellulolyticus</i> in complex with cellotetraose. <b>1996</b> , 35, 10648-60	223
1988	Structure of staphylococcal alpha-hemolysin, a heptameric transmembrane pore. <b>1996</b> , 274, 1859-66	1967
1987	Trimeric assembly and three-dimensional structure model of the FACIT collagen COL1-NC1 junction from CD and NMR analysis. <b>1996</b> , 35, 9647-60	32
1986	Three-dimensional solution structure of <i>Saccharomyces cerevisiae</i> reduced iso-1-cytochrome c. <b>1996</b> , 35, 13788-96	85
1985	Flavin reductase P: structure of a dimeric enzyme that reduces flavin. <b>1996</b> , 35, 13531-9	86
1984	X-ray crystal structure of human acidic fibroblast growth factor. <b>1996</b> , 35, 2086-94	124
1983	High-resolution solution structure of basic fibroblast growth factor determined by multidimensional heteronuclear magnetic resonance spectroscopy. <b>1996</b> , 35, 13552-61	54
1982	Structure of 3 alpha-hydroxysteroid/dihydrodiol dehydrogenase complexed with NADP <sup>+</sup> . <b>1996</b> , 35, 10702-11	101
1981	Kinetic and X-ray structural studies of a mutant <i>Escherichia coli</i> alkaline phosphatase (His-412-->Gln) at one of the zinc binding sites. <b>1996</b> , 35, 2394-402	17
1980	Crystal structure of an antagonist mutant of human growth hormone, G120R, in complex with its receptor at 2.9 Å resolution. <b>1996</b> , 271, 32197-203	70
1979	Identification of surface residues mediating tissue factor binding and catalytic function of the serine protease factor VIIa. <b>1996</b> , 93, 14379-84	170
1978	Crystal structure of <i>Bacillus licheniformis</i> α-Amylase at 1.7 Å resolution. <b>1996</b> , 12, 163-170	1
1977	Cocrystal structure of YY1 bound to the adeno-associated virus P5 initiator. <b>1996</b> , 93, 13577-82	159
1976	Chaperone activity and structure of monomeric polypeptide binding domains of GroEL. <b>1996</b> , 93, 15024-9	123
1975	High resolution NMR solution structure of the leucine zipper domain of the c-Jun homodimer. <b>1996</b> , 271, 13663-7	85



1974	NMR characterization and solution structure determination of the oxidized cytochrome c7 from <i>Desulfuromonas acetoxidans</i> . <b>1996</b> , 93, 14396-400	49
1973	Crystal structure of the secretory form of membrane-associated human carbonic anhydrase IV at 2.8-Å resolution. <b>1996</b> , 93, 13589-94	134
1972	A site-directed mutagenesis of pro-urokinase which substantially reduces its intrinsic activity. <b>1996</b> , 35, 14070-6	30
1971	Phosphoglycerate mutase from <i>Schizosaccharomyces pombe</i> : development of an expression system and characterisation of three histidine mutants of the enzyme. <b>1996</b> , 1296, 69-75	14
1970	Intermediate trapping and laue X-ray diffraction: potential for enzyme mechanism, dynamics, and inhibitor screening. <b>1996</b> , 70, 215-56	13
1969	Patterns and conformations of commonly occurring supersecondary structures (basic motifs) in protein data bank. <b>1996</b> , 15, 675-90	23
1968	Solution structure of the DNA-binding domain of the tomato heat-stress transcription factor HSF24. <b>1996</b> , 236, 911-21	49
1967	Crystal structure of the bifunctional soybean Bowman-Birk inhibitor at 0.28-nm resolution. Structural peculiarities in a folded protein conformation. <b>1996</b> , 242, 122-31	77
1966	Crystal structure and amino acid sequence of <i>Wolinella succinogenes</i> L-asparaginase. <b>1996</b> , 241, 201-7	76
1965	Multiple solution conformations of the integrin-binding cyclic pentapeptide cyclo(-Ser-D-Leu-Asp-Val-Pro-). Analysis of the (phi, psi) space available to cyclic pentapeptides. <b>1996</b> , 242, 352-62	26
1964	The dynamics and binding of a Type III antifreeze protein in water and on ice. <b>1996</b> , 388, 65-77	13
1963	Structure of the regulatory domain of scallop myosin at 2 Å resolution: implications for regulation. <b>1996</b> , 4, 21-32	199
1962	Crystal structure of the ternary complex of mouse lung carbonyl reductase at 1.8 Å resolution: the structural origin of coenzyme specificity in the short-chain dehydrogenase/reductase family. <b>1996</b> , 4, 33-45	203
1961	The structure of the substrate-free form of MurB, an essential enzyme for the synthesis of bacterial cell walls. <b>1996</b> , 4, 47-54	59
1960	The crystal structure of ribosomal protein L14 reveals an important organizational component of the translational apparatus. <b>1996</b> , 4, 55-66	60
1959	Crystal structures of nucleoside 2-deoxyribosyltransferase in native and ligand-bound forms reveal architecture of the active site. <b>1996</b> , 4, 97-107	44
1958	The structure of simian virus 40 refined at 3.1 Å resolution. <b>1996</b> , 4, 165-82	268
1957	Crystal structures of murine polyomavirus in complex with straight-chain and branched-chain sialyloligosaccharide receptor fragments. <b>1996</b> , 4, 183-94	156

1956	Structure of a dehydratase-isomerase from the bacterial pathway for biosynthesis of unsaturated fatty acids: two catalytic activities in one active site. <b>1996</b> , 4, 253-64	218
1955	The crystal structure of endoglucanase CelA, a family 8 glycosyl hydrolase from <i>Clostridium thermocellum</i> . <b>1996</b> , 4, 265-75	153
1954	Protein-protein interactions in the pyruvate dehydrogenase multienzyme complex: dihydrolipoamide dehydrogenase complexed with the binding domain of dihydrolipoamide acetyltransferase. <b>1996</b> , 4, 277-86	110
1953	Crystal structure of firefly luciferase throws light on a superfamily of adenylate-forming enzymes. <b>1996</b> , 4, 287-98	515
1952	Crystal structure of the yeast cell-cycle control protein, p13suc1, in a strand-exchanged dimer. <b>1996</b> , 4, 299-309	27
1951	The crystal structure of peanut peroxidase. <b>1996</b> , 4, 311-21	248
1950	Structure of rat procathepsin B: model for inhibition of cysteine protease activity by the proregion. <b>1996</b> , 4, 405-16	162
1949	The 1.1 Å crystal structure of the neuronal acetylcholine receptor antagonist, alpha-conotoxin PnIA from <i>Conus pennaceus</i> . <b>1996</b> , 4, 417-23	93
1948	Aromatic interactions define the binding of the alphavirus spike to its nucleocapsid. <b>1996</b> , 4, 519-29	95
1947	The crystal structure of bacteriophage Q beta at 3.5 Å resolution. <b>1996</b> , 4, 543-54	165
1946	The structure of elongation factor G in complex with GDP: conformational flexibility and nucleotide exchange. <b>1996</b> , 4, 555-65	126
1945	The solution structure of human thioredoxin complexed with its target from Ref-1 reveals peptide chain reversal. <b>1996</b> , 4, 613-20	149
1944	Crystal structure of a new heat-labile enterotoxin, LT-IIb. <b>1996</b> , 4, 665-78	63
1943	Crystal structure of a phosphatase-resistant mutant of sporulation response regulator Spo0F from <i>Bacillus subtilis</i> . <b>1996</b> , 4, 679-90	65
1942	Solution structure and peptide binding of the SH3 domain from human Fyn. <b>1996</b> , 4, 705-14	86
1941	Crystal structure of transaldolase B from <i>Escherichia coli</i> suggests a circular permutation of the alpha/beta barrel within the class I aldolase family. <b>1996</b> , 4, 715-24	78
1940	Crystal structures of reduced, oxidized, and mutated human thioredoxins: evidence for a regulatory homodimer. <b>1996</b> , 4, 735-51	325
1939	Substrate binding is required for assembly of the active conformation of the catalytic site in Ntn amidotransferases: evidence from the 1.8 Å crystal structure of the glutaminase domain of glucosamine 6-phosphate synthase. <b>1996</b> , 4, 801-10	126

1938	Mechanism of cyanogenesis: the crystal structure of hydroxynitrile lyase from <i>Hevea brasiliensis</i> . <b>1996</b> , 4, 811-22	100
1937	Insights into specificity of cleavage and mechanism of cell entry from the crystal structure of the highly specific <i>Aspergillus</i> ribotoxin, restrictocin. <b>1996</b> , 4, 837-52	86
1936	Crystal structure of a eukaryotic (pea seedling) copper-containing amine oxidase at 2.2 Å resolution. <b>1996</b> , 4, 943-55	233
1935	The solution structure of the bovine S100B protein dimer in the calcium-free state. <b>1996</b> , 4, 1041-52	123
1934	Crystal structure of UDP-N-acetylglucosamine enolpyruvyltransferase, the target of the antibiotic fosfomycin. <b>1996</b> , 4, 1065-75	82
1933	Structural evidence for specific S8-RNA and S8-protein interactions within the 30S ribosomal subunit: ribosomal protein S8 from <i>Bacillus stearothermophilus</i> at 1.9 Å resolution. <b>1996</b> , 4, 1093-104	61
1932	An alpha to beta conformational switch in EF-Tu. <b>1996</b> , 4, 1153-9	182
1931	Crystal structure of the ternary complex of 1,3,8-trihydroxynaphthalene reductase from <i>Magnaporthe grisea</i> with NADPH and an active-site inhibitor. <b>1996</b> , 4, 1161-70	75
1930	Structures of the extracellular domain of the type I tumor necrosis factor receptor. <b>1996</b> , 4, 1251-62	131
1929	The structure of the C-terminal domain of methionine synthase: presenting S-adenosylmethionine for reductive methylation of B12. <b>1996</b> , 4, 1263-75	106
1928	Structure of the GDP-Pi complex of Gly203-->Ala gamma1: a mimic of the ternary product complex of gamma-catalyzed GTP hydrolysis. <b>1996</b> , 4, 1277-90	53
1927	Small structural changes account for the high thermostability of 1[4Fe-4S] ferredoxin from the hyperthermophilic bacterium <i>Thermotoga maritima</i> . <b>1996</b> , 4, 1291-301	107
1926	The crystal structure of a class II fructose-1,6-bisphosphate aldolase shows a novel binuclear metal-binding active site embedded in a familiar fold. <b>1996</b> , 4, 1303-15	100
1925	A pancreatic lipase with a phospholipase A1 activity: crystal structure of a chimeric pancreatic lipase-related protein 2 from guinea pig. <b>1996</b> , 4, 1363-74	93
1924	Phi/psi-chology: Ramachandran revisited. <b>1996</b> , 4, 1395-400	478
1923	The UmuD' protein filament and its potential role in damage induced mutagenesis. <b>1996</b> , 4, 1401-12	40
1922	The structure of glucose-fructose oxidoreductase from <i>Zymomonas mobilis</i> : an osmoprotective periplasmic enzyme containing non-dissociable NADP. <b>1996</b> , 4, 1413-28	80
1921	Crystal structure of a fungal elicitor secreted by <i>Phytophthora cryptogea</i> , a member of a novel class of plant necrotic proteins. <b>1996</b> , 4, 1429-39	84

1920	Substrate mimicry in the active center of a mammalian alpha-amylase: structural analysis of an enzyme-inhibitor complex. <b>1996</b> , 4, 1441-52	123
1919	Zinc mediated dimer of human interferon-alpha 2b revealed by X-ray crystallography. <b>1996</b> , 4, 1453-63	209
1918	A model of Ca(2+)-free calmodulin binding to unconventional myosins reveals how calmodulin acts as a regulatory switch. <b>1996</b> , 4, 1475-90	96
1917	The structural basis for pyrophosphatase catalysis. <b>1996</b> , 4, 1491-508	115
1916	Towards the complete structural characterization of a protein folding pathway: the structures of the denatured, transition and native states for the association/folding of two complementary fragments of cleaved chymotrypsin inhibitor 2. Direct evidence for a nucleation-condensation mechanism. <b>1996</b> , 1, 189-208	36
1915	Structural investigation of the complexation properties between horse spleen apoferritin and metalloporphyrins. <b>1996</b> , 24, 314-21	21
1914	Refined structures of bobwhite quail lysozyme uncomplexed and complexed with the HyHEL-5 Fab fragment. <b>1996</b> , 26, 55-65	23
1913	An extended sampling of the configurational space of HPr from E. coli. <b>1996</b> , 26, 314-22	78
1912	Structure and dynamics of the DNA binding protein HU from Bacillus stearothermophilus by NMR spectroscopy. <b>1996</b> , 40, 553-9	23
1911	Knowledge-based modeling of a legume lectin and docking of the carbohydrate ligand: the Ulex europaeus lectin I and its interaction with fucose. <b>1996</b> , 14, 322-7, 363-4	17
1910	Structure in solution of a four-helix lipid binding protein. <b>1996</b> , 5, 13-23	111
1909	The crystal structure of trypanothione reductase from the human pathogen Trypanosoma cruzi at 2.3 Å resolution. <b>1996</b> , 5, 52-61	78
1908	Structure-based modeling of the ligand binding domain of the human cell surface receptor CD23 and comparison of two independently derived molecular models. <b>1996</b> , 5, 240-7	12
1907	BSTI, a trypsin inhibitor from skin secretions of Bombina bombina related to protease inhibitors of nematodes. <b>1996</b> , 5, 357-62	63
1906	The structure of bovine mitochondrial adenylate kinase: comparison with isoenzymes in other compartments. <b>1996</b> , 5, 434-41	49
1905	Solution structure and lipid binding of a nonspecific lipid transfer protein extracted from maize seeds. <b>1996</b> , 5, 565-77	100
1904	Structure of a secreted aspartic protease from C. albicans complexed with a potent inhibitor: implications for the design of antifungal agents. <b>1996</b> , 5, 640-52	84
1903	Crystal structure of cod liver class I alcohol dehydrogenase: substrate pocket and structurally variable segments. <b>1996</b> , 5, 663-71	42

1902	Two crystal structures of the leupeptin-trypsin complex. <b>1996</b> , 5, 752-8	35
1901	Extremely thermostable L(+)-lactate dehydrogenase from <i>Thermotoga maritima</i> : cloning, characterization, and crystallization of the recombinant enzyme in its tetrameric and octameric state. <b>1996</b> , 5, 862-73	17
1900	An unusual route to thermostability disclosed by the comparison of <i>Thermus thermophilus</i> and <i>Escherichia coli</i> inorganic pyrophosphatases. <b>1996</b> , 5, 1014-25	60
1899	Improving the quality of NMR and crystallographic protein structures by means of a conformational database potential derived from structure databases. <b>1996</b> , 5, 1067-80	180
1898	The crystal structure of TGF-beta 3 and comparison to TGF-beta 2: implications for receptor binding. <b>1996</b> , 5, 1261-71	127
1897	Cytochrome c3 from <i>Desulfovibrio gigas</i> : crystal structure at 1.8 Å resolution and evidence for a specific calcium-binding site. <b>1996</b> , 5, 1342-54	74
1896	Experimentally observed conformation-dependent geometry and hidden strain in proteins. <b>1996</b> , 5, 1406-20	214
1895	A novel complex of a phenolic derivative with insulin: structural features related to the T->R transition. <b>1996</b> , 5, 1502-11	41
1894	Crystal structures of the active site mutant (Arg-243->Ala) in the T and R allosteric states of pig kidney fructose-1,6-bisphosphatase expressed in <i>Escherichia coli</i> . <b>1996</b> , 5, 1541-53	12
1893	Crystal structure of a biologically inactive mutant of toxic shock syndrome toxin-1 at 2.5 Å resolution. <b>1996</b> , 5, 1737-41	9
1892	Crystal structure of the 2[4Fe-4S] ferredoxin from <i>Chromatium vinosum</i> : evolutionary and mechanistic inferences for [3/4Fe-4S] ferredoxins. <b>1996</b> , 5, 1765-75	61
1891	The 1.8-Å X-ray structure of the <i>Escherichia coli</i> PotD protein complexed with spermidine and the mechanism of polyamine binding. <b>1996</b> , 5, 1984-90	50
1890	Crystal structure analyses of uncomplexed ecotin in two crystal forms: implications for its function and stability. <b>1996</b> , 5, 2236-47	25
1889	Evidence for an active T-state pig kidney fructose 1,6-bisphosphatase: interface residue Lys-42 is important for allosteric inhibition and AMP cooperativity. <b>1996</b> , 5, 2333-42	20
1888	Crystal structure of dUTP pyrophosphatase from feline immunodeficiency virus. <b>1996</b> , 5, 2429-37	72
1887	Insights into the molecular basis of thermal stability from the structure determination of <i>Pyrococcus furiosus</i> glutamate dehydrogenase. <b>1996</b> , 18, 105-17	48
1886	Structural transitions during activation and ligand binding in hexadecameric Rubisco inferred from the crystal structure of the activated unliganded spinach enzyme. <b>1996</b> , 3, 95-101	90
1885	Crystallographic observation of a covalent catalytic intermediate in a beta-glycosidase. <b>1996</b> , 3, 149-54	142

1884	The 2.4 Å crystal structure of the bacterial chaperonin GroEL complexed with ATP gamma S. <b>1996</b> , 3, 170-7	211
1883	The X-ray structures of two mutant crystallin domains shed light on the evolution of multi-domain proteins. <b>1996</b> , 3, 267-74	33
1882	Structure based design and characterization of peptides that inhibit IgE binding to its high-affinity receptor. <b>1996</b> , 3, 419-26	77
1881	The structure of <i>Desulfovibrio vulgaris</i> rubrerythrin reveals a unique combination of rubredoxin-like FeS <sub>4</sub> and ferritin-like diiron domains. <b>1996</b> , 3, 539-46	118
1880	Inhibitory conformation of the reactive loop of alpha 1-antitrypsin. <b>1996</b> , 3, 676-81	208
1879	Novel mechanism for defective receptor binding of apolipoprotein E2 in type III hyperlipoproteinemia. <b>1996</b> , 3, 718-22	105
1878	Ras/Rap effector specificity determined by charge reversal. <b>1996</b> , 3, 723-9	189
1877	The crystal structure of a llama heavy chain variable domain. <b>1996</b> , 3, 752-7	121
1876	Crystal structure of turnip yellow mosaic virus. <b>1996</b> , 3, 771-81	105
1875	C2 domain conformational changes in phospholipase C-delta 1. <b>1996</b> , 3, 788-95	100
1874	Crystal structure of a camel single-domain VH antibody fragment in complex with lysozyme. <b>1996</b> , 3, 803-11	383
1873	Three-dimensional structure of human cyclin H, a positive regulator of the CDK-activating kinase. <b>1996</b> , 3, 849-55	57
1872	Domain swapping creates a third putative combining site in bovine odorant binding protein dimer. <b>1996</b> , 3, 863-7	174
1871	Crystal structures of <i>Toxoplasma gondii</i> HGXPRTase reveal the catalytic role of a long flexible loop. <b>1996</b> , 3, 881-7	88
1870	Crystal structure of <i>Aplysia</i> ADP ribosyl cyclase, a homologue of the bifunctional ectozyme CD38. <b>1996</b> , 3, 957-64	127
1869	A leucine-rich repeat variant with a novel repetitive protein structural motif. <b>1996</b> , 3, 991-4	42
1868	Structural similarity between TAFs and the heterotetrameric core of the histone octamer. <b>1996</b> , 380, 316-22	232
1867	Crystal structure of the kinesin motor domain reveals a structural similarity to myosin. <b>1996</b> , 380, 550-5	577

1866	Crystal structure of the motor domain of the kinesin-related motor ncd. <b>1996</b> , 380, 555-9	335
1865	Structure of the UmuD' protein and its regulation in response to DNA damage. <b>1996</b> , 380, 727-30	152
1864	Structure and mutational analysis of Rab GDP-dissociation inhibitor. <b>1996</b> , 381, 42-8	153
1863	Structure of Bordetella pertussis virulence factor P.69 pertactin. <b>1996</b> , 381, 90-2	259
1862	Structural basis for inhibition of receptor protein-tyrosine phosphatase-alpha by dimerization. <b>1996</b> , 382, 555-9	297
1861	Unique fold and active site in cytomegalovirus protease. <b>1996</b> , 383, 275-9	151
1860	Three-dimensional structure of human cytomegalovirus protease. <b>1996</b> , 383, 279-82	146
1859	Crystal structure of a T-cell receptor beta-chain complexed with a superantigen. <b>1996</b> , 384, 188-92	265
1858	Interacting residues in the extracellular region of the common beta subunit of the human granulocyte-macrophage colony-stimulating factor, interleukin (IL)-3, and IL-5 receptors involved in constitutive activation. <b>1996</b> , 271, 29707-14	39
1857	Refined crystal structures of guanine nucleotide complexes of adenylosuccinate synthetase from Escherichia coli. <b>1996</b> , 271, 15407-13	22
1856	A common structural basis for the inhibition of ribulose 1,5-bisphosphate carboxylase by 4-carboxyarabinitol 1,5-bisphosphate and xylulose 1,5-bisphosphate. <b>1996</b> , 271, 32894-9	26
1855	Ligand binding to integrin alphaIIb beta3 is dependent on a MIDAS-like domain in the beta3 subunit. <b>1996</b> , 271, 21978-84	141
1854	Crystal Structure of S-Adenosylmethionine Synthetase. <b>1996</b> , 271, 136-147	90
1853	A structure of the complex between concanavalin A and methyl-3,6-di-O-(alpha-D-mannopyranosyl)-alpha-D-mannopyranoside reveals two binding modes. <b>1996</b> , 271, 30614-8	57
1852	Crystal structure of PotD, the primary receptor of the polyamine transport system in Escherichia coli. <b>1996</b> , 271, 9519-25	73
1851	Self Assembling Organic Nanotubes. <b>1996</b> , 181-188	1
1850	Structural basis of trimannoside recognition by concanavalin A. <b>1996</b> , 271, 972-6	232
1849	Active site structural features for chemically modified forms of rhodanese. <b>1996</b> , 271, 21054-61	41

1848	A discontinuous eight-amino acid epitope in human interleukin-3 binds the alpha-chain of its receptor. <b>1996</b> , 271, 31922-8	17
1847	The crystallographic structure of phytohemagglutinin-L. <b>1996</b> , 271, 20479-85	88
1846	The Co-crystal structure of staphylococcal enterotoxin type A with Zn <sup>2+</sup> at 2.7 Å resolution. Implications for major histocompatibility complex class II binding. <b>1996</b> , 271, 32212-6	41
1845	Crystal structure of arcelin-5, a lectin-like defense protein from <i>Phaseolus vulgaris</i> . <b>1996</b> , 271, 32796-802	25
1844	Ligand specificity of brain lipid-binding protein. <b>1996</b> , 271, 24711-9	142
1843	An efficient method for sampling the essential subspace of proteins. <b>1996</b> , 13, 615-25	234
1842	New insights on DNA recognition by ets proteins from the crystal structure of the PU.1 ETS domain-DNA complex. <b>1996</b> , 271, 23329-37	72
1841	Structural analysis of monosaccharide recognition by rat liver mannose-binding protein. <b>1996</b> , 271, 663-74	133
1840	Phosphorylation events associated with different states of activation of a hepatic cardiolipin/protease-activated protein kinase. Structural identity to the protein kinase N-type protein kinases. <b>1996</b> , 271, 32233-40	31
1839	Entrapment of 6-thiophosphoryl-IMP in the active site of crystalline adenylosuccinate synthetase from <i>Escherichia coli</i> . <b>1997</b> , 272, 15200-5	28
1838	Crystal structure of murine/human Ubc9 provides insight into the variability of the ubiquitin-conjugating system. <b>1997</b> , 272, 21381-7	107
1837	Model building and refinement practice. <b>1997</b> , 277, 208-30	232
1836	Refinement and Comparisons of the Crystal Structures of Pig Cytosolic Aspartate Aminotransferase and Its Complex with 2-Methylaspartate. <b>1997</b> , 272, 17293-17302	80
1835	<i>Trimeresurus stejnegeri</i> snake venom plasminogen activator. Site-directed mutagenesis and molecular modeling. <b>1997</b> , 272, 20531-7	49
1834	Isolation, cloning, sequence analysis and X-ray structure of dimethyl sulfoxide/trimethylamine N-oxide reductase from <i>Rhodobacter capsulatus</i> . <b>1997</b> , 378, 293-302	2
1833	Biochemical and crystallographic analyses of a portal mutant of the adipocyte lipid-binding protein. <b>1997</b> , 272, 9793-801	27
1832	Structure of cardiac muscle troponin C unexpectedly reveals a closed regulatory domain. <b>1997</b> , 272, 18216-21	157
1831	X-ray structure of human class IV sigma sigma alcohol dehydrogenase. Structural basis for substrate specificity. <b>1997</b> , 272, 18558-63	62



1830	Secretion of a novel, developmentally regulated fatty acid-binding protein into the perivitelline fluid of the parasitic nematode, <i>Ascaris suum</i> . <b>1997</b> , 272, 9933-41	58
1829	A model for the activation of the epidermal growth factor receptor kinase involvement of an asymmetric dimer?. <b>1997</b> , 36, 3826-36	31
1828	Crystal structure at 1.1 Å resolution of alpha-conotoxin Pn1B: comparison with alpha-conotoxins Pn1A and GI. <b>1997</b> , 36, 11323-30	80
1827	Mouse mast cell protease 9, a novel member of the chromosome 14 family of serine proteases that is selectively expressed in uterine mast cells. <b>1997</b> , 272, 29158-66	51
1826	The crystal structure of the liver fatty acid-binding protein. A complex with two bound oleates. <b>1997</b> , 272, 7140-50	203
1825	Structural mapping of the active site specificity determinants of human tissue-type plasminogen activator. Implications for the design of low molecular weight substrates and inhibitors. <b>1997</b> , 272, 21713-9	59
1824	The X-ray structure of the PurR-guanine-purF operator complex reveals the contributions of complementary electrostatic surfaces and a water-mediated hydrogen bond to corepressor specificity and binding affinity. <b>1997</b> , 272, 22648-53	42
1823	Crystal structure of rat Bcl-xL. Implications for the function of the Bcl-2 protein family. <b>1997</b> , 272, 27886-92	97
1822	Three-dimensional structure of L-2-haloacid dehalogenase from <i>Xanthobacter autotrophicus</i> GJ10 complexed with the substrate-analogue formate. <b>1997</b> , 272, 33015-22	89
1821	Examination of substrate binding in thiamin diphosphate-dependent transketolase by protein crystallography and site-directed mutagenesis. <b>1997</b> , 272, 1864-9	84
1820	A single chain Fv fragment of P-glycoprotein-specific monoclonal antibody C219. Design, expression, and crystal structure at 2.4 Å resolution. <b>1997</b> , 272, 29784-9	25
1819	Crystal Structure Refinement Incorporating Chemical Information. <b>1997</b> , 219-230	7
1818	The first step of aminoacylation at the atomic level in histidyl-tRNA synthetase. <b>1997</b> , 94, 7144-9	94
1817	The solution structure of the N-terminal domain of alpha2-macroglobulin receptor-associated protein. <b>1997</b> , 94, 7521-5	44
1816	Human argininosuccinate lyase: a structural basis for intragenic complementation. <b>1997</b> , 94, 9063-8	99
1815	Structure of the thrombin complex with triabin, a lipocalin-like exosite-binding inhibitor derived from a triatomine bug. <b>1997</b> , 94, 11845-50	109
1814	Atomic structure of a thermostable subdomain of HIV-1 gp41. <b>1997</b> , 94, 12303-8	507
1813	The crystal structure of human interferon beta at 2.2-Å resolution. <b>1997</b> , 94, 11813-8	183

1812	The structure of mitogen-activated protein kinase p38 at 2.1-A resolution. <b>1997</b> , 94, 2327-32	254
1811	Identification of a second aryl phosphate-binding site in protein-tyrosine phosphatase 1B: a paradigm for inhibitor design. <b>1997</b> , 94, 13420-5	386
1810	Vascular endothelial growth factor: crystal structure and functional mapping of the kinase domain receptor binding site. <b>1997</b> , 94, 7192-7	367
1809	Unique features in the structure of the complex between HIV-1 reverse transcriptase and the bis(heteroaryl)piperazine (BHAP) U-90152 explain resistance mutations for this nonnucleoside inhibitor. <b>1997</b> , 94, 3984-9	173
1808	Structural mimicry of a native protein by a minimized binding domain. <b>1997</b> , 94, 10080-5	124
1807	Collaborative Computational Project, number 4: providing programs for protein crystallography. <b>1997</b> , 277, 620-33	154
1806	The anticoagulant activation of antithrombin by heparin. <b>1997</b> , 94, 14683-8	618
1805	Structural basis for dual excitation and photoisomerization of the <i>Aequorea victoria</i> green fluorescent protein. <b>1997</b> , 94, 2306-11	617
1804	Structures of competitive inhibitor complexes of protocatechuate 3,4-dioxygenase: multiple exogenous ligand binding orientations within the active site. <b>1997</b> , 36, 10039-51	81
1803	Crystal structure of cardiotoxin V from Taiwan cobra venom: pH-dependent conformational change and a novel membrane-binding motif identified in the three-finger loops of P-type cardiotoxin. <b>1997</b> , 36, 2403-13	49
1802	Crystal structures of substrate and substrate analog complexes of protocatechuate 3,4-dioxygenase: endogenous Fe <sup>3+</sup> ligand displacement in response to substrate binding. <b>1997</b> , 36, 10052-66	154
1801	Catalytic domain structure of vampire bat plasminogen activator: a molecular paradigm for proteolysis without activation cleavage. <b>1997</b> , 36, 13483-93	41
1800	Structure of the carboxy-terminal fragment of the apo-biotin carboxyl carrier subunit of <i>Escherichia coli</i> acetyl-CoA carboxylase. <b>1997</b> , 36, 15089-100	68
1799	The structure of L-aspartate ammonia-lyase from <i>Escherichia coli</i> . <b>1997</b> , 36, 9136-44	80
1798	The <i>Streptomyces lividans</i> family 12 endoglucanase: construction of the catalytic cre, expression, and X-ray structure at 1.75 Å resolution. <b>1997</b> , 36, 16032-9	52
1797	A response regulatory protein with the site of phosphorylation blocked by an arginine interaction: crystal structure of Spo0F from <i>Bacillus subtilis</i> . <b>1997</b> , 36, 12739-45	42
1796	Structures of wild-type chloromet and L103N hydroxomet <i>Thermotoga zostericola</i> myohemerythrins at 1.8 Å resolution. <b>1997</b> , 36, 7044-9	27
1795	Chemical synthesis, structural modeling, and biological activity of the epidermal growth factor-like domain of human cripto. <b>1997</b> , 36, 3837-45	26

1794	The structure of the superantigen exfoliative toxin A suggests a novel regulation as a serine protease. <b>1997</b> , 36, 1559-66	120
1793	The Concept of Solvent Compatibility and Its Impact on Protein Stability and Activity Enhancement in Nonaqueous Solvents. <b>1997</b> , 119, 9939-9948	28
1792	Binding of formamides to liver alcohol dehydrogenase. <b>1997</b> , 36, 3522-7	57
1791	Phospholipase A2 engineering. Structural and functional roles of the highly conserved active site residue aspartate-99. <b>1997</b> , 36, 3104-14	48
1790	Solution structure for Pandinus toxin K-alpha (PiTX-K alpha), a selective blocker of A-type potassium channels. <b>1997</b> , 36, 2763-71	18
1789	Characterization of the unbound 2[Fe4S4]-ferredoxin-like photosystem I subunit PsaC from the Cyanobacterium synechococcus elongatus. <b>1997</b> , 36, 13629-37	17
1788	The crystal structure of <i>Citrobacter freundii</i> tyrosine phenol-lyase complexed with 3-(4'-hydroxyphenyl)propionic acid, together with site-directed mutagenesis and kinetic analysis, demonstrates that arginine 381 is required for substrate specificity. <b>1997</b> , 36, 6502-10	73
1787	Atomic resolution (0.94 Å) structure of <i>Clostridium acidurici</i> ferredoxin. Detailed geometry of [4Fe-4S] clusters in a protein. <b>1997</b> , 36, 16065-73	124
1786	Tyrosine and tryptophan structure markers in hemoglobin ultraviolet resonance Raman spectra: mode assignments via subunit-specific isotope labeling of recombinant protein. <b>1997</b> , 36, 15701-12	91
1785	Flexibility of liver alcohol dehydrogenase in stereoselective binding of 3-butylthiolane 1-oxides. <b>1997</b> , 36, 382-9	55
1784	Active site plasticity in D-amino acid oxidase: a crystallographic analysis. <b>1997</b> , 36, 5853-60	79
1783	Identification of catalytically important residues in yeast transketolase. <b>1997</b> , 36, 15643-9	65
1782	Structure of the <i>Aspergillus oryzae</i> alpha-amylase complexed with the inhibitor acarbose at 2.0 Å resolution. <b>1997</b> , 36, 10837-45	191
1781	The crystal structure of zinc-containing ferredoxin from the thermoacidophilic archaeon <i>Sulfolobus</i> sp. strain 7. <b>1997</b> , 36, 1505-13	33
1780	Structure and function of the xenobiotic substrate-binding site and location of a potential non-substrate-binding site in a class pi glutathione S-transferase. <b>1997</b> , 36, 9690-702	89
1779	Electrostatic mechanism for DNA bending by bZIP proteins. <b>1997</b> , 36, 10033-8	39
1778	Molecular simulation of dynorphin A-(1-10) binding to extracellular loop 2 of the kappa-opioid receptor. A model for receptor activation. <b>1997</b> , 40, 3254-62	74
1777	Crystal structure at 2.0 Å resolution of phosphoribosyl anthranilate isomerase from the hyperthermophile <i>Thermotoga maritima</i> : possible determinants of protein stability. <b>1997</b> , 36, 6009-16	93

1776	Structure of bacterial luciferase beta 2 homodimer: implications for flavin binding. <b>1997</b> , 36, 665-72	15
1775	Structure of carbamoyl phosphate synthetase: a journey of 96 Å from substrate to product. <b>1997</b> , 36, 6305-16	302
1774	Crystal structure of the Escherichia coli peptide deformylase. <b>1997</b> , 36, 13904-9	118
1773	The three-dimensional structure of the human Pi class glutathione transferase P1-1 in complex with the inhibitor ethacrynic acid and its glutathione conjugate. <b>1997</b> , 36, 576-85	111
1772	Crystal structure of a polyhistidine-tagged recombinant catalytic subunit of cAMP-dependent protein kinase complexed with the peptide inhibitor PKI(5-24) and adenosine. <b>1997</b> , 36, 4438-48	104
1771	Crystal structure of a class I ubiquitin conjugating enzyme (Ubc7) from Saccharomyces cerevisiae at 2.9 angstroms resolution. <b>1997</b> , 36, 1621-7	61
1770	Peptide ligands of pp60(c-src) SH2 domains: a thermodynamic and structural study. <b>1997</b> , 36, 6283-93	90
1769	Solution structure of phenol hydroxylase protein component P2 determined by NMR spectroscopy. <b>1997</b> , 36, 495-504	43
1768	Crystal structure of Escherichia coli xanthine phosphoribosyltransferase. <b>1997</b> , 36, 4125-34	72
1767	Definition of the switch surface in the solution structure of Cdc42Hs. <b>1997</b> , 36, 8755-66	87
1766	Structure of a selectin-like mutant of mannose-binding protein complexed with sialylated and sulfated Lewis(x) oligosaccharides. <b>1997</b> , 36, 979-88	86
1765	High-resolution NMR structure and backbone dynamics of the Bacillus subtilis response regulator, Spo0F: implications for phosphorylation and molecular recognition. <b>1997</b> , 36, 10015-25	62
1764	Structural and biochemical characterization of the GTPgammaS-, GDP.Pi-, and GDP-bound forms of a GTPase-deficient Gly42 --> Val mutant of Galpha1. <b>1997</b> , 36, 15660-9	61
1763	Mechanism of direct coupling between binding and induced structural change in regulatory calcium binding proteins. <b>1997</b> , 36, 4386-92	116
1762	Solution structure of the 30 kDa N-terminal domain of enzyme I of the Escherichia coli phosphoenolpyruvate:sugar phosphotransferase system by multidimensional NMR. <b>1997</b> , 36, 2517-30	159
1761	Multifunctional role of Tyr 108 in the catalytic mechanism of human glutathione transferase P1-1. Crystallographic and kinetic studies on the Y108F mutant enzyme. <b>1997</b> , 36, 6207-17	58
1760	Refined structure, DNA binding studies, and dynamics of the bacteriophage Pf3 encoded single-stranded DNA binding protein. <b>1997</b> , 36, 9120-35	25
1759	Three-dimensional structure of tetrahydrodipicolinate N-succinyltransferase. <b>1997</b> , 36, 489-94	64

1758	Calcium-induced structural transition in the regulatory domain of human cardiac troponin C. <b>1997</b> , 36, 12138-46	177
1757	Tertiary structure of RBD2 and backbone dynamics of RBD1 and RBD2 of the human U1A protein determined by NMR spectroscopy. <b>1997</b> , 36, 10393-405	38
1756	Structural comparison of the enzymatically active and inactive forms of delta crystallin and the role of histidine 91. <b>1997</b> , 36, 14012-22	31
1755	Insight into signal transduction: structural alterations in transmembrane helices probed by multi-1 ns molecular dynamics simulations. <b>1997</b> , 15, 555-72	19
1754	The entropic penalty of ordered water accounts for weaker binding of the antibiotic novobiocin to a resistant mutant of DNA gyrase: a thermodynamic and crystallographic study. <b>1997</b> , 36, 9663-73	200
1753	Solution structure of oxidized horse heart cytochrome c. <b>1997</b> , 36, 9867-77	282
1752	Influenza neuraminidase inhibitors possessing a novel hydrophobic interaction in the enzyme active site: design, synthesis, and structural analysis of carbocyclic sialic acid analogues with potent anti-influenza activity. <b>1997</b> , 119, 681-90	952
1751	Crystal structures of ribonuclease A complexes with 5'-diphosphoadenosine 3'-phosphate and 5'-diphosphoadenosine 2'-phosphate at 1.7 Å resolution. <b>1997</b> , 36, 5578-88	77
1750	Free R value: cross-validation in crystallography. <b>1997</b> , 277, 366-96	228
1749	Active site cavity of herpesvirus proteases revealed by the crystal structure of herpes simplex virus protease/inhibitor complex. <b>1997</b> , 36, 14023-9	67
1748	Structure of the chromatin binding (chromo) domain from mouse modifier protein 1. <b>1997</b> , 16, 2473-81	140
1747	Crystal structure of the complex of bovine pancreatic phospholipase A2 with the inhibitor 1-hexadecyl-3-(trifluoroethyl)-sn-glycero-2-phosphomethanol. <b>1997</b> , 36, 14186-91	47
1746	Mutagenesis of the histidine ligand in human lactoferrin: iron binding properties and crystal structure of the histidine-253-->methionine mutant. <b>1997</b> , 36, 341-6	40
1745	X-ray structure of motor and neck domains from rat brain kinesin. <b>1997</b> , 36, 16155-65	164
1744	Discrete backbone disorder in the nuclear magnetic resonance structure of apo intestinal fatty acid-binding protein: implications for the mechanism of ligand entry. <b>1997</b> , 36, 1450-60	157
1743	X-ray structures of the MgADP, MgATPgammaS, and MgAMPPNP complexes of the Dictyostelium discoideum myosin motor domain. <b>1997</b> , 36, 11619-28	188
1742	Comparison of two independent crystal structures of human dihydrofolate reductase ternary complexes reduced with nicotinamide adenine dinucleotide phosphate and the very tight-binding inhibitor PT523. <b>1997</b> , 36, 13897-903	52
1741	Crystal structure of Tritrichomonas foetus inosine-5'-monophosphate dehydrogenase and the enzyme-product complex. <b>1997</b> , 36, 10666-74	55

1740	Structure of the endoglucanase I from <i>Fusarium oxysporum</i> : native, cellobiose, and 3,4-epoxybutyl beta-D-cellobioside-inhibited forms, at 2.3 Å resolution. <b>1997</b> , 36, 5902-11	80
1739	Refined structure of an intact IgG2a monoclonal antibody. <b>1997</b> , 36, 1581-97	380
1738	Structural insights into the evolution of an antibody combining site. <b>1997</b> , 276, 1665-9	500
1737	Crystal structure of human BPI and two bound phospholipids at 2.4 angstrom resolution. <b>1997</b> , 276, 1861-4	317
1736	Structure and function of a squalene cyclase. <b>1997</b> , 277, 1811-5	397
1735	Toroidal structure of lambda-exonuclease. <b>1997</b> , 277, 1824-7	184
1734	The structure of nitric oxide synthase oxygenase domain and inhibitor complexes. <b>1997</b> , 278, 425-31	321
1733	Crystal structure of the catalytic domains of adenylyl cyclase in a complex with G $\alpha$ .GTP $\gamma$ S. <b>1997</b> , 278, 1907-16	638
1732	Crystal structure of the adenylyl cyclase activator G $\alpha$ . <b>1997</b> , 278, 1943-7	260
1731	Immune versus natural selection: antibody aldolases with enzymic rates but broader scope. <b>1997</b> , 278, 2085-92	357
1730	Crystal structure of protein farnesyltransferase at 2.25 angstrom resolution. <b>1997</b> , 275, 1800-4	329
1729	Ligand-induced domain movement in pyruvate kinase: structure of the enzyme from rabbit muscle with Mg <sup>2+</sup> , K <sup>+</sup> , and L-phospholactate at 2.7 Å resolution. <b>1997</b> , 345, 199-206	74
1728	Towards a molecular understanding of phase separation in the lens: a comparison of the X-ray structures of two high T <sub>c</sub> gamma-crystallins, gammaE and gammaF, with two low T <sub>c</sub> gamma-crystallins, gammaB and gammaD. <b>1997</b> , 65, 609-30	38
1727	A natural antibody missing a cysteine in VH: consequences for thermodynamic stability and folding. <b>1997</b> , 265, 161-72	117
1726	<i>Streptomyces griseus</i> aminopeptidase: X-ray crystallographic structure at 1.75 Å resolution. <b>1997</b> , 265, 620-36	108
1725	Structure of human chi chi alcohol dehydrogenase: a glutathione-dependent formaldehyde dehydrogenase. <b>1997</b> , 265, 330-43	84
1724	Structure and mechanism of a sub-family of enzymes related to N-acetylneuraminase lyase. <b>1997</b> , 266, 381-99	96
1723	X-ray structure at 1.76 Å resolution of a polypeptide phospholipase A2 inhibitor. <b>1997</b> , 266, 160-72	21

1722	The amino-terminal residues in the crystal structure of connective tissue activating peptide-III (des10) block the ELR chemotactic sequence. <b>1997</b> , 266, 367-80	20
1721	Structure of maltoporin from <i>Salmonella typhimurium</i> ligated with a nitrophenyl-maltotrioxide. <b>1997</b> , 266, 761-75	125
1720	Crystal structure of the gramicidin/potassium thiocyanate complex. <b>1997</b> , 266, 963-77	49
1719	Solution structure of the albumin-binding GA module: a versatile bacterial protein domain. <b>1997</b> , 266, 859-65	68
1718	Crystal structure of a ternary complex of D-2-hydroxyisocaproate dehydrogenase from <i>Lactobacillus casei</i> , NAD <sup>+</sup> and 2-oxoisocaproate at 1.9 Å resolution. <b>1997</b> , 267, 640-60	56
1717	Crystal structure of glutamate dehydrogenase from the hyperthermophilic eubacterium <i>Thermotoga maritima</i> at 3.0 Å resolution. <b>1997</b> , 267, 916-32	142
1716	High-resolution solution structure of human pNR-2/pS2: a single trefoil motif protein. <b>1997</b> , 267, 418-32	59
1715	Solution structure of recombinant human interleukin-6. <b>1997</b> , 268, 468-81	65
1714	Structure of TcpG, the DsbA protein folding catalyst from <i>Vibrio cholerae</i> . <b>1997</b> , 268, 137-46	64
1713	Three-dimensional structure of an Fab-peptide complex: structural basis of HIV-1 protease inhibition by a monoclonal antibody. <b>1997</b> , 267, 1207-22	51
1712	Characterization of long-range structure in the denatured state of staphylococcal nuclease. II. Distance restraints from paramagnetic relaxation and calculation of an ensemble of structures. <b>1997</b> , 268, 170-84	270
1711	The three-dimensional structure of flavodoxin reductase from <i>Escherichia coli</i> at 1.7 Å resolution. <b>1997</b> , 268, 147-57	122
1710	Assembly of protein tertiary structures from fragments with similar local sequences using simulated annealing and Bayesian scoring functions. <b>1997</b> , 268, 209-25	1108
1709	Apoprotein structure in the LH2 complex from <i>Rhodospseudomonas acidophila</i> strain 10050: modular assembly and protein pigment interactions. <b>1997</b> , 268, 412-23	169
1708	Crystal structure of the aspartic proteinase from <i>Rhizomucor miehei</i> at 2.15 Å resolution. <b>1997</b> , 268, 449-59	38
1707	Comparison of the three-dimensional structures of recombinant human H and horse L ferritins at high resolution. <b>1997</b> , 268, 424-48	277
1706	Crystal structures of the free and liganded form of an esterolytic catalytic antibody. <b>1997</b> , 268, 390-400	59
1705	Solution structure of R-elafin, a specific inhibitor of elastase. <b>1997</b> , 268, 666-77	44

1704	Atomic resolution (1.0 Å) crystal structure of <i>Fusarium solani</i> cutinase: stereochemical analysis. <b>1997</b> , 268, 779-99	191
1703	The crystal structure of seleno-glutathione peroxidase from human plasma at 2.9 Å resolution. <b>1997</b> , 268, 869-85	142
1702	The rational construction of an antibody against cystatin: lessons from the crystal structure of an artificial Fab fragment. <b>1997</b> , 268, 934-51	15
1701	Molecular structure of the lipoamide dehydrogenase domain of a surface antigen from <i>Neisseria meningitidis</i> . <b>1997</b> , 269, 129-41	49
1700	Protein folding simulations with genetic algorithms and a detailed molecular description. <b>1997</b> , 269, 240-59	114
1699	Crystal structure of an oligomer of proteolytic zymogens: detailed conformational analysis of the bovine ternary complex and implications for their activation. <b>1997</b> , 269, 861-80	24
1698	Dual conformations of a T cell receptor V alpha homodimer: implications for variability in V alpha V beta domain association. <b>1997</b> , 269, 385-94	18
1697	The 1.8 Å crystal structure of winged bean albumin 1, the major albumin from <i>Psophocarpus tetragonolobus</i> (L.) DC. <b>1997</b> , 269, 881-91	24
1696	Crystal structure of the C-terminal tetrad repeat from synexin (annexin VII) of <i>Dictyostelium discoideum</i> . <b>1997</b> , 270, 79-88	25
1695	The crystal structure of an Fe-superoxide dismutase from the hyperthermophile <i>Aquifex pyrophilus</i> at 1.9 Å resolution: structural basis for thermostability. <b>1997</b> , 270, 259-74	112
1694	Three-dimensional structure of the DNA-binding domain of the fructose repressor from <i>Escherichia coli</i> by 1H and 15N NMR. <b>1997</b> , 270, 496-510	34
1693	Crystal structure of cytoplasmic <i>Escherichia coli</i> peptidyl-prolyl isomerase: evidence for decreased mobility of loops upon complexation. <b>1997</b> , 271, 258-65	26
1692	<i>Thermus thermophilus</i> cytochrome-c552: A new highly thermostable cytochrome-c structure obtained by MAD phasing. <b>1997</b> , 271, 629-44	80
1691	Crystal structure of the bacteriochlorophyll a protein from <i>Chlorobium tepidum</i> . <b>1997</b> , 271, 456-71	181
1690	Crystal structure of the beta-glycosidase from the hyperthermophilic archeon <i>Sulfolobus solfataricus</i> : resilience as a key factor in thermostability. <b>1997</b> , 271, 789-802	220
1689	The X-ray structure of the DNA-binding domain from the <i>Saccharomyces cerevisiae</i> cell-cycle transcription factor Mbp1 at 2.1 Å resolution. <b>1997</b> , 272, 1-8	53
1688	The high resolution crystal structure of deoxyhemoglobin S. <b>1997</b> , 272, 398-407	134
1687	High-resolution solution NMR structure of the Z domain of staphylococcal protein A. <b>1997</b> , 272, 573-90	126



1686	Structure and mechanism of L-fucose isomerase from <i>Escherichia coli</i> . <b>1997</b> , 273, 256-68	66
1685	Solution structure of the first three zinc fingers of TFIIIA bound to the cognate DNA sequence: determinants of affinity and sequence specificity. <b>1997</b> , 273, 183-206	171
1684	Refined X-ray crystallographic structure of the poliovirus 3C gene product. <b>1997</b> , 273, 1032-47	166
1683	Validation of protein models from C $\alpha$ coordinates alone. <b>1997</b> , 273, 371-6	135
1682	Solution structure of the I gamma subdomain of the Mu end DNA-binding domain of phage Mu transposase. <b>1997</b> , 273, 19-25	32
1681	The 1.6 Å crystal structure of the AraC sugar-binding and dimerization domain complexed with D-fucose. <b>1997</b> , 273, 226-37	53
1680	Charges, hydrogen bonds, and correlated motions in the 1 Å resolution refined structure of the mating pheromone Er-1 from <i>Euplotes raikovi</i> . <b>1997</b> , 273, 479-500	10
1679	X-ray crystal structure and solution fluorescence characterization of Mg $\cdot$ 2'(3')-O-(N-methylanthraniloyl) nucleotides bound to the <i>Dictyostelium discoideum</i> myosin motor domain. <b>1997</b> , 274, 394-407	48
1678	The crystal structure of a type I cohesin domain at 1.7 Å resolution. <b>1997</b> , 273, 701-13	81
1677	The 1.8 Å crystal structure of the dimeric peroxisomal 3-ketoacyl-CoA thiolase of <i>Saccharomyces cerevisiae</i> : implications for substrate binding and reaction mechanism. <b>1997</b> , 273, 714-28	98
1676	Neutralizing epitopes on the extracellular interferon gamma receptor (IFN $\gamma$ R) alpha-chain characterized by homolog scanning mutagenesis and X-ray crystal structure of the A6 fab-IFN $\gamma$ R1-108 complex. <b>1997</b> , 273, 882-97	26
1675	Crystallization, structural determination and analysis of a novel parasite vaccine candidate: <i>Fasciola hepatica</i> glutathione S-transferase. <b>1997</b> , 273, 857-72	48
1674	Structure of the fifth EGF-like domain of thrombomodulin: An EGF-like domain with a novel disulfide-bonding pattern. <b>1997</b> , 273, 913-26	28
1673	The structures of human glutathione transferase P1-1 in complex with glutathione and various inhibitors at high resolution. <b>1997</b> , 274, 84-100	158
1672	Crystal structure of annexin V with its ligand K-201 as a calcium channel activity inhibitor. <b>1997</b> , 274, 16-20	50
1671	The RNA binding domain of ribosomal protein L11: three-dimensional structure of the RNA-bound form of the protein and its interaction with 23 S rRNA. <b>1997</b> , 274, 101-13	52
1670	Three-dimensional structure of diferric bovine lactoferrin at 2.8 Å resolution. <b>1997</b> , 274, 222-36	312
1669	Structure of dihydrodipicolinate synthase of <i>Nicotiana glauca</i> reveals novel quaternary structure. <b>1997</b> , 274, 608-21	71

1668	Unique structural features of the monomeric Cu,Zn superoxide dismutase from Escherichia coli, revealed by X-ray crystallography. <b>1997</b> , 274, 408-20	73
1667	Cloning, sequencing, crystallization and X-ray structure of glutathione S-transferase-III from Zea mays var. mutin: a leading enzyme in detoxification of maize herbicides. <b>1997</b> , 274, 577-87	70
1666	Crystal structure of herbicide-detoxifying maize glutathione S-transferase-I in complex with lactoylglutathione: evidence for an induced-fit mechanism. <b>1997</b> , 274, 446-53	91
1665	The three-dimensional structures of a polysaccharide binding antibody to Cryptococcus neoformans and its complex with a peptide from a phage display library: implications for the identification of peptide mimotopes. <b>1997</b> , 274, 622-34	71
1664	Crystal structure of acidic seminal fluid protein (aSFP) at 1.9 Å resolution: a bovine polypeptide of the spermadhesin family. <b>1997</b> , 274, 650-60	35
1663	The 2.4 Å resolution crystal structure of boar seminal plasma PSP-I/PSP-II: a zona pellucida-binding glycoprotein heterodimer of the spermadhesin family built by a CUB domain architecture. <b>1997</b> , 274, 635-49	69
1662	The 2.35 Å crystal structure of the inactivated form of chicken Src: a dynamic molecule with multiple regulatory interactions. <b>1997</b> , 274, 757-75	223
1661	Solution structure of human p8MTCP1, a cysteine-rich protein encoded by the MTCP1 oncogene, reveals a new alpha-helical assembly motif. <b>1997</b> , 274, 801-15	23
1660	The crystal structure of the complex of concanavalin A with 4'-methylumbelliferyl-alpha-D-glucopyranoside. <b>1997</b> , 118, 23-30	39
1659	The crystal structure of a Fab fragment to the melanoma-associated GD2 ganglioside. <b>1997</b> , 119, 6-16	37
1658	De novo protein design: fully automated sequence selection. <b>1997</b> , 278, 82-7	953
1657	Redox-dependent structural changes in the nitrogenase P-cluster. <b>1997</b> , 36, 1181-7	437
1656	Crystal structure of the complex of diphtheria toxin with an extracellular fragment of its receptor. <b>1997</b> , 1, 67-78	83
1655	Structure of RGS4 bound to AlF4--activated G(i alpha1): stabilization of the transition state for GTP hydrolysis. <b>1997</b> , 89, 251-61	696
1654	Core structure of gp41 from the HIV envelope glycoprotein. <b>1997</b> , 89, 263-73	1767
1653	X-ray crystallography reveals a large conformational change during guanyl transfer by mRNA capping enzymes. <b>1997</b> , 89, 545-53	239
1652	Structure of a cholesterol-binding, thiol-activated cytolysin and a model of its membrane form. <b>1997</b> , 89, 685-92	412
1651	Structure of an enzyme required for aminoglycoside antibiotic resistance reveals homology to eukaryotic protein kinases. <b>1997</b> , 89, 887-95	217

1650	Cocrystal structure of the messenger RNA 5' cap-binding protein (eIF4E) bound to 7-methyl-GDP. <b>1997</b> , 89, 951-61	574
1649	Protein-protein communication: structural model of the repression complex formed by CytR and the global regulator CRP. <b>1997</b> , 89, 1101-9	33
1648	Structural adaptations in the specialized bacteriophage T4 co-chaperonin Gp31 expand the size of the Anfinsen cage. <b>1997</b> , 90, 361-71	90
1647	Activation mechanism of the MAP kinase ERK2 by dual phosphorylation. <b>1997</b> , 90, 859-69	643
1646	Cloning and crystal structure of hematopoietic prostaglandin D synthase. <b>1997</b> , 90, 1085-95	226
1645	The structure of ClpP at 2.3 Å resolution suggests a model for ATP-dependent proteolysis. <b>1997</b> , 91, 447-56	512
1644	Crystal structure at 1.7 Å resolution of VEGF in complex with domain 2 of the Flt-1 receptor. <b>1997</b> , 91, 695-704	432
1643	Crystallographic analysis of anti-p24 (HIV-1) monoclonal antibody cross-reactivity and polyspecificity. <b>1997</b> , 91, 811-20	110
1642	Molecular basis of sulfite oxidase deficiency from the structure of sulfite oxidase. <b>1997</b> , 91, 973-83	438
1641	The crystal structure of plasma gelsolin: implications for actin severing, capping, and nucleation. <b>1997</b> , 90, 661-70	246
1640	Insights into multistep phosphorelay from the crystal structure of the C-terminal HPT domain of ArcB. <b>1997</b> , 88, 717-23	137
1639	Three-dimensional structure of <i>Serratia marcescens</i> nuclease at 1.7 Å resolution and mechanism of its action. <b>1997</b> , 412, 217-22	24
1638	Amino acid sequence and three-dimensional structure of the Tn-specific isolectin B4 from <i>Vicia villosa</i> . <b>1997</b> , 412, 190-6	21
1637	Influence of a NH <sub>2</sub> -terminal extension on the activity of KTX2, a K <sup>+</sup> channel blocker purified from <i>Androctonus australis</i> scorpion venom. <b>1997</b> , 417, 123-9	20
1636	The glutathione conjugate of ethacrynic acid can bind to human pi class glutathione transferase P1-1 in two different modes. <b>1997</b> , 419, 32-6	45
1635	Molecular and biochemical studies on the hypoxanthine-guanine phosphoribosyltransferases of the pathogenic haemoflagellates. <b>1997</b> , 27, 203-13	31
1634	[16] SHELXL: High-resolution refinement. <b>1997</b> , 319-343	1940
1633	Slow-binding inhibition of <i>Escherichia coli</i> cystathionine beta-lyase by L-aminoethoxyvinylglycine: a kinetic and X-ray study. <b>1997</b> , 36, 12633-43	60

1632	Structure of the proteasome activator REGalpha (PA28alpha). <b>1997</b> , 390, 639-43	160
1631	Modeling of anti-nucleosome immunoglobulin Fv domains: analysis of electrostatic interactions. <b>1997</b> , 34, 793-807	8
1630	Variable domain structure of kappaIV human light chain Len: high homology to the murine light chain McPC603. <b>1997</b> , 34, 1291-301	32
1629	Characterization of a Schistosoma mansoni gene encoding a homologue of the Y-box binding protein. <b>1997</b> , 198, 5-16	22
1628	Crystal structures of the copper and nickel complexes of RNase A: metal-induced interprotein interactions and identification of a novel copper binding motif. <b>1997</b> , 94, 9620-5	20
1627	Degradation of C1-Inhibitor by Plasmin: Implications for the Control of Inflammatory Processes. <b>1997</b> , 3, 385-396	29
1626	Catalytic mechanism of the adenylyl and guanylyl cyclases: modeling and mutational analysis. <b>1997</b> , 94, 13414-9	239
1625	X-ray structures of a hydrolytic antibody and of complexes elucidate catalytic pathway from substrate binding and transition state stabilization through water attack and product release. <b>1997</b> , 94, 7857-61	56
1624	Crystal structure of varicella-zoster virus protease. <b>1997</b> , 94, 2874-9	64
1623	The 2.0-A resolution crystal structure of a trimeric antibody fragment with noncognate VH-VL domain pairs shows a rearrangement of VH CDR3. <b>1997</b> , 94, 9637-42	70
1622	Solution structure of the ribosomal RNA binding protein S15 from Thermus thermophilus. <b>1997</b> , 4, 20-3	57
1621	Product binding and role of the C-terminal region in class I D-fructose 1,6-bisphosphate aldolase. <b>1997</b> , 4, 36-9	104
1620	Structure of acetylcholinesterase complexed with the nootropic alkaloid, (-)-huperzine A. <b>1997</b> , 4, 57-63	343
1619	The structure of MCP-1 in two crystal forms provides a rare example of variable quaternary interactions. <b>1997</b> , 4, 64-9	130
1618	The solution structure of a specific GAGA factor-DNA complex reveals a modular binding mode. <b>1997</b> , 4, 122-32	171
1617	The structure of the cytochrome p450BM-3 haem domain complexed with the fatty acid substrate, palmitoleic acid. <b>1997</b> , 4, 140-6	397
1616	Crystal structure of a calponin homology domain. <b>1997</b> , 4, 175-9	95
1615	Solution structure of the carbohydrate-binding B-subunit homopentamer of verotoxin VT-1 from E. coli. <b>1997</b> , 4, 190-3	35

1614	Crystal structure of the two RNA binding domains of human hnRNP A1 at 1.75 Å resolution. <b>1997</b> , 4, 215-22	106
1613	The first structure of an aldehyde dehydrogenase reveals novel interactions between NAD and the Rossmann fold. <b>1997</b> , 4, 317-26	249
1612	Structure of human IgM rheumatoid factor Fab bound to its autoantigen IgG Fc reveals a novel topology of antibody-antigen interaction. <b>1997</b> , 4, 374-81	186
1611	Structure of coagulation factors IX/X-binding protein, a heterodimer of C-type lectin domains. <b>1997</b> , 4, 438-41	110
1610	Defining long range order in NMR structure determination from the dependence of heteronuclear relaxation times on rotational diffusion anisotropy. <b>1997</b> , 4, 443-9	155
1609	The structure of I-Crel, a group I intron-encoded homing endonuclease. <b>1997</b> , 4, 468-76	106
1608	A molecular clamp in the crystal structure of the N-terminal domain of the yeast Hsp90 chaperone. <b>1997</b> , 4, 477-82	193
1607	Structure of a calpain Ca(2+)-binding domain reveals a novel EF-hand and Ca(2+)-induced conformational changes. <b>1997</b> , 4, 532-8	162
1606	The structure of a novel insecticidal neurotoxin, omega-atracotoxin-HV1, from the venom of an Australian funnel web spider. <b>1997</b> , 4, 559-66	149
1605	Solution structure of the N-terminal zinc binding domain of HIV-1 integrase. <b>1997</b> , 4, 567-77	273
1604	Crystal structure of tyrosine hydroxylase at 2.3 Å and its implications for inherited neurodegenerative diseases. <b>1997</b> , 4, 578-85	218
1603	Crystal structure of the RAG1 dimerization domain reveals multiple zinc-binding motifs including a novel zinc binuclear cluster. <b>1997</b> , 4, 586-91	121
1602	Crystal structure at 2.8 Å resolution of anabolic ornithine transcarbamylase from Escherichia coli. <b>1997</b> , 4, 622-5	35
1601	Crystal structure of the streptococcal superantigen SPE-C: dimerization and zinc binding suggest a novel mode of interaction with MHC class II molecules. <b>1997</b> , 4, 635-43	95
1600	Crystal structure of RhoA-GDP and its functional implications. <b>1997</b> , 4, 699-703	138
1599	Crystal structure of the molybdate binding protein ModA. <b>1997</b> , 4, 703-7	65
1598	Structure of translation factor eIF4E bound to m7GDP and interaction with 4E-binding protein. <b>1997</b> , 4, 717-24	309
1597	Use of dipolar <sup>1</sup> H- <sup>15</sup> N and <sup>1</sup> H- <sup>13</sup> C couplings in the structure determination of magnetically oriented macromolecules in solution. <b>1997</b> , 4, 732-8	408

1596	The crystal structures of two spermadhesins reveal the CUB domain fold. <b>1997</b> , 4, 783-8	110
1595	Structure and mechanism of endo/exocellulase E4 from <i>Thermomonospora fusca</i> . <b>1997</b> , 4, 810-8	309
1594	Crystal structure of nitric oxide reductase from denitrifying fungus <i>Fusarium oxysporum</i> . <b>1997</b> , 4, 827-32	152
1593	Structure of the collagen-binding domain from a <i>Staphylococcus aureus</i> adhesin. <b>1997</b> , 4, 833-8	122
1592	Crystal structure of DNA photolyase from <i>Anacystis nidulans</i> . <b>1997</b> , 4, 887-91	174
1591	Crystal structure of the unique RNA-binding domain of the influenza virus NS1 protein. <b>1997</b> , 4, 896-9	108
1590	Crystal structure of estrogen sulphotransferase. <b>1997</b> , 4, 904-8	237
1589	Crystal structure of the catalytic domain of human phenylalanine hydroxylase reveals the structural basis for phenylketonuria. <b>1997</b> , 4, 995-1000	148
1588	Crystal structure of colicin Ia. <b>1997</b> , 385, 461-4	224
1587	Structure of the adenylyl cyclase catalytic core. <b>1997</b> , 386, 247-53	336
1586	Structure of ADP x AIF4(-)-stabilized nitrogenase complex and its implications for signal transduction. <b>1997</b> , 387, 370-6	452
1585	Crystallographic structure of the T domain-DNA complex of the Brachyury transcription factor. <b>1997</b> , 389, 884-8	280
1584	Bacterial lipases for biotechnological applications. <b>1997</b> , 3, 3-12	67
1583	PDBsum: a Web-based database of summaries and analyses of all PDB structures. <b>1997</b> , 22, 488-90	448
1582	Crystal structure of common type acylphosphatase from bovine testis. <b>1997</b> , 5, 69-79	86
1581	The novel acidophilic structure of the killer toxin from halotolerant yeast demonstrates remarkable folding similarity with a fungal killer toxin. <b>1997</b> , 5, 81-94	35
1580	Crystal structure of a thermostable <i>Bacillus</i> DNA polymerase I large fragment at 2.1 Å resolution. <b>1997</b> , 5, 95-108	141
1579	The DNA-binding domain of OmpR: crystal structures of a winged helix transcription factor. <b>1997</b> , 5, 109-24	210

1578	Crystal structure of a 30 kDa C-terminal fragment from the gamma chain of human fibrinogen. <b>1997, 5, 125-38</b>	217
1577	The crystal structure of a triacylglycerol lipase from <i>Pseudomonas cepacia</i> reveals a highly open conformation in the absence of a bound inhibitor. <b>1997, 5, 173-85</b>	275
1576	The structure of an energy-coupling protein from bacteria, IIBcellobiose, reveals similarity to eukaryotic protein tyrosine phosphatases. <b>1997, 5, 217-25</b>	39
1575	Barley lipid-transfer protein complexed with palmitoyl CoA: the structure reveals a hydrophobic binding site that can expand to fit both large and small lipid-like ligands. <b>1997, 5, 291-306</b>	119
1574	Crystal structure of carboxypeptidase G2, a bacterial enzyme with applications in cancer therapy. <b>1997, 5, 337-47</b>	183
1573	Crystal structure of the DNA-binding domain of Mbp1, a transcription factor important in cell-cycle control of DNA synthesis. <b>1997, 5, 349-58</b>	39
1572	Solution structure of a type 2 module from fibronectin: implications for the structure and function of the gelatin-binding domain. <b>1997, 5, 359-70</b>	90
1571	A cohesin domain from <i>Clostridium thermocellum</i> : the crystal structure provides new insights into cellulosome assembly. <b>1997, 5, 381-90</b>	104
1570	The refined structure of human rhinovirus 16 at 2.15 Å resolution: implications for the viral life cycle. <b>1997, 5, 427-41</b>	136
1569	A mechanism for toxin insertion into membranes is suggested by the crystal structure of the channel-forming domain of colicin E1. <b>1997, 5, 443-58</b>	132
1568	Bovine beta-lactoglobulin at 1.8 Å resolution—still an enigmatic lipocalin. <b>1997, 5, 481-95</b>	629
1567	Unusual structure of the oxygen-binding site in the dimeric bacterial hemoglobin from <i>Vitreoscilla</i> sp. <b>1997, 5, 497-507</b>	118
1566	The crystal structure of rhamnogalacturonase A from <i>Aspergillus aculeatus</i> : a right-handed parallel beta helix. <b>1997, 5, 533-44</b>	124
1565	Solution structure of the sodium channel antagonist conotoxin GS: a new molecular caliper for probing sodium channel geometry. <b>1997, 5, 571-83</b>	46
1564	A 'specificity' pocket inferred from the crystal structures of the complexes of aldose reductase with the pharmaceutically important inhibitors tolrestat and sorbinil. <b>1997, 5, 601-12</b>	218
1563	A modulator of rho family G proteins, rhoGDI, binds these G proteins via an immunoglobulin-like domain and a flexible N-terminal arm. <b>1997, 5, 623-33</b>	98
1562	Formylmethanofuran: tetrahydromethanopterin formyltransferase from <i>Methanopyrus kandleri</i> - new insights into salt-dependence and thermostability. <b>1997, 5, 635-46</b>	65
1561	Solution structure of the granular starch binding domain of <i>Aspergillus niger</i> glucoamylase bound to beta-cyclodextrin. <b>1997, 5, 647-61</b>	162

1560	Crystal structure of nitrile hydratase reveals a novel iron centre in a novel fold. <b>1997</b> , 5, 691-9	267
1559	Structure of mitochondrial aldehyde dehydrogenase: the genetic component of ethanol aversion. <b>1997</b> , 5, 701-11	297
1558	Triosephosphate isomerase from <i>Plasmodium falciparum</i> : the crystal structure provides insights into antimalarial drug design. <b>1997</b> , 5, 751-61	122
1557	The structure of enzyme IIAlactose from <i>Lactococcus lactis</i> reveals a new fold and points to possible interactions of a multicomponent system. <b>1997</b> , 5, 775-88	40
1556	Structure of bacteriophage T4 fibritin: a segmented coiled coil and the role of the C-terminal domain. <b>1997</b> , 5, 789-98	180
1555	The structure of <i>Staphylococcus aureus</i> epidermolytic toxin A, an atypic serine protease, at 1.7 Å resolution. <b>1997</b> , 5, 813-24	80
1554	The crystal structure of the nucleotide-free alpha 3 beta 3 subcomplex of F1-ATPase from the thermophilic <i>Bacillus PS3</i> is a symmetric trimer. <b>1997</b> , 5, 825-36	226
1553	Crystal structure of phosphoadenylyl sulphate (PAPS) reductase: a new family of adenine nucleotide alpha hydrolases. <b>1997</b> , 5, 895-906	50
1552	A binary complex of the catalytic subunit of cAMP-dependent protein kinase and adenosine further defines conformational flexibility. <b>1997</b> , 5, 921-35	113
1551	Antibody fragment Fv4155 bound to two closely related steroid hormones: the structural basis of fine specificity. <b>1997</b> , 5, 937-48	39
1550	Structure of poliovirus type 2 Lansing complexed with antiviral agent SCH48973: comparison of the structural and biological properties of three poliovirus serotypes. <b>1997</b> , 5, 961-78	89
1549	Human ornithine aminotransferase complexed with L-canaline and gabaculine: structural basis for substrate recognition. <b>1997</b> , 5, 1067-75	67
1548	N-terminal arm exchange is observed in the 2.15 Å crystal structure of oxidized nitrite reductase from <i>Pseudomonas aeruginosa</i> . <b>1997</b> , 5, 1157-71	133
1547	The structure of ribosomal protein S7 at 1.9 Å resolution reveals a beta-hairpin motif that binds double-stranded nucleic acids. <b>1997</b> , 5, 1187-98	61
1546	The crystal structure of bovine bile salt activated lipase: insights into the bile salt activation mechanism. <b>1997</b> , 5, 1209-18	88
1545	Structure of mouse 7S NGF: a complex of nerve growth factor with four binding proteins. <b>1997</b> , 5, 1275-85	55
1544	The crystal structure of vascular endothelial growth factor (VEGF) refined to 1.93 Å resolution: multiple copy flexibility and receptor binding. <b>1997</b> , 5, 1325-38	204
1543	The coupling of light-induced electron transfer and proton uptake as derived from crystal structures of reaction centres from <i>Rhodospseudomonas viridis</i> modified at the binding site of the secondary quinone, QB. <b>1997</b> , 5, 1339-59	194



1542	The crystal structure of HIV-1 Nef protein bound to the Fyn kinase SH3 domain suggests a role for this complex in altered T cell receptor signaling. <b>1997</b> , 5, 1361-72	188
1541	The crystal structure of Escherichia coli purine nucleoside phosphorylase: a comparison with the human enzyme reveals a conserved topology. <b>1997</b> , 5, 1373-83	118
1540	The class II MHC protein HLA-DR1 in complex with an endogenous peptide: implications for the structural basis of the specificity of peptide binding. <b>1997</b> , 5, 1385-96	133
1539	The role of DNA in the mechanism of NFkappaB dimer formation: crystal structures of the dimerization domains of the p50 and p65 subunits. <b>1997</b> , 5, 1427-36	69
1538	Structure of the complex of leech-derived tryptase inhibitor (LDTI) with trypsin and modeling of the LDTI-tryptase system. <b>1997</b> , 5, 1465-74	28
1537	Crystal structure of ferrochelatase: the terminal enzyme in heme biosynthesis. <b>1997</b> , 5, 1501-10	162
1536	The structure of versutoxin (delta-atracotoxin-Hv1) provides insights into the binding of site 3 neurotoxins to the voltage-gated sodium channel. <b>1997</b> , 5, 1525-35	108
1535	Crystal structure of carboxylesterase from Pseudomonas fluorescens, an alpha/beta hydrolase with broad substrate specificity. <b>1997</b> , 5, 1571-84	93
1534	Solution structure and proposed binding mechanism of a novel potassium channel toxin kappa-conotoxin PVIIA. <b>1997</b> , 5, 1585-97	82
1533	High-resolution polypeptide structure in a lamellar phase lipid environment from solid state NMR derived orientational constraints. <b>1997</b> , 5, 1655-69	252
1532	Unusual ligand structure in Ni-Fe active center and an additional Mg site in hydrogenase revealed by high resolution X-ray structure analysis. <b>1997</b> , 5, 1671-80	341
1531	Structures of four Ca <sup>2+</sup> -bound troponin C at 2.0 Å resolution: further insights into the Ca <sup>2+</sup> -switch in the calmodulin superfamily. <b>1997</b> , 5, 1695-711	150
1530	Homology modelling of an antimicrobial protein, Ace-AMP1, from lipid transfer protein structures. <b>1997</b> , 2, 183-92	15
1529	Denaturation and reactivation of dimeric human glutathione reductase--an assay for folding inhibitors. <b>1997</b> , 245, 273-82	31
1528	Three-dimensional structure in solution of the N-terminal lipoyl domain of the pyruvate dehydrogenase complex from Azotobacter vinelandii. <b>1997</b> , 244, 352-60	40
1527	1.8-Å crystal structure of the catalytic domain of human neutrophil collagenase (matrix metalloproteinase-8) complexed with a peptidomimetic hydroxamate primed-side inhibitor with a distinct selectivity profile. <b>1997</b> , 247, 356-63	64
1526	A determination of the solution conformation of secretoneurin, a neuropeptide originating from the processing of secretogranin II, by 1H-NMR and restrained molecular dynamics. <b>1997</b> , 246, 665-73	13
1525	The bioactive conformation of neuropeptide Y analogues at the human Y <sub>2</sub> -receptor. <b>1997</b> , 247, 1019-28	16

1524	Structure, catalysis and supramolecular assembly of adenylate kinase from maize. <b>1997</b> , 250, 326-31	36
1523	Solution structure of reduced microsomal rat cytochrome b5. <b>1997</b> , 249, 270-9	25
1522	Examination of the thiamin diphosphate binding site in yeast transketolase by site-directed mutagenesis. <b>1997</b> , 244, 646-52	40
1521	Proton nuclear magnetic resonance studies on huwentoxin-I from the venom of the spider <i>Selenocosmia huwena</i> : 2. Three-dimensional structure in solution. <b>1997</b> , 16, 565-74	51
1520	Crystal structure of a prolonged-acting insulin with albumin-binding properties. <b>1997</b> , 36, 2826-31	71
1519	<sup>1</sup> H and <sup>15</sup> N NMR assignment and solution structure of the SH3 domain of spectrin: comparison of unrefined and refined structure sets with the crystal structure. <b>1997</b> , 9, 347-57	50
1518	Three-dimensional structure of the Hck SH2 domain in solution. <b>1997</b> , 10, 263-72	19
1517	The crystal structure of the designed trimeric coiled coil coil-VaLd: implications for engineering crystals and supramolecular assemblies. <b>1997</b> , 6, 80-8	128
1516	Crystal structure of the reduced Schiff-base intermediate complex of transaldolase B from <i>Escherichia coli</i> : mechanistic implications for class I aldolases. <b>1997</b> , 6, 119-24	60
1515	Crystal structure of cutinase covalently inhibited by a triglyceride analogue. <b>1997</b> , 6, 275-86	73
1514	Complete <sup>1</sup> H, <sup>13</sup> C, and <sup>15</sup> N NMR resonance assignments and secondary structure of human glutaredoxin in the fully reduced form. <b>1997</b> , 6, 383-90	10
1513	Importance of van der Waals contact between Glu 35 and Trp 109 to the catalytic action of human lysozyme. <b>1997</b> , 6, 473-6	7
1512	Crystal structure of the hydroxylase component of methane monooxygenase from <i>Methylosinus trichosporium</i> OB3b. <b>1997</b> , 6, 556-68	231
1511	A 3D model for the measles virus receptor CD46 based on homology modeling, Monte Carlo simulations, and hemagglutinin binding studies. <b>1997</b> , 6, 588-97	22
1510	Mutations of fumarase that distinguish between the active site and a nearby dicarboxylic acid binding site. <b>1997</b> , 6, 834-42	36
1509	Characterization of the allosteric binding pocket of human liver fructose-1,6-bisphosphatase by protein crystallography and inhibitor activity studies. <b>1997</b> , 6, 971-82	24
1508	Predicted structure of the extracellular region of ligand-gated ion-channel receptors shows SH2-like and SH3-like domains forming the ligand-binding site. <b>1997</b> , 6, 983-98	32
1507	Structural basis for the negative allostery between Ca(2+)- and Mg(2+)-binding in the intracellular Ca(2+)-receptor calbindin D9k. <b>1997</b> , 6, 1139-47	59

1506	The uncharged surface features surrounding the active site of Escherichia coli DsbA are conserved and are implicated in peptide binding. <b>1997</b> , 6, 1148-56	72
1505	Structural studies of the streptavidin binding loop. <b>1997</b> , 6, 1157-66	162
1504	Refined structures of three crystal forms of toxic shock syndrome toxin-1 and of a tetramutant with reduced activity. <b>1997</b> , 6, 1220-7	20
1503	The co-crystal structure of unliganded bovine alpha-thrombin and prethrombin-2: movement of the Tyr-Pro-Pro-Trp segment and active site residues upon ligand binding. <b>1997</b> , 6, 1438-48	35
1502	The X-ray structure of a mutant eye lens beta B2-crystallin with truncated sequence extensions. <b>1997</b> , 6, 1612-20	23
1501	The effect of denaturants on protein structure. <b>1997</b> , 6, 1727-33	95
1500	Crystal structures of bovine chymotrypsin and trypsin complexed to the inhibitor domain of Alzheimer's amyloid beta-protein precursor (APPI) and basic pancreatic trypsin inhibitor (BPTI): engineering of inhibitors with altered specificities. <b>1997</b> , 6, 1806-24	115
1499	Solution structure of drosomycin, the first inducible antifungal protein from insects. <b>1997</b> , 6, 1878-84	132
1498	Molecular modeling of CD28 and three-dimensional analysis of residue conservation in the CD28/CD152 family. <b>1997</b> , 15, 135-9, 108-11	14
1497	A structural model of the human thrombopoietin receptor complex. <b>1997</b> , 15, 170-8, 185-8	18
1496	Crystal structure of the bovine alpha-chymotrypsin:Kunitz inhibitor complex. An example of multiple protein:protein recognition sites. <b>1997</b> , 10, 26-35	37
1495	Assessment of comparative modeling in CASP2. <b>1997</b> , 29, 14-28	80
1494	Successful ab initio prediction of the tertiary structure of NK-lysin using multiple sequences and recognized supersecondary structural motifs. <b>1997</b> , 29, 185-191	66
1493	Evaluation of comparative protein structure modeling by MODELLER-3. <b>1997</b> , 29, 50-58	168
1492	Model building by comparison: A combination of expert knowledge and computer automation. <b>1997</b> , 29, 59-67	7
1491	Crystal structure of a recombinant form of the maltodextrin-binding protein carrying an inserted sequence of a B-cell epitope from the preS2 region of hepatitis B virus. <b>1997</b> , 27, 1-8	10
1490	Homology model for the human GSTT2 Theta class glutathione transferase. <b>1997</b> , 27, 118-30	17
1489	Comparative modeling of the three-dimensional structure of the calmodulin-related TCH2 protein from Arabidopsis. <b>1997</b> , 27, 144-53	16

1488	Construction and analysis of a detailed three-dimensional model of the ligand binding domain of the human B cell receptor CD40. <b>1997</b> , 27, 59-70	19
1487	Homology modeling of rabbit prolactin hormone complexed with its receptor. <b>1997</b> , 27, 459-468	7
1486	Structure prediction and fold recognition for the ferrocyclase family of proteins. <b>1997</b> , 27, 517-522	7
1485	NADP-dependent enzymes. I: Conserved stereochemistry of cofactor binding. <b>1997</b> , 28, 10-28	161
1484	The high-resolution crystal structure of a 24-kDa gyrase B fragment from <i>E. coli</i> complexed with one of the most potent coumarin inhibitors, clorobiocin. <b>1997</b> , 28, 41-52	119
1483	Refined solution structure of the anti-mammal and anti-insect LqqIII scorpion toxin: comparison with other scorpion toxins. <b>1997</b> , 28, 360-74	31
1482	Bactericidal antibody recognition of a PorA epitope of <i>Neisseria meningitidis</i> : Crystal structure of a Fab fragment in complex with a fluorescein-conjugated peptide. <b>1997</b> , 29, 113-125	28
1481	Structural basis of the properties of an industrially relevant thermophilic xylanase. <b>1997</b> , 29, 77-86	80
1480	Prediction of protein conformational freedom from distance constraints. <b>1997</b> , 29, 240-51	219
1479	Solution structure of maurotoxin, a scorpion toxin from <i>Scorpio maurus</i> , with high affinity for voltage-gated potassium channels. <b>1997</b> , 29, 321-333	78
1478	Solution structure of TsKapa, a charybdotoxin-like scorpion toxin from <i>Tityus serrulatus</i> with high affinity for apamin-sensitive Ca(2+)-activated K <sup>+</sup> channels. <b>1997</b> , 29, 359-69	35
1477	Theoretical investigation of IL-6 multiprotein receptor assembly. <b>1997</b> , 29, 528-548	9
1476	Improvements and extensions in the conformational database potential for the refinement of NMR and X-ray structures of proteins and nucleic acids. <b>1997</b> , 125, 171-7	170
1475	Re-engineering the diiron site in rubrerythrin towards that in ribonucleotide reductase. <b>1997</b> , 263, 255-262	12
1474	An inactive pancreatic lipase-related protein is activated into a triglyceride-lipase by mutagenesis based on the 3-D structure. <b>1998</b> , 93, 103-14	12
1473	Refinement of the three-dimensional structures of cytochrome c3 from <i>Desulfovibrio vulgaris</i> Hildenborough at 1.67 Å resolution and from <i>Desulfovibrio desulfuricans</i> ATCC 27774 at 1.6 Å resolution. <b>1998</b> , 273, 213-224	46
1472	The NMR solution structure and characterization of pH dependent chemical shifts of the beta-elicitin, cryptogein. <b>1998</b> , 12, 523-34	29
1471	Enzymes harboring unnatural amino acids: mechanistic and structural analysis of the enhanced catalytic activity of a glutathione transferase containing 5-fluorotryptophan. <b>1998</b> , 37, 6286-94	59

1470	Structural and theoretical studies suggest domain movement produces an active conformation of thymidine phosphorylase. <b>1998</b> , 281, 285-99	64
1469	Structure of an XRCC1 BRCT domain: a new protein-protein interaction module. <b>1998</b> , 17, 6404-11	196
1468	Structure-based design and synthesis of lipophilic 2,4-diamino-6-substituted quinazolines and their evaluation as inhibitors of dihydrofolate reductases and potential antitumor agents. <b>1998</b> , 41, 3426-34	58
1467	Structure of phage fr capsids with a deletion in the FG loop: implications for viral assembly. <b>1998</b> , 249, 80-8	17
1466	Structure of the metal-ion-activated diphtheria toxin repressor/tox operator complex. <b>1998</b> , 394, 502-6	158
1465	Solution structure of a protein inhibitor of neuronal nitric oxide synthase. <b>1998</b> , 5, 965-9	46
1464	An antagonist peptide-EPO receptor complex suggests that receptor dimerization is not sufficient for activation. <b>1998</b> , 5, 993-1004	177
1463	Heme packing motifs revealed by the crystal structure of the tetra-heme cytochrome c554 from <i>Nitrosomonas europaea</i> . <b>1998</b> , 5, 1005-12	79
1462	Structure of the outer membrane protein A transmembrane domain. <b>1998</b> , 5, 1013-7	398
1461	Structure of a heparin-linked biologically active dimer of fibroblast growth factor. <b>1998</b> , 393, 812-7	331
1460	Crystal structure of a bacteriophage T7 DNA replication complex at 2.2 Å resolution. <b>1998</b> , 391, 251-8	1115
1459	Comparison of X-ray and NMR structures for the Antennapedia homeodomain-DNA complex. <b>1998</b> , 5, 692-7	115
1458	NMR structure of human erythropoietin and a comparison with its receptor bound conformation. <b>1998</b> , 5, 861-6	146
1457	Solution structure of the cellular factor BAF responsible for protecting retroviral DNA from autointegration. <b>1998</b> , 5, 903-9	99
1456	Crystal structure of the ATP-binding subunit of an ABC transporter. <b>1998</b> , 396, 703-7	632
1455	The atomic structure of the bluetongue virus core. <b>1998</b> , 395, 470-8	488
1454	Crystal structure of a hepatitis delta virus ribozyme. <b>1998</b> , 395, 567-74	660
1453	DNA binding and cleavage by the nuclear intron-encoded homing endonuclease I-PpoI. <b>1998</b> , 394, 96-101	193

1452	Three-dimensional structure of the Stat3beta homodimer bound to DNA. <b>1998</b> , 394, 145-51	707
1451	Cross-enzyme inhibition by gabexate mesylate: formulation and reactivity study. <b>1998</b> , 87, 1335-40	11
1450	Crystal structure of asparagine synthetase reveals a close evolutionary relationship to class II aminoacyl-tRNA synthetase. <b>1998</b> , 5, 15-9	65
1449	Antigen distortion allows influenza virus to escape neutralization. <b>1998</b> , 5, 119-23	97
1448	Crystal structure of an RNA aptamer-protein complex at 2.8 A resolution. <b>1998</b> , 5, 133-9	118
1447	The structural basis of phage display elucidated by the crystal structure of the N-terminal domains of g3p. <b>1998</b> , 5, 140-7	94
1446	Crystal structure of the von Willebrand factor A1 domain in complex with the function blocking NMC-4 Fab. <b>1998</b> , 5, 189-94	90
1445	Conformational adaptation of agonists to the human nuclear receptor RAR gamma. <b>1998</b> , 5, 199-202	123
1444	Crystal structure of aspartate decarboxylase at 2.2 A resolution provides evidence for an ester in protein self-processing. <b>1998</b> , 5, 289-93	79
1443	Crystal structure of the hCASK PDZ domain reveals the structural basis of class II PDZ domain target recognition. <b>1998</b> , 5, 317-25	149
1442	Structure determination of selenomethionyl S-adenosylhomocysteine hydrolase using data at a single wavelength. <b>1998</b> , 5, 369-76	99
1441	Crystal structure of a novel human peroxidase enzyme at 2.0 A resolution. <b>1998</b> , 5, 400-6	321
1440	The structure of PurR mutant L54M shows an alternative route to DNA kinking. <b>1998</b> , 5, 436-41	17
1439	Design, structure and stability of a hyperthermophilic protein variant. <b>1998</b> , 5, 470-5	289
1438	A new DNA-binding motif in the Skn-1 binding domain-DNA complex. <b>1998</b> , 5, 484-91	46
1437	Comparison of the conformations of two intact monoclonal antibodies with hinges. <b>1998</b> , 163, 35-43	36
1436	Structures of Cdc42 bound to the active and catalytically compromised forms of Cdc42GAP. <b>1998</b> , 5, 1047-52	158
1435	Analysis of the structure and substrate binding of Phormidium lapideum alanine dehydrogenase. <b>1998</b> , 5, 561-7	68

1434	Solution structure of cyanovirin-N, a potent HIV-inactivating protein. <b>1998</b> , 5, 571-8	220
1433	The X-ray structure of a cobalamin biosynthetic enzyme, cobalt-precorrin-4 methyltransferase. <b>1998</b> , 5, 585-92	53
1432	Crystal structure and active site location of N-(1-D-carboxylethyl)-L-norvaline dehydrogenase. <b>1998</b> , 5, 593-601	29
1431	NMR structure of a parallel homotrimeric coiled coil. <b>1998</b> , 5, 687-91	34
1430	Ambiguous NOEs and automated NOE assignment. <b>1998</b> , 32, 107-139	185
1429	Homology predicted structure and comparison with the secondary structure from NMR data for plastocyanin for the cyanobacterium <i>Synechocystis</i> sp. PCC 6803. <b>1998</b> , 275-276, 73-89	5
1428	A molecular model for the d chain of the giant haemoglobin from <i>Lumbricus terrestris</i> and its implications for subunit assembly. <b>1998</b> , 1383, 130-42	10
1427	Homology models for the PERB11 multigene family. <b>1998</b> , 3, 27-37	2
1426	Reading protein sequences backwards. <b>1998</b> , 3, 79-85	40
1425	Energy strain in three-dimensional protein structures. <b>1998</b> , 3, 259-69	34
1424	Non-homology knowledge-based prediction of the papain prosegment folding pattern: a description of plausible folding and activation mechanisms. <b>1998</b> , 3, 271-84	6
1423	The mechanism of regulation of hexokinase: new insights from the crystal structure of recombinant human brain hexokinase complexed with glucose and glucose-6-phosphate. <b>1998</b> , 6, 39-50	107
1422	Crystal structure of porcine cathepsin H determined at 2.1 Å resolution: location of the mini-chain C-terminal carboxyl group defines cathepsin H aminopeptidase function. <b>1998</b> , 6, 51-61	145
1421	Crystal structure of p14TCL1, an oncogene product involved in T-cell prolymphocytic leukemia, reveals a novel beta-barrel topology. <b>1998</b> , 6, 147-55	42
1420	The 3-D structure of a folate-dependent dehydrogenase/cyclohydrolase bifunctional enzyme at 1.5 Å resolution. <b>1998</b> , 6, 173-82	61
1419	A novel calcium-sensitive switch revealed by the structure of human S100B in the calcium-bound form. <b>1998</b> , 6, 211-22	116
1418	The three-dimensional structure of Ca(2+)-bound calyculin: implications for Ca(2+)-signal transduction by S100 proteins. <b>1998</b> , 6, 223-31	109
1417	New aspects of electron transfer revealed by the crystal structure of a truncated bovine adrenodoxin, Adx(4-108). <b>1998</b> , 6, 269-80	150

1416	Activation of <i>Bacillus licheniformis</i> alpha-amylase through a disorder->order transition of the substrate-binding site mediated by a calcium-sodium-calcium metal triad. <b>1998</b> , 6, 281-92	201
1415	Human theta class glutathione transferase: the crystal structure reveals a sulfate-binding pocket within a buried active site. <b>1998</b> , 6, 309-22	139
1414	The structure of the <i>Escherichia coli</i> phosphotransferase IIAmannitol reveals a novel fold with two conformations of the active site. <b>1998</b> , 6, 377-88	47
1413	Conformational variability of the N-terminal helix in the structure of ribosomal protein S15. <b>1998</b> , 6, 429-38	46
1412	How glutaminyl-tRNA synthetase selects glutamine. <b>1998</b> , 6, 439-49	114
1411	Structure and control of pyridoxal phosphate dependent allosteric threonine deaminase. <b>1998</b> , 6, 465-75	161
1410	EF-hands at atomic resolution: the structure of human psoriasis (S100A7) solved by MAD phasing. <b>1998</b> , 6, 477-89	93
1409	Structure of a microbial homologue of mammalian platelet-activating factor acetylhydrolases: <i>Streptomyces exfoliatus</i> lipase at 1.9 A resolution. <b>1998</b> , 6, 511-9	89
1408	Structure of an aromatic-ring-hydroxylating dioxygenase-naphthalene 1,2-dioxygenase. <b>1998</b> , 6, 571-86	454
1407	Crystal structure of the receptor-binding domain of alpha 2-macroglobulin. <b>1998</b> , 6, 595-604	40
1406	The crystal structure of phenol hydroxylase in complex with FAD and phenol provides evidence for a concerted conformational change in the enzyme and its cofactor during catalysis. <b>1998</b> , 6, 605-17	126
1405	Interfering with the inhibitory mechanism of serpins: crystal structure of a complex formed between cleaved plasminogen activator inhibitor type 1 and a reactive-centre loop peptide. <b>1998</b> , 6, 627-36	92
1404	Barley alpha-amylase bound to its endogenous protein inhibitor BASI: crystal structure of the complex at 1.9 A resolution. <b>1998</b> , 6, 649-59	114
1403	Co-crystal structure of sterol regulatory element binding protein 1a at 2.3 A resolution. <b>1998</b> , 6, 661-72	102
1402	Validation tools: can they indicate the information content of macromolecular crystal structures?. <b>1998</b> , 6, 685-90	18
1401	A mixed disulfide bond in bacterial glutathione transferase: functional and evolutionary implications. <b>1998</b> , 6, 721-34	134
1400	Crystal structures of reduced and oxidized DsbA: investigation of domain motion and thiolate stabilization. <b>1998</b> , 6, 757-67	141
1399	Lactate dehydrogenase from the hyperthermophilic bacterium <i>thermotoga maritima</i> : the crystal structure at 2.1 A resolution reveals strategies for intrinsic protein stabilization. <b>1998</b> , 6, 769-81	108



1398	The structure and function of antiameobin I, a proline-rich membrane-active polypeptide. <b>1998</b> , 6, 783-92	65
1397	Bovine F1-ATPase covalently inhibited with 4-chloro-7-nitrobenzofurazan: the structure provides further support for a rotary catalytic mechanism. <b>1998</b> , 6, 831-7	83
1396	The additivity of substrate fragments in enzyme-ligand binding. <b>1998</b> , 6, 839-48	72
1395	Crystal structure of a colicin N fragment suggests a model for toxicity. <b>1998</b> , 6, 863-74	120
1394	Crystal structure of the C2 domain from protein kinase C-delta. <b>1998</b> , 6, 885-94	95
1393	The structural basis of lipid interactions in lipovitellin, a soluble lipoprotein. <b>1998</b> , 6, 895-909	130
1392	A novel strategy for inhibition of alpha-amylases: yellow meal worm alpha-amylase in complex with the Ragi bifunctional inhibitor at 2.5 A resolution. <b>1998</b> , 6, 911-21	118
1391	The crystal structure of dienoyl-CoA isomerase at 1.5 A resolution reveals the importance of aspartate and glutamate sidechains for catalysis. <b>1998</b> , 6, 957-70	80
1390	Structure of 3-isopropylmalate dehydrogenase in complex with 3-isopropylmalate at 2.0 A resolution: the role of Glu88 in the unique substrate-recognition mechanism. <b>1998</b> , 6, 971-82	62
1389	Crystal structure of JNK3: a kinase implicated in neuronal apoptosis. <b>1998</b> , 6, 983-91	170
1388	Involvement of the C terminus in intramolecular nitrogen channeling in glucosamine 6-phosphate synthase: evidence from a 1.6 A crystal structure of the isomerase domain. <b>1998</b> , 6, 1047-55	89
1387	Structural basis of inhibitor selectivity in MAP kinases. <b>1998</b> , 6, 1117-28	395
1386	A novel deamido-NAD <sup>+</sup> -binding site revealed by the trapped NAD-adenylate intermediate in the NAD <sup>+</sup> synthetase structure. <b>1998</b> , 6, 1129-40	41
1385	VEGF and the Fab fragment of a humanized neutralizing antibody: crystal structure of the complex at 2.4 A resolution and mutational analysis of the interface. <b>1998</b> , 6, 1153-67	234
1384	Structural basis of activity and subunit recognition in G protein heterotrimers. <b>1998</b> , 6, 1169-83	84
1383	Amino-acid sequence and three-dimensional structure of the Staphylococcus aureus metalloproteinase at 1.72 A resolution. <b>1998</b> , 6, 1185-93	77
1382	The crystal structure of the novel snake venom plasminogen activator TSV-PA: a prototype structure for snake venom serine proteinases. <b>1998</b> , 6, 1195-206	94
1381	Structure of translation initiation factor 5A from Pyrobaculum aerophilum at 1.75 A resolution. <b>1998</b> , 6, 1207-14	98

1380	Crystal structure of the phosphatidylethanolamine-binding protein from bovine brain: a novel structural class of phospholipid-binding proteins. <b>1998</b> , 6, 1255-65	90
1379	The crystal structure of nitrophorin 4 at 1.5 Å resolution: transport of nitric oxide by a lipocalin-based heme protein. <b>1998</b> , 6, 1315-27	109
1378	Crystal structure of the NK1 fragment of human hepatocyte growth factor at 2.0 Å resolution. <b>1998</b> , 6, 1383-93	57
1377	Structure of the protein kinase C beta phospholipid-binding C2 domain complexed with Ca <sup>2+</sup> . <b>1998</b> , 6, 1395-405	151
1376	Structural comparisons of calponin homology domains: implications for actin binding. <b>1998</b> , 6, 1419-31	122
1375	GDP-4-keto-6-deoxy-D-mannose epimerase/reductase from <i>Escherichia coli</i> , a key enzyme in the biosynthesis of GDP-L-fucose, displays the structural characteristics of the RED protein homology superfamily. <b>1998</b> , 6, 1453-65	56
1374	Ligand size is a major determinant of specificity in periplasmic oxyanion-binding proteins: the 1.2 Å resolution crystal structure of <i>Azotobacter vinelandii</i> ModA. <b>1998</b> , 6, 1529-39	56
1373	Sheep liver cytosolic aldehyde dehydrogenase: the structure reveals the basis for the retinal specificity of class 1 aldehyde dehydrogenases. <b>1998</b> , 6, 1541-51	181
1372	The crystal structure of pneumococcal surface antigen PsaA reveals a metal-binding site and a novel structure for a putative ABC-type binding protein. <b>1998</b> , 6, 1553-61	191
1371	CD and NMR structural characterization of ceratotoxins, natural peptides with antimicrobial activity. <b>1998</b> , 39, 653-664	3
1370	Transfer of a protein binding epitope to a minimal designed peptide. <b>1998</b> , 47, 265-75	6
1369	The structural basis of MHC control of collagen-induced arthritis; binding of the immunodominant type II collagen 256-270 glycopeptide to H-2Aq and H-2Ap molecules. <b>1998</b> , 28, 755-67	73
1368	Crystal structures and properties of de novo circularly permuted 1,3-1,4-beta-glucanases. <b>1998</b> , 30, 155-67	27
1367	Conformation of the sebacyl beta1Lys82-beta2Lys82 crosslink in T-state human hemoglobin. <b>1998</b> , 30, 309-20	5
1366	Crystal structure of the disulfide-stabilized Fv fragment of anticancer antibody B1: Conformational influence of an engineered disulfide bond. <b>1998</b> , 31, 128-138	18
1365	Evidence of new cadmium binding sites in recombinant horse L-chain ferritin by anomalous Fourier difference map calculation. <b>1998</b> , 31, 477-485	25
1364	First partial three-dimensional model of human monoamine oxidase A. <b>1998</b> , 32, 97-110	7
1363	Role of water in plasticity, stability, and action of proteins: the crystal structures of lysozyme at very low levels of hydration. <b>1998</b> , 32, 229-40	77

1362	Recognition of single-stranded DNA by nuclease P1: High resolution crystal structures of complexes with substrate analogs. <b>1998</b> , 32, 414-424	88
1361	Reactivation of the totally inactive pancreatic lipase RP1 by structure-predicted point mutations. <b>1998</b> , 32, 523-531	47
1360	Crystal structures of HLA-A*0201 complexed with antigenic peptides with either the amino- or carboxyl-terminal group substituted by a methyl group. <b>1998</b> , 33, 97-106	35
1359	Kinetic steps for alpha-helix formation. <b>1998</b> , 33, 343-57	42
1358	A homology model for the human theta-class glutathione transferase T1-1. <b>1998</b> , 33, 444-54	16
1357	Structural basis of increased resistance to thermal denaturation induced by single amino acid substitution in the sequence of beta-glucosidase A from <i>Bacillus polymyxa</i> . <b>1998</b> , 33, 567-76	25
1356	Röntgenstrukturanalyse großer Biomoleküle. <b>1998</b> , 32, 22-33	1
1355	Structural study on hen egg-white lysozyme crystals grown in gravity and microgravity. <b>1998</b> , 41, 238-44	2
1354	Substrate specificity of prostate-specific antigen (PSA). <b>1998</b> , 5, 475-88	81
1353	Role of the microcin B17 propeptide in substrate recognition: solution structure and mutational analysis of McbA1-26. <b>1998</b> , 5, 217-28	43
1352	Engineering multi-domain redox proteins containing flavodoxin as bio-transformer: preparatory studies by rational design. <b>1998</b> , 13, 675-85	20
1351	Active-site mobility in human immunodeficiency virus, type 1, protease as demonstrated by crystal structure of A28S mutant. <b>1998</b> , 7, 300-5	18
1350	X-ray structures of three interface mutants of gammaB-crystallin from bovine eye lens. <b>1998</b> , 7, 611-8	15
1349	Crystal structure of glycosylasparaginase from <i>Flavobacterium meningosepticum</i> . <b>1998</b> , 7, 774-81	27
1348	Complex of NS3 protease and NS4A peptide of BK strain hepatitis C virus: a 2.2 Å resolution structure in a hexagonal crystal form. <b>1998</b> , 7, 837-47	217
1347	Thermodynamic and structural consequences of flexible loop deletion by circular permutation in the streptavidin-biotin system. <b>1998</b> , 7, 848-59	65
1346	Molecular dynamics simulations of hydrophobic collapse of ubiquitin. <b>1998</b> , 7, 860-74	79
1345	LIF receptor-gp130 interaction investigated by homology modeling: implications for LIF binding. <b>1998</b> , 7, 886-96	13

1344	The structure of a glycogen phosphorylase glucopyranose spirohydantoin complex at 1.8 Å resolution and 100 K: the role of the water structure and its contribution to binding. <b>1998</b> , 7, 915-27	80
1343	Solution structure and dynamics of a designed monomeric variant of the lambda Cro repressor. <b>1998</b> , 7, 983-93	9
1342	Hinge bending within the cytokine receptor superfamily revealed by the 2.4 Å crystal structure of the extracellular domain of rabbit tissue factor. <b>1998</b> , 7, 1106-15	18
1341	The role of polar interactions in the molecular recognition of CD40L with its receptor CD40. <b>1998</b> , 7, 1124-35	64
1340	Crystal structure of human cathepsin S. <b>1998</b> , 7, 1294-302	64
1339	Crystal structure of apo-glycine N-methyltransferase (GNMT). <b>1998</b> , 7, 1326-31	24
1338	Crystal structure of <i>Saccharomyces cerevisiae</i> cytosolic aspartate aminotransferase. <b>1998</b> , 7, 1380-7	28
1337	Crystal structure of an engineered Cro monomer bound nonspecifically to DNA: possible implications for nonspecific binding by the wild-type protein. <b>1998</b> , 7, 1485-94	27
1336	Improving the binding affinity of an antibody using molecular modeling and site-directed mutagenesis. <b>1998</b> , 7, 1671-80	6
1335	Binding of a substrate analog to a domain swapping protein: X-ray structure of the complex of bovine seminal ribonuclease with uridylyl(2',5')adenosine. <b>1998</b> , 7, 1691-9	34
1334	Quantitative evaluation of the chicken lysozyme epitope in the HyHEL-10 Fab complex: free energies and kinetics. <b>1998</b> , 7, 1868-74	35
1333	The structure of serine hydroxymethyltransferase as modeled by homology and validated by site-directed mutagenesis. <b>1998</b> , 7, 1976-82	7
1332	Differences between the electronic environments of reduced and oxidized <i>Escherichia coli</i> DsbA inferred from heteronuclear magnetic resonance spectroscopy. <b>1998</b> , 7, 2065-80	12
1331	Structure of the xylanase from <i>Penicillium simplicissimum</i> . <b>1998</b> , 7, 2081-8	83
1330	Crystal structure of spinach plastocyanin at 1.7 Å resolution. <b>1998</b> , 7, 2099-105	93
1329	Structure of betaine aldehyde dehydrogenase at 2.1 Å resolution. <b>1998</b> , 7, 2106-17	133
1328	The functional importance of structural differences between the mannitol-specific IIA <sub>mannitol</sub> and the regulatory IIA <sub>nitrogen</sub> . <b>1998</b> , 7, 2210-6	8
1327	Determinants of strand register in antiparallel beta-sheets of proteins. <b>1998</b> , 7, 2287-300	163

1326	Effects of pressure on the structure of metmyoglobin: molecular dynamics predictions for pressure unfolding through a molten globule intermediate. <b>1998</b> , 7, 2301-13	19
1325	Solution structure of barley lipid transfer protein complexed with palmitate. Two different binding modes of palmitate in the homologous maize and barley nonspecific lipid transfer proteins. <b>1998</b> , 7, 2490-8	93
1324	Crystal structure of the effector-binding domain of the trehalose-repressor of Escherichia coli, a member of the LacI family, in its complexes with inducer trehalose-6-phosphate and noninducer trehalose. <b>1998</b> , 7, 2511-21	34
1323	Crystal structure of two quaternary complexes of dethiobiotin synthetase, enzyme-MgADP-ALF3-diaminopelargonic acid and enzyme-MgADP-dethiobiotin-phosphate; implications for catalysis. <b>1998</b> , 7, 2560-6	18
1322	Solution structure of the His12 --> Cys mutant of the N-terminal zinc binding domain of HIV-1 integrase complexed to cadmium. <b>1998</b> , 7, 2669-74	37
1321	Homology modelling and molecular dynamics aided analysis of ligand complexes demonstrates functional properties of lipid-transfer proteins encoded by the barley low-temperature-inducible gene family, blt4. <b>1998</b> , 14, 523-33	18
1320	Evidence for new non-steroidal human aromatase inhibitors and comparison with equine aromatase inhibition for an understanding of the mammalian active site. <b>1998</b> , 33, 451-462	27
1319	Gene organization and chromosome location of the neural-specific RNA binding protein Elavl4. <b>1998</b> , 208, 139-45	17
1318	Structural differences between HLA-DQ molecules associated with myasthenia gravis characterized by molecular modeling. <b>1998</b> , 85, 102-5	13
1317	Potent dipeptide inhibitors of the pp60c-src SH2 domain. <b>1998</b> , 41, 1894-908	24
1316	Molecular modeling studies on binding of bFGF to heparin and its receptor FGFR1. <b>1998</b> , 15, 1009-27	17
1315	Structure of the shiga-like toxin I B-pentamer complexed with an analogue of its receptor Gb3. <b>1998</b> , 37, 1777-88	377
1314	Three-dimensional structure of a human Fab with high affinity for tetanus toxoid. <b>1998</b> , 3, 253-70	41
1313	Messages from ultrahigh resolution crystal structures. <b>1998</b> , 8, 730-7	62
1312	Validation of protein models derived from experiment. <b>1998</b> , 8, 631-9	155
1311	Crystal structures of two I-Ad-peptide complexes reveal that high affinity can be achieved without large anchor residues. <b>1998</b> , 8, 319-29	214
1310	Structural basis of 2C TCR allorecognition of H-2Ld peptide complexes. <b>1998</b> , 8, 553-62	146
1309	The crystal structure of H-2Dd MHC class I complexed with the HIV-1-derived peptide P18-I10 at 2.4 Å resolution: implications for T cell and NK cell recognition. <b>1998</b> , 9, 199-208	64

1308	Three-dimensional structure of the complex between a T cell receptor beta chain and the superantigen staphylococcal enterotoxin B. <b>1998</b> , 9, 807-16	172
1307	Structural features impose tight peptide binding specificity in the nonclassical MHC molecule HLA-E. <b>1998</b> , 1, 531-41	165
1306	Crystal structure of the N-terminal domain of sialoadhesin in complex with 3' sialyllactose at 1.85 A resolution. <b>1998</b> , 1, 719-28	244
1305	The structure of VanX reveals a novel amino-dipeptidase involved in mediating transposon-based vancomycin resistance. <b>1998</b> , 2, 75-84	85
1304	DNA recognition and cleavage by the LAGLIDADG homing endonuclease I-Crel. <b>1998</b> , 2, 469-76	144
1303	Formation of a novel four-helix bundle and molecular recognition sites by dimerization of a response regulator phosphotransferase. <b>1998</b> , 2, 485-93	103
1302	Crystal structure of the Ebola virus membrane fusion subunit, GP2, from the envelope glycoprotein ectodomain. <b>1998</b> , 2, 605-16	366
1301	Crystal structure of an octameric RuvA-Holliday junction complex. <b>1998</b> , 2, 361-72	108
1300	The three-dimensional structures of two toxins from snake venom throw light on the anticoagulant and neurotoxic sites of phospholipase A2. <b>1998</b> , 36, 75-92	61
1299	Crystal structure of piratoxin-I: a calcium-independent, myotoxic phospholipase A2-homologue from <i>Bothrops pirajai</i> venom. <b>1998</b> , 36, 1395-406	34
1298	Crystal structure of a G:T/U mismatch-specific DNA glycosylase: mismatch recognition by complementary-strand interactions. <b>1998</b> , 92, 117-29	222
1297	The unusual active site of Gal6/bleomycin hydrolase can act as a carboxypeptidase, aminopeptidase, and peptide ligase. <b>1998</b> , 93, 103-9	52
1296	Crystal structure of the thermosome, the archaeal chaperonin and homolog of CCT. <b>1998</b> , 93, 125-38	375
1295	Solution structure of the RAIDD CARD and model for CARD/CARD interaction in caspase-2 and caspase-9 recruitment. <b>1998</b> , 94, 171-80	282
1294	Crystal structure of the signal sequence binding subunit of the signal recognition particle. <b>1998</b> , 94, 181-91	244
1293	Crystal structure of a GCN5-related N-acetyltransferase: <i>Serratia marcescens</i> aminoglycoside 3-N-acetyltransferase. <b>1998</b> , 94, 439-49	211
1292	Crystal structure of the hexamerization domain of N-ethylmaleimide-sensitive fusion protein. <b>1998</b> , 94, 525-36	285
1291	Crystal structure of a vertebrate smooth muscle myosin motor domain and its complex with the essential light chain: visualization of the pre-power stroke state. <b>1998</b> , 94, 559-71	614

1290	The crystal structure of the IkappaBalpha/NF-kappaB complex reveals mechanisms of NF-kappaB inactivation. <b>1998</b> , 95, 759-70	522
1289	Three-dimensional structure of an evolutionarily conserved N-terminal domain of syntaxin 1A. <b>1998</b> , 94, 841-9	268
1288	Crystal structure of a human alkylbase-DNA repair enzyme complexed to DNA: mechanisms for nucleotide flipping and base excision. <b>1998</b> , 95, 249-58	252
1287	Crystal structure of the Dbl and pleckstrin homology domains from the human Son of sevenless protein. <b>1998</b> , 95, 259-68	202
1286	Crystal structure of a murine alpha-class glutathione S-transferase involved in cellular defense against oxidative stress. <b>1998</b> , 422, 285-90	15
1285	Trypanosoma cruzi glycosomal glyceraldehyde-3-phosphate dehydrogenase: structure, catalytic mechanism and targeted inhibitor design. <b>1998</b> , 424, 131-5	66
1284	Elucidation of the cause for reduced activity of abnormal human plasmin containing an Ala55-Thr mutation: importance of highly conserved Ala55 in serine proteases. <b>1998</b> , 425, 448-52	9
1283	Demonstration of a tandem pair of complement protein modules in GABA(B) receptor 1a. <b>1998</b> , 432, 103-8	57
1282	Multiple crystal forms of hexokinase I: new insights regarding conformational dynamics, subunit interactions, and membrane association. <b>1998</b> , 434, 42-6	16
1281	Archaeal cold-adapted proteins: structural and evolutionary analysis of the elongation factor 2 proteins from psychrophilic, mesophilic and thermophilic methanogens. <b>1998</b> , 439, 281-6	40
1280	A third fibronectin type III domain in the extracellular region of the insulin receptor family. <b>1998</b> , 441, 331-6	24
1279	Disruption of Escherichia coli transaldolase into catalytically active monomers: evidence against half-of-the-sites mechanism. <b>1998</b> , 441, 247-50	12
1278	The structure of SAICAR synthase: an enzyme in the de novo pathway of purine nucleotide biosynthesis. <b>1998</b> , 6, 363-76	40
1277	Structure of the Escherichia coli RNA polymerase alpha subunit amino-terminal domain. <b>1998</b> , 281, 262-6	83
1276	Kinetic analysis and X-ray structure of haloalkane dehalogenase with a modified halide-binding site. <b>1998</b> , 37, 15013-23	49
1275	Structural basis for the recognition of carbohydrates by human galectin-7. <b>1998</b> , 37, 13930-40	166
1274	Native carboxypeptidase A in a new crystal environment reveals a different conformation of the important tyrosine 248. <b>1998</b> , 37, 16555-64	52
1273	The structure of the monomeric porcine odorant binding protein sheds light on the domain swapping mechanism. <b>1998</b> , 37, 7913-8	115

1272	Structure and mechanism of action and inhibition of steroid dehydrogenase enzymes involved in hypertension. <b>1998</b> , 24, 521-9	8
1271	Homology model for the ligand-binding domain of the human estrogen receptor. <b>1998</b> , 15, 841-51	12
1270	Crystal structure of the arcelin-1 dimer from <i>Phaseolus vulgaris</i> at 1.9-A resolution. <b>1998</b> , 273, 12914-22	31
1269	Three dimensional structure of the soybean agglutinin Gal/GalNAc complexes by homology modeling. <b>1998</b> , 15, 853-60	21
1268	Ca <sup>2+</sup> binding and conformational changes in a calmodulin domain. <b>1998</b> , 37, 13744-54	61
1267	Two high-resolution crystal structures of the recombinant N-lobe of human transferrin reveal a structural change implicated in iron release. <b>1998</b> , 37, 7919-28	224
1266	Trypanosomal nucleoside hydrolase. A novel mechanism from the structure with a transition-state inhibitor. <b>1998</b> , 37, 6277-85	77
1265	Tertiary structures of amyloidogenic and non-amyloidogenic transthyretin variants: new model for amyloid fibril formation. <b>1998</b> , 5, 175-87	41
1264	Fast-reacting thiols in rat hemoglobins can intercept damaging species in erythrocytes more efficiently than glutathione. <b>1998</b> , 273, 19198-206	49
1263	High resolution crystal structure of pyruvate decarboxylase from <i>Zymomonas mobilis</i> . Implications for substrate activation in pyruvate decarboxylases. <b>1998</b> , 273, 20196-204	135
1262	Crystal structure of the complex between VEGF and a receptor-blocking peptide. <b>1998</b> , 37, 17765-72	54
1261	Crystal structure of tyrosine hydroxylase with bound cofactor analogue and iron at 2.3 A resolution: self-hydroxylation of Phe300 and the pterin-binding site. <b>1998</b> , 37, 13437-45	125
1260	Mutational and crystallographic analyses of interfacial residues in annexin V suggest direct interactions with phospholipid membrane components. <b>1998</b> , 37, 8004-10	48
1259	Crystal structure of 4-oxalocrotonate tautomerase inactivated by 2-oxo-3-pentynoate at 2.4 A resolution: analysis and implications for the mechanism of inactivation and catalysis. <b>1998</b> , 37, 14692-700	70
1258	Reassessment of acarbose as a transition state analogue inhibitor of cyclodextrin glycosyltransferase. <b>1998</b> , 37, 17192-8	55
1257	Solution structures of the Ca <sup>2+</sup> -free and Ca <sup>2+</sup> -bound C2A domain of synaptotagmin I: does Ca <sup>2+</sup> induce a conformational change?. <b>1998</b> , 37, 16106-15	201
1256	Solution structure of calcium-bound rat S100B(beta-beta) as determined by nuclear magnetic resonance spectroscopy,. <b>1998</b> , 37, 2729-40	156
1255	Solution structure of oxidized cytochrome c6 from the green alga <i>Monoraphidium braunii</i> . <b>1998</b> , 37, 4831-43	37



1254	Approaching the transition state in the crystal structure of a phosphoribosyltransferase. <b>1998</b> , 37, 17120-7	78
1253	The crystal structure of benzoylformate decarboxylase at 1.6 Å resolution: diversity of catalytic residues in thiamin diphosphate-dependent enzymes. <b>1998</b> , 37, 9918-30	158
1252	NMR solution structure of the oxidized form of MerP, a mercuric ion binding protein involved in bacterial mercuric ion resistance. <b>1998</b> , 37, 9316-22	44
1251	Crystal structure of the zinc-dependent beta-lactamase from <i>Bacillus cereus</i> at 1.9 Å resolution: binuclear active site with features of a mononuclear enzyme. <b>1998</b> , 37, 12404-11	219
1250	Structure of human adenosine kinase at 1.5 Å resolution. <b>1998</b> , 37, 15607-20	170
1249	High-resolution crystal structures of human hemoglobin with mutations at tryptophan 37β: structural basis for a high-affinity T-state. <b>1998</b> , 37, 4358-73	49
1248	Evidence for an induced-fit mechanism operating in pi class glutathione transferases. <b>1998</b> , 37, 9912-7	53
1247	Ca <sup>2+</sup> -dependent structural changes in C-type mannose-binding proteins. <b>1998</b> , 37, 17965-76	65
1246	Evolution of enzymatic activities in the enolase superfamily: crystal structure of (D)-glucarate dehydratase from <i>Pseudomonas putida</i> . <b>1998</b> , 37, 14358-68	34
1245	Homology model for oncostatin M based on NMR structural data. <b>1998</b> , 37, 10581-8	9
1244	Structure and interaction site of the regulatory domain of troponin-C when complexed with the 96-148 region of troponin-I. <b>1998</b> , 37, 12419-30	53
1243	Possible arrangement of the five domains in human complement factor I as determined by a combination of X-ray and neutron scattering and homology modeling. <b>1998</b> , 37, 13918-29	32
1242	Mutation and modeling analysis of the <i>Saccharomyces cerevisiae</i> Swi6 ankyrin repeats. <b>1998</b> , 37, 4437-50	12
1241	The 1.1 Å resolution crystal structure of [Tyr15]Epl, a novel alpha-conotoxin from <i>Conus episcopatus</i> , solved by direct methods. <b>1998</b> , 37, 11425-33	46
1240	Solution structure of the N-terminal EGF-like domain from human factor VII. <b>1998</b> , 37, 10605-15	23
1239	NMR study suggests a major role for Arg111 in maintaining the structure and dynamical properties of type II human cellular retinoic acid binding protein. <b>1998</b> , 37, 13021-32	12
1238	Discrepancies between the NMR and X-ray structures of uncomplexed barstar: analysis suggests that packing densities of protein structures determined by NMR are unreliable. <b>1998</b> , 37, 6958-66	63
1237	Nuclear magnetic resonance solution structure of the plasminogen-activator protein staphylokinase. <b>1998</b> , 37, 10635-42	22

1236	X-ray crystal structure of glycinamide ribonucleotide synthetase from <i>Escherichia coli</i> . <b>1998</b> , 37, 15647-62	49
1235	NarL dimerization? Suggestive evidence from a new crystal form. <b>1998</b> , 37, 3665-76	67
1234	Protein farnesyltransferase: structure and implications for substrate binding. <b>1998</b> , 37, 7907-12	80
1233	Structure of Thrombin Inhibited by Aeruginosin 298-A From a Blue-Green Alga. <b>1998</b> , 120, 597-598	48
1232	Novel water-mediated hydrogen bonds as the structural basis for the low oxygen affinity of the blood substitute candidate rHb(alpha 96Val-->Trp). <b>1998</b> , 37, 9258-65	25
1231	Solution structure of oxidized rat microsomal cytochrome b5 in the presence of 2 M guanidinium chloride: monitoring the early steps in protein unfolding. <b>1998</b> , 37, 17082-92	18
1230	Crystal structure of ErmC', an rRNA methyltransferase which mediates antibiotic resistance in bacteria. <b>1998</b> , 37, 7103-12	90
1229	The reduction potential of cytochrome b5 is modulated by its exposed heme edge. <b>1998</b> , 37, 1485-94	78
1228	Interaction site for soluble cytochromes on the tetraheme cytochrome subunit bound to the bacterial photosynthetic reaction center mapped by site-directed mutagenesis. <b>1998</b> , 37, 11732-44	29
1227	Three-dimensional models of estrogen receptor ligand binding domain complexes, based on related crystal structures and mutational and structure-activity relationship data. <b>1998</b> , 41, 1803-14	56
1226	Nuclear magnetic resonance structural and ligand binding studies of BLBC, a two-domain fragment of barley lectin. <b>1998</b> , 37, 116-28	22
1225	RT loop flexibility enhances the specificity of Src family SH3 domains for HIV-1 Nef. <b>1998</b> , 37, 14683-91	111
1224	Ligand-induced conformational change in transferrins: crystal structure of the open form of the N-terminal half-molecule of human transferrin. <b>1998</b> , 37, 13978-86	169
1223	Solution structure of the catalytic domain of human stromelysin-1 complexed to a potent, nonpeptidic inhibitor. <b>1998</b> , 37, 14048-56	36
1222	X-ray crystal structure of the yeast Kar3 motor domain complexed with Mg.ADP to 2.3 A resolution. <b>1998</b> , 37, 1769-76	91
1221	Structural studies of wild-type and mutant reaction centers from an antenna-deficient strain of <i>Rhodobacter sphaeroides</i> : monitoring the optical properties of the complex from bacterial cell to crystal. <b>1998</b> , 37, 4740-50	79
1220	Conformational changes occurring upon reduction and NO binding in nitrite reductase from <i>Pseudomonas aeruginosa</i> . <b>1998</b> , 37, 13987-96	82
1219	NMR solution structure of a cytoplasmic surface loop of the human red cell anion transporter, band 3. <b>1998</b> , 37, 11670-8	19

1218	Structure of the hexapeptide xenobiotic acetyltransferase from <i>Pseudomonas aeruginosa</i> . <b>1998</b> , 37, 6689-96	83
1217	Movement of a loop in domain 3 of aerolysin is required for channel formation. <b>1998</b> , 37, 741-6	34
1216	The solution structure of oxidized rat microsomal cytochrome b5. <b>1998</b> , 37, 173-84	82
1215	Preferred Conformation of C-Lactose at the Free and Peanut Lectin Bound States. <b>1998</b> , 120, 11297-11303	70
1214	Modulation of the redox potentials of FMN in <i>Desulfovibrio vulgaris</i> flavodoxin: thermodynamic properties and crystal structures of glycine-61 mutants. <b>1998</b> , 37, 8405-16	57
1213	Stereochemical course of enzymatic enolpyruvyl transfer and catalytic conformation of the active site revealed by the crystal structure of the fluorinated analogue of the reaction tetrahedral intermediate bound to the active site of the C115A mutant of MurA. <b>1998</b> , 37, 2572-7	62
1212	Solution structure of murine macrophage inflammatory protein-2. <b>1998</b> , 37, 8303-13	34
1211	A 1.4 Å crystal structure for the hypoxanthine phosphoribosyltransferase of <i>Trypanosoma cruzi</i> . <b>1998</b> , 37, 15066-75	58
1210	Crystal structures of the G protein Gi alpha 1 complexed with GDP and Mg <sup>2+</sup> : a crystallographic titration experiment. <b>1998</b> , 37, 14376-85	79
1209	Structure and ligand binding determinants of the recombinant kringle 5 domain of human plasminogen. <b>1998</b> , 37, 3258-71	85
1208	NMR solution structure of type II human cellular retinoic acid binding protein: implications for ligand binding. <b>1998</b> , 37, 12727-36	34
1207	Prion protein selectively binds copper(II) ions. <b>1998</b> , 37, 7185-93	469
1206	Biochemical characterization and crystallographic structure of an <i>Escherichia coli</i> protein from the phosphotriesterase gene family. <b>1998</b> , 37, 5096-106	56
1205	Unanticipated inhibition of the metallo-beta-lactamase from <i>Bacteroides fragilis</i> by 4-morpholineethanesulfonic acid (MES): a crystallographic study at 1.85-Å resolution. <b>1998</b> , 37, 6791-800	120
1204	The origin of differences in the physical properties of the equilibrium forms of cytochrome b5 revealed through high-resolution NMR structures and backbone dynamic analyses. <b>1998</b> , 37, 8289-302	42
1203	Structure of the bis(Mg <sup>2+</sup> )-ATP-oxalate complex of the rabbit muscle pyruvate kinase at 2.1 Å resolution: ATP binding over a barrel. <b>1998</b> , 37, 6247-55	116
1202	Genomic organization and structure of alpha-hydroxynitrile lyase in cassava ( <i>Manihot esculenta</i> Crantz). <b>1998</b> , 356, 107-16	8
1201	Primary structure and molecular modeling of mistletoe lectin I from <i>Viscum album</i> . <b>1998</b> , 247, 367-72	23

1200	Organic solvent binding to crystalline subtilisin1 in mostly aqueous media and in the neat solvents. <b>1998</b> , 248, 273-7	19
1199	Characterization of a cytochrome P450 from the acidothermophilic archaea <i>Sulfolobus solfataricus</i> . <b>1998</b> , 252, 166-72	92
1198	Homology models of the C domains of blood coagulation factors V and VIII: a proposed membrane binding mode for FV and FVIII C2 domains. <b>1998</b> , 24, 448-61	42
1197	Crystal structure of the cyanobacterial metallothionein repressor SmtB: a model for metalloregulatory proteins. <b>1998</b> , 275, 337-46	130
1196	The 2.15 Å crystal structure of a triple mutant plastocyanin from the cyanobacterium <i>Synechocystis</i> sp. PCC 6803. <b>1998</b> , 275, 327-36	39
1195	Wild-type alpha 1-antitrypsin is in the canonical inhibitory conformation. <b>1998</b> , 275, 419-25	127
1194	Crystal structure of beta-glucosidase A from <i>Bacillus polymyxa</i> : insights into the catalytic activity in family 1 glycosyl hydrolases. <b>1998</b> , 275, 491-502	153
1193	Kunitz-type soybean trypsin inhibitor revisited: refined structure of its complex with porcine trypsin reveals an insight into the interaction between a homologous inhibitor from <i>Erythrina caffra</i> and tissue-type plasminogen activator. <b>1998</b> , 275, 347-63	204
1192	Dissecting histidine interactions of ribonuclease T1 with asparagine and glutamine replacements: analysis of double mutant cycles at one position. <b>1998</b> , 275, 651-61	10
1191	The effects of steric mutations on the structure of type III antifreeze protein and its interaction with ice. <b>1998</b> , 275, 515-25	72
1190	The crystal structure of enoyl-CoA hydratase complexed with octanoyl-CoA reveals the structural adaptations required for binding of a long chain fatty acid-CoA molecule. <b>1998</b> , 275, 847-59	99
1189	Crystal structure of the lysozyme from bacteriophage lambda and its relationship with V and C-type lysozymes. <b>1998</b> , 276, 151-64	44
1188	The mechanism of an inhibitory antibody on TF-initiated blood coagulation revealed by the crystal structures of human tissue factor, Fab 5G9 and TF.G9 complex. <b>1998</b> , 275, 873-94	105
1187	Who checks the checkers? Four validation tools applied to eight atomic resolution structures. EU 3-D Validation Network. <b>1998</b> , 276, 417-36	106
1186	Solution structure of the glycosylated second type 2 module of fibronectin. <b>1998</b> , 276, 177-87	50
1185	Crystal structure of the IIB subunit of a fructose permease (IIBLev) from <i>Bacillus subtilis</i> . <b>1998</b> , 276, 591-602	38
1184	Rice non-specific lipid transfer protein: the 1.6 Å crystal structure in the unliganded state reveals a small hydrophobic cavity. <b>1998</b> , 276, 437-48	117
1183	The 2.3 Å X-ray crystal structure of <i>S. cerevisiae</i> phosphoglycerate mutase. <b>1998</b> , 276, 449-59	49

1182	The solution structure of the complex of <i>Lactobacillus casei</i> dihydrofolate reductase with methotrexate. <b>1998</b> , 277, 119-34	35
1181	Crystal structure of tryptophanase. <b>1998</b> , 276, 603-23	102
1180	Solution structure of the C-terminal SH2 domain of the p85 alpha regulatory subunit of phosphoinositide 3-kinase. <b>1998</b> , 276, 461-78	46
1179	Carbohydrate specificity and quaternary association in basic winged bean lectin: X-ray analysis of the lectin at 2.5 A resolution. <b>1998</b> , 276, 787-96	60
1178	Crystal structure of microbial superantigen staphylococcal enterotoxin B at 1.5 A resolution: implications for superantigen recognition by MHC class II molecules and T-cell receptors. <b>1998</b> , 277, 61-79	108
1177	The crystal structure of bikunin from the inter-alpha-inhibitor complex: a serine protease inhibitor with two Kunitz domains. <b>1998</b> , 276, 955-66	58
1176	Crystal structure of human recombinant ornithine aminotransferase. <b>1998</b> , 277, 81-102	88
1175	Generation of ligand binding sites in T4 lysozyme by deficiency-creating substitutions. <b>1998</b> , 277, 467-85	39
1174	The solution structure of the Leu22-->Val mutant AREA DNA binding domain complexed with a TGATAG core element defines a role for hydrophobic packing in the determination of specificity. <b>1998</b> , 277, 621-34	37
1173	The solution structure of a fungal AREA protein-DNA complex: an alternative binding mode for the basic carboxyl tail of GATA factors. <b>1998</b> , 277, 605-20	59
1172	Determination of the structure of oxidised <i>Desulfovibrio africanus</i> ferredoxin I by 1H NMR spectroscopy and comparison of its solution structure with its crystal structure. <b>1998</b> , 277, 683-706	25
1171	Kinetic and X-ray structural studies of three mutant <i>E. coli</i> alkaline phosphatases: insights into the catalytic mechanism without the nucleophile Ser102. <b>1998</b> , 277, 647-62	50
1170	Equine infectious anemia virus transactivator is a homeodomain-type protein. <b>1998</b> , 277, 749-55	8
1169	Structural diversity of leucine-rich repeat proteins. <b>1998</b> , 277, 519-27	445
1168	Crystal structure of a functional unit from Octopus hemocyanin. <b>1998</b> , 278, 855-70	342
1167	Assessing protein structures with a non-local atomic interaction energy. <b>1998</b> , 277, 1141-52	419
1166	Crystal structure of yellow meal worm alpha-amylase at 1.64 A resolution. <b>1998</b> , 278, 617-28	104
1165	Structural and functional analysis of the 1:1 growth hormone:receptor complex reveals the molecular basis for receptor affinity. <b>1998</b> , 277, 1111-28	252

1164	The mechanism of the elongation and branching reaction of poly(ADP-ribose) polymerase as derived from crystal structures and mutagenesis. <b>1998</b> , 278, 57-65	136
1163	Solution structure of the human Hck SH3 domain and identification of its ligand binding site. <b>1998</b> , 278, 253-65	28
1162	Structural changes in the region directly adjacent to the DNA-binding helix highlight a possible mechanism to explain the observed changes in the sequence-specific binding of winged helix proteins. <b>1998</b> , 278, 293-9	63
1161	Structure of <i>Azotobacter vinelandii</i> 7Fe ferredoxin at 1.35 Å resolution and determination of the [Fe-S] bonds with 0.01 Å accuracy. <b>1998</b> , 278, 629-39	37
1160	Crystal structure of apo-cellular retinoic acid-binding protein type II (R111M) suggests a mechanism of ligand entry. <b>1998</b> , 278, 641-53	36
1159	Structural studies of binding site tryptophan mutants in the high-affinity streptavidin-biotin complex. <b>1998</b> , 279, 211-21	70
1158	The three-dimensional structure of the nitrogen regulatory protein IIANtr from <i>Escherichia coli</i> . <b>1998</b> , 279, 245-55	30
1157	Crystal structure of ribosomal protein S8 from <i>Thermus thermophilus</i> reveals a high degree of structural conservation of a specific RNA binding site. <b>1998</b> , 279, 233-44	28
1156	Determination of the three-dimensional solution structure of <i>Raphanus sativus</i> antifungal protein 1 by 1H NMR. <b>1998</b> , 279, 257-70	137
1155	Conformational changes of the Tet repressor induced by tetracycline trapping. <b>1998</b> , 279, 439-47	105
1154	Ribosomal proteins S5 and L6: high-resolution crystal structures and roles in protein synthesis and antibiotic resistance. <b>1998</b> , 279, 873-88	55
1153	Structural investigation of the cofactor-free chloroperoxidases. <b>1998</b> , 279, 889-900	148
1152	Quality assessment of NMR structures: a statistical survey. <b>1998</b> , 281, 149-64	98
1151	A bisubstrate analog induces unexpected conformational changes in phosphoglycerate kinase from <i>Trypanosoma brucei</i> . <b>1998</b> , 279, 1137-48	40
1150	Crystal structure of lambda-Cro bound to a consensus operator at 3.0 Å resolution. <b>1998</b> , 280, 137-51	78
1149	Refined structure of Cro repressor protein from bacteriophage lambda suggests both flexibility and plasticity. <b>1998</b> , 280, 129-36	44
1148	Crystal structure of a human embryonic haemoglobin: the carbonmonoxy form of gower II (alpha2 epsilon2) haemoglobin at 2.9 Å resolution. <b>1998</b> , 280, 475-84	19
1147	1.8 Å crystal structure of the major NAD(P)H:FMN oxidoreductase of a bioluminescent bacterium, <i>Vibrio fischeri</i> : overall structure, cofactor and substrate-analog binding, and comparison with related flavoproteins. <b>1998</b> , 280, 259-73	74

1146	The 2.5 Å resolution structure of the jcl42 Fab fragment/HPr complex. <b>1998</b> , 280, 829-45	30
1145	Conformational variability in structures of the nitrogenase iron proteins from <i>Azotobacter vinelandii</i> and <i>Clostridium pasteurianum</i> . <b>1998</b> , 280, 669-85	129
1144	High-resolution solution structure of the retinoid X receptor DNA-binding domain. <b>1998</b> , 281, 271-84	54
1143	Insights into the mechanism of heterodimerization from the 1H-NMR solution structure of the c-Myc-Max heterodimeric leucine zipper. <b>1998</b> , 281, 165-81	88
1142	A single mutation in the regulatory chain of <i>Escherichia coli</i> aspartate transcarbamoylase results in an extreme T-state structure. <b>1998</b> , 281, 121-34	21
1141	Crystal structure of the truncated cubic core component of the <i>Escherichia coli</i> 2-oxoglutarate dehydrogenase multienzyme complex. <b>1998</b> , 280, 655-68	61
1140	A pH-dependent stabilization of an active site loop observed from low and high pH crystal structures of mutant monomeric glycinamide ribonucleotide transformylase at 1.8 to 1.9 Å. <b>1998</b> , 281, 485-99	39
1139	A structural basis for transition-state stabilization in antibody-catalyzed hydrolysis: crystal structures of an abzyme at 1.8 Å resolution. <b>1998</b> , 281, 501-11	41
1138	Structural basis for the binding of an anti-cytochrome c antibody to its antigen: crystal structures of FabE8-cytochrome c complex to 1.8 Å resolution and FabE8 to 2.26 Å resolution. <b>1998</b> , 281, 301-22	67
1137	Solution structure of <i>Desulfovibrio vulgaris</i> (Hildenborough) ferrocycytochrome c3: structural basis for functional cooperativity. <b>1998</b> , 281, 719-39	54
1136	GlnK, a PII-homologue: structure reveals ATP binding site and indicates how the T-loops may be involved in molecular recognition. <b>1998</b> , 282, 149-65	139
1135	Combined biophysical and biochemical information confirms arrangement of transmembrane helices visible from the three-dimensional map of frog rhodopsin. <b>1998</b> , 281, 741-54	51
1134	Crystal structure of agkistrodotoxin, a phospholipase A2-type presynaptic neurotoxin from <i>agkistrodon halys pallas</i> . <b>1998</b> , 282, 1-11	41
1133	The structure of a trimeric archaeal adenylate kinase. <b>1998</b> , 282, 167-79	60
1132	Regulation of hexokinase I: crystal structure of recombinant human brain hexokinase complexed with glucose and phosphate. <b>1998</b> , 282, 345-57	80
1131	A comparison of the crystallographic structures of two catalytic antibodies with esterase activity. <b>1998</b> , 282, 1033-41	33
1130	Three-dimensional structure of O-acetylserine sulfhydrylase from <i>Salmonella typhimurium</i> . <b>1998</b> , 283, 121-33	179
1129	Cofilin and gelsolin segment-1: molecular dynamics simulation and biochemical analysis predict a similar actin binding mode. <b>1998</b> , 282, 921-32	60

1128	Structures of free and complexed forms of Escherichia coli xanthine-guanine phosphoribosyltransferase. <b>1998</b> , 282, 875-89	55
1127	A 2.8 Å resolution structure of 6-phosphogluconate dehydrogenase from the protozoan parasite Trypanosoma brucei: comparison with the sheep enzyme accounts for differences in activity with coenzyme and substrate analogues. <b>1998</b> , 282, 667-81	50
1126	The 1.25 Å resolution refinement of the cholera toxin B-pentamer: evidence of peptide backbone strain at the receptor-binding site. <b>1998</b> , 282, 1043-59	148
1125	Crystal structure of carbonic anhydrase from Neisseria gonorrhoeae and its complex with the inhibitor acetazolamide. <b>1998</b> , 283, 301-10	90
1124	The solution structure of a cytotoxic ribonuclease from the oocytes of Rana catesbeiana (bullfrog). <b>1998</b> , 283, 231-44	26
1123	Implications for function and therapy of a 2.9 Å structure of binary-complexed antithrombin. <b>1998</b> , 283, 9-14	94
1122	Structures of native and complexed complement factor D: implications of the atypical His57 conformation and self-inhibitory loop in the regulation of specific serine protease activity. <b>1998</b> , 282, 1061-81	56
1121	Three-dimensional structure of H-2Dd complexed with an immunodominant peptide from human immunodeficiency virus envelope glycoprotein 120. <b>1998</b> , 283, 179-91	61
1120	Differences in the intersubunit contacts in triosephosphate isomerase from two closely related pathogenic trypanosomes. <b>1998</b> , 283, 193-203	61
1119	Structure of the complex between the HIV-1 nucleocapsid protein NCp7 and the single-stranded pentanucleotide d(ACGCC). <b>1998</b> , 283, 419-34	131
1118	Conformational differences of an immunosuppressant peptolide in a single crystal and in a crystal complex with human cyclophilin A. <b>1998</b> , 283, 451-61	14
1117	Crystal structure of methionine aminopeptidase from hyperthermophile, Pyrococcus furiosus. <b>1998</b> , 284, 101-24	129
1116	Engrailed homeodomain-DNA complex at 2.2 Å resolution: a detailed view of the interface and comparison with other engrailed structures. <b>1998</b> , 284, 351-61	105
1115	Crystal structure of oxidized trimethylamine N-oxide reductase from Shewanella massilia at 2.5 Å resolution. <b>1998</b> , 284, 435-47	148
1114	Crystal structures of a rat anti-CD52 (CAMPATH-1) therapeutic antibody Fab fragment and its humanized counterpart. <b>1998</b> , 284, 85-99	26
1113	The molecular mechanism of pneumolysin, a virulence factor from Streptococcus pneumoniae. <b>1998</b> , 284, 449-61	94
1112	A synthetic holliday junction is sandwiched between two tetrameric Mycobacterium leprae RuvA structures in solution: new insights from neutron scattering contrast variation and modelling. <b>1998</b> , 284, 385-400	17
1111	Ligand-induced conformational change in penicillin acylase. <b>1998</b> , 284, 463-75	93



1110	Crossreactivity, efficiency and catalytic specificity of an esterase-like antibody. <b>1998</b> , 284, 741-50	10
1109	Structure and functional implications of the polymerase active site region in a complex of HIV-1 RT with a double-stranded DNA template-primer and an antibody Fab fragment at 2.8 A resolution. <b>1998</b> , 284, 1095-111	302
1108	Crystal structure at 1.95 A resolution of the breast tumour-specific antibody SM3 complexed with its peptide epitope reveals novel hypervariable loop recognition. <b>1998</b> , 284, 713-28	61
1107	Conformational analysis of the first observed non-proline cis-peptide bond occurring within the complementarity determining region (CDR) of an antibody. <b>1998</b> , 284, 549-55	21
1106	Crystal structure of GCN4-pIQI, a trimeric coiled coil with buried polar residues. <b>1998</b> , 284, 859-65	84
1105	Three-dimensional structure of human tissue inhibitor of metalloproteinases-2 at 2.1 A resolution. <b>1998</b> , 284, 1133-40	80
1104	Stepping through an RNA structure: A novel approach to conformational analysis. <b>1998</b> , 284, 1465-78	110
1103	Crystal structure of the E2 DNA-binding domain from human papillomavirus type 16: implications for its DNA binding-site selection mechanism. <b>1998</b> , 284, 1479-89	83
1102	The R78K and D117E active-site variants of <i>Saccharomyces cerevisiae</i> soluble inorganic pyrophosphatase: structural studies and mechanistic implications. <b>1998</b> , 284, 1565-80	18
1101	The X-ray structure of <i>Escherichia coli</i> enoyl reductase with bound NAD <sup>+</sup> at 2.1 A resolution. <b>1998</b> , 284, 1529-46	47
1100	Sequence profile of the parallel beta helix in the pectate lyase superfamily. <b>1998</b> , 122, 223-35	38
1099	Ab initio modeling and molecular dynamics simulation of the alpha 1b-adrenergic receptor activation. <b>1998</b> , 14, 302-17	35
1098	Solution structure of Ace-AMP1, a potent antimicrobial protein extracted from onion seeds. Structural analogies with plant nonspecific lipid transfer proteins. <b>1998</b> , 37, 3623-37	92
1097	Refined atomic model of the four-layer aggregate of the tobacco mosaic virus coat protein at 2.4-A resolution. <b>1998</b> , 74, 604-15	90
1096	Static and dynamic roles of extracellular loops in G-protein-coupled receptors: a mechanism for sequential binding of thyrotropin-releasing hormone to its receptor. <b>1998</b> , 74, 1087-100	43
1095	Identification of the ice-binding surface on a type III antifreeze protein with a "flatness function" algorithm. <b>1998</b> , 74, 2142-51	115
1094	Inhibitor and NAD <sup>+</sup> binding to poly(ADP-ribose) polymerase as derived from crystal structures and homology modeling. <b>1998</b> , 37, 3893-900	188
1093	Structural basis of the Tanford transition of bovine beta-lactoglobulin. <b>1998</b> , 37, 14014-23	432

1092	Solution NMR structure and backbone dynamics of the major cold-shock protein (CspA) from <i>Escherichia coli</i> : evidence for conformational dynamics in the single-stranded RNA-binding site. <b>1998</b> , 37, 10881-96	98
1091	Structure of nitric oxide synthase oxygenase dimer with pterin and substrate. <b>1998</b> , 279, 2121-6	624
1090	Crystal structure and evolution of a transfer RNA splicing enzyme. <b>1998</b> , 280, 279-84	122
1089	Enzyme structure with two catalytic sites for double-sieve selection of substrate. <b>1998</b> , 280, 578-82	319
1088	Structure of the <i>Bacillus agaradherans</i> family 5 endoglucanase at 1.6 Å and its cellobiose complex at 2.0 Å resolution. <b>1998</b> , 37, 1926-32	84
1087	Role of a dynamic loop in cation activation and allosteric regulation of recombinant porcine fructose-1,6-bisphosphatase. <b>1998</b> , 37, 11441-50	55
1086	Structure-based redesign of corepressor specificity of the <i>Escherichia coli</i> purine repressor by substitution of residue 190. <b>1998</b> , 37, 971-82	14
1085	Structure-activity relationship studies of novel carbocyclic influenza neuraminidase inhibitors. <b>1998</b> , 41, 2451-60	276
1084	Allostery in rabbit pyruvate kinase: development of a strategy to elucidate the mechanism. <b>1998</b> , 37, 15266-76	27
1083	Thermophilic xylanase from <i>Thermomyces lanuginosus</i> : high-resolution X-ray structure and modeling studies. <b>1998</b> , 37, 13475-85	129
1082	Biochemical and structural analysis of the IgE binding sites on ara h1, an abundant and highly allergenic peanut protein. <b>1998</b> , 273, 13753-9	191
1081	Identification of CD44 residues important for hyaluronan binding and delineation of the binding site. <b>1998</b> , 273, 338-43	140
1080	Crystal structure of Taq DNA polymerase in complex with an inhibitory Fab: the Fab is directed against an intermediate in the helix-coil dynamics of the enzyme. <b>1998</b> , 95, 12562-7	24
1079	Triose-phosphate isomerase (TIM) of the psychrophilic bacterium <i>Vibrio marinus</i> . Kinetic and structural properties. <b>1998</b> , 273, 2199-206	111
1078	Primary and tertiary structures of the Fab fragment of a monoclonal anti-E-selectin 7A9 antibody that inhibits neutrophil attachment to endothelial cells. <b>1998</b> , 273, 11770-5	10
1077	Structural basis for inactivating mutations and pH-dependent activity of avian sarcoma virus integrase. <b>1998</b> , 273, 32685-9	18
1076	Crystal structure of the catalytic domain of protein-tyrosine phosphatase SHP-1. <b>1998</b> , 273, 28199-207	95
1075	Insights into the molecular basis of salt tolerance from the study of glutamate dehydrogenase from <i>Halobacterium salinarum</i> . <b>1998</b> , 273, 9023-30	43

1074	Comparison of x-ray crystal structures of an acyl-enzyme intermediate of subtilisin Carlsberg formed in anhydrous acetonitrile and in water. <b>1998</b> , 95, 12918-23	47
1073	PHOTOSYNTHETIC CYTOCHROMES <i>c</i> IN CYANOBACTERIA, ALGAE, AND PLANTS. <b>1998</b> , 49, 397-425	82
1072	1.85-Å resolution crystal structure of human ornithine transcarbamoylase complexed with N-phosphonacetyl-L-ornithine. Catalytic mechanism and correlation with inherited deficiency. <b>1998</b> , 273, 34247-54	54
1071	Crystal structure of human RhoA in a dominantly active form complexed with a GTP analogue. <b>1998</b> , 273, 9656-66	154
1070	Crystal structure of the human ubiquitin-like protein NEDD8 and interactions with ubiquitin pathway enzymes. <b>1998</b> , 273, 34983-91	156
1069	Structure of barley grain peroxidase refined at 1.9-Å resolution. A plant peroxidase reversibly inactivated at neutral pH. <b>1998</b> , 273, 2241-8	71
1068	Mode of binding of anti-P-glycoprotein antibody MRK-16 to its antigen. A crystallographic and molecular modeling study. <b>1998</b> , 273, 25413-9	13
1067	Structure of a biological oxygen sensor: a new mechanism for heme-driven signal transduction. <b>1998</b> , 95, 15177-82	351
1066	The use of computational chemistry in the study of sex steroid biosynthesis. <b>1998</b> , 24, 541-7	6
1065	X-ray crystal structure of the human galectin-3 carbohydrate recognition domain at 2.1-Å resolution. <b>1998</b> , 273, 13047-52	315
1064	Addressing the tertiary structure of human parathyroid hormone-(1-34). <b>1998</b> , 273, 10420-7	90
1063	The rub family of ubiquitin-like proteins. Crystal structure of Arabidopsis rub1 and expression of multiple rubs in Arabidopsis. <b>1998</b> , 273, 34976-82	71
1062	Detailed comparison of two molecular models of the human CD40 ligand with an x-ray structure and critical assessment of model-based mutagenesis and residue mapping studies. <b>1998</b> , 273, 24603-9	24
1061	Protein structure prediction and design. <b>1998</b> , 4, 177-214	5
1060	Crystal structure of recombinant soybean beta-amylase complexed with beta-cyclodextrin. <b>1998</b> , 273, 19859-65	36
1059	Crystal structures of Flavobacterium glycosylasparaginase. An N-terminal nucleophile hydrolase activated by intramolecular proteolysis. <b>1998</b> , 273, 20205-12	48
1058	Crystal structure of barley 1,3-1,4-beta-glucanase at 2.0-Å resolution and comparison with Bacillus 1,3-1,4-beta-glucanase. <b>1998</b> , 273, 3438-46	31
1057	Engineering of cyclodextrin product specificity and pH optima of the thermostable cyclodextrin glycosyltransferase from Thermoanaerobacterium thermosulfurigenes EM1. <b>1998</b> , 273, 5771-9	84

1056	Characterization of interactions between the anti-apoptotic protein BAG-1 and Hsc70 molecular chaperones. <b>1998</b> , 273, 22506-14	92
1055	The three-dimensional structure of aspergillus niger pectin lyase B at 1.7-A resolution. <b>1998</b> , 116, 69-80	96
1054	Structure-based minimization of transforming growth factor-alpha (TGF-alpha) through NMR analysis of the receptor-bound ligand. Design, solution structure, and activity of TGF-alpha 8-50. <b>1998</b> , 273, 27357-63	12
1053	Structure and activity of rat pancreatic lipase-related protein 2. <b>1998</b> , 273, 32121-8	70
1052	Conformational correction mechanisms aiding antigen recognition by a humanized antibody. <b>1998</b> , 187, 479-85	28
1051	New enzyme lineages by subdomain shuffling. <b>1998</b> , 95, 9813-8	49
1050	Crystal structure of a calcium-phospholipid binding domain from cytosolic phospholipase A2. <b>1998</b> , 273, 1596-604	223
1049	Structural and functional characterization of Streptomyces plicatus beta-N-acetylhexosaminidase by comparative molecular modeling and site-directed mutagenesis. <b>1998</b> , 273, 19618-24	56
1048	Solution structure of eotaxin, a chemokine that selectively recruits eosinophils in allergic inflammation. <b>1998</b> , 273, 22471-9	80
1047	Solution conformation of the synthetic bovine proenkephalin-A209-237 by 1H NMR spectroscopy. <b>1998</b> , 273, 33517-23	11
1046	Structural studies of ribosomal proteins. <b>1998</b> , 379, 795-805	9
1045	Crystal structure of HLA-DR2 (DRA*0101, DRB1*1501) complexed with a peptide from human myelin basic protein. <b>1998</b> , 188, 1511-20	254
1044	Evidence for subsites in the galectins involved in sugar binding at the nonreducing end of the central galactose of oligosaccharide ligands: sequence analysis, homology modeling and mutagenesis studies of hamster galectin-3. <b>1998</b> , 8, 45-57	57
1043	Cloning and analysis of the genes for a novel electron-transferring flavoprotein from Megasphaera elsdenii. Expression and characterization of the recombinant protein. <b>1998</b> , 273, 21015-24	24
1042	Structural homology between the Rap30 DNA-binding domain and linker histone H5: implications for preinitiation complex assembly. <b>1998</b> , 95, 9117-22	61
1041	Crystal structure of troponin C in complex with troponin I fragment at 2.3-A resolution. <b>1998</b> , 95, 4847-52	199
1040	Crystal structures of two tropinone reductases: different reaction stereospecificities in the same protein fold. <b>1998</b> , 95, 4876-81	113
1039	Solution structure of SpoIIAA, a phosphorylatable component of the system that regulates transcription factor sigmaF of Bacillus subtilis. <b>1998</b> , 95, 5067-71	54

1038	Photoactive yellow protein: a structural prototype for the three-dimensional fold of the PAS domain superfamily. <b>1998</b> , 95, 5884-90	222
1037	Crystal structure of MTCP-1: implications for role of TCL-1 and MTCP-1 in T cell malignancies. <b>1998</b> , 95, 3413-8	31
1036	Structure and mechanism of a proline-specific aminopeptidase from Escherichia coli. <b>1998</b> , 95, 3472-7	157
1035	Residue-specific bioincorporation of non-natural, biologically active amino acids into proteins as possible drug carriers: structure and stability of the per-thiaproline mutant of annexin V. <b>1998</b> , 95, 455-9	78
1034	Cloning, Recombinant Expression and Characterization of Wild Type-105-Trp-Calmodulin of the Green Alga Mougeotia scalaris. <b>1998</b> , 111, 346-353	5
1033	Molecular Modeling of Ligand and Mutation Sites of the Type A Domains of Human von Willebrand Factor and Their Relevance to von Willebrand's Disease. <b>1998</b> , 91, 2032-2044	68
1032	Distinct Metal Environment in Fe-Substituted Manganese Superoxide Dismutase Provides a Structural Basis of Metal Specificity. <b>1998</b> , 120, 9684-9685	53
1031	Crystal structure of 2,5-diketo-D-gluconic acid reductase A complexed with NADPH at 2.1-A resolution. <b>1998</b> , 95, 6768-73	49
1030	Delta3,5-delta2,4-dienoyl-CoA isomerase from rat liver. Molecular characterization. <b>1998</b> , 273, 349-55	46
1029	The crystal structure of a 3D domain-swapped dimer of RNase A at a 2.1-A resolution. <b>1998</b> , 95, 3437-42	171
1028	Translation elongation factor 2 is part of the target for a new family of antifungals. <b>1998</b> , 42, 2694-9	66
1027	Structure of a complex between a cap analogue and mRNA guanylyl transferase demonstrates the structural chemistry of RNA capping. <b>1998</b> , 95, 1505-10	54
1026	Light-activated rhodopsin induces structural binding motif in G protein alpha subunit. <b>1998</b> , 95, 4270-5	158
1025	Crystal structure of the Saccharomyces cerevisiae ubiquitin-conjugating enzyme Rad6 at 2.6 A resolution. <b>1998</b> , 273, 6271-6	56
1024	Structure of the complex of Maclura pomifera agglutinin and the T-antigen disaccharide, Galbeta1,3GalNAc. <b>1998</b> , 273, 6312-8	80
1023	Solution structure of the cytohesin-1 (B2-1) Sec7 domain and its interaction with the GTPase ADP ribosylation factor 1. <b>1998</b> , 95, 7909-14	43
1022	Structure and function of the Bacillus hybrid enzyme GluXyn-1: native-like jellyroll fold preserved after insertion of autonomous globular domain. <b>1998</b> , 95, 6613-8	64
1021	Structural basis for recognition of phosphorylated high mannose oligosaccharides by the cation-dependent mannose 6-phosphate receptor. <b>1999</b> , 274, 29889-96	48

1020	Man alpha1-2 Man alpha-OMe-concanavalin A complex reveals a balance of forces involved in carbohydrate recognition. <b>1999</b> , 9, 539-45	60
1019	Identification of mimotope peptides which bind to the mycotoxin deoxynivalenol-specific monoclonal antibody. <b>1999</b> , 65, 3279-86	51
1018	Amino acid neighbours and detailed conformational analysis of cysteines in proteins. <b>1999</b> , 12, 535-48	136
1017	Trench-shaped binding sites promote multiple classes of interactions between collagen and the adherence receptors, alpha(1)beta(1) integrin and Staphylococcus aureus cna MSCRAMM. <b>1999</b> , 274, 24906-13	82
1016	Molecular modeling of single polypeptide chain of calcium-binding protein p26olf from dimeric S100B(beta-beta). <b>1999</b> , 12, 395-405	14
1015	Probing the substrate specificity of the intracellular brain platelet-activating factor acetylhydrolase. <b>1999</b> , 12, 693-700	25
1014	Molecular modeling of the amyloid-beta-peptide using the homology to a fragment of triosephosphate isomerase that forms amyloid in vitro. <b>1999</b> , 12, 959-66	11
1013	Analysis of the reaction mechanism and substrate specificity of haloalkane dehalogenases by sequential and structural comparisons. <b>1999</b> , 12, 989-98	53
1012	Definition and transfer of a serological epitope specific for peptide-empty forms of MHC class I. <b>1999</b> , 11, 1897-906	53
1011	Kappa light chain-associated Fanconi's syndrome: molecular analysis of monoclonal immunoglobulin light chains from patients with and without intracellular crystals. <b>1999</b> , 12, 363-9	48
1010	Structure of Ustilago maydis killer toxin KP6 alpha-subunit. A multimeric assembly with a central pore. <b>1999</b> , 274, 20425-31	19
1009	Antibody C219 recognizes an alpha-helical epitope on P-glycoprotein. <b>1999</b> , 96, 13679-84	42
1008	Bactericidal antibody recognition of meningococcal PorA by induced fit. Comparison of liganded and unliganded Fab structures. <b>1999</b> , 274, 1495-501	24
1007	Crystal structure of SQD1, an enzyme involved in the biosynthesis of the plant sulfolipid headgroup donor UDP-sulfoquinovose. <b>1999</b> , 96, 13097-102	62
1006	Crystal structure of a dimeric chymotrypsin inhibitor 2 mutant containing an inserted glutamine repeat. <b>1999</b> , 96, 1257-61	58
1005	A structural snapshot of an intermediate on the streptavidin-biotin dissociation pathway. <b>1999</b> , 96, 8384-9	57
1004	Homology modeling of the multicopper oxidase Fet3 gives new insights in the mechanism of iron transport in yeast. <b>1999</b> , 12, 895-7	16
1003	Protein threading by PROSPECT: a prediction experiment in CASP3. <b>1999</b> , 12, 899-907	15

1002	Stereoselective carveol dehydrogenase from <i>Rhodococcus erythropolis</i> DCL14. A novel nicotinoprotein belonging to the short chain dehydrogenase/reductase superfamily. <b>1999</b> , 274, 26296-304	43
1001	The high resolution crystal structure of recombinant <i>Crithidia fasciculata</i> tryparedoxin-I. <b>1999</b> , 274, 25613-22	56
1000	SCOP: a Structural Classification of Proteins database. <b>1999</b> , 27, 254-6	191
999	Crystal structure of hen apo-ovotransferrin. Both lobes adopt an open conformation upon loss of iron. <b>1999</b> , 274, 28445-52	54
998	Structure and characterization of <i>Ectothiorhodospira vacuolata</i> cytochrome b(558), a prokaryotic homologue of cytochrome b(5). <b>1999</b> , 274, 35614-20	33
997	Graphical representation of the salient conformational features of protein residues. <b>1999</b> , 12, 523-6	3
996	Crystal structure of <i>Bacillus subtilis</i> YabJ, a purine regulatory protein and member of the highly conserved YjgF family. <b>1999</b> , 96, 13074-9	67
995	Crystal structure of neuropsin, a hippocampal protease involved in kindling epileptogenesis. <b>1999</b> , 274, 4220-4	46
994	A structural explanation for the retinal specificity of class 1 ALDH enzymes. <b>1999</b> , 463, 27-38	8
993	Alpha-helix nucleation by a calcium-binding peptide loop. <b>1999</b> , 96, 903-8	69
992	Atomic resolution crystal structure of hydroxynitrile lyase from <i>Hevea brasiliensis</i> . <b>1999</b> , 380, 993-1000	43
991	Local electrostatic optimization in proteins. <b>1999</b> , 12, 727-35	4
990	The accessory subunit of mtDNA polymerase shares structural homology with aminoacyl-tRNA synthetases: implications for a dual role as a primer recognition factor and processivity clamp. <b>1999</b> , 96, 9527-32	73
989	Asparagine and glutamine rotamers: B-factor cutoff and correction of amide flips yield distinct clustering. <b>1999</b> , 96, 400-5	41
988	Solution structure of Apaf-1 CARD and its interaction with caspase-9 CARD: a structural basis for specific adaptor/caspase interaction. <b>1999</b> , 96, 11265-70	127
987	The structural and functional analysis of the hemoglobin D component from chicken. <b>1999</b> , 274, 6411-20	41
986	Alternative structural state of transferrin. The crystallographic analysis of iron-loaded but domain-opened ovotransferrin N-lobe. <b>1999</b> , 274, 10190-4	49
985	Complete mapping of divergent amino acids responsible for differential ligand binding of folate receptors alpha and beta. <b>1999</b> , 274, 11086-91	56

984	Site-directed mutagenesis of cytochrome c6 from <i>Synechocystis</i> sp. PCC 6803. The heme protein possesses a negatively charged area that may be isofunctional with the acidic patch of plastocyanin. <b>1999</b> , 274, 13292-7	42
983	The acid-labile subunit of the serum insulin-like growth factor-binding protein complexes. Structural determination by molecular modeling and electron microscopy. <b>1999</b> , 274, 23328-32	39
982	Effect of species differences on stromelysin-1 (MMP-3) inhibitor potency. An explanation of inhibitor selectivity using homology modeling and chimeric proteins. <b>1999</b> , 274, 24881-7	13
981	Crystal structure of anti-Hen egg white lysozyme antibody (HyHEL-10) Fv-antigen complex. Local structural changes in the protein antigen and water-mediated interactions of Fv-antigen and light chain-heavy chain interfaces. <b>1999</b> , 274, 27623-31	58
980	Inhibitor binding studies on enoyl reductase reveal conformational changes related to substrate recognition. <b>1999</b> , 274, 30811-7	50
979	NMR solution structure of domain 1 of human annexin I shows an autonomous folding unit. <b>1999</b> , 274, 2971-7	12
978	Structural and ligand binding analysis of recombinant blo t 13 allergen from <i>Blomia tropicalis</i> mite, a fatty acid binding protein. <b>1999</b> , 119, 181-4	26
977	Crystal structure of carboxylase reaction-oriented ribulose 1, 5-bisphosphate carboxylase/oxygenase from a thermophilic red alga, <i>Galdieria partita</i> . <b>1999</b> , 274, 15655-61	48
976	Crystal structure of chitosanase from <i>Bacillus circulans</i> MH-K1 at 1.6-A resolution and its substrate recognition mechanism. <b>1999</b> , 274, 30818-25	80
975	Molecular dynamics simulations of a protein-protein dimer: particle-mesh Ewald electrostatic model yields far superior results to standard cutoff model. <b>1999</b> , 16, 1205-18	60
974	Site-directed mutagenesis of cytochrome c(6) from <i>Anabaena</i> species PCC 7119. Identification of surface residues of the heme protein involved in photosystem I reduction. <b>1999</b> , 274, 33565-70	36
973	Structural analysis at 2.2 Å of orthorhombic crystals presents the asymmetry of the allophycocyanin-linker complex, AP.LC7.8, from phycobilisomes of <i>Mastigocladus laminosus</i> . <b>1999</b> , 96, 1363-8	124
972	Crystal structure of human gastric lipase and model of lysosomal acid lipase, two lipolytic enzymes of medical interest. <b>1999</b> , 274, 16995-7002	128
971	Crystal structure of human T cell leukemia virus type 1 gp21 ectodomain crystallized as a maltose-binding protein chimera reveals structural evolution of retroviral transmembrane proteins. <b>1999</b> , 96, 4319-24	192
970	Nucleoside hydrolase from <i>Leishmania major</i> . Cloning, expression, catalytic properties, transition state inhibitors, and the 2.5-Å crystal structure. <b>1999</b> , 274, 21114-20	90
969	Structure of Gialpha1.GppNHp, autoinhibition in a galpha protein-substrate complex. <b>1999</b> , 274, 16669-72	45
968	From residue matching patterns to protein folding topographies: general model and bovine pancreatic trypsin inhibitor. <b>1999</b> , 96, 12991-6	27
967	Structure of human factor VIIa and its implications for the triggering of blood coagulation. <b>1999</b> , 96, 8925-30	148



966	Crystal structure determinations of oxidized and reduced pseudoazurins from <i>Achromobacter cycloclastes</i> . Concerted movement of copper site in redox forms with the rearrangement of hydrogen bond at a remote histidine. <b>1999</b> , 274, 17845-52	40
965	Dengue virus NS3 serine protease. Crystal structure and insights into interaction of the active site with substrates by molecular modeling and structural analysis of mutational effects. <b>1999</b> , 274, 5573-80	84
964	Structure of the complex between the antibiotic cerulenin and its target, beta-ketoacyl-acyl carrier protein synthase. <b>1999</b> , 274, 6031-4	155
963	Convergent evolution of <i>Trichomonas vaginalis</i> lactate dehydrogenase from malate dehydrogenase. <b>1999</b> , 96, 6285-90	93
962	Evolution of a light-harvesting protein by addition of new subunits and rearrangement of conserved elements: crystal structure of a cryptophyte phycoerythrin at 1.63-Å resolution. <b>1999</b> , 96, 8901-6	102
961	The cyclization mechanism of cyclodextrin glycosyltransferase (CGTase) as revealed by a gamma-cyclodextrin-CGTase complex at 1.8-Å resolution. <b>1999</b> , 274, 34868-76	101
960	Solution structure of the major alpha-amylase inhibitor of the crop plant amaranth. <b>1999</b> , 274, 20473-8	35
959	Optical detection of cytochrome P450 by sensitizer-linked substrates. <b>1999</b> , 96, 12987-90	55
958	Molecular recognition of lipid antigens by T cell receptors. <b>1999</b> , 189, 195-205	152
957	Structure of the subunit c oligomer in the F1Fo ATP synthase: model derived from solution structure of the monomer and cross-linking in the native enzyme. <b>1999</b> , 96, 7785-90	102
956	Crystal structure of cardosin A, a glycosylated and Arg-Gly-Asp-containing aspartic proteinase from the flowers of <i>Cynara cardunculus</i> L. <b>1999</b> , 274, 27694-701	73
955	The X-ray Structure of Epoxide Hydrolase from <i>Agrobacterium radiobacter</i> AD1. <b>1999</b> , 274, 14579-14586	140
954	N- and C-terminal residues combine in the fusion-pH influenza hemagglutinin HA(2) subunit to form an N cap that terminates the triple-stranded coiled coil. <b>1999</b> , 96, 8967-72	251
953	Functional and structural studies of wild type SOX9 and mutations causing campomelic dysplasia. <b>1999</b> , 274, 24023-30	85
952	Effectors of the stringent response target the active site of <i>Escherichia coli</i> adenylosuccinate synthetase. <b>1999</b> , 274, 17505-10	33
951	Crystal structures of zinc-free and -bound heme domain of human inducible nitric-oxide synthase. Implications for dimer stability and comparison with endothelial nitric-oxide synthase. <b>1999</b> , 274, 21276-84	155
950	The cytochrome c oxidase from <i>Paracoccus denitrificans</i> does not change the metal center ligation upon reduction. <b>1999</b> , 274, 33296-9	112
949	Territrem B, a tremorgenic mycotoxin that inhibits acetylcholinesterase with a noncovalent yet irreversible binding mechanism. <b>1999</b> , 274, 34916-23	30

948	Engineering the substrate specificity of the Abl tyrosine kinase. <b>1999</b> , 274, 4995-5003	20
947	Crystal structures of intermediates in the dehalogenation of haloalkanoates by L-2-haloacid dehalogenase. <b>1999</b> , 274, 30672-8	65
946	Catalysis and specificity in enzymatic glycoside hydrolysis: a 2,5B conformation for the glycosyl-enzyme intermediate revealed by the structure of the Bacillus agaradhaerens family 11 xylanase. <b>1999</b> , 6, 483-92	106
945	Comparative molecular field analysis (CoMFA) and docking studies of non-nucleoside HIV-1 RT inhibitors (NNIs). <b>1999</b> , 7, 2283-92	58
944	Scorpion alpha-like toxins, toxic to both mammals and insects, differentially interact with receptor site 3 on voltage-gated sodium channels in mammals and insects. <b>1999</b> , 11, 975-85	42
943	High-resolution solution structure of gurmarin, a sweet-taste-suppressing plant polypeptide. <b>1999</b> , 264, 525-33	26
942	The crystal structure of a wheat nonspecific lipid transfer protein (ns-LTP1) complexed with two molecules of phospholipid at 2.1 Å resolution. <b>1999</b> , 264, 562-8	108
941	Design and evaluation of novel bivalent thrombin inhibitors based on amidinophenylalanines. <b>1999</b> , 265, 598-605	18
940	A proton-NMR investigation of the fully reduced cytochrome c7 from Desulfuromonas acetoxidans. Comparison between the reduced and the oxidized forms. <b>1999</b> , 266, 634-43	26
939	Solution structure of a new hypothalamic neuropeptide, human hypocretin-2/orexin-B. <b>1999</b> , 266, 831-9	54
938	Solution structure of a recombinant mouse major urinary protein. <b>1999</b> , 266, 1210-8	40
937	Characterization and modelling of VanT: a novel, membrane-bound, serine racemase from vancomycin-resistant Enterococcus gallinarum BM4174. <b>1999</b> , 31, 1653-64	65
936	The whey acidic protein family: a new signature motif and three-dimensional structure by comparative modeling. <b>1999</b> , 17, 106-13, 134-6	111
935	Structure of the Janus-faced C2B domain of rabphilin. <b>1999</b> , 1, 106-12	60
934	Structure-based identification of a novel NTPase from Methanococcus jannaschii. <b>1999</b> , 6, 691-6	116
933	Crystal structure of the copper chaperone for superoxide dismutase. <b>1999</b> , 6, 724-9	155
932	The tetramerization domain of the Mnt repressor consists of two right-handed coiled coils. <b>1999</b> , 6, 755-9	46
931	Structure of chalcone synthase and the molecular basis of plant polyketide biosynthesis. <b>1999</b> , 6, 775-84	470

930	Functional changes in the structure of the SRP GTPase on binding GDP and Mg <sup>2+</sup> GDP. <b>1999</b> , 6, 793-801	72
929	Crystal structure of hemopexin reveals a novel high-affinity heme site formed between two beta-propeller domains. <b>1999</b> , 6, 926-31	195
928	Evolution and mechanism from structures of an ADP-ribosylating toxin and NAD complex. <b>1999</b> , 6, 932-6	207
927	Structure and mechanism of the glycyl radical enzyme pyruvate formate-lyase. <b>1999</b> , 6, 969-75	159
926	Structural basis for recognition of the tra mRNA precursor by the Sex-lethal protein. <b>1999</b> , 398, 579-85	324
925	Structure of the C-terminal domain of FliG, a component of the rotor in the bacterial flagellar motor. <b>1999</b> , 400, 472-5	93
924	Four-helical-bundle structure of the cytoplasmic domain of a serine chemotaxis receptor. <b>1999</b> , 400, 787-92	397
923	Crystal structure of nerve growth factor in complex with the ligand-binding domain of the TrkA receptor. <b>1999</b> , 401, 184-8	313
922	Structure of the C2 domain of human factor VIII at 1.5 Å resolution. <b>1999</b> , 402, 439-42	300
921	Crystal structure of the novel aspartic proteinase zymogen proplasmepsin II from plasmodium falciparum. <b>1999</b> , 6, 32-7	55
920	Crystal structure of recombinant bovine neurocalcin. <b>1999</b> , 6, 80-8	90
919	The crystal structure of a complex of p11 with the annexin II N-terminal peptide. <b>1999</b> , 6, 89-95	230
918	Solution structure of the 40,000 Mr phosphoryl transfer complex between the N-terminal domain of enzyme I and HPr. <b>1999</b> , 6, 166-73	171
917	Crystal structure of the MAPK phosphatase Pyst1 catalytic domain and implications for regulated activation. <b>1999</b> , 6, 174-81	133
916	Crystal structure of a scavenger receptor cysteine-rich domain sheds light on an ancient superfamily. <b>1999</b> , 6, 228-32	139
915	Structural characterization of nitric oxide synthase isoforms reveals striking active-site conservation. <b>1999</b> , 6, 233-42	345
914	Structural and mechanistic basis of immunity toward endonuclease colicins. <b>1999</b> , 6, 243-52	148
913	Directed evolution of thymidine kinase for AZT phosphorylation using DNA family shuffling. <b>1999</b> , 17, 259-64	106

912	Open conformation of a flavocytochrome c3 fumarate reductase. <b>1999</b> , 6, 1104-7	61
911	Crystal structure of transhydrogenase domain III at 1.2 Å resolution. <b>1999</b> , 6, 1126-31	55
910	Quaternary changes in topoisomerase II may direct orthogonal movement of two DNA strands. <b>1999</b> , 6, 322-6	123
909	A cis proline turn linking two beta-hairpin strands in the solution structure of an antibody-bound HIV-1III <sub>B</sub> V3 peptide. <b>1999</b> , 6, 331-5	50
908	Crystal structure of brefeldin A esterase, a bacterial homolog of the mammalian hormone-sensitive lipase. <b>1999</b> , 6, 340-5	128
907	Structures of the M2 channel-lining segments from nicotinic acetylcholine and NMDA receptors by NMR spectroscopy. <b>1999</b> , 6, 374-9	284
906	Autoinhibition by an internal nuclear localization signal revealed by the crystal structure of mammalian importin alpha. <b>1999</b> , 6, 388-97	303
905	Solution structure of the extended neuronal nitric oxide synthase PDZ domain complexed with an associated peptide. <b>1999</b> , 6, 417-21	124
904	Structure of the arginine repressor from <i>Bacillus stearothermophilus</i> . <b>1999</b> , 6, 427-32	61
903	X-ray structures along the reaction pathway of cyclodextrin glycosyltransferase elucidate catalysis in the alpha-amylase family. <b>1999</b> , 6, 432-6	311
902	The crystal structure of HasA, a hemophore secreted by <i>Serratia marcescens</i> . <b>1999</b> , 6, 516-20	164
901	A novel two-chain proteinase inhibitor generated by circularization of a multidomain precursor protein. <b>1999</b> , 6, 526-30	48
900	A complex of influenza hemagglutinin with a neutralizing antibody that binds outside the virus receptor binding site. <b>1999</b> , 6, 530-4	136
899	Structure, specificity and CDR mobility of a class II restricted single-chain T-cell receptor. <b>1999</b> , 6, 574-81	75
898	The 2.0 Å structure of human hypoxanthine-guanine phosphoribosyltransferase in complex with a transition-state analog inhibitor. <b>1999</b> , 6, 588-93	130
897	Structure of the human adenovirus serotype 2 fiber head domain at 1.5 Å resolution. <b>1999</b> , 262, 333-43	82
896	Prediction of three-dimensional structure and mapping of conformational epitopes of envelope glycoprotein of Japanese encephalitis virus. <b>1999</b> , 261, 31-42	92
895	The refined crystal structure of cowpea mosaic virus at 2.8 Å resolution. <b>1999</b> , 265, 20-34	227

894	Three-dimensional structure of Selenocosmia huwena lectin-I (SHL-I) from the venom of the spider Selenocosmia huwena by 2D-NMR. <b>1999</b> , 18, 609-17	39
893	Allosteric inhibition of glycogen phosphorylase a by the potential antidiabetic drug 3-isopropyl 4-(2-chlorophenyl)-1,4-dihydro-1-ethyl-2-methyl-pyridine-3,5,6-tricarboxylate. <b>1999</b> , 8, 1930-45	43
892	Solution structure of the receptor tyrosine kinase EphB2 SAM domain and identification of two distinct homotypic interaction sites. <b>1999</b> , 8, 1954-61	69
891	Crystal structure of penicillin G acylase from the Bro1 mutant strain of <i>Providencia rettgeri</i> . <b>1999</b> , 8, 1971-81	45
890	Three-dimensional structures of enzyme-substrate complexes of the hydroxynitrile lyase from <i>Hevea brasiliensis</i> . <b>1999</b> , 8, 1990-2000	62
889	Crystal structure of the EF-hand parvalbumin at atomic resolution (0.91 Å) and at low temperature (100 K). Evidence for conformational multistates within the hydrophobic core. <b>1999</b> , 8, 2194-204	39
888	Ternary complex structure of human HGPRTase, PRPP, Mg <sup>2+</sup> , and the inhibitor HPP reveals the involvement of the flexible loop in substrate binding. <b>1999</b> , 8, 1023-31	58
887	The 2.1 Å structure of an elicitor-ergosterol complex: a recent addition to the Sterol Carrier Protein family. <b>1999</b> , 8, 1191-9	66
886	<i>Sulfolobus acidocaldarius</i> inorganic pyrophosphatase: structure, thermostability, and effect of metal ion in an archaeal pyrophosphatase. <b>1999</b> , 8, 1218-31	31
885	The Schiff base complex of yeast 5-aminolaevulinic acid dehydratase with laevulinic acid. <b>1999</b> , 8, 1250-6	44
884	The Ubp6 family of deubiquitinating enzymes contains a ubiquitin-like domain: SUB. <b>1999</b> , 8, 1268-75	17
883	The crystal structure of a bacterial, bifunctional 5,10 methylene-tetrahydrofolate dehydrogenase/cyclohydrolase. <b>1999</b> , 8, 1342-9	30
882	X-ray crystallographic analysis of the structural basis for the interactions of pokeweed antiviral protein with its active site inhibitor and ribosomal RNA substrate analogs. <b>1999</b> , 8, 1765-72	51
881	Homology modeling and active-site residues probing of the thermophilic <i>Alicyclobacillus acidocaldarius</i> esterase 2. <b>1999</b> , 8, 1789-96	30
880	NMR structure and metal interactions of the CopZ copper chaperone. <b>1999</b> , 274, 22597-603	104
879	NMR spectroscopy reveals common structural features of the birch pollen allergen Bet v 1 and the cherry allergen Pru a 1. <b>1999</b> , 17, 449-464	23
878	Solution structure of the histidine-containing phosphocarrier protein from <i>Staphylococcus carnosus</i> . <b>1999</b> , 17, 465-480	12
877	Three-dimensional structure of $\beta$ -conotoxin EI determined by <sup>1</sup> H NMR spectroscopy. <b>1999</b> , 6, 199-207	2

876	Investigation of the binding interactions of progesterone using muteins of the human progesterone receptor ligand binding domain designed on the basis of a three-dimensional protein model. <b>1999</b> , 1429, 391-400	18
875	A single domain thermophilic xylanase can bind insoluble xylan: evidence for surface aromatic clusters. <b>1999</b> , 1433, 110-21	25
874	Crystal structure at 1.63 Å resolution of the native form of porcine beta-trypsin: revealing an acetate ion binding site and functional water network. <b>1999</b> , 1435, 7-21	9
873	Inhibition of tumor necrosis factor-alpha (TNF-alpha)/TNF-alpha receptor binding by structural analogues of suramin. <b>1999</b> , 58, 851-9	37
872	A preliminary comparison of structural models for catalytic intermediates of acetylcholinesterase. <b>1999</b> , 119-120, 43-52	25
871	The solution structure of VAT-N reveals a 'missing link' in the evolution of complex enzymes from a simple betaalphanbetabeta element. <b>1999</b> , 9, 1158-68	90
870	Crystal structure of colicin E3 immunity protein: an inhibitor of a ribosome-inactivating RNase. <b>1999</b> , 7, 1365-72	12
869	Diverse structural solutions to catalysis in a family of antibodies. <b>1999</b> , 7, 1385-93	19
868	Crystal structure of Escherichia coli PurE, an unusual mutase in the purine biosynthetic pathway. <b>1999</b> , 7, 1395-406	41
867	The crystal structure of the minus-end-directed microtubule motor protein ncd reveals variable dimer conformations. <b>1999</b> , 7, 1407-16	47
866	Crystal structure of the RNA-dependent RNA polymerase of hepatitis C virus. <b>1999</b> , 7, 1417-26	352
865	Binding of non-catalytic ATP to human hexokinase I highlights the structural components for enzyme-membrane association control. <b>1999</b> , 7, 1427-37	37
864	Crystal structure of Escherichia coli lytic transglycosylase Slt35 reveals a lysozyme-like catalytic domain with an EF-hand. <b>1999</b> , 7, 1167-80	68
863	Crystal structure of an archaeobacterial DNA polymerase. <b>1999</b> , 7, 1189-99	81
862	High-resolution structure of the conger eel galectin, congerin I, in lactose-liganded and ligand-free forms: emergence of a new structure class by accelerated evolution. <b>1999</b> , 7, 1223-33	45
861	The second type II module from human matrix metalloproteinase 2: structure, function and dynamics. <b>1999</b> , 7, 1235-45	45
860	The crystal structure of methenyltetrahydromethanopterin cyclohydrolase from the hyperthermophilic archaeon Methanopyrus kandleri. <b>1999</b> , 7, 1257-68	41
859	A biosynthetic thiolase in complex with a reaction intermediate: the crystal structure provides new insights into the catalytic mechanism. <b>1999</b> , 7, 1279-90	68

858	Structure of the Escherichia coli TolB protein determined by MAD methods at 1.95 Å resolution. <b>1999</b> , 7, 1291-300	64
857	The structure of the outer membrane protein OmpX from Escherichia coli reveals possible mechanisms of virulence. <b>1999</b> , 7, 1301-9	257
856	Helianthus tuberosus lectin reveals a widespread scaffold for mannose-binding lectins. <b>1999</b> , 7, 1473-82	95
855	Conformational changes induced by phosphorylation of the FixJ receiver domain. <b>1999</b> , 7, 1505-15	177
854	Structural transitions in the FixJ receiver domain. <b>1999</b> , 7, 1517-26	50
853	The crystal structure of coxsackievirus A9: new insights into the uncoating mechanisms of enteroviruses. <b>1999</b> , 7, 1527-38	78
852	The structure of the signal receiver domain of the Arabidopsis thaliana ethylene receptor ETR1. <b>1999</b> , 7, 1547-56	89
851	An archetypical extradiol-cleaving catecholic dioxygenase: the crystal structure of catechol 2,3-dioxygenase (metapyrocatechase) from Pseudomonas putida mt-2. <b>1999</b> , 7, 25-34	159
850	Structure of the adenylation domain of an NAD <sup>+</sup> -dependent DNA ligase. <b>1999</b> , 7, 35-42	76
849	The crystal structure of plasminogen activator inhibitor 2 at 2.0 Å resolution: implications for serpin function. <b>1999</b> , 7, 43-54	48
848	Crystal structure of the first dissimilatory nitrate reductase at 1.9 Å solved by MAD methods. <b>1999</b> , 7, 65-79	257
847	Crystal structure of Trypanosoma cruzi trypanothione reductase in complex with trypanothione, and the structure-based discovery of new natural product inhibitors. <b>1999</b> , 7, 81-9	181
846	The crystal structure of the DNase domain of colicin E7 in complex with its inhibitor Im7 protein. <b>1999</b> , 7, 91-102	176
845	The structure of active serpin 1K from Manduca sexta. <b>1999</b> , 7, 103-9	62
844	The primary and three-dimensional structures of a nine-haem cytochrome c from Desulfovibrio desulfuricans ATCC 27774 reveal a new member of the Hmc family. <b>1999</b> , 7, 119-30	71
843	Three-dimensional structure of a barley beta-D-glucan exohydrolase, a family 3 glycosyl hydrolase. <b>1999</b> , 7, 179-90	194
842	A new proposal for urease mechanism based on the crystal structures of the native and inhibited enzyme from Bacillus pasteurii: why urea hydrolysis costs two nickels. <b>1999</b> , 7, 205-16	392
841	X-ray structure of pyrrolidone carboxyl peptidase from the hyperthermophilic archaeon Thermococcus litoralis. <b>1999</b> , 7, 237-44	56

- 840 Crystal structure of a viral cyclin, a positive regulator of cyclin-dependent kinase 6. **1999**, 7, 245-54 29
- 839 Crystal structure of the trimeric alpha-helical coiled-coil and the three lectin domains of human lung surfactant protein D. **1999**, 7, 255-64 114
- 838 A 30-angstrom-long U-shaped catalytic tunnel in the crystal structure of polyamine oxidase. **1999**, 7, 265-76 153
- 837 Structure of acetylcholinesterase complexed with E2020 (Aricept): implications for the design of new anti-Alzheimer drugs. **1999**, 7, 297-307 571
- 836 The crystal structure of methylglyoxal synthase from *Escherichia coli*. **1999**, 7, 309-17 34
- 835 Crystal structure of the kinase domain of human vascular endothelial growth factor receptor 2: a key enzyme in angiogenesis. **1999**, 7, 319-30 159
- 834 The crystal structure of pyroglutamyl peptidase I from *Bacillus amyloliquefaciens* reveals a new structure for a cysteine protease. **1999**, 7, 399-411 31
- 833 Chloroplast NADP-malate dehydrogenase: structural basis of light-dependent regulation of activity by thiol oxidation and reduction. **1999**, 7, 461-75 83
- 832 Crystal structure of 6-hydroxymethyl-7,8-dihydropterin pyrophosphokinase, a potential target for the development of novel antimicrobial agents. **1999**, 7, 489-96 60
- 831 Crystal structure of an aminoglycoside 6'-N-acetyltransferase: defining the GCN5-related N-acetyltransferase superfamily fold. **1999**, 7, 497-507 127
- 830 The 2.7 Å crystal structure of deoxygenated hemoglobin from the sea lamprey (*Petromyzon marinus*): structural basis for a lowered oxygen affinity and Bohr effect. **1999**, 7, 517-26 31
- 829 Removal of the bridging ligand atom at the Ni-Fe active site of [NiFe] hydrogenase upon reduction with H<sub>2</sub>, as revealed by X-ray structure analysis at 1.4 Å resolution. **1999**, 7, 549-56 304
- 828 The crystal structure of a reduced [NiFeSe] hydrogenase provides an image of the activated catalytic center. **1999**, 7, 557-66 405
- 827 Structure of mammalian ornithine decarboxylase at 1.6 Å resolution: stereochemical implications of PLP-dependent amino acid decarboxylases. **1999**, 7, 567-81 135
- 826 The crystal structure of human S-adenosylmethionine decarboxylase at 2.25 Å resolution reveals a novel fold. **1999**, 7, 583-95 69
- 825 Crystal structure of the Atx1 metallochaperone protein at 1.02 Å resolution. **1999**, 7, 605-17 211
- 824 Crystal structure of the ATPase domain of translation initiation factor 4A from *Saccharomyces cerevisiae*--the prototype of the DEAD box protein family. **1999**, 7, 671-9 102
- 823 Pyruvate formate lyase is structurally homologous to type I ribonucleotide reductase. **1999**, 7, 733-44 36



822	Structure of L-aspartate oxidase: implications for the succinate dehydrogenase/fumarate reductase oxidoreductase family. <b>1999</b> , 7, 745-56	76
821	Crystal structure of mammalian purple acid phosphatase. <b>1999</b> , 7, 757-67	152
820	Structure of the specificity domain of the Dorsal homologue Gambif1 bound to DNA. <b>1999</b> , 7, 841-52	24
819	Crystal structure of phenylalanine-regulated 3-deoxy-D-arabino-heptulosonate-7-phosphate synthase from <i>Escherichia coli</i> . <b>1999</b> , 7, 865-75	105
818	Glutamate mutase from <i>Clostridium cochlearium</i> : the structure of a coenzyme B12-dependent enzyme provides new mechanistic insights. <b>1999</b> , 7, 891-902	201
817	Identification of the <i>Archaeoglobus fulgidus</i> endonuclease III DNA interaction surface using heteronuclear NMR methods. <b>1999</b> , 7, 919-30	13
816	Crystal structure of an aromatic ring opening dioxygenase LigAB, a protocatechuate 4,5-dioxygenase, under aerobic conditions. <b>1999</b> , 7, 953-65	149
815	Crystal structure of <i>Pseudomonas fluorescens</i> 4-hydroxyphenylpyruvate dioxygenase: an enzyme involved in the tyrosine degradation pathway. <b>1999</b> , 7, 977-88	120
814	Coagulation factor IXa: the relaxed conformation of Tyr99 blocks substrate binding. <b>1999</b> , 7, 989-96	113
813	Specific inhibition of insect alpha-amylases: yellow meal worm alpha-amylase in complex with the amaranth alpha-amylase inhibitor at 2.0 Å resolution. <b>1999</b> , 7, 1079-88	74
812	The three-dimensional structure of caspase-8: an initiator enzyme in apoptosis. <b>1999</b> , 7, 1125-33	121
811	The atomic-resolution structure of human caspase-8, a key activator of apoptosis. <b>1999</b> , 7, 1135-43	146
810	X-ray crystal structure of aminoimidazole ribonucleotide synthetase (PurM), from the <i>Escherichia coli</i> purine biosynthetic pathway at 2.5 Å resolution. <b>1999</b> , 7, 1155-66	61
809	The structure of an entire noncovalent immunoglobulin kappa light-chain dimer (Bence-Jones protein) reveals a weak and unusual constant domains association. <b>1999</b> , 260, 192-9	25
808	Crystal structure of a hybrid between ribonuclease A and bovine seminal ribonuclease--the basic surface, at 2.0 Å resolution. <b>1999</b> , 260, 176-82	8
807	The three-dimensional structure of Asp189Ser trypsin provides evidence for an inherent structural plasticity of the protease. <b>1999</b> , 263, 20-6	28
806	Free Energy Analysis of Protein-DNA Binding: The EcoRI Endonuclease-DNA Complex. <b>1999</b> , 151, 333-357	96
805	Probing the disulfide folding pathway of insulin-like growth factor-I. <b>1999</b> , 62, 693-703	26

804	Model building by comparison at CASP3: Using expert knowledge and computer automation. <b>1999</b> , 37, 47-54	107
803	An iterative structure-assisted approach to sequence alignment and comparative modeling. <b>1999</b> , 37, 55-60	29
802	Structural basis for the activity of two muconate cycloisomerase variants toward substituted muconates. <b>1999</b> , 34, 125-136	20
801	Structure of catalase HPII from <i>Escherichia coli</i> at 1.9 Å resolution. <b>1999</b> , 34, 155-66	51
800	Homology modeling and substrate binding study of human CYP4A11 enzyme. <b>1999</b> , 34, 403-415	34
799	Solution structure of potassium channel-inhibiting scorpion toxin Lq2. <b>1999</b> , 34, 417-26	14
798	Molecular dynamics and accuracy of NMR structures: Effects of error bounds and data removal. <b>1999</b> , 34, 453-463	20
797	Modeling of acanthoxin A1, a PLA2 enzyme from the venom of the common death adder ( <i>Acanthopis antarcticus</i> ). <b>1999</b> , 35, 80-8	6
796	Validation of NMR side-chain conformations by packing calculations. <b>1999</b> , 35, 184-94	6
795	Knowledge-based interaction potentials for proteins. <b>1999</b> , 36, 54-67	47
794	Probing the modelled structure of Wheatwin1 by controlled proteolysis and sequence analysis of unfractionated digestion mixtures. <b>1999</b> , 36, 192-204	11
793	X-ray crystallographic studies of the denaturation of ribonuclease S. <b>1999</b> , 36, 282-294	12
792	High resolution structure and sequence of <i>T. aurantiacus</i> Xylanase I: Implications for the evolution of thermostability in family 10 xylanases and enzymes with $\beta$ barrel architecture. <b>1999</b> , 36, 295-306	65
791	A database method for automated map interpretation in protein crystallography. <b>1999</b> , 36, 526-541	10
790	Solution structure and RNA-binding activity of the N-terminal leucine-repeat region of hepatitis delta antigen. <b>1999</b> , 37, 121-9	27
789	Theoretical study of the electrostatically driven step of receptor-G protein recognition. <b>1999</b> , 37, 145-156	29
788	Homology modeling and substrate binding study of human CYP2C9 enzyme. <b>1999</b> , 37, 176-90	32
787	Homology modeling and substrate binding study of human CYP2C18 and CYP2C19 enzymes. <b>1999</b> , 37, 204-17	12

786	The three-dimensional solution structure of <i>Aesculus hippocastanum</i> antimicrobial protein 1 determined by 1H nuclear magnetic resonance. <b>1999</b> , 37, 388-403	52
785	Validation of nuclear magnetic resonance structures of proteins and nucleic acids: hydrogen geometry and nomenclature. <b>1999</b> , 37, 404-16	20
784	The crystal structure of triosephosphate isomerase (TIM) from <i>Thermotoga maritima</i> : A comparative thermostability structural analysis of ten different TIM structures. <b>1999</b> , 37, 441-453	119
783	Crystal structure of a thermophilic alcohol dehydrogenase substrate complex suggests determinants of substrate specificity and thermostability. <b>1999</b> , 37, 619-27	52
782	A structural model for the <i>rolA</i> protein and its interaction with DNA. <b>1999</b> , 37, 697-708	18
781	Insights into the mechanisms of catalysis and heterotropic regulation of <i>Escherichia coli</i> aspartate transcarbamoylase based upon a structure of the enzyme complexed with the bisubstrate analogue N-phosphonacetyl-L-aspartate at 2.1 Å. <b>1999</b> , 37, 729-742	61
780	Comparison of the three-dimensional structures of a humanized and a chimeric Fab of an anti-gamma-interferon antibody. <b>1999</b> , 12, 19-32	23
779	X-ray structure of ornithine decarboxylase from <i>Trypanosoma brucei</i> : the native structure and the structure in complex with alpha-difluoromethylornithine. <b>1999</b> , 38, 15174-84	129
778	COMPUTATIONAL TECHNIQUES. <b>1999</b> , 91-cp1	2
777	Novel approach to predicting P450-mediated drug metabolism: development of a combined protein and pharmacophore model for CYP2D6. <b>1999</b> , 42, 1515-24	190
776	Crystal structures of alpha-mercaptoacyldipeptides in the thermolysin active site: structural parameters for a Zn monodentation or bidentation in metalloendopeptidases. <b>1999</b> , 38, 12569-76	42
775	The crystal structure of a 2-fluorocellotriosyl complex of the <i>Streptomyces lividans</i> endoglucanase CelB2 at 1.2 Å resolution. <b>1999</b> , 38, 4826-33	49
774	Crystal structures of aged phosphorylated acetylcholinesterase: nerve agent reaction products at the atomic level. <b>1999</b> , 38, 7032-9	248
773	Solution structure and dynamics of the CX3C chemokine domain of fractalkine and its interaction with an N-terminal fragment of CX3CR1. <b>1999</b> , 38, 1402-14	128
772	Crystal structure of histidine ammonia-lyase revealing a novel polypeptide modification as the catalytic electrophile. <b>1999</b> , 38, 5355-61	192
771	Biochemical characterization and crystal structure determination of human heart short chain L-3-hydroxyacyl-CoA dehydrogenase provide insights into catalytic mechanism. <b>1999</b> , 38, 5786-98	80
770	Structure-based design, synthesis, and X-ray crystallography of a high-affinity antagonist of the Grb2-SH2 domain containing an asparagine mimetic. <b>1999</b> , 42, 2358-63	51
769	Conformationally constrained butyrophenones with mixed dopaminergic (D(2)) and serotonergic (5-HT(2A), 5-HT(2C)) affinities: synthesis, pharmacology, 3D-QSAR, and molecular modeling of (aminoalkyl)benzo- and -thienocycloalkanones as putative atypical antipsychotics. <b>1999</b> , 42, 2774-97	33

768	The 2.1 Å structure of a cysteine protease with proline specificity from ginger rhizome, <i>Zingiber officinale</i> . <b>1999</b> , 38, 11624-33	54
767	Crystallographic evidence for preformed dimers of erythropoietin receptor before ligand activation. <b>1999</b> , 283, 987-90	545
766	X-ray crystallographic structure of the Norwalk virus capsid. <b>1999</b> , 286, 287-90	698
765	Domain movement in gelsolin: a calcium-activated switch. <b>1999</b> , 286, 1939-42	127
764	Implication of tubby proteins as transcription factors by structure-based functional analysis. <b>1999</b> , 286, 2119-25	159
763	Crystal structure of <i>Thermotoga maritima</i> ribosome recycling factor: a tRNA mimic. <b>1999</b> , 286, 2349-52	160
762	Structure of a fructose-1,6-bis(phosphate) aldolase liganded to its natural substrate in a cleavage-defective mutant at 2.3 Å. <b>1999</b> , 38, 12655-64	49
761	Molecular modeling of an active loop structure in lysozyme. Sequence effects or crystal packing?. <b>1999</b> , 16, 873-89	1
760	Identification of the calcium binding site and a novel ytterbium site in blood coagulation factor XIII by x-ray crystallography. <b>1999</b> , 274, 4917-23	81
759	Quantitative structure-activity relationship of human neutrophil collagenase (MMP-8) inhibitors using comparative molecular field analysis and X-ray structure analysis. <b>1999</b> , 42, 1908-20	78
758	The solution structure and dynamics of an Arc repressor mutant reveal premelting conformational changes related to DNA binding. <b>1999</b> , 38, 6035-42	19
757	Solution structures of the C-terminal domain of cardiac troponin C free and bound to the N-terminal domain of cardiac troponin I. <b>1999</b> , 38, 8313-22	46
756	Pi7, an orphan peptide from the scorpion <i>Pandinus imperator</i> : a 1H-NMR analysis using a nano-NMR Probe. <b>1999</b> , 38, 16756-65	29
755	Comparison of the structures of beta amyloid peptide (25-35) and substance P in trifluoroethanol/water solution. <b>1999</b> , 17, 381-91	24
754	Androctonin, a novel antimicrobial peptide from scorpion <i>Androctonus australis</i> : solution structure and molecular dynamics simulations in the presence of a lipid monolayer. <b>1999</b> , 17, 367-80	38
753	Tumor suppressor INK4: determination of the solution structure of p18INK4C and demonstration of the functional significance of loops in p18INK4C and p16INK4A. <b>1999</b> , 38, 2930-40	38
752	Crystal structure of invasin: a bacterial integrin-binding protein. <b>1999</b> , 286, 291-5	238
751	Muscle fatty acid-binding protein. <b>1999</b> , 1441, 94-105	21

750	Crystal structure of an MHC class I presented glycopeptide that generates carbohydrate-specific CTL. <b>1999</b> , 10, 51-61	110
749	Crystal structures of two H-2Db/glycopeptide complexes suggest a molecular basis for CTL cross-reactivity. <b>1999</b> , 10, 63-74	116
748	Triggering cell death: the crystal structure of Apo2L/TRAIL in a complex with death receptor 5. <b>1999</b> , 4, 563-71	360
747	The structural basis of Rho effector recognition revealed by the crystal structure of human RhoA complexed with the effector domain of PKN/PRK1. <b>1999</b> , 4, 793-803	146
746	Cap-dependent translation initiation in eukaryotes is regulated by a molecular mimic of eIF4G. <b>1999</b> , 3, 707-16	406
745	The crystal structure of the human hepatitis B virus capsid. <b>1999</b> , 3, 771-80	520
744	Identification of a homologue of CD59 in a cyclostome: implications for the evolutionary development of the complement system. <b>1999</b> , 23, 1-14	14
743	Molecular evolution and structural analyses of the spike glycoprotein from Brazilian SARS-CoV-2 genomes: the impact of selected mutations.. <b>2022</b> , 1-19	0
742	Professor Dame Janet Thornton to receive 'The FEBS Journal Open Science Award'.. <b>2022</b> ,	1
741	Exploring the antihyperglycemic potential of tetrapeptides devised from AdMc1 different receptor proteins inhibition using in silico approaches.. <b>2022</b> , 36, 3946320221103120	3
740	Multistage and transmission-blocking tubulin targeting potent antimalarial discovered from the open access MMV Pathogen Box.	
739	High prevalence of an alpha variant lineage with a premature stop codon in ORF7a in Iraq, winter 2020-2021. <b>2022</b> , 17, e0267295	1
738	The involvement of CYP1A2 in biodegradation of dioxins in pigs. <b>2022</b> , 17, e0267162	
737	Multicopper oxidase enzymes from <i>Chrysoporthe cubensis</i> improve the saccharification yield of sugarcane bagasse. <b>2022</b> ,	
736	Virtual Quasi-2D Intermediates as Building Blocks for Plausible Structural Models of Amyloid Fibrils from Proteins with Complex Topologies: A Case Study of Insulin.	0
735	Deciphering the role of S-adenosyl homocysteine nucleosidase in quorum sensing mediated biofilm formation. <b>2022</b> , 23,	
734	Artonin F Induces the Ubiquitin-Proteasomal Degradation of c-Met and Decreases Akt-mTOR Signaling. <b>2022</b> , 15, 633	
733	Identification of some dietary flavonoids as potential inhibitors of TMPRSS2 through protein-ligand interaction studies and binding free energy calculations.	0

732	In Search of Synergistic Insect Repellents: Modeling of Muscarinic GPCR Interactions with Classical and Bitopic Photoactive Ligands. <b>2022</b> , 27, 3280	0
731	Characterization of the Cell Wall Component through Thermogravimetric Analysis and Its Relationship with an Expansin-like Protein in <i>Deschampsia antarctica</i> . <b>2022</b> , 23, 5741	0
730	Characterization of proteome wide antigenic epitopes to design proteins specific and proteome-wide ensemble vaccines against heartland virus using structural vaccinology and immune simulation approaches. <b>2022</b> , 168, 105592	1
729	Insilico structure based drug design approach to find potential hits in ventilator-associated pneumonia caused by <i>Pseudomonas aeruginosa</i> . <b>2022</b> , 146, 105597	
728	Orthopalladated N,N-Dimethyl-1-Phenethylamine Compounds Containing 2,6-Lutidine: Synthesis, DNA Binding Studies and Cytotoxicity Evaluation.	
727	Novel Etodolac Derivatives as Eukaryotic Elongation Factor 2 Kinase (eEF2K) Inhibitors for Targeted Cancer Therapy.	0
726	Molecular dynamics simulations of the conformational plasticity in the active pocket of salt-inducible kinase 2 (SIK2) multi-state binding with bosutinib. <b>2022</b> , 20, 2574-2586	1
725	Substantiation of propitious Bnzybiotic from two novel bacteriophages isolated from a wastewater treatment plant in Qatar. <b>2022</b> , 12,	0
724	Antimalarial phytochemicals as potential inhibitors of SARS-CoV-2 guanine N7-methyltransferase (nsp 14): an integrated computational approach. 1-23	
723	Exploring the molecular interaction of Pheniramine with <i>Enterococcus faecalis</i> Homoserine Kinase: In-silico and in vitro studies.	
722	Deciphering the structural and functional impact of Q657L mutation in NLRC4 using computational methods. 1-16	
721	Reactive Human Plasma Glutathione Peroxidase Mutant with Diselenide Bond Succeeds in Tetramer Formation. <b>2022</b> , 11, 1083	
720	Molecular dynamics and intrinsic disorder analysis of the SARS-CoV-2 Nsp1 structural changes caused by substitution and deletion mutations. 1-10	2
719	Inhibition of Arenaviridae nucleoprotein exonuclease by bisphosphonate. <b>2022</b> , 9,	
718	GenNBPSeg: Online web server to generate Never Born Protein Sequences using Toeplitz Matrix Approach with Structure Analysis. <b>2022</b> , 17,	0
717	Genome-Wide Identification, In Silico Characterization of AtCOP1-Targeting Regulatory Proteins Network and their Expression Profiling in The COP1 Downregulated <i>Arabidopsis thaliana</i> .	
716	An Insight Based on Computational Analysis of the Interaction between the Receptor-Binding Domain of the Omicron Variants and Human Angiotensin-Converting Enzyme 2. <b>2022</b> , 11, 797	1
715	Dual transcriptome based reconstruction of <i>Salmonella</i> -human integrated metabolic network to screen potential drug targets. <b>2022</b> , 17, e0268889	0

- 714 In silico comparative structural and compositional analysis of glycoproteins of RSV to study the nature of stability and transmissibility of RSV A.
- 713 Molecular Modelling and Docking Analysis of Filarial Targets by using New Lead Compounds identified from *Psoralea corylifolia* and *Mimusops elengi*. **2022**, 11,
- 712 Identification of Therapeutic Targets in an Emerging Gastrointestinal Pathogen *Campylobacter ureolyticus* and Possible Intervention through Natural Products. **2022**, 11, 680 1
- 711 In Silico Analysis and Functional Characterization of Antimicrobial and Insecticidal Vicilin from Moth Bean (*Vigna aconitifolia* (Jacq.) Marechal) Seeds. **2022**, 27, 3251 0
- 710 tREPs-A New Class of Functional tRNA-Encoded Peptides. 0
- 709 Insecticidal Activity of Organic Extracts of *Solidago graminifolia* and Its Main Metabolites (Quercetin and Chlorogenic Acid) against *Spodoptera frugiperda*: An In Vitro and In Silico Approach. **2022**, 27, 3325 1
- 708 In silico investigation of cytochrome bc1 molecular inhibition mechanism against *Trypanosoma cruzi*.
- 707 In silico SARS-CoV-2 vaccine development for Omicron strain using reverse vaccinology. 0
- 706 Combined in Silico Prediction Methods, Molecular Dynamic Simulation, and Molecular Docking of FOXG1 Missense Mutations: Effect on FoxG1 Structure and Its Interactions with DNA and Bmi-1 Protein. 0
- 705 Articulating Target-Mining Techniques to Disinter Alzheimer's Specific Targets for Drug Repurposing. **2022**, 106931
- 704 A pragmatic pharmacophore informatics strategy to discover new potent inhibitors against pim-3.
- 703 Staufen-2 functions as a cofactor for enhanced Rev-mediated nucleocytoplasmic trafficking of HIV-1 genomic RNA via the CRM1 pathway. 0
- 702 Engineering globins for efficient biodegradation of malachite green: two case studies of myoglobin and neuroglobin. **2022**, 12, 18654-18660
- 701 Expression, Purification, and In Silico Characterization of *Mycobacterium smegmatis* Alternative Sigma Factor SigB. **2022**, 2022, 1-11 0
- 700 Molecular mechanism of interaction between fatty acid delta 6 desaturase and acyl-CoA by computational prediction. **2022**, 12,
- 699 Antiproliferative efficacy of the antioxidant bioactive compounds of defatted seeds of *Azadirachta indica* and *Momordica charantia* against the regulatory function of tumor suppressor gene inducing oral carcinoma. 1-15
- 698 Identification of homozygous missense variant in SIX5 gene underlying recessive nonsyndromic hearing impairment. **2022**, 17, e0268078
- 697 P450 gene duplication and divergence led to the evolution of dual novel functions and insecticide cross-resistance in the brown planthopper *Nilaparvata lugens*. **2022**, 18, e1010279 1

- 696 Deletion of the Loop Linking Two Domains of Exo-Inulinase InuAMN8 Diminished the Enzymatic Thermo-Halo-Alcohol Tolerance. 13,
- 695 Crystal structure of mevalonate 3,5-bisphosphate decarboxylase reveals insight into the evolution of decarboxylases in the mevalonate metabolic pathways. **2022**, 102111 1
- 694 Computer-Aided Design of  $\beta$ -L-Rhamnosidase to Increase the Synthesis Efficiency of Icariside I. 10,
- 693 Molecular Docking and In Silico Simulation of *Trichinella spiralis* Membrane-Associated Progesterone Receptor Component 2 (Ts-MAPRC2) and Its Interaction with Human PGRMC1. **2022**, 2022, 1-10
- 692 Dendronized Polymeric Biomaterial for Loading, Stabilization, and Targeted Cytosolic Delivery of microRNA in Cancer Cells.
- 691 The complex of Fas-associated factor 1 with Hsp70 stabilizes the adherens junction integrity by suppressing RhoA activation. 1
- 690 Evaluation of the inhibitory potential of Valproic acid against histone deacetylase of *Leishmania donovani* and computational studies of Valproic acid derivatives. 1-18
- 689 Insights into the structural peculiarities of the N-terminal and receptor binding domains of the spike protein from the SARS-CoV-2 Omicron variant. **2022**, 105735 2
- 688 Application of Phytochemicals To Combat Fungal Pathogens of Pulses: An Approach toward Inhibition of Fungal Propagation and Invasin Activity.
- 687 Development of New Potential Inhibitors of  $\beta$  Integrins through In Silico Methods Screening and Computational Validation. **2022**, 12, 932 1
- 686 Structural and Mechanistic Insights into *Mycobacterium abscessus* Aspartate Decarboxylase PanD and a Pyrazinoic Acid-Derived Inhibitor. 0
- 685 A Lipoate-Protein Ligase Is Required for De Novo Lipoyl-Protein Biosynthesis in the Hyperthermophilic Archaeon *Thermococcus kodakarensis*.
- 684 Prediction and expression analysis of deleterious nonsynonymous SNPs of Arabidopsis ACD11 gene by combining computational algorithms and molecular docking approach. **2022**, 18, e1009539
- 683 Homology Modeling and Molecular Docking Approaches for the Proposal of Novel Insecticides against the African Malaria Mosquito (*Anopheles gambiae*). **2022**, 27, 3846
- 682 First Data on *Ornithodoros moubata* Aquaporins: Structural, Phylogenetic and Immunogenic Characterisation as Vaccine Targets. **2022**, 11, 694 1
- 681 Designing of potent anti-diabetic molecules by targeting SIK2 using computational approaches.
- 680 AlphaFold Models of Small Proteins Rival the Accuracy of Solution NMR Structures. 9, 1
- 679 Insights from a computational analysis of the SARS-CoV-2 Omicron variant: Host-pathogen interaction, pathogenicity, and possible drug therapeutics. **2022**, 10, 0



- 678 QSAR, homology modeling, and docking simulation on SARS-CoV-2 and pseudomonas aeruginosa inhibitors, ADMET, and molecular dynamic simulations to find a possible oral lead candidate. **2022**, 20, 0
- 677 An in silico approach towards identification of novel drug targets in Klebsiella oxytoca. **2022**, 100998
- 676 In Silico Molecular Dynamics of Griseofulvin and Its Derivatives Revealed Potential Therapeutic Applications for COVID-19. **2022**, 23, 6889 2
- 675 Development of Multi-epitope Based Subunit Vaccine Against Crimean-Congo Hemorrhagic Fever Virus Using Reverse Vaccinology Approach. **2022**, 28, 0
- 674 An Immunoinformatics Prediction of Novel Multi-Epitope Vaccines Candidate Against Surface Antigens of Nipah Virus. **2022**, 28, 0
- 673 Molecular docking and simulation studies to prove the antimicrobial property of cowpea extract. 32-43
- 672 In Silico Docking of Nematode  $\beta$ Tubulins With Benzimidazoles Points to Gene Expression and Orthologue Variation as Factors in Anthelmintic Resistance. 3,
- 671 Structure-Functional Characteristics of the Svx Protein—the Virulence Factor of the Phytopathogenic Bacterium Pectobacterium atrosepticum. **2022**, 23, 6914 0
- 670 Structural Insight into Terminal Galactose Recognition by Two Non-HBGA Binding GI.3 Noroviruses.
- 669 Improvement of Fusel Alcohol Production by Engineering of the Yeast Branched-Chain Amino Acid Aminotransaminase. 1
- 668 Proteomic analysis of adipose tissue revealing differentially abundant proteins in highly efficient mid-lactating dairy cows. **2022**, 12,
- 667 Ex vivo, in vitro, and in silico approaches to unveil the mechanisms underlying vasorelaxation effect of Mentha Longifolia (L.) in porcine coronary artery. **2022**, 153, 113298
- 666 Designing and development of phthalimides as potent anti-tubulin hybrid molecules against malaria. **2022**, 239, 114534 0
- 665 Extracts of selected Lamiaceae species as promising antidiabetics: Chemical profiling, in vitro and in silico approach combined with dynamical modeling. **2022**, 186, 115200 0
- 664 Structural Protein Effects Underpinning Cognitive Developmental Delay of the PURA p.Phe233del Mutation Modelled by Artificial Intelligence and the Hybrid Quantum Mechanics/Molecular Mechanics Framework. **2022**, 12, 871 0
- 663 Resveratrol and Its Natural Analogues Inhibit RNA Dependant RNA Polymerase (RdRp) of Rhizopus oryzae in Mucormycosis through Computational Investigations. 1-18 1
- 662 In Silico Designed Multi-Epitope Immunogen  $\beta$ pme-VAC/LGCM-2022—May Induce Both Cellular and Humoral Immunity against Treponema pallidum Infection. **2022**, 10, 1019 0
- 661 Binding of the M. tuberculosis EccC ATPase double hexameric ring to the EsxAB virulence factor is enhanced by ATP.

- 660 Point mutations that boost aromatic amino acid production and CO<sub>2</sub> assimilation in plants. **2022**, 8, 0
- 659 Ancient whale rhodopsin reconstructs dim-light vision over a major evolutionary transition: Implications for ancestral diving behavior. **2022**, 119, 1
- 658 A unique antigen against SARS-CoV-2, *Acinetobacter baumannii*, and *Pseudomonas aeruginosa*. **2022**, 12, 0
- 657 Design of a Multi-epitope Vaccine against Chicken Anemia Virus Disease. **2022**, 14, 1456 0
- 656 N-linked glycosylation enhances hemagglutinin stability in avian H5N6 influenza virus to promote adaptation in mammals. **2022**, 1, 1
- 655 Structural Characterization of L-Galactose Dehydrogenase: An Essential Enzyme for Vitamin C Biosynthesis. 0
- 654 Scorpion Neurotoxin Syb-prII-1 Exerts Analgesic Effect through Nav1.8 Channel and MAPKs Pathway. **2022**, 23, 7065
- 653 Identification of phytochemicals from *Eclipta alba* and assess their potentiality against Hepatitis C virus envelope glycoprotein: virtual screening, docking, and molecular dynamics simulation study. 1-17 1
- 652 In silico and experimental validation of a new modified arginine-rich cell penetrating peptide for plasmid DNA delivery. **2022**, 122005 0
- 651 A multi-epitope vaccine designed against blood-stage of malaria: an immunoinformatic and structural approach. **2022**, 12, 1
- 650 Glycosylation of Aromatic Glycosides by a Promiscuous Glycosyltransferase UGT71BD1 from *Cistanche tubulosa*. 2
- 649 Homology modeling, virtual screening, molecular docking, molecular dynamic (MD) simulation, and ADMET approaches for identification of natural anti-Parkinson agents targeting MAO-B protein. **2022**, 136803 1
- 648 Identification of HPr kinase/phosphorylase inhibitors: novel antimicrobials against resistant *Enterococcus faecalis*.
- 647 Biochemical characterization and structure-based in silico screening of potent inhibitor molecules against the 1 cys peroxiredoxin of bacterioferritin comigratory protein family from *Candidatus Liberibacter asiaticus*. 1-13
- 646 Structure Prediction, Evaluation, and Validation of GPR18 Lipid Receptor Using Free Programs. **2022**, 23, 7917
- 645 Synthesis (Z) vs (E) Selectivity, Antifungal Activity against *Fusarium oxysporum*, and Structure-Based Virtual Screening of Novel Schiff Bases Derived from L-Tryptophan. **2022**, 7, 24714-24726 0
- 644 Structural Validation by the G-Factor Properly Regulates Boost Potentials Imposed in Conformational Sampling of Proteins. 1
- 643 Structural Analysis of Ino2p/Ino4p Mutual Interactions and Their Binding Interface with Promoter DNA. **2022**, 23, 7600

- 642 Proteome Exploration of *Legionella pneumophila* To Identify Novel Therapeutics: a Hierarchical Subtractive Genomics and Reverse Vaccinology Approach. ○
- 641 Thermostability engineering of industrial enzymes through structure modification. ○
- 640 Phytochemical composition, biological propensities, and in-silico studies of *Crateva adansonii* DC.: A natural source of bioactive compounds. **2022**, 101890 ○
- 639 Functional Characterization of a 2OGD Involved in Abietane-Type Diterpenoids Biosynthetic Pathway in *Salvia miltiorrhiza*. 13, ○
- 638 A Novel Anti-CD22 scFv.Bim Fusion Protein Effectively Induces Apoptosis in Malignant B cells and Promotes Cytotoxicity.
- 637 Structural and Dynamics Studies of the Spcas9 Variant Provide Insights into the Regulatory Role of the REC1 Domain. **2022**, 12, 8687-8697 1
- 636 In silico analyses of leptin and leptin receptor of spotted snakehead *Channa punctata*. **2022**, 17, e0270881 ○
- 635 Vietnamese *Dalbergia tonkinensis*: A Promising Source of Mono- and Bifunctional Vasodilators. **2022**, 27, 4505 ○
- 634 Development of a Multi-Epitope Vaccine for *Mycoplasma hyopneumoniae* and Evaluation of Its Immune Responses in Mice and Piglets. **2022**, 23, 7899 2
- 633 In silico structural and functional characterization of *Antheraea mylitta* cocoonase. **2022**, 20, ○
- 632 Biophysical and modeling-based approach for the identification of inhibitors against DOHH from *Leishmania donovani*.
- 631 Pharmacophore modelling, docking and molecular dynamic simulation studies in the discovery of potential human renin inhibitors. **2022**, 108272 ○
- 630 The C-Terminal Acidic Tail Modulates the Anticancer Properties of HMGB1. **2022**, 23, 7865
- 629 Multistage and transmission-blocking tubulin targeting potent antimalarial discovered from the open access MMV Pathogen Box. **2022**, 115154 1
- 628 Integration of In Silico Strategies for Drug Repositioning towards P38 $\beta$  Mitogen-Activated Protein Kinase (MAPK) at the Allosteric Site. **2022**, 14, 1461 ○
- 627 In Silico Comparative Structural and Residue Interaction Network Analysis of MATE Efflux Proteins in *P. aeruginosa* and *S. aureus*.
- 626 A Selective Adenylyl Cyclase 1 Inhibitor Relieves Pain Without Causing Tolerance. 13,
- 625 Cloning and Characterization of *Drosophila melanogaster* Juvenile Hormone Epoxide Hydrolases (JEH) and Their Promoters. **2022**, 12, 991

624	Comparative molecular dynamics analyses on PIK3CA hotspot mutations with PI3K $\beta$ -specific inhibitors and ATP. <b>2022</b> , 99, 107726	0
623	Characterization of novel nuclease and protease activities among Leptospiral immunoglobulin-like proteins. <b>2022</b> , 727, 109349	0
622	Genome-wide identification and analysis of HECT E3 ubiquitin ligase gene family in <i>Ruditapes philippinarum</i> and their involvement in the response to heat stress and <i>Vibrio anguillarum</i> infection. <b>2022</b> , 43, 101012	0
621	Complete structure elucidation of a functional form of the <i>Bacillus thuringiensis</i> Cry4Ba Endotoxin: Insights into toxin-induced transmembrane pore architecture. <b>2022</b> , 620, 158-164	0
620	Non-active site mutations in the HIV protease: Diminished drug binding affinity is achieved through modulating the hydrophobic sliding mechanism. <b>2022</b> , 217, 27-41	
619	<i>C. elegans</i> ribosomal protein S3 protects against H <sub>2</sub> O <sub>2</sub> -induced DNA damage and suppresses spontaneous mutations in yeast. <b>2022</b> , 117, 103359	
618	In-silico functional and structural annotation of hypothetical protein from <i>Klebsiella pneumoniae</i> : A potential drug target. <b>2022</b> , 116, 108262	5
617	Mechanism of the distinct toxicity level of imidacloprid and thiacloprid against honey bees: An in silico study based on cytochrome P450 9Q3. <b>2022</b> , 116, 108257	
616	Anti-Metalloprotease P-I Single-Domain Antibodies: Tools for Next-Generation Snakebite Antivenoms. <b>2022</b> , 2022, 1-17	0
615	Multi-epitope-based vaccine design by exploring antigenic potential among leptospiral lipoproteins using comprehensive immunoinformatics and structure-based approaches.	0
614	Wheat Grain Proteins: Past, Present and Future.	0
613	Structural insights into the RNA interaction with Yam bean Mosaic virus (coat protein) from <i>Pachyrhizus erosus</i> using bioinformatics approach. <b>2022</b> , 17, e0270534	1
612	Modifying Thermostability and Reusability of Hyperthermophilic Mannanase by Immobilization on Glutaraldehyde Cross-Linked Chitosan Beads. <b>2022</b> , 12, 999	0
611	Probing the interaction between selected furan derivatives and porcine myofibrillar proteins by spectroscopic and molecular docking approaches. <b>2022</b> , 133776	0
610	Divergent evolution of extreme production of variant plant monounsaturated fatty acids. <b>2022</b> , 119,	0
609	In silico analysis of a Skp1 protein homolog from the human pathogen <i>E. histolytica</i> .	
608	Design and evaluation of pyrimidine derivatives as potent inhibitors of ABCG2, a breast cancer resistance protein. <b>2022</b> , 12,	1
607	Pharmacophore-based virtual screening, molecular docking and molecular dynamics simulations study for the identification of LIM kinase-1 inhibitors. 1-15	1

- 606 Robust Construction of Voronoi Diagrams of Spherical Balls in Three-Dimensional Space. **2022**, 103374 ○
- 605 Data collection from crystals grown in microfluidic droplets. **2022**, 78, ○
- 604 Vaccinomics strategy to design an epitope peptide vaccine against *Helicobacter pylori*. **2022**, 121, 380-395 ○
- 603 Mechanism of polyhydroxy alcohol-mediated curing on moisture migration of minced pork tenderloin: On the basis of molecular docking. **2022**, 15, 100401 1
- 602 Structural, functional, and molecular docking analyses of microbial cutinase enzymes against polyurethane monomers. **2022**, 3, 100063 1
- 601 Impact of Sucralose on Environmental Bacteria: Mechanistic Insights from Molecular Modeling. **2022**, 358-368
- 600 Synoeca-MP: New insights into its mechanism of action by using NMR and molecular dynamics simulations approach.
- 599 Human TMPRSS2 non-catalytic ectodomain and SARS-CoV-2 S2' subunit interaction mediated SARS-CoV-2 endocytosis: a model proposal with virtual screening for potential drug molecules to inhibit this interaction. 1-12
- 598 Computational insights on molecular interactions of acifran with GPR109A and GPR109B. **2022**, 28, ○
- 597 Structural assembly of the nucleic-acid-binding Thp3Csn12Bem1 complex functioning in mRNA splicing. **2022**, 50, 8882-8897 1
- 596 Imidazole and nitroimidazole derivatives as NADH -fumarate reductase inhibitors: Density functional theory studies, homology modeling, and molecular docking. **2022**, 43, 1573-1595 ○
- 595 Design of Multi-Epitope Vaccine for *Staphylococcus saprophyticus*: Pan-Genome and Reverse Vaccinology Approach. **2022**, 10, 1192 ○
- 594 Is the Glycoprotein Responsible for the Differences in Dispersal Rates between Lettuce Necrotic Yellows Virus Subgroups?. **2022**, 14, 1574
- 593 In silico analysis of enzymes involved in mycosporine-like amino acids biosynthesis in *Euhalothece* sp.: Structural and functional characterization. **2022**, 66, 102806 2
- 592 Designing a Humanized Immunotoxin Based on HER2 Specific scFv and DFF40 Toxin Against Breast Cancer: An In-Silico Study. **2022**, 28,
- 591 Structure based virtual screening and molecular dynamics of natural anti-biofilm compounds against SagS response regulator/sensor kinase in *Pseudomonas aeruginosa*. 1-16 ○
- 590 Anti-apoptotic Bcl-2 protein in apo and holo conformation anchored to the membrane: comparative molecular dynamics simulations. 1-15
- 589 Novel Scaffolds for Modulation of NOD2 Identified by Pharmacophore-Based Virtual Screening. **2022**, 12, 1054 1

588 Modulation of KV4.3-KCHIP2 Channels by IQM-266: Role of DPP6 and KCNE2. **2022**, 23, 9170

587 Structure-based in silico design and in vitro acaricidal activity assessment of Acacia nilotica and Psidium guajava extracts against Sarcoptes scabiei var. cuniculi. 1

586 Using deep learning predictions of inter-residue distances for model validation.

585 Exploring whole proteome to contrive multi-epitope-based vaccine for NeoCoV: An immunoinformatics and in-silico approach. 13, 0

584 Structural and functional insights into the candidate genes associated with different developmental stages of flag leaf in bread wheat (*Triticum aestivum* L.). 13, 0

583 Structural Characterization of Human Heat Shock Protein 90 N-Terminal Domain and Its Variants K112R and K112A in Complex with a Potent 1,2,3-Triazole-Based Inhibitor. **2022**, 23, 9458

582 Homology Modeling and Analysis of Vacuolar Aspartyl Protease from a Novel Yeast Expression Host *Meyerozyma guilliermondii* Strain SO.

581 A key residue of plant ABC transporter modulates access path geometry and phenylpropanoid substrate selectivity.

580 Insight into the structural basis of the dual inhibitory mode of Lima bean (*Phaseolus lunatus*) serine protease inhibitor.

579 Computational Biology of BRCA2 in Male Breast Cancer, through Prediction of Probable nsSNPs, and Hit Identification. 0

578 A processive GH9 family endoglucanase of *Bacillus licheniformis* and the role of its carbohydrate-binding domain. 0

577 Immunoinformatics-Aided Analysis of RSV Fusion and Attachment Glycoproteins to Design a Potent Multi-Epitope Vaccine. **2022**, 10, 1381 0

576 A C2 domain containing plasma membrane protein of *Plasmodium falciparum* merozoites mediates calcium-dependent binding and invasion to host erythrocytes. **2022**, 0

575 Melianone inhibits Secreted Aspartic Proteases (SAP), a virulence factor during hyphal formation in *Candida albicans*.. **2022**, 18,

574 Inhibition of mutationally activated HER2.

573 Dynamic study of small toxic hydrophobic proteins PepA1 and PepG1 of *Staphylococcus aureus*. **2022**, 0

572 Engineering an autonomous VH domain to modulate intracellular pathways and to interrogate the eIF4F complex. **2022**, 13, 1

571 A novel homozygous missense substitution p.Thr313Ile in the PDE6B gene underlies autosomal recessive retinitis pigmentosa in a consanguineous Pakistani family.

- 570 Protein engineering of carbonyl reductases for asymmetric synthesis of ticagrelor precursor (1S)-2-chloro-1-(3,4-difluorophenyl)ethanol. **2022**, 108600
- 569 In silico analysis of the C-terminal domain of big defensin from the Pacific oyster. 1-13
- 568 In silico structural homology modeling and functional characterization of Mycoplasma gallisepticum variable lipoprotein hemagglutinin proteins. 9,
- 567 Crystal structures of Schistosoma mansoni histone deacetylase 8 reveal a novel binding site for allosteric inhibitors.. **2022**, 102375 ○
- 566 Structural analysis unravels the functional promiscuity of Quinolone synthase-mediated polyketide biosynthesis in Aegle marmelos Correa.
- 565 Identification of key interactions of benzimidazole resistance-associated amino acid mutations in Ascaris ßubulins by molecular docking simulations. **2022**, 12,
- 564 Docking and molecular dynamics studies of human ezrin protein with a modelled SARS-CoV-2 endodomain and their interaction with potential invasion inhibitors. **2022**, 102277
- 563 A novel causative functional mutation in GATA6 gene is responsible for familial dilated cardiomyopathy as supported by in silico functional analysis. **2022**, 12,
- 562 Investigating the functional role of a buried interchain aromatic cluster in Escherichia coli GrpE dimer.
- 561 Development of a new chemo-enzymatic catalytic route for synthesis of (S)-2-chlorophenylglycine. **2022**,
- 560 Engineering an ß-rhamnosidase from Aspergillus niger for efficient conversion of rutin substrate. **2022**, 186, 108572 ○
- 559 Dynamic recognition of naloxone, morphine and endomorphin1 in the same pocket of ß-opioid receptors. 9, 1
- 558 Modeling of MT. P495, an mRNA-based vaccine against the phosphate-binding protein PstS1 of Mycobacterium tuberculosis.
- 557 In Silico Interactions of the Components from the Schinus terebinthifolius Extract with Human Tyrosinase. **2022**, 87, ○
- 556 Subtractive genomics profiling for potential drug targets identification against Moraxella catarrhalis. **2022**, 17, e0273252 ○
- 555 Genetic characterization of the visual pigments of the red-eared turtle (Trachemys scripta elegans) and computational predictions of the spectral sensitivity. **2022**, 100141 ○
- 554 Ab initio modelling of an essential mammalian protein: Transcription Termination Factor 1 (TTF1). 1-10 1
- 553 Von Hippel- Lindau (VHL) disease and VHL-associated tumors in Indian subjects: VHL gene testing in a resource constraint setting. **2022**, 23,

552	The Flexible, Extended Coil of the PDZ-Binding Motif of the Three Deadly Human Coronavirus E Proteins Plays a Role in Pathogenicity. <b>2022</b> , 14, 1707	
551	Analgesic Conotoxin Binding Site on the Human GABAB Receptor. MOLPHARM-AR-2022-000543	0
550	Novel Labdane Diterpenes-Based Synthetic Derivatives: Identification of a Bifunctional Vasodilator That Inhibits CaV1.2 and Stimulates KCa1.1 Channels. <b>2022</b> , 20, 515	1
549	Pharmacological and In Silico Analysis of Oat Avenanthramides as EGFR Inhibitors: Effects on EGF-Induced Lung Cancer Cell Growth and Migration. <b>2022</b> , 23, 8534	2
548	Plant catalase in silico characterization and phylogenetic analysis with structural modeling. <b>2022</b> , 20,	
547	Therapeutic capability of selected medicinal plants' bioactive constituents against the mutant ovarian TP53 gene; A computational approach..	
546	CoVM2: Molecular Biological Data Integration of SARS-CoV-2 Proteins in a Macro-to-Micro Method. <b>2022</b> , 12, 1067	
545	Drug Repurposing Based on Protozoan Proteome: In Vitro Evaluation of In Silico Screened Compounds against <i>Toxoplasma gondii</i> . <b>2022</b> , 14, 1634	0
544	Immunoinformatics-guided designing of epitope-based subunit vaccine from Pilus assembly protein of <i>Acinetobacter baumannii</i> bacteria. <b>2022</b> , 508, 113325	5
543	The drp-1-mediated mitochondrial fission inhibitor mdivi-1 impacts the function of ion channels and pathways underpinning vascular smooth muscle tone. <b>2022</b> , 203, 115205	
542	Most frequently harboured missense variants of hACE2 across different populations exhibit varying patterns of binding interaction with spike glycoproteins of emerging SARS-CoV-2 of different lineages. <b>2022</b> , 148, 105903	
541	Insight into glucocorticoids glucosylation by glucosyltransferase: A combined experimental and in-silico approach. <b>2022</b> , 289, 106875	
540	Biosynthesis and characterization of <i>Serratia marcescens</i> derived silver nanoparticles: Investigating its antibacterial, anti-biofilm potency and molecular docking analysis with biofilm-associated proteins. <b>2022</b> , 365, 120094	0
539	Computational study of the conformational ensemble of CX3C chemokine receptor 1 (CX3CR1) and its interactions with antagonist and agonist ligands. <b>2022</b> , 117, 108278	
538	ATP-site inhibitors induce unique conformations of the acute myeloid leukemia-associated Src-family kinase, Fgr. <b>2022</b> ,	0
537	Structural and Functional Annotation and Molecular Docking Analysis of a Hypothetical Protein from <i>Neisseria gonorrhoeae</i> : An In-Silico Approach. <b>2022</b> , 2022, 1-12	2
536	Bioinformatics analysis of Muscovy duck parvovirus REP and VP1 proteins. 1-16	0
535	Novel tricyclic small molecule inhibitors of Nicotinamide N-methyltransferase for the treatment of metabolic disorders. <b>2022</b> , 12,	1



534	In-silico designing of a multi-epitope vaccine against SARS-CoV2 and studying the interaction of the vaccine with Alpha, Beta, Delta, and Omicron variants of concern. <b>2022</b> , 19,	0
533	Integrating in silico and in vivo approach for investigating the role of polyherbal oil in prevention and treatment of COVID-19 infection. <b>2022</b> , 367, 110179	1
532	Novel bi-functional thermostable chimeric enzyme for feasible xylo-oligosaccharides production from agro-industrial wastes. <b>2022</b> , 122, 331-340	0
531	Bioinformatics pipeline unveils genetic variability to synthetic vaccine design for Indian SARS-CoV-2 genomes. <b>2022</b> , 112, 109224	0
530	A subtractive proteomics and immunoinformatics approach towards designing a potential multi-epitope vaccine against pathogenic <i>Listeria monocytogenes</i> . <b>2022</b> , 172, 105782	2
529	MlaC belongs to a unique class of non-canonical substrate-binding proteins and follows a novel phospholipid-binding mechanism. <b>2022</b> , 214, 107896	0
528	Benchmark dataset for the Voronoi diagram of 3D spherical balls. <b>2022</b> , 45, 108605	0
527	PIPs from <i>Fragaria vesca</i> : A structural analysis of native and mutated protein. <b>2022</b> , 117, 108310	0
526	Comparative analyses of <i>Theobroma cacao</i> and <i>T. grandiflorum</i> mitogenomes reveal conserved gene content embedded within complex and plastic structures. <b>2023</b> , 849, 146904	0
525	Structural and functional insights into the glycoside hydrolase family 30 xylanase of the rumen bacterium <i>Ruminococcus flavefaciens</i> . <b>2023</b> , 1272, 134155	0
524	Fragment-based design of $\beta$ -cyanoacrylates and $\beta$ -cyanoacrylamides targeting Dengue and Zika NS2B/NS3 proteases.	1
523	Molecular Interactions Associated with Coagulation of Organic Pollutants by 2S Albumin of Plant Proteins: A Computational Approach.	0
522	HGDiscovery: An online tool providing functional and phenotypic information on novel variants of homogentisate 1,2- dioxigenase. <b>2022</b> , 4, 271-277	0
521	Analysis of a novel class A $\beta$ -lactamase OKP-B-6 of <i>Klebsiella quasipneumoniae</i> : structural characterisation and interaction with commercially available drugs. 117,	0
520	Screening of Pathogenic Missense Single Nucleotide Variants From LHPP Gene Associated With the Hepatocellular Carcinoma: An In silico Approach. <b>2022</b> , 16, 117793222211155	0
519	Identification of 4-acrylamido-N-(pyridazin-3-yl)benzamide as anti-COVID-19 compound: a DFTB, molecular docking, and molecular dynamics study. <b>2022</b> , 12, 24178-24186	0
518	Biochemical, structural, and computational studies of a $\beta$ -carbonic anhydrase from the pathogenic bacterium <i>Burkholderia pseudomallei</i> . <b>2022</b> , 20, 4185-4194	2
517	Prediction and validation of host-pathogen interactions by a versatile inference approach using <i>Aspergillus fumigatus</i> as a case study. <b>2022</b> , 20, 4225-4237	0

516	Zymography assisted quick purification, characterization and inhibition analysis of <i>K. pneumoniae</i> alkaline phosphatase by mercury and thiohydroxal compounds. <b>2023</b> , 201, 106185	0
515	In-depth analysis of the interactions of various aryl hydrocarbon receptor ligands from a computational perspective. <b>2023</b> , 118, 108339	0
514	In silico prediction of the animal susceptibility and virtual screening of natural compounds against SARS-CoV-2: Molecular dynamics simulation based analysis. 13,	0
513	Homology modeling of human BAP1 and analysis of its binding properties through molecular docking and molecular dynamics simulation. 1-16	0
512	Identification of long-chain alkane-degrading (LadA) monooxygenases in <i>Aspergillus flavus</i> via in silico analysis. 13,	0
511	In silico identification of potential drug-like molecules against G glycoprotein of Nipah virus by molecular docking, DFT studies, and molecular dynamic simulation. 1-15	0
510	Structural study of the uPA-nafamostat complex reveals a covalent inhibitory mechanism of nafamostat. <b>2022</b> ,	0
509	Phenolic Profile, Antioxidant and Enzyme Inhibitory Activities of Leaves from Two Cassia and Two Senna Species. <b>2022</b> , 27, 5590	4
508	Structural basis of lipoprotein recognition by the bacterial Lol trafficking chaperone LolA. <b>2022</b> , 119,	2
507	Structure of the hypothetical protein TTHA1873 from <i>Thermus thermophilus</i> . <b>2022</b> , 78, 338-346	0
506	Biocomputational characterisation of MBO_200107 protein of <i>Mycobacterium tuberculosis</i> variant caprae: a molecular docking and simulation study. 1-20	0
505	Deciphering the mechanisms of zinc tolerance in the cyanobacterium <i>Anabaena sphaerica</i> and its zinc bioremediation potential.	0
504	In silico designing of a novel epitope-based candidate vaccine against <i>Streptococcus pneumoniae</i> with introduction of a new domain of PepO as adjuvant. <b>2022</b> , 20,	0
503	Immunoinformatics Studies and Design of a Potential Multi-Epitope Peptide Vaccine to Combat the Fatal Visceral Leishmaniasis. <b>2022</b> , 10, 1598	2
502	In Vitro Antimicrobial Screening of Benzoylthioureas: Synthesis, Antibacterial Activity toward <i>Streptococcus agalactiae</i> and Molecular Docking Study. <b>2022</b> , 7,	0
501	In silico study on the Hepatitis E virus RNA Helicase and its inhibition by silvestrol, rocaglamide and other flavagline compounds. <b>2022</b> , 12,	0
500	Genome mining of <i>Fusarium</i> reveals structural and functional diversity of pectin lyases: a bioinformatics approach. <b>2022</b> , 12,	0
499	Structural changes and adaptative evolutionary constraints in FLOWERING LOCUS T and TERMINAL FLOWER1-like genes of flowering plants. 13,	0

498	Comprehensive Molecular Interaction Studies to Construe the Repellent/Kill Activity of Geraniol During Binding Event Against <i>Aedes aegypti</i> Proteins.	1
497	Solvation Effects, Reactivity Studies and Molecular Dynamics of Two Phosphonic Acids □ Theoretical Investigation. 1-15	0
496	Promotion of Bladder Cancer Cell Metastasis by 2-Mercaptobenzothiazole via Its Activation of Aryl Hydrocarbon Receptor Transcription: Molecular Dynamics Simulations, Cell-Based Assays, and Machine Learning-Driven Prediction. <b>2022</b> , 56, 13254-13263	1
495	Novel multi epitope-based vaccine against monkeypox virus: vaccinomic approach. <b>2022</b> , 12,	3
494	Identification of Potential IgE-Binding Epitopes Contributing to the Cross-Reactivity of the Major Cupressaceae Pectate-Lyase Pollen Allergens (Group 1). <b>2022</b> , 2, 106-118	0
493	Chaperonin activity of Plasmodium prefoldin complex is essential to guard proteotoxic stress response and presents a new target for drug discovery.	0
492	Drug repurposing and sequence analysis in S-glycoprotein variants reveals critical signature patterns and destabilization of receptor-binding domain in omicron variant. 1-18	0
491	Bioinformatic-based approach for mutagenesis of plant immune Tm-22 receptor to confer resistance against tomato brown rugose fruit virus (ToBRFV). 13,	0
490	Combined Structural Analysis and Molecular Dynamics Reveal Penicillin-Binding Protein Inhibition Mode with $\beta$ -Lactones.	1
489	Gain of function studies on predicted host receptors for white spot virus. <b>2022</b> ,	0
488	<i>Giardia duodenalis</i> : Flavohemoglobin is involved in drug biotransformation and resistance to albendazole. <b>2022</b> , 18, e1010840	0
487	Molecular basis for thermal stability and affinity in a VHH : contribution of the framework region and its influence in the conformation of the CDR3.	0
486	A multidisciplinary approach disclosing unexplored Aflatoxin B1 roles in severe impairment of vitamin D mechanisms of action.	0
485	ADRA2B and HTR1A: An updated study of the biogenic amine receptors reveals novel conserved motifs which play key role in Mental Disorders.	0
484	Comprehensive analysis predicting effects of deleterious SNPs of human progesterone receptor gene on its structure and functions: a computational approach. 1-16	0
483	Unique Structural Fold of LonBA Protease from <i>Bacillus subtilis</i> , a Member of a Newly Identified Subfamily of Lon Proteases. <b>2022</b> , 23, 11425	0
482	In-silico comparative modeling and interaction studies of PRSV proteins - Accelerated towards dissection of structure based evolutionary divergence and functional interaction of virus within the host.	0
481	In silico and In vitro Analysis of <i>Nigella sativa</i> Bioactives Against Chorismate Synthase of <i>Listeria monocytogenes</i> : a Target Protein for Biofilm Inhibition.	0

- 480 Molecular insight into *Aspergillus oryzae*  $\beta$ -mannanase interacting with mannotriose revealed by molecular dynamic simulation study. **2022**, 17, e0268333 ○
- 479 Synthesis, biological evaluation and molecular modeling studies of novel 1,2,3-triazole-linked menadione-furan derivatives as P2X7 inhibitors. ○
- 478 Mechanism of enhanced sensitivity of mutated  $\beta$ -adrenergic-like octopamine receptor to amitraz in honeybee *Apis mellifera* : An insight from MD simulations. ○
- 477 Lumateperone Interact with S-Protein of Ebola Virus and TIM-1 of Human Cell Membrane: Insights from Computational Studies. **2022**, 12, 8820 ○
- 476 Computational insights into diverse aspects of glutathione S-transferase gene family in *Papaver somniferum*. ○
- 475 Characterization of B-box family genes and their expression profiles under abiotic stresses in the *Melilotus albus*. 13, ○
- 474 Design, Synthesis, and Herbicidal Activity of Naphthalimide $\beta$ -royl Hybrids as Potent Transketolase Inhibitors. 2 ○
- 473 The evolutionary advantage of an aromatic clamp in plant family 3 glycoside exo-hydrolases. **2022**, 13, ○
- 472 Structural and functional characterization of Cas2 of CRISPR-Cas subtype I-C lacking the CRISPR component. 9, ○
- 471 Group housing enhances mating and increases the sensitization of chemical cues in *Bactrocera dorsalis*. ○
- 470 Structural heterogeneity and precision of implications drawn from cryo-electron microscopy structures: SARS-CoV-2 spike-protein mutations as a test case. ○
- 469 A genetically encoded BRET-based SARS-CoV-2 Mpro protease activity sensor. **2022**, 5, ○
- 468 Bioinformatic analysis of SIRT7 sequence and structure. 1-11 ○
- 467 Discovery and Development of First-in-Class ACKR3/CXCR7 Superagonists for Platelet Degranulation Modulation. ○
- 466 Analysis of glutathione-S-transferases from larvae of *Galleria mellonella* (Lepidoptera, Pyralidae) with potential alkaloid detoxification function. 13, ○
- 465 Copper(II) iodide complex with 4-Pyridinecarboxaldehyde ligand: Synthesis, spectroscopic characterisation, AIM and NCI analysis combined with molecular docking and antibacterial activity studies. **2022**, 134279 ○
- 464 A single exon-encoded *Theileria parva* strain Muguga cysteine protease (ThpCP): Molecular modelling and characterisation. **2022**, ○
- 463 Microbial volatile organic compounds 2-heptanol and acetoin control *Fusarium crown and root rot* of tomato. ○

- 462 *Toxoplasma gondii* importin B shows weak auto-inhibition. 0
- 461 Crystal structure of a Burkholderia peptidase and modification of the substrate-binding site for enhanced hydrolytic activity toward gluten-derived pro-immunogenic peptides. **2022**, 0
- 460 Functional characterization of a DNA-dependent AAA ATPase in a F-cluster mycobacteriophage. **2022**, 198957 0
- 459 Identification of resistance gene analogs of the NBS-LRR family through transcriptome probing and in silico prediction of the expressome of *Dalbergia sissoo* under dieback disease stress. 13, 1
- 458 Identification of natural small molecule modulators of MurB from *Salmonella Enterica* Serovar Typhi Ty2 strain using computational and biophysical approaches. 0
- 457 Immunoinformatic Design of a Putative Multi-Epitope Vaccine Candidate Against *Trypanosoma brucei gambiense*. **2022**, 1
- 456 Molecular Dynamic Simulation of Neurexin1 Mutations Associated with Mental Disorder. 0
- 455 Loss-of-function of triacylglycerol lipases are associated with low flour rancidity in pearl millet [*Pennisetum glaucum* (L.) R. Br.]. 13, 0
- 454 Evaluating the role of trypsin in silk degumming: An in silico approach. **2022**, 359, 35-47 1
- 453 Bioinformatic Characterization of a Kappa-Carrageenase from *Pseudomonas fluorescens*. **2022**, 6, 33-39 0
- 452 In silico investigation of the role of vitamins in cancer therapy through inhibition of MCM7 oncoprotein. **2022**, 12, 31004-31015 0
- 451 Engineering of a Baeyer-Villiger Monooxygenase reveals key residues for asymmetric oxidation of omeprazole sulfide. 0
- 450 Efficient Synthesis of Fluorinated Derivatives from Isolated 24-Ethyl cholest-5-en-3 $\beta$ l: Characterization, Quantum Chemical Calculations by DFT and Molecular Docking. **2022**, 34, 2947-2954 0
- 449 In vivo developmental studies of *Helicoverpa armigera* and in silico molecular interactions with trypsin reveal the bio-insecticidal potential of trypsin inhibitor (SSTI) isolated from *Solanum surattense*. **2022**, 0
- 448 Does Generic Cyclic Kinase Insert Domain of Receptor Tyrosine Kinase KIT Clone Its Native Homologue?. **2022**, 23, 12898 0
- 447 Crystal structure of an L-type lectin domain from archaea. 0
- 446 Insights into molecular docking and dynamics to reveal therapeutic potential of natural compounds against P53 protein. 1-20 1
- 445 Phylogenomic analysis of 20S proteasome gene family reveals stress-responsive patterns in rapeseed (*Brassica napus* L.). 13, 0

- 444 Molecular modeling, molecular dynamics simulation, and essential dynamics analysis of grancalcin: An upregulated biomarker in experimental autoimmune encephalomyelitis mice. **2022**, 8, e11232 ○
- 443 Designing of Peptide Based Multi-Epitope Vaccine Construct against Gallbladder Cancer Using Immunoinformatics and Computational Approaches. **2022**, 10, 1850 ○
- 442 Predicted Structure and Functions of the Prototypic Alphaherpesvirus Herpes Simplex Virus Type-1 UL37 Tegument Protein. **2022**, 14, 2189 1
- 441 Exploring the Factors which Result in Cytochrome P450 Catalyzed Desaturation Versus Hydroxylation. ○
- 440 Pharmacophore Modeling Using Machine Learning for Screening the BloodBrain Barrier Permeation of Xenobiotics. **2022**, 19, 13471 ○
- 439 Structural analysis of PpSP15 and PsSP9 sand fly salivary proteins designed with a self-cleavable linker as a live vaccine candidate against cutaneous leishmaniasis. **2022**, 15, ○
- 438 Cloning and characterization of *Aedes aegypti* juvenile hormone epoxide hydrolases (JHEHs). ○
- 437 Uncovering the antimalarial potential of toad venoms through a bioassay-guided fractionation process. **2022**, ○
- 436 Envelope Glycoprotein based multi-epitope vaccine against a co-infection of Human Herpesvirus 5 and Human Herpesvirus 6 using in silico strategies. ○
- 435 The determination of the effect(s) of solute carrier family 22-member 2 (SLC22A2) haplotype variants on drug binding via molecular dynamic simulation systems. **2022**, 12, ○
- 434 Cloning and characterization of AiiA, an acylhomoserine lactonase from *Bacillus cereus* RC1 to control soft rot causing pathogen *Lelliottia amnigena* RCE. **2022**, 204, ○
- 433 SARS-CoV-2 Variants Show a Gradual Declining Pathogenicity and Pro-Inflammatory Cytokine Stimulation, an Increasing Antigenic and Anti-Inflammatory Cytokine Induction, and Rising Structural Protein Instability: A Minimal Number Genome-Based Approach. 1
- 432 In Silico Structural Analysis of Serine Carboxypeptidase Nf314, a Potential Drug Target in *Naegleria fowleri* Infections. **2022**, 23, 12203 ○
- 431 Immunoinformatics-Based Identification of B and T Cell Epitopes in RNA-Dependent RNA Polymerase of SARS-CoV-2. **2022**, 10, 1660 1
- 430 Computational identification and experimental validation of anti-filarial lead molecules targeting metal binding/substrate channel residues of Cu/Zn SOD1 from *Wuchereria bancrofti*. 1-14 ○
- 429 In Silico Analysis on the Interaction of Haloacid Dehalogenase from *Bacillus cereus* IndB1 with 2-Chloroalkanoic Acid Substrates. **2022**, 2022, 1-9 ○
- 428 Computational Modeling of Virally-encoded Ion Channel Structure. ○
- 427 Computational analysis revealed Triamcinolone acetonide produced by *Bacillus velezensis* YEBBR6 as having antagonistic activity against *Fusarium oxysporum* f. sp. *cubense*. ○

426	Designing a novel SOX9 based multi-epitope vaccine to combat metastatic triple-negative breast cancer using immunoinformatics approach.	1
425	Structural studies of the phosphoribosyltransferase involved in cobamide biosynthesis in methanogenic archaea and cyanobacteria. <b>2022</b> , 12,	0
424	Molecular interactions of PCSK9 with an inhibitory nanobody, CAP1 and HLA-C: functional regulation of LDLR levels.	0
423	Structure and Dynamics of Human Chemokine CCL16Implications for Biological Activity. <b>2022</b> , 12, 1588	0
422	A novel allosteric site employs a conserved inhibition mechanism in human kidney-type glutaminase.	0
421	Identification and molecular modeling of novel endogenous activator proteins of Sirt-1: an in silico study. 1-16	0
420	Functional Characterization and Synthetic Application of Is2-SDR, a Novel Thermostable and Promiscuous Ketoreductase from a Hot Spring Metagenome. <b>2022</b> , 23, 12153	0
419	Huangqi Guizhi Wuwu decoction in peripheral neurotoxicity treatment using network pharmacology and molecular docking. <b>2022</b> , 101, e31281	0
418	An in silico analysis of rpoB mutations to affect Chlamydia trachomatis sensitivity to rifamycin. <b>2022</b> , 20,	0
417	Influence of C107R mutation from hepatitis B virus genotype H on in vitro hepatitis B surface antigen detection and IFN- $\alpha$ treatment.	0
416	Engineering of Microbial Substrate Promiscuous CYP105A5 for Improving the Flavonoid Hydroxylation. <b>2022</b> , 12, 1157	0
415	Phenotype-based drug screening: An in vivo strategy to classify and identify the chemical compounds modulating zebrafish M-cell regeneration. 9,	0
414	Design of a Chimeric Multi-Epitope Vaccine (CMEV) against Both Leishmania martiniquensis and Leishmania orientalis Parasites Using Immunoinformatic Approaches. <b>2022</b> , 11, 1460	0
413	Dimerization of the C-type lectin-like receptor CD93 promotes its binding to Multimerin-2 in endothelial cells. <b>2022</b> ,	0
412	Identification and functional annotation of hypothetical protein from the core genome of Orientia tsutsugamushi towards designing a novel drug target.	0
411	Comparative homology of Pleurotus ostreatus laccase enzyme: Swiss model or Modeller?. 1-14	0
410	PDBsum 1 : a standalone program for generating PDBsum analyses.	0
409	Designing an Epitope-Based Peptide Vaccine Derived from RNA-Dependent RNA Polymerase (RdRp) against Dengue Virus Serotype 2. <b>2022</b> , 10, 1734	0

408	Computationally Guided Enzymatic Studies on Schizochytrium-Sourced Malonyl-CoA:ACP Transacylase. <b>2022</b> , 70, 13922-13934	2
407	Designing, characterization, and immune stimulation of a novel multi-epitopic peptide-based potential vaccine candidate against monkeypox virus through screening its whole genome encoded proteins: An immunoinformatics approach. <b>2022</b> , 50, 102481	1
406	Emulation of the structure of the Saposin protein fold by a lung surfactant peptide construct of surfactant Protein B. <b>2022</b> , 17, e0276787	0
405	BACTERIAL NADQ (COG4111) IS A NUDIX-LIKE, ATP-RESPONSIVE REGULATOR OF NAD BIOSYNTHESIS. <b>2022</b> , 107917	0
404	GLB-3: A resilient, cysteine-rich, membrane-tethered globin expressed in the reproductive and nervous system of <i>Caenorhabditis elegans</i> . <b>2022</b> , 112063	0
403	Integrated Bioinformatics-Based Subtractive Genomics Approach to Decipher the Therapeutic Drug Target and Its Possible Intervention against Brucellosis. <b>2022</b> , 9, 633	1
402	AmyJ33, a truncated amylase with improved catalytic properties.	0
401	Immuno-informatics profiling of monkeypox virus cell surface binding protein for designing a next generation multi-valent peptide-based vaccine. 13,	2
400	Engineering Human Neuroglobin into a Cytochrome c -Like Protein with a Single Thioether Bond in Non-native State.	0
399	A multilayer dynamic perturbation analysis method for predicting ligand-protein interactions. <b>2022</b> , 23,	0
398	Anonaine from <i>Annona crassiflora</i> inhibits glutathione S-transferase and improves cypermethrin activity on <i>Rhipicephalus (Boophilus) microplus</i> (Canestrini, 1887). <b>2022</b> , 243, 108398	0
397	Theoretical evaluation of the malathion and its chemical derivatives interaction with cytosolic phospholipase A2 from zebrafish. <b>2023</b> , 311, 136984	0
396	Unveiling the potential of <i>Lichtheimia ramosa</i> AJP11 for myco-transformation of polystyrene sulfonate and its driving molecular mechanism. <b>2023</b> , 325, 116579	0
395	In silico assessment of missense point mutations on human cathelicidin LL-37. <b>2023</b> , 118, 108368	0
394	In silico design of fusion keratinocyte growth factor containing collagen-binding domain for tissue engineering application. <b>2023</b> , 118, 108351	1
393	Isolation and Computational Characterization of Glutathione Peroxidase Gene from an Aquatic Fern - <i>Salvinia molesta</i> .	0
392	Abyssomicin W and Neoabyssomicin B are potential inhibitors of New Delhi Metallo-β-Lactamase-1 (NDM -1): A computational approach. <b>2022</b> , 0	0
391	Subtractive proteomic analysis for identification of potential drug targets and vaccine candidates against <i>Burkholderia pseudomallei</i> K96243. <b>2022</b> , 35, 101127	0



390	Identification and in-vitro analysis of potential proteasome inhibitors targeting PSM $\beta$ for multiple myeloma. <b>2023</b> , 157, 113963	0
389	Further studies on nicotianamine aminotransferase (NAAT) genes involved in biofortification in bread wheat ( <i>Triticum aestivum</i> L.). <b>2023</b> , 33, 100389	0
388	In silico characterization, molecular docking, and dynamic simulation of a novel fungal cell-death suppressing effector, MoRlpA as potential cathepsin B-like cysteine protease inhibitor during rice blast infection. 1-18	0
387	Identification of potential candidate vaccines against <i>Mycobacterium ulcerans</i> based on the major facilitator superfamily transporter protein. 13,	0
386	Structural insight into the activation of an <i>Arabidopsis</i> organellar C-to-U RNA editing enzyme by active site complementation.	0
385	In silico investigation of organometallic complexes for identification of RNase A inhibitor. <b>2022</b> , 122556	0
384	Mutational analysis of phospholipase C epsilon 1 gene in Egyptian children with steroid-resistant nephrotic syndrome. <b>2022</b> , 23,	0
383	Crystal Structure of <i>Schizosaccharomyces pombe</i> Rho1 Reveals Its Evolutionary Relationship with Other Rho GTPases. <b>2022</b> , 11, 1627	0
382	Screening and Identification of Natural Product-Like Compounds as Potential Antibacterial Agents Targeting FemC of <i>Staphylococcus aureus</i> : An in-Silico Approach. <b>2022</b> , 7,	2
381	Peptides for Coating TiO <sub>2</sub> Implants: An In Silico Approach. <b>2022</b> , 23, 14048	0
380	Targeting <i>Acanthamoeba</i> proteins interaction with flavonoids of Propolis extract by in vitro and in silico studies for promising therapeutic effects. 11, 1274	0
379	Investigation of the Enzymes Required for the Biosynthesis of 2,3-Diacetamido-2,3-dideoxy-d-glucuronic acid in <i>Psychrobacter cryohalolentis</i> K5 T.	0
378	Common recognition topology of mex transporters of <i>Pseudomonas aeruginosa</i> revealed by molecular modelling. 13,	1
377	Identification and characterization of RuvBL DNA helicase genes for tolerance against abiotic stresses in bread wheat ( <i>Triticum aestivum</i> L.).	0
376	Proteome-Based Investigation Identified Potential Drug Repurposable Small Molecules Against Monkeypox Disease.	1
375	Pose, duplicate, then elaborate: Steps towards increased affinity for inhibitors targeting the specificity surface of the Pim-1 kinase. <b>2022</b> , 114914	0
374	Mce1R of <i>Mycobacterium tuberculosis</i> prefers long-chain fatty acids as specific ligands: a computational study.	0
373	Comparison and Functional Analysis of Odorant-Binding Proteins and Chemosensory Proteins in Two Closely Related Thrips Species, <i>Frankliniella occidentalis</i> and <i>Frankliniella intonsa</i> (Thysanoptera: Thripidae) Based on Antennal Transcriptome Analysis. <b>2022</b> , 23, 13900	0

372	Computational prediction of B and T-cell epitopes of Kyasanur Forest Disease virus marker proteins towards the development of precise diagnosis and potent subunit vaccine. 1-20	0
371	Structural and evolutionary insights into the multidomain galectin from the red abalone <i>Haliotis rufescens</i> with specificity for sulfated glycans. <b>2022</b> ,	0
370	Immunoprophylactic properties of the <i>Corynebacterium pseudotuberculosis</i> -derived MBP:PLD:CP40 fusion protein.	1
369	Structural basis for ubiquitylation by HOIL-1.	0
368	A novel hybrid biocatalyst from immobilized Eversa <sup>®</sup> Transform 2.0 lipase and its application in biolubricant synthesis. 1-22	2
367	Estimation of Drug-Target Residence Time by Targeted Molecular Dynamics Simulations.	0
366	Design of a multi-epitope protein as a subunit vaccine against lumpy skin disease using an immunoinformatics approach. <b>2022</b> , 12,	2
365	Genomic analysis of <i>Paenibacillus</i> sp. MDMC362 from the Merzouga desert leads to the identification of a potentially thermostable catalase.	0
364	Structural Basis for (2R,3R)-Taxifolin Binding and Reaction Products to the Bacterial Chalcone Isomerase of <i>Eubacterium ramulus</i> . <b>2022</b> , 27, 7909	0
363	Orthopalladated N,N-Dimethyl-1-Phenethylamine Compounds Containing 2,6-Lutidine: Synthesis, Dna Binding Studies and Cytotoxicity Evaluation. <b>2022</b> , 116185	0
362	Allosteric Inhibition of Neutral Sphingomyelinase 2 (nSMase2) by DPTIP: From Antiflaviviral Activity to Deciphering Its Binding Site through In Silico Studies and Experimental Validation. <b>2022</b> , 23, 13935	1
361	The protein conformational basis of isoflavone biosynthesis. <b>2022</b> , 5,	0
360	In silico analysis of koranimine, a cyclic imine compound from <i>Peribacillus frigiditolerans</i> reveals potential nematocidal activity. <b>2022</b> , 12,	0
359	Deciphering the role of endophytic microbiome in postharvest diseases management of fruits: Opportunity areas in commercial up-scale production. 13,	0
358	Virtual screening and cheminformatics descriptors uncover insecticidal molecular mechanisms besides plant essential oils' action..	0
357	A novel thioredoxin glutathione reductase from evolutionary ancient metazoan Hydra. <b>2022</b> , 637, 23-31	0
356	Comparative computational study to augment UbiA prenyltransferases inherent in purple photosynthetic bacteria cultured from mangrove microbial mats in Qatar for coenzyme Q10 biosynthesis.. <b>2022</b> , 36, e00775	0
355	Multimodal approach to characterize the tetrameric form of human PML-RBCC domain and ATO-mediated conformational changes. <b>2022</b> , 223, 468-478	0

- 354 Identification of novel inhibitors of high affinity iron permease (FTR1) through implementing pharmacokinetics index to fight against black fungus: An in silico approach. **2022**, 106, 105385 1
- 353 In silico analysis of a novel protein in CAR T- cell therapy for the treatment of hematologic cancer through molecular modelling, docking, and dynamics approach. **2022**, 151, 106285 0
- 352 Designing a humanized immunotoxin based on DELTA-stichotoxin-Hmg2a toxin: an in silico study. **2022**, 28, 0
- 351 Exploiting ELIOT for Scaffold-Repurposing Opportunities: TRIM33 a Possible Novel E3 Ligase to Expand the Toolbox for PROTAC Design. **2022**, 23, 14218 0
- 350 Virtual screening and computational simulation analysis of antimicrobial photodynamic therapy using propolis-benzofuran A to control of Monkeypox. **2022**, 103208 0
- 349 Exploring the mechanism of compromised thermostability of aromatic l-amino acid decarboxylase from *Bacillus atrophaeus* through comparative molecular dynamics simulations. **2023**, 1219, 113972 0
- 348 Molecular evolution and structural analyses of proteins involved in metabolic pathways of volatile organic compounds in *Petunia hybrida* (Solanaceae). **2023**, 46, 0
- 347 Isolation and characterization of glycoprotein (CNP) isolated from *Cocos nucifera* L. nutshell and its immunomodulatory role on macrophage activation. **2023**, 100, 105380 0
- 346 HbADF4, an actin-depolymerizing factor, regulates latex flow by modulating actin dynamics in rubber tree. **2023**, 192, 116111 0
- 345 First evidence of a serine arginine protein kinase (SRPK) in *leishmania braziliensis* and its potential as therapeutic target. **2023**, 238, 106801 0
- 344 One-step production of biodiesel by wet *Escherichia coli* cells expressing a non-specific and methanol-resistant lipase. **2023**, 125, 75-83 0
- 343 Unveiling the membrane bound dihydroorotate: Quinone oxidoreductase from *Staphylococcus aureus*. **2023**, 1864, 148948 0
- 342 Piperidine-based natural products targeting Type IV pili antivirulence: A computational approach. **2023**, 119, 108382 0
- 341 Deletion of the ATP20 gene in *Ustilago maydis* produces an unstable dimer of F1FO-ATP synthase associated with a decrease in mitochondrial ATP synthesis and a high H<sub>2</sub>O<sub>2</sub> production. **2023**, 1864, 148950 0
- 340 Tools for protein structure prediction and for molecular docking applied to enzyme active site analysis: A case study using a BAHD hydroxycinnamoyltransferase. **2022**, 0
- 339 Computational analysis of fusion protein of anti-HER2 scFv and alpha luffin: A new immunotoxin protein for HER2 positive cancers. 58, 0
- 338 Electrostatic Interactions Are the Primary Determinant of the Binding Affinity of SARS-CoV-2 Spike RBD to ACE2: A Computational Case Study of Omicron Variants. **2022**, 23, 14796 1
- 337 Optimization of 1,2,4-Triazole-3-thiones toward Broad-Spectrum Metallo-β-lactamase Inhibitors Showing Potent Synergistic Activity on VIM- and NDM-1-Producing Clinical Isolates. **2022**, 65, 16392-16419 0

- 336 Understanding the in silico aspects of bacterial catabolic cascade for styrene degradation. 0
- 335 Ligand-Based Discovery of a Small Molecule as Inhibitor of  $\beta$ Synuclein Amyloid Formation. **2022**, 23, 14844 1
- 334 Protein Structure Validation Derives a Smart Conformational Search in a Physically Relevant Configurational Subspace. **2022**, 62, 6217-6227 0
- 333 The Scaffold Immunophilin FKBP51 Is a Phosphoprotein That Undergoes Dynamic Mitochondrial-Nuclear Shuttling. **2022**, 11, 3771 0
- 332 Structural Studies of Bypass of Forespore Protein C from Bacillus Subtilis to Reveal Its Inhibitory Molecular Mechanism for SpoIVB. **2022**, 12, 1530 0
- 331 Structural insight to human Retinoid X receptor alpha-Thyroid hormone receptor beta heterodimer by molecular modelling and MD-simulation studies: role of conserved water molecules. 1-12 0
- 330 Using deep-learning predictions of inter-residue distances for model validation. **2022**, 78, 1412-1427 0
- 329 Molecular Cloning, Expression, Sequence Characterization and Structural Insight of Bubalus bubalis Growth Hormone-Receptor. 0
- 328 Bioinsecticidal activity of actinomycete secondary metabolites against the acetylcholinesterase of the legume insect pest Acyrthosiphon pisum: a computational study. **2022**, 20, 0
- 327 Unveiling Attributes of Human 15-Lipoxygenase-1 as a Potential Candidate for Prostate Cancer Drug Development Using in Silico Approaches. 1-13 0
- 326 Genomic landscape of the emerging XDR Salmonella Typhi for mining druggable targets clpP, hisH, folP and gpml and screening of novel TCM inhibitors, molecular docking and simulation analyses. 0
- 325 Characterization of SARS-CoV-2 Isolate (MZ558159) Reported from India for in Silico Drug Designing. **2022**, 8, 175-188 0
- 324 Asn215Ser, Ala143Thr, and Arg112Cys variants in  $\beta$ galactosidase A protein confer stability loss in Fabry disease. 1-10 0
- 323 Finding inhibitor from phytochemicals for novel target Glycosyltransferase family 62 protein in Trichophyton rubrum using insilico study. 0
- 322 Exploration of natural product database for the identification of potent inhibitor against IDH2 mutational variants for glioma therapy. **2023**, 29, 0
- 321 Pathogen-driven gene expression patterns lead to a novel approach to the identification of common therapeutic targets. **2022**, 12, 0
- 320  $\beta$ Amino carbonyl derivatives: Synthesis, Molecular Docking, ADMET, Molecular Dynamic and Herbicidal studies.. **2022**, 7, 3
- 319 Identification, Characterization and Expression Profiling of the RS Gene Family during the Withering Process of White Tea in the Tea Plant (Camellia sinensis) Reveal the Transcriptional Regulation of CsRS8. **2023**, 24, 202 0

- 318 In silico analysis of peroxidase from *Luffa acutangula*. **2023**, 13, ○
- 317 The novel anti-cancer feature of Brazzein through activating of hTLR5 by integration of biological evaluation: molecular docking and molecular dynamics simulation. **2022**, 12, ○
- 316 NlugOBP8 in *Nilaparvata lugens* Involved in the Perception of Two Terpenoid Compounds from Rice Plant. ○
- 315 The laccase of *Myrothecium roridum* VKM F-3565: a new look at the fungal laccase tolerance to neutral alkaline conditions. ○
- 314 In silico analysis of NHP2 membrane protein, a novel vaccine candidate present in the RD7 region of *Mycobacterium tuberculosis*. ○
- 313 Molecular Modeling, Virtual Screening, and Molecular Dynamics for *Leishmania infantum* Methionyl-tRNA Synthetase. ○
- 312 Resolution of Racemic Aryloxy-Propan-2-yl Acetates via Lipase-Catalyzed Hydrolysis: Preparation of Enantiomerically Pure/Enantioenriched Mexiletine Intermediates and Analogs. **2022**, 12, 1566 ○
- 311 Pharmacoinformatic approach to identify potential phytochemicals against SARS-CoV-2 spike receptor-binding domain in native and variants of concern. ○
- 310 The Highly Potent AhR Agonist Picoberin Modulates Hh-Dependent Osteoblast Differentiation. **2022**, 65, 16268-16289 ○
- 309 Cross-Feeding and Enzymatic Catabolism for Mannan-Oligosaccharide Utilization by the Butyrate-Producing Gut Bacterium *Roseburia hominis* A2-183. **2022**, 10, 2496 ○
- 308 Structural and functional mapping of ars gene cluster in *Deinococcus indicus* DR1. **2022**, ○
- 307 Unconventional interactions of the TRPV4 ion channel with beta-adrenergic receptor ligands. **2023**, 6, e202201704 ○
- 306 Cell-Permeable PROTAC Degradors against KEAP1 Efficiently Suppress Hepatic Stellate Cell Activation through the Antioxidant and Anti-Inflammatory Pathway. ○
- 305 Quinolinyln Enaminone derivatives exhibit leishmanicidal activity against *Leishmania donovani* by impairing the mitochondrial electron transport chain complex and inducing ROS-mediated programmed cell death. ○
- 304 Quinoxalinones as A Novel Inhibitor Scaffold for EGFR (L858R/T790M/C797S) Tyrosine Kinase: Molecular Docking, Biological Evaluations, and Computational Insights. **2022**, 27, 8901 ○
- 303 Temperature-Dependent StructureFunction Properties of Bacterial Xylose Isomerase Enzyme for Food Applications: An In Silico Study. **2022**, 4, 1317-1329 ○
- 302 Structure and Dynamics of the Unassembled Nucleoprotein of Rabies Virus in Complex with Its Phosphoprotein Chaperone Module. **2022**, 14, 2813 ○
- 301 Bioactive compounds from *Pandanous fascicularis* as potential therapeutic candidate to tackle hepatitis a inhibition: Docking and molecular dynamics simulation study. 1-17 2

- 300 Global Analysis of Plasmodium falciparum Dihydropteroate Synthase Variants Associated with Sulfadoxine Resistance Reveals Variant Distribution and Mechanisms of Resistance:A Computational-Based Study. **2023**, 28, 145 ○
- 299 IMIDAZONAPHTHYRIDINE EFFECTS ON CHIKUNGUNYA VIRUS REPLICATION: ANTIVIRAL ACTIVITY BY DEPENDENT AND INDEPENDENT OF INTERFERON TYPE 1 PATHWAYS. **2022**, 199029 ○
- 298 Structure elucidation of Staphylococcus capitis lipase. Molecular dynamics simulations to investigate the effects of calcium and zinc ions on the structural stability. 1-13 ○
- 297 Evaluation of Candidatus Liberibacter Asiaticus Efflux Pump Inhibition by Antimicrobial Peptides. **2022**, 27, 8729 ○
- 296 Computational Exploration of Anti-cancer Potential of Flavonoids against Cyclin-Dependent Kinase 8: An In Silico Molecular Docking and Dynamic Approach. 1
- 295 Tissue specific expression of Bacterial cellulose synthase (Bcs) genes improves Cotton fiber length and strength. **2022**, 111576 ○
- 294 In silico identification and characterization of potential druggable targets among hypothetical proteins of Leptospira interrogans serovar Copenhageni: a comprehensive bioinformatics approach. 1-21 ○
- 293 Potential antiviral peptides targeting the SARS-CoV-2 spike protein. **2022**, 23, 1
- 292 Structural Evaluation and Conformational Dynamics of ZNF141T474I Mutation Provoking Postaxial Polydactyly Type A. **2022**, 9, 749 1
- 291 A Biologically Active Chromone from Bomarea setacea ( alstroemeriaceae ): Leishmanicidal, Antioxidant and Multilevel Computational Studies. **2022**, 7, ○
- 290 Insights into the role of the cobalt(III)-thiosemicarbazone complex as a potential inhibitor of the Chikungunya virus nsP4. ○
- 289 In Silico Profiling of Non-Synonymous SNPs of Fat Mass and Obesity- Associated Gene: Possible impacts on the treatment of Non-Alcoholic Fatty Liver Disease. ○
- 288 Bioinformatics Designing and Molecular Modelling of a Universal mRNA Vaccine for SARS-CoV-2 Infection. **2022**, 10, 2107 ○
- 287 Substrate profiling of the metalloproteinase ovastacin [Implications for its physiological function in mammalian fertilization. ○
- 286 Destabilizers of the thymidylate synthase homodimer accelerate its proteasomal degradation and inhibit cancer growth. 11, ○
- 285 Leucine 434 is essential for docosahexaenoic acid-induced augmentation of L-glutamate transporter current. **2022**, 102793 ○
- 284 In silico study reveals unconventional interactions between MDC1 of DDR and Beclin-1 of autophagy. ○
- 283 Potential inhibitors of FemC to combat Staphylococcus aureus: virtual screening, molecular docking, dynamics simulation, and MM-PBSA analysis. 1-12 ○

- 282 EII Tubulin Levels Determine the Neurotoxicity Induced by Colchicine-Site Binding Agent Indibulin. ○
- 281 Bactericidal Properties of Proline-Rich *Aedes aegypti* Trypsin Modulating Oostatic Factor (AeaTMOF). **2023**, 13, 19 ○
- 280 AC81 Is a Putative Disulfide Isomerase Involved in Baculoviral Disulfide Bond Formation. **2022**, 96, ○
- 279 Molecular interaction studies of thymol via molecular dynamic simulations and free energy calculations using multi-target approach against *Aedes aegypti* proteome to decipher its role as mosquito repellent. 1-16 ○
- 278 Substitution of PINK1 Gly411 modulates substrate receptivity and turnover. 1-22 1
- 277 In Vitro Inhibition of SARS-CoV-2 Infection by Bromhexine hydrochloride. ○
- 276 Molecular characterization of glutor-GLUT interaction and prediction of glutorβ drug-likeness: implications for its utility as an antineoplastic agent. 1-12 ○
- 275 The ChaC1 active site: Defining the residues and determining the role of ChaC1 -exclusive residues in the structural and functional stability. ○
- 274 Molecular interactions of PCSK9 with an inhibitory nanobody, CAP1 and HLA-C: Functional regulation of LDLR levels. **2022**, 101662 ○
- 273 A novel structurally identified epitope delivered by macrophage membrane-coated PLGA nanoparticles elicits protection against *Pseudomonas aeruginosa*. **2022**, 20, ○
- 272 Anti-amoebic effects of synthetic acridine-9(10H)-one against brain-eating amoebae. **2023**, 106824 ○
- 271 Genome-wide identification, evolution and transcriptome analysis of GRAS gene family in Chinese chestnut (*Castanea mollissima*). 13, ○
- 270 Identification and In Silico Analysis of a Homozygous Nonsense Variant in TGM1 Gene Segregating with Congenital Ichthyosis in a Consanguineous Family. **2023**, 59, 103 ○
- 269 Salmonella-mediated oral delivery of multiple-target vaccine constructs with conserved and variable regions of SARS-CoV-2 protect against the Delta and Omicron variants in hamster. **2023**, 105101 ○
- 268 Conservation and divergence of the G-interfaces of *Drosophila melanogaster* septins. ○
- 267 In-silico multi-epitope vaccine candidate against type-1 parainfluenza virus. ○
- 266 Molecular Modeling of an Anti-DNA Autoantibody (V-88) and Mapping of Its V Region Epitopes Recognized by Heterologous and Autoimmune Antibodies. **1998**, 161, 2944-2952 1
- 265 Binding of Longer Peptides to the H-2Kb Heterodimer Is Restricted to Peptides Extended at Their C Terminus: Refinement of the Inherent MHC Class I Peptide Binding Criteria. **1999**, 163, 4434-4441 11

- 264 Insights into pyrrolysine function from structures of a trimethylamine methyltransferase and its corrinoid protein complex. **2023**, 6, ○
- 263 Selene-Ethylenelacticamides and N-Aryl-Propanamides as Broad-Spectrum Leishmanicidal Agents. **2023**, 12, 136 ○
- 262 Comparative genomics and interactomics of polyadenylation factors for the prediction of new parasite targets: *Entamoeba histolytica* as a working model. ○
- 261 Reducing the Immunogenicity of Pulchellin A-Chain, Ribosome-Inactivating Protein Type 2, by Computational Protein Engineering for Potential New Immunotoxins. **2023**, 6, 85-101 ○
- 260 In silico design of a promiscuous chimeric multi-epitope vaccine against *Mycobacterium tuberculosis*. **2023**, ○
- 259 Identification of a novel P2X7 antagonist using structure-based virtual screening. 13, ○
- 258 Validation of novel catechol derivatives as potent *Escherichia coli* MetAP inhibitors using Molecular Docking and Molecular Dynamics Simulation. ○
- 257 Decoding whole genome of *Anoxybacillus rupiensis* TPH1 isolated from Tatapani hot spring, India and giving insight into bioremediation ability of TPH1 via heavy metals and azo dyes. **2023**, 104027 ○
- 256 Resolving colistin resistance and heteroresistance in *Enterobacter* species. **2023**, 14, ○
- 255 Design of a potential Sema4A based multi-epitope vaccine to combat triple-negative breast cancer: An immunoinformatic approach. ○
- 254 An immunoinformatic approach towards development of a potent and effective multi-epitope vaccine against monkeypox virus (MPXV). 1-14 ○
- 253 Partial characterization of purified glycoprotein from nutshell of *Arachis hypogea* L. towards macrophage activation and leishmanicidal activity. ○
- 252 Structural basis for ubiquitylation by HOIL-1. 9, ○
- 251 Structural Basis for the IgE-Binding Cross-Reacting Epitopic Peptides of Cup s 3, a PR-5 Thaumatin-like Protein Allergen from Common Cypress (*Cupressus sempervirens*) Pollen. **2023**, 3, 11-24 ○
- 250 Novel high-risk missense mutations identification in FAT4 gene causing Hennekam syndrome and Van Maldergem syndrome 2 through molecular dynamics simulation. **2023**, 37, 101160 ○
- 249 The pathogenic effect of SNPs on structure and function of human TLR4 using a computational approach. 1-14 ○
- 248 Novel CaLB-like Lipase Found Using ProspectBIO, a Software for Genome-Based Bioprospection. **2023**, 12, 6 ○
- 247 Synthesis, Biological Evaluation and Molecular Modeling Studies of Naphthoquinone Sulfonamides and Sulfonate Ester Derivatives as P2X7 Inhibitors. **2023**, 28, 590 ○



- 246 The structure of the high-affinity nickel-binding site in the Ni,Zn-HypA $\alpha$ reE2 complex. ○
- 245 Computational design of prospective molecular targets for Burkholderia cepacia complex by molecular docking and dynamic simulation studies. ○
- 244 The Association between Genetic Variations and Morphology-based Brain Networks Changes in Alzheimer's Disease. ○
- 243 Modulation of the IKS channel by PIP2 requires two binding sites per monomer. **2023**, 3, 100073 ○
- 242 New simulation insights on the structural transition mechanism of Bovine Rhodopsin activation. ○
- 241 Structural and functional analysis of a tandem repeat galacturonic acid-binding lectin from the sea hare *Aplysia californica*. **2023**, 132, 108513 ○
- 240 Silibinin chronic treatment in a rat model of Parkinson disease: A comprehensive in-vivo evaluation and in silico molecular modeling. **2023**, 175517 1
- 239 How well do semiempirical QM methods describe the structure of proteins?. 1
- 238 Comprehensive molecular analysis identifies eight novel variants in XY females with disorders of sex development. ○
- 237 In silico drug screen reveals potential competitive MTHFR inhibitors for clinical repurposing. 1-14 ○
- 236 Antileishmanial Activity of *Clinanthus milagroanthus* S. Leiva & Meerow (Amaryllidaceae) Collected in Peru. **2023**, 12, 322 ○
- 235 Molecular Dynamics Simulations Reveal Novel Interacting Regions of Human Prion Protein to *Brucella abortus* Hsp60 Protein. ○
- 234 Biochemical characterization, substrate and stereoselectivity of an outer surface putative  $\beta$  hydrolase from the pathogenic *Leptospira*. **2023**, 229, 803-813 ○
- 233 Ensemble-based, high-throughput virtual screening of potential inhibitor targeting putative farnesol dehydrogenase of *Metisa plana* (Lepidoptera: Psychidae). **2023**, 103, 107811 ○
- 232 New insights into the substrate inhibition of human 17 $\beta$ hydroxysteroid dehydrogenase type 1. **2023**, 228, 106246 ○
- 231 Structure of the complex of camel peptidoglycan recognition protein-S with hexanoic acid reveals novel features of the versatile ligand-binding site at the dimeric interface. **2023**, 1871, 140887 ○
- 230 Attenuation of fluoride-induced hepatorenal oxidative stress by ferulic acid in vivo: An approach with in-silico analysis and interaction informatics of ferulic acid. **2023**, 77, 127133 ○
- 229 An Immunoinformatics Approach to Design a Potent Multi-Epitope Vaccine against Asia-1 Genotype of Crimean-Congo Haemorrhagic Fever Virus Using the Structural Glycoproteins as a Target. **2023**, 11, 61 ○

228	Structural and Functional Characterization of Novel Phosphotyrosine Phosphatase Protein from <i>Drosophila melanogaster</i> (Pupal Retina). <b>2023</b> , 8, 1937-1945	○
227	Vibrational spectroscopic, electronic influences, reactivity analysis and molecular docking studies of 2-Fluoro-4-iodo-5-methylpyridine. <b>2023</b> , 56, 14-27	○
226	Studies of the symmetric binding mode of daclatasvir and analogs using a new homology model of HCV NS5A GT-4a. <b>2023</b> , 29,	○
225	Design of a multi-epitope vaccine against <i>Haemophilus parasuis</i> based on pan-genome and immunoinformatics approaches. 9,	○
224	In silico detection and characterization of novel virulence proteins of the emerging poultry pathogen <i>Gallibacterium anatis</i> . <b>2022</b> , 20, e41	○
223	Antimicrobial resistance in <i>Klebsiella pneumoniae</i> : identification of bacterial DNA adenine methyltransferase as a novel drug target from hypothetical proteins using subtractive genomics. <b>2022</b> , 20, e47	○
222	In silico design and evaluation of a novel mRNA vaccine against BK virus: a reverse vaccinology approach.	1
221	Functional, and phylogenetic analysis of maleylacetate reductase of <i>Pseudomonas</i> sp strain PNP3: An in-silico approach. <b>2022</b> , 10, 1331-1343	○
220	Comparative analysis of Cf-4 and Cf-19 in tomato ( <i>Solanum lycopersicum</i> ) [A bioinformatics study. <b>2017</b> , 87,	○
219	Herbivory-inducible lipid-transfer proteins (LTPs) of <i>Cicer arietinum</i> as potential human allergens. 1-17	○
218	Deciphering the interaction mechanism of natural actives against larval proteins of <i>Aedes aegypti</i> to identify potential larvicides: a computational biology analysis. 1-23	○
217	In silico analysis of NHP2 membrane protein, a novel vaccine candidate present in the RD7 region of <i>Mycobacterium tuberculosis</i> .	○
216	Blind Assessment of Monomeric AlphaFold2 Protein Structure Models with Experimental NMR Data.	○
215	Mitochondrial Genome Alterations, Cytochrome C Oxidase Activity, and Oxidative Stress: Implications in Primary Open-angle Glaucoma. <b>2023</b> , 16, 158-165	○
214	Immunoinformatics Approach to Design a Multi-Epitope Nanovaccine against <i>Leishmania</i> Parasite: Elicitation of Cellular Immune Responses. <b>2023</b> , 11, 304	○
213	Identification of Quorum Quenching N-Acyl Homoserine Lactonases from <i>Priestia aryabhatai</i> J1D and <i>Bacillus cereus</i> G Isolated from the Rhizosphere. <b>2023</b> , 80,	○
212	Identification of thrombin inhibiting antithrombin-III like protein from <i>Punica granatum</i> using in silico approach and invitro validation of thrombin inhibition activity in crude protein. 1-13	○
211	In silico profiling of nonsynonymous SNPs of fat mass and obesity-associated gene: possible impacts on the treatment of non-alcoholic fatty liver disease. <b>2023</b> , 22,	○

- 210 Characterization and expression of domains of Alphaherpesvirus bovine 1/5 envelope glycoproteins B in *Komagataella phaffii*. **2023**, 19, ○
- 209 Identification of potential inhibitor molecule against MabA protein of *Mycobacterium leprae* by integrated in silico approach. 1-16 ○
- 208 Genomic landscape of the emerging XDR *Salmonella* Typhi for mining druggable targets clpP, hisH, folP and gpml and screening of novel TCM inhibitors, molecular docking and simulation analyses. **2023**, 23, ○
- 207 Characterizing inhibitors of human AP endonuclease 1. **2023**, 18, e0280526 ○
- 206 Effector protein Hcp2a of avian pathogenic *Escherichia coli* interacts with the endoplasmic reticulum associated RPL23 protein of chicken DF-1 fibroblasts. **2023**, 54, ○
- 205 Structure and functional determinants of Rad6Bre1 subunits in the histone H2B ubiquitin-conjugating complex. ○
- 204 Application of Molecular Simulation Methods in Food Science: Status and Prospects. ○
- 203 A Wider and Deeper Peptide-Binding Groove for the Class I Molecules from B15 Compared with B19 Chickens Correlates with Relative Resistance to Marek's Disease. ○
- 202 Proteomics analysis reveals three potential cacao target that interacts with *Moniliophthora perniciosa* NEP during witches broom disease. **2023**, 101946 ○
- 201 Molecular docking and simulation studies against nucleoside diphosphate kinase (NDK) of *Pseudomonas aeruginosa* with secondary metabolite identified by genome mining from *paenibacillus himensis*. 1-10 ○
- 200 An immunoinformatics and structural vaccinology study to design a multi-epitope vaccine against *Staphylococcus aureus* infection. ○
- 199 In silico investigation of cytochrome bc1 molecular inhibition mechanism against *Trypanosoma cruzi*. **2023**, 17, e0010545 ○
- 198 Combining protein and metabolic engineering to achieve green biosynthesis of 12EO-Glc-PPD in *Saccharomyces cerevisiae*. 1
- 197 The glycine N-acyltransferases, GLYAT and GLYATL1, contribute to the detoxification of isovaleryl-CoA - an in-silico and in vitro validation. **2023**, 21, 1236-1248 ○
- 196 Homology Modeling of Carbonic Anhydrase from *Dunaliella Viridis*. ○
- 195 Discovery of N-l-Lactoyl-l-Trp as a Bitterness Masker via Structure-Based Virtual Screening and a Sensory Approach. **2023**, 71, 2082-2093 ○
- 194 Molecular interaction modeling of carbon nanotubes and fullerene toward prioritized targets of SARS-CoV-2 by computer-aided screening and docking studies. **2023**, 157-179 ○
- 193 Characterization of the Technofunctional Properties and Three-Dimensional Structure Prediction of 11S Globulins from Amaranth (*Amaranthus hypochondriacus* L.) Seeds. **2023**, 12, 461 1

- 192 Computational design and structure dynamics analysis of bifunctional chimera of endoxylanase from *Clostridium thermocellum* and xylosidase from *Bacteroides ovatus*. **2023**, 13, ○
- 191 In Vitro Structure-Activity Relationship Study of a Novel Octapeptide Angiotensin-I Converting Enzyme (ACE) Inhibitor from the Freshwater Mussel *Lamellidens marginalis*. **2023**, 29, ○
- 190 Role of hinge motion and ATP dynamics in factors for inversion stimulation FIS protein deduced while targeting drug resistant *Orientia tsutsugamushi*. **2023**, 120, 108425 ○
- 189 In silico Investigation of Immulina Glycosidic Residues as Immunostimulants by Targeting *Penaeus monodon* Shrimp Toll-Receptor 9. **2022**, ○
- 188 Easy Not Easy: Comparative Modeling with High-Sequence Identity Templates. **2023**, 83-100 ○
- 187 Media optimization, extraction, purification and characterization of exopolysaccharide from *Fusarium proliferatum*: A novel source bioactive polysaccharide. **2023**, 5, 100923 ○
- 186 S-Adenosyl-L-Homocysteine Exhibits Potential Antiviral Activity Against Dengue Virus Serotype-3 (DENV-3) in Bangladesh: A Viroinformatics-Based Approach. **2023**, 17, 117793222311582 ○
- 185 Structural and functional characterization of 1-deoxy-D-xylulose-5-phosphate synthase (DXS) from *Acinetobacter baumannii*: identification of promising lead molecules from virtual screening, molecular docking and molecular dynamics simulations. 1-14 ○
- 184 Towards characterizing of *Enterocytozoon hepatopenaei* (EHP) spore wall proteins with feature identification and analogy modeling. **2023**, 38, 101215 ○
- 183 Structural and functional characterization of RNA dependent RNA polymerase of *Macrobrachium rosenbergii* nodavirus (MnRdRp). 1-13 ○
- 182 Design of a potential Sema4A-based multi-epitope vaccine to combat triple-negative breast cancer: an immunoinformatic approach. **2023**, 40, ○
- 181 Identification of Natural Lead Compounds against Hemagglutinin-Esterase Surface Glycoprotein in Human Coronaviruses Investigated via MD Simulation, Principal Component Analysis, Cross-Correlation, H-Bond Plot and MMGBSA. **2023**, 11, 793 1
- 180 Molecular cloning, characterization and 3D modelling of spotted snakehead fbn1 C-terminal region encoding asprosin and expression analysis of fbn1. **2023**, 13, ○
- 179 Peptide Models of the Cytoplasmic Tail of Influenza A/H1N1 Virus Hemagglutinin Expand Understanding its pH-Dependent Modes of Interaction with Matrix Protein M1. ○
- 178 Coumarin-Based Compounds as Inhibitors of Tyrosinase/Tyrosine Hydroxylase: Synthesis, Kinetic Studies, and In Silico Approaches. **2023**, 24, 5216 ○
- 177 Toward overcoming pyrethroid resistance in mosquito control: the role of sodium channel blocker insecticides. ○
- 176 Structural evidence of the conversion of nitric oxide (NO) to nitrite ion (NO<sub>2</sub><sup>-</sup>) by lactoperoxidase (LPO): Structure of the complex of LPO with NO<sub>2</sub><sup>-</sup> at 1.89 Å resolution. ○
- 175 Structural modeling and analyses of genetic variations in the human XPC nucleotide excision repair protein. 1-28 ○

- 174 Structure and interactions of the phloem lectin (phloem protein 2) Cus17 from *Cucumis sativus*. **2023**, 31, 464-479.e5 ○
- 173 Designing of multi-epitope peptide vaccine against *Acinetobacter baumannii* through combined immunoinformatics and protein interaction based approaches. ○
- 172 Genome-wide identification of PR10 family members and expression profile analysis of PvPR10 in common bean (*Phaseolus vulgaris* L.) in response to hormones and several abiotic stress conditions. ○
- 171 Structure-based design of promising natural products to inhibit thymidylate kinase from Monkeypox virus and validation using free energy calculations. **2023**, 158, 106797 ○
- 170 Carboxymuconolactone decarboxylase is a prospective molecular target for multi-drug resistant *Acinetobacter baumannii*-computational modeling, molecular docking and dynamic simulation studies. **2023**, 157, 106793 ○
- 169 In silico structural exploration of serine protease from a CTG-clade yeast *Meyerozyma guilliermondii* strain SO. **2023**, 668, 115092 ○
- 168 Ergosterol influences activity of succinic dehydrogenase in tomato and barley. **2023**, 156, 131-143 ○
- 167 Directed targeting of B-cell maturation antigen-specific CAR T cells by bioinformatic approaches: From in-silico to in-vitro. **2023**, 228, 152376 ○
- 166 Novel pro-and eukaryotic expression plasmid expressing omicron antigens delivered via *Salmonella* elicited MHC class I and II based protective immunity. **2023**, 357, 404-416 ○
- 165 In silico characterization of Ajmaline biosynthesis pathway genes in plants. **2023**, 34, 100420 ○
- 164 Molecular characterization, putative structure and function, and expression profile of OAS1 gene in the endometrium of goats (*Capra hircus*). **2023**, 23, 100760 ○
- 163 Emerging contaminant triclosan incites endocrine disruption, reproductive impairments and oxidative stress in the commercially important carp, *Catla* (*Labeo catla*): An insight through molecular, histopathological and bioinformatic approach. **2023**, 268, 109605 ○
- 162 Phylogenetic distribution, structural analysis and interaction of nucleotide excision repair proteins in cyanobacteria. **2023**, 126, 103487 ○
- 161 Selective vitamins as potential options for dietary therapeutic interventions: In silico and In vitro insights from mutant C terminal fragment of FGA. **2023**, 230, 106290 ○
- 160 Identification of Potent Small-Molecule PCSK9 Inhibitors Based on Quantitative Structure-Activity Relationship, Pharmacophore Modeling, and Molecular Docking Procedure. **2023**, 48, 101660 ○
- 159 Purinergic approach to effective glioma treatment with temozolomide reveals enhanced anti-cancer effects mediated by P2X7 receptor. **2023**, 106, 110641 ○
- 158 Computational docking investigation of phytocompounds from bergamot essential oil against *Serratia marcescens* protease and FabI: Alternative pharmacological strategy. **2023**, 104, 107829 ○
- 157 Discovery of a spirocyclic 3-bromo-4,5-dihydroisoxazole covalent inhibitor of hGAPDH with antiproliferative activity against pancreatic cancer cells. **2023**, 254, 115286 ○

- 156 The plant specialized metabolite epicatechin-3-gallate (EC3G) perturbs lipid metabolism and attenuates fat accumulation in pigeonpea pod borer, *Helicoverpa armigera*. **2023**, 231, 123325 ○
- 155 Biochemical Characterization of a GH46 Chitosanase Provides Insights into the Novel Digestion Specificity. **2023**, 71, 2038-2048 ○
- 154 Revisiting the Ramachandran plot based on statistical analysis of static and dynamic characteristics of protein structures. **2023**, 215, 107939 ○
- 153 In silico design of a multi-epitope vaccine against the spike and the nucleocapsid proteins of the Omicron variant of SARS-CoV-2. 1-15 ○
- 152 Engineering of xylanases for the development of biotechnologically important characteristics. **2023**, 120, 1171-1188 ○
- 151 Key regulators in the architecture of substrate access/egress channels in mammalian cytochromes P450 governing flexibility in substrate oxyfunctionalization. **2023**, 241, 112150 ○
- 150 ACW-02 an Acridine Triazolidine Derivative Presents Antileishmanial Activity Mediated by DNA Interaction and Immunomodulation. **2023**, 16, 204 ○
- 149 Cloning and Molecular Characterization of the pHID Gene Involved in the Biosynthesis of Bhloroglucinolide Compound with Antibiotic Properties from Plant Growth Promoting Bacteria *Pseudomonas* spp.. **2023**, 12, 260 2
- 148 Exploring staphylococcal superantigens to design a potential multi-epitope vaccine against *Staphylococcus aureus*: an in-silico reverse vaccinology approach. 1-15 ○
- 147 Structure of pyridoxal 5'-phosphate-bound D-threonine aldolase from *Chlamydomonas reinhardtii*. **2023**, 79, 31-37 ○
- 146 Investigation of biological activities of two cultivars of *Cicer arietinum* proteins mass associated with Alzheimer's disease. ○
- 145 Functional analysis of metalloenzymes from human gut microbiota and their role in ulcerative colitis. **2023**, 134, ○
- 144 Impacts of Sourdough Technology on the Availability of Celiac Peptides from Wheat Hard End Gliadins: In Silico Approach. **2023**, 3, 39-57 ○
- 143 Multiple-P450 Gene Co-Up-Regulation in the Development of Permethrin Resistance in the House Fly, *Musca domestica*. **2023**, 24, 3170 ○
- 142 I329L: A Dual Action Viral Antagonist of TLR Activation Encoded by the African Swine Fever Virus (ASFV). **2023**, 15, 445 ○
- 141 Host-Erythrocytic Sphingosine-1-Phosphate Regulates Plasmodium Histone Deacetylase Activity and Exhibits Epigenetic Control over Cell Death and Differentiation. **2023**, 11, ○
- 140 Targeting *Acanthamoeba* proteins interaction with flavonoids of Propolis extract by in vitro and in silico studies for promising therapeutic effects. 11, 1274 ○
- 139 Exploration of Candidate Genes Involved in the Biosynthesis, Regulation and Recognition of the Male-Produced Aggregation Pheromone of *Halyomorpha halys*. **2023**, 14, 163 ○

- 138 Engineering the kinetic stability of a ß-refoil protein by tuning its topological complexity. 10, ○
- 137 Designing of new tetrahydro-ß-carboline-based ABCG2 inhibitors using 3D-QSAR, molecular docking, and DFT tools. 1-12 ○
- 136 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 ○
- 135 Investigation of Multi-Subunit Mycobacterium tuberculosis DNA-Directed RNA Polymerase and Its Rifampicin Resistant Mutants. **2023**, 24, 3313 ○
- 134 Identification of the molecular determinants of antagonist potency in the allosteric binding pocket of human P2X4. 14, ○
- 133 Neutron Reflectometry and Molecular Simulations Demonstrate HIV-1 Nef Homodimer Formation on Model Lipid Bilayers. **2023**, 435, 168009 ○
- 132 Immunoinformatics Study: Multi-Epitope Based Vaccine Design from SARS-CoV-2 Spike Glycoprotein. **2023**, 11, 399 ○
- 131 Arginine transportation mechanism through cationic amino acid transporter 1: insights from molecular dynamics studies. 1-15 ○
- 130 Reversal of the unique Q493R mutation increases the affinity of Omicron S1-RBD for ACE2. **2023**, 21, 1966-1977 ○
- 129 Challenges in antibody structure prediction. **2023**, 15, ○
- 128 Characterisation of the Putative Antigenic Genes of the Outer Membrane Proteins of Pasteurella multocida B:2 Strain PMTB2.1 through in silico Analysis. **2022**, 46, 277-313 ○
- 127 Integration of immunoinformatics and cheminformatics to design and evaluate a multipeptide vaccine against Klebsiella pneumoniae and Pseudomonas aeruginosa coinfection. 10, ○
- 126 Structural analysis of human G-protein-coupled receptor 17 ligand binding sites. **2023**, 124, 533-544 ○
- 125 SNP based analysis depicts phenotypic variability in heme oxygenase-1 protein. **2023**, ○
- 124 A computational investigation on Rho-related GTP-binding protein RhoB through molecular modeling and molecular dynamics simulation study. ○
- 123 Engineered Glycosidase for Significantly Improved Production of Naturally Rare Vina-Ginsenoside R7. **2023**, 71, 3852-3861 ○
- 122 Sarbecoviruses of British Horseshoe Bats; Sequence Variation and Epidemiology. ○
- 121 Site-Specific Phosphorylation of RTK KIT Kinase Insert Domain: Interactome Landscape Perspectives. **2023**, 1, 39-71 ○

- 120 Molecular docking approaches of biomolecules extracted from red seaweed *Kappaphycus alvarezii* against hemolysin protein of bioluminescence disease-causing bacteria *Vibrio harveyi*. ○
- 119 Altering the Regioselectivity of T1 Lipase from *Geobacillus zalihae* toward sn-3 Acylglycerol Using a Rational Design Approach. **2023**, 13, 416 ○
- 118 ECEL1 novel mutation in arthrogryposis type 5D : A molecular dynamic simulation study. ○
- 117 Surface display of pancreatic lipase inhibitor peptides by engineered *Saccharomyces boulardii*: Potential as an anti-obesity probiotic. **2023**, 102, 105458 ○
- 116 Deciphering local adaptation of native Indian cattle (*Bos indicus*) breeds using landscape genomics and in-silico prediction of deleterious SNP effects on protein structure and function. **2023**, 13, ○
- 115 Sequence assignment validation in protein crystal structure models with checkMySequence. ○
- 114 Structural organization of RDGB (retinal degeneration B), a multi-domain lipid transfer protein: a molecular modelling and simulation based approach. 1-15 ○
- 113 Structural modelling and dynamics of full-length of TLR10 sheds light on possible modes of dimerization, ligand binding and mechanism of action. **2023**, 5, 100097 ○
- 112 Structural basis for the dual GTPase specificity of the DOCK10 guanine nucleotide exchange factor. **2023**, 653, 12-20 ○
- 111 Allosteric modulation of conserved motifs and helices in 5HT2BR: Advances drug discovery and therapeutic approach towards drug resistant epilepsy. 1-14 ○
- 110 Computational approaches screening DNA aptamers against conserved outer membrane protein W of *Vibrio cholerae* O1- an investigation expanding the potential for point-of-care detection with aptasensors. 1-12 ○
- 109 Identification of B and T Cell Epitopes to Design an Epitope-Based Peptide Vaccine against the Cell Surface Binding Protein of Monkeypox Virus: An Immunoinformatics Study. **2023**, 2023, 1-14 ○
- 108 Anastrozole-mediated modulation of mitochondrial activity by inhibition of mitochondrial permeability transition pore opening: an initial perspective. 1-17 ○
- 107 Computational investigation of honeybee venom proteins as potential Omicron SARS-CoV-2 inhibitors. **2023**, 94, 3-10 ○
- 106 Alleviation of arthritis through prevention of neutrophil extracellular traps by an orally available inhibitor of protein arginine deiminase 4. **2023**, 13, ○
- 105 Designing multi-epitope vaccine against important colorectal cancer (CRC) associated pathogens based on immunoinformatics approach. **2023**, 24, ○
- 104 Immunoinformatics design of multi-epitope vaccine using OmpA, OmpD and enterotoxin against non-typhoidal salmonellosis. **2023**, 24, ○
- 103 Immunoinformatics-aided design of a new multi-epitope vaccine adjuvanted with domain 4 of pneumolysin against *Streptococcus pneumoniae* strains. **2023**, 24, ○



102	Solution structure of the DNA binding domain of Arabidopsis transcription factor WRKY11. <b>2023</b> , 653, 133-139	0
101	Designing a Next-Generation Multiepitope-Based Vaccine against Staphylococcus aureus Using Reverse Vaccinology Approaches. <b>2023</b> , 12, 376	0
100	Insights into the binding mechanism of ascorbic acid and violaxanthin with violaxanthin de-epoxidase (VDE) and chlorophycean violaxanthin de-epoxidase (CVDE) enzymes.	0
99	In silico analysis of highly disordered human IRS1 protein 3D structure to uncover new target for Metformin to ameliorate diabetes.	0
98	Characterization of a New Glucose-Tolerant GH1 $\beta$ Glycosidase from Aspergillus fumigatus with Transglycosylation Activity. <b>2023</b> , 24, 4489	0
97	Million-atom molecular dynamics simulations reveal the interfacial interactions and assembly of plant PSII-LHCII supercomplex. <b>2023</b> , 13, 6699-6712	0
96	Molecular Simulation Study on the Interaction between Porcine CR1-like and C3b. <b>2023</b> , 28, 2183	0
95	Atomic resolution structure of a DNA-binding histone protein from the bacterium Bdellovibrio bacteriovorus.	0
94	Tip60's Novel RNA-Binding Function Modulates Alternative Splicing of Pre-mRNA Targets Implicated in Alzheimer's Disease. <b>2023</b> , 43, 2398-2423	0
93	1,3-Benzodioxole Tagged Lidocaine Based Ionic Liquids as Anticancer Drug: Synthesis, Characterization and In Silico Study. <b>2023</b> , 8,	0
92	Potential effect of luteolin, epiafzelechin, and albigenin on rats under cadmium-induced inflammatory insult: In silico and in vivo approach. 11,	0
91	Computational design of fusion proteins against ErbB2-amplified tumors inspired by ricin toxin. 10,	0
90	In silico design of a polypeptide as a vaccine candidate against ascariasis. <b>2023</b> , 13,	0
89	Therapeutic capability of selected medicinal plants' bioactive constituents against the mutant ovarian TP53 gene; a computational approach. <b>2023</b> , 5, 8-32	0
88	Structural Characterization of the Chlorophyllide a Oxygenase (CAO) Enzyme Through an In Silico Approach. <b>2023</b> , 91, 225-235	0
87	The dynamic nature of netrin-1 and the structural basis for glycosaminoglycan fragment-induced filament formation. <b>2023</b> , 14,	1
86	Adding New Scientific Evidences on the Pharmaceutical Properties of Pelargonium quercetorum Agnew Extracts by Using In Vitro and In Silico Approaches. <b>2023</b> , 12, 1132	1
85	Charge-changing point mutations in the E protein of tick-borne encephalitis virus. <b>2023</b> , 168,	0

- 84 Structure modelling of odorant receptor from *Aedes aegypti* and identification of potential repellent molecules. **2023**, 21, 2204-2214 ○
- 83 In Silico Exploration of Microtubule Agent Griseofulvin and Its Derivatives Interactions with Different Human  $\beta$ Tubulin Isoforms. **2023**, 28, 2384 ○
- 82 NMR structure of emfourin, a novel protein metalloprotease inhibitor: Insights into the mechanism of action. **2023**, 299, 104585 ○
- 81 In Silico-Based Structural Evaluation to Categorize the Pathogenicity of Mutations Identified in the RAD Class of Proteins. **2023**, 8, 10266-10277 ○
- 80 Molecular cloning and production of recombinant Pcal\_0672, a family GH57 glycoside hydrolase from *Pyrobaculum calidifontis*. ○
- 79 Rational design of mini protein mimicking uricase: Encapsulation in ZIF -8 for uric acid detection. ○
- 78 Performance of Eversa Transform 2.0 Lipase in Ester Production Using Babassu Oil (*Orbignya sp.*) and Tucuman Oil (*Astrocaryum vulgare*): A Comparative Study between Liquid and Immobilized Forms in Fe<sub>3</sub>O<sub>4</sub> Nanoparticles. **2023**, 13, 571 1
- 77 Combinatorial interactions among natural structural variants of Brassica SOC1 promoters and SVP depict conservation of binding affinity despite molecular diversity. ○
- 76 Computational Analysis and Experimental Testing of the Molecular Mode of Action of Gatastatin and Its Derivatives. **2023**, 15, 1714 ○
- 75 Biochemical Characterization of an Endoglucanase GH7 from Thermophile *Thermothielavioides terrestris* Expressed on *Aspergillus nidulans*. **2023**, 13, 582 ○
- 74 Identification and characterization of molecular entities differentially expressed in bacteria genome upon treatment with glyphosate shock. **2023**, 9, e13868 ○
- 73 Design of a multi-epitopic vaccine against Epstein-Barr virus via computer-based methods. 14, ○
- 72 Insight into biosorption of hexavalent chromium using isolated species *Aspergillus Proliferans* LA: A systemic and In silico studies. **2023**, 7, 83 ○
- 71 Antimicrobial Potential of Betulinic Acid and Investigation of the Mechanism of Action against Nuclear and Metabolic Enzymes with Molecular Modeling. **2023**, 12, 449 ○
- 70 Discovering and Designing a Chimeric Hyperthermophilic Chitinase for Crystalline Chitin Degradation. **2023**, 11, 4690-4698 ○
- 69 <em>In silico</em> screening of potential compounds from begonia genus as 3CL protease (3CL pro) SARS-CoV-2 inhibitors. ○
- 68 Functional metagenomics uncovers nitrile-hydrolysing enzymes in a coal metagenome. 10, ○
- 67 A computational therapeutic evaluation of 5-Fluorouracil and different phytochemicals in view of dynamic behavior with native and mutated protein related to colon cancer. **2023**, ○

- 66 Targeting Ras-binding domain of ELMO1 by computational nanobody design. **2023**, 6, ○
- 65 Cancer mutations rewire the RNA methylation specificity of METTL3-METTL14. ○
- 64 Template-Based Modelling of the Structure of Fungal Effector Proteins. ○
- 63 In silico characterization of differentially expressed short-read nucleotide sequences identified in dieback stress-induced transcriptomic analysis reveals their role as antimicrobial peptides. 14, ○
- 62 A novel homozygous synonymous splicing variant in SELENOI gene causes spastic paraplegia 81. ○
- 61 Elucidating the molecular mechanisms of essential oils' insecticidal action using a novel cheminformatics protocol. **2023**, 13, ○
- 60 Drug repurposing for Mpox: Discovery of small molecules as potential inhibitors against DNA-dependent RNA polymerase using molecular modeling approach. ○
- 59 Evaluation of SNPs from human IGFBP6 associated with gene expression: an in-silico study. 1-13 ○
- 58 Restriction of access to the central cavity is a major contributor to substrate selectivity in plant ABCG transporters. **2023**, 80, ○
- 57 Protein Homology Modeling for Effective Drug Design. **2023**, 329-337 ○
- 56 A novel homozygous missense substitution p.Thr313Ile in the PDE6B gene underlies autosomal recessive retinitis pigmentosa in a consanguineous Pakistani family. **2023**, 23, ○
- 55 Homology Modeling of Transporter Proteins. **2023**, 247-264 ○
- 54 Unraveling the Aquaporin-3 Inhibitory Effect of Rottlerin by Experimental and Computational Approaches. **2023**, 24, 6004 ○
- 53 Ensemble of structure and ligand-based classification models for hERG liability profiling. 14, ○
- 52 H<sub>2</sub>S-generating cytosolic L-cysteine desulfhydrase (LCD) and mitochondrial D-cysteine desulfhydrase (DCD) from sweet pepper (*Capsicum annuum* L.) are regulated during fruit ripening and by nitric oxide (NO). ○
- 51 Exploring and targeting potential druggable antimicrobial resistance targets ArgS, SecY and MurA in *Staphylococcus sciuri* with TCM inhibitors through subtractive genomics strategy. ○
- 50 Exploring biogenic chalcones as DprE1 inhibitors for antitubercular activity via in silico approach. **2023**, 29, ○
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- 30 A Computational Biology Study on the Structure and Dynamics Determinants of Thermal Stability of the Chitosanase from *Aspergillus fumigatus*. **2023**, 24, 6671 ○
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- 6 In silico structural and functional characterization of hypothetical proteins from Monkeypox virus. **2023**, 21, ○
- 5 An mRNA-Based Multiple Antigenic Gene Expression System Delivered by Engineered Salmonella for Severe Fever with Thrombocytopenia Syndrome and Assessment of Its Immunogenicity and Protection Using a Human DC-SIGN-Transduced Mouse Model. **2023**, 15, 1339 ○
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- 2 Molecular cloning and in silico analysis of chalcone isomerase from *Polygonum minus*. ○
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