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#	Paper	IF	Citations
2271	Computational Investigations of the Interaction between the Cell Membrane and Nanoparticles Coated with a Pulmonary Surfactant.		
2270	StructureActivity Relationship Studies and Molecular Modeling of Naphthalene-Based Sphingosine Kinase 2 Inhibitors.		
2269	Molecular Occupancy of Nanodot Arrays.		
2268	Repurposing of a Nucleoside Scaffold from Adenosine Receptor Agonists to Opioid Receptor Antagonists.		
2267	Measurement of Roundness and Sphericity Parameters Using an Electronic Particle Size Analyzer. **1967**, Vol. 37,		3
2266	Packing of alpha-helices: geometrical constraints and contact areas. *Journal of Molecular Biology*, **1978**, 119, 537-55	6.5	342
2265	A general method to assess similarity of protein structures, with applications to T4 bacteriophage lysozyme. **1978**, 75, 2180-4		65
2264	Space-filling models of kinase clefts and conformation changes. **1979**, 204, 375-80		273
2263	Packing defects, cavities, volume fluctuations, and access to the interior of proteins. Including some general comments on surface area and protein structure. **1979**, 44, 47-63		143
2262	Hydrodynamics and protein hydration. **1979**, 196, 165-77		261
2261	Structure of a bacteriochlorophyll a-protein from the green photosynthetic bacterium Prosthecochloris aestuarii. *Journal of Molecular Biology*, **1979**, 131, 259-85	6.5	259
2260	Protein folding: evaluation of some simple rules for the assembly of helices into tertiary structures with myoglobin as an example. *Journal of Molecular Biology*, **1979**, 132, 275-88	6.5	146
2259	Nuclear magnetic relaxation study on the interaction of glycyl-L-tyrosine with manganese-carboxypeptidase A in solution. *Journal of Biochemistry*, **1979**, 86, 1001-11	3.1	1
2258	Description of the quaternary structure of tetrameric proteins. Forms that show either right-handed or left-handed symmetry at the subunit level. **1980**, 187, 297-302		2
2257	Model for haptoglobin heavy chain based upon structural homology. **1980**, 77, 3393-7		88
2256	Towards a quantum-chemical representation of enzyme activity. A scrf pce cndo/2 study of the ladh proton relay system. **1980**, 72, 334-341		26
2255	A method for constrained energy minimization of macromolecules. **1980**, 1, 266-274		51

2254	Local hydrophobicity stabilizes secondary structures in proteins. **1980**, 19, 1617-28		67
2253	Modification of the apparent radius of gyration of cytochrome c by the distribution of counterions in solution. **1980**, 19, 1887-1897		4
2252	NMR analyses of molecular conformations and conformational equilibria with the lanthanide probe method. **1980**, 14, 67-111		99
2251	Immunochemical properties of abnormal hemoglobins C-Harlem (beta 6 Glu replaced by Val, beta 73 Asp replaced by Asn), S (beta 6 Glu replaced by Val), Korle Bu (beta 73 Asp replaced by Asn), Vancouver (beta 73 Asp replaced by Tyr), and Mobile (beta 73 Asp replaced by Val). **1980**, 624, 286-92		4
2250	Analysis and prediction of protein beta-sheet structures by a combinatorial approach. **1980**, 285, 378-82		112
2249	Structure of southern bean mosaic virus at 2.8 A resolution. **1980**, 286, 33-9		386
2248	Molecular dynamics of ferrocytochrome c. **1980**, 286, 304-5		42
2247	Structural and functional diversity in 4-alpha-helical proteins. **1980**, 287, 82-4		224
2246	The effect of hGH on hypothalamic-pituitary-thyroid function in patients with pituitary dwarfism. **1980**, 93, 13-9		15
2245	Yeast tRNAPhe conformation wheels: a novel probe of the monoclinic and orthorhombic models. **1980**, 8, 2307-29		17
2244	Logical analysis of the mechanism of protein folding. V. Packing game simulation of alpha/beta proteins. *Journal of Molecular Biology*, **1980**, 138, 797-832	6.5	16
2243	Structure of a complex between yeast hexokinase A and glucose. I. Structure determination and refinement at 3.5 A resolution. *Journal of Molecular Biology*, **1980**, 140, 183-209	6.5	86
2242	Packing of alpha-helices onto beta-pleated sheets and the anatomy of alpha/beta proteins. *Journal of Molecular Biology*, **1980**, 143, 95-128	6.5	104
2241	On the use of chemically derived distance constraints in the prediction of protein structure with myoglobin as an example. *Journal of Molecular Biology*, **1980**, 137, 9-22	6.5	61
2240	A systematic approach to the comparison of protein structures. *Journal of Molecular Biology*, **1980**, 140, 77-99	6.5	91
2239	Quantitative analysis of structural domains in protein. **1980**, 32, 213-5		9
2238	Configuron dependence on translation of specific codon pairs. I. Helical regions of human alpha and beta globins. **1980**, 97, 868-74		
2237	Proton nuclear magnetic resonance studies of human immunoglobulins: conformation of the hinge region of the IgG1 immunoglobulin. **1980**, 19, 5130-5		24

2236	Computation of enzyme-substrate specificity. **1981**, 20, 1730-43		17
2235	Computation of peptide-protein interactions. Catalysis by chymotrypsin: prediction of relative substrate reactivities. **1981**, 103, 107-110		17
2234	Electrostatic contributions to the energetics of dimer-tetramer assembly in human hemoglobin: pH dependence and effect of specifically bound chloride ions. **1981**, 20, 7439-49		37
2233	Refined crystal structure of gamma-chymotrypsin at 1.9 A resolution. Comparison with other pancreatic serine proteases. *Journal of Molecular Biology*, **1981**, 148, 449-79	6.5	142
2232	An examination of the expected degree of sequence similarity that might arise in proteins that have converged to similar conformational states. The impact of such expectations on the search for homology between the structurally similar domains of rhodanese. *Journal of Molecular Biology*, **1981**, 151, 179-97	6.5	46
2231	Crystallographic structure of Rhodospirillum molischianum ferricytochrome c' at 2.5 A resolution. *Journal of Molecular Biology*, **1981**, 153, 399-424	6.5	75
2230	Hydrogen exchange from identified regions of the S-protein component of ribonuclease as a function of temperature, pH, and the binding of S-peptide. *Journal of Molecular Biology*, **1981**, 145, 835-51	6.5	53
2229	Conformational and geometrical properties of beta-sheets in proteins. I. Parallel beta-sheets. *Journal of Molecular Biology*, **1981**, 146, 101-17	6.5	61
2228	Conformational and geometrical properties of beta-sheets in proteins. II. Antiparallel and mixed beta-sheets. *Journal of Molecular Biology*, **1981**, 146, 119-41	6.5	62
2227	1H nuclear magnetic resonance study of the histidine residues of insulin. *Journal of Molecular Biology*, **1981**, 150, 609-13	6.5	29
2226	A reassessment of the structure of Paracoccus cytochrome c-550. *Journal of Molecular Biology*, **1981**, 147, 351-6	6.5	42
2225	Molecular dynamics of ferrocytochrome c. Magnitude and anisotropy of atomic displacements. *Journal of Molecular Biology*, **1981**, 153, 1087-109	6.5	134
2224	Disulphide bridges in globular proteins. *Journal of Molecular Biology*, **1981**, 151, 261-87	6.5	703
2223	Analysis of the tertiary structure of protein beta-sheet sandwiches. *Journal of Molecular Biology*, **1981**, 148, 253-72	6.5	94
2222	Binding of hydroxamic acid inhibitors to crystalline thermolysin suggests a pentacoordinate zinc intermediate in catalysis. **1981**, 20, 6912-20		221
2221	Location of structural domains in protein. **1981**, 20, 6544-52		128
2220	An inhomogeneous self-consistent reaction field theory of protein core effects. Towards a quantum scheme for describing enzyme reactions. **1981**, 75, 3624-3635		85
2219	Rotation of sickle cells in homogeneous magnetic fields. **1981**, 36, 443-7		12

2218	Folding units in globular proteins. **1981**, 78, 4304-8	120
2217	Relative orientation of close-packed beta-pleated sheets in proteins. **1981**, 78, 4146-50	95
2216	Energy Surface of Protein Molecule in the Conformational Phase Space. **1981**, 50, 261-269	2
2215	GRAMPS - A graphics language interpreter for real-time, interactive, three-dimensional picture editing and animation. **1981**, 15, 133-142	70
2214	Orientation of oxygen in oxyhaemoproteins and its implications for haem catabolism. **1981**, 289, 93-5	29
2213	Location of domains in globular proteins. **1981**, 291, 85-7	66
2212	Intramolecular flexibility in phenylalanine transfer RNA. **1981**, 294, 286-7	43
2211	Structure of vitamin D-dependent calcium-binding protein from bovine intestine. **1981**, 294, 327-32	299
2210	Dipoles of the alpha-helix and beta-sheet: their role in protein folding. **1981**, 294, 532-6	277
2209	Real-time color graphics in studies of molecular interactions. **1981**, 211, 661-6	213
2208	GRAMPS - A graphics language interpreter for real-time, interactive, three-dimensional picture editing and animation. **1981**,	5
2207	Application of Ring Current Calculations to the Proton NMR of Proteins and Transfer RNA. **1982**, 193-336	68
2206	Computer-generated schematic diagrams of protein structures. **1982**, 216, 539-40	188
2205	alpha-Helix dipole model and electrostatic stabilization of 4-alpha-helical proteins. **1982**, 79, 4545-9	122
2204	Amino acid sequence homology among the 2-hydroxy acid dehydrogenases: mitochondrial and cytoplasmic malate dehydrogenases form a homologous system with lactate dehydrogenase. **1982**, 79, 6166-70	124
2203	Structural similarity in the DNA-binding domains of catabolite gene activator and cro repressor proteins. **1982**, 79, 3097-100	165
2202	Electrostatic potential molecular surfaces. **1982**, 79, 3754-8	288
2201	Slow structural changes shown by the 3-nitrotyrosine-237 residue in pig heart [Tyr(3NO2)237] lactate dehydrogenase. **1982**, 201, 465-71	30

2200	A computergraphical method of describing the shapes of subunit interfaces of oligomers. Analysis of the quaternary structure of concanavalin A and of prealbumin. **1982**, 205, 353-9		5
2199	Elementary Patterns in Protein-Nucleic Acid Interactions. IV. Crystal Structure of 3-(Adenin-9-yl)propionamide : 1-Methylthymine (1 : 1) Complex Dihydrate. **1982**, 55, 2734-2738		12
2198	A conformational approach to the study of the dynamics of enzyme inhibition: studies on thermolysin. **1982**, 4, 130-136		6
2197	A structural model for the chromophore-binding domain of ovine rhodopsin. **1982**, 4, 263-268		71
2196	Sequential resonance assignments in protein 1H nuclear magnetic resonance spectra. Computation of sterically allowed proton-proton distances and statistical analysis of proton-proton distances in single crystal protein conformations. *Journal of Molecular Biology*, **1982**, 155, 321-46	6.5	517
2195	Analysis and prediction of the packing of alpha-helices against a beta-sheet in the tertiary structure of globular proteins. *Journal of Molecular Biology*, **1982**, 156, 821-62	6.5	128
2194	Evolution of proteins formed by beta-sheets. I. Plastocyanin and azurin. *Journal of Molecular Biology*, **1982**, 160, 309-23	6.5	121
2193	Evolution of proteins formed by beta-sheets. II. The core of the immunoglobulin domains. *Journal of Molecular Biology*, **1982**, 160, 325-42	6.5	259
2192	Structure of thermolysin refined at 1.6 A resolution. *Journal of Molecular Biology*, **1982**, 160, 623-39	6.5	430
2191	On the problem of comparing protein structures. Development and applications of a new method for the assessment of structural similarities of polypeptide conformations. *Journal of Molecular Biology*, **1982**, 156, 359-88	6.5	46
2190	Crystallographic study of the binding of a trifluoroacetyl dipeptide anilide inhibitor with elastase. *Journal of Molecular Biology*, **1982**, 162, 645-58	6.5	55
2189	Reactivity of ferric Aplysia and sperm whale myoglobins towards imidazole. X-ray and binding study. *Journal of Molecular Biology*, **1982**, 158, 305-15	6.5	89
2188	Crystallographic refinement and atomic models of two different forms of citrate synthase at 2.7 and 1.7 A resolution. *Journal of Molecular Biology*, **1982**, 158, 111-52	6.5	481
2187	Crystallization and preliminary crystallographic analysis at low resolution of the allosteric L-lactate dehydrogenase from Lactobacillus casei. *Journal of Molecular Biology*, **1982**, 162, 819-38	6.5	18
2186	Three-dimensional structure of the complex between pancreatic secretory trypsin inhibitor (Kazal type) and trypsinogen at 1.8 A resolution. Structure solution, crystallographic refinement and preliminary structural interpretation. *Journal of Molecular Biology*, **1982**, 162, 839-68	6.5	177
2185	Role of local induced-fit of Ser 195 in beta-trypsin: a molecular orbital study. **1982**, 139, 181-4		4
2184	Determination and analysis of the 2 A-structure of copper, zinc superoxide dismutase. *Journal of Molecular Biology*, **1982**, 160, 181-217	6.5	879
2183	Protein conformation from electron spin relaxation data. **1982**, 38, 299-310		115

2182	Correspondence of homologies in amino acid sequence and tertiary structure of protein molecules. **1982**, 701, 242-52	46
2181	Phase extension and refinement. II. Application to metmyoglobin 2.0 Å data. **1982**, 38, 117-122	5
2180	The maximum determinant method and the maximum entropy method. **1982**, 38, 122-128	20
2179	On the evaluation of root-mean-square errors in atomic coordinates in protein crystallography. **1982**, 38, 432-438	4
2178	Interference effects among variants. **1982**, 38, 438-442	3
2177	The chiroptical properties of proteins. III. Adenylate kinase. **1982**, 21, 547-63	6
2176	Normal vibrations of proteins: glucagon. **1982**, 21, 711-4	60
2175	Equilibrium folding and unfolding pathways for a model protein. **1982**, 21, 1333-63	31
2174	The role of the environment around the catalytic triad in α-trypsin: A molecular orbital study. **1982**, 11, 322-327	5
2173	The pKa value of His 57-Asp 102 couple in the active site of bovine pancreatic beta-trypsin: a molecular orbital study. **1982**, 99, 759-75	7
2172	Molecular graphics on microcomputers. **1982**, 10, 104-107	4
2171	Structure-function relationship of [2Fe-2S] ferredoxins and design of a model molecule. **1982**, 15, 243-57	39
2170	Conformational analysis by bond orbitals with delocalization corrections: Rotation of the ser-195 side chain in α-chymotrypsin. **1982**, 22, 929-938	12
2169	Conformation of terminal regions in proteins. **1982**, 298, 296-7	15
2168	Electrostatic orientation during electron transfer between flavodoxin and cytochrome c. **1983**, 301, 169-71	114
2167	Prediction of super-secondary structure in proteins. **1983**, 301, 540-2	97
2166	Structure of trimeric haemerythrin. **1983**, 303, 86-8	43
2165	Interior turns in globular proteins. **1983**, 304, 654-7	47

2164	Analytical molecular surface calculation. **1983**, 16, 548-558	1954
2163	Prediction of three-dimensional structure of plant lectins from the domains of concanavalin A. **1983**, 743, 212-8	19
2162	Assessment of secondary-structure prediction of proteins. Comparison of computerized Chou-Fasman method with others. **1983**, 748, 285-99	88
2161	On the electrostatic properties of papain in relation to its enzymatic activity. **1983**, 24, 353-371	20
2160	Equilibrium folding pathways for model proteins. **1983**, 30, 549-559	2
2159	Determination of the Raman tensor of the haem group in myoglobin by resonance Raman scattering in solution and single crystals. **1983**, 10, 257-273	9
2158	Equilibrium folding-unfolding pathways of model proteins: effect of myoglobin-heme contacts. **1983**, 22, 79-85	6
2157	Dictionary of protein secondary structure: pattern recognition of hydrogen-bonded and geometrical features. **1983**, 22, 2577-637	11842
2156	Bond orbital framework for rapid calculation of environmental effects on molecular potential surfaces. **1983**, 96, 499-501	37
2155	Electron microscopy of tRNA crystals. **1983**, 12, 201-211	4
2154	An ellipsoidal approximation of protein shape. **1983**, 1, 30-38	81
2153	Colour stereo space-filling representations of Ribonuclease- mononucleotide interactions. **1983**, 1, 68-70	4
2152	A toolkit for computational molecular biology I: packing and unpacking of protein coordinate sets. **1983**, 1, 118-121	3
2151	Proteins and polypeptides computer graphics for space-filling model representations. **1983**, 7, 67-74	7
2150	Comparison of protein electrostatic potential along the catalytic triad of serine proteinases. **1983**, 103, 349-56	35
2149	Conformational properties of the neurotoxins and cytotoxins isolated from Elapid snake venoms. **1983**, 14, 113-71	179
2148	Protein engineering. **1983**, 219, 666-71	151
2147	Structural analysis of the inhibition of thermolysin by an active-site-directed irreversible inhibitor. **1983**, 22, 236-40	42

2146	Amino and carboxy-terminal regions in globular proteins. *Journal of Molecular Biology*, **1983**, 167, 443-60	6.5	178
2145	Three-dimensional reconstruction and averaging of 50 S ribosomal subunits of Escherichia coli from electron micrographs. *Journal of Molecular Biology*, **1983**, 163, 431-50	6.5	50
2144	Representation of short and long-range handedness in protein structures by signed distance maps. *Journal of Molecular Biology*, **1983**, 163, 613-21	6.5	23
2143	Solvent-accessible surfaces of proteins and nucleic acids. **1983**, 221, 709-13		2405
2142	Insulinomimetic homology of concanavalin A. **1983**, 10, 223-8		1
2141	How good are predictions of protein secondary structure?. **1983**, 155, 179-82		292
2140	Adaptation of plasminogen activator sequences to known protease structures. **1983**, 157, 219-23		54
2139	Ion-pairs in proteins. *Journal of Molecular Biology*, **1983**, 168, 867-85	6.5	599
2138	Anomalous x-ray scattering from terbium-labeled parvalbumin in solution. **1983**, 41, 287-92		36
2137	Structure of the complex of Streptomyces griseus protease B and the third domain of the turkey ovomucoid inhibitor at 1.8-A resolution. **1983**, 22, 4420-33		210
2136	A 1H nOe and CD study of the salt-concentration dependence of the structure of d(G-C). **1983**, 11, 3779-93		12
2135	Modular structural units, exons, and function in chicken lysozyme. **1983**, 80, 1964-8		132
2134	Crystal Structure of Adenine-1-(2-Carboxyethyl)uracil (1 : 1) Complex. A Model for Interactions of Amino Acid Side Chains with Nucleic Acid Base Pair. **1983**, 56, 2234-2237		13
2133	Three-dimensional structure of fungal proteinase K reveals similarity to bacterial subtilisin.. **1984**, 3, 1311-1314		68
2132	Computer analysis and structure prediction of nucleic acids and proteins. **1984**, 12, 417-28		50
2131	Effect of configuration of the inhibitors on the mode of binding to the enzyme, thermolysin. **1984**, 2, 29-40		2
2130	An iterative approach to placing counterions around DNA. **1984**, 1, 1525-33		13
2129	Fractal Analysis of Tertiary Structure of Protein Molecule. **1984**, 53, 2162-2171		29

2128	Structural and functional aspects of domain motions in proteins. **1984**, 15, 291-384		209
2127	The binding of 2,3-diphosphoglycerate to haemoglobin: A student exercise in modelling protein-ligand interactions. **1984**, 12, 65-68		
2126	A new approach to illustrating electrostatic molecular surfaces. **1984**, 2, 14-17		16
2125	CDA: an interactive program for the comparative analysis of crystal structure coordinate data. **1984**, 2, 70-78		1
2124	VENUS a program to display protein structure using raster colour graphics. **1984**, 2, 79-82		7
2123	O?s and N?s close contacts in serine proteinases. **1984**, 125, 159-165		2
2122	3.2 structure of the copper-containing, oxygen-carrying protein Panulirus interruptus haemocyanin. **1984**, 309, 23-29		351
2121	The reactivity of anti-peptide antibodies is a function of the atomic mobility of sites in a protein. **1984**, 312, 127-34		460
2120	The catalytic mechanism of serine proteases: single proton versus double proton transfer. **1984**, 107, 329-38		7
2119	Improvement of protein phases by coarse model modification. **1984**, 40, 269-277		24
2118	A method for the systematic comparison of the three-dimensional structures of proteins and some results. **1984**, 40, 600-610		33
2117	On integrating the techniques of direct methods and isomorphous replacement. III. The three-phase invariant for the native and two-derivative case. **1984**, 40, 646-651		3
2116	Charge interactions of cytochrome c with cytochrome c oxidase. **1984**, 16, 1059-64		5
2115	Conformational analysis by scaled energy embedding. **1984**, 5, 548-554		19
2114	The analysis of protein structures: New insights from a growing data base. **1984**, 1, 105-110		2
2113	Buried surface area, conformational entropy, and protein stability. **1984**, 23, 1605-20		58
2112	Structure-activity relationships of sulfonamide drugs and human carbonic anhydrase C: modeling of inhibitor molecules into the receptor site of the enzyme with an interactive computer graphics display. *Journal of Pharmaceutical Sciences*, **1984**, 73, 352-8	3.9	24
2111	Structural implications of primary sequences from a family of Balbiani ring-encoded proteins in Chironomus. **1984**, 20, 296-303		35

2110	Protein-protein recognition: method for finding complementary surfaces of interacting proteins. **1984**, 111, 17-30		26
2109	The spatial structure of the axially bound methionine in solution conformations of horse ferrocytochrome c and Pseudomonas aeruginosa ferrocytochrome c551 by 1H NMR. **1984**, 11, 3-15		25
2108	Hydrogen bonding in globular proteins. **1984**, 44, 97-179		1422
2107	Pyridoxal phosphate modified cytochromes c. Identification and electron transfer properties. **1984**, 765, 329-39		11
2106	FFT method to compute solution X-ray scattering curves. **1984**, 66, 121-6		5
2105	Electrostatic effects in water-accessible regions of proteins. **1984**, 23, 3887-3891		123
2104	Binding of N-carboxymethyl dipeptide inhibitors to thermolysin determined by X-ray crystallography: a novel class of transition-state analogues for zinc peptidases. **1984**, 23, 5724-9		150
2103	Substrate-cofactor interactions for glycogen phosphorylase b: a binding study in the crystal with heptenitol and heptulose 2-phosphate. **1984**, 23, 5862-73		66
2102	A fast method of comparing protein structures. **1984**, 168, 97-102		21
2101	Modelling the ATP-binding site of oncogene products, the epidermal growth factor receptor and related proteins. **1984**, 175, 387-92		111
2100	Proline-containing beta-turns in peptides and proteins: analysis of structural data on globular proteins. **1984**, 232, 482-95		16
2099	Polypeptide secondary structure determination by nuclear magnetic resonance observation of short proton-proton distances. *Journal of Molecular Biology*, **1984**, 180, 715-40	6.5	658
2098	Calibration of the angular dependence of the amide proton-C alpha proton coupling constants, 3JHN alpha, in a globular protein. Use of 3JHN alpha for identification of helical secondary structure. *Journal of Molecular Biology*, **1984**, 180, 741-51	6.5	885
2097	An analysis of incorrectly folded protein models. Implications for structure predictions. *Journal of Molecular Biology*, **1984**, 177, 787-818	6.5	267
2096	Twisted hyperboloid (Strophoid) as a model of beta-barrels in proteins. *Journal of Molecular Biology* , **1984**, 177, 567-73	6.5	37
2095	Role of catalytic residues in the formation of a tetrahedral adduct in the acylation reaction of bovine beta-trypsin. A molecular orbital study. *Journal of Molecular Biology*, **1984**, 179, 103-23	6.5	19
2094	Mechanisms of domain closure in proteins. *Journal of Molecular Biology*, **1984**, 174, 175-91	6.5	162
2093	Recognition of super-secondary structure in proteins. *Journal of Molecular Biology*, **1984**, 173, 487-514	6.5	110

2092	On the environment of ionizable groups in globular proteins. *Journal of Molecular Biology*, **1984**, 173, 515-21	6.5	140
2091	Refined structure of cytochrome c3 at 1.8 A resolution. *Journal of Molecular Biology*, **1984**, 172, 109-39	6.5	280
2090	Intrahelical hydrogen bonding of serine, threonine and cysteine residues within alpha-helices and its relevance to membrane-bound proteins. *Journal of Molecular Biology*, **1984**, 175, 75-81	6.5	235
2089	Protein dynamics. **1984**, 47, 1-46		227
2088	The hydrophobic moment detects periodicity in protein hydrophobicity. **1984**, 81, 140-4		772
2087	On the use of sequence homologies to predict protein structure: identical pentapeptides can have completely different conformations. **1984**, 81, 1075-8		335
2086	Allosteric interactions of glycogen phosphorylase b. A crystallographic study of glucose 6-phosphate and inorganic phosphate binding to di-imidate-cross-linked phosphorylase b. **1984**, 218, 45-60		31
2085	Computer graphics of large macromolecules. **1985**, 13, 793-5		8
2084	Automatic recognition of domains in globular proteins. **1985**, 115, 430-40		13
2083	Normal modes for specific motions of macromolecules: application to the hinge-bending mode of lysozyme. **1985**, 82, 4995-9		296
2082	Structural invariants of antigen binding: comparison of immunoglobulin VL-VH and VL-VL domain dimers. **1985**, 82, 4592-6		81
2081	Influence of solvent accessibility and intermolecular contacts on atomic mobilities in hemerythrins. **1985**, 82, 1104-7		68
2080	Identical short peptide sequences in unrelated proteins can have different conformations: a testing ground for theories of immune recognition. **1985**, 82, 5255-9		145
2079	Crystal and molecular structure of chymotrypsin inhibitor 2 from barley seeds in complex with subtilisin Novo. **1985**, 82, 7242-6		115
2078	Three-dimensional structure of beta 2-microglobulin. **1985**, 82, 4225-9		151
2077	The 2-A resolution structure of a thermostable ribonuclease A chemically cross-linked between lysine residues 7 and 41. **1985**, 82, 8473-7		19
2076	Solution of the embedding problem and decomposition of symmetric matrices. **1985**, 82, 2197-201		30
2075	Molecular structure of human renin and its gene.. **1985**, 61, 257-260		1

2074	Searching for interacting surfaces of proteins--the improved method. **1985**, 116, 607-12	7
2073	Surface electrostatic potentials on macromolecules in a monopole approximation: a computer program and an application to cytochromes. **1985**, 115, 571-593	25
2072	The catalytic mechanism of serine proteases II: The effect of the protein environment in the alpha-chymotrypsin proton relay system. **1985**, 112, 783-98	25
2071	Structure of the calcium regulatory muscle protein troponin-C at 2.8 A resolution. **1985**, 313, 653-9	595
2070	Sulphate sequestered in the sulphate-binding protein of Salmonella typhimurium is bound solely by hydrogen bonds. **1985**, 314, 257-60	409
2069	Beta-hairpin families in globular proteins. **1985**, 316, 170-4	522
2068	Cooperative dimeric and tetrameric clam haemoglobins are novel assemblages of myoglobin folds. **1985**, 316, 277-80	96
2067	Visualization of electrostatic recognition by enzymes for their ligands and cofactors. **1985**, 3, 2-11	35
2066	Interactive program for investigation of protein structures based on 1H NMR experiments. **1985**, 3, 79-83	40
2065	Reasoning about protein topology using the logic programming language PROLOG. **1985**, 3, 151-157	43
2064	A low cost system for the graphical display of space-filling models of proteins. **1985**, 9, 301-315	3
2063	Statistical analysis of the physical properties of the 20 naturally occurring amino acids. **1985**, 4, 23-55	262
2062	Relation between sequence similarity and structural similarity in proteins. Role of important properties of amino acids. **1985**, 4, 265-297	55
2061	Molecular surface Triangulation. **1985**, 18, 499-505	150
2060	Energy difference associated with proline isomerization in ribonuclease A. **1985**, 830, 109-12	9
2059	Ionization of tyrosine residues in horse-heart ferricytochrome c and its guanidinated and acetylated-guanidinated derivatives. **1985**, 828, 325-35	4
2058	A direct-methods solution to the phase problem in the single isomorphous replacement case: theoretical basis and initial applications. **1985**, 41, 571-577	27
2057	Structure of a serine protease from rat mast cells determined from twinned crystals by isomorphous and molecular replacement. **1985**, 41, 139-147	25

2056	The crystal and molecular structure of the third domain of silver pheasant ovomucoid (OMSVP3). **1985**, 147, 387-95	103
2055	Erabutoxin b. Initial protein refinement and sequence analysis at 0.140-nm resolution. **1985**, 153, 521-7	42
2054	Energetics of multihelix interactions in protein folding: application to myoglobin. **1985**, 24, 1271-91	21
2053	Simulation of the diffusion-controlled reaction between superoxide and superoxide dismutase. I. Simple models. **1985**, 24, 1323-36	61
2052	Molecular recognition. I. Automatic identification of topographic surface features. **1985**, 24, 1613-27	34
2051	Structural analysis of carboxypeptidase A and its complexes with inhibitors as a basis for modeling enzyme recognition and specificity. **1985**, 24, 1721-58	56
2050	Amino acid composition and hydrophobicity patterns of protein domains correlate with their structures. **1985**, 24, 1995-2023	45
2049	Fast approximations for accessible surface area and molecular volume of protein segments. **1985**, 24, 2511-9	12
2048	On the correlation of S-S and C-S raman bands frequencies and intensities with conformations of disulfide bridges in proteins. **1985**, 3, 185-96	10
2047	MOLECULAR DESIGNER: an interactive program for the display of protein structure on the IBM-PC. **1985**, 1, 177-81	
2046	Structural model for the trialkyltin binding site on cat hemoglobin. **1985**, 3, 579-84	11
2045	Three-dimensional structure of human renin. **1985**, 7, 3-12	123
2044	Dynamics of substrate binding to copper zinc superoxide dismutase. **1985**, 89, 1072-1074	62
2043	Fractal surfaces of proteins. **1985**, 230, 1163-5	183
2042	Electron spin relaxation rates in nitrosyl ferrous myoglobin. **1985**, 82, 2828-2830	3
2041	Fractal and spectral dimensions of biopolymer chains: Solvent studies of electron spin relaxation rates in myoglobin azide. **1985**, 82, 4699-4706	58
2040	Aromatic-aromatic interaction: a mechanism of protein structure stabilization. **1985**, 229, 23-8	2171
2039	Hydrophobicity of amino acid residues in globular proteins. **1985**, 229, 834-8	983

2038	Chapter 5 Protein crystallography. **1985**, 11, 347-415		2
2037	Interaction of pyrophosphate moieties with .alpha.-helixes in dinucleotide-binding proteins. **1985**, 24, 1346-1357		491
2036	X-ray crystallographic structure of the light-harvesting biliprotein C-phycocyanin from the thermophilic cyanobacterium Mastigocladus laminosus and its resemblance to globin structures. *Journal of Molecular Biology*, **1985**, 184, 257-77	6.5	346
2035	The active center of catalase. *Journal of Molecular Biology*, **1985**, 185, 21-37	6.5	366
2034	Low-frequency motions in protein molecules. Beta-sheet and beta-barrel. **1985**, 48, 289-97		105
2033	The role of the alpha-helix dipole in protein function and structure. **1985**, 45, 149-95		444
2032	Refined structure of alpha-lytic protease at 1.7 A resolution. Analysis of hydrogen bonding and solvent structure. *Journal of Molecular Biology*, **1985**, 184, 479-502	6.5	158
2031	Intron/exon structure of the chicken pyruvate kinase gene. **1985**, 40, 81-90		144
2030	Crystal structure of Azotobacter cytochrome c5 at 2.5 A resolution. *Journal of Molecular Biology*, **1985**, 184, 279-95	6.5	68
2029	Helix movements and the reconstruction of the haem pocket during the evolution of the cytochrome c family. *Journal of Molecular Biology*, **1985**, 182, 151-8	6.5	67
2028	Bovine chymotrypsinogen A X-ray crystal structure analysis and refinement of a new crystal form at 1.8 A resolution. *Journal of Molecular Biology*, **1985**, 185, 595-624	6.5	215
2027	Simulation of conformational changes in 2 Zn insulin. *Journal of Molecular Biology*, **1985**, 181, 317-22	6.5	26
2026	Interactions between an alpha-helix and a beta-sheet. Energetics of alpha/beta packing in proteins. *Journal of Molecular Biology*, **1985**, 186, 591-609	6.5	66
2025	Structure of ferricytochrome c' from Rhodospirillum molischianum at 1.67 A resolution. *Journal of Molecular Biology*, **1985**, 186, 627-43	6.5	173
2024	Domain association in immunoglobulin molecules. The packing of variable domains. *Journal of Molecular Biology*, **1985**, 186, 651-63	6.5	349
2023	Quantitation of the immunogenic potential of protein antigens. **1985**, 22, 1243-54		12
2022	Radial distributions of water□water distances in protein crystals. **1985**, 7, 223-225		4
2021	Electrostatic complementarity between the catalytic triad and the protein environment in serine proteinases. **1985**, 123, 413-419		6

2020	Modelling active site response towards changes in the protein-core of serine proteases. Aa CNDO/2□NDO SCRF study of subtilisin and thiosubtilisin. **1985**, 123, 67-84	11
2019	Quantum chemical conformational analysis of the catalytic triad in □chymotrypsin. **1985**, 123, 85-95	14
2018	Study of ethanol-lysozyme interactions using neutron diffraction. **1985**, 24, 5862-9	45
2017	Estimation of effective interresidue contact energies from protein crystal structures: quasi-chemical approximation. **1985**, 18, 534-552	1307
2016	Inactivation of chymotrypsin by 5-benzyl-6-chloro-2-pyrone: 13C NMR and X-ray diffraction analyses of the inactivator-enzyme complex. **1985**, 24, 64-8	33
2015	Common structural framework of the two Ca2+/Mg2+ binding loops of troponin C and other Ca2+ binding proteins. **1985**, 24, 5298-302	108
2014	Crystallization and structure at 3.2 □resolution of a terbium parvalbumin. **1985**, 182, 103-106	8
2013	Amino-aromatic interactions in proteins. **1986**, 203, 139-43	621
2012	Reduction in potency and reversal of left-shifting activity of BW12C with the major and minor components of chicken hemoglobin. **1986**, 209, 129-33	
2011	Oscillations of trypsinogen activation. **1986**, 23, 269-76	3
2010	Prediction of protein structural class by discriminant analysis. **1986**, 874, 205-15	79
2009	Recognition and interactions controlling the assemblies of beta barrel domains. **1986**, 49, 191-206	41
2008	A model of the Fc of immunoglobulin E. **1986**, 23, 1063-75	45
2007	Ionic association in water: from atoms to enzymes. **1986**, 482, 210-21	15
2006	Vibrational spectroscopy and conformation of peptides, polypeptides, and proteins. **1986**, 38, 181-364	2207
2005	Internal cavities and buried waters in globular proteins. **1986**, 25, 3619-25	258
2004	Long-range electron transfer in heme proteins. **1986**, 233, 948-52	293
2003	Hydrogen-1 nuclear magnetic resonance investigation of Clostridium pasteurianum rubredoxin: previously unobserved signals. **1986**, 25, 50-4	15

2002	Static accessibility model of protein antigenicity: the case of scorpion neurotoxin. **1986**, 25, 6748-54		28
2001	Electrostatic analysis of the interaction of cytochrome c with native and dimethyl ester heme substituted cytochrome b5. **1986**, 25, 7085-91		91
2000	Location of antigenic epitopes on antibody molecules. *Journal of Molecular Biology*, **1986**, 189, 715-21	6.5	56
1999	Construction of an atomic model for tropomyosin and implications for interactions with actin. *Journal of Molecular Biology*, **1986**, 192, 128-31	6.5	49
1998	X-ray structure and refinement of carbon-monoxy (Fe II)-myoglobin at 1.5 A resolution. *Journal of Molecular Biology*, **1986**, 192, 133-54	6.5	495
1997	Kinetics of electron transfer between cytochromes c' and the semiquinones of free flavin and clostridial flavodoxin. **1986**, 25, 1383-90		39
1996	An improved approach to the analysis of drug-protein binding by distance geometry. **1986**, 134, 415-28		
1995	Identification and analysis of extended strands and □sheets in globular proteins. **1986**, 8, 89-96		3
1994	Comparison of intramolecular packing of a protein in native and □holten globule□states. **1986**, 8, 226-230		45
1993	Mn2+-probe ESR method for the analyses of the dissociation of charged residues on the surface of immunoglobulins. **1986**, 23, 285-90		7
1992	Antibody Fab assembly: the interface residues between CH1 and CL. **1986**, 23, 951-60		26
1991	Phosphocholine binding immunoglobulin Fab McPC603. An X-ray diffraction study at 2.7 A. *Journal of Molecular Biology*, **1986**, 190, 593-604	6.5	579
1990	Identification of protein sequence homology by consensus template alignment. *Journal of Molecular Biology*, **1986**, 188, 233-58	6.5	270
1989	Refined models for computer calculations in protein engineering. Calibration and testing of atomic potential functions compatible with more efficient calculations. *Journal of Molecular Biology*, **1986**, 188, 259-81	6.5	51
1988	Location of □ontinuous□antigenic determinants in the protruding regions of proteins.. **1986**, 5, 409-413		211
1987	X-ray crystal structure of the complex of human leukocyte elastase (PMN elastase) and the third domain of the turkey ovomucoid inhibitor.. **1986**, 5, 2453-2458		218
1986	Refined 1.2 A crystal structure of the complex formed between subtilisin Carlsberg and the inhibitor eglin c. Molecular structure of eglin and its detailed interaction with subtilisin.. **1986**, 5, 813-818		125
1985	Using known substructures in protein model building and crystallography.. **1986**, 5, 819-822		595

1984	The folding type of a protein is relevant to the amino acid composition. *Journal of Biochemistry*, **1986**, 99, 153-62	3.1	361
1983	The relation between the divergence of sequence and structure in proteins.. **1986**, 5, 823-826		1635
1982	Theoretical prediction and experimental measurement of the bile-pigment isomer pattern obtained from degradation of catalase haem. **1986**, 236, 303-6		9
1981	Four classes of beta-hairpins in proteins. **1986**, 240, 289-92		99
1980	A preliminary three-dimensional structure of angiogenin. **1986**, 83, 1965-9		63
1979	Antigenic determinants in proteins coincide with surface regions accessible to large probes (antibody domains). **1986**, 83, 226-30		251
1978	Subgroups of variable region genes of beta chains of T-cell receptors for antigen. **1986**, 83, 4461-3		44
1977	Evolutionary origin of autoreactive determinants (autogens). **1986**, 83, 2521-5		19
1976	The relation of ion pairs to protein hydration: An IR spectroscopic and X-ray crystallographic survey. **1986**, 25, 317-335		13
1975	Spermine-nucleic acid interactions: a theoretical study. **1986**, 25, 375-92		43
1974	Molecular cartography of globular proteins with application to antigenic sites. **1986**, 25, 863-83		55
1973	Peptide-bond distortions and the curvature of alpha-helices. **1986**, 25, 1087-93		31
1972	Shape complementarity at the hemoglobin alpha 1 beta 1 subunit interface. **1986**, 25, 1229-47		190
1971	Evolutionary similarity among peptide segments is a basis for prediction of protein folding. **1986**, 25, 1565-77		42
1970	Prediction of protein structural class from the amino acid sequence. **1986**, 25, 1659-72		160
1969	The distribution of charged groups in proteins. **1986**, 25, 1717-33		119
1968	5-(N-Arylnortropan-3-yl)- and 5-(N-Arylpiperidin-4-yl)-2,4-diaminopyrimidines. Novel Inhibitors of Dihydrofolate Reductase. **1986**, 69, 887-897		5
1967	Approaches to Synthetic Vaccines Design of Epitope-Containing Amphiphilic Peptides Matching the Antigenic Structure in the Native Protein. **1986**, 69, 985-995		14

1966	Spatial geometric arrangements of disulfide-crosslinked loops in proteins. **1986**, 7, 67-88	32
1965	Spatially constrained minimization of macromolecules. **1986**, 7, 165-175	38
1964	Interactive program for visualization and modelling of proteins, nucleic acids and small molecules. **1986**, 4, 82-87	136
1963	Plotting protein surfaces. **1986**, 4, 93-96	6
1962	Comprehensive molecular modelling system. **1986**, 4, 134-142	9
1961	Visualization of energetics and conformations from molecular computer simulations. **1986**, 4, 203-207	6
1960	Measurement of protein surface shape by solid angles. **1986**, 4, 3-6	95
1959	Origin of low-frequency motions in biological macromolecules. A view of recent progress in the quasi-continuity model. **1986**, 25, 105-16	32
1958	A computer program for normal-coordinate calculations of a polypeptide chain with any conformation and length. **1986**, 143, 445-448	5
1957	The catalytic mechanism of serine proteases. III. An Indo-ISCRF study of the methylacetate docking in alpha-chymotrypsin. **1986**, 118, 45-59	9
1956	Thermal motion of whole protein molecules in protein solids. **1986**, 121, 73-88	21
1955	The galactan-binding immunoglobulin Fab J539: an X-ray diffraction study at 2.6-A resolution. **1986**, 1, 74-80	167
1954	An algorithm for determining the conformation of polypeptide segments in proteins by systematic search. **1986**, 1, 146-63	246
1953	Predicting antibody hypervariable loop conformations. II: Minimization and molecular dynamics studies of MCPC603 from many randomly generated loop conformations. **1986**, 1, 342-62	197
1952	Molecular structure of an aspartic proteinase zymogen, porcine pepsinogen, at 1.8 A resolution. **1986**, 319, 33-8	294
1951	Continuous and discontinuous protein antigenic determinants. **1986**, 322, 747-8	471
1950	Alpha-lactalbumin possesses a novel calcium binding loop. **1986**, 324, 84-7	213
1949	The deposition of crystallographic results: current problems and their causes. **1986**, 42, 1671-1675	1

1948	Molecular speleology: the exploration of crevices in proteins for prediction of binding sites, design of drugs and analysis of surface recognition. **1986**, 42, 83-85	8
1947	Crystallographic structural analysis of phosphoramidates as inhibitors and transition-state analogs of thermolysin. **1986**, 157, 261-8	98
1946	The pH and redox-state dependence of the copper site in azurin from Pseudomonas aeruginosa as studied by EXAFS. **1986**, 873, 214-27	34
1945	Amino acid sequence homology applied to the prediction of protein secondary structures, and joint prediction with existing methods. **1986**, 871, 45-54	80
1944	Using Prolog to represent and reason about protein structure. **1986**, 536-543	4
1943	Potential metal-binding domains in nucleic acid binding proteins. **1986**, 232, 485-7	1083
1942	Visualization of the entire surface of a protein by cartographic projection. **1986**, 2, 265-8	
1941	Loops in globular proteins: a novel category of secondary structure. **1986**, 234, 849-55	509
1940	PROPHET, a national computing resource for life science research. **1986**, 14, 21-4	4
1939	Molecular dynamics of a cytochrome c-cytochrome b5 electron transfer complex. **1987**, 238, 794-7	166
1938	Inhibition of serine proteinases by tetra-p-amidinophenoxy-neo-pentane: thermodynamic and molecular modeling study. **1987**, 2, 23-30	7
1937	Perspectives on antigenicity and idiotypy. **1987**, 2, 339-56	14
1936	Approaching a complete classification of protein secondary structure. **1987**, 5, 689-704	27
1935	Agreement between single crystal X-ray and molecular mechanical sugar ring conformations. **1987**, 5, 513-37	8
1934	Preparation and characterization in solution of oligonucleotides alkylated by activated carcinogenic polycyclic aromatic hydrocarbons. **1987**, 5, 615-37	7
1933	Nucleic acid model building: the multiple backbone solutions associated with a given base morphology. **1987**, 4, 895-938	61
1932	A stereochemical model of the transpeptidation complex. **1987**, 4, 729-44	15
1931	Bacterial resistance to beta-lactam antibiotics: crystal structure of beta-lactamase from Staphylococcus aureus PC1 at 2.5 A resolution. **1987**, 236, 694-701	359

1930	Molecular structure of troponin C and its implications for the Ca2+ triggering of muscle contraction. **1987**, 139, 610-32		15
1929	Pig pancreatic anhydro-elastase. Role of the serine-195 hydroxy group in the binding of inhibitors and substrate. **1987**, 242, 267-73		3
1928	Binding of a reduced peptide inhibitor to the aspartic proteinase from Rhizopus chinensis: implications for a mechanism of action. **1987**, 84, 7009-13		292
1927	Molecular structure of mammalian neuropeptide Y: analysis by molecular cloning and computer-aided comparison with crystal structure of avian homologue. **1987**, 84, 2532-6		173
1926	Three-dimensional structure of a genetically engineered variant of porcine growth hormone. **1987**, 84, 6434-7		401
1925	Three-dimensional structure of an antibody-antigen complex. **1987**, 84, 8075-9		561
1924	Tertiary templates for proteins. Use of packing criteria in the enumeration of allowed sequences for different structural classes. *Journal of Molecular Biology*, **1987**, 193, 775-91	6.5	1366
1923	Interior and surface of monomeric proteins. *Journal of Molecular Biology*, **1987**, 196, 641-56	6.5	784
1922	Rat submaxillary gland serine protease, tonin. Structure solution and refinement at 1.8 A resolution. *Journal of Molecular Biology*, **1987**, 195, 373-96	6.5	121
1921	Crystal and molecular structures of the complex of alpha-chymotrypsin with its inhibitor turkey ovomucoid third domain at 1.8 A resolution. *Journal of Molecular Biology*, **1987**, 195, 397-418	6.5	235
1920	Refinement of the crystal structure of wheat germ agglutinin isolectin 2 at 1.8 A resolution. *Journal of Molecular Biology*, **1987**, 194, 501-29	6.5	88
1919	The tertiary structure of azurin from Pseudomonas denitrificans as determined by Cu resonant diffraction using synchrotron radiation. *Journal of Molecular Biology*, **1987**, 196, 413-9	6.5	38
1918	Hydrophobicity and residue-residue contacts in globular proteins. **1987**, 9, 39-48		13
1917	Sidechain rotational isomerization in proteins. Dynamic simulation with solvent surroundings. **1987**, 51, 637-41		26
1916	Interpretation of fluorescence decays in proteins using continuous lifetime distributions. **1987**, 51, 925-36		283
1915	Canonical structures for the hypervariable regions of immunoglobulins. *Journal of Molecular Biology*, **1987**, 196, 901-17	6.5	1195
1914	Calculations of electrostatic properties in proteins. Analysis of contributions from induced protein dipoles. *Journal of Molecular Biology*, **1987**, 198, 721-35	6.5	120
1913	High-resolution crystal structure of cytochrome P450cam. *Journal of Molecular Biology*, **1987**, 195, 687-700	6.5	1283

1912	WAALSURF: Molecular graphics on a personal computer. **1987**, 11, 449-458		5
1911	Hydrophobic cluster analysis: an efficient new way to compare and analyse amino acid sequences. **1987**, 224, 149-55		508
1910	The geometries of interacting arginine-carboxyls in proteins. **1987**, 224, 161-71		85
1909	Correlation among sites of limited proteolysis, enzyme accessibility and segmental mobility. **1987**, 211, 185-9		59
1908	The hydration of protein secondary structures. **1987**, 213, 423-7		25
1907	The effect of ethylenediamine chemical modification of plastocyanin on the rate of cytochrome f oxidation and P-700+ reduction. **1987**, 894, 386-98		71
1906	Third type of secondary structure: noncooperative mobile conformation. Protein Data Bank analysis. **1987**, 146, 934-8		34
1905	A novel supersecondary structure in globular proteins comprising the collagen-like helix and beta-turn. *Journal of Molecular Biology*, **1987**, 198, 705-9	6.5	10
1904	Isolation and structure of a covalent cross-link adduct between mitomycin C and DNA. **1987**, 235, 1204-8		406
1903	Refined crystal structure of dogfish M4 apo-lactate dehydrogenase. *Journal of Molecular Biology*, **1987**, 198, 445-67	6.5	178
1902	Correlation between calculated local stability and hydrogen exchange rates in proteins. *Journal of Molecular Biology*, **1987**, 198, 339-49	6.5	17
1901	Analysis of side-chain orientations in homologous proteins. *Journal of Molecular Biology*, **1987**, 196, 175-88	6.5	128
1900	Structure of myohemerythrin in the azidomet state at 1.7/1.3 A resolution. *Journal of Molecular Biology*, **1987**, 197, 273-96	6.5	367
1899	A strategy for the rapid multiple alignment of protein sequences. Confidence levels from tertiary structure comparisons. *Journal of Molecular Biology*, **1987**, 198, 327-37	6.5	412
1898	Structure and refinement at 1.8 A resolution of the aspartic proteinase from Rhizopus chinensis. *Journal of Molecular Biology*, **1987**, 196, 877-900	6.5	196
1897	Analysis of sequence-similar pentapeptides in unrelated protein tertiary structures. Strategies for protein folding and a guide for site-directed mutagenesis. *Journal of Molecular Biology*, **1987**, 197, 331-48	6.5	114
1896	Protein structures in solution by nuclear magnetic resonance and distance geometry. The polypeptide fold of the basic pancreatic trypsin inhibitor determined using two different algorithms, DISGEO and DISMAN. *Journal of Molecular Biology*, **1987**, 196, 611-39	6.5	596
1895	Prediction of protein secondary structure and active sites using the alignment of homologous sequences. *Journal of Molecular Biology*, **1987**, 195, 957-61	6.5	375

1894	Analysis of the relationship between side-chain conformation and secondary structure in globular proteins. *Journal of Molecular Biology*, **1987**, 198, 295-310	6.5	404
1893	The pAR5 mutation and the allosteric mechanism of Escherichia coli aspartate carbamoyltransferase.. **1987**, 6, 2843-2847		15
1892	Energy minimization and molecular dynamics studies of Asn-102 elastase. **1987**, 1, 211-7		7
1891	Strategic approaches to drug design. I. An integrated software framework for molecular modelling. **1987**, 1, 31-51		300
1890	Spin density distribution in oxygen-liganded model heme proteins: Predictions of 17O hyperfine broadening of ESR spectra of metmyoglobin, cytochrome c peroxidase, catalase, and cytochrome P450. **1987**, 32, 75-83		0
1889	Continuous compact protein domains. **1987**, 2, 90-110		27
1888	Determination of three-dimensional protein structures from nuclear magnetic resonance data using fragments of known structures. **1987**, 2, 188-201		29
1887	Calculation of coordinates from incomplete and incorrect distance data. **1987**, 38, 1-9		2
1886	Molecular graphics in the study of the calcium-binding sites of carp parvalbumin and other proteins. **1987**, 5, 113-116		0
1885	An efficient newton-like method for molecular mechanics energy minimization of large molecules. **1987**, 8, 1016-1024		785
1884	Crystal Structure and Conformation of Short Linear Peptides. Part V. N-Benzyloxycarbonyl-Glycyl-Glycyl-L-Proline. **1987**, 96, 437-441		
1883	Prediction of the folding of short polypeptide segments by uniform conformational sampling. **1987** , 26, 137-68		411
1882	Conformation of DNA in solution: CD calculations based on crystal structures of B- and Z-DNA fragments. **1987**, 26, 457-61		7
1881	A new approach to the problem of docking two molecules: the ellipsoid algorithm. **1987**, 26, 777-93		43
1880	Prediction of protein--ligand interactions: the complex of porcine pancreatic elastase with a valine-derived benzoxazinone. **1987**, 26, 1207-25		
1879	Conformational constraints of amino acid side chains in alpha-helices. **1987**, 26, 1273-86		53
1878	Proline-induced constraints in alpha-helices. **1987**, 26, 1587-600		100
1877	Predicting antibody hypervariable loop conformation. I. Ensembles of random conformations for ringlike structures. **1987**, 26, 2053-85		239

1876	Using CAD to design receptor targetting of potent drugs. **1987**, 19, 91-94	1
1875	Perq interactive molecular modelling system. **1987**, 5, 63-70	2
1874	Expert system for protein engineering: its application in the study of chloramphenicol acetyltransferase and avian pancreatic polypeptide. **1987**, 5, 8-17	25
1873	Pharmacophoric pattern matching in files of 3D chemical structures: evaluation of search performance. **1987**, 5, 41-48	67
1872	Prediction of the structure of proteins using related structures, energy minimization and computer graphics. **1987**, 5, 133-140	13
1871	Beta-bulges within loops as recurring features of protein structure. **1987**, 911, 261-5	28
1870	Secondary structure predictions and medium range interactions. **1987**, 916, 200-4	139
1869	Inhibition of phosphorylcholine binding to antibodies using synthetic peptides. **1987**, 325, 168-71	5
1868	Stabilization of charges on isolated ionic groups sequestered in proteins by polarized peptide units. **1987**, 329, 561-4	110
1867	The high-resolution X-ray crystal structure of the complex formed between subtilisin Carlsberg and eglin c, an elastase inhibitor from the leech Hirudo medicinalis. Structural analysis, subtilisin structure and interface geometry. **1987**, 166, 673-92	258
1866	A toolkit for computational molecular biology. III. MICRYFON □a (fairly) general program for input of protein coordinate files. **1987**, 20, 488-490	1
1865	A certain lack of co-ordination. **1987**, 5, 59-60	
1864	A phased translation function. **1988**, 21, 490-495	103
1863	RIBBON: a stereo cartoon drawing program for proteins. **1988**, 21, 572-576	168
1862	18th Sir Hans Krebs lecture. Knowledge-based protein modelling and design. **1988**, 172, 513-20	211
1861	NMR studies of the conformations of leghemoglobins from soybean and lupin. **1988**, 178, 419-35	14
1860	Zymogen activation: effect of peptides sequentially related to the bovine beta-trypsin N-terminus on Kazal inhibitor and benzamidine binding to bovine trypsinogen. **1988**, 1, 130-7	8
1859	Conformational analysis and computer graphics in drug research. **1988**, 8, 1-25	16

1858	Effect of discrete distribution of ions on B- and Z-DNA: a theoretical investigation. **1988**, 27, 187-200	9
1857	Simulation of the diffusion-controlled reaction between superoxide and superoxide dismutase. II. Detailed models. **1988**, 27, 251-69	80
1856	Structural and energetic parameters of Ca2+ binding to peptides and proteins. **1988**, 27, 1865-86	27
1855	Analysis, design and modification of loop regions in proteins. **1988**, 8, 63-9	84
1854	YETI: An interactive molecular mechanics program for small-molecule protein complexes. **1988**, 9, 269-280	53
1853	A fast, direct algorithm for the least-squares fitting of two sets of atomic coordinates of macromolecular structures. **1988**, 9, 596-599	3
1852	Brownian dynamics simulation of protein association. **1988**, 1, 291-311	45
1851	Molecular modeling of protein structure and function: a bioinformatic approach. **1988**, 1, 323-41	5
1850	Computer-aided molecular modelling: research study or research tool?. **1988**, 2, 179-89	6
1849	Crystallographic modelling. **1988**, 2, 225-33	15
1848	Molecular modeling and dynamics of neuropeptide Y. **1988**, 2, 55-63	30
1847	Orientation and structure-building role of the water molecules bound at the contact surface of the dihydrofolate reductase-methotrexate complex. **1988**, 2, 65-76	10
1846	Comparative review of molecular modelling software for personal computers. **1988**, 2, 81-90	7
1845	Analysis of the biomacromolecular architecture of eukaryotic and prokaryotic serine proteases. **1988**, 3, 127-137	1
1844	LOPAL and SCAMP: techniques for the comparison and display of protein structures. **1988**, 6, 190-196	17
1843	Energetics of charge-charge interactions in proteins. **1988**, 3, 32-52	258
1842	Identification of structural motifs from protein coordinate data: secondary structure and first-level supersecondary structure. **1988**, 3, 71-84	341
1841	Calculation of the total electrostatic energy of a macromolecular system: solvation energies, binding energies, and conformational analysis. **1988**, 4, 7-18	724

1840	Criteria that discriminate between native proteins and incorrectly folded models. **1988**, 4, 19-30	173
1839	Oligopeptide biases in protein sequences and their use in predicting protein coding regions in nucleotide sequences. **1988**, 4, 99-122	235
1838	Comparative molecular model building of two serine proteinases from cytotoxic T lymphocytes. **1988**, 4, 190-204	75
1837	Helix lap-joints as ion-binding sites: DNA-binding motifs and Ca-binding "EF hands" are related by charge and sequence reversal. **1988**, 4, 229-39	30
1836	Structural alignment and analysis of two distantly related proteins: Aplysia limacina myoglobin and sea lamprey globin. **1988**, 4, 240-50	9
1835	Electrostatics and molecular recognition. **1988**, 34, 85-93	1
1834	Continuum electrostatics and hydration phenomena. **1988**, 34, 103-118	20
1833	Nonlinear methods for discrimination and their application to classification of protein structures. **1988**, 130, 461-8	6
1832	Protein Folding: New Twists. **1988**, 6, 167-171	7
1831	Liquid-like movements in crystalline insulin. **1988**, 332, 659-62	111
1830	Identification of predictive sequence motifs limited by protein structure data base size. **1988**, 335, 45-9	158
1829	Elbow motion in the immunoglobulins involves a molecular ball-and-socket joint. **1988**, 335, 188-90	149
1828	A protein sequence/structure database. Protein Engineering Club Database Group. **1988**, 335, 745-6	81
1827	Structure and assembly of protocatechuate 3,4-dioxygenase. **1988**, 336, 403-5	279
1826	The MIDAS database system. **1988**, 6, 2-12	24
1825	The MIDAS display system. **1988**, 6, 13-27	852
1824	Context-free spheres: A new method for rapid CPK image generation. **1988**, 6, 149-154	9
1823	MANOSK: A graphics program for analyzing and modeling molecular structure and functions. **1988**, 6, 155-160	31

1822	Description of molecular surface shape using Fourier descriptors. **1988**, 6, 104-108	71
1821	Calculating CPK images on a UNIX workstation. **1988**, 6, 109-111	2
1820	The formation of protein secondary structure. Its connection with amino acid sequence. **1988**, 31, 139-42	7
1819	Low-frequency collective motion in biomacromolecules and its biological functions. **1988**, 30, 3-48	308
1818	The reconstruction of helical particles with variable pitch. **1988**, 26, 255-70	32
1817	Electrostatic catalysis in enzymes. **1988**, 47, 281-287	12
1816	Interactive display of the subunit and chain structure of proteins on a microcomputer. **1988**, 16, 165-166	
1815	A molecular graphics suite of programs for a microcomputer to display molecules from cambridge crystallographic data files and the alpha-carbon backbone of proteins from protein data bank crystal files. **1988**, 12, 65-82	3
1814	Electrostatic features of molecular recognition by cyclic urea mimics of chymotrypsin. **1988**, 210, 151-162	8
1813	A biological macromolecule crystallization database: A basis for a crystallization strategy. **1988**, 90, 51-59	69
1812	Molecular factors stabilizing protein crystals. **1988**, 90, 273-282	33
1811	A program for semi-automatic sequential resonance assignments in protein 1H nuclear magnetic resonance spectra. **1988**, 76, 400-415	7
1810	A study on the quaternary structure change of hemoglobin in the ligation process. **1988**, 956, 243-55	4
1809	Improvements in a secondary structure prediction method based on a search for local sequence homologies and its use as a model building tool. **1988**, 955, 283-95	90
1808	Prediction of the location of structural domains in globular proteins. **1988**, 7, 427-71	60
1807	Prediction of probable pathways of folding in globular proteins. **1988**, 7, 491-507	16
1806	Segmentation of a protein into structural elements: analysis and classification of segments. **1988**, 7, 509-25	2
1805	The refined crystal structure of subtilisin Carlsberg at 2.5 A resolution. **1988**, 2, 271-6	91

1804	Structural comparison of two serine proteinase-protein inhibitor complexes: Eglin-C-subtilisin Carlsberg and CI-2-subtilisin Novo. **1988**, 27, 6582-6598		331
1803	Determination of the quaternary structural states of bovine casein by small-angle X-ray scattering: submicellar and micellar forms. **1988**, 266, 548-61		49
1802	Protein dynamics and distance determination by NOE measurements. **1988**, 236, 71-6		54
1801	Protein secondary structure and homology by neural networks. The alpha-helices in rhodopsin. **1988**, 241, 223-8		135
1800	Distributions of water around amino acid residues in proteins. *Journal of Molecular Biology*, **1988**, 202, 637-57	6.5	207
1799	Electrostatic effects of charge perturbations introduced by metal oxidation in proteins. A theoretical analysis. *Journal of Molecular Biology*, **1988**, 203, 507-10	6.5	68
1798	Amino acid substitutions in structurally related proteins. A pattern recognition approach. Determination of a new and efficient scoring matrix. *Journal of Molecular Biology*, **1988**, 204, 1019-29	6.5	282
1797	Analysis and prediction of the different types of beta-turn in proteins. *Journal of Molecular Biology*, **1988**, 203, 221-32	6.5	896
1796	Refined crystal structure of troponin C from turkey skeletal muscle at 2.0 A resolution. *Journal of Molecular Biology*, **1988**, 203, 761-79	6.5	302
1795	Effect of hydrostatic pressure on the solvent in crystals of hen egg-white lysozyme. *Journal of Molecular Biology*, **1988**, 200, 401-10	6.5	59
1794	Helix geometry in proteins. *Journal of Molecular Biology*, **1988**, 201, 601-19	6.5	922
1793	Serine hydrolase-phosphyl ester interactions: Molecular modeling. **1988**, 170, 159-169		12
1792	Calculation of proton transfers in hydrogen bonding interactions with semi-empirical MNDO/H. **1988**, 179, 153-163		6
1791	Simple determination of water orientation around hydrated molecules. **1988**, 181, 361-375		10
1790	General architecture of the alpha-helical globule. *Journal of Molecular Biology*, **1988**, 204, 749-69	6.5	125
1789	Structural analysis of polymers of sickle cell hemoglobin. I. Sickle hemoglobin fibers. *Journal of Molecular Biology*, **1988**, 199, 315-31	6.5	61
1788	Amino acid preferences for specific locations at the ends of alpha helices. **1988**, 240, 1648-52		1337
1787	Three-dimensional model of stellacyanin and its implications for electron transfer reactivity. *Journal of Molecular Biology*, **1988**, 204, 407-15	6.5	16

1786	Yeast iso-1-cytochrome c. A 2.8 A resolution three-dimensional structure determination. *Journal of Molecular Biology*, **1988**, 199, 295-314	6.5	122
1785	Studies of specificity and catalysis in trypsin by structural analysis of site-directed mutants. **1988**, 8, 225-36		17
1784	Quantum mechanical modeling of aspartic proteinase interactions: difference in binding of diastereomeric statine models. **1988**, 157, 450-6		3
1783	. **1988**, 8, 42-50		68
1782	Crystal structure of neutral protease from Bacillus cereus refined at 3.0 A resolution and comparison with the homologous but more thermostable enzyme thermolysin. *Journal of Molecular Biology*, **1988**, 199, 525-37	6.5	116
1781	Refined crystal structure of Streptomyces griseus trypsin at 1.7 A resolution. *Journal of Molecular Biology*, **1988**, 200, 523-51	6.5	109
1780	Crystal structure determination and refinement of pike 4.10 parvalbumin (minor component from Esox lucius). *Journal of Molecular Biology*, **1988**, 202, 349-53	6.5	46
1779	1H nuclear magnetic resonance study of the protonation behaviour of the histidine residues and the electron self-exchange reaction of azurin from Alcaligenes denitrificans. *Journal of Molecular Biology*, **1988**, 200, 189-99	6.5	52
1778	One type of gamma-turn, rather than the other gives rise to chain-reversal in proteins. *Journal of Molecular Biology*, **1988**, 204, 777-82	6.5	168
1777	X-ray diffraction studies of 14-filament models of deoxygenated sickle cell hemoglobin fibers. II. Models based on the deoxygenated sickle hemoglobin crystal structure. *Journal of Molecular Biology*, **1988**, 200, 141-50	6.5	2
1776	Recurring loop motif in proteins that occurs in right-handed and left-handed forms. Its relationship with alpha-helices and beta-bulge loops. *Journal of Molecular Biology*, **1988**, 199, 503-11	6.5	63
1775	Surface, subunit interfaces and interior of oligomeric proteins. *Journal of Molecular Biology*, **1988**, 204, 155-64	6.5	590
1774	Helix signals in proteins. **1988**, 240, 1632-41		630
1773	The chemistry and mechanism of antibody binding to protein antigens. **1988**, 43, 1-98		160
1772	A sequence motif in many polymerases. **1988**, 16, 9909-16		363
1771	The first sequenced normal hemoglobin lacking histidine in position 146 of the beta-chains. The primary structures of the major and minor hemoglobin components of the great crested newt (Triturus cristatus, Urodela, Amphibia). **1988**, 369, 1343-60		2
1770	Response:Crystallographic Citations. **1988**, 242, 347-348		
1769	Crystallographic citations. **1988**, 242, 347-8		

1768	A multivariate analysis method for discriminating protein secondary structural segments. **1988**, 2, 87-92		20
1767	Structure of antibody-antigen complexes: implications for immune recognition. **1988**, 43, 99-132		172
1766	Microcomputer-based three-dimensional stereoscopic macromolecular graphics display. **1988**, 4, 193-6		
1765	Three-dimensional structure of d(GGGATCCC) in the crystalline state. **1988**, 16, 7799-816		44
1764	A protein secondary structure prediction scheme for the IBM PC and compatibles. **1988**, 4, 473-7		6
1763	Turn of promotor DNA by cAMP receptor protein characterized by bead model simulation of rotational diffusion. **1988**, 5, 819-37		20
1762	Intermolecular nuclear Overhauser effect and atomic pair potential approaches to wheat germ agglutinin-sugar binding. **1988**, 6, 593-608		5
1761	A rigorous basepair oriented description of DNA structures. **1988**, 6, 397-420		30
1760	A simple qualitative representation of polypeptide chain folds: comparison of protein tertiary structures. **1988**, 5, 1267-79		34
1759	PROPHET--a national computing resource for life science research. **1988**, 16, 1873-5		8
1758	Brownian dynamics of cytochrome c and cytochrome c peroxidase association. **1988**, 241, 67-70		268
1757	Energetics of the structure of the four-alpha-helix bundle in proteins. **1988**, 85, 4295-9		123
1756	Model-building study of the combining sites of two antibodies to alpha (1----6)dextran. **1988**, 85, 6885-9		50
1755	Purification, sequence, and model structure of charybdotoxin, a potent selective inhibitor of calcium-activated potassium channels. **1988**, 85, 3329-33		269
1754	The electrostatic fields in the active-site clefts of actinidin and papain. **1988**, 254, 235-8		33
1753	Characteristic thermodynamic properties of hydrated water for 20 amino acid residues in globular proteins. *Journal of Biochemistry*, **1988**, 104, 433-9	3.1	26
1752	The Fractal Nature of Molecule-Surface Chemical Activities and Physical Interactions in Porous Materials. **1988**, 39, 421-432		7
1751	Viral cysteine proteases are homologous to the trypsin-like family of serine proteases: structural and functional implications. **1988**, 85, 7872-6		354

1750	Proposed structure for the zinc-binding domains from transcription factor IIIA and related proteins. **1988**, 85, 99-102		385
1749	Structural principles of parallel beta-barrels in proteins. **1988**, 85, 3338-42		82
1748	Protein engineering of antibody binding sites: recovery of specific activity in an anti-digoxin single-chain Fv analogue produced in Escherichia coli. **1988**, 85, 5879-83		1297
1747	The 2.5 A X-ray crystal structure of the acid-stable proteinase inhibitor from human mucous secretions analysed in its complex with bovine alpha-chymotrypsin.. **1988**, 7, 345-351		173
1746	The 2.0 A X-ray crystal structure of chicken egg white cystatin and its possible mode of interaction with cysteine proteinases.. **1988**, 7, 2593-2599		446
1745	X-ray study of baker's yeast lipoamide dehydrogenase at 4.5 A resolution by molecular replacement method. *Journal of Biochemistry*, **1988**, 103, 463-9	3.1	23
1744	Predicting Mechanism and Activity. **1989**, 26-36		1
1743	Nobel lecture. A structural basis of light energy and electron transfer in biology.. **1989**, 8, 2125-2147		45
1742	An automatic search for similar spatial arrangements of alpha-helices and beta-strands in globular proteins. **1989**, 6, 1045-60		23
1741	Modelling the polypeptide backbone with 'spare parts' from known protein structures. **1989**, 2, 335-45		153
1740	Preliminary Analysis of Water Molecule Distributions in Proteins. *Molecular Simulation*, **1989**, 3, 167-182 2		4
1739	Investigations on the convergence rate of the thermodynamic and structural parameters from Monte Carlo simulations of aqueous solutions of methanol and methylamine. **1989**, 91, 3707-3715		14
1738	Inhibition of serine proteinases by p-carbethoxyphenyl esters of epsilon-guanidino- and epsilon-amino caproic acid: thermodynamic and molecular modeling study. **1989**, 2, 249-59		3
1737	Thermal stability and cross-linking of Hb New York [beta 113(G15)Val----Glu]. **1989**, 13, 147-56		11
1736	Structure of recombinant human renin, a target for cardiovascular-active drugs, at 2.5 A resolution. **1989**, 243, 1346-51		215
1735	Searching techniques for databases of protein secondary structures. **1989**, 15, 287-298		12
1734	Amino-acid sequences and functional differentiation of hemoglobins A and D from swift (Apus apus, Apodiformes). **1989**, 370, 1197-207		11
1733	Water-inserted alpha-helical segments implicate reverse turns as folding intermediates. **1989**, 244, 1333-7		208

1732	Electrostatic interactions in proteins. A theoretical analysis of lysozyme ionization. **1989**, 999, 1-6	42
1731	Structure-function relationships in the inorganic salt-induced precipitation of alpha-chymotrypsin. **1989**, 995, 231-45	42
1730	Structural studies on bio-active compounds. Part XV. Structure-activity relationships for pyrimethamine and a series of diaminopyrimidine analogues versus bacterial dihydrofolate reductase. **1989**, 995, 21-7	14
1729	GENPRO: automatic generation of Prolog clause files for knowledge-based systems in the biomedical sciences. **1989**, 28, 207-14	1
1728	Nobel lecture. A structural basis of light energy and electron transfer in biology. **1989**, 9, 635-73	10
1727	MolDraw: Molecular graphics for the Macintosh. **1989**, 2, 65-71	36
1726	GEOM: a new tool for molecular modelling based on distance geometry calculations with NMR data. **1989**, 3, 195-210	16
1725	A molecular modeling study on binding of drugs to calmodulin. **1989**, 3, 101-9	9
1724	Resonance Raman characterization of heme Fe(IV)=O groups of intermediates of yeast cytochrome C peroxidase and lactoperoxidase. **1989**, 214, 27-41	60
1723	CRYST a system to display 3D images of crystal structure, symmetry operations and crystal forms. **1989**, 22, 633-639	5
1722	Cauchy distribution, intensity statistics and phases of reflections from crystal planes. **1989**, 45, 314-319	5
1721	Simultaneous search for symmetry-related molecules in cross-rotation functions. **1989**, 45, 309-314	
1720	Nucleotide sequence of the glyceraldehyde-3-phosphate dehydrogenase gene from the mesophilic methanogenic archaebacteria Methanobacterium bryantii and Methanobacterium formicicum. Comparison with the respective gene structure of the closely related extreme thermophile Methanothermus fervidus. **1989**, 179, 405-13	50
1719	Electron transport in sulfate-reducing bacteria. Molecular modeling and NMR studies of the rubredoxin--tetraheme-cytochrome-c3 complex. **1989**, 185, 695-700	35
1718	Algorithm for rapid calculation of excluded volume of large molecules. **1989**, 10, 376-379	40
1717	Pattern recognition in the prediction of protein structure. I. Tripeptide conformational probabilities calculated from the amino acid sequence. **1989**, 10, 770-797	53
1716	Pattern recognition in the prediction of protein structure. II. Chain conformation from a probability-directed search procedure. **1989**, 10, 798-816	37
1715	Pattern recognition in the prediction of protein structure. III. An importance-sampling minimization procedure. **1989**, 10, 817-831	31

1714	Model-building of Fnr and FixK DNA-binding domains suggests a basis for specific DNA recognition. **1989**, 2, 114-21	20
1713	Eine strukturelle Grundlage f□ die □bertragung von Lichtenergie und Elektronen in der Biologie (Nobel-Vortrag). **1989**, 101, 849-871	120
1712	Some observations on conserved polar side chains in immunoglobulin V-domains. **1989**, 21, 227-32	5
1711	Some observations on the replacement of the conserved amino acid residues of immunoglobulin domains. **1989**, 21, 1033-7	2
1710	Molecular dynamics of the alpha-helical epitope of a novel synthetic lipopeptide foot-and-mouth disease virus vaccine. **1989**, 28, 499-512	13
1709	Solvation thermodynamics of biopolymers. I. Separation of the volume and surface interactions with estimates for proteins. **1989**, 28, 1309-25	27
1708	Solvation thermodynamics of biopolymers. II. Correlations between functional groups. **1989**, 28, 1327-37	13
1707	Superoxide dismutase: fluctuations in the structure and solvation of the active site channel studied by molecular dynamics simulation. **1989**, 28, 2085-96	26
1706	The coordination polyhedron of Ca2+, Cd2+ in parvalbumin. **1989**, 163, 5-7	10
1705	Brownian simulation of cytochrome c551 association and electron self-exchange. **1989**, 41, 207-222	8
1704	Modeling loop structures in proteins and nucleic acids: an RNA stem-loop. **1989**, 7, 186-95	9
1703	A rapid method for comparing and matching the spherical parameter surfaces of molecules and other irregular objects. **1989**, 7, 130-7	26
1702	Rapid geometric searching in protein structures. **1989**, 7, 48-53	19
1701	Protein-protein interactions on the surface of immunoglobulin molecules. **1989**, 7, 60-63	10
1700	□HOODRAW□n interactive molecular graphics program (PC/XT/AT) to display small molecules complexed with protein fragments selected from the protein data bank. **1989**, 13, 387-394	1
1699	Defining the axis of a helix. **1989**, 13, 185-189	55
1698	Solubility-activity relationships in the inorganic salt-induced precipitation of □chymotrypsin. **1989**, 11, 264-276	30
1697	Consequences of magnetization transfer on the determination of solution structures of proteins. **1989**, 83, 267-278	6

1696	Thermitase, a thermostable subtilisin: comparison of predicted and experimental structures and the molecular cause of thermostability. **1989**, 5, 22-37	44
1695	Electrostatic interactions in the assembly of Escherichia coli aspartate transcarbamylase. **1989**, 5, 66-77	12
1694	Structural basis of hierarchical multiple substates of a protein. II: Monte Carlo simulation of native thermal fluctuations and energy minimization. **1989**, 5, 104-12	35
1693	Rapid calculation of the solution scattering profile from a macromolecule of known structure. **1989** , 5, 149-55	48
1692	Secondary structural analysis of retrovirus integrase: characterization by circular dichroism and empirical prediction methods. **1989**, 5, 156-65	20
1691	Rebuilding flavodoxin from C alpha coordinates: a test study. **1989**, 5, 170-82	87
1690	The crystal structure of the ternary complex of staphylococcal nuclease, Ca2+, and the inhibitor pdTp, refined at 1.65 A. **1989**, 5, 183-201	233
1689	PKB: a program system and data base for analysis of protein structure. **1989**, 5, 233-47	23
1688	Molecular dynamics effects on protein electrostatics. **1989**, 5, 313-21	57
1687	Describing protein structure: a general algorithm yielding complete helicoidal parameters and a unique overall axis. **1989**, 6, 46-60	117
1686	Computational and site-specific mutagenesis analyses of the asymmetric charge distribution on calmodulin. **1989**, 6, 70-85	53
1685	Comparing short protein substructures by a method based on backbone torsion angles. **1989**, 6, 155-67	32
1684	Structural determinants of the conformations of medium-sized loops in proteins. **1989**, 6, 382-94	75
1683	Use of restrained molecular dynamics in water to determine three-dimensional protein structure: prediction of the three-dimensional structure of Ecballium elaterium trypsin inhibitor II. **1989**, 6, 405-17	64
1682	The surface area of monomeric proteins: significance of power law behavior. **1989**, 6, 418-23	13
1681	Electrostatic complementarity in molecular aggregates. 9: Protein-ligand complexes. **1989**, 35, 215-221	11
1680	Three-dimensional structure of aspartyl protease from human immunodeficiency virus HIV-1. **1989**, 337, 615-20	812
1679	The three-dimensional structure of foot-and-mouth disease virus at 2.9 A resolution. **1989**, 337, 709-16	765

1678	Transfer of a beta-turn structure to a new protein context. **1989**, 339, 73-6		91
1677	Protein structure alignment. *Journal of Molecular Biology*, **1989**, 208, 1-22	6.5	563
1676	Crystal structure of muconolactone isomerase at 3.3 A resolution. *Journal of Molecular Biology*, **1989**, 205, 557-71	6.5	29
1675	On the molecular nature of "restrictive" antigenic elements present on major histocompatibility complex (MHC) proteins. **1989**, 140, 145-58		3
1674	Molecular dynamics refinement of a thermitase-eglin-c complex at 1.98 A resolution and comparison of two crystal forms that differ in calcium content. *Journal of Molecular Biology*, **1989**, 210, 347-67	6.5	97
1673	Refined structure of baboon alpha-lactalbumin at 1.7 A resolution. Comparison with C-type lysozyme. *Journal of Molecular Biology*, **1989**, 208, 99-127	6.5	280
1672	A polypeptide chain-refolding event occurs in the Gly82 variant of yeast iso-1-cytochrome c. *Journal of Molecular Biology*, **1989**, 210, 313-22	6.5	36
1671	Prediction of Protein Structural Classes from Amino Acid Compositions. **1989**, 549-586		103
1670	The Hydrophobicity Profile. **1989**, 625-633		10
1669	Tertiary Structure Prediction. **1989**, 647-705		30
1668	Principles and Patterns of Protein Conformation. **1989**, 1-98		227
1667	Molecular dynamics of tryptophan in ribonuclease-T1. II. Correlations with fluorescence. **1989**, 56, 43-66		35
1666	Electrostatic and steric control of electron self-exchange in cytochromes c, c551, and b5. **1989**, 56, 339-51		50
1665	Evidence for ligand-induced conformational changes in proteins from phosphorescence spectroscopy. **1989**, 56, 353-60		15
1664	Distance dependence of the tryptophan-disulfide interaction at the triplet level from pulsed phosphorescence studies on a model system. **1989**, 56, 361-7		35
1663	Models of binding of 4'-nitrophenyl alpha-D-mannopyranoside to the lectin concanavalin A. **1989**, 11, 17-22		6
1662	Construction of side-chains in homology modelling. Application to the C-terminal lobe of rhizopuspepsin. *Journal of Molecular Biology*, **1989**, 210, 785-811	6.5	87
1661	X-ray structure of lipoamide dehydrogenase from Azotobacter vinelandii determined by a combination of molecular and isomorphous replacement techniques. *Journal of Molecular Biology*, **1989**, 206, 365-79	6.5	86

1660	Investigating protein-protein interaction surfaces using a reduced stereochemical and electrostatic model. *Journal of Molecular Biology*, **1989**, 206, 381-95	6.5	45
1659	Engineering protein thermal stability. Sequence statistics point to residue substitutions in alpha-helices. *Journal of Molecular Biology*, **1989**, 206, 397-406	6.5	273
1658	Pseudo 2-fold symmetry in the copper-binding domain of arthropodan haemocyanins. Possible implications for the evolution of oxygen transport proteins. *Journal of Molecular Biology*, **1989**, 206, 531-46	6.5	77
1657	Periplasmic binding protein structure and function. Refined X-ray structures of the leucine/isoleucine/valine-binding protein and its complex with leucine. *Journal of Molecular Biology*, **1989**, 206, 171-91	6.5	234
1656	Structure of the L-leucine-binding protein refined at 2.4 A resolution and comparison with the Leu/Ile/Val-binding protein structure. *Journal of Molecular Biology*, **1989**, 206, 193-207	6.5	98
1655	Conformation of beta-hairpins in protein structures. A systematic classification with applications to modelling by homology, electron density fitting and protein engineering. *Journal of Molecular Biology*, **1989**, 206, 759-77	6.5	460
1654	Crystal structure of recombinant human interleukin-1 beta at 2.0 A resolution. *Journal of Molecular Biology*, **1989**, 209, 779-91	6.5	178
1653	Three-dimensional structure of cyclodextrin glycosyltransferase from Bacillus circulans at 3.4 A resolution. *Journal of Molecular Biology*, **1989**, 209, 793-800	6.5	59
1652	Biomedical science and the third world. Under the volcano. Trypanothione reductase. **1989**, 569, 193-200		9
1651	Electrical potentials in trypsin isozymes. **1989**, 28, 9918-26		72
1650	On the attribution of binding energy in antigen-antibody complexes McPC 603, D1.3, and HyHEL-5. **1989**, 28, 4735-49		384
1649	Crystallographic characterization and three-dimensional model of yeast Cu,Zn superoxide dismutase. **1989**, 160, 677-81		9
1648	Crystal structure of thermitase from Thermoactinomyces vulgaris at 2.2 A resolution. **1989**, 244, 208-12		11
1647	Possible role of some groups in the structure and function of HIV-1 protease as revealed by molecular modeling studies. **1989**, 247, 118-22		19
1646	A theoretical study of the acidification of the rhinovirus capsid. **1989**, 257, 403-7		8
1645	Structure of spheroidene in the photosynthetic reaction center from Y Rhodobacter sphaeroides. **1989**, 258, 47-50		116
1644	Recognition of functional regions in primary structures using a set of property patterns. **1989**, 257, 191-5		15
1643	A template based method of pattern matching in protein sequences. **1989**, 54, 159-252		19

1642	Structure of bovine immunoglobulin constant region heavy chain gamma 1 and gamma 2 genes. **1989**, 26, 841-50		52
1641	Analysis of structure-function relationships of neuropeptide Y using molecular dynamics simulations and pharmacological activity and binding measurements. **1989**, 25, 295-313		28
1640	Contributions of left-handed helical residues to the structure and stability of bacteriophage T4 lysozyme. *Journal of Molecular Biology*, **1989**, 210, 181-93	6.5	46
1639	A comparison of the CHARMM, AMBER and ECEPP potentials for peptides. II. Phi-psi maps for N-acetyl alanine N'-methyl amide: comparisons, contrasts and simple experimental tests. **1989**, 7, 421-53		152
1638	Structural origins of high-affinity biotin binding to streptavidin. **1989**, 243, 85-8		1013
1637	Protein motifs and data-base searching. **1989**, 14, 300-4		47
1636	A relational database of protein structures designed for flexible enquiries about conformation. **1989**, 2, 431-42		40
1635	A method to identify distinctive charge configurations in protein sequences, with application to human herpesvirus polypeptides. *Journal of Molecular Biology*, **1989**, 205, 165-77	6.5	36
1634	Comparison of the refined crystal structures of two wheat germ isolectins. *Journal of Molecular Biology*, **1989**, 209, 475-87	6.5	41
1633	Aplysia limacina myoglobin. Crystallographic analysis at 1.6 A resolution. *Journal of Molecular Biology*, **1989**, 205, 529-44	6.5	131
1632	Structure of tyrosyl-tRNA synthetase refined at 2.3 A resolution. Interaction of the enzyme with the tyrosyl adenylate intermediate. *Journal of Molecular Biology*, **1989**, 208, 83-98	6.5	356
1631	Crystal structure of hexameric haemocyanin from Panulirus interruptus refined at 3.2 A resolution. *Journal of Molecular Biology*, **1989**, 209, 249-79	6.5	343
1630	Resonance Raman studies of oriented chromophores: Metmyoglobin single crystals. **1989**, 90, 3015-3032		23
1629	Electrostatic fields in the active sites of lysozymes. **1989**, 86, 5361-5		44
1628	Stabilization of phage T4 lysozyme by engineered disulfide bonds. **1989**, 86, 6562-6		235
1627	Evolution of a bifunctional enzyme: 6-phosphofructo-2-kinase/fructose-2,6-bisphosphatase. **1989**, 86, 9642-6		101
1626	Interaction of glyceraldehyde-3-phosphate dehydrogenase with AMP as studied by means of a spin-labeled analog. **1989**, 370, 1245-52		3
1625	Protein secondary structure prediction with a neural network. **1989**, 86, 152-6		380

1624	Structure of human neutrophil elastase in complex with a peptide chloromethyl ketone inhibitor at 1.84-A resolution. **1989**, 86, 7-11	232
1623	Significant structural and functional change of an antigen-binding site by a distant amino acid substitution: proposal of a structural mechanism. **1989**, 86, 5532-6	51
1622	Structure of an antibody-antigen complex: crystal structure of the HyHEL-10 Fab-lysozyme complex. **1989**, 86, 5938-42	422
1621	Searching for pharmacophores in large coordinate data bases and its use in drug design. **1989**, 86, 8165-9	58
1620	Crystal structure analysis of auromomycin apoprotein (macromomycin) shows importance of protein side chains to chromophore binding selectivity. **1989**, 86, 6587-91	33
1619	Topological distribution of four-alpha-helix bundles. **1989**, 86, 6592-6	175
1618	Three-dimensional structure of Fab R19.9, a monoclonal murine antibody specific for the p-azobenzenearsonate group. **1989**, 86, 607-11	79
1617	Changing activity of ribonuclease A during adsorption: a molecular explanation. **1989**, 86, 8392-6	77
1616	Modeling antibody hypervariable loops: a combined algorithm. **1989**, 86, 9268-72	175
1615	Destabilization of an alpha-helix-bundle protein by helix dipoles. **1989**, 86, 1524-8	65
1614	A relational database of protein structure. **1989**, 17, 845-7	1
1613	The human genome project: approaches to the automation of sequence data input. **1989**, 17, 847-50	0
1612	The Standard Molecular Data Format (SMD Format) as an Integration Tool in Computer Chemistry. **1989**, 105-117	
1611	Antibody remodeling: a general solution to the design of a metal-coordination site in an antibody binding pocket. **1990**, 87, 6654-8	105
1610	Long-range electron exchange measured in proteins by quenching of tryptophan phosphorescence. **1990**, 87, 5099-103	46
1609	Structural comparisons of the native and reactive-centre-cleaved forms of alpha 1-antitrypsin by neutron- and X-ray-scattering in solution. **1990**, 267, 203-12	52
1608	Nucleotide sequences and three-dimensional modelling of the VH and VL domains of two human monoclonal antibodies specific for the D antigen of the human Rh-blood-group system. **1990**, 268, 135-40	25
1607	Protein sequence database. **1990**, 183, 31-49	43

1606	Knowledge-based prediction of protein structures. **1990**, 147, 85-100	21
1605	The tryptophan synthase multienzyme complex: exploring structure-function relationships with X-ray crystallography and mutagenesis. **1990**, 8, 27-32	32
1604	A serine protease triad forms the catalytic centre of a triacylglycerol lipase. **1990**, 343, 767-70	1098
1603	Structure of human pancreatic lipase. **1990**, 343, 771-4	1086
1602	Another catalytic triad?. **1990**, 346, 225	25
1601	Amino acid sequences around the pyridoxal-5'-phosphate-binding sites of phenol hydroxylase. **1990** , 187, 225-8	8
1600	E. Antonini Plenary lecture. A structural basis of light energy and electron transfer in biology. **1990**, 187, 283-305	40
1599	Structural features of neutral protease from Bacillus subtilis deduced from model-building and limited proteolysis experiments. **1990**, 189, 221-7	29
1598	Recognition of different nucleotide-binding sites in primary structures using a property-pattern approach. **1990**, 191, 347-58	48
1597	The highly resolved excess electron distance distribution of biopolymers in solution □calculation from intermediate-angle X-ray scattering and interpretation. **1990**, 23, 26-34	4
1596	PAP: a protein analysis package. **1990**, 23, 434-436	8
1595	ABSCOR: a scaling and absorption correction program for the FAST area detector diffractometer. **1990**, 23, 436-439	35
1594	Intensity-based domain refinement of oriented but unpositioned molecular replacement models. **1990**, 46 (Pt 5), 352-9	15
1593	Temperature factor of silicon by powder neutron diffraction. **1990**, 46, 435-437	5
1592	Phase effects in three-beam grazing-incidence X-ray diffraction. **1990**, 46, 567-576	2
1591	Determination of the crystal structure of recombinant pig myoglobin by molecular replacement and its refinement. **1990**, 46 (Pt 3), 370-7	7
1590	Structures of six terminally substituted [n]staffanes, n = 1□. **1990**, 46, 377-389	16
1589	Molecular-replacement structure determination of two different antibody:antigen complexes. **1990**, 46 (Pt 3), 418-25	4

1588	Structure of belladonna mottle virus: cross-rotation function studies with southern bean mosaic virus. **1990**, 46, 562-567	3
1587	Structure of 1,2-dinitrobenzene. **1990**, 46, 567-572	12
1586	Refinement of glucose isomerase from Streptomyces albus at 1.65 A with data from an imaging plate. **1990**, 46 (Pt 6), 833-41	30
1585	Symmetry and subunit arrangement of tobacco necrosis virus (TNV). **1990**, 46, 855-860	3
1584	The rates of photolysis of the four individual tryptophan residues in UV exposed calf gamma-II crystallin. **1990**, 51, 363-8	27
1583	Space-group frequencies of proteins and of organic compounds with more than one formula unit in the asymmetric unit. **1990**, 46, 725-730	58
1582	Functional and NMR studies of Hb Sassari (Asp-126 alpha----His); role of the inter-subunit contacts in the affinity control of human hemoglobin. **1990**, 1041, 250-3	5
1581	Evaluation of neural network performance by receiver operating characteristic (ROC) analysis: examples from the biotechnology domain. **1990**, 32, 73-80	26
1580	Metadata-based generation and management of knowledgebases from molecular biological databases. **1990**, 32, 115-23	5
1579	Testing of insulin hexamer-stabilizing ligands using theoretical binding, microcalorimetry, and nuclear magnetic resonance (NMR) line broadening techniques. **1990**, 7, 600-5	1
1578	Recognition of secondary-structure elements in 3D TOCSY-NOESY spectra of proteins. Interpretation of 3D cross-peak amplitudes. **1990**, 86, 453-469	5
1577	DOCKing ligands into receptors: The test case of □chymotrypsin. **1990**, 3, 713-722	11
1576	A PROLOG approach to analysing protein structure. **1990**, 3, 739-756	5
1575	Molecular anatomy: phyletic relationships derived from three-dimensional structures of proteins. **1990**, 30, 43-59	91
1574	On the nature of antibody combining sites: unusual structural features that may confer on these sites an enhanced capacity for binding ligands. **1990**, 7, 112-24	207
1573	Modeling of the human intercellular adhesion molecule-1, the human rhinovirus major group receptor. **1990**, 7, 227-33	51
1572	Identification of protein folds: matching hydrophobicity patterns of sequence sets with solvent accessibility patterns of known structures. **1990**, 7, 257-64	92
1571	ALMA, an editor for large sequence alignments. **1990**, 7, 291-5	28

1570	Comparative modeling methods: application to the family of the mammalian serine proteases. **1990**, 7, 317-34	355
1569	The building of protein structures from alpha-carbon coordinates. **1990**, 7, 366-77	67
1568	Molecular interactions in protein crystals: solvent accessible surface and stability. **1990**, 8, 1-5	39
1567	Revised 2.3 A structure of porcine pepsin: evidence for a flexible subdomain. **1990**, 8, 62-81	116
1566	The three-dimensional structure of recombinant bovine chymosin at 2.3 A resolution. **1990**, 8, 82-101	114
1565	Comparison of the structures of globins and phycocyanins: evidence for evolutionary relationship. **1990**, 8, 133-55	81
1564	HERA--a program to draw schematic diagrams of protein secondary structures. **1990**, 8, 203-12	92
1563	Plastic adaptation toward mutations in proteins: structural comparison of thymidylate synthases. **1990**, 8, 315-33	133
1562	Three-dimensional structures of complexes of Lathyrus ochrus isolectin I with glucose and mannose: fine specificity of the monosaccharide-binding site. **1990**, 8, 365-76	113
1561	Comparison of the X-ray structure of baboon alpha-lactalbumin and the tertiary predicted computer models of human alpha-lactalbumin. **1990**, 4, 369-79	8
1560	Modeling of protease I collagenolytic enzyme from the fiddler crab Uca pugilator. **1990**, 4, 107-16	1
1559	A rapid method of protein structure alignment. **1990**, 147, 517-51	115
1558	1H-NMR stereospecific assignments by conformational data-base searches. **1990**, 29, 813-22	97
1557	Solvent effect on binding thermodynamics of biopolymers. **1990**, 29, 901-19	28
1556	A 1.8 A resolution potential function for protein folding. **1990**, 29, 1479-89	46
1555	Statistical descriptors for the size and shape of globular proteins. **1990**, 29, 1745-54	12
1554	Analysis of side-chain conformational distributions in neutrophil peptide-5 NMR structures. **1990**, 29, 1807-22	8
1553	Conformational studies on peptides with proline in the right-handed alpha-helical region. **1990**, 30, 287-98	61

1552	Protein structure prediction using a combination of sequence homology and global energy minimization I. Global energy minimization of surface loops. **1990**, 11, 121-151	62
1551	Macromodel□n integrated software system for modeling organic and bioorganic molecules using molecular mechanics. **1990**, 11, 440-467	3405
1550	Computing the electric potential of biomolecules: Application of a new method of molecular surface triangulation. **1990**, 11, 603-622	80
1549	Interaction of the peptide CF3-Leu-Ala-NH-C6H4-CF3 (TFLA) with porcine pancreatic elastase. X-ray studies at 1.8 A. **1990**, 3, 36-44	19
1548	X-ray crystal structure of the bovine alpha-chymotrypsin/eglin c complex at 2.6 A resolution. **1990**, 3, 163-8	10
1547	Protein interactions with immobilized transition metal ions: quantitative evaluations of variations in affinity and binding capacity. **1990**, 191, 160-8	64
1546	A theorem on amplitudes of thermal atomic fluctuations in large molecules assuming specific conformations calculated by normal mode analysis. **1990**, 35, 105-12	45
1545	Bovine trypsinogen activation. A thermodynamic study. **1990**, 37, 355-62	11
1544	PASS: simple molecular graphics system for personal computers. **1990**, 8, 207-11	2
1543	Automated three-dimensional model building. **1990**, 8, 234-235	
1542	Peptide mechanics. **1990**, 8, 235	
1541	A new tool for the qualitative and quantitative analysis of protein surfaces using B-spline and density of surface neighborhood. **1990**, 8, 133-40, 146	21
1540	RAMBLE: a conformational search program. **1990**, 8, 156-62	14
1539	Protein modeling of human prorenin using the molecular dynamics method. **1990**, 8, 163-7, 150	14
1538	A two-path recursive relational database structure for molecular information systems. **1990**, 8, 2-10	2
1537	WHAT IF: a molecular modeling and drug design program. **1990**, 8, 52-6, 29	2930
1536	Symmetry and crystallography: new facilities in the graphic software MANOSK. **1990**, 8, 108-10, 92	1
1535	Aspartate aminotransferase: investigation of the active sites. **1990**, 8, 111-5, 92-3	3

1534	Introduction to three-dimensional chemical structure handling. **1990**, 3, 527-530		2
1533	3D database searching and de novo construction methods in molecular design. **1990**, 3, 697-711		33
1532	Knowledge acquisition from crystallographic databases: Towards a knowledge-based approach to molecular scene analysis. **1990**, 3, 757-774		12
1531	MARDIGRAS-A procedure for matrix analysis of relaxation for discerning geometry of an aqueous structure. **1990**, 87, 475-487		31
1530	Hydrophilicity of proteins and DNA. **1990**, 237, 63-73		5
1529	Three-dimensional structure determination of an anti-2-phenyloxazolone antibody: the role of somatic mutation and heavy/light chain pairing in the maturation of an immune response.. **1990**, 9, 3807-3814		111
1528	S-class cytochromes c have a variety of folding patterns: structure of cytochrome c-553 from Desulfovibrio vulgaris determined by the multi-wavelength anomalous dispersion method. *Journal of Biochemistry*, **1990**, 108, 701-3	3.1	37
1527	The refined 2.4 A X-ray crystal structure of recombinant human stefin B in complex with the cysteine proteinase papain: a novel type of proteinase inhibitor interaction.. **1990**, 9, 1939-1947		373
1526	How Trp repressor binds to its operator.. **1990**, 9, 1963-1967		52
1525	Selenomethionyl proteins produced for analysis by multiwavelength anomalous diffraction (MAD): a vehicle for direct determination of three-dimensional structure.. **1990**, 9, 1665-1672		796
1524	New services of the EMBL Data Library. **1990**, 18, 4319-23		17
1523	The Thermal Stability of Hb O-Indonesia [β16(GH4)Glu->Lys]. **1990**, 14, 641-646		4
1522	Using molecular dynamics simulations on crambin to evaluate the suitability of different continuum dielectric and hydrogen atom models for protein simulations. **1990**, 7, 1019-41		15
1521	Secondary structure prediction for the spectrin 106-amino acid segment, and a proposed model for tertiary structure. **1990**, 8, 55-62		7
1520	Mapping the CD4 binding site for human immunodeficiency virus by alanine-scanning mutagenesis. **1990**, 87, 7150-4		152
1519	Chapter 11 Site-Directed Computer-Aided Drug Design: Progress Towards the Design of Novel Lead Compounds Using Molecular Lattices. **1990**, 6, 117-132		
1518	Protein model structure evaluation using the solvation free energy of folding. **1990**, 87, 3240-3		101
1517	Incorporation of crystallographic temperature factors in the statistical analysis of protein tertiary structures. **1990**, 3, 649-57		10

1516	Hydroxyl hydrogen conformations in trypsin determined by the neutron diffraction solvent difference map method: relative importance of steric and electrostatic factors in defining hydrogen-bonding geometries. **1990**, 87, 4468-72	26
1515	Domain communication in the dynamical structure of human immunodeficiency virus 1 protease. **1990**, 87, 8864-8	110
1514	A single amino acid substitution in the variable region of the light chain specifically blocks immunoglobulin secretion. **1990**, 87, 8135-9	76
1513	Design and synthesis of a peptide having chymotrypsin-like esterase activity. **1990**, 248, 1544-7	195
1512	A joint 2D NMR and theoretical investigation of Ca2+ binding loops III and IV of calmodulin. **1990**, 7, 1003-18	1
1511	Predicting surface exposure of amino acids from protein sequence. **1990**, 3, 659-65	85
1510	Phylogenetic relationships from three-dimensional protein structures. **1990**, 183, 670-90	55
1509	Sequence dependent effects in methylphosphonate deoxyribonucleotide double and triple helical complexes. **1990**, 18, 3545-55	88
1508	Molecular Switching Transitions In Biological Macromolecules.	
1507	Structure of chymotrypsin-trifluoromethyl ketone inhibitor complexes: comparison of slowly and rapidly equilibrating inhibitors. **1990**, 29, 7600-7	120
1506	Role of lysine-54 in determining cofactor specificity and binding in human dihydrofolate reductase. **1990**, 29, 8063-9	18
1505	Proposed mechanism for the condensation reaction of citrate synthase: 1.9-.ANG. structure of the ternary complex with oxaloacetate and carboxymethyl coenzyme A. **1990**, 29, 2213-2219	104
1504	Quenching of the amidolytic activity of one-chain tissue-type plasminogen activator by mutation of lysine-416. **1990**, 29, 3451-7	33
1503	Global energy minimization by rotational energy embedding. **1990**, 30, 222-7	29
1502	De novo design, expression, and characterization of Felix: a four-helix bundle protein of native-like sequence. **1990**, 249, 884-91	390
1501	Local variability and base sequence effects in DNA crystal structures. **1990**, 8, 539-72	52
1500	Histidine-40 of ribonuclease T1 acts as base catalyst when the true catalytic base, glutamic acid-58, is replaced by alanine. **1990**, 29, 9064-72	104
1499	Sequential 1H NMR assignments and secondary structure of aponeocarzinostatin in solution. **1990**, 29, 8401-9	26

1498	Designs for a broad substrate specificity keto acid dehydrogenase. **1990**, 29, 8587-91		67
1497	Conformations of folded proteins in restricted spaces. **1990**, 29, 3287-94		213
1496	Geometry of interaction of metal ions with histidine residues in protein structures. **1990**, 4, 57-63		115
1495	Competitor analogs for defined T cell antigens: peptides incorporating a putative binding motif and polyproline or polyglycine spacers. **1990**, 60, 63-72		75
1494	Protein-protein recognition and the association of immunoglobulin constant domains. *Journal of Molecular Biology*, **1990**, 216, 965-73	6.5	28
1493	Modeling of globular proteins. A distance-based data search procedure for the construction of insertion/deletion regions and Pro----non-Pro mutations. *Journal of Molecular Biology*, **1990**, 216, 991-1016	6.5	54
1492	Diffraction diagnosis of protein folding in gap junction connexons. **1990**, 57, 1025-36		43
1491	Excluded volume approximation to protein-solvent interaction. The solvent contact model. **1990**, 57, 1103-7		66
1490	Deoxymyoglobin studied by the conformational normal mode analysis. I. Dynamics of globin and the heme-globin interaction. *Journal of Molecular Biology*, **1990**, 216, 95-109	6.5	66
1489	Identification of native protein folds amongst a large number of incorrect models. The calculation of low energy conformations from potentials of mean force. *Journal of Molecular Biology*, **1990**, 216, 167-80	6.5	278
1488	Framework residue 71 is a major determinant of the position and conformation of the second hypervariable region in the VH domains of immunoglobulins. *Journal of Molecular Biology*, **1990**, 215, 175-82	6.5	218
1487	Preliminary crystal structure analysis of an Fab specific for a Salmonella O-polysaccharide antigen. *Journal of Molecular Biology*, **1990**, 215, 489-92	6.5	11
1486	2.2 A resolution structure analysis of two refined N-acetylneuraminyl-lactose--wheat germ agglutinin isolectin complexes. *Journal of Molecular Biology*, **1990**, 215, 635-51	6.5	151
1485	Characterization of the binding sites of protein L11 and the L10.(L12)4 pentameric complex in the GTPase domain of 23 S ribosomal RNA from Escherichia coli. *Journal of Molecular Biology*, **1990**, 213, 275-88	6.5	126
1484	Conformational and geometrical properties of idealized beta-barrels in proteins. *Journal of Molecular Biology*, **1990**, 213, 315-26	6.5	45
1483	Automatic definition of recurrent local structure motifs in proteins. *Journal of Molecular Biology*, **1990**, 213, 327-36	6.5	98
1482	Relations between protein sequence and structure and their significance. *Journal of Molecular Biology*, **1990**, 213, 337-50	6.5	51
1481	Calculation of conformational ensembles from potentials of mean force. An approach to the knowledge-based prediction of local structures in globular proteins. *Journal of Molecular Biology*, **1990**, 213, 859-83	6.5	956

1480	A common pentapeptide conformation occurs in viral acid proteases and other proteins. *Journal of Molecular Biology*, **1990**, 216, 201-6	6.5	3
1479	Machine learning approach for the prediction of protein secondary structure. *Journal of Molecular Biology*, **1990**, 216, 441-57	6.5	86
1478	The entropic tension of protein loops. *Journal of Molecular Biology*, **1990**, 216, 459-65	6.5	13
1477	Hydrogen bond stereochemistry in protein structure and function. *Journal of Molecular Biology*, **1990**, 215, 457-71	6.5	250
1476	Kinetics of disulfide bond reduction in alpha-lactalbumin by dithiothreitol and molecular basis of superreactivity of the Cys6-Cys120 disulfide bond. **1990**, 29, 8240-9		130
1475	An investigation of oligopeptides linking domains in protein tertiary structures and possible candidates for general gene fusion. *Journal of Molecular Biology*, **1990**, 211, 943-58	6.5	237
1474	Novel method for the rapid evaluation of packing in protein structures. *Journal of Molecular Biology* , **1990**, 211, 959-74	6.5	130
1473	Evolution of protein cores. Constraints in point mutations as observed in globin tertiary structures. *Journal of Molecular Biology*, **1990**, 211, 975-88	6.5	49
1472	Definition of general topological equivalence in protein structures. A procedure involving comparison of properties and relationships through simulated annealing and dynamic programming. *Journal of Molecular Biology*, **1990**, 212, 403-28	6.5	477
1471	Molecular and crystal structures of monoclinic porcine pepsin refined at 1.8 A resolution. *Journal of Molecular Biology*, **1990**, 214, 143-70	6.5	242
1470	Improvements in protein secondary structure prediction by an enhanced neural network. *Journal of Molecular Biology*, **1990**, 214, 171-82	6.5	626
1469	X-ray analyses of aspartic proteinases. II. Three-dimensional structure of the hexagonal crystal form of porcine pepsin at 2.3 A resolution. *Journal of Molecular Biology*, **1990**, 214, 199-222	6.5	211
1468	Occurrence and role of cis peptide bonds in protein structures. *Journal of Molecular Biology*, **1990**, 214, 253-60	6.5	452
1467	Crystallization and preliminary X-ray crystallographic studies of benzamidine-inhibited trypsin from the North Atlantic salmon (Salmo salar). *Journal of Molecular Biology*, **1990**, 214, 355-8	6.5	13
1466	X-ray crystal structure determination and refinement at 1.9 A resolution of isolectin I from the seeds of Lathyrus ochrus. *Journal of Molecular Biology*, **1990**, 214, 571-84	6.5	86
1465	Molecular structure of flavocytochrome b2 at 2.4 A resolution. *Journal of Molecular Biology*, **1990**, 212, 837-63	6.5	310
1464	Protruding domain of tomato bushy stunt virus coat protein is a hitherto unrecognized class of jellyroll conformation. *Journal of Molecular Biology*, **1990**, 212, 7-9	6.5	11
1463	Use of techniques derived from graph theory to compare secondary structure motifs in proteins. *Journal of Molecular Biology*, **1990**, 212, 151-66	6.5	179

1462	Crystal structure of thioredoxin from Escherichia coli at 1.68 A resolution. *Journal of Molecular Biology*, **1990**, 212, 167-84	6.5	532
1461	Calcium binding in alpha-amylases: an X-ray diffraction study at 2.1-A resolution of two enzymes from Aspergillus. **1990**, 29, 6244-9		302
1460	Random mutagenesis used to probe the structure and function of Bacillus stearothermophilus alpha-amylase. **1990**, 3, 181-91		70
1459	Hydrophobic cluster analysis: procedures to derive structural and functional information from 2-D-representation of protein sequences. **1990**, 72, 555-74		298
1458	Modelling of poliovirus. HIV-1 antigen chimaeras. **1990**, 271, 194-8		20
1457	Mapping the copper ligands of Cu,Zn superoxide dismutase by nuclear Overhauser enhancement of the isotropically shifted 1H-NMR lines of the Cu,Co derivative. **1990**, 261, 231-6		11
1456	Modulation of the affinity of aspartic proteases by the mutated residues in active site models. **1990** , 261, 241-4		12
1455	Assignment of imidazole resonances from two-dimensional proton NMR spectra of bovine Cu,Zn superoxide dismutase. Evidence for similar active site conformation in the oxidized and reduced enzyme. **1990**, 263, 127-30		9
1454	Prediction of prolyl residues in cis-conformation in protein structures on the basis of the amino acid sequence. **1990**, 277, 159-63		43
1453	Crystal structure of an alkaline protease from Bacillus alcalophilus at 2.4 A resolution. **1990**, 274, 57-60		9
1452	Computer simulation of zinc finger motifs from cellular nucleic acid binding protein and their interaction with consensus DNA sequences. **1990**, 274, 217-22		1
1451	Modeling of the electrostatic potential field of plastocyanin. **1990**, 277, 241-54		38
1450	Chemical modification of spinach plastocyanin using 4-chloro-3,5-dinitrobenzoic acid: characterization of four singly-modified forms. **1990**, 1016, 107-14		18
1449	All fifteen possible arrangements of three disulfide bridges in proteins are known. **1990**, 172, 1364-70		11
1448	High-resolution refinement of yeast iso-1-cytochrome c and comparisons with other eukaryotic cytochromes c. *Journal of Molecular Biology*, **1990**, 214, 527-55	6.5	375
1447	Protein folding and chain collapse. **1990**, 29, 1823-1833		7
1446	Hydrophobicity of amino acid subgroups in proteins. **1990**, 8, 6-13		126
1445	An envelope-based approach for direct phase determination of macromolecular structures. **1990**, 46 (Pt 11), 915-22		3

1444	High-resolution three-dimensional structure of horse heart cytochrome c. *Journal of Molecular Biology*, **1990**, 214, 585-95	6.5	940
1443	Crystal structure of thermitase at 1.4 A resolution. *Journal of Molecular Biology*, **1990**, 214, 261-79	6.5	122
1442	Generation of a lysosomal enzyme targeting signal in the secretory protein pepsinogen. **1990**, 63, 281-91		143
1441	Prediction of protein side-chain conformation by packing optimization. *Journal of Molecular Biology* , **1991**, 217, 373-88	6.5	244
1440	Influence of proline residues on protein conformation. *Journal of Molecular Biology*, **1991**, 218, 397-412	6.5	966
1439	Molecular recognition. Conformational analysis of limited proteolytic sites and serine proteinase protein inhibitors. *Journal of Molecular Biology*, **1991**, 220, 507-30	6.5	340
1438	Cooperative ligand reorientations in cytochrome c3: a molecular dynamics simulation. **1991**, 1058, 83-4		1
1437	The interaction of nitrotyrosine-83 plastocyanin with cytochromes f and c: pH dependence and the effect of an additional negative charge on plastocyanin. **1991**, 1056, 166-72		29
1436	Oncostatin M stimulates urokinase-type plasminogen activator activity in human synovial fibroblasts. **1991**, 180, 652-9		42
1435	On alpha-helices terminated by glycine. 1. Identification of common structural features. **1991**, 180, 660-5		32
1434	On alpha-helices terminated by glycine. 2. Recognition by sequence patterns. **1991**, 180, 666-72		13
1433	A possible procedure for reducing the immunogenicity of antibody variable domains while preserving their ligand-binding properties. **1991**, 28, 489-98		146
1432	Structures of deoxy and oxy hemerythrin at 2.0 A resolution. *Journal of Molecular Biology*, **1991**, 218, 583-93	6.5	197
1431	Structural aspects of metal liganding to functional groups in proteins. **1991**, 42, 1-76		357
1430	Modelling by homology. **1991**, 1, 219-223		18
1429	Molecular modeling in food research: technology and techniques. **1991**, 2, 110-115		7
1428	The three-dimensional structure of the aspartyl protease from the HIV-1 isolate BRU. **1991**, 73, 1391-6		167
1427	Experimentally verifying molecular dynamics simulations through fluorescence anisotropy measurements. **1991**, 30, 1173-9		33

1426	Binding of the bovine and porcine pancreatic secretory trypsin inhibitor (Kazal) to human leukocyte elastase: a thermodynamic study. **1991**, 5, 207-13		3
1425	Structural basis for the inactivation of the P54 mutant of beta-lactamase from Staphylococcus aureus PC1. **1991**, 30, 9503-9		68
1424	Effects of point mutations in a hinge region on the stability, folding, and enzymatic activity of Escherichia coli dihydrofolate reductase. **1991**, 30, 7801-9		36
1423	Crystallization and structure determination to 2.5-A resolution of the oxidized [2Fe-2S] ferredoxin isolated from Anabaena 7120. **1991**, 30, 4126-31		178
1422	Structure of the IIA domain of the glucose permease of Bacillus subtilis at 2.2-A resolution. **1991**, 30, 9583-94		92
1421	Conformational stability, folding, and ligand-binding affinity of single-chain Fv immunoglobulin fragments expressed in Escherichia coli. **1991**, 30, 10117-25		145
1420	Does helix dipole have any role in binding metal ions in protein structures?. **1991**, 290, 387-90		4
1419	Structural properties of human carbonic anhydrase II at pH 9.5. **1991**, 181, 579-84		15
1418	A model for histone H5-DNA interaction: simultaneous minor and major groove binding. **1991**, 174, 898-902		6
1417	Correct intron splicing generates a new type of a putative zinc-binding domain in a transcriptional activator of Aspergillus nidulans. **1991**, 280, 11-6		43
1416	An extension of secondary structure prediction towards the prediction of tertiary structure. **1991**, 280, 141-6		12
1415	A structure-derived sequence pattern for the detection of type I copper binding domains in distantly related proteins. **1991**, 279, 73-8		38
1414	Simple techniques for the quantification of protein secondary structure by 1H NMR spectroscopy. **1991**, 293, 72-80		89
1413	High-resolution solution structure of reduced French bean plastocyanin and comparison with the crystal structure of poplar plastocyanin. *Journal of Molecular Biology*, **1991**, 221, 533-55	6.5	104
1412	Crystal structure of human alpha-lactalbumin at 1.7 A resolution. *Journal of Molecular Biology*, **1991** , 221, 571-81	6.5	205
1411	Beta-breakers: an aperiodic secondary structure. *Journal of Molecular Biology*, **1991**, 221, 603-13	6.5	43
1410	Serpin tertiary structure transformation. *Journal of Molecular Biology*, **1991**, 221, 615-21	6.5	148
1409	Analysis of protein main-chain solvation as a function of secondary structure. *Journal of Molecular Biology*, **1991**, 221, 669-91	6.5	65

1408	Prediction of protein backbone conformation based on seven structure assignments. Influence of local interactions. *Journal of Molecular Biology*, **1991**, 221, 961-79	6.5	180
1407	X-ray structure of human relaxin at 1 5 *Journal of Molecular Biology*, **1991**, 221, 15-21	6.5	5
1406	Protein docking and complementarity. *Journal of Molecular Biology*, **1991**, 221, 327-46	6.5	264
1405	Relationship between nuclear magnetic resonance chemical shift and protein secondary structure. *Journal of Molecular Biology*, **1991**, 222, 311-33	6.5	1720
1404	Refined 1.83 A structure of trypanosomal triosephosphate isomerase crystallized in the presence of 2.4 M-ammonium sulphate. A comparison with the structure of the trypanosomal triosephosphate isomerase-glycerol-3-phosphate complex. *Journal of Molecular Biology*, **1991**, 220, 995-1015	6.5	148
1403	Ionic interactions with parvalbumins. Crystal structure determination of pike 4.10 parvalbumin in four different ionic environments. *Journal of Molecular Biology*, **1991**, 220, 1017-39	6.5	129
1402	Molecular basis of co-operativity in protein folding. *Journal of Molecular Biology*, **1991**, 222, 687-98	6.5	81
1401	Construction of new ligand binding sites in proteins of known structure. I. Computer-aided modeling of sites with pre-defined geometry. *Journal of Molecular Biology*, **1991**, 222, 763-85	6.5	214
1400	A simplified mechanical model of proteins tested on the globin fold. *Journal of Molecular Biology*, **1991**, 222, 805-17	6.5	9
1399	Generalized protein tertiary structure recognition using associative memory Hamiltonians. *Journal of Molecular Biology*, **1991**, 222, 1013-34	6.5	65
1398	Refined crystal structure of Cd, Zn metallothionein at 2.0 esolution. *Journal of Molecular Biology*, **1991**, 221, 1269-1293	6.5	11
1397	X-ray analyses of aspartic proteinases IV. *Journal of Molecular Biology*, **1991**, 221, 1295-1309	6.5	4
1396	Model for the structure of formaldehyde dehydrogenase based on alcohol dehydrogenase. **1991**, 13, 73-6		5
1395	A totally synthetic histidine-2 ferredoxin: thermal stability and redox properties. **1991**, 30, 11669-76		30
1394	Structural biology of zinc. **1991**, 42, 281-355		284
1393	Lysozyme revisited: crystallographic evidence for distortion of an N-acetylmuramic acid residue bound in site D. *Journal of Molecular Biology*, **1991**, 220, 401-24	6.5	245
1392	X-ray analysis of the single chain B29-A1 peptide-linked insulin molecule. A completely inactive analogue. *Journal of Molecular Biology*, **1991**, 220, 425-33	6.5	196
1391	Molecular structure of cytochrome c2 isolated from Rhodobacter capsulatus determined at 2.5 A resolution. *Journal of Molecular Biology*, **1991**, 220, 673-85	6.5	89

1390	Structures of met and azidomet hemerythrin at 1.66 A resolution. *Journal of Molecular Biology*, **1991**, 220, 723-37	6.5	101
1389	Amino acid similarity coefficients for protein modeling and sequence alignment derived from main-chain folding angles. *Journal of Molecular Biology*, **1991**, 219, 481-97	6.5	50
1388	Analysis of protein loop closure. Two types of hinges produce one motion in lactate dehydrogenase. *Journal of Molecular Biology*, **1991**, 220, 133-49	6.5	150
1387	Side-chain clusters in protein structures and their role in protein folding. *Journal of Molecular Biology*, **1991**, 220, 151-71	6.5	92
1386	Refined crystal structure of beta-lactamase from Staphylococcus aureus PC1 at 2.0 A resolution. *Journal of Molecular Biology*, **1991**, 217, 701-19	6.5	207
1385	Suggestions for "safe" residue substitutions in site-directed mutagenesis. *Journal of Molecular Biology*, **1991**, 217, 721-9	6.5	345
1384	Refined crystal structures of subtilisin novo in complex with wild-type and two mutant eglins. Comparison with other serine proteinase inhibitor complexes. *Journal of Molecular Biology*, **1991**, 217, 353-71	6.5	72
1383	Is the hydrophobic effect stabilizing or destabilizing in proteins? The contribution of disulphide bonds to protein stability. *Journal of Molecular Biology*, **1991**, 217, 389-98	6.5	157
1382	Structure, function and properties of antibody binding sites. *Journal of Molecular Biology*, **1991**, 217, 133-51	6.5	388
1381	Refined structure of porcine pepsinogen at 1.8 A resolution. *Journal of Molecular Biology*, **1991**, 219, 671-92	6.5	96
1380	Reaction mechanism of alkaline phosphatase based on crystal structures. Two-metal ion catalysis. *Journal of Molecular Biology*, **1991**, 218, 449-64	6.5	821
1379	X-ray crystal structure of the ferric sperm whale myoglobin: imidazole complex at 2.0 A resolution. *Journal of Molecular Biology*, **1991**, 217, 409-12	6.5	60
1378	"Soft docking": matching of molecular surface cubes. *Journal of Molecular Biology*, **1991**, 219, 79-102	6.5	360
1377	Protein folding. Effect of packing density on chain conformation. *Journal of Molecular Biology*, **1991**, 219, 109-22	6.5	89
1376	Crystal structure of a barnase-d(GpC) complex at 1.9 A resolution. *Journal of Molecular Biology*, **1991**, 219, 123-32	6.5	84
1375	Database algorithm for generating protein backbone and side-chain co-ordinates from a C alpha trace application to model building and detection of co-ordinate errors. *Journal of Molecular Biology*, **1991**, 218, 183-94	6.5	301
1374	Comparison of the crystal structures of a flavodoxin in its three oxidation states at cryogenic temperatures. *Journal of Molecular Biology*, **1991**, 218, 195-208	6.5	187
1373	Structural mechanism for glycogen phosphorylase control by phosphorylation and AMP. *Journal of Molecular Biology*, **1991**, 218, 233-60	6.5	220

1372	Sequence space soup of proteins and copolymers. **1991**, 95, 3775-3787	168
1371	Arginine-mediated RNA recognition: the arginine fork. **1991**, 252, 1167-71	614
1370	Molecular dynamics simulations of the unfolding of an alpha-helical analogue of ribonuclease A S-peptide in water. **1991**, 30, 3864-71	207
1369	Atomic structure of acetylcholinesterase from Torpedo californica: a prototypic acetylcholine-binding protein. **1991**, 253, 872-9	2413
1368	A method to identify protein sequences that fold into a known three-dimensional structure. **1991**, 253, 164-70	2411
1367	Calcium-binding sites in proteins: a structural perspective. **1991**, 42, 77-144	178
1366	Crystal structure of haloalkane dehalogenase: an enzyme to detoxify halogenated alkanes.. **1991**, 10, 1297-1302	151
1365	Crystal structure of Penicillium citrinum P1 nuclease at 2.8 A resolution.. **1991**, 10, 1607-1618	203
1364	Histidine pKa shifts accompanying the inactivating Asp121----Asn substitution in a semisynthetic bovine pancreatic ribonuclease. **1991**, 88, 8116-20	33
1363	Predicting protein secondary structure based on amino acid sequence. **1991**, 202, 31-44	64
1362	Pattern-based approaches to protein structure prediction. **1991**, 202, 252-68	9
1361	Combined procedures of distance geometry and molecular dynamics for determining protein structure from nuclear magnetic resonance data. **1991**, 202, 268-300	13
1360	Molecular modeling and dynamics of biologically active peptides: application to neuropeptide Y. **1991**, 202, 449-70	3
1359	X-ray crystallographic analysis of free and antigen-complexed Fab fragments to investigate structural basis of immune recognition. **1991**, 203, 153-76	37
1358	Perspectives on non-heme iron protein chemistry. **1991**, 42, 199-280	59
1357	Molecular modeling of antibody combining sites. **1991**, 203, 121-53	46
1356	A soluble, single-chain T-cell receptor fragment endowed with antigen-combining properties. **1991**, 88, 8646-50	73
1355	Calculation of protein conformation as an assembly of stable overlapping segments: application to bovine pancreatic trypsin inhibitor. **1991**, 88, 3661-5	47

1354	Effects of amino acid substitution on three-dimensional structure: an X-ray analysis of cytochrome c3 from Desulfovibrio vulgaris Hildenborough at 2 A resolution. *Journal of Biochemistry*, **1991**, 110, 532-40	56
1353	The Effect of a Protein Environment on the Proposed Activation Mechanism of the Histamine H2-Receptor. **1991**, 31, 409-421	2
1352	Structure and topological symmetry of the glyphosate target 5-enolpyruvylshikimate-3-phosphate synthase: a distinctive protein fold. **1991**, 88, 5046-50	137
1351	Identification of the major pregnancy-specific antigens of cattle and sheep as inactive members of the aspartic proteinase family. **1991**, 88, 10247-51	165
1350	Water structure in cubic insulin crystals. **1991**, 88, 622-6	61
1349	.	1
1348	The 2.0 Å Crystal Structure of Cyanide Metmyoglobin Reconstituted with 5,10,15,20-Tetrapropylhemin. **1991**, 64, 821-828	11
1347	Structure-function relationships in the cysteine proteinases actinidin, papain and papaya proteinase omega. Three-dimensional structure of papaya proteinase omega deduced by knowledge-based modelling and active-centre characteristics determined by two-hydronic-state reactivity probe kinetics and kinetics of catalysis. **1991**, 280 (Pt 1), 79-92	53
1346	Clefts and binding sites in protein receptors. **1991**, 202, 126-56	14
1345	Molecular interstitial skeleton. **1991**, 15, 37-45	8
1344	Superposition of three-dimensional objects: A fast and numerically stable algorithm for the calculation of the matrix of optimal rotation. **1991**, 15, 73-78	30
1343	Protein interactions with surface-immobilized metal ions: structure-dependent variations in affinity and binding capacity with temperature and urea concentration. **1991**, 42, 105-18	32
1342	Structure prediction and modelling. **1991**, 2, 512-9	6
1341	A molecular dynamics simulation of the C-terminal fragment of the L7/L12 ribosomal protein in solution. **1991**, 158, 501-512	21
1340	Visualization of structural similarity in proteins. **1991**, 9, 169-74, 163-4	15
1339	Crepe-ribbon representation for protein structures: comparison of phospholipases A2. **1991**, 9, 3-10, 33	4
1338	Molecular modeling on the Commodore Amiga. **1991**, 9, 24-6, 36	2
1337	Number of residues in a sphere around a certain residue can be used as a hydrophobic penalty function of proteins. **1991**, 9, 78-84, 95-6	2

1336	Program for the visualization of inorganic crystals. **1991**, 9, 85-90, 97-9	3
1335	Stereo viewing on the PC/AT with EGA graphics. **1991**, 9, 111-4	6
1334	Vibrational studies of the disulfied group in proteins part IV. SS and CS stretch frequencies of known peptide and protein disulfide bridges. **1991**, 250, 89-102	26
1333	Crystallization of basic proteins by ion pairing. **1991**, 110, 20-25	54
1332	The crystal packing interactions of two different crystal forms of bovine Ribonuclease A. **1991**, 110, 119-130	12
1331	Active site interactions in hydrated trypsin-organophosphate adducts: a yeti molecular mechanics study. **1991**, 226, 99-110	12
1330	Comparative study of the charge distribution in tetravalent carbonyl transients and organophosphorus adducts of trypsin. **1991**, 233, 335-342	7
1329	The utility of the four-dimensional ramachandran map for the description of peptide conformations. **1991**, 232, 291-319	30
1328	Chaos-theoretical analysis of possible structural quantities for globular proteins. **1991**, 1079, 73-8	2
1327	Amino acid sequence and molecular modelling of a thermostable two (4Fe-4S) ferredoxin from the archaebacterium Methanococcus thermolithotrophicus. **1991**, 1076, 79-85	12
1326	Acid denatured apo-cytochrome c is a random coil: evidence from small-angle X-ray scattering and dynamic light scattering. **1991**, 1078, 289-95	58
1325	Protein sequences--homologies and motifs. **1991**, 9, 300-2	4
1324	Protein hydration in aqueous solution. **1991**, 254, 974-80	728
1323	A model for interfacial activation in lipases from the structure of a fungal lipase-inhibitor complex. **1991**, 351, 491-4	1021
1322	Ser-His-Glu triad forms the catalytic site of the lipase from Geotrichum candidum. **1991**, 351, 761-4	499
1321	Molecular characterization of the gor gene encoding glutathione reductase from Pseudomonas aeruginosa: determinants of substrate specificity among pyridine nucleotide-disulphide oxidoreductases. **1991**, 5, 163-171	29
1320	AUTOMR: an automatic processing program system for the molecular replacement method. **1991**, 24, 1063-1066	9
1319	TELS: least-squares solution of the structure-invariant equations. **1991**, 47, 484-490	3

1318	An independent crystallographic refinement of porcine phospholipase A2 at 2.4 A resolution. **1991**, 47 (Pt 4), 558-9	10
1317	Use of molecular replacement in the solution of an immunoglobulin Fab fragment structure. **1991**, 47 (Pt 4), 549-55	3
1316	Solution of the structure of Aspergillus niger acid alpha-amylase by combined molecular replacement and multiple isomorphous replacement methods. **1991**, 47 (Pt 4), 527-35	43
1315	Structure and molecular model refinement of Aspergillus oryzae (TAKA) alpha-amylase: an application of the simulated-annealing method. **1991**, 47 (Pt 4), 535-44	85
1314	Complex between the subtilisin from a mesophilic bacterium and the leech inhibitor eglin-C. **1991**, 47 (Pt 5), 707-30	44
1313	Structure solution and molecular dynamics refinement of the yeast Cu,Zn enzyme superoxide dismutase. **1991**, 47 (Pt 6), 918-27	20
1312	Proton-NMR studies of the effects of ionic strength and pH on the hyperfine-shifted resonances and phenylalanine-82 environment of three species of mitochondrial ferricytochrome c. **1991**, 197, 631-41	18
1311	Fluorescence study of the conformational properties of myoglobin structure. 2. pH- and ligand-induced conformational changes in ferric- and ferrousmyoglobins. **1991**, 198, 233-9	10
1310	Conserved amino acid sequences among plant proteins sorted to protein bodies and plant vacuoles. Can they play a role in protein sorting?. **1991**, 199, 441-50	11
1309	Isolation, characterization, cDNA cloning and gene expression of an avian transthyretin. Implications for the evolution of structure and function of transthyretin in vertebrates. **1991**, 200, 679-87	68
1308	Global analysis of the time-resolved fluorescence of alpha- chymotrypsinogen A and alpha-chymotrypsin powders as a function of hydration. **1991**, 53, 57-63	11
1307	Computer localization of some Gm markers on the surface of the Fc region of human immunoglobulin G. **1991**, 99, 661-6	
1306	Electrostatics and diffusion of molecules in solution: simulations with the University of Houston Brownian dynamics program. **1991**, 62, 187-197	440
1305	Redox properties of 2[4Fe?4S] ferredoxins. **1991**, 251, 27-33	38
1304	Protein secondary structure from Fourier transform infrared spectroscopy: a data base analysis. **1991**, 194, 89-100	138
1303	Standard-geometry chains fitted to X-ray derived structures: Validation of the rigid-geometry approximation. I. Chain closure through a limited search of [bopl]conformations. **1991**, 12, 505-526	46
1302	Determination of molecular topology and atomic hybridization states from heavy atom coordinates. **1991**, 12, 891-898	25
1301	Detection of cavities in a set of interpenetrating spheres. **1991**, 12, 918-922	29

1300	Toward accurate transferable electrostatic models for polypeptides: A distributed multipole study of blocked amino acid residue charge distributions. **1991**, 12, 1187-1197	42
1299	Prediction of the rotational diffusion behavior of biopolymers on the basis of their solution or crystal structure. **1991**, 31, 149-60	18
1298	Effects of limited input distance constraints upon the distance geometry algorithm. **1991**, 31, 1049-64	17
1297	Binding mode of azide to ferric Aplysia limacina myoglobin. Crystallographic analysis at 1.9 A resolution. **1991**, 4, 1-6	29
1296	Binding of the neuroleptic drug haloperidol to a monoclonal antibody: refinement of the binding site molecular model using canonical structures. **1991**, 4, 7-15	8
1295	Cytokine conformations: predictive studies. **1991**, 4, 63-75	24
1294	Binding of the recombinant proteinase inhibitor eglin c from leech Hirudo medicinalis to serine (pro)enzymes: a comparative thermodynamic study. **1991**, 4, 113-9	15
1293	PLEC: a program for building, modelling and optimizing polypeptide structures. **1991**, 64, 131-139	
1292	A fast unbiased comparison of protein structures by means of the Needleman-Wunsch algorithm. **1991**, 32, 340-54	22
1291	Molecular recognition: models for drug design. **1991**, 47, 1148-61	5
1290	Structure and function of channels and channelogs as studied by computational chemistry. **1991**, 119, 109-32	31
1289	Statistical analysis of double NOE transfer pathways in proteins as measured in 3D NOE-NOE spectroscopy. **1991**, 1, 421-38	6
1288	Automatic creation of drug candidate structures based on receptor structure. Starting point for artificial lead generation.. **1991**, 47, 8985-8990	138
1287	Predicted three-dimensional structure of the protease inhibitor domain of the Alzheimer's disease beta-amyloid precursor. **1991**, 9, 1-11	8
1286	Distribution and complementarity of hydropathy in multisubunit proteins. **1991**, 9, 37-55	82
1285	Database of homology-derived protein structures and the structural meaning of sequence alignment. **1991**, 9, 56-68	1411
1284	Weak correlation between predictive power of individual sequence patterns and overall prediction accuracy in proteins. **1991**, 9, 69-78	31
1283	Hydrogen bonds involving sulfur atoms in proteins. **1991**, 9, 99-107	196

1282	A metal-mediated hydride shift mechanism for xylose isomerase based on the 1.6 A Streptomyces rubiginosus structures with xylitol and D-xylose. **1991**, 9, 153-73	177
1281	The crystal structure of the "open" and the "closed" conformation of the flexible loop of trypanosomal triosephosphate isomerase. **1991**, 10, 33-49	79
1280	The crystal structure of staphylococcal nuclease refined at 1.7 A resolution. **1991**, 10, 92-105	232
1279	Modeling conformational change in macromolecules as an elastic deformation. **1991**, 10, 162-70	2
1278	Secondary structure-based profiles: use of structure-conserving scoring tables in searching protein sequence databases for structural similarities. **1991**, 10, 229-39	135
1277	Detection of common three-dimensional substructures in proteins. **1991**, 11, 52-8	170
1276	SESAM: a relational database for structure and sequence of macromolecules. **1991**, 11, 59-76	37
1275	A model for human cardiac troponin C and for modulation of its Ca2+ affinity by drugs. **1991**, 11, 79-94	30
1274	Molecular dynamics simulations of the cytochrome c3-rubredoxin complex from Desulfovibrio vulgaris. **1991**, 11, 142-52	14
1273	A 175-psec molecular dynamics simulation of camphor-bound cytochrome P-450cam. **1991**, 11, 184-204	67
1272	Analysis of the steric strain in the polypeptide backbone of protein molecules. **1991**, 11, 223-9	202
1271	Protein-protein recognition analyzed by docking simulation. **1991**, 11, 271-80	134
1270	Computer design of bioactive molecules: a method for receptor-based de novo ligand design. **1991**, 11, 314-28	200
1269	Distance-constraint approach to higher-order structures of globular proteins with empirically determined distances between amino acid residues. **1991**, 10, 233-43	5
1268	Investigation of a physical basis for conformational similarity in proteins. **1991**, 10, 273-85	3
1267	A molecular model for the active site of S-adenosyl-L-homocysteine hydrolase. **1991**, 5, 213-34	13
1266	A machine learning approach to computer-aided molecular design. **1991**, 5, 617-28	28
1265	Calmodulin structure and function: Implication of arginine in the compaction related to ligand binding. **1991**, 1, 231-247	21

1264	The inclusion of electrostatic hydration energies in molecular mechanics calculations. **1991**, 5, 5-20	88
1263	Converter: a program to convert crystallographic coordinates among different molecular graphics standards on PC-IBM platforms. **1991**, 7, 395-6	
1262	A new approach to the rapid determination of protein side chain conformations. **1991**, 8, 1267-89	284
1261	Conformation of beta hairpins in protein structures: classification and diversity in homologous structures. **1991**, 202, 59-82	74
1260	Changes in activity of porcine phospholipase A2 brought about by charge engineering of a major structural element to alter stability. **1991**, 4, 929-34	7
1259	Three-dimensional structures of acidic and basic fibroblast growth factors. **1991**, 251, 90-3	366
1258	Comparisons of the sequences, 3-D structures and mechanisms of pepsin-like and retroviral aspartic proteinases. **1991**, 306, 443-53	10
1257	Studies on a Dimeric Aspartic Protease from a Single Domain of Pepsin. **1991**, 239-248	
1256	Structural models of ribonuclease H domains in reverse transcriptases from retroviruses. **1991**, 19, 1817-23	37
1255	The application of SSADM to modelling the logical structure of proteins. **1991**, 7, 515-24	1
1254	Stabilization of functional proteins by introduction of multiple disulfide bonds. **1991**, 202, 336-56	84
1253	SMGWS 2: improved microcomputer-based three-dimensional stereoscopic macromolecular graphics display. **1991**, 7, 107-8	
1252	Molecular packing and morphology of protein crystals. **1991**, 24, 105-110	14
1251	Diffusion-controlled enzymatic reactions. **1991**, 202, 473-97	54
1250	The EMBL data library. **1991**, 19 Suppl, 2227-30	44
1249	Static and dynamic properties of a new lattice model of polypeptide chains. **1991**, 94, 3978-3985	54
1248	Relationships among serine hydrolases: evidence for a common structural motif in triacylglyceride lipases and esterases. **1991**, 69, 842-51	131
1247	Direct phase determination of large macromolecular crystals using three-beam x-ray interference. **1991**, 67, 3113-3116	18

1246	Prediction of the thermodynamics of protein unfolding: the helix-coil transition of poly(L-alanine). **1991**, 88, 2859-63	71
1245	Three-dimensional structure of human basic fibroblast growth factor, a structural homolog of interleukin 1 beta. **1991**, 88, 3446-50	226
1244	Comparative modeling of homologous proteins. **1991**, 202, 239-52	57
1243	The protein-folding problem: the native fold determines packing, but does packing determine the native fold?. **1991**, 88, 4195-9	87
1242	Protonation of interacting residues in a protein by a Monte Carlo method: application to lysozyme and the photosynthetic reaction center of Rhodobacter sphaeroides. **1991**, 88, 5804-8	291
1241	The conformational analysis of serine protease inhibitors and its applications for drug design. **1992**, 5, 331-8	4
1240	The combination of symbolic and numerical computation for three-dimensional modeling of RNA. **1991**, 253, 1255-60	168
1239	Analysis of active site motions from a 175 picosecond molecular dynamics simulation of camphor-bound cytochrome P450cam. **1991**, 9, 187-203	25
1238	Structure of the calcium-dependent lectin domain from a rat mannose-binding protein determined by MAD phasing. **1991**, 254, 1608-15	518
1237	The primary structure of the hemoglobin from the Australian ghost bat (Macroderma gigas, Microchiroptera). **1991**, 372, 1089-95	1
1236	A "living fossil" sequence: primary structure of the coelacanth (Latimeria chalumnae) hemoglobin--evolutionary and functional aspects. **1991**, 372, 599-612	8
1235	.	
1234	Comparative modeling of proteins in the design of novel renin inhibitors. **1991**, 26, 77-127	37
1233	Structurally homologous ligand binding of integrin Mac-1 and viral glycoprotein C receptors. **1991**, 254, 1200-2	41
1232	Electronic data publishing and GenBank. **1991**, 252, 1273-7	64
1231	Atomic structure of the DNA repair [4Fe-4S] enzyme endonuclease III. **1992**, 258, 434-40	289
1230	. **1992**,	2
1229	Computational Approaches to Modeling and Analyzing Thermostability in Proteins. **1992**, 153-173	2

1228	Three dimensional structure of a natural auto antibody □A predicted model of the antigen binding site. **1992**,	
1227	ADSP--a new package for computational sequence analysis. **1992**, 8, 451-9	10
1226	Crystal structure of an engineered subtilisin inhibitor complexed with bovine trypsin. **1992**, 89, 4407-11	22
1225	Some aspects of structural studies on aspartic proteinases. **1992**, 52, 31-38	1
1224	Construction of a dictionary of sequence motifs that characterize groups of related proteins. **1992**, 5, 479-88	32
1223	The EMBL Data Library. **1992**, 20 Suppl, 2071-4	46
1222	Identification of an E-selectin region critical for carbohydrate recognition and cell adhesion. **1992**, 119, 215-27	151
1221	3 Nsec molecular dynamics simulation of the protein ubiquitin and comparison with X-ray crystal and solution NMR structures. **1992**, 9, 935-49	14
1220	An efficient automated computer vision based technique for detection of three dimensional structural motifs in proteins. **1992**, 9, 769-89	69
1219	Induction of autoantibodies to human enzymes following viral infection: a biologically relevant hypothesis. **1992**, 30, 449-54	
1218	Membrane fusion. **1992**, 258, 917-24	675
1217	Relationships between sequence and structure for the four-alpha-helix bundle tertiary motif in proteins. **1992**, 5, 739-48	28
1216	Generation and analysis of random point mutations in an antibody CDR2 sequence: many mutated antibodies lose their ability to bind antigen. **1992**, 176, 855-66	57
1215	Discretized model of proteins. I. Monte Carlo study of cooperativity in homopolypeptides. **1992**, 97, 9412-9426	105
1214	Inhibition of human alpha-, beta- and gamma-thrombin by mono-, bis-, tris- and tetra-benzamidine structures: thermodynamic study. **1992**, 6, 131-9	5
1213	Structural aspects of recognition motifs contributing to autoimmune responses. **1992**, 11, 199-206	2
1212	Role of loop-helix interactions in stabilizing four-helix bundle proteins. **1992**, 89, 7315-9	55
1211	Humanization of an anti-p185HER2 antibody for human cancer therapy. **1992**, 89, 4285-9	1468

1210	Protein tertiary structure recognition using optimized Hamiltonians with local interactions. **1992**, 89, 9029-33	202
1209	Hydrophobicity and structural classes in proteins. **1992**, 5, 373-5	77
1208	Loops and secondary structure mimetics: development and applications in basic science and rational drug design. **1992**, 10, 773-8	32
1207	Structural Aspects of Intermolecular Interactions. **1992**, 211, 75-88	5
1206	Synthetic analogues of chymostatin. Inhibition of chymotrypsin and Streptomyces griseus proteinase A. **1992**, 286 (Pt 2), 475-80	13
1205	A non-glycosylated extracellular superoxide dismutase variant. **1992**, 288 (Pt 2), 451-6	38
1204	Side-chain entropy opposes alpha-helix formation but rationalizes experimentally determined helix-forming propensities. **1992**, 89, 5937-41	268
1203	Optimal protein-folding codes from spin-glass theory. **1992**, 89, 4918-22	311
1202	Sequence-structure matching in globular proteins: application to supersecondary and tertiary structure determination. **1992**, 89, 12098-102	121
1201	Comparison of protein structures determined by NMR in solution and by X-ray diffraction in single crystals. **1992**, 25, 325-77	78
1200	Effects of compact volume and chain stiffness on the conformations of native proteins. **1992**, 89, 6614-8	42
1199	Conversion of acetylcholinesterase to butyrylcholinesterase: modeling and mutagenesis. **1992**, 89, 10827-31	273
1198	Singlet-state information on proteins from triplet-state data. **1992**, 1640, 478	
1197	A lattice model for protein structure prediction at low resolution. **1992**, 89, 2536-40	182
1196	Protein hydration in aqueous solution. **1992**, 35-45	53
1195	Detection of secondary structure elements in proteins by hydrophobic cluster analysis. **1992**, 5, 629-35	112
1194	Three-dimensional profiles for analysing protein sequence□structure relationships. **1992**, 93, 25-34	26
1193	1.67-A X-ray structure of the B2 immunoglobulin-binding domain of streptococcal protein G and comparison to the NMR structure of the B1 domain. **1992**, 31, 10449-57	96

1192	Incorporation of a stabilizing Ca(2+)-binding loop into subtilisin BPN'. **1992**, 31, 7796-801	81
1191	. **1992**, 12, 23-32	7
1190	Arginine residues as stabilizing elements in proteins. **1992**, 31, 2239-53	196
1189	NMR characterization of a diamagnetic model of unliganded alpha chains from human hemoglobin. **1992**, 74, 845-51	2
1188	The three-dimensional structure of a glutathione S-transferase from the mu gene class. Structural analysis of the binary complex of isoenzyme 3-3 and glutathione at 2.2-A resolution. **1992**, 31, 10169-84	394
1187	The contribution of halogen atoms to protein-ligand interactions. **1992**, 14, 193-7	12
1186	Electrostatic fields in antibodies and antibody/antigen complexes. **1992**, 58, 203-24	83
1185	Lessons from analyzing protein structures. **1992**, 2, 888-894	19
1184	Primary structure of immunoglobulins through evolution. **1992**, 2, 422-431	34
1183	The latent tendencies of PAI-1. **1992**, 17, 49-50	11
1182	The HIV-1 protease as a therapeutic target for AIDS. **1992**, 8, 153-64	310
1181	The Rhizobium leguminosarum biovar phaseoli glnT gene, encoding glutamine synthetase III. **1992**, 119, 1-8	26
1180	Physicochemical and structural implications for molecular recognition in immobilized metal affinity chromatography. **1992**, 4, 14-24	5
1179	Proteins designed for challenging environments and catalysis in organic solvents. **1992**, 2, 559-568	6
1178	Introducing strong metal-binding sites onto surfaces of proteins for facile and efficient metal-affinity purifications. **1992**, 4, 25-40	19
1177	Hemoglobin Dallas (alpha 97(G4)Asn-->Lys): functional characterization of a high oxygen affinity natural mutant. **1992**, 1180, 15-20	2
1176	Alteration in molecular structure which results in disease: the Met-30 variant of human plasma transthyretin. **1992**, 1139, 9-16	22
1175	The structure of human mitochondrial manganese superoxide dismutase reveals a novel tetrameric interface of two 4-helix bundles. **1992**, 71, 107-18	416

1174	Structural modeling of the human erythrocyte bisphosphoglycerate mutase. **1992**, 74, 519-26	7
1173	Simulation of the thermal denaturation of hen egg white lysozyme: trapping the molten globule state. **1992**, 31, 7745-8	141
1172	Three Dimensional Structure of Acetylcholinesterase. **1992**, 95-107	9
1171	Model calculations on the amide-I infrared bands of globular proteins. **1992**, 96, 3379-3387	407
1170	Extracting information on folding from the amino acid sequence: accurate predictions for protein regions with preferred conformation in the absence of tertiary interactions. **1992**, 31, 10226-38	106
1169	The nucleic acid database. A comprehensive relational database of three-dimensional structures of nucleic acids. **1992**, 63, 751-9	869
1168	Strong electrostatic loop-helix interactions in bundle motif protein structures. **1992**, 63, 682-8	17
1167	Looking at proteins: representations, folding, packing, and design. Biophysical Society National Lecture, 1992. **1992**, 63, 1186-1209	99
1166	Multisite association by recombinant proteins can enhance binding selectivity. Preferential removal of immune complexes from serum by immobilized truncated FB analogues of the B domain from staphylococcal protein A. **1992**, 62, 87-91	16
1165	Protein structure prediction based on statistical potential. **1992**, 62, 104-6	17
1164	Computer models of a new deoxy-sickle cell hemoglobin fiber based on x-ray diffraction data. **1992**, 61, 1638-46	1
1163	Modeling of antibody combining sites: Goals, expectations, and realities. **1992**, 1, 65-70	2
1162	Homology modeling of antibody combining sites. **1992**, 1, 71-79	1
1161	Antibody modeling using the conformational search program CONGEN. **1992**, 1, 96-106	23
1160	Antibody modeling: Beyond homology. **1992**, 1, 126-136	21
1159	On the use of minimization from many randomly generated loop structures in modeling antibody combining sites. **1992**, 1, 137-146	13
1158	Similarity searching in databases of three-dimensional molecules and macromolecules. **1992**, 32, 617-30	34
1157	Protein engineering of xylose (glucose) isomerase from Actinoplanes missouriensis. 1. Crystallography and site-directed mutagenesis of metal binding sites. **1992**, 31, 5449-58	121

1156	1H NMR assignments and secondary structure of human beta 2-microglobulin in solution. **1992**, 31, 8906-15	59
1155	Extracting information on folding from the amino acid sequence: consensus regions with preferred conformation in homologous proteins. **1992**, 31, 10239-49	50
1154	Crystallographic analysis of transition-state mimics bound to penicillopepsin: phosphorus-containing peptide analogues. **1992**, 31, 5201-14	60
1153	Mambin, a potent glycoprotein IIb-IIIa antagonist and platelet aggregation inhibitor structurally related to the short neurotoxins. **1992**, 31, 4766-72	111
1152	A segment-based approach to protein secondary structure prediction. **1992**, 31, 983-93	45
1151	Proteolysis of an active site peptide of lactate dehydrogenase by human immunodeficiency virus type 1 protease. **1992**, 31, 10153-68	35
1150	Hepatitis A virus 3C proteinase substrate specificity. **1992**, 31, 7862-9	62
1149	Multidomain binding of transforming growth factor alpha to the epidermal growth factor receptor. **1992**, 31, 9546-54	18
1148	Construction of a stable dimer of Bacillus stearothermophilus lactate dehydrogenase. **1992**, 31, 8307-14	26
1147	Similarities in melittin functional group reactivities during self-association and association with lipid bilayers. **1992**, 31, 5698-704	6
1146	Buried water in homologous serine proteases. **1992**, 31, 12785-91	105
1145	Mutation of the heme-binding crevice of flavocytochrome b2 from Saccharomyces cerevisiae: altered heme potential and absence of redox cooperativity between heme and FMN centers. **1992**, 31, 11376-82	15
1144	Homology-derived three-dimensional structure prediction of Candida cylindracea lipase. **1992**, 1165, 129-33	10
1143	Can enzymes adopt a self-inhibited form? Results of x-ray crystallographic studies of chymosin. **1992**, 184, 1074-81	28
1142	Structural study and preliminary crystallographic data for the hemoglobin from reindeer (Rangifer tarandus tarandus). **1992**, 187, 1063-70	3
1141	Crystal structure of peroxynitrite-modified bovine Cu,Zn superoxide dismutase. **1992**, 299, 350-5	70
1140	Effects of NO2-modification of Tyr83 on the reactivity of spinach plastocyanin with cytochrome f. **1992**, 1099, 35-44	15
1139	The path of a protein chain can be approximated by the conformation dictated by interpeptide ionic bridges. **1992**, 302, 57-60	

1138	Three-dimensional structural resemblance between leucine aminopeptidase and carboxypeptidase A revealed by graph-theoretical techniques. **1992**, 303, 48-52		42
1137	Do antigenic peptides have a unique sense of direction inside the MHC binding groove? A molecular modelling study. **1992**, 303, 224-8		4
1136	Applying machine learning methods for finding significant amino acid properties in proteins. **1992**, 297, 241-6		5
1135	The fifth Datta Lecture. Structural similarities between the aspartate receptor of bacterial chemotaxis and the trp repressor of E. coli. Implications for transmembrane signaling. **1992**, 307, 3-9		28
1134	Concepts in protein folding. **1992**, 307, 10-3		12
1133	Three-dimensional structure of catalase from Micrococcus lysodeikticus at 1.5 A resolution. **1992**, 312, 127-31		75
1132	Asp537, Asp812 are essential and Lys631, His811 are catalytically significant in bacteriophage T7 RNA polymerase activity. *Journal of Molecular Biology*, **1992**, 226, 37-45	6.5	73
1131	Crystal structure solution and refinement of the semisynthetic cobalt-substituted bovine erythrocyte superoxide dismutase at 2.0 A resolution. *Journal of Molecular Biology*, **1992**, 226, 227-38	6.5	46
1130	A 500 ps molecular dynamics simulation study of interleukin-1 beta in water. Correlation with nuclear magnetic resonance spectroscopy and crystallography. *Journal of Molecular Biology*, **1992**, 226, 239-50	6.5	166
1129	Towards an understanding of the arginine-aspartate interaction. *Journal of Molecular Biology*, **1992**, 226, 251-62	6.5	98
1128	X-ray structure determination of telokin, the C-terminal domain of myosin light chain kinase, at 2.8 A resolution. *Journal of Molecular Biology*, **1992**, 227, 840-51	6.5	143
1127	Prediction of protein folding pathways. *Journal of Molecular Biology*, **1992**, 227, 901-16	6.5	28
1126	Oxidation state-dependent conformational changes in cytochrome c. *Journal of Molecular Biology*, **1992**, 223, 959-76	6.5	364
1125	Structural details of ribonuclease H from Escherichia coli as refined to an atomic resolution. *Journal of Molecular Biology*, **1992**, 223, 1029-52	6.5	211
1124	Role of B13 Glu in insulin assembly. The hexamer structure of recombinant mutant (B13 Glu-->Gln) insulin. *Journal of Molecular Biology*, **1992**, 228, 1163-76	6.5	48
1123	Structure of cobalt carbonic anhydrase complexed with bicarbonate. *Journal of Molecular Biology*, **1992**, 228, 1212-8	6.5	77
1122	Refined crystal structure of a recombinant immunoglobulin domain and a complementarity-determining region 1-grafted mutant. *Journal of Molecular Biology*, **1992**, 225, 739-53	6.5	59
1121	Crystal structure of yeast Cu,Zn superoxide dismutase. Crystallographic refinement at 2.5 A resolution. *Journal of Molecular Biology*, **1992**, 225, 791-809	6.5	110

1120	Docking by least-squares fitting of molecular surface patterns. *Journal of Molecular Biology*, **1992**, 225, 849-58	6.5	84
1119	Comparison of the refined crystal structures of liganded and unliganded chicken, yeast and trypanosomal triosephosphate isomerase. *Journal of Molecular Biology*, **1992**, 224, 1115-26	6.5	96
1118	The interdependence of protein surface topography and bound water molecules revealed by surface accessibility and fractal density measures. *Journal of Molecular Biology*, **1992**, 228, 13-22	6.5	116
1117	Evaluation of the sequence template method for protein structure prediction. Discrimination of the (beta/alpha)8-barrel fold. *Journal of Molecular Biology*, **1992**, 228, 170-87	6.5	32
1116	Three-dimensional structure of an Fv from a human IgM immunoglobulin. *Journal of Molecular Biology*, **1992**, 228, 188-207	6.5	81
1115	Crystallization, structure determination and least-squares refinement to 1.75 A resolution of the fatty-acid-binding protein isolated from Manduca sexta L. *Journal of Molecular Biology*, **1992**, 228, 208-19	6.5	48
1114	Anatomy and evolution of proteins displaying the viral capsid jellyroll topology. *Journal of Molecular Biology*, **1992**, 228, 220-42	6.5	54
1113	Crystal packing in six crystal forms of pancreatic ribonuclease. *Journal of Molecular Biology*, **1992**, 228, 243-51	6.5	67
1112	New algorithm to model protein-protein recognition based on surface complementarity. Applications to antibody-antigen docking. *Journal of Molecular Biology*, **1992**, 228, 277-97	6.5	144
1111	Nuclear magnetic resonance solution structure of the alpha-neurotoxin from the black mamba (Dendroaspis polylepis polylepis). *Journal of Molecular Biology*, **1992**, 227, 1118-35	6.5	33
1110	Structure of native and apo carbonic anhydrase II and structure of some of its anion-ligand complexes. *Journal of Molecular Biology*, **1992**, 227, 1192-204	6.5	462
1109	Analysis of non-polar regions in proteins. *Journal of Molecular Biology*, **1992**, 224, 629-38	6.5	15
1108	Taxonomy and conformational analysis of loops in proteins. *Journal of Molecular Biology*, **1992**, 224, 685-99	6.5	122
1107	Structure-derived hydrophobic potential. Hydrophobic potential derived from X-ray structures of globular proteins is able to identify native folds. *Journal of Molecular Biology*, **1992**, 224, 725-32	6.5	160
1106	Structure determination and refinement of bovine lens leucine aminopeptidase and its complex with bestatin. *Journal of Molecular Biology*, **1992**, 224, 113-40	6.5	192
1105	Three-dimensional structure of porcine pancreatic procarboxypeptidase A. A comparison of the A and B zymogens and their determinants for inhibition and activation. *Journal of Molecular Biology*, **1992**, 224, 141-57	6.5	109
1104	Refined crystal structure of ascorbate oxidase at 1.9 A resolution. *Journal of Molecular Biology*, **1992**, 224, 179-205	6.5	420
1103	Crystal structure of the alkaline proteinase Savinase from Bacillus lentus at 1.4 A resolution. *Journal of Molecular Biology*, **1992**, 223, 427-45	6.5	140

1102	beta-Trefoil fold. Patterns of structure and sequence in the Kunitz inhibitors interleukins-1 beta and 1 alpha and fibroblast growth factors. *Journal of Molecular Biology*, **1992**, 223, 531-43	6.5	290
1101	Crystal structure of the complex between carboxypeptidase A and the biproduct analog inhibitor L-benzylsuccinate at 2.0 A resolution. *Journal of Molecular Biology*, **1992**, 223, 573-8	6.5	49
1100	Refined crystal structure of the influenza virus N9 neuraminidase-NC41 Fab complex. *Journal of Molecular Biology*, **1992**, 227, 122-48	6.5	203
1099	Structure determination and analysis of yeast iso-2-cytochrome c and a composite mutant protein. *Journal of Molecular Biology*, **1992**, 227, 160-76	6.5	43
1098	Domain closure in mitochondrial aspartate aminotransferase. *Journal of Molecular Biology*, **1992**, 227, 197-213	6.5	172
1097	Topology fingerprint approach to the inverse protein folding problem. *Journal of Molecular Biology*, **1992**, 227, 227-38	6.5	317
1096	Structure of scorpion toxin variant-3 at 1.2 A resolution. *Journal of Molecular Biology*, **1992**, 227, 239-52	6.5	75
1095	Molecular basis of co-operativity in protein folding. III. Structural identification of cooperative folding units and folding intermediates. *Journal of Molecular Biology*, **1992**, 227, 293-306	6.5	172
1094	Model for the differential stabilities of rhinovirus and poliovirus to mild acidic pH, based on electrostatics calculations. *Journal of Molecular Biology*, **1992**, 223, 247-57	6.5	21
1093	Evolutionary conservativeness of electric field in the Cu,Zn superoxide dismutase active site. Evidence for co-ordinated mutation of charged amino acid residues. *Journal of Molecular Biology*, **1992**, 223, 337-42	6.5	70
1092	The crystal structure of the Bacillus lentus alkaline protease, subtilisin BL, at 1.4 A resolution. *Journal of Molecular Biology*, **1992**, 228, 580-95	6.5	35
1091	Structural consequences of sequence patterns in the fingerprint region of the nucleotide binding fold. Implications for nucleotide specificity. *Journal of Molecular Biology*, **1992**, 228, 662-71	6.5	142
1090	Three-dimensional structure of the high-potential iron-sulfur protein isolated from the purple phototrophic bacterium Rhodocyclus tenuis determined and refined at 1.5 A resolution. *Journal of Molecular Biology*, **1992**, 228, 672-86	6.5	95
1089	Pyrrolidine ring puckering in cis and trans-proline residues in proteins and polypeptides. Different puckers are favoured in certain situations. *Journal of Molecular Biology*, **1992**, 228, 725-34	6.5	130
1088	Recognition of distantly related protein sequences using conserved motifs and neural networks. *Journal of Molecular Biology*, **1992**, 228, 951-62	6.5	27
1087	Characterization of "native" apomyoglobin by molecular dynamics simulation. *Journal of Molecular Biology*, **1992**, 227, 375-80	6.5	58
1086	Ribose and glucose-galactose receptors. Competitors in bacterial chemotaxis. *Journal of Molecular Biology*, **1992**, 227, 418-40	6.5	29
1085	Three-dimensional structures of bulge-containing DNA fragments. *Journal of Molecular Biology*, **1992**, 225, 397-431	6.5	85

1084	X-ray structure refinement and comparison of three forms of mitochondrial aspartate aminotransferase. *Journal of Molecular Biology*, **1992**, 225, 495-517	6.5	192
1083	Accurate modeling of protein conformation by automatic segment matching. *Journal of Molecular Biology*, **1992**, 226, 507-33	6.5	526
1082	Proline cis-trans isomers in calbindin D9k observed by X-ray crystallography. *Journal of Molecular Biology*, **1992**, 223, 601-6	6.5	130
1081	Crystal structure of the unique parvalbumin component from muscle of the leopard shark (Triakis semifasciata). The first X-ray study of an alpha-parvalbumin. *Journal of Molecular Biology*, **1992**, 223, 705-20	6.5	48
1080	Three-dimensional structure of acylphosphatase. Refinement and structure analysis. *Journal of Molecular Biology*, **1992**, 224, 427-40	6.5	122
1079	Analysis of insertions/deletions in protein structures. *Journal of Molecular Biology*, **1992**, 224, 461-71	6.5	205
1078	Common spatial arrangements of backbone fragments in homologous and non-homologous proteins. *Journal of Molecular Biology*, **1992**, 225, 5-9	6.5	97
1077	Evaluation of protein models by atomic solvation preference. *Journal of Molecular Biology*, **1992**, 225, 93-105	6.5	186
1076	Crystal and molecular structure of the bovine alpha-chymotrypsin-eglin c complex at 2.0 A resolution. *Journal of Molecular Biology*, **1992**, 225, 107-23	6.5	90
1075	1.7 A X-ray structure of the periplasmic ribose receptor from Escherichia coli. *Journal of Molecular Biology*, **1992**, 225, 155-75	6.5	133
1074	New triple-helical model for the shaft of the adenovirus fibre. *Journal of Molecular Biology*, **1992**, 226, 1073-84	6.5	69
1073	Refined 2.3 A X-ray crystal structure of bovine thrombin complexes formed with the benzamidine and arginine-based thrombin inhibitors NAPAP, 4-TAPAP and MQPA. A starting point for improving antithrombotics. *Journal of Molecular Biology*, **1992**, 226, 1085-99	6.5	189
1072	Hydrogen bonding in globular proteins. *Journal of Molecular Biology*, **1992**, 226, 1143-59	6.5	366
1071	Contacts between Tet repressor and tet operator revealed by new recognition specificities of single amino acid replacement mutants. *Journal of Molecular Biology*, **1992**, 226, 1257-70	6.5	42
1070	Immunoglobulin VH clan and family identity predicts variable domain structure and may influence antigen binding.. **1992**, 11, 603-609		134
1069	A three-dimensional model of the Photosystem II reaction centre of Pisum sativum. **1992**, 34, 287-300		167
1068	The computer program LUDI: a new method for the de novo design of enzyme inhibitors. **1992**, 6, 61-78		615
1067	LUDI: rule-based automatic design of new substituents for enzyme inhibitor leads. **1992**, 6, 593-606		335

1066	Computational simulations of the conformational behaviour of the adhesive proteins RGDS fragment. **1992**, 6, 113-30	6
1065	Predicting the product specificity and coupling of cytochrome P450cam. **1992**, 6, 449-60	56
1064	Similarity screening of molecular data sets. **1992**, 6, 513-20	18
1063	Streptokinase is a flexible multi-domain protein. **1992**, 20, 355-61	35
1062	Structure-function relationship for the highly toxic crotoxin from Crotalus durissus terrificus. **1992**, 21, 199-205	5
1061	The kinemage: a tool for scientific communication. **1992**, 1, 3-9	175
1060	Calculation of the free energy of association for protein complexes. **1992**, 1, 169-81	274
1059	Environment-specific amino acid substitution tables: tertiary templates and prediction of protein folds. **1992**, 1, 216-26	236
1058	Atomic solvation parameters applied to molecular dynamics of proteins in solution. **1992**, 1, 227-35	453
1057	Direct observation by X-ray analysis of the tetrahedral "intermediate" of aspartic proteinases. **1992** , 1, 322-8	100
1056	Selection of representative protein data sets. **1992**, 1, 409-17	639
1055	The refined 1.9-A X-ray crystal structure of D-Phe-Pro-Arg chloromethylketone-inhibited human alpha-thrombin: structure analysis, overall structure, electrostatic properties, detailed active-site geometry, and structure-function relationships. **1992**, 1, 426-71	530
1054	Assembly of polypeptide and protein backbone conformations from low energy ensembles of short fragments: development of strategies and construction of models for myoglobin, lysozyme, and thymosin beta 4. **1992**, 1, 625-40	39
1053	Intramolecular interactions in pancreatic ribonucleases. **1992**, 1, 1050-60	7
1052	Molecular dynamics studies of a DNA-binding protein: 1. A comparison of the trp repressor and trp aporepressor aqueous simulations. **1992**, 1, 1173-84	20
1051	Molecular dynamics studies of a DNA-binding protein: 2. An evaluation of implicit and explicit solvent models for the molecular dynamics simulation of the Escherichia coli trp repressor. **1992**, 1, 1185-205	93
1050	Correlation functions as a tool for protein modeling and structure analysis. **1992**, 1, 1269-78	24
1049	Structure of the oxidized long-chain flavodoxin from Anabaena 7120 at 2 A resolution. **1992**, 1, 1413-27	98

1048	Modeling the antigen combining site of an anti-dinitrophenyl antibody, ANO2. **1992**, 1, 1465-76	17
1047	X-ray crystal structures of the oxidized and reduced forms of the rubredoxin from the marine hyperthermophilic archaebacterium Pyrococcus furiosus. **1992**, 1, 1494-507	227
1046	Internal water molecules and H-bonding in biological macromolecules: a review of structural features with functional implications. **1992**, 1, 1543-62	173
1045	Comprehensive sequence analysis of the 182 predicted open reading frames of yeast chromosome III. **1992**, 1, 1677-90	98
1044	A database of protein structure families with common folding motifs. **1992**, 1, 1691-8	171
1043	Functional implications of interleukin-1 beta based on the three-dimensional structure. **1992**, 12, 10-23	71
1042	Correlations of atomic movements in lysozyme crystals. **1992**, 12, 145-57	65
1041	Domain flexibility in aspartic proteinases. **1992**, 12, 158-70	98
1040	Solvent structure in crystals of trypsin determined by X-ray and neutron diffraction. **1992**, 12, 203-22	88
1039	Analysis of solvent structure in proteins using neutron D2O-H2O solvent maps: pattern of primary and secondary hydration of trypsin. **1992**, 12, 223-36	65
1038	A method for determining the positions of polar hydrogens added to a protein structure that maximizes protein hydrogen bonding. **1992**, 12, 266-77	33
1037	Recurrent alpha beta loop structures in TIM barrel motifs show a distinct pattern of conserved structural features. **1992**, 12, 299-313	37
1036	Analysis of protein sheet topologies by graph theoretical methods. **1992**, 12, 314-23	44
1035	Stereochemical quality of protein structure coordinates. **1992**, 12, 345-64	1269
1034	The molecular structure of UDP-galactose 4-epimerase from Escherichia coli determined at 2.5 A resolution. **1992**, 12, 372-81	92
1033	Use of conditional probabilities for determining relationships between amino acid sequence and protein secondary structure. **1992**, 12, 382-99	14
1032	The high-resolution crystal structure of porcine pepsinogen. **1992**, 13, 1-25	88
1031	Structures of complexes of rhizopuspepsin with pepstatin and other statine-containing inhibitors. **1992**, 13, 195-205	33

1030	A multiple-start Monte Carlo docking method. **1992**, 13, 206-22	187
1029	Monte Carlo docking of oligopeptides to proteins. **1992**, 13, 223-30	81
1028	Common features of the conformations of antigen-binding loops in immunoglobulins and application to modeling loop conformations. **1992**, 13, 231-45	61
1027	Detection of native-like models for amino acid sequences of unknown three-dimensional structure in a data base of known protein conformations. **1992**, 13, 258-71	210
1026	A systematic search for protein signature sequences. **1992**, 14, 16-28	25
1025	Variability of conformations at crystal contacts in BPTI represent true low-energy structures: correspondence among lattice packing and molecular dynamics structures. **1992**, 14, 65-74	63
1024	Structural effects induced by mutagenesis affected by crystal packing factors: the structure of a 30-51 disulfide mutant of basic pancreatic trypsin inhibitor. **1992**, 14, 75-87	34
1023	A structural model for human dihydrolipoamide dehydrogenase. **1992**, 14, 88-101	22
1022	Fast structure alignment for protein databank searching. **1992**, 14, 139-67	126
1021	Fast and simple Monte Carlo algorithm for side chain optimization in proteins: application to model building by homology. **1992**, 14, 213-23	133
1020	Multiple protein sequence alignment from tertiary structure comparison: assignment of global and residue confidence levels. **1992**, 14, 309-23	542
1019	Crystal structure of human immunoglobulin fragment Fab New refined at 2.0 A resolution. **1992**, 14, 363-71	54
1018	Structural studies of the retroviral proteinase from avian myeloblastosis associated virus. **1992**, 14, 382-91	19
1017	Folding protein alpha-carbon chains into compact forms by Monte Carlo methods. **1992**, 14, 409-20	72
1016	Generation of a substructure library for the description and classification of protein secondary structure. I. Overview of the methods and results. **1992**, 14, 430-9	25
1015	Generation of a substructure library for the description and classification of protein secondary structure. II. Application to spectra-structure correlations in Fourier transform infrared spectroscopy. **1992**, 14, 440-50	29
1014	Application of a directed conformational search for generating 3-D coordinates for protein structures from alpha-carbon coordinates. **1992**, 14, 465-74	28
1013	Modeling the anti-CEA antibody combining site by homology and conformational search. **1992**, 14, 483-98	98

1012	An augmented ribbon model of protein structure. **1992**, 11, 47-63	3
1011	Similarity between average distance maps of structurally homologous proteins. **1992**, 11, 305-20	4
1010	Protein folding in the cell. **1992**, 355, 33-45	3834
1009	Crystal structure of the cell-binding B oligomer of verotoxin-1 from E. coli. **1992**, 355, 748-50	280
1008	Assessment of protein models with three-dimensional profiles. **1992**, 356, 83-5	2511
1007	The dead-end elimination theorem and its use in protein side-chain positioning. **1992**, 356, 539-42	601
1006	A new approach to protein fold recognition. **1992**, 358, 86-9	1079
1005	Structure of astacin and implications for activation of astacins and zinc-ligation of collagenases. **1992**, 358, 164-7	304
1004	Structure of porphobilinogen deaminase reveals a flexible multidomain polymerase with a single catalytic site. **1992**, 359, 33-9	187
1003	Molecular structure of the acyl-enzyme intermediate in beta-lactam hydrolysis at 1.7 A resolution. **1992**, 359, 700-5	549
1002	Crystal structure of TFIID TATA-box binding protein. **1992**, 360, 40-6	391
1001	Structure of a C-type mannose-binding protein complexed with an oligosaccharide. **1992**, 360, 127-34	879
1000	The three-dimensional structure of an intact monoclonal antibody for canine lymphoma. **1992**, 360, 369-72	198
999	Theoretical and practical aspects of antigenized antibodies. **1992**, 130, 125-50	15
998	Spectroscopic properties of the nitric oxide derivative of ferrous man, horse, and ruminant hemoglobins: a comparative study. **1992**, 45, 31-7	11
997	Surface properties of mussel adhesive protein component films. **1992**, 13, 1000-8	45
996	An interactive FORTRAN program for three-dimensional molecular visualization. **1992**, 16, 265-266	
995	NOE R factors and structural refinement using FIRM, an iterative relaxation matrix program. **1992**, 98, 283-298	3

994 VisiCoor: a simple program for visualization of proteins. **1992**, 10, 25-8, 21-2

993 A crystallographic molecular lattice builder applied to model lipid bilayers. **1992**, 10, 29-32, 23

992 Automated site-directed drug design: a method for the generation of general three-dimensional molecular graphs. **1992**, 10, 131-43 18

991 XELE--a polypeptide model-building program for a graphics workstation. **1992**, 10, 185-9, 165 2

990 PROBIT: a statistical approach to modeling proteins from partial coordinate data using substructure libraries. **1992**, 10, 124-6 18

989 Using a RIBBON program to illustrate lipid bilayer packing. **1992**, 10, 253-6

988 The compact domain conformation of human Glu-plasminogen in solution. **1992**, 1159, 155-61 36

987 Molecular modeling of the 3-D structure of cytochrome P-450scc. **1992**, 1160, 281-6 43

986 Hydrogen bond network of cytochrome P-450cam: a network connecting the heme group with helix K. **1992**, 1122, 41-4 13

985 Molecular biological databases--present and future. **1992**, 10, 61-6 12

984 A method for determining overall protein fold from NMR distance restraints. **1992**, 2, 535-543 8

983 TIRF of salt and surface effects on protein adsorption. **1992**, 148, 469-484 54

982 The inertia-equivalent ellipsoid: a link between atomic structure and low-resolution models of small globular proteins determined by small-angle X-ray scattering. **1992**, 25, 181-191 15

981 The database BIOSCAT: a tool for structure research by scattering and hydrodynamic methods. **1992**, 25, 803-806 5

980 Structure determination of a dimeric form of erabutoxin-b, crystallized from a thiocyanate solution. **1992**, 48 (Pt 4), 520-31 19

979 Highly conserved, potential cleavage sites about the desetopes of MHC class I and class II molecules. **1992**, 39, 26-31

978 The aconitase of Escherichia coli. Nucleotide sequence of the aconitase gene and amino acid sequence similarity with mitochondrial aconitases, the iron-responsive-element-binding protein and isopropylmalate isomerases. **1992**, 204, 599-609 59

977 Crystal structure of NAD-dependent formate dehydrogenase. **1992**, 206, 441-52 49

976	The binding of triazine herbicides to the photosynthetic reaction center of Rhodopseudomonas viridis. Energy minimization studies. **1992**, 206, 685-90	10
975	A correlation-coefficient method to predicting protein-structural classes from amino acid compositions. **1992**, 207, 429-3	52
974	The structure of neutral protease from Bacillus cereus at 0.2-nm resolution. **1992**, 207, 781-91	62
973	Molecular dynamics study of a complex between the human histocompatibility antigen HLA-A2 and the IMP58-66 nonapeptide from influenza virus matrix protein. **1992**, 208, 101-13	40
972	Crystal structure of carboxypeptidase T from Thermoactinomyces vulgaris. **1992**, 208, 281-8	57
971	Recombinant chicken egg white cystatin variants of the QLVSG region. **1992**, 209, 837-45	56
970	A weighting method for predicting protein structural class from amino acid composition. **1992**, 210, 747-9	25
969	Crystallographic studies of the binding of protonated and unprotonated inhibitors to carbonic anhydrase using hydrogen sulphide and nitrate anions. **1992**, 210, 867-71	58
968	Molecular Modeling of the Class I Human Histocompatibility Molecule HLA-A2 Presenting an Allele-Specific Nonapeptide from Influenza Matrix Protein. **1992**, 31, 886-890	7
967	Development of an extended simulated annealing method: application to the modeling of complementary determining regions of immunoglobulins. **1992**, 32, 33-43	68
966	Vibrational studies of the disulfide group in proteins. Part V. Correlation of SS stretch frequencies with the CCSS dihedral angle in known protein disulfide bridges. **1992**, 32, 321-6	19
965	Hydrophobic interaction between globin helices. **1992**, 32, 477-90	13
964	Theoretical determination of conformational paths in citrate synthase. **1992**, 32, 561-74	29
963	Shape distributions of protein topography. **1992**, 32, 1215-36	43
962	Analysis of the effectiveness of proline substitutions and glycine replacements in increasing the stability of phage T4 lysozyme. **1992**, 32, 1431-41	60
961	The shapes of backbones of chain molecules: Three-dimensional characterization by spherical shape maps. **1992**, 32, 1609-1621	39
960	MSEED: A program for the rapid analytical determination of accessible surface areas and their derivatives. **1992**, 13, 1-11	134
959	Probing the conformational space available to inhibitors in the thermolysin active site using Monte Carlo/energy minimization techniques. **1992**, 13, 214-228	46

958	Standard-geometry chains fitted to X-ray derived structures: Validation of the rigid-geometry approximation. II. Systematic searches for short loops in proteins: Applications to bovine pancreatic ribonuclease A and human lysozyme. **1992**, 13, 329-350	25
957	Molecular docking using shape descriptors. **1992**, 13, 380-397	348
956	Efficient algorithm for the reconstruction of a protein backbone from the □carbon coordinates. **1992**, 13, 443-456	46
955	Automated docking with grid-based energy evaluation. **1992**, 13, 505-524	770
954	Conformational analysis of flexible ligands in macromolecular receptor sites. **1992**, 13, 730-748	171
953	Warum Pentose- und nicht Hexose-Nucleins□ren?? Teil I. Einleitung und Problemstellung, Konformationsanalyse f□ Oligonucleotid-Ketten aus 2?,3?-Dideoxyglucopyranosyl-Bausteinen (□Homo-DNS)□sowie Betrachtungen zur Konformation von A- und B-DNS. **1992**, 75, 218-259	148
952	Vibrational studies of the disulfide group in proteins. VII. Normal mode analysis of the Raman spectra of erabutoxin, □I crystallin and immunoglobulin. **1992**, 23, 517-521	16
951	Binding of the Kunitz-type trypsin inhibitor DE-3 from Erythrina caffra seeds to serine proteinases: a comparative study. **1992**, 5, 105-14	10
950	Methoden der multiplen Peptidsynthese und ihre Anwendungen. **1992**, 104, 375-391	58
949	Molek□dynamiksimulation f□ ein allelspezifisches virales Nonapeptid aus dem Influenza-Matrix-protein in der Bindungstasche eines menschlichen MHC-Klasse-I-Proteins. **1992**, 104, 928-931	3
948	An expanded nomenclature scheme for labeling peptide fragmentations and its use with 'AMASS', a computer program for generating all possible fragment ion structures from known precursors. **1993**, 22, 31-44	10
947	Application of distance geometry to the proton assignment problem. **1993**, 33, 107-15	24
946	Necessary conditions for avoiding incorrect polypeptide folds in conformational search by energy minimization. **1993**, 33, 173-92	12
945	Approximation and characterization of molecular surfaces. **1993**, 33, 219-29	103
944	Shape analysis of molecular surfaces. **1993**, 33, 231-8	63
943	Conformational preference functions for predicting helices in membrane proteins. **1993**, 33, 255-73	36
942	Molecular dynamics of sickle and normal hemoglobins. **1993**, 33, 735-42	10
941	The hydration of proteins in nearly anhydrous organic solvent suspensions. **1993**, 33, 1213-24	40

940	The loop problem in proteins: a Monte Carlo simulated annealing approach. **1993**, 33, 1271-86	32
939	Energetics of the disulfide bridge: An ab initio study. **1993**, 33, 1591-1603	7
938	Effect of fluorochrome location in protein A on sensing efficiency of IgG. **1993**, 42, 37-42	8
937	Conformational and energetic effects of truncating nonbonded interactions in an aqueous protein dynamics simulation. **1993**, 14, 295-311	90
936	Yammp: Development of a molecular mechanics program using the modular programming method. **1993**, 14, 455-470	36
935	The ethylene group as a peptide bond mimicking unit: A theoretical conformational analysis. **1993**, 14, 471-477	3
934	A critical comparison of search algorithms applied to the optimization of protein side-chain conformations. **1993**, 14, 790-798	61
933	Lattice representations of globular proteins: How good are they?. **1993**, 14, 1194-1202	77
932	Improved strategy in analytic surface calculation for molecular systems: Handling of singularities and computational efficiency. **1993**, 14, 1272-1280	176
931	Optimization of primers for cloning libraries of mouse immunoglobulin genes using the polymerase chain reaction. **1993**, 23, 206-11	77
930	Actin filament structure probed with monoclonal antibodies. **1993**, 25, 73-86	7
929	Inhibitors of aspartyl proteinases. **1993**, 13, 731-78	48
928	PLIM: a protein-ligand interaction modeller. **1993**, 6, 111-5	6
927	From crystals to enzymes: simple models of molecular recognition. **1993**, 6, 187-94	1
926	Protein three-dimensional structure generation with an empirical hydrophobic penalty function. **1993**, 11, 222-32, 234	3
925	Graphical representations of the class I MHC cleft. **1993**, 11, 174-9, 187	4
924	Modeling and solution structure probing of the HIV-1 TAR stem-loop. **1993**, 11, 92-7, 124	12
923	SETOR: hardware-lighted three-dimensional solid model representations of macromolecules. **1993**, 11, 134-8, 127-8	1140

922	Tyrosine hypochromism and absence of tyrosine-tryptophan energy transfer in phospholipase A2 and ribonuclease T1. **1993**, 171, 231-236	5
921	Conformational classification of short backbone fragments in globular proteins and its use for coding backbone conformations. **1993**, 47, 163-178	5
920	Self-similarity of Mn(II)-induced trypsin activity oscillations. Experimental evidence. **1993**, 52, 131-8	4
919	Analysis of hydrogen bonds in peptides, based on the hydration affinity of amides. **1993**, 297, 115-126	9
918	Amide modes of reverse turns. **1993**, 5, 143-173	15
917	Structural and functional aspects of RGD-containing protein antagonists of glycoprotein IIb-IIIa. **1993**, 4, 438-45	49
916	Synthesis of peptides containing a sulfinamide or a sulfonamide transition-state isostere. **1993**, 49, 1133-1150	67
915	GenStar: a method for de novo drug design. **1993**, 7, 23-43	103
914	Hydrophilic surface maps of channel-forming peptides: analysis of amphipathic helices. **1993**, 22, 269-77	15
913	Predicting secondary structures of membrane proteins with neural networks. **1993**, 22, 41-51	26
912	Intrinsic nature of the three-dimensional structure of proteins as determined by distance geometry with good sampling properties. **1993**, 3, 19-40	31
911	A preliminary 3D model for cytochrome P450 2D6 constructed by homology model building. **1993**, 7, 281-9	48
910	Stereochemistry of charged nitrogen-aromatic interactions and its involvement in ligand-receptor binding. **1993**, 7, 173-82	37
909	PROGEN: an automated modelling algorithm for the generation of complete protein structures from the alpha-carbon atomic coordinates. **1993**, 7, 199-224	9
908	Applications of electrospray mass spectrometry to studies on the structural properties of ribonuclease A and ribonuclease B. **1993**, 7, 332-335	11
907	Gaussian neighborhood: a new measure of accessibility for residues of protein molecules. **1993**, 15, 50-61	6
906	Crystallographic analysis of Thr-200-->His human carbonic anhydrase II and its complex with the substrate, HCO3-. **1993**, 15, 80-7	85
905	On the calculation of pKas in proteins. **1993**, 15, 252-65	489

904	Multiple-site titration and molecular modeling: two rapid methods for computing energies and forces for ionizable groups in proteins. **1993**, 15, 266-82	254
903	Theoretical studies of relaxation of a monomeric subunit of HIV-1 protease in water using molecular dynamics. **1993**, 15, 374-84	19
902	Packing and recognition of protein structural elements: a new approach applied to the 4-helix bundle of myohemerythrin. **1993**, 15, 413-25	15
901	A novel computer modeling approach to the structures of small bioactive peptides: the structure of gonadotropin releasing hormone. **1993**, 16, 48-56	23
900	Prediction of protein folding class from amino acid composition. **1993**, 16, 79-91	60
899	Picosecond timescale rigid-helix and side-chain motions in deoxymyoglobin. **1993**, 16, 141-54	45
898	Calcium-independent subtilisin by design. **1993**, 16, 205-13	43
897	Surface motifs by a computer vision technique: searches, detection, and implications for protein-ligand recognition. **1993**, 16, 278-92	63
896	Improved calculations of compactness and a reevaluation of continuous compact units. **1993**, 16, 293-300	17
895	Conformational deformation in deoxymyoglobin by hydrostatic pressure. **1993**, 16, 327-40	51
894	An analysis of the conformational paths of citrate synthase. **1993**, 16, 393-407	12
893	Molecular basis of cooperativity in protein folding. IV. CORE: a general cooperative folding model. **1993**, 17, 111-23	26
892	Structural relationships of homologous proteins as a fundamental principle in homology modeling. **1993**, 17, 138-51	81
891	Conformational analysis of protein structures derived from NMR data. **1993**, 17, 232-51	64
890	Crystal structure of the complex of human alpha-thrombin and nonhydrolyzable bifunctional inhibitors, hirutonin-2 and hirutonin-6. **1993**, 17, 252-65	34
889	A calculation strategy for the structure determination of symmetric dimers by 1H NMR. **1993**, 17, 297-309	301
888	A reduced representation of proteins for use in restraint satisfaction calculations. **1993**, 17, 310-24	14
887	Crystal structure of Escherichia coli RNase HI in complex with Mg2+ at 2.8 A resolution: proof for a single Mg(2+)-binding site. **1993**, 17, 337-46	131

886	Recognition of errors in three-dimensional structures of proteins. **1993**, 17, 355-62	1679
885	A method to recognize distant repeats in protein sequences. **1993**, 17, 391-41	59
884	Crystallographic studies and primary structure of the antitumor monoclonal CC49 Fab'. **1993**, 17, 438-43	3
883	Disulfide bonding patterns and protein topologies. **1993**, 2, 41-54	46
882	Modeling alpha-helical transmembrane domains: the calculation and use of substitution tables for lipid-facing residues. **1993**, 2, 55-70	127
881	Exploration of subsite binding specificity of human cathepsin D through kinetics and rule-based molecular modeling. **1993**, 2, 264-76	80
880	Structural analysis based on state-space modeling. **1993**, 2, 305-14	140
879	Reconstruction of protein conformations from estimated positions of the C alpha coordinates. **1993**, 2, 315-24	25
878	Controlling the regiospecificity and coupling of cytochrome P450cam: T185F mutant increases coupling and abolishes 3-hydroxynorcamphor product. **1993**, 2, 357-65	28
877	Structure of Paramecium tetraurelia calmodulin at 1.8 A resolution. **1993**, 2, 436-47	70
876	Modeling the structure of Pyrococcus furiosus rubredoxin by homology to other X-ray structures. **1993**, 2, 640-9	12
875	Investigations of the thermostability of rubredoxin models using molecular dynamics simulations. **1993**, 2, 650-65	14
874	Reduced representation model of protein structure prediction: statistical potential and genetic algorithms. **1993**, 2, 762-85	181
873	Catching a common fold. **1993**, 2, 877-83	83
872	Families and the structural relatedness among globular proteins. **1993**, 2, 884-99	72
871	Molecular dynamics simulations and rigid body (TLS) analysis of aspartate carbamoyltransferase: evidence for an uncoupled R state. **1993**, 2, 927-35	19
870	Representing an ensemble of NMR-derived protein structures by a single structure. **1993**, 2, 936-44	35
869	Effects of alanine substitutions in alpha-helices of sperm whale myoglobin on protein stability. **1993**, 2, 1099-105	44

868	Crystal structure to 2.45 A resolution of a monoclonal Fab specific for the Brucella A cell wall polysaccharide antigen. **1993**, 2, 1106-13	59
867	Cross-validation of protein structural class prediction using statistical clustering and neural networks. **1993**, 2, 1171-82	80
866	Prediction of the three-dimensional structures of the nerve growth factor and epidermal growth factor binding proteins (kallikreins) and an hypothetical structure of the high molecular weight complex of epidermal growth factor with its binding protein. **1993**, 2, 1229-41	11
865	The structure and function of omega loop A replacements in cytochrome c. **1993**, 2, 1429-40	20
864	Modeling of protein loops by simulated annealing. **1993**, 2, 1502-10	82
863	Verification of protein structures: patterns of nonbonded atomic interactions. **1993**, 2, 1511-9	2259
862	Identification, classification, and analysis of beta-bulges in proteins. **1993**, 2, 1574-90	176
861	Confidence limits on the branching order of phylogenetic trees. **1993**, 2, 1686-96	4
860	Knowledge-based model building of proteins: concepts and examples. **1993**, 2, 1798-810	97
859	Comparison of conformational characteristics in structurally similar protein pairs. **1993**, 2, 1811-26	160
858	Toward computational determination of peptide-receptor structure. **1993**, 2, 1827-43	28
857	Aldehyde dehydrogenases: widespread structural and functional diversity within a shared framework. **1993**, 2, 1890-900	164
856	Structural argument for N-terminal initiation of protein folding. **1993**, 2, 1989-91	23
855	Thermodynamics of BPTI folding. **1993**, 2, 2028-36	92
854	Origins of structural diversity within sequentially identical hexapeptides. **1993**, 2, 2134-45	89
853	Classification of doubly wound nucleotide binding topologies using automated loop searches. **1993**, 2, 2146-53	34
852	Prediction of protein folding pathways: Bovine pancreatic trypsin inhibitor. **1993**, 11, S67-71	1
851	Protein secondary structure conformations and associated hydrophobicity scales. **1993**, 14, 35-45	7

850	Strategies for selecting mutation sites for methionine enhancement in the bean seed storage protein phaseolin. **1993**, 12, 545-60	30
849	A new approach to predicting protein folding types. **1993**, 12, 169-78	27
848	Investigating the s-2 subsite selectivity of alkaline proteases in hydrolysis of diastereo-peptide esters and molecular-modeling interpretation. **1993**, 1, 361-7	2
847	Recognition by Max of its cognate DNA through a dimeric b/HLH/Z domain. **1993**, 363, 38-45	658
846	The role of turns in the structure of an alpha-helical protein. **1993**, 364, 355-8	103
845	Co-crystal structure of the HNF-3/fork head DNA-recognition motif resembles histone H5. **1993**, 364, 412-20	1121
844	An SH2-SH3 domain hybrid. **1993**, 364, 765	24
843	Structure and function of endoglucanase V. **1993**, 365, 362-4	126
842	Crystal structure of the DsbA protein required for disulphide bond formation in vivo. **1993**, 365, 464-8	361
841	Co-crystal structure of TBP recognizing the minor groove of a TATA element. **1993**, 365, 520-7	994
840	Tandem binding in crystals of a trp repressor/operator half-site complex. **1993**, 366, 178-82	146
839	Amino/aromatic interactions. **1993**, 366, 413-413	48
838	Recurrence of a binding motif?. **1993**, 362, 299	23
837	Structure of a major immunogenic site on foot-and-mouth disease virus. **1993**, 362, 566-8	313
836	Probing the S-1? subsite selectivity of an industrial alkaline protease in anhydrous t-butanol. **1993**, 3, 727-733	7
835	Myelin P0-glycoprotein: predicted structure and interactions of extracellular domain. **1993**, 61, 1987-95	32
834	On the mechanism of energy transfer to Tb3+ ions in proteins. A time-resolved luminescence study of the Tb-elastase complex. **1993**, 211, 467-73	8
833	Crystallographic studies of azide binding to human carbonic anhydrase II. **1993**, 213, 507-15	19

832	Crystal structure of apo-neocarzinostatin at 0.15-nm resolution. **1993**, 213, 737-41	37
831	Binding of bovine pancreatic trypsin inhibitor to heparin binding protein/CAP37/azurocidin. Interaction between a Kunitz-type inhibitor and a proteolytically inactive serine proteinase homologue. **1993**, 214, 271-9	17
830	Sequential assignment of proton resonances in the NMR spectrum of Zn-substituted alpha chains from human hemoglobin. Ligand-induced tertiary changes in the heme pocket. **1993**, 214, 383-93	5
829	Site specificity of glycation of horse liver alcohol dehydrogenase in vitro. **1993**, 215, 567-72	36
828	Electrostatic evidence for the activation of the glutathione thiol by Tyr7 in pi-class glutathione transferases. **1993**, 215, 663-70	51
827	Structural requirements for processing of pro-adipokinetic hormone I. **1993**, 217, 905-11	15
826	Complexes of the polyamines spermine, spermidine and putrescine with alpha-lactalbumins. **1993**, 218, 303-9	6
825	Quality control of protein models: directional atomic contact analysis. **1993**, 26, 47-60	243
824	Protein symmetry: metric and crystal (a precautionary note). **1993**, 26, 68-70	
823	The FROG PC series: programs for electron-density and model investigations for proteins. **1993**, 26, 291-294	14
822	PROCHECK: a program to check the stereochemical quality of protein structures. **1993**, 26, 283-291	17966
821	Comparison of radiation-induced decay and structure refinement from X-ray data collected from lysozyme crystals at low and ambient temperatures. **1993**, 26, 309-319	33
820	GEOM□a program to assess the reliability of a protein model. **1993**, 26, 495-496	1
819	TLSANL: TLS parameter-analysis program for segmented anisotropic refinement of macromolecular structures. **1993**, 26, 622-624	81
818	Methods used in the structure determination of foot-and-mouth disease virus. **1993**, 49 (Pt 1), 45-55	31
817	The asymmetric unit of X-ray intensity data of the seven crystal systems. **1993**, 49, 369-371	2
816	The use of protein homologues in the rotation function. **1993**, 49 (Pt 2), 306-15	3
815	New techniques for the determination of the scale and overall isotropic temperature factors. **1993**, 49, 389-398	4

814	On the doublet phase sums of isomorphous data sets. **1993**, 49, 359-369	1
813	On the relation between the diffraction ratio, the doublet values and the reliability of the triplet estimates. **1993**, 49, 350-358	1
812	On direct-methods phase information from differences between isomorphous structure factors. **1993**, 49, 557-569	7
811	Complex of ribonuclease from Streptomyces aureofaciens with 2'-GMP at 1.7 A resolution. **1993**, 49, 257-71	15
810	Assessment of phase accuracy by cross validation: the free R value. Methods and applications. **1993** , 49, 24-36	368
809	Phasing macromolecular structures via structure-invariant algebra. **1993**, 49, 3-8	2
808	Molecular scene analysis: the integration of direct-methods and artificial-intelligence strategies for solving protein crystal structure. **1993**, 49, 168-78	7
807	Protein single-crystal diffraction with 5 A synchrotron X-rays at the sulfur K-absorption edge. **1993**, 49, 308-10	9
806	Structure determination and refinement of benzamidine-inhibited trypsin from the North Atlantic salmon (Salmo salar) at 1.82 A resolution. **1993**, 49, 318-30	4
805	Crystallographic analyses of an active HIV-1 ribonuclease H domain show structural features that distinguish it from the inactive form. **1993**, 49, 423-7	15
804	Structure of triosephosphate isomerase from Escherichia coli determined at 2.6 A resolution. **1993**, 49, 403-17	48
803	Orientation of non-crystallographic symmetry axes in protein crystals. **1993**, 49, 505-12	13
802	PRISM: topologically constrained phased refinement for macromolecular crystallography. **1993**, 49, 429-39	17
801	Refined structure of cadmium-substituted concanavalin A at 2.0 A resolution. **1993**, 49, 561-71	20
800	Structure of recombinant bovine interferon-gamma at 3.0 A resolution. **1993**, 49, 513-21	8
799	Location of haem in bacterioferritin of E. coli. **1993**, 49, 597-600	5
798	Structure of the crystalline complex of cytidylic acid (2'-CMP) with ribonuclease at 1.6 A resolution. Conservation of solvent sites in RNase-A high-resolution structures. **1993**, 49, 541-7	29
797	Executive Secretary. **1993**, 49, 427-427	

796	Peptides secondary structure prediction with neural networks: a criterion for building appropriate learning sets. **1993**, 40, 1114-21	11
795	Symptomatic type II protein C deficiency caused by a missense mutation (Gly 381-->Ser) in the substrate-binding pocket. **1993**, 84, 285-9	15
794	A molecular model of the serine protease domain of activated protein C: application to the study of missense mutations causing protein C deficiency. **1993**, 84, 290-300	21
793	HYDRO: a program for protein hydropathy predictions. **1993**, 41, 121-9	2
792	Recurring structural motifs in proteins with different functions. **1993**, 3, 131-9	43
791	Structural similarity of DNA-binding domains of bacteriophage repressors and the globin core. **1993**, 3, 141-8	160
790	A method for predicting protein structure from sequence. **1993**, 3, 414-23	73
789	New folds for all-beta proteins. **1993**, 1, 217-22	67
788	Major antigen-induced domain rearrangements in an antibody. **1993**, 1, 83-93	201
787	Alpha plus beta folds revisited: some favoured motifs. **1993**, 1, 105-20	142
786	Peptide models 4. Topological features of molecular mechanics and ab initio 2D-ramachandran maps. **1993**, 288, 161-179	66
785	Statistical potentials and learning methods to evaluate protein models: application to the coiled-coil tropomyosin. **1993**, 286, 47-54	1
784	A complete set of conformational elements defining secondary structures of proteins. **1993**, 286, 75-85	9
783	Molecular modelling and epitope prediction of gp29 from lymphatic filariae. **1993**, 58, 145-53	14
782	Dynamic structural and functional relationships in recombinant plasminogen activator inhibitor-1 (rPAI-1). **1993**, 1202, 221-9	24
781	Molecular dynamics simulation of a phospholipase A2-substrate complex. **1993**, 1162, 135-42	17
780	Selective oxidation of Met-192 in bovine alpha-chymotrypsin. Effect on catalytic and inhibitor binding properties. **1993**, 1161, 201-8	6
779	Physical and conformational properties of staphylokinase in solution. **1993**, 1161, 244-8	27

778	Extracting the information--sequence analysis software design evolves. **1993**, 11, 223-7		2
777	Antigen recognition and targeted delivery by the single-chain Fv. **1993**, 22, 189-224		26
776	Three-dimensional structure of acetylcholinesterase and of its complexes with anticholinesterase drugs. *Chemico-Biological Interactions*, **1993**, 87, 187-97	5	82
775	Molecular bases for heme:ligand recognition in sperm whale (Physeter Catodon) andAplysia limacine myoglobin. **1993**, 4, 65-73		5
774	Ariel: an information system for AIDS research. **1993**, 31 Suppl, S12-6		0
773	Finding the lowest free energy conformation of a protein is an NP-hard problem: proof and implications. **1993**, 55, 1183-98		104
772	Structure-based design of inhibitors of purine nucleoside phosphorylase. 1. 9-(arylmethyl) derivatives of 9-deazaguanine. **1993**, 36, 55-69		125
771	atomium-a Python structure parser. **2020**, 36, 2750-2754		7
770	Redundancy-weighting the PDB for detailed secondary structure prediction using deep-learning models. **2020**, 36, 3733-3738		2
769	Allantoin, a Potential Metabolite That Promotes AMPK Phosphorylation and Suppresses Cholesterol Biosynthesis Via the Mevalonate Pathway and Bloch Pathway. **2020**, 191, 226-244		1
768	Genome re-seqeunce and analysis of Burkholderia glumae strain AU6208 and evidence of toxoflavin: A potential bacterial toxin. **2020**, 86, 107245		1
767	analysis of Calcium Dependent Protein Kinase 6 of Cr through molecular modeling, docking, and dynamics simulation study. **2021**, 39, 5461-5470		2
766	Non-conventional force fields for applications in spectroscopy and chemical reaction dynamics. **2020**, 153, 010901		10
765	Probe into a multi-protein prokaryotic organelle using thermal scanning assay reveals distinct properties of the core and the shell. **2020**, 1864, 129680		2
764	Mobility of water and of protein atoms at the protein-water interface, monitored by anisotropic atomic displacement parameters, are largely uncorrelated. **2020**, 52, 435-443		2
763	Applications of water molecules for analysis of macromolecule properties. **2020**, 18, 355-365		10
762	Exploring the computational methods for protein-ligand binding site prediction. **2020**, 18, 417-426		33
761	Water-Intake and Water-Molecule Paths to the Active Site of Secretory Phospholipase A Studied Using MD Simulations and the Tracking Tool AQUA-DUCT. **2020**, 124, 1881-1891		1

760	Semisynthesis of ursolic acid-2-(2-thienylidene)-oxadiazole hybrid molecule and an evaluation of its COX inhibition property. **2020**, 57, 2048-2055		3
759	Identification and Molecular Characterization of a Pellino Protein in Kuruma Prawn () in Response to White Spot Syndrome Virus and Infection. **2020**, 21,		5
758	Protein X-ray Crystallography and Drug Discovery. *Molecules*, **2020**, 25,	4.8	41
757	What are the current limits on determination of protonation state using neutron macromolecular crystallography?. **2020**, 634, 225-255		
756	Self-Parametrizing System-Focused Atomistic Models. **2020**, 16, 1646-1665		18
755	Association of HLA-A*11:01 with Sulfonamide-Related Severe Cutaneous Adverse Reactions in Japanese Patients. **2020**, 140, 1659-1662.e6		7
754	Nanoparticle translocation across the lung surfactant film regulated by grafting polymers. **2020**, 12, 3931-3940		5
753	Best practices for high data-rate macromolecular crystallography (HDRMX). **2020**, 7, 014302		5
752	Calculating the absolute binding free energy of the insulin dimer in an explicit solvent.. **2020**, 10, 790-800		7
751	Computational Advances in Bio and Medical Sciences. **2020**,		
750	Structure and biological evaluation of pyridine-2-carboxamidine copper(II) complex resulting from N'-(4-nitrophenylsulfonyloxy)2-pyridine-carboxamidoxime. **2020**, 208, 111085		6
749	Molecular dynamics simulations in photosynthesis. **2020**, 144, 273-295		25
748	Kinetic and structural characterization of therapeutic albumin chemical functionalization using complementary mass spectrometry techniques. **2020**, 185, 113242		2
747	The Identification of Metal Ion Ligand-Binding Residues by Adding the Reclassified Relative Solvent Accessibility. **2020**, 11, 214		3
746	Cloning, expression, homology modelling and molecular dynamics simulation of four domain-containing ⊟amylase from Streptomyces griseus. **2021**, 39, 2152-2163		7
745	Synthesis of new morpholine containing 3-amido-9-ethylcarbazole derivative and studies on its biophysical interactions with calf thymus DNA/HSA. **2021**, 39, 1561-1571		4
744	Erythroxylum pungens Tropane Alkaloids: GC-MS Analysis and the Bioactive Potential of 3-(2-methylbutyryloxy)tropan-6,7-diol in Zebrafish (Danio rerio). **2021**, 87, 177-186		1
743	In vitro and in silico evaluation of the inhibitory effect of a curcumin-based oxovanadium (IV) complex on alkaline phosphatase activity and bacterial biofilm formation. **2021**, 105, 147-168		6

742	Molecular dynamics provides new insights into the mechanism of calcium signal transduction and interdomain interactions in cardiac troponin. **2021**, 11, 1841-1853		0
741	Searching for a Better Match between Protein Secondary Structure Definitions and Protein FTIR Spectra. **2021**, 93, 1561-1568		10
740	Investigation of C-glycosylated apigenin and luteolin derivatives effects on protein tyrosine phosphatase 1B inhibition with molecular and cellular approaches. **2021**, 17, 100141		3
739	LAHMA: structure analysis through local annotation of homology-matched amino acids. *Acta Crystallographica Section D: Structural Biology*, **2021**, 77, 28-40	5.5	2
738	In silico and in vitro anti-AChE activity investigations of constituents from Mytragyna speciosa for Alzheimer's disease treatment. **2021**, 35, 325-336		1
737	Role of water in the determination of protonation states of titratable residues. **2021**, 27, 61		0
736	The Protein Data Bank Archive. **2021**, 2305, 3-21		12
735	Recent advances in de novo protein design: Principles, methods, and applications. *Journal of Biological Chemistry*, **2021**, 296, 100558	5.4	29
734	Amino acid side chain contribution to protein FTIR spectra: impact on secondary structure evaluation. **2021**, 50, 641-651		4
733	Structural effects driven by rare point mutations in amylin hormone, the type II diabetes-associated peptide.		
732	FTIR Imaging of Protein Microarrays for High Throughput Secondary Structure Determination. **2021** , 93, 3733-3741		13
731	Integrating structure-based machine learning and co-evolution to investigate specificity in plant sesquiterpene synthases. **2021**, 17, e1008197		1
730	Advanced strategies for development of vaccines against human bacterial pathogens. **2021**, 37, 67		1
729	FRAGSITE: A Fragment-Based Approach for Virtual Ligand Screening. **2021**, 61, 2074-2089		8
728	Protein modeling. **2021**,		
727	How anisotropic and isotropic atomic displacement parameters monitor protein covalent bonds rigidity: isotropic B-factors underestimate bond rigidity. **2021**, 53, 779-782		1
726	Spike mutation T403R allows bat coronavirus RaTG13 to use human ACE2.		0
725	Prospects of Tensor-Based Numerical Modeling of the Collective Electrostatics in Many-Particle Systems. **2021**, 61, 864-886		1

724	Automated Construction of Quantum-Classical Hybrid Models. **2021**, 17, 3797-3813		8
723	Thermodynamic profile and molecular modeling of the interaction between Grb2 dimer and flavonoids Rutin and Morin. **2021**, 1234, 130164		1
722	Molecular structure, vibrational spectroscopic, frontier molecular orbital and natural bond orbital analysis of anti-cancer drug 6-chloro-3- pyridine carbonitrile. 1-18		2
721	Open-access data: A cornerstone for artificial intelligence approaches to protein structure prediction. **2021**, 29, 515-520		3
720	Virtual screening of potential anticancer drugs based on microbial products. **2021**,		1
719	Phytochemicals from Nigerian medicinal plants modulate therapeutically-relevant diabetes targets: insight from computational direction. 1		1
718	Protein-structure prediction revolutionized. **2021**, 596, 487-488		8
717	Structural effects driven by rare point mutations in amylin hormone, the type II diabetes-associated peptide. **2021**, 1865, 129935		
716	Unraveling the binding mechanism of an Oxovanadium(IV) - Curcumin complex on albumin, DNA and DNA gyrase by in vitro and in silico studies and evaluation of its hemocompatibility. **2021**, 221, 111402		0
715	Investigating the Mechanism of Herba in the Treatment of Colorectal Cancer by Network Pharmacology and Molecular Docking. **2021**, 2021, 3905367		2
714	DeepPocket: Ligand Binding Site Detection and Segmentation using 3D Convolutional Neural Networks. **2021**,		8
713	In-vitro Cytotoxicity and In-silico Insights of the Multi-target Anticancer Candidates from Haplophyllum tuberculatum. **2021**, 4, 192-201		
712	Chalcogen Bonds Involving Selenium in Protein Structures. *ACS Chemical Biology*, **2021**, 16, 1622-1627	4.9	7
711	Decline of protein structure rigidity with interatomic distance. **2021**, 22, 466		
710	Cassava mosaic virus in Africa: Functional analysis of virus coat proteins based on evolutionary processes and protein structure. **2021**, 24, 101239		2
709	A molecular docking study of human STEAP2 for the discovery of new potential anti-prostate cancer chemotherapeutic candidates.		
708	Interaction of Thymine DNA Glycosylase with Oxidised 5-Methyl-cytosines in Their Amino- and Imino-Forms. *Molecules*, **2021**, 26,	4.8	0
707	Protein Structural Denaturation Evaluated by MCR-ALS of Protein Microarray FTIR Spectra. **2021**, 93, 13441-13449		3

706	A differential subcellular localization of two copper transporters from the COPT family suggests distinct roles in copper homeostasis in Physcomitrium patens. **2021**, 167, 459-469	2
705	VASPKIT: A user-friendly interface facilitating high-throughput computing and analysis using VASP code. **2021**, 267, 108033	434
704	Intrinsically disordered proteins: Chronology of a discovery. **2021**, 279, 106694	3
703	Python for Chemists. **2022**,	
702	3-State Protein Secondary Structure Prediction based on SCOPe Classes. 64,	0
701	Distant homology recognition using structural classification of proteins. **1997**, 29, 105-112	8
700	Assessment of comparative modeling in CASP2. **1997**, 29, 14-28	9
699	Successful ab initio prediction of the tertiary structure of NK-lysin using multiple sequences and recognized supersecondary structural motifs. **1997**, 29, 185-191	13
698	Ab initio folding of proteins using restraints derived from evolutionary information. **1999**, 37, 177-185	32
697	Model building by comparison at CASP3: Using expert knowledge and computer automation. **1999**, 37, 47-54	25
696	Virtual Screening. **2003**, 243-279	3
695	X-ray crystallography of proteins. **1994**, 37, 1-72	4
694	Computer Graphics and Molecular Modeling in the Analysis of Synthetic Targets. 1-85	4
693	Metal-Binding Domains in Nucleic Acid-Binding and Gene-Regulatory Proteins. 143-185	20
692	Zinc Endoproteases: A Structural Superfamily. 73-88	2
691	Design and Diversity Analysis of Compound Libraries for Lead Discovery. **1999**, 409-439	4
690	Adsorption of proteins onto charged surfaces: A Monte Carlo approach with explicit ions. **1996**, 17, 1783-1803	20
689	A new method for side-chain conformation prediction using a Hopfield network and reproduced rotamers. **1996**, 17, 1667-1683	5

688	Thermal-induced unfolding domains in aldolase identified by amide hydrogen exchange and mass spectrometry. **1996**, 5, 1282-9	25
687	Protein clefts in molecular recognition and function. **1996**, 5, 2438-52	291
686	Evolution of beta-amylase: patterns of variation and conservation in subfamily sequences in relation to parsimony mechanisms. **1996**, 25, 456-72	26
685	Receptor-Based Prediction of Binding Affinities. **2002**, 35-61	6
684	In vitro and in silico affinity fingerprints: Finding similarities beyond structural classes. **2000**, 231-244	3
683	Predicting binding modes, binding affinities and Hot spots for protein-ligand complexes using a knowledge-based scoring function. **2000**, 115-144	1
682	The Structures of Photosynthetic Reaction Centers from Purple Bacteria as Revealed by X-Ray Crystallography. **1995**, 503-526	1
681	Plastocyanin: Structure, Location, Diffusion and Electron Transfer Mechanisms. **1996**, 413-429	4
680	3 Structure of ribonucleases. 3001-3006	1
679	Bidirectional Dynamics for Protein Secondary Structure Prediction. **2000**, 80-104	17
678	Improving Profile-Profile Alignments via Log Average Scoring. **2001**, 11-26	8
677	A CLP Approach to the Protein Side-Chain Placement Problem. **2001**, 479-493	5
676	An artificial life model for predicting the tertiary structure of unknown proteins that emulates the folding process. **1995**, 862-875	6
675	Computing with evolving proteins. **1998**, 207-215	2
674	The Role of Structural Water Molecules in Protein Saccharide Complexes. **1993**, 321-337	7
673	Hydration of Amino Acids in Protein Crystals. **1993**, 63-97	1
672	Water Structure of Crystallized Proteins: High-Resolution Studies. **1993**, 98-147	3
671	Computer Modelling and Information Technology. **1991**, 253-289	3

670	Membrane Protein Structure Prediction. **2009**, 91-111	1
669	Aplysia limacina Myoglobin: Molecular Bases for Ligand Binding. **1991**, 161-170	1
668	Molecular Modeling with Substructure Libraries Derived from Known Protein Structures. **1990**, 175-188	7
667	The Chemistry of Antigen-Antibody Union. **1985**, 243-258	2
666	Crystal structure analysis of subtilisin BPN' mutants engineered for studying thermal stability. **1996** , 379, 159-69	7
665	Crystallographic study of eglin-C binding to thermitase. **1996**, 379, 5-9	1
664	Three dimensional structure of the antibiotic bacitracin A complexed to two different subtilisin proteases: novel mode of enzyme inhibition. **1996**, 379, 29-41	9
663	Comparative anatomy of phospholipase A2 structures. **1990**, 279, 23-36	3
662	The GOR Method for Predicting Secondary Structures in Proteins. **1989**, 417-465	37
661	A new way of looking at aspartic proteinase structures: a comparison of pepsin structure to other aspartic proteinases in the near active site region. **1995**, 362, 19-32	6
660	Activated dynamics of flap opening in HIV-1 protease. **1995**, 362, 455-60	10
659	A Model of Butyrylcholinesterase Based on the X-Ray Structure of Acetylcholinesterase Indicates Differences in Specificity. **1992**, 189-194	2
658	Proton Transfer Pathways in the Reaction Center of Rhodobacter Sphaeroides: A Computational Study. **1992**, 363-374	12
657	Structural constraints on residue substitution. **1992**, 14, 231-49	3
656	Gaussian-Based Approaches to Protein-Structure Similarity. **2000**, 83-88	1
655	Tryptophans in membrane proteins. X-ray crystallographic analyses. **1999**, 467, 789-99	35
654	Theoretical and Computer Analysis of Protein Primary Sequences: Structure Comparison and Prediction. **1988**, 21-65	4
653	Inhibitor binding induces structural changes in porcine pepsin. **1991**, 306, 9-21	11

652	Functional implications of the three-dimensional structure of bovine chymosin. **1991**, 306, 23-37	10
651	The Dead-End Elimination Theorem: A New Approach to the Side-Chain Packing Problem. **1994**, 307-337	12
650	In Search of Protein Folds. **1994**, 353-407	2
649	Computational Complexity, Protein Structure Prediction, and the Levinthal Paradox. **1994**, 433-506	18
648	Multiple-Start Monte Carlo Docking of Flexible Ligands. **1994**, 71-108	10
647	Charged-particle transport in biomolecular media: the third generation. **1994**, 63, 77-91; discussion 91-2	1
646	Hydrogen Bonding Models: Their Relevance to Molecular Modeling. **1996**, 119-141	2
645	Comments on some present and future problems in protein structure. **1984**, 27, 1-24	2
644	Thermodynamic strategies for rational protein and drug design. **1995**, 7, 219-41	10
643	Applications of Knowledge Based Mean Fields in the Determination of Protein Structures. **1994**, 297-315	2
642	Domains and Modules of Proteins. **1993**, 229-232	1
641	Synthetic Protein Surface Domains as Bioactive Stationary Phases. **1993**, 277-312	1
640	SPOT-Seq-RNA: predicting protein-RNA complex structure and RNA-binding function by fold recognition and binding affinity prediction. **2014**, 1137, 119-30	26
639	Fusion RNAs in crystallographic studies of double-stranded RNA from trypanosome RNA editing. **2015**, 1240, 191-216	1
638	Crystallization: digging into the past to learn lessons for the future. **2015**, 1261, 141-56	4
637	Modeling and predicting RNA three-dimensional structures. **2015**, 1269, 101-21	5
636	CATH-Gene3D: Generation of the Resource and Its Use in Obtaining Structural and Functional Annotations for Protein Sequences. **2017**, 1558, 79-110	15
635	Databases, Repositories, and Other Data Resources in Structural Biology. **2017**, 1607, 643-665	4

634	Identifying and Overcoming Crystal Pathologies: Disorder and Twinning. **2017**, 1607, 185-217	3
633	The role and application of in silico docking in chemical genomics research. **2005**, 310, 63-91	1
632	Receptor flexibility for large-scale in silico ligand screens: chances and challenges. **2008**, 443, 353-64	3
631	Improving pairwise sequence alignment between distantly related proteins. **2007**, 395, 255-68	1
630	Determination of antibody structures. **2014**, 1131, 395-406	2
629	Forecasting Model for the Annual Growth of Cryogenic Electron Microscopy Data. **2020**, 147-158	1
628	Patterns of Sequence Variation in Families of Homologous Proteins. **1991**, 373-385	3
627	Lysozyme: a model enzyme in protein crystallography. **1996**, 75, 185-222	41
626	More Reliable Protein NMR Peak Assignment via Improved 2-Interval Scheduling. **2003**, 580-592	1
625	Stochastic Conformational Roadmaps for Computing Ensemble Properties of Molecular Motion. **2004**, 131-147	4
624	Structure and function of CD44: characteristic molecular features and analysis of the hyaluronan binding site. **2001**, 33, 85-103	5
623	Molecular architecture of helicoidal proteinaceous eggshells. **1992**, 19, 115-86	10
622	Visual Analysis of Biomolecular Surfaces. **2008**, 237-255	5
621	Classification of Complex Molecules. **2009**, 243-315	3
620	A Grid-Based Hybrid Hierarchical Genetic Algorithm for Protein Structure Prediction. **2010**, 291-319	2
619	A New Method for the Fast Solution of Protein-3D-Structures, Combining Experiments and Bioinformatics. **2002**, 59-78	1
618	Chemical Fragmentation Approach to the Quantum Chemical Description of Extended Systems. **1991**, 1-49	6
617	Chemical Fragmentation Approach to the Quantum Chemical Description of Extended Systems. **1991**, 1-49	2

616	The role of the protein in the stabilization of the charge separated states in photosynthetic reaction centers. **1996**, 133-141	1
615	New Insights into the X-Ray Structure of the Reaction Center from Rhodopseudomonas viridis. **1996**, 23-35	5
614	Molecular Dynamics Simulations of Proteins and Protein-Protein Complexes. **1990**, 68-84	3
613	The Helix-Turn-Helix Motif and the Cro Repressor. **1992**, 85-95	2
612	The Human Genome and High Performance Computing in Molecular Biology. **1992**, 32-48	3
611	From Sequence Similarity to Structural Homology of Proteins. **1993**, 15-28	1
610	Formbasierte Suche nach komplementären 3D-Oberflächen in einer Protein-Datenbank. **1995**, 373-382	2
609	Structure and Selectivity of Ca-Binding Sites in Proteins: The 5-Fold Site in an Icosahedral Virus. **1990**, 283-299	3
608	Structure and Function of Bovine Lens Aminopeptidase and Comparison with Homologous Aminopeptidases. **1996**, 21-67	6
607	Structure and Assembly of the Channel-Forming Aeromonas Toxin Aerolysin. **1996**, 79-95	1
606	Molecular Modeling of the Nicotinic Acetylcholine Receptor. **1998**, 85-108	3
605	The structure of an immunodominant loop on foot and mouth disease virus, serotype O1, determined under reducing conditions. **1994**, 9, 51-8	7
604	Model-Building and Reduction of Model Bias in Electron Density Maps. **2013**, 193-203	1
603	Reverse Monte Carlo Study of Diffuse Scattering from a Frustrated Protein System. **2013**, 243-251	1
602	Computer modelling and drug design. **1992**, 133-162	1
601	Ion Selectivity and Molecular Structure of Binding Sites and Channels in Icosahedral Viruses. **1988**, 27-50	6
600	Approaches to the Multiple-Minima Problem in Conformational Energy Calculations on Polypeptides and Proteins. **1988**, 1-14	11
599	MOIL-View A Program for Visualization of Structure and Dynamics of Biomolecules and STO A Program for Computing Stochastic Paths. **1995**, 241-265	38

598	Binding of Cations and Protons in the Active Site of Acetylcholinesterase. **1995**, 25-37	4
597	Defining molecular similarity and complementarity for drug design. **1995**, 1-23	1
596	Similarity-searching and clustering algorithms for processing databases of two-dimensional and three-dimensional chemical structures. **1995**, 110-137	7
595	Time scales and fluctuations of protein dynamics: metmyoglobin in aqueous solution. **1993**, 168-193	1
594	Computer Modeling of Constrained Peptide Systems. **1992**, 17-38	1
593	Peptide Conformational Potential Energy Surfaces and their Relevance to Protein Folding. **1992**, 39-82	2
592	3-D Structure of Acetylcholinesterase and Complexes of it with Anticholinesterase Agents. **1992**, 161-175	4
591	Protein Structure Prediction and Neural Networks. **1991**, 991-1015	2
590	Systematic Study of Crystal Packing. **1999**, 251-262	4
589	Molecular Modeling of Globular Proteins : Strategy 1D => 3D: Secondary Structures and Epitopes. **1997**, 121-150	3
588	PROTEP: A Program for Graph-Theoretic Similarity Searching of the 3-D Structures in the Protein Data Bank. **1995**, 123-140	2
587	Homology Modeling of Horseradish Peroxidase. **1995**, 75-93	4
586	Monte Carlo lattice dynamics and the prediction of protein folds. **1997**, 395-429	4
585	Gaussian shape methods. **1997**, 150-176	12
584	Modeling protonation equilibria in biomolecules. **1997**, 199-222	6
583	Inhibition of PTP1B by farnesylated 2-arylbenzofurans isolated from Morus alba root bark: unraveling the mechanism of inhibition based on in vitro and in silico studies. **2020**, 43, 961-975	7
582	Predictions of Protein Secondary and Tertiary Structure. **1994**, 203-232	1
581	Learning an Objective Alphabet of Amino Acid Conformations in Protein11By acceptance of this article, the publisher and/or recipient acknowledges the U.S. Government's right to retain a nonexclusive, royalty-free license in and to any copyright covering this paper. This research was supported by the Northwest College and University Association for Science (Washington State University) under grant DE-FG06-89ER-75522 with the U.S. Department of Energy.. **1993**, 541-548	3

580	Interactive Graphics in Medicinal Chemistry. **1980**, 9, 267-298		10
579	The Effects of Local Environments on the Pattern of Amino-Acid Substitution in Homologous Prote Instructures: the Role of Side-Chain to Main-Chain Van Der Waals Interactions. **1994**, 405-412		1
578	A Photographic Essay of Porphyrins and Related Macrocycles**Dedicated to the memory of Walter C. Hamilton who provided help, facilities, and encouragement, leading to several computer graphics techniques employed in this chapter.. **1978**, 513-529		4
577	Applications of Crystallographic Databases in Molecular Design. **1990**, 261-281		2
576	SOLUTION STRUCTURE OF TGFBY 2D 1H NMR AND MOLECULAR MODELLING. **1989**, 223-232		1
575	THE SEQUENCE ATTRIBUTES METHOD FOR DETERMINING CORRELATIONS BETWEEN AMINO ACID SEQUENCE AND PROTEIN SECONDARY STRUCTURE. **1990**, 405-415		1
574	Knowledge-Based Protein Modelling: Human Plasma Kallikrein and Human Neutrophil Defensin. **1990**, 567-574		2
573	Energy profiles for ion permeation in pentameric protein channels: from viruses to receptor channels. **1990**, 1, 195-211		6
572	Crosslinked enzyme crystals (CLECs)as immobilized enzyme particles. **1993**, 47, 63-73		3
571	Use of Information Technology in the Search for New PET Tracers. **1998**, 267-271		2
570	Genetic Algorithms for Chemical Structure Handling and Molecular Recognition. **1996**, 211-242		3
569	Crystallographic Studies of Ribonuclease Complexes. **1997**, 305-VI		6
568	PROTEIN MOTIFS AND DATA-BASE SEARCHING. **1990**, 153-161		3
567	Crystal structure of ribonuclease A.d(ApTpApApG) complex. Direct evidence for extended substrate recognition.. *Journal of Biological Chemistry*, **1994**, 269, 21526-21531	5.4	102
566	Structure of ribonuclease A derivative II at 2.1-A resolution.. *Journal of Biological Chemistry*, **1994**, 269, 19707-19712	5.4	12
565	Crystal structure of RNase T1 complexed with the product nucleotide 3GMP. Structural evidence for direct interaction of histidine 40 and glutamic acid 58 with the 2hydroxyl group of the ribose. *Journal of Biological Chemistry*, **1994**, 269, 17531-17536	5.4	28
564	A model for the Ca2+-induced conformational transition of troponin C. A trigger for muscle contraction.. *Journal of Biological Chemistry*, **1986**, 261, 2638-2644	5.4	240
563	Interaction of a legume lectin with two components of the bacterial cell wall. A crystallographic study. *Journal of Biological Chemistry*, **1994**, 269, 9429-9435	5.4	30

562	Intrapeptide regulation of protein kinase C.. *Journal of Biological Chemistry*, **1994**, 269, 8383-8387	5.4	95
561	CA/TG sequence at the 5' end of oligo(A)-tracts strongly modulates DNA curvature.. *Journal of Biological Chemistry*, **1994**, 269, 7824-7833	5.4	52
560	Electrostatic interactions in sperm whale myoglobin. Site specificity, roles in structural elements, and external electrostatic potential distributions.. *Journal of Biological Chemistry*, **1985**, 260, 14070-14082	5.4	26
559	Refined crystal structure of deoxyhemoglobin S. I. Restrained least-squares refinement at 3.0-A resolution.. *Journal of Biological Chemistry*, **1985**, 260, 8272-8279	5.4	77
558	Sequencing and modeling of anti-DNA immunoglobulin Fv domains. Comparison with crystal structures.. *Journal of Biological Chemistry*, **1994**, 269, 3623-3632	5.4	44
557	Electrostatic modification at the amino termini of hemoglobin A.. *Journal of Biological Chemistry*, **1994**, 269, 2796-2804	5.4	3
556	Topology of an amiloride-binding protein.. *Journal of Biological Chemistry*, **1994**, 269, 2805-2813	5.4	13
555	Protein-polysaccharide interactions. A monoclonal antibody specific for the capsular polysaccharide of Cryptococcus neoformans.. *Journal of Biological Chemistry*, **1994**, 269, 1858-1864	5.4	19
554	Interactions and spatial arrangement of spin-labeled NAD+ bound to glyceraldehyde-3-phosphate dehydrogenase. Comparison of EPR and X-ray modeling data.. *Journal of Biological Chemistry*, **1984**, 259, 9717-9728	5.4	29
553	Molecular anatomy of the antibody binding site.. *Journal of Biological Chemistry*, **1983**, 258, 14433-14437	5.4	97
552	X-ray structure of a (alpha-Man(1-3)beta-Man(1-4)GlcNAc)-lectin complex at 2.1-A resolution. The role of water in sugar-lectin interaction.. *Journal of Biological Chemistry*, **1990**, 265, 18161-18165	5.4	77
551	Characterization of anti-Z-DNA antibody binding sites on Z-DNA by nuclear magnetic resonance spectroscopy.. *Journal of Biological Chemistry*, **1990**, 265, 18608-18614	5.4	11
550	Characterization of an active single polypeptide form of the human immunodeficiency virus type 1 protease.. *Journal of Biological Chemistry*, **1990**, 265, 17348-17354	5.4	58
549	Inclusion body formation and protein stability in sequence variants of interleukin-1 beta.. *Journal of Biological Chemistry*, **1993**, 268, 18053-18061	5.4	91
548	Molecular model of the extracellular lectin-like domain in CD69.. *Journal of Biological Chemistry*, **1994**, 269, 32457-32463	5.4	22
547	Models for the complexes formed between cytochrome b5 and the subunits of methemoglobin.. *Journal of Biological Chemistry*, **1983**, 258, 7369-7373	5.4	78
546	L-3-hydroxyacyl coenzyme A dehydrogenase. The location of NAD binding sites and the bilobal subunit structure.. *Journal of Biological Chemistry*, **1983**, 258, 2383-2389	5.4	7
545	The presence of a histidine-aspartic acid pair in the active site of 2-hydroxyacid dehydrogenases. X-ray refinement of cytoplasmic malate dehydrogenase.. *Journal of Biological Chemistry*, **1983**, 258, 472-482	5.4	128

544	The crystal structure of pea lectin at 6-A resolution.. *Journal of Biological Chemistry*, **1982**, 257, 13278-13282	5.4	18
543	Crystal structures of Escherichia coli and Lactobacillus casei dihydrofolate reductase refined at 1.7 A resolution. I. General features and binding of methotrexate.. *Journal of Biological Chemistry*, **1982**, 257, 13650-13662	5.4	566
542	An atomic model for protein-protein phosphoryl group transfer.. *Journal of Biological Chemistry*, **1992**, 267, 24819-24823	5.4	39
541	Stabilization of Escherichia coli ribonuclease H by introduction of an artificial disulfide bond.. *Journal of Biological Chemistry*, **1991**, 266, 6038-6044	5.4	75
540	The crystal structure of a lysine 49 phospholipase A2 from the venom of the cottonmouth snake at 2.0-A resolution.. *Journal of Biological Chemistry*, **1990**, 265, 17649-17656	5.4	87
539	The 2.0-A resolution structure of Escherichia coli histidine-containing phosphocarrier protein HPr. A redetermination.. *Journal of Biological Chemistry*, **1993**, 268, 22490-22501	5.4	81
538	Structural comparison of sulfodiimine and sulfonamide inhibitors in their complexes with zinc enzymes.. *Journal of Biological Chemistry*, **1992**, 267, 19192-19197	5.4	20
537	Structure-function relationships in the activation of platelet thrombin receptors by receptor-derived peptides.. *Journal of Biological Chemistry*, **1992**, 267, 6081-6085	5.4	233
536	Probing protein-protein interactions. The ribose-binding protein in bacterial transport and chemotaxis.. *Journal of Biological Chemistry*, **1994**, 269, 30206-30211	5.4	73
535	The structure of human lymphotoxin (tumor necrosis factor-beta) at 1.9-A resolution.. *Journal of Biological Chemistry*, **1992**, 267, 2119-2122	5.4	142
534	Influence of the chemical nature of side chain at beta 108 of hemoglobin A on the modulation of the oxygen affinity by chloride ions. Low oxygen affinity variants of human hemoglobin expressed in transgenic pigs: hemoglobins Presbyterian and Yoshizuka.. *Journal of Biological Chemistry*, **1994**, 269, 27692-27699	5.4	20
533	Conserved waters in legume lectin crystal structures. The importance of bound water for the sequence-structure relationship within the legume lectin family.. *Journal of Biological Chemistry*, **1994**, 269, 26722-26733	5.4	53
532	The binding site on human immunoglobulin E for its high affinity receptor. *Journal of Biological Chemistry*, **1994**, 269, 26368-26373	5.4	138
531	Crystal structure of oxygenated Scapharca dimeric hemoglobin at 1.7-A resolution.. *Journal of Biological Chemistry*, **1994**, 269, 25259-25267	5.4	35
530	Cocrystals of yeast cytochrome c peroxidase and horse heart cytochrome c.. *Journal of Biological Chemistry*, **1987**, 262, 13881-13884	5.4	36
529	X-ray structure of a biantennary octasaccharide-lectin complex refined at 2.3-A resolution.. *Journal of Biological Chemistry*, **1992**, 267, 197-203	5.4	99
528	Structural changes that accompany the reduced catalytic efficiency of two semisynthetic ribonuclease analogs.. *Journal of Biological Chemistry*, **1992**, 267, 247-256	5.4	26
527	Mechanism of molecular recognition. Structural aspects of 3,3'-diiodo-L-thyronine binding to human serum transthyretin.. *Journal of Biological Chemistry*, **1992**, 267, 353-357	5.4	55

526	Lysosomal enzyme phosphorylation. II. Protein recognition determinants in either lobe of procathepsin D are sufficient for phosphorylation of both the amino and carboxyl lobe oligosaccharides. *Journal of Biological Chemistry*, **1992**, 267, 23349-23356	5.4	49
525	Phosphorylation of Asn-linked oligosaccharides located at novel sites on the lysosomal enzyme cathepsin D. *Journal of Biological Chemistry*, **1992**, 267, 23357-23363	5.4	32
524	Three-dimensional models of four mouse mast cell chymases. Identification of proteoglycan binding regions and protease-specific antigenic epitopes.. *Journal of Biological Chemistry*, **1993**, 268, 9023-9034	5.4	88
523	Dissociation of heparin-dependent thrombin and factor Xa inhibitory activities of antithrombin-III by mutations in the reactive site.. *Journal of Biological Chemistry*, **1993**, 268, 9035-9040	5.4	24
522	Kinetic analysis of a mutant (His107→Tyr) responsible for human carbonic anhydrase II deficiency syndrome.. *Journal of Biological Chemistry*, **1993**, 268, 4775-4779	5.4	12
521	Crystallographic refinement of lignin peroxidase at 2 A.. *Journal of Biological Chemistry*, **1993**, 268, 4429-4440	5.4	317
520	The x-ray crystal structure refinements of normal human transthyretin and the amyloidogenic Val-30→Met variant to 1.7-A resolution.. *Journal of Biological Chemistry*, **1993**, 268, 2416-2424	5.4	159
519	X-ray crystal structure of the Ala-109→Thr variant of human transthyretin which produces euthyroid hyperthyroxinemia.. *Journal of Biological Chemistry*, **1993**, 268, 2425-2430	5.4	44
518	Effects of gene mutations in lipoprotein and hepatic lipases as interpreted by a molecular model of the pancreatic triglyceride lipase.. *Journal of Biological Chemistry*, **1991**, 266, 23112-23119	5.4	65
517	Mapping and molecular modeling of a recognition domain for lysosomal enzyme targeting.. *Journal of Biological Chemistry*, **1991**, 266, 23365-23372	5.4	59
516	Structure of a recombinant calmodulin from Drosophila melanogaster refined at 2.2-A resolution.. *Journal of Biological Chemistry*, **1991**, 266, 21375-21380	5.4	99
515	Crystal structure of recombinant rabbit interferon-gamma at 2.7-A resolution.. *Journal of Biological Chemistry*, **1991**, 266, 21791-21797	5.4	53
514	The molecular structure of the high potential iron-sulfur protein isolated from Ectothiorhodospira halophila determined at 2.5-A resolution.. *Journal of Biological Chemistry*, **1991**, 266, 18660-18667	5.4	72
513	Characterization of a recombinant single-chain molecule comprising the variable domains of a monoclonal antibody specific for human fibrin fragment D-dimer.. *Journal of Biological Chemistry*, **1991**, 266, 16343-16349	5.4	38
512	Modification of human hemoglobin by glutathione. III. Perturbations of hemoglobin conformation analyzed by computer modeling.. *Journal of Biological Chemistry*, **1986**, 261, 14717-14724	5.4	19
511	The adenine nucleotide binding site on yeast hexokinase PII. Affinity labeling of Lys-111 by pyridoxal 5→diphospho-5→adenosine.. *Journal of Biological Chemistry*, **1988**, 263, 7907-7912	5.4	20
510	Haloperidol binding to monoclonal antibodies. Predictions of three-dimensional combining site structure via computer modeling.. *Journal of Biological Chemistry*, **1988**, 263, 4064-4074	5.4	14
509	Identification of ADP in the iron-sulfur flavoprotein trimethylamine dehydrogenase.. *Journal of Biological Chemistry*, **1988**, 263, 3075-3078	5.4	30

508	Cloning, expression, and site-directed mutagenesis of chicken skeletal muscle troponin C.. *Journal of Biological Chemistry*, **1988**, 263, 2371-2376	5.4	63
507	The Structure of Tumor Necrosis Factor-at 2.6 Resolution. *Journal of Biological Chemistry*, **1989**, 264, 17595-17605	5.4	389
506	Photolabeling of Calmodulin with Basic, Amphiphilic Helical Peptides Containing p-Benzoylphenylalanine. *Journal of Biological Chemistry*, **1989**, 264, 14571-14578	5.4	72
505	2.8-A Structure of penicillin-sensitive D-alanyl carboxypeptidase-transpeptidase from Streptomyces R61 and complexes with beta-lactams.. *Journal of Biological Chemistry*, **1985**, 260, 6449-6458	5.4	63
504	Electrostatic interactions during electron transfer reactions between c-type cytochromes and flavodoxin.. *Journal of Biological Chemistry*, **1985**, 260, 5568-5573	5.4	62
503	Complex formation between flavodoxin and cytochrome c. Cross-linking studies.. *Journal of Biological Chemistry*, **1985**, 260, 5175-5178	5.4	15
502	Affinity labeling of dihydrofolate reductase with an antifolate glyoxal.. *Journal of Biological Chemistry*, **1985**, 260, 1465-1474	5.4	9
501	Crystal structure of yeast cytochrome c peroxidase refined at 1.7-A resolution.. *Journal of Biological Chemistry*, **1984**, 259, 13027-13036	5.4	553
500	A Proton Nuclear Magnetic Resonance and Nuclear Overhauser Effect (NOE) Study of Human Plasma Prealbumin, Including the Development and Application to Spectral Assignment of a Combined Ring Current Shift and NOE Prediction Program. *Journal of Biological Chemistry*, **1989**, 264, 2003-2012	5.4	8
499	Crystal structure of Escherichia coli CheY refined at 1.7-A resolution. *Journal of Biological Chemistry*, **1991**, 266, 15511-15519	5.4	247
498	Electrostatic orientation of the electron-transfer complex between plastocyanin and cytochrome c. *Journal of Biological Chemistry*, **1991**, 266, 13431-13441	5.4	81
497	Structural characterization of heme ligation in the His64Tyr variant of myoglobin.. *Journal of Biological Chemistry*, **1994**, 269, 12606-12610	5.4	21
496	The 2.4-crystal structure of Scapharca dimeric hemoglobin. *Journal of Biological Chemistry*, **1989**, 264, 21052-21061	5.4	60
495	Mutagenesis of human acetylcholinesterase. Identification of residues involved in catalytic activity and in polypeptide folding.. *Journal of Biological Chemistry*, **1992**, 267, 17640-17648	5.4	125
494	A molecular model of RGD ligands. Antibody D gene segments that direct specificity for the integrin alpha IIb beta 3.. *Journal of Biological Chemistry*, **1992**, 267, 18085-18092	5.4	53
493	The crystallographic structure of the protease from human immunodeficiency virus type 2 with two synthetic peptidic transition state analog inhibitors. *Journal of Biological Chemistry*, **1993**, 268, 13103-13109	5.4	63
492	A proton nuclear magnetic resonance and molecular modeling study of cardiac troponin C. Calcium dependence and aromatic spectral assignments.. *Journal of Biological Chemistry*, **1990**, 265, 9754-9763	5.4	5
491	Structure of wheat serine carboxypeptidase II at 3.5-A resolution. A new class of serine proteinase.. *Journal of Biological Chemistry*, **1990**, 265, 6528-6531	5.4	80

490	Experimental and theoretical evidence supporting the role of Gly363 in blood coagulation factor IXa (Gly193 in chymotrypsin) for proper activation of the proenzyme.. *Journal of Biological Chemistry*, **1990**, 265, 2956-2961	5.4	14
489	Altering the mouth of a hydrophobic pocket. Structure and kinetics of human carbonic anhydrase II mutants at residue Val-121.. *Journal of Biological Chemistry*, **1991**, 266, 17320-17325	5.4	107
488	Chimeric L6 anti-tumor antibody. Genomic construction, expression, and characterization of the antigen binding site.. *Journal of Biological Chemistry*, **1992**, 267, 15552-15558	5.4	27
487	Crystal structure of a wheat germ agglutinin/glycophorin-sialoglycopeptide receptor complex. Structural basis for cooperative lectin-cell binding.. *Journal of Biological Chemistry*, **1992**, 267, 14345-14352	5.4	103
486	Chloride ion independence of the Bohr effect in a mutant human hemoglobin beta (V1M+H2deleted).. *Journal of Biological Chemistry*, **1994**, 269, 23965-23969	5.4	32
485	A study of the electron paramagnetic resonance properties of single monoclinic crystals of bovine superoxide dismutase.. *Journal of Biological Chemistry*, **1982**, 257, 336-344	5.4	38
484	Inhibition of carbonic anhydrases I and II by N-unsubstituted carbamate esters.. *Journal of Biological Chemistry*, **1992**, 267, 25044-25050	5.4	6
483	Structural and functional importance of a conserved hydrogen bond network in human carbonic anhydrase II.. *Journal of Biological Chemistry*, **1993**, 268, 27458-27466	5.4	62
482	Identification of a secondary Fc gamma RI binding site within a genetically engineered human IgG antibody.. *Journal of Biological Chemistry*, **1993**, 268, 25124-25131	5.4	18
481	Three-dimensional structure of the tryptophan synthase alpha 2 beta 2 multienzyme complex from Salmonella typhimurium.. *Journal of Biological Chemistry*, **1988**, 263, 17857-17871	5.4	555
480	The refined structure of vitamin D-dependent calcium-binding protein from bovine intestine. Molecular details, ion binding, and implications for the structure of other calcium-binding proteins.. *Journal of Biological Chemistry*, **1986**, 261, 8761-8777	5.4	256
479	Restrained least squares refinement of native (calcium) and cadmium-substituted carp parvalbumin using X-ray crystallographic data at 1.6-Å resolution. *Journal of Biological Chemistry*, **1989**, 264, 16620-16628	5.4	86
478	Positively charged amino acid residues located similarly in sea anemone and scorpion toxins. *Journal of Biological Chemistry*, **1994**, 269, 16785-16788	5.4	52
477	Kinetic and modeling studies of subsites S4-S3' of Moloney murine leukemia virus protease. *Journal of Biological Chemistry*, **1994**, 269, 16795-16801	5.4	25
476	Crystal structures of ribonuclease HI active site mutants from Escherichia coli.. *Journal of Biological Chemistry*, **1993**, 268, 22092-22099	5.4	31
475	The x-ray structure of the periplasmic galactose binding protein from Salmonella typhimurium at 3.0-A resolution.. *Journal of Biological Chemistry*, **1983**, 258, 7991-7997	5.4	38
474	Structure and phospholipid transfer activity of human PLTP: analysis by molecular modeling and site-directed mutagenesis. **1999**, 40, 1123-1130		50
473	Chapter 4 The binding of ions to proteins. **1999**, 99-152		2

472	Towards the routine use of in silico screenings for drug discovery using metabolic modelling. **2020**, 48, 955-969		7
471	CXC chemokines connective tissue activating peptide-III and neutrophil activating peptide-2 are heparin/heparan sulfate-degrading enzymes. *Journal of Biological Chemistry*, **1995**, 270, 3268-77	5.4	83
470	PBxplore: a tool to analyze local protein structure and deformability with protein Blocks.		1
469	Evolution of an enzyme conformational ensemble guides design of an efficient biocatalyst.		5
468	Automated map sharpening by maximization of detail and connectivity.		6
467	Real-space refinement in Phenix for cryo-EM and crystallography.		8
466	End-to-end differentiable learning of protein structure.		10
465	New tools for the analysis and validation of Cryo-EM maps and atomic models.		4
464	Parsers, Data Structures and Algorithms for Macromolecular Analysis Toolkit (MAT): Design and Implementation.		1
463	Evolution of Aminoacyl-tRNA Synthetases Analysis of Unique Domain Architectures and Phylogenetic Trees Reveals a Complex History of Horizontal Gene Transfer Events. **1999**, 9, 689-710		196
462	From deep TLS validation to ensembles of atomic models built from elemental motions. **2015**, 71, 1668-83		11
461	The geometry of Niggli reduction: - search of alternative unit cells. **2014**, 47, 360-364		14
460	Acceleratingk-nearest-neighbor searches. **2016**, 49, 1471-1477		2
459	The data universe of structural biology. **2020**, 7, 630-638		8
458	Gold Standard for macromolecular crystallography diffraction data. **2020**, 7, 784-792		2
457	Evaluation of models determined by neutron diffraction and proposed improvements to their validation and deposition. *Acta Crystallographica Section D: Structural Biology*, **2018**, 74, 800-813	5.5	10
456	Automated map sharpening by maximization of detail and connectivity. *Acta Crystallographica Section D: Structural Biology*, **2018**, 74, 545-559	5.5	132
455	Real-space refinement in PHENIX for cryo-EM and crystallography. *Acta Crystallographica Section D: Structural Biology*, **2018**, 74, 531-544	5.5	917

454	New tools for the analysis and validation of cryo-EM maps and atomic models. *Acta Crystallographica Section D: Structural Biology*, **2018**, 74, 814-840	5.5	291
453	Macromolecular structure determination using X-rays, neutrons and electrons: recent developments in Phenix. *Acta Crystallographica Section D: Structural Biology*, **2019**, 75, 861-877	5.5	1527
452	Cleavage of the iron-methionine bond in c-type cytochromes: crystal structure of oxidized and reduced cytochrome c(2) from Rhodopseudomonas palustris and its ammonia complex. **2002**, 11, 6-17		26
451	Proton-NMR studies show that the Thr-102 mutant of yeast iso-1-cytochrome c is a typical member of the eukaryotic cytochrome c family. **1988**, 177, 167-77		28
450	1H and 15N Resonance Assignments and Structure of the N-Terminal Domain of Escherichia coli Initiation Factor 3. **1995**, 228, 395-402		36
449	X-ray structures of human neutrophil collagenase complexed with peptide hydroxamate and peptide thiol inhibitors. Implications for substrate binding and rational drug design. **1995**, 228, 830-41		156
448	Structural and Functional Conservation in Response Regulators. 53-64		22
447	Functional characterization of pediocin PA-1 binding to liposomes in the absence of a protein receptor and its relationship to a predicted tertiary structure. **1997**, 63, 524-31		80
446	The Haemophilus influenzae HtrA protein is a protective antigen. **1998**, 66, 899-906		39
445	Intermonomer disulfide bonds impair the fusion activity of influenza virus hemagglutinin. **1992**, 66, 4940-50		91
444	Homolog-scanning mutagenesis reveals poliovirus receptor residues important for virus binding and replication. **1994**, 68, 2578-88		61
443	Structure-based identification of an inducer of the low-pH conformational change in the influenza virus hemagglutinin: irreversible inhibition of infectivity. **1997**, 71, 8808-20		86
442	Poliovirus Sabin type 1 neutralization epitopes recognized by immunoglobulin A monoclonal antibodies. **1997**, 71, 6905-12		18
441	Conformational Flexibility of Bovine Pancreatic Ribonuclease A. **1983**, 52, 4407-4416		1
440	A Computational Approach towards the Understanding of Plasmodium falciparum Multidrug Resistance Protein 1. **2013**, 2013, 437168		4
439	Evidence of antigen receptor-influenced oligoclonal B lymphocyte expansion in the synovium of a patient with longstanding rheumatoid arthritis. **1994**, 93, 361-70		42
438	Structural characteristics of human salivary statherin: a model for boundary lubrication at the enamel surface. **1993**, 4, 363-70		34
437	Defining an Antigenic Epitope on Platelet Factor 4 Associated With Heparin-Induced Thrombocytopenia. **1998**, 92, 3250-3259		7

436	Mutations in the gene encoding neutrophil elastase in congenital and cyclic neutropenia. **2000**, 96, 2317-2322	10
435	Protein Sequence Analysis and Prediction of Secondary Structural Features. **2004**, 99-185	1
434	Immobilized metal-ion affinity chromatography. **2002**,	2
433	Nucleic Acid Simulations. **2001**,	1
432	How to Employ Proteins in Nonaqueous Environments. **2001**,	1
431	Information. **1998**, 88-107	1
430	Structure–function relationships of A-, F- and V-ATPases. **2001**, 204, 2597-2605	84
429	Dipeptidyl peptidase-IV inhibitors used in type-2 diabetes inhibit a phospholipase C: a case of promiscuous scaffolds in proteins. **2013**, 2, 286	5
428	In silico Analysis of Interactions between HLA-A*31:01 and carbamazepine-related Compounds. **2016**, 16, 5-8	1
427	In silico Analysis of Interactions between Nevirapine-related Compounds, HLA-B*14:02 and T-cell Receptor . **2016**, 16, 9-12	2
426	Evolutionary and Functional Relationships in the Truncated Hemoglobin Family. **2016**, 12, e1004701	23
425	Local alignment refinement using structural assessment. **2008**, 3, e2645	4
424	A comparative structural bioinformatics analysis of the insulin receptor family ectodomain based on phylogenetic information. **2008**, 3, e3667	38
423	Coexistence of flexibility and stability of proteins: an equation of state. **2009**, 4, e7296	19
422	Modeling-dependent protein characterization of the rice aldehyde dehydrogenase (ALDH) superfamily reveals distinct functional and structural features. **2010**, 5, e11516	41
421	Structural analysis of prolyl oligopeptidases using molecular docking and dynamics: insights into conformational changes and ligand binding. **2011**, 6, e26251	22
420	A conformational switch in the active site of BT_2972, a methyltransferase from an antibiotic resistant pathogen B. thetaiotaomicron. **2011**, 6, e27543	1
419	Active site detection by spatial conformity and electrostatic analysis--unravelling a proteolytic function in shrimp alkaline phosphatase. **2011**, 6, e28470	34

418	The zinc dyshomeostasis hypothesis of Alzheimer's disease. **2012**, 7, e33552	107
417	BCL::Fold--de novo prediction of complex and large protein topologies by assembly of secondary structure elements. **2012**, 7, e49240	38
416	Alternative splice variants in TIM barrel proteins from human genome correlate with the structural and evolutionary modularity of this versatile protein fold. **2013**, 8, e70582	7
415	Can natural proteins designed with 'inverted' peptide sequences adopt native-like protein folds?. **2014**, 9, e107647	7
414	An integrative approach to the study of filamentous oligomeric assemblies, with application to RecA. **2015**, 10, e0116414	10
413	HbAHP-25, an In-Silico Designed Peptide, Inhibits HIV-1 Entry by Blocking gp120 Binding to CD4 Receptor. **2015**, 10, e0124839	6
412	Analyses of the Sequence and Structural Properties Corresponding to Pentapeptide and Large Palindromes in Proteins. **2015**, 10, e0139568	2
411	ENTPRISE: An Algorithm for Predicting Human Disease-Associated Amino Acid Substitutions from Sequence Entropy and Predicted Protein Structures. **2016**, 11, e0150965	18
410	Investigating the Role of Loop C Hydrophilic Residue 'T244' in the Binding Site of β1 GABAC Receptors via Site Mutation and Partial Agonism. **2016**, 11, e0156618	4
409	Insights on the mechanism of action of immunostimulants in relation to their pharmacological potency. The effects of imidazoquinolines on TLR8. **2017**, 12, e0178846	5
408	Class IA PI3Ks regulate subcellular and functional dynamics of IDO1. **2020**, 21, e49756	12
407	Exploring the interactions of the RAS family in the human protein network and their potential implications in RAS-directed therapies. **2016**, 7, 75810-75826	4
406	Carnitine palmitoyl transferase-1A (CPT1A): a new tumor specific target in human breast cancer. **2016**, 7, 19982-96	47
405	A Fhit-mimetic peptide suppresses annexin A4-mediated chemoresistance to paclitaxel in lung cancer cells. **2016**, 7, 29927-36	9
404	An Improved Integration of Template-Based and Template-Free Protein Structure Modeling Methods and its Assessment in CASP11. **2015**, 22, 586-93	9
403	Progress in protein crystallography. **2016**, 23, 201-10	18
402	An overview of computational life science databases & exchange formats of relevance to chemical biology research. **2013**, 16, 189-98	8
401	Protein-Protein Interactions of Phosphodiesterases. **2019**, 19, 555-564	1

400	Shining Light on an mGlu5 Photoswitchable NAM: A Theoretical Perspective. **2016**, 14, 441-54	12
399	Design, Synthesis and Anxiolytic Activity Evaluation of N-Acyltryptophanyl- Containing Dipeptides, Potential TSPO Ligands. **2019**, 15, 383-399	3
398	Consensus prediction of protein conformational disorder from amino acidic sequence. **2008**, 2, 1-5	8
397	Systematic comparison of crystal and NMR protein structures deposited in the protein data bank. **2010**, 4, 83-95	52
396	Macromolecular crystallographic estructure refinement. **2015**, 191, a219	3
395	Graph Applications in Chemoinformatics and Structural Bioinformatics. 1126-1157	1
394	Predicting Multi-Component Protein Assemblies Using an Ant Colony Approach. **2012**, 3, 19-31	2
393	Human butyrylcholinesterase knock-out equivalent: Potential to assess role in Alzheimer disease. **2012**, 01, 1-11	1
392	Interaction of Hemoglobin with Binuclearcationic Tetranitrosyl Iron Complex with Penicillamine. Cations Binding Sites. **2015**, 05, 169-178	2
391	A Brief Overview of a Few Popular and Important Protein Databases. **2012**, 02, 115-120	5
390	Correctness and accuracy of template-based modeled single chain fragment variable (scFv) protein anti-breast cancer cell line (MCF-7). **2013**, 03, 183-194	6
389	Attractive Sulfur...Interaction between Fluorinated Dimethyl Sulfur (FDMS) and Benzene. **2007**, 28, 959-964	18
388	Molecular Dynamics Free Energy Simulation Study to Rationalize the Relative Activities of PPAR Agonists. **2008**, 29, 363-371	6
387	Functional annotation of hypothetical proteins - A review. **2006**, 1, 335-8	60
386	CARON--average RMSD of NMR structure ensembles. **2009**, 4, 132-3	6
385	Insight towards the conserved water mediated recognition of catalytic and structural Zn(+2) ions in human Matrix Metalloproteinase-8 enzyme: A study by MD-simulation methods. **2013**, 9, 126-33	3
384	Computational protein structure modeling and analysis of UV-B stress protein in Synechocystis PCC 6803. **2013**, 9, 639-44	1
383	Three dimensional (3D) structure prediction and substrate-protein interaction study of the chitin binding protein CBP24 from B. thuringiensis. **2013**, 9, 725-9	6

382	Inferences from the ADMET analysis of predicted inhibitors to Follicle Stimulating Hormone in the context of infertility. **2013**, 9, 788-91		7
381	Design and evaluation of chalconeimine derivatives as □amylase inhibitors. **2019**, 15, 523-529		4
380	Virtual screening of Indonesian herbal database as HIV-1 reverse transcriptase inhibitor. **2012**, 8, 1206-10		11
379	The role of CDK5 and GSK3B kinases in hyperphosphorylation of microtubule associated protein tau (MAPT) in Alzheimer's disease. **2013**, 9, 1023-30		29
378	Comparative Modeling of Protein Structure-Progress and Prospects. **1989**, 94, 79-84		8
377	The Protein Data Bank: Current Status and Future Challenges. **1996**, 101, 231-241		18
376	The Biological Macromolecule Crystallization Database and NASA Protein Crystal Growth Archive. **1996**, 101, 309-20		15
375	Variability of DNA structure and protein-nucleic acid reconginition. **2010**, 26, 360-372		9
374	Building bridges between cellular and molecular structural biology. **2017**, 6,		9
373	PBxplore: a tool to analyze local protein structure and deformability with Protein Blocks. **2017**, 5, e4013		18
372	structural and functional prediction of African swine fever virus protein-B263R reveals features of a TATA-binding protein. **2018**, 6, e4396		7
371	Macrosphelide A Exhibits a Specific Anti-Cancer Effect by Simultaneously Inactivating ENO1, ALDOA, and FH. *Pharmaceuticals*, **2021**, 14,	5.2	1
370	Hydrogen-Bonding Hotspots as an Aid for Site-Directed Drug Design. **2000**, 410-411		
369	Common Structural Elements in the Architecture of the Cofactor-Binding Domains in Unrelated Families of Pyridoxal Phosphate-Dependent Enzymes. **2000**, 123-128		
368	Ab Initio Calculations Related to Glucagon. **2000**, 83-96		
367	Adenovirus Proteinase-Antiviral Target for Triple-Combination Therapy on a Single Enzyme: Potential Inhibitor-Binding Sites. **2000**, 145-158		
366	Receptor-Based Molecular Diversity: Analysis of HIV Protease Inhibitors. **2000**, 442-443		
365	Collection Views: Dynamically Composed Views Which Inherit Behaviour. **2000**, 102-121		1

364	Global Optimization and Sampling in the Context of Tertiary Structure Prediction: A Comparison of Two Algorithms. **2000**, 57-71	
363	Design And Development Of Small-molecule Inhibitor Of Tumor Necrosis Factor-. **2000**,	
362	Including biological literature improves homology search. **2001**, 374-83	7
361	Automated Identification of Three-Dimensional Common Structural Features of Proteins.. **2001**, 7, 161-170	5
360	Introduction. **2001**,	
359	Computer Aided Drug Design. **2001**,	1
358	Structure Information. **2001**, 345-360	
357	Computer Modeling of Protein Structure. **2001**,	
356	Secondary Structural Prediction Of Proteins.	
355	Structural Molecular Biology The New Perspective for Regional Science. **2002**, 373-382	
354	Structure Databases.	
353	Molecular Dynamics Simulations: A Tool for Drug Design. **2002**, 181-209	
352	Construction of a Three-Dimensional Motif Dictionary for Protein Structural Data Mining. **2002**, 17, 608-613	1
351	Protein Structure.	
350	Efficient Computational Algorithms for Fast Electrostatics and Molecular Docking. **2002**, 411-441	
349	Conformational changes in HIV-1 protease: molecular dynamic simulation study in picoseond and nanosecond timescales. **2002**, 18, 117-123	1
348	Conformational Search: Proteins.	
347	Molecular Docking and Structure-based Design.	

346 Protein Data Bank (PDB): A Database of 3D Structural Information of Biological Macromolecules.

345 Conformational Flexibility in 3D Structure Searching.

344 Protein Force Fields. 1

343 Structure Representation.

342 Protein Structure Prediction in 1D, 2D, and 3D.

341 Three-dimensional Structure Searching.

340 Pharmacophore and Drug Discovery.

339 Identifying Flat Regions and Slabs in Protein Structures. **2003**, 83-97

338 MOLDA for Protein Modeling: A Molecular Modeling Program for Biological Molecules.. **2003**, 2, 143-148

337 Development of Multifunctional Object-Oriented Program Library for Molecular Simulation and Structure Analysis.. **2003**, 2, 7-16

336 Environment-dependent and position-specific frequencies of amino acid occurrences in .ALPHA.-helices. **2003**, 3, 58-77

335 Application of Evolutionary Computation to Protein Folding. **2003**, 915-940

334 Structure, Energetics, and Spectroscopy of Models for Enzyme Cofactors. **2003**, 163-175

333 Application of Evolutionary Computation to Protein Folding with Specialized Operators. **2003**, 163-191 2

332 Bioinformatik. **2003**, 143-212 0

331 Methods of Computational Genomics. **2004**, 279-342

330 Protein Data Bank (PDB).

329 Protein Data Bank (PDB). **2004**,

328	Ontological Foundation for Protein Data Models. **2005**, 916-925	1
327	Analysis of the Effects of Multiple Sequence Alignments in Protein Secondary Structure Prediction. **2005**, 128-140	
326	Protein□ligand Interactions: Knowledge-Based Methods.	
325	Factors D and B. **2005**, 91-110	
324	Computer modelling of the immunoreactive conformation of the HIV-RF immunodominant epitope. **2005**, 21, 165-173	
323	Towards Semantic Interoperability of Protein Data Sources. **2006**, 1835-1843	2
322	Theoretical and empirical approaches to protein-structure prediction and analysis. **1991**, 35, 1-86	3
321	Protein Three-Dimensional Structure Validation. **2007**, 507-530	
320	Resources and Infrastructure for Structural Bioinformatics. **2007**, 207-227	
319	Protein Structure Prediction as a Systems Problem. **2007**, 177-206	
318	The Protein as a Supermolecule: The Architecture of a (β□ Barrel. 235-309	
317	Calcium binding to skeletal muscle troponin C and the regulation of muscle contraction. **1986**, 122, 120-44	4
316	Comparative analysis of protein three-dimensional structures and an approach to the inverse folding problem. **1991**, 161, 28-36; discussion 37-51	2
315	Modelling antibody combining sites: a review. **1991**, 159, 55-69; discussion 69-71	
314	Structure Information. 345-360	
313	Databases in Biochemistry and Molecular Biology. 756-793	
312	Current Trends in Biomedical Data and Applications. **2009**, 1-9	
311	Protein structure databases. **2010**, 609, 59-82	

310 Computational Scale Linking in Biological Protein Materials. **2010**, 491-531

309 Multiscale Modeling of Biological Protein Materials Deformation and Failure. **2010**, 473-533

308 Digital archives for molecular microscopy. **2010**,

307 Comparative sequence and structural analyses of neuroserpin. **2010**,

306 Ballast: A Ball-Based Algorithm for Structural Motifs. **2012**, 79-93 1

305 3D Structure and Drug Design. **2012**, 145-158

304 Crystallographic Maps and Models at Low and at Subatomic Resolutions. **2013**, 221-230

303 Neural Networks in Bioinformatics. **2013**, 505-525

302 Protein Three-Dimensional Structure Validation. **2013**,

301 Crystallographic Structure Refinement in a Nutshell. **2013**, 211-219 1

300 Systems Toxicology Approaches. **2013**, 121-139

299 Analysis of conformational flexibility of loop 110-120 of protein tyrosine phosphatase 1B. **2013**, 85, 73-80

298 Computational Evaluation of Protein Energy Functions. **2014**, 288-299

297 Exact Protein Structure Classification Using the Maximum Contact Map Overlap Metric. **2014**, 262-273 1

296 Structural Implications for Macromolecular Recognition and Redesign. **1973**, 41-69

295 Data base requirements for graphical applications in biochemistry. **1980**, 263-284 1

294 Coordinate Transformations. **1981**, 24-72

293 Packing Densities and Iron-Sulfur Proteins. **1982**, 361-364

292	Strain and Electrostatic Contributions to Cooperativity in Hemoglobin. **1982**, 211-215	
291	R□tgenstrukturanalyse □eine computer-abh□gige Methode. **1984**, 173-206	
290	Variability, Modelling and Prediction of □Hairpins with Reference to the Immunoglobulin Fold. **1985**, 23-31	
289	R□tgenstrukturanalyseeine computer□bh□gige Methode. **1985**, 173-206	
288	Comparative Structures of Mouse Antibody Combining Sites. **1985**, 51-60	
287	X-ray Diffraction Methods for the Analysis of Metalloproteins. **1986**, 215-259	
286	Programme zur Auswertung kristallographischer Daten in Datenbanken. **1987**, 113-117	
285	Electron Density Fitting with Computer Graphics: A Review and a Glimpse. **1987**, 125-130	2
284	Molecular Graphics in the Study of the Calcium-Binding Sites of Carp Parvalbumin and Other Proteins. **1987**, 113-116	
283	Spectral Dimensions of Paramagnetic Proteins. **1987**, 210-223	
282	Prediction of Protein Structure from Amino Acid Sequence. **1987**, 141-149	
281	Preferred Residue Interactions in Protein Subunit and Domain Interfaces. **1989**, 370-378	
280	The Use of Structural Templates in Protein Backbone Modeling. **1989**, 94, 65-78	
279	Prediction of Packing of Secondary Structure. **1989**, 467-548	1
278	Resonance Raman Spectroscopic Characterization of the Oxidation of the Horseradish Peroxidase Active Site. **1989**, 31-42	1
277	MOLCAD □Neue Entwicklungen von Molecular Modelling Software f□Superworkstations. **1989**, 357-361	
276	Knowledge-Based Protein Modeling and the Design of Novel Molecules. **1990**, 209-227	
275	E. Antonini Plenary Lecture A structural basis of light energy and electron transfer in biology. **1990**, 25-47	

274 Human Immunodeficiency Virus (Type 1) Protease: Enzymology and Three-Dimensional Structure of a New AIDS Drug Target. **1990**, 321-334

273 PROTEIN STRUCTURE PREDICTION. **1990**, 557-565

272 Crystallographic determination of protein structure. **1990**, 14, 111-29

271 Subunit Interactions and the Function of Tumor Necrosis Factor. **1990**, 383-394

270 Chemical Modification of the Lysine Residues on Plastocyanin and the Effect on Cytochrome f.. **1990**, 2213-2216

269 Inhibitor Design from Known Structures. **1990**, 200-210

268 Preferred Interaction Patterns from Crystallographic Databases. **1990**, 229-253 1

267 Information Systems and Databases as Alternatives. **1990**, 18, 83-89 5

266 Protein and peptide functionaly important regions search method by aminoacid sequence. **1990**, 6, 36-42

265 Tools for Molecular Graphics Depictions of Lipid Structures. **1991**, 40-51

264 COMPUTER AIDED DESIGN OF ARTIFICIAL PROTEINS. **1991**, 417-422 0

263 A novel crepe ribbon representation for protein structures. **1991**, 325-329

262 Design and synthesis of chymohelizyme-1, a peptide having chymotrypsin-like catalytic activity. **1991**, 574-576

261 General Considerations on Methods for Studying Molecular Structures and Electron Density Distributions. **1991**, 1-5

260 Computational and database retrieval approaches for determining polypeptide conformation. **1991**, 260-265

259 The Main Structure Databanks in Molecular Science. **1991**, 157-172

258 Patterns of Sequence and 3-D Structure Variation in Families of Homologous Proteins: Lessons for Tertiary Templates and Comparative Modelling. **1992**, 189-204

257 Protein Structure Prediction and Neural Networks. **1992**, 1151-1154

256	Comparative molecular modeling of the active subunit of human kininase I. **1992**, 38 (Pt 1), 368-75	
255	Secondary and Supersecondary Motifs in Protein Structures. **1992**, 141-155	
254	Chaos- theoretical Analysis of Protein Structures. **1993**, 1259-1262	
253	Advanced Computer Applications in Protein Engineering. **1993**, 1161-1164	
252	The most frequent SARFs (Spatial ARrangements of backbone Fragments) in protein structures. **1993**, 1255-1257	
251	Modeling three-dimensional structure and electrostatics of alkali-stable cyclomaltodextrin glucanotransferase. **1993**, 47, 291-298	1
250	The expansion of core group interaction that drives protein folding: A hypothesis based on the cytochrome c fragment complex. **1993**, 199-203	1
249	Estimation of the Mechanism of Peptide Binding to HLA Class II Molecules. **1993**, 377-381	
248	Sequence Patterns that Characterize Protein Families with a Common Fold. **1993**, 221-227	
247	Techniques for conformational searches of peptides and proteins. **1993**, 1241-1246	
246	Classification of conformations of short peptide backbone fragments by principal component analysis and it's use to code protein backbone structures. **1993**, 1251-1254	
245	Representation and Searching of 3-D Protein Structures. **1993**, 273-292	0
244	Conformational deformation in deoxymyoglobin by hydrostatic pressure. **1993**, 1215-1218	
243	Prediction of regions with well defined conformational preferences in proteins, and their relevance to protein folding. **1993**, 1229-1235	
242	Application of computational neural networks to the prediction of protein structural features. **1993** , 15, 1-19	1
241	The crystal structure of EcoRV endonuclease and of its complexes with cognate and non-cognate DNA fragments. **1993**, 12, 1781-95	152
240	Data Based Modeling of Proteins. **1994**, 277-296	
239	Extraction and Characterisation of Molecular Surface Knobs and Holes for the Study of Complex Formation. **1994**, 389-396	

238	Molecular approaches to the design of chemical crop protection agents. **1994**, 41-67		
237	Humanization of Monoclonal Antibodies. **1994**, 105-134		1
236	Steps Towards Predicting the Structure of Membrane Proteins. **1994**, 239-252		
235	An object-oriented database of protein structure data. **1994**, 336-350		
234	An Adaptive Branch-and-Bound Minimization Method Based on Dynamic Programming. **1994**, 409-432		0
233	Conformational Search and Protein Folding. **1994**, 125-163		0
232	Structure-Function Modeling in Blood Coagulation: Interfaces, Biology and Chemistry. **1994**, 139-148		
231	Protein Fold Families and Structural Motifs. **1994**, 253-275		
230	Design of an Auto-associative Neural Network with Hidden Layer Activations that were used to Reclassify Local Protein Structures. **1994**, 397-404		
229	Combining computation with database access in biomolecular computing. **1994**, 317-335		5
228	Machine Learning for Protein Structure Prediction. **1994**, 384-390		0
227	Identical mutations at corresponding positions in two homologous proteins with nonidentical effects. *Journal of Biological Chemistry*, **1994**, 269, 11196-11200	5.4	6
226	The Role of the Protein in Stabilizing the Charge Separated States in Bacterial Photosynthesis. **1995**, 407-411		
225	The Role of Structure-Based Ligand Design in Industrial Pharmaceutical Research. **1995**, 187-206		
224	Dynamic Domains: A Simple Method of Analysing Structural Movements in Proteins. **1995**, 137-149		
223	Applications of Empirical Amino Acid Potential Functions. **1995**, 151-166		
222	The Docking of Cytochrome f with Plastocyanin: Three Possible Complexes. **1995**, 1707-1710		
221	The Sedoheptulose Bisphosphatase of Chlamydomonas Reinhardtii Contains a Potential Inter-Domain Disulphide and is Redox-Sensitive. **1995**, 3963-3966		

220	R□tgenstrahlen in der Biochemie. **1995**, 402-426	
219	Modelling the Interactions of Protein Side-Chains. **1995**, 119-135	1
218	Molekulare Bioinformatik. **1996**, 83-111	2
217	Shiga Toxin. **1996**, 173-190	2
216	Molecular Modelling - An Introduction. **1996**, 181-199	
215	Hydroxyl and water molecule orientations in trypsin: comparison to molecular dynamic structures. **1996**, 64, 273-87	
214	Biology and Biochemistry. **1996**,	
213	Industrial Protein X-Ray Crystallography: An Overview. **1996**, 1-19	
212	The Nucleic Acid Database: Present and Future. **1996**, 101, 243-257	0
211	Computational tools for structure-based design. **1997**, 433-450	
210	The Role of the Protein in Modulating Cofactor Electrochemistry in Proteins: The Calculation of Electrostatic Forces. **1997**, 361-390	
209	Chapter The secondary structure of proteins. **1997**, 99-136	
208	Data Management for Ligand-Based Drug Design. **1997**, 205-230	
207	Oligonucleotide Aptamers as Specific Targeting Devices in Diagnostics and Therapy. **1997**, 135-159	
206	Chapter 4 Computational methods relating protein sequence and structure. **1997**, 165-268	
205	Professional Gambling. **1997**, 79-119	
204	3D Similarity search by shape approximation. **1997**, 9-28	3
203	Roles of zinc and magnesium ions in enzymes. **1998**, 227-279	1

202 A Theoretical Study on the Measurability of Bijvoet Differences in Macromolecular Crystals. **1998**, 199-209

201 Molecular Recognition of Anionic Species: Hydrogenbonding Properties of Sulfate Andthiocyanate. **1998**, 523-525

200 New Tools for Drug Design Based on Protein Ligand Recognition Principles. **1998**, 97-118

199 Molecular Scene Analysis and Its Role in Protein Structure Determination. **1998**, 339-359

198 Recursive, object-oriented structures for molecular modeling. **1998**, 18, 2-8

197 The Carboxyl-Terminal Region of Protein C Is Essential for Its Secretion. **1998**, 91, 3784-3791 2

196 The Development and Application of Knowledge-Based Approaches to Molecular Design. **1999**, 243-260

195 New Techniques for the Construction of Residue Potentials for Protein Folding. **1999**, 212-224

194 Monosaccharides: geometry and dynamics. **1999**, 1-46 2

193 Canavalin. **1999**, 241-257

192 Computer modeling of protein, nucleic acid, and drug structures. **1999**, 475-505

191 Computational Biology:: The Fundamentals of Sequence-Based Techniques. **2014**, 1-28

190 PREMONITION - Preprocessing motifs in protein structures for search acceleration. 3, 217 3

189 Brownian dynamics simulation of peptides with the University of Houston Brownian Dynamics (UHBD) program. **2015**, 1268, 75-87

188 Insight into the Intermolecular Recognition Mechanism between HLA-A*24:02 and Antitumor Peptides against Breast Cancer. **2015**, 15, 1-4

187 Concluding Remarks. **2015**, 143-148

186 Explaining the Closure of Calculated HOMO-LUMO Gaps in Biomolecular Systems. **2015**, 95-110

185 Mutual Interaction Study Between DnaK-GroEL-FtSH with Heat Shock Regulator σ32 to Explain Prokaryotic Heat Shock Regulation. **2015**, 55-61

184	The Computational Analysis of Protein Ligand Docking with Diverse Genetic Algorithm Parameters. **2015**, 129-135		
183	Perspectives and Pitfalls in Nucleic Acids Crystallography. **2016**, 1320, 3-8		2
182	Molecular Modeling and Its Applications in Protein Engineering. **2016**, 281-306		1
181	Online Molecular Docking Resources. **2016**, 360-379		
180	X-Ray Crystallography. **2016**, 489-622		
179	Production of a Locus- and Allele-Specific Monoclonal Antibody for the Characterization of SLA-1*0401 mRNA and Protein Expression Levels in MHC-Defined Microminipigs. **2016**, 11, e0164995		2
178	Online Molecular Docking Resources. **2017**, 941-959		
177	Sequential eviction of crowded nucleoprotein complexes by the RecBCD molecular motor.		
176	Serial Crystallography with Multi-stage Merging oi 1000 of Images.		2
175	End-to-End Differentiable Learning of Protein Structure. *SSRN Electronic Journal*,	1	1
174	Desenvolvimento de nanodispositivos baseados em biomolculas: abordagens computacionais. **2018**, 118-155		
173	Biophysical Mechanism of the SAHA Inhibition of Zn²⁺-Histone Deacetylase-Like Protein (FB188 HDAH) Assessed via Crystal Structure Analysis. **2018**, 08, 91-114		
172	Map segmentation, automated model-building and their application to the Cryo-EM Model Challenge.		
171	pNeRF: Parallelized Conversion from Internal to Cartesian Coordinates.		
170	An Analysis of Characterized Plant Sesquiterpene Synthases.		
169	Methods of Structure Determination. **2019**, 193-209		
168	In silico analysis of interactions of flucloxacillin and its metabolites with HLA-B*57:01 . **2019**, 19, 1-4		
167	Comparative MD simulations and advanced analytics based studies on wild-type and hot-spot mutant A59G HRas.		

166	CoCoPRED: coiled-coil protein structural feature prediction from amino acid sequence using deep neural networks. **2021**,		
165	Data- and diversity-driven development of a Shotgun crystallization screen using the Protein Data Bank. *Acta Crystallographica Section D: Structural Biology*, **2021**, 77, 1437-1450	5.5	2
164	A simple technique to classify diffraction data from dynamic proteins according to individual polymorphs.		
163	Structures and energetics of darunavir and active site amino acids of native and mutant HIV‐1 protease: a computational study. 1		0
162	Extra Virgin Olive Oil consumption from Mild Cognitive Impairment patients attenuates oxidative and nitrative stress reflecting on the reduction of the PARP levels and DNA damage. **2021**, 156, 111621		2
161	Integrating structure-based machine learning and co-evolution to investigate specificity in plant sesquiterpene synthases.		
160	Structural Classification of Complex Molecules by Artificial Intelligence Techniques. 25-91		1
159	Graph Applications in Chemoinformatics and Structural Bioinformatics. 386-420		
158	Investigation of non-corrin cobalt(II)-containing sites in protein structures of the Protein Data Bank. **2013**, 69, 176-183		
157	Prion protein structure and pathology of transmissible spongiform encephalopathies (TSE). **1999**, 330-334		
156	A recursive algorithm for efficient combinatorial library docking. **2000**, 63-81		
155	Modifications of the scoring function in FlexX for virtual screening applications. **2000**, 83-98		
154	The Structure of Reaction Centers from Purple Bacteria. **1999**, 99-122		
153	References for 3. 3082-3087		
152	A Symmetry-Free Subspace for Ab initio Protein Folding Simulations. **2008**, 128-139		1
151	Protein Structure and Its Folding Rate. **2008**, 273-301		
150	A multimodal neural network with single-state predictions for protein secondary structure. **2004**, 8, 168-173		
149	Cu, Zn Superoxide dismutase: distorted active site binds substrate without significant energetic cost. **2006**, 115, 27		

148	Protein tertiary structure recognition using optimized associative memory Hamiltonians.	1
147	Computer-simulated density models of polymers of sickle hemoglobin. **1986**, 44, 178-179	
146	Natural Cystatin C fragments inhibit GPR15-mediated HIV and SIV infection without interfering with GPR15L signaling.	
145	Comparative MD simulations and advanced analytics based studies on wild-type and hot-spot mutant A59G HRas. **2020**, 15, e0234836	
144	Preparation and characterization of monoclonal antibodies recognizing two CD4 isotypes of Microminipigs. **2020**, 15, e0242572	1
143	Lithium-Protein Interactions: Analysis of Lithium-Containing Protein Crystal Structures Deposited in the Protein Data Bank. **2020**, 27, 763-769	0
142	Insights into the functional architecture of the catalytic center of a maize beta-glucosidase Zm-p60.1. **2001**, 127, 973-85	10
141	OWL--a non-redundant composite protein sequence database. **1994**, 22, 3574-7	90
140	The HSSP database of protein structure-sequence alignments. **1994**, 22, 3597-9	32
139	The FSSP database of structurally aligned protein fold families. **1994**, 22, 3600-9	205
138	The SBASE protein domain library, release 3.0: a collection of annotated protein sequence segments. **1994**, 22, 3610-5	21
137	Characterization of two distinct MHC class II binding sites in the superantigen staphylococcal enterotoxin A. **1995**, 14, 2978-86	42
136	Crystal structure of the superantigen staphylococcal enterotoxin type A. **1995**, 14, 3292-301	56
135	Crystal structure of the phosphatidylinositol-specific phospholipase C from Bacillus cereus in complex with myo-inositol. **1995**, 14, 3855-63	38
134	PI 3-kinase: structural and functional analysis of intersubunit interactions. **1994**, 13, 511-21	102
133	Generation of interleukin-6 receptor antagonists by molecular-modeling guided mutagenesis of residues important for gp130 activation. **1994**, 13, 1357-67	28
132	A single amino acid substitution in the exoplasmic domain of the human growth hormone (GH) receptor confers familial GH resistance (Laron syndrome) with positive GH-binding activity by abolishing receptor homodimerization. **1994**, 13, 1386-95	16
131	Integrin LFA-1 alpha subunit contains an ICAM-1 binding site in domains V and VI. **1994**, 13, 1790-8	11

130	Crystal structure of the adenovirus DNA binding protein reveals a hook-on model for cooperative DNA binding. **1994**, 13, 2994-3002	28
129	The binding epitopes of neurotrophin-3 to its receptors trkC and gp75 and the design of a multifunctional human neurotrophin. **1994**, 13, 5896-909	23
128	Evolutionary link between glycogen phosphorylase and a DNA modifying enzyme. **1995**, 14, 1287-93	17
127	Three-dimensional structure of the bifunctional protein PCD/DCoH, a cytoplasmic enzyme interacting with transcription factor HNF1. **1995**, 14, 2034-42	14
126	Crystal structure of a theta-class glutathione transferase. **1995**, 14, 2133-43	53
125	Enhancement and destruction of antibody function by somatic mutation: unequal occurrence is controlled by V gene combinatorial associations. **1995**, 14, 2784-94	7
124	Nobel lecture. A structural basis of light energy and electron transfer in biology. **1989**, 8, 2125-47	7
123	The structure of the saccharide-binding site of concanavalin A. **1989**, 8, 2189-93	43
122	OB(oligonucleotide/oligosaccharide binding)-fold: common structural and functional solution for non-homologous sequences. **1993**, 12, 861-7	331
121	Common features in DNA recognition helices of eukaryotic transcription factors. **1993**, 12, 3221-6	20
120	First structure of a snake venom metalloproteinase: a prototype for matrix metalloproteinases/collagenases. **1993**, 12, 4151-7	43
119	Expression of conformationally constrained adhesion peptide in an antibody CDR loop and inhibition of natural killer cell cytotoxic activity by an antibody antigenized with the RGD motif. **1993**, 12, 4375-84	7
118	Crystal structure of the human adenovirus proteinase with its 11 amino acid cofactor. **1996**, 15, 1778-83	33
117	Crystal structure of a bacterial family-III cellulose-binding domain: a general mechanism for attachment to cellulose. **1996**, 15, 5739-51	112
116	Crystal structure of haloalkane dehalogenase: an enzyme to detoxify halogenated alkanes. **1991**, 10, 1297-302	37
115	Crystal structure of Penicillium citrinum P1 nuclease at 2.8 A resolution. **1991**, 10, 1607-18	33
114	The 2.5 A X-ray crystal structure of the acid-stable proteinase inhibitor from human mucous secretions analysed in its complex with bovine alpha-chymotrypsin. **1988**, 7, 345-51	45
113	The 2.0 A X-ray crystal structure of chicken egg white cystatin and its possible mode of interaction with cysteine proteinases. **1988**, 7, 2593-9	120

112	The three-dimensional structure of the seed storage protein phaseolin at 3 A resolution. **1990**, 9, 9-15	36
111	Selenomethionyl proteins produced for analysis by multiwavelength anomalous diffraction (MAD): a vehicle for direct determination of three-dimensional structure. **1990**, 9, 1665-72	340
110	The refined 2.4 A X-ray crystal structure of recombinant human stefin B in complex with the cysteine proteinase papain: a novel type of proteinase inhibitor interaction. **1990**, 9, 1939-47	120
109	How Trp repressor binds to its operator. **1990**, 9, 1963-7	23
108	Three-dimensional structure determination of an anti-2-phenyloxazolone antibody: the role of somatic mutation and heavy/light chain pairing in the maturation of an immune response. **1990**, 9, 3807-14	30
107	The pAR5 mutation and the allosteric mechanism of Escherichia coli aspartate carbamoyltransferase. **1987**, 6, 2843-7	4
106	Immunoglobulin VH clan and family identity predicts variable domain structure and may influence antigen binding. **1992**, 11, 603-9	46
105	Three-dimensional crystal structure of recombinant murine interferon-beta. **1992**, 11, 3193-201	28
104	Three-dimensional structure of fungal proteinase K reveals similarity to bacterial subtilisin. **1984**, 3, 1311-4	15
103	Location of 'continuous' antigenic determinants in the protruding regions of proteins. **1986**, 5, 409-13	77
102	Refined 1.2 A crystal structure of the complex formed between subtilisin Carlsberg and the inhibitor eglin c. Molecular structure of eglin and its detailed interaction with subtilisin. **1986**, 5, 813-8	23
101	Using known substructures in protein model building and crystallography. **1986**, 5, 819-22	174
100	The relation between the divergence of sequence and structure in proteins. **1986**, 5, 823-6	660
99	X-ray crystal structure of the complex of human leukocyte elastase (PMN elastase) and the third domain of the turkey ovomucoid inhibitor. **1986**, 5, 2453-8	56
98	Crystal structure of the catalytic core domain of the family 6 cellobiohydrolase II, Cel6A, from Humicola insolens, at 1.92 A resolution. **1999**, 337 (Pt 2), 297-304	20
97	Variable domain-linked oligosaccharides of a human monoclonal IgG: structure and influence on antigen binding. **1999**, 338 (Pt 2), 529-38	16
96	Aldolase A Ins(1,4,5)P3-binding domains as determined by site-directed mutagenesis. **1999**, 341 (Pt 3), 805-12	4
95	Oligomerization reduces heparin affinity but enhances receptor binding of fibroblast growth factor 2. **2000**, 345 Pt 1, 107-13	7

94	Structure and function of Humicola insolens family 6 cellulases: structure of the endoglucanase, Cel6B, at 1.6 A resolution. **2000**, 348 Pt 1, 201-7		19
93	Crystal structure of the NADP+-dependent aldehyde dehydrogenase from Vibrio harveyi: structural implications for cofactor specificity and affinity. **2000**, 349 Pt 3, 853-61		29
92	Looking at proteins: representations, folding, packing, and design. Biophysical Society National Lecture, 1992. **1992**, 63, 1185-209		54
91	Successful molecular dynamics simulation of the zinc-bound farnesyltransferase using the cationic dummy atom approach. **2000**, 9, 1857-65		97
90	Pyramidalization of backbone carbonyl carbon atoms in proteins. **2000**, 9, 2038-42		25
89	Bioinformatics in support of molecular medicine. **1998**, 53-61		8
88	Delivering bioinformatics training: bridging the gaps between computer science and biomedicine. **2002**, 220-4		
87	Computer applications for prediction of protein-protein interactions and rational drug design. **2009** , 2, 101-23		9
86	Possible Function of the ribT Gene of Bacillus subtilis: Theoretical Prediction, Cloning, and Expression. **2014**, 6, 106-9		1
85	Isolation and characterization of a dihydrofolate reductase gene mutation in methotrexate-resistant Drosophila cells. *Gene Expression*, **1996**, 6, 231-9	3.4	4
84	Spike residue 403 affects binding of coronavirus spikes to human ACE2. *Nature Communications*, **2021**, 12, 6855	17.4	3
83	Investigation of microcystin conformation and binding towards PPP1 by molecular dynamics simulation. *Chemico-Biological Interactions*, **2021**, 109766	5	0
82	Structural biology is solved - now what?. *Nature Methods*, **2022**, 19, 24-26	21.6	2
81	Unraveling the Structural Development of Peptide-Coordinated Iron-Sulfur Clusters: Prebiotic Evolution and Biosynthetic Strategies. *Chinese Journal of Chemistry*,	4.9	0
80	Comparison of Glycoside Hydrolase family 3 β-xylosidases from basidiomycetes and ascomycetes reveals evolutionarily distinct xylan degradation systems.. *Journal of Biological Chemistry*, **2022**, 101670	5.4	2
79	Beta-and gamma-turns in proteins revisited: a new set of amino acid turn-type dependent positional preferences and potentials. *Journal of Biosciences*, **2000**, 25, 143-56	2.3	41
78	A simple technique to classify diffraction data from dynamic proteins according to individual polymorphs.. *Acta Crystallographica Section D: Structural Biology*, **2022**, 78, 268-277	5.5	1
77	Water Distribution on Protein Surface of the Lyophilized Proteins with Different Topography Studied by Molecular Dynamics Simulations.. *Journal of Pharmaceutical Sciences*, **2022**,	3.9	

76	Antifungal activity of 2-Chloro-N-phenylacetamide, docking and molecular dynamics studies against clinical isolates of Candida tropicalis and Candida parapsilosis.. *Journal of Applied Microbiology*, **2022**,	4.7	1
75	Structural and Biophysical Analysis of the Phytochelatin-Synthase-Like Enzyme from sp. Shows That Its Protease Activity is Sensitive to the Redox State of the Substrate.. *ACS Chemical Biology*, **2022**,	4.9	0
74	Developing Community Resources for Nucleic Acid Structures.. *Life*, **2022**, 12,	3	1
73	Fifty years of Protein Data Bank in the Journal of Biochemistry. *Journal of Biochemistry*, **2021**,	3.1	
72	A topology approach towards modeling activities and properties on a biomolecular surface. **2021**,		1
71	Large-Scale Screening Reveals That Geometric Structure Matters More Than Electronic Structure in the Bioinspired Catalyst Design of Formate Dehydrogenase Mimics. *ACS Catalysis*, **2022**, 12, 383-396	13.1	0
70	Synthesis, structural, spectroscopic and docking studies on (E)-1-Ferrocenyl-3-phenyl□propen-1-one by the density functional theory. *Molecular Simulation*, **2022**, 48, 387-402	2	
69	Structural Bases for Hesperetin Derivatives: Inhibition of Protein Tyrosine Phosphatase 1B, Kinetics Mechanism and Molecular Docking Study.. *Molecules*, **2021**, 26,	4.8	2
68	Determinants of Spike Infectivity, Processing and Neutralization in SARS-CoV-2 Omicron subvariants BA.1 and BA.2.		1
67	Data_Sheet_1.doc. **2020**,		
66	Data_Sheet_2.doc. **2020**,		
65	Data_Sheet_3.doc. **2020**,		
64	Data_Sheet_4.zip. **2020**,		
63	Table_1.doc. **2020**,		
62	DataSheet_1.xlsx. **2019**,		
61	DataSheet_2.xlsx. **2019**,		
60	DataSheet_3.xlsx. **2019**,		
59	DataSheet_4.xlsx. **2019**,		

58	DataSheet_5.xlsx. **2019**,		
57	Presentation_1.pdf. **2019**,		
56	Molecular Principles, Components, Technology, and Concepts: Proteins Protein Domains: Structure, Function, and Methods. **2022**,		
55	Advancement of Computer-Aided Design Software and Simulation Tools for Nucleic Acid Nanostructures and DNA Origami. **2022**, 75-99		
54	In silico approaches to develop herbal acaricides against R. (Boophilus) Microplus and In vitro Anti-Tick activities of selected medicinal plants. *Saudi Journal of Biological Sciences*, **2022**, 29, 103302	4	1
53	Inhibitory effect of thymoquinone from Nigella sativa against SARS-CoV-2 main protease. An in-silico study.. *Brazilian Journal of Biology*, **2022**, 84, e250667	1.5	2
52	Investigation of the interaction between anticancer drug ibrutinib and double-stranded DNA by electrochemical and molecular docking techniques. *Microchemical Journal*, **2022**, 180, 107622	4.8	0
51	Determinants of Spike Infectivity, Processing and Neutralization in SARS-CoV-2 Omicron Subvariants BA.1 and BA.2. *SSRN Electronic Journal*,	1	
50	An experimental and theoretical study of ROS scavenging by organosulfur compounds from garlic: In silico analysis of metabolic pathways and interactions on CYP2E1. *Journal of Sulfur Chemistry*, 1-23	2.3	1
49	Surveying non-visual arrestins reveals allosteric interactions between functional sites.		
48	A Molecular Docking Study of Human STEAP2 for the Discovery of New Potential Anti-Prostate Cancer Chemotherapeutic Candidates. *Frontiers in Bioinformatics*, **2022**, 2,		
47	Response : Crystallographic Citations. **1988**, 242, 347-348		0
46	Response : Crystallographic Citations. **1988**, 242, 347-347		0
45	Response : Crystallographic Citations. **1988**, 242, 347-348		0
44	Modelling active site response towards changes in the protein-core of serine proteases. A CNDO/2 NDO SCRF study of subtilisin and thiosubtilisin. **1985**, 24, 67-84		0
43	Quantum chemical conformational analysis of the catalytic triad in hymotrypsin. **1985**, 24, 85-95		0
42	Collective Variable for Metadynamics Derived From AlphaFold Output. *Frontiers in Molecular Biosciences*, 9,	5.6	0
41	Therapeutic Inhibitors: Natural Product Options through Computer-Aided Drug Design.		

40	Survey of the Intermolecular Disulfide Bonds Observed in Protein Crystal Structures Deposited in the Protein Data Bank. *Life*, **2022**, 12, 986	3	
39	Serial crystallography with multi-stage merging of thousands of images. *Acta Crystallographica Section F, Structural Biology Communications*, **2022**, 78, 281-288	1.1	0
38	Palladium(II) Complexes of Substituted Salicylaldehydes: Synthesis, Characterization and Investigation of Their Biological Profile. *Pharmaceuticals*, **2022**, 15, 886	5.2	0
37	Determinants of Spike Infectivity, Processing and Neutralization in SARS-CoV-2 Omicron subvariants BA.1 and BA.2. *Cell Host and Microbe*, **2022**,	23.4	6
36	Emerging Role of Structural and Systems Biology in Anticancer Therapeutics. **2022**, 97-114		
35	Homology modeling and virtual characterization of cytochrome c nitrite reductase (NrfA) in three model bacteria responsible for short-circuit pathway, DNRA in the terrestrial nitrogen cycle. **2022**, 38,		
34	On the Molecular Driving Force of Protein–Protein Association. **2022**, 2, 240-247		
33	Recognition in the Domain of Molecular Chirality: From Noncovalent Interactions to Separation of Enantiomers. **2022**, 122, 13235-13400		7
32	CEMIP (HYBID , KIAA1199): Structure, function and expression in health and disease.		1
31	Bovine Serum Amine Oxidase and Polyamine Analogues: Chemical Synthesis and Biological Evaluation Integrated with Molecular Docking and 3-D QSAR Studies. **2022**, 62, 3910-3927		
30	Surveying non-visual arrestins reveals allosteric interactions between functional sites.		
29	Polypharmacology in Old Drug Rediscovery: Drug Repurposing. **2022**, 535-592		0
28	PDBmsA: An online tool for PDB file splitting and interactive molecular visualization.		0
27	Neural Network for Screening Active Sites on Proteins. **2022**, 225-246		0
26	In silico evaluation of Philippine Natural Products against SARS-CoV-2 Main Protease. **2022**, 28,		0
25	Drug Repurposing Based on Machine Learning. **2022**, 143-164		0
24	Identification of a novel class of cyclic penta-peptides against hepatitis C virus as p7 channel blockers. **2022**, 20, 5902-5910		0
23	Interplay between hydrogen and chalcogen bonds in cysteine.		0

22	CAT: A Compound Attachment Tool for the Construction of Composite Chemical Compounds.	0
21	Variance-Reduced Randomized Kaczmarz Algorithm In Xfel Single-Particle Imaging Phase Retrieval. **2022**,	0
20	In Silico Approach for the Evaluation of the Potential Antiviral Activity of Extra Virgin Olive Oil (EVOO) Bioactive Constituents Oleuropein and Oleocanthal on Spike Therapeutic Drug Target of SARS-CoV-2. **2022**, 27, 7572	1
19	Chalcogen bonds formed by protein sulfur atoms in proteins. A survey of high-resolution structures deposited in the protein data bank. 1-7	0
18	Randomized Kaczmarz Method for Single-Particle X-Ray Image Phase Retrieval. **2022**, 1-16	0
17	Storing and structuring big data in histological research (vertebrates) using a relational database in SQL. **2022**, 13, 207-212	0
16	Computer-Aided Drug Design: An Update. **2023**, 123-152	1
15	Species-Based Differences in Mechanical Properties, Cytocompatibility, and Printability of Methacrylated Collagen Hydrogels. **2022**, 23, 5137-5147	1
14	The Contribution of Hydrophobic Interactions to Conformational Changes of Inward/Outward Transmembrane Transport Proteins. **2022**, 12, 1212	0
13	Investigating the Anticancer Activity of G-Rh1 Using In Silico and In Vitro Studies (A549 Lung Cancer Cells). **2022**, 27, 8311	1
12	A Peptides Prediction Methodology with Fragments and CNN for Tertiary Structure Based on GRSA2. **2022**, 11, 729	0
11	A catalyst acceleration platform toward realizing the energy transition. **2022**, 5, 4179-4186	0
10	Methyl jasmonate induces selaginellin accumulation in Selaginella convoluta. **2023**, 19,	0
9	Synthesis, crystal structure, DFT, Hirshfeld surface analysis, energy framework, docking and molecular dynamic simulations of (E)-4-(4-methylbenzyl)-6-styrylpyridazin-3(2H)-one as anticancer agent. 1-20	0
8	IgM Heavy Chain Complementarity-Determining Region 3 Diversity Is Constrained by Genetic and Somatic Mechanisms Until Two Months After Birth. **1999**, 162, 6060-6070	21
7	Identifying Potential Molecular Targets in Fungi Based on (Dis)Similarities in Binding Site Architecture with Proteins of the Human Pharmacolome. **2023**, 28, 692	0
6	Inhibition of Cancer Cell Proliferation and Bacterial Growth by Silver(I) Complexes Bearing a CH3-Substituted Thiadiazole-Based Thioamide. **2023**, 28, 336	0
5	A geometric and topological analysis of the binding behavior of Intrinsically Disordered Proteins. **2022**,	0

4	Computer Simulation Techniques for Modelling Statics and Dynamics of Nanoscale Structures. **2014**, 230-299	0
3	Highlights in TMPRSS2 inhibition mechanism with guanidine derivatives approved drugs for COVID-19 treatment. 1-15	0
2	Randomized Kaczmarz Method for Single Particle X-Ray Image Phase Retrieval. **2023**, 1273-1288	0
1	In vitropharmacological profile of KW-6356, a novel adenosine A2Areceptor antagonist/inverse agonist. MOLPHARM-AR-2022-000633	0