Design of a novel globular protein fold with atomic-level accuracy

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#	Paper	IF	Citations
1397	The Rosetta All-Atom Energy Function for Macromolecular Modeling and Design.		
1396	Multiple Synthetic Routes to the Mini-Protein Omomyc and Coiled-Coil Domain Truncations.		
1395	Structural biology. Learning to speak the language of proteins. *Science*, **2003**, 302, 1347-8	33.3	2
1394	Computational design of receptors for an organophosphate surrogate of the nerve agent soman. **2004**, 101, 7907-12		89
1393	FamClash: a method for ranking the activity of engineered enzymes. **2004**, 101, 4142-7		61
1392	Protein Sequence Optimization: Theory, Practice, and Fundamental Impossibility. **2004**, 2, 1-10		4
1391	De novo design of catalytic proteins. **2004**, 101, 11566-70		274
1390	Paradigms for computational nucleic acid design. **2004**, 32, 1392-403		145
1389	Improvement of comparative model accuracy by free-energy optimization along principal components of natural structural variation. **2004**, 101, 15346-51		59
1388	From computational quantum chemistry to computational biology: experiments and computations are (full) partners. **2004**, 1, P23-6		4
1387	Developing optimal non-linear scoring function for protein design. **2004**, 20, 3080-98		28
1386	ICBS: a database of interactions between protein chains mediated by beta-sheet formation. **2004**, 20, 2767-77		50
1385	A new hydrogen-bonding potential for the design of protein-RNA interactions predicts specific contacts and discriminates decoys. **2004**, 32, 5147-62		62
1384	Biochemistry. De novo design of an enzyme. *Science*, **2004**, 304, 1916-7	33.3	13
1383	Searching for folded proteins in vitro and in silico. **2004**, 271, 1615-22		23
1382	Ten thousand interactions for the molecular biologist. **2004**, 22, 1317-21		169
1381	A novel ADP- and zinc-binding fold from function-directed in vitro evolution. **2004**, 11, 382-3		50

1380	Computational redesign of protein-protein interaction specificity. **2004**, 11, 371-9		254
1379	10 residue folded peptide designed by segment statistics. **2004**, 12, 1507-18		230
1378	Exploring folding free energy landscapes using computational protein design. *Current Opinion in Structural Biology*, **2004**, 14, 89-95	8.1	84
1377	Simulating protein evolution in sequence and structure space. *Current Opinion in Structural Biology*, **2004**, 14, 202-7	8.1	81
1376	Development of novel statistical potentials for protein fold recognition. *Current Opinion in Structural Biology*, **2004**, 14, 225-32	8.1	104
1375	Advances in computational protein design. *Current Opinion in Structural Biology*, **2004**, 14, 487-94	8.1	78
1374	Protein structure prediction and analysis using the Robetta server. **2004**, 32, W526-31		1239
1373	Some fundamental aspects of building protein structures from fragment libraries. *Protein Science*, **2004**, 13, 1636-50	6.3	34
1372	Chemical synthesis of TASP arrays and their application in protein design. **2004**, 8, 219-29		16
1371	A portable allosteric mechanism. *Proteins: Structure, Function and Bioinformatics*, **2004**, 57, 9-11	4.2	9
1370	Ab initio prediction of the three-dimensional structure of a de novo designed protein: a double-blind case study. *Proteins: Structure, Function and Bioinformatics*, **2005**, 58, 560-70	4.2	46
1369	Computational challenges in combinatorial library design for protein engineering. **2004**, 50, 262-272		27
1368	Combinatorial approaches to novel proteins. **2004**, 5, 177-82		11
1367	Protein Design at the Crossroads of Biotechnology, Chemistry, and Evolution. Proceedings of the 86th International Titisee Conference. Titisee, Germany, 23-27 October 2002. **2004**, 5, 143-239		
1366	Evolutionary optimization of a nonbiological ATP binding protein for improved folding stability. **2004**, 11, 865-74		23
1365	Computational design of protein-protein interactions. **2004**, 8, 91-7		187
1364	Novel methods for directed evolution of enzymes: quality, not quantity. **2004**, 15, 291-7		196
1363	Novel forms of chemical protein diversity -- in nature and in the laboratory. **2004**, 15, 607-14		36

1362	Site-directed protein recombination as a shortest-path problem. **2004**, 17, 589-94		51
1361	7 Computational protein design and discovery. **2004**, 100, 195-236		7
1360	Quantitative characterization of protein structure: application to a novel ββα fold. **2004**, 28, 1608-1614		9
1359	Simulated evolution of emergent chiral structures in polyalanine. **2004**, 126, 14459-67		26
1358	Evolution and evolvability of proteins in the laboratory. **2004**, 101, 3997-8		
1357	Investigating protein folding, misfolding and nonnative states: experimental and theoretical methods. **2004**, 34, 1-3		2
1356	Experimental investigation of protein folding and misfolding. **2004**, 34, 4-14		110
1355	Characterization of the folding energy landscapes of computer generated proteins suggests high folding free energy barriers and cooperativity may be consequences of natural selection. **2004**, 338, 573-83		83
1354	Structural test of the parameterized-backbone method for protein design. **2004**, 342, 289-97		22
1353	Detection and structure determination of an equilibrium unfolding intermediate of Rd-apocytochrome b562: native fold with non-native hydrophobic interactions. **2004**, 343, 1477-85		27
1352	A simple physical model for the prediction and design of protein-DNA interactions. **2004**, 344, 59-70		86
1351	Computational design of a biologically active enzyme. *Science*, **2004**, 304, 1967-71	33.3	244
1350	Protein structure prediction using Rosetta. **2004**, 383, 66-93		1142
1349	Functional engineered channels and pores (Review). **2004**, 21, 209-20		172
1348	Future Directions for the Chemical Industry. **2005**, 329-360		
1347	Chapter 18 Computationally Assisted Protein Design. **2005**, 245-253		1
1346	Biochemie 2004. **2005**, 53, 273-280		0
1345	Ab initio structure prediction. **2005**,		

1344	Protein components for nanodevices. **2005**, 9, 576-84		88
1343	Electrostatics in computational protein design. **2005**, 9, 622-6		98
1342	Computational methods for protein design and protein sequence variability: biased Monte Carlo and replica exchange. **2005**, 401, 205-210		33
1341	E2 conjugating enzymes must disengage from their E1 enzymes before E3-dependent ubiquitin and ubiquitin-like transfer. **2005**, 12, 933-4		117
1340	Engineering novel binding proteins from nonimmunoglobulin domains. **2005**, 23, 1257-68		536
1339	Natural-like function in artificial WW domains. *Nature*, **2005**, 437, 579-83	50.4	196
1338	Design of a heterospecific, tetrameric, 21-residue miniprotein with mixed alpha/beta structure. **2005**, 13, 225-34		33
1337	The nitty-gritty of protein interactions. **2005**, 13, 1737-8		2
1336	Protein folding and the organization of the protein topology universe. **2005**, 30, 13-9		95
1335	Assessing local structural perturbations in proteins. **2005**, 6, 226		2
1334	Simulated folding in polypeptides of diversified molecular tacticity: implications for protein folding and de novo design. **2005**, 78, 96-105		19
1333	Effects of segment substitution on the structure and stability of immunoglobulin G binding domain of streptococcal protein G. **2005**, 79, 9-17		
1332	Research challenges, opportunities and synergism in systems engineering and computational biology. **2005**, 51, 1872-1884		27
1331	Progress and challenges in high-resolution refinement of protein structure models. *Proteins: Structure, Function and Bioinformatics*, **2005**, 59, 15-29	4.2	130
1330	Protein design simulations suggest that side-chain conformational entropy is not a strong determinant of amino acid environmental preferences. *Proteins: Structure, Function and Bioinformatics*, **2006**, 62, 739-48	4.2	29
1329	. **2005**,		36
1328	[The >: can one predict the structure of proteins?]. **2005**, 21, 609-12		
1327	. **2005**,		9

1326	Improvement in protein functional site prediction by distinguishing structural and functional constraints on protein family evolution using computational design. **2005**, 33, 5861-7		69
1325	A multi-objective evolutionary approach to peptide structure redesign and stabilization. **2005**,		
1324	An active enzyme constructed from a 9-amino acid alphabet. **2005**, 280, 37742-6		80
1323	Rotamer-Pair Energy Calculations Using a Trie Data Structure. **2005**, 389-400		9
1322	New directions in the study of Peptide h-bonds and Peptide solvation. **2005**, 72, ix-xii		2
1321	Protein structure estimation from minimal restraints using Rosetta. **2005**, 394, 244-60		27
1320	Coarse-graining protein energetics in sequence variables. **2005**, 95, 148103		18
1319	A segment of cold shock protein directs the folding of a combinatorial protein. **2005**, 102, 1396-401		27
1318	Hairpin folding rates reflect mutations within and remote from the turn region. **2005**, 102, 15483-7		88
1317	Algorithms in Bioinformatics. **2005**,		4
1316	Massive sequence perturbation of a small protein. **2005**, 102, 14988-93		25
1315	Three-stage prediction of protein beta-sheets by neural networks, alignments and graph algorithms. **2005**, 21 Suppl 1, i75-84		91
1314	Specificity versus stability in computational protein design. **2005**, 102, 12724-9		118
1313	Sequence optimization and designability of enzyme active sites. **2005**, 102, 12035-40		16
1312	CAMPO, SCR_FIND and CHC_FIND: a suite of web tools for computational structural biology. **2005**, 33, W50-5		17
1311	Design of combinatorial protein libraries of optimal size. *Proteins: Structure, Function and Bioinformatics*, **2005**, 60, 769-77	4.2	22
1310	Progress in modeling of protein structures and interactions. *Science*, **2005**, 310, 638-42	33.3	244
1309	Design of a calcium-binding protein with desired structure in a cell adhesion molecule. **2005**, 127, 2085-93		57

1308	Overview of molecular dynamics techniques and early scientific results from the Blue Gene project. **2005**, 49, 475-487		9
1307	Practical lessons from protein structure prediction. **2005**, 33, 1874-91		97
1306	Specificity and biomineralization activities of Ti-binding peptide-1 (TBP-1). **2005**, 21, 3090-5		194
1305	Design of amphiphilic protein maquettes: controlling assembly, membrane insertion, and cofactor interactions. *Biochemistry*, **2005**, 44, 12329-43	3.2	57
1304	A residue-pairwise generalized born scheme suitable for protein design calculations. **2005**, 109, 22667-73		36
1303	Laboratory-directed protein evolution. **2005**, 69, 373-92		147
1302	De novo design of a redox-active minimal rubredoxin mimic. **2005**, 127, 5804-5		114
1301	Recapitulation of protein family divergence using flexible backbone protein design. **2005**, 346, 631-44		62
1300	Energy functions for protein design: adjustment with protein-protein complex affinities, models for the unfolded state, and negative design of solubility and specificity. **2005**, 347, 203-27		171
1299	Comprehensive analysis of protein folding activation thermodynamics reveals a universal behavior violated by kinetically stable proteases. **2005**, 347, 355-66		49
1298	Evolutionary protein stabilization in comparison with computational design. **2005**, 351, 1160-8		33
1297	Design of lambda Cro fold: solution structure of a monomeric variant of the de novo protein. **2005**, 354, 801-14		14
1296	Finding the fittest fold: using the evolutionary record to design new proteins. **2005**, 122, 832-4		5
1295	Searching for hypothetical proteins: theory and practice based upon original data and literature. **2005**, 77, 90-127		141
1294	One- and two-body decomposable Poisson-Boltzmann methods for protein design calculations. *Protein Science*, **2005**, 14, 1293-304	6.3	45
1293	Action-at-a-distance interactions enhance protein binding affinity. *Protein Science*, **2005**, 14, 1363-9	6.3	29
1292	Functionalized foldamers: synthesis and characterization of a glycosylated beta-peptide 314-helix conveying the TN-antigen. **2005**, 3, 1359-61		28
1291	The design of coiled-coil structures and assemblies. **2005**, 70, 79-112		422

1290	Computational thermostabilization of an enzyme. *Science*, **2005**, 308, 857-60	33.3	303
1289	Introduction to Chemoinformatics in Drug Discovery □A Personal View. **2005**, 1-22		1
1288	Toward high-resolution de novo structure prediction for small proteins. *Science*, **2005**, 309, 1868-71	33.3	686
1287	Bioinformatics and Drug Discovery. **2006**,		1
1286	In silico protein design: fitting sequence onto structure. *Methods in Molecular Biology*, **2006**, 316, 359-74	1.4	5
1285	Protein Design. **2006**,		
1284	Protein folding thermodynamics and dynamics: where physics, chemistry, and biology meet. **2006**, 106, 1559-88		294
1283	Computer-based design of novel protein structures. **2006**, 35, 49-65		107
1282	IPRO: an iterative computational protein library redesign and optimization procedure. **2006**, 90, 4167-80		45
1281	A computational study of nucleosomal DNA flexibility. **2006**, 91, 4121-32		65
1280	Repeat protein architectures predicted by a continuum representation of fold space. *Protein Science*, **2006**, 15, 753-60	6.3	10
1279	In vitro evolution of proteins. **2006**, 101, 449-56		48
1278	Mechanisms of protein assembly: lessons from minimalist models. **2006**, 39, 135-42		77
1277	Design of functional ferritin-like proteins with hydrophobic cavities. **2006**, 128, 6611-9		52
1276	Femtomolar Zn(II) affinity in a peptide-based ligand designed to model thiolate-rich metalloprotein active sites. **2006**, 45, 9941-58		47
1275	Protein folding pathways studied by pulsed- and native-state hydrogen exchange. **2006**, 106, 1757-68		53
1274	Computational design of a single amino acid sequence that can switch between two distinct protein folds. **2006**, 128, 1154-61		147
1273	Rational design of new binding specificity by simultaneous mutagenesis of calmodulin and a target peptide. *Biochemistry*, **2006**, 45, 12547-59	3.2	32

1272	Structure-based prediction of bZIP partnering specificity. **2006**, 355, 1125-42		55
1271	Contribution of electrostatic interactions, compactness and quaternary structure to protein thermostability: lessons from structural genomics of Thermotoga maritima. **2006**, 356, 547-57		117
1270	Recapitulation and design of protein binding peptide structures and sequences. **2006**, 357, 917-27		48
1269	Massive sequence perturbation of the Raf ras binding domain reveals relationships between sequence conservation, secondary structure propensity, hydrophobic core organization and stability. **2006**, 362, 151-71		7
1268	Mis-translation of a computationally designed protein yields an exceptionally stable homodimer: implications for protein engineering and evolution. **2006**, 362, 1004-24		26
1267	Machine learning and the prediction of protein structure: the state of the art. **2006**, 359-370		
1266	After-Action of the Ideas of I.M. Lifshitz in Polymer and Biopolymer Physics. 189-210		2
1265	Protein Modeling. **2006**,		
1264	Chemical Complementation. **2006**, 183-219		
1263	The Challenges of Making Useful Protein-Ligand Free Energy Predictions for Drug Discovery. **2006**, 321-351		3
1262	Computer Simulations in Pharmacokinetics and Pharmacodynamics: Rediscovering Systems Physiology in the 21st Century. **2006**, 513-528		
1261	MUMBO: a protein-design approach to crystallographic model building and refinement. **2006**, 62, 648-58		15
1260	Site-directed combinatorial construction of chimaeric genes: general method for optimizing assembly of gene fragments. *Proteins: Structure, Function and Bioinformatics*, **2006**, 64, 629-42	4.2	14
1259	Criteria for downhill protein folding: calorimetry, chevron plot, kinetic relaxation, and single-molecule radius of gyration in chain models with subdued degrees of cooperativity. *Proteins: Structure, Function and Bioinformatics*, **2006**, 65, 373-91	4.2	63
1258	Structural refinement of protein segments containing secondary structure elements: Local sampling, knowledge-based potentials, and clustering. *Proteins: Structure, Function and Bioinformatics*, **2006**, 65, 463-79	4.2	33
1257	ROSETTALIGAND: protein-small molecule docking with full side-chain flexibility. *Proteins: Structure, Function and Bioinformatics*, **2006**, 65, 538-48	4.2	336
1256	Structural and dynamical properties of manganese catalase and the synthetic protein DF1 and their implication for reactivity from classical molecular dynamics calculations. *Proteins: Structure, Function and Bioinformatics*, **2006**, 65, 317-30	4.2	19
1255	Surface hydrophobic groups, stability, and flip-flopping in lattice proteins. *Proteins: Structure, Function and Bioinformatics*, **2007**, 66, 321-41	4.2	3

1254	Advances in protein structure prediction and de novo protein design: A review. **2006**, 61, 966-988		175
1253	Identifying the interacting positions of a protein using Boolean learning and support vector machines. **2006**, 30, 268-79		3
1252	Elucidation of conserved long-range interaction networks in proteins and their significance in determining protein topology. **2006**, 368, 595-606		14
1251	Genetic selection for protein solubility enabled by the folding quality control feature of the twin-arginine translocation pathway. *Protein Science*, **2006**, 15, 449-58	6.3	107
1250	CIRSE: a solvation energy estimator compatible with flexible protein docking and design applications. *Protein Science*, **2006**, 15, 1579-96	6.3	10
1249	Affinity enhancement of an in vivo matured therapeutic antibody using structure-based computational design. *Protein Science*, **2006**, 15, 949-60	6.3	137
1248	A composite score for predicting errors in protein structure models. *Protein Science*, **2006**, 15, 1653-66	6.3	141
1247	Simple electrostatic model improves designed protein sequences. *Protein Science*, **2006**, 15, 2014-8	6.3	15
1246	Configurational-bias sampling technique for predicting side-chain conformations in proteins. *Protein Science*, **2006**, 15, 2029-39	6.3	28
1245	Intelligent design: the de novo engineering of proteins with specified functions. **2006**, 3045-51		60
1244	The promise of synthetic biology. **2006**, 73, 735-9		51
1243	Design of protein conformational switches. *Current Opinion in Structural Biology*, **2006**, 16, 525-30	8.1	95
1242	Knowledge-based potentials in protein design. *Current Opinion in Structural Biology*, **2006**, 16, 508-13	8.1	74
1241	High-resolution structural validation of the computational redesign of human U1A protein. **2006**, 14, 847-56		19
1240	Directed evolution of metabolic pathways. **2006**, 24, 28-38		55
1239	A designed well-folded monomeric four-helix bundle protein prepared by Fmoc solid-phase peptide synthesis and native chemical ligation. **2006**, 12, 1436-47		5
1238	Removal of kinetic traps and enhanced protein folding by strategic substitution of amino acids in a model alpha-helical hairpin peptide. **2006**, 81, 167-78		16
1237	Computational design of proteins stereochemically optimized in size, stability, and folding speed. **2006**, 83, 122-34		7

1236	Dramatic performance enhancements for the FASTER optimization algorithm. **2006**, 27, 1071-5		49
1235	Rapid detection of similarity in protein structure and function through contact metric distances. **2006**, 34, e152		27
1234	Consensus design as a tool for engineering repeat proteins. *Methods in Molecular Biology*, **2006**, 340, 151-70	1.4	40
1233	Sequence search methods and scoring functions for the design of protein structures. *Methods in Molecular Biology*, **2006**, 340, 183-206	1.4	1
1232	Electrostatic design of protein-protein association rates. *Methods in Molecular Biology*, **2006**, 340, 235-49	1.4	31
1231	Computational protein design: a novel path to future protein drugs. **2006**, 12, 3973-97		31
1230	Active Sites by Computational Protein Design. **2006**,		3
1229	A Monte Carlo sampling method of amino acid sequences adaptable to given main-chain atoms in the proteins. **2006**, 140, 543-52		
1228	Sampling realistic protein conformations using local structural bias. *PLoS Computational Biology*, **2006**, 2, e131	5	66
1227	Emergence of protein fold families through rational design. *PLoS Computational Biology*, **2006**, 2, e85	5	167
1226	Wiggle-predicting functionally flexible regions from primary sequence. *PLoS Computational Biology*, **2006**, 2, e90	5	25
1225	Prediction and design of macromolecular structures and interactions. **2006**, 361, 459-63		53
1224	Bioinformatic challenges for the next decade(s). **2006**, 361, 525-7		7
1223	Biochemistry. Loop grafting and the origins of enzyme species. *Science*, **2006**, 311, 475-6	33.3	53
1222	Shaping up the protein folding funnel by local interaction: lesson from a structure prediction study. **2006**, 103, 3141-6		57
1221	Structural and computational characterization of the SHV-1 beta-lactamase-beta-lactamase inhibitor protein interface. **2006**, 281, 26745-53		42
1220	RosettaDesign server for protein design. **2006**, 34, W235-8		154
1219	Combinatorial methods for small-molecule placement in computational enzyme design. **2006**, 103, 16710-5		94

1218	Common attributes of native-state structures of proteins, disordered proteins, and amyloid. **2006**, 103, 6883-8		44
1217	Voltage sensor conformations in the open and closed states in ROSETTA structural models of K(+) channels. **2006**, 103, 7292-7		196
1216	Protein Design. 267-289		0
1215	Nonnatural protein-protein interaction-pair design by key residues grafting. **2007**, 104, 5330-5		67
1214	Positive and negative design in stability and thermal adaptation of natural proteins. *PLoS Computational Biology*, **2007**, 3, e52	5	94
1213	Design of multi-specificity in protein interfaces. *PLoS Computational Biology*, **2007**, 3, e164	5	87
1212	Creating functional artificial proteins. **2007**, 8, 3-18		23
1211	Novel formulations for the sequence selection problem in de novo protein design with flexible templates. **2007**, 22, 51-71		23
1210	Single-molecule force spectroscopy reveals a mechanically stable protein fold and the rational tuning of its mechanical stability. **2007**, 104, 9278-83		95
1209	Local Protein Structures. **2007**, 2, 165-202		64
1208	Engineering enzymes for biocatalysis. **2007**, 1, 1-9		45
1207	Control of Polypeptide Chain Folding and Assembly. 147-171		3
1206	Knowledge-Based Energy Functions for Computational Studies of Proteins. **2007**, 71-123		7
1205	Functional residues serve a dominant role in mediating the cooperativity of the protein ensemble. **2007**, 104, 4347-52		63
1204	Computationally designed libraries of fluorescent proteins evaluated by preservation and diversity of function. **2007**, 104, 48-53		74
1203	High-resolution design of a protein loop. **2007**, 104, 17668-73		97
1202	Computational Enzymology: Insights into Enzyme Mechanism and Catalysis from Modelling. **2007**, 275-304		
1201	Protein structural codes and nucleation sites for protein folding. **2007**, 16, 392-404		6

1200	Dead-end elimination with backbone flexibility. **2007**, 23, i185-94		65
1199	De Novo Structure Prediction: Methods and Applications. 389-418		1
1198	Neoceptors: reengineering GPCRs to recognize tailored ligands. **2007**, 28, 111-6		25
1197	The highly cooperative folding of small naturally occurring proteins is likely the result of natural selection. **2007**, 128, 613-24		117
1196	Exploiting elements of transcriptional machinery to enhance protein stability. **2007**, 366, 103-16		11
1195	High-resolution structural and thermodynamic analysis of extreme stabilization of human procarboxypeptidase by computational protein design. **2007**, 366, 1209-21		79
1194	The stability effects of protein mutations appear to be universally distributed. **2007**, 369, 1318-32		295
1193	Modeling backbone flexibility to achieve sequence diversity: the design of novel alpha-helical ligands for Bcl-xL. **2007**, 371, 1099-117		70
1192	Structure-based protocol for identifying mutations that enhance protein-protein binding affinities. **2007**, 371, 1392-404		84
1191	Full-sequence computational design and solution structure of a thermostable protein variant. **2007**, 372, 1-6		57
1190	Electrostatic contributions to the stability of the GCN4 leucine zipper structure. **2007**, 374, 206-19		44
1189	Bioengineering novel in vitro metabolic pathways using synthetic biology. **2007**, 10, 246-53		44
1188	A minimal TrpRS catalytic domain supports sense/antisense ancestry of class I and II aminoacyl-tRNA synthetases. **2007**, 25, 851-62		67
1187	Designing biological systems. **2007**, 21, 242-54		113
1186	A rational route to probing membrane proteins. **2007**, 8, 214		5
1185	Role of protons in the thermodynamic contribution of a Zn(II)-Cys4 site toward metalloprotein stability. *Biochemistry*, **2007**, 46, 3745-58	3.2	37
1184	Computational Methods for Protein Structure Prediction and Modeling. **2007**,		5
1183	Probing the mechanical stability of proteins using the atomic force microscope. **2007**, 35, 1564-8		27

1182	Biology by design: reduction and synthesis of cellular components and behaviour. **2007**, 4, 607-23		48
1181	Engineering proteins with tailored nanomechanical properties: a single molecule approach. **2007**, 5, 3399-406		20
1180	Structure prediction of protein-solid surface interactions reveals a molecular recognition motif of statherin for hydroxyapatite. **2007**, 129, 13713-22		103
1179	Structural insights into the evolution of a non-biological protein: importance of surface residues in protein fold optimization. **2007**, 2, e467		15
1178	Introduction to Computer-Assisted Drug Design Overview and Perspective for the Future. **2007**, 13-41		
1177	Computational protein design promises to revolutionize protein engineering. **2007**, 42, 31, 33, 35 passim		26
1176	Agent-based protein structure prediction. **2007**, 3, 183-197		8
1175	Future Trends. 1651-1686		
1174	Rescue of degradation-prone mutants of the FK506-rapamycin binding (FRB) protein with chemical ligands. **2007**, 8, 1162-9		29
1173	Hybrid peptides: expanding the beta turn in peptide hairpins by the insertion of beta-, gamma-, and delta-residues. **2007**, 13, 5917-26		52
1172	Maintaining solvent accessible surface area under rotamer substitution for protein design. **2007**, 28, 1336-41		10
1171	An object-oriented library for computational protein design. **2007**, 28, 2378-88		32
1170	Understanding the folding and stability of a zinc finger-based full sequence design protein with replica exchange molecular dynamics simulations. *Proteins: Structure, Function and Bioinformatics*, **2007**, 67, 338-49	4.2	20
1169	Atomic contacts in protein structures. A detailed analysis of atomic radii, packing, and overlaps. *Proteins: Structure, Function and Bioinformatics*, **2007**, 68, 595-601	4.2	26
1168	Computing van der Waals energies in the context of the rotamer approximation. *Proteins: Structure, Function and Bioinformatics*, **2007**, 68, 863-78	4.2	20
1167	A tetrapeptide fragment-based design method results in highly stable artificial proteins. *Proteins: Structure, Function and Bioinformatics*, **2007**, 68, 839-49	4.2	14
1166	Critical assessment of methods of protein structure prediction-Round VII. *Proteins: Structure, Function and Bioinformatics*, **2007**, 69 Suppl 8, 3-9	4.2	189
1165	Using quantum mechanics to improve estimates of amino acid side chain rotamer energies. *Proteins: Structure, Function and Bioinformatics*, **2008**, 71, 1637-46	4.2	23

1164	Computational design of antibody-affinity improvement beyond in vivo maturation. **2007**, 25, 1171-6		253
1163	High-resolution structure prediction and the crystallographic phase problem. *Nature*, **2007**, 450, 259-64	50.4	262
1162	FliK regulates flagellar hook length as an internal ruler. **2007**, 64, 1404-15		78
1161	Potential energy functions for protein design. *Current Opinion in Structural Biology*, **2007**, 17, 199-204	8.1	118
1160	The protein folding problem: when will it be solved?. *Current Opinion in Structural Biology*, **2007**, 17, 342-8	8.1	182
1159	Miniaturizing chemistry and biology in microdroplets. **2007**, 1773-88		155
1158	Protein fabrication automation. *Protein Science*, **2007**, 16, 379-90	6.3	52
1157	Structure of a designed, right-handed coiled-coil tetramer containing all biological amino acids. *Protein Science*, **2007**, 16, 2224-32	6.3	18
1156	Protein engineering: opportunities and challenges. **2007**, 75, 1225-32		48
1155	Chimeric Protein Engineering. **2007**, 13, 151-160		7
1154	Computational design of digital and memory biological devices. **2007**, 1, 183-95		19
1153	Using the Rosetta algorithm and selected inter-residue distances to predict protein structure. **2008** , 108, 2793-2802		2
1152	Computational design and experimental study of tighter binding peptides to an inactivated mutant of HIV-1 protease. *Proteins: Structure, Function and Bioinformatics*, **2008**, 70, 678-94	4.2	38
1151	Protein model quality assessment prediction by combining fragment comparisons and a consensus C(alpha) contact potential. *Proteins: Structure, Function and Bioinformatics*, **2008**, 71, 1211-8	4.2	30
1150	Relationship between energy distribution and fold stability: Insights from molecular dynamics simulations of native and mutant proteins. *Proteins: Structure, Function and Bioinformatics*, **2008**, 72, 660-72	4.2	45
1149	Refining homology models by combining replica-exchange molecular dynamics and statistical potentials. *Proteins: Structure, Function and Bioinformatics*, **2008**, 72, 1171-88	4.2	65
1148	The NMR solution structure of the artificial protein M7 matches the computationally designed model. *Proteins: Structure, Function and Bioinformatics*, **2008**, 72, 1104-7	4.2	7
1147	Predicting helix orientation for coiled-coil dimers. *Proteins: Structure, Function and Bioinformatics*, **2008**, 72, 1048-65	4.2	34

1146	Searching combinatorial libraries for native proteins with novel folds. **2008**, 9, 1361-3		4
1145	Computational protein design: software implementation, parameter optimization, and performance of a simple model. **2008**, 29, 1092-102		26
1144	An improved pairwise decomposable finite-difference Poisson-Boltzmann method for computational protein design. **2008**, 29, 1153-62		26
1143	Reference energy extremal optimization: a stochastic search algorithm applied to computational protein design. **2008**, 29, 1762-71		8
1142	Back to the future: ribonuclease A. **2008**, 90, 259-77		74
1141	An effective strategy for the design of proteins with enhanced mechanical stability. **2008**, 47, 6900-3		24
1140	Artificial enzymes made to order: combination of computational design and directed evolution. **2008**, 47, 7802-3		24
1139	Mechanical Engineering of Elastomeric Proteins: Toward Designing New Protein Building Blocks for Biomaterials. **2008**, 18, 2643-2657		37
1138	An Effective Strategy for the Design of Proteins with Enhanced Mechanical Stability. **2008**, 120, 7006-7009		
1137	Künstliche Enzyme maßgeschneidert: Kombination von Computerdesign und gerichteter Evolution. **2008**, 120, 7918-7920		1
1136	OPUS-Rota: a fast and accurate method for side-chain modeling. *Protein Science*, **2008**, 17, 1576-85	6.3	47
1135	Structural characterization of partially folded intermediates of apomyoglobin H64F. *Protein Science* , **2008**, 17, 313-21	6.3	15
1134	Macromolecular modeling with rosetta. **2008**, 77, 363-82		693
1133	Protein design by directed evolution. **2008**, 37, 153-73		309
1132	Chemical gene synthesis: strategies, softwares, error corrections, and applications. **2008**, 32, 522-40		52
1131	Kemp elimination catalysts by computational enzyme design. *Nature*, **2008**, 453, 190-5	50.4	977
1130	Computational biochemistry: old enzymes, new tricks. *Nature*, **2008**, 453, 164-6	50.4	11
1129	Do-it-yourself enzymes. **2008**, 4, 273-5		19

1128	Breaking the barriers of translation. **2008**, 4, 275-6		2
1127	Computational design of four-helix bundle proteins that bind nonbiological cofactors. **2008**, 24, 74-9		7
1126	Exploration of twin-arginine translocation for expression and purification of correctly folded proteins in Escherichia coli. **2008**, 1, 403-15		25
1125	Synthetic biology through biomolecular design and engineering. *Current Opinion in Structural Biology*, **2008**, 18, 491-8	8.1	76
1124	Structure prediction of domain insertion proteins from structures of individual domains. **2008**, 16, 513-27		17
1123	Ab initio folding of proteins with all-atom discrete molecular dynamics. **2008**, 16, 1010-8		241
1122	Computer-based redesign of a beta sandwich protein suggests that extensive negative design is not required for de novo beta sheet design. **2008**, 16, 1799-805		34
1121	Targeting metastable coiled-coil domains by computational design. **2008**, 130, 12038-44		20
1120	Toward full-sequence de novo protein design with flexible templates for human beta-defensin-2. **2008**, 94, 584-99		42
1119	Stabilization provided by neighboring strands is critical for the mechanical stability of proteins. **2008**, 95, 3935-42		32
1118	Oligo(N-aryl glycines): a new twist on structured peptoids. **2008**, 130, 16622-32		165
1117	Biomimicry of surfactant protein C. **2008**, 41, 1409-17		30
1116	Computational design of protein therapeutics. **2008**, 5, e43-8		23
1115	Quantum mechanical design of enzyme active sites. **2008**, 73, 889-99		47
1114	Protein sequence and structure alignments within one framework. **2008**, 3, 4		9
1113	Directing noble metal ion chemistry within a designed ferritin protein. *Biochemistry*, **2008**, 47, 12729-39	3.2	79
1112	Computational De Novo Peptide and Protein Design: Rigid Templates versus Flexible Templates. **2008**, 47, 993-1001		25
1111	OPUS-PSP: an orientation-dependent statistical all-atom potential derived from side-chain packing. **2008**, 376, 288-301		141

1110	Design of protein-ligand binding based on the molecular-mechanics energy model. **2008**, 380, 415-24		38
1109	A simple model of backbone flexibility improves modeling of side-chain conformational variability. **2008**, 380, 757-74		60
1108	Backrub-like backbone simulation recapitulates natural protein conformational variability and improves mutant side-chain prediction. **2008**, 380, 742-56		232
1107	Peptide and protein building blocks for synthetic biology: from programming biomolecules to self-organized biomolecular systems. **2008**, 3, 38-50		195
1106	The protein folding problem. **2008**, 37, 289-316		722
1105	Protein design with L- and D-alpha-amino acid structures as the alphabet. **2008**, 41, 1301-8		64
1104	Characterizing the first steps of amyloid formation for the ccbeta peptide. **2008**, 112, 9998-10004		11
1103	Caching of a chameleon segment facilitates folding of a protein with end-to-end beta-sheet. **2008**, 112, 15134-9		11
1102	Selecting folded proteins from a library of secondary structural elements. **2008**, 130, 176-85		15
1101	De novo computational design of retro-aldol enzymes. *Science*, **2008**, 319, 1387-91	33.3	892
1100	MedusaScore: an accurate force field-based scoring function for virtual drug screening. *Journal of Chemical Information and Modeling*, **2008**, 48, 1656-62	6.1	131
1099	Crystal structure of an extensively simplified variant of bovine pancreatic trypsin inhibitor in which over one-third of the residues are alanines. **2008**, 105, 15334-9		26
1098	NMR-detected conformational exchange observed in a computationally designed variant of protein Gbeta1. **2008**, 21, 577-87		5
1097	Simulation of Top7-CFr: a transient helix extension guides folding. **2008**, 105, 8004-7		42
1096	Algorithm for backrub motions in protein design. **2008**, 24, i196-204		63
1095	Reconstruction of protein backbones from the BriX collection of canonical protein fragments. *PLoS Computational Biology*, **2008**, 4, e1000083	5	39
1094	Intramolecular cohesion of coils mediated by phenylalanine--glycine motifs in the natively unfolded domain of a nucleoporin. *PLoS Computational Biology*, **2008**, 4, e1000145	5	43
1093	Two-dimensional surface display of functional groups on a beta-helical antifreeze protein scaffold. **2008**, 21, 107-14		8

1092 A computational framework to empower probabilistic protein design. **2008**, 24, i214-22 18

1091 PVS: a web server for protein sequence variability analysis tuned to facilitate conserved epitope discovery. **2008**, 36, W35-41 125

1090 On the role of a conserved, potentially helix-breaking residue in the tRNA-binding alpha-helix of archaeal CCA-adding enzymes. **2008**, 14, 1284-9 2

1089 An antibody loop replacement design feasibility study and a loop-swapped dimer structure. **2009**, 22, 93-101 8

1088 THE DIFFERENTIAL GEOMETRY OF PROTEINS AND ITS APPLICATIONS TO STRUCTURE DETERMINATION. **2008**, 03, 77-101 9

1087 Minimal models for proteins and RNA from folding to function. **2008**, 84, 203-50 37

1086 Conformation of a coarse-grained protein chain (an aspartic acid protease) model in effective solvent by a bond-fluctuating Monte Carlo simulation. **2008**, 77, 031902 6

1085 Evolution of Protein Folds. **2008**, 131-151 5

1084 Computational Protein Design. **2008**, 401-423

1083 Proteindesign und -engineering. **2008**, 56, 298-301

1082 Protein design at room temperature: the role of side□hain conformational entropy. **2008**,

1081 . **2009**, 14

1080 . **2009**, 7

1079 Bibliography. 374-439

1078 References in Figure Legends. 440-442

1077 . **2009**, 1

1076 A man-made ATP-binding protein evolved independent of nature causes abnormal growth in bacterial cells. **2009**, 4, e7385 5

1075 Probabilistic models and machine learning in structural bioinformatics. **2009**, 18, 505-26 13

1074	Engineering an ultra-stable affinity reagent based on Top7. **2009**, 22, 325-32		17
1073	Computational structure-based redesign of enzyme activity. **2009**, 106, 3764-9		167
1072	Rationally designed integrin beta3 mutants stabilized in the high affinity conformation. **2009**, 284, 3917-24		32
1071	Computational design of ligand binding is not a solved problem. **2009**, 106, 18491-6		78
1070	Simultaneous prediction of protein folding and docking at high resolution. **2009**, 106, 18978-83		127
1069	Alteration of enzyme specificity by computational loop remodeling and design. **2009**, 106, 9215-20		104
1068	Thermostable variants of cocaine esterase for long-time protection against cocaine toxicity. **2009**, 75, 318-23		72
1067	Incorporating receptor flexibility in the molecular design of protein interfaces. **2009**, 22, 575-86		12
1066	Fact and Fantasy in Nanotech Imagery. **2009**, 42, 52-57		7
1065	Electrostatic contributions to the stabilities of native proteins and amyloid complexes. **2009**, 466, 233-58		10
1064	A correspondence between solution-state dynamics of an individual protein and the sequence and conformational diversity of its family. *PLoS Computational Biology*, **2009**, 5, e1000393	5	60
1063	Residue energy and mobility in sequence to global structure and dynamics of a HIV-1 protease (1DIFA) by a coarse-grained Monte Carlo simulation. *Journal of Chemical Physics*, **2009**, 130, 044906	3.9	10
1062	Splicing of designer exons reveals unexpected complexity in pre-mRNA splicing. **2009**, 15, 367-76		31
1061	Evolution of protein modularity. *Current Opinion in Structural Biology*, **2009**, 19, 335-40	8.1	35
1060	TransCent: computational enzyme design by transferring active sites and considering constraints relevant for catalysis. **2009**, 10, 54		6
1059	Vps-C complexes: gatekeepers of endolysosomal traffic. **2009**, 21, 543-51		182
1058	Synthetic Life: Ethobricks for a New Biology. 273-285		
1057	De Novo Design of a Motif. **2009**, 121, 3351-3353		2

1056	Rotamer optimization for protein design through MAP estimation and problem-size reduction. **2009**, 30, 1923-45		20
1055	SHARPEN-systematic hierarchical algorithms for rotamers and proteins on an extended network. **2009**, 30, 999-1005		13
1054	Cluster expansion models for flexible-backbone protein energetics. **2009**, 30, 2402-13		15
1053	An efficient algorithm for multistate protein design based on FASTER. **2010**, 31, 904-16		38
1052	Computational design of protein-ligand binding: modifying the specificity of asparaginyl-tRNA synthetase. **2010**, 31, 1273-86		10
1051	De novo design of a beta alpha beta motif. **2009**, 48, 3301-3		35
1050	Backbone flexibility in computational protein design. **2009**, 20, 420-8		84
1049	Computational study of the heterodimerization between mu and delta receptors. **2009**, 23, 321-32		29
1048	Mechanical signaling on the single protein level studied using steered molecular dynamics. **2009**, 55, 141-52		26
1047	Emergent strategies for inverse molecular design. **2009**, 52, 1769-1776		9
1046	Structural determinants of protein folding. **2009**, 66, 2341-61		17
1045	Computational protein design with side-chain conformational entropy. *Proteins: Structure, Function and Bioinformatics*, **2009**, 74, 176-91	4.2	20
1044	Structural determinants of species-selective substrate recognition in human and Drosophila serotonin transporters revealed through computational docking studies. *Proteins: Structure, Function and Bioinformatics*, **2009**, 74, 630-42	4.2	50
1043	Building alternate protein structures using the elastic network model. *Proteins: Structure, Function and Bioinformatics*, **2009**, 74, 682-700	4.2	20
1042	Fragment-based local statistical potentials derived by combining an alphabet of protein local structures with secondary structures and solvent accessibilities. *Proteins: Structure, Function and Bioinformatics*, **2009**, 74, 820-36	4.2	16
1041	Simulated tempering yields insight into the low-resolution Rosetta scoring functions. *Proteins: Structure, Function and Bioinformatics*, **2009**, 74, 777-88	4.2	22
1040	Evaluation of an inverse molecular design algorithm in a model binding site. *Proteins: Structure, Function and Bioinformatics*, **2009**, 75, 168-86	4.2	8
1039	Improving NMR protein structure quality by Rosetta refinement: a molecular replacement study. *Proteins: Structure, Function and Bioinformatics*, **2009**, 75, 147-67	4.2	54

1038	Accurate prediction for atomic-level protein design and its application in diversifying the near-optimal sequence space. *Proteins: Structure, Function and Bioinformatics*, **2009**, 75, 682-705	4.2	15
1037	Multi-constraint computational design suggests that native sequences of germline antibody H3 loops are nearly optimal for conformational flexibility. *Proteins: Structure, Function and Bioinformatics*, **2009**, 75, 846-58	4.2	45
1036	All-atom chain-building by optimizing MODELLER energy function using conformational space annealing. *Proteins: Structure, Function and Bioinformatics*, **2009**, 75, 1010-23	4.2	37
1035	X-ray vs. NMR structures as templates for computational protein design. *Proteins: Structure, Function and Bioinformatics*, **2009**, 77, 97-110	4.2	33
1034	Computational protein design as a tool for fold recognition. *Proteins: Structure, Function and Bioinformatics*, **2009**, 77, 139-58	4.2	24
1033	Improved prediction of protein side-chain conformations with SCWRL4. *Proteins: Structure, Function and Bioinformatics*, **2009**, 77, 778-95	4.2	902
1032	Structural understanding of stabilization patterns in engineered bispecific Ig-like antibody molecules. *Proteins: Structure, Function and Bioinformatics*, **2009**, 77, 832-41	4.2	32
1031	Relating protein conformational changes to packing efficiency and disorder. *Protein Science*, **2009**, 18, 1230-40	6.3	8
1030	Motif-directed flexible backbone design of functional interactions. *Protein Science*, **2009**, 18, 1293-305	6.3	24
1029	Computational design of Candida boidinii xylose reductase for altered cofactor specificity. *Protein Science*, **2009**, 18, 2125-38	6.3	76
1028	Selection and structural analysis of de novo proteins from an alpha3beta3 genetic library. *Protein Science*, **2009**, 18, 384-98	6.3	13
1027	Prospects for de novo phasing with de novo protein models. **2009**, 65, 169-75		32
1026	Inverse tuning of metal binding affinity and protein stability by altering charged coordination residues in designed calcium binding proteins. **2009**, 2, 11		8
1025	An effective all-atom potential for proteins. **2009**, 2, 2		58
1024	Rational design of a structural and functional nitric oxide reductase. *Nature*, **2009**, 462, 1079-82	50.4	200
1023	Computer-aided design of functional protein interactions. **2009**, 5, 797-807		131
1022	Solubility-dependent structural formation of a 25-residue, natively unfolded protein, induced by addition of a seven-residue peptide fragment. **2009**, 276, 2336-47		
1021	Automatic protein structure prediction system enabling rapid and accurate model building for enzyme screening. **2009**, 45, 218-225		4

1020	Order Up! The Custom Enzyme Shop Is Open for Business. **2009**, 16, 795-796		
1019	Computer simulation of proteins: thermodynamics and structure prediction. **2009**, 51, 33-40		3
1018	Assessing computational methods for predicting protein stability upon mutation: good on average but not in the details. **2009**, 22, 553-60		267
1017	Factors that affect the degree of twist in beta-sheet structures: a molecular dynamics simulation study of a cross-beta filament of the GNNQQNY peptide. **2009**, 113, 1728-37		54
1016	Synthesis at the interface of chemistry and biology. **2009**, 131, 12497-515		82
1015	Protein design based on parallel dimensional reduction. *Journal of Chemical Information and Modeling*, **2009**, 49, 1261-71	6.1	5
1014	The interstrand amino acid pairs play a significant role in determining the parallel or antiparallel orientation of beta-strands. **2009**, 386, 537-43		12
1013	RosettaLigand docking with full ligand and receptor flexibility. **2009**, 385, 381-92		309
1012	Sampling bottlenecks in de novo protein structure prediction. **2009**, 393, 249-60		80
1011	Structural basis for exquisite specificity of affinity clamps, synthetic binding proteins generated through directed domain-interface evolution. **2009**, 392, 1221-31		40
1010	Native topology of the designed protein Top7 is not conducive to cooperative folding. **2009**, 96, L25-7		27
1009	Solution- and adsorbed-state structural ensembles predicted for the statherin-hydroxyapatite system. **2009**, 96, 3082-91		49
1008	De Novo Design of Proteins. **2009**, 207-248		1
1007	Genome and proteome annotation: organization, interpretation and integration. **2009**, 6, 129-47		36
1006	The influence of protein dynamics on the success of computational enzyme design. **2009**, 131, 14111-5		52
1005	Computational Approaches in Peptide and Protein Design: An Overview. **2009**, 5-48		2
1004	Challenges in the computational design of proteins. **2009**, 6 Suppl 4, S477-91		41
1003	Protein design in biological networks: from manipulating the input to modifying the output. **2009**, 22, 537-42		22

1002	The Tumbleweed: towards a synthetic proteinmotor. **2009**, 3, 204-12		32
1001	Adsorption of peptides (A3, Flg, Pd2, Pd4) on gold and palladium surfaces by a coarse-grained Monte Carlo simulation. **2009**, 11, 1989-2001		82
1000	Protein design by sampling an undirected graphical model of residue constraints. **2009**, 6, 506-16		9
999	Rational design of peptide-based building blocks for nanoscience and synthetic biology. **2009**, 143, 305-17; discussion 359-72		30
998	Knowledge-based Protein Design. **2009**,		
997	Search Algorithms. **2009**,		
996	Modulating Protein Structure. **2009**,		
995	Recent progress in protein drug design and discovery with a focus on novel approaches to the development of anti-cocaine medications. **2009**, 1, 515-28		25
994	Future Challenges Of Computational Protein Design. **2009**,		2
993	Computational methods for de novo protein design and its applications to the human immunodeficiency virus 1, purine nucleoside phosphorylase, ubiquitin specific protease 7, and histone demethylases. **2010**, 11, 264-78		17
992	Proteins: sequence to structure and function--current status. **2010**, 11, 498-514		47
991	Conformational Search for the Protein Native State. **2010**, 431-452		2
990	Modeling Mutations in Proteins Using Medusa and Discrete Molecule Dynamics. **2010**, 453-476		0
989	Zinc-finger hydrolase: Computational selection of a linker and a sequence towards metal activation with a synthetic protein. **2010**, 18, 8270-6		11
988	Minimal formulation of joint motion for biomechanisms. **2010**, 62, 291-303		46
987	Designing ensembles in conformational and sequence space to characterize and engineer proteins. *Current Opinion in Structural Biology*, **2010**, 20, 377-84	8.1	22
986	Computational design of epitope-scaffolds allows induction of antibodies specific for a poorly immunogenic HIV vaccine epitope. **2010**, 18, 1116-26		168
985	Protein structure modelling and evaluation based on a 4-distance description of side-chain interactions. **2010**, 11, 374		23

984	De novo design of a non-natural fold for an iron-sulfur protein: alpha-helical coiled-coil with a four-iron four-sulfur cluster binding site in its central core. **2010**, 1797, 406-13		55
983	Generating artificial homologous proteins according to the representative family character in molecular mechanics properties--an attempt in validating an underlying rule of protein evolution. **2010**, 584, 1059-65		3
982	Fast determination of the optimal rotational matrix for macromolecular superpositions. **2010**, 31, 1561-3		78
981	A gradient-directed Monte Carlo approach for protein design. **2010**, 31, 2164-8		12
980	Identifying and reducing error in cluster-expansion approximations of protein energies. **2010**, 31, 2900-14		11
979	Protein Recognition. **2010**, 505-532		
978	Potential hydrophobic interaction between two cysteines in interior hydrophobic region improves thermostability of a family 11 xylanase from Neocallimastix patriciarum. **2010**, 105, 861-70		42
977	Prediction of the parallel/antiparallel orientation of beta-strands using amino acid pairing preferences and support vector machines. **2010**, 263, 360-8		24
976	Molecular basis of the structural stability of a Top7-based scaffold at extreme pH and temperature conditions. **2010**, 28, 755-65		8
975	Design strategies for the creation of artificial metalloenzymes. **2010**, 14, 184-99		115
974	Conformational diversity and computational enzyme design. **2010**, 14, 676-82		29
973	Selecting sequences that fold into a defined 3D structure: A new approach for protein design based on molecular dynamics and energetics. **2010**, 146, 76-84		14
972	Development of thermostable lipase B from Candida antarctica (CalB) through in silico design employing B-factor and RosettaDesign. **2010**, 47, 1-5		43
971	Stacking and energetic contribution of aromatic islands at the binding interface of antibody proteins. **2010**, 6 Suppl 1, S1		11
970	Prediction of structures of zinc-binding proteins through explicit modeling of metal coordination geometry. *Protein Science*, **2010**, 19, 494-506	6.3	36
969	Cysteine-free Rop: a four-helix bundle core mutant has wild-type stability and structure but dramatically different unfolding kinetics. *Protein Science*, **2010**, 19, 670-9	6.3	11
968	An exciting but challenging road ahead for computational enzyme design. *Protein Science*, **2010**, 19, 1817-9	6.3	128
967	Design of multispecific protein sequences using probabilistic graphical modeling. *Proteins: Structure, Function and Bioinformatics*, **2010**, 78, 530-47	4.2	15

966	Computational exploration of the network of sequence flow between protein structures. *Proteins: Structure, Function and Bioinformatics*, **2010**, 78, 985-1003	4.2	19
965	Computational design of second-site suppressor mutations at protein-protein interfaces. *Proteins: Structure, Function and Bioinformatics*, **2010**, 78, 1055-65	4.2	30
964	De novo backbone scaffolds for protein design. *Proteins: Structure, Function and Bioinformatics*, **2010**, 78, 1311-25	4.2	31
963	Improving computational protein design by using structure-derived sequence profile. *Proteins: Structure, Function and Bioinformatics*, **2010**, 78, 2338-48	4.2	20
962	Protein-protein interactions and selection: generation of molecule-binding proteins on the basis of tertiary structural information. **2010**, 277, 2006-14		8
961	Designing artificial enzymes by intuition and computation. **2010**, 2, 15-24		193
960	A decade of chemical biology. **2010**, 6, 847-54		20
959	A score of the ability of a three-dimensional protein model to retrieve its own sequence as a quantitative measure of its quality and appropriateness. **2010**, 5, e12483		9
958	SPRINT: side-chain prediction inference toolbox for multistate protein design. **2010**, 26, 2466-7		11
957	Characterizing the regularity of tetrahedral packing motifs in protein tertiary structure. **2010**, 26, 3059-66		10
956	Design of an HA2-based Escherichia coli expressed influenza immunogen that protects mice from pathogenic challenge. **2010**, 107, 13701-6		177
955	Modulation of integrin activation by an entropic spring in the {beta}-knee. **2010**, 285, 32954-32966		26
954	Specificity in computational protein design. **2010**, 285, 31095-9		13
953	Experimental library screening demonstrates the successful application of computational protein design to large structural ensembles. **2010**, 107, 19838-43		53
952	Design and directed evolution of a dideoxy purine nucleoside phosphorylase. **2010**, 23, 607-16		19
951	OptCDR: a general computational method for the design of antibody complementarity determining regions for targeted epitope binding. **2010**, 23, 849-58		50
950	Predicting resistance mutations using protein design algorithms. **2010**, 107, 13707-12		96
949	Competition between native topology and nonnative interactions in simple and complex folding kinetics of natural and designed proteins. **2010**, 107, 2920-5		80

948	Design of a non-glycosylated outer domain-derived HIV-1 gp120 immunogen that binds to CD4 and induces neutralizing antibodies. **2010**, 285, 27100-27110		32
947	Minimalist design of water-soluble cross-beta architecture. **2010**, 107, 3469-74		20
946	PyRosetta: a script-based interface for implementing molecular modeling algorithms using Rosetta. **2010**, 26, 689-91		333
945	Particle Swarm Optimization for multimodal combinatorial problems and its application to protein design. **2010**,		1
944	The protein-protein interface evolution acts in a similar way to antibody affinity maturation. **2010**, 285, 3865-3871		17
943	Combined use of experimental and computational screens to characterize protein stability. **2010**, 23, 799-807		5
942	RosettaBackrub--a web server for flexible backbone protein structure modeling and design. **2010**, 38, W569-75		94
941	The challenge of designing scientific discovery games. **2010**,		67
940	Globular structure of a human immunodeficiency virus-1 protease (1DIFA dimer) in an effective solvent medium by a Monte Carlo simulation. *Journal of Chemical Physics*, **2010**, 132, 125101	3.9	15
939	How do amino acid mismatches affect the outcome of hematopoietic cell transplants?. **2010**,		1
938	Molecular recognition and drug-lead identification: what can molecular simulations tell us?. **2010**, 17, 25-41		31
937	Staphylococcal surface display in combinatorial protein engineering and epitope mapping of antibodies. **2010**, 4, 171-82		22
936	De novo design of peptide-calcite biomineralization systems. **2010**, 132, 12252-62		43
935	Mechanisms of protein evolution and their application to protein engineering. **2007**, 75, 193-239, xii-xiii		22
934	Novel enzymes through design and evolution. **2007**, 75, 241-94, xiii		14
933	Folding simulations of a de novo designed protein with a betaalphabeta fold. **2010**, 98, 321-9		13
932	Computational design of chimeric protein libraries for directed evolution. *Methods in Molecular Biology*, **2010**, 673, 175-88	1.4	3
931	Development of a rotamer library for use in beta-peptide foldamer computational design. **2010**, 132, 7312-20		30

930	Practically useful: what the Rosetta protein modeling suite can do for you. *Biochemistry*, **2010**, 49, 2987-98	3.2	298
929	Computational design and elaboration of a de novo heterotetrameric alpha-helical protein that selectively binds an emissive abiological (porphinato)zinc chromophore. **2010**, 132, 3997-4005		50
928	Controllable synthetic molecular channels: biomimetic ammonia switch. **2010**, 114, 1174-9		9
927	Three-dimensional structures reveal multiple ADP/ATP binding modes for a synthetic class of artificial proteins. *Biochemistry*, **2010**, 49, 8689-99		2
926	Computational predictions of the mutant behavior of AraC. **2010**, 398, 462-70		5
925	Computational design of a PAK1 binding protein. **2010**, 400, 257-70		61
924	Structure-based prediction of the peptide sequence space recognized by natural and synthetic PDZ domains. **2010**, 402, 460-74		84
923	Computational design of a chain-specific tetracycline repressor heterodimer. **2010**, 403, 371-85		6
922	Engineering signal transduction pathways. **2010**, 140, 33-47		94
921	Computational protein design, from single domain soluble proteins to membrane proteins. **2010**, 39, 2071-82		21
920	Computational enzymology. **2010**, 46, 2354-72		90
919	Zipper-Like Unfolding of β-Sheets Accessed by Pioneer Water Molecules: Atomic Resolution of Forced Unfold Reveals Different Mechanisms for Parallel and Antiparallel Motifs. **2010**, 1, 1341-1345		2
918	Directed Evolution of Enzymes. **2010**, 723-749		2
917	The EVB as a quantitative tool for formulating simulations and analyzing biological and chemical reactions. **2010**, 145, 71-106		77
916	Bioinspired organic chemistry. **2010**, 106, 447		3
915	A de novo peptide hexamer with a mutable channel. **2011**, 7, 935-41		144
914	Protein Structure Design and Engineering. **2011**,		
913	Computational design of the sequence and structure of a protein-binding peptide. **2011**, 133, 4190-2		41

912	Computational design of a collagen A:B:C-type heterotrimer. **2011**, 133, 15260-3		44
911	Design and characterization of stabilized derivatives of human CD4D12 and CD4D1. *Biochemistry*, **2011**, 50, 7891-900	3.2	11
910	A new way to see RNA. **2011**, 44, 433-66		16
909	Sampling Protein Energy Landscapes The Quest for Efficient Algorithms. **2011**, 209-230		2
908	Computational Design of New Protein Catalysts. **2011**, 241-266		1
907	Algorithm discovery by protein folding game players. **2011**, 108, 18949-53		289
906	Computational design and biophysical characterization of aggregation-resistant point mutations for D crystallin illustrate a balance of conformational stability and intrinsic aggregation propensity. *Biochemistry*, **2011**, 50, 628-39	3.2	41
905	Protein Nanomechanics. **2011**, 227-261		2
904	Computational Protein Design. **2011**, 325-342		
903	Advances in TNF Family Research. **2011**,		3
902	Bayesian models and algorithms for protein sheet prediction. **2011**, 8, 395-409		21
901	Computational design approaches and tools for synthetic biology. **2011**, 3, 97-108		65
900	Combined application of cheminformatics- and physical force field-based scoring functions improves binding affinity prediction for CSAR data sets. *Journal of Chemical Information and Modeling*, **2011**, 51, 2027-35	6.1	23
899	Biomolecularmodeling and simulation: a field coming of age. **2011**, 44, 191-228		119
898	Structure-based design of non-natural amino-acid inhibitors of amyloid fibril formation. *Nature*, **2011**, 475, 96-100	50.4	341
897	Towards artificial metallonucleases for gene therapy: recent advances and new perspectives. **2011**, 3, 1935-66		18
896	Cooperativity, local-nonlocal coupling, and nonnative interactions: principles of protein folding from coarse-grained models. **2011**, 62, 301-26		163
895	A de novo protein binding pair by computational design and directed evolution. **2011**, 42, 250-60		141

894	Statistical mechanics analysis of sparse data. **2011**, 173, 541-8	14
893	Computational protein design using flexible backbone remodeling and resurfacing: case studies in structure-based antigen design. **2011**, 405, 284-97	51
892	Alternate states of proteins revealed by detailed energy landscape mapping. **2011**, 405, 607-18	207
891	Computational protein design and large-scale assessment by I-TASSER structure assembly simulations. **2011**, 407, 764-76	32
890	Characterizing the existing and potential structural space of proteins by large-scale multiple loop permutations. **2011**, 408, 585-95	21
889	Triosephosphate isomerase by consensus design: dramatic differences in physical properties and activity of related variants. **2011**, 413, 195-208	50
888	Redesign of the PAK1 autoinhibitory domain for enhanced stability and affinity in biosensor applications. **2011**, 413, 513-22	8
887	Hotspot-centric de novo design of protein binders. **2011**, 413, 1047-62	32
886	Approaches for probing the sequence space of substrates recognized by molecular chaperones. **2011**, 53, 318-24	
885	Protein folds and protein folding. **2011**, 24, 11-9	41
884	Computational design of a thermostable mutant of cocaine esterase via molecular dynamics simulations. **2011**, 9, 4138-43	20
883	Four small puzzles that Rosetta doesn't solve. **2011**, 6, e20044	54
882	RosettaScripts: a scripting language interface to the Rosetta macromolecular modeling suite. **2011**, 6, e20161	311
881	Anchored design of protein-protein interfaces. **2011**, 6, e20872	49
880	Microarray generation of thousand-member oligonucleotide libraries. **2011**, 6, e24906	11
879	Can enzyme engineering benefit from the modulation of protein motions? Lessons learned from NMR relaxation dispersion experiments. **2011**, 18, 336-43	13
878	Rational and Combinatorial Methods to Create Designer Protein Interfaces. **2011**, 161-179	
877	Towards structure-based protein drug design. **2011**, 39, 1382-6, suppl 1 p following 1386	22

876	Protein folding: To knot or not to knot?. **2011**, 10, 84-6		15
875	Material witness: Carbon tailoring. **2011**, 10, 86		2
874	Computational design of protein-ligand interfaces: potential in therapeutic development. **2011**, 29, 159-66		14
873	Recent advances in computational protein design. *Current Opinion in Structural Biology*, **2011**, 21, 467-728.1		71
872	Theoretical and computational protein design. **2011**, 62, 129-49		119
871	Computational design of virus-like protein assemblies on carbon nanotube surfaces. *Science*, **2011**, 332, 1071-6	33.3	178
870	Chapter 14:Redox Active Protein Maquettes: Multi-functional Green Enzymes**2011**, 408-425		
869	Computational design of proteins targeting the conserved stem region of influenza hemagglutinin. *Science*, **2011**, 332, 816-21	33.3	441
868	The empirical valence bond model: theory and applications. **2011**, 1, 30-45		130
867	Molecular size scaling in families of protein native folds. **2011**, 49, 1493-1506		7
866	hHSS1: a novel secreted factor and suppressor of glioma growth located at chromosome 19q13.33. **2011**, 102, 197-211		13
865	Mapping the distribution of packing topologies within protein interiors shows predominant preference for specific packing motifs. **2011**, 12, 195		15
864	Conformational analysis and design of cross-strand disulfides in antiparallel sheets. *Proteins: Structure, Function and Bioinformatics*, **2011**, 79, 244-60	4.2	24
863	Automated minimization of steric clashes in protein structures. *Proteins: Structure, Function and Bioinformatics*, **2011**, 79, 261-70	4.2	258
862	Accounting for conformational entropy in predicting binding free energies of protein-protein interactions. *Proteins: Structure, Function and Bioinformatics*, **2011**, 79, 444-62	4.2	41
861	Computational protein design with a generalized Born solvent model: application to Asparaginyl-tRNA synthetase. *Proteins: Structure, Function and Bioinformatics*, **2011**, 79, 3448-68	4.2	19
860	De novo protein structure prediction by dynamic fragment assembly and conformational space annealing. *Proteins: Structure, Function and Bioinformatics*, **2011**, 79, 2403-17	4.2	46
859	Restricted sidechain plasticity in the structures of native proteins and complexes. *Protein Science*, **2011**, 20, 753-7	6.3	37

858	Assessment of flexible backbone protein design methods for sequence library prediction in the therapeutic antibody Herceptin-HER2 interface. *Protein Science*, **2011**, 20, 1082-9	6.3	27
857	High-resolution structure prediction of a circular permutation loop. *Protein Science*, **2011**, 20, 1929-34	6.3	3
856	Optical detection of protein in complex media with plasmonic nanoparticle dimers. **2011**, 7, 1993-7		37
855	Designing New Proteins. **2011**, 473-490		
854	Terminierung des Amyloid-Reißverschlusses durch Design. **2011**, 123, 11489-11491		
853	Terminating the amyloid zipper by design. **2011**, 50, 11293-4		2
852	Peptoids at the 7th Summit: toward macromolecular systems engineering. **2011**, 96, 537-44		4
851	Engineering protein switches: sensors, regulators, and spare parts for biology and biotechnology. **2011**, 12, 353-61		38
850	Optimizing non-natural protein function with directed evolution. **2011**, 15, 201-10		213
849	Novel proteins: from fold to function. **2011**, 15, 421-6		55
848	Thermostabilization of Bacillus circulans xylanase: computational optimization of unstable residues based on thermal fluctuation analysis. **2011**, 151, 56-65		91
847	Computational design of intermolecular stability and specificity in protein self-assembly. **2011**, 487, 575-93		7
846	Systematic placement of structural water molecules for improved scoring of protein-ligand interactions. **2011**, 24, 777-89		36
845	The effect of using a polarizable solvent model upon the folding equilibrium of different peptides. **2011**, 109, 493-506		18
844	The denatured state dictates the topology of two proteins with almost identical sequence but different native structure and function. **2011**, 286, 3863-72		34
843	Production of secretory and extracellular N-linked glycoproteins in Escherichia coli. **2011**, 77, 871-81		93
842	Extensive protein and DNA backbone sampling improves structure-based specificity prediction for C2H2 zinc fingers. **2011**, 39, 4564-76		34
841	Experimental illumination of a fitness landscape. **2011**, 108, 7896-901		212

840	Computational design of a symmetric homodimer using β-strand assembly. **2011**, 108, 20562-7		63
839	Improved sequence-based prediction of strand residues. **2011**, 9, 67-89		4
838	High-precision, in vitro validation of the sequestration mechanism for generating ultrasensitive dose-response curves in regulatory networks. *PLoS Computational Biology*, **2011**, 7, e1002171	5	39
837	Computational design of an endo-1,4-beta-xylanase ligand binding site. **2011**, 24, 503-16		16
836	Catalytic residues and a predicted structure of tetrahydrobiopterin-dependent alkylglycerol mono-oxygenase. **2012**, 443, 279-86		16
835	Structure-based design for high-hanging vaccine fruits. **2012**, 114, 33-50		6
834	Exploring objective functions and cross-terms in the optimization of an energy function for protein design. **2012**,		
833	Astrophysics: Cosmic explosions in the young Universe. *Nature*, **2012**, 491, 205-6	50.4	1
832	Canonical and micro-canonical analysis of folding of trpzip2: an all-atom replica exchange Monte Carlo simulation study. *Journal of Chemical Physics*, **2012**, 137, 045103	3.9	7
831	Calibration of Boltzmann distribution priors in Bayesian data analysis. **2012**, 86, 066705		3
830	The plant proteome folding project: structure and positive selection in plant protein families. **2012**, 4, 360-71		13
829	Chameleonicity and folding of the C-fragment of TOP7. **2012**, 97, 68003		6
828	Design of DNA Origami Machines and Mechanisms. **2012**,		1
827	Computational Biology. **2012**,		1
826	The protein-folding problem, 50 years on. *Science*, **2012**, 338, 1042-6	33.3	940
825	Principles for designing ideal protein structures. *Nature*, **2012**, 491, 222-7	50.4	391
824	Structural biology: A toolbox for protein design. *Nature*, **2012**, 491, 204-5	50.4	6
823	Engineering a thermoregulated intein-modified xylanase into maize for consolidated lignocellulosic biomass processing. **2012**, 30, 1131-6		69

822	Engineering and Application of Genetically Encoded Calcium Indicators. **2012**, 125-147		1
821	Human antibodies that neutralize HIV-1: identification, structures, and B cell ontogenies. **2012**, 37, 412-25		364
820	Rational Design of Enzymes. **2012**, 89-117		22
819	Domain-swapped dimeric structure of a stable and functional de novo four-helix bundle protein, WA20. **2012**, 116, 6789-97		26
818	Improved Statistical Sampling and Accuracy with Accelerated Molecular Dynamics on Rotatable Torsions. **2012**, 8, 4004-12		30
817	Novel protease inhibitors via computational redesign of subtilisin BPN' propeptide. *Biochemistry*, **2012**, 51, 8247-55	3.2	2
816	Computational approaches for rational design of proteins with novel functionalities. **2012**, 2, e201209002		38
815	Dynamics in Sequence Space for RNA Secondary Structure Design. **2012**, 8, 3663-70		17
814	Squaring the circle in peptide assembly: from fibers to discrete nanostructures by de novo design. **2012**, 134, 15457-67		77
813	AWSEM-MD: protein structure prediction using coarse-grained physical potentials and bioinformatically based local structure biasing. **2012**, 116, 8494-503		184
812	Computational design of self-assembling register-specific collagen heterotrimers. *Nature Communications*, **2012**, 3, 1087	17.4	40
811	Design of Escherichia coli-expressed stalk domain immunogens of H1N1 hemagglutinin that protect mice from lethal challenge. **2012**, 86, 13434-44		62
810	The spatial architecture of protein function and adaptation. *Nature*, **2012**, 491, 138-42	50.4	319
809	Structural analyses of covalent enzyme-substrate analog complexes reveal strengths and limitations of de novo enzyme design. **2012**, 415, 615-25		47
808	Inhibition of amyloid formation. **2012**, 421, 441-65		210
807	Structures of the HIN domain:DNA complexes reveal ligand binding and activation mechanisms of the AIM2 inflammasome and IFI16 receptor. **2012**, 36, 561-71		352
806	Relationship between stability and flexibility in the most flexible region of Photinus pyralis luciferase. **2012**, 1824, 350-8		28
805	Role of the biomolecular energy gap in protein design, structure, and evolution. **2012**, 149, 262-73		83

804	Efficient sampling of protein conformational space using fast loop building and batch minimization on highly parallel computers. **2012**, 33, 2483-91		28
803	Multistate approaches in computational protein design. *Protein Science*, **2012**, 21, 1241-52	6.3	51
802	BetaSearch: a new method for querying -residue motifs. **2012**, 5, 391		1
801	The RNA Folding Problems: Different Levels of sRNA Structure Prediction. **2012**, 91-117		5
800	Prescriptive peptide design. **2012**, 190-237		
799	Carbohydrate recognition by the antiviral lectin cyanovirin-N. **2012**, 134, 19639-51		17
798	Computational design by evolving folds and assemblies over the alphabet in L- and D- amino acids. **2012**, 2, 3242		4
797	A basis set of de novo coiled-coil peptide oligomers for rational protein design and synthetic biology. **2012**, 1, 240-50		159
796	Computational design of an gliadin peptidase. **2012**, 134, 20513-20		83
795	Collective dynamics differentiates functional divergence in protein evolution. *PLoS Computational Biology*, **2012**, 8, e1002428	5	23
794	Rapid calculation of protein pKa values using Rosetta. **2012**, 103, 587-595		51
793	Designing proteins from simple motifs: opportunities in Top-Down Symmetric Deconstruction. *Current Opinion in Structural Biology*, **2012**, 22, 442-50	8.1	23
792	Squaring theory with practice in RNA design. *Current Opinion in Structural Biology*, **2012**, 22, 457-66	8.1	25
791	Hemoprotein Models. **2012**, 235-305		
790	Chapter 9:Coarse-grain Protein Models. **2012**, 219-248		1
789	Biomimetic and Bioinspired Self-Assembled Peptide Nanostructures. **2012**,		
788	Bayesian Methods in Structural Bioinformatics. **2012**,		18
787	Genetically Encoded Functional Indicators. **2012**,		2

786	Protein design using continuous rotamers. *PLoS Computational Biology*, **2012**, 8, e1002335	5	75
785	Prediction of mutational tolerance in HIV-1 protease and reverse transcriptase using flexible backbone protein design. *PLoS Computational Biology*, **2012**, 8, e1002639	5	17
784	Incorporation of noncanonical amino acids into Rosetta and use in computational protein-peptide interface design. **2012**, 7, e32637		71
783	Using RosettaLigand for small molecule docking into comparative models. **2012**, 7, e50769		33
782	Random coil to globular thermal response of a protein (H3.1) with three knowledge-based coarse-grained potentials. **2012**, 7, e49352		12
781	Evolution of the Protein Repertoire. **2012**,		
780	The linear interaction energy method for the prediction of protein stability changes upon mutation. *Proteins: Structure, Function and Bioinformatics*, **2012**, 80, 111-25	4.2	25
779	A divide-and-conquer approach to determine the Pareto frontier for optimization of protein engineering experiments. *Proteins: Structure, Function and Bioinformatics*, **2012**, 80, 790-806	4.2	27
778	Computational protein design with explicit consideration of surface hydrophobic patches. *Proteins: Structure, Function and Bioinformatics*, **2012**, 80, 825-38	4.2	48
777	Robust design and optimization of retroaldol enzymes. *Protein Science*, **2012**, 21, 717-26	6.3	125
776	Mimicking the action of folding chaperones by Hamiltonian replica-exchange molecular dynamics simulations: application in the refinement of de novo models. *Proteins: Structure, Function and Bioinformatics*, **2012**, 80, 1744-54	4.2	12
775	An energy-based conformer library for side chain optimization: improved prediction and adjustable sampling. *Proteins: Structure, Function and Bioinformatics*, **2012**, 80, 2218-34	4.2	14
774	Predicting self-assembly: from empirism to determinism. **2012**, 41, 3713-30		158
773	Engineering synthetic recursive pathways to generate non-natural small molecules. **2012**, 8, 518-26		46
772	Protein folding simplicity in complexity. **2012**, 524, 379-391		14
771	A Designed Functional Metalloenzyme that Reduces O2 to H2O with Over One Thousand Turnovers. **2012**, 124, 5687-5690		14
770	A designed functional metalloenzyme that reduces O2 to H2O with over one thousand turnovers. **2012**, 51, 5589-92		89
769	Nature versus nurture: developing enzymes that function under extreme conditions. **2012**, 3, 77-102		140

768	A fluorogenic red fluorescent protein heterodimer. **2012**, 19, 353-60		63
767	Empirical and computational design of iron-sulfur cluster proteins. **2012**, 1817, 1256-62		27
766	Protein model discrimination using mutational sensitivity derived from deep sequencing. **2012**, 20, 371-81		62
765	Increasing sequence diversity with flexible backbone protein design: the complete redesign of a protein hydrophobic core. **2012**, 20, 1086-96		45
764	Helix stabilized, thermostable, and protease-resistant self-assembled peptide nanostructures as potential inhibitors of protein-protein interactions. **2013**, 14, 2684-9		25
763	Funneling and frustration in the energy landscapes of some designed and simplified proteins. *Journal of Chemical Physics*, **2013**, 139, 121908	3.9	25
762	Computational Protein Design for Synthetic Biology. **2013**, 101-122		3
761	Computational design of protein-protein interactions. *Current Opinion in Structural Biology*, **2013**, 23, 903-10	8.1	46
760	Atomistic description of the folding of a dimeric protein. **2013**, 117, 12935-42		37
759	Metalloprotein Design. **2013**, 565-593		10
758	Remodeling a □peptide bundle. **2013**, 4, 319-324		16
757	Establishing catalytic activity on an artificial (β)8-barrel protein designed from identical half-barrels. **2013**, 587, 2798-805		7
756	Structure-based redesign of proteins for minimal T-cell epitope content. **2013**, 34, 879-91		15
755	Evaluating the conformation and binding interface of cap-binding proteins and complexes via ultraviolet photodissociation mass spectrometry. **2013**, 12, 5867-77		9
754	Interplay of hydrogen bonds and n->π* interactions in proteins. **2013**, 135, 18682-8		95
753	Minireview: applied structural bioinformatics in proteomics. **2013**, 32, 505-11		9
752	Forcefield_PTM: Charge and AMBER Forcefield Parameters for Frequently Occurring Post-Translational Modifications. **2013**, 9, 5653-5674		68
751	De Novo Computational Protein Design. **2013**, 467-493		

750	Computational design of a protein-based enzyme inhibitor. **2013**, 425, 3563-75		71
749	Mining tertiary structural motifs for assessment of designability. **2013**, 523, 21-40		16
748	Multistate protein design using CLEVER and CLASSY. **2013**, 523, 171-90		17
747	Emerging themes in the computational design of novel enzymes and protein-protein interfaces. **2013**, 587, 1147-54		41
746	Scientific benchmarks for guiding macromolecular energy function improvement. **2013**, 523, 109-43		164
745	Computational protein design: the Proteus software and selected applications. **2013**, 34, 2472-84		38
744	De novo design of immunoreactive conformation-specific HIV-1 epitopes based on Top7 scaffold. **2013**, 3, 11790		7
743	ATP sequestration by a synthetic ATP-binding protein leads to novel phenotypic changes in Escherichia coli. **2013**, 8, 451-63		4
742	An integrated approach to extreme thermostabilization and affinity maturation of an antibody. **2013**, 26, 151-64		40
741	Building synthetic gene circuits from combinatorial libraries: screening and selection strategies. **2013**, 9, 1559-67		26
740	Computational protein design suggests that human PCNA-partner interactions are not optimized for affinity. *Proteins: Structure, Function and Bioinformatics*, **2013**, 81, 341-8	4.2	8
739	FAM3B PANDER and FAM3C ILEI represent a distinct class of signaling molecules with a non-cytokine-like fold. **2013**, 21, 306-13		17
738	New designed protein assemblies. **2013**, 17, 940-5		26
737	Generating thermal stable variants of protein domains through phage display. **2013**, 60, 38-45		13
736	Computational and theoretical methods for protein folding. *Biochemistry*, **2013**, 52, 8601-24	3.2	42
735	Fundamental challenges in mechanistic enzymology: progress toward understanding the rate enhancements of enzymes. *Biochemistry*, **2013**, 52, 2050-67	3.2	55
734	Energy functions in de novo protein design: current challenges and future prospects. **2013**, 42, 315-35		61
733	Proline editing: a general and practical approach to the synthesis of functionally and structurally diverse peptides. Analysis of steric versus stereoelectronic effects of 4-substituted prolines on conformation within peptides. **2013**, 135, 4333-63		117

732	Doing molecular biophysics: finding, naming, and picturing signal within complexity. **2013**, 42, 1-28		17
731	Computational enzyme design. **2013**, 52, 5700-25		351
730	Constructing manmade enzymes for oxygen activation. **2013**, 42, 3136-50		19
729	Designing functional metalloproteins: from structural to catalytic metal sites. **2013**, 257, 2565-2588		96
728	Design of a single-chain polypeptide tetrahedron assembled from coiled-coil segments. **2013**, 9, 362-6		224
727	Rational HIV immunogen design to target specific germline B cell receptors. *Science*, **2013**, 340, 711-6	33.3	519
726	AutoBioCAD: full biodesign automation of genetic circuits. **2013**, 2, 230-6		40
725	Evolution of a designed retro-aldolase leads to complete active site remodeling. **2013**, 9, 494-8		186
724	Folding of Top7 in unbiased all-atom Monte Carlo simulations. *Proteins: Structure, Function and Bioinformatics*, **2013**, 81, 1446-56	4.2	15
723	The how's and why's of protein folding intermediates. **2013**, 531, 14-23		39
722	Small-molecule ligand docking into comparative models with Rosetta. **2013**, 8, 1277-98		116
721	In vitro and in vivo characterization of designed immunogens derived from the CD-helix of the stem of influenza hemagglutinin. *Proteins: Structure, Function and Bioinformatics*, **2013**, 81, 1759-75	4.2	10
720	A simple probabilistic model of multibody interactions in proteins. *Proteins: Structure, Function and Bioinformatics*, **2013**, 81, 1340-50	4.2	5
719	Evolution-based design of proteins. **2013**, 523, 213-35		30
718	Protein Structure Modeling with Rosetta: Case Studies in Structure Prediction and Enzyme Repurposing. **2013**, 353-362		
717	Folding the proteome. **2013**, 38, 337-44		77
716	Design of protein catalysts. **2013**, 82, 447-70		150
715	A population-based evolutionary search approach to the multiple minima problem in de novo protein structure prediction. **2013**, 13 Suppl 1, S4		15

714	Expanded explorations into the optimization of an energy function for protein design. **2013**, 10, 1176-87		5
713	Accelerating protein tertiary structure analysis based on FPGA. **2013**,		
712	Dead-end elimination with perturbations (DEEPer): a provable protein design algorithm with continuous sidechain and backbone flexibility. *Proteins: Structure, Function and Bioinformatics*, **2013**, 81, 18-39	4.2	70
711	Using the RosettaSurface algorithm to predict protein structure at mineral surfaces. **2013**, 532, 343-66		20
710	Computational protein design quantifies structural constraints on amino acid covariation. *PLoS Computational Biology*, **2013**, 9, e1003313	5	25
709	An evolution-based approach to De Novo protein design and case study on Mycobacterium tuberculosis. *PLoS Computational Biology*, **2013**, 9, e1003298	5	39
708	Human germline antibody gene segments encode polyspecific antibodies. *PLoS Computational Biology*, **2013**, 9, e1003045	5	55
707	Rational design of a ligand-controlled protein conformational switch. **2013**, 110, 6800-4		86
706	Advancing Methods for Biomolecular Crystallography. **2013**,		1
705	Protein design by fusion: implications for protein structure prediction and evolution. **2013**, 69, 2451-60		3
704	Advances in Rosetta structure prediction for difficult molecular-replacement problems. **2013**, 69, 2202-8		18
703	EvoDesign: De novo protein design based on structural and evolutionary profiles. **2013**, 41, W273-80		36
702	An internal ligand-bound, metastable state of a leukocyte integrin, X2. **2013**, 203, 629-42		57
701	Computerbasiertes Enzymdesign. **2013**, 125, 5810-5836		37
700	Structure of the absent in melanoma 2 (AIM2) pyrin domain provides insights into the mechanisms of AIM2 autoinhibition and inflammasome assembly. **2013**, 288, 13225-35		113
699	Protein WISDOM: a workbench for in silico de novo design of biomolecules. **2013**,		18
698	Statistical Analysis of Terminal Extensions of Protein Strand Pairs. **2013**, 2013, 909436		3
697	The PyRosetta Toolkit: a graphical user interface for the Rosetta software suite. **2013**, 8, e66856		23

696	Octarellin VI: using rosetta to design a putative artificial (β/α)8 protein. **2013**, 8, e71858		20
695	RosettaEPR: rotamer library for spin label structure and dynamics. **2013**, 8, e72851		33
694	Applying physics-based scoring to calculate free energies of binding for single amino acid mutations in protein-protein complexes. **2013**, 8, e82849		116
693	Principles for Designing Ideal Protein Structures. **2013**, 53, 190-193		3
692	Design of a zinc-finger hydrolase with a synthetic β protein. **2014**, 9, e96234		3
691	Systematic Analysis of Large Enzyme Families: Identification of Specificity- and Selectivity-Determining Hotspots. **2014**, 6, 944-950		15
690	Rational design of heterodimeric protein using domain swapping for myoglobin. **2015**, 54, 511-5		18
689	Frustration in biomolecules. **2014**, 47, 285-363		168
688	Computational redesign of metalloenzymes for catalyzing new reactions. *Methods in Molecular Biology*, **2014**, 1216, 265-73	1.4	2
687	A kinetic mechanism for in vivo protein folding. **2014**, 10,		2
686	A "fuzzy"-logic language for encoding multiple physical traits in biomolecules. **2014**, 426, 4125-4138		16
685	De novo design and experimental characterization of ultrashort self-associating peptides. *PLoS Computational Biology*, **2014**, 10, e1003718	5	29
684	Modeling Non-Native Interactions in Designed Proteins. **2014**, 54, 1230-1240		16
683	Pairwise decomposition of an MMGBSA energy function for computational protein design. **2014**, 35, 1371-87		32
682	Motif-directed redesign of enzyme specificity. *Protein Science*, **2014**, 23, 312-20	6.3	8
681	Designing cooperativity into the designed protein Top7. *Proteins: Structure, Function and Bioinformatics*, **2014**, 82, 364-74	4.2	7
680	Centenary Award and Sir Frederick Gowland Hopkins Memorial Lecture. Protein folding, structure prediction and design. **2014**, 42, 225-9		25
679	Learning To Fold Proteins Using Energy Landscape Theory. **2014**, 54, 1311-1337		44

678	Computational design of novel enzymes without cofactors. *Methods in Molecular Biology*, **2014**, 1216, 197-210	1.4	9
677	Computational design of metalloproteins. *Methods in Molecular Biology*, **2014**, 1216, 233-49	1.4	4
676	Biophysics of protein evolution and evolutionary protein biophysics. **2014**, 11, 20140419		144
675	Protein Design. *Methods in Molecular Biology*, **2014**,	1.4	
674	Biophysical highlights from 54 years of macromolecular crystallography. **2014**, 106, 510-25		9
673	Enhanced Sampling for Biomolecular Simulations. **2014**, 249-267		1
672	All-Atom Monte Carlo Simulations of Protein Folding and Aggregation. **2014**, 433-444		2
671	Understanding thermal adaptation of enzymes through the multistate rational design and stability prediction of 100 adenylate kinases. **2014**, 22, 218-29		27
670	Backbone flexibility of CDR3 and immune recognition of antigens. **2014**, 426, 1583-99		14
669	Protein design: toward functional metalloenzymes. **2014**, 114, 3495-578		329
668	Princeton_TIGRESS: protein geometry refinement using simulations and support vector machines. *Proteins: Structure, Function and Bioinformatics*, **2014**, 82, 794-814	4.2	21
667	Assessment of protein side-chain conformation prediction methods in different residue environments. *Proteins: Structure, Function and Bioinformatics*, **2014**, 82, 1971-84	4.2	25
666	Rational design of topographical helix mimics as potent inhibitors of protein-protein interactions. **2014**, 136, 7877-88		91
665	An integrated approach for thermal stabilization of a mesophilic adenylate kinase. *Proteins: Structure, Function and Bioinformatics*, **2014**, 82, 1947-59	4.2	11
664	Protein NMR structures refined with Rosetta have higher accuracy relative to corresponding X-ray crystal structures. **2014**, 136, 1893-906		47
663	Proof of principle for epitope-focused vaccine design. *Nature*, **2014**, 507, 201-6	50.4	365
662	Computational design of a pH-sensitive IgG binding protein. **2014**, 111, 675-80		57
661	Computational design of water-soluble □helical barrels. *Science*, **2014**, 346, 485-8	33.3	244

660	De Novo Designed Copper -Helical Peptides: From Design to Function. **2014**, 2014, 2177-2193		10
659	Predicting evolutionary site variability from structure in viral proteins: buriedness, packing, flexibility, and design. **2014**, 79, 130-42		31
658	Protein design with a comprehensive statistical energy function and boosted by experimental selection for foldability. *Nature Communications*, **2014**, 5, 5330	17.4	47
657	Urzymology: experimental access to a key transition in the appearance of enzymes. **2014**, 289, 30213-30220		33
656	Computational and biochemical docking of the irreversible cocaine analog RTI 82 directly demonstrates ligand positioning in the dopamine transporter central substrate-binding site. **2014**, 289, 29712-27		21
655	CHARMM-GUI PDB manipulator for advanced modeling and simulations of proteins containing nonstandard residues. *Advances in Protein Chemistry and Structural Biology*, **2014**, 96, 235-65	5.3	96
654	Intelligent Computing in Bioinformatics. **2014**,		3
653	Predicting enzymatic reactivity: from theory to design. **2014**, 4, 407-421		27
652	Improving the accuracy of protein stability predictions with multistate design using a variety of backbone ensembles. *Proteins: Structure, Function and Bioinformatics*, **2014**, 82, 771-84	4.2	36
651	Hierarchical cascades of instability govern the mechanics of coiled coils: helix unfolding precedes coil unzipping. **2014**, 107, 477-484		10
650	Improved stability and half-life of fluorinated phosphotriesterase using Rosetta. **2014**, 15, 1761-4		9
649	A computational approach to enzyme design: predicting -aminotransferase catalytic activity using docking and MM-GBSA scoring. *Journal of Chemical Information and Modeling*, **2014**, 54, 2334-46	6.1	62
648	Evolution and design of protein structure by folding nucleus symmetric expansion. **2014**, 22, 1377-84		16
647	Automatic NOESY assignment in CS-RASREC-Rosetta. **2014**, 59, 147-59		11
646	A computationally designed inhibitor of an Epstein-Barr viral Bcl-2 protein induces apoptosis in infected cells. **2014**, 157, 1644-1656		96
645	Improving computational efficiency and tractability of protein design using a piecemeal approach. A strategy for parallel and distributed protein design. **2014**, 30, 1138-1145		5
644	Self-assembled bionanostructures: proteins following the lead of DNA nanostructures. **2014**, 12, 4		40
643	A proposed mechanism for the promotion of prion conversion involving a strictly conserved tyrosine residue in the -2 loop of PrPC. **2014**, 289, 10660-10667		31

642	Hyperglycosylated stable core immunogens designed to present the CD4 binding site are preferentially recognized by broadly neutralizing antibodies. **2014**, 88, 14002-16		28
641	Design of net-charged abc-type collagen heterotrimers. **2014**, 185, 163-7		7
640	Stereoselective inhibition of serotonin transporters by antimalarial compounds. **2014**, 73, 98-106		9
639	Merging molecular mechanism and evolution: theory and computation at the interface of biophysics and evolutionary population genetics. *Current Opinion in Structural Biology*, **2014**, 26, 84-91	8.1	62
638	Influenza hemagglutinin stem-fragment immunogen elicits broadly neutralizing antibodies and confers heterologous protection. **2014**, 111, E2514-23		135
637	An accurate binding interaction model in de novo computational protein design of interactions: if you build it, they will bind. **2014**, 185, 136-46		12
636	Recent Advances in De Novo Protein Design. **2014**, 207-232		
635	Encyclopedia of Applied and Computational Mathematics. **2015**, 863-865		
634	Utilizing Markov Chains to Model Ion Channel Sequence Variation and Kinetics. **2015**, 123-132		
633	Encyclopedia of Applied and Computational Mathematics. **2015**, 1007-1014		
632	Substrate Phage Display. **2015**, 222-245		
631	Antibody-Based Technologies for Environmental Biodetection. **2015**, 2.3.1-1-2.3.1-12		
630	Distinguishing proteins from arbitrary amino acid sequences. *Scientific Reports*, **2015**, 5, 7972	4.9	4
629	On statistical energy functions for biomolecular modeling and design. **2015**, 3, 157-167		3
628	Encyclopedia of Applied and Computational Mathematics. **2015**, 940-951		0
627	Artificial Diiron Enzymes with a De Novo Designed Four-Helix Bundle Structure. **2015**, 2015, 3371-3390		50
626	AbDesign: An algorithm for combinatorial backbone design guided by natural conformations and sequences. *Proteins: Structure, Function and Bioinformatics*, **2015**, 83, 1385-406	4.2	55
625	Effects of Non-Natural Amino Acid Incorporation into the Enzyme Core Region on Enzyme Structure and Function. *International Journal of Molecular Sciences*, **2015**, 16, 22735-53	6.3	4

624	Design of Protein Multi-specificity Using an Independent Sequence Search Reduces the Barrier to Low Energy Sequences. *PLoS Computational Biology*, **2015**, 11, e1004300	5	25
623	Enhancements to the Rosetta Energy Function Enable Improved Identification of Small Molecules that Inhibit Protein-Protein Interactions. **2015**, 10, e0140359		16
622	Constrained versus unconstrained folding free-energy landscapes. **2015**, 113, 2905-2912		2
621	Protein design: Past, present, and future. **2015**, 104, 334-50		32
620	Better theoretical models and protein design experiments can help to understand protein folding. **2015**, 6, 202-4		1
619	BetaProbe: A probability based method for predicting beta sheet topology using integer programming. **2015**,		3
618	RNA-Redesign: a web server for fixed-backbone 3D design of RNA. **2015**, 43, W498-501		6
617	Single-Point Mutation with a Rotamer Library Toolkit: Toward Protein Engineering. *Journal of Chemical Information and Modeling*, **2015**, 55, 2657-71	6.1	5
616	Encyclopedia of Applied and Computational Mathematics. **2015**, 850-856		
615	Encyclopedia of Applied and Computational Mathematics. **2015**, 881-886		
614	Encyclopedia of Applied and Computational Mathematics. **2015**, 886-894		7
613	Encyclopedia of Applied and Computational Mathematics. **2015**, 839-841		2
612	Encyclopedia of Applied and Computational Mathematics. **2015**, 923-925		
611	Nucleic acid aptamers in cancer research, diagnosis and therapy. **2015**, 44, 1240-56		165
610	Assessing protein conformational sampling and structural stability via de novo design and molecular dynamics simulations. **2015**, 103, 351-61		5
609	Structure-based design of combinatorial mutagenesis libraries. *Protein Science*, **2015**, 24, 895-908	6.3	11
608	Combined covalent-electrostatic model of hydrogen bonding improves structure prediction with Rosetta. **2015**, 11, 609-22		163
607	Quality Assessment of Predicted Protein Models Using Energies Calculated by the Fragment Molecular Orbital Method. **2015**, 34, 97-104		12

606	MetREx: a protein design approach for the exploration of sequence-reactivity relationships in metalloenzymes. **2015**, 36, 553-63		1
605	De novo protein structure determination from near-atomic-resolution cryo-EM maps. **2015**, 12, 335-8		131
604	Structural and dynamic properties that govern the stability of an engineered fibronectin type III domain. **2015**, 28, 67-78		28
603	Discriminating between stabilizing and destabilizing protein design mutations via recombination and simulation. **2015**, 28, 259-67		10
602	Functional Class I and II Amino Acid-activating Enzymes Can Be Coded by Opposite Strands of the Same Gene. **2015**, 290, 19710-25		44
601	De novo protein design: how do we expand into the universe of possible protein structures?. *Current Opinion in Structural Biology*, **2015**, 33, 16-26	8.1	125
600	Self-Assembling Nano-Architectures Created from a Protein Nano-Building Block Using an Intermolecularly Folded Dimeric de Novo Protein. **2015**, 137, 11285-93		75
599	Combined Crystal Structure of a Type I Cohesin: MUTATION AND AFFINITY BINDING STUDIES REVEAL STRUCTURAL DETERMINANTS OF COHESIN-DOCKERIN SPECIFICITIES. **2015**, 290, 16215-25		9
598	Computational redesign of the lipid-facing surface of the outer membrane protein OmpA. **2015**, 112, 9632-7		21
597	Design of ordered two-dimensional arrays mediated by noncovalent protein-protein interfaces. *Science*, **2015**, 348, 1365-8	33.3	173
596	Ribosome. Mechanical force releases nascent chain-mediated ribosome arrest in vitro and in vivo. *Science*, **2015**, 348, 457-60	33.3	148
595	Automated determination of fibrillar structures by simultaneous model building and fiber diffraction refinement. **2015**, 12, 679-84		4
594	Increasing the stability of the bacteriophage endolysin PlyC using rationale-based FoldX computational modeling. **2015**, 28, 85-92		23
593	Towards the computational design of protein post-translational regulation. **2015**, 23, 2877-82		17
592	Computational treatment of metalloproteins. **2015**, 119, 5945-56		14
591	Toward the Computational Design of Artificial Metalloenzymes: From Protein□igand Docking to Multiscale Approaches. **2015**, 5, 2469-2480		42
590	The Self-Association of Graphane Is Driven by London Dispersion and Enhanced Orbital Interactions. **2015**, 11, 1621-30		36
589	Toward Computationally Designed Self-Reporting Biosensors Using Leave-One-Out Green Fluorescent Protein. *Biochemistry*, **2015**, 54, 6263-73	3.2	6

588	Control over overall shape and size in de novo designed proteins. **2015**, 112, E5478-85		75
587	Prediction of Stable Globular Proteins Using Negative Design with Non-native Backbone Ensembles. **2015**, 23, 2011-21		19
586	Massively parallel sampling of lattice proteins reveals foundations of thermal adaptation. *Journal of Chemical Physics*, **2015**, 143, 055101	3.9	2
585	Design of symmetric TIM barrel proteins from first principles. **2015**, 16, 18		21
584	Algorithm to design inhibitors using stereochemically mixed l,d polypeptides: Validation against HIV protease. **2015**, 81, 410-7		1
583	InteractiveROSETTA: a graphical user interface for the PyRosetta protein modeling suite. **2015**, 31, 4023-5		11
582	Protein stability: computation, sequence statistics, and new experimental methods. *Current Opinion in Structural Biology*, **2015**, 33, 161-8	8.1	90
581	Bayesian evidence and model selection. **2015**, 47, 50-67		41
580	Crystal structure of designed PX domain from cytokine-independent survival kinase and implications on evolution-based protein engineering. **2015**, 191, 197-206		9
579	Guaranteed Discrete Energy Optimization on Large Protein Design Problems. **2015**, 11, 5980-9		44
578	SIRAH: a structurally unbiased coarse-grained force field for proteins with aqueous solvation and long-range electrostatics. **2015**, 11, 723-39		84
577	The Iterative Protein Redesign and Optimization (IPRO) suite of programs. **2015**, 36, 251-63		27
576	Computational de novo design of a self-assembling peptide with predefined structure. **2015**, 427, 550-62		15
575	A general computational approach for repeat protein design. **2015**, 427, 563-75		63
574	Rational protein design: developing next-generation biological therapeutics and nanobiotechnological tools. **2015**, 7, 330-41		9
573	Insight into a molecular interaction force supporting peptide backbones and its implication to protein loops and folding. **2015**, 33, 1957-72		4
572	Computational modeling of membrane proteins. *Proteins: Structure, Function and Bioinformatics*, **2015**, 83, 1-24	4.2	69
571	Rational Design of Heterodimeric Protein using Domain Swapping for Myoglobin. **2015**, 127, 521-525		6

570	Deterministic model of biomolecular networks with stimuli-responsive properties. **2015**, 26, 921-930		9
569	Computational de novo design of a four-helix bundle protein--DND_4HB. *Protein Science*, **2015**, 24, 434-45	6.3	16
568	Structure-based inhibition of protein-protein interactions. **2015**, 94, 480-8		37
567	Towards designing new nano-scale protein architectures. **2016**, 60, 315-324		4
566	From Mollusks to Medicine: A Venomics Approach for the Discovery and Characterization of Therapeutics from Terebridae Peptide Toxins. **2016**, 8, 117		29
565	The Folding of de Novo Designed Protein DS119 via Molecular Dynamics Simulations. *International Journal of Molecular Sciences*, **2016**, 17,	6.3	1
564	Use of an Improved Matching Algorithm to Select Scaffolds for Enzyme Design Based on a Complex Active Site Model. **2016**, 11, e0156559		12
563	Using Evolution to Guide Protein Engineering: The Devil IS in the Details. **2016**, 111, 10-8		27
562	Improving hybrid statistical and physical forcefields through local structure enumeration. *Protein Science*, **2016**, 25, 1525-34	6.3	5
561	Protein side chain conformation predictions with an MMGBSA energy function. *Proteins: Structure, Function and Bioinformatics*, **2016**, 84, 803-19	4.2	17
560	Molprobity's ultimate rotamer-library distributions for model validation. *Proteins: Structure, Function and Bioinformatics*, **2016**, 84, 1177-89	4.2	69
559	Introduction of a polar core into the de novo designed protein Top7. *Protein Science*, **2016**, 25, 1299-307	6.3	4
558	Protein rethreading: A novel approach to protein design. *Scientific Reports*, **2016**, 6, 26847	4.9	3
557	Perspective: Evolutionary design of granular media and block copolymer patterns. **2016**, 4, 053209		25
556	Simplification of complexity in protein molecular systems by grouping amino acids: a view from physics. **2016**, 1, 444-466		3
555	Computational design of proteins with novel structure and functions. **2016**, 25, 018702		1
554	Beyond the outer limits of nature by directed evolution. *Biotechnology Advances*, **2016**, 34, 754-767	17.8	37
553	The unexpected structure of the designed protein Octarellin V.1 forms a challenge for protein structure prediction tools. **2016**, 195, 19-30		11

552	Structure-Based Identification of HDAC8 Non-histone Substrates. **2016**, 24, 458-68		31
551	Algorithms for protein design. *Current Opinion in Structural Biology*, **2016**, 39, 16-26	8.1	47
550	Protein backbone ensemble generation explores the local structural space of unseen natural homologs. **2016**, 32, 1454-61		4
549	Protein Folding and Structure Prediction from the Ground Up: The Atomistic Associative Memory, Water Mediated, Structure and Energy Model. **2016**, 120, 8557-65		22
548	An intramolecular disulfide bond designed in myoglobin fine-tunes both protein structure and peroxidase activity. **2016**, 600, 47-55		19
547	Rosetta and the Design of Ligand Binding Sites. *Methods in Molecular Biology*, **2016**, 1414, 47-62	1.4	18
546	Design of structurally distinct proteins using strategies inspired by evolution. *Science*, **2016**, 352, 687-90	33.3	93
545	De novo design of protein homo-oligomers with modular hydrogen-bond network-mediated specificity. *Science*, **2016**, 352, 680-7	33.3	194
544	PROTEIN DESIGN. Inspired by nature. *Science*, **2016**, 352, 657-8	33.3	8
543	Designed Repeat Proteins as Building Blocks for Nanofabrication. **2016**, 940, 61-81		13
542	Computational Redesign of Thioredoxin Is Hypersensitive toward Minor Conformational Changes in the Backbone Template. **2016**, 428, 4361-4377		13
541	Protocols for Molecular Modeling with Rosetta3 and RosettaScripts. *Biochemistry*, **2016**, 55, 4748-63	3.2	118
540	Smart Materials for DNA-Based Nanoconstructions. **2016**, 21-60		
539	Rational design of TNF□binding proteins based on the de novo designed protein DS119. *Protein Science*, **2016**, 25, 2066-2075	6.3	5
538	Synthetic beta-solenoid proteins with the fragment-free computational design of a beta-hairpin extension. **2016**, 113, 10346-51		19
537	Proteins of well-defined structures can be designed without backbone readjustment by a statistical model. **2016**, 196, 350-357		8
536	Therapeutic Potential of Foldamers: From Chemical Biology Tools To Drug Candidates?. **2016**, 59, 9599-9621		94
535	The coming of age of de novo protein design. *Nature*, **2016**, 537, 320-7	50.4	697

534	Balancing Selectivity and Efficacy of Bispecific Epidermal Growth Factor Receptor (EGFR) □-MET Antibodies and Antibody-Drug Conjugates. **2016**, 291, 25106-25119		42
533	Smoothing a rugged protein folding landscape by sequence-based redesign. *Scientific Reports*, **2016**, 6, 33958	4.9	16
532	Protein engineering by highly parallel screening of computationally designed variants. **2016**, 2, e1600692		21
531	Computational protein design with backbone plasticity. **2016**, 44, 1523-1529		14
530	Oligooxopiperazines as Topographical Helix Mimetics. **2016**, 1-24		1
529	Tertiary alphabet for the observable protein structural universe. **2016**, 113, E7438-E7447		34
528	Folding and Stabilization of Native-Sequence-Reversed Proteins. *Scientific Reports*, **2016**, 6, 25138	4.9	3
527	Boosting protein stability with the computational design of □-sheet surfaces. *Protein Science*, **2016**, 25, 702-10	6.3	10
526	Toward high-resolution computational design of the structure and function of helical membrane proteins. **2016**, 23, 475-80		21
525	Structural constraints-based evaluation of immunogenic avirulent toxins from Clostridium botulinum C2 and C3 toxins as subunit vaccines. **2016**, 44, 17-27		7
524	Coarse-Grained Protein Models and Their Applications. **2016**, 116, 7898-936		489
523	Why reinvent the wheel? Building new proteins based on ready-made parts. *Protein Science*, **2016**, 25, 1179-87	6.3	28
522	Intermediate divergence levels maximize the strength of structure-sequence correlations in enzymes and viral proteins. *Protein Science*, **2016**, 25, 1341-53	6.3	4
521	The role of negative selection in protein evolution revealed through the energetics of the native state ensemble. *Proteins: Structure, Function and Bioinformatics*, **2016**, 84, 435-47	4.2	6
520	Structural Characterizations of the Fas Receptor and the Fas-Associated Protein with Death Domain Interactions. **2016**, 35, 51-60		7
519	Designer protein delivery: From natural to engineered affinity-controlled release systems. *Science*, **2016**, 351, aac4750	33.3	104
518	Controlling Allosteric Networks in Proteins. **2016**, 116, 6463-87		135
517	Generating, Maintaining, and Exploiting Diversity in a Memetic Algorithm for Protein Structure Prediction. **2016**, 24, 577-607		28

516	De Novo Proteins with Life-Sustaining Functions Are Structurally Dynamic. **2016**, 428, 399-411		24
515	A new structural model of Alzheimer's Aβ42 fibrils based on electron paramagnetic resonance data and Rosetta modeling. **2016**, 194, 61-7		41
514	Computational Tools Applied to Enzyme Design□a review. **2016**, 1,		8
513	Turning statistical physics models into materials design engines. **2016**, 113, 34-9		51
512	Characterization of the Domain Orientations of E. coli 5'-Nucleotidase by Fitting an Ensemble of Conformers to DEER Distance Distributions. **2016**, 24, 43-56		14
511	Protein sequence design and its applications. *Current Opinion in Structural Biology*, **2016**, 37, 71-80	8.1	8
510	De novo design of a four-fold symmetric TIM-barrel protein with atomic-level accuracy. **2016**, 12, 29-34		151
509	Online Design. **2016**, 73-85		
508	The Automated Design of Materials Far From Equilibrium. **2016**,		2
507	Structure-function discrepancy in Clostridium botulinum C3 toxin for its rational prioritization as a subunit vaccine. **2016**, 34, 1317-29		10
506	Engineering Transcriptional Regulator Effector Specificity Using Computational Design and In Vitro Rapid Prototyping: Developing a Vanillin Sensor. **2016**, 5, 287-95		63
505	Protein-Protein Interaction for the De Novo Design of Cyclin-Dependent Kinase Peptide Inhibitors. *Methods in Molecular Biology*, **2016**, 1336, 59-66	1.4	
504	Fast, cheap and out of control--Insights into thermodynamic and informatic constraints on natural protein sequences from de novo protein design. **2016**, 1857, 485-492		8
503	Efficient dynamic programming algorithm with prior knowledge for protein□strand alignment. **2017**, 417, 43-50		2
502	A Non-natural Protein Rescues Cells Deleted for a Key Enzyme in Central Metabolism. **2017**, 6, 694-700		19
501	Computational design of an epitope-specific Keap1 binding antibody using hotspot residues grafting and CDR loop swapping. *Scientific Reports*, **2017**, 7, 41306	4.9	15
500	Principles for designing proteins with cavities formed by curved□sheets. *Science*, **2017**, 355, 201-206	33.3	82
499	Insights from molecular dynamics simulations for computational protein design. **2017**, 2, 9-33		98

498	Molecular Engineering of Enzymes. **2017**, 47-80		
497	A four-helix bundle DNA nanostructure with binding pockets for pyrimidine nucleotides. **2017**, 9, 7047-7054		5
496	Computational protein design: a review. **2017**, 29, 143001		27
495	Geometric Principles for Designing Highly Symmetric Self-Assembling Protein Nanomaterials. **2017**, 46, 23-42		71
494	Overcoming an optimization plateau in the directed evolution of highly efficient nerve agent bioscavengers. **2017**, 30, 333-345		41
493	Hidden Markov model and Chapman Kolmogrov for protein structures prediction from images. **2017**, 68, 231-244		20
492	Hydrogen/Deuterium Exchange Mass Spectrometry of Human Green Opsin Reveals a Conserved Pro-Pro Motif in Extracellular Loop 2 of Monostable Visual G Protein-Coupled Receptors. *Biochemistry*, **2017**, 56, 2338-2348	3.2	5
491	The Rosetta All-Atom Energy Function for Macromolecular Modeling and Design. **2017**, 13, 3031-3048		486
490	The ribosome destabilizes native and non-native structures in a nascent multidomain protein. *Protein Science*, **2017**, 26, 1439-1451	6.3	29
489	Foldit Standalone: a video game-derived protein structure manipulation interface using Rosetta. **2017**, 33, 2765-2767		44
488	Residue-centric modeling and design of saccharide and glycoconjugate structures. **2017**, 38, 276-287		31
487	Computational Protein Design. *Methods in Molecular Biology*, **2017**,	1.4	5
486	Computational Protein Design Under a Given Backbone Structure with the ABACUS Statistical Energy Function. *Methods in Molecular Biology*, **2017**, 1529, 217-226	1.4	10
485	The Framework of Computational Protein Design. *Methods in Molecular Biology*, **2017**, 1529, 3-19	1.4	4
484	An Evolution-Based Approach to De Novo Protein Design. *Methods in Molecular Biology*, **2017**, 1529, 243-264	1.4	9
483	Achievements and Challenges in Computational Protein Design. *Methods in Molecular Biology*, **2017**, 1529, 21-94	1.4	8
482	Design of self-assembling transmembrane helical bundles to elucidate principles required for membrane protein folding and ion transport. **2017**, 372,		17
481	Metamorphic Proteins: Emergence of Dual Protein Folds from One Primary Sequence. *Biochemistry*, **2017**, 56, 2971-2984	3.2	36

480	Protein design: from computer models to artificial intelligence. **2017**, 7, e1318		15
479	Cofactor specificity switch in Shikimate dehydrogenase by rational design and consensus engineering. **2017**, 30, 533-541		8
478	Bioconjugation and Active Site Design of Enzymes Using Non-natural Amino Acids. **2017**, 56, 6535-6547		9
477	Outperforming Nature Catalysts: Designing Metalloenzymes for Chemical Synthesis. **2017**, 89-122		0
476	Synthetic Protein Switches: Theoretical and Experimental Considerations. *Methods in Molecular Biology*, **2017**, 1596, 3-25	1.4	3
475	The Unique Domain Forms a Fuzzy Intramolecular Complex in Src Family Kinases. **2017**, 25, 630-640.e4		38
474	Automated protein design: Landmarks and operational principles. **2017**, 125, 24-35		9
473	On-chip integration of droplet microfluidics and nanostructure-initiator mass spectrometry for enzyme screening. **2017**, 17, 323-331		33
472	Multistate Computational Protein Design with Backbone Ensembles. *Methods in Molecular Biology*, **2017**, 1529, 161-179	1.4	14
471	In silico methods for design of biological therapeutics. **2017**, 131, 33-65		36
470	Principles for computational design of binding antibodies. **2017**, 114, 10900-10905		73
469	Health Informatics Data Analysis. **2017**,		
468	De novo design of covalently constrained mesosize protein scaffolds with unique tertiary structures. **2017**, 114, 10852-10857		44
467	Design of coiled-coil protein-origami cages that self-assemble in vitro and in vivo. **2017**, 35, 1094-1101		89
466	Rational design of proteins that exchange on functional timescales. **2017**, 13, 1280-1285		54
465	Protein sheet prediction using an efficient dynamic programming algorithm. **2017**, 70, 142-155		4
464	De novo design of a hyperstable non-natural protein-ligand complex with sub- accuracy. **2017**, 9, 1157-1164		60
463	Rules for connectivity of secondary structure elements in protein: Two-layer sandwiches. *Protein Science*, **2017**, 26, 2257-2267	6.3	2

462	Full Protein Sequence Redesign with an MMGBSA Energy Function. **2017**, 13, 4932-4943		8
461	A component analysis of the free energies of folding of 35 proteins: A consensus view on the thermodynamics of folding at the molecular level. **2017**, 38, 2791-2801		8
460	Proteins. **2017**, 59-92		
459	Protein Engineering. **2017**, 113-127		
458	Limiting the valence: advancements and new perspectives on patchy colloids, soft functionalized nanoparticles and biomolecules. **2017**, 19, 19847-19868		50
457	Advances in design of protein folds and assemblies. **2017**, 40, 65-71		20
456	Protein design by multiobjective optimization. **2017**,		3
455	How the stability of a folded protein depends on interfacial water properties and residue-residue interactions. **2017**, 245, 129-139		18
454	Cyclic oligomer design with de novo □proteins. *Protein Science*, **2017**, 26, 2187-2194	6.3	7
453	Searching for the Pareto frontier in multi-objective protein design. **2017**, 9, 339-344		4
452	Design and applications of a clamp for Green Fluorescent Protein with picomolar affinity. *Scientific Reports*, **2017**, 7, 16292	4.9	30
451	The influence of disulfide bonds on the mechanical stability of proteins is context dependent. **2017**, 292, 13374-13380		21
450	Complex binding pathways determine the regeneration of mammalian green cone opsin with a locked retinal analogue. **2017**, 292, 10983-10997		8
449	Inverse statistical problems: from the inverse Ising problem to data science. **2017**, 66, 197-261		125
448	Role of Water in the Selection of Stable Proteins at Ambient and Extreme Thermodynamic Conditions. **2017**, 7,		12
447	Recurring sequence-structure motifs in (β□barrel proteins and experimental optimization of a chimeric protein designed based on such motifs. **2017**, 1865, 165-175		4
446	Protein Engineering Techniques. **2017**,		7
445	Computational tools for the evaluation of laboratory-engineered biocatalysts. **2016**, 53, 284-297		67

444	Rational design of cholesterol oxidase for efficient bioresolution of cholestane skeleton substrates. *Scientific Reports*, **2017**, 7, 16375	4.9	7
443	Protein's number of beta-sheets prediction using structural features. **2017**,		0
442	Flexible Proteins at the Origin of Life. **2017**, 7,		8
441	BetaCon. **2017**,		1
440	4.14 Rational and Combinatorial Methods to Create Designer Protein Interfaces. **2017**, 221-247		1
439	A cyber-linked undergraduate research experience in computational biomolecular structure prediction and design. *PLoS Computational Biology*, **2017**, 13, e1005837	5	7
438	A critical analysis of computational protein design with sparse residue interaction graphs. *PLoS Computational Biology*, **2017**, 13, e1005346	5	1
437	Rosetta:MSF: a modular framework for multi-state computational protein design. *PLoS Computational Biology*, **2017**, 13, e1005600	5	29
436	Data driven flexible backbone protein design. *PLoS Computational Biology*, **2017**, 13, e1005722	5	8
435	High-resolution global peptide-protein docking using fragments-based PIPER-FlexPepDock. *PLoS Computational Biology*, **2017**, 13, e1005905	5	58
434	Protein Structure Prediction and Homology Modeling. **2017**, 120-144		
433	Disentangling polydispersity in the PCNA-p15PAF complex, a disordered, transient and multivalent macromolecular assembly. **2017**, 45, 1501-1515		28
432	Exploring the effects of sparse restraints on protein structure prediction. *Proteins: Structure, Function and Bioinformatics*, **2018**, 86, 248-262	4.2	0
431	Automated design evolution of stereochemically randomized protein foldamers. **2018**, 15, 036001		3
430	Deconvolving the Fate of Carbon in Coastal Sediments. **2018**, 45, 4134-4142		14
429	Computational Protein Design with Deep Learning Neural Networks. *Scientific Reports*, **2018**, 8, 6349	4.9	72
428	Self-Assembling Supramolecular Nanostructures Constructed from de Novo Extender Protein Nanobuilding Blocks. **2018**, 7, 1381-1394		21
427	Protocols for Requirement-Driven Protein Design in the Rosetta Modeling Program. *Journal of Chemical Information and Modeling*, **2018**, 58, 895-901	6.1	12

426	Probing Molecular Basis for Constructing Interface Bionanostructures. **2018**, 61, 1125-1138		
425	Holistic Approach to Partial Covalent Interactions in Protein Structure Prediction and Design with Rosetta. *Journal of Chemical Information and Modeling*, **2018**, 58, 1021-1036	6.1	1
424	Understanding the roles of functional peptides in designing apatite and silica nanomaterials biomimetically using NMR techniques. **2018**, 33, 44-52		10
423	Structural heterogeneity and dynamics in protein evolution and design. *Current Opinion in Structural Biology*, **2018**, 48, 157-163	8.1	26
422	Combining Rosetta with molecular dynamics (MD): A benchmark of the MD-based ensemble protein design. **2018**, 203, 54-61		12
421	Principles of Protein Stability and Their Application in Computational Design. **2018**, 87, 105-129		106
420	Beyond Thermodynamic Constraints: Evolutionary Sampling Generates Realistic Protein Sequence Variation. **2018**, 208, 1387-1395		6
419	Common fibrillar spines of amyloid-β and human islet amyloid polypeptide revealed by microelectron diffraction and structure-based inhibitors. **2018**, 293, 2888-2902		31
418	A computational method for the design of nested proteins by loop-directed domain insertion. *Proteins: Structure, Function and Bioinformatics*, **2018**, 86, 354-369	4.2	1
417	TetraBASE: A Side Chain-Independent Statistical Energy for Designing Realistically Packed Protein Backbones. *Journal of Chemical Information and Modeling*, **2018**, 58, 430-442	6.1	2
416	Are natural proteins special? Can we do that?. *Current Opinion in Structural Biology*, **2018**, 48, 124-132	8.1	12
415	Applying graph theory to protein structures: an Atlas of coiled coils. **2018**, 34, 3316-3323		6
414	Recent advances in automated protein design and its future challenges. **2018**, 13, 587-604		12
413	Accurately Predicting Disordered Regions of Proteins Using Rosetta ResidueDisorder Application. **2018**, 122, 3920-3930		10
412	Computational design of membrane proteins using RosettaMembrane. *Protein Science*, **2018**, 27, 341-355	6.3	13
411	Web-accessible molecular modeling with Rosetta: The Rosetta Online Server that Includes Everyone (ROSIE). *Protein Science*, **2018**, 27, 259-268	6.3	32
410	Conformationally constrained peptides target the allosteric kinase dimer interface and inhibit EGFR activation. **2018**, 26, 1167-1173		11
409	Elfin: An algorithm for the computational design of custom three-dimensional structures from modular repeat protein building blocks. **2018**, 201, 100-107		6

408	Type-III secretion pore formed by flagellar protein FliP. **2018**, 107, 94-103		18
407	Polymer Families and Their Extended Activities. **2018**, 89-137		
406	Integration of molecular dynamics simulation and hotspot residues grafting for de novo scFv design against Salmonella Typhi TolC protein. **2018**, 31, e2695		3
405	Hierarchical design of artificial proteins and complexes toward synthetic structural biology. **2018**, 10, 391-410		21
404	Inverse statistical physics of protein sequences: a key issues review. *Reports on Progress in Physics*, **2018**, 81, 032601	14.4	90
403	Improving the Thermostability and Catalytic Efficiency of the Subunit-Fused Nitrile Hydratase by Semi-Rational Engineering. **2018**, 10, 1370-1375		17
402	Design of metalloproteins and novel protein folds using variational autoencoders. *Scientific Reports* , **2018**, 8, 16189	4.9	50
401	Rosetta FunFolDes - A general framework for the computational design of functional proteins. *PLoS Computational Biology*, **2018**, 14, e1006623	5	20
400	Computational Design of Epitope-Specific Functional Antibodies. **2018**, 25, 2121-2131.e5		32
399	Toward a Halophenol Dehalogenase from Iodotyrosine Deiodinase via Computational Design. **2018**, 8, 11783-11793		4
398	Design of highly active double-pseudoknotted ribozymes: a combined computational and experimental study. **2019**, 47, 29-42		3
397	An adaptive geometric search algorithm for macromolecular scaffold selection. **2018**, 31, 345-354		
396	Editorial overview: The many facets of protein design: from self-assembled materials to vaccines. *Current Opinion in Structural Biology*, **2018**, 51, iv-vi	8.1	
395	Simple yet functional phosphate-loop proteins. **2018**, 115, E11943-E11950		44
394	Energy Landscape of the Designed Protein Top7. **2018**, 122, 12282-12291		7
393	Strategies for designing non-natural enzymes and binders. **2018**, 47, 67-76		28
392	Mutational Basin-Hopping: Combined Structure and Sequence Optimization for Biomolecules. **2018** , 9, 6169-6173		9
391	Energy Landscapes of Macromolecules with Unique 3D Structures. **2018**, 63, 485-496		4

390	iCFN: an efficient exact algorithm for multistate protein design. **2018**, 34, i811-i820		15
389	De novo design of a non-local β-sheet protein with high stability and accuracy. **2018**, 25, 1028-1034		54
388	Bioinformation Discovery. **2018**,		1
387	De novo design of a fluorescence-activating β-barrel. *Nature*, **2018**, 561, 485-491	50.4	156
386	Antibody Affinity Maturation by Computational Design. *Methods in Molecular Biology*, **2018**, 1827, 15-34	1.4	14
385	Approaching protein design with multisite λ-dynamics: Accurate and scalable mutational folding free energies in T4 lysozyme. *Protein Science*, **2018**, 27, 1910-1922	6.3	11
384	Peptide and protein nanotechnology into the 2020s: beyond biology. **2018**, 47, 3391-3394		31
383	Blind prediction of noncanonical RNA structure at atomic accuracy. **2018**, 4, eaar5316		25
382	Flagella-mediated secretion of a novel cytotoxin affecting both vertebrate and invertebrate hosts. *Communications Biology*, **2018**, 1, 59	6.7	23
381	RosettaAntibodyDesign (RAbD): A general framework for computational antibody design. *PLoS Computational Biology*, **2018**, 14, e1006112	5	53
380	QM/MM Description of Newly Selected Catalytic Bioscavengers Against Organophosphorus Compounds Revealed Reactivation Stimulus Mediated by Histidine Residue in the Acyl-Binding Loop. **2018**, 9, 834		6
379	Computer-aided design of amino acid-based therapeutics: a review. **2018**, 12, 1239-1254		19
378	Folding up and Moving on-Nascent Protein Folding on the Ribosome. **2018**, 430, 4580-4591		24
377	Essentials of de novo protein design: Methods and applications. **2018**, 8, e1374		22
376	Binary addition in a living cell based on riboregulation. **2018**, 14, e1007548		4
375	Computational protein design-the next generation tool to expand synthetic biology applications. **2018**, 52, 145-152		25
374	Engineering altered protein-DNA recognition specificity. **2018**, 46, 4845-4871		24
373	Contact Potential for Structure Prediction of Proteins and Protein Complexes from Potts Model. **2018**, 115, 809-821		12

372	Computational Design To Reduce Conformational Flexibility and Aggregation Rates of an Antibody Fab Fragment. **2018**, 15, 3079-3092		15
371	Integrating linear optimization with structural modeling to increase HIV neutralization breadth. *PLoS Computational Biology*, **2018**, 14, e1005999	5	4
370	IDeAS: automated design tool for hetero-chiral protein folds. **2018**, 15, 066005		5
369	Protein Design. **2019**, 644-651		1
368	Redox Engineering of Cytochrome c using DNA Nanostructure-Based Charged Encapsulation and Spatial Control. **2019**, 11, 13874-13880		17
367	Synthetic sequence entanglement augments stability and containment of genetic information in cells. *Science*, **2019**, 365, 595-598	33.3	28
366	Advances in protein structure prediction and design. **2019**, 20, 681-697		215
365	Interplay of Protein Disorder in Retinoic Acid Receptor Heterodimer and Its Corepressor Regulates Gene Expression. **2019**, 27, 1270-1285.e6		25
364	Towards functional de novo designed proteins. **2019**, 52, 102-111		39
363	76: A designed antimicrobial peptide to combat carbapenem- and tigecycline-resistant. **2019**, 5, eaax1946		34
362	Targeting trimeric transmembrane domain 5 of oncogenic latent membrane protein 1 using a computationally designed peptide. **2019**, 10, 7584-7590		5
361	General Methodology to Identify the Minimum Alphabet Size for Heteropolymer Design. **2019**, 2, 1900031		5
360	Designing protein structures and complexes with the molecular modeling program Rosetta. **2019**, 294, 19436-19443		13
359	Substrate-imprinted docking of Agrobacterium tumefaciens uronate dehydrogenase for increased substrate selectivity. **2019**, 140, 1214-1225		4
358	Inverse design of charged colloidal particle interactions for self assembly into specified crystal structures. *Journal of Chemical Physics*, **2019**, 151, 084109	3.9	11
357	The computational protein designers. *Nature*, **2019**, 571, 585-587	50.4	7
356	B-SIDER: Computational Algorithm for the Design of Complementary Sheet Sequences. *Journal of Chemical Information and Modeling*, **2019**, 59, 4504-4511	6.1	2
355	Sibe: a computation tool to apply protein sequence statistics to predict folding and design in silico. **2019**, 20, 455		4

354	The influence of biotinylation on the ability of a computer designed protein to detect B-cells producing anti-HIV-1 2F5 antibodies. **2019**, 93, 107442		1
353	Computational design of structured loops for new protein functions. **2019**, 400, 275-288		16
352	Secondary Forces in Protein Folding. **2019**, 14, 1677-1686		44
351	Computational Modeling of Designed Ankyrin Repeat Protein Complexes with Their Targets. **2019**, 431, 2852-2868		2
350	rstoolbox - a Python library for large-scale analysis of computational protein design data and structural bioinformatics. **2019**, 20, 240		11
349	Thermal-response of a protein (hHv1) by a coarse-grained MC and all-atom MD computer simulations. **2019**, 527, 121310		2
348	Validation of protein backbone structures calculated from NMR angular restraints using Rosetta. **2019**, 73, 229-244		7
347	Methods for the Refinement of Protein Structure 3D Models. *International Journal of Molecular Sciences*, **2019**, 20,	6.3	32
346	Feature Design for Protein Interface Hotspots Using KFC2 and Rosetta. **2019**, 177-197		
345	Networks of electrostatic and hydrophobic interactions modulate the complex folding free energy surface of a designed protein. **2019**, 116, 6806-6811		16
344	Research in Data Science. **2019**,		
343	Unraveling the structural elements of pH sensitivity and substrate binding in the human zinc transporter SLC39A2 (ZIP2). **2019**, 294, 8046-8063		10
342	Directed Assembly of Homopentameric Cholera Toxin B-Subunit Proteins into Higher-Order Structures Using Coiled-Coil Appendages. **2019**, 141, 5211-5219		9
341	De Novo Design of Four-Helix Bundle Metalloproteins: One Scaffold, Diverse Reactivities. **2019**, 52, 1148-1159		66
340	Redesign of a novel D-allulose 3-epimerase from Staphylococcus aureus for thermostability and efficient biocatalytic production of D-allulose. **2019**, 18, 59		28
339	Computational Redesign of PD-1 Interface for PD-L1 Ligand Selectivity. **2019**, 27, 829-836.e3		10
338	Random Forest Refinement of the KECSA2 Knowledge-Based Scoring Function for Protein Decoy Detection. *Journal of Chemical Information and Modeling*, **2019**, 59, 1919-1929	6.1	9
337	Domain topology, stability, and translation speed determine mechanical force generation on the ribosome. **2019**, 116, 5523-5532		27

336	What has de novo protein design taught us about protein folding and biophysics?. *Protein Science*, **2019**, 28, 678-683	6.3	81
335	Applications of Fluorescent Protein-Based Sensors in Bioimaging. **2019**, 149-183		1
334	Toward the computational design of protein crystals with improved resolution. *Acta Crystallographica Section D: Structural Biology*, **2019**, 75, 1015-1027	5.5	2
333	Consistency principle for protein design. **2019**, 16, 304-309		5
332	Molecular dynamics simulations suggest stabilizing mutations in a de novo designed protein. **2019**, 32, 317-329		4
331	The importance of catalytic promiscuity for enzyme design and evolution. **2019**, 3, 687-705		90
330	Computational design of Bacillus licheniformis RN-01 levansucrase for control of the chain length of levan-type fructooligosaccharides. **2019**, 140, 1239-1248		14
329	Affinity maturation and characterization of the ofatumumab monoclonal antibody. **2019**, 120, 940-950		16
328	Variable Neighborhood Search with Cost Function Networks To Solve Large Computational Protein Design Problems. *Journal of Chemical Information and Modeling*, **2019**, 59, 127-136	6.1	5
327	Superfunneled Energy Landscape of Protein Evolution Unifies the Principles of Protein Evolution, Folding, and Design. **2019**, 122, 018103		5
326	Protein model discrimination attempts using mutational sensitivity, predicted secondary structure, and model quality information. *Proteins: Structure, Function and Bioinformatics*, **2019**, 87, 326-336	4.2	5
325	ORAI1 channel gating and selectivity is differentially altered by natural mutations in the first or third transmembrane domain. **2019**, 597, 561-582		25
324	A structural homology approach for computational protein design with flexible backbone. **2019**, 35, 2418-2426		4
323	Computational Design of Synthetic Enzymes. **2019**, 119, 6613-6630		79
322	Dynamically Tunable, Macroscopic Molecular Networks Enabled by Cellular Synthesis of 4-Arm Star-like Proteins. **2020**, 2, 233-249		19
321	The Role of Protein Engineering in Biomedical Applications of Mammalian Synthetic Biology. **2020**, 16, e1903093		8
320	From directed evolution to computational enzyme engineering review. **2020**, 66, e16847		31
319	EvoEF2: accurate and fast energy function for computational protein design. **2020**, 36, 1135-1142		33

318	Comparison of Rosetta flexible-backbone computational protein design methods on binding interactions. *Proteins: Structure, Function and Bioinformatics*, **2020**, 88, 206-226	4.2	20
317	Identification of Protein Functional Regions. **2020**, 21, 335-347		0
316	Peptide science: A "rule model" for new generations of peptidomimetics. **2020**, 102, 35-74		13
315	An efficient single pot DNA recombination method for protein library generation. **2020**, 146, 661-667		
314	Toward the Accuracy and Speed of Protein Side-Chain Packing: A Systematic Study on Rotamer Libraries. *Journal of Chemical Information and Modeling*, **2020**, 60, 410-420	6.1	5
313	A general-purpose protein design framework based on mining sequence-structure relationships in known protein structures. **2020**, 117, 1059-1068		30
312	Computer-based Engineering of Thermostabilized Antibody Fragments. **2020**, 66, e16864		4
311	A De Novo Designed Esterase with p-Nitrophenyl Acetate Hydrolysis Activity. *Molecules*, **2020**, 25,	4.8	2
310	Assessing multiple score functions in Rosetta for drug discovery. **2020**, 15, e0240450		7
309	Redesigning HVEM Interface for Selective Binding to LIGHT, BTLA, and CD160. **2020**, 28, 1197-1205.e2		5
308	Influenza Hemagglutinin Head Domain Mimicry by Rational Design. **2020**, 39, 434-448		1
307	Tight and specific lanthanide binding in a de novo TIM barrel with a large internal cavity designed by symmetric domain fusion. **2020**, 117, 30362-30369		17
306	Robust folding of a de novo designed ideal protein even with most of the core mutated to valine. **2020**, 117, 31149-31156		8
305	Physics-Based Computational Protein Design: An Update. **2020**, 124, 10637-10648		7
304	Deep Learning in Protein Structural Modeling and Design. **2020**, 1, 100142		52
303	Hybrid MC/MD for protein design. *Journal of Chemical Physics*, **2020**, 153, 054113	3.9	2
302	Using physical features of protein core packing to distinguish real proteins from decoys. *Protein Science*, **2020**, 29, 1931-1944	6.3	1
301	Synergetic integration of computer-aided design, experimental synthesis, and self-assembly for the rational design of peptide/protein nanofibrils. **2020**, 219-239		

300	IPRO+/-: Computational Protein Design Tool Allowing for Insertions and Deletions. **2020**, 28, 1344-1357.e4		3
299	Can proteins be truly designed sans function?. *Science*, **2020**, 369, 1166-1167	33.3	
298	Expanding the space of protein geometries by computational design of de novo fold families. *Science*, **2020**, 369, 1132-1136	33.3	28
297	Enhanced DNA repair by DNA photolyase bearing an artificial light-harvesting chromophore. **2020**, 48, 10076-10086		4
296	De Novo Protein Design Using the Blueprint Builder in Rosetta. **2020**, 102, e116		0
295	Crystal structure of a novel fold protein Gp72 from the freshwater cyanophage Mic1. *Proteins: Structure, Function and Bioinformatics*, **2020**, 88, 1226-1232	4.2	0
294	The emerging role of computational design in peptide macrocycle drug discovery. **2020**, 15, 833-852		15
293	The advent of de novo proteins for cancer immunotherapy. **2020**, 56, 119-128		5
292	Specificity and affinity of the N-terminal residues in staphylocoagulase in binding to prothrombin. **2020**, 295, 5614-5625		3
291	Recent Advances and Promises in Nitrile Hydratase: From Mechanism to Industrial Applications. **2020**, 8, 352		18
290	Fluorescent Imaging in Medicinal Chemistry. **2020**,		1
289	Different potential of mean force of two-state protein GB1 and downhill protein gpW revealed by molecular dynamics simulation. **2020**, 29, 078701		1
288	Practically useful protein-design methods combining phylogenetic and atomistic calculations. *Current Opinion in Structural Biology*, **2020**, 63, 58-64	8.1	16
287	DeCoDe: degenerate codon design for complete protein-coding DNA libraries. **2020**, 36, 3357-3364		4
286	DenseCPD: Improving the Accuracy of Neural-Network-Based Computational Protein Sequence Design with DenseNet. *Journal of Chemical Information and Modeling*, **2020**, 60, 1245-1252	6.1	10
285	De novo Protein Structure Prediction by Coupling Contact with Distance Profile. **2020**, PP,		1
284	A physics-based energy function allows the computational redesign of a PDZ domain. *Scientific Reports*, **2020**, 10, 11150	4.9	3
283	Pair Potentials as Machine Learning Features. **2020**, 16, 5385-5400		1

282	Structural proteomics, electron cryo-microscopy and structural modeling approaches in bacteria-human protein interactions. **2020**, 209, 265-275		8
281	protein design, a retrospective. **2020**, 53, e3		66
280	Rational design of affinity ligands for bioseparation. **2020**, 1619, 460871		10
279	Deep learning methods in protein structure prediction. **2020**, 18, 1301-1310		80
278	Experimentally-driven protein structure modeling. **2020**, 220, 103777		14
277	Dynamics, a Powerful Component of Current and Future in Silico Approaches for Protein Design and Engineering. *International Journal of Molecular Sciences*, **2020**, 21,	6.3	6
276	Enzyme engineering strategies for catalytic activity in wide pH range. **2020**, 91-101		
275	Identification and Analysis of Natural Building Blocks for Evolution-Guided Fragment-Based Protein Design. **2020**, 432, 3898-3914		14
274	Enabling protein-hosted organocatalytic transformations. **2020**, 10, 16147-16161		4
273	Perturbing the energy landscape for improved packing during computational protein design. *Proteins: Structure, Function and Bioinformatics*, **2021**, 89, 436-449	4.2	22
272	Arming Yourself for The In Silico Protein Design Revolution. **2021**, 39, 651-664		2
271	Bioinformatics and Chemometrics for Discovering Biologically Active Peptides From Food Proteins. **2021**, 482-494		0
270	Stabilizing the closed SARS-CoV-2 spike trimer. *Nature Communications*, **2021**, 12, 244	17.4	60
269	Computationally grafting an IgE epitope onto a scaffold: Implications for a pan anti-allergy vaccine design. **2021**, 19, 4738-4750		0
268	Rosetta design with co-evolutionary information retains protein function. *PLoS Computational Biology*, **2021**, 17, e1008568	5	1
267	A clinically relevant polymorphism in the Na/taurocholate cotransporting polypeptide (NTCP) occurs at a rheostat position. **2021**, 296, 100047		4
266	Bottom-up de novo design of functional proteins with complex structural features. **2021**, 17, 492-500		25
265	Recent advances in de novo protein design: Principles, methods, and applications. **2021**, 296, 100558		29

264	Mutation Maker, An Open Source Oligo Design Platform for Protein Engineering. **2021**, 10, 357-370		2
263	A Rosetta-based protein design protocol converging to natural sequences. *Journal of Chemical Physics*, **2021**, 154, 074114	3.9	1
262	Generating functional protein variants with variational autoencoders. *PLoS Computational Biology*, **2021**, 17, e1008736	5	24
261	Biosupramolecular Systems: Integrating Cues into Responses. **2021**, 143, 4467-4482		13
260	100th Anniversary of Macromolecular Science Viewpoint: Data-Driven Protein Design.. **2021**, 10, 327-340		5
259	Evolution as a Guide to Designing Amino Acid Alphabets. *International Journal of Molecular Sciences* , **2021**, 22,	6.3	5
258	Protein sequence design by conformational landscape optimization. **2021**, 118,		29
257	The symmetric designer protein Pizza as a scaffold for metal coordination. *Proteins: Structure, Function and Bioinformatics*, **2021**, 89, 945	4.2	2
256	Type III secretion system effector proteins are mechanically labile. **2021**, 118,		4
255	Nanoscale programming of cellular and physiological phenotypes: inorganic meets organic programming. **2021**, 7, 15		1
254	Designed Hairpins Inhibit LDH5 Oligomerization and Enzymatic Activity. **2021**, 64, 3767-3779		3
253	The Role of Rigid Residues in Modulating TEM-1 Lactamase Function and Thermostability. *International Journal of Molecular Sciences*, **2021**, 22,	6.3	1
252	De novo sequence redesign of a functional Ras-binding domain globally inverted the surface charge distribution and led to extreme thermostability. **2021**, 118, 2031-2042		2
251	Sampling of Structure and Sequence Space of Small Protein Folds.		4
250	Crystal structures of Scone, pseudosymmetric folding of a symmetric designer protein.		
249	Residue-based pharmacophore approaches to study protein-protein interactions. *Current Opinion in Structural Biology*, **2021**, 67, 205-211	8.1	2
248	PyRosetta Jupyter Notebooks Teach Biomolecular Structure Prediction and Design.. **2021**, 2, 108-122		1
247	Uncovering the modified immunopeptidome reveals insights into principles of PTM-driven antigenicity.		0

246	Protlego: A Python package for the analysis and design of chimeric proteins. **2021**,		6
245	A strategy for proline and glycine mutations to proteins with alchemical free energy calculations. **2021**, 42, 1088-1094		3
244	Current directions in combining simulation-based macromolecular modeling approaches with deep learning. **2021**, 16, 1025-1044		3
243	Step-by-step design of proteins for small molecule interaction: A review on recent milestones. *Protein Science*, **2021**, 30, 1502-1520	6.3	1
242	XENet: Using a new graph convolution to accelerate the timeline for protein design on quantum computers.		
241	Modifying the catalytic preference of alpha-amylase toward n-alkanes for bioremediation purposes using in silico strategies. **2021**, 42, 1540-1551		1
240	Deep learning techniques have significantly impacted protein structure prediction and protein design. *Current Opinion in Structural Biology*, **2021**, 68, 194-207	8.1	16
239	High-Fidelity Sequence-Selective Duplex Formation by Recognition-Encoded Melamine Oligomers. **2021**, 143, 8669-8678		3
238	RosettaSurf - a surface-centric computational design approach.		
237	Computational and experimental assessment of backbone templates for computational protein design.		
236	Role of backbone strain in de novo design of complex α/β protein structures. *Nature Communications*, **2021**, 12, 3921	17.4	9
235	Deep representation learning improves prediction of LacI-mediated transcriptional repression. **2021**, 118,		1
234	Panx1 channels promote both anti- and pro-seizure-like activities in the zebrafish via p2rx7 receptors and ATP signaling.		
233	A Brief History of De Novo Protein Design: Minimal, Rational, and Computational. **2021**, 433, 167160		9
232	Principles and Methods in Computational Membrane Protein Design. **2021**, 433, 167154		2
231	Lattice protein design using Bayesian learning. **2021**, 104, 014404		0
230	Accurately positioning functional residues with robotics-inspired computational protein design.		
229	Design of complicated all-β protein structures.		0

228	The register shift rules for β-motifs for de novo protein design. **2021**, 16, e0256895		1
227	Exploration of novel α/β protein folds through de novo design.		2
226	Gastrobodies are engineered antibody mimetics resilient to pepsin and hydrochloric acid. *Communications Biology*, **2021**, 4, 960	6.7	1
225	De Novo protein design by an energy function based on series expansion in distance and orientation dependence. **2021**,		0
224	Using AlphaFold for Rapid and Accurate Fixed Backbone Protein Design.		4
223	LM-GVP: A Generalizable Deep Learning Framework for Protein Property Prediction from Sequence and Structure.		0
222	XENet: Using a new graph convolution to accelerate the timeline for protein design on quantum computers. *PLoS Computational Biology*, **2021**, 17, e1009037	5	2
221	Mechanism for the Unfolding of the TOP7 Protein in Steered Molecular Dynamics Simulations as Revealed by Mutual Information Analysis. *Frontiers in Molecular Biosciences*, **2021**, 8, 696609	5.6	0
220	Computational and Experimental Assessment of Backbone Templates for Computational Redesign of the Thioredoxin Fold. **2021**, 125, 11141-11149		1
219	A Novel Human Antibody, HF, against HER2/erb-B2 Obtained by a Computer-Aided Antibody Design Method. **2021**,		
218	Spread of Gamma (P.1) sub-lineages carrying Spike mutations close to the furin cleavage site and deletions in the N-terminal domain drives ongoing transmission of SARS-CoV-2 in Amazonas, Brazil.		4
217	Multiobjective heuristic algorithm for protein design in a quantified continuous sequence space. **2021**, 19, 2575-2587		1
216	Molecular flexibility in computational protein design: an algorithmic perspective. **2021**, 34,		6
215	Single molecule force spectroscopy reveals the context dependent folding pathway of the C-terminal fragment of Top7. **2020**, 12, 2876-2884		5
214	Computational design of TNF ligand-based protein therapeutics. **2011**, 691, 521-34		1
213	Design and Fabrication of DNA Origami Mechanisms and Machines. **2012**, 487-500		2
212	Methods for library-scale computational protein design. *Methods in Molecular Biology*, **2014**, 1216, 129-59	1.4	3
211	Flexible Backbone Methods for Predicting and Designing Peptide Specificity. *Methods in Molecular Biology*, **2017**, 1561, 173-187	1.4	3

210	Overcoming the Key Challenges in De Novo Protein Design: Enhancing Computational Efficiency and Incorporating True Backbone Flexibility. **2008**, 133-183	1
209	On-the-Fly Rotamer Pair Energy Evaluation in Protein Design. **2008**, 343-354	4
208	Computational Design in Synthetic Biology. **2009**, 49-63	1
207	The Inverse Protein Folding Problem: Protein Design and Structure Prediction in the Genomic Era. **2012**, 121-140	1
206	Directed Evolution of Enzymes. **2010**, 654-673	1
205	ATOMISTIC MODELING OF PROTEIN ADSORPTION TO CERAMIC BIOMATERIALS IN WATER: A FIRST STEP TOWARD REALISTIC SIMULATION OF THE BIOMATERIALS SURFACE IN VIVO. **2006**, 173-194	1
204	Development and applications of artificial symmetrical proteins. **2020**, 18, 3959-3968	3
203	Chapter 4:Computational Design of Protein Function. 87-107	6
202	ISAMBARD: an open-source computational environment for biomolecular analysis, modelling and design. **2017**, 33, 3043-3050	25
201	High-resolution global peptide-protein docking using fragments-based PIPER-FlexPepDock.	2
200	RosettaAntibodyDesign (RAbD): A General Framework for Computational Antibody Design.	2
199	Protein Sequence Design with a Learned Potential.	11
198	A bottom-up approach for the de novo design of functional proteins.	3
197	Generating functional protein variants with variational autoencoders.	5
196	De novo design of high-affinity antibody variable regions (Fv) against the SARS-CoV-2 spike protein.	2
195	Stabilizing the Closed SARS-CoV-2 Spike Trimer.	3
194	Protein sequence design by explicit energy landscape optimization.	4
193	RamaNet: Computational de novo helical protein backbone design using a long short-term memory generative neural network.	4

192	Designing Peptides on a Quantum Computer.		13
191	A Framework for Scientific Discovery through Video Games.		12
190	The total absolute curvature of open curves in E^{3}. **2008**, 52,		4
189	RamaNet: Computational de novo helical protein backbone design using a long short-term memory generative adversarial neural network. 9, 298		2
188	RamaNet: Computational de novo helical protein backbone design using a long short-term memory generative neural network. 9, 298		7
187	The role of local backrub motions in evolved and designed mutations. *PLoS Computational Biology*, **2012**, 8, e1002629	5	24
186	Principles and Overview of Sampling Methods for Modeling Macromolecular Structure and Dynamics. *PLoS Computational Biology*, **2016**, 12, e1004619	5	124
185	The roles of entropy and kinetics in structure prediction. **2009**, 4, e5840		7
184	Computational protein design: validation and possible relevance as a tool for homology searching and fold recognition. **2010**, 5, e10410		16
183	Nonnative interactions in coupled folding and binding processes of intrinsically disordered proteins. **2010**, 5, e15375		34
182	Predicting the tolerated sequences for proteins and protein interfaces using RosettaBackrub flexible backbone design. **2011**, 6, e20451		73
181	A generic program for multistate protein design. **2011**, 6, e20937		74
180	Generalized fragment picking in Rosetta: design, protocols and applications. **2011**, 6, e23294		131
179	RosettaRemodel: a generalized framework for flexible backbone protein design. **2011**, 6, e24109		200
178	A Pareto-optimal refinement method for protein design scaffolds. **2013**, 8, e59004		120
177	Alternative computational protocols for supercharging protein surfaces for reversible unfolding and retention of stability. **2013**, 8, e64363		50
176	Bayesian weighting of statistical potentials in NMR structure calculation. **2014**, 9, e100197		4
175	Kinetic and sequence-structure-function analysis of LinB enzyme variants with and hexachlorocyclohexane. **2014**, 9, e103632		4

174	How structure defines affinity in protein-protein interactions. **2014**, 9, e110085		46
173	Transferable coarse-grained potential for de novo protein folding and design. **2014**, 9, e112852		19
172	A Framework to Simplify Combined Sampling Strategies in Rosetta. **2015**, 10, e0138220		10
171	Enhancing the Thermostability of Serratia plymuthica Sucrose Isomerase Using B-Factor-Directed Mutagenesis. **2016**, 11, e0149208		21
170	Mapping the Geometric Evolution of Protein Folding Motor. **2016**, 11, e0163993		7
169	Diversity of protein structures and difficulties in fold recognition: the curious case of protein G. **2009**, 1, 69		8
168	Regulating and Programming Biological Systems With Modular Molecular Parts. **2012**, 39, 119-125		1
167	HLA mismatches and hematopoietic cell transplantation: structural simulations assess the impact of changes in peptide binding specificity on transplant outcome. **2011**, 7, 4		6
166	Impact of the Protein Data Bank Across Scientific Disciplines. **2020**, 19, 25		9
165	Amino-acid site variability among natural and designed proteins. **2013**, 1, e211		13
164	Recording of cellular physiological histories along optically readable self-assembling protein chains.		1
163	Modularity-based parallel protein design algorithm with an implementation using shared memory programming. *Proteins: Structure, Function and Bioinformatics*, **2021**,	4.2	1
162	AlphaDesign: A de novo protein design framework based on AlphaFold.		9
161	De Novo Design of .LAMBDA. Cro Fold. **2007**, 47, 185-189		
160	Chemical Complementation Assays. 183		
159	Interpreting The Observed Substrate Selectivity And The Product Regioselectivity In Orf2-Catalyzed Prenylation From X-Ray Structures. **2009**, 351-375		
158	Tools and Techniques. **2009**, 65-77		
157	Thermostable Proteins. 1		

156 Protein Folding, Structure Prediction and the Principle of Protein Architecture. **2010**, 50, 210-211 1

155 Recent Advances inDe NovoProtein Design. 207-232

154 Mechanics of Proteins and Tailored Mechanics of Engineered Proteins. **2011**, 47-82

153 Introduction. **2012**, 1-3

152 Proteins made to order. *Nature*, 50.4

151 Predicting the Outer/Inner BetaStrands in Protein Beta Sheets Based on the Random Forest Algorithm. **2014**, 1-9 1

150 Nanomechanics of Single Biomacromolecules. **2014**, 1077-1123

149 Protein Structure Prediction. 33-66

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147 Protein Structure Refinement Algorithms. 83-108

146 Framework. 9-31

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144 Bibliography. 111

143 Protein Design. 67-82

142 Introduction. 1-4

141 Related Literature. 5-8

140 Introduction. **2016**, 1-14

139 Scoring Functions for Predicting Structure and Binding of Proteins. **2016**, 29-78

138	Generating the Fancy Protein Basket with De Novo and Combinatorial Approaches. **2017**, 85-102	
137	An Adaptive Geometric Search Algorithm for Macromolecular Scaffold Selection.	
136	Global Nonlinear Fitness Function for Protein Structures. **2017**, 1-35	
135	Rational design of proteins that exchange on functional timescales.	
134	Beyond thermodynamic constraints: Evolutionary sampling generates realistic protein sequence variation.	
133	Tools and Techniques. **2018**, 75-94	
132	Sibe: a computation tool to apply protein sequence statistics to folding and design.	
131	Rosetta FunFolDes a general framework for the computational design of functional proteins.	1
130	rstoolbox: management and analysis of computationally designed structural ensembles.	1
129	Interplay of protein disorder in retinoic acid receptor heterodimer and its corepressor regulates gene expression.	
128	A general-purpose protein design framework based on mining sequence-structure relationships in known protein structures.	1
127	Design Guidelines For Sequestration Feedback Networks.	
126	Enhanced Sampling for Biomolecular Simulations. **2019**, 257-280	0
125	Domain topology, stability, and translation speed determine mechanical force generation on the ribosome.	1
124	Design of Self-Assembling Molecules and Boundary Value Problem for Flows on a Space of <i>n</i>-Simplices. **2019**, 10, 907-946	1
123	Feature Design for Protein Interface hotspots using KFC2 and Rosetta.	
122	B-SIDER: Computational Algorithm for the Design of Complementary sheet Sequences.	
121	Molecular Determinants of conotoxin KIIIA Interaction with the Human Voltage-Gated Sodium Channel NaV1.7.	

120	Toward computational design of protein crystals with improved resolution.	
119	Combining statistical and neural network approaches to derive energy functions for completely flexible protein backbone design.	
118	Comparison of Rosetta flexible-backbone computational protein design methods on binding interactions.	
117	Cloning, phylogenetic research, and prokaryotic expression study of the metabolic detoxification gene in Matsuda. **2019**, 7, e7641	
116	DeCoDe: degenerate codon design for complete protein-coding DNA libraries.	
115	A physics-based energy function allows the computational redesign of a PDZ domain.	1
114	Consistency Principle for Protein Design. **2020**, 60, 325-330	
113	Expanding the space of protein geometries by computational design of de novo fold families.	
112	Mutation Maker, An Open Source Oligo Design Platform for Protein Engineering.	
111	A clinically-relevant polymorphism in the Na+/taurocholate cotransporting polypeptide (NTCP) occurs at a rheostat position.	1
110	The biophysical basis of protein domain compatibility.	0
109	Nascent SecM chain interacts with outer ribosomal surface to stabilize translation arrest. **2020**, 477, 557-566	0
108	Protein Nanostructures with Purpose-Designed Properties in Biotechnology and Medicine. **2020**, 71-89	1
107	Encyclopedia of Biophysics. **2020**, 1-7	
106	Proteus software for physics-based protein design.	1
105	Monte-Carlo Methods in Studies of Protein Folding and Evolution. **2006**, 563-593	
104	Protlego: A Python package for the analysis and design of chimeric proteins.	0
103	RamaNet: Computational de novo helical protein backbone design using a long short-term memory generative neural network. 9, 298	1

102	Computationally Grafting an IgE Epitope onto a Scaffold: Implications for a Pan Anti-Allergy Vaccine Design.		
101	Ofatumumab Monoclonal Antibody Affinity Maturation Through in silico Modeling. **2018**, 22, 180-92		10
100	Fold2Seq: A Joint Sequence(1D)-Fold(3D) Embedding-based Generative Model for Protein Design. **2021**, 139, 1261-1271		0
99	Discussion Commemorating the 60th Anniversary of SEIBUTSU BUTSURI III: Concepts and Perspectives in Biophysics. **2021**, 61, 410-418		
98	Assessing and enhancing foldability in designed proteins.		0
97	State-Targeting Stabilization of Adenosine A Receptor by Fusing a Custom-Made De Novo Designed Helical Protein. *International Journal of Molecular Sciences*, **2021**, 22,	6.3	2
96	Surface Engineering of Top7 to Facilitate Structure Determination.. *International Journal of Molecular Sciences*, **2022**, 23,	6.3	
95	Structural DNA nanotechnology: Immobile Holliday junctions to artificial robots.. *Current Topics in Medicinal Chemistry*, **2022**,	3	1
94	Active site center redesign increases protein stability preserving catalysis.		
93	Incorporation of metal-chelating unnatural amino acids into halotag for allylic deamination. *Journal of Organometallic Chemistry*, **2022**, 962, 122272	2.3	2
92	Research progress of glucoamylase with industrial potential.. *Journal of Food Biochemistry*, **2022**, e14099	3.3	2
91	De Novo Peptide and Protein Design Using Generative Adversarial Networks: An Update.. *Journal of Chemical Information and Modeling*, **2022**,	6.1	3
90	A backbone-centred energy function of neural networks for protein design.. *Nature*, **2022**,	50.4	4
89	Probing ion channel functional architecture and domain recombination compatibility by massively parallel domain insertion profiling. *Nature Communications*, **2021**, 12, 7114	17.4	3
88	Protein Symmetry, Function and Stability. **2022**,		
87	Advances in the Computational Design of Small-Molecule-Controlled Protein-Based Circuits for Synthetic Biology. *Proceedings of the IEEE*, **2022**, 1-16	14.3	2
86	Structural Prediction of Peptide-MHC Binding Modes.. *Methods in Molecular Biology*, **2022**, 2405, 245-282	1.4	1
85	From 4-arm star proteins to diverse stimuli-responsive molecular networks enabled by orthogonal genetically encoded click chemistries. *Polymer Chemistry*,	4.9	1

84	Algorithms for protein design.. *Advances in Protein Chemistry and Structural Biology*, **2022**, 130, 1-38	5.3	0
83	Computational Design of Miniprotein Binders.. *Methods in Molecular Biology*, **2022**, 2405, 361-382	1.4	0
82	Can the Jigsaw Puzzle Model of Protein Folding Re-assemble a Hydrophobic Core?. *Proteins: Structure, Function and Bioinformatics*, **2022**,	4.2	0
81	Spread of Gamma (P.1) Sub-Lineages Carrying Spike Mutations Close to the Furin Cleavage Site and Deletions in the N-Terminal Domain Drives Ongoing Transmission of SARS-CoV-2 in Amazonas, Brazil.. *Microbiology Spectrum*, **2022**, 10, e0236621	8.9	3
80	Interactions between Artificial Channel Protein, Water Molecules, and Ions Based on Theoretical Approaches. *Symmetry*, **2022**, 14, 691	2.7	1
79	RosettaSurf-A surface-centric computational design approach.. *PLoS Computational Biology*, **2022**, 18, e1009178	5	0
78	Advances in Rational Protein Engineering toward Functional Architectures and Their Applications in Food Science.. *Journal of Agricultural and Food Chemistry*, **2022**,	5.7	1
77	Transient Water Wires Mediate Selective Proton Conduction in Designed Channel Proteins.		
76	What Have We Learned from Design of Function in Large Proteins?. *Biodesign Research*, **2022**, 2022, 1-11	3.1	2
75	The X-ray crystallography phase problem solved thanks to AlphaFold and RoseTTAFold models: a case-study report.. *Acta Crystallographica Section D: Structural Biology*, **2022**, 78, 517-531	5.5	1
74	Protein design via deep learning.. *Briefings in Bioinformatics*, **2022**,	13.4	1
73	Optogenetic tools for microbial synthetic biology.. *Biotechnology Advances*, **2022**, 107953	17.8	0
72	Computational design of novel protein-protein interactions - An overview on methodological approaches and applications.. *Current Opinion in Structural Biology*, **2022**, 74, 102370	8.1	2
71	Computational Design of Peptides with Improved Recognition of the Focal Adhesion Kinase FAT Domain.. *Methods in Molecular Biology*, **2022**, 2405, 383-402	1.4	
70	Knowledge-Based Unfolded State Model for Protein Design.. *Methods in Molecular Biology*, **2022**, 2405, 403-424	1.4	
69	De Novo Design of Immunoglobulin-like Domains.		0
68	Generative power of a protein language model trained on multiple sequence alignments.		0
67	De Novo Protein Design Using Flexible Templates. **2008**, 638-643		1

66	Presentation_1.PDF. **2018**,		
65	LM-GVP: an extensible sequence and structure informed deep learning framework for protein property prediction.. *Scientific Reports*, **2022**, 12, 6832	4.9	0
64	Design and Engineering of Miniproteins. *ACS Bio & Med Chem Au*,		1
63	Tertiary motifs as building blocks for the design of protein-binding peptides. *Protein Science*, **2022**, 31,	6.3	0
62	Biotin-painted proteins have thermodynamic stability switched by kinetic folding routes. *Journal of Chemical Physics*,	3.9	0
61	Panx1 channels promote both anti- and pro-seizure-like activities in the zebrafish via p2rx7 receptors and ATP signaling.. *Communications Biology*, **2022**, 5, 472	6.7	0
60	Prediction of allosterically acting mutations using MD simulations and Rosetta.		
59	Tau Aggregation Inhibiting Peptides as Potential Therapeutics for Alzheimer Disease. *Cellular and Molecular Neurobiology*,	4.6	1
58	The Structural Rule Distinguishing a Superfold: A Case Study of Ferredoxin Fold and the Reverse Ferredoxin Fold. *Molecules*, **2022**, 27, 3547	4.8	
57	Transcriptome-wide mapping reveals a diverse dihydrouridine landscape including mRNA. *PLoS Biology*, **2022**, 20, e3001622	9.7	0
56	High-throughput discovery of TRAF6-interacting peptides identifies determinants of positive and negative design and shows known and candidate human interaction partner motifs are not optimized for affinity.		
55	Improved Repeat Protein Stability by Combined Consensus and Computational Protein Design. *Biochemistry*,	3.2	0
54	Key aspects of the past 30 Years of protein design. *Reports on Progress in Physics*,	14.4	1
53	Predicting the locations of cryptic pockets from single protein structures using the PocketMiner graph neural network.		0
52	Accurate and efficient protein sequence design through learning concise local environment of residues.		
51	A Method for Assessing the Robustness of Protein Structures by Randomizing Packing Interactions. *Frontiers in Molecular Biosciences*, 9,	5.6	
50	Protein as evolvable functionally-constrained amorphous matter.		
49	Rotamer-free protein sequence design based on deep learning and self-consistency. *Nature Computational Science*, **2022**, 2, 451-462		0

48	Computational design of peptides to target NaV1.7 channel with high potency and selectivity for the treatment of pain.	
47	Ferrous iron uptake via IRT1/ZIP evolved at least twice in green plants.	
46	Design of Peptides that Fold and Self-Assemble on Graphite.	0
45	Immunostimulatory Polymers as Adjuvants, Immunotherapies, and Delivery Systems. **2022**, 55, 6913-6937	1
44	Assessing and enhancing foldability in designed proteins. **2022**, 31,	1
43	Active site center redesign increases protein stability preserving catalysis in thioredoxin. **2022**, 31,	0
42	Protein Design: From the Aspect of Water Solubility and Stability.	7
41	Protein scaffolds in human clinics. **2022**, 61, 108032	1
40	Computational Methods for Peptide Macrocycle Drug Design. **2022**, 79-161	0
39	Protein–protein interaction prediction with deep learning: A comprehensive review. **2022**, 20, 5316-5341	0
38	Recurrent neural network model for identifying epilepsy based neurological auditory disorder. **2023**, 91-105	0
37	Configurational entropy, transition rates, and optimal interactions for rapid folding in coarse-grained model proteins. **2022**, 157, 125101	0
36	De novo design and Rosetta-based assessment of high-affinity antibody variable regions (Fv) against the SARS-CoV -2 spike receptor binding domain (RBD).	0
35	Differential regulation of insulin signaling by monomeric and oligomeric amyloid beta-peptide.	0
34	Biotinylation Eliminates the Intermediate State of Top7 Designed with an HIV-1 Epitope. **2022**, 126, 7331-7342	0
33	Identifying well-folded de novo proteins in the new era of accurate structure prediction. 9,	0
32	De novo design of immunoglobulin-like domains. **2022**, 13,	0
31	Post-translational modifications reshape the antigenic landscape of the MHC I immunopeptidome in tumors.	0

30	Molecular determinants of TRAF6 binding specificity suggest that native interaction partners are not optimized for affinity. **2022**, 31,	0
29	Design and optimization of enzymatic activity in a de novo □barrel scaffold. **2022**, 31,	0
28	Time-resolved Spectroscopic Mapping of Vibrational Energy Flow in Proteins: Understanding Thermal Diffusion at the Nanoscale.	0
27	Computational protein design with data-driven approaches: Recent developments and perspectives.	0
26	An efficient method to predict protein thermostability in alanine mutation. **2022**, 24, 29629-29639	0
25	Sampling of structure and sequence space of small protein folds. **2022**, 13,	0
24	Design of artificial enzymes: insights into protein scaffolds.	0
23	Broadly applicable and accurate protein design by integrating structure prediction networks and diffusion generative models.	1
22	Language models generalize beyond natural proteins.	0
21	Coordinate-Dependent Drift-Diffusion Reveals the Kinetic Intermediate Traps of Top7-Based Proteins.	0
20	De novo protein backbone generation based on diffusion with structured priors and adversarial training.	0
19	A high-level programming language for generative protein design.	0
18	Protein as evolvable functionally constrained amorphous matter. **2022**, 47,	0
17	De novo protein design by inversion of the AlphaFold structure prediction network.	0
16	Computational design of constitutively active cGAS.	0
15	Computational design of peptides to target NaV1.7 channel with high potency and selectivity for the treatment of pain. 11,	0
14	A probabilistic view of protein stability, conformational specificity, and design.	0
13	Structural features of sensory two component systems: a synthetic biology perspective. **2023**, 480, 127-140	0

12	Protein Structure Determination using Sparse NMR Data. **2012**, 84-110	0
11	Protein Engineering Methods to Design Protein Therapeutics. **2023**, 49-100	0
10	Designing artificial pathways for improving chemical production. **2023**, 64, 108119	0
9	Generative power of a protein language model trained on multiple sequence alignments. 12,	0
8	Quantitative comparison of protein-protein interaction interface using physicochemical feature-based descriptors of surface patches. 10,	0
7	Predicting binding affinity changes from long-distance mutations using molecular dynamics simulations and Rosetta.	0
6	Network of hotspot interactions cluster tau amyloid folds. **2023**, 14,	0
5	Computational Insights into the Allosteric Modulation of a Phthalate-Degrading Hydrolase by Distal Mutations. **2023**, 13, 443	0
4	Computational design of a cyclic peptide that inhibits the CTLA4 immune checkpoint.	0
3	Molecular determinants of Ɛconotoxin KIIIA interaction with the human voltage-gated sodium channel NaV1.7. 14,	0
2	Computational Protein Design for COVID-19 Research and Emerging Therapeutics.	0
1	De novodesign of stable proteins that efficaciously inhibit oncogenic G proteins.	0