Sandor Vajda

List of Publications by Year
in descending order

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184	16,306	27035	20625
papers	citations	58	120
		h-index	g-index

194	194	194	17607
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Side-chain Packing Using SE(3)-Transformer. Pacific Symposium on Biocomputing Pacific Symposium on Biocomputing, 2022, 27, 46-55.	0.7	0
2	FTMove: A Web Server for Detection and Analysis of Cryptic and Allosteric Binding Sites by Mapping Multiple Protein Structures. Journal of Molecular Biology, 2022, 434, 167587.	2.0	12
3	Elucidation of protein function using computational docking and hotspot analysis by ClusPro and FTMap. Acta Crystallographica Section D: Structural Biology, 2022, 78, 690-697.	1.1	3
4	Mapping the binding sites of challenging drug targets. Current Opinion in Structural Biology, 2022, 75, 102396.	2.6	8
5	API Development Increases Access to Shared Computing Resources at Boston University. Journal of Software Engineering and Applications, 2022, 15, 197-207.	0.8	3
6	Conservation of binding properties in protein models. Computational and Structural Biotechnology Journal, 2021, 19, 2549-2566.	1.9	2
7	Improved cluster ranking in proteinâ€“protein docking using a regression approach. Computational and Structural Biotechnology Journal, 2021, 19, 2269-2278.	1.9	6
8	Progress toward improved understanding of antibody maturation. Current Opinion in Structural Biology, 2021, 67, 226-231.	2.6	12
9	Exploring protein hotspots by optimized fragment pharmacophores. Nature Communications, 2021, 12, 3201.	5.8	28
10	Assessing the binding properties of <scp>CASP14</scp> targets and models. Proteins: Structure, Function and Bioinformatics, 2021, 89, 1922-1939.	1.5	11
11	Prediction of protein assemblies, the next frontier: The <scp>CASP14â€CAPRI</scp> experiment. Proteins: Structure, Function and Bioinformatics, 2021, 89, 1800-1823.	1.5	73
12	Side-chain Packing Using SE(3)-Transformer. , 2021, , .		2
13	ClusPro LigTBM: Automated Template-based Small Molecule Docking. Journal of Molecular Biology, 2020, 432, 3404-3410.	2.0	17
14	Modeling betaâ€sheet peptideâ€protein interactions: Rosetta FlexPepDock in CAPRI rounds 38â€45. Proteins: Structure, Function and Bioinformatics, 2020, 88, 1037-1049.	1.5	10
15	Interaction Energetics and Druggability of the Proteinâ€“Protein Interaction between Kelch-like ECH-Associated Protein 1 (KEAP1) and Nuclear Factor Erythroid 2 Like 2 (Nrf2). Biochemistry, 2020, 59, 563-581.	1.2	28
16	Structure-Based Analysis of Cryptic-Site Opening. Structure, 2020, 28, 223-235.e2.	1.6	13
17	Performance and Its Limits in Rigid Body Protein-Protein Docking. Structure, 2020, 28, 1071-1081.e3.	1.6	306
18	Benchmark Sets for Binding Hot Spot Identification in Fragment-Based Ligand Discovery. Journal of Chemical Information and Modeling, 2020, 60, 6612-6623.	2.5	10

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19	ClusPro in rounds 38 to 45 of CAPRI: Toward combining templateâ€based methods with free docking. Proteins: Structure, Function and Bioinformatics, 2020, 88, 1082-1090.	1.5	5
20	Templateâ€based modeling by ClusPro in CASP13 and the potential for using coâ€evolutionary information in docking. Proteins: Structure, Function and Bioinformatics, 2019, 87, 1241-1248.	1.5	15
21	Blind prediction of homoâ€and heteroâ€protein complexes: The CASP13â€CAPRI experiment. Proteins: Structure, Function and Bioinformatics, 2019, 87, 1200-1221.	1.5	99
22	Amidino-Rocaglates: A Potent Class of eIF4A Inhibitors. Cell Chemical Biology, 2019, 26, 1586-1593.e3.	2.5	45
23	What method to use for proteinâ€“protein docking?. Current Opinion in Structural Biology, 2019, 55, 1-7.	2.6	83
24	Kinase Atlas: Druggability Analysis of Potential Allosteric Sites in Kinases. Journal of Medicinal Chemistry, 2019, 62, 6512-6524.	2.9	52
25	Why Some Targets Benefit from beyond Rule of Five Drugs. Journal of Medicinal Chemistry, 2019, 62, 10005-10025.	2.9	75
26	Analysis of tractable allosteric sites in G protein-coupled receptors. Scientific Reports, 2019, 9, 6180.	1.6	31
27	Discovery of Macrocyclic Inhibitors of Apurinic/Apyrimidinic Endonuclease 1. Journal of Medicinal Chemistry, 2019, 62, 1971-1988.	2.9	12
28	Structure-based Druggability Assessment of Anti-virulence Targets from Pseudomonas aeruginosa. Current Protein and Peptide Science, 2019, 20, 1189-1203.	0.7	9
29	Mapping global protein contacts. Science, 2019, 365, 120-121.	6.0	1
30	Mapping global protein contacts. Science, 2019, 365, 120-121.	6.0	3
31	Protein docking refinement by convex underestimation in the low-dimensional subspace of encounter complexes. Scientific Reports, 2018, 8, 5896.	1.6	5
32	Exploring the structural origins of cryptic sites on proteins. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E3416-E3425.	3.3	96
33	Cryptic binding sites on proteins: definition, detection, and druggability. Current Opinion in Chemical Biology, 2018, 44, 1-8.	2.8	119
34	A benchmark testing ground for integrating homology modeling and protein docking. Proteins: Structure, Function and Bioinformatics, 2017, 85, 10-16.	1.5	29
35	The ClusPro web server for proteinâ€“protein docking. Nature Protocols, 2017, 12, 255-278.	5.5	1,959
36	New additions to the <scp>C</scp>lus<scp>P</scp>ro server motivated by <scp>CAPRI</scp>. Proteins: Structure, Function and Bioinformatics, 2017, 85, 435-444.	1.5	395

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37	ClusPro-DC: Dimer Classification by the Cluspro Server for Proteinâ€“Protein Docking. Journal of Molecular Biology, 2017, 429, 372-381.	2.0	36
38	Focused gridâ€based resampling for protein docking and mapping. Journal of Computational Chemistry, 2016, 37, 961-970.	1.5	6
39	Prediction of homoprotein and heteroprotein complexes by protein docking and templateâ€based modeling: A CASPâ€CAPRI experiment. Proteins: Structure, Function and Bioinformatics, 2016, 84, 323-348.	1.5	148
40	Proteinâ€“protein docking by fast generalized Fourier transforms on 5D rotational manifolds. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, E4286-93.	3.3	43
41	Quantifying the chameleonic properties of macrocycles and other high-molecular-weight drugs. Drug Discovery Today, 2016, 21, 712-717.	3.2	185
42	Challenges in structural approaches to cell modeling. Journal of Molecular Biology, 2016, 428, 2943-2964.	2.0	51
43	Accounting for pairwise distance restraints in FFT-based proteinâ€“protein docking. Bioinformatics, 2016, 32, 3342-3344.	1.8	38
44	Accounting for observed small angle Xâ€ray scattering profile in the proteinâ€“protein docking server cluspro. Journal of Computational Chemistry, 2015, 36, 1568-1572.	1.5	27
45	Conservation and Covariance in Small Bacterial Phosphoglycosyltransferases Identify the Functional Catalytic Core. Biochemistry, 2015, 54, 7326-7334.	1.2	30
46	Energy Minimization on Manifolds for Docking Flexible Molecules. Journal of Chemical Theory and Computation, 2015, 11, 1063-1076.	2.3	24
47	The Impact of Side-Chain Packing on Protein Docking Refinement. Journal of Chemical Information and Modeling, 2015, 55, 872-881.	2.5	15
48	New Frontiers in Druggability. Journal of Medicinal Chemistry, 2015, 58, 9063-9088.	2.9	93
49	Ligand deconstruction: Why some fragment binding positions are conserved and others are not. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, E2585-94.	3.3	61
50	The FTMap family of web servers for determining and characterizing ligand-binding hot spots of proteins. Nature Protocols, 2015, 10, 733-755.	5.5	496
51	Lessons from Hot Spot Analysis for Fragment-Based Drug Discovery. Trends in Pharmacological Sciences, 2015, 36, 724-736.	4.0	58
52	Fragments and hot spots in drug discovery. Oncotarget, 2015, 6, 18740-18741.	0.8	5
53	Fragmentâ€based Drug Discovery Targeting KEAP1/Nrf2 Binding. FASEB Journal, 2015, 29, 712.20.	0.2	1
54	Optimization on the space of rigid and flexible motions: An alternative manifold optimization approach. , 2014, 2014, 5825-5830.		1

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55	Evidence of Conformational Selection Driving the Formation of Ligand Binding Sites in Protein-Protein Interfaces. PLoS Computational Biology, 2014, 10, e1003872.	1.5	22
56	Ligand Binding and Activation of PPAR Î³ by Firemaster ^{Â®} 550: Effects on Adipogenesis and Osteogenesis in Vitro. Environmental Health Perspectives, 2014, 122, 1225-1232.	2.8	167
57	A Subspace Semi-Definite programming-based Underestimation (SSDU) method for stochastic global optimization in protein docking. , 2014, 2014, 4623-4628.		1
58	Insights into the Architecture of the eIF2BÎ±/Î²/Î´ Regulatory Subcomplex. Biochemistry, 2014, 53, 3432-3445.	1.2	32
59	Blind prediction of interfacial water positions in CAPRI. Proteins: Structure, Function and Bioinformatics, 2014, 82, 620-632.	1.5	50
60	Docking Server for the Identification of Heparin Binding Sites on Proteins. Journal of Chemical Information and Modeling, 2014, 54, 2068-2078.	2.5	56
61	How proteins bind macrocycles. Nature Chemical Biology, 2014, 10, 723-731.	3.9	329
62	Efficient Maintenance and Update of Nonbonded Lists in Macromolecular Simulations. Journal of Chemical Theory and Computation, 2014, 10, 4449-4454.	2.3	2
63	In Silico Identification of an Aryl Hydrocarbon Receptor Antagonist with Biological Activity In Vitro and In Vivo. Molecular Pharmacology, 2014, 86, 593-608.	1.0	45
64	Stimulators of translation identified during a small molecule screening campaign. Analytical Biochemistry, 2014, 447, 6-14.	1.1	4
65	Encounter complexes and dimensionality reduction in proteinâ€“protein association. ELife, 2014, 3, e01370.	2.8	61
66	How good is automated protein docking?. Proteins: Structure, Function and Bioinformatics, 2013, 81, 2159-2166.	1.5	570
67	Sampling and scoring: A marriage made in heaven. Proteins: Structure, Function and Bioinformatics, 2013, 81, 1874-1884.	1.5	58
68	Comprehensive Experimental and Computational Analysis of Binding Energy Hot Spots at the NF-ÎºB Essential Modulator/IKKÎ² Proteinâ€“Protein Interface. Journal of the American Chemical Society, 2013, 135, 6242-6256.	6.6	44
69	FTFlex: accounting for binding site flexibility to improve fragment-based identification of druggable hot spots. Bioinformatics, 2013, 29, 1218-1219.	1.8	30
70	Flexible refinement of protein-ligand docking on manifolds. , 2013, , 1392-1397.		2
71	A new distributed algorithm for side-chain positioning in the process of protein docking. , 2013, , 739-744.		3
72	Community-wide evaluation of methods for predicting the effect of mutations on protein-protein interactions. Proteins: Structure, Function and Bioinformatics, 2013, 81, 1980-1987.	1.5	87

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73	Application of asymmetric statistical potentials to antibodyâ€“protein docking. Bioinformatics, 2012, 28, 2608-2614.	1.8	156
74	Computational mapping reveals dramatic effect of Hoogsteen breathing on duplex DNA reactivity with formaldehyde. Nucleic Acids Research, 2012, 40, 7644-7652.	6.5	37
75	A new approach to rigid body minimization with application to molecular docking. , 2012, , 2983-2988.		4
76	FTMAP: extended protein mapping with user-selected probe molecules. Nucleic Acids Research, 2012, 40, W271-W275.	6.5	130
77	Rigid Body Energy Minimization on Manifolds for Molecular Docking. Journal of Chemical Theory and Computation, 2012, 8, 4374-4380.	2.3	22
78	A message passing approach to Side Chain Positioning with applications in protein docking refinement. , 2012, , 2310-2315.		3
79	Analysis of Protein Binding Sites by Computational Solvent Mapping. Methods in Molecular Biology, 2012, 819, 13-27.	0.4	19
80	Hot Spot Analysis for Driving the Development of Hits into Leads in Fragment-Based Drug Discovery. Journal of Chemical Information and Modeling, 2012, 52, 199-209.	2.5	52
81	Minimal ensembles of side chain conformers for modeling proteinâ€“protein interactions. Proteins: Structure, Function and Bioinformatics, 2012, 80, 591-601.	1.5	26
82	Relationship between Hot Spot Residues and Ligand Binding Hot Spots in Proteinâ€“Protein Interfaces. Journal of Chemical Information and Modeling, 2012, 52, 2236-2244.	2.5	99
83	FTSite: high accuracy detection of ligand binding sites on unbound protein structures. Bioinformatics, 2012, 28, 286-287.	1.8	189
84	Robust Identification of Binding Hot Spots Using Continuum Electrostatics: Application to Hen Egg-White Lysozyme. Journal of the American Chemical Society, 2011, 133, 20668-20671.	6.6	28
85	Analysis of Binding Site Hot Spots on the Surface of Ras GTPase. Journal of Molecular Biology, 2011, 413, 773-789.	2.0	139
86	Blocking eIF4E-eIF4G Interaction as a Strategy To Impair Coronavirus Replication. Journal of Virology, 2011, 85, 6381-6389.	1.5	93
87	Reversing chemoresistance by small molecule inhibition of the translation initiation complex eIF4F. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 1046-1051.	3.3	153
88	Structural conservation of druggable hot spots in proteinâ€“protein interfaces. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 13528-13533.	3.3	220
89	Where does amantadine bind to the influenza virus M2 proton channel?. Trends in Biochemical Sciences, 2010, 35, 471-475.	3.7	41
90	Domain motion and interdomain hot spots in a multidomain enzyme. Protein Science, 2010, 19, 1662-1672.	3.1	21

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91	Achieving reliability and high accuracy in automated protein docking: Cluspro, PIPER, SDU, and stability analysis in CAPRI rounds 13â€“19. Proteins: Structure, Function and Bioinformatics, 2010, 78, 3124-3130.	1.5	211
92	Fragment-based identification of druggable â€˜hot spotsâ€™ of proteins using Fourier domain correlation techniques. Bioinformatics, 2009, 25, 621-627.	1.8	402
93	Convergence and combination of methods in proteinâ€“protein docking. Current Opinion in Structural Biology, 2009, 19, 164-170.	2.6	195
94	Detection of ligand binding hot spots on protein surfaces via fragment-based methods: application to DJ-1 and glucocerebrosidase. Journal of Computer-Aided Molecular Design, 2009, 23, 491-500.	1.3	77
95	Structural insights into recognition of Î²2â€glycoprotein I by the lipoprotein receptors. Proteins: Structure, Function and Bioinformatics, 2009, 77, 940-949.	1.5	9
96	Binding Hot Spots and Amantadine Orientation in the Influenza A Virus M2 Proton Channel. Biophysical Journal, 2009, 97, 2846-2853.	0.2	39
97	The Structural Basis of Pregnane X Receptor Binding Promiscuity. Biochemistry, 2009, 48, 11572-11581.	1.2	70
98	Identification of Druggable Hot Spots on Proteins and in Proteinâ€“ Protein Interfaces. , 2009, , 253-280.		0
99	Discrimination of nearâ€native structures in proteinâ€“protein docking by testing the stability of local minima. Proteins: Structure, Function and Bioinformatics, 2008, 72, 993-1004.	1.5	41
100	Novel Druggable Hot Spots in Avian Influenza Neuraminidase H5N1 Revealed by Computational Solvent Mapping of a Reduced and Representative Receptor Ensemble. Chemical Biology and Drug Design, 2008, 71, 106-116.	1.5	97
101	DARS (Decoys As the Reference State) Potentials for Protein-Protein Docking. Biophysical Journal, 2008, 95, 4217-4227.	0.2	141
102	Accelerating and focusing proteinâ€“protein docking correlations using multi-dimensional rotational FFT generating functions. Bioinformatics, 2008, 24, 1865-1873.	1.8	175
103	Protein Docking by the Underestimation of Free Energy Funnels in the Space of Encounter Complexes. PLoS Computational Biology, 2008, 4, e1000191.	1.5	41
104	SDU: A Semidefinite Programming-Based Underestimation Method for Stochastic Global Optimization in Protein Docking. IEEE Transactions on Automatic Control, 2007, 52, 664-676.	3.6	20
105	Ensemble Modeling of Substrate Binding to Cytochromes P450:Â Analysis of Catalytic Differences between CYP1A Orthologsâ€,â€¡. Biochemistry, 2007, 46, 2640-2654.	1.2	45
106	Engineering a novel, stable dimeric streptavidin with lower isoelectric point. Journal of Biotechnology, 2007, 128, 213-225.	1.9	14
107	Optimizing noisy funnel-like functions on the euclidean group with applications to protein docking. , 2007, , .		2
108	Exploring the Binding Sites of the Haloalkane Dehalogenase DhlA from Xanthobacter autotrophicus GJ10. Biochemistry, 2007, 46, 9239-9249.	1.2	20

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109	Identification of Hot Spots within Druggable Binding Regions by Computational Solvent Mapping of Proteins. Journal of Medicinal Chemistry, 2007, 50, 1231-1240.	2.9	125
110	Docking with PIPER and refinement with SDU in rounds 6â€“11 of CAPRI. Proteins: Structure, Function and Bioinformatics, 2007, 69, 734-742.	1.5	12
111	ClusPro: Performance in CAPRI rounds 6â€“11 and the new server. Proteins: Structure, Function and Bioinformatics, 2007, 69, 781-785.	1.5	77
112	Computational Screening of Phthalate Monoesters for Binding to PPARÎ³. Chemical Research in Toxicology, 2006, 19, 999-1009.	1.7	29
113	Computational Solvent Mapping Reveals the Importance of Local Conformational Changes for Broad Substrate Specificity in Mammalian Cytochromes P450â€. Biochemistry, 2006, 45, 9393-9407.	1.2	35
114	Protein-protein docking with reduced potentials by exploiting multi-dimensional energy funnels. , 2006, 2006, 5330-3.		4
115	PIPER: An FFT-based protein docking program with pairwise potentials. Proteins: Structure, Function and Bioinformatics, 2006, 65, 392-406.	1.5	714
116	Clustering of domains of functionally related enzymes in the interaction database PRECISE by the generation of primary sequence patterns. Journal of Molecular Graphics and Modelling, 2006, 24, 426-433.	1.3	0
117	Classification of protein complexes based on the biophysics of association. FASEB Journal, 2006, 20, A851.	0.2	0
118	Characterization of protein-ligand interaction sites using experimental and computational methods. Current Opinion in Drug Discovery & Development, 2006, 9, 354-62.	1.9	29
119	Classification of protein complexes based on docking difficulty. Proteins: Structure, Function and Bioinformatics, 2005, 60, 176-180.	1.5	52
120	Performance of the first protein docking server ClusPro in CAPRI rounds 3-5. Proteins: Structure, Function and Bioinformatics, 2005, 60, 239-244.	1.5	30
121	Exploring the Binding Site Structure of the PPARÎ³ Ligand-Binding Domain by Computational Solvent Mapping. Biochemistry, 2005, 44, 1193-1209.	1.2	71
122	Optimal Clustering for Detecting Near-Native Conformations in Protein Docking. Biophysical Journal, 2005, 89, 867-875.	0.2	119
123	Consensus alignment server for reliable comparative modeling with distant templates. Nucleic Acids Research, 2004, 32, W50-W54.	6.5	10
124	PRECISE: a Database of Predicted and Consensus Interaction Sites in Enzymes. Nucleic Acids Research, 2004, 33, D206-D211.	6.5	11
125	Anchor residues in protein-protein interactions. Proceedings of the National Academy of Sciences of the United States of America, 2004, 101, 11287-11292.	3.3	327
126	Proteinâ€“protein docking: is the glass half-full or half-empty?. Trends in Biotechnology, 2004, 22, 110-116.	4.9	106

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127	ClusPro: an automated docking and discrimination method for the prediction of protein complexes. Bioinformatics, 2004, 20, 45-50.	1.8	809
128	ClusPro: a fully automated algorithm for protein-protein docking. Nucleic Acids Research, 2004, 32, W96-W99.	6.5	717
129	Improved mapping of protein binding sites. Journal of Computer-Aided Molecular Design, 2003, 17, 173-186.	1.3	22
130	Algorithms for computational solvent mapping of proteins. Proteins: Structure, Function and Bioinformatics, 2003, 51, 340-351.	1.5	53
131	CAPRI: A Critical Assessment of PRedicted Interactions. Proteins: Structure, Function and Bioinformatics, 2003, 52, 2-9.	1.5	586
132	Combination of scoring functions improves discrimination in protein-protein docking. Proteins: Structure, Function and Bioinformatics, 2003, 53, 840-854.	1.5	37
133	Identification of Substrate Binding Sites in Enzymes by Computational Solvent Mapping. Journal of Molecular Biology, 2003, 332, 1095-1113.	2.0	69
134	Homology Modeling of Proteins Using Multiple Models and Consensus Sequence Alignment. Lecture Notes in Computer Science, 2003, , 389-401.	1.0	0
135	Computational mapping identifies the binding sites of organic solvents on proteins. Proceedings of the National Academy of Sciences of the United States of America, 2002, 99, 4290-4295.	3.3	115
136	Inversion of Noise-Free Laplace Transforms: Towards a Standardized Set of Test Problems. Inverse Problems in Science and Engineering, 2002, 10, 467-483.	0.5	30
137	Proteinâ€“protein association kinetics and protein docking. Current Opinion in Structural Biology, 2002, 12, 36-40.	2.6	107
138	A Streptavidin Mutant Useful for Directed Immobilization on Solid Surfaces. Bioconjugate Chemistry, 2001, 12, 1000-1004.	1.8	43
139	Dynamical View of the Positions of Key Side Chains in Protein-Protein Recognition. Biophysical Journal, 2001, 80, 635-642.	0.2	88
140	Continuum electrostatic analysis of preferred solvation sites around proteins in solution. , 2000, 38, 176-188.		17
141	Scoring docked conformations generated by rigid-body protein-protein docking. Proteins: Structure, Function and Bioinformatics, 2000, 40, 525-537.	1.5	112
142	Discrimination of near-native protein structures from misfolded models by empirical free energy functions. Proteins: Structure, Function and Bioinformatics, 2000, 41, 518-534.	1.5	68
143	Kinetics of Desolvation-Mediated Proteinâ€“Protein Binding. Biophysical Journal, 2000, 78, 1094-1105.	0.2	141
144	Discrimination of near-native protein structures from misfolded models by empirical free energy functions. , 2000, 41, 518.		2

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145	Free Energy Landscapes of Encounter Complexes in Protein-Protein Association. Biophysical Journal, 1999, 76, 1166-1178.	0.2	181
146	The waters of life. Journal of the Franklin Institute, 1998, 335, 213-240.	1.9	4
147	Predicted and trifluoroethanol-induced Î±-helicity of polypeptides. , 1998, 39, 367-376.		30
148	Selecting nearâ€native conformations in homology modeling: The role of molecular mechanics and solvation terms. Protein Science, 1998, 7, 1772-1780.	3.1	22
149	Genetic engineering of streptavidin, a versatile affinity tag. Biomedical Applications, 1998, 715, 85-91.	1.7	41
150	Empirical potentials and functions for protein folding and binding. Current Opinion in Structural Biology, 1997, 7, 222-228.	2.6	136
151	Empirical free energy calculation: Comparison to calorimetric data. Protein Science, 1997, 6, 1976-1984.	3.1	29
152	Properties and Applications of Genetically Engineered Streptavidins. , 1997, , 295-301.		1
153	Molecular Engineering of Streptavidin. Annals of the New York Academy of Sciences, 1996, 799, 383-390.	1.8	20
154	Empirical free energy as a target function in docking and design: application to HIV-1 protease inhibitors. FEBS Letters, 1996, 384, 87-91.	1.3	21
155	Peptide docking using dynamic programming. , 1996, 17, 418-428.		21
156	Prediction of protein complexes using empirical free energy functions. Protein Science, 1996, 5, 614-626.	3.1	91
157	Free energy mapping of class I MHC molecules and structural determination of bound peptides. Protein Science, 1996, 5, 1272-1281.	3.1	52
158	Streptavidins with intersubunit crosslinks have enhanced stability. Nature Biotechnology, 1996, 14, 1007-1011.	9.4	57
159	Predicted and trifluoroethanol-induced Î±-helicity of polypeptides. , 1996, 39, 367.		14
160	Flexible docking of peptides to class I major-histocompatibility-complex receptors. Genetic Analysis, Techniques and Applications, 1995, 12, 1-21.	1.5	36
161	Extracting hydrophobicity parameters from solute partition and protein mutation/unfolding experiments. Protein Engineering, Design and Selection, 1995, 8, 1081-1092.	1.0	26
162	Identifiability and Distinguishability of General Reaction Systems. The Journal of Physical Chemistry, 1994, 98, 5265-5271.	2.9	45

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163	Finite-state and reduced-parameter representations of protein backbone conformations. Journal of Computational Chemistry, 1994, 15, 300-312.	1.5	4
164	Identifiability and indistinguishability of nonlinear pharmacokinetic models. Journal of Pharmacokinetics and Pharmacodynamics, 1994, 22, 229-251.	0.6	29
165	Indistinguishability for a class of nonlinear compartmental models. Mathematical Biosciences, 1994, 119, 77-95.	0.9	9
166	Effect of Conformational Flexibility and Solvation on Receptor-Ligand Binding Free Energies. Biochemistry, 1994, 33, 13977-13988.	1.2	160
167	An Adaptive Branch-and-Bound Minimization Method Based on Dynamic Programming. , 1994, , 409-432.		1
168	Generalized parametric sensitivity: Application to a CSTR. Chemical Engineering Science, 1993, 48, 2453-2461.	1.9	6
169	Loop closure via bond scaling and relaxation. Journal of Computational Chemistry, 1993, 14, 556-565.	1.5	48
170	The binding domain structure of retinoblastomaâ€binding proteins. Protein Science, 1993, 2, 155-164.	3.1	18
171	Determining protein loop conformation using scalingâ€relaxation techniques. Protein Science, 1993, 2, 1242-1248.	3.1	69
172	Toward computational determination of peptideâ€receptor structure. Protein Science, 1993, 2, 1827-1843.	3.1	32
173	The local information content of the protein structural database. FEBS Letters, 1993, 322, 143-146.	1.3	7
174	Computing the Structure of Bound Peptides. Journal of Molecular Biology, 1993, 234, 515-521.	2.0	66
175	Parametric sensitivity and self-similarity in thermal explosion theory. Chemical Engineering Science, 1992, 47, 1063-1078.	1.9	50
176	Determining minimum energy conformations of polypeptides by dynamic programming. Biopolymers, 1990, 29, 1755-1772.	1.2	55
177	Global identifiability of the parameters of nonlinear systems with specified inputs: A comparison of methods. Mathematical Biosciences, 1990, 102, 41-73.	0.9	127
178	Similarity transformation approach to identifiability analysis of nonlinear compartmental models. Mathematical Biosciences, 1989, 93, 217-248.	0.9	187
179	Parameter space boundaries for unidentifiable compartmental models. Mathematical Biosciences, 1989, 97, 27-60.	0.9	14
180	Numerical deconvolution using system identification methods. Journal of Pharmacokinetics and Pharmacodynamics, 1988, 16, 85-107.	0.6	25

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182	Analysis of unique structural identifiability via submodels. Mathematical Biosciences, 1984, 71, 125-146.	0.9	13
183	Structural equivalence of linear systems and compartmental models. Mathematical Biosciences, 1981, 55, 39-64.	0.9	39
184	ON STRUCTURAL EQUIVALENCE OF COMPARTMENTAL MODELS. , 1981, , 157-168.		1