Maxim Totrov

List of Publications by Year
in descending order

47 papers	6,926 citations	159585 30 h-index	223800 46 g-index
49 all docs	49 docs citations	49 times ranked	6625 citing authors

#	Article	IF	Citations
1	ICM?A new method for protein modeling and design: Applications to docking and structure prediction from the distorted native conformation. Journal of Computational Chemistry, 1994, 15, 488-506.	3.3	1,502
2	Biased Probability Monte Carlo Conformational Searches and Electrostatic Calculations for Peptides and Proteins. Journal of Molecular Biology, 1994, 235, 983-1002.	4.2	901
3	Flexible ligand docking to multiple receptor conformations: a practical alternative. Current Opinion in Structural Biology, 2008, 18, 178-184.	5.7	456
4	Pocketome via Comprehensive Identification and Classification of Ligand Binding Envelopes. Molecular and Cellular Proteomics, 2005, 4, 752-761.	3.8	350
5	High-throughput docking for lead generation. Current Opinion in Chemical Biology, 2001, 5, 375-382.	6.1	339
6	Flexible proteinâ€“ligand docking by global energy optimization in internal coordinates. Proteins: Structure, Function and Bioinformatics, 1997, 29, 215-220.	2.6	334
7	Docking and scoring with ICM: the benchmarking results and strategies for improvement. Journal of Computer-Aided Molecular Design, 2012, 26, 675-686.	2.9	290
8	Identification of Proteinâ€“Protein Interaction Sites from Docking Energy Landscapes. Journal of Molecular Biology, 2004, 335, 843-865.	4.2	276
9	ICM-DISCO docking by global energy optimization with fully flexible side-chains. Proteins: Structure, Function and Bioinformatics, 2003, 52, 113-117.	2.6	183
10	Soft protein-protein docking in internal coordinates. Protein Science, 2009, 11, 280-291.	7.6	175
11	Four-Dimensional Docking: A Fast and Accurate Account of Discrete Receptor Flexibility in Ligand Docking. Journal of Medicinal Chemistry, 2009, 52, 397-406.	6.4	172
12	Nuclear Hormone Receptor Targeted Virtual Screening. Journal of Medicinal Chemistry, 2003, 46, 3045-3059.	6.4	170
13	Homology modeling by the ICM method. Proteins: Structure, Function and Bioinformatics, 1995, 23, 403-414.	2.6	160
14	Conserved structural elements in the V3 crown of HIV-1 gp120. Nature Structural and Molecular Biology, 2010, 17, 955-961.	8.2	147
15	Prediction of the binding energy for small molecules, peptides and proteins. Journal of Molecular Recognition, 1999, 12, 177-190.	2.1	146
16	Flexible proteinâ€“ligand docking by global energy optimization in internal coordinates. Proteins: Structure, Function and Bioinformatics, 1997, 29, 215-220.	2.6	139
17	Detailed ab initio prediction of lysozymeâ€“antibody complex with 1.6 Ã… accuracy. Nature Structural and Molecular Biology, 1994, 1, 259-263.	8.2	123
18	Rapid boundary element solvation electrostatics calculations in folding simulations: Successful folding of a 23-residue peptide. Biopolymers, 2001, 60, 124-133.	2.4	115

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19	Atomic Property Fields: Generalized 3D Pharmacophoric Potential for Automated Ligand Superposition, Pharmacophore Elucidation and 3D QSAR. Chemical Biology and Drug Design, 2008, 71, 15-27.	3.2	104
20	A new method for ligand docking to flexible receptors by dual alanine scanning and refinement (SCARE). Journal of Computer-Aided Molecular Design, 2008, 22, 311-325.	2.9	74
21	Development of a new physicsâ€based internal coordinate mechanics force field and its application to protein loop modeling. Proteins: Structure, Function and Bioinformatics, 2011, 79, 477-498.	2.6	73
22	Ab InitioFolding of Peptides by the Optimal-Bias Monte Carlo Minimization Procedure. Journal of Computational Physics, 1999, 151, 402-421.	3.8	65
23	Homology modeling with internal coordinate mechanics: Deformation zone mapping and improvements of models via conformational search. Proteins: Structure, Function and Bioinformatics, 1997, 29, 29-37.	2.6	58
24	Cross-Clade HIV-1 Neutralizing Antibodies Induced with V3-Scaffold Protein Immunogens following Priming with gp120 DNA. Journal of Virology, 2011, 85, 9887-9898.	3.4	54
25	Improving CAPRI predictions: Optimized desolvation for rigid-body docking. Proteins: Structure, Function and Bioinformatics, 2005, 60, 308-313.	2.6	45
26	Flexible proteinâ€“ligand docking by global energy optimization in internal coordinates. Proteins: Structure, Function and Bioinformatics, 1997, 29, 215-220.	2.6	44
27	Structure-guided design and immunological characterization of immunogens presenting the HIV-1 gp120 V3 loop on a CTB scaffold. Virology, 2010, 405, 513-523.	2.4	42
28	Homology modeling with internal coordinate mechanics: Deformation zone mapping and improvements of models via conformational search. Proteins: Structure, Function and Bioinformatics, 1997, 29, 29-37.	2.6	40
29	Ligand-biased ensemble receptor docking (LigBEnD): a hybrid ligand/receptor structure-based approach. Journal of Computer-Aided Molecular Design, 2018, 32, 187-198.	2.9	39
30	Multimeric Epitope-Scaffold HIV Vaccines Target V1V2 and Differentially Tune Polyfunctional Antibody Responses. Cell Reports, 2019, 28, 877-895.e6.	6.4	36
31	Derivation of sensitive discrimination potential for virtual ligand screening. , 1999, , .		30
32	Functional Antibody Response Against V1V2 and V3 of HIV gp120 in the VAX003 and VAX004 Vaccine Trials. Scientific Reports, 2018, 8, 542.	3.3	30
33	ICFF: A new method to incorporate implicit flexibility into an internal coordinate force field. Journal of Computational Chemistry, 2003, 24, 254-265.	3.3	28
34	Ligand binding site superposition and comparison based on Atomic Property Fields: identification of distant homologues, convergent evolution and PDB-wide clustering of binding sites. BMC Bioinformatics, 2011, 12, S35.	2.6	28
35	Accurate and efficient generalized born model based on solvent accessibility: Derivation and application for LogP octanol/water prediction and flexible peptide docking. Journal of Computational Chemistry, 2004, 25, 609-619.	3.3	25
36	Hybrid receptor structure/ligand-based docking and activity prediction in ICM: development and evaluation in D3R Grand Challenge 3. Journal of Computer-Aided Molecular Design, 2019, 33, 35-46.	2.9	16

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37	Protein-RNA Docking Using ICM. Journal of Chemical Theory and Computation, 2018, 14, 4971-4984.	5.3	15
38	Estimated Secondary Structure Propensities within V1/V2 Region of HIV gp120 Are an Important Global Antibody Neutralization Sensitivity Determinant. PLoS ONE, 2014, 9, e94002.	2.5	13
39	Efficient parallelization of the energy, surface, and derivative calculations for internal coordinate mechanics. Journal of Computational Chemistry, 1994, 15, 1105-1112.	3.3	11
40	Macrocycle modeling in ICM: benchmarking and evaluation in D3R Grand Challenge 4. Journal of Computer-Aided Molecular Design, 2019, 33, 1057-1069.	2.9	8
41	Loop Simulations. Methods in Molecular Biology, 2011, 857, 207-229.	0.9	6
42	HIV p24 as Scaffold for Presenting Conformational HIV Env Antigens. PLoS ONE, 2012, 7, e43318.	2.5	6
43	Acetylcholinesterase of the sand fly, Phlebotomus papatasi (Scopoli): construction, expression and biochemical properties of the G119S orthologous mutant. Parasites and Vectors, 2014, 7, 577.	2.5	6
44	All-Atom Internal Coordinate Mechanics (ICM) Force Field for Hexopyranoses and Glycoproteins. Journal of Chemical Theory and Computation, 2015, 11, 2167-2186.	5.3	6
45	An HIV Vaccine Targeting the V2 Region of the HIV Envelope Induces a Highly Durable Polyfunctional Fc-Mediated Antibody Response in Rhesus Macaques. Journal of Virology, 2020, 94, .	3.4	6
46	Mosquito Acetylcholinesterase as a Target for Novel Phenyl-Substituted Carbamates. International Journal of Environmental Research and Public Health, 2019, 16, 1500.	2.6	4
47	Prediction of the binding energy for small molecules, peptides and proteins. , 1999, 12, 177.		1