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	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
2	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
3	Multimeric Epitope-Scaffold HIV Vaccines Target V1V2 and Differentially Tune Polyfunctional Antibody Responses. Cell Reports, 2019, 28, 877-895.e6.	6.4	36
4	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
5	Mosquito Acetylcholinesterase as a Target for Novel Phenyl-Substituted Carbamates. International Journal of Environmental Research and Public Health, 2019, 16, 1500.	2.6	4
6	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
7	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
8	Protein-RNA Docking Using ICM. Journal of Chemical Theory and Computation, 2018, 14, 4971-4984.	5.3	15
9	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
10	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
11	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
12	HIV p24 as Scaffold for Presenting Conformational HIV Env Antigens. PLoS ONE, 2012, 7, e43318.	2.5	6
13	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
14	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
15	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
16	Loop Simulations. Methods in Molecular Biology, 2011, 857, 207-229.	0.9	6
17	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
18	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

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19	Conserved structural elements in the V3 crown of HIV-1 gp120. Nature Structural and Molecular Biology, 2010, 17, 955-961.	8.2	147
20	Soft protein-protein docking in internal coordinates. Protein Science, 2009, 11, 280-291.	7.6	175
21	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
22	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
23	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
24	Flexible ligand docking to multiple receptor conformations: a practical alternative. Current Opinion in Structural Biology, 2008, 18, 178-184.	5.7	456
25	Improving CAPRI predictions: Optimized desolvation for rigid-body docking. Proteins: Structure, Function and Bioinformatics, 2005, 60, 308-313.	2.6	45
26	Pocketome via Comprehensive Identification and Classification of Ligand Binding Envelopes. Molecular and Cellular Proteomics, 2005, 4, 752-761.	3.8	350
27	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
28	Identification of Proteinâ€“Protein Interaction Sites from Docking Energy Landscapes. Journal of Molecular Biology, 2004, 335, 843-865.	4.2	276
29	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
30	ICM-DISCO docking by global energy optimization with fully flexible side-chains. Proteins: Structure, Function and Bioinformatics, 2003, 52, 113-117.	2.6	183
31	Nuclear Hormone Receptor Targeted Virtual Screening. Journal of Medicinal Chemistry, 2003, 46, 3045-3059.	6.4	170
32	High-throughput docking for lead generation. Current Opinion in Chemical Biology, 2001, 5, 375-382.	6.1	339
33	Rapid boundary element solvation electrostatics calculations in folding simulations: Successful folding of a 23-residue peptide. Biopolymers, 2001, 60, 124-133.	2.4	115
34	Derivation of sensitive discrimination potential for virtual ligand screening. , 1999, , .		30
35	Ab InitioFolding of Peptides by the Optimal-Bias Monte Carlo Minimization Procedure. Journal of Computational Physics, 1999, 151, 402-421.	3.8	65
36	Prediction of the binding energy for small molecules, peptides and proteins. Journal of Molecular Recognition, 1999, 12, 177-190.	2.1	146

#	Article	IF	Citations
37	Prediction of the binding energy for small molecules, peptides and proteins. , 1999, 12, 177.		1
38	Flexible proteinâ€“ligand docking by global energy optimization in internal coordinates. Proteins: Structure, Function and Bioinformatics, 1997, 29, 215-220.	2.6	334
39	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
40	Flexible proteinâ€“ligand docking by global energy optimization in internal coordinates. Proteins: Structure, Function and Bioinformatics, 1997, 29, 215-220.	2.6	44
41	Flexible proteinâ€“ligand docking by global energy optimization in internal coordinates. Proteins: Structure, Function and Bioinformatics, 1997, 29, 215-220.	2.6	139
42	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
43	Homology modeling by the ICM method. Proteins: Structure, Function and Bioinformatics, 1995, 23, 403-414.	2.6	160
44	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
45	Efficient parallelization of the energy, surface, and derivative calculations for internal coordinate mechanics. Journal of Computational Chemistry, 1994, 15, 1105-1112.	3.3	11
46	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
47	Biased Probability Monte Carlo Conformational Searches and Electrostatic Calculations for Peptides and Proteins. Journal of Molecular Biology, 1994, 235, 983-1002.	4.2	901