Garrett M Morris

List of Publications by Year
in descending order

74 papers	34,745 citations	147566 31 h-index	98622 67 g-index
101 all docs	101 docs citations	101 times ranked	37975 citing authors

#	Article	IF	Citations
1	AutoDock4 and AutoDockTools4: Automated docking with selective receptor flexibility. Journal of Computational Chemistry, 2009, 30, 2785-2791.	1.5	16,850
2	Automated docking using a Lamarckian genetic algorithm and an empirical binding free energy function. , 1998, 19, 1639-1662.		8,897
3	A semiempirical free energy force field with charge-based desolvation. Journal of Computational Chemistry, 2007, 28, 1145-1152.	1.5	1,854
4	Automated docking of flexible ligands: Applications of autodock. , 1996, 9, 1-5.		1,284
5	Distributed automated docking of flexible ligands to proteins: Parallel applications of AutoDock 2.4. Journal of Computer-Aided Molecular Design, 1996, 10, 293-304.	1.3	907
6	Crystal Structure of a Neutralizing Human IgG Against HIV-1: A Template for Vaccine Design. Science, 2001, 293, 1155-1159.	6.0	870
7	Using AutoDock for Ligandâ€Receptor Docking. Current Protocols in Bioinformatics, 2008, 24, Unit 8.14.	25.8	573
8	Molecular Docking. Methods in Molecular Biology, 2008, 443, 365-382.	0.4	551
9	Automated docking to multiple target structures: Incorporation of protein mobility and structural water heterogeneity in AutoDock. Proteins: Structure, Function and Bioinformatics, 2002, 46, 34-40.	1.5	394
10	Target Flexibility: An Emerging Consideration in Drug Discovery and Design. Journal of Medicinal Chemistry, 2008, 51, 6237-6255.	2.9	280
11	Freely Available Conformer Generation Methods: How Good Are They?. Journal of Chemical Information and Modeling, 2012, 52, 1146-1158.	2.5	178
12	Rapid and Accurate Prediction and Scoring of Water Molecules in Protein Binding Sites. PLoS ONE, 2012, 7, e32036.	1.1	149
13	The prospects of quantum computing in computational molecular biology. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1481.	6.2	108
14	Active site binding modes of curcumin in HIV-1 protease and integrase. Bioorganic and Medicinal Chemistry Letters, 2005, 15, 3364-3368.	1.0	97
15	Automated docking of ligands to an artificial active site: augmenting crystallographic analysis with computer modeling. Journal of Computer-Aided Molecular Design, 2003, 17, 525-536.	1.3	81
16	ElectroShape: fast molecular similarity calculations incorporating shape, chirality and electrostatics. Journal of Computer-Aided Molecular Design, 2010, 24, 789-801.	1.3	77
17	Conformational Changes in Nitric Oxide Synthases Induced by Chlorzoxazone and Nitroindazoles:â€‰ Crystallographic and Computational Analyses of Inhibitor Potency. Biochemistry, 2002, 41, 13915-13925.	1.2	63
18	A Dynamic Model of HIV Integrase Inhibition and Drug Resistance. Journal of Molecular Biology, 2010, 397, 600-615.	2.0	63

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19	Learning from the ligand: using ligand-based features to improve binding affinity prediction. Bioinformatics, 2020, 36, 758-764.	1.8	60
20	Crystal Structures of the Inactive D30N Mutant of Feline Immunodeficiency Virus Protease Complexed with a Substrate and an Inhibitorâ€,â€¡. Biochemistry, 1997, 36, 10696-10708.	1.2	57
21	Development of a New Type of Protease Inhibitors, Efficacious against FIV and HIV Variants. Journal of the American Chemical Society, 1999, 121, 1145-1155.	6.6	56
22	Discovery of SARS-CoV-2 M^{pro} peptide inhibitors from modelling substrate and ligand binding. Chemical Science, 2021, 12, 13686-13703.	3.7	54
23	Structural mapping of CD134 residues critical for interaction with feline immunodeficiency virus. Nature Structural and Molecular Biology, 2005, 12, 60-66.	3.6	51
24	Mechanistic and structural requirements for active site labeling of phosphoglycerate mutase by spiroepoxides. Molecular BioSystems, 2007, 3, 495.	2.9	46
25	Functional Proteomic and Structural Insights into Molecular Recognition in the Nitrilase Family Enzymes. Biochemistry, 2008, 47, 13514-13523.	1.2	45
26	Assessing the Role of Polarization in Docking. Journal of Physical Chemistry A, 2008, 112, 12157-12163.	1.1	42
27	One Size Does Not Fit All: The Limits of Structure-Based Models in Drug Discovery. Journal of Chemical Theory and Computation, 2013, 9, 4266-4274.	2.3	41
28	Improving the accuracy of ultrafast ligand-based screening: incorporating lipophilicity into ElectroShape as an extra dimension. Journal of Computer-Aided Molecular Design, 2011, 25, 785-790.	1.3	39
29	Bayesian optimization for conformer generation. Journal of Cheminformatics, 2019, 11, 32.	2.8	37
30	Automated Docking with Protein Flexibility in the Design of Femtomolar â€œClick Chemistryâ€•Inhibitors of Acetylcholinesterase. Journal of Chemical Information and Modeling, 2013, 53, 898-906.	2.5	36
31	Characterization of the SARS-CoV-2 ExoN (nsp14ExoNâ€“nsp10) complex: implications for its role in viral genome stability and inhibitor identification. Nucleic Acids Research, 2022, 50, 1484-1500.	6.5	36
32	Electron transport in cytochromes P-450 by covalent switching. Proceedings of the Royal Society B: Biological Sciences, 1991, 245, 43-51.	1.2	32
33	Structural studies of FIV and HIV-1 proteases complexed with an efficient inhibitor of FIV protease. , 2000, 38, 29-40.		32
34	Crystal Structure of an Intact Human IgG: Antibody Asymmetry, Flexibility, and a Guide for HIV-1 Vaccine Design. Advances in Experimental Medicine and Biology, 2003, 535, 55-66.	0.8	32
35	Alteration of Substrate and Inhibitor Specificity of Feline Immunodeficiency Virus Protease. Journal of Virology, 2000, 74, 4710-4720.	1.5	31
36	Defining HIV-1 Protease Substrate Selectivity. Current Drug Targets Infectious Disorders, 2002, 2, 37-50.	2.1	29

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37	The emerging role of cloud computing in molecular modelling. Journal of Molecular Graphics and Modelling, 2013, 44, 177-187.	1.3	29
38	Understanding Conformational Entropy in Small Molecules. Journal of Chemical Theory and Computation, 2021, 17, 2099-2106.	2.3	29
39	Learning protein-ligand binding affinity with atomic environment vectors. Journal of Cheminformatics, 2021, 13, 59.	2.8	29
40	The active site of cytochrome P-450 nifedipine oxidase: a model-building study. Journal of Molecular Graphics, 1989, 7, 206-211.	1.7	28
41	Viral Evolution in Response to the Broad-Based Retroviral Protease Inhibitor TL-3. Journal of Virology, 2001, 75, 9502-9508.	1.5	28
42	Understanding the Structural Requirements for Activators of the Kef Bacterial Potassium Efflux System. Biochemistry, 2014, 53, 1982-1992.	1.2	25
43	Molecular modelling of the sterol C-14 demethylase of Saccharomyces cerevisiae. Biochemical Society Transactions, 1991, 19, 793-795.	1.6	24
44	Molecular Determinants of Binding to the Plasmodium Subtilisin-like Protease 1. Journal of Chemical Information and Modeling, 2013, 53, 573-583.	2.5	24
45	Mapping of the CXCR4 Binding Site within Variable Region 3 of the Feline Immunodeficiency Virus Surface Glycoprotein. Journal of Virology, 2008, 82, 9134-9142.	1.5	23
46	Structural Basis for Distinctions between Substrate and Inhibitor Specificities for Feline Immunodeficiency Virus and Human Immunodeficiency Virus Proteases. Journal of Virology, 2003, 77, 6589-6600.	1.5	22
47	Structural Insights into the Mechanisms of Drug Resistance in HIV-1 Protease NL4-3. Journal of Molecular Biology, 2006, 356, 967-981.	2.0	22
48	Molecular analysis of the feline immunodeficiency virus protease: generation of a novel form of the protease by autoproteolysis and construction of cleavage-resistant proteases. Journal of Virology, 1997, 71, 5505-5511.	1.5	22
49	Understanding Ring Puckering in Small Molecules and Cyclic Peptides. Journal of Chemical Information and Modeling, 2021, 61, 743-755.	2.5	20
50	Scoring Functions for Protein-Ligand Binding Affinity Prediction Using Structure-based Deep Learning: A Review. Frontiers in Bioinformatics, 0, 2, .	1.0	20
51	Design and synthesis of broad-Based mono- and bi- cyclic inhibitors of FIV and HIV proteases. Bioorganic and Medicinal Chemistry, 2003, 11, 2025-2040.	1.4	19
52	Molecular similarity including chirality. Journal of Molecular Graphics and Modelling, 2009, 28, 368-370.	1.3	19
53	Shapeâ€based similarity searching in chemical databases. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2013, 3, 226-241.	6.2	19
54	The matching of protein sequences using color intrasequence homology displays. Journal of Molecular Graphics, 1988, 6, 135-140.	1.7	18

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55	Evolutionary analysis of HIV-1 protease inhibitors: Methods for design of inhibitors that evade resistance. Proteins: Structure, Function and Bioinformatics, 2002, 48, 63-74.	1.5	17
56	Recognition templates for predicting adenylate-binding sites in proteins. Journal of Molecular Biology, 2001, 314, 1245-1255.	2.0	16
57	Exploration of Piperidinols as Potential Antitubercular Agents. Molecules, 2014, 19, 16274-16290.	1.7	16
58	Improved Evolutionary Hybrids for Flexible Ligand Docking in AutoDock. Nonconvex Optimization and Its Applications, 2000, , 209-229.	0.1	16
59	Model of the ?L?2 integrin I-domain/ICAM-1 DI interface suggests that subtle changes in loop orientation determine ligand specificity. Proteins: Structure, Function and Bioinformatics, 2002, 48, 151-160.	1.5	15
60	Packaging HIV Virion Components through Dynamic Equilibria of a Human tRNA Synthetase. Journal of Physical Chemistry B, 2010, 114, 16273-16279.	1.2	15
61	Comparison of ultraâ€fast 2<scp>D</scp> and 3<scp>D</scp> ligand and target descriptors for side effect prediction and network analysis in polypharmacology. British Journal of Pharmacology, 2013, 170, 557-567.	2.7	15
62	Coevolutionary analysis of resistance-evading peptidomimetic inhibitors of HIV-1 protease. Proceedings of the National Academy of Sciences of the United States of America, 1999, 96, 1369-1374.	3.3	14
63	BOKEI: Bayesian optimization using knowledge of correlated torsions and expected improvement for conformer generation. Physical Chemistry Chemical Physics, 2020, 22, 5211-5219.	1.3	14
64	Coevolution and subsite decomposition for the design of resistance-evading HIV-1 protease inhibitors 1 1Edited by F. E. Cohen. Journal of Molecular Biology, 1999, 287, 77-92.	2.0	13
65	Learning from Docked Ligands: Ligand-Based Features Rescue Structure-Based Scoring Functions When Trained on Docked Poses. Journal of Chemical Information and Modeling, 2022, 62, 5329-5341.	2.5	10
66	Ligity: A Non-Superpositional, Knowledge-Based Approach to Virtual Screening. Journal of Chemical Information and Modeling, 2019, 59, 2600-2616.	2.5	9
67	Automated docking of flexible ligands: Applications of autodock. , 1996, 9, 1.		7
68	Seeing our way to drug design. Journal of Computer - Aided Molecular Design, 1993, 1, 329-344.	1.0	6
69	Investigating the potential for a limited quantum speedup on protein lattice problems. New Journal of Physics, 0, , .	1.2	6
70	Bibliography of theoretical calculations in molecular pharmacology. Journal of Molecular Graphics, 1987, 5, 211-222.	1.7	5
71	Computational Coevolution of Antiviral Drug Resistance. Artificial Life, 1998, 4, 41-59.	1.0	3
72	Mining for medicines â€“ in silico. Trends in Biotechnology, 2001, 19, 123-124.	4.9	2

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73	Chapter 7. Docking and Virtual Screening. RSC Drug Discovery Series, 2012, , 171-194.	0.2	0
74	Assessment of a probabilistic framework for combining structure- and ligand-based virtual screening. Journal of Cheminformatics, 2012, 4, .	2.8	0