Garrett M Morris

List of Publications by Year in Descending Order

78 papers	26,420 citations	28 h-index	101 g-index
101 ext. papers	30,426 ext. citations	6.3 avg, IF	6.64 L-index

#	Paper	IF	Citations
78	Characterization of the SARS-CoV-2 ExoN (nsp14ExoN-nsp10) complex: implications for its role in viral genome stability and inhibitor identification.. *Nucleic Acids Research*, **2022**,	20.1	4
77	Understanding Conformational Entropy in Small Molecules. *Journal of Chemical Theory and Computation*, **2021**, 17, 2099-2106	6.4	6
76	Understanding Ring Puckering in Small Molecules and Cyclic Peptides. *Journal of Chemical Information and Modeling*, **2021**, 61, 743-755	6.1	9
75	Learning protein-ligand binding affinity with atomic environment vectors. *Journal of Cheminformatics*, **2021**, 13, 59	8.6	6
74	Discovery of SARS-CoV-2 M peptide inhibitors from modelling substrate and ligand binding. *Chemical Science*, **2021**, 12, 13686-13703	9.4	14
73	The prospects of quantum computing in computational molecular biology. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2021**, 11, e1481	7.9	28
72	BOKEI: Bayesian optimization using knowledge of correlated torsions and expected improvement for conformer generation. *Physical Chemistry Chemical Physics*, **2020**, 22, 5211-5219	3.6	6
71	Learning from the ligand: using ligand-based features to improve binding affinity prediction. *Bioinformatics*, **2020**, 36, 758-764	7.2	25
70	Ligity: A Non-Superpositional, Knowledge-Based Approach to Virtual Screening. *Journal of Chemical Information and Modeling*, **2019**, 59, 2600-2616	6.1	8
69	Bayesian optimization for conformer generation. *Journal of Cheminformatics*, **2019**, 11, 32	8.6	20
68	Understanding the structural requirements for activators of the Kef bacterial potassium efflux system. *Biochemistry*, **2014**, 53, 1982-92	3.2	20
67	Exploration of piperidinols as potential antitubercular agents. *Molecules*, **2014**, 19, 16274-90	4.8	12
66	The emerging role of cloud computing in molecular modelling. *Journal of Molecular Graphics and Modelling*, **2013**, 44, 177-87	2.8	23
65	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	6.4	31
64	Shape-based similarity searching in chemical databases. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2013**, 3, 226-241	7.9	16
63	Automated docking with protein flexibility in the design of femtomolar "click chemistry" inhibitors of acetylcholinesterase. *Journal of Chemical Information and Modeling*, **2013**, 53, 898-906	6.1	33
62	Molecular determinants of binding to the Plasmodium subtilisin-like protease 1. *Journal of Chemical Information and Modeling*, **2013**, 53, 573-83	6.1	23

61	Comparison of ultra-fast 2D and 3D ligand and target descriptors for side effect prediction and network analysis in polypharmacology. *British Journal of Pharmacology*, **2013**, 170, 557-67	8.6	11
60	Assessment of a probabilistic framework for combining structure- and ligand-based virtual screening. *Journal of Cheminformatics*, **2012**, 4,	8.6	78
59	Freely available conformer generation methods: how good are they?. *Journal of Chemical Information and Modeling*, **2012**, 52, 1146-58	6.1	128
58	Rapid and accurate prediction and scoring of water molecules in protein binding sites. *PLoS ONE*, **2012**, 7, e32036	3.7	124
57	Improving the accuracy of ultrafast ligand-based screening: incorporating lipophilicity into ElectroShape as an extra dimension. *Journal of Computer-Aided Molecular Design*, **2011**, 25, 785-90	4.2	28
56	Packaging HIV virion components through dynamic equilibria of a human tRNA synthetase. *Journal of Physical Chemistry B*, **2010**, 114, 16273-9	3.4	13
55	A dynamic model of HIV integrase inhibition and drug resistance. *Journal of Molecular Biology*, **2010** , 397, 600-15	6.5	52
54	ElectroShape: fast molecular similarity calculations incorporating shape, chirality and electrostatics. *Journal of Computer-Aided Molecular Design*, **2010**, 24, 789-801	4.2	60
53	AutoDock4 and AutoDockTools4: Automated docking with selective receptor flexibility. *Journal of Computational Chemistry*, **2009**, 30, 2785-91	3.5	11655
52	Molecular similarity including chirality. *Journal of Molecular Graphics and Modelling*, **2009**, 28, 368-70	2.8	17
51	Molecular docking. *Methods in Molecular Biology*, **2008**, 443, 365-82	1.4	307
50	Using AutoDock for ligand-receptor docking. *Current Protocols in Bioinformatics*, **2008**, Chapter 8, Unit 8.14	24.2	340
49	Functional proteomic and structural insights into molecular recognition in the nitrilase family enzymes. *Biochemistry*, **2008**, 47, 13514-23	3.2	43
48	Target flexibility: an emerging consideration in drug discovery and design. *Journal of Medicinal Chemistry*, **2008**, 51, 6237-55	8.3	244
47	Assessing the role of polarization in docking. *Journal of Physical Chemistry A*, **2008**, 112, 12157-63	2.8	36
46	Mapping of the CXCR4 binding site within variable region 3 of the feline immunodeficiency virus surface glycoprotein. *Journal of Virology*, **2008**, 82, 9134-42	6.6	21
45	Mechanistic and structural requirements for active site labeling of phosphoglycerate mutase by spiroepoxides. *Molecular BioSystems*, **2007**, 3, 495-506		42
44	A semiempirical free energy force field with charge-based desolvation. *Journal of Computational Chemistry*, **2007**, 28, 1145-52	3.5	1602

43	Structural insights into the mechanisms of drug resistance in HIV-1 protease NL4-3. *Journal of Molecular Biology*, **2006**, 356, 967-81	6.5	22
42	Structural mapping of CD134 residues critical for interaction with feline immunodeficiency virus. *Nature Structural and Molecular Biology*, **2005**, 12, 60-6	17.6	45
41	Active site binding modes of curcumin in HIV-1 protease and integrase. *Bioorganic and Medicinal Chemistry Letters*, **2005**, 15, 3364-8	2.9	78
40	Automated docking of ligands to an artificial active site: augmenting crystallographic analysis with computer modeling. *Journal of Computer-Aided Molecular Design*, **2003**, 17, 525-36	4.2	74
39	Design and synthesis of broad-based mono- and bi- cyclic inhibitors of FIV and HIV proteases. *Bioorganic and Medicinal Chemistry*, **2003**, 11, 2025-40	3.4	18
38	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	3.6	32
37	Structural basis for distinctions between substrate and inhibitor specificities for feline immunodeficiency virus and human immunodeficiency virus proteases. *Journal of Virology*, **2003**, 77, 6589-600	6.6	19
36	Defining HIV-1 protease substrate selectivity. *Current Drug Targets Infectious Disorders*, **2002**, 2, 37-50		28
35	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	4.2	341
34	Evolutionary analysis of HIV-1 protease inhibitors: Methods for design of inhibitors that evade resistance. *Proteins: Structure, Function and Bioinformatics*, **2002**, 48, 63-74	4.2	17
33	Model of the alphaLbeta2 integrin I-domain/ICAM-1 DI interface suggests that subtle changes in loop orientation determine ligand specificity. *Proteins: Structure, Function and Bioinformatics*, **2002**, 48, 151-60	4.2	15
32	Conformational changes in nitric oxide synthases induced by chlorzoxazone and nitroindazoles: crystallographic and computational analyses of inhibitor potency. *Biochemistry*, **2002**, 41, 13915-25	3.2	53
31	Mining for medicines in silico. *Trends in Biotechnology*, **2001**, 19, 123-124	15.1	2
30	Crystal structure of a neutralizing human IGG against HIV-1: a template for vaccine design. *Science*, **2001**, 293, 1155-9	33.3	764
29	Viral evolution in response to the broad-based retroviral protease inhibitor TL-3. *Journal of Virology* , **2001**, 75, 9502-8	6.6	28
28	Recognition templates for predicting adenylate-binding sites in proteins. *Journal of Molecular Biology*, **2001**, 314, 1245-55	6.5	16
27	Structural studies of FIV and HIV-1 proteases complexed with an efficient inhibitor of FIV protease. *Proteins: Structure, Function and Bioinformatics*, **2000**, 38, 29-40	4.2	27
26	Alteration of substrate and inhibitor specificity of feline immunodeficiency virus protease. *Journal of Virology*, **2000**, 74, 4710-20	6.6	28

25	Protein-Ligand Docking. *Methods and Principles in Medicinal Chemistry*, **2000**, 31-48	0.4	16
24	Improved Evolutionary Hybrids for Flexible Ligand Docking in AutoDock. *Nonconvex Optimization and Its Applications*, **2000**, 209-229		12
23	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, 1369-74	11.5	14
22	Development of a New Type of Protease Inhibitors, Efficacious against FIV and HIV Variants. *Journal of the American Chemical Society*, **1999**, 121, 1145-1155	16.4	51
21	Coevolution and subsite decomposition for the design of resistance-evading HIV-1 protease inhibitors. *Journal of Molecular Biology*, **1999**, 287, 77-92	6.5	13
20	Automated docking using a Lamarckian genetic algorithm and an empirical binding free energy function **1998**, 19, 1639-1662		7548
19	Computational coevolution of antiviral drug resistance. *Artificial Life*, **1998**, 4, 41-59	1.4	3
18	Crystal structures of the inactive D30N mutant of feline immunodeficiency virus protease complexed with a substrate and an inhibitor. *Biochemistry*, **1997**, 36, 10696-708	3.2	55
17	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, 5505-11	6.6	21
16	Automated docking of flexible ligands: applications of AutoDock. *Journal of Molecular Recognition*, **1996**, 9, 1-5	2.6	1057
15	Distributed automated docking of flexible ligands to proteins: parallel applications of AutoDock 2.4. *Journal of Computer-Aided Molecular Design*, **1996**, 10, 293-304	4.2	796
14	Automated docking of flexible ligands: Applications of autodock **1996**, 9, 1		6
13	Seeing our way to drug design. *Journal of Computer - Aided Molecular Design*, **1993**, 1, 329-344		5
12	Molecular modelling of the sterol C-14 demethylase of Saccharomyces cerevisiae. *Biochemical Society Transactions*, **1991**, 19, 793-5	5.1	21
11	Electron transport in cytochromes P-450 by covalent switching. *Proceedings of the Royal Society B: Biological Sciences*, **1991**, 245, 43-51	4.4	26
10	The active site of cytochrome P-450 nifedipine oxidase: a model-building study. *Journal of Molecular Graphics*, **1989**, 7, 206-11		25
9	The matching of protein sequences using color intrasequence homology displays. *Journal of Molecular Graphics*, **1988**, 6, 135-140		17
8	Bibliography of theoretical calculations in molecular pharmacology. *Journal of Molecular Graphics*, **1987**, 5, 211-222		4

7	Learning Protein-Ligand Binding Affinity with Atomic Environment Vectors		2
6	SuCOS is Better than RMSD for Evaluating Fragment Elaboration and Docking Poses		4
5	Characterisation of the SARS-CoV-2 ExoN (nsp14ExoN-nsp10) complex: implications for its role in viral genome stability and inhibitor identification		6
4	COVID Moonshot: Open Science Discovery of SARS-CoV-2 Main Protease Inhibitors by Combining Crowdsourcing, High-Throughput Experiments, Computational Simulations, and Machine Learning		18
3	Discovery of SARS-CoV-2 Mpro Peptide Inhibitors from Modelling Substrate and Ligand Binding		1
2	Investigating the potential for a limited quantum speedup on protein lattice problems. *New Journal of Physics*,	2.9	2
1	Scoring Functions for Protein-Ligand Binding Affinity Prediction Using Structure-based Deep Learning: A Review. *Frontiers in Bioinformatics*,2,		1