Markus A Lill

List of Publications by Citations

89 papers	2,740 citations	29 h-index	50 g-index
99 ext. papers	3,103 ext. citations	4.5 avg, IF	5.67 L-index

#	Paper	IF	Citations
89	Computer-aided drug design platform using PyMOL. *Journal of Computer-Aided Molecular Design*, **2011**, 25, 13-9	4.2	278
88	Combining protein modeling and 6D-QSAR. Simulating the binding of structurally diverse ligands to the estrogen receptor. *Journal of Medicinal Chemistry*, **2005**, 48, 3700-3	8.3	145
87	Long-chain carboxychromanols, metabolites of vitamin E, are potent inhibitors of cyclooxygenases. *Proceedings of the National Academy of Sciences of the United States of America*, **2008**, 105, 20464-9	11.5	139
86	Proton shuttle in green fluorescent protein studied by dynamic simulations. *Proceedings of the National Academy of Sciences of the United States of America*, **2002**, 99, 2778-81	11.5	131
85	Multi-dimensional QSAR in drug discovery. *Drug Discovery Today*, **2007**, 12, 1013-7	8.8	116
84	Integrating structure-based and ligand-based approaches for computational drug design. *Future Medicinal Chemistry*, **2011**, 3, 735-50	4.1	101
83	Metrics for measuring distances in configuration spaces. *Journal of Chemical Physics*, **2013**, 139, 184118	3.9	96
82	Potential Inhibitors for Novel Coronavirus Protease Identified by Virtual Screening of 606 Million Compounds. *International Journal of Molecular Sciences*, **2020**, 21,	6.3	96
81	Challenges predicting ligand-receptor interactions of promiscuous proteins: the nuclear receptor PXR. *PLoS Computational Biology*, **2009**, 5, e1000594	5	94
80	Dynamic water networks in cytochrome C oxidase from Paracoccus denitrificans investigated by molecular dynamics simulations. *Biophysical Journal*, **2004**, 86, 1873-89	2.9	89
79	Molecular dynamics simulation of proton transport with quantum mechanically derived proton hopping rates (Q-HOP MD). *Journal of Chemical Physics*, **2001**, 115, 7993-8005	3.9	80
78	Efficient incorporation of protein flexibility and dynamics into molecular docking simulations. *Biochemistry*, **2011**, 50, 6157-69	3.2	78
77	Substrate tunnels in enzymes: structure-function relationships and computational methodology. *Proteins: Structure, Function and Bioinformatics*, **2015**, 83, 599-611	4.2	77
76	The challenge of predicting drug toxicity in silico. *Basic and Clinical Pharmacology and Toxicology*, **2006**, 99, 195-208	3.1	59
75	Raptor: combining dual-shell representation, induced-fit simulation, and hydrophobicity scoring in receptor modeling: application toward the simulation of structurally diverse ligand sets. *Journal of Medicinal Chemistry*, **2004**, 47, 6174-86	8.3	56
74	WATsite: hydration site prediction program with PyMOL interface. *Journal of Computational Chemistry*, **2014**, 35, 1255-60	3.5	51
73	Prediction of small-molecule binding to cytochrome P450 3A4: flexible docking combined with multidimensional QSAR. *ChemMedChem*, **2006**, 1, 73-81	3.7	50

72	Impact of induced fit on ligand binding to the androgen receptor: a multidimensional QSAR study to predict endocrine-disrupting effects of environmental chemicals. *Journal of Medicinal Chemistry*, **2005**, 48, 5666-74	8.3	43
71	Virtual screening in drug design. *Methods in Molecular Biology*, **2013**, 993, 1-12	1.4	37
70	Extensive rigid analogue design maps the binding conformation of potent N-benzylphenethylamine 5-HT2A serotonin receptor agonist ligands. *ACS Chemical Neuroscience*, **2013**, 4, 96-109	5.7	36
69	Novel ligands for the chemokine receptor-3 (CCR3): a receptor-modeling study based on 5D-QSAR. *Journal of Medicinal Chemistry*, **2005**, 48, 1515-27	8.3	36
68	Utilizing experimental data for reducing ensemble size in flexible-protein docking. *Journal of Chemical Information and Modeling*, **2012**, 52, 187-98	6.1	34
67	Decision Making in Structure-Based Drug Discovery: Visual Inspection of Docking Results. *Journal of Medicinal Chemistry*, **2021**, 64, 2489-2500	8.3	34
66	Protein pharmacophore selection using hydration-site analysis. *Journal of Chemical Information and Modeling*, **2012**, 52, 1046-60	6.1	33
65	Compact parameter set for fast estimation of proton transfer rates. *Journal of Chemical Physics*, **2001**, 114, 1125-1132	3.9	33
64	PharmDock: a pharmacophore-based docking program. *Journal of Cheminformatics*, **2014**, 6, 14	8.6	31
63	Simulating alpha/beta selectivity at the human thyroid hormone receptor: consensus scoring using multidimensional QSAR. *ChemMedChem*, **2007**, 2, 78-87	3.7	30
62	Kinetics of the initial steps of G protein-coupled receptor-mediated cellular signaling revealed by single-molecule imaging. *ChemPhysChem*, **2005**, 6, 1633-40	3.2	30
61	Induced fit docking, and the use of QM/MM methods in docking. *Drug Discovery Today: Technologies* , **2013**, 10, e411-8	7.1	29
60	Reaction rates for proton transfer over small barriers and connection to transition state theory. *Journal of Chemical Physics*, **2001**, 115, 7985-7992	3.9	27
59	Accounting for Environmental Effects in ab Initio Calculations of Proton Transfer Barriers. *Journal of Physical Chemistry A*, **2000**, 104, 8283-8289	2.8	26
58	Including ligand-induced protein flexibility into protein tunnel prediction. *Journal of Computational Chemistry*, **2014**, 35, 1748-56	3.5	25
57	Significant enhancement of docking sensitivity using implicit ligand sampling. *Journal of Chemical Information and Modeling*, **2011**, 51, 693-706	6.1	23
56	Potentially increasing the metabolic stability of drug candidates via computational site of metabolism prediction by CYP2C9: The utility of incorporating protein flexibility via an ensemble of structures. *European Journal of Medicinal Chemistry*, **2011**, 46, 3953-63	6.8	22
55	Exploring the potential of protein-based pharmacophore models in ligand pose prediction and ranking. *Journal of Chemical Information and Modeling*, **2013**, 53, 1179-90	6.1	21

54	In silico prediction of harmful effects triggered by drugs and chemicals. *Toxicology and Applied Pharmacology*, **2005**, 207, 398-407	4.6	21
53	Solvent interaction energy calculations on molecular dynamics trajectories: increasing the efficiency using systematic frame selection. *Journal of Chemical Information and Modeling*, **2011**, 51, 2680-9	6.1	20
52	Combining structure- and ligand-based approaches to improve site of metabolism prediction in CYP2C9 substrates. *Pharmaceutical Research*, **2015**, 32, 986-1001	4.5	19
51	Stabilization of an unusual salt bridge in ubiquitin by the extra C-terminal domain of the proteasome-associated deubiquitinase UCH37 as a mechanism of its exo specificity. *Biochemistry*, **2013**, 52, 3564-78	3.2	19
50	Mapping the catechol binding site in dopamine D receptors: synthesis and evaluation of two parallel series of bicyclic dopamine analogues. *ChemMedChem*, **2011**, 6, 1024-40	3.7	17
49	Rubiscolins are naturally occurring G protein-biased delta opioid receptor peptides. *European Neuropsychopharmacology*, **2019**, 29, 450-456	1.2	17
48	Combining 4D pharmacophore generation and multidimensional QSAR: modeling ligand binding to the bradykinin B2 receptor. *Journal of Chemical Information and Modeling*, **2006**, 46, 2135-45	6.1	16
47	In silico prediction of receptor-mediated environmental toxic phenomena-application to endocrine disruption. *SAR and QSAR in Environmental Research*, **2005**, 16, 149-69	3.5	16
46	Mixed-model QSAR at the glucocorticoid receptor: predicting the binding mode and affinity of psychotropic drugs. *ChemMedChem*, **2009**, 4, 100-9	3.7	15
45	Elucidating the multiple roles of hydration for accurate protein-ligand binding prediction via deep learning. *Communications Chemistry*, **2020**, 3,	6.3	14
44	Ensemble generation and the influence of protein flexibility on geometric tunnel prediction in cytochrome P450 enzymes. *PLoS ONE*, **2014**, 9, e99408	3.7	14
43	Single-molecule study of molecular mobility in the cytoplasm of Escherichia coli. *Physical Review E*, **2012**, 86, 021907	2.4	14
42	Probing the steric space at the floor of the D1 dopamine receptor orthosteric binding domain: 7 7 8 and 8methyl substituted dihydrexidine analogues. *Journal of Medicinal Chemistry*, **2011**, 54, 5508-21	8.3	14
41	Single hepatitis-B virus core capsid binding to individual nuclear pore complexes in Hela cells. *Biophysical Journal*, **2006**, 91, 3123-30	2.9	13
40	Ranking protein-protein docking results using steered molecular dynamics and potential of mean force calculations. *Journal of Computational Chemistry*, **2016**, 37, 1861-5	3.5	13
39	Analysis of factors influencing hydration site prediction based on molecular dynamics simulations. *Journal of Chemical Information and Modeling*, **2014**, 54, 2987-95	6.1	12
38	Structural transitions and interactions in the early stages of human glucagon amyloid fibrillation. *Biophysical Journal*, **2015**, 108, 937-948	2.9	12
37	New computational method for prediction of interacting protein loop regions. *Proteins: Structure, Function and Bioinformatics*, **2010**, 78, 1748-59	4.2	12

36	From Crystal Structures and Their Analysis to the in silico Prediction of Toxic Phenomena. *Helvetica Chimica Acta*, **2003**, 86, 1554-1568	2	12
35	Flexibility of PCNA-protein interface accommodates differential binding partners. *PLoS ONE*, **2014**, 9, e102481	3.7	12
34	Molecular Determinants of the Differential Modulation of Ca1.2 and Ca1.3 by Nifedipine and FPL 64176. *Molecular Pharmacology*, **2018**, 94, 973-983	4.3	11
33	A bifunctional colchicinoid that binds to the androgen receptor. *Molecular Cancer Therapeutics*, **2007**, 6, 2328-36	6.1	11
32	Efficient and Accurate Hydration Site Profiling for Enclosed Binding Sites. *Journal of Chemical Information and Modeling*, **2018**, 58, 2183-2188	6.1	10
31	Inhibitors for Novel Coronavirus Protease Identified by Virtual Screening of 687 Million Compounds		9
30	WATsite2.0 with PyMOL Plugin: Hydration Site Prediction and Visualization. *Methods in Molecular Biology*, **2017**, 1611, 123-134	1.4	9
29	Fibpredictor: a computational method for rapid prediction of amyloid fibril structures. *Journal of Molecular Modeling*, **2016**, 22, 206	2	9
28	Optimization of a 1,3,4-oxadiazole series for inhibition of Ca/calmodulin-stimulated activity of adenylyl cyclases 1 and 8 for the treatment of chronic pain. *European Journal of Medicinal Chemistry* , **2019**, 162, 568-585	6.8	9
27	Role of computational methods in pharmaceutical sciences. *Methods in Molecular Biology*, **2012**, 929, 21-48	1.4	8
26	Analogues of doxanthrine reveal differences between the dopamine D1 receptor binding properties of chromanoisoquinolines and hexahydrobenzo[a]phenanthridines. *European Journal of Medicinal Chemistry*, **2012**, 48, 97-107	6.8	7
25	Predicting flexible loop regions that interact with ligands: the challenge of accurate scoring. *Proteins: Structure, Function and Bioinformatics*, **2012**, 80, 246-60	4.2	7
24	Modeling of Halogen-Protein Interactions in Co-Solvent Molecular Dynamics Simulations. *Journal of Chemical Information and Modeling*, **2019**, 59, 38-42	6.1	6
23	Molecular Modeling Evaluation of the Enantiomers of a Novel Adenylyl Cyclase 2 Inhibitor. *Journal of Chemical Information and Modeling*, **2017**, 57, 322-334	6.1	5
22	Virtual test kits for predicting harmful effects triggered by drugs and chemicals mediated by specific proteins. *ALTEX: Alternatives To Animal Experimentation*, **2005**, 22, 123-34	4.3	5
21	Improving Atom-Type Diversity and Sampling in Cosolvent Simulations Using Dynamics. *Journal of Chemical Theory and Computation*, **2019**, 15, 3272-3287	6.4	4
20	Confined Mobility of TonB and FepA in Escherichia coli Membranes. *PLoS ONE*, **2016**, 11, e0160862	3.7	4
19	Computational Assessment of Combination Therapy of Androgen Receptor-Targeting Compounds. *Journal of Chemical Information and Modeling*, **2021**, 61, 1001-1009	6.1	4

18	Discovery of Inhibitors for Proliferating Cell Nuclear Antigen Using a Computational-Based Linked-Multiple-Fragment Screen. *ACS Omega*, **2019**, 4, 15181-15196	3.9	3
17	Calculation of Thermodynamic Properties of Bound Water Molecules. *Methods in Molecular Biology*, **2018**, 1762, 389-402	1.4	3
16	In Silico Drug Discovery and Design **2013**,		3
15	Are distance-dependent statistical potentials considering three interacting bodies superior to two-body statistical potentials for protein structure prediction?. *Journal of Bioinformatics and Computational Biology*, **2014**, 12, 1450022	1	3
14	Multi-Dimensional QSAR in Drug Discovery: Probing Ligand Alignment and Induced Fit - Application to GPCRs and Nuclear Receptors. *Current Computer-Aided Drug Design*, **2005**, 1, 307-324	1.4	3
13	Dissecting the Influence of Protein Flexibility on the Location and Thermodynamic Profile of Explicit Water Molecules in Protein-Ligand Binding. *Journal of Chemical Theory and Computation*, **2016**, 12, 4578-92	6.4	3
12	Conformational Changes of Thyroid Receptors in Response to Antagonists. *Journal of Chemical Information and Modeling*, **2021**, 61, 1010-1019	6.1	3
11	Potential Inhibitors for Novel Coronavirus Protease Identified by Virtual Screening of 606 Million Compounds		2
10	Application of information theory to a three-body coarse-grained representation of proteins in the PDB: insights into the structural and evolutionary roles of residues in protein structure. *Proteins: Structure, Function and Bioinformatics*, **2014**, 82, 3450-65	4.2	1
9	Towards a Realistic Representation in Surface-Based Pseudoreceptor Modeling: a PDB-Wide Analysis of Binding Pockets. *Molecular Informatics*, **2012**, 31, 259-71	3.8	1
8	Computational Modeling of Receptor-Mediated Toxicity315-351		1
7	Evaluation of Xa inhibitors as potential inhibitors of the SARS-CoV-2 Mpro protease.. *PLoS ONE*, **2022**, 17, e0262482	3.7	1
6	Computational Selectivity Assessment of Protease Inhibitors against SARS-CoV-2. *International Journal of Molecular Sciences*, **2021**, 22,	6.3	1
5	Internet laboratory for predicting harmful effects triggered by drugs and chemicals--a progress report. *ALTEX: Alternatives To Animal Experimentation*, **2003**, 20, 85-91	4.3	1
4	Integrating structure-and ligand-based approaches for computer-aided drug design **2013**, 190-202		
3	Ligand pathways in estrogen-related receptors.. *Journal of Biomolecular Structure and Dynamics*, **2022**, 1-10	3.6	
2	Computer Simulation Meets Molecular Biology **2003**, 87-98		
1	Docking 3-phenyltropane analogs into an ensemble of serotonin transporter homology model conformations. *FASEB Journal*, **2011**, 25, 1083.2	0.9	