Matthias Rarey

List of Publications by Year in Descending Order

142 papers	9,464 citations	42 h-index	96 g-index
159 ext. papers	10,865 ext. citations	6 avg, IF	6.27 L-index

#	Paper	IF	Citations
142	Analyzing Structural Features of Proteins from Deep-Sea Organisms.. *Proteins: Structure, Function and Bioinformatics*, **2022**,	4.2	1
141	X-ray screening identifies active site and allosteric inhibitors of SARS-CoV-2 main protease. *Science*, **2021**, 372, 642-646	33.3	95
140	LSLOpt: An open-source implementation of the step-length controlled LSL-BFGS algorithm. *Journal of Computational Chemistry*, **2021**, 42, 1095-1100	3.5	0
139	GeoMine: interactive pattern mining of protein-ligand interfaces in the Protein Data Bank. *Bioinformatics*, **2021**, 37, 424-425	7.2	2
138	Topological Similarity Search in Large Combinatorial Fragment Spaces. *Journal of Chemical Information and Modeling*, **2021**, 61, 238-251	6.1	5
137	Disconnected Maximum Common Substructures under Constraints. *Journal of Chemical Information and Modeling*, **2021**, 61, 167-178	6.1	4
136	Maximum Common Substructure Searching in Combinatorial Make-on-Demand Compound Spaces. *Journal of Chemical Information and Modeling*, **2021**,	6.1	4
135	SMARTS.plus - A Toolbox for Chemical Pattern Design. *Molecular Informatics*, **2020**, 39, e2000216	3.8	2
134	A Consistent Scheme for Gradient-Based Optimization of ProteinLigand Poses. *Journal of Chemical Information and Modeling*, **2020**, 60, 6502-6522	6.1	8
133	Shape-Based Descriptors for Efficient Structure-Based Fragment Growing. *Journal of Chemical Information and Modeling*, **2020**, 60, 6269-6281	6.1	1
132	ProteinsPlus: interactive analysis of protein-ligand binding interfaces. *Nucleic Acids Research*, **2020**, 48, W48-W53	20.1	37
131	Comparing Molecular Patterns Using the Example of SMARTS: Theory and Algorithms. *Journal of Chemical Information and Modeling*, **2019**, 59, 2560-2571	6.1	14
130	Comparing Molecular Patterns Using the Example of SMARTS: Applications and Filter Collection Analysis. *Journal of Chemical Information and Modeling*, **2019**, 59, 2572-2586	6.1	7
129	In Need of Bias Control: Evaluating Chemical Data for Machine Learning in Structure-Based Virtual Screening. *Journal of Chemical Information and Modeling*, **2019**, 59, 947-961	6.1	104
128	Machine Learning in Drug Discovery. *Journal of Chemical Information and Modeling*, **2019**, 59, 945-946	6.1	24
127	Conformator: A Novel Method for the Generation of Conformer Ensembles. *Journal of Chemical Information and Modeling*, **2019**, 59, 731-742	6.1	26
126	StructureProfiler: an all-in-one tool for 3D protein structure profiling. *Bioinformatics*, **2019**, 35, 874-876	7.2	2

125	Connected Subgraph Fingerprints: Representing Molecules Using Exhaustive Subgraph Enumeration. *Journal of Chemical Information and Modeling*, **2019**, 59, 4625-4635	6.1	3
124	NAOMInext - Synthetically feasible fragment growing in a structure-based design context. *European Journal of Medicinal Chemistry*, **2019**, 163, 747-762	6.8	4
123	Prediction, Analysis, and Comparison of Active Sites **2018**, 283-311		1
122	Structure-Based Virtual Screening **2018**, 313-331		3
121	Placement of Water Molecules in Protein Structures: From Large-Scale Evaluations to Single-Case Examples. *Journal of Chemical Information and Modeling*, **2018**, 58, 1625-1637	6.1	22
120	Exploring Structure-Activity Relationships with Three-Dimensional Matched Molecular Pairs-A Review. *ChemMedChem*, **2018**, 13, 482-489	3.7	6
119	RingDecomposerLib: An Open-Source Implementation of Unique Ring Families and Other Cycle Bases. *Journal of Chemical Information and Modeling*, **2017**, 57, 122-126	6.1	6
118	Index-Based Searching of Interaction Patterns in Large Collections of Protein-Ligand Interfaces. *Journal of Chemical Information and Modeling*, **2017**, 57, 148-158	6.1	10
117	High-Quality Dataset of Protein-Bound Ligand Conformations and Its Application to Benchmarking Conformer Ensemble Generators. *Journal of Chemical Information and Modeling*, **2017**, 57, 529-539	6.1	39
116	Large-Scale Analysis of Hydrogen Bond Interaction Patterns in Protein-Ligand Interfaces. *Journal of Medicinal Chemistry*, **2017**, 60, 4245-4257	8.3	35
115	Prediction of protein mutation effects based on dehydration and hydrogen bonding - A large-scale study. *Proteins: Structure, Function and Bioinformatics*, **2017**, 85, 1550-1566	4.2	
114	Ligand-based virtual screening under partial shape constraints. *Journal of Computer-Aided Molecular Design*, **2017**, 31, 335-347	4.2	5
113	Benchmarking Commercial Conformer Ensemble Generators. *Journal of Chemical Information and Modeling*, **2017**, 57, 2719-2728	6.1	51
112	Computational Macrocyclization: From de novo Macrocycle Generation to Binding Affinity Estimation. *ChemMedChem*, **2017**, 12, 1866-1872	3.7	19
111	Estimating Electron Density Support for Individual Atoms and Molecular Fragments in X-ray Structures. *Journal of Chemical Information and Modeling*, **2017**, 57, 2437-2447	6.1	41
110	NAOMInova: Interactive Geometric Analysis of Noncovalent Interactions in Macromolecular Structures. *Journal of Chemical Information and Modeling*, **2017**, 57, 2132-2142	6.1	3
109	From cheminformatics to structure-based design: Web services and desktop applications based on the NAOMI library. *Journal of Biotechnology*, **2017**, 261, 207-214	3.7	2
108	ProteinsPlus: a web portal for structure analysis of macromolecules. *Nucleic Acids Research*, **2017**, 45, W337-W343	20.1	80

107	mRAISE: an alternative algorithmic approach to ligand-based virtual screening. *Journal of Computer-Aided Molecular Design*, **2016**, 30, 583-94	4.2	9
106	Supporting Biocatalysis Research with Structural Bioinformatics **2016**, 71-100		1
105	FSees: Customized Enumeration of Chemical Subspaces with Limited Main Memory Consumption. *Journal of Chemical Information and Modeling*, **2016**, 56, 1641-53	6.1	6
104	11th German Conference on Chemoinformatics (GCC 2015) : Fulda, Germany. 8-10 November 2015. *Journal of Cheminformatics*, **2016**, 8, 18	8.6	
103	Linker-Region Modified Derivatives of the Deoxyhypusine Synthase Inhibitor CNI-1493 Suppress HIV-1 Replication. *Archiv Der Pharmazie*, **2016**, 349, 91-103	4.3	4
102	SIENA: Efficient Compilation of Selective Protein Binding Site Ensembles. *Journal of Chemical Information and Modeling*, **2016**, 56, 248-59	6.1	27
101	Feasibility of Active Machine Learning for Multiclass Compound Classification. *Journal of Chemical Information and Modeling*, **2016**, 56, 12-20	6.1	30
100	Torsion Library Reloaded: A New Version of Expert-Derived SMARTS Rules for Assessing Conformations of Small Molecules. *Journal of Chemical Information and Modeling*, **2016**, 56, 1-5	6.1	25
99	The Art of Compiling Protein Binding Site Ensembles. *Molecular Informatics*, **2016**, 35, 593-598	3.8	4
98	UNICON: A Powerful and Easy-to-Use Compound Library Converter. *Journal of Chemical Information and Modeling*, **2016**, 56, 1105-11	6.1	16
97	ASCONA: Rapid Detection and Alignment of Protein Binding Site Conformations. *Journal of Chemical Information and Modeling*, **2015**, 55, 1747-56	6.1	11
96	Evidence of water molecules--a statistical evaluation of water molecules based on electron density. *Journal of Chemical Information and Modeling*, **2015**, 55, 771-83	6.1	40
95	MONA 2: A Light Cheminformatics Platform for Interactive Compound Library Processing. *Journal of Chemical Information and Modeling*, **2015**, 55, 2071-8	6.1	22
94	Discriminative Chemical Patterns: Automatic and Interactive Design. *Journal of Chemical Information and Modeling*, **2015**, 55, 1535-46	6.1	10
93	In silico design, synthesis, and screening of novel deoxyhypusine synthase inhibitors targeting HIV-1 replication. *ChemMedChem*, **2014**, 9, 940-52	3.7	8
92	Facing the challenges of structure-based target prediction by inverse virtual screening. *Journal of Chemical Information and Modeling*, **2014**, 54, 1676-86	6.1	56
91	The valence state combination model: a generic framework for handling tautomers and protonation states. *Journal of Chemical Information and Modeling*, **2014**, 54, 756-66	6.1	14
90	An integrated approach to knowledge-driven structure-based virtual screening. *Journal of Computer-Aided Molecular Design*, **2014**, 28, 927-39	4.2	7

89	Elucidating protein-protein interactions using the HYDE scoring function. *Journal of Cheminformatics*, **2014**, 6,	8.6	78
88	Accessing Open PHACTS: interactive exploration of compounds and targets from the semantic web. *Journal of Cheminformatics*, **2014**, 6,	8.6	78
87	Protein□gand interaction databases: advanced tools to mine activity data and interactions on a structural level. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2014**, 4, 562-575	7.9	8
86	Benchmark data sets for structure-based computational target prediction. *Journal of Chemical Information and Modeling*, **2014**, 54, 2261-74	6.1	17
85	Exploiting structural information for drug-target assessment. *Future Medicinal Chemistry*, **2014**, 6, 319-31	4.1	19
84	Protoss: a holistic approach to predict tautomers and protonation states in protein-ligand complexes. *Journal of Cheminformatics*, **2014**, 6, 12	8.6	98
83	Force-field-based minimizations of protein-ligand complexes in the blink of an eye. *Journal of Cheminformatics*, **2013**, 5,	8.6	78
82	Visualisierung komplexer, molekularer Zusammenh□ge. *BioSpektrum*, **2013**, 19, 146-148	0.1	
81	Interactive design of generic chemical patterns. *Drug Discovery Today*, **2013**, 18, 651-8	8.8	12
80	Coping with Combinatorial Space in Molecular Design **2013**, 325-347		3
79	CONFECT: conformations from an expert collection of torsion patterns. *ChemMedChem*, **2013**, 8, 1690-700	3.7	21
78	A consistent description of HYdrogen bond and DEhydration energies in protein-ligand complexes: methods behind the HYDE scoring function. *Journal of Computer-Aided Molecular Design*, **2013**, 27, 15-29	4.2	158
77	Reading PDB: perception of molecules from 3D atomic coordinates. *Journal of Chemical Information and Modeling*, **2013**, 53, 76-87	6.1	19
76	Predicting enzymatic function from global binding site descriptors. *Proteins: Structure, Function and Bioinformatics*, **2013**, 81, 479-89	4.2	11
75	Torsion angle preferences in druglike chemical space: a comprehensive guide. *Journal of Medicinal Chemistry*, **2013**, 56, 2016-28	8.3	83
74	Fast protein binding site comparison via an index-based screening technology. *Journal of Chemical Information and Modeling*, **2013**, 53, 411-22	6.1	18
73	Protein pocket and ligand shape comparison and its application in virtual screening. *Journal of Computer-Aided Molecular Design*, **2013**, 27, 511-24	4.2	20
72	Searching for recursively defined generic chemical patterns in nonenumerated fragment spaces. *Journal of Chemical Information and Modeling*, **2013**, 53, 1676-88	6.1	9

71	Scientific competency questions as the basis for semantically enriched open pharmacological space development. *Drug Discovery Today*, **2013**, 18, 843-52	8.8	40
70	MONA - Interactive manipulation of molecule collections. *Journal of Cheminformatics*, **2013**, 5, 38	8.6	20
69	A flexible-hydrogen interaction model for protein-ligand docking. *Journal of Cheminformatics*, **2012**, 4,	8.6	78
68	Some thoughts on the "A" in computer-aided molecular design. *Journal of Computer-Aided Molecular Design*, **2012**, 26, 113-4	4.2	1
67	TFD: Torsion Fingerprints as a new measure to compare small molecule conformations. *Journal of Chemical Information and Modeling*, **2012**, 52, 1499-512	6.1	27
66	Perspectives from Medicinal Chemistry **2012**, 217-230		2
65	Searching for substructures in fragment spaces. *Journal of Chemical Information and Modeling*, **2012** , 52, 3181-9	6.1	5
64	Computational biotechnology: prediction of competitive substrate inhibition of enzymes by buffer compounds with protein-ligand docking. *Journal of Biotechnology*, **2012**, 161, 391-401	3.7	12
63	Evaluation of deoxyhypusine synthase inhibitors targeting BCR-ABL positive leukemias. *Investigational New Drugs*, **2012**, 30, 2274-83	4.3	9
62	Design of combinatorial libraries for the exploration of virtual hits from fragment space searches with LoFT. *Journal of Chemical Information and Modeling*, **2012**, 52, 373-9	6.1	7
61	Fast force field-based optimization of protein-ligand complexes with graphics processor. *Journal of Computational Chemistry*, **2012**, 33, 2554-65	3.5	11
60	The Internet as Scientific Knowledge Base: Navigating the Chem-Bio Space. *Molecular Informatics*, **2012**, 31, 543-546	3.8	4
59	Combining global and local measures for structure-based druggability predictions. *Journal of Chemical Information and Modeling*, **2012**, 52, 360-72	6.1	237
58	Unique ring families: a chemically meaningful description of molecular ring topologies. *Journal of Chemical Information and Modeling*, **2012**, 52, 2013-21	6.1	16
57	Systematic benchmark of substructure search in molecular graphs - From Ullmann to VF2. *Journal of Cheminformatics*, **2012**, 4, 13	8.6	23
56	Nearly no Scoring Function Without a Hansch-Analysis. *Molecular Informatics*, **2012**, 31, 503-7	3.8	3
55	Substantial improvements in large-scale redocking and screening using the novel HYDE scoring function. *Journal of Computer-Aided Molecular Design*, **2012**, 26, 701-23	4.2	84
54	DoGSiteScorer: a web server for automatic binding site prediction, analysis and druggability assessment. *Bioinformatics*, **2012**, 28, 2074-5	7.2	231

53	Improving similarity-driven library design: customized matching and regioselective feature trees. *Journal of Chemical Information and Modeling*, **2011**, 51, 2156-63	6.1	4
52	NAOMI: on the almost trivial task of reading molecules from different file formats. *Journal of Chemical Information and Modeling*, **2011**, 51, 3199-207	6.1	39
51	Maximum common subgraph isomorphism algorithms and their applications in molecular science: a review. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2011**, 1, 68-79	7.9	50
50	De novo design by pharmacophore-based searches in fragment spaces. *Journal of Computer-Aided Molecular Design*, **2011**, 25, 931-45	4.2	13
49	Consistent two-dimensional visualization of protein-ligand complex series. *Journal of Cheminformatics*, **2011**, 3, 21	8.6	5
48	Flat and Easy: 2D Depiction of Protein-Ligand Complexes. *Molecular Informatics*, **2011**, 30, 12-9	3.8	3
47	From activity cliffs to target-specific scoring models and pharmacophore hypotheses. *ChemMedChem*, **2011**, 6, 1630-9, 1533	3.7	39
46	LoFT: similarity-driven multiobjective focused library design. *Journal of Chemical Information and Modeling*, **2010**, 50, 1-21	6.1	34
45	Analyzing the topology of active sites: on the prediction of pockets and subpockets. *Journal of Chemical Information and Modeling*, **2010**, 50, 2041-52	6.1	111
44	From structure diagrams to visual chemical patterns. *Journal of Chemical Information and Modeling*, **2010**, 50, 1529-35	6.1	43
43	Drawing the PDB: Protein-Ligand Complexes in Two Dimensions. *ACS Medicinal Chemistry Letters*, **2010**, 1, 540-5	4.3	192
42	In Pursuit of Fully Flexible Protein-Ligand Docking: Modeling the Bilateral Mechanism of Binding. *Molecular Informatics*, **2010**, 29, 164-73	3.8	17
41	PoseView -- molecular interaction patterns at a glance. *Journal of Cheminformatics*, **2010**, 2,	8.6	44
40	Second-generation de novo design: a view from a medicinal chemist perspective. *Journal of Computer-Aided Molecular Design*, **2009**, 23, 593-602	4.2	25
39	Fast automated placement of polar hydrogen atoms in protein-ligand complexes. *Journal of Cheminformatics*, **2009**, 1, 13	8.6	35
38	Conformational sampling for large-scale virtual screening: accuracy versus ensemble size. *Journal of Chemical Information and Modeling*, **2009**, 49, 2303-11	6.1	26
37	Beyond the virtual screening paradigm: structure-based searching for new lead compounds. *Journal of Chemical Information and Modeling*, **2009**, 49, 800-9	6.1	29
36	Modeling of metal interaction geometries for protein-ligand docking. *Proteins: Structure, Function and Bioinformatics*, **2008**, 71, 1237-54	4.2	50

35	Towards an integrated description of hydrogen bonding and dehydration: decreasing false positives in virtual screening with the HYDE scoring function. *ChemMedChem*, **2008**, 3, 885-97	3.7	122
34	On the art of compiling and using 'drug-like' chemical fragment spaces. *ChemMedChem*, **2008**, 3, 1503-7	3.7	121
33	SwiFT: an index structure for reduced graph descriptors in virtual screening and clustering. *Journal of Chemical Information and Modeling*, **2007**, 47, 1341-53	6.1	10
32	From modeling to medicinal chemistry: automatic generation of two-dimensional complex diagrams. *ChemMedChem*, **2007**, 2, 853-60	3.7	61
31	TrixX: structure-based molecule indexing for large-scale virtual screening in sublinear time. *Journal of Computer-Aided Molecular Design*, **2007**, 21, 223-38	4.2	17
30	Exploring fragment spaces under multiple physicochemical constraints. *Journal of Computer-Aided Molecular Design*, **2007**, 21, 327-40	4.2	12
29	Recore: a fast and versatile method for scaffold hopping based on small molecule crystal structure conformations. *Journal of Chemical Information and Modeling*, **2007**, 47, 390-9	6.1	109
28	FlexNovo: structure-based searching in large fragment spaces. *ChemMedChem*, **2006**, 1, 854-68	3.7	51
27	Molecular complexes at a glance: automated generation of two-dimensional complex diagrams. *Bioinformatics*, **2006**, 22, 1710-6	7.2	224
26	Fully automated flexible docking of ligands into flexible synthetic receptors using forward and inverse docking strategies. *Journal of Chemical Information and Modeling*, **2006**, 46, 903-11	6.1	23
25	Multiple-ligand-based virtual screening: methods and applications of the MTree approach. *Journal of Medicinal Chemistry*, **2005**, 48, 6575-84	8.3	38
24	Novel technologies for virtual screening. *Drug Discovery Today*, **2004**, 9, 27-34	8.8	153
23	FlexX-Scan: fast, structure-based virtual screening. *Proteins: Structure, Function and Bioinformatics*, **2004**, 57, 504-17	4.2	55
22	Automated drawing of structural molecular formulas under constraints. *Journal of Chemical Information and Computer Sciences*, **2004**, 44, 1065-78		50
21	Flexible docking under pharmacophore type constraints. *Journal of Computer-Aided Molecular Design*, **2002**, 16, 129-49	4.2	139
20	Similarity searching in large combinatorial chemistry spaces. *Journal of Computer-Aided Molecular Design*, **2001**, 15, 497-520	4.2	104
19	Detailed analysis of scoring functions for virtual screening. *Journal of Medicinal Chemistry*, **2001**, 44, 1035-42	5.9	451
18	FlexE: efficient molecular docking considering protein structure variations. *Journal of Molecular Biology*, **2001**, 308, 377-95	6.5	408

17	Small Molecule Docking and Scoring. *Reviews in Computational Chemistry*, **2001**, 1-60		64
16	A recursive algorithm for efficient combinatorial library docking. *Journal of Computer - Aided Molecular Design*, **2000**, 20, 63-81		29
15	The particle concept: placing discrete water molecules during protein-ligand docking predictions. *Proteins: Structure, Function and Bioinformatics*, **1999**, 34, 17-28	4.2	176
14	Evaluation of the FLEXX incremental construction algorithm for protein-ligand docking. *Proteins: Structure, Function and Bioinformatics*, **1999**, 37, 228-41	4.2	677
13	Two-stage method for protein-ligand docking. *Journal of Medicinal Chemistry*, **1999**, 42, 4422-33	8.3	81
12	The particle concept: placing discrete water molecules during protein-ligand docking predictions **1999**, 34, 17		4
11	Evaluation of the FLEXX incremental construction algorithm for protein□gand docking **1999**, 37, 228		3
10	Feature trees: a new molecular similarity measure based on tree matching. *Journal of Computer-Aided Molecular Design*, **1998**, 12, 471-90	4.2	245
9	Multiple automatic base selection: protein-ligand docking based on incremental construction without manual intervention. *Journal of Computer-Aided Molecular Design*, **1997**, 11, 369-84	4.2	156
8	CASP2 experiences with docking flexible ligands using FLEXX. *Proteins: Structure, Function and Bioinformatics*, **1997**, 29, 221-225	4.2	41
7	CASP2 experiences with docking flexible ligands using FLEXX. *Proteins: Structure, Function and Bioinformatics*, **1997**, 29, 221-225	4.2	4
6	CASP2 experiences with docking flexible ligands using FlexX. *Proteins: Structure, Function and Bioinformatics*, **1997**, Suppl 1, 221-5	4.2	14
5	A fast flexible docking method using an incremental construction algorithm. *Journal of Molecular Biology*, **1996**, 261, 470-89	6.5	2332
4	Placement of medium-sized molecular fragments into active sites of proteins. *Journal of Computer-Aided Molecular Design*, **1996**, 10, 41-54	4.2	157
3	Docking and Scoring for Structure-based Drug Design541-599		5
2	Catalytic cleavage of HEAT and subsequent covalent binding of the tetralone moiety by the SARS-CoV-2 main protease		2
1	Inhibition of SARS-CoV-2 main protease by allosteric drug-binding		6