Matthias Rarey

List of Publications by Year
in descending order

146	11,892	57758	30087
papers	citations	44 h-index	103 g-index

159	159	159	9968
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	A Fast Flexible Docking Method using an Incremental Construction Algorithm. Journal of Molecular Biology, 1996, 261, 470-489.	4.2	2,609
2	Evaluation of the FLEXX incremental construction algorithm for protein-ligand docking. Proteins: Structure, Function and Bioinformatics, 1999, 37, 228-241.	2.6	776
3	Detailed Analysis of Scoring Functions for Virtual Screening. Journal of Medicinal Chemistry, 2001, 44, 1035-1042.	6.4	495
4	FlexE: efficient molecular docking considering protein structure variations1 1Edited by J. Thornton. Journal of Molecular Biology, 2001, 308, 377-395.	4.2	451
5	DoGSiteScorer: a web server for automatic binding site prediction, analysis and druggability assessment. Bioinformatics, 2012, 28, 2074-2075.	4.1	381
6	Combining Global and Local Measures for Structure-Based Druggability Predictions. Journal of Chemical Information and Modeling, 2012, 52, 360-372.	5.4	346
7	Molecular complexes at a glance: automated generation of two-dimensional complex diagrams. Bioinformatics, 2006, 22, 1710-1716.	4.1	337
8	Feature trees: a new molecular similarity measure based on tree matching. , 1998, 12, 471-490.		283
9	X-ray screening identifies active site and allosteric inhibitors of SARS-CoV-2 main protease. Science, 2021, 372, 642-646.	12.6	240
10	On the Art of Compiling and Using 'Drugâ€Like' Chemical Fragment Spaces. ChemMedChem, 2008, 3, 1503-1507.	3.2	231
11	A consistent description of HYdrogen bond and DEhydration energies in proteinâ€“ligand complexes: methods behind the HYDE scoring function. Journal of Computer-Aided Molecular Design, 2013, 27, 15-29.	2.9	231
12	Drawing the PDB: Proteinâ˜Ligand Complexes in Two Dimensions. ACS Medicinal Chemistry Letters, 2010, 1, 540-545.	2.8	223
13	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.	5.4	196
14	The particle concept: placing discrete water molecules during protein-ligand docking predictions. Proteins: Structure, Function and Bioinformatics, 1999, 34, 17-28.	2.6	187
15	Analyzing the Topology of Active Sites: On the Prediction of Pockets and Subpockets. Journal of Chemical Information and Modeling, 2010, 50, 2041-2052.	5.4	184
16	Placement of medium-sized molecular fragments into active sites of proteins. Journal of Computer-Aided Molecular Design, 1996, 10, 41-54.	2.9	178
17	Multiple automatic base selection: protein-ligand docking based on incremental construction without manual intervention. Journal of Computer-Aided Molecular Design, 1997, 11, 369-384.	2.9	178
18	Novel technologies for virtual screening. Drug Discovery Today, 2004, 9, 27-34.	6.4	168

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19	Towards an Integrated Description of Hydrogen Bonding and Dehydration: Decreasing False Positives in Virtual Screening with the HYDE Scoring Function. ChemMedChem, 2008, 3, 885-897.	3.2	168
20	ProteinsPlus: a web portal for structure analysis of macromolecules. Nucleic Acids Research, 2017, 45, W337-W343.	14.5	158
21	Flexible docking under pharmacophore type constraints. Journal of Computer-Aided Molecular Design, 2002, 16, 129-149.	2.9	157
22	Protoss: a holistic approach to predict tautomers and protonation states in protein-ligand complexes. Journal of Cheminformatics, 2014, 6, 12.	6.1	141
23	ProteinsPlus: interactive analysis of proteinâ€“ligand binding interfaces. Nucleic Acids Research, 2020, 48, W48-W53.	14.5	135
24	Recore:â€‰ A Fast and Versatile Method for Scaffold Hopping Based on Small Molecule Crystal Structure Conformations. Journal of Chemical Information and Modeling, 2007, 47, 390-399.	5.4	132
25	Similarity searching in large combinatorial chemistry spaces. , 2001, 15, 497-520.		124
26	Substantial improvements in large-scale redocking and screening using the novel HYDE scoring function. Journal of Computer-Aided Molecular Design, 2012, 26, 701-723.	2.9	114
27	Torsion Angle Preferences in Druglike Chemical Space: A Comprehensive Guide. Journal of Medicinal Chemistry, 2013, 56, 2016-2028.	6.4	106
28	Automated Drawing of Structural Molecular Formulas under Constraints. Journal of Chemical Information and Computer Sciences, 2004, 44, 1065-1078.	2.8	90
29	Small Molecule Docking and Scoring. Reviews in Computational Chemistry, 2001, , 1-60.	1.5	88
30	Benchmarking Commercial Conformer Ensemble Generators. Journal of Chemical Information and Modeling, 2017, 57, 2719-2728.	5.4	88
31	Two-Stage Method for Proteinâ^'Ligand Docking. Journal of Medicinal Chemistry, 1999, 42, 4422-4433.	6.4	86
32	From Modeling to Medicinal Chemistry: Automatic Generation of Two-Dimensional Complex Diagrams. ChemMedChem, 2007, 2, 853-860.	3.2	79
33	FlexX-Scan: Fast, structure-based virtual screening. Proteins: Structure, Function and Bioinformatics, 2004, 57, 504-517.	2.6	77
34	Facing the Challenges of Structure-Based Target Prediction by Inverse Virtual Screening. Journal of Chemical Information and Modeling, 2014, 54, 1676-1686.	5.4	68
35	Estimating Electron Density Support for Individual Atoms and Molecular Fragments in X-ray Structures. Journal of Chemical Information and Modeling, 2017, 57, 2437-2447.	5.4	68
36	PoseView -- molecular interaction patterns at a glance. Journal of Cheminformatics, 2010, 2, .	6.1	67

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37	FlexNovo: Structure-Based Searching in Large Fragment Spaces. ChemMedChem, 2006, 1, 854-868.	3.2	64
38	Maximum common subgraph isomorphism algorithms and their applications in molecular science: a review. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 68-79.	14.6	62
39	Modeling of metal interaction geometries for proteinâ€“ligand docking. Proteins: Structure, Function and Bioinformatics, 2008, 71, 1237-1254.	2.6	60
40	Large-Scale Analysis of Hydrogen Bond Interaction Patterns in Proteinâ€“Ligand Interfaces. Journal of Medicinal Chemistry, 2017, 60, 4245-4257.	6.4	58
41	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.	5.4	57
42	Fast automated placement of polar hydrogen atoms in protein-ligand complexes. Journal of Cheminformatics, 2009, 1, 13.	6.1	56
43	From Structure Diagrams to Visual Chemical Patterns. Journal of Chemical Information and Modeling, 2010, 50, 1529-1535.	5.4	56
44	NAOMI: On the Almost Trivial Task of Reading Molecules from Different File formats. Journal of Chemical Information and Modeling, 2011, 51, 3199-3207.	5.4	52
45	CASP2 experiences with docking flexible ligands using FLEXX. Proteins: Structure, Function and Bioinformatics, 1997, 29, 221-225.	2.6	51
46	Evidence of Water Moleculesâ€”A Statistical Evaluation of Water Molecules Based on Electron Density. Journal of Chemical Information and Modeling, 2015, 55, 771-783.	5.4	49
47	Conformator: A Novel Method for the Generation of Conformer Ensembles. Journal of Chemical Information and Modeling, 2019, 59, 731-742.	5.4	49
48	Exploration of Ultralarge Compound Collections for Drug Discovery. Journal of Chemical Information and Modeling, 2022, 62, 2021-2034.	5.4	46
49	Scientific competency questions as the basis for semantically enriched open pharmacological space development. Drug Discovery Today, 2013, 18, 843-852.	6.4	44
50	From Activity Cliffs to Targetâ€Specific Scoring Models and Pharmacophore Hypotheses. ChemMedChem, 2011, 6, 1630-1639.	3.2	43
51	Machine Learning in Drug Discovery. Journal of Chemical Information and Modeling, 2019, 59, 945-946.	5.4	43
52	Multiple-Ligand-Based Virtual Screening:Â Methods and Applications of the MTree Approach. Journal of Medicinal Chemistry, 2005, 48, 6575-6584.	6.4	40
53	SIENA: Efficient Compilation of Selective Protein Binding Site Ensembles. Journal of Chemical Information and Modeling, 2016, 56, 248-259.	5.4	39
54	TFD: Torsion Fingerprints As a New Measure To Compare Small Molecule Conformations. Journal of Chemical Information and Modeling, 2012, 52, 1499-1512.	5.4	38

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55	Feasibility of Active Machine Learning for Multiclass Compound Classification. Journal of Chemical Information and Modeling, 2016, 56, 12-20.	5.4	37
56	LoFT: Similarity-Driven Multiobjective Focused Library Design. Journal of Chemical Information and Modeling, 2010, 50, 1-21.	5.4	35
57	ProteinsPlus: a comprehensive collection of web-based molecular modeling tools. Nucleic Acids Research, 2022, 50, W611-W615.	14.5	35
58	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.	5.4	34
59	A recursive algorithm for efficient combinatorial library docking. Journal of Computer - Aided Molecular Design, 2000, 20, 63-81.	1.0	32
60	A Consistent Scheme for Gradient-Based Optimization of Proteinâ€“Ligand Poses. Journal of Chemical Information and Modeling, 2020, 60, 6502-6522.	5.4	32
61	Beyond the Virtual Screening Paradigm: Structure-Based Searching for New Lead Compounds. Journal of Chemical Information and Modeling, 2009, 49, 800-809.	5.4	31
62	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.	5.4	30
63	TrixX: structure-based molecule indexing for large-scale virtual screening in sublinear time. Journal of Computer-Aided Molecular Design, 2007, 21, 223-238.	2.9	29
64	CONFECT: Conformations from an Expert Collection of Torsion Patterns. ChemMedChem, 2013, 8, 1690-1700.	3.2	29
65	Conformational Sampling for Large-Scale Virtual Screening: Accuracy versus Ensemble Size. Journal of Chemical Information and Modeling, 2009, 49, 2303-2311.	5.4	28
66	MONA 2: A Light Cheminformatics Platform for Interactive Compound Library Processing. Journal of Chemical Information and Modeling, 2015, 55, 2071-2078.	5.4	28
67	Second-generation de novo design: a view from a medicinal chemist perspective. Journal of Computer-Aided Molecular Design, 2009, 23, 593-602.	2.9	27
68	Reading PDB: Perception of Molecules from 3D Atomic Coordinates. Journal of Chemical Information and Modeling, 2013, 53, 76-87.	5.4	27
69	Exploiting structural information for drug-target assessment. Future Medicinal Chemistry, 2014, 6, 319-331.	2.3	27
70	Systematic benchmark of substructure search in molecular graphs - From Ullmann to VF2. Journal of Cheminformatics, 2012, 4, 13.	6.1	26
71	MONA â€“ Interactive manipulation of molecule collections. Journal of Cheminformatics, 2013, 5, 38.	6.1	26
72	UNICON: A Powerful and Easy-to-Use Compound Library Converter. Journal of Chemical Information and Modeling, 2016, 56, 1105-1111.	5.4	26

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73	Protein pocket and ligand shape comparison and its application in virtual screening. Journal of Computer-Aided Molecular Design, 2013, 27, 511-524.	2.9	25
74	Computational Macrocyclization: From deâ€...novo Macrocycle Generation to Binding Affinity Estimation. ChemMedChem, 2017, 12, 1866-1872.	3.2	25
75	Comparing Molecular Patterns Using the Example of SMARTS: Theory and Algorithms. Journal of Chemical Information and Modeling, 2019, 59, 2560-2571.	5.4	25
76	Fully Automated Flexible Docking of Ligands into Flexible Synthetic Receptors Using Forward and Inverse Docking Strategies. Journal of Chemical Information and Modeling, 2006, 46, 903-911.	5.4	24
77	Topological Similarity Search in Large Combinatorial Fragment Spaces. Journal of Chemical Information and Modeling, 2021, 61, 238-251.	5.4	24
78	Maximum Common Substructure Searching in Combinatorial Make-on-Demand Compound Spaces. Journal of Chemical Information and Modeling, 2022, 62, 2133-2150.	5.4	23
79	Editorial: Method and Data Sharing and Reproducibility of Scientific Results. Journal of Chemical Information and Modeling, 2020, 60, 5868-5869.	5.4	22
80	Fast Protein Binding Site Comparison via an Index-Based Screening Technology. Journal of Chemical Information and Modeling, 2013, 53, 411-422.	5.4	21
81	Machine Learning in Drug Discovery. Journal of Chemical Information and Modeling, 2018, 58, 1723-1724.	5.4	21
82	Benchmark Data Sets for Structure-Based Computational Target Prediction. Journal of Chemical Information and Modeling, 2014, 54, 2261-2274.	5.4	20
83	Interpretation of Structureâ€“Activity Relationships in Real-World Drug Design Data Sets Using Explainable Artificial Intelligence. Journal of Chemical Information and Modeling, 2022, 62, 447-462.	5.4	20
84	In Pursuit of Fully Flexible Proteinâ€Ligand Docking: Modeling the Bilateral Mechanism of Binding. Molecular Informatics, 2010, 29, 164-173.	2.5	19
85	De novo design by pharmacophore-based searches in fragment spaces. Journal of Computer-Aided Molecular Design, 2011, 25, 931-945.	2.9	17
86	Fast force fieldâ€based optimization of proteinâ€“ligand complexes with graphics processor. Journal of Computational Chemistry, 2012, 33, 2554-2565.	3.3	17
87	Unique Ring Families: A Chemically Meaningful Description of Molecular Ring Topologies. Journal of Chemical Information and Modeling, 2012, 52, 2013-2021.	5.4	17
88	Interactive design of generic chemical patterns. Drug Discovery Today, 2013, 18, 651-658.	6.4	17
89	An integrated approach to knowledge-driven structure-based virtual screening. Journal of Computer-Aided Molecular Design, 2014, 28, 927-939.	2.9	16
90	Index-Based Searching of Interaction Patterns in Large Collections of Proteinâ€“Ligand Interfaces. Journal of Chemical Information and Modeling, 2017, 57, 148-158.	5.4	16

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91	Exploring fragment spaces under multiple physicochemical constraints. Journal of Computer-Aided Molecular Design, 2007, 21, 327-340.	2.9	15
92	Computational biotechnology: Prediction of competitive substrate inhibition of enzymes by buffer compounds with proteinâ€“ligand docking. Journal of Biotechnology, 2012, 161, 391-401.	3.8	15
93	The Valence State Combination Model: A Generic Framework for Handling Tautomers and Protonation States. Journal of Chemical Information and Modeling, 2014, 54, 756-766.	5.4	15
94	ASCONA: Rapid Detection and Alignment of Protein Binding Site Conformations. Journal of Chemical Information and Modeling, 2015, 55, 1747-1756.	5.4	15
95	Comparing Molecular Patterns Using the Example of SMARTS: Applications and Filter Collection Analysis. Journal of Chemical Information and Modeling, 2019, 59, 2572-2586.	5.4	15
96	Proteinâ€“ligand interaction databases: advanced tools to mine activity data and interactions on a structural level. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 562-575.	14.6	14
97	Connected Subgraph Fingerprints: Representing Molecules Using Exhaustive Subgraph Enumeration. Journal of Chemical Information and Modeling, 2019, 59, 4625-4635.	5.4	14
98	CASP2 experiences with docking flexible ligands using FLEXX. Proteins: Structure, Function and Bioinformatics, 1997, 29, 221-225.	2.6	14
99	SwiFT:â€‰ An Index Structure for Reduced Graph Descriptors in Virtual Screening and Clustering. Journal of Chemical Information and Modeling, 2007, 47, 1341-1353.	5.4	13
100	Predicting enzymatic function from global binding site descriptors. Proteins: Structure, Function and Bioinformatics, 2013, 81, 479-489.	2.6	13
101	Comparison of Combinatorial Fragment Spaces and Its Application to Ultralarge Make-on-Demand Compound Catalogs. Journal of Chemical Information and Modeling, 2022, 62, 553-566.	5.4	13
102	Searching for Recursively Defined Generic Chemical Patterns in Nonenumerated Fragment Spaces. Journal of Chemical Information and Modeling, 2013, 53, 1676-1688.	5.4	12
103	What is the potential of structure-based target prediction methods?. Future Medicinal Chemistry, 2014, 6, 1987-1989.	2.3	11
104	Discriminative Chemical Patterns: Automatic and Interactive Design. Journal of Chemical Information and Modeling, 2015, 55, 1535-1546.	5.4	11
105	mRAISE: an alternative algorithmic approach to ligand-based virtual screening. Journal of Computer-Aided Molecular Design, 2016, 30, 583-594.	2.9	11
106	In silico Design, Synthesis, and Screening of Novel Deoxyhypusine Synthase Inhibitors Targeting HIVâ€1 Replication. ChemMedChem, 2014, 9, 940-952.	3.2	10
107	NAOMInext â€“ Synthetically feasible fragment growing in a structure-based design context. European Journal of Medicinal Chemistry, 2019, 163, 747-762.	5.5	10
108	Evaluation of deoxyhypusine synthase inhibitors targeting BCR-ABL positive leukemias. Investigational New Drugs, 2012, 30, 2274-2283.	2.6	9

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109	SMARTS.plus â€“ A Toolbox for Chemical Pattern Design. Molecular Informatics, 2020, 39, e2000216.	2.5	9
110	GeoMine: interactive pattern mining of proteinâ€“ligand interfaces in the Protein Data Bank. Bioinformatics, 2021, 37, 424-425.	4.1	9
111	Exploring Structureâ€“Activity Relationships with Threeâ€Dimensional Matched Molecular Pairsâ€”A Review. ChemMedChem, 2018, 13, 482-489.	3.2	9
112	Searching for Substructures in Fragment Spaces. Journal of Chemical Information and Modeling, 2012, 52, 3181-3189.	5.4	8
113	Design of Combinatorial Libraries for the Exploration of Virtual Hits from Fragment Space Searches with LoFT. Journal of Chemical Information and Modeling, 2012, 52, 373-379.	5.4	7
114	FSees: Customized Enumeration of Chemical Subspaces with Limited Main Memory Consumption. Journal of Chemical Information and Modeling, 2016, 56, 1641-1653.	5.4	7
115	RingDecomposerLib: An Open-Source Implementation of Unique Ring Families and Other Cycle Bases. Journal of Chemical Information and Modeling, 2017, 57, 122-126.	5.4	7
116	Searching Geometric Patterns in Protein Binding Sites and Their Application to Data Mining in Protein Kinase Structures. Journal of Medicinal Chemistry, 2022, 65, 1384-1395.	6.4	7
117	Improving Similarity-Driven Library Design: Customized Matching and Regioselective Feature Trees. Journal of Chemical Information and Modeling, 2011, 51, 2156-2163.	5.4	6
118	The Internet as Scientific Knowledge Base: Navigating the Chemâ€Bio Space. Molecular Informatics, 2012, 31, 543-546.	2.5	6
119	Linkerâ€Region Modified Derivatives of the Deoxyhypusine Synthase Inhibitor CNIâ€1493 Suppress HIVâ€1 Replication. Archiv Der Pharmazie, 2016, 349, 91-103.	4.1	6
120	Special Issue on Reaction Informatics and Chemical Space. Journal of Chemical Information and Modeling, 2022, 62, 2009-2010.	5.4	6
121	Calculating and Optimizing Physicochemical Property Distributions of Large Combinatorial Fragment Spaces. Journal of Chemical Information and Modeling, 2022, 62, 2800-2810.	5.4	6
122	Docking and Scoring for Structure-based Drug Design. , 0, , 541-599.		5
123	Consistent two-dimensional visualization of protein-ligand complex series. Journal of Cheminformatics, 2011, 3, 21.	6.1	5
124	Ligand-based virtual screening under partial shape constraints. Journal of Computer-Aided Molecular Design, 2017, 31, 335-347.	2.9	5
125	From cheminformatics to structure-based design: Web services and desktop applications based on the NAOMI library. Journal of Biotechnology, 2017, 261, 207-214.	3.8	5
126	Shape-Based Descriptors for Efficient Structure-Based Fragment Growing. Journal of Chemical Information and Modeling, 2020, 60, 6269-6281.	5.4	5

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127	Disconnected Maximum Common Substructures under Constraints. Journal of Chemical Information and Modeling, 2021, 61, 167-178.	5.4	5
128	Nearly no Scoring Function Without a Hanschâ€Analysis. Molecular Informatics, 2012, 31, 503-507.	2.5	4
129	The Art of Compiling Protein Binding Site Ensembles. Molecular Informatics, 2016, 35, 593-598.	2.5	4
130	NAOMInova: Interactive Geometric Analysis of Noncovalent Interactions in Macromolecular Structures. Journal of Chemical Information and Modeling, 2017, 57, 2132-2142.	5.4	4
131	StructureProfiler: an all-in-one tool for 3D protein structure profiling. Bioinformatics, 2019, 35, 874-876.	4.1	4
132	CASP2 experiences with docking flexible ligands using FLEXX. Proteins: Structure, Function and Bioinformatics, 1997, 29, 221-225.	2.6	4
133	The particle concept: placing discrete water molecules during proteinâ€ligand docking predictions. Proteins: Structure, Function and Bioinformatics, 1999, 34, 17-28.	2.6	4
134	The Torsion Library: Semiautomated Improvement of Torsion Rules with SMARTScompare. Journal of Chemical Information and Modeling, 2022, 62, 1644-1653.	5.4	4
135	Flat and Easy: 2D Depiction of Proteinâ€Ligand Complexes. Molecular Informatics, 2011, 30, 12-19.	2.5	3
136	Call for Papers for the Special Issue: From Reaction Informatics to Chemical Space. Journal of Chemical Information and Modeling, 2021, 61, 1531-1532.	5.4	3
137	Evaluation of the FLEXX incremental construction algorithm for proteinâ€“ligand docking. , 1999, 37, 228.		3
138	<scp>LSLOpt</scp>: An <scp>openâ€source</scp> implementation of the <scp>stepâ€length</scp> controlled <scp>LSLâ€BFGS</scp> algorithm. Journal of Computational Chemistry, 2021, 42, 1095-1100.	3.3	2
139	Analyzing structural features of proteins from deepâ€sea organisms. Proteins: Structure, Function and Bioinformatics, 2022, 90, 1521-1537.	2.6	2
140	Some thoughts on the â€œAâ€•in computer-aided molecular design. Journal of Computer-Aided Molecular Design, 2012, 26, 113-114.	2.9	1
141	11th German Conference on Chemoinformatics (GCC 2015). Journal of Cheminformatics, 2016, 8, 18.	6.1	1
142	A flexible-hydrogen interaction model for protein-ligand docking. Journal of Cheminformatics, 2012, 4, .	6.1	0
143	Force-field-based minimizations of protein-ligand complexes in the blink of an eye. Journal of Cheminformatics, 2013, 5, .	6.1	0
144	Elucidating protein-protein interactions using the HYDE scoring function. Journal of Cheminformatics, 2014, 6, .	6.1	0

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145	Accessing Open PHACTS: interactive exploration of compounds and targets from the semantic web. Journal of Cheminformatics, 2014, 6, .	6.1	0
146	Prediction of protein mutation effects based on dehydration and hydrogen bonding â€“ A largeâ€scale study. Proteins: Structure, Function and Bioinformatics, 2017, 85, 1550-1566.	2.6	0