Gisbert Schneider

List of Publications by Year
in descending order

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429 papers	24,326 citations	10351 72 h-index	11288 136 g-index
515 all docs	515 docs citations	515 times ranked	21586 citing authors

#	Article	IF	Citations
1	Designing antimicrobial peptides: form follows function. Nature Reviews Drug Discovery, 2012, 11, 37-51.	21.5	1,578
2	Counting on natural products for drug design. Nature Chemistry, 2016, 8, 531-541.	6.6	879
3	Computer-based de novo design of drug-like molecules. Nature Reviews Drug Discovery, 2005, 4, 649-663.	21.5	756
4	â€œScaffold-Hoppingâ€•by Topological Pharmacophore Search: A Contribution to Virtual Screening. Angewandte Chemie - International Edition, 1999, 38, 2894-2896.	7.2	629
5	Deep Learning in Drug Discovery. Molecular Informatics, 2016, 35, 3-14.	1.4	502
6	Concepts of Artificial Intelligence for Computer-Assisted Drug Discovery. Chemical Reviews, 2019, 119, 10520-10594.	23.0	499
7	Comparison of Support Vector Machine and Artificial Neural Network Systems for Drug/Nondrug Classification. Journal of Chemical Information and Computer Sciences, 2003, 43, 1882-1889.	2.8	487
8	Automating drug discovery. Nature Reviews Drug Discovery, 2018, 17, 97-113.	21.5	456
9	Virtual screening: an endless staircase?. Nature Reviews Drug Discovery, 2010, 9, 273-276.	21.5	445
10	Drug discovery with explainable artificial intelligence. Nature Machine Intelligence, 2020, 2, 573-584.	8.3	411
11	Rethinking drug design in the artificial intelligence era. Nature Reviews Drug Discovery, 2020, 19, 353-364.	21.5	394
12	Predicting drug metabolism: experiment and/or computation?. Nature Reviews Drug Discovery, 2015, 14, 387-404.	21.5	355
13	Generative Recurrent Networks for De Novo Drug Design. Molecular Informatics, 2018, 37, 1700111.	1.4	305
14	PocketPicker: analysis of ligand binding-sites with shape descriptors. Chemistry Central Journal, 2007, 1, 7.	2.6	278
15	Virtual screening and fast automated docking methods. Drug Discovery Today, 2002, 7, 64-70.	3.2	275
16	Scaffold Architecture and Pharmacophoric Properties of Natural Products and Trade Drugs:Â Application in the Design of Natural Product-Based Combinatorial Libraries. ACS Combinatorial Science, 2001, 3, 284-289.	3.3	270
17	Development of a Virtual Screening Method for Identification of â€œFrequent Hittersâ€•in Compound Libraries. Journal of Medicinal Chemistry, 2002, 45, 137-142.	2.9	270
18	Helicobacter pylori HtrA is a new secreted virulence factor that cleaves Eâ€cadherin to disrupt intercellular adhesion. EMBO Reports, 2010, 11, 798-804.	2.0	264

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19	Virtual screening and fast automated docking methods. Drug Discovery Today, 2002, 7, 64-70.	3.2	249
20	De Novo Design of Bioactive Small Molecules by Artificial Intelligence. Molecular Informatics, 2018, 37, 1700153.	1.4	246
21	Optimized Particle Swarm Optimization (OPSO) and its application to artificial neural network training. BMC Bioinformatics, 2006, 7, 125.	1.2	226
22	De novo design of molecular architectures by evolutionary assembly of drug-derived building blocks. Journal of Computer-Aided Molecular Design, 2000, 14, 487-494.	1.3	218
23	Scaffold diversity of natural products: inspiration for combinatorial library design. Natural Product Reports, 2008, 25, 892.	5.2	200
24	Deciphering apicoplast targeting signals â€“ feature extraction from nuclear-encoded precursors of Plasmodium falciparum apicoplast proteins. Gene, 2001, 280, 19-26.	1.0	199
25	Identifying the macromolecular targets of de novo-designed chemical entities through self-organizing map consensus. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 4067-4072.	3.3	196
26	DOGS: Reaction-Driven de novo Design of Bioactive Compounds. PLoS Computational Biology, 2012, 8, e1002380.	1.5	193
27	Artificial neural networks for computer-based molecular design. Progress in Biophysics and Molecular Biology, 1998, 70, 175-222.	1.4	189
28	Dual-display of small molecules enables the discovery of ligand pairs and facilitates affinity maturation. Nature Chemistry, 2015, 7, 241-249.	6.6	181
29	Active-learning strategies in computer-assisted drug discovery. Drug Discovery Today, 2015, 20, 458-465.	3.2	169
30	A Virtual Screening Method for Prediction of the hERG Potassium Channel Liability of Compound Libraries. ChemBioChem, 2002, 3, 455.	1.3	168
31	Recurrent Neural Network Model for Constructive Peptide Design. Journal of Chemical Information and Modeling, 2018, 58, 472-479.	2.5	165
32	Distinct Roles of Secreted HtrA Proteases from Gram-negative Pathogens in Cleaving the Junctional Protein and Tumor Suppressor E-cadherin. Journal of Biological Chemistry, 2012, 287, 10115-10120.	1.6	150
33	The rational design of amino acid sequences by artificial neural networks and simulated molecular evolution: de novo design of an idealized leader peptidase cleavage site. Biophysical Journal, 1994, 66, 335-344.	0.2	140
34	Support vector machine applications in bioinformatics. Applied Bioinformatics, 2003, 2, 67-77.	1.7	137
35	An Unusual ERAD-Like Complex Is Targeted to the Apicoplast ofPlasmodium falciparum. Eukaryotic Cell, 2009, 8, 1134-1145.	3.4	136
36	Scaffold-Hopping: How Far Can You Jump?. QSAR and Combinatorial Science, 2006, 25, 1162-1171.	1.5	135

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37	Chemically Advanced Template Search (CATS) for Scaffoldâ€Hopping and Prospective Target Prediction for â€˜Orphanâ€™ Molecules. Molecular Informatics, 2013, 32, 133-138.	1.4	132
38	Collection of Bioactive Reference Compounds for Focused Library Design. QSAR and Combinatorial Science, 2003, 22, 713-718.	1.5	128
39	Artificial intelligence in drug discovery: recent advances and future perspectives. Expert Opinion on Drug Discovery, 2021, 16, 949-959.	2.5	128
40	A critical overview of computational approaches employed for COVID-19 drug discovery. Chemical Society Reviews, 2021, 50, 9121-9151.	18.7	128
41	De Novo Drug Design. Methods in Molecular Biology, 2010, 672, 299-323.	0.4	125
42	De Novo Design at the Edge of Chaos. Journal of Medicinal Chemistry, 2016, 59, 4077-4086.	2.9	124
43	Properties and prediction of mitochondrial transit peptides from Plasmodium falciparum. Molecular and Biochemical Parasitology, 2003, 132, 59-66.	0.5	120
44	Revealing the macromolecular targets of complex natural products. Nature Chemistry, 2014, 6, 1072-1078.	6.6	114
45	Self-Organizing Maps in Drug Discovery: Compound Library Design, Scaffold-Hopping, Repurposing. Current Medicinal Chemistry, 2009, 16, 258-266.	1.2	111
46	Generative molecular design in low data regimes. Nature Machine Intelligence, 2020, 2, 171-180.	8.3	111
47	Prediction of Type III Secretion Signals in Genomes of Gram-Negative Bacteria. PLoS ONE, 2009, 4, e5917.	1.1	108
48	modlAMP: Python for antimicrobial peptides. Bioinformatics, 2017, 33, 2753-2755.	1.8	106
49	Flux (1):Â A Virtual Synthesis Scheme for Fragment-Based de Novo Design. Journal of Chemical Information and Modeling, 2006, 46, 699-707.	2.5	101
50	Bidirectional Molecule Generation with Recurrent Neural Networks. Journal of Chemical Information and Modeling, 2020, 60, 1175-1183.	2.5	101
51	Advances in the prediction of protein targeting signals. Proteomics, 2004, 4, 1571-1580.	1.3	99
52	Automated De Novo Drug Design: Are We Nearly There Yet?. Angewandte Chemie - International Edition, 2019, 58, 10792-10803.	7.2	99
53	Feature-extraction from endopeptidase cleavage sites in mitochondrial targeting peptides. , 1998, 30, 49-60.		98
54	Geometric deep learning on molecular representations. Nature Machine Intelligence, 2021, 3, 1023-1032.	8.3	98

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55	Discovery of Smallâ€Molecule Interleukinâ€2 Inhibitors from a DNAâ€Encoded Chemical Library. Chemistry - A European Journal, 2012, 18, 7729-7737.	1.7	94
56	A Collection of Robust Organic Synthesis Reactions for In Silico Molecule Design. Journal of Chemical Information and Modeling, 2011, 51, 3093-3098.	2.5	92
57	Identification and functional analysis of cyclooxygenase-1 as a molecular target of boswellic acids. Biochemical Pharmacology, 2008, 75, 503-513.	2.0	89
58	Comparison of correlation vector methods for ligand-based similarity searching. Journal of Computer-Aided Molecular Design, 2003, 17, 687-698.	1.3	87
59	Properties and Architecture of Drugs and Natural Products Revisited. Current Chemical Biology, 2007, 1, 115-127.	0.2	87
60	Virtual Screening for Bioactive Molecules by Evolutionary De Novo Design. Angewandte Chemie - International Edition, 2000, 39, 4130-4133.	7.2	86
61	Scaffold-Hopping Potential of Ligand-Based Similarity Concepts. ChemMedChem, 2006, 1, 181-185.	1.6	86
62	Accessing New Chemical Entities through Microfluidic Systems. Angewandte Chemie - International Edition, 2014, 53, 5750-5758.	7.2	86
63	Privileged Structures Revisited. Angewandte Chemie - International Edition, 2017, 56, 7971-7974.	7.2	85
64	Simple 2,4-Diacylphloroglucinols as Classic Transient Receptor Potential-6 Activatorsâ€"Identification of a Novel Pharmacophore. Molecular Pharmacology, 2010, 77, 368-377.	1.0	84
65	Processing and classification of chemical data inspired by insect olfaction. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 20285-20289.	3.3	81
66	Voyages to the (un)known: adaptive design of bioactive compounds. Trends in Biotechnology, 2009, 27, 18-26.	4.9	80
67	Prediction of Hepatic Metabolic Clearance. Clinical Pharmacokinetics, 2001, 40, 553-563.	1.6	79
68	Pseudoreceptor models in drug design: bridging ligand- and receptor-based virtual screening. Nature Reviews Drug Discovery, 2008, 7, 667-677.	21.5	78
69	Identification of E-cadherin signature motifs functioning as cleavage sites for Helicobacter pylori HtrA. Scientific Reports, 2016, 6, 23264.	1.6	77
70	Combining in Vitro and in Vivo Pharmacokinetic Data for Prediction of Hepatic Drug Clearance in Humans by Artificial Neural Networks and Multivariate Statistical Techniques. Journal of Medicinal Chemistry, 1999, 42, 5072-5076.	2.9	76
71	Multiâ€Objective Molecular De Novo Design by Adaptive Fragment Prioritization. Angewandte Chemie - International Edition, 2014, 53, 4244-4248.	7.2	76
72	Trends in Virtual Combinatorial Library Design. Current Medicinal Chemistry, 2002, 9, 2095-2101.	1.2	75

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73	Prediction of Extracellular Proteases of the Human Pathogen Helicobacter pylori Reveals Proteolytic Activity of the Hp1018/19 Protein HtrA. PLoS ONE, 2008, 3, e3510.	1.1	75
74	Active learning for computational chemogenomics. Future Medicinal Chemistry, 2017, 9, 381-402.	1.1	75
75	Peptide design by artificial neural networks and computer-based evolutionary search. Proceedings of the National Academy of Sciences of the United States of America, 1998, 95, 12179-12184.	3.3	74
76	Ligand-Based Combinatorial Design of Selective Purinergic Receptor (A2A) Antagonists Using Self-Organizing Maps. ACS Combinatorial Science, 2003, 5, 233-237.	3.3	73
77	Identification of Human Cathepsin G As a Functional Target of Boswellic Acids from the Anti-Inflammatory Remedy Frankincense. Journal of Immunology, 2009, 183, 3433-3442.	0.4	72
78	Nonlinear dimensionality reduction and mapping of compound libraries for drug discovery. Journal of Molecular Graphics and Modelling, 2012, 34, 108-117.	1.3	72
79	Identification of Natural-Product-Derived Inhibitors of 5-Lipoxygenase Activity by Ligand-Based Virtual Screening. Journal of Medicinal Chemistry, 2007, 50, 2640-2646.	2.9	70
80	Characterisation of worldwide Helicobacter pylori strains reveals genetic conservation and essentiality of serine protease HtrA. Molecular Microbiology, 2016, 99, 925-944.	1.2	70
81	Tuning artificial intelligence on the de novo design of natural-product-inspired retinoid X receptor modulators. Communications Chemistry, 2018, 1, .	2.0	69
82	Flux (2):â€‰ Comparison of Molecular Mutation and Crossover Operators for Ligand-Based de Novo Design. Journal of Chemical Information and Modeling, 2007, 47, 656-667.	2.5	68
83	Common non-epigenetic drugs as epigenetic modulators. Trends in Molecular Medicine, 2013, 19, 742-753.	3.5	68
84	Membranolytic anticancer peptides. MedChemComm, 2016, 7, 2232-2245.	3.5	68
85	Extraction and Visualization of Potential Pharmacophore Points Using Support Vector Machines:Â Application to Ligand-Based Virtual Screening for COX-2 Inhibitors. Journal of Medicinal Chemistry, 2005, 48, 6997-7004.	2.9	67
86	The molecular mechanism of the inhibition by licofelone of the biosynthesis of 5â€lipoxygenase products. British Journal of Pharmacology, 2007, 152, 471-480.	2.7	67
87	Designing Anticancer Peptides by Constructive Machine Learning. ChemMedChem, 2018, 13, 1300-1302.	1.6	67
88	Combining Onâ€Chip Synthesis of a Focused Combinatorial Library with Computational Target Prediction Reveals Imidazopyridine GPCR Ligands. Angewandte Chemie - International Edition, 2014, 53, 582-585.	7.2	66
89	Kernel Approach to Molecular Similarity Based on Iterative Graph Similarity. Journal of Chemical Information and Modeling, 2007, 47, 2280-2286.	2.5	64
90	Phenotype-based high-content chemical library screening identifies statins as inhibitors of in vivo lymphangiogenesis. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, E2665-74.	3.3	64

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91	Species-specific Inhibition of APOBEC3C by the Prototype Foamy Virus Protein Bet. Journal of Biological Chemistry, 2009, 284, 5819-5826.	1.6	63
92	2,4-Diaminopyrimidines as histamine H4 receptor ligandsâ€"Scaffold optimization and pharmacological characterization. Bioorganic and Medicinal Chemistry, 2009, 17, 7186-7196.	1.4	63
93	Context-Based Identification of Protein-Protein Interfaces and â€œHot-Spotâ€•Residues. Chemistry and Biology, 2011, 18, 344-353.	6.2	63
94	Advancing drug discovery via GPU-based deep learning. Expert Opinion on Drug Discovery, 2018, 13, 579-582.	2.5	62
95	Concept of Combinatorial De Novo Design of Drugâ€like Molecules by Particle Swarm Optimization. Chemical Biology and Drug Design, 2008, 72, 16-26.	1.5	61
96	SVM-Based Feature Selection for Characterization of Focused Compound Collections. Journal of Chemical Information and Computer Sciences, 2004, 44, 993-999.	2.8	60
97	Hyperforin is a novel type of 5-lipoxygenase inhibitor with high efficacy in vivo. Cellular and Molecular Life Sciences, 2009, 66, 2759-2771.	2.4	60
98	Enabling future drug discovery by de novo design. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 742-759.	6.2	60
99	From Machine Learning to Natural Product Derivatives that Selectively Activate Transcription Factor PPARÎ³. ChemMedChem, 2010, 5, 191-194.	1.6	58
100	Aminothiazole-Featured Pirinixic Acid Derivatives As Dual 5-Lipoxygenase and Microsomal Prostaglandin E₂ Synthase-1 Inhibitors with Improved Potency and Efficiency in Vivo. Journal of Medicinal Chemistry, 2013, 56, 9031-9044.	2.9	58
101	Local structural motifs of protein backbones are classified by self-organizing neural networks. Protein Engineering, Design and Selection, 1996, 9, 833-842.	1.0	55
102	Multi-objective active machine learning rapidly improves structureâ€“activity models and reveals new proteinâ€“protein interaction inhibitors. Chemical Science, 2016, 7, 3919-3927.	3.7	55
103	Predicting Compound Selectivity by Self-Organizing Maps: Cross-Activities of Metabotropic Glutamate Receptor Antagonists. ChemMedChem, 2006, 1, 1066-1068.	1.6	54
104	SmiLib v2.0: A Java-Based Tool for Rapid Combinatorial Library Enumeration. QSAR and Combinatorial Science, 2007, 26, 407-410.	1.5	54
105	Revealing the Macromolecular Targets of Fragmentâ€Like Natural Products. Angewandte Chemie - International Edition, 2015, 54, 10516-10520.	7.2	54
106	Neural networks are useful tools for drug design. Neural Networks, 2000, 13, 15-16.	3.3	53
107	A Hierarchical Clustering Approach for Large Compound Libraries. Journal of Chemical Information and Modeling, 2005, 45, 807-815.	2.5	53
108	Inhibitors of Helicobacter pylori Protease HtrA Found by â€˜Virtual Ligandâ€™ Screening Combat Bacterial Invasion of Epithelia. PLoS ONE, 2011, 6, e17986.	1.1	52

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109	Combining generative artificial intelligence and on-chip synthesis for de novo drug design. Science Advances, 2021, 7, .	4.7	52
110	Mapping of protein surface cavities and prediction of enzyme class by a self-organizing neural network. Protein Engineering, Design and Selection, 2000, 13, 83-88.	1.0	51
111	Fuzzy Pharmacophore Models from Molecular Alignments for Correlation-Vector-Based Virtual Screening. Journal of Medicinal Chemistry, 2004, 47, 4653-4664.	2.9	51
112	Impact of Conformational Flexibility on Three-Dimensional Similarity Searching Using Correlation Vectors. Journal of Chemical Information and Modeling, 2006, 46, 2324-2332.	2.5	51
113	Crystal structures of mouse class II alcohol dehydrogenase reveal determinants of substrate specificity and catalytic efficiency 1 1Edited by J. Thornton. Journal of Molecular Biology, 2000, 302, 441-453.	2.0	50
114	Development of artificial neural filters for pattern recognition in protein sequences. Journal of Molecular Evolution, 1993, 36, 586-595.	0.8	49
115	Adhesion, Invasion, and Agglutination Mediated by Two Trimeric Autotransporters in the Human Uropathogen Proteus mirabilis. Infection and Immunity, 2010, 78, 4882-4894.	1.0	49
116	Dimerization of human 5-lipoxygenase. Biological Chemistry, 2011, 392, 1097-1111.	1.2	49
117	Structureâ€“Activity Relationship of Nonacidic Quinazolinone Inhibitors of Human Microsomal Prostaglandin Synthase 1 (mPGESÂ1). Journal of Medicinal Chemistry, 2012, 55, 3792-3803.	2.9	49
118	Scaffold Hopping by â€œFuzzyâ€•Pharmacophores and its Application to RNA Targets. ChemBioChem, 2007, 8, 1932-1936.	1.3	48
119	Standardization of WT1 mRNA quantitation for minimal residual disease monitoring in childhood AML and implications of WT1 gene mutations: a European multicenter study. Leukemia, 2009, 23, 1472-1479.	3.3	48
120	Extending the Structureâ€“Activity Relationship of Anthranilic Acid Derivatives As Farnesoid X Receptor Modulators: Development of a Highly Potent Partial Farnesoid X Receptor Agonist. Journal of Medicinal Chemistry, 2014, 57, 8035-8055.	2.9	48
121	A neural network model for the prediction of membraneâ€spanning amino acid sequences. Protein Science, 1994, 3, 1597-1601.	3.1	47
122	Automated de novo molecular design by hybrid machine intelligence and rule-driven chemical synthesis. Nature Machine Intelligence, 2019, 1, 307-315.	8.3	47
123	Mind and machine in drug design. Nature Machine Intelligence, 2019, 1, 128-130.	8.3	45
124	Coloring Molecules with Explainable Artificial Intelligence for Preclinical Relevance Assessment. Journal of Chemical Information and Modeling, 2021, 61, 1083-1094.	2.5	45
125	Predicting olfactory receptor neuron responses from odorant structure. Chemistry Central Journal, 2007, 1, 11.	2.6	44
126	Identification and Validation of a Potent Typeâ€…II Inhibitor of Inactive Poloâ€like Kinaseâ€…1. ChemMedChem, 2009, 4, 1806-1809.	1.6	44

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127	Benzodioxoles: Novel Cannabinoid-1 Receptor Inverse Agonists for the Treatment of Obesity. Journal of Medicinal Chemistry, 2008, 51, 2115-2127.	2.9	43
128	Form follows function: Shape analysis of protein cavities for receptorâ€based drug design. Proteomics, 2009, 9, 451-459.	1.3	43
129	From Complex Natural Products to Simple Synthetic Mimetics by Computational De Novo Design. Angewandte Chemie - International Edition, 2016, 55, 6789-6792.	7.2	42
130	Native Electrospray Ionization Mass Spectrometry Reveals Multiple Facets of Aptamerâ€“Ligand Interactions: From Mechanism to Binding Constants. Journal of the American Chemical Society, 2018, 140, 7486-7497.	6.6	42
131	Scaffold hopping from natural products to synthetic mimetics by holistic molecular similarity. Communications Chemistry, 2018, 1, .	2.0	42
132	The State of the Art of Chemical Biology. ChemBioChem, 2009, 10, 16-29.	1.3	41
133	Chapter 10 Analysis and prediction of mitochondrial targeting peptides. Methods in Cell Biology, 2001, 65, 175-187.	0.5	40
134	Binding to Large Enzyme Pockets: Smallâ€Molecule Inhibitors of Trypanothione Reductase. ChemMedChem, 2014, 9, 1880-1891.	1.6	40
135	In silico design and optimization of selective membranolytic anticancer peptides. Scientific Reports, 2019, 9, 11282.	1.6	40
136	Beam Search for Automated Design and Scoring of Novel ROR Ligands with Machine Intelligence**. Angewandte Chemie - International Edition, 2021, 60, 19477-19482.	7.2	40
137	Model structure of APOBEC3C reveals a binding pocket modulating ribonucleic acid interaction required for encapsidation. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 12079-12084.	3.3	39
138	Multidimensional Deâ€...Novo Design Reveals 5â€HT_{2B} Receptorâ€Selective Ligands. Angewandte Chemie - International Edition, 2015, 54, 1551-1555.	7.2	39
139	Hybrid Network Model for â€œDeep Learningâ€•of Chemical Data: Application to Antimicrobial Peptides. Molecular Informatics, 2017, 36, 1600011.	1.4	39
140	Bacterial serine protease HtrA as a promising new target for antimicrobial therapy?. Cell Communication and Signaling, 2017, 15, 4.	2.7	39
141	A Computational Method for Unveiling the Target Promiscuity of Pharmacologically Active Compounds. Angewandte Chemie - International Edition, 2017, 56, 11520-11524.	7.2	39
142	Computer-Assisted Discovery of Retinoid X Receptor Modulating Natural Products and Isofunctional Mimetics. Journal of Medicinal Chemistry, 2018, 61, 5442-5447.	2.9	39
143	New Inhibitors of the Tat-TAR RNA Interaction Found with a â€œFuzzyâ€•Pharmacophore Model. ChemBioChem, 2005, 6, 1119-1125.	1.3	38
144	Coactosin-like protein functions as a stabilizing chaperone for 5-lipoxygenase: role of tryptophan 102. Biochemical Journal, 2010, 425, 265-274.	1.7	38

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145	Neighborhoodâ€Preserving Visualization of Adaptive Structureâ€“Activity Landscapes: Application to Drug Discovery. Angewandte Chemie - International Edition, 2011, 50, 11633-11636.	7.2	38
146	Reaction-driven de novo design, synthesis and testing of potential type II kinase inhibitors. Future Medicinal Chemistry, 2011, 3, 415-424.	1.1	37
147	Structural properties of so-called NSAIDâ€“phospholipid-complexes. European Journal of Pharmaceutical Sciences, 2011, 44, 103-116.	1.9	37
148	Probing the Bioactivity-Relevant Chemical Space of Robust Reactions and Common Molecular Building Blocks. Journal of Chemical Information and Modeling, 2012, 52, 1167-1178.	2.5	37
149	Immunosuppressive Small Molecule Discovered by Structureâ€Based Virtual Screening for Inhibitors of Proteinâ€“Protein Interactions. Angewandte Chemie - International Edition, 2012, 51, 258-261.	7.2	37
150	Fragmentâ€Based Deâ€...Novo Design Reveals a Smallâ€Molecule Inhibitor of Helicobacter Pylori HtrA. Angewandte Chemie - International Edition, 2015, 54, 10244-10248.	7.2	37
151	QMugs, quantum mechanical properties of drug-like molecules. Scientific Data, 2022, 9, .	2.4	37
152	A fast virtual screening filter for cytochrome P450â€...3A4 inhibition liability of compound libraries. QSAR and Combinatorial Science, 2002, 21, 249-256.	1.4	36
153	Architecture, function and prediction of long signal peptides. Briefings in Bioinformatics, 2009, 10, 569-578.	3.2	36
154	Homology Model Adjustment and Ligand Screening with a Pseudoreceptor of the Human Histamine H₄ Receptor. ChemMedChem, 2009, 4, 820-827.	1.6	36
155	Biological impact of freezing Plk1 in its inactive conformation in cancer cells. Cell Cycle, 2010, 9, 761-774.	1.3	36
156	De novo design of anticancer peptides by ensemble artificial neural networks. Journal of Molecular Modeling, 2019, 25, 112.	0.8	36
157	Graph Kernels for Molecular Similarity. Molecular Informatics, 2010, 29, 266-273.	1.4	35
158	SMILIB: Rapid Assembly of Combinatorial Libraries in SMILES Notation. QSAR and Combinatorial Science, 2003, 22, 719-721.	1.5	34
159	Status of HTS Data Mining Approaches. QSAR and Combinatorial Science, 2004, 23, 207-213.	1.5	34
160	Virtual Screening for Selective Allosteric mGluR1 Antagonists and Structureâ€“Activity Relationship Investigations for Coumarine Derivatives. ChemMedChem, 2007, 2, 1763-1773.	1.6	34
161	Nonacidic Inhibitors of Human Microsomal Prostaglandin Synthase 1 (mPGES 1) Identified by a Multistep Virtual Screening Protocol. Journal of Medicinal Chemistry, 2010, 53, 911-915.	2.9	34
162	De-orphaning the marine natural product (Â±)-marinopyrrole A by computational target prediction and biochemical validation. Chemical Communications, 2017, 53, 2272-2274.	2.2	34

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163	Scaffoldâ€Hopping Cascade Yields Potent Inhibitors of 5â€Lipoxygenase. ChemMedChem, 2008, 3, 1535-1538.	1.6	33
164	Scrutinizing MHC-I Binding Peptides and Their Limits of Variation. PLoS Computational Biology, 2013, 9, e1003088.	1.5	33
165	Spotting and designing promiscuous ligands for drug discovery. Chemical Communications, 2016, 52, 1135-1138.	2.2	33
166	Peptide design in machina: development of artificial mitochondrial protein precursor cleavage sites by simulated molecular evolution. Biophysical Journal, 1995, 68, 434-447.	0.2	32
167	How many potentially secreted proteins are contained in a bacterial genome?. Gene, 1999, 237, 113-121.	1.0	32
168	Detection and assessment of near-zero delays in neuronal spiking activity. Journal of Neuroscience Methods, 2006, 152, 97-106.	1.3	32
169	Shapelets: Possibilities and limitations of shape-based virtual screening. Journal of Computational Chemistry, 2008, 29, 108-114.	1.5	32
170	Structureâ€Based Pharmacophore Screening for Naturalâ€Productâ€Derived PPARÎ³ Agonists. ChemBioChem, 2009, 10, 75-78.	1.3	32
171	Multidimensional Design of Anticancer Peptides. Angewandte Chemie - International Edition, 2015, 54, 10370-10374.	7.2	32
172	Feature-extraction from endopeptidase cleavage sites in mitochondrial targeting peptides. Proteins: Structure, Function and Bioinformatics, 1998, 30, 49-60.	1.5	32
173	Molecular Query Language (MQL)A Context-Free Grammar for Substructure Matching. Journal of Chemical Information and Modeling, 2007, 47, 295-301.	2.5	31
174	De novo design â€“ hop(p)ing against hope. Drug Discovery Today: Technologies, 2013, 10, e453-e460.	4.0	31
175	Deorphaning the Macromolecular Targets of the Natural Anticancer Compound Doliculide. Angewandte Chemie - International Edition, 2016, 55, 12408-12411.	7.2	31
176	Machine Learning Estimates of Natural Product Conformational Energies. PLoS Computational Biology, 2014, 10, e1003400.	1.5	30
177	Deorphaning Pyrrolopyrazines as Potent Multiâ€Target Antimalarial Agents. Angewandte Chemie - International Edition, 2014, 53, 7079-7084.	7.2	30
178	De Novo Fragment Design for Drug Discovery and Chemical Biology. Angewandte Chemie - International Edition, 2015, 54, 15079-15083.	7.2	30
179	Generative Models for Artificiallyâ€Intelligent Molecular Design. Molecular Informatics, 2018, 37, 1880131.	1.4	30
180	From Virtual to Real Screening for D3 Dopamine Receptor Ligands. ChemBioChem, 2005, 6, 997-999.	1.3	29

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