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	De Novo Molecular Design with Chemical Language Models. Methods in Molecular Biology, 2022, 2390, 207-232.	0.4	3
2	Perplexity-Based Molecule Ranking and Bias Estimation of Chemical Language Models. Journal of Chemical Information and Modeling, 2022, 62, 1199-1206.	2.5	8
3	Î”-Quantum machine-learning for medicinal chemistry. Physical Chemistry Chemical Physics, 2022, 24, 10775-10783.	1.3	21
4	Identification of novel off targets of baricitinib and tofacitinib by machine learning with a focus on thrombosis and viral infection. Scientific Reports, 2022, 12, 7843.	1.6	5
5	Translating from Proteins to Ribonucleic Acids for Ligandâ€binding Site Detection. Molecular Informatics, 2022, 41, .	1.4	3
6	TBIO-08. The molecular basis for rational targeting of FGFR-driven growth and invasiveness in pediatric brain tumors. Neuro-Oncology, 2022, 24, i184-i184.	0.6	0
7	QMugs, quantum mechanical properties of drug-like molecules. Scientific Data, 2022, 9, .	2.4	37
8	Engineering of a functional Î³-tocopherol transfer protein. Redox Biology, 2021, 38, 101773.	3.9	5
9	Molecular Scaffold Hopping via Holistic Molecular Representation. Methods in Molecular Biology, 2021, 2266, 11-35.	0.4	4
10	Coloring Molecules with Explainable Artificial Intelligence for Preclinical Relevance Assessment. Journal of Chemical Information and Modeling, 2021, 61, 1083-1094.	2.5	45
11	Artificial intelligence in drug discovery: recent advances and future perspectives. Expert Opinion on Drug Discovery, 2021, 16, 949-959.	2.5	128
12	POS0091â€…OFF-TARGET PROFILING OF JANUS KINASE (JAK) INHIBITORS IN RHEUMATOID ARTHRITIS: A COMPUTER-BASED APPROACH FOR DRUG SAFETY STUDIES AND REPURPOSING. Annals of the Rheumatic Diseases, 2021, 80, 255.2-255.	0.5	0
13	Combining generative artificial intelligence and on-chip synthesis for de novo drug design. Science Advances, 2021, 7, .	4.7	52
14	Learning from Nature: From a Marine Natural Product to Synthetic Cyclooxygenaseâ€1 Inhibitors by Automated De Novo Design. Advanced Science, 2021, 8, e2100832.	5.6	17
15	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
16	High-mass MALDI-MS unravels ligand-mediated G proteinâ€“coupling selectivity to GPCRs. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	9
17	Beamâ€Search zum automatisierten Entwurf und Scoring neuer RORâ€Liganden mithilfe maschineller Intelligenz**. Angewandte Chemie, 2021, 133, 19626-19632.	1.6	1
18	Bioaffinity Screening with a Rapid and Sample-Efficient Autosampler for Native Electrospray Ionization Mass Spectrometry. Analytical Chemistry, 2021, 93, 13342-13350.	3.2	3

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19	A critical overview of computational approaches employed for COVID-19 drug discovery. Chemical Society Reviews, 2021, 50, 9121-9151.	18.7	128
20	Computer-Aided Design and Synthesis of a New Class of PEX14 Inhibitors: Substituted 2,3,4,5-Tetrahydrobenzo[F][1,4]oxazepines as Potential New Trypanocidal Agents. Journal of Chemical Information and Modeling, 2021, 61, 5256-5268.	2.5	1
21	Geometric deep learning on molecular representations. Nature Machine Intelligence, 2021, 3, 1023-1032.	8.3	98
22	Identification of Synthetic Activators of Cancer Cell Migration by Hybrid Deep Learning. ChemBioChem, 2020, 21, 500-507.	1.3	1
23	Bidirectional Molecule Generation with Recurrent Neural Networks. Journal of Chemical Information and Modeling, 2020, 60, 1175-1183.	2.5	101
24	Rethinking drug design in the artificial intelligence era. Nature Reviews Drug Discovery, 2020, 19, 353-364.	21.5	394
25	Structural insights into the interaction of botulinum neurotoxin a with its neuronal receptor SV2C. Toxicon, 2020, 175, 36-43.	0.8	3
26	Drug discovery with explainable artificial intelligence. Nature Machine Intelligence, 2020, 2, 573-584.	8.3	411
27	Morphing of Amphipathic Helices to Explore the Activity and Selectivity of Membranolytic Antimicrobial Peptides. Biochemistry, 2020, 59, 3772-3781.	1.2	4
28	Introducing the CSP Analyzer: A novel Machine Learning-based application for automated analysis of two-dimensional NMR spectra in NMR fragment-based screening. Computational and Structural Biotechnology Journal, 2020, 18, 603-611.	1.9	13
29	Virtual Screening and Design with Machine Intelligence Applied to Pimâ€1 Kinase Inhibitors. Molecular Informatics, 2020, 39, e2000109.	1.4	7
30	Filovirus Antiviral Activity of Cationic Amphiphilic Drugs Is Associated with Lipophilicity and Ability To Induce Phospholipidosis. Antimicrobial Agents and Chemotherapy, 2020, 64, .	1.4	13
31	Generative molecular design in low data regimes. Nature Machine Intelligence, 2020, 2, 171-180.	8.3	111
32	Shape Similarity by Fractal Dimensionality: An Application in the de novo Design of (â˜)â€Englerin A Mimetics. ChemMedChem, 2020, 15, 566-570.	1.6	6
33	Interaction analysis of glycoengineered antibodies with CD16a: a native mass spectrometry approach. MAbs, 2020, 12, 1736975.	2.6	7
34	A novel FRET peptide assay reveals efficient Helicobacter pylori HtrA inhibition through zinc and copper binding. Scientific Reports, 2020, 10, 10563.	1.6	19
35	AI reflections in 2019. Nature Machine Intelligence, 2020, 2, 2-9.	8.3	6
36	In silico design and optimization of selective membranolytic anticancer peptides. Scientific Reports, 2019, 9, 11282.	1.6	40

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37	Concepts of Artificial Intelligence for Computer-Assisted Drug Discovery. Chemical Reviews, 2019, 119, 10520-10594.	23.0	499
38	Automated de novo molecular design by hybrid machine intelligence and rule-driven chemical synthesis. Nature Machine Intelligence, 2019, 1, 307-315.	8.3	47
39	Machine learning models for hydrogen bond donor and acceptor strengths using large and diverse training data generated by first-principles interaction free energies. Journal of Cheminformatics, 2019, 11, 59.	2.8	19
40	Identifizierung von Chemokinliganden durch biochemische Rezeptorfragmentierung und simulierte Peptidevolution. Angewandte Chemie, 2019, 131, 7212-7216.	1.6	0
41	SIG-02. RATIONAL TARGETING OF PRO-INVASIVE FGFR SIGNALING IN MEDULLOBLASTOMA. Neuro-Oncology, 2019, 21, ii113-ii113.	0.6	1
42	Identification of Chemokine Ligands by Biochemical Fragmentation and Simulated Peptide Evolution. Angewandte Chemie - International Edition, 2019, 58, 7138-7142.	7.2	2
43	Design of Naturalâ€Productâ€Inspired Multitarget Ligands by Machine Learning. ChemMedChem, 2019, 14, 1129-1134.	1.6	27
44	De novo design of anticancer peptides by ensemble artificial neural networks. Journal of Molecular Modeling, 2019, 25, 112.	0.8	36
45	Automated De Novo Drug Design: Are We Nearly There Yet?. Angewandte Chemie - International Edition, 2019, 58, 10792-10803.	7.2	99
46	Automated De Novo Drug Design: Are We Nearly There Yet?. Angewandte Chemie, 2019, 131, 10906-10917.	1.6	12
47	Mind and machine in drug design. Nature Machine Intelligence, 2019, 1, 128-130.	8.3	45
48	De novo Molecular Design with Generative Long Short-term Memory. Chimia, 2019, 73, 1006.	0.3	15
49	Synthetic Activators of Cell Migration Designed by Constructive Machine Learning. ChemistryOpen, 2019, 8, 1303-1308.	0.9	9
50	Discovery of Novel Molecular Frameworks of Farnesoidâ€...X Receptor Modulators by Ensemble Machine Learning. ChemistryOpen, 2019, 8, 3-3.	0.9	2
51	Discovery of Novel Molecular Frameworks of Farnesoidâ€...X Receptor Modulators by Ensemble Machine Learning. ChemistryOpen, 2019, 8, 7-14.	0.9	2
52	In Silico Target Prediction for Small Molecules. Methods in Molecular Biology, 2019, 1888, 273-309.	0.4	19
53	Simulated Molecular Evolution for Anticancer Peptide Design. Angewandte Chemie - International Edition, 2019, 58, 1674-1678.	7.2	20
54	Simulated Molecular Evolution for Anticancer Peptide Design. Angewandte Chemie, 2019, 131, 1688-1692.	1.6	0

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55	Gaussian Process Regression Models for the Prediction of Hydrogen Bond Acceptor Strengths. Molecular Informatics, 2019, 38, 1800115.	1.4	10
56	[Special Issue for Honor Award dedicating to Prof Kimito Funatsu]Molecular Design With Long Short-Term Memory Networks. Journal of Computer Aided Chemistry, 2019, 20, 35-42.	0.3	0
57	Generative Models for Artificiallyâ€intelligent Molecular Design. Molecular Informatics, 2018, 37, 1880131.	1.4	30
58	Advancing drug discovery via GPU-based deep learning. Expert Opinion on Drug Discovery, 2018, 13, 579-582.	2.5	62
59	Designing Anticancer Peptides by Constructive Machine Learning. ChemMedChem, 2018, 13, 1300-1302.	1.6	67
60	Cheminformatics and the Mean. Molecular Informatics, 2018, 37, 1880132.	1.4	1
61	Recurrent Neural Network Model for Constructive Peptide Design. Journal of Chemical Information and Modeling, 2018, 58, 472-479.	2.5	165
62	De Novo Design of Bioactive Small Molecules by Artificial Intelligence. Molecular Informatics, 2018, 37, 1700153.	1.4	246
63	Total Synthesis of Ripostatin B and Structureâ€“Activity Relationship Studies on Ripostatin Analogs. Journal of Organic Chemistry, 2018, 83, 7150-7172.	1.7	22
64	Binding Specificities of Nanobodyâ€¢Membrane Protein Complexes Obtained from Chemical Cross-Linking and High-Mass MALDI Mass Spectrometry. Analytical Chemistry, 2018, 90, 5306-5313.	3.2	15
65	Generative Recurrent Networks for De Novo Drug Design. Molecular Informatics, 2018, 37, 1700111.	1.4	305
66	Automating drug discovery. Nature Reviews Drug Discovery, 2018, 17, 97-113.	21.5	456
67	Scaffold-Hopping from Synthetic Drugs by Holistic Molecular Representation. Scientific Reports, 2018, 8, 16469.	1.6	24
68	Tuning artificial intelligence on the de novo design of natural-product-inspired retinoid X receptor modulators. Communications Chemistry, 2018, 1, .	2.0	69
69	MetScore: Site of Metabolism Prediction Beyond Cytochrome P450 Enzymes. ChemMedChem, 2018, 13, 2281-2289.	1.6	21
70	Polypharmacological Drugâ^'target Inference for Chemogenomics. Molecular Informatics, 2018, 37, e1800050.	1.4	7
71	Combined Proteomic and In Silico Target Identification Reveal a Role for 5-Lipoxygenase in Developmental Signaling Pathways. Cell Chemical Biology, 2018, 25, 1095-1106.e23.	2.5	13
72	Quantification of hydrolyzed peptides and proteins by amino acid fluorescence. Journal of Peptide Science, 2018, 24, e3113.	0.8	11

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73	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
74	Lipophilicity prediction of peptides and peptide derivatives by consensus machine learning. MedChemComm, 2018, 9, 1538-1546.	3.5	17
75	Scaffold hopping from natural products to synthetic mimetics by holistic molecular similarity. Communications Chemistry, 2018, 1, .	2.0	42
76	Scaffold hopping from synthetic RXR modulators by virtual screening and de novo design. MedChemComm, 2018, 9, 1289-1292.	3.5	19
77	Computer-Assisted Discovery of Retinoid X Receptor Modulating Natural Products and Isofunctional Mimetics. Journal of Medicinal Chemistry, 2018, 61, 5442-5447.	2.9	39
78	Hybrid Network Model for â€œDeep Learningâ€•of Chemical Data: Application to Antimicrobial Peptides. Molecular Informatics, 2017, 36, 1600011.	1.4	39
79	Big Data and Deep Learning: A New Age of Molecular Informatics?. Molecular Informatics, 2017, 36, 1780132.	1.4	3
80	De novo Drug Design â€“ Ye olde Scoring Problem Revisited. Molecular Informatics, 2017, 36, 1681031.	1.4	12
81	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
82	Bacterial serine protease HtrA as a promising new target for antimicrobial therapy?. Cell Communication and Signaling, 2017, 15, 4.	2.7	39
83	modlAMP: Python for antimicrobial peptides. Bioinformatics, 2017, 33, 2753-2755.	1.8	106
84	Exploring the Structural Space of the Galectinâ€1â€“Ligand Interaction. ChemBioChem, 2017, 18, 1477-1481.	1.3	7
85	Privileged Structures Revisited. Angewandte Chemie - International Edition, 2017, 56, 7971-7974.	7.2	85
86	Active learning for computational chemogenomics. Future Medicinal Chemistry, 2017, 9, 381-402.	1.1	75
87	Site of Metabolism Prediction Based on abâ€…initio Derived Atom Representations. ChemMedChem, 2017, 12, 606-612.	1.6	23
88	Macromolecular target prediction by self-organizing feature maps. Expert Opinion on Drug Discovery, 2017, 12, 271-277.	2.5	26
89	Discovery of a Novel Inhibitor of the Hedgehog Signaling Pathway through Cellâ€based Compound Discovery and Target Prediction. Angewandte Chemie, 2017, 129, 13201-13205.	1.6	7
90	Discovery of a Novel Inhibitor of the Hedgehog Signaling Pathway through Cellâ€based Compound Discovery and Target Prediction. Angewandte Chemie - International Edition, 2017, 56, 13021-13025.	7.2	22

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91	A Computational Method for Unveiling the Target Promiscuity of Pharmacologically Active Compounds. Angewandte Chemie - International Edition, 2017, 56, 11520-11524.	7.2	39
92	Peptideâ€“Membrane Interaction between Targeting and Lysis. ACS Chemical Biology, 2017, 12, 2254-2259.	1.6	12
93	Privilegierte Strukturen neu betrachtet. Angewandte Chemie, 2017, 129, 8079-8083.	1.6	8
94	A Computational Method for Unveiling the Target Promiscuity of Pharmacologically Active Compounds. Angewandte Chemie, 2017, 129, 11678-11682.	1.6	7
95	Rational Design of Membraneâ€Poreâ€Forming Peptides. Small, 2017, 13, 1701316.	5.2	24
96	Characterisation of anticancer peptides at the single-cell level. Lab on A Chip, 2017, 17, 2933-2940.	3.1	26
97	Matrixâ€based Molecular Descriptors for Prospective Virtual Compound Screening. Molecular Informatics, 2017, 36, 1600091.	1.4	18
98	Scoring of de novo Designed Chemical Entities by Macromolecular Target Prediction. Molecular Informatics, 2017, 36, 1600110.	1.4	5
99	New use of an old drug: inhibition of breast cancer stem cells by benztropine mesylate. Oncotarget, 2017, 8, 1007-1022.	0.8	22
100	Characterisation of worldwide Helicobacter pylori strains reveals genetic conservation and essentiality of serine protease HtrA. Molecular Microbiology, 2016, 99, 925-944.	1.2	70
101	Counting on natural products for drug design. Nature Chemistry, 2016, 8, 531-541.	6.6	879
102	Sparse Neural Network Models of Antimicrobial Peptideâ€Activity Relationships. Molecular Informatics, 2016, 35, 606-614.	1.4	15
103	Deorphaning the Macromolecular Targets of the Natural Anticancer Compound Doliculide. Angewandte Chemie - International Edition, 2016, 55, 12408-12411.	7.2	31
104	Designing Multiâ€target Compound Libraries with Gaussian Process Models. Molecular Informatics, 2016, 35, 192-198.	1.4	9
105	Deep Learning in Drug Discovery. Molecular Informatics, 2016, 35, 3-14.	1.4	502
106	Molecular Informatics: From Models to Systems and Beyond. Molecular Informatics, 2016, 35, 2-2.	1.4	0
107	Identification of E-cadherin signature motifs functioning as cleavage sites for Helicobacter pylori HtrA. Scientific Reports, 2016, 6, 23264.	1.6	77
108	Membranolytic anticancer peptides. MedChemComm, 2016, 7, 2232-2245.	3.5	68

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109	Deorphaning the Macromolecular Targets of the Natural Anticancer Compound Doliculide. Angewandte Chemie, 2016, 128, 12596-12599.	1.6	3
110	Coping with Complexity in Ligand-Based De Novo Design. ACS Symposium Series, 2016, , 143-158.	0.5	1
111	Calcium binding protects E-cadherin from cleavage by Helicobacter pylori HtrA. Gut Pathogens, 2016, 8, 29.	1.6	29
112	Von komplexen Naturstoffen zu synthetisch leicht zugÃnglichen Mimetika mithilfe von computergestÃ¼ztem Deâ€novoâ€Design. Angewandte Chemie, 2016, 128, 6901-6904.	1.6	11
113	From Complex Natural Products to Simple Synthetic Mimetics by Computational De Novo Design. Angewandte Chemie - International Edition, 2016, 55, 6789-6792.	7.2	42
114	Robust molecular representations for modelling and design derived from atomic partial charges. Chemical Communications, 2016, 52, 681-684.	2.2	25
115	De Novo Design at the Edge of Chaos. Journal of Medicinal Chemistry, 2016, 59, 4077-4086.	2.9	124
116	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
117	Spotting and designing promiscuous ligands for drug discovery. Chemical Communications, 2016, 52, 1135-1138.	2.2	33
118	The quantum chemical search for novel materials and the issue of data processing: The InfoMol project. Journal of Computational Science, 2016, 15, 65-73.	1.5	5
119	Attractors in Sequence Space: Peptide Morphing by Directed Simulated Evolution. Molecular Informatics, 2015, 34, 709-714.	1.4	5
120	Computer-assisted quantification of motile and invasive capabilities of cancer cells. Scientific Reports, 2015, 5, 15338.	1.6	23
121	Aryl Bisâ€Sulfonamide Inhibitors of IspF from Arabidopsis thaliana and Plasmodium falciparum. ChemMedChem, 2015, 10, 2090-2098.	1.6	15
122	De Novo Fragment Design for Drug Discovery and Chemical Biology. Angewandte Chemie - International Edition, 2015, 54, 15079-15083.	7.2	30
123	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
124	Revealing the Macromolecular Targets of Fragmentâ€Like Natural Products. Angewandte Chemie - International Edition, 2015, 54, 10516-10520.	7.2	54
125	Structural insights on cholesterol endosynthesis: Binding of squalene and 2,3-oxidosqualene to supernatant protein factor. Journal of Structural Biology, 2015, 190, 261-270.	1.3	21
126	Systems Approaches and Big Data in Molecular Informatics. Molecular Informatics, 2015, 34, 2-2.	1.4	2

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127	Unraveling the Activation Mechanism of Taspase1 which Controls the Oncogenic AF4â€“MLL Fusion Protein. EBioMedicine, 2015, 2, 386-395.	2.7	9
128	Dual-display of small molecules enables the discovery of ligand pairs and facilitates affinity maturation. Nature Chemistry, 2015, 7, 241-249.	6.6	181
129	Multidimensional Deâ€...Novo Design Reveals 5â€HT_{2B} Receptorâ€Selective Ligands. Angewandte Chemie - International Edition, 2015, 54, 1551-1555.	7.2	39
130	In Silico Screening. , 2015, , 141-160.		1
131	Chemography of Natural Product Space. Planta Medica, 2015, 81, 429-435.	0.7	23
132	Fragmentation of GW4064 led to a highly potent partial farnesoid X receptor agonist with improved drug-like properties. Bioorganic and Medicinal Chemistry, 2015, 23, 3490-3498.	1.4	15
133	Predicting drug metabolism: experiment and/or computation?. Nature Reviews Drug Discovery, 2015, 14, 387-404.	21.5	355
134	Repurposing de novo designed entities reveals phosphodiesterase 3B and cathepsin L modulators. Chemical Communications, 2015, 51, 7478-7481.	2.2	10
135	Multidimensional Design of Anticancer Peptides. Angewandte Chemie - International Edition, 2015, 54, 10370-10374.	7.2	32
136	Boswellic acids target the human immune system-modulating antimicrobial peptide LL-37. Pharmacological Research, 2015, 102, 53-60.	3.1	14
137	Active-learning strategies in computer-assisted drug discovery. Drug Discovery Today, 2015, 20, 458-465.	3.2	169
138	In Silico Adoption of an Orphan Nuclear Receptor NR4A1. PLoS ONE, 2015, 10, e0135246.	1.1	6
139	Flashback Forward: Reaction-Driven De Novo Design of Bioactive Compounds. Synlett, 2014, 25, 170-178.	1.0	14
140	Machine Learning Estimates of Natural Product Conformational Energies. PLoS Computational Biology, 2014, 10, e1003400.	1.5	30
141	Coping with Polypharmacology by Computational Medicinal Chemistry. Chimia, 2014, 68, 648.	0.3	6
142	Piloting the Membranolytic Activities of Peptides with a Selfâ€organizing Map. ChemBioChem, 2014, 15, 2225-2231.	1.3	8
143	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
144	Binding to Large Enzyme Pockets: Smallâ€Molecule Inhibitors of Trypanothione Reductase. ChemMedChem, 2014, 9, 1880-1891.	1.6	40

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145	Future De Novo Drug Design. Molecular Informatics, 2014, 33, 397-402.	1.4	28
146	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
147	Accessing New Chemical Entities through Microfluidic Systems. Angewandte Chemie - International Edition, 2014, 53, 5750-5758.	7.2	86
148	Molecular Informatics Going â€œFully Onlineâ€• Molecular Informatics, 2014, 33, 2-2.	1.4	1
149	Fractal Dimensions of Macromolecular Structures. Molecular Informatics, 2014, 33, 588-596.	1.4	12
150	Revealing the macromolecular targets of complex natural products. Nature Chemistry, 2014, 6, 1072-1078.	6.6	114
151	Inhibiting Helicobacter pylori HtrA protease by addressing a computationally predicted allosteric ligand binding site. Chemical Science, 2014, 5, 3583.	3.7	29
152	Multiâ€Objective Molecular De Novo Design by Adaptive Fragment Prioritization. Angewandte Chemie - International Edition, 2014, 53, 4244-4248.	7.2	76
153	Vanillin-derived antiproliferative compounds influence Plk1 activity. Bioorganic and Medicinal Chemistry Letters, 2014, 24, 5063-5069.	1.0	14
154	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
155	Peptide lineup against Gram-negative bacterial infection â€“ first-in-class peptide inhibitor of H. pylori HtrA. Journal of Cheminformatics, 2014, 6, .	2.8	0
156	Target prediction by cascaded self-organizing maps for ligand de-orphaning and side-effect investigation. Journal of Cheminformatics, 2014, 6, .	2.8	1
157	Identification of pirinixic acid derivatives bearing a 2-aminothiazole moiety combines dual PPARÎ±/Î³ activation and dual 5-LO/mPGES-1 inhibition. Bioorganic and Medicinal Chemistry Letters, 2014, 24, 3757-3763.	1.0	13
158	Targeting Dynamic Pockets of HIV-1 Protease by Structure-Based Computational Screening for Allosteric Inhibitors. Journal of Chemical Information and Modeling, 2014, 54, 987-991.	2.5	29
159	Anthranilic acid derivatives as novel ligands for farnesoid X receptor (FXR). Bioorganic and Medicinal Chemistry, 2014, 22, 2447-2460.	1.4	27
160	Deorphaning Pyrrolopyrazines as Potent Multiâ€Target Antimalarial Agents. Angewandte Chemie - International Edition, 2014, 53, 7079-7084.	7.2	30
161	Breaking the data barrier in computational medicinal chemistry. Future Medicinal Chemistry, 2014, 6, 245-246.	1.1	2
162	Combinatorial chemistry by ant colony optimization. Future Medicinal Chemistry, 2014, 6, 267-280.	1.1	16

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163	Steering Target Selectivity and Potency by Fragmentâ€Based De Novo Drug Design. Angewandte Chemie - International Edition, 2013, 52, 10006-10009.	7.2	23
164	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
165	Exhaustive Proteome Mining for Functional MHC-I Ligands. ACS Chemical Biology, 2013, 8, 1876-1881.	1.6	12
166	Common non-epigenetic drugs as epigenetic modulators. Trends in Molecular Medicine, 2013, 19, 742-753.	3.5	68
167	Drugs by Numbers: Reactionâ€Driven De Novo Design of Potent and Selective Anticancer Leads. Angewandte Chemie - International Edition, 2013, 52, 4676-4681.	7.2	22
168	Editorial: Sustained Success of Molecular Informatics. Molecular Informatics, 2013, 32, 3-3.	1.4	0
169	De novo design â€“ hop(p)ing against hope. Drug Discovery Today: Technologies, 2013, 10, e453-e460.	4.0	31
170	Computational Resources for MHC Ligand Identification. Molecular Informatics, 2013, 32, 326-336.	1.4	8
171	De novo design and optimization of Aurora A kinase inhibitors. Chemical Science, 2013, 4, 1229.	3.7	23
172	Quinolin-4(1H)-imines are Potent Antiplasmodial Drugs Targeting the Liver Stage of Malaria. Journal of Medicinal Chemistry, 2013, 56, 4811-4815.	2.9	21
173	Synthesis and pharmacological characterization of benzenesulfonamides as dual species inhibitors of human and murine mPGES-1. Bioorganic and Medicinal Chemistry, 2013, 21, 7874-7883.	1.4	18
174	Adaptive Peptide Design. Chimia, 2013, 67, 859-863.	0.3	4
175	Scrutinizing MHC-I Binding Peptides and Their Limits of Variation. PLoS Computational Biology, 2013, 9, e1003088.	1.5	33
176	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
177	Pharmacophore Alignment Search Tool (PhAST): Significance Assessment of Chemical Similarity. Molecular Informatics, 2013, 32, 625-646.	1.4	2
178	DOGS: Reaction-Driven de novo Design of Bioactive Compounds. PLoS Computational Biology, 2012, 8, e1002380.	1.5	193
179	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
180	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

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181	From Theory to Bench Experiment by Computer-assisted Drug Design. Chimia, 2012, 66, 120.	0.3	5
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