JÃ¼rgen Bajorath

List of Publications by Year
in descending order

573 papers	20,094 citations	26567 56 h-index	19690 117 g-index
662 all docs	662 docs citations	662 times ranked	13876 citing authors

#	Article	IF	Citations
1	Fine-tuning of a generative neural network for designing multi-target compounds. Journal of Computer-Aided Molecular Design, 2022, 36, 363-371.	1.3	8
2	Structure- and Similarity-Based Survey of Allosteric Kinase Inhibitors, Activators, and Closely Related Compounds. Journal of Medicinal Chemistry, 2022, 65, 922-934.	2.9	33
3	Systematic identification of activity cliffs with dualâ€atom replacements and their rationalization on the basis of singleâ€atom replacement analogs and Xâ€ray structures. Chemical Biology and Drug Design, 2022, 99, 308-319.	1.5	0
4	Approach for the Design of Covalent Protein Kinase Inhibitors via Focused Deep Generative Modeling. Molecules, 2022, 27, 570.	1.7	8
5	AI in Life Science Research â€“ The Road Ahead. Artificial Intelligence in the Life Sciences, 2022, 2, 100030.	1.6	0
6	Deep Machine Learning for Computer-Aided Drug Design. Frontiers in Drug Discovery, 2022, 2, .	1.1	8
7	Evolution of Support Vector Machine and Regression Modeling in Chemoinformatics and Drug Discovery. Journal of Computer-Aided Molecular Design, 2022, 36, 355-362.	1.3	44
8	Artificial intelligence in interdisciplinary life science and drug discovery research. Future Science OA, 2022, 8, FSO792.	0.9	8
9	Introducing a Chemically Intuitive Core-Substituent Fingerprint Designed to Explore Structural Requirements for Effective Similarity Searching and Machine Learning. Molecules, 2022, 27, 2331.	1.7	5
10	Differentiating Inhibitors of Closely Related Protein Kinases with Single- or Multi-Target Activity via Explainable Machine Learning and Feature Analysis. Biomolecules, 2022, 12, 557.	1.8	5
11	Understanding uncertainty in deep learning builds confidence. Artificial Intelligence in the Life Sciences, 2022, 2, 100033.	1.6	0
12	New Horizons in Drug Discovery - Understanding and Advancing Different Types of Kinase Inhibitors: Seven Years in Kinase Inhibitor Research with Impressive Achievements and New Future Prospects. Journal of Medicinal Chemistry, 2022, 65, 891-892.	2.9	9
13	Machine Learning in Chemoinformatics and Medicinal Chemistry. Annual Review of Biomedical Data Science, 2022, 5, 43-65.	2.8	8
14	From traditional to data-driven medicinal chemistry: A case study. Drug Discovery Today, 2022, 27, 2065-2070.	3.2	2
15	Publication Criteria and Requirements for Studies on Protein Kinase Inhibitorsâ”€What Is Expected?. Journal of Medicinal Chemistry, 2022, 65, 6973-6974.	2.9	10
16	DeepAS â€“ Chemical language model for the extension of active analogue series. Bioorganic and Medicinal Chemistry, 2022, 66, 116808.	1.4	5
17	Deep learning of proteinâ€“ligand interactionsâ€”Remembering the actors. Artificial Intelligence in the Life Sciences, 2022, 2, 100037.	1.6	1
18	Computational method for the systematic alignment of analogue series with structure-activity relationship transfer potential across different targets. European Journal of Medicinal Chemistry, 2022, 239, 114558.	2.6	3

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19	Explainable machine learning for medicinal chemistry: exploring multi-target compounds. Future Medicinal Chemistry, 2022, 14, 1171-1173.	1.1	2
20	Prediction of Promiscuity Cliffs Using Machine Learning. Molecular Informatics, 2021, 40, 2000196.	1.4	6
21	Introducing the metacore concept for multi-target ligand design. RSC Medicinal Chemistry, 2021, 12, 628-635.	1.7	5
22	Predicting Isoform-Selective Carbonic Anhydrase Inhibitors via Machine Learning and Rationalizing Structural Features Important for Selectivity. ACS Omega, 2021, 6, 4080-4089.	1.6	8
23	Evaluation of multi-target deep neural network models for compound potency prediction under increasingly challenging test conditions. Journal of Computer-Aided Molecular Design, 2021, 35, 285-295.	1.3	10
24	Prediction of activity cliffs on the basis of images using convolutional neural networks. Journal of Computer-Aided Molecular Design, 2021, 35, 1157-1164.	1.3	11
25	Systematic comparison of competitive and allosteric kinase inhibitors reveals common structural characteristics. European Journal of Medicinal Chemistry, 2021, 214, 113206.	2.6	6
26	Evolution of assay interference concepts in drug discovery. Expert Opinion on Drug Discovery, 2021, 16, 719-721.	2.5	13
27	Adapting the DeepSARM approach for dual-target ligand design. Journal of Computer-Aided Molecular Design, 2021, 35, 587-600.	1.3	5
28	Machine learning reveals that structural features distinguishing promiscuous and non-promiscuous compounds depend on target combinations. Scientific Reports, 2021, 11, 7863.	1.6	14
29	Data set of competitive and allosteric protein kinase inhibitors confirmed by X-ray crystallography. Data in Brief, 2021, 35, 106816.	0.5	4
30	Rationality over fashion and hype in drug design. F1000Research, 2021, 10, 397.	0.8	23
31	Structured data sets of compounds with multi-target and corresponding single-target activity from biological assays. Future Science OA, 2021, 7, FSO685.	0.9	2
32	Structural characteristics of compounds with multitarget activity. Future Drug Discovery, 2021, 3, .	0.8	6
33	Systematic assessment of structure-promiscuity relationships between different types of kinase inhibitors. Bioorganic and Medicinal Chemistry, 2021, 41, 116226.	1.4	3
34	Minimal screening requirements for identifying highly promiscuous kinase inhibitors. Future Medicinal Chemistry, 2021, 13, 1083-1085.	1.1	1
35	Feature importance correlation from machine learning indicates functional relationships between proteins and similar compound binding characteristics. Scientific Reports, 2021, 11, 14245.	1.6	18
36	State-of-the-art of artificial intelligence in medicinal chemistry. Future Science OA, 2021, 7, FSO702.	0.9	21

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37	Compound dataset and custom code for deep generative multi-target compound design. Future Science OA, 2021, 7, FSO715.	0.9	4
38	Development of curcumin-based amyloid Î² aggregation inhibitors for Alzheimer's disease using the SAR matrix approach. Bioorganic and Medicinal Chemistry, 2021, 46, 116357.	1.4	6
39	Chemistry-centric explanation of machine learning models. Artificial Intelligence in the Life Sciences, 2021, 1, 100009.	1.6	3
40	R-group replacement database for medicinal chemistry. Future Science OA, 2021, 7, FSO742.	0.9	5
41	Systematic mapping of R-group space enables the generation of an R-group replacement system for medicinal chemistry. European Journal of Medicinal Chemistry, 2021, 225, 113771.	2.6	6
42	Informatics for Chemistry, Biology, and Biomedical Sciences. Journal of Chemical Information and Modeling, 2021, 61, 26-35.	2.5	42
43	Comprehensive analysis of R-groups in medicinal chemistry. Future Medicinal Chemistry, 2021, , .	1.1	0
44	Searchable database of frequent R-groups in medicinal chemistry and their preferred replacements. Data in Brief, 2021, 39, 107456.	0.5	0
45	Data-Driven Analysis of Fluorination of Ligands of Aminergic G Protein Coupled Receptors. Biomolecules, 2021, 11, 1647.	1.8	2
46	Explainable machine learning predictions of dual-target compounds reveal characteristic structural features. Scientific Reports, 2021, 11, 21594.	1.6	11
47	Learning functional group chemistry from molecular images leads to accurate prediction of activity cliffs. Artificial Intelligence in the Life Sciences, 2021, 1, 100022.	1.6	2
48	Impact of Artificial Intelligence on Compound Discovery, Design, and Synthesis. ACS Omega, 2021, 6, 33293-33299.	1.6	16
49	Iterative DeepSARM modeling for compound optimization. Artificial Intelligence in the Life Sciences, 2021, 1, 100015.	1.6	1
50	Second-Generation Artificial Intelligence Approaches for Life Science Research. Artificial Intelligence in the Life Sciences, 2021, 1, 100026.	1.6	0
51	Explainable Machine Learning for Property Predictions in Compound Optimization. Journal of Medicinal Chemistry, 2021, 64, 17744-17752.	2.9	34
52	Interpretation of Compound Activity Predictions from Complex Machine Learning Models Using Local Approximations and Shapley Values. Journal of Medicinal Chemistry, 2020, 63, 8761-8777.	2.9	178
53	Machine Learning Models for Accurate Prediction of Kinase Inhibitors with Different Binding Modes. Journal of Medicinal Chemistry, 2020, 63, 8738-8748.	2.9	34
54	Introducing a new category of activity cliffs combining different compound similarity criteria. RSC Medicinal Chemistry, 2020, 11, 132-141.	1.7	10

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55	Promiscuity analysis of a kinase panel screen with designated p38 alpha inhibitors. European Journal of Medicinal Chemistry, 2020, 187, 112004.	2.6	3
56	Data structures for computational compound promiscuity analysis and exemplary applications to inhibitors of the human kinome. Journal of Computer-Aided Molecular Design, 2020, 34, 1-10.	1.3	8
57	Exploring structure-promiscuity relationships using dual-site promiscuity cliffs and corresponding single-site analogs. Bioorganic and Medicinal Chemistry, 2020, 28, 115238.	1.4	2
58	Activity cliffs produced by single-atom modification of active compounds: Systematic identification and rationalization based on X-ray structures. European Journal of Medicinal Chemistry, 2020, 207, 112846.	2.6	5
59	Quantitative Comparison of Three-Dimensional Activity Landscapes of Compound Data Sets Based upon Topological Features. ACS Omega, 2020, 5, 24111-24117.	1.6	2
60	DeepCOMO: from structure-activity relationship diagnostics to generative molecular design using the compound optimization monitor methodology. Journal of Computer-Aided Molecular Design, 2020, 34, 1207-1218.	1.3	7
61	Data set of activity cliffs with single-atom modification and associated X-ray structure information for medicinal and computational chemistry applications. Data in Brief, 2020, 33, 106364.	0.5	0
62	Evidence for the presence of core structure-dependent activity cliffs. Future Medicinal Chemistry, 2020, 12, 1451-1455.	1.1	0
63	New Horizons in Drug Discovery - Understanding and Advancing Kinase Inhibitors. Journal of Medicinal Chemistry, 2020, 63, 7921-7922.	2.9	4
64	N-Sulfonyl dipeptide nitriles as inhibitors of human cathepsin S: In silico design, synthesis and biochemical characterization. Bioorganic and Medicinal Chemistry Letters, 2020, 30, 127420.	1.0	4
65	Identifying representative kinases for inhibitor evaluation via systematic analysis of compound-based target relationships. European Journal of Medicinal Chemistry, 2020, 204, 112641.	2.6	4
66	From Qualitative to Quantitative Analysis of Activity and Property Landscapes. Journal of Chemical Information and Modeling, 2020, 60, 5873-5880.	2.5	11
67	Memory-assisted reinforcement learning for diverse molecular de novo design. Journal of Cheminformatics, 2020, 12, 68.	2.8	53
68	Global Assessment of Substituents on the Basis of Analogue Series. Journal of Medicinal Chemistry, 2020, 63, 15013-15020.	2.9	7
69	Activity landscape image analysis using convolutional neural networks. Journal of Cheminformatics, 2020, 12, 34.	2.8	11
70	Kinase inhibitor data set for systematic analysis of representative kinases across the human kinome. Data in Brief, 2020, 32, 106189.	0.5	5
71	Computational Method for Quantitative Comparison of Activity Landscapes on the Basis of Image Data. Molecules, 2020, 25, 3952.	1.7	1
72	Compounds with multitarget activity: structure-based analysis and machine learning. Future Drug Discovery, 2020, 2, .	0.8	7

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73	Prediction of an MMP-1 inhibitor activity cliff using the SAR matrix approach and its experimental validation. Scientific Reports, 2020, 10, 14710.	1.6	9
74	Analysis of Biological Screening Compounds with Single- or Multi-Target Activity via Diagnostic Machine Learning. Biomolecules, 2020, 10, 1605.	1.8	13
75	Systematic Data Analysis and Diagnostic Machine Learning Reveal Differences between Compounds with Single- and Multitarget Activity. Molecular Pharmaceutics, 2020, 17, 4652-4666.	2.3	14
76	Interpretation of machine learning models using shapley values: application to compound potency and multi-target activity predictions. Journal of Computer-Aided Molecular Design, 2020, 34, 1013-1026.	1.3	248
77	Increasing the public activity cliff knowledge base with new categories of activity cliffs. Future Science OA, 2020, 6, FSO472.	0.9	2
78	Advances in exploring activity cliffs. Journal of Computer-Aided Molecular Design, 2020, 34, 929-942.	1.3	18
79	Assessing the information content of structural and proteinâ€“ligand interaction representations for the classification of kinase inhibitor binding modes via machine learning and active learning. Journal of Cheminformatics, 2020, 12, 36.	2.8	14
80	Deep SAR matrix: SAR matrix expansion for advanced analog design using deep learning architectures. Future Drug Discovery, 2020, 2, .	0.8	11
81	Simplified activity cliff network representations with high interpretability and immediate access to SAR information. Journal of Computer-Aided Molecular Design, 2020, 34, 943-952.	1.3	1
82	Integrating computational lead optimization diagnostics with analog design and candidate selection. Future Science OA, 2020, 6, FSO451.	0.9	6
83	Mapping the S1 and S1â€™ subsites of cysteine proteases with new dipeptidyl nitrile inhibitors as trypanocidal agents. PLoS Neglected Tropical Diseases, 2020, 14, e0007755.	1.3	11
84	Biological Activity Profiles of Multitarget Ligands from X-ray Structures. Molecules, 2020, 25, 794.	1.7	2
85	X-ray Structure-Based Chemoinformatic Analysis Identifies Promiscuous Ligands Binding to Proteins from Different Classes with Varying Shapes. International Journal of Molecular Sciences, 2020, 21, 3782.	1.8	7
86	Artificial Intelligence in Drug Discovery: Into the Great Wide Open. Journal of Medicinal Chemistry, 2020, 63, 8651-8652.	2.9	40
87	Computational Method for Structure-Based Analysis of SAR Transfer. Journal of Medicinal Chemistry, 2020, 63, 1388-1396.	2.9	4
88	Computational method for the identification of third generation activity cliffs. MethodsX, 2020, 7, 100793.	0.7	5
89	Systematic Exploration of Activity Cliffs Containing Privileged Substructures. Molecular Pharmaceutics, 2020, 17, 979-989.	2.3	5
90	Current Trends, Overlooked Issues, and Unmet Challenges in Virtual Screening. Journal of Chemical Information and Modeling, 2020, 60, 4112-4115.	2.5	34

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91	QSAR without borders. Chemical Society Reviews, 2020, 49, 3525-3564.	18.7	427
92	The SAR Matrix Method and an Artificially Intelligent Variant for the Identification and Structural Organization of Analog Series, SAR Analysis, and Compound Design. Molecular Informatics, 2020, 39, e2000045.	1.4	9
93	From SAR Diagnostics to Compound Design: Development Chronology of the Compound Optimization Monitor (COMO) Method. Molecular Informatics, 2020, 39, 2000046.	1.4	4
94	Inhibitor bias in luciferase-based luminescence assays. Future Science OA, 2020, 6, FSO594.	0.9	4
95	ccbmlib â€“ a Python package for modeling Tanimoto similarity value distributions. F1000Research, 2020, 9, 100.	0.8	11
96	ccbmlib â€“ a Python package for modeling Tanimoto similarity value distributions. F1000Research, 2020, 9, 100.	0.8	5
97	Combining structural and bioactivity-based fingerprints improves prediction performance and scaffoldÂhopping capability. Journal of Cheminformatics, 2019, 11, 54.	2.8	28
98	Data structures for compound promiscuity analysis: promiscuity cliffs, pathways and promiscuity hubs formed by inhibitors of the human kinome. Future Science OA, 2019, 5, FSO404.	0.9	3
99	Evaluation of different virtual screening strategies on the basis of compound sets with characteristic core distributions and dissimilarity relationships. Journal of Computer-Aided Molecular Design, 2019, 33, 729-743.	1.3	4
100	Forward-looking perspective on publishing in drug discovery. Future Drug Discovery, 2019, 1, FDD2.	0.8	2
101	Can Cysteine Protease Cross-Class Inhibitors Achieve Selectivity?. Journal of Medicinal Chemistry, 2019, 62, 10497-10525.	2.9	47
102	Introducing a new category of activity cliffs with chemical modifications at multiple sites and rationalizing contributions of individual substitutions. Bioorganic and Medicinal Chemistry, 2019, 27, 3605-3612.	1.4	12
103	Second-generation activity cliffs identified on the basis of target set-dependent potency difference criteria. Future Medicinal Chemistry, 2019, 11, 379-394.	1.1	12
104	Identification of Compounds That Interfere with Highâ€Throughput Screening Assay Technologies. ChemMedChem, 2019, 14, 1795-1802.	1.6	21
105	A general approach for retrosynthetic molecular core analysis. Journal of Cheminformatics, 2019, 11, 61.	2.8	8
106	Method for Systematic Analogue Search Using the Mega SAR Matrix Database. Journal of Chemical Information and Modeling, 2019, 59, 3727-3734.	2.5	5
107	Evolving Concept of Activity Cliffs. ACS Omega, 2019, 4, 14360-14368.	1.6	76
108	Large-Scale Comparison of Alternative Similarity Search Strategies with Varying Chemical Information Contents. ACS Omega, 2019, 4, 15304-15311.	1.6	7

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109	Computational chemical biology on the rise. Future Medicinal Chemistry, 2019, 11, 1-3.	1.1	5
110	Promiscuous Ligands from Experimentally Determined Structures, Binding Conformations, and Protein Family-Dependent Interaction Hotspots. ACS Omega, 2019, 4, 1729-1737.	1.6	18
111	Systematic identification of target set-dependent activity cliffs. Future Science OA, 2019, 5, FSO363.	0.9	7
112	The Future Is Now: Artificial Intelligence in Drug Discovery. Journal of Medicinal Chemistry, 2019, 62, 5249-5249.	2.9	3
113	Exploration of Target Synergy in Cancer Treatment by Cell-Based Screening Assay and Network Propagation Analysis. Journal of Chemical Information and Modeling, 2019, 59, 3072-3079.	2.5	1
114	Integrating the Structureâ€“Activity Relationship Matrix Method with Molecular Grid Maps and Activity Landscape Models for Medicinal Chemistry Applications. ACS Omega, 2019, 4, 7061-7069.	1.6	19
115	Prediction of Different Classes of Promiscuous and Nonpromiscuous Compounds Using Machine Learning and Nearest Neighbor Analysis. ACS Omega, 2019, 4, 6883-6890.	1.6	18
116	Duality of activity cliffs in drug discovery. Expert Opinion on Drug Discovery, 2019, 14, 517-520.	2.5	13
117	Systematic computational identification of promiscuity cliff pathways formed by inhibitors of the human kinome. Journal of Computer-Aided Molecular Design, 2019, 33, 559-572.	1.3	8
118	Recent Progress in Structure-Based Evaluation of Compound Promiscuity. ACS Omega, 2019, 4, 2758-2765.	1.6	17
119	Multitask Machine Learning for Classifying Highly and Weakly Potent Kinase Inhibitors. ACS Omega, 2019, 4, 4367-4375.	1.6	49
120	Compound optimization monitor (COMO) method for computational evaluation of progress in medicinal chemistry projects. Future Drug Discovery, 2019, 1, FDD15.	0.8	5
121	Identifying Promiscuous Compounds with Activity against Different Target Classes. Molecules, 2019, 24, 4185.	1.7	17
122	Exploring Alternative Strategies for the Identification of Potent Compounds Using Support Vector Machine and Regression Modeling. Journal of Chemical Information and Modeling, 2019, 59, 983-992.	2.5	7
123	Virtual Screening with Generative Topographic Maps: How Many Maps Are Required?. Journal of Chemical Information and Modeling, 2019, 59, 564-572.	2.5	20
124	Systematic Extraction of Analogue Series from Large Compound Collections Using a New Computational Compoundâ€“Core Relationship Method. ACS Omega, 2019, 4, 1027-1032.	1.6	56
125	Cathepsin B: Active site mapping with peptidic substrates and inhibitors. Bioorganic and Medicinal Chemistry, 2019, 27, 1-15.	1.4	47
126	Three-Dimensional Activity Landscape Models of Different Design and Their Application to Compound Mapping and Potency Prediction. Journal of Chemical Information and Modeling, 2019, 59, 993-1004.	2.5	9

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127	Repositioning the Chemical Information Science Gateway. F1000Research, 2019, 8, 976.	0.8	2
128	[Special Issue for Honor Award dedicating to Prof Kimito Funatsu]Exploring Polypharmacology and Molecular Promiscuity. Journal of Computer Aided Chemistry, 2019, 20, 43-46.	0.3	0
129	Identification of 4â€arylâ€1 Hâ€pyrrole[2,3â€b]pyridine derivatives for the development of new Bâ€Raf inhibitors. Chemical Biology and Drug Design, 2018, 92, 1382-1386.	1.5	3
130	Combining Similarity Searching and Network Analysis for the Identification of Active Compounds. ACS Omega, 2018, 3, 3768-3777.	1.6	10
131	Evaluation of Kinase Inhibitor Selectivity Using Cellâ€based Profiling Data. Molecular Informatics, 2018, 37, e1800024.	1.4	2
132	Exploring Selectivity of Multikinase Inhibitors across the Human Kinome. ACS Omega, 2018, 3, 1147-1153.	1.6	14
133	Computational method for estimating progression saturation of analog series. RSC Advances, 2018, 8, 5484-5492.	1.7	12
134	Design of a tripartite network for the prediction of drug targets. Journal of Computer-Aided Molecular Design, 2018, 32, 321-330.	1.3	8
135	Design of an Activity-Based Probe for Human Neutrophil Elastase: Implementation of the Lossen Rearrangement To Induce FÃ¶rster Resonance Energy Transfers. Biochemistry, 2018, 57, 742-752.	1.2	28
136	Application of Generative Autoencoder in De Novo Molecular Design. Molecular Informatics, 2018, 37, 1700123.	1.4	276
137	X-ray Structures of Targetâ€“Ligand Complexes Containing Compounds with Assay Interference Potential. Journal of Medicinal Chemistry, 2018, 61, 1276-1284.	2.9	22
138	Series of screening compounds with high hit rates for the exploration of multi-target activities and assay interference. Future Science OA, 2018, 4, FSO279.	0.9	2
139	X-ray-Structure-Based Identification of Compounds with Activity against Targets from Different Families and Generation of Templates for Multitarget Ligand Design. ACS Omega, 2018, 3, 106-111.	1.6	19
140	Extracting Compound Profiling Matrices from Screening Data. ACS Omega, 2018, 3, 4706-4712.	1.6	10
141	Prediction of Compound Profiling Matrices Using Machine Learning. ACS Omega, 2018, 3, 4713-4723.	1.6	32
142	Reconciling Selectivity Trends from a Comprehensive Kinase Inhibitor Profiling Campaign with Known Activity Data. ACS Omega, 2018, 3, 3113-3119.	1.6	12
143	Redundancy in two major compound databases. Drug Discovery Today, 2018, 23, 1183-1186.	3.2	8
144	Rationalizing Promiscuity Cliffs. ChemMedChem, 2018, 13, 490-494.	1.6	14

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145	Machine Learning Distinguishes with High Accuracy between Pan-Assay Interference Compounds That Are Promiscuous or Represent Dark Chemical Matter. Journal of Medicinal Chemistry, 2018, 61, 10255-10264.	2.9	25
146	Computational Analysis of Kinase Inhibitors Identifies Promiscuity Cliffs across the Human Kinome. ACS Omega, 2018, 3, 17295-17308.	1.6	25
147	Computational Assessment of Chemical Saturation of Analogue Series under Varying Conditions. ACS Omega, 2018, 3, 15799-15808.	1.6	9
148	Computational Method to Evaluate Progress in Lead Optimization. Journal of Medicinal Chemistry, 2018, 61, 10895-10900.	2.9	18
149	Prediction of Compound Profiling Matrices, Part II: Relative Performance of Multitask Deep Learning and Random Forest Classification on the Basis of Varying Amounts of Training Data. ACS Omega, 2018, 3, 12033-12040.	1.6	20
150	Data-Driven Exploration of Selectivity and Off-Target Activities of Designated Chemical Probes. Molecules, 2018, 23, 2434.	1.7	9
151	SAR Matrix Method for Large-Scale Analysis of Compound Structureâ€“Activity Relationships and Exploration of Multitarget Activity Spaces. Methods in Molecular Biology, 2018, 1825, 339-352.	0.4	2
152	Mapping Biological Activities to Different Types of Molecular Scaffolds: Exemplary Application to Protein Kinase Inhibitors. Methods in Molecular Biology, 2018, 1825, 327-337.	0.4	1
153	Collection of analog series-based scaffolds from public compound sources. Future Science OA, 2018, 4, FSO287.	0.9	8
154	Data analytics and deep learning in medicinal chemistry. Future Medicinal Chemistry, 2018, 10, 1541-1543.	1.1	5
155	Exploring ensembles of bioactive or virtual analogs of X-ray ligands for shape similarity searching. Journal of Computer-Aided Molecular Design, 2018, 32, 759-767.	1.3	2
156	Improving the utility of molecular scaffolds for medicinal and computational chemistry. Future Medicinal Chemistry, 2018, 10, 1645-1648.	1.1	13
157	Computationally derived compound profiling matrices. Future Science OA, 2018, 4, FSO327.	0.9	0
158	A Hybrid Virtual Screening Protocol Based on Binding Mode Similarity. Methods in Molecular Biology, 2018, 1824, 165-175.	0.4	3
159	Foundations of data-driven medicinal chemistry. Future Science OA, 2018, 4, FSO320.	0.9	10
160	Rationalizing the Formation of Activity Cliffs in Different Compound Data Sets. ACS Omega, 2018, 3, 7736-7744.	1.6	16
161	Computational design of new molecular scaffolds for medicinal chemistry, part II: generalization of analog series-based scaffolds. Future Science OA, 2018, 4, FSO267.	0.9	8
162	Identification and analysis of promiscuity cliffs formed by bioactive compounds and experimental implications. RSC Advances, 2017, 7, 58-66.	1.7	15

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163	Structure-Promiscuity Relationship Puzzlesâ€"Extensively Assayed Analogs with Large Differences in Target Annotations. AAPS Journal, 2017, 19, 856-864.	2.2	14
164	Influence of Varying Training Set Composition and Size on Support Vector Machine-Based Prediction of Active Compounds. Journal of Chemical Information and Modeling, 2017, 57, 710-716.	2.5	27
165	Systematic analysis of structural and activity relationships between conventional hierarchical and analog series-based scaffolds. RSC Advances, 2017, 7, 18718-18723.	1.7	3
166	How Frequently Are Pan-Assay Interference Compounds Active? Large-Scale Analysis of Screening Data Reveals Diverse Activity Profiles, Low Global Hit Frequency, and Many Consistently Inactive Compounds. Journal of Medicinal Chemistry, 2017, 60, 3879-3886.	2.9	97
167	Application of a New Scaffold Concept for Computational Target Deconvolution of Chemical Cancer Cell Line Screens. ACS Omega, 2017, 2, 1463-1468.	1.6	14
168	Privileged Structural Motif Detection and Analysis Using Generative Topographic Maps. Journal of Chemical Information and Modeling, 2017, 57, 1218-1232.	2.5	9
169	Compound Data Mining for Drug Discovery. Methods in Molecular Biology, 2017, 1526, 247-256.	0.4	9
170	Is scaffold hopping a reliable indicator for the ability of computational methods to identify structurally diverse active compounds?. Journal of Computer-Aided Molecular Design, 2017, 31, 603-608.	1.3	2
171	Computational scaffold hopping: cornerstone for the future of drug design?. Future Medicinal Chemistry, 2017, 9, 629-631.	1.1	25
172	Compound Ranking Based on Fuzzy Three-Dimensional Similarity Improves the Performance of Docking into Homology Models of G-Protein-Coupled Receptors. ACS Omega, 2017, 2, 2583-2592.	1.6	6
173	Identifying relationships between unrelated pharmaceutical target proteins on the basis of shared active compounds. Future Science OA, 2017, 3, FSO212.	0.9	4
174	A Fluorescentâ€Labeled Phosphono Bisbenzguanidine As an Activityâ€Based Probe for Matriptase. Chemistry - A European Journal, 2017, 23, 5205-5209.	1.7	12
175	Entering the â€˜big dataâ€™ era in medicinal chemistry: molecular promiscuity analysis revisited. Future Science OA, 2017, 3, FSO179.	0.9	53
176	Molecular Similarity Concepts for Informatics Applications. Methods in Molecular Biology, 2017, 1526, 231-245.	0.4	28
177	Tracing compound pathways using chemical space networks. MedChemComm, 2017, 8, 376-384.	3.5	5
178	Mapping of inhibitors and activity data to the human kinome and exploring promiscuity from a ligand and target perspective. Chemical Biology and Drug Design, 2017, 89, 834-845.	1.5	16
179	Modeling Tanimoto Similarity Value Distributions and Predicting Search Results. Molecular Informatics, 2017, 36, 1600131.	1.4	15
180	Recent Advances in Scaffold Hopping. Journal of Medicinal Chemistry, 2017, 60, 1238-1246.	2.9	213

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181	Dark chemical matter in public screening assays and derivation of target hypotheses. MedChemComm, 2017, 8, 2100-2104.	3.5	6
182	Support Vector Machine Classification and Regression Prioritize Different Structural Features for Binary Compound Activity and Potency Value Prediction. ACS Omega, 2017, 2, 6371-6379.	1.6	75
183	From birdâ€™s eye views to molecular communities: two-layered visualization of structureâ€“activity relationships in large compound data sets. Journal of Computer-Aided Molecular Design, 2017, 31, 961-977.	1.3	5
184	Promiscuity of inhibitors of human protein kinases at varying data confidence levels and test frequencies. RSC Advances, 2017, 7, 41265-41271.	1.7	20
185	Activity profiles of analog series containing pan assay interference compounds. RSC Advances, 2017, 7, 35638-35647.	1.7	24
186	From activity cliffs to promiscuity cliffs. Future Science OA, 2017, 3, FSO227.	0.9	3
187	Exploring Structural Relationships between Bioactive and Commercial Chemical Space and Developing Target Hypotheses for Compound Acquisition. ACS Omega, 2017, 2, 7760-7766.	1.6	2
188	Heat shock protein 90 and serine/threonine kinase B-Raf inhibitors have overlapping chemical space. RSC Advances, 2017, 7, 31069-31074.	1.7	17
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