Jrgen Bajorath

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

545 papers	15,586 citations	51 h-index	103 g-index
662 ext. papers	17,900 ext. citations	5 avg, IF	7.47 L-index

#	Paper	IF	Citations
545	AI in Life Science Research The Road Ahead. *Artificial Intelligence in the Life Sciences*, **2022**, 2, 100030		
544	Evolution of Support Vector Machine and Regression Modeling in Chemoinformatics and Drug Discovery.. *Journal of Computer-Aided Molecular Design*, **2022**, 1	4.2	5
543	Artificial intelligence in interdisciplinary life science and drug discovery research.. *Future Science OA* , **2022**, 8, FSO792	2.7	0
542	Understanding uncertainty in deep learning builds confidence. *Artificial Intelligence in the Life Sciences*, **2022**, 2, 100033		
541	DeepAS - Chemical language model for the extension of active analogue series.. *Bioorganic and Medicinal Chemistry*, **2022**, 66, 116808	3.4	0
540	Deep learning of protein ligand interactions Remembering the actors. *Artificial Intelligence in the Life Sciences*, **2022**, 2, 100037		
539	Explainable machine learning predictions of dual-target compounds reveal characteristic structural features. *Scientific Reports*, **2021**, 11, 21594	4.9	1
538	Learning Functional Group Chemistry from Molecular Images Leads to Accurate Prediction of Activity Cliffs. *Artificial Intelligence in the Life Sciences*, **2021**, 100022		0
537	Impact of Artificial Intelligence on Compound Discovery, Design, and Synthesis.. *ACS Omega*, **2021**, 6, 33293-33299	3.9	3
536	Iterative DeepSARM Modeling for Compound Optimization. *Artificial Intelligence in the Life Sciences* , **2021**, 100015		
535	Second-generation artificial intelligence approaches for life science research. *Artificial Intelligence in the Life Sciences*, **2021**, 1, 100026		
534	Searchable database of frequent R-groups in medicinal chemistry and their preferred replacements. *Data in Brief*, **2021**, 39, 107456	1.2	
533	Informatics for Chemistry, Biology, and Biomedical Sciences. *Journal of Chemical Information and Modeling*, **2021**, 61, 26-35	6.1	15
532	Prediction of activity cliffs on the basis of images using convolutional neural networks. *Journal of Computer-Aided Molecular Design*, **2021**, 35, 1157-1164	4.2	1
531	Systematic comparison of competitive and allosteric kinase inhibitors reveals common structural characteristics. *European Journal of Medicinal Chemistry*, **2021**, 214, 113206	6.8	2
530	Adapting the DeepSARM approach for dual-target ligand design. *Journal of Computer-Aided Molecular Design*, **2021**, 35, 587-600	4.2	3
529	Machine learning reveals that structural features distinguishing promiscuous and non-promiscuous compounds depend on target combinations. *Scientific Reports*, **2021**, 11, 7863	4.9	6

528	Data set of competitive and allosteric protein kinase inhibitors confirmed by X-ray crystallography. *Data in Brief*, **2021**, 35, 106816	1.2	1
527	Rationality over fashion and hype in drug design. *F1000Research*, **2021**, 10,	3.6	7
526	Fine-tuning of a generative neural network for designing multi-target compounds. *Journal of Computer-Aided Molecular Design*, **2021**, 1	4.2	2
525	Structured data sets of compounds with multi-target and corresponding single-target activity from biological assays. *Future Science OA*, **2021**, 7, FSO685	2.7	1
524	Structural characteristics of compounds with multitarget activity. *Future Drug Discovery*, **2021**, 3, FDD60	2	2
523	Systematic assessment of structure-promiscuity relationships between different types of kinase inhibitors. *Bioorganic and Medicinal Chemistry*, **2021**, 41, 116226	3.4	1
522	Feature importance correlation from machine learning indicates functional relationships between proteins and similar compound binding characteristics. *Scientific Reports*, **2021**, 11, 14245	4.9	5
521	Prediction of Promiscuity Cliffs Using Machine Learning. *Molecular Informatics*, **2021**, 40, e2000196	3.8	5
520	Introducing the metacore concept for multi-target ligand design. *RSC Medicinal Chemistry*, **2021**, 12, 628-635	3.5	1
519	Predicting Isoform-Selective Carbonic Anhydrase Inhibitors via Machine Learning and Rationalizing Structural Features Important for Selectivity. *ACS Omega*, **2021**, 6, 4080-4089	3.9	4
518	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	4.2	2
517	Compound dataset and custom code for deep generative multi-target compound design. *Future Science OA*, **2021**, 7, FSO715	2.7	4
516	Development of curcumin-based amyloid β aggregation inhibitors for Alzheimer's disease using the SAR matrix approach. *Bioorganic and Medicinal Chemistry*, **2021**, 46, 116357	3.4	3
515	Chemistry-Centric Explanation of Machine Learning Models. *Artificial Intelligence in the Life Sciences* , **2021**, 1, 100009		0
514	R-group replacement database for medicinal chemistry. *Future Science OA*, **2021**, 7, FSO742	2.7	1
513	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	6.8	3
512	Structure- and Similarity-Based Survey of Allosteric Kinase Inhibitors, Activators, and Closely Related Compounds. *Journal of Medicinal Chemistry*, **2021**,	8.3	6
511	Explainable Machine Learning for Property Predictions in Compound Optimization.. *Journal of Medicinal Chemistry*, **2021**, 64, 17744-17752	8.3	2

510	Systematic Data Analysis and Diagnostic Machine Learning Reveal Differences between Compounds with Single- and Multitarget Activity. *Molecular Pharmaceutics*, **2020**, 17, 4652-4666	5.6	11
509	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	4.2	60
508	Increasing the public activity cliff knowledge base with new categories of activity cliffs. *Future Science OA*, **2020**, 6, FSO472	2.7	2
507	Advances in exploring activity cliffs. *Journal of Computer-Aided Molecular Design*, **2020**, 34, 929-942	4.2	5
506	Assessing the information content of structural and protein-ligand interaction representations for the classification of kinase inhibitor binding modes via machine learning and active learning. *Journal of Cheminformatics*, **2020**, 12, 36	8.6	8
505	Deep SAR matrix: SAR matrix expansion for advanced analog design using deep learning architectures. *Future Drug Discovery*, **2020**, 2, FDD36	2	7
504	Simplified activity cliff network representations with high interpretability and immediate access to SAR information. *Journal of Computer-Aided Molecular Design*, **2020**, 34, 943-952	4.2	1
503	Integrating computational lead optimization diagnostics with analog design and candidate selection. *Future Science OA*, **2020**, 6, FSO451	2.7	3
502	Mapping the S1 and S1' subsites of cysteine proteases with new dipeptidyl nitrile inhibitors as trypanocidal agents. *PLoS Neglected Tropical Diseases*, **2020**, 14, e0007755	4.8	8
501	Biological Activity Profiles of Multitarget Ligands from X-ray Structures. *Molecules*, **2020**, 25,	4.8	1
500	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,	6.3	6
499	Computational Method for Structure-Based Analysis of SAR Transfer. *Journal of Medicinal Chemistry*, **2020**, 63, 1388-1396	8.3	1
498	Computational method for the identification of third generation activity cliffs. *MethodsX*, **2020**, 7, 100793	1.9	3
497	Systematic Exploration of Activity Cliffs Containing Privileged Substructures. *Molecular Pharmaceutics*, **2020**, 17, 979-989	5.6	4
496	Current Trends, Overlooked Issues, and Unmet Challenges in Virtual Screening. *Journal of Chemical Information and Modeling*, **2020**, 60, 4112-4115	6.1	10
495	QSAR without borders. *Chemical Society Reviews*, **2020**, 49, 3525-3564	58.5	196
494	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	3.8	4
493	From SAR Diagnostics to Compound Design: Development Chronology of the Compound Optimization Monitor (COMO) Method. *Molecular Informatics*, **2020**, 39, e2000046	3.8	4

492	ccbmlib - a Python package for modeling Tanimoto similarity value distributions. *F1000Research*, **2020**, 9,	3.6	3
491	ccbmlib – a Python package for modeling Tanimoto similarity value distributions. *F1000Research*, **2020**, 9, 100	3.6	2
490	Introducing a new category of activity cliffs combining different compound similarity criteria. *RSC Medicinal Chemistry*, **2020**, 11, 132-141	3.5	5
489	Promiscuity analysis of a kinase panel screen with designated p38 alpha inhibitors. *European Journal of Medicinal Chemistry*, **2020**, 187, 112004	6.8	3
488	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	4.2	6
487	Exploring structure-promiscuity relationships using dual-site promiscuity cliffs and corresponding single-site analogs. *Bioorganic and Medicinal Chemistry*, **2020**, 28, 115238	3.4	2
486	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	6.8	4
485	Quantitative Comparison of Three-Dimensional Activity Landscapes of Compound Data Sets Based upon Topological Features. *ACS Omega*, **2020**, 5, 24111-24117	3.9	1
484	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	4.2	4
483	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	1.2	
482	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	2.9	2
481	Identifying representative kinases for inhibitor evaluation via systematic analysis of compound-based target relationships. *European Journal of Medicinal Chemistry*, **2020**, 204, 112641	6.8	1
480	From Qualitative to Quantitative Analysis of Activity and Property Landscapes. *Journal of Chemical Information and Modeling*, **2020**, 60, 5873-5880	6.1	5
479	Memory-assisted reinforcement learning for diverse molecular de novo design. *Journal of Cheminformatics*, **2020**, 12, 68	8.6	20
478	Global Assessment of Substituents on the Basis of Analogue Series. *Journal of Medicinal Chemistry*, **2020**, 63, 15013-15020	8.3	3
477	Activity landscape image analysis using convolutional neural networks. *Journal of Cheminformatics*, **2020**, 12, 34	8.6	5
476	Kinase inhibitor data set for systematic analysis of representative kinases across the human kinome. *Data in Brief*, **2020**, 32, 106189	1.2	1
475	Computational Method for Quantitative Comparison of Activity Landscapes on the Basis of Image Data. *Molecules*, **2020**, 25,	4.8	1

474	Compounds with multitarget activity: structure-based analysis and machine learning. *Future Drug Discovery*, **2020**, 2, FDD44	2	6
473	Prediction of an MMP-1 inhibitor activity cliff using the SAR matrix approach and its experimental validation. *Scientific Reports*, **2020**, 10, 14710	4.9	4
472	Analysis of Biological Screening Compounds with Single- or Multi-Target Activity via Diagnostic Machine Learning. *Biomolecules*, **2020**, 10,	5.9	8
471	Interpretation of Compound Activity Predictions from Complex Machine Learning Models Using Local Approximations and Shapley Values. *Journal of Medicinal Chemistry*, **2020**, 63, 8761-8777	8.3	48
470	Machine Learning Models for Accurate Prediction of Kinase Inhibitors with Different Binding Modes. *Journal of Medicinal Chemistry*, **2020**, 63, 8738-8748	8.3	20
469	A general approach for retrosynthetic molecular core analysis. *Journal of Cheminformatics*, **2019**, 11, 61	8.6	6
468	Method for Systematic Analogue Search Using the Mega SAR Matrix Database. *Journal of Chemical Information and Modeling*, **2019**, 59, 3727-3734	6.1	5
467	Evolving Concept of Activity Cliffs. *ACS Omega*, **2019**, 4, 14360-14368	3.9	30
466	Large-Scale Comparison of Alternative Similarity Search Strategies with Varying Chemical Information Contents. *ACS Omega*, **2019**, 4, 15304-15311	3.9	2
465	Computational chemical biology on the rise. *Future Medicinal Chemistry*, **2019**, 11, 1-3	4.1	5
464	Promiscuous Ligands from Experimentally Determined Structures, Binding Conformations, and Protein Family-Dependent Interaction Hotspots. *ACS Omega*, **2019**, 4, 1729-1737	3.9	13
463	Systematic identification of target set-dependent activity cliffs. *Future Science OA*, **2019**, 5, FSO363	2.7	5
462	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	6.1	1
461	Integrating the Structure–Activity Relationship Matrix Method with Molecular Grid Maps and Activity Landscape Models for Medicinal Chemistry Applications. *ACS Omega*, **2019**, 4, 7061-7069	3.9	13
460	Prediction of Different Classes of Promiscuous and Nonpromiscuous Compounds Using Machine Learning and Nearest Neighbor Analysis. *ACS Omega*, **2019**, 4, 6883-6890	3.9	14
459	Systematic computational identification of promiscuity cliff pathways formed by inhibitors of the human kinome. *Journal of Computer-Aided Molecular Design*, **2019**, 33, 559-572	4.2	8
458	Recent Progress in Structure-Based Evaluation of Compound Promiscuity. *ACS Omega*, **2019**, 4, 2758-2765	3.9	12
457	Combining structural and bioactivity-based fingerprints improves prediction performance and scaffold hopping capability. *Journal of Cheminformatics*, **2019**, 11, 54	8.6	17

456	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	2.7	3
455	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	4.2	4
454	Forward-looking perspective on publishing in drug discovery. *Future Drug Discovery*, **2019**, 1, FDD2	2	2
453	Can Cysteine Protease Cross-Class Inhibitors Achieve Selectivity?. *Journal of Medicinal Chemistry*, **2019**, 62, 10497-10525	8.3	31
452	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	3.4	10
451	Second-generation activity cliffs identified on the basis of target set-dependent potency difference criteria. *Future Medicinal Chemistry*, **2019**, 11, 379-394	4.1	7
450	Identification of Compounds That Interfere with High-Throughput Screening Assay Technologies. *ChemMedChem*, **2019**, 14, 1795-1802	3.7	15
449	[Special Issue for Honor Award dedicating to Prof Kimito Funatsu]Exploring Polypharmacology and Molecular Promiscuity. *Journal of Computer Aided Chemistry*, **2019**, 20, 43-46	0.2	
448	Multitask Machine Learning for Classifying Highly and Weakly Potent Kinase Inhibitors. *ACS Omega*, **2019**, 4, 4367-4375	3.9	23
447	Compound optimization monitor (COMO) method for computational evaluation of progress in medicinal chemistry projects. *Future Drug Discovery*, **2019**, 1, FDD15	2	4
446	Identifying Promiscuous Compounds with Activity against Different Target Classes. *Molecules*, **2019**, 24,	4.8	10
445	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	6.1	6
444	Virtual Screening with Generative Topographic Maps: How Many Maps Are Required?. *Journal of Chemical Information and Modeling*, **2019**, 59, 564-572	6.1	13
443	Systematic Extraction of Analogue Series from Large Compound Collections Using a New Computational Compound-Core Relationship Method. *ACS Omega*, **2019**, 4, 1027-1032	3.9	36
442	Cathepsin B: Active site mapping with peptidic substrates and inhibitors. *Bioorganic and Medicinal Chemistry*, **2019**, 27, 1-15	3.4	29
441	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	6.1	9
440	Identification of 4-aryl-1H-pyrrole[2,3-b]pyridine derivatives for the development of new B-Raf inhibitors. *Chemical Biology and Drug Design*, **2018**, 92, 1382-1386	2.9	1
439	Combining Similarity Searching and Network Analysis for the Identification of Active Compounds. *ACS Omega*, **2018**, 3, 3768-3777	3.9	5

438	Evaluation of Kinase Inhibitor Selectivity Using Cell-based Profiling Data. *Molecular Informatics*, **2018**, 37, e1800024	3.8	2
437	Exploring Selectivity of Multikinase Inhibitors across the Human Kinome. *ACS Omega*, **2018**, 3, 1147-1153	3.9	13
436	Computational method for estimating progression saturation of analog series.. *RSC Advances*, **2018**, 8, 5484-5492	3.7	10
435	Design of a tripartite network for the prediction of drug targets. *Journal of Computer-Aided Molecular Design*, **2018**, 32, 321-330	4.2	6
434	Design of an Activity-Based Probe for Human Neutrophil Elastase: Implementation of the Lossen Rearrangement To Induce Förster Resonance Energy Transfers. *Biochemistry*, **2018**, 57, 742-752	3.2	20
433	Application of Generative Autoencoder in De Novo Molecular Design. *Molecular Informatics*, **2018**, 37, 1700123	3.8	174
432	X-ray Structures of Target-Ligand Complexes Containing Compounds with Assay Interference Potential. *Journal of Medicinal Chemistry*, **2018**, 61, 1276-1284	8.3	18
431	Series of screening compounds with high hit rates for the exploration of multi-target activities and assay interference. *Future Science OA*, **2018**, 4, FSO279	2.7	1
430	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	3.9	16
429	Extracting Compound Profiling Matrices from Screening Data. *ACS Omega*, **2018**, 3, 4706-4712	3.9	8
428	Prediction of Compound Profiling Matrices Using Machine Learning. *ACS Omega*, **2018**, 3, 4713-4723	3.9	23
427	Reconciling Selectivity Trends from a Comprehensive Kinase Inhibitor Profiling Campaign with Known Activity Data. *ACS Omega*, **2018**, 3, 3113-3119	3.9	12
426	Redundancy in two major compound databases. *Drug Discovery Today*, **2018**, 23, 1183-1186	8.8	5
425	Rationalizing Promiscuity Cliffs. *ChemMedChem*, **2018**, 13, 490-494	3.7	12
424	Improving the utility of molecular scaffolds for medicinal and computational chemistry. *Future Medicinal Chemistry*, **2018**, 10, 1645-1648	4.1	6
423	A Hybrid Virtual Screening Protocol Based on Binding Mode Similarity. *Methods in Molecular Biology* , **2018**, 1824, 165-175	1.4	2
422	Rationalizing the Formation of Activity Cliffs in Different Compound Data Sets. *ACS Omega*, **2018**, 3, 7736-7744	3.9	13
421	Computational design of new molecular scaffolds for medicinal chemistry, part II: generalization of analog series-based scaffolds. *Future Science OA*, **2018**, 4, FSO267	2.7	8

420	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	8.3	19
419	Computational Analysis of Kinase Inhibitors Identifies Promiscuity Cliffs across the Human Kinome. *ACS Omega*, **2018**, 3, 17295-17308	3.9	16
418	Computational Assessment of Chemical Saturation of Analogue Series under Varying Conditions. *ACS Omega*, **2018**, 3, 15799-15808	3.9	7
417	Computational Method to Evaluate Progress in Lead Optimization. *Journal of Medicinal Chemistry*, **2018**, 61, 10895-10900	8.3	11
416	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	3.9	12
415	Data-Driven Exploration of Selectivity and Off-Target Activities of Designated Chemical Probes. *Molecules*, **2018**, 23,	4.8	7
414	SAR Matrix Method for Large-Scale Analysis of Compound Structure-Activity Relationships and Exploration of Multitarget Activity Spaces. *Methods in Molecular Biology*, **2018**, 1825, 339-352	1.4	2
413	Mapping Biological Activities to Different Types of Molecular Scaffolds: Exemplary Application to Protein Kinase Inhibitors. *Methods in Molecular Biology*, **2018**, 1825, 327-337	1.4	1
412	Collection of analog series-based scaffolds from public compound sources. *Future Science OA*, **2018**, 4, FSO287	2.7	5
411	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	4.2	2
410	Identification and analysis of promiscuity cliffs formed by bioactive compounds and experimental implications. *RSC Advances*, **2017**, 7, 58-66	3.7	15
409	Structure-Promiscuity Relationship Puzzles-Extensively Assayed Analogs with Large Differences in Target Annotations. *AAPS Journal*, **2017**, 19, 856-864	3.7	13
408	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	6.1	18
407	Systematic analysis of structural and activity relationships between conventional hierarchical and analog series-based scaffolds. *RSC Advances*, **2017**, 7, 18718-18723	3.7	3
406	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	8.3	79
405	Application of a New Scaffold Concept for Computational Target Deconvolution of Chemical Cancer Cell Line Screens. *ACS Omega*, **2017**, 2, 1463-1468	3.9	12
404	Privileged Structural Motif Detection and Analysis Using Generative Topographic Maps. *Journal of Chemical Information and Modeling*, **2017**, 57, 1218-1232	6.1	6
403	Compound Data Mining for Drug Discovery. *Methods in Molecular Biology*, **2017**, 1526, 247-256	1.4	8

402	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	4.2	2
401	Algorithmic Chemoinformatics **2017**, 393-448		
400	Design of Diverse and Focused Compound Libraries **2017**, 83-101		2
399	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	3.9	4
398	Identifying relationships between unrelated pharmaceutical target proteins on the basis of shared active compounds. *Future Science OA*, **2017**, 3, FSO212	2.7	3
397	A Fluorescent-Labeled Phosphono Bisbenzguanidine As an Activity-Based Probe for Matriptase. *Chemistry - A European Journal*, **2017**, 23, 5205-5209	4.8	11
396	Entering the 'big data' era in medicinal chemistry: molecular promiscuity analysis revisited. *Future Science OA*, **2017**, 3, FSO179	2.7	39
395	Molecular Similarity Concepts for Informatics Applications. *Methods in Molecular Biology*, **2017**, 1526, 231-245	1.4	21
394	Tracing compound pathways using chemical space networks. *MedChemComm*, **2017**, 8, 376-384	5	4
393	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	2.9	14
392	Modeling Tanimoto Similarity Value Distributions and Predicting Search Results. *Molecular Informatics*, **2017**, 36, 1600131	3.8	9
391	Recent Advances in Scaffold Hopping. *Journal of Medicinal Chemistry*, **2017**, 60, 1238-1246	8.3	131
390	Dark chemical matter in public screening assays and derivation of target hypotheses. *MedChemComm*, **2017**, 8, 2100-2104	5	4
389	Support Vector Machine Classification and Regression Prioritize Different Structural Features for Binary Compound Activity and Potency Value Prediction. *ACS Omega*, **2017**, 2, 6371-6379	3.9	36
388	From bird's eye views to molecular communities: two-layered visualization of structure-activity relationships in large compound data sets. *Journal of Computer-Aided Molecular Design*, **2017**, 31, 961-977	4.2	4
387	Exploring differential evolution for inverse QSAR analysis. *F1000Research*, **2017**, 6,	3.6	4
386	Promiscuity of inhibitors of human protein kinases at varying data confidence levels and test frequencies. *RSC Advances*, **2017**, 7, 41265-41271	3.7	20
385	Activity profiles of analog series containing pan assay interference compounds. *RSC Advances*, **2017**, 7, 35638-35647	3.7	20

384	From activity cliffs to promiscuity cliffs. *Future Science OA*, **2017**, 3, FSO227	2.7	3
383	Exploring Structural Relationships between Bioactive and Commercial Chemical Space and Developing Target Hypotheses for Compound Acquisition. *ACS Omega*, **2017**, 2, 7760-7766	3.9	2
382	Heat shock protein 90 and serine/threonine kinase B-Raf inhibitors have overlapping chemical space. *RSC Advances*, **2017**, 7, 31069-31074	3.7	12
381	Representation and identification of activity cliffs. *Expert Opinion on Drug Discovery*, **2017**, 12, 879-883	6.2	31
380	Characterization of P2X4 receptor agonists and antagonists by calcium influx and radioligand binding studies. *Biochemical Pharmacology*, **2017**, 125, 41-54	6	34
379	Charting Biologically Relevant Spirocyclic Compound Space. *Chemistry - A European Journal*, **2017**, 23, 703-710	4.8	75
378	Isonicotinohydrazones as inhibitors of alkaline phosphatase and ecto-5'-nucleotidase. *Chemical Biology and Drug Design*, **2017**, 89, 365-370	2.9	19
377	Virtual Screening for Dual Hsp90/B-Raf Inhibitors. *Methods in Pharmacology and Toxicology*, **2017**, 355-365	1.1	
376	Assessing Scaffold Diversity of Kinase Inhibitors Using Alternative Scaffold Concepts and Estimating the Scaffold Hopping Potential for Different Kinases. *Molecules*, **2017**, 22,	4.8	9
375	Exploring differential evolution for inverse QSAR analysis. *F1000Research*, **2017**, 6, 1285	3.6	7
374	Towards a systematic assessment of assay interference: Identification of extensively tested compounds with high assay promiscuity. *F1000Research*, **2017**, 6,	3.6	4
373	Towards a systematic assessment of assay interference: Identification of extensively tested compounds with high assay promiscuity. *F1000Research*, **2017**, 6, 1505	3.6	4
372	Exploring sets of molecules from patents and relationships to other active compounds in chemical space networks. *Journal of Computer-Aided Molecular Design*, **2017**, 31, 779-788	4.2	4
371	Prediction of Activity Cliffs Using Condensed Graphs of Reaction Representations, Descriptor Recombination, Support Vector Machine Classification, and Support Vector Regression. *Journal of Chemical Information and Modeling*, **2016**, 56, 1631-40	6.1	18
370	Exploring Molecular Promiscuity from a Ligand and Target Perspective. *ACS Symposium Series*, **2016** , 19-34	0.4	1
369	Predicting bioactive conformations and binding modes of macrocycles. *Journal of Computer-Aided Molecular Design*, **2016**, 30, 841-849	4.2	12
368	Evaluation of bisbenzamidines as inhibitors for matriptase-2. *Bioorganic and Medicinal Chemistry Letters*, **2016**, 26, 3741-5	2.9	6
367	Hierarchical Analysis of Bioactive Matched Molecular Pairs, Encoded Chemical Transformations, and Associated Substructures. *Molecular Informatics*, **2016**, 35, 483-488	3.8	4

366	Maximum common substructure-based Tversky index: an asymmetric hybrid similarity measure. *Journal of Computer-Aided Molecular Design*, **2016**, 30, 523-31	4.2	8
365	Analog series-based scaffolds: computational design and exploration of a new type of molecular scaffolds for medicinal chemistry. *Future Science OA*, **2016**, 2, FSO149	2.7	24
364	Highly Promiscuous Small Molecules from Biological Screening Assays Include Many Pan-Assay Interference Compounds but Also Candidates for Polypharmacology. *Journal of Medicinal Chemistry* , **2016**, 59, 10285-10290	8.3	33
363	Limiting the Number of Potential Binding Modes by Introducing Symmetry into Ligands: Structure-Based Design of Inhibitors for Trypsin-Like Serine Proteases. *Chemistry - A European Journal*, **2016**, 22, 610-25	4.8	7
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