Jrgen Bajorath

List of Publications by Citations

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	Docking and scoring in virtual screening for drug discovery: methods and applications. *Nature Reviews Drug Discovery*, **2004**, 3, 935-49	64.1	2083
544	Integration of virtual and high-throughput screening. *Nature Reviews Drug Discovery*, **2002**, 1, 882-94	64.1	615
543	Polypharmacology: challenges and opportunities in drug discovery. *Journal of Medicinal Chemistry*, **2014**, 57, 7874-87	8.3	571
542	Molecular similarity analysis in virtual screening: foundations, limitations and novel approaches. *Drug Discovery Today*, **2007**, 12, 225-33	8.8	362
541	Molecular similarity in medicinal chemistry. *Journal of Medicinal Chemistry*, **2014**, 57, 3186-204	8.3	326
540	Current trends in ligand-based virtual screening: molecular representations, data mining methods, new application areas, and performance evaluation. *Journal of Chemical Information and Modeling*, **2010**, 50, 205-16	6.1	269
539	Exploring activity cliffs in medicinal chemistry. *Journal of Medicinal Chemistry*, **2012**, 55, 2932-42	8.3	242
538	QSAR without borders. *Chemical Society Reviews*, **2020**, 49, 3525-3564	58.5	196
537	Quo vadis, virtual screening? A comprehensive survey of prospective applications. *Journal of Medicinal Chemistry*, **2010**, 53, 8461-7	8.3	186
536	Selected concepts and investigations in compound classification, molecular descriptor analysis, and virtual screening. *Journal of Chemical Information and Computer Sciences*, **2001**, 41, 233-45		184
535	Application of Generative Autoencoder in De Novo Molecular Design. *Molecular Informatics*, **2018**, 37, 1700123	3.8	174
534	State-of-the-art in ligand-based virtual screening. *Drug Discovery Today*, **2011**, 16, 372-6	8.8	160
533	MMP-Cliffs: systematic identification of activity cliffs on the basis of matched molecular pairs. *Journal of Chemical Information and Modeling*, **2012**, 52, 1138-45	6.1	157
532	SAR index: quantifying the nature of structure-activity relationships. *Journal of Medicinal Chemistry*, **2007**, 50, 5571-8	8.3	151
531	Activity landscape representations for structure-activity relationship analysis. *Journal of Medicinal Chemistry*, **2010**, 53, 8209-23	8.3	148
530	Navigating structure-activity landscapes. *Drug Discovery Today*, **2009**, 14, 698-705	8.8	145
529	Recent progress in understanding activity cliffs and their utility in medicinal chemistry. *Journal of Medicinal Chemistry*, **2014**, 57, 18-28	8.3	138

528	Recent Advances in Scaffold Hopping. *Journal of Medicinal Chemistry*, **2017**, 60, 1238-1246	8.3	131
527	Structure-activity relationship anatomy by network-like similarity graphs and local structure-activity relationship indices. *Journal of Medicinal Chemistry*, **2008**, 51, 6075-84	8.3	129
526	New methodologies for ligand-based virtual screening. *Current Pharmaceutical Design*, **2005**, 11, 1189-202	3.3	118
525	Compound promiscuity: what can we learn from current data?. *Drug Discovery Today*, **2013**, 18, 644-50	8.8	115
524	Combinatorial preferences affect molecular similarity/diversity calculations using binary fingerprints and Tanimoto coefficients. *Journal of Chemical Information and Computer Sciences*, **2000**, 40, 163-6		108
523	Similarity searching. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2011**, 1, 260-282	7.9	91
522	Virtual screening methods that complement HTS. *Combinatorial Chemistry and High Throughput Screening*, **2004**, 7, 259-69	1.3	86
521	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
520	Scaffold hopping using two-dimensional fingerprints: true potential, black magic, or a hopeless endeavor? Guidelines for virtual screening. *Journal of Medicinal Chemistry*, **2010**, 53, 5707-15	8.3	78
519	Computational Exploration of Molecular Scaffolds in Medicinal Chemistry. *Journal of Medicinal Chemistry*, **2016**, 59, 4062-76	8.3	75
518	Charting Biologically Relevant Spirocyclic Compound Space. *Chemistry - A European Journal*, **2017**, 23, 703-710	4.8	75
517	Computational analysis of ligand relationships within target families. *Current Opinion in Chemical Biology*, **2008**, 12, 352-8	9.7	75
516	Lessons learned from molecular scaffold analysis. *Journal of Chemical Information and Modeling*, **2011**, 51, 1742-53	6.1	73
515	Rationalizing three-dimensional activity landscapes and the influence of molecular representations on landscape topology and the formation of activity cliffs. *Journal of Chemical Information and Modeling*, **2010**, 50, 1021-33	6.1	72
514	Development of potent and selective inhibitors of ecto-5'-nucleotidase based on an anthraquinone scaffold. *Journal of Medicinal Chemistry*, **2010**, 53, 2076-86	8.3	72
513	SARANEA: a freely available program to mine structure-activity and structure-selectivity relationship information in compound data sets. *Journal of Chemical Information and Modeling*, **2010**, 50, 68-78	6.1	70
512	Local structural changes, global data views: graphical substructure-activity relationship trailing. *Journal of Medicinal Chemistry*, **2011**, 54, 2944-51	8.3	70
511	Design and evaluation of a molecular fingerprint involving the transformation of property descriptor values into a binary classification scheme. *Journal of Chemical Information and Computer Sciences*, **2003**, 43, 1151-7		69

510	The future of virtual compound screening. *Chemical Biology and Drug Design*, **2013**, 81, 33-40	2.9	63
509	Identification of the first low-molecular-weight inhibitors of matriptase-2. *Journal of Medicinal Chemistry*, **2010**, 53, 5523-35	8.3	63
508	Support vector machines for drug discovery. *Expert Opinion on Drug Discovery*, **2014**, 9, 93-104	6.2	61
507	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
506	Data structures and computational tools for the extraction of SAR information from large compound sets. *Drug Discovery Today*, **2010**, 15, 630-9	8.8	60
505	Profile scaling increases the similarity search performance of molecular fingerprints containing numerical descriptors and structural keys. *Journal of Chemical Information and Computer Sciences*, **2003**, 43, 1218-25		60
504	Database searching for compounds with similar biological activity using short binary bit string representations of molecules. *Journal of Chemical Information and Computer Sciences*, **1999**, 39, 881-6		60
503	Large-scale similarity search profiling of ChEMBL compound data sets. *Journal of Chemical Information and Modeling*, **2011**, 51, 1831-9	6.1	59
502	Support-vector-machine-based ranking significantly improves the effectiveness of similarity searching using 2D fingerprints and multiple reference compounds. *Journal of Chemical Information and Modeling*, **2008**, 48, 742-6	6.1	57
501	Advancing the activity cliff concept. *F1000Research*, **2013**, 2, 199	3.6	55
500	Chemical substitutions that introduce activity cliffs across different compound classes and biological targets. *Journal of Chemical Information and Modeling*, **2010**, 50, 1248-56	6.1	55
499	Similarity-potency trees: a method to search for SAR information in compound data sets and derive SAR rules. *Journal of Chemical Information and Modeling*, **2010**, 50, 1395-409	6.1	55
498	Ligand prediction for orphan targets using support vector machines and various target-ligand kernels is dominated by nearest neighbor effects. *Journal of Chemical Information and Modeling*, **2009**, 49, 2155-67	6.1	55
497	Molecular similarity analysis uncovers heterogeneous structure-activity relationships and variable activity landscapes. *Chemistry and Biology*, **2007**, 14, 489-97		54
496	Fingerprint scaling increases the probability of identifying molecules with similar activity in virtual screening calculations. *Journal of Chemical Information and Computer Sciences*, **2001**, 41, 746-53		53
495	Integrating structure- and ligand-based virtual screening: comparison of individual, parallel, and fused molecular docking and similarity search calculations on multiple targets. *ChemMedChem*, **2008**, 3, 1566-71	3.7	52
494	Searching for target-selective compounds using different combinations of multiclass support vector machine ranking methods, kernel functions, and fingerprint descriptors. *Journal of Chemical Information and Modeling*, **2009**, 49, 582-92	6.1	51
493	Current compound coverage of the kinome. *Journal of Medicinal Chemistry*, **2015**, 58, 30-40	8.3	50

492	Polypharmacology directed compound data mining: identification of promiscuous chemotypes with different activity profiles and comparison to approved drugs. *Journal of Chemical Information and Modeling*, **2010**, 50, 2112-8	6.1	50
491	Ligand prediction from protein sequence and small molecule information using support vector machines and fingerprint descriptors. *Journal of Chemical Information and Modeling*, **2009**, 49, 767-79	6.1	50
490	Matched molecular pairs derived by retrosynthetic fragmentation. *MedChemComm*, **2014**, 5, 64-67	5	49
489	Evaluation of descriptors and mini-fingerprints for the identification of molecules with similar activity. *Journal of Chemical Information and Computer Sciences*, **2000**, 40, 1227-34		48
488	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
487	Synthesis, biological evaluation and molecular docking of N-phenyl thiosemicarbazones as urease inhibitors. *Bioorganic Chemistry*, **2015**, 61, 51-7	5.1	47
486	From structure-activity to structure-selectivity relationships: quantitative assessment, selectivity cliffs, and key compounds. *ChemMedChem*, **2009**, 4, 1864-73	3.7	47
485	Differential Shannon Entropy as a sensitive measure of differences in database variability of molecular descriptors. *Journal of Chemical Information and Computer Sciences*, **2001**, 41, 1060-6		47
484	Active compounds from a diverse library of triazolothiadiazole and triazolothiadiazine scaffolds: synthesis, crystal structure determination, cytotoxicity, cholinesterase inhibitory activity, and binding mode analysis. *Bioorganic and Medicinal Chemistry*, **2014**, 22, 6163-73	3.4	46
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482	Extending the activity cliff concept: structural categorization of activity cliffs and systematic identification of different types of cliffs in the ChEMBL database. *Journal of Chemical Information and Modeling*, **2012**, 52, 1806-11	6.1	44
481	Design of multitarget activity landscapes that capture hierarchical activity cliff distributions. *Journal of Chemical Information and Modeling*, **2011**, 51, 258-66	6.1	44
480	Chemical space networks: a powerful new paradigm for the description of chemical space. *Journal of Computer-Aided Molecular Design*, **2014**, 28, 795-802	4.2	43
479	BindingDB and ChEMBL: online compound databases for drug discovery. *Expert Opinion on Drug Discovery*, **2011**, 6, 683-7	6.2	43
478	Molecular scaffolds with high propensity to form multi-target activity cliffs. *Journal of Chemical Information and Modeling*, **2010**, 50, 500-10	6.1	42
477	Systematic computational analysis of structure-activity relationships: concepts, challenges and recent advances. *Future Medicinal Chemistry*, **2009**, 1, 451-66	4.1	42
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475	Computational Method for the Systematic Identification of Analog Series and Key Compounds Representing Series and Their Biological Activity Profiles. *Journal of Medicinal Chemistry*, **2016**, 59, 7667-76	8.3	42

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473	Matched molecular pair analysis of small molecule microarray data identifies promiscuity cliffs and reveals molecular origins of extreme compound promiscuity. *Journal of Medicinal Chemistry*, **2012**, 55, 10220-8	8.3	41
472	Systematic analysis of public domain compound potency data identifies selective molecular scaffolds across druggable target families. *Journal of Medicinal Chemistry*, **2010**, 53, 752-8	8.3	41
471	Emerging chemical patterns: a new methodology for molecular classification and compound selection. *Journal of Chemical Information and Modeling*, **2006**, 46, 2502-14	6.1	41
470	From activity cliffs to activity ridges: informative data structures for SAR analysis. *Journal of Chemical Information and Modeling*, **2011**, 51, 1848-56	6.1	40
469	Entering the 'big data' era in medicinal chemistry: molecular promiscuity analysis revisited. *Future Science OA*, **2017**, 3, FSO179	2.7	39
468	Exploring compound promiscuity patterns and multi-target activity spaces. *Computational and Structural Biotechnology Journal*, **2014**, 9, e201401003	6.8	39
467	Prediction of activity cliffs using support vector machines. *Journal of Chemical Information and Modeling*, **2012**, 52, 2354-65	6.1	39
466	Virtual compound screening in drug discovery. *Future Medicinal Chemistry*, **2012**, 4, 593-602	4.1	39
465	Comparison of 2D fingerprint methods for multiple-template similarity searching on compound activity classes of increasing structural diversity. *ChemMedChem*, **2007**, 2, 208-17	3.7	39
464	Coumarin-thiazole and -oxadiazole derivatives: Synthesis, bioactivity and docking studies for aldose/aldehyde reductase inhibitors. *Bioorganic Chemistry*, **2016**, 68, 177-86	5.1	39
463	A coumarin-labeled vinyl sulfone as tripeptidomimetic activity-based probe for cysteine cathepsins. *ChemBioChem*, **2014**, 15, 955-9	3.8	37
462	Virtual screening identifies novel sulfonamide inhibitors of ecto-5'-nucleotidase. *Journal of Medicinal Chemistry*, **2012**, 55, 6576-81	8.3	37
461	Determining the Degree of Promiscuity of Extensively Assayed Compounds. *PLoS ONE*, **2016**, 11, e0153873	3.7	37
460	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
459	Chemoinformatics: a view of the field and current trends in method development. *Bioorganic and Medicinal Chemistry*, **2012**, 20, 5317-23	3.4	36
458	Large-scale exploration of bioisosteric replacements on the basis of matched molecular pairs. *Future Medicinal Chemistry*, **2011**, 3, 425-36	4.1	36
457	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

456	Analysis of structure-based virtual screening studies and characterization of identified active compounds. *Future Medicinal Chemistry*, **2012**, 4, 603-13	4.1	35
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454	Characterization of P2X4 receptor agonists and antagonists by calcium influx and radioligand binding studies. *Biochemical Pharmacology*, **2017**, 125, 41-54	6	34
453	Improving the search performance of extended connectivity fingerprints through activity-oriented feature filtering and application of a bit-density-dependent similarity function. *ChemMedChem*, **2009**, 4, 540-8	3.7	34
452	Molecular similarity analysis and virtual screening by mapping of consensus positions in binary-transformed chemical descriptor spaces with variable dimensionality. *Journal of Chemical Information and Computer Sciences*, **2004**, 44, 21-9		34
451	Recursive median partitioning for virtual screening of large databases. *Journal of Chemical Information and Computer Sciences*, **2003**, 43, 182-8		34
450	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
449	What is the likelihood of an active compound to be promiscuous? Systematic assessment of compound promiscuity on the basis of PubChem confirmatory bioassay data. *AAPS Journal*, **2013**, 15, 808-15	3.7	33
448	Computer-aided drug discovery. *F1000Research*, **2015**, 4,	3.6	33
447	Growth of ligand-target interaction data in ChEMBL is associated with increasing and activity measurement-dependent compound promiscuity. *Journal of Chemical Information and Modeling*, **2012**, 52, 2550-8	6.1	33
446	Similarity searching using fingerprints of molecular fragments involved in protein-ligand interactions. *Journal of Chemical Information and Modeling*, **2008**, 48, 2308-12	6.1	33
445	Design and evaluation of a novel class-directed 2D fingerprint to search for structurally diverse active compounds. *Journal of Chemical Information and Modeling*, **2006**, 46, 2515-26	6.1	33
444	Accurate partitioning of compounds belonging to diverse activity classes. *Journal of Chemical Information and Computer Sciences*, **2002**, 42, 757-64		33
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438	Representation and identification of activity cliffs. *Expert Opinion on Drug Discovery*, **2017**, 12, 879-883	6.2	31
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436	Targeting multifunctional proteins by virtual screening: structurally diverse cytohesin inhibitors with differentiated biological functions. *ACS Chemical Biology*, **2010**, 5, 839-49	4.9	31
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432	Assessment of molecular similarity from the analysis of randomly generated structural fragment populations. *Journal of Chemical Information and Modeling*, **2006**, 46, 1937-44	6.1	30
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429	Molecular fingerprint recombination: generating hybrid fingerprints for similarity searching from different fingerprint types. *ChemMedChem*, **2009**, 4, 1859-63	3.7	29
428	Ligand-target interaction-based weighting of substructures for virtual screening. *Journal of Chemical Information and Modeling*, **2008**, 48, 1955-64	6.1	29
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425	Cathepsin B: Active site mapping with peptidic substrates and inhibitors. *Bioorganic and Medicinal Chemistry*, **2019**, 27, 1-15	3.4	29
424	Three-Dimensional Similarity in Molecular Docking: Prioritizing Ligand Poses on the Basis of Experimental Binding Modes. *Journal of Chemical Information and Modeling*, **2016**, 56, 580-7	6.1	28
423	A homogeneous fluorescence resonance energy transfer system for monitoring the activation of a protein switch in real time. *Journal of the American Chemical Society*, **2011**, 133, 8372-9	16.4	28
422	Exploration of structure-activity relationship determinants in analogue series. *Journal of Medicinal Chemistry*, **2009**, 52, 3212-24	8.3	28
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418	Novel structural hybrids of pyrazolobenzothiazines with benzimidazoles as cholinesterase inhibitors. *European Journal of Medicinal Chemistry*, **2014**, 78, 106-17	6.8	27
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415	Inhibition of human leukocyte elastase by brunsvicamides a-C: cyanobacterial cyclic peptides. *ChemMedChem*, **2009**, 4, 1425-9	3.7	27
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413	Chemical database mining through entropy-based molecular similarity assessment of randomly generated structural fragment populations. *Journal of Chemical Information and Modeling*, **2007**, 47, 59-68	6.1	27
412	Activity-relevant similarity values for fingerprints and implications for similarity searching. *F1000Research*, **2016**, 5,	3.6	27
411	Design and characterization of chemical space networks for different compound data sets. *Journal of Computer-Aided Molecular Design*, **2015**, 29, 113-25	4.2	26
410	Systematic identification and classification of three-dimensional activity cliffs. *Journal of Chemical Information and Modeling*, **2012**, 52, 1490-8	6.1	26
409	Combining cluster analysis, feature selection and multiple support vector machine models for the identification of human ether-a-go-go related gene channel blocking compounds. *Chemical Biology and Drug Design*, **2009**, 73, 17-25	2.9	26
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407	Mapping algorithms for molecular similarity analysis and ligand-based virtual screening: design of DynaMAD and comparison with MAD and DMC. *Journal of Chemical Information and Modeling*, **2006**, 46, 1623-34	6.1	26
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404	Monitoring the Progression of Structure-Activity Relationship Information during Lead Optimization. *Journal of Medicinal Chemistry*, **2016**, 59, 4235-44	8.3	25
403	Computational polypharmacology analysis of the heat shock protein 90 interactome. *Journal of Chemical Information and Modeling*, **2015**, 55, 676-86	6.1	25

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396	A distance function for retrieval of active molecules from complex chemical space representations. *Journal of Chemical Information and Modeling*, **2006**, 46, 1094-7	6.1	24
395	Partitioning methods for the identification of active molecules. *Current Medicinal Chemistry*, **2003**, 10, 707-15	4.3	24
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392	Lessons learned from the design of chemical space networks and opportunities for new applications. *Journal of Computer-Aided Molecular Design*, **2016**, 30, 191-208	4.2	23
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384	Multitask Machine Learning for Classifying Highly and Weakly Potent Kinase Inhibitors. *ACS Omega*, **2019**, 4, 4367-4375	3.9	23
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378	Bayesian screening for active compounds in high-dimensional chemical spaces combining property descriptors and molecular fingerprints. *Chemical Biology and Drug Design*, **2008**, 71, 8-14	2.9	22
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373	Prediction of compounds with closely related activity profiles using weighted support vector machine linear combinations. *Journal of Chemical Information and Modeling*, **2013**, 53, 791-801	6.1	21
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370	Systematic artifacts in support vector regression-based compound potency prediction revealed by statistical and activity landscape analysis. *PLoS ONE*, **2015**, 10, e0119301	3.7	21
369	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
368	Promiscuity of inhibitors of human protein kinases at varying data confidence levels and test frequencies. *RSC Advances*, **2017**, 7, 41265-41271	3.7	20
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