

# Johannes Kirchmair

## List of Publications by Citations

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129  
papers

4,193  
citations

35  
h-index

61  
g-index

150  
ext. papers

4,826  
ext. citations

5  
avg, IF

5.72  
L-index

#	Paper	IF	Citations
129	Evaluation of the performance of 3D virtual screening protocols: RMSD comparisons, enrichment assessments, and decoy selection--what can we learn from earlier mistakes?. <i>Journal of Computer-Aided Molecular Design</i> , <b>2008</b> , 22, 213-28	4.2	278
128	Predicting drug metabolism: experiment and/or computation?. <i>Nature Reviews Drug Discovery</i> , <b>2015</b> , 14, 387-404	64.1	255
127	From in silico target prediction to multi-target drug design: current databases, methods and applications. <i>Journal of Proteomics</i> , <b>2011</b> , 74, 2554-74	3.9	214
126	Computational prediction of metabolism: sites, products, SAR, P450 enzyme dynamics, and mechanisms. <i>Journal of Chemical Information and Modeling</i> , <b>2012</b> , 52, 617-48	6.1	212
125	How to optimize shape-based virtual screening: choosing the right query and including chemical information. <i>Journal of Chemical Information and Modeling</i> , <b>2009</b> , 49, 678-92	6.1	164
124	Comparative performance assessment of the conformational model generators omega and catalyst: a large-scale survey on the retrieval of protein-bound ligand conformations. <i>Journal of Chemical Information and Modeling</i> , <b>2006</b> , 46, 1848-61	6.1	151
123	Comparative analysis of protein-bound ligand conformations with respect to catalyst's conformational space subsampling algorithms. <i>Journal of Chemical Information and Modeling</i> , <b>2005</b> , 45, 422-30	6.1	125
122	Influenza neuraminidase: a druggable target for natural products. <i>Natural Product Reports</i> , <b>2012</b> , 29, 11-36	15.1	116
121	CAESAR: a new conformer generation algorithm based on recursive buildup and local rotational symmetry consideration. <i>Journal of Chemical Information and Modeling</i> , <b>2007</b> , 47, 1923-32	6.1	105
120	Antiviral potential and molecular insight into neuraminidase inhibiting diarylheptanoids from <i>Alpinia katsumadai</i> . <i>Journal of Medicinal Chemistry</i> , <b>2010</b> , 53, 778-86	8.3	101
119	Data Resources for the Computer-Guided Discovery of Bioactive Natural Products. <i>Journal of Chemical Information and Modeling</i> , <b>2017</b> , 57, 2099-2111	6.1	99
118	The Protein Data Bank (PDB), its related services and software tools as key components for in silico guided drug discovery. <i>Journal of Medicinal Chemistry</i> , <b>2008</b> , 51, 7021-40	8.3	81
117	Quantifying the shifts in physicochemical property space introduced by the metabolism of small organic molecules. <i>Journal of Cheminformatics</i> , <b>2013</b> , 5,	8.6	78
116	Enhancing drug discovery through in silico screening: strategies to increase true positives retrieval rates. <i>Current Medicinal Chemistry</i> , <b>2008</b> , 15, 2040-53	4.3	72
115	Structure-based virtual screening for the discovery of natural inhibitors for human rhinovirus coat protein. <i>Journal of Medicinal Chemistry</i> , <b>2008</b> , 51, 842-51	8.3	70
114	The challenges involved in modeling toxicity data in silico: a review. <i>Current Pharmaceutical Design</i> , <b>2012</b> , 18, 1266-91	3.3	67
113	Fast and efficient in silico 3D screening: toward maximum computational efficiency of pharmacophore-based and shape-based approaches. <i>Journal of Chemical Information and Modeling</i> , <b>2007</b> , 47, 2182-96	6.1	64

112	Computational methods and tools to predict cytochrome P450 metabolism for drug discovery. <i>Chemical Biology and Drug Design</i> , <b>2019</b> , 93, 377-386	2.9	62
111	Discovery of novel PPAR ligands by a virtual screening approach based on pharmacophore modeling, 3D shape, and electrostatic similarity screening. <i>Journal of Medicinal Chemistry</i> , <b>2008</b> , 51, 6303-17	8.2	60
110	Pharmacophore modeling and parallel screening for PPAR ligands. <i>Journal of Computer-Aided Molecular Design</i> , <b>2007</b> , 21, 575-90	4.2	58
109	Identification of HIV-1 reverse transcriptase dual inhibitors by a combined shape-, 2D-fingerprint- and pharmacophore-based virtual screening approach. <i>European Journal of Medicinal Chemistry</i> , <b>2012</b> , 50, 216-29	6.8	55
108	Benchmarking Commercial Conformer Ensemble Generators. <i>Journal of Chemical Information and Modeling</i> , <b>2017</b> , 57, 2719-2728	6.1	51
107	Discovery of nonsteroidal 17beta-hydroxysteroid dehydrogenase 1 inhibitors by pharmacophore-based screening of virtual compound libraries. <i>Journal of Medicinal Chemistry</i> , <b>2008</b> , 51, 4188-99	8.3	51
106	Characterization of the Chemical Space of Known and Readily Obtainable Natural Products. <i>Journal of Chemical Information and Modeling</i> , <b>2018</b> , 58, 1518-1532	6.1	50
105	Novel pharmacological chaperones that correct phenylketonuria in mice. <i>Human Molecular Genetics</i> , <b>2012</b> , 21, 1877-87	5.6	50
104	Hit Dexter 2.0: Machine-Learning Models for the Prediction of Frequent Hitters. <i>Journal of Chemical Information and Modeling</i> , <b>2019</b> , 59, 1030-1043	6.1	50
103	One concept, three implementations of 3D pharmacophore-based virtual screening: distinct coverage of chemical search space. <i>Journal of Chemical Information and Modeling</i> , <b>2010</b> , 50, 1241-7	6.1	46
102	GLORY: Generator of the Structures of Likely Cytochrome P450 Metabolites Based on Predicted Sites of Metabolism. <i>Frontiers in Chemistry</i> , <b>2019</b> , 7, 402	5	43
101	Discovery of prenylated flavonoids with dual activity against influenza virus and <i>Streptococcus pneumoniae</i> . <i>Scientific Reports</i> , <b>2016</b> , 6, 27156	4.9	41
100	Fast MEtabolizer (FAME): A rapid and accurate predictor of sites of metabolism in multiple species by endogenous enzymes. <i>Journal of Chemical Information and Modeling</i> , <b>2013</b> , 53, 2896-907	6.1	41
99	Synthesis, semipreparative HPLC separation, biological evaluation, and 3D-QSAR of hydrazothiazole derivatives as human monoamine oxidase B inhibitors. <i>Bioorganic and Medicinal Chemistry</i> , <b>2010</b> , 18, 5063-70	3.4	41
98	Morphinans and isoquinolines: acetylcholinesterase inhibition, pharmacophore modeling, and interaction with opioid receptors. <i>Bioorganic and Medicinal Chemistry</i> , <b>2010</b> , 18, 5071-80	3.4	40
97	High-Quality Dataset of Protein-Bound Ligand Conformations and Its Application to Benchmarking Conformer Ensemble Generators. <i>Journal of Chemical Information and Modeling</i> , <b>2017</b> , 57, 529-539	6.1	39
96	Critical comparison of virtual screening methods against the MUV data set. <i>Journal of Chemical Information and Modeling</i> , <b>2009</b> , 49, 2168-78	6.1	38
95	FAME 2: Simple and Effective Machine Learning Model of Cytochrome P450 Regioselectivity. <i>Journal of Chemical Information and Modeling</i> , <b>2017</b> , 57, 1832-1846	6.1	36

94	FAME 3: Predicting the Sites of Metabolism in Synthetic Compounds and Natural Products for Phase 1 and Phase 2 Metabolic Enzymes. <i>Journal of Chemical Information and Modeling</i> , <b>2019</b> , 59, 3400-3412	6.1	34
93	Development of anti-viral agents using molecular modeling and virtual screening techniques. <i>Infectious Disorders - Drug Targets</i> , <b>2011</b> , 11, 64-93	1.1	33
92	Cheminformatics in Natural Product-based Drug Discovery. <i>Molecular Informatics</i> , <b>2020</b> , 39, e2000171	3.8	33
91	NP-Scout: Machine Learning Approach for the Quantification and Visualization of the Natural Product-Likeness of Small Molecules. <i>Biomolecules</i> , <b>2019</b> , 9,	5.9	31
90	Dual Acting Neuraminidase Inhibitors Open New Opportunities to Disrupt the Lethal Synergism between <i>Streptococcus pneumoniae</i> and Influenza Virus. <i>Frontiers in Microbiology</i> , <b>2016</b> , 7, 357	5.7	31
89	Computer-guided approach to access the anti-influenza activity of licorice constituents. <i>Journal of Natural Products</i> , <b>2014</b> , 77, 563-70	4.9	30
88	Identification of chemically diverse, novel inhibitors of 17 $\beta$ -hydroxysteroid dehydrogenase type 3 and 5 by pharmacophore-based virtual screening. <i>Journal of Steroid Biochemistry and Molecular Biology</i> , <b>2011</b> , 125, 148-61	5.1	30
87	Novel neuraminidase inhibitors: identification, biological evaluation and investigations of the binding mode. <i>Future Medicinal Chemistry</i> , <b>2011</b> , 3, 437-50	4.1	30
86	Discovery of novel CB2 receptor ligands by a pharmacophore-based virtual screening workflow. <i>Journal of Medicinal Chemistry</i> , <b>2009</b> , 52, 369-78	8.3	30
85	Synthesis and biological assessment of novel 2-thiazolylhydrazones and computational analysis of their recognition by monoamine oxidase B. <i>European Journal of Medicinal Chemistry</i> , <b>2012</b> , 48, 284-95	6.8	29
84	How do metabolites differ from their parent molecules and how are they excreted?. <i>Journal of Chemical Information and Modeling</i> , <b>2013</b> , 53, 354-67	6.1	29
83	Disruption of the viral polymerase complex assembly as a novel approach to attenuate influenza A virus. <i>Journal of Biological Chemistry</i> , <b>2011</b> , 286, 8414-8424	5.4	28
82	Antipneumococcal activity of neuraminidase inhibiting artocarpin. <i>International Journal of Medical Microbiology</i> , <b>2015</b> , 305, 289-97	3.7	27
81	Predicting Cyclooxygenase Inhibition by Three-Dimensional Pharmacophoric Profiling. Part I: Model Generation, Validation and Applicability in Ethnopharmacology. <i>Molecular Informatics</i> , <b>2010</b> , 29, 75-86	3.8	27
80	Conformator: A Novel Method for the Generation of Conformer Ensembles. <i>Journal of Chemical Information and Modeling</i> , <b>2019</b> , 59, 731-742	6.1	26
79	Hit Dexter: A Machine-Learning Model for the Prediction of Frequent Hitters. <i>ChemMedChem</i> , <b>2018</b> , 13, 564-571	3.7	26
78	Pyrazolopyrimidines: Potent Inhibitors Targeting the Capsid of Rhino- and Enteroviruses. <i>ChemMedChem</i> , <b>2015</b> , 10, 1629-34	3.7	26
77	Validation strategies for target prediction methods. <i>Briefings in Bioinformatics</i> , <b>2020</b> , 21, 791-802	13.4	26

76	Cytochrome P450 site of metabolism prediction from 2D topological fingerprints using GPU accelerated probabilistic classifiers. <i>Journal of Cheminformatics</i> , <b>2014</b> , 6, 29	8.6	25
75	Anti-cancer Drug Development: Computational Strategies to Identify and Target Proteins Involved in Cancer Metabolism. <i>Current Pharmaceutical Design</i> , <b>2013</b> , 19, 532-577	3.3	24
74	Discovery of novel cathepsin S inhibitors by pharmacophore-based virtual high-throughput screening. <i>Journal of Chemical Information and Modeling</i> , <b>2008</b> , 48, 1693-705	6.1	23
73	Computational approaches for skin sensitization prediction. <i>Critical Reviews in Toxicology</i> , <b>2018</b> , 48, 738-760	3.6	22
72	Thienoquinolines as novel disruptors of the PKC/RACK2 protein-protein interaction. <i>Journal of Medicinal Chemistry</i> , <b>2014</b> , 57, 3235-46	8.3	20
71	GLORYx: Prediction of the Metabolites Resulting from Phase 1 and Phase 2 Biotransformations of Xenobiotics. <i>Chemical Research in Toxicology</i> , <b>2021</b> , 34, 286-299	4	20
70	Interface dynamics explain assembly dependency of influenza neuraminidase catalytic activity. <i>Journal of Biomolecular Structure and Dynamics</i> , <b>2015</b> , 33, 104-20	3.6	19
69	Modulators of protein-protein interactions: novel approaches in targeting protein kinases and other pharmaceutically relevant biomolecules. <i>Current Topics in Medicinal Chemistry</i> , <b>2011</b> , 11, 1305-19	3	19
68	N-thiadiazole-4-hydroxy-2-quinolone-3-carboxamides bearing heteroaromatic rings as novel antibacterial agents: Design, synthesis, biological evaluation and target identification. <i>European Journal of Medicinal Chemistry</i> , <b>2020</b> , 188, 112022	6.8	19
67	Complementary assays helping to overcome challenges for identifying neuraminidase inhibitors. <i>Future Virology</i> , <b>2015</b> , 10, 77-88	2.4	17
66	NERDD: a web portal providing access to in silico tools for drug discovery. <i>Bioinformatics</i> , <b>2020</b> , 36, 1291-1292	12.92	16
65	Applications of integrated data mining methods to exploring natural product space for acetylcholinesterase inhibitors. <i>Combinatorial Chemistry and High Throughput Screening</i> , <b>2010</b> , 13, 54-66	1.3	16
64	Aryl Bis-Sulfonamide Inhibitors of IspF from <i>Arabidopsis thaliana</i> and <i>Plasmodium falciparum</i> . <i>ChemMedChem</i> , <b>2015</b> , 10, 2090-8	3.7	15
63	Natural products against acute respiratory infections: Strategies and lessons learned. <i>Journal of Ethnopharmacology</i> , <b>2020</b> , 248, 112298	5	15
62	Cryo-EM structure of pleconaril-resistant rhinovirus-B5 complexed to the antiviral OBR-5-340 reveals unexpected binding site. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2019</b> , 116, 19109-19115	11.5	14
61	Similarity-Based Methods and Machine Learning Approaches for Target Prediction in Early Drug Discovery: Performance and Scope. <i>International Journal of Molecular Sciences</i> , <b>2020</b> , 21,	6.3	14
60	Sequence-specific positions of water molecules at the interface between DNA and minor groove binders. <i>ChemPhysChem</i> , <b>2008</b> , 9, 2766-71	3.2	13
59	Tackling Antimicrobial Resistance with Small Molecules Targeting LsrK: Challenges and Opportunities. <i>Journal of Medicinal Chemistry</i> , <b>2020</b> , 63, 15243-15257	8.3	12

58	Discovery of Bioactive Natural Products for the Treatment of Acute Respiratory Infections - An Integrated Approach. <i>Planta Medica</i> , <b>2018</b> , 84, 684-695	3.1	11
57	Hydrogen-bonding patterns of minor groove-binder-DNA complexes reveal criteria for discovery of new scaffolds. <i>Journal of Chemical Information and Modeling</i> , <b>2009</b> , 49, 1063-9	6.1	11
56	Alignment-Based Prediction of Sites of Metabolism. <i>Journal of Chemical Information and Modeling</i> , <b>2017</b> , 57, 1258-1264	6.1	10
55	Scope of 3D Shape-Based Approaches in Predicting the Macromolecular Targets of Structurally Complex Small Molecules Including Natural Products and Macrocyclic Ligands. <i>Journal of Chemical Information and Modeling</i> , <b>2020</b> , 60, 2858-2875	6.1	10
54	Discovery and Characterization of Diazenylaryl Sulfonic Acids as Inhibitors of Viral and Bacterial Neuraminidases. <i>Frontiers in Microbiology</i> , <b>2017</b> , 8, 205	5.7	10
53	Molecular mechanism of a specific capsid binder resistance caused by mutations outside the binding pocket. <i>Antiviral Research</i> , <b>2015</b> , 123, 138-45	10.8	9
52	Chapter 3:Pharmacophore-based Virtual Screening in Drug Discovery <b>2008</b> , 76-119		9
51	Consideration of Water and Solvation Effects in Virtual Screening. <i>Methods and Principles in Medicinal Chemistry</i> , <b>2011</b> , 263-289	0.4	8
50	Anti-cancer drug development: computational strategies to identify and target proteins involved in cancer metabolism. <i>Current Pharmaceutical Design</i> , <b>2013</b> , 19, 532-77	3.3	8
49	Skin Doctor: Machine Learning Models for Skin Sensitization Prediction that Provide Estimates and Indicators of Prediction Reliability. <i>International Journal of Molecular Sciences</i> , <b>2019</b> , 20,	6.3	7
48	Barbituric acid derivative BAS 02104951 inhibits PKC $\alpha$ /PKC $\beta$ /PKC $\gamma$ /RACK2 interaction, Elk-1 phosphorylation in HeLa and PKC $\delta$ and $\epsilon$ translocation in PC3 cells following TPA-induction. <i>Journal of Biochemistry</i> , <b>2011</b> , 149, 331-6	3.1	7
47	Rationality over fashion and hype in drug design. <i>F1000Research</i> , <b>2021</b> , 10,	3.6	7
46	Resources for Chemical, Biological, and Structural Data on Natural Products. <i>Progress in the Chemistry of Organic Natural Products</i> , <b>2019</b> , 110, 37-71	1.9	6
45	INH14, a Small-Molecule Urea Derivative, Inhibits the IKK $\beta$ -Dependent TLR Inflammatory Response. <i>ChemBioChem</i> , <b>2019</b> , 20, 710-717	3.8	6
44	HDAC3i-Finder: A Machine Learning-based Computational Tool to Screen for HDAC3 Inhibitors. <i>Molecular Informatics</i> , <b>2021</b> , 40, e2000105	3.8	6
43	How Diverse Are the Protein-Bound Conformations of Small-Molecule Drugs and Cofactors?. <i>Frontiers in Chemistry</i> , <b>2018</b> , 6, 68	5	5
42	Metabolite Detection and Profiling. <i>Methods and Principles in Medicinal Chemistry</i> , <b>2014</b> , 485-498	0.4	5
41	Software for Metabolism Prediction. <i>Methods and Principles in Medicinal Chemistry</i> , <b>2014</b> , 27-52	0.4	5

40	Experimental Approaches to Analysis of Reactions of Cytochrome P450 Enzymes. <i>Methods and Principles in Medicinal Chemistry</i> , <b>2014</b> , 199-220	0.4	5
39	ALADDIN: Docking Approach Augmented by Machine Learning for Protein Structure Selection Yields Superior Virtual Screening Performance. <i>Molecular Informatics</i> , <b>2020</b> , 39, e1900103	3.8	5
38	ChemBioSim: Enhancing Conformal Prediction of In Vivo Toxicity by Use of Predicted Bioactivities. <i>Journal of Chemical Information and Modeling</i> , <b>2021</b> , 61, 3255-3272	6.1	5
37	Skin Doctor CP: Conformal Prediction of the Skin Sensitization Potential of Small Organic Molecules. <i>Chemical Research in Toxicology</i> , <b>2021</b> , 34, 330-344	4	5
36	QM/MM Studies of Structure and Reactivity of Cytochrome P450 Enzymes: Methodology and Selected Applications. <i>Methods and Principles in Medicinal Chemistry</i> , <b>2014</b> , 133-178	0.4	4
35	Knowledge-Based Approaches for Predicting the Sites and Products of Metabolism. <i>Methods and Principles in Medicinal Chemistry</i> , <b>2014</b> , 293-318	0.4	4
34	Online Databases and Web Servers for Drug Metabolism Research. <i>Methods and Principles in Medicinal Chemistry</i> , <b>2014</b> , 53-74	0.4	4
33	Structure-Based Methods for Predicting the Sites and Products of Metabolism. <i>Methods and Principles in Medicinal Chemistry</i> , <b>2014</b> , 243-264	0.4	4
32	The Challenges Involved in Modeling Toxicity Data In Silico: A Review. <i>Current Drug Metabolism</i> , <b>2012</b> , 18, 1266-1291	3.5	4
31	G392E neuroserpin causing the dementia FENIB is secreted from cells but is not synaptotoxic. <i>Scientific Reports</i> , <b>2021</b> , 11, 8766	4.9	4
30	Platform for determining the inhibition profile of neuraminidase inhibitors in an influenza virus N1 background. <i>Journal of Virological Methods</i> , <b>2016</b> , 237, 192-199	2.6	4
29	Phenylethylene glycol-derived LpxC inhibitors with diverse Zn <sup>2+</sup> -binding groups. <i>Tetrahedron</i> , <b>2019</b> , 75, 486-509	2.4	4
28	Cytochrome P450 Substrate Recognition and Binding. <i>Methods and Principles in Medicinal Chemistry</i> , <b>2014</b> , 103-132	0.4	3
27	Structure and Dynamics of Human Drug-Metabolizing Cytochrome P450 Enzymes. <i>Methods and Principles in Medicinal Chemistry</i> , <b>2014</b> , 75-102	0.4	3
26	Support Vector Machine (SVM) Models for Predicting Inhibitors of the 3SProcessing Step of HIV-1 Integrase. <i>Molecular Informatics</i> , <b>2013</b> , 32, 811-26	3.8	3
25	In Silico Models to Predict the Perturbation of Molecular Initiating Events Related to Thyroid Hormone Homeostasis. <i>Chemical Research in Toxicology</i> , <b>2021</b> , 34, 396-411	4	3
24	CYPlebrity: Machine learning models for the prediction of inhibitors of cytochrome P450 enzymes. <i>Bioorganic and Medicinal Chemistry</i> , <b>2021</b> , 46, 116388	3.4	3
23	Analysis of the FLVR motif of SHIP1 and its importance for the protein stability of SH2 containing signaling proteins. <i>Cellular Signalling</i> , <b>2019</b> , 63, 109380	4.9	2

22	Prediction of Phosphoglycoprotein (P-gp)-Mediated Disposition in Early Drug Discovery. <i>Methods and Principles in Medicinal Chemistry</i> , <b>2014</b> , 373-396	0.4	2
21	Reactivity-Based Approaches and Machine Learning Methods for Predicting the Sites of Cytochrome P450-Mediated Metabolism. <i>Methods and Principles in Medicinal Chemistry</i> , <b>2014</b> , 265-292	0.4	2
20	Metabolism in Drug Development. <i>Methods and Principles in Medicinal Chemistry</i> , <b>2014</b> , 1-26	0.4	2
19	Computational Free Energy Methods for Ascertaining Ligand Interaction with Metabolizing Enzymes. <i>Methods and Principles in Medicinal Chemistry</i> , <b>2014</b> , 179-198	0.4	2
18	CYPstrate: A Set of Machine Learning Models for the Accurate Classification of Cytochrome P450 Enzyme Substrates and Non-Substrates. <i>Molecules</i> , <b>2021</b> , 26,	4.8	2
17	Consideration of predicted small-molecule metabolites in computational toxicology		2
16	Pharmacophore-Based Methods for Predicting the Inhibition and Induction of Metabolic Enzymes. <i>Methods and Principles in Medicinal Chemistry</i> , <b>2014</b> , 351-372	0.4	1
15	Predicting Toxic Effects of Metabolites. <i>Methods and Principles in Medicinal Chemistry</i> , <b>2014</b> , 397-412	0.4	1
14	In Vitro Approaches to Study Drug-Drug Interactions. <i>Methods and Principles in Medicinal Chemistry</i> , <b>2014</b> , 441-484	0.4	1
13	Antibacterial activity of xylose-derived LpxC inhibitors - Synthesis, biological evaluation and molecular docking studies. <i>Bioorganic Chemistry</i> , <b>2021</b> , 107, 104603	5.1	1
12	BonMOLife: Small-Sized Libraries of Readily Purchasable Compounds, Optimized to Produce Genuine Hits in Biological Screens across the Protein Space. <i>International Journal of Molecular Sciences</i> , <b>2021</b> , 22,	6.3	1
11	Predicting the Skin Sensitization Potential of Small Molecules with Machine Learning Models Trained on Biologically Meaningful Descriptors. <i>Pharmaceuticals</i> , <b>2021</b> , 14,	5.2	1
10	AKT1 and PTEN show the highest affinities among phosphoinositide binding proteins for the second messengers PtdIns(3,4,5)P and PtdIns(3,4)P. <i>Biochemical and Biophysical Research Communications</i> , <b>2021</b> , 568, 110-115	3.4	1
9	Computational Applications in Secondary Metabolite Discovery (CAISMD): an online workshop. <i>Journal of Cheminformatics</i> , <b>2021</b> , 13, 64	8.6	1
8	Molecular Interaction Fields for Predicting the Sites and Products of Metabolism. <i>Methods and Principles in Medicinal Chemistry</i> , <b>2014</b> , 221-242	0.4	0
7	Azepine-Indole Alkaloids From Modulate 5-HT Receptors and Prevent Protein Toxicity in Transgenic .. <i>Frontiers in Neuroscience</i> , <b>2022</b> , 16, 826289	5.1	0
6	Studying and mitigating the effects of data drifts on ML model performance at the example of chemical toxicity data.. <i>Scientific Reports</i> , <b>2022</b> , 12, 7244	4.9	0
5	11th German Conference on Chemoinformatics (GCC 2015) : Fulda, Germany. 8-10 November 2015. <i>Journal of Cheminformatics</i> , <b>2016</b> , 8, 18	8.6	



- 4 Quantitative Structure-Activity Relationship (QSAR) Methods for the Prediction of Substrates, Inhibitors, and Inducers of Metabolic Enzymes. *Methods and Principles in Medicinal Chemistry*, **2014**, 319-350 0.4
- 3 In Vitro Models for Metabolism: Applicability for Research on Food Bioactives. *Methods and Principles in Medicinal Chemistry*, **2014**, 413-440 0.4
- 2 Anti-cancer Drug Development: Computational Strategies to Identify and Target Proteins Involved in Cancer Metabolism. *Current Pharmaceutical Design*, **2012**, 19, 532-577 3.3
- 1 Computational prediction of frequent hitters in target-based and cell-based assays. *Artificial Intelligence in the Life Sciences*, **2021**, 1, 100007