Johannes Kirchmair

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.

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	Azepine-Indole Alkaloids From Modulate 5-HT Receptors and Prevent Protein Toxicity in Transgenic .. *Frontiers in Neuroscience*, **2022**, 16, 826289	5.1	0
128	Studying and mitigating the effects of data drifts on ML model performance at the example of chemical toxicity data.. *Scientific Reports*, **2022**, 12, 7244	4.9	0
127	G392E neuroserpin causing the dementia FENIB is secreted from cells but is not synaptotoxic. *Scientific Reports*, **2021**, 11, 8766	4.9	4
126	Rationality over fashion and hype in drug design. *F1000Research*, **2021**, 10,	3.6	7
125	ChemBioSim: Enhancing Conformal Prediction of In Vivo Toxicity by Use of Predicted Bioactivities. *Journal of Chemical Information and Modeling*, **2021**, 61, 3255-3272	6.1	5
124	GLORYx: Prediction of the Metabolites Resulting from Phase 1 and Phase 2 Biotransformations of Xenobiotics. *Chemical Research in Toxicology*, **2021**, 34, 286-299	4	20
123	HDAC3i-Finder: A Machine Learning-based Computational Tool to Screen for HDAC3 Inhibitors. *Molecular Informatics*, **2021**, 40, e2000105	3.8	6
122	In Silico Models to Predict the Perturbation of Molecular Initiating Events Related to Thyroid Hormone Homeostasis. *Chemical Research in Toxicology*, **2021**, 34, 396-411	4	3
121	Skin Doctor CP: Conformal Prediction of the Skin Sensitization Potential of Small Organic Molecules. *Chemical Research in Toxicology*, **2021**, 34, 330-344	4	5
120	Antibacterial activity of xylose-derived LpxC inhibitors - Synthesis, biological evaluation and molecular docking studies. *Bioorganic Chemistry*, **2021**, 107, 104603	5.1	1
119	BonMOLiFe: Small-Sized Libraries of Readily Purchasable Compounds, Optimized to Produce Genuine Hits in Biological Screens across the Protein Space. *International Journal of Molecular Sciences*, **2021**, 22,	6.3	1
118	CYPstrate: A Set of Machine Learning Models for the Accurate Classification of Cytochrome P450 Enzyme Substrates and Non-Substrates. *Molecules*, **2021**, 26,	4.8	2
117	Predicting the Skin Sensitization Potential of Small Molecules with Machine Learning Models Trained on Biologically Meaningful Descriptors. *Pharmaceuticals*, **2021**, 14,	5.2	1
116	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. *Biochemical and Biophysical Research Communications*, **2021**, 568, 110-115	3.4	1
115	CYPlebrity: Machine learning models for the prediction of inhibitors of cytochrome P450 enzymes. *Bioorganic and Medicinal Chemistry*, **2021**, 46, 116388	3.4	3
114	Computational Applications in Secondary Metabolite Discovery (CAiSMD): an online workshop. *Journal of Cheminformatics*, **2021**, 13, 64	8.6	1
113	Computational prediction of frequent hitters in target-based and cell-based assays. *Artificial Intelligence in the Life Sciences*, **2021**, 1, 100007		

112	NERDD: a web portal providing access to in silico tools for drug discovery. *Bioinformatics*, **2020**, 36, 1291-1292	7.4	16
111	Tackling Antimicrobial Resistance with Small Molecules Targeting LsrK: Challenges and Opportunities. *Journal of Medicinal Chemistry*, **2020**, 63, 15243-15257	8.3	12
110	Scope of 3D Shape-Based Approaches in Predicting the Macromolecular Targets of Structurally Complex Small Molecules Including Natural Products and Macrocyclic Ligands. *Journal of Chemical Information and Modeling*, **2020**, 60, 2858-2875	6.1	10
109	Similarity-Based Methods and Machine Learning Approaches for Target Prediction in Early Drug Discovery: Performance and Scope. *International Journal of Molecular Sciences*, **2020**, 21,	6.3	14
108	ALADDIN: Docking Approach Augmented by Machine Learning for Protein Structure Selection Yields Superior Virtual Screening Performance. *Molecular Informatics*, **2020**, 39, e1900103	3.8	5
107	N-thiadiazole-4-hydroxy-2-quinolone-3-carboxamides bearing heteroaromatic rings as novel antibacterial agents: Design, synthesis, biological evaluation and target identification. *European Journal of Medicinal Chemistry*, **2020**, 188, 112022	6.8	19
106	Cheminformatics in Natural Product-based Drug Discovery. *Molecular Informatics*, **2020**, 39, e2000171	3.8	33
105	Validation strategies for target prediction methods. *Briefings in Bioinformatics*, **2020**, 21, 791-802	13.4	26
104	Natural products against acute respiratory infections: Strategies and lessons learned. *Journal of Ethnopharmacology*, **2020**, 248, 112298	5	15
103	Cryo-EM structure of pleconaril-resistant rhinovirus-B5 complexed to the antiviral OBR-5-340 reveals unexpected binding site. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 19109-19115	11.5	14
102	Skin Doctor: Machine Learning Models for Skin Sensitization Prediction that Provide Estimates and Indicators of Prediction Reliability. *International Journal of Molecular Sciences*, **2019**, 20,	6.3	7
101	NP-Scout: Machine Learning Approach for the Quantification and Visualization of the Natural Product-Likeness of Small Molecules. *Biomolecules*, **2019**, 9,	5.9	31
100	GLORY: Generator of the Structures of Likely Cytochrome P450 Metabolites Based on Predicted Sites of Metabolism. *Frontiers in Chemistry*, **2019**, 7, 402	5	43
99	Conformator: A Novel Method for the Generation of Conformer Ensembles. *Journal of Chemical Information and Modeling*, **2019**, 59, 731-742	6.1	26
98	Analysis of the FLVR motif of SHIP1 and its importance for the protein stability of SH2 containing signaling proteins. *Cellular Signalling*, **2019**, 63, 109380	4.9	2
97	FAME 3: Predicting the Sites of Metabolism in Synthetic Compounds and Natural Products for Phase 1 and Phase 2 Metabolic Enzymes. *Journal of Chemical Information and Modeling*, **2019**, 59, 3400-3412	6.1	34
96	Resources for Chemical, Biological, and Structural Data on Natural Products. *Progress in the Chemistry of Organic Natural Products*, **2019**, 110, 37-71	1.9	6
95	Phenylethylene glycol-derived LpxC inhibitors with diverse Zn2+-binding groups. *Tetrahedron*, **2019**, 75, 486-509	2.4	4

94	INH14, a Small-Molecule Urea Derivative, Inhibits the IKK-Dependent TLR Inflammatory Response. *ChemBioChem*, **2019**, 20, 710-717	3.8	6
93	Computational methods and tools to predict cytochrome P450 metabolism for drug discovery. *Chemical Biology and Drug Design*, **2019**, 93, 377-386	2.9	62
92	Hit Dexter 2.0: Machine-Learning Models for the Prediction of Frequent Hitters. *Journal of Chemical Information and Modeling*, **2019**, 59, 1030-1043	6.1	50
91	Hit Dexter: A Machine-Learning Model for the Prediction of Frequent Hitters. *ChemMedChem*, **2018**, 13, 564-571	3.7	26
90	Discovery of Bioactive Natural Products for the Treatment of Acute Respiratory Infections - An Integrated Approach. *Planta Medica*, **2018**, 84, 684-695	3.1	11
89	Characterization of the Chemical Space of Known and Readily Obtainable Natural Products. *Journal of Chemical Information and Modeling*, **2018**, 58, 1518-1532	6.1	50
88	How Diverse Are the Protein-Bound Conformations of Small-Molecule Drugs and Cofactors?. *Frontiers in Chemistry*, **2018**, 6, 68	5	5
87	Computational approaches for skin sensitization prediction. *Critical Reviews in Toxicology*, **2018**, 48, 738-760	5.7	22
86	High-Quality Dataset of Protein-Bound Ligand Conformations and Its Application to Benchmarking Conformer Ensemble Generators. *Journal of Chemical Information and Modeling*, **2017**, 57, 529-539	6.1	39
85	Alignment-Based Prediction of Sites of Metabolism. *Journal of Chemical Information and Modeling*, **2017**, 57, 1258-1264	6.1	10
84	Benchmarking Commercial Conformer Ensemble Generators. *Journal of Chemical Information and Modeling*, **2017**, 57, 2719-2728	6.1	51
83	Data Resources for the Computer-Guided Discovery of Bioactive Natural Products. *Journal of Chemical Information and Modeling*, **2017**, 57, 2099-2111	6.1	99
82	FAME 2: Simple and Effective Machine Learning Model of Cytochrome P450 Regioselectivity. *Journal of Chemical Information and Modeling*, **2017**, 57, 1832-1846	6.1	36
81	Discovery and Characterization of Diazenylaryl Sulfonic Acids as Inhibitors of Viral and Bacterial Neuraminidases. *Frontiers in Microbiology*, **2017**, 8, 205	5.7	10
80	Discovery of prenylated flavonoids with dual activity against influenza virus and Streptococcus pneumoniae. *Scientific Reports*, **2016**, 6, 27156	4.9	41
79	11th German Conference on Chemoinformatics (GCC 2015) : Fulda, Germany. 8-10 November 2015. *Journal of Cheminformatics*, **2016**, 8, 18	8.6	
78	Dual Acting Neuraminidase Inhibitors Open New Opportunities to Disrupt the Lethal Synergism between Streptococcus pneumoniae and Influenza Virus. *Frontiers in Microbiology*, **2016**, 7, 357	5.7	31
77	Platform for determining the inhibition profile of neuraminidase inhibitors in an influenza virus N1 background. *Journal of Virological Methods*, **2016**, 237, 192-199	2.6	4

76	Predicting drug metabolism: experiment and/or computation?. *Nature Reviews Drug Discovery*, **2015**, 14, 387-404	64.1	255
75	Antipneumococcal activity of neuraminidase inhibiting artocarpin. *International Journal of Medical Microbiology*, **2015**, 305, 289-97	3.7	27
74	Complementary assays helping to overcome challenges for identifying neuraminidase inhibitors. *Future Virology*, **2015**, 10, 77-88	2.4	17
73	Molecular mechanism of a specific capsid binder resistance caused by mutations outside the binding pocket. *Antiviral Research*, **2015**, 123, 138-45	10.8	9
72	Pyrazolopyrimidines: Potent Inhibitors Targeting the Capsid of Rhino- and Enteroviruses. *ChemMedChem*, **2015**, 10, 1629-34	3.7	26
71	Aryl Bis-Sulfonamide Inhibitors of IspF from Arabidopsis thaliana and Plasmodium falciparum. *ChemMedChem*, **2015**, 10, 2090-8	3.7	15
70	Interface dynamics explain assembly dependency of influenza neuraminidase catalytic activity. *Journal of Biomolecular Structure and Dynamics*, **2015**, 33, 104-20	3.6	19
69	Thienoquinolines as novel disruptors of the PKC/RACK2 protein-protein interaction. *Journal of Medicinal Chemistry*, **2014**, 57, 3235-46	8.3	20
68	Computer-guided approach to access the anti-influenza activity of licorice constituents. *Journal of Natural Products*, **2014**, 77, 563-70	4.9	30
67	QM/MM Studies of Structure and Reactivity of Cytochrome P450 Enzymes: Methodology and Selected Applications. *Methods and Principles in Medicinal Chemistry*, **2014**, 133-178	0.4	4
66	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	
65	Prediction of Phosphoglycoprotein (P-gp)-Mediated Disposition in Early Drug Discovery. *Methods and Principles in Medicinal Chemistry*, **2014**, 373-396	0.4	2
64	Knowledge-Based Approaches for Predicting the Sites and Products of Metabolism. *Methods and Principles in Medicinal Chemistry*, **2014**, 293-318	0.4	4
63	Online Databases and Web Servers for Drug Metabolism Research. *Methods and Principles in Medicinal Chemistry*, **2014**, 53-74	0.4	4
62	Pharmacophore-Based Methods for Predicting the Inhibition and Induction of Metabolic Enzymes. *Methods and Principles in Medicinal Chemistry*, **2014**, 351-372	0.4	1
61	Structure-Based Methods for Predicting the Sites and Products of Metabolism. *Methods and Principles in Medicinal Chemistry*, **2014**, 243-264	0.4	4
60	Predicting Toxic Effects of Metabolites. *Methods and Principles in Medicinal Chemistry*, **2014**, 397-412	0.4	1
59	In Vitro Models for Metabolism: Applicability for Research on Food Bioactives. *Methods and Principles in Medicinal Chemistry*, **2014**, 413-440	0.4	

58	Metabolite Detection and Profiling. *Methods and Principles in Medicinal Chemistry*, **2014**, 485-498	0.4	5
57	In Vitro Approaches to Study DrugDrug Interactions. *Methods and Principles in Medicinal Chemistry*, **2014**, 441-484	0.4	1
56	Cytochrome P450 site of metabolism prediction from 2D topological fingerprints using GPU accelerated probabilistic classifiers. *Journal of Cheminformatics*, **2014**, 6, 29	8.6	25
55	Cytochrome P450 Substrate Recognition and Binding. *Methods and Principles in Medicinal Chemistry* , **2014**, 103-132	0.4	3
54	Reactivity-Based Approaches and Machine Learning Methods for Predicting the Sites of Cytochrome P450-Mediated Metabolism. *Methods and Principles in Medicinal Chemistry*, **2014**, 265-292	0.4	2
53	Metabolism in Drug Development. *Methods and Principles in Medicinal Chemistry*, **2014**, 1-26	0.4	2
52	Software for Metabolism Prediction. *Methods and Principles in Medicinal Chemistry*, **2014**, 27-52	0.4	5
51	Structure and Dynamics of Human Drug-Metabolizing Cytochrome P450 Enzymes. *Methods and Principles in Medicinal Chemistry*, **2014**, 75-102	0.4	3
50	Computational Free Energy Methods for Ascertaining Ligand Interaction with Metabolizing Enzymes. *Methods and Principles in Medicinal Chemistry*, **2014**, 179-198	0.4	2
49	Experimental Approaches to Analysis of Reactions of Cytochrome P450 Enzymes. *Methods and Principles in Medicinal Chemistry*, **2014**, 199-220	0.4	5
48	Molecular Interaction Fields for Predicting the Sites and Products of Metabolism. *Methods and Principles in Medicinal Chemistry*, **2014**, 221-242	0.4	0
47	Quantifying the shifts in physicochemical property space introduced by the metabolism of small organic molecules. *Journal of Cheminformatics*, **2013**, 5,	8.6	78
46	How do metabolites differ from their parent molecules and how are they excreted?. *Journal of Chemical Information and Modeling*, **2013**, 53, 354-67	6.1	29
45	FAst MEtabolizer (FAME): A rapid and accurate predictor of sites of metabolism in multiple species by endogenous enzymes. *Journal of Chemical Information and Modeling*, **2013**, 53, 2896-907	6.1	41
44	Support Vector Machine (SVM) Models for Predicting Inhibitors of the 3SProcessing Step of HIV-1 Integrase. *Molecular Informatics*, **2013**, 32, 811-26	3.8	3
43	Anti-cancer Drug Development: Computational Strategies to Identify and Target Proteins Involved in Cancer Metabolism. *Current Pharmaceutical Design*, **2013**, 19, 532-577	3.3	24
42	Anti-cancer drug development: computational strategies to identify and target proteins involved in cancer metabolism. *Current Pharmaceutical Design*, **2013**, 19, 532-77	3.3	8
41	Synthesis and biological assessment of novel 2-thiazolylhydrazones and computational analysis of their recognition by monoamine oxidase B. *European Journal of Medicinal Chemistry*, **2012**, 48, 284-95	6.8	29

40	Identification of HIV-1 reverse transcriptase dual inhibitors by a combined shape-, 2D-fingerprint- and pharmacophore-based virtual screening approach. *European Journal of Medicinal Chemistry*, **2012**, 50, 216-29	6.8	55
39	Influenza neuraminidase: a druggable target for natural products. *Natural Product Reports*, **2012**, 29, 11-36	15.1	116
38	Novel pharmacological chaperones that correct phenylketonuria in mice. *Human Molecular Genetics* , **2012**, 21, 1877-87	5.6	50
37	Computational prediction of metabolism: sites, products, SAR, P450 enzyme dynamics, and mechanisms. *Journal of Chemical Information and Modeling*, **2012**, 52, 617-48	6.1	212
36	The Challenges Involved in Modeling Toxicity Data In Silico: A Review. *Current Drug Metabolism*, **2012**, 18, 1266-1291	3.5	4
35	The challenges involved in modeling toxicity data in silico: a review. *Current Pharmaceutical Design*, **2012**, 18, 1266-91	3.3	67
34	Anti-cancer Drug Development: Computational Strategies to Identify and Target Proteins Involved in Cancer Metabolism. *Current Pharmaceutical Design*, **2012**, 19, 532-577	3.3	
33	Consideration of Water and Solvation Effects in Virtual Screening. *Methods and Principles in Medicinal Chemistry*, **2011**, 263-289	0.4	8
32	From in silico target prediction to multi-target drug design: current databases, methods and applications. *Journal of Proteomics*, **2011**, 74, 2554-74	3.9	214
31	Identification of chemically diverse, novel inhibitors of 17β-hydroxysteroid dehydrogenase type 3 and 5 by pharmacophore-based virtual screening. *Journal of Steroid Biochemistry and Molecular Biology*, **2011**, 125, 148-61	5.1	30
30	Barbituric acid derivative BAS 02104951 inhibits PKCα/PKCβ/PKCβ/RACK2 interaction, Elk-1 phosphorylation in HeLa and PKCβ and α translocation in PC3 cells following TPA-induction. *Journal of Biochemistry*, **2011**, 149, 331-6	3.1	7
29	Novel neuraminidase inhibitors: identification, biological evaluation and investigations of the binding mode. *Future Medicinal Chemistry*, **2011**, 3, 437-50	4.1	30
28	Development of anti-viral agents using molecular modeling and virtual screening techniques. *Infectious Disorders - Drug Targets*, **2011**, 11, 64-93	1.1	33
27	Modulators of protein-protein interactions: novel approaches in targeting protein kinases and other pharmaceutically relevant biomolecules. *Current Topics in Medicinal Chemistry*, **2011**, 11, 1305-19	3	19
26	Disruption of the viral polymerase complex assembly as a novel approach to attenuate influenza A virus. *Journal of Biological Chemistry*, **2011**, 286, 8414-8424	5.4	28
25	One concept, three implementations of 3D pharmacophore-based virtual screening: distinct coverage of chemical search space. *Journal of Chemical Information and Modeling*, **2010**, 50, 1241-7	6.1	46
24	Antiviral potential and molecular insight into neuraminidase inhibiting diarylheptanoids from Alpinia katsumadai. *Journal of Medicinal Chemistry*, **2010**, 53, 778-86	8.3	101
23	Applications of integrated data mining methods to exploring natural product space for acetylcholinesterase inhibitors. *Combinatorial Chemistry and High Throughput Screening*, **2010**, 13, 54-66	1.3	16

22	Predicting Cyclooxygenase Inhibition by Three-Dimensional Pharmacophoric Profiling. Part I: Model Generation, Validation and Applicability in Ethnopharmacology. *Molecular Informatics*, **2010**, 29, 75-86	3.8	27
21	Synthesis, semipreparative HPLC separation, biological evaluation, and 3D-QSAR of hydrazothiazole derivatives as human monoamine oxidase B inhibitors. *Bioorganic and Medicinal Chemistry*, **2010**, 18, 5063-70	3.4	41
20	Morphinans and isoquinolines: acetylcholinesterase inhibition, pharmacophore modeling, and interaction with opioid receptors. *Bioorganic and Medicinal Chemistry*, **2010**, 18, 5071-80	3.4	40
19	Hydrogen-bonding patterns of minor groove-binder-DNA complexes reveal criteria for discovery of new scaffolds. *Journal of Chemical Information and Modeling*, **2009**, 49, 1063-9	6.1	11
18	Critical comparison of virtual screening methods against the MUV data set. *Journal of Chemical Information and Modeling*, **2009**, 49, 2168-78	6.1	38
17	How to optimize shape-based virtual screening: choosing the right query and including chemical information. *Journal of Chemical Information and Modeling*, **2009**, 49, 678-92	6.1	164
16	Discovery of novel CB2 receptor ligands by a pharmacophore-based virtual screening workflow. *Journal of Medicinal Chemistry*, **2009**, 52, 369-78	8.3	30
15	Discovery of novel PPAR ligands by a virtual screening approach based on pharmacophore modeling, 3D shape, and electrostatic similarity screening. *Journal of Medicinal Chemistry*, **2008**, 51, 6303-17	8.3	60
14	Structure-based virtual screening for the discovery of natural inhibitors for human rhinovirus coat protein. *Journal of Medicinal Chemistry*, **2008**, 51, 842-51	8.3	70
13	Discovery of nonsteroidal 17beta-hydroxysteroid dehydrogenase 1 inhibitors by pharmacophore-based screening of virtual compound libraries. *Journal of Medicinal Chemistry*, **2008**, 51, 4188-99	8.3	51
12	The Protein Data Bank (PDB), its related services and software tools as key components for in silico guided drug discovery. *Journal of Medicinal Chemistry*, **2008**, 51, 7021-40	8.3	81
11	Discovery of novel cathepsin S inhibitors by pharmacophore-based virtual high-throughput screening. *Journal of Chemical Information and Modeling*, **2008**, 48, 1693-705	6.1	23
10	Enhancing drug discovery through in silico screening: strategies to increase true positives retrieval rates. *Current Medicinal Chemistry*, **2008**, 15, 2040-53	4.3	72
9	Evaluation of the performance of 3D virtual screening protocols: RMSD comparisons, enrichment assessments, and decoy selection--what can we learn from earlier mistakes?. *Journal of Computer-Aided Molecular Design*, **2008**, 22, 213-28	4.2	278
8	Sequence-specific positions of water molecules at the interface between DNA and minor groove binders. *ChemPhysChem*, **2008**, 9, 2766-71	3.2	13
7	Chapter 3:Pharmacophore-based Virtual Screening in Drug Discovery **2008**, 76-119		9
6	Fast and efficient in silico 3D screening: toward maximum computational efficiency of pharmacophore-based and shape-based approaches. *Journal of Chemical Information and Modeling*, **2007**, 47, 2182-96	6.1	64
5	Pharmacophore modeling and parallel screening for PPAR ligands. *Journal of Computer-Aided Molecular Design*, **2007**, 21, 575-90	4.2	58

4	CAESAR: a new conformer generation algorithm based on recursive buildup and local rotational symmetry consideration. *Journal of Chemical Information and Modeling*, **2007**, 47, 1923-32	6.1	105
3	Comparative performance assessment of the conformational model generators omega and catalyst: a large-scale survey on the retrieval of protein-bound ligand conformations. *Journal of Chemical Information and Modeling*, **2006**, 46, 1848-61	6.1	151
2	Comparative analysis of protein-bound ligand conformations with respect to catalyst's conformational space subsampling algorithms. *Journal of Chemical Information and Modeling*, **2005**, 45, 422-30	6.1	125
1	Consideration of predicted small-molecule metabolites in computational toxicology		2