Johannes Kirchmair

List of Publications by Year
in descending order

118 papers	5,355 citations	76294 40 h-index	91828 69 g-index
150 all docs	150 docs citations	150 times ranked	6219 citing authors

#	Article	IF	Citations
1	Predicting drug metabolism: experiment and/or computation?. Nature Reviews Drug Discovery, 2015, 14, 387-404.	21.5	355
2	Evaluation of the performance of 3D virtual screening protocols: RMSD comparisons, enrichment assessments, and decoy selectionâ€"What can we learn from earlier mistakes?. Journal of Computer-Aided Molecular Design, 2008, 22, 213-228.	1.3	330
3	Computational Prediction of Metabolism: Sites, Products, SAR, P450 Enzyme Dynamics, and Mechanisms. Journal of Chemical Information and Modeling, 2012, 52, 617-648.	2.5	246
4	From in silico target prediction to multi-target drug design: Current databases, methods and applications. Journal of Proteomics, 2011, 74, 2554-2574.	1.2	243
5	How To Optimize Shape-Based Virtual Screening: Choosing the Right Query and Including Chemical Information. Journal of Chemical Information and Modeling, 2009, 49, 678-692.	2.5	178
6	Comparative Performance Assessment of the Conformational Model Generators Omega and Catalyst:Â A Large-Scale Survey on the Retrieval of Protein-Bound Ligand Conformations. Journal of Chemical Information and Modeling, 2006, 46, 1848-1861.	2.5	159
7	Comparative Analysis of Protein-Bound Ligand Conformations with Respect to Catalyst's Conformational Space Subsampling Algorithms. Journal of Chemical Information and Modeling, 2005, 45, 422-430.	2.5	148
8	Influenza neuraminidase: A druggable target for natural products. Natural Product Reports, 2012, 29, 11-36.	5.2	146
9	Data Resources for the Computer-Guided Discovery of Bioactive Natural Products. Journal of Chemical Information and Modeling, 2017, 57, 2099-2111.	2.5	131
10	CAESAR:â€‰ A New Conformer Generation Algorithm Based on Recursive Buildup and Local Rotational Symmetry Consideration. Journal of Chemical Information and Modeling, 2007, 47, 1923-1932.	2.5	119
11	Antiviral Potential and Molecular Insight into Neuraminidase Inhibiting Diarylheptanoids from Alpinia katsumadai. Journal of Medicinal Chemistry, 2010, 53, 778-786.	2.9	114
12	Computational methods and tools to predict cytochrome P450 metabolism for drug discovery. Chemical Biology and Drug Design, 2019, 93, 377-386.	1.5	109
13	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, 7021-7040.	2.9	91
14	Benchmarking Commercial Conformer Ensemble Generators. Journal of Chemical Information and Modeling, 2017, 57, 2719-2728.	2.5	88
15	Structure-Based Virtual Screening for the Discovery of Natural Inhibitors for Human Rhinovirus Coat Protein. Journal of Medicinal Chemistry, 2008, 51, 842-851.	2.9	83
16	Characterization of the Chemical Space of Known and Readily Obtainable Natural Products. Journal of Chemical Information and Modeling, 2018, 58, 1518-1532.	2.5	81
17	Cheminformatics in Natural Productâ€based Drug Discovery. Molecular Informatics, 2020, 39, e2000171.	1.4	81
18	The Challenges Involved in Modeling Toxicity Data In Silico: A Review. Current Pharmaceutical Design, 2012, 18, 1266-1291.	0.9	80

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19	Enhancing Drug Discovery Through In Silico Screening: Strategies to Increase True Positives Retrieval Rates. Current Medicinal Chemistry, 2008, 15, 2040-2053.	1.2	76
20	Hit Dexter 2.0: Machine-Learning Models for the Prediction of Frequent Hitters. Journal of Chemical Information and Modeling, 2019, 59, 1030-1043.	2.5	70
21	Fast and Efficient in Silico 3D Screening:â€‰ Toward Maximum Computational Efficiency of Pharmacophore-Based and Shape-Based Approaches. Journal of Chemical Information and Modeling, 2007, 47, 2182-2196.	2.5	69
22	Pharmacophore modeling and parallel screening for PPAR ligands. Journal of Computer-Aided Molecular Design, 2007, 21, 575-590.	1.3	65
23	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, 6303-6317.	2.9	65
24	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, 216-229.	2.6	63
25	Discovery of prenylated flavonoids with dual activity against influenza virus and Streptococcus pneumoniae. Scientific Reports, 2016, 6, 27156.	1.6	63
26	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.	2.5	60
27	Novel pharmacological chaperones that correct phenylketonuria in mice. Human Molecular Genetics, 2012, 21, 1877-1887.	1.4	58
28	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.	2.5	57
29	GLORY: Generator of the Structures of Likely Cytochrome P450 Metabolites Based on Predicted Sites of Metabolism. Frontiers in Chemistry, 2019, 7, 402.	1.8	57
30	FAME 2: Simple and Effective Machine Learning Model of Cytochrome P450 Regioselectivity. Journal of Chemical Information and Modeling, 2017, 57, 1832-1846.	2.5	56
31	Discovery of Nonsteroidal 17Î²-Hydroxysteroid Dehydrogenase 1 Inhibitors by Pharmacophore-Based Screening of Virtual Compound Libraries. Journal of Medicinal Chemistry, 2008, 51, 4188-4199.	2.9	55
32	One Concept, Three Implementations of 3D Pharmacophore-Based Virtual Screening: Distinct Coverage of Chemical Search Space. Journal of Chemical Information and Modeling, 2010, 50, 1241-1247.	2.5	54
33	GLORYx: Prediction of the Metabolites Resulting from Phase 1 and Phase 2 Biotransformations of Xenobiotics. Chemical Research in Toxicology, 2021, 34, 286-299.	1.7	51
34	Conformator: A Novel Method for the Generation of Conformer Ensembles. Journal of Chemical Information and Modeling, 2019, 59, 731-742.	2.5	49
35	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, 2896-2907.	2.5	47
36	Morphinans and isoquinolines: Acetylcholinesterase inhibition, pharmacophore modeling, and interaction with opioid receptors. Bioorganic and Medicinal Chemistry, 2010, 18, 5071-5080.	1.4	46

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37	NERDD: a web portal providing access to in silico tools for drug discovery. Bioinformatics, 2020, 36, 1291-1292.	1.8	46
38	Synthesis, semipreparative HPLC separation, biological evaluation, and 3D-QSAR of hydrazothiazole derivatives as human monoamine oxidase B inhibitors. Bioorganic and Medicinal Chemistry, 2010, 18, 5063-5070.	1.4	44
39	Development of Anti-Viral Agents Using Molecular Modeling and Virtual Screening Techniques. Infectious Disorders - Drug Targets, 2011, 11, 64-93.	0.4	43
40	NP-Scout: Machine Learning Approach for the Quantification and Visualization of the Natural Product-Likeness of Small Molecules. Biomolecules, 2019, 9, 43.	1.8	43
41	Critical Comparison of Virtual Screening Methods against the MUV Data Set. Journal of Chemical Information and Modeling, 2009, 49, 2168-2178.	2.5	42
42	Validation strategies for target prediction methods. Briefings in Bioinformatics, 2020, 21, 791-802.	3.2	42
43	Computer-Guided Approach to Access the Anti-influenza Activity of Licorice Constituents. Journal of Natural Products, 2014, 77, 563-570.	1.5	38
44	Dual Acting Neuraminidase Inhibitors Open New Opportunities to Disrupt the Lethal Synergism between Streptococcus pneumoniae and Influenza Virus. Frontiers in Microbiology, 2016, 7, 357.	1.5	38
45	Computational approaches for skin sensitization prediction. Critical Reviews in Toxicology, 2018, 48, 738-760.	1.9	38
46	Discovery of Novel CB₂ Receptor Ligands by a Pharmacophore-Based Virtual Screening Workflow. Journal of Medicinal Chemistry, 2009, 52, 369-378.	2.9	37
47	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.	2.6	36
48	Novel neuraminidase inhibitors: identification, biological evaluation and investigations of the binding mode. Future Medicinal Chemistry, 2011, 3, 437-450.	1.1	34
49	Hit Dexter: A Machineâ€Learning Model for the Prediction of Frequent Hitters. ChemMedChem, 2018, 13, 564-571.	1.6	34
50	Predicting Cyclooxygenase Inhibition by Threeâ€Dimensional Pharmacophoric Profiling. Part I: Model Generation, Validation and Applicability in Ethnopharmacology. Molecular Informatics, 2010, 29, 75-86.	1.4	33
51	Identification of chemically diverse, novel inhibitors of 17Î²-hydroxysteroid dehydrogenase type 3 and 5 by pharmacophore-based virtual screening. Journal of Steroid Biochemistry and Molecular Biology, 2011, 125, 148-161.	1.2	33
52	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, 284-295.	2.6	33
53	How Do Metabolites Differ from Their Parent Molecules and How Are They Excreted?. Journal of Chemical Information and Modeling, 2013, 53, 354-367.	2.5	33
54	Pyrazolopyrimidines: Potent Inhibitors Targeting the Capsid of Rhinoâ€and Enteroviruses. ChemMedChem, 2015, 10, 1629-1634.	1.6	33

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55	Antipneumococcal activity of neuraminidase inhibiting artocarpin. International Journal of Medical Microbiology, 2015, 305, 289-297.	1.5	32
56	Natural products against acute respiratory infections: Strategies and lessons learned. Journal of Ethnopharmacology, 2020, 248, 112298.	2.0	32
57	Disruption of the Viral Polymerase Complex Assembly as a Novel Approach to Attenuate Influenza A Virus. Journal of Biological Chemistry, 2011, 286, 8414-8424.	1.6	31
58	Anti-cancer Drug Development: Computational Strategies to Identify and Target Proteins Involved in Cancer Metabolism. Current Pharmaceutical Design, 2013, 19, 532-577.	0.9	30
59	Thienoquinolines as Novel Disruptors of the PKCÎµ/RACK2 Proteinâ€“Protein Interaction. Journal of Medicinal Chemistry, 2014, 57, 3235-3246.	2.9	26
60	Cytochrome P450 site of metabolism prediction from 2D topological fingerprints using GPU accelerated probabilistic classifiers. Journal of Cheminformatics, 2014, 6, 29.	2.8	26
61	Discovery of Novel Cathepsin S Inhibitors by Pharmacophore-Based Virtual High-Throughput Screening. Journal of Chemical Information and Modeling, 2008, 48, 1693-1705.	2.5	25
62	Interface dynamics explain assembly dependency of influenza neuraminidase catalytic activity. Journal of Biomolecular Structure and Dynamics, 2015, 33, 104-120.	2.0	24
63	Similarity-Based Methods and Machine Learning Approaches for Target Prediction in Early Drug Discovery: Performance and Scope. International Journal of Molecular Sciences, 2020, 21, 3585.	1.8	24
64	Complementary assays helping to overcome challenges for identifying neuraminidase inhibitors. Future Virology, 2015, 10, 77-88.	0.9	23
65	Rationality over fashion and hype in drug design. F1000Research, 2021, 10, 397.	0.8	23
66	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.	3.3	22
67	Tackling Antimicrobial Resistance with Small Molecules Targeting LsrK: Challenges and Opportunities. Journal of Medicinal Chemistry, 2020, 63, 15243-15257.	2.9	21
68	In Silico Models to Predict the Perturbation of Molecular Initiating Events Related to Thyroid Hormone Homeostasis. Chemical Research in Toxicology, 2021, 34, 396-411.	1.7	20
69	Modulators of Protein-Protein Interactions â€“ Novel Approaches in Targeting Protein Kinases and Other Pharmaceutically Relevant Biomolecules. Current Topics in Medicinal Chemistry, 2011, 11, 1305-1319.	1.0	19
70	Applications of Integrated Data Mining Methods to Exploring Natural Product Space for Acetylcholinesterase Inhibitors. Combinatorial Chemistry and High Throughput Screening, 2010, 13, 54-66.	0.6	18
71	Discovery of Bioactive Natural Products for the Treatment of Acute Respiratory Infections â€“ An Integrated Approach. Planta Medica, 2018, 84, 684-695.	0.7	18
72	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.	2.5	18

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73	Ring systems in natural products: structural diversity, physicochemical properties, and coverage by synthetic compounds. Natural Product Reports, 2022, 39, 1544-1556.	5.2	18
74	HDAC3iâ€Finder: A Machine Learningâ€based Computational Tool to Screen for HDAC3 Inhibitors. Molecular Informatics, 2021, 40, e2000105.	1.4	16
75	CYPlebrity: Machine learning models for the prediction of inhibitors of cytochrome P450 enzymes. Bioorganic and Medicinal Chemistry, 2021, 46, 116388.	1.4	16
76	Aryl Bisâ€Sulfonamide Inhibitors of IspF from Arabidopsis thaliana and Plasmodium falciparum. ChemMedChem, 2015, 10, 2090-2098.	1.6	15
77	Skin Doctor: Machine Learning Models for Skin Sensitization Prediction that Provide Estimates and Indicators of Prediction Reliability. International Journal of Molecular Sciences, 2019, 20, 4833.	1.8	15
78	Sequenceâ€Specific Positions of Water Molecules at the Interface between DNA and Minor Groove Binders. ChemPhysChem, 2008, 9, 2766-2771.	1.0	14
79	Molecular mechanism of a specific capsid binder resistance caused by mutations outside the binding pocket. Antiviral Research, 2015, 123, 138-145.	1.9	14
80	Discovery and Characterization of Diazenylaryl Sulfonic Acids as Inhibitors of Viral and Bacterial Neuraminidases. Frontiers in Microbiology, 2017, 8, 205.	1.5	13
81	ChemBioSim: Enhancing Conformal Prediction of In Vivo Toxicity by Use of Predicted Bioactivities. Journal of Chemical Information and Modeling, 2021, 61, 3255-3272.	2.5	13
82	Hydrogen-Bonding Patterns of Minor Groove-Binderâ"DNA Complexes Reveal Criteria for Discovery of New Scaffolds. Journal of Chemical Information and Modeling, 2009, 49, 1063-1069.	2.5	11
83	Alignment-Based Prediction of Sites of Metabolism. Journal of Chemical Information and Modeling, 2017, 57, 1258-1264.	2.5	11
84	Skin Doctor CP: Conformal Prediction of the Skin Sensitization Potential of Small Organic Molecules. Chemical Research in Toxicology, 2021, 34, 330-344.	1.7	11
85	Pharmacophore-based Virtual Screening in Drug Discovery. , 2008, , 76-119.		10
86	Barbituric acid derivative BAS 02104951 inhibits PKCÂ, PKCÂ, PKCÂ/RACK2 interaction, Elk-1 phosphorylation in HeLa and PKCÂ and Â translocation in PC3 cells following TPA-induction. Journal of Biochemistry, 2011, 149, 331-336.	0.9	9
87	Anti-cancer drug development: computational strategies to identify and target proteins involved in cancer metabolism. Current Pharmaceutical Design, 2013, 19, 532-77.	0.9	9
88	PAIN(S) relievers for medicinal chemists: how computational methods can assist in hit evaluation. Future Medicinal Chemistry, 2018, 10, 1533-1535.	1.1	8
89	Phenylethylene glycol-derived LpxC inhibitors with diverse Zn2+-binding groups. Tetrahedron, 2019, 75, 486-509.	1.0	8
90	INH14, a Smallâ€Molecule Urea Derivative, Inhibits the IKKÎ±/Î²â€Dependent TLR Inflammatory Response. ChemBioChem, 2019, 20, 710-717.	1.3	8

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91	ALADDIN: Docking Approach Augmented by Machine Learning for Protein Structure Selection Yields Superior Virtual Screening Performance. Molecular Informatics, 2020, 39, e1900103.	1.4	8
92	Platform for determining the inhibition profile of neuraminidase inhibitors in an influenza virus N1 background. Journal of Virological Methods, 2016, 237, 192-199.	1.0	7
93	How Diverse Are the Protein-Bound Conformations of Small-Molecule Drugs and Cofactors?. Frontiers in Chemistry, 2018, 6, 68.	1.8	7
94	G392E neuroserpin causing the dementia FENIB is secreted from cells but is not synaptotoxic. Scientific Reports, 2021, 11, 8766.	1.6	7
95	Predicting the Skin Sensitization Potential of Small Molecules with Machine Learning Models Trained on Biologically Meaningful Descriptors. Pharmaceuticals, 2021, 14, 790.	1.7	7
96	Consideration of predicted small-molecule metabolites in computational toxicology. , 2022, 1, 158-172.		7
97	Resources for Chemical, Biological, and Structural Data on Natural Products. Progress in the Chemistry of Organic Natural Products, 2019, 110, 37-71.	0.8	6
98	Discovery ofN-quinazolinone-4-hydroxy-2-quinolone-3-carboxamides as DNA gyrase B-targeted antibacterial agents. Journal of Enzyme Inhibition and Medicinal Chemistry, 2022, 37, 1620-1631.	2.5	6
99	Molecular Informatics in Natural Products Research. Molecular Informatics, 2020, 39, e2000206.	1.4	5
100	Antibacterial activity of xylose-derived LpxC inhibitors â€“ Synthesis, biological evaluation and molecular docking studies. Bioorganic Chemistry, 2021, 107, 104603.	2.0	5
101	CYPstrate: A Set of Machine Learning Models for the Accurate Classification of Cytochrome P450 Enzyme Substrates and Non-Substrates. Molecules, 2021, 26, 4678.	1.7	5
102	AKT1 and PTEN show the highest affinities among phosphoinositide binding proteins for the second messengers PtdIns(3,4,5)P3 and PtdIns(3,4)P2. Biochemical and Biophysical Research Communications, 2021, 568, 110-115.	1.0	5
103	Studying and mitigating the effects of data drifts on ML model performance at the example of chemical toxicity data. Scientific Reports, 2022, 12, 7244.	1.6	5
104	The Challenges Involved in Modeling Toxicity Data In Silico: A Review. Current Drug Metabolism, 2012, 18, 1266-1291.	0.7	4
105	Analysis of the FLVR motif of SHIP1 and its importance for the protein stability of SH2 containing signaling proteins. Cellular Signalling, 2019, 63, 109380.	1.7	4
106	Support Vector Machine (SVM) Models for Predicting Inhibitors of the 3â€² Processing Step of HIVâ€1 Integrase. Molecular Informatics, 2013, 32, 811-826.	1.4	3
107	Computational Applications in Secondary Metabolite Discovery (CAiSMD): an online workshop. Journal of Cheminformatics, 2021, 13, 64.	2.8	3
108	Computational prediction of frequent hitters in target-based and cell-based assays. Artificial Intelligence in the Life Sciences, 2021, 1, 100007.	1.6	3

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109	BonMOLiÃ¨re: 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, 7773.	1.8	2
110	Azepine-Indole Alkaloids From Psychotria nemorosa Modulate 5-HT2A Receptors and Prevent in vivo Protein Toxicity in Transgenic Caenorhabditis elegans. Frontiers in Neuroscience, 2022, 16, 826289.	1.4	2
111	Development and Experimental Validation of Regularized Machine Learning Models Detecting New, Structurally Distinct Activators of PXR. Cells, 2022, 11, 1253.	1.8	2
112	11th German Conference on Chemoinformatics (GCC 2015). Journal of Cheminformatics, 2016, 8, 18.	2.8	1
113	Mechanism of BIP-4 mediated inhibition of InsP3Kinase-A. Bioscience Reports, 2021, 41, .	1.1	1
114	Maximizing the Performance of Similarity-Based Virtual Screening Methods by Generating Synergy from the Integration of 2D and 3D Approaches. International Journal of Molecular Sciences, 2022, 23, 7747.	1.8	1
115	Comparative Analysis of Protein-Bound Ligand Conformations with Respect to Catalystâ€²s Conformational Space Subsampling Algorithms.. ChemInform, 2005, 36, no.	0.1	0
116	Quantifying the shifts in physicochemical property space introduced by the metabolism of small organic molecules. Journal of Cheminformatics, 2013, 5, .	2.8	0
117	Editorial for the Special Section "Artificial Intelligence in Drug Discovery". Drug Discovery Today: Technologies, 2019, 32-33, 1-2.	4.0	0
118	Anti-cancer Drug Development: Computational Strategies to Identify and Target Proteins Involved in Cancer Metabolism. Current Pharmaceutical Design, 2012, 19, 532-577.	0.9	0