Sean Ekins

List of Publications by Year
in descending order

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351 papers	16,811 citations	11651 70 h-index	30087 103 g-index
439 all docs	439 docs citations	439 times ranked	14617 citing authors

#	Article	IF	Citations
1	In silico pharmacology for drug discovery: methods for virtual ligand screening and profiling. British Journal of Pharmacology, 2007, 152, 9-20.	5.4	522
2	Exploiting machine learning for end-to-end drug discovery and development. Nature Materials, 2019, 18, 435-441.	27.5	334
3	Three-Dimensional Quantitative Structure-Activity Relationship for Inhibition of Human Ether-a-Go-Go-Related Gene Potassium Channel. Journal of Pharmacology and Experimental Therapeutics, 2002, 301, 427-434.	2.5	282
4	In silico pharmacology for drug discovery: applications to targets and beyond. British Journal of Pharmacology, 2007, 152, 21-37.	5.4	269
5	In silico repositioning of approved drugs for rare and neglected diseases. Drug Discovery Today, 2011, 16, 298-310.	6.4	269
6	Comparison of Deep Learning With Multiple Machine Learning Methods and Metrics Using Diverse Drug Discovery Data Sets. Molecular Pharmaceutics, 2017, 14, 4462-4475.	4.6	249
7	Progress in predicting human ADME parameters in silico. Journal of Pharmacological and Toxicological Methods, 2000, 44, 251-272.	0.7	240
8	Pathway Mapping Tools for Analysis of High Content Data. , 2007, 356, 319-350.		206
9	Application of Three-Dimensional Quantitative Structure-Activity Relationships of P-Glycoprotein Inhibitors and Substrates. Molecular Pharmacology, 2002, 61, 974-981.	2.3	204
10	The Next Era: Deep Learning in Pharmaceutical Research. Pharmaceutical Research, 2016, 33, 2594-2603.	3.5	180
11	Three-Dimensional Quantitative Structure-Activity Relationships of Inhibitors of P-Glycoprotein. Molecular Pharmacology, 2002, 61, 964-973.	2.3	179
12	Techniques: Application of systems biology to absorption, distribution, metabolism, excretion and toxicity. Trends in Pharmacological Sciences, 2005, 26, 202-209.	8.7	179
13	Present and future in vitro approaches for drug metabolism. Journal of Pharmacological and Toxicological Methods, 2000, 44, 313-324.	0.7	169
14	THE ROLE OF CYP2B6 IN HUMAN XENOBIOTIC METABOLISM*. Drug Metabolism Reviews, 1999, 31, 719-754.	3.6	168
15	A bibliometric review of drug repurposing. Drug Discovery Today, 2018, 23, 661-672.	6.4	163
16	A Pharmacophore for Human Pregnane X Receptor Ligands. Drug Metabolism and Disposition, 2002, 30, 96-99.	3.3	160
17	Design, Synthesis, Cytoselective Toxicity, Structureâ€“Activity Relationships, and Pharmacophore of Thiazolidinone Derivatives Targeting Drug-Resistant Lung Cancer Cells. Journal of Medicinal Chemistry, 2008, 51, 1242-1251.	6.4	155
18	In vitro and pharmacophore insights into CYP3A enzymes. Trends in Pharmacological Sciences, 2003, 24, 161-166.	8.7	145

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19	Predicting undesirable drug interactions with promiscuous proteins in silico. Drug Discovery Today, 2004, 9, 276-285.	6.4	144
20	Human Pregnane X Receptor Antagonists and Agonists Define Molecular Requirements for Different Binding Sites. Molecular Pharmacology, 2007, 72, 592-603.	2.3	143
21	Rapid Identification of P-glycoprotein Substrates and Inhibitors. Drug Metabolism and Disposition, 2006, 34, 1976-1984.	3.3	136
22	Cross-reactivity of steroid hormone immunoassays: clinical significance and two-dimensional molecular similarity prediction. BMC Clinical Pathology, 2014, 14, 33.	1.8	132
23	A novel method for generation of signature networks as biomarkers from complex high throughput data. Toxicology Letters, 2005, 158, 20-29.	0.8	129
24	A critical overview of computational approaches employed for COVID-19 drug discovery. Chemical Society Reviews, 2021, 50, 9121-9151.	38.1	128
25	Novel web-based tools combining chemistry informatics, biology and social networks for drug discovery. Drug Discovery Today, 2009, 14, 261-270.	6.4	126
26	Algorithms for network analysis in systems-ADME/Tox using the MetaCore and MetaDrug platforms. Xenobiotica, 2006, 36, 877-901.	1.1	125
27	Pharmacophore modeling of cytochromes P450. Advanced Drug Delivery Reviews, 2002, 54, 367-383.	13.7	123
28	Comparing Multiple Machine Learning Algorithms and Metrics for Estrogen Receptor Binding Prediction. Molecular Pharmaceutics, 2018, 15, 4361-4370.	4.6	120
29	Non-classical transpeptidases yield insight into new antibacterials. Nature Chemical Biology, 2017, 13, 54-61.	8.0	116
30	Influence of Molecular Structure on Substrate Binding to the Human Organic Cation Transporter, hOCT1. Molecular Pharmacology, 2003, 63, 489-498.	2.3	110
31	A COMBINED APPROACH TO DRUG METABOLISM AND TOXICITY ASSESSMENT. Drug Metabolism and Disposition, 2006, 34, 495-503.	3.3	108
32	The importance of discerning shape in molecular pharmacology. Trends in Pharmacological Sciences, 2009, 30, 138-147.	8.7	106
33	A Predictive Ligand-Based Bayesian Model for Human Drug-Induced Liver Injury. Drug Metabolism and Disposition, 2010, 38, 2302-2308.	3.3	106
34	Challenges Predicting Ligand-Receptor Interactions of Promiscuous Proteins: The Nuclear Receptor PXR. PLoS Computational Biology, 2009, 5, e1000594.	3.2	102
35	Towards a gold standard: regarding quality in public domain chemistry databases and approaches to improving the situation. Drug Discovery Today, 2012, 17, 685-701.	6.4	102
36	Pharmacophore-based discovery of ligands for drug transporters. Advanced Drug Delivery Reviews, 2006, 58, 1431-1450.	13.7	101

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37	Molecular Determinants of Substrate/Inhibitor Binding to the Human and Rabbit Renal Organic Cation Transporters hOCT2 and rbOCT2. Molecular Pharmacology, 2005, 67, 1067-1077.	2.3	96
38	Evolution of promiscuous nuclear hormone receptors: LXR, FXR, VDR, PXR, and CAR. Molecular and Cellular Endocrinology, 2011, 334, 39-48.	3.2	96
39	New Predictive Models for Bloodâ€“Brain Barrier Permeability of Drug-like Molecules. Pharmaceutical Research, 2008, 25, 1836-1845.	3.5	95
40	Open Source Bayesian Models. 1. Application to ADME/Tox and Drug Discovery Datasets. Journal of Chemical Information and Modeling, 2015, 55, 1231-1245.	5.4	95
41	GENERATION AND VALIDATION OF RAPID COMPUTATIONAL FILTERS FOR CYP2D6 AND CYP3A4. Drug Metabolism and Disposition, 2003, 31, 1077-1080.	3.3	94
42	Examination of purported probes of human CYP2B6. Pharmacogenetics and Genomics, 1997, 7, 165-179.	5.7	93
43	A ligand-based approach to understanding selectivity of nuclear hormone receptors PXR, CAR, FXR, LXRalpha, and LXRbeta. Pharmaceutical Research, 2002, 19, 1788-1800.	3.5	93
44	Dual use of artificial-intelligence-powered drug discovery. Nature Machine Intelligence, 2022, 4, 189-191.	16.0	93
45	Evolution of pharmacologic specificity in the pregnane X receptor. BMC Evolutionary Biology, 2008, 8, 103.	3.2	92
46	Effects of Antipsychotic Drugs on Ito, INa, Isus, IK1, and hERG: QT Prolongation, Structure Activity Relationship, and Network Analysis. Pharmaceutical Research, 2006, 23, 1133-1143.	3.5	91
47	Evolution of the bile salt nuclear receptor FXR in vertebrates*. Journal of Lipid Research, 2008, 49, 1577-1587.	4.2	91
48	Progress in computational toxicology. Journal of Pharmacological and Toxicological Methods, 2014, 69, 115-140.	0.7	91
49	Comparative Pharmacophore Modeling of Organic Anion Transporting Polypeptides: A Meta-Analysis of Rat Oatp1a1 and Human OATP1B1. Journal of Pharmacology and Experimental Therapeutics, 2005, 314, 533-541.	2.5	90
50	Repurposing Quaternary Ammonium Compounds as Potential Treatments for COVID-19. Pharmaceutical Research, 2020, 37, 104.	3.5	90
51	Computational Models for Drug Inhibition of the Human Apical Sodium-Dependent Bile Acid Transporter. Molecular Pharmaceutics, 2009, 6, 1591-1603.	4.6	89
52	A quality alert and call for improved curation of public chemistry databases. Drug Discovery Today, 2011, 16, 747-750.	6.4	88
53	Insights for Human Ether-a-Go-Go-Related Gene Potassium Channel Inhibition Using Recursive Partitioning and Kohonen and Sammon Mapping Techniques. Journal of Medicinal Chemistry, 2006, 49, 5059-5071.	6.4	87
54	Bayesian Models Leveraging Bioactivity and Cytotoxicity Information for Drug Discovery. Chemistry and Biology, 2013, 20, 370-378.	6.0	87

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55	Structureâ€“Activity Relationship for FDA Approved Drugs As Inhibitors of the Human Sodium Taurocholate Cotransporting Polypeptide (NTCP). Molecular Pharmaceutics, 2013, 10, 1008-1019.	4.6	86
56	Towards a new age of virtual ADME/TOX and multidimensional drug discovery. Journal of Computer-Aided Molecular Design, 2002, 16, 381-401.	2.9	85
57	Evolving molecules using multi-objective optimization: applying to ADME/Tox. Drug Discovery Today, 2010, 15, 451-460.	6.4	85
58	Using Open Source Computational Tools for Predicting Human Metabolic Stability and Additional Absorption, Distribution, Metabolism, Excretion, and Toxicity Properties. Drug Metabolism and Disposition, 2010, 38, 2083-2090.	3.3	83
59	Comparing and Validating Machine Learning Models for Mycobacterium tuberculosis Drug Discovery. Molecular Pharmaceutics, 2018, 15, 4346-4360.	4.6	83
60	Past, Present, and Future Applications of Precision-Cut Liver Slices for in Vitro Xenobiotic Metabolism. Drug Metabolism Reviews, 1996, 28, 591-623.	3.6	82
61	Computational databases, pathway and cheminformatics tools for tuberculosis drug discovery. Trends in Microbiology, 2011, 19, 65-74.	7.7	82
62	DÃ©jÃ vu: Stimulating open drug discovery for SARS-CoV-2. Drug Discovery Today, 2020, 25, 928-941.	6.4	81
63	A collaborative database and computational models for tuberculosis drug discovery. Molecular BioSystems, 2010, 6, 840.	2.9	80
64	Machine learning models identify molecules active against the Ebola virus in vitro. F1000Research, 2015, 4, 1091.	1.6	80
65	Computational prediction of human drug metabolism. Expert Opinion on Drug Metabolism and Toxicology, 2005, 1, 303-324.	3.3	78
66	Discovery of Novel Antimalarial Compounds Enabled by QSAR-Based Virtual Screening. Journal of Chemical Information and Modeling, 2013, 53, 475-492.	5.4	77
67	Assessment of Substrate-Dependent Ligand Interactions at the Organic Cation Transporter OCT2 Using Six Model Substrates. Molecular Pharmacology, 2018, 94, 1057-1068.	2.3	77
68	Modeling of active transport systems. Advanced Drug Delivery Reviews, 2002, 54, 329-354.	13.7	76
69	Chemical target and pathway toxicity mechanisms defined in primary human cell systems. Journal of Pharmacological and Toxicological Methods, 2010, 61, 3-15.	0.7	75
70	Three-Dimensional Quantitative Structure Activity Relationship for Cyp2d6 Substrates. QSAR and Combinatorial Science, 2002, 21, 357-368.	1.2	74
71	Shape Signatures: New Descriptors for Predicting Cardiotoxicity In Silico. Chemical Research in Toxicology, 2008, 21, 1304-1314.	3.3	74
72	Molecular Determinants of Ligand Selectivity for the Human Multidrug and Toxin Extruder Proteins MATE1 and MATE2-K. Journal of Pharmacology and Experimental Therapeutics, 2012, 341, 743-755.	2.5	74

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73	Machine Learning Models and Pathway Genome Data Base for Trypanosoma cruzi Drug Discovery. PLoS Neglected Tropical Diseases, 2015, 9, e0003878.	3.0	74
74	Open Source Bayesian Models. 2. Mining a â€œBig Datasetâ€•To Create and Validate Models with ChEMBL. Journal of Chemical Information and Modeling, 2015, 55, 1246-1260.	5.4	73
75	A Comprehensive in Vitro and in Silico Analysis of Antibiotics That Activate Pregnane X Receptor and Induce CYP3A4 in Liver and Intestine. Drug Metabolism and Disposition, 2008, 36, 1689-1697.	3.3	72
76	Thiophenecarboxamide Derivatives Activated by EthA Kill Mycobacterium tuberculosis by Inhibiting the CTP Synthetase PyrG. Chemistry and Biology, 2015, 22, 917-927.	6.0	72
77	Analysis and hit filtering of a very large library of compounds screened against Mycobacterium tuberculosis. Molecular BioSystems, 2010, 6, 2316-2324.	2.9	69
78	Opportunities and challenges using artificial intelligence in ADME/Tox. Nature Materials, 2019, 18, 418-422.	27.5	69
79	In silico approaches to predicting drug metabolism, toxicology and beyond. Biochemical Society Transactions, 2003, 31, 611-614.	3.4	68
80	PXR and the regulation of apoA1 and HDL-cholesterol in rodents. Pharmacological Research, 2004, 50, 237-246.	7.1	68
81	In Vitro and Pharmacophore-Based Discovery of Novel hPEPT1 Inhibitors. Pharmaceutical Research, 2005, 22, 512-517.	3.5	68
82	Computational Discovery of Novel Low Micromolar Human Pregnane X Receptor Antagonists. Molecular Pharmacology, 2008, 74, 662-672.	2.3	68
83	Intrinsic Disorder in Nuclear Hormone Receptors. Journal of Proteome Research, 2008, 7, 4359-4372.	3.7	67
84	Machine Learning Methods and Docking for Predicting Human Pregnane X Receptor Activation. Chemical Research in Toxicology, 2008, 21, 1457-1467.	3.3	65
85	Optimizing Higher Throughput Methods to Assess Drug-Drug Interactions for CYP1A2, CYP2C9, CYP2C19, CYP2D6, rCYP2D6, and CYP3A4 In Vitro Using a Single Point IC50. Journal of Biomolecular Screening, 2002, 7, 373-382.	2.6	64
86	Computational Approaches That Predict Metabolic Intermediate Complex Formation with CYP3A4 (+b5). Drug Metabolism and Disposition, 2007, 35, 1466-1475.	3.3	63
87	Precompetitive preclinical ADME/Tox data: set it free on the web to facilitate computational model building and assist drug development. Lab on A Chip, 2010, 10, 13-22.	6.0	63
88	CATMoS: Collaborative Acute Toxicity Modeling Suite. Environmental Health Perspectives, 2021, 129, 47013.	6.0	63
89	STRUCTURAL BIOLOGY AND FUNCTION OF SOLUTE TRANSPORTERS: IMPLICATIONS FOR IDENTIFYING AND DESIGNING SUBSTRATES. Drug Metabolism Reviews, 2002, 34, 709-750.	3.6	62
90	Application of in silico approaches to predicting drugâ€“drug interactions. Journal of Pharmacological and Toxicological Methods, 2001, 45, 65-69.	0.7	61

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91	Computational Models to Assign Biopharmaceutics Drug Disposition Classification from Molecular Structure. Pharmaceutical Research, 2007, 24, 2249-2262.	3.5	61
92	Using molecular similarity to highlight the challenges of routine immunoassay-based drug of abuse/toxicology screening in emergency medicine. BMC Emergency Medicine, 2009, 9, 5.	1.9	60
93	Ligand specificity and evolution of liver X receptors. Journal of Steroid Biochemistry and Molecular Biology, 2008, 110, 83-94.	2.5	58
94	Bacterial Peptide Recognition and Immune Activation Facilitated by Human Peptide Transporter PEPT2. American Journal of Respiratory Cell and Molecular Biology, 2008, 39, 536-542.	2.9	58
95	Elucidating the â€˜Jekyll and Hydeâ€™ Nature of PXR: The Case for Discovering Antagonists or Allosteric Antagonists. Pharmaceutical Research, 2009, 26, 1807-1815.	3.5	58
96	Future directions for drug transporter modelling. Xenobiotica, 2007, 37, 1152-1170.	1.1	57
97	Essential Metabolites of Mycobacterium tuberculosis and Their Mimics. MBio, 2011, 2, e00301-10.	4.1	56
98	Machine learning models identify molecules active against the Ebola virus in vitro. F1000Research, 2015, 4, 1091.	1.6	56
99	Repurposing the Ebola and Marburg Virus Inhibitors Tilorone, Quinacrine, and Pyronaridine: In Vitro Activity against SARS-CoV-2 and Potential Mechanisms. ACS Omega, 2021, 6, 7454-7468.	3.5	56
100	KOHONEN MAPS FOR PREDICTION OF BINDING TO HUMAN CYTOCHROME P450 3A4. Drug Metabolism and Disposition, 2004, 32, 1183-1189.	3.3	55
101	Systems-ADME/Tox: Resources and network approaches. Journal of Pharmacological and Toxicological Methods, 2006, 53, 38-66.	0.7	55
102	Comparing Machine Learning Algorithms for Predicting Drug-Induced Liver Injury (DILI). Molecular Pharmaceutics, 2020, 17, 2628-2637.	4.6	55
103	Integrated in Silicoâ^'in Vitro Strategy for Addressing Cytochrome P450 3A4 Time-Dependent Inhibition. Chemical Research in Toxicology, 2010, 23, 664-676.	3.3	54
104	Ten Simple Rules of Live Tweeting at Scientific Conferences. PLoS Computational Biology, 2014, 10, e1003789.	3.2	54
105	A common feature pharmacophore for FDA-approved drugs inhibiting the Ebola virus. F1000Research, 2014, 3, 277.	1.6	54
106	Hybrid Scoring and Classification Approaches to Predict Human Pregnane X Receptor Activators. Pharmaceutical Research, 2009, 26, 1001-1011.	3.5	53
107	Reaching Out to Collaborators: Crowdsourcing for Pharmaceutical Research. Pharmaceutical Research, 2010, 27, 393-395.	3.5	52
108	Quantitative Structure Activity Relationships for the Glucuronidation of Simple Phenols by Expressed Human UGT1A6 and UGT1A9. Drug Metabolism and Disposition, 2002, 30, 734-738.	3.3	51

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109	Enhancing Hit Identification in Mycobacterium tuberculosis Drug Discovery Using Validated Dual-Event Bayesian Models. PLoS ONE, 2013, 8, e63240.	2.5	51
110	Efficacy of Tilorone Dihydrochloride against Ebola Virus Infection. Antimicrobial Agents and Chemotherapy, 2018, 62, .	3.2	51
111	Halogenated ligands and their interactions with amino acids: Implications for structureâ€“activity and structureâ€“toxicity relationships. Journal of Molecular Graphics and Modelling, 2008, 27, 170-177.	2.4	50
112	Targeting Mycobacterium tuberculosis Topoisomerase I by Small-Molecule Inhibitors. Antimicrobial Agents and Chemotherapy, 2015, 59, 1549-1557.	3.2	50
113	Open drug discovery for the Zika virus. F1000Research, 2016, 5, 150.	1.6	50
114	A NOVEL METHOD FOR VISUALIZING NUCLEAR HORMONE RECEPTOR NETWORKS RELEVANT TO DRUG METABOLISM. Drug Metabolism and Disposition, 2005, 33, 474-481.	3.3	49
115	Ebola Virus Bayesian Machine Learning Models Enable New in Vitro Leads. ACS Omega, 2019, 4, 2353-2361.	3.5	49
116	Multiple Machine Learning Comparisons of HIV Cell-based and Reverse Transcriptase Data Sets. Molecular Pharmaceutics, 2019, 16, 1620-1632.	4.6	49
117	Finding Promiscuous Old Drugs for New Uses. Pharmaceutical Research, 2011, 28, 1785-1791.	3.5	48
118	Combining Computational Methods for Hit to Lead Optimization in Mycobacterium Tuberculosis Drug Discovery. Pharmaceutical Research, 2014, 31, 414-435.	3.5	48
119	The Aâ€“Z of Zika drug discovery. Drug Discovery Today, 2018, 23, 1833-1847.	6.4	48
120	The Natural Product Eugenol Is an Inhibitor of the Ebola Virus In Vitro. Pharmaceutical Research, 2019, 36, 104.	3.5	47
121	Three-Dimensional Quantitative Structure-Permeability Relationship Analysis for a Series of Inhibitors of Rhinovirus Replication. Journal of Chemical Information and Computer Sciences, 2001, 41, 1578-1586.	2.8	46
122	Comprehensive Computational Assessment of ADME Properties Using Mapping Techniques. Current Drug Discovery Technologies, 2005, 2, 99-113.	1.2	46
123	Molecular Characterization of CYP2B6 Substrates. Current Drug Metabolism, 2008, 9, 363-373.	1.2	46
124	Inhibition of Mycobacterium tuberculosis topoisomerase I by m-AMSA, a eukaryotic type II topoisomerase poison. Biochemical and Biophysical Research Communications, 2014, 446, 916-920.	2.1	46
125	Mobile apps for chemistry in the world of drug discovery. Drug Discovery Today, 2011, 16, 928-939.	6.4	44
126	Computational mapping tools for drug discovery. Drug Discovery Today, 2009, 14, 767-775.	6.4	43

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127	Troubleshooting computational methods in drug discovery. Journal of Pharmacological and Toxicological Methods, 2010, 61, 67-75.	0.7	43
128	Predicting Mouse Liver Microsomal Stability with â€œPrunedâ€•Machine Learning Models and Public Data. Pharmaceutical Research, 2016, 33, 433-449.	3.5	43
129	QUANTITATIVE STRUCTURE-METABOLISM RELATIONSHIP MODELING OF METABOLIC N-DEALKYLATION REACTION RATES. Drug Metabolism and Disposition, 2004, 32, 1111-1120.	3.3	42
130	Identification and Validation of Novel Human Pregnane X Receptor Activators among Prescribed Drugs via Ligand-Based Virtual Screening. Drug Metabolism and Disposition, 2011, 39, 337-344.	3.3	42
131	Applications and Limitations of In Silico Models in Drug Discovery. Methods in Molecular Biology, 2012, 910, 87-124.	0.9	42
132	Repurposing the antimalarial pyronaridine tetraphosphate to protect against Ebola virus infection. PLoS Neglected Tropical Diseases, 2019, 13, e0007890.	3.0	42
133	Quantum Machine Learning Algorithms for Drug Discovery Applications. Journal of Chemical Information and Modeling, 2021, 61, 2641-2647.	5.4	42
134	The Major Human Pregnane X Receptor (PXR) Splice Variant, PXR.2, Exhibits Significantly Diminished Ligand-Activated Transcriptional Regulation. Drug Metabolism and Disposition, 2009, 37, 1295-1304.	3.3	41
135	Looking Back to the Future: Predicting in Vivo Efficacy of Small Molecules versus Mycobacterium tuberculosis. Journal of Chemical Information and Modeling, 2014, 54, 1070-1082.	5.4	41
136	A multitarget approach to drug discovery inhibiting Mycobacterium tuberculosis PyrG and PanK. Scientific Reports, 2018, 8, 3187.	3.3	41
137	Chemoinformatic Methods for Predicting Interference in Drug of Abuse/Toxicology Immunoassays. Clinical Chemistry, 2009, 55, 1203-1213.	3.2	39
138	The evolution of farnesoid X, vitamin D, and pregnane X receptors: insights from the green-spotted pufferfish (Tetraodon nigriviridis) and other non-mammalian species. BMC Biochemistry, 2011, 12, 5.	4.4	39
139	Incorporating Green Chemistry Concepts into Mobile Chemistry Applications and Their Potential Uses. ACS Sustainable Chemistry and Engineering, 2013, 1, 8-13.	6.7	39
140	Tilorone: a Broad-Spectrum Antiviral Invented in the USA and Commercialized in Russia and beyond. Pharmaceutical Research, 2020, 37, 71.	3.5	39
141	Dispensing Processes Impact Apparent Biological Activity as Determined by Computational and Statistical Analyses. PLoS ONE, 2013, 8, e62325.	2.5	39
142	Molecular Cloning, Expression, and Characterization of CYP2D17 from Cynomolgus Monkey Liver. Archives of Biochemistry and Biophysics, 1999, 372, 189-196.	3.0	38
143	Development of Computational Models for Enzymes, Transporters, Channels, and Receptors Relevant to ADME/Tox. Reviews in Computational Chemistry, 2004, , 333-415.	1.5	38
144	Human Immunodeficiency Virus Protease Inhibitors Interact with ATP Binding Cassette Transporter 4/Multidrug Resistance Protein 4: A Basis for Unanticipated Enhanced Cytotoxicity. Molecular Pharmacology, 2013, 84, 361-371.	2.3	38

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145	Molecular Similarity Methods for Predicting Cross-Reactivity With Therapeutic Drug Monitoring Immunoassays. Therapeutic Drug Monitoring, 2009, 31, 337-344.	2.0	37
146	Illustrating and homology modeling the proteins of the Zika virus. F1000Research, 2016, 5, 275.	1.6	37
147	Synergistic Lethality of a Binary Inhibitor of Mycobacterium tuberculosis KasA. MBio, 2018, 9, .	4.1	37
148	High Throughput and Computational Repurposing for Neglected Diseases. Pharmaceutical Research, 2019, 36, 27.	3.5	37
149	Prediction of Human Drug Metabolizing Enzyme Induction. Current Drug Metabolism, 2003, 4, 381-391.	1.2	37
150	Methods for Predicting Human Drug Metabolism. Advances in Clinical Chemistry, 2007, 43, 131-176.	3.7	36
151	Novel Inhibitors of Human Organic Cation/Carnitine Transporter (hOCTN2) via Computational Modeling and In Vitro Testing. Pharmaceutical Research, 2009, 26, 1890-1900.	3.5	36
152	When pharmaceutical companies publish large datasets: an abundance of riches or fool's gold?. Drug Discovery Today, 2010, 15, 812-815.	6.4	36
153	Multifaceted roles of ultra-rare and rare disease patients/parents in drug discovery. Drug Discovery Today, 2013, 18, 1043-1051.	6.4	36
154	Are Bigger Data Sets Better for Machine Learning? Fusing Single-Point and Dual-Event Dose Response Data for Mycobacterium tuberculosis. Journal of Chemical Information and Modeling, 2014, 54, 2157-2165.	5.4	36
155	Validating New Tuberculosis Computational Models with Public Whole Cell Screening Aerobic Activity Datasets. Pharmaceutical Research, 2011, 28, 1859-1869.	3.5	35
156	A Virtual Screen Discovers Novel, Fragment-Sized Inhibitors of Mycobacterium tuberculosis InhA. Journal of Chemical Information and Modeling, 2015, 55, 645-659.	5.4	35
157	A hybrid approach to advancing quantitative prediction of tissue distribution of basic drugs in human. Toxicology and Applied Pharmacology, 2011, 250, 194-212.	2.8	34
158	Bayesian models for screening and TB Mobile for target inference with Mycobacterium tuberculosis. Tuberculosis, 2014, 94, 162-169.	1.9	34
159	A Phenotypic Based Target Screening Approach Delivers New Antitubercular CTP Synthetase Inhibitors. ACS Infectious Diseases, 2017, 3, 428-437.	3.8	34
160	Why Wait? The Case for Treating Tuberculosis with Inhaled Drugs. Pharmaceutical Research, 2019, 36, 166.	3.5	34
161	Evaluation of Computational Docking to Identify Pregnane X Receptor Agonists in the ToxCast Database. Environmental Health Perspectives, 2010, 118, 1412-1417.	6.0	33
162	In silico methods for predicting drugâ€“drug interactions with cytochrome P-450s, transporters and beyond. Advanced Drug Delivery Reviews, 2015, 86, 46-60.	13.7	33

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163	Repurposing Approved Drugs as Inhibitors of Kv7.1 and Nav1.8 to Treat Pitt Hopkins Syndrome. Pharmaceutical Research, 2019, 36, 137.	3.5	33
164	Back to the future: Advances in development of broad-spectrum capsid-binding inhibitors of enteroviruses. European Journal of Medicinal Chemistry, 2019, 178, 606-622.	5.5	33
165	Small molecules with antiviral activity against the Ebola virus. F1000Research, 2015, 4, 38.	1.6	33
166	OpenZika: An IBM World Community Grid Project to Accelerate Zika Virus Drug Discovery. PLoS Neglected Tropical Diseases, 2016, 10, e0005023.	3.0	33
167	Reengineering the pharmaceutical industry by crash-testing molecules. Drug Discovery Today, 2005, 10, 1191-1200.	6.4	32
168	Open Drug Discovery Teams: A Chemistry Mobile App for Collaboration. Molecular Informatics, 2012, 31, 585-597.	2.5	32
169	A generalizable pre-clinical research approach for orphan disease therapy. Orphanet Journal of Rare Diseases, 2012, 7, 39.	2.7	32
170	Four disruptive strategies for removing drug discovery bottlenecks. Drug Discovery Today, 2013, 18, 265-271.	6.4	32
171	New target prediction and visualization tools incorporating open source molecular fingerprints for TB Mobile 2.0. Journal of Cheminformatics, 2014, 6, 38.	6.1	32
172	Molecular dynamics simulations of Zika virus NS3 helicase: Insights into RNA binding site activity. Biochemical and Biophysical Research Communications, 2017, 492, 643-651.	2.1	32
173	Tilorone, a Broad-Spectrum Antiviral for Emerging Viruses. Antimicrobial Agents and Chemotherapy, 2020, 64, .	3.2	32
174	Remdesivir and EIDD-1931 Interact with Human Equilibrative Nucleoside Transporters 1 and 2: Implications for Reaching SARS-CoV-2 Viral Sanctuary Sites. Molecular Pharmacology, 2021, 100, 548-557.	2.3	32
175	Quantitative Structure Activity Relationship for Inhibition of Human Organic Cation/Carnitine Transporter. Molecular Pharmaceutics, 2010, 7, 2120-2131.	4.6	31
176	Machine Learning Models Identify Inhibitors of SARS-CoV-2. Journal of Chemical Information and Modeling, 2021, 61, 4224-4235.	5.4	31
177	Application of data mining approaches to drug delivery. Advanced Drug Delivery Reviews, 2006, 58, 1409-1430.	13.7	30
178	Industrializing rare disease therapy discovery and development. Nature Biotechnology, 2017, 35, 117-118.	17.5	30
179	Repurposing Quinacrine against Ebola Virus Infection In Vivo. Antimicrobial Agents and Chemotherapy, 2019, 63, .	3.2	30
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