

Sean Ekins

List of Publications by Year in descending order

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Version: 2024-02-01

351
papers

16,811
citations

11639

70
h-index

30058

103
g-index

439
all docs

439
docs citations

439
times ranked

14617
citing authors

#	ARTICLE	IF	CITATIONS
1	Knowledge-based approaches to drug discovery for rare diseases. <i>Drug Discovery Today</i> , 2022, 27, 490-502.	3.2	15
2	<i>Mycobacterium abscessus</i> drug discovery using machine learning. <i>Tuberculosis</i> , 2022, 132, 102168.	0.8	5
3	Response to Comments on "Remdesivir and EIDD-1931 Interact with Human Equilibrative Nucleoside Transporters 1 and 2: Implications for Reaching SARS-CoV-2 Viral Sanctuary Sites". <i>Molecular Pharmacology</i> , 2022, 101, 121-122.	1.0	1
4	Chalcones from <i>Angelica keiskei</i> (ashitaba) inhibit key Zika virus replication proteins. <i>Bioorganic Chemistry</i> , 2022, 120, 105649.	2.0	13
5	The commoditization of AI for molecule design. <i>Artificial Intelligence in the Life Sciences</i> , 2022, 2, 100031.	1.6	4
6	Dual use of artificial-intelligence-powered drug discovery. <i>Nature Machine Intelligence</i> , 2022, 4, 189-191.	8.3	93
7	Machine Learning Models for <i>Mycobacterium tuberculosis</i> In Vitro Activity: Prediction and Target Visualization. <i>Molecular Pharmaceutics</i> , 2022, 19, 674-689.	2.3	8
8	Pyronaridine Protects against SARS-CoV-2 Infection in Mouse. <i>ACS Infectious Diseases</i> , 2022, 8, 1147-1160.	1.8	14
9	MegaSyn: Integrating Generative Molecular Design, Automated Analog Designer, and Synthetic Viability Prediction. <i>ACS Omega</i> , 2022, 7, 18699-18713.	1.6	13
10	Lack of an Effect of Polysorbate 80 on Intestinal Drug Permeability in Humans. <i>Pharmaceutical Research</i> , 2022, 39, 1881-1890.	1.7	7
11	<i>Rickettsia</i> Aglow: A Fluorescence Assay and Machine Learning Model to Identify Inhibitors of Intracellular Infection. <i>ACS Infectious Diseases</i> , 2022, 8, 1280-1290.	1.8	2
12	A teachable moment for dual-use. <i>Nature Machine Intelligence</i> , 2022, 4, 607-607.	8.3	6
13	Dispirotriperazine-core compounds, their biological activity with a focus on broad antiviral property, and perspectives in drug design (mini-review). <i>European Journal of Medicinal Chemistry</i> , 2021, 211, 113014.	2.6	13
14	Predicting Drug Interactions with Human Equilibrative Nucleoside Transporters 1 and 2 Using Functional Knockout Cell Lines and Bayesian Modeling. <i>Molecular Pharmacology</i> , 2021, 99, 147-162.	1.0	15
15	Enzyme Replacement Therapy for Mucopolysaccharidosis IIID using Recombinant Human β -N-Acetylglucosamine-6-Sulfatase in Neonatal Mice. <i>Molecular Pharmaceutics</i> , 2021, 18, 214-227.	2.3	8
16	Bioactivity Comparison across Multiple Machine Learning Algorithms Using over 5000 Datasets for Drug Discovery. <i>Molecular Pharmaceutics</i> , 2021, 18, 403-415.	2.3	25
17	Using Bibliometric Analysis and Machine Learning to Identify Compounds Binding to Sialidase-1. <i>ACS Omega</i> , 2021, 6, 3186-3193.	1.6	11
18	A Machine Learning Strategy for Drug Discovery Identifies Anti-Schistosomal Small Molecules. <i>ACS Infectious Diseases</i> , 2021, 7, 406-420.	1.8	18

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19	The Antiviral Drug Tilorone Is a Potent and Selective Inhibitor of Acetylcholinesterase. <i>Chemical Research in Toxicology</i> , 2021, 34, 1296-1307.	1.7	15
20	Devising effective enzyme replacement therapy for infantile onset neuronal ceroid lipofuscinosis (CLN1 disease). <i>Molecular Genetics and Metabolism</i> , 2021, 132, S28.	0.5	2
21	Repurposing the Ebola and Marburg Virus Inhibitors Tilorone, Quinacrine, and Pyronaridine: <i>In Vitro</i> Activity against SARS-CoV-2 and Potential Mechanisms. <i>ACS Omega</i> , 2021, 6, 7454-7468.	1.6	56
22	Flavonoids from <i>Pterogyne nitens</i> as Zika virus NS2B-NS3 protease inhibitors. <i>Bioorganic Chemistry</i> , 2021, 109, 104719.	2.0	26
23	CATMoS: Collaborative Acute Toxicity Modeling Suite. <i>Environmental Health Perspectives</i> , 2021, 129, 47013.	2.8	63
24	Discovery of 5-Nitro-6-thiocyanatopyrimidines as Inhibitors of <i>Cryptococcus neoformans</i> and <i>Cryptococcus gattii</i> . <i>ACS Medicinal Chemistry Letters</i> , 2021, 12, 774-781.	1.3	5
25	Multiple Computational Approaches for Predicting Drug Interactions with Human Equilibrative Nucleoside Transporter 1. <i>Drug Metabolism and Disposition</i> , 2021, 49, 479-489.	1.7	9
26	Quantum Machine Learning Algorithms for Drug Discovery Applications. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 2641-2647.	2.5	42
27	Comparing the Pfizer Central Nervous System Multiparameter Optimization Calculator and a BBB Machine Learning Model. <i>ACS Chemical Neuroscience</i> , 2021, 12, 2247-2253.	1.7	9
28	Metabolomic and transcriptomic analysis reveals endogenous substrates and metabolic adaptation in rats lacking <i>Abcg2</i> and <i>Abcb1a</i> transporters. <i>PLoS ONE</i> , 2021, 16, e0253852.	1.1	6
29	Development of Machine Learning Models and the Discovery of a New Antiviral Compound against Yellow Fever Virus. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 3804-3813.	2.5	16
30	Cationic Compounds with SARS-CoV-2 Antiviral Activity and Their Interaction with Organic Cation Transporter/Multidrug and Toxin Extruder Secretory Transporters. <i>Journal of Pharmacology and Experimental Therapeutics</i> , 2021, 379, 96-107.	1.3	7
31	Machine Learning Models Identify Inhibitors of SARS-CoV-2. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 4224-4235.	2.5	31
32	Bayesian Modeling and Intrabacterial Drug Metabolism Applied to Drug-Resistant <i>Staphylococcus aureus</i> . <i>ACS Infectious Diseases</i> , 2021, 7, 2508-2521.	1.8	8
33	Defending Antiviral Cationic Amphiphilic Drugs That May Cause Drug-Induced Phospholipidosis. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 4125-4130.	2.5	14
34	Remdesivir and EIDD-1931 Interact with Human Equilibrative Nucleoside Transporters 1 and 2: Implications for Reaching SARS-CoV-2 Viral Sanctuary Sites. <i>Molecular Pharmacology</i> , 2021, 100, 548-557.	1.0	32
35	Recent advances in drug repurposing using machine learning. <i>Current Opinion in Chemical Biology</i> , 2021, 65, 74-84.	2.8	28
36	A critical overview of computational approaches employed for COVID-19 drug discovery. <i>Chemical Society Reviews</i> , 2021, 50, 9121-9151.	18.7	128

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37	UV-adVISor: Attention-Based Recurrent Neural Networks to Predict UV-Vis Spectra. <i>Analytical Chemistry</i> , 2021, 93, 16076-16085.	3.2	9
38	Antitubercular Triazines: Optimization and Intrabacterial Metabolism. <i>Cell Chemical Biology</i> , 2020, 27, 172-185.e11.	2.5	22
39	Comparison of Machine Learning Models for the Androgen Receptor. <i>Environmental Science & Technology</i> , 2020, 54, 13690-13700.	4.6	17
40	Evaluation of Assay Central Machine Learning Models for Rat Acute Oral Toxicity Prediction. <i>ACS Sustainable Chemistry and Engineering</i> , 2020, 8, 16020-16027.	3.2	15
41	Machine Learning for Discovery of GSK3 β Inhibitors. <i>ACS Omega</i> , 2020, 5, 26551-26561.	1.6	22
42	Pruned Machine Learning Models to Predict Aqueous Solubility. <i>ACS Omega</i> , 2020, 5, 16562-16567.	1.6	15
43	Collaborating to Fight COVID-19. <i>Genetic Engineering and Biotechnology News</i> , 2020, 40, 12-13.	0.1	0
44	Machine Learning Platform to Discover Novel Growth Inhibitors of <i>Neisseria gonorrhoeae</i> . <i>Pharmaceutical Research</i> , 2020, 37, 141.	1.7	7
45	Pyronaridine tetrphosphate efficacy against Ebola virus infection in guinea pig. <i>Antiviral Research</i> , 2020, 181, 104863.	1.9	16
46	Computational Approaches to Identify Molecules Binding to Mycobacterium tuberculosis KasA. <i>ACS Omega</i> , 2020, 5, 29935-29942.	1.6	8
47	Comparing Machine Learning Models for Aromatase (P450 19A1). <i>Environmental Science & Technology</i> , 2020, 54, 15546-15555.	4.6	5
48	Repurposing Pyramax $\text{\textcircled{R}}$, quinacrine and tilorone as treatments for Ebola virus disease. <i>Antiviral Research</i> , 2020, 182, 104908.	1.9	20
49	Toward the Target: Tilorone, Quinacrine, and Pyronaridine Bind to Ebola Virus Glycoprotein. <i>ACS Medicinal Chemistry Letters</i> , 2020, 11, 1653-1658.	1.3	15
50	Synergistic drug combinations and machine learning for drug repurposing in chordoma. <i>Scientific Reports</i> , 2020, 10, 12982.	1.6	27
51	The past, present and future of RNA respiratory viruses: influenza and coronaviruses. <i>Pathogens and Disease</i> , 2020, 78, .	0.8	7
52	Machine Learning Models for Estrogen Receptor Bioactivity and Endocrine Disruption Prediction. <i>Environmental Science & Technology</i> , 2020, 54, 12202-12213.	4.6	28
53	Comparing Machine Learning Algorithms for Predicting Drug-Induced Liver Injury (DILI). <i>Molecular Pharmaceutics</i> , 2020, 17, 2628-2637.	2.3	55
54	Repurposing Quaternary Ammonium Compounds as Potential Treatments for COVID-19. <i>Pharmaceutical Research</i> , 2020, 37, 104.	1.7	90

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55	Tilorone: a Broad-Spectrum Antiviral Invented in the USA and Commercialized in Russia and beyond. <i>Pharmaceutical Research</i> , 2020, 37, 71.	1.7	39
56	Molecule Property Analyses of Active Compounds for <i>Mycobacterium tuberculosis</i> . <i>Journal of Medicinal Chemistry</i> , 2020, 63, 8917-8955.	2.9	19
57	Repurposing the Dihydropyridine Calcium Channel Inhibitor Nicardipine as a Nav1.8 Inhibitor In Vivo for Pitt Hopkins Syndrome. <i>Pharmaceutical Research</i> , 2020, 37, 127.	1.7	7
58	Tilorone, a Broad-Spectrum Antiviral for Emerging Viruses. <i>Antimicrobial Agents and Chemotherapy</i> , 2020, 64, .	1.4	32
59	DÃ©jÃ© vu: Stimulating open drug discovery for SARS-CoV-2. <i>Drug Discovery Today</i> , 2020, 25, 928-941.	3.2	81
60	Cheminformatics Analysis and Modeling with MacrolactoneDB. <i>Scientific Reports</i> , 2020, 10, 6284.	1.6	15
61	Repurposing Approved Drugs as Inhibitors of Kv7.1 and Nav1.8 to Treat Pitt Hopkins Syndrome. <i>Pharmaceutical Research</i> , 2019, 36, 137.	1.7	33
62	Intrabacterial Metabolism Obscures the Successful Prediction of an InhA Inhibitor of <i>Mycobacterium tuberculosis</i> . <i>ACS Infectious Diseases</i> , 2019, 5, 2148-2163.	1.8	16
63	Why Wait? The Case for Treating Tuberculosis with Inhaled Drugs. <i>Pharmaceutical Research</i> , 2019, 36, 166.	1.7	34
64	Repurposing Quinacrine against Ebola Virus Infection In Vivo. <i>Antimicrobial Agents and Chemotherapy</i> , 2019, 63, .	1.4	30
65	Ebola Virus Bayesian Machine Learning Models Enable New in Vitro Leads. <i>ACS Omega</i> , 2019, 4, 2353-2361.	1.6	49
66	Transparency in Decision Modelling: What, Why, Who and How?. <i>Pharmacoeconomics</i> , 2019, 37, 1355-1369.	1.7	28
67	Back to the future: Advances in development of broad-spectrum capsid-binding inhibitors of enteroviruses. <i>European Journal of Medicinal Chemistry</i> , 2019, 178, 606-622.	2.6	33
68	Novel ketamine analogues cause a false positive phencyclidine immunoassay. <i>Annals of Clinical Biochemistry</i> , 2019, 56, 598-607.	0.8	5
69	The Natural Product Eugenol Is an Inhibitor of the Ebola Virus In Vitro. <i>Pharmaceutical Research</i> , 2019, 36, 104.	1.7	47
70	Opportunities and challenges using artificial intelligence in ADME/Tox. <i>Nature Materials</i> , 2019, 18, 418-422.	13.3	69
71	Exploiting machine learning for end-to-end drug discovery and development. <i>Nature Materials</i> , 2019, 18, 435-441.	13.3	334
72	Accidental intoxications in toddlers: lack of cross-reactivity of vilazodone and its urinary metabolite M17 with drug of abuse screening immunoassays. <i>BMC Clinical Pathology</i> , 2019, 19, 2.	1.8	2

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73	New targets for HIV drug discovery. <i>Drug Discovery Today</i> , 2019, 24, 1139-1147.	3.2	18
74	High-throughput screening and Bayesian machine learning for copper-dependent inhibitors of <i>Staphylococcus aureus</i> . <i>Metallomics</i> , 2019, 11, 696-706.	1.0	30
75	Multiple Machine Learning Comparisons of HIV Cell-based and Reverse Transcriptase Data Sets. <i>Molecular Pharmaceutics</i> , 2019, 16, 1620-1632.	2.3	49
76	A diarylamine derived from anthranilic acid inhibits ZIKV replication. <i>Scientific Reports</i> , 2019, 9, 17703.	1.6	15
77	Repurposing the antimalarial pyronaridine tetraphosphate to protect against Ebola virus infection. <i>PLoS Neglected Tropical Diseases</i> , 2019, 13, e0007890.	1.3	42
78	High Throughput and Computational Repurposing for Neglected Diseases. <i>Pharmaceutical Research</i> , 2019, 36, 27.	1.7	37
79	Halogen Substitution Influences Ketamine Metabolism by Cytochrome P450 2B6: In Vitro and Computational Approaches. <i>Molecular Pharmaceutics</i> , 2019, 16, 898-906.	2.3	30
80	A rapid method for estimation of the efficacy of potential antimicrobials in humans and animals by agar diffusion assay. <i>Chemical Biology and Drug Design</i> , 2019, 93, 1021-1025.	1.5	6
81	Comparing and Validating Machine Learning Models for <i>Mycobacterium tuberculosis</i> Drug Discovery. <i>Molecular Pharmaceutics</i> , 2018, 15, 4346-4360.	2.3	83
82	Data Mining and Computational Modeling of High-Throughput Screening Datasets. <i>Methods in Molecular Biology</i> , 2018, 1755, 197-221.	0.4	7
83	A multitarget approach to drug discovery inhibiting <i>Mycobacterium tuberculosis</i> PyrG and Pank. <i>Scientific Reports</i> , 2018, 8, 3187.	1.6	41
84	A bibliometric review of drug repurposing. <i>Drug Discovery Today</i> , 2018, 23, 661-672.	3.2	163
85	Efficacy of Tilorone Dihydrochloride against Ebola Virus Infection. <i>Antimicrobial Agents and Chemotherapy</i> , 2018, 62, .	1.4	51
86	Computational drug discovery for the Zika virus. <i>Brazilian Journal of Pharmaceutical Sciences</i> , 2018, 54, .	1.2	6
87	Synergistic Lethality of a Binary Inhibitor of <i>Mycobacterium tuberculosis</i> KasA. <i>MBio</i> , 2018, 9, .	1.8	37
88	Characterization of new, efficient <i>Mycobacterium tuberculosis</i> topoisomerase-I inhibitors and their interaction with human ABC multidrug transporters. <i>PLoS ONE</i> , 2018, 13, e0202749.	1.1	4
89	The “Z” of Zika drug discovery. <i>Drug Discovery Today</i> , 2018, 23, 1833-1847.	3.2	48
90	Naïve Bayesian Models for Vero Cell Cytotoxicity. <i>Pharmaceutical Research</i> , 2018, 35, 170.	1.7	25

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91	Comparing Multiple Machine Learning Algorithms and Metrics for Estrogen Receptor Binding Prediction. <i>Molecular Pharmaceutics</i> , 2018, 15, 4361-4370.	2.3	120
92	Doing it All - How Families are Reshaping Rare Disease Research. <i>Pharmaceutical Research</i> , 2018, 35, 192.	1.7	8
93	The EU approved antimalarial pyronaridine shows antitubercular activity and synergy with rifampicin, targeting RNA polymerase. <i>Tuberculosis</i> , 2018, 112, 98-109.	0.8	12
94	Assessment of Substrate-Dependent Ligand Interactions at the Organic Cation Transporter OCT2 Using Six Model Substrates. <i>Molecular Pharmacology</i> , 2018, 94, 1057-1068.	1.0	77
95	Machine learning and docking models for <i>Mycobacterium tuberculosis</i> topoisomerase I. <i>Tuberculosis</i> , 2017, 103, 52-60.	0.8	21
96	Industrializing rare disease therapy discovery and development. <i>Nature Biotechnology</i> , 2017, 35, 117-118.	9.4	30
97	A Phenotypic Based Target Screening Approach Delivers New Antitubercular CTP Synthetase Inhibitors. <i>ACS Infectious Diseases</i> , 2017, 3, 428-437.	1.8	34
98	Rosuvastatin and Atorvastatin Are Ligands of the Human Constitutive Androstane Receptor/Retinoid X Receptor Complex. <i>Drug Metabolism and Disposition</i> , 2017, 45, 974-976.	1.7	11
99	Molecular dynamics simulations of Zika virus NS3 helicase: Insights into RNA binding site activity. <i>Biochemical and Biophysical Research Communications</i> , 2017, 492, 643-651.	1.0	32
100	A summary of some EU funded Tuberculosis drug discovery collaborations. <i>Drug Discovery Today</i> , 2017, 22, 479-480.	3.2	2
101	Enabling Anyone to Translate Clinically Relevant Ideas to Therapies. <i>Pharmaceutical Research</i> , 2017, 34, 1-6.	1.7	15
102	Addressing the Metabolic Stability of Antituberculars through Machine Learning. <i>ACS Medicinal Chemistry Letters</i> , 2017, 8, 1099-1104.	1.3	13
103	Ahead of Our Time: Collaboration in Modeling Then and Now. <i>Pharmacoeconomics</i> , 2017, 35, 975-976.	1.7	14
104	Comparison of Deep Learning With Multiple Machine Learning Methods and Metrics Using Diverse Drug Discovery Data Sets. <i>Molecular Pharmaceutics</i> , 2017, 14, 4462-4475.	2.3	249
105	Non-classical transpeptidases yield insight into new antibacterials. <i>Nature Chemical Biology</i> , 2017, 13, 54-61.	3.9	116
106	Raising awareness of the importance of funding for tuberculosis small-molecule research. <i>Drug Discovery Today</i> , 2017, 22, 487-491.	3.2	12
107	Learning from the past for TB drug discovery in the future. <i>Drug Discovery Today</i> , 2017, 22, 534-545.	3.2	24
108	Collaborative drug discovery for More Medicines for Tuberculosis (MM4TB). <i>Drug Discovery Today</i> , 2017, 22, 555-565.	3.2	12

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109	The new alchemy: Online networking, data sharing and research activity distribution tools for scientists. <i>F1000Research</i> , 2017, 6, 1315.	0.8	4
110	Illustrating and homology modeling the proteins of the Zika virus. <i>F1000Research</i> , 2016, 5, 275.	0.8	37
111	Open drug discovery for the Zika virus. <i>F1000Research</i> , 2016, 5, 150.	0.8	50
112	The Next Era: Deep Learning in Pharmaceutical Research. <i>Pharmaceutical Research</i> , 2016, 33, 2594-2603.	1.7	180
113	Lack of Influence of Substrate on Ligand Interaction with the Human Multidrug and Toxin Extruder, MATE1. <i>Molecular Pharmacology</i> , 2016, 90, 254-264.	1.0	19
114	Predictive modeling targets thymidylate synthase ThyX in <i>Mycobacterium tuberculosis</i> . <i>Scientific Reports</i> , 2016, 6, 27792.	1.6	25
115	Machine Learning Model Analysis and Data Visualization with Small Molecules Tested in a Mouse Model of <i>Mycobacterium tuberculosis</i> Infection (2014-2015). <i>Journal of Chemical Information and Modeling</i> , 2016, 56, 1332-1343.	2.5	23
116	Open Source Bayesian Models. 3. Composite Models for Prediction of Binned Responses. <i>Journal of Chemical Information and Modeling</i> , 2016, 56, 275-285.	2.5	14
117	Incentives for Starting Small Companies Focused on Rare and Neglected Diseases. <i>Pharmaceutical Research</i> , 2016, 33, 809-815.	1.7	7
118	Predicting Mouse Liver Microsomal Stability with "Pruned" Machine Learning Models and Public Data. <i>Pharmaceutical Research</i> , 2016, 33, 433-449.	1.7	43
119	Thermodynamic Proxies to Compensate for Biases in Drug Discovery Methods. <i>Pharmaceutical Research</i> , 2016, 33, 194-205.	1.7	20
120	Illustrating and homology modeling the proteins of the Zika virus. <i>F1000Research</i> , 2016, 5, 275.	0.8	25
121	OpenZika: An IBM World Community Grid Project to Accelerate Zika Virus Drug Discovery. <i>PLoS Neglected Tropical Diseases</i> , 2016, 10, e0005023.	1.3	33
122	Shedding Light on Synergistic Chemical Genetic Connections with Machine Learning. <i>Cell Systems</i> , 2015, 1, 377-379.	2.9	2
123	Modeling error in experimental assays using the bootstrap principle: understanding discrepancies between assays using different dispensing technologies. <i>Journal of Computer-Aided Molecular Design</i> , 2015, 29, 1073-1086.	1.3	12
124	Machine Learning Models and Pathway Genome Data Base for <i>Trypanosoma cruzi</i> Drug Discovery. <i>PLoS Neglected Tropical Diseases</i> , 2015, 9, e0003878.	1.3	74
125	Open Source Bayesian Models. 2. Mining a "Big Dataset" To Create and Validate Models with ChEMBL. <i>Journal of Chemical Information and Modeling</i> , 2015, 55, 1246-1260.	2.5	73
126	Open Source Bayesian Models. 1. Application to ADME/Tox and Drug Discovery Datasets. <i>Journal of Chemical Information and Modeling</i> , 2015, 55, 1231-1245.	2.5	95

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127	Phoenix Nest: Starting a small company focused on Sanfilippo syndrome. <i>Molecular Genetics and Metabolism</i> , 2015, 114, S40-S41.	0.5	0
128	A Virtual Screen Discovers Novel, Fragment-Sized Inhibitors of <i>Mycobacterium tuberculosis</i> InhA. <i>Journal of Chemical Information and Modeling</i> , 2015, 55, 645-659.	2.5	35
129	Targeting <i>Mycobacterium tuberculosis</i> Topoisomerase I by Small-Molecule Inhibitors. <i>Antimicrobial Agents and Chemotherapy</i> , 2015, 59, 1549-1557.	1.4	50
130	Evolution of a thienopyrimidine antitubercular relying on medicinal chemistry and metabolomics insights. <i>Tetrahedron Letters</i> , 2015, 56, 3246-3250.	0.7	27
131	Making Transporter Models for Drug-Drug Interaction Prediction Mobile. <i>Drug Metabolism and Disposition</i> , 2015, 43, 1642-1645.	1.7	13
132	Thiophenecarboxamide Derivatives Activated by EthA Kill <i>Mycobacterium tuberculosis</i> by Inhibiting the CTP Synthetase PyrG. <i>Chemistry and Biology</i> , 2015, 22, 917-927.	6.2	72
133	FDA approved drugs as potential Ebola treatments. <i>F1000Research</i> , 2015, 4, 48.	0.8	13
134	Machines first, humans second: on the importance of algorithmic interpretation of open chemistry data. <i>Journal of Cheminformatics</i> , 2015, 7, 9.	2.8	26
135	In silico methods for predicting drug-drug interactions with cytochrome P-450s, transporters and beyond. <i>Advanced Drug Delivery Reviews</i> , 2015, 86, 46-60.	6.6	33
136	A brief review of recent Charcot-Marie-Tooth research and priorities. <i>F1000Research</i> , 2015, 4, 53.	0.8	28
137	Parallel Worlds of Public and Commercial Bioactive Chemistry Data. <i>Journal of Medicinal Chemistry</i> , 2015, 58, 2068-2076.	2.9	28
138	Databases and collaboration require standards for human stem cell research. <i>Drug Discovery Today</i> , 2015, 20, 247-254.	3.2	4
139	A substrate pharmacophore for the human sodium taurocholate co-transporting polypeptide. <i>International Journal of Pharmaceutics</i> , 2015, 478, 88-95.	2.6	25
140	Quantitative NTCP pharmacophore and lack of association between DILI and NTCP Inhibition. <i>European Journal of Pharmaceutical Sciences</i> , 2015, 66, 1-9.	1.9	29
141	Machine learning models identify molecules active against the Ebola virus in vitro. <i>F1000Research</i> , 2015, 4, 1091.	0.8	56
142	Small molecules with antiviral activity against the Ebola virus. <i>F1000Research</i> , 2015, 4, 38.	0.8	33
143	Finding small molecules for the "next Ebola"™. <i>F1000Research</i> , 2015, 4, 58.	0.8	17
144	Finding small molecules for the "next Ebola"™. <i>F1000Research</i> , 2015, 4, 58.	0.8	14

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145	Machine learning models identify molecules active against the Ebola virus in vitro. F1000Research, 2015, 4, 1091.	0.8	80
146	Combining Metabolite-Based Pharmacophores with Bayesian Machine Learning Models for Mycobacterium tuberculosis Drug Discovery. PLoS ONE, 2015, 10, e0141076.	1.1	14
147	Ten Simple Rules of Live Tweeting at Scientific Conferences. PLoS Computational Biology, 2014, 10, e1003789.	1.5	54
148	Hacking into the granuloma: Could antibody antibiotic conjugates be developed for TB?. Tuberculosis, 2014, 94, 715-716.	0.8	3
149	Curing TB with open science. Tuberculosis, 2014, 94, 183-185.	0.8	3
150	Bayesian models for screening and TB Mobile for target inference with Mycobacterium tuberculosis. Tuberculosis, 2014, 94, 162-169.	0.8	34
151	Computational Models for Neglected Diseases: Gaps and Opportunities. Pharmaceutical Research, 2014, 31, 271-277.	1.7	18
152	No Activation of Human Pregnane X Receptor by Hyperforin-Related Phloroglucinols. Journal of Pharmacology and Experimental Therapeutics, 2014, 348, 393-400.	1.3	11
153	Inhibition of Mycobacterium tuberculosis topoisomerase I by m-AMSA, a eukaryotic type II topoisomerase poison. Biochemical and Biophysical Research Communications, 2014, 446, 916-920.	1.0	46
154	Progress in computational toxicology. Journal of Pharmacological and Toxicological Methods, 2014, 69, 115-140.	0.3	91
155	Computational Prediction and Validation of an Expert's Evaluation of Chemical Probes. Journal of Chemical Information and Modeling, 2014, 54, 2996-3004.	2.5	22
156	Looking Back to the Future: Predicting <i>in Vivo</i> Efficacy of Small Molecules versus <i>Mycobacterium tuberculosis</i> . Journal of Chemical Information and Modeling, 2014, 54, 1070-1082.	2.5	41
157	Are Bigger Data Sets Better for Machine Learning? Fusing Single-Point and Dual-Event Dose Response Data for <i>Mycobacterium tuberculosis</i> . Journal of Chemical Information and Modeling, 2014, 54, 2157-2165.	2.5	36
158	Cross-reactivity of steroid hormone immunoassays: clinical significance and two-dimensional molecular similarity prediction. BMC Clinical Pathology, 2014, 14, 33.	1.8	132
159	New target prediction and visualization tools incorporating open source molecular fingerprints for TB Mobile 2.0. Journal of Cheminformatics, 2014, 6, 38.	2.8	32
160	Bigger data, collaborative tools and the future of predictive drug discovery. Journal of Computer-Aided Molecular Design, 2014, 28, 997-1008.	1.3	22
161	Combining Computational Methods for Hit to Lead Optimization in Mycobacterium Tuberculosis Drug Discovery. Pharmaceutical Research, 2014, 31, 414-435.	1.7	48
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