Sean Ekins

List of Publications by Year
in descending order

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351 papers	16,811 citations	11608 70 h-index	30010 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. Drug Discovery Today, 2022, 27, 490-502.	3.2	15
2	Mycobacterium abscessus drug discovery using machine learning. Tuberculosis, 2022, 132, 102168.	0.8	5
3	Response to Comments on â€œRemdesivir and EIDD-1931 Interact with Human Equilibrative Nucleoside Transporters 1 and 2: Implications for Reaching SARS-CoV-2 Viral Sanctuary Sitesâ€. Molecular Pharmacology, 2022, 101, 121-122.	1.0	1
4	Chalcones from Angelica keiskei (ashitaba) inhibit key Zika virus replication proteins. Bioorganic Chemistry, 2022, 120, 105649.	2.0	13
5	The commoditization of AI for molecule design. Artificial Intelligence in the Life Sciences, 2022, 2, 100031.	1.6	4
6	Dual use of artificial-intelligence-powered drug discovery. Nature Machine Intelligence, 2022, 4, 189-191.	8.3	93
7	Machine Learning Models for Mycobacterium tuberculosisÂ In Vitro Activity: Prediction and Target Visualization. Molecular Pharmaceutics, 2022, 19, 674-689.	2.3	8
8	Pyronaridine Protects against SARS-CoV-2 Infection in Mouse. ACS Infectious Diseases, 2022, 8, 1147-1160.	1.8	14
9	MegaSyn: Integrating Generative Molecular Design, Automated Analog Designer, and Synthetic Viability Prediction. ACS Omega, 2022, 7, 18699-18713.	1.6	13
10	Lack of an Effect of Polysorbate 80 on Intestinal Drug Permeability in Humans. Pharmaceutical Research, 2022, 39, 1881-1890.	1.7	7
11	Rickettsia Aglow: A Fluorescence Assay and Machine Learning Model to Identify Inhibitors of Intracellular Infection. ACS Infectious Diseases, 2022, 8, 1280-1290.	1.8	2
12	A teachable moment for dual-use. Nature Machine Intelligence, 2022, 4, 607-607.	8.3	6
13	Dispirotripiperazine-core compounds, their biological activity with a focus on broad antiviral property, and perspectives in drug design (mini-review). European Journal of Medicinal Chemistry, 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. Molecular Pharmacology, 2021, 99, 147-162.	1.0	15
15	Enzyme Replacement Therapy for Mucopolysaccharidosis IIID using Recombinant Human Î±-N-Acetylglucosamine-6-Sulfatase in Neonatal Mice. Molecular Pharmaceutics, 2021, 18, 214-227.	2.3	8
16	Bioactivity Comparison across Multiple Machine Learning Algorithms Using over 5000 Datasets for Drug Discovery. Molecular Pharmaceutics, 2021, 18, 403-415.	2.3	25
17	Using Bibliometric Analysis and Machine Learning to Identify Compounds Binding to Sialidase-1. ACS Omega, 2021, 6, 3186-3193.	1.6	11
18	A Machine Learning Strategy for Drug Discovery Identifies Anti-Schistosomal Small Molecules. ACS Infectious Diseases, 2021, 7, 406-420.	1.8	18

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

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37	UV-adVISor: Attention-Based Recurrent Neural Networks to Predict UVâ€“Vis Spectra. Analytical Chemistry, 2021, 93, 16076-16085.	3.2	9
38	Antitubercular Triazines: Optimization and Intrabacterial Metabolism. Cell Chemical Biology, 2020, 27, 172-185.e11.	2.5	22
39	Comparison of Machine Learning Models for the Androgen Receptor. Environmental Science & Technology, 2020, 54, 13690-13700.	4.6	17
40	Evaluation of Assay Central Machine Learning Models for Rat Acute Oral Toxicity Prediction. ACS Sustainable Chemistry and Engineering, 2020, 8, 16020-16027.	3.2	15
41	Machine Learning for Discovery of GSK3Î² Inhibitors. ACS Omega, 2020, 5, 26551-26561.	1.6	22
42	Pruned Machine Learning Models to Predict Aqueous Solubility. ACS Omega, 2020, 5, 16562-16567.	1.6	15
43	Collaborating to Fight COVID-19. Genetic Engineering and Biotechnology News, 2020, 40, 12-13.	0.1	0
44	Machine Learning Platform to Discover Novel Growth Inhibitors of Neisseria gonorrhoeae. Pharmaceutical Research, 2020, 37, 141.	1.7	7
45	Pyronaridine tetraphosphate efficacy against Ebola virus infection in guinea pig. Antiviral Research, 2020, 181, 104863.	1.9	16
46	Computational Approaches to Identify Molecules Binding to Mycobacterium tuberculosis KasA. ACS Omega, 2020, 5, 29935-29942.	1.6	8
47	Comparing Machine Learning Models for Aromatase (P450 19A1). Environmental Science & Technology, 2020, 54, 15546-15555.	4.6	5
48	Repurposing PyramaxÂ®, quinacrine and tilorone as treatments for Ebola virus disease. Antiviral Research, 2020, 182, 104908.	1.9	20
49	Toward the Target: Tilorone, Quinacrine, and Pyronaridine Bind to Ebola Virus Glycoprotein. ACS Medicinal Chemistry Letters, 2020, 11, 1653-1658.	1.3	15
50	Synergistic drug combinations and machine learning for drug repurposing in chordoma. Scientific Reports, 2020, 10, 12982.	1.6	27
51	The past, present and future of RNA respiratory viruses: influenza and coronaviruses. Pathogens and Disease, 2020, 78, .	0.8	7
52	Machine Learning Models for Estrogen Receptor Bioactivity and Endocrine Disruption Prediction. Environmental Science & Technology, 2020, 54, 12202-12213.	4.6	28
53	Comparing Machine Learning Algorithms for Predicting Drug-Induced Liver Injury (DILI). Molecular Pharmaceutics, 2020, 17, 2628-2637.	2.3	55
54	Repurposing Quaternary Ammonium Compounds as Potential Treatments for COVID-19. Pharmaceutical Research, 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. Pharmaceutical Research, 2020, 37, 71.	1.7	39
56	Molecule Property Analyses of Active Compounds for Mycobacterium tuberculosis. Journal of Medicinal Chemistry, 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. Pharmaceutical Research, 2020, 37, 127.	1.7	7
58	Tilorone, a Broad-Spectrum Antiviral for Emerging Viruses. Antimicrobial Agents and Chemotherapy, 2020, 64, .	1.4	32
59	DÃ©jÃ vu: Stimulating open drug discovery for SARS-CoV-2. Drug Discovery Today, 2020, 25, 928-941.	3.2	81
60	Cheminformatics Analysis and Modeling with MacrolactoneDB. Scientific Reports, 2020, 10, 6284.	1.6	15
61	Repurposing Approved Drugs as Inhibitors of Kv7.1 and Nav1.8 to Treat Pitt Hopkins Syndrome. Pharmaceutical Research, 2019, 36, 137.	1.7	33
62	Intrabacterial Metabolism Obscures the Successful Prediction of an InhA Inhibitor of Mycobacterium tuberculosis. ACS Infectious Diseases, 2019, 5, 2148-2163.	1.8	16
63	Why Wait? The Case for Treating Tuberculosis with Inhaled Drugs. Pharmaceutical Research, 2019, 36, 166.	1.7	34
64	Repurposing Quinacrine against Ebola Virus Infection In Vivo. Antimicrobial Agents and Chemotherapy, 2019, 63, .	1.4	30
65	Ebola Virus Bayesian Machine Learning Models Enable New in Vitro Leads. ACS Omega, 2019, 4, 2353-2361.	1.6	49
66	Transparency in Decision Modelling: What, Why, Who and How?. Pharmacoeconomics, 2019, 37, 1355-1369.	1.7	28
67	Back to the future: Advances in development of broad-spectrum capsid-binding inhibitors of enteroviruses. European Journal of Medicinal Chemistry, 2019, 178, 606-622.	2.6	33
68	Novel ketamine analogues cause a false positive phencyclidine immunoassay. Annals of Clinical Biochemistry, 2019, 56, 598-607.	0.8	5
69	The Natural Product Eugenol Is an Inhibitor of the Ebola Virus In Vitro. Pharmaceutical Research, 2019, 36, 104.	1.7	47
70	Opportunities and challenges using artificial intelligence in ADME/Tox. Nature Materials, 2019, 18, 418-422.	13.3	69
71	Exploiting machine learning for end-to-end drug discovery and development. Nature Materials, 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. BMC Clinical Pathology, 2019, 19, 2.	1.8	2

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

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91	Comparing Multiple Machine Learning Algorithms and Metrics for Estrogen Receptor Binding Prediction. Molecular Pharmaceutics, 2018, 15, 4361-4370.	2.3	120
92	Doing it All - How Families are Reshaping Rare Disease Research. Pharmaceutical Research, 2018, 35, 192.	1.7	8
93	The EU approved antimalarial pyronaridine shows antitubercular activity and synergy with rifampicin, targeting RNA polymerase. Tuberculosis, 2018, 112, 98-109.	0.8	12
94	Assessment of Substrate-Dependent Ligand Interactions at the Organic Cation Transporter OCT2 Using Six Model Substrates. Molecular Pharmacology, 2018, 94, 1057-1068.	1.0	77
95	Machine learning and docking models for Mycobacterium tuberculosis topoisomerase I. Tuberculosis, 2017, 103, 52-60.	0.8	21
96	Industrializing rare disease therapy discovery and development. Nature Biotechnology, 2017, 35, 117-118.	9.4	30
97	A Phenotypic Based Target Screening Approach Delivers New Antitubercular CTP Synthetase Inhibitors. ACS Infectious Diseases, 2017, 3, 428-437.	1.8	34
98	Rosuvastatin and Atorvastatin Are Ligands of the Human Constitutive Androstane Receptor/Retinoid X Receptor Î± Complex. Drug Metabolism and Disposition, 2017, 45, 974-976.	1.7	11
99	Molecular dynamics simulations of Zika virus NS3 helicase: Insights into RNA binding site activity. Biochemical and Biophysical Research Communications, 2017, 492, 643-651.	1.0	32
100	A summary of some EU funded Tuberculosis drug discovery collaborations. Drug Discovery Today, 2017, 22, 479-480.	3.2	2
101	Enabling Anyone to Translate Clinically Relevant Ideas to Therapies. Pharmaceutical Research, 2017, 34, 1-6.	1.7	15
102	Addressing the Metabolic Stability of Antituberculars through Machine Learning. ACS Medicinal Chemistry Letters, 2017, 8, 1099-1104.	1.3	13
103	Ahead of Our Time: Collaboration in Modeling Then and Now. Pharmacoeconomics, 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. Molecular Pharmaceutics, 2017, 14, 4462-4475.	2.3	249
105	Non-classical transpeptidases yield insight into new antibacterials. Nature Chemical Biology, 2017, 13, 54-61.	3.9	116
106	Raising awareness of the importance of funding for tuberculosis small-molecule research. Drug Discovery Today, 2017, 22, 487-491.	3.2	12
107	Learning from the past for TB drug discovery in the future. Drug Discovery Today, 2017, 22, 534-545.	3.2	24
108	Collaborative drug discovery for More Medicines for Tuberculosis (MM4TB). Drug Discovery Today, 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. F1000Research, 2017, 6, 1315.	0.8	4
110	Illustrating and homology modeling the proteins of the Zika virus. F1000Research, 2016, 5, 275.	0.8	37
111	Open drug discovery for the Zika virus. F1000Research, 2016, 5, 150.	0.8	50
112	The Next Era: Deep Learning in Pharmaceutical Research. Pharmaceutical Research, 2016, 33, 2594-2603.	1.7	180
113	Lack of Influence of Substrate on Ligand Interaction with the Human Multidrug and Toxin Extruder, MATE1. Molecular Pharmacology, 2016, 90, 254-264.	1.0	19
114	Predictive modeling targets thymidylate synthase ThyX in Mycobacterium tuberculosis. Scientific Reports, 2016, 6, 27792.	1.6	25
115	Machine Learning Model Analysis and Data Visualization with Small Molecules Tested in a Mouse Model of Mycobacterium tuberculosis Infection (2014â€“2015). Journal of Chemical Information and Modeling, 2016, 56, 1332-1343.	2.5	23
116	Open Source Bayesian Models. 3. Composite Models for Prediction of Binned Responses. Journal of Chemical Information and Modeling, 2016, 56, 275-285.	2.5	14
117	Incentives for Starting Small Companies Focused on Rare and Neglected Diseases. Pharmaceutical Research, 2016, 33, 809-815.	1.7	7
118	Predicting Mouse Liver Microsomal Stability with â€œPrunedâ€•Machine Learning Models and Public Data. Pharmaceutical Research, 2016, 33, 433-449.	1.7	43
119	Thermodynamic Proxies to Compensate for Biases in Drug Discovery Methods. Pharmaceutical Research, 2016, 33, 194-205.	1.7	20
120	Illustrating and homology modeling the proteins of the Zika virus. F1000Research, 2016, 5, 275.	0.8	25
121	OpenZika: An IBM World Community Grid Project to Accelerate Zika Virus Drug Discovery. PLoS Neglected Tropical Diseases, 2016, 10, e0005023.	1.3	33
122	Shedding Light on Synergistic Chemical Genetic Connections with Machine Learning. Cell Systems, 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. Journal of Computer-Aided Molecular Design, 2015, 29, 1073-1086.	1.3	12
124	Machine Learning Models and Pathway Genome Data Base for Trypanosoma cruzi Drug Discovery. PLoS Neglected Tropical Diseases, 2015, 9, e0003878.	1.3	74
125	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.	2.5	73
126	Open Source Bayesian Models. 1. Application to ADME/Tox and Drug Discovery Datasets. Journal of Chemical Information and Modeling, 2015, 55, 1231-1245.	2.5	95

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127	Phoenix Nest: Starting a small company focused on Sanfilippo syndrome. Molecular Genetics and Metabolism, 2015, 114, S40-S41.	0.5	0
128	A Virtual Screen Discovers Novel, Fragment-Sized Inhibitors of Mycobacterium tuberculosis InhA. Journal of Chemical Information and Modeling, 2015, 55, 645-659.	2.5	35
129	Targeting Mycobacterium tuberculosis Topoisomerase I by Small-Molecule Inhibitors. Antimicrobial Agents and Chemotherapy, 2015, 59, 1549-1557.	1.4	50
130	Evolution of a thienopyrimidine antitubercular relying on medicinal chemistry and metabolomics insights. Tetrahedron Letters, 2015, 56, 3246-3250.	0.7	27
131	Making Transporter Models for Drugâ€“Drug Interaction Prediction Mobile. Drug Metabolism and Disposition, 2015, 43, 1642-1645.	1.7	13
132	Thiophenecarboxamide Derivatives Activated by EthA Kill Mycobacterium tuberculosis by Inhibiting the CTP Synthetase PyrG. Chemistry and Biology, 2015, 22, 917-927.	6.2	72
133	FDA approved drugs as potential Ebola treatments. F1000Research, 2015, 4, 48.	0.8	13
134	Machines first, humans second: on the importance of algorithmic interpretation of open chemistry data. Journal of Cheminformatics, 2015, 7, 9.	2.8	26
135	In silico methods for predicting drugâ€“drug interactions with cytochrome P-450s, transporters and beyond. Advanced Drug Delivery Reviews, 2015, 86, 46-60.	6.6	33
136	A brief review of recent Charcot-Marie-Tooth research and priorities. F1000Research, 2015, 4, 53.	0.8	28
137	Parallel Worlds of Public and Commercial Bioactive Chemistry Data. Journal of Medicinal Chemistry, 2015, 58, 2068-2076.	2.9	28
138	Databases and collaboration require standards for human stem cell research. Drug Discovery Today, 2015, 20, 247-254.	3.2	4
139	A substrate pharmacophore for the human sodium taurocholate co-transporting polypeptide. International Journal of Pharmaceutics, 2015, 478, 88-95.	2.6	25
140	Quantitative NTCP pharmacophore and lack of association between DILI and NTCP Inhibition. European Journal of Pharmaceutical Sciences, 2015, 66, 1-9.	1.9	29
141	Machine learning models identify molecules active against the Ebola virus in vitro. F1000Research, 2015, 4, 1091.	0.8	56
142	Small molecules with antiviral activity against the Ebola virus. F1000Research, 2015, 4, 38.	0.8	33
143	Finding small molecules for the â€˜next Ebolaâ€™. F1000Research, 2015, 4, 58.	0.8	17
144	Finding small molecules for the â€˜next Ebolaâ€™. F1000Research, 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 Expertâ€™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 in Vivo Efficacy of Small Molecules versus Mycobacterium tuberculosis. 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 Mycobacterium tuberculosis. 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
162	Using cheminformatics to predict cross reactivity of â€œdesigner drugsâ€•to their currently available immunoassays. Journal of Cheminformatics, 2014, 6, 22.	2.8	23

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163	Minding the gaps in tuberculosis research. Drug Discovery Today, 2014, 19, 1279-1282.	3.2	7
164	Recommendations to enable drug development for inherited neuropathies: Charcot-Marie-Tooth and Giant Axonal Neuropathy. F1000Research, 2014, 3, 83.	0.8	7
165	Collaboration for rare disease drug discovery research. F1000Research, 2014, 3, 261.	0.8	22
166	A common feature pharmacophore for FDA-approved drugs inhibiting the Ebola virus. F1000Research, 2014, 3, 277.	0.8	54
167	Collecting rare diseases. F1000Research, 2014, 3, 260.	0.8	0
168	TB Mobile: a mobile app for anti-tuberculosis molecules with known targets. Journal of Cheminformatics, 2013, 5, 13.	2.8	29
169	Incorporating Green Chemistry Concepts into Mobile Chemistry Applications and Their Potential Uses. ACS Sustainable Chemistry and Engineering, 2013, 1, 8-13.	3.2	39
170	Fusing Dual-Event Data Sets for Mycobacterium tuberculosis Machine Learning Models and Their Evaluation. Journal of Chemical Information and Modeling, 2013, 53, 3054-3063.	2.5	29
171	Multifaceted roles of ultra-rare and rare disease patients/parents in drug discovery. Drug Discovery Today, 2013, 18, 1043-1051.	3.2	36
172	Challenges and recommendations for obtaining chemical structures of industry-provided repurposing candidates. Drug Discovery Today, 2013, 18, 58-70.	3.2	24
173	Novel diaryl ureas with efficacy in a mouse model of malaria. Bioorganic and Medicinal Chemistry Letters, 2013, 23, 1022-1025.	1.0	22
174	Discovery of Novel Antimalarial Compounds Enabled by QSAR-Based Virtual Screening. Journal of Chemical Information and Modeling, 2013, 53, 475-492.	2.5	77
175	Bayesian Models Leveraging Bioactivity and Cytotoxicity Information for Drug Discovery. Chemistry and Biology, 2013, 20, 370-378.	6.2	87
176	Computational Approaches and Collaborative Drug Discovery for Trypanosomal Diseases. , 2013, , 81-102.		3
177	The Collaborative Drug Discovery (CDD) Database. Methods in Molecular Biology, 2013, 993, 139-154.	0.4	25
178	Computational Models for Tuberculosis Drug Discovery. Methods in Molecular Biology, 2013, 993, 245-262.	0.4	19
179	Four disruptive strategies for removing drug discovery bottlenecks. Drug Discovery Today, 2013, 18, 265-271.	3.2	32
180	Structureâ€“Activity Relationship for FDA Approved Drugs As Inhibitors of the Human Sodium Taurocholate Cotransporting Polypeptide (NTCP). Molecular Pharmaceutics, 2013, 10, 1008-1019.	2.3	86

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181	Novel Yeast-based Strategy Unveils Antagonist Binding Regions on the Nuclear Xenobiotic Receptor PXR. Journal of Biological Chemistry, 2013, 288, 13655-13668.	1.6	28
182	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.	1.0	38
183	Enhancing Hit Identification in Mycobacterium tuberculosis Drug Discovery Using Validated Dual-Event Bayesian Models. PLoS ONE, 2013, 8, e63240.	1.1	51
184	LASSO-ing Potential Nuclear Receptor Agonists and Antagonists: A New Computational Method for Database Screening. Journal of Computational Medicine, 2013, 2013, 1-8.	0.3	2
185	Cheminformatics workflows using mobile apps. Chem-Bio Informatics Journal, 2013, 13, 1-18.	0.1	12
186	Dispensing Processes Impact Apparent Biological Activity as Determined by Computational and Statistical Analyses. PLoS ONE, 2013, 8, e62325.	1.1	39
187	Why Open Drug Discovery Needs Four Simple Rules for Licensing Data and Models. PLoS Computational Biology, 2012, 8, e1002706.	1.5	17
188	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.	1.3	74
189	Ligand- and Structure-Based Pregnane X Receptor Models. Methods in Molecular Biology, 2012, 929, 359-375.	0.4	14
190	Computational Modeling to Accelerate the Identification of Substrates and Inhibitors for Transporters That Affect Drug Disposition. Clinical Pharmacology and Therapeutics, 2012, 92, 661-665.	2.3	22
191	Open Drug Discovery Teams: A Chemistry Mobile App for Collaboration. Molecular Informatics, 2012, 31, 585-597.	1.4	32
192	A generalizable pre-clinical research approach for orphan disease therapy. Orphanet Journal of Rare Diseases, 2012, 7, 39.	1.2	32
193	Applications and Limitations of In Silico Models in Drug Discovery. Methods in Molecular Biology, 2012, 910, 87-124.	0.4	42
194	Disruptive Strategies for Removing Drug Discovery Bottlenecks. Nature Precedings, 2012, , .	0.1	1
195	Redefining Cheminformatics with Intuitive Collaborative Mobile Apps. Molecular Informatics, 2012, 31, 569-584.	1.4	25
196	Combining Cheminformatics Methods and Pathway Analysis to Identify Molecules with Whole-Cell Activity Against Mycobacterium Tuberculosis. Pharmaceutical Research, 2012, 29, 2115-2127.	1.7	28
197	A Substrate Pharmacophore for the Human Organic Cation/Carnitine Transporter Identifies Compounds Associated with Rhabdomyolysis. Molecular Pharmaceutics, 2012, 9, 905-913.	2.3	16
198	Bottlenecks Caused by Software Gaps in miRNA and RNAi Research. Pharmaceutical Research, 2012, 29, 1717-1721.	1.7	0

#	Article	IF	Citations
199	Towards a gold standard: regarding quality in public domain chemistry databases and approaches to improving the situation. Drug Discovery Today, 2012, 17, 685-701.	3.2	102
200	Activation of a tunicate (Ciona intestinalis) xenobiotic receptor orthologue by both natural toxins and synthetic toxicants. Toxicon, 2012, 59, 365-372.	0.8	25
201	Accessing, Using, and Creating Chemical Property Databases for Computational Toxicology Modeling. Methods in Molecular Biology, 2012, 929, 221-241.	0.4	7
202	Evolution of promiscuous nuclear hormone receptors: LXR, FXR, VDR, PXR, and CAR. Molecular and Cellular Endocrinology, 2011, 334, 39-48.	1.6	96
203	Computational databases, pathway and cheminformatics tools for tuberculosis drug discovery. Trends in Microbiology, 2011, 19, 65-74.	3.5	82
204	A hybrid approach to advancing quantitative prediction of tissue distribution of basic drugs in human. Toxicology and Applied Pharmacology, 2011, 250, 194-212.	1.3	34
205	In silico repositioning of approved drugs for rare and neglected diseases. Drug Discovery Today, 2011, 16, 298-310.	3.2	269
206	Alternative business models for drug discovery. Drug Discovery Today, 2011, 16, 643-645.	3.2	10
207	A quality alert and call for improved curation of public chemistry databases. Drug Discovery Today, 2011, 16, 747-750.	3.2	88
208	Mobile apps for chemistry in the world of drug discovery. Drug Discovery Today, 2011, 16, 928-939.	3.2	44
209	Validating New Tuberculosis Computational Models with Public Whole Cell Screening Aerobic Activity Datasets. Pharmaceutical Research, 2011, 28, 1859-1869.	1.7	35
210	Finding Promiscuous Old Drugs for New Uses. Pharmaceutical Research, 2011, 28, 1785-1791.	1.7	48
211	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
212	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.	1.7	42
213	Essential Metabolites of Mycobacterium tuberculosis and Their Mimics. MBio, 2011, 2, e00301-10.	1.8	56
214	Quantitative Structure Activity Relationship for Inhibition of Human Organic Cation/Carnitine Transporter. Molecular Pharmaceutics, 2010, 7, 2120-2131.	2.3	31
215	Reaching Out to Collaborators: Crowdsourcing for Pharmaceutical Research. Pharmaceutical Research, 2010, 27, 393-395.	1.7	52
216	Chemical Space: Missing Pieces in Cheminformatics. Pharmaceutical Research, 2010, 27, 2035-2039.	1.7	18

#	Article	IF	Citations
217	Chemical target and pathway toxicity mechanisms defined in primary human cell systems. Journal of Pharmacological and Toxicological Methods, 2010, 61, 3-15.	0.3	75
218	Troubleshooting computational methods in drug discovery. Journal of Pharmacological and Toxicological Methods, 2010, 61, 67-75.	0.3	43
219	Evolving molecules using multi-objective optimization: applying to ADME/Tox. Drug Discovery Today, 2010, 15, 451-460.	3.2	85
220	When pharmaceutical companies publish large datasets: an abundance of riches or fool's gold?. Drug Discovery Today, 2010, 15, 812-815.	3.2	36
221	Why we should be vigilant: Drug cytotoxicity observed with in vitro transporter inhibition studies. Biochemical Pharmacology, 2010, 80, 1087-1092.	2.0	11
222	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.	1.7	83
223	A Predictive Ligand-Based Bayesian Model for Human Drug-Induced Liver Injury. Drug Metabolism and Disposition, 2010, 38, 2302-2308.	1.7	106
224	Evaluation of Computational Docking to Identify Pregnane X Receptor Agonists in the ToxCast Database. Environmental Health Perspectives, 2010, 118, 1412-1417.	2.8	33
225	Targeting Drug Transporters â€“ Combining In Silico and In Vitro Approaches to Predict In Vivo. Methods in Molecular Biology, 2010, 637, 65-103.	0.4	17
226	Two farnesoid X receptor alpha isoforms in Japanese medaka (Oryzias latipes) are differentially activated in vitro. Aquatic Toxicology, 2010, 98, 245-255.	1.9	18
227	A collaborative database and computational models for tuberculosis drug discovery. Molecular BioSystems, 2010, 6, 840.	2.9	80
228	Analysis and hit filtering of a very large library of compounds screened against Mycobacterium tuberculosis. Molecular BioSystems, 2010, 6, 2316-2324.	2.9	69
229	Integrated in Silicoâ^'in Vitro Strategy for Addressing Cytochrome P450 3A4 Time-Dependent Inhibition. Chemical Research in Toxicology, 2010, 23, 664-676.	1.7	54
230	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.	3.1	63
231	Meta-analysis of molecular property patterns and filtering of public datasets of antimalarial â€œhitsâ€• and drugs. MedChemComm, 2010, 1, 325.	3.5	23
232	Time for Cooperation in Health Economics among the Modelling Community. Pharmacoeconomics, 2010, 28, 609-613.	1.7	20
233	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.	1.7	41
234	Challenges Predicting Ligand-Receptor Interactions of Promiscuous Proteins: The Nuclear Receptor PXR. PLoS Computational Biology, 2009, 5, e1000594.	1.5	102

#	Article	IF	Citations
235	Novel web-based tools combining chemistry informatics, biology and social networks for drug discovery. Drug Discovery Today, 2009, 14, 261-270.	3.2	126
236	Understanding nuclear receptors using computational methods. Drug Discovery Today, 2009, 14, 486-494.	3.2	29
237	Computational mapping tools for drug discovery. Drug Discovery Today, 2009, 14, 767-775.	3.2	43
238	Competitive collaboration in the pharmaceutical and biotechnology industry. Drug Discovery Today, 2009, 14, 1079-1081.	3.2	21
239	Hybrid Scoring and Classification Approaches to Predict Human Pregnane X Receptor Activators. Pharmaceutical Research, 2009, 26, 1001-1011.	1.7	53
240	A Turning Point For Bloodâ€“Brain Barrier Modeling. Pharmaceutical Research, 2009, 26, 1283-1284.	1.7	11
241	Elucidating the â€˜Jekyll and Hydeâ€™ Nature of PXR: The Case for Discovering Antagonists or Allosteric Antagonists. Pharmaceutical Research, 2009, 26, 1807-1815.	1.7	58
242	Novel Inhibitors of Human Organic Cation/Carnitine Transporter (hOCTN2) via Computational Modeling and In Vitro Testing. Pharmaceutical Research, 2009, 26, 1890-1900.	1.7	36
243	Predicting Inhibitors of Acetylcholinesterase by Regression and Classification Machine Learning Approaches with Combinations of Molecular Descriptors. Pharmaceutical Research, 2009, 26, 2216-2224.	1.7	26
244	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.	0.7	60
245	Computational Models for Drug Inhibition of the Human Apical Sodium-Dependent Bile Acid Transporter. Molecular Pharmaceutics, 2009, 6, 1591-1603.	2.3	89
246	The importance of discerning shape in molecular pharmacology. Trends in Pharmacological Sciences, 2009, 30, 138-147.	4.0	106
247	Chemoinformatic Methods for Predicting Interference in Drug of Abuse/Toxicology Immunoassays. Clinical Chemistry, 2009, 55, 1203-1213.	1.5	39
248	Molecular Similarity Methods for Predicting Cross-Reactivity With Therapeutic Drug Monitoring Immunoassays. Therapeutic Drug Monitoring, 2009, 31, 337-344.	1.0	37
249	Computer- Aided Decision Making from Drug Discovery to Pharmacoeconomics. Drug Discovery Series, 2009, , 209-226.	0.1	0
250	New Predictive Models for Bloodâ€“Brain Barrier Permeability of Drug-like Molecules. Pharmaceutical Research, 2008, 25, 1836-1845.	1.7	95
251	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.	1.3	50
252	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.	2.9	155

#	Article	IF	Citations
253	Evolution of pharmacologic specificity in the pregnane X receptor. BMC Evolutionary Biology, 2008, 8, 103.	3.2	92
254	Shape Signatures: New Descriptors for Predicting Cardiotoxicity In Silico. Chemical Research in Toxicology, 2008, 21, 1304-1314.	1.7	74
255	Ligand specificity and evolution of liver X receptors. Journal of Steroid Biochemistry and Molecular Biology, 2008, 110, 83-94.	1.2	58
256	Machine Learning Methods and Docking for Predicting Human Pregnane X Receptor Activation. Chemical Research in Toxicology, 2008, 21, 1457-1467.	1.7	65
257	A retrospective randomized study of asthma control in the US: results of the CHARIOT study. Current Medical Research and Opinion, 2008, 24, 3443-3452.	0.9	25
258	Intrinsic Disorder in Nuclear Hormone Receptors. Journal of Proteome Research, 2008, 7, 4359-4372.	1.8	67
259	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.	1.7	72
260	Evolution of the bile salt nuclear receptor FXR in vertebrates*. Journal of Lipid Research, 2008, 49, 1577-1587.	2.0	91
261	Combined Computational Metabolite Prediction and Automated Structure-Based Analysis of Mass Spectrometric Data. Toxicology Mechanisms and Methods, 2008, 18, 243-250.	1.3	23
262	Computational Discovery of Novel Low Micromolar Human Pregnane X Receptor Antagonists. Molecular Pharmacology, 2008, 74, 662-672.	1.0	68
263	Bacterial Peptide Recognition and Immune Activation Facilitated by Human Peptide Transporter PEPT2. American Journal of Respiratory Cell and Molecular Biology, 2008, 39, 536-542.	1.4	58
264	Molecular Characterization of CYP2B6 Substrates. Current Drug Metabolism, 2008, 9, 363-373.	0.7	46
265	Pathway Mapping Tools for Analysis of High Content Data. , 2007, 356, 319-350.		206
266	Computational Approaches That Predict Metabolic Intermediate Complex Formation with CYP3A4 (+b5). Drug Metabolism and Disposition, 2007, 35, 1466-1475.	1.7	63
267	Classification of Metabolites with Kernel-Partial Least Squares (K-PLS). Drug Metabolism and Disposition, 2007, 35, 325-327.	1.7	28
268	Three-Dimensional Quantitative Structure-Activity Relationship Analysis of Human CYP51 Inhibitors. Drug Metabolism and Disposition, 2007, 35, 493-500.	1.7	17
269	Future directions for drug transporter modelling. Xenobiotica, 2007, 37, 1152-1170.	0.5	57
270	Methods for Predicting Human Drug Metabolism. Advances in Clinical Chemistry, 2007, 43, 131-176.	1.8	36

#	Article	IF	Citations
271	Human Pregnane X Receptor Antagonists and Agonists Define Molecular Requirements for Different Binding Sites. Molecular Pharmacology, 2007, 72, 592-603.	1.0	143
272	In silico pharmacology for drug discovery: methods for virtual ligand screening and profiling. British Journal of Pharmacology, 2007, 152, 9-20.	2.7	522
273	In silico pharmacology for drug discovery: applications to targets and beyond. British Journal of Pharmacology, 2007, 152, 21-37.	2.7	269
274	Improving the drug selection and development process for combination devices. Drug Discovery Today, 2007, 12, 844-852.	3.2	21
275	Computational Models to Assign Biopharmaceutics Drug Disposition Classification from Molecular Structure. Pharmaceutical Research, 2007, 24, 2249-2262.	1.7	61
276	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.	2.9	87
277	Rapid Identification of P-glycoprotein Substrates and Inhibitors. Drug Metabolism and Disposition, 2006, 34, 1976-1984.	1.7	136
278	Systems Approaches for Pharmaceutical Research and Development. , 2006, , 139-165.		3
279	Computer Methods for Predicting Drug Metabolism. , 2006, , 443-468.		2
280	Algorithms for network analysis in systems-ADME/Tox using the MetaCore and MetaDrug platforms. Xenobiotica, 2006, 36, 877-901.	0.5	125
281	Application of data mining approaches to drug delivery. Advanced Drug Delivery Reviews, 2006, 58, 1409-1430.	6.6	30
282	Pharmacophore-based discovery of ligands for drug transporters. Advanced Drug Delivery Reviews, 2006, 58, 1431-1450.	6.6	101
283	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.	1.7	91
284	Systems-ADME/Tox: Resources and network approaches. Journal of Pharmacological and Toxicological Methods, 2006, 53, 38-66.	0.3	55
285	A COMBINED APPROACH TO DRUG METABOLISM AND TOXICITY ASSESSMENT. Drug Metabolism and Disposition, 2006, 34, 495-503.	1.7	108
286	Systems Biology: Applications in Drug Discovery. , 2005, , 123-183.		15
287	Reengineering the pharmaceutical industry by crash-testing molecules. Drug Discovery Today, 2005, 10, 1191-1200.	3.2	32
288	In Vitro and Pharmacophore-Based Discovery of Novel hPEPT1 Inhibitors. Pharmaceutical Research, 2005, 22, 512-517.	1.7	68

#	Article	IF	Citations
289	Molecular Determinants of Substrate/Inhibitor Binding to the Human and Rabbit Renal Organic Cation Transporters hOCT2 and rbOCT2. Molecular Pharmacology, 2005, 67, 1067-1077.	1.0	96
290	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.	1.3	90
291	A NOVEL METHOD FOR VISUALIZING NUCLEAR HORMONE RECEPTOR NETWORKS RELEVANT TO DRUG METABOLISM. Drug Metabolism and Disposition, 2005, 33, 474-481.	1.7	49
292	Comprehensive Computational Assessment of ADME Properties Using Mapping Techniques. Current Drug Discovery Technologies, 2005, 2, 99-113.	0.6	46
293	Computational prediction of human drug metabolism. Expert Opinion on Drug Metabolism and Toxicology, 2005, 1, 303-324.	1.5	78
294	Techniques: Application of systems biology to absorption, distribution, metabolism, excretion and toxicity. Trends in Pharmacological Sciences, 2005, 26, 202-209.	4.0	179
295	A novel method for generation of signature networks as biomarkers from complex high throughput data. Toxicology Letters, 2005, 158, 20-29.	0.4	129
296	Predicting undesirable drug interactions with promiscuous proteins in silico. Drug Discovery Today, 2004, 9, 276-285.	3.2	144
297	KOHONEN MAPS FOR PREDICTION OF BINDING TO HUMAN CYTOCHROME P450 3A4. Drug Metabolism and Disposition, 2004, 32, 1183-1189.	1.7	55
298	QUANTITATIVE STRUCTURE-METABOLISM RELATIONSHIP MODELING OF METABOLIC N-DEALKYLATION REACTION RATES. Drug Metabolism and Disposition, 2004, 32, 1111-1120.	1.7	42
299	PXR and the regulation of apoA1 and HDL-cholesterol in rodents. Pharmacological Research, 2004, 50, 237-246.	3.1	68
300	Development of Computational Models for Enzymes, Transporters, Channels, and Receptors Relevant to ADME/Tox. Reviews in Computational Chemistry, 2004, , 333-415.	1.5	38
301	In vitro and pharmacophore insights into CYP3A enzymes. Trends in Pharmacological Sciences, 2003, 24, 161-166.	4.0	145
302	Influence of Molecular Structure on Substrate Binding to the Human Organic Cation Transporter, hOCT1. Molecular Pharmacology, 2003, 63, 489-498.	1.0	110
303	GENERATION AND VALIDATION OF RAPID COMPUTATIONAL FILTERS FOR CYP2D6 AND CYP3A4. Drug Metabolism and Disposition, 2003, 31, 1077-1080.	1.7	94
304	In silico approaches to predicting drug metabolism, toxicology and beyond. Biochemical Society Transactions, 2003, 31, 611-614.	1.6	68
305	Prediction of Human Drug Metabolizing Enzyme Induction. Current Drug Metabolism, 2003, 4, 381-391.	0.7	37
306	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.	1.3	282

#	Article	IF	Citations
307	STRUCTURAL BIOLOGY AND FUNCTION OF SOLUTE TRANSPORTERS: IMPLICATIONS FOR IDENTIFYING AND DESIGNING SUBSTRATES. Drug Metabolism Reviews, 2002, 34, 709-750.	1.5	62
308	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
309	Application of Three-Dimensional Quantitative Structure-Activity Relationships of P-Glycoprotein Inhibitors and Substrates. Molecular Pharmacology, 2002, 61, 974-981.	1.0	204
310	Three-Dimensional Quantitative Structure-Activity Relationships of Inhibitors of P-Glycoprotein. Molecular Pharmacology, 2002, 61, 964-973.	1.0	179
311	A Pharmacophore for Human Pregnane X Receptor Ligands. Drug Metabolism and Disposition, 2002, 30, 96-99.	1.7	160
312	The PXR crystal structure: the end of the beginning. Trends in Pharmacological Sciences, 2002, 23, 49-50.	4.0	27
313	Modeling of active transport systems. Advanced Drug Delivery Reviews, 2002, 54, 329-354.	6.6	76
314	Pharmacophore modeling of cytochromes P450. Advanced Drug Delivery Reviews, 2002, 54, 367-383.	6.6	123
315	Integrating computer-based de novo drug design and multidimensional filtering for desirable drugs. Targets, 2002, 1, 196-205.	0.3	19
316	Three-Dimensional Quantitative Structure Activity Relationship for Cyp2d6 Substrates. QSAR and Combinatorial Science, 2002, 21, 357-368.	1.4	74
317	Quantitative Structure Activity Relationships for the Glucuronidation of Simple Phenols by Expressed Human UGT1A6 and UGT1A9. Drug Metabolism and Disposition, 2002, 30, 734-738.	1.7	51
318	Towards a new age of virtual ADME/TOX and multidimensional drug discovery. Journal of Computer-Aided Molecular Design, 2002, 16, 381-401.	1.3	85
319	A ligand-based approach to understanding selectivity of nuclear hormone receptors PXR, CAR, FXR, LXRalpha, and LXRbeta. Pharmaceutical Research, 2002, 19, 1788-1800.	1.7	93
320	Optimizing Higher Throughput Methods to Assess Drug-Drug Interactions for CYP1A2, CYP2C9, CYP2C19, CYP2D6, rCYP2D6, and CYP3A4 <I>In Vitro</I> Using a Single Point IC₅₀. Journal of Biomolecular Screening, 2002, 7, 373-382.	2.6	1
321	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
322	Application of in silico approaches to predicting drugâ€“drug interactions. Journal of Pharmacological and Toxicological Methods, 2001, 45, 65-69.	0.3	61
323	Progress in predicting human ADME parameters in silico. Journal of Pharmacological and Toxicological Methods, 2000, 44, 251-272.	0.3	240
324	Present and future in vitro approaches for drug metabolism. Journal of Pharmacological and Toxicological Methods, 2000, 44, 313-324.	0.3	169

#	Article	IF	Citations
325	Towards a new age of virtual ADME/TOX and multidimensional drug discovery. Molecular Diversity, 2000, 5, 255-275.	2.1	25
326	THE ROLE OF CYP2B6 IN HUMAN XENOBIOTIC METABOLISM*. Drug Metabolism Reviews, 1999, 31, 719-754.	1.5	168
327	Molecular Cloning, Expression, and Characterization of CYP2D17 from Cynomolgus Monkey Liver. Archives of Biochemistry and Biophysics, 1999, 372, 189-196.	1.4	38
328	In Vitro Metabolism. , 1999, , 363-399.		15
329	Examination of purported probes of human CYP2B6. Pharmacogenetics and Genomics, 1997, 7, 165-179.	5.7	93
330	Past, Present, and Future Applications of Precision-Cut Liver Slices for in Vitro Xenobiotic Metabolism. Drug Metabolism Reviews, 1996, 28, 591-623.	1.5	82
331	Applications of QSAR Methods to Ion Channels. , 0, , 353-389.		8
332	Applications of QSAR to Enzymes Involved in Toxicology. , 0, , 277-293.		3
333	Computational Approaches for Assessment of Toxicity: A Historical Perspective and Current Status. , 0, , 183-215.		6
334	Physiologically Based Pharmacokinetic and Pharmacodynamic Modeling. , 0, , 33-69.		4
335	Crystal Structures of Toxicology Targets. , 0, , 469-519.		1
336	Novel Applications of Kernelâ€“Partial Least Squares to Modeling a Comprehensive Array of Properties for Drug Discovery. , 0, , 403-432.		10
337	Application of Interpretable Models to ADME/TOX Problems. , 0, , 581-597.		0
338	Strategies for Using Computational Toxicology Methods in Pharmaceutical R&D. , 0, , 545-579.		3
339	Computational Modeling of Receptor-Mediated Toxicity. , 0, , 315-351.		1
340	QSAR Studies on Drug Transporters Involved in Toxicology. , 0, , 295-314.		4
341	An Introduction to Toxicology and Its Methodologies. , 0, , 1-20.		2
342	Current QSAR Techniques for Toxicology. , 0, , 217-238.		5

#	Article	IF	Citations
343	High-Throughput Protein-Based Technologies and Computational Models for Drug Development, Efficacy, and Toxicity. , 0, , 29-52.		4
344	Systems Pharmacology, Biomarkers, and Biomolecular Networks. , 0, , 75-113.		0
345	Computational Systems Biology Modeling of Dosimetry and Cellular Response Pathways. , 0, , 155-173.		0
346	Regulation of Gene Expression by Small, Non-Coding RNAs: Practical Applications. , 0, , 327-347.		0
347	Machine learning models identify molecules active against the Ebola virus in vitro. F1000Research, 0, 4, 1091.	0.8	14
348	Evolution of Electronic Laboratory Notebooks. , 0, , 301-320.		3
349	Collaborative Innovation: Essential Foundation of Scientific Discovery. , 0, , 19-37.		1
350	Need for Collaborative Technologies in Drug Discovery. , 0, , 1-18.		0
351	Machine Learning for Discovery of New ADORA Modulators. Frontiers in Pharmacology, 0, 13, .	1.6	3