Tudor I Oprea

List of Publications by Year in descending order

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232 papers	21,646 citations	10979 71 h-index	11601 135 g-index
297 all docs	297 docs citations	297 times ranked	22387 citing authors

#	Article	IF	Citations
1	A comprehensive map of molecular drug targets. Nature Reviews Drug Discovery, 2017, 16, 19-34.	21.5	1,608
2	Is There a Difference between Leads and Drugs? A Historical Perspective. Journal of Chemical Information and Computer Sciences, 2001, 41, 1308-1315.	2.8	738
3	Virtual and biomolecular screening converge on a selective agonist for GPR30. Nature Chemical Biology, 2006, 2, 207-212.	3.9	730
4	The Design of Leadlike Combinatorial Libraries. Angewandte Chemie - International Edition, 1999, 38, 3743-3748.	7.2	719
5	Estrogen Signaling through the Transmembrane G Proteinâ€“Coupled Receptor GPR30. Annual Review of Physiology, 2008, 70, 165-190.	5.6	539
6	Property distribution of drug-related chemical databases. , 2000, 14, 251-264.		537
7	BDDCS Applied to Over 900 Drugs. AAPS Journal, 2011, 13, 519-547.	2.2	532
8	Pursuing the leadlikeness concept in pharmaceutical research. Current Opinion in Chemical Biology, 2004, 8, 255-263.	2.8	513
9	BDDCS, the Rule of 5 and drugability. Advanced Drug Delivery Reviews, 2016, 101, 89-98.	6.6	475
10	In vivo effects of a GPR30 antagonist. Nature Chemical Biology, 2009, 5, 421-427.	3.9	461
11	Distribution and characterization of estrogen receptor G protein-coupled receptor 30 in the rat central nervous system. Journal of Endocrinology, 2007, 193, 311-321.	1.2	433
12	QSAR without borders. Chemical Society Reviews, 2020, 49, 3525-3564.	18.7	427
13	G Proteinâ€“Coupled Receptor 30 (GPR30) Mediates Gene Expression Changes and Growth Response to 17Î²-Estradiol and Selective GPR30 Ligand G-1 in Ovarian Cancer Cells. Cancer Research, 2007, 67, 1859-1866.	0.4	383
14	Chemography:Â The Art of Navigating in Chemical Space. ACS Combinatorial Science, 2001, 3, 157-166.	3.3	320
15	Temporal disease trajectories condensed from population-wide registry data covering 6.2 million patients. Nature Communications, 2014, 5, 4022.	5.8	289
16	VALIDATE:Â A New Method for the Receptor-Based Prediction of Binding Affinities of Novel Ligands. Journal of the American Chemical Society, 1996, 118, 3959-3969.	6.6	278
17	Pharos: Collating protein information to shed light on the druggable genome. Nucleic Acids Research, 2017, 45, D995-D1002.	6.5	271
18	Unexplored therapeutic opportunities in the human genome. Nature Reviews Drug Discovery, 2018, 17, 317-332.	21.5	263

#	Article	IF	Citations
19	Integrating virtual screening in lead discovery. Current Opinion in Chemical Biology, 2004, 8, 349-358.	2.8	256
20	Identification of a GPER/GPR30 antagonist with improved estrogen receptor counterselectivity. Journal of Steroid Biochemistry and Molecular Biology, 2011, 127, 358-366.	1.2	254
21	Novel Chemical Space Exploration via Natural Products. Journal of Medicinal Chemistry, 2009, 52, 1953-1962.	2.9	248
22	Drug repurposing from an academic perspective. Drug Discovery Today: Therapeutic Strategies, 2011, 8, 61-69.	0.5	240
23	The significance of acid/base properties in drug discovery. Chemical Society Reviews, 2013, 42, 485-496.	18.7	236
24	DrugCentral: online drug compendium. Nucleic Acids Research, 2017, 45, D932-D939.	6.5	215
25	Drug Repurposing: Far Beyond New Targets for Old Drugs. AAPS Journal, 2012, 14, 759-763.	2.2	212
26	Ligand-Based Identification of Environmental Estrogens. Chemical Research in Toxicology, 1996, 9, 1240-1248.	1.7	208
27	Interactive exploration of chemical space with Scaffold Hunter. Nature Chemical Biology, 2009, 5, 581-583.	3.9	207
28	The G Proteinâ€“Coupled Receptor GPR30 Inhibits Proliferation of Estrogen Receptorâ€“Positive Breast Cancer Cells. Cancer Research, 2010, 70, 1184-1194.	0.4	204
29	How many rare diseases are there?. Nature Reviews Drug Discovery, 2020, 19, 77-78.	21.5	204
30	Flow cytometry for high-throughput, high-content screening. Current Opinion in Chemical Biology, 2004, 8, 392-398.	2.8	196
31	Therapies for rare diseases: therapeutic modalities, progress and challenges ahead. Nature Reviews Drug Discovery, 2020, 19, 93-111.	21.5	190
32	Three-dimensional QSAR of human immunodeficiency virus (I) protease inhibitors. 1. A CoMFA study employing experimentally-determined alignment rules. Journal of Medicinal Chemistry, 1993, 36, 4152-4160.	2.9	186
33	Current trends in lead discovery: are we looking for the appropriate properties?. Journal of Computer-Aided Molecular Design, 2002, 16, 325-334.	1.3	183
34	QSAR Modeling of the Bloodâ€“Brain Barrier Permeability for Diverse Organic Compounds. Pharmaceutical Research, 2008, 25, 1902-1914.	1.7	163
35	Optimization of CAMD techniques 3. Virtual screening enrichment studies: a help or hindrance in tool selection?. Journal of Computer-Aided Molecular Design, 2008, 22, 169-178.	1.3	163
36	Quantifying the Relationships among Drug Classes. Journal of Chemical Information and Modeling, 2008, 48, 755-765.	2.5	160

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37	In silico toxicology protocols. Regulatory Toxicology and Pharmacology, 2018, 96, 1-17.	1.3	159
38	Understanding drugâ€likeness. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 760-781.	6.2	152
39	In vitro differentiation of human mesenchymal stem cells to epithelial lineage. Journal of Cellular and Molecular Medicine, 2007, 11, 502-508.	1.6	147
40	Modulation of Bitter Taste Perception by a Small Molecule hTAS2R Antagonist. Current Biology, 2010, 20, 1104-1109.	1.8	142
41	A Novel Approach for Predicting P-Glycoprotein (ABCB1) Inhibition Using Molecular Interaction Fields. Journal of Medicinal Chemistry, 2011, 54, 1740-1751.	2.9	141
42	Microbial Efflux Pump Inhibition: Tactics and Strategies. Current Pharmaceutical Design, 2011, 17, 1291-1302.	0.9	140
43	The ins and outs of GPR30: A transmembrane estrogen receptor. Journal of Steroid Biochemistry and Molecular Biology, 2008, 109, 350-353.	1.2	136
44	Advancing Biological Understanding and Therapeutics Discovery with Small-Molecule Probes. Cell, 2015, 161, 1252-1265.	13.5	135
45	Three-dimensional quantitative structure-activity relationship of human immunodeficiency virus (I) protease inhibitors. 2. Predictive power using limited exploration of alternate binding modes. Journal of Medicinal Chemistry, 1994, 37, 2206-2215.	2.9	134
46	Characterization of a Cdc42 Protein Inhibitor and Its Use as a Molecular Probe. Journal of Biological Chemistry, 2013, 288, 8531-8543.	1.6	134
47	Systems chemical biology. Nature Chemical Biology, 2007, 3, 447-450.	3.9	129
48	Bioactivity-guided mapping and navigation of chemical space. Nature Chemical Biology, 2009, 5, 585-592.	3.9	129
49	DrugCentral 2021 supports drug discovery and repositioning. Nucleic Acids Research, 2021, 49, D1160-D1169.	6.5	129
50	A critical overview of computational approaches employed for COVID-19 drug discovery. Chemical Society Reviews, 2021, 50, 9121-9151.	18.7	128
51	Identification of a functional water channel in cytochrome P450 enzymes. Proceedings of the National Academy of Sciences of the United States of America, 1997, 94, 2133-2138.	3.3	125
52	GPR30: a novel therapeutic target in estrogen-related disease. Trends in Pharmacological Sciences, 2008, 29, 116-123.	4.0	122
53	A crowdsourcing evaluation of the NIH chemical probes. Nature Chemical Biology, 2009, 5, 441-447.	3.9	111
54	TCRD and Pharos 2021: mining the human proteome for disease biology. Nucleic Acids Research, 2021, 49, D1334-D1346.	6.5	109

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55	DrugCentral 2018: an update. Nucleic Acids Research, 2019, 47, D963-D970.	6.5	104
56	Associating Drugs, Targets and Clinical Outcomes into an Integrated Network Affords a New Platform for Computerâ€Aided Drug Repurposing. Molecular Informatics, 2011, 30, 100-111.	1.4	100
57	Virtual Screening in Lead Discovery: A Viewpoint. Molecules, 2002, 7, 51-62.	1.7	98
58	Lead-like, drug-like or â€œPub-likeâ€: how different are they?. Journal of Computer-Aided Molecular Design, 2007, 21, 113-119.	1.3	98
59	Integration of Virtual Screening with High-Throughput Flow Cytometry to Identify Novel Small Molecule Formylpeptide Receptor Antagonists. Molecular Pharmacology, 2005, 68, 1301-1310.	1.0	94
60	hERG Classification Model Based on a Combination of Support Vector Machine Method and GRIND Descriptors. Molecular Pharmaceutics, 2008, 5, 117-127.	2.3	91
61	Toward minimalistic modeling of oral drug absorption. Journal of Molecular Graphics and Modelling, 1999, 17, 261-274.	1.3	89
62	Computational and Practical Aspects of Drug Repositioning. Assay and Drug Development Technologies, 2015, 13, 299-306.	0.6	89
63	Chemical space navigation in lead discovery. Current Opinion in Chemical Biology, 2002, 6, 384-389.	2.8	88
64	Badapple: promiscuity patterns from noisy evidence. Journal of Cheminformatics, 2016, 8, 29.	2.8	85
65	Expression of estrogen receptor GPR30 in the rat spinal cord and in autonomic and sensory ganglia. Journal of Neuroscience Research, 2009, 87, 1610-1619.	1.3	83
66	Intracellular Cannabinoid Type 1 (CB1) Receptors Are Activated by Anandamide. Journal of Biological Chemistry, 2011, 286, 29166-29174.	1.6	83
67	Pharmacokinetically Based Mapping Device for Chemical Space Navigation. ACS Combinatorial Science, 2002, 4, 258-266.	3.3	82
68	An automated PLS search for biologically relevant QSAR descriptors. Journal of Computer-Aided Molecular Design, 2004, 18, 437-449.	1.3	79
69	BDDCS Class Prediction for New Molecular Entities. Molecular Pharmaceutics, 2012, 9, 570-580.	2.3	78
70	Will Artificial Intelligence for Drug Discovery Impact Clinical Pharmacology?. Clinical Pharmacology and Therapeutics, 2020, 107, 780-785.	2.3	77
71	A Competitive Nucleotide Binding Inhibitor: In Vitro Characterization of Rab7 GTPase Inhibition. ACS Chemical Biology, 2012, 7, 1095-1108.	1.6	76
72	ChemProt-3.0: a global chemical biology diseases mapping. Database: the Journal of Biological Databases and Curation, 2016, 2016, bav123.	1.4	75

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73	Rapid Evaluation of Synthetic and Molecular Complexity for in Silico Chemistry. Journal of Chemical Information and Modeling, 2005, 45, 1237-1243.	2.5	74
74	ChemProt: a disease chemical biology database. Nucleic Acids Research, 2011, 39, D367-D372.	6.5	71
75	Strategies for Compound Selection. Current Drug Discovery Technologies, 2004, 1, 211-220.	0.6	71
76	Novel derivatives of 1,3,4-oxadiazoles are potent mitostatic agents featuring strong microtubule depolymerizing activity in the sea urchin embryo and cell culture assays. European Journal of Medicinal Chemistry, 2010, 45, 1683-1697.	2.6	70
77	High-Throughput Flow Cytometry to Detect Selective Inhibitors of ABCB1, ABCC1, and ABCG2 Transporters. Assay and Drug Development Technologies, 2008, 6, 263-276.	0.6	67
78	Improving the prediction of the brain disposition for orally administered drugs using BDDCS. Advanced Drug Delivery Reviews, 2012, 64, 95-109.	6.6	65
79	Surface Descriptors for Proteinâ˜'Ligand Affinity Prediction. Journal of Medicinal Chemistry, 2003, 46, 25-33.	2.9	64
80	High-Throughput Screening with HyperCytÂ® Flow Cytometry to Detect Small Molecule Formylpeptide Receptor Ligands. Journal of Biomolecular Screening, 2005, 10, 374-382.	2.6	63
81	Drug target ontology to classify and integrate drug discovery data. Journal of Biomedical Semantics, 2017, 8, 50.	0.9	63
82	Three-dimensional quantitative structure-activity relationships of steroid aromatase inhibitors. Journal of Computer-Aided Molecular Design, 1996, 10, 186-200.	1.3	59
83	Exemestane's 17-hydroxylated metabolite exerts biological effects as an androgen. Molecular Cancer Therapeutics, 2007, 6, 2817-2827.	1.9	58
84	Fluorescent substrates for flow cytometric evaluation of efflux inhibition in ABCB1, ABCC1, and ABCG2 transporters. Analytical Biochemistry, 2013, 437, 77-87.	1.1	57
85	Artificial intelligence, drug repurposing and peer review. Nature Biotechnology, 2020, 38, 1127-1131.	9.4	56
86	Current trends in lead discovery: are we looking for the appropriate properties?. Molecular Diversity, 2000, 5, 199-208.	2.1	55
87	Target, chemical and bioactivity databases â€“ integration is key. Drug Discovery Today: Technologies, 2006, 3, 357-365.	4.0	53
88	Activation of dioxin response element (DRE)-associated genes by benzo(a)pyrene 3,6-quinone and benzo(a)pyrene 1,6-quinone in MCF-10A human mammary epithelial cells. Toxicology and Applied Pharmacology, 2007, 221, 203-214.	1.3	52
89	Chemical information management in drug discovery: optimizing the computational and combinatorial chemistry interfaces11Color Plates for this article are on page 541.. Journal of Molecular Graphics and Modelling, 2000, 18, 512-524.	1.3	51
90	ChemProt-2.0: visual navigation in a disease chemical biology database. Nucleic Acids Research, 2012, 41, D464-D469.	6.5	50

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91	Estrogen Rapidly Modulates 5-Hydroxytrytophan-Induced Visceral Hypersensitivity via GPR30 in Rats. Gastroenterology, 2009, 137, 1040-1050.	0.6	48
92	Oncology exploration: charting cancer medicinal chemistry space. Drug Discovery Today, 2006, 11, 149-159.	3.2	46
93	Linking Pharmacology to Clinical Reports: Cyclobenzaprine and Its Possible Association With Serotonin Syndrome. Clinical Pharmacology and Therapeutics, 2011, 90, 662-665.	2.3	46
94	A novel receptor cross-talk between the ATP receptor P2Y2 and formyl peptide receptors reactivates desensitized neutrophils to produce superoxide. Experimental Cell Research, 2014, 323, 209-217.	1.2	46
95	Discovery of a specific inhibitor of human GLUT5 by virtual screening and in vitro transport evaluation. Scientific Reports, 2016, 6, 24240.	1.6	45
96	A machine learning platform to estimate anti-SARS-CoV-2 activities. Nature Machine Intelligence, 2021, 3, 527-535.	8.3	45
97	AlphaFold illuminates half of the dark human proteins. Current Opinion in Structural Biology, 2022, 74, 102372.	2.6	45
98	Scaffold Topologies. 2. Analysis of Chemical Databases. Journal of Chemical Information and Modeling, 2008, 48, 1311-1324.	2.5	44
99	Scaffold Topologies. 1. Exhaustive Enumeration up to Eight Rings. Journal of Chemical Information and Modeling, 2008, 48, 1304-1310.	2.5	43
100	Virtual and In Vitro Antiviral Screening Revive Therapeutic Drugs for COVID-19. ACS Pharmacology and Translational Science, 2020, 3, 1278-1292.	2.5	43
101	Emerging trends in the discovery of natural product antibacterials. Current Opinion in Pharmacology, 2013, 13, 678-687.	1.7	42
102	The leukocyte chemotactic receptor FPR2, but not the closely related FPR1, is sensitive to cell-penetrating pepducins with amino acid sequences descending from the third intracellular receptor loop. Biochimica Et Biophysica Acta - Molecular Cell Research, 2013, 1833, 1914-1923.	1.9	42
103	A Scaffoldâ€Treeâ€Merging Strategy for Prospective Bioactivity Annotation of Î³â€Pyrones. Angewandte Chemie - International Edition, 2010, 49, 3666-3670.	7.2	41
104	Crowdsourced mapping of unexplored target space of kinase inhibitors. Nature Communications, 2021, 12, 3307.	5.8	41
105	Highly efficient synthesis and characterization of the GPR30-selective agonist G-1 and related tetrahydroquinoline analogs. Organic and Biomolecular Chemistry, 2010, 8, 2252.	1.5	40
106	A Chemogenomic Analysis of Ionization Constantsâ€"Implications for Drug Discovery. ChemMedChem, 2013, 8, 242-255.	1.6	40
107	A Novel Pharmacologic Activity of Ketorolac for Therapeutic Benefit in Ovarian Cancer Patients. Clinical Cancer Research, 2015, 21, 5064-5072.	3.2	40
108	Exploring the dark genome: implications for precision medicine. Mammalian Genome, 2019, 30, 192-200.	1.0	40

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109	Virtual screening applications: a study of ligand-based methods and different structure representations in four different scenarios. Journal of Computer-Aided Molecular Design, 2007, 21, 617-640.	1.3	38
110	Theoretical and Practical Aspects of Three-Dimensional Quantitative Structure-Activity Relationships. Reviews in Computational Chemistry, 2007, , 127-182.	1.5	37
111	Novel Activities of Select NSAID R-Enantiomers against Rac1 and Cdc42 GTPases. PLoS ONE, 2015, 10, e0142182.	1.1	36
112	CFP-10 from Mycobacterium tuberculosis Selectively Activates Human Neutrophils through a Pertussis Toxin-Sensitive Chemotactic Receptor. Infection and Immunity, 2015, 83, 205-213.	1.0	36
113	Transporterâ€Mediated Efflux Influences CNS Side Effects: ABCB1, from Antitarget to Target. Molecular Informatics, 2010, 29, 16-26.	1.4	35
114	G protein-coupled estrogen receptor 1-mediated effects in the rat myometrium. American Journal of Physiology - Cell Physiology, 2011, 301, C1262-C1269.	2.1	35
115	Mechanisms of G Protein-Coupled Estrogen Receptor-Mediated Spinal Nociception. Journal of Pain, 2012, 13, 742-754.	0.7	35
116	Receptor-based prediction of binding affinities. Journal of Computer - Aided Molecular Design, 1998, 9/11, 35-61.	1.0	34
117	Deciphering the Plasma Proteome of Type 2 Diabetes. Diabetes, 2020, 69, 2766-2778.	0.3	34
118	Dissociation of I Domain and Global Conformational Changes in LFA-1:Â Refinement of Small Molecule-I Domain Structureâ˜Activity Relationshipsâ€. Biochemistry, 2005, 44, 4322-4331.	1.2	33
119	Biomolecular screening of formylpeptide receptor ligands with a sensitive, quantitative, high-throughput flow cytometry platform. Nature Protocols, 2006, 1, 59-66.	5.5	33
120	Cross-Pharmacology Analysis of G Protein-Coupled Receptors. Current Topics in Medicinal Chemistry, 2011, 11, 1956-1963.	1.0	33
121	How to Illuminate the Druggable Genome Using Pharos. Current Protocols in Bioinformatics, 2020, 69, e92.	25.8	33
122	Duplex highâ€throughput flow cytometry screen identifies two novel formylpeptide receptor family probes. Cytometry Part A: the Journal of the International Society for Analytical Cytology, 2009, 75A, 253-263.	1.1	32
123	P2Y2 receptor signaling in neutrophils is regulated from inside by a novel cytoskeleton-dependent mechanism. Experimental Cell Research, 2015, 336, 242-252.	1.2	31
124	Comparison of the Minimal Steric Difference (MTD) and Comparative Molecular Field Analysis (CoMFA) Methods for Analysis of Binding of Steroids to Carrier Proteins. QSAR and Combinatorial Science, 1993, 12, 21-26.	1.4	30
125	High-throughput flow cytometry for drug discovery. Expert Opinion on Drug Discovery, 2007, 2, 685-696.	2.5	30
126	The CARLSBAD Database: A Confederated Database of Chemical Bioactivities. Database: the Journal of Biological Databases and Curation, 2013, 2013, bat044.	1.4	30

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127	Diseases 2.0: a weekly updated database of diseaseâ€“gene associations from text mining and data integration. Database: the Journal of Biological Databases and Curation, 2022, 2022, .	1.4	30
128	Ligand-Based Virtual Screening by Novelty Detection with Self-Organizing Maps. Journal of Chemical Information and Modeling, 2007, 47, 2044-2062.	2.5	29
129	High-Throughput Screening for Daunorubicin-Mediated Drug Resistance Identifies Mometasone Furoate as a Novel ABCB1-Reversal Agent. Journal of Biomolecular Screening, 2008, 13, 185-193.	2.6	29
130	Targeting the Transposase Domain of the DNA Repair Component Metnase to Enhance Chemotherapy. Cancer Research, 2012, 72, 6200-6208.	0.4	29
131	Discovery of a Novel Selective PPARÎ³ Ligand with Partial Agonist Binding Properties by Integrated in Silico/in Vitro Work Flow. Journal of Chemical Information and Modeling, 2013, 53, 923-937.	2.5	29
132	Multiconformational Minimal Steric Difference. Structure-Acetylcholinesterase Hydrolysis Rates Relations for Acetic Acid Esters. QSAR and Combinatorial Science, 1993, 12, 367-372.	1.4	28
133	2D QSAR and similarity studies on cruzain inhibitors aimed at improving selectivity over cathepsin L. Bioorganic and Medicinal Chemistry, 2008, 16, 838-853.	1.4	28
134	Detection of Intracellular Granularity Induction in Prostate Cancer Cell Lines by Small Molecules Using the HyperCytÂ® High-Throughput Flow Cytometry System. Journal of Biomolecular Screening, 2009, 14, 596-609.	2.6	28
135	Model-Free Drug-Likeness from Fragments. Journal of Chemical Information and Modeling, 2010, 50, 1387-1394.	2.5	28
136	A Different Method for Steric Field Evaluation in CoMFA Improves Model Robustness. Journal of Chemical Information and Computer Sciences, 1997, 37, 1162-1170.	2.8	27
137	TIN-X: target importance and novelty explorer. Bioinformatics, 2017, 33, 2601-2603.	1.8	27
138	Solid-Phase Synthesis of Libraries Generated from a 4-Phenyl-2-carboxy-piperazine Scaffoldâ€. ACS Combinatorial Science, 2001, 3, 546-553.	3.3	26
139	On the information content of 2D and 3D descriptors for QSAR. Journal of the Brazilian Chemical Society, 2002, 13, 811.	0.6	26
140	Discovery of Selective Probes and Antagonists for G Protein-Coupled Receptors FPR/FPRL1 and GPR30. Current Topics in Medicinal Chemistry, 2009, 9, 1227-1236.	1.0	25
141	QSAR studies of disperse azo dyes. Towards the negation of the pharmacophore theory of dye-fiber interaction?. Dyes and Pigments, 1997, 33, 41-64.	2.0	24
142	iPHACE: integrative navigation in pharmacological space. Bioinformatics, 2010, 26, 985-986.	1.8	24
143	High-Throughput Screen for the Chemical Inhibitors of Antiapoptotic Bcl-2 Family Proteins by Multiplex Flow Cytometry. Assay and Drug Development Technologies, 2011, 9, 465-474.	0.6	24
144	Proteomic analysis defines kinase taxonomies specific for subtypes of breast cancer. Oncotarget, 2018, 9, 15480-15497.	0.8	24

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145	Post-High-Throughput Screening Analysis: An Empirical Compound Prioritization Scheme. Journal of Biomolecular Screening, 2005, 10, 419-426.	2.6	23
146	Small molecule inhibitors of hantavirus infection. Bioorganic and Medicinal Chemistry Letters, 2010, 20, 7085-7091.	1.0	23
147	Bradycardic effects mediated by activation of G proteinâ€coupled estrogen receptor in rat nucleus ambiguus. Experimental Physiology, 2013, 98, 679-691.	0.9	23
148	Integration of virtual and physical screening. Drug Discovery Today: Technologies, 2006, 3, 377-385.	4.0	22
149	An Overview of the Challenges in Designing, Integrating, and Delivering BARD: A Public Chemical-Biology Resource and Query Portal for Multiple Organizations, Locations, and Disciplines. Journal of Biomolecular Screening, 2014, 19, 614-627.	2.6	22
150	Chronic obstructive pulmonary disease phenotypes using cluster analysis of electronic medical records. Health Informatics Journal, 2018, 24, 394-409.	1.1	22
151	State of the Art and Uses for the Biopharmaceutics Drug Disposition Classification System (BDDCS): New Additions, Revisions, and Citation References. AAPS Journal, 2022, 24, 37.	2.2	22
152	CACHE (Critical Assessment of Computational Hit-finding Experiments): A publicâ€“private partnership benchmarking initiative to enable the development of computational methods for hit-finding. Nature Reviews Chemistry, 2022, 6, 287-295.	13.8	22
153	Surrogate data â€“ a secure way to share corporate data. Journal of Computer-Aided Molecular Design, 2005, 19, 749-764.	1.3	21
154	MTDâ^'PLS:â€‰ A PLS Variant of the Minimal Topologic Difference Method. III. Mapping Interactions between Estradiol Derivatives and the Alpha Estrogenic Receptor. Journal of Chemical Information and Modeling, 2005, 45, 1275-1281.	2.5	20
155	High-Throughput Multiplex Flow Cytometry Screening for Botulinum Neurotoxin Type A Light Chain Protease Inhibitors. Assay and Drug Development Technologies, 2010, 8, 37-46.	0.6	20
156	A Selective ATP-Binding Cassette Subfamily G Member 2 Efflux Inhibitor Revealed via High-Throughput Flow Cytometry. Journal of Biomolecular Screening, 2013, 18, 26-38.	2.6	20
157	Computational Systems Chemical Biology. Methods in Molecular Biology, 2011, 672, 459-488.	0.4	19
158	Descriptor collision and confusion: Toward the design of descriptors to mask chemical structures. Journal of Computer-Aided Molecular Design, 2005, 19, 625-635.	1.3	18
159	Conformational mAb as a Tool for Integrin Ligand Discovery. Assay and Drug Development Technologies, 2009, 7, 507-515.	0.6	18
160	Machine learning prediction and tau-based screening identifies potential Alzheimerâ€™s disease genes relevant to immunity. Communications Biology, 2022, 5, 125.	2.0	18
161	MTD-PLS: A PLS-Based Variant of the MTD Method. A 3D-QSAR Analysis of Receptor Affinities for a Series of Halogenated Dibenzoxin and Biphenyl Derivatives. SAR and QSAR in Environmental Research, 2001, 12, 75-92.	1.0	17
162	A systems chemical biology study of malate synthase and isocitrate lyase inhibition in Mycobacterium tuberculosis during active and NRP growth. Computational Biology and Chemistry, 2013, 47, 167-180.	1.1	17

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163	FRET detection of lymphocyte functionâ€“associated antigen-1 conformational extension. Molecular Biology of the Cell, 2015, 26, 43-54.	0.9	17
164	A pepducin designed to modulate P2Y 2 R function interacts with FPR2 in human neutrophils and transfers ATP to an NADPH-oxidase-activating ligand through a receptor cross-talk mechanism. Biochimica Et Biophysica Acta - Molecular Cell Research, 2016, 1863, 1228-1237.	1.9	17
165	Diabetes mellitus risk for 102 drugs and drug combinations used in patients with bipolar disorder. Psychoneuroendocrinology, 2020, 112, 104511.	1.3	17
166	Ligand-directed targeting of lymphatic vessels uncovers mechanistic insights in melanoma metastasis. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 2521-2526.	3.3	16
167	A Novel Flow Cytometric HTS Assay Reveals Functional Modulators of ATP Binding Cassette Transporter ABCB6. PLoS ONE, 2012, 7, e40005.	1.1	15
168	An Automated High-Throughput Cell-Based Multiplexed Flow Cytometry Assay to Identify Novel Compounds to Target Candida albicans Virulence-Related Proteins. PLoS ONE, 2014, 9, e110354.	1.1	15
169	Impact of similarity threshold on the topology of molecular similarity networks and clustering outcomes. Journal of Cheminformatics, 2016, 8, 16.	2.8	15
170	Chemical Database Preparation for Compound Acquisition or Virtual Screening. , 2006, 316, 375-388.		14
171	A non-peptide receptor inhibitor with selectivity for one of the neutrophil formyl peptide receptors, FPR 1. Biochemical Pharmacology, 2012, 83, 1655-1662.	2.0	14
172	Off-Patent Drug Repositioning. Journal of Chemical Information and Modeling, 2020, 60, 5746-5753.	2.5	14
173	Antibacterial Activity of Pepducins, Allosterical Modulators of Formyl Peptide Receptor Signaling. Antimicrobial Agents and Chemotherapy, 2014, 58, 2985-2988.	1.4	13
174	Activation of Rho Family GTPases by Small Molecules. ACS Chemical Biology, 2018, 13, 1514-1524.	1.6	13
175	A Selective Ligand for Estrogen Receptor Proteins Discriminates Rapid and Genomic Signaling. Cell Chemical Biology, 2019, 26, 1692-1702.e5.	2.5	13
176	Rapid Estimation of Hydrophobicity for Virtual Combinatorial Library Analysis. SAR and QSAR in Environmental Research, 2001, 12, 129-141.	1.0	12
177	Glossary of terms used in computational drug design, part II (IUPAC Recommendations 2015). Pure and Applied Chemistry, 2016, 88, 239-264.	0.9	12
178	High-Throughput Flow Cytometry Screening of Multidrug Efflux Systems. Methods in Molecular Biology, 2018, 1700, 293-318.	0.4	12
179	Identification of new GLUT2-selective inhibitors through in silico ligand screening and validation in eukaryotic expression systems. Scientific Reports, 2021, 11, 13751.	1.6	12
180	Novel drug targets in 2019. Nature Reviews Drug Discovery, 2020, 19, 300-300.	21.5	12

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