List of Publications by Year in descending order

Source: https://exaly.com/author-pdf/6001108/publications.pdf Version: 2024-02-01



#	Article	IF	CITATIONS
1	DisGeNET: a comprehensive platform integrating information on human disease-associated genes and variants. Nucleic Acids Research, 2017, 45, D833-D839.	6.5	1,865
2	The DisGeNET knowledge platform for disease genomics: 2019 update. Nucleic Acids Research, 2020, 48, D845-D855.	6.5	1,083
3	DisGeNET: a discovery platform for the dynamical exploration of human diseases and their genes. Database: the Journal of Biological Databases and Curation, 2015, 2015, bav028-bav028.	1.4	847
4	Adverse outcome pathways: opportunities, limitations and open questions. Archives of Toxicology, 2017, 91, 3477-3505.	1.9	282
5	The DisGeNET cytoscape app: Exploring and visualizing disease genomics data. Computational and Structural Biotechnology Journal, 2021, 19, 2960-2967.	1.9	221
6	DisGeNET: a Cytoscape plugin to visualize, integrate, search and analyze gene–disease networks. Bioinformatics, 2010, 26, 2924-2926.	1.8	180
7	Pathway databases and tools for their exploitation: benefits, current limitations and challenges. Molecular Systems Biology, 2009, 5, 290.	3.2	173
8	Gene-Disease Network Analysis Reveals Functional Modules in Mendelian, Complex and Environmental Diseases. PLoS ONE, 2011, 6, e20284.	1.1	153
9	Role of UEV-1, an Inactive Variant of the E2 UbiquitinConjugating Enzymes, in In Vitro Differentiation and Cell Cycle Behavior of HT-29-M6 Intestinal Mucosecretory Cells. Molecular and Cellular Biology, 1998, 18, 576-589.	1.1	142
10	Mental health impact of the first wave of COVID-19 pandemic on Spanish healthcare workers: A large cross-sectional survey. Revista De PsiquiatrÃa Y Salud Mental, 2021, 14, 90-105.	1.0	133
11	Membrane cholesterol access into a G-protein-coupled receptor. Nature Communications, 2017, 8, 14505.	5.8	129
12	Induced Effects of Sodium Ions on Dopaminergic G-Protein Coupled Receptors. PLoS Computational Biology, 2010, 6, e1000884.	1.5	93
13	GPCRmd uncovers the dynamics of the 3D-GPCRome. Nature Methods, 2020, 17, 777-787.	9.0	90
14	Membrane omega-3 fatty acids modulate the oligomerisation kinetics of adenosine A2A and dopamine D2 receptors. Scientific Reports, 2016, 6, 19839.	1.6	89
15	Four simple recommendations to encourage best practices in research software. F1000Research, 2017, 6, 876.	0.8	88
16	A Multiscale Simulation System for the Prediction of Drug-Induced Cardiotoxicity. Journal of Chemical Information and Modeling, 2011, 51, 483-492.	2.5	86
17	Anchorâ^'GRIND:Â Filling the Gap between Standard 3D QSAR and the GRid-INdependent Descriptors. Journal of Medicinal Chemistry, 2005, 48, 2687-2694.	2.9	84
18	PsyGeNET: a knowledge platform on psychiatric disorders and their genes. Bioinformatics, 2015, 31, 3075-3077.	1.8	79

#	Article	IF	CITATIONS
19	Comparison of the effects of amiodarone versus metoprolol on the frequency of ventricular arrhythmias and on mortality after acute myocardial infarction. American Journal of Cardiology, 1993, 72, 1243-1248.	0.7	78
20	Incorporating Molecular Shape into the Alignment-free GRid-INdependent Descriptors. Journal of Medicinal Chemistry, 2004, 47, 2805-2815.	2.9	78
21	Mesenteric infarction: an analysis of 83 patients with prognostic studies in 44 cases undergoing a massive small-bowel resection. British Journal of Surgery, 2005, 75, 544-548.	0.1	75
22	Surgical Wound Infections: Prospective Study of 4,468 Clean Wounds. Infection Control, 1987, 8, 277-280.	0.5	71
23	Thirtyâ€day suicidal thoughts and behaviors among hospital workers during the first wave of the Spain COVIDâ€19 outbreak. Depression and Anxiety, 2021, 38, 528-544.	2.0	70
24	Detecting Signs of Depression in Tweets in Spanish: Behavioral and Linguistic Analysis. Journal of Medical Internet Research, 2019, 21, e14199.	2.1	66
25	Automatic search for maximum similarity between molecular electrostatic potential distributions. Journal of Computer-Aided Molecular Design, 1991, 5, 371-380.	1.3	64
26	Personalized Respiratory Medicine: Exploring the Horizon, Addressing the Issues. Summary of a BRN-AJRCCM Workshop Held in Barcelona on June 12, 2014. American Journal of Respiratory and Critical Care Medicine, 2015, 191, 391-401.	2.5	61
27	Identifying temporal patterns in patient disease trajectories using dynamic time warping: A population-based study. Scientific Reports, 2018, 8, 4216.	1.6	61
28	3D-QSAR methods on the basis of ligand-receptor complexes. Application of COMBINE and GRID/GOLPE methodologies to a series of CYP1A2 ligands. Journal of Computer-Aided Molecular Design, 2000, 14, 341-353.	1.3	59
29	The eTOX Data-Sharing Project to Advance in Silico Drug-Induced Toxicity Prediction. International Journal of Molecular Sciences, 2014, 15, 21136-21154.	1.8	56
30	Legacy data sharing to improve drug safety assessment: the eTOX project. Nature Reviews Drug Discovery, 2017, 16, 811-812.	21.5	56
31	New Serotonin 5-HT2A, 5-HT2B, and 5-HT2CReceptor Antagonists:Â Synthesis, Pharmacology, 3D-QSAR, and Molecular Modeling of (Aminoalkyl)benzo and Heterocycloalkanones. Journal of Medicinal Chemistry, 2002, 45, 54-71.	2.9	53
32	DisGeNET-RDF: harnessing the innovative power of the Semantic Web to explore the genetic basis of diseases. Bioinformatics, 2016, 32, 2236-2238.	1.8	52
33	Multiâ€Receptor Binding Profile of Clozapine and Olanzapine: A Structural Study Based on the New β ₂ Adrenergic Receptor Template. ChemMedChem, 2008, 3, 1194-1198.	1.6	51
34	Applicability Domain Analysis (ADAN): A Robust Method for Assessing the Reliability of Drug Property Predictions. Journal of Chemical Information and Modeling, 2014, 54, 1500-1511.	2.5	51
35	Inroads to Predict in Vivo Toxicology—An Introduction to the eTOX Project. International Journal of Molecular Sciences, 2012, 13, 3820-3846.	1.8	50
36	MEPSIM: A computational package for analysis and comparison of molecular electrostatic potentials. Journal of Computer-Aided Molecular Design, 1993, 7, 337-347.	1.3	48

#	Article	IF	CITATIONS
37	Network medicine analysis of COPD multimorbidities. Respiratory Research, 2014, 15, 111.	1.4	48
38	Improving data and knowledge management to better integrate health care and research. Journal of Internal Medicine, 2013, 274, 321-328.	2.7	44
39	Distinction between Asymptomatic Monoclonal B-cell Lymphocytosis with Cyclin D1 Overexpression and Mantle Cell Lymphoma: From Molecular Profiling to Flow Cytometry. Clinical Cancer Research, 2014, 20, 1007-1019.	3.2	44
40	A Knowledge-Driven Approach to Extract Disease-Related Biomarkers from the Literature. BioMed Research International, 2014, 2014, 1-11.	0.9	42
41	Drug-Induced Acute Myocardial Infarction: Identifying â€~Prime Suspects' from Electronic Healthcare Records-Based Surveillance System. PLoS ONE, 2013, 8, e72148.	1.1	41
42	Design, Synthesis, and Structureâ´'Activity Relationships of 1-,3-,8-, and 9-Substituted-9-deazaxanthines at the Human A2BAdenosine Receptor. Journal of Medicinal Chemistry, 2006, 49, 282-299.	2.9	37
43	Synthesis and Atypical Antipsychotic Profile of Some 2-(2-Piperidinoethyl)benzocycloalkanones as Analogs of Butyrophenone. Journal of Medicinal Chemistry, 1994, 37, 2564-2573.	2.9	36
44	The EUâ€ADR Web Platform: delivering advanced pharmacovigilance tools. Pharmacoepidemiology and Drug Safety, 2013, 22, 459-467.	0.9	36
45	Validation of the medical expert system PNEUMON-IA. Journal of Biomedical Informatics, 1992, 25, 511-526.	0.7	35
46	Conformationally Constrained Butyrophenones with Mixed Dopaminergic (D2) and Serotoninergic (5-HT2A, 5-HT2C) Affinities:  Synthesis, Pharmacology, 3D-QSAR, and Molecular Modeling of (Aminoalkyl)benzo- and -thienocycloalkanones as Putative Atypical Antipsychotics. Journal of Medicinal Chemistry, 1999, 42, 2774-2797.	2.9	35
47	Synthesis, binding affinity and SAR of new benzolactam derivatives as dopamine D3 receptor ligands. Bioorganic and Medicinal Chemistry Letters, 2009, 19, 1773-1778.	1.0	35
48	Three-dimensional modelling of human cytochrome P450 1A2 and its interaction with caffeine and MeIQ. Journal of Computer-Aided Molecular Design, 1997, 11, 395-408.	1.3	34
49	Automatic Filtering and Substantiation of Drug Safety Signals. PLoS Computational Biology, 2012, 8, e1002457.	1.5	34
50	Quantum chemical study of the molecular patterns of MAO inhibitors and substrates. International Journal of Quantum Chemistry, 1983, 23, 1627-1641.	1.0	33
51	Quantum chemical structure-activity relationships on \hat{l}^2 -carbolines as natural monoamine oxidase inhibitors. International Journal of Quantum Chemistry, 1983, 23, 1643-1652.	1.0	33
52	Molecular and clinical diseasome of comorbidities in exacerbated COPD patients. European Respiratory Journal, 2015, 46, 1001-1010.	3.1	32
53	Proximal Pathway Enrichment Analysis for Targeting Comorbid Diseases via Network Endopharmacology. Pharmaceuticals, 2018, 11, 61.	1.7	32
54	GUILDify v2.0: A Tool to Identify Molecular Networks Underlying Human Diseases, Their Comorbidities and Their Druggable Targets. Journal of Molecular Biology, 2019, 431, 2477-2484.	2.0	32

#	Article	IF	CITATIONS
55	OSIRISv1.2: A named entity recognition system for sequence variants of genes in biomedical literature. BMC Bioinformatics, 2008, 9, 84.	1.2	31
56	comoRbidity: an R package for the systematic analysis of disease comorbidities. Bioinformatics, 2018, 34, 3228-3230.	1.8	31
57	Relationships between the activity of some H2-receptor agonists of histamine and their ab initio molecular electrostatic potential (MEP) and electron density comparison coefficients. European Journal of Medicinal Chemistry, 1988, 23, 7-10.	2.6	30
58	In silico models in drug development: where we are. Current Opinion in Pharmacology, 2018, 42, 111-121.	1.7	30
59	On the Ceneration of Catalytic Antibodies by Transition State Analogues. ChemBioChem, 2003, 4, 277-285.	1.3	29
60	Detection of New Biased Agonists for the Serotonin 5-HT _{2A} Receptor: Modeling and Experimental Validation. Molecular Pharmacology, 2015, 87, 740-746.	1.0	29
61	Genetic and functional characterization of disease associations explains comorbidity. Scientific Reports, 2017, 7, 6207.	1.6	28
62	In Silico QT and APD Prolongation Assay for Early Screening of Drug-Induced Proarrhythmic Risk. Journal of Chemical Information and Modeling, 2018, 58, 867-878.	2.5	28
63	Retinoic acid formation from retinol in the human gastric mucosa: role of class IV alcohol dehydrogenase and its relevance to morphological changes. American Journal of Physiology - Renal Physiology, 2005, 289, G429-G433.	1.6	27
64	1-, 3- and 8-substituted-9-deazaxanthines as potent and selective antagonists at the human A2B adenosine receptor. Bioorganic and Medicinal Chemistry, 2008, 16, 2852-2869.	1.4	27
65	Knowledge engineering for health: A new discipline required to bridge the "ICT gap―between research and healthcare. Human Mutation, 2012, 33, 797-802.	1.1	27
66	Modeling Complexes of Transmembrane Proteins: Systematic Analysis of ProteinProtein Docking Tools. Molecular Informatics, 2013, 32, 717-733.	1.4	27
67	A Dynamic View of Molecular Switch Behavior at Serotonin Receptors: Implications for Functional Selectivity. PLoS ONE, 2014, 9, e109312.	1.1	27
68	Novel Insights into Biased Agonism at G Protein-Coupled Receptors and their Potential for Drug Design. Current Pharmaceutical Design, 2013, 19, 5156-5166.	0.9	27
69	Unconditional convergence in SCF theory: a general level shift technique. Chemical Physics Letters, 1977, 47, 581-583.	1.2	26
70	QF2004B, a potential antipsychotic butyrophenone derivative with similar pharmacological properties to clozapine. Neuropharmacology, 2006, 51, 251-262.	2.0	26
71	Synthesis, Binding Affinity, and Molecular Docking Analysis of New Benzofuranone Derivatives as Potential Antipsychotics. Journal of Medicinal Chemistry, 2008, 51, 6085-6094.	2.9	26
72	Quantitative comparison of molecular electrostatic potential distributions from several semiempirical andab initiowave functions. Journal of Computational Chemistry, 1993, 14, 922-927.	1.5	24

#	Article	IF	CITATIONS
73	Validation of the Medical Expert System RENOIR. Journal of Biomedical Informatics, 1994, 27, 456-471.	0.7	24
74	From SNPs to pathways: integration of functional effect of sequence variations on models of cell signalling pathways. BMC Bioinformatics, 2009, 10, S6.	1.2	24
75	Novel approaches for modeling of the A1 adenosine receptor and its agonist binding site. Proteins: Structure, Function and Bioinformatics, 2004, 54, 705-715.	1.5	23
76	Multistructure 3D-QSAR Studies on a Series of Conformationally Constrained Butyrophenones Docked into a New Homology Model of the 5-HT2A Receptor. Journal of Medicinal Chemistry, 2007, 50, 3242-3255.	2.9	23
77	Synthesis, 3Dâ€QSAR, and Structural Modeling of Benzolactam Derivatives with Binding Affinity for the D ₂ and D ₃ Receptors. ChemMedChem, 2010, 5, 1300-1317.	1.6	23
78	OSIRIS: a tool for retrieving literature about sequence variants. Bioinformatics, 2006, 22, 2567-2569.	1.8	22
79	eTOXlab, an open source modeling framework for implementing predictive models in production environments. Journal of Cheminformatics, 2015, 7, 8.	2.8	22
80	Novel insights on the structural determinants of clozapine and olanzapine multi-target binding profiles. European Journal of Medicinal Chemistry, 2014, 77, 91-95.	2.6	21
81	Mental health impact of the first wave of COVID-19 pandemic on Spanish healthcare workers: A large cross-sectional survey. Revista De PsiquiatrÃa Y Salud Mental (English Edition), 2021, 14, 90-105.	0.2	21
82	Neuronal nicotinic receptor agonists: a multi-approach development of the pharmacophore. Journal of Computer-Aided Molecular Design, 2001, 15, 859-872.	1.3	20
83	Ligands of Neuronal Nicotinic Acetylcholine Receptor (nAChR): Inferences from the Hansch and 3-D Quantitative Structure-Activity Relationship (QSAR) Models. Current Medicinal Chemistry, 2002, 9, 1-29.	1.2	20
84	Maximum electrostatic similarity between biomolecules optimizing both relative positions and conformations. Computational and Theoretical Chemistry, 1991, 230, 437-446.	1.5	19
85	Knowledge environments representing molecular entities for the virtual physiological human. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2008, 366, 3091-3110.	1.6	19
86	A Chemocentric Approach to the Identification of Cancer Targets. PLoS ONE, 2012, 7, e35582.	1.1	19
87	Publishing DisGeNET as nanopublications. Semantic Web, 2016, 7, 519-528.	1.1	18
88	Network, Transcriptomic and Genomic Features Differentiate Genes Relevant for Drug Response. Frontiers in Genetics, 2018, 9, 412.	1,1	18
89	Proyecto de biomarcadores y perfiles clÃnicos personalizados en la enfermedad pulmonar obstructiva crónica (proyecto BIOMEPOC). Archivos De Bronconeumologia, 2019, 55, 93-99.	0.4	18
90	Comorbidity between Alzheimer's disease and major depression: a behavioural and transcriptomic characterization study in mice. Alzheimer's Research and Therapy, 2021, 13, 73.	3.0	18

#	Article	IF	CITATIONS
91	Synthesis, Affinity at 5-HT2A, 5-HT2B and 5-HT2C Serotonin Receptors and Structure-Activity Relationships of a Series of Cyproheptadine Analogues Chemical and Pharmaceutical Bulletin, 1997, 45, 842-848.	0.6	17
92	Integrative Modeling Strategies for Predicting Drug Toxicities at the eTOX Project. Molecular Informatics, 2015, 34, 477-484.	1.4	17
93	The eTRANSAFE Project on Translational Safety Assessment through Integrative Knowledge Management: Achievements and Perspectives. Pharmaceuticals, 2021, 14, 237.	1.7	17
94	The VATAM guidelines. International Journal of Medical Informatics, 1999, 56, 107-115.	1.6	16
95	Continuing education and community pharmacists in Galicia: a study of opinions. International Journal of Clinical Pharmacy, 2004, 26, 173-177.	1.4	15
96	IDENTIFYING GENE-SPECIFIC VARIATIONS IN BIOMEDICAL TEXT. Journal of Bioinformatics and Computational Biology, 2007, 05, 1277-1296.	0.3	15
97	Nanoinformatics: developing new computing applications for nanomedicine. Computing (Vienna/New) Tj ETQq1	l 0.78431 3.2	4 _I gBT /Ov€
98	Gathering and Exploring Scientific Knowledge in Pharmacovigilance. PLoS ONE, 2013, 8, e83016.	1.1	15
99	Synthesis, adenosine receptor binding and 3D-QSAR of 4-substituted 2-(2′-furyl)-1,2,4-triazolo[1,5-a]quinoxalines. Bioorganic and Medicinal Chemistry, 2008, 16, 2103-2113.	1.4	14
100	Electrostatic corrections to extended Hýckel theory. International Journal of Quantum Chemistry, 1977, 11, 271-276.	1.0	13
101	The Impact of Computer Science in Molecular Medicine: Enabling High- Throughput Research. Current Topics in Medicinal Chemistry, 2013, 13, 526-575.	1.0	13
102	Hepatotoxicity prediction by systems biology modeling of disturbed metabolic pathways using gene expression data. ALTEX: Alternatives To Animal Experimentation, 2017, 34, 219-234.	0.9	13
103	MIPSIM: similarity analysis of molecular interaction potentials. Bioinformatics, 2000, 16, 568-569.	1.8	12
104	Integrative knowledge management to enhance pharmaceutical R&D. Nature Reviews Drug Discovery, 2014, 13, 239-240.	21.5	12
105	Quantitative Structure-Activity Relationships on MAO Substrates by Means of Quantum Chemical Properties. QSAR and Combinatorial Science, 1986, 5, 54-57.	1.4	11
106	Introducing medical students to medical informatics. Medical Education, 1993, 27, 479-483.	1.1	11
107	Text mining and expert curation to develop a database on psychiatric diseases and their genes. Database: the Journal of Biological Databases and Curation, 2017, 2017, .	1.4	11
108	An ensemble learning approach for modeling the systems biology of drug-induced injury. Biology Direct, 2021, 16, 5.	1.9	11

#	Article	IF	CITATIONS
109	Comparative Analysis of Putative Agonist-Binding Modes in the Human A1 Adenosine Receptor. ChemBioChem, 2004, 5, 841-849.	1.3	10
110	A Novel Multilevel Statistical Method for the Study of the Relationships between Multireceptorial Binding Affinity Profiles and In Vivo Endpoints. Molecular Pharmacology, 2010, 77, 149-158.	1.0	10
111	Development of an Infrastructure for the Prediction of Biological Endpoints in Industrial Environments. Lessons Learned at the eTOX Project. Frontiers in Pharmacology, 2018, 9, 1147.	1.6	10
112	Comparison of biomolecules on the basis of Molecular Interaction Potentials. Journal of the Brazilian Chemical Society, 2002, 13, 795-799.	0.6	10
113	Toward a unifying strategy for the structure-based prediction of toxicological endpoints. Archives of Toxicology, 2016, 90, 2445-2460.	1.9	9
114	Flame: an open source framework for model development, hosting, and usage in production environments. Journal of Cheminformatics, 2021, 13, 31.	2.8	9
115	Four-month incidence of suicidal thoughts and behaviors among healthcare workers after the first wave of the Spain COVID-19 pandemic. Journal of Psychiatric Research, 2022, 149, 10-17.	1.5	9
116	Use of alignment-free molecular descriptors in diversity analysis and optimal sampling of molecular libraries. Molecular Diversity, 2000, 6, 135-147.	2.1	8
117	Information technology in community pharmacies for supporting responsible self-medication. American Journal of Health-System Pharmacy, 2000, 57, 1601-1603.	0.5	8
118	Conformationally constrained butyrophenones as new pharmacological tools to study 5-HT2A and 5-HT2C receptor behaviours. European Journal of Medicinal Chemistry, 2003, 38, 433-440.	2.6	8
119	The eTOX Library of Public Resources for in Silico Toxicity Prediction. Molecular Informatics, 2013, 32, 24-35.	1.4	8
120	Discussion of "The New Role of Biomedical Informatics in the Age of Digital Medicine― Methods of Information in Medicine, 2016, 55, 403-421.	0.7	8
121	A system-level analysis of patient disease trajectories based on clinical, phenotypic and molecular similarities. Bioinformatics, 2021, 37, 1435-1443.	1.8	8
122	The Challenge of the Effective Implementation of FAIR Principles in Biomedical Research. Methods of Information in Medicine, 2020, 59, 117-118.	0.7	7
123	Cyproheptadine Analogues: Synthesis, Antiserotoninergic Activity, and Structure-Activity Relationships. Journal of Pharmaceutical Sciences, 1993, 82, 1090-1093.	1.6	6
124	Towards a MIP-based alignment and docking in computer-aided drug design. Proteins: Structure, Function and Bioinformatics, 2004, 56, 585-594.	1.5	6
125	Viva Europa, a Land of Excellence in Research and Innovation for Health and Wellbeing. Progress in Preventive Medicine (New York, N Y), 2017, 2, e006.	0.7	6
126	Antiserotoninergic Activity of 2-Aminoethylbenzocyclanones in Rat Aorta: Structure-Activity Relationships. Journal of Pharmaceutical Sciences, 1993, 82, 513-517.	1.6	5

#	Article	IF	CITATIONS
127	Theoretical Study on the Metabolism of Caffeine by Cytochrome P-450 1A2 and its Inhibition. QSAR and Combinatorial Science, 1994, 13, 281-284.	1.4	5
128	Inventory of validation approaches in selected health telematics projects. International Journal of Medical Informatics, 1999, 56, 87-96.	1.6	5
129	Controlling for Chance Agreement in the Validation of Medical Expert Systems with No Gold Standard: PNEUMON-IA and RENOIR Revisited. Journal of Biomedical Informatics, 2000, 33, 380-397.	0.7	5
130	The BIOMEPOC Project: Personalized Biomarkers and Clinical Profiles in Chronic Obstructive Pulmonary Disease. Archivos De Bronconeumologia, 2019, 55, 93-99.	0.4	5
131	ISOTOPE: ISOform-guided prediction of epiTOPEs in cancer. PLoS Computational Biology, 2021, 17, e1009411.	1.5	5
132	The ELIXIR Human Copy Number Variations Community: building bioinformatics infrastructure for research. F1000Research, 2020, 9, 1229.	0.8	5
133	Statistical errors in software. International Journal of Epidemiology, 1988, 17, 931-931.	0.9	4
134	Effects of longâ€ŧerm treatment with metoprolol and hydrochlorothiazide on plasma lipids and lipoproteins. Journal of Internal Medicine, 1990, 228, 323-331.	2.7	4
135	Validating spongia, an expert system for sponge identification. Expert Systems With Applications, 1999, 16, 379-384.	4.4	4
136	Distant collaboration in drug discovery: the LINK3D project. Journal of Computer-Aided Molecular Design, 2002, 16, 809-818.	1.3	4
137	An automated tool for obtaining QSAR-ready series of compounds using semantic web technologies. Bioinformatics, 2018, 34, 131-133.	1.8	4
138	Generating Modeling Data From Repeat-Dose Toxicity Reports. Toxicological Sciences, 2018, 162, 287-300.	1.4	4
139	Molecular Diversity Sample Generation on the Basis of Quantum-Mechanical Computations and Principal Component Analysis. Combinatorial Chemistry and High Throughput Screening, 2002, 5, 49-57.	0.6	3
140	ELIXIR and Toxicology: a community in development. F1000Research, 0, 10, 1129.	0.8	3
141	Clinical-Based and Expert Selection of Terms Related to Depression for Twitter Streaming and Language Analysis. Studies in Health Technology and Informatics, 2020, 270, 921-925.	0.2	3
142	Extended Hückel theory of hydrogen-molecule interactions. International Journal of Quantum Chemistry, 1975, 9, 1021-1031.	1.0	2
143	The role of solvation in redox processes. Chemical Physics Letters, 1979, 62, 255-258.	1.2	2
144	Differential effects of 2'-deoxyguanosine on peripheral blood mononuclear cell proliferation in healthy donors and Hashimoto's thyroiditis patients. Cell Proliferation, 1996, 29, 513-521.	2.4	2

#	Article	IF	CITATIONS
145	Hepatotoxicity Prediction by Systems Biology Modeling of Disturbed Metabolic Pathways Using Gene Expression Data. Methods in Molecular Biology, 2018, 1800, 505-518.	0.4	2
146	Title is missing!. Journal of Computer-Aided Molecular Design, 2001, 15, 1153-1153.	1.3	1
147	Comparison of electrostatic similarity approaches applied to a series of ketanserin analogues with 5-HT2A antagonistic activity. QSAR and Combinatorial Science, 1998, 17, 199-204.	1.4	1
148	Service Oriented Architecture for Biomedical Collaborative Research. Lecture Notes in Computer Science, 2005, , 252-261.	1.0	1
149	Exploring the Association of Cancer and Depression in Electronic Health Records: Combining Encoded Diagnosis and Mining Free-Text Clinical Notes. JMIR Cancer, 2022, 8, e39003.	0.9	1
150	Influence of pH on the Binding of Diphenylmethylenepiperidines by 5-HT2B Receptors in Rat Stomach Fundus Chemical and Pharmaceutical Bulletin, 2002, 50, 395-398.	0.6	0
151	Pharmacophore Development for the Interaction of Cytochrome P450 1A2 with Its Substrates and Inhibitors. , 2000, , 141-146.		0
152	Development and Validation of an In Silico Rabbit Purkinje Cell Action Potential Model: A Step Towards a Drug Safety Testing Tool. , 0, , .		0
153	Evaluating Behavioral and Linguistic Changes During Drug Treatment for Depression Using Tweets in Spanish: Pairwise Comparison Study. Journal of Medical Internet Research, 2020, 22, e20920.	2.1	0
154	Development of In Silico Methods for Toxicity Prediction in Collaboration Between Academia and the Pharmaceutical Industry. Methods in Molecular Biology, 2022, 2425, 119-131.	0.4	0