JosÃ© L Medina Franco

List of Publications by Year
in descending order

255	8,390	47006	74163
papers	citations	47	75
		h-index	g-index

290	290	290	8134
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Shifting from the single to the multitarget paradigm in drug discovery. Drug Discovery Today, 2013, 18, 495-501.	6.4	384
2	Recognizing Pitfalls in Virtual Screening: A Critical Review. Journal of Chemical Information and Modeling, 2012, 52, 867-881.	5.4	358
3	Novel and selective DNA methyltransferase inhibitors: Docking-based virtual screening and experimental evaluation. Bioorganic and Medicinal Chemistry, 2010, 18, 822-829.	3.0	165
4	Nanaomycin A Selectively Inhibits DNMT3B and Reactivates Silenced Tumor Suppressor Genes in Human Cancer Cells. Molecular Cancer Therapeutics, 2010, 9, 3015-3023.	4.1	154
5	Synthesis and Biochemical Evaluation of Î”²-Isoxazoline Derivatives as DNA Methyltransferase 1 Inhibitors. Journal of Medicinal Chemistry, 2011, 54, 7663-7677.	6.4	154
6	Characterization of Activity Landscapes Using 2D and 3D Similarity Methods: Consensus Activity Cliffs. Journal of Chemical Information and Modeling, 2009, 49, 477-491.	5.4	145
7	Activity cliffs in drug discovery: Dr Jekyll or Mr Hyde?. Drug Discovery Today, 2014, 19, 1069-1080.	6.4	140
8	Chemoinformatic Analysis of Combinatorial Libraries, Drugs, Natural Products, and Molecular Libraries Small Molecule Repository. Journal of Chemical Information and Modeling, 2009, 49, 1010-1024.	5.4	138
9	Expanding the medicinally relevant chemical space with compound libraries. Drug Discovery Today, 2012, 17, 718-726.	6.4	136
10	Natural products as DNA methyltransferase inhibitors: a computer-aided discovery approach. Molecular Diversity, 2011, 15, 293-304.	3.9	132
11	Visualization of the Chemical Space in Drug Discovery. Current Computer-Aided Drug Design, 2008, 4, 322-333.	1.2	131
12	A critical overview of computational approaches employed for COVID-19 drug discovery. Chemical Society Reviews, 2021, 50, 9121-9151.	38.1	128
13	Integrating Virtual Screening and Combinatorial Chemistry for Accelerated Drug Discovery. Combinatorial Chemistry and High Throughput Screening, 2011, 14, 475-487.	1.1	122
14	Editorial: In silico Methods for Drug Design and Discovery. Frontiers in Chemistry, 2020, 8, 612.	3.6	117
15	A comparative study of flavonoid analogues on streptozotocinâ€“nicotinamide induced diabetic rats: Quercetin as a potential antidiabetic agent acting via 11Î²-Hydroxysteroid dehydrogenase type 1 inhibition. European Journal of Medicinal Chemistry, 2010, 45, 2606-2612.	5.5	114
16	Strategies for the Use of Mixture-Based Synthetic Combinatorial Libraries: Scaffold Ranking, Direct Testing In Vivo, and Enhanced Deconvolution by Computational Methods. ACS Combinatorial Science, 2008, 10, 3-19.	3.3	108
17	Antidiabetic activity of some pentacyclic acid triterpenoids, role of PTPâ€“1B: In vitro, in silico, and in vivo approaches. European Journal of Medicinal Chemistry, 2011, 46, 2243-2251.	5.5	107
18	The many roles of molecular complexity in drug discovery. Drug Discovery Today, 2017, 22, 120-126.	6.4	107

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19	Molecular Modeling and Molecular Dynamics Studies of Hydralazine with Human DNA Methyltransferaseâ€...1. ChemMedChem, 2009, 4, 792-799.	3.2	104
20	In Silico ADME/Tox Profiling of Natural Products: A Focus on BIOFACQUIM. ACS Omega, 2020, 5, 16076-16084.	3.5	88
21	Structureâ€“activity relationships of benzimidazole derivatives as antiparasitic agents: Dual activity-difference (DAD) maps. MedChemComm, 2011, 2, 44-49.	3.4	80
22	Advances in the computational development of DNA methyltransferase inhibitors. Drug Discovery Today, 2011, 16, 418-425.	6.4	80
23	Molecular dynamics simulations of human DNA methyltransferase 3B with selective inhibitor nanaomycin A. Journal of Structural Biology, 2011, 176, 185-191.	2.8	77
24	Natural product drug discovery in the artificial intelligence era. Chemical Science, 2022, 13, 1526-1546.	7.4	75
25	Molecular Scaffold Analysis of Natural Products Databases in the Public Domain. Chemical Biology and Drug Design, 2012, 80, 717-724.	3.2	74
26	Combinatorial Libraries As a Tool for the Discovery of Novel, Broad-Spectrum Antibacterial Agents Targeting the ESKAPE Pathogens. Journal of Medicinal Chemistry, 2015, 58, 3340-3355.	6.4	74
27	The prince and the pauper. A tale of anticancer targeted agents. Molecular Cancer, 2008, 7, 82.	19.2	73
28	Homology modeling, docking and structure-based pharmacophore of inhibitors of DNA methyltransferase. Journal of Computer-Aided Molecular Design, 2011, 25, 555-567.	2.9	70
29	A Similarityâ€based Dataâ€fusion Approach to the Visual Characterization and Comparison of Compound Databases. Chemical Biology and Drug Design, 2007, 70, 393-412.	3.2	67
30	Toward Drug Repurposing in Epigenetics: Olsalazine as a Hypomethylating Compound Active in a Cellular Context. ChemMedChem, 2014, 9, 560-565.	3.2	67
31	DataWarrior: an evaluation of the open-source drug discovery tool. Expert Opinion on Drug Discovery, 2019, 14, 335-341.	5.0	67
32	The impact of chemoinformatics on drug discovery in the pharmaceutical industry. Expert Opinion on Drug Discovery, 2020, 15, 293-306.	5.0	67
33	Molecular basis for benzimidazole resistance from a novel Î²-tubulin binding site model. Journal of Molecular Graphics and Modelling, 2013, 45, 26-37.	2.4	61
34	Scanning Structureâ€“Activity Relationships with Structureâ€“Activity Similarity and Related Maps: From Consensus Activity Cliffs to Selectivity Switches. Journal of Chemical Information and Modeling, 2012, 52, 2485-2493.	5.4	60
35	Computational Drug Design Methodsâ€”Current and Future Perspectives. , 2019, , 19-44.		60
36	Visualization of Molecular Fingerprints. Journal of Chemical Information and Modeling, 2011, 51, 1552-1563.	5.4	59

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37	Consensus Models of Activity Landscapes with Multiple Chemical, Conformer, and Property Representations. Journal of Chemical Information and Modeling, 2011, 51, 1259-1270.	5.4	58
38	BIOFACQUIM: A Mexican Compound Database of Natural Products. Biomolecules, 2019, 9, 31.	4.0	58
39	Towards a systematic characterization of the antiprotozoal activity landscape of benzimidazole derivatives. Bioorganic and Medicinal Chemistry, 2010, 18, 7380-7391.	3.0	57
40	Consensus Diversity Plots: a global diversity analysis of chemical libraries. Journal of Cheminformatics, 2016, 8, 63.	6.1	56
41	Systematic Extraction of Analogue Series from Large Compound Collections Using a New Computational Compoundâ€“Core Relationship Method. ACS Omega, 2019, 4, 1027-1032.	3.5	56
42	Multitarget Structureâ€“Activity Relationships Characterized by Activity-Difference Maps and Consensus Similarity Measure. Journal of Chemical Information and Modeling, 2011, 51, 2427-2439.	5.4	54
43	Towards the identification of the binding site of benzimidazoles to Î²-tubulin of Trichinella spiralis: Insights from computational and experimental data. Journal of Molecular Graphics and Modelling, 2013, 41, 12-19.	2.4	54
44	Extended connectivity interaction features: improving binding affinity prediction through chemical description. Bioinformatics, 2021, 37, 1376-1382.	4.1	54
45	Molecular Modeling of Inhibitors of Human DNA Methyltransferase with a Crystal Structure. Advances in Protein Chemistry and Structural Biology, 2012, 87, 219-247.	2.3	53
46	Density Functional Theory and Electrochemical Studies: Structureâ€“Efficiency Relationship on Corrosion Inhibition. Journal of Chemical Information and Modeling, 2015, 55, 2391-2402.	5.4	53
47	Discovery and development of DNA methyltransferase inhibitors using in silico approaches. Drug Discovery Today, 2015, 20, 569-577.	6.4	53
48	Effects of Cyclic Lipodepsipeptide Structural Modulation on Stability, Antibacterial Activity, and Human Cell Toxicity. ChemMedChem, 2012, 7, 871-882.	3.2	52
49	Database fingerprint (DFP): an approach to represent molecular databases. Journal of Cheminformatics, 2017, 9, 9.	6.1	51
50	Activity Cliffs: Facts or Artifacts?. Chemical Biology and Drug Design, 2013, 81, 553-556.	3.2	49
51	Inhibitors of HMG-CoA Reductase: Current and Future Prospects. Mini-Reviews in Medicinal Chemistry, 2009, 9, 1272-1283.	2.4	47
52	Benzotriazoles and Indazoles Are Scaffolds with Biological Activity against Entamoeba histolytica. Journal of Biomolecular Screening, 2011, 16, 862-868.	2.6	47
53	Balancing novelty with confined chemical space in modern drug discovery. Expert Opinion on Drug Discovery, 2014, 9, 151-165.	5.0	47
54	Molecular Modeling Studies of the Novel Inhibitors of DNA Methyltransferases SGI-1027 and CBC12: Implications for the Mechanism of Inhibition of DNMTs. PLoS ONE, 2013, 8, e62152.	2.5	46

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55	Chemical Space and Diversity of the NuBBE Database: A Chemoinformatic Characterization. Journal of Chemical Information and Modeling, 2019, 59, 74-85.	5.4	46
56	Scaffold Diversity of Fungal Metabolites. Frontiers in Pharmacology, 2017, 8, 180.	3.5	45
57	Open chemoinformatic resources to explore the structure, properties and chemical space of molecules. RSC Advances, 2017, 7, 54153-54163.	3.6	45
58	Analysis of a large food chemical database: chemical space, diversity, and complexity. F1000Research, 2018, 7, 993.	1.6	43
59	Chemoinformatic expedition of the chemical space of fungal products. Future Medicinal Chemistry, 2016, 8, 1399-1412.	2.3	42
60	Ivermectin as an inhibitor of cancer stemâ€‘like cells. Molecular Medicine Reports, 2018, 17, 3397-3403.	2.4	42
61	Informatics for Chemistry, Biology, and Biomedical Sciences. Journal of Chemical Information and Modeling, 2021, 61, 26-35.	5.4	42
62	Resveratrol-salicylate derivatives as selective DNMT3 inhibitors and anticancer agents. Journal of Enzyme Inhibition and Medicinal Chemistry, 2016, 31, 695-703.	5.2	40
63	Platform for Unified Molecular Analysis: PUMA. Journal of Chemical Information and Modeling, 2017, 57, 1735-1740.	5.4	40
64	Vasorelaxant activity of some structurally related triterpenic acids from Phoradendron reichenbachianum (Viscaceae) mainly by NO production: Ex vivo and in silico studies. FÃ¬toterapÃ¬Ã¢, 2012, 83, 1023-1029.	2.2	39
65	Chemoinformatic Analysis of GRAS (Generally Recognized as Safe) Flavor Chemicals and Natural Products. PLoS ONE, 2012, 7, e50798.	2.5	37
66	Ribavirin as a tri-targeted antitumor repositioned drug. Oncology Reports, 2015, 33, 2384-2392.	2.6	37
67	Exploring the chemical space and the bioactivity profile of lactams: a chemoinformatic study. RSC Advances, 2019, 9, 27105-27116.	3.6	37
68	Inhibitors of DNA Methyltransferases From Natural Sources: A Computational Perspective. Frontiers in Pharmacology, 2018, 9, 1144.	3.5	36
69	Acoplamiento Molecular: Avances Recientes y Retos. TIP Revista Especializada En Ciencias QuÃmico-BiolÃ³gicas, 0, 21, .	0.3	36
70	Insights from pharmacological similarity of epigenetic targets in epipolypharmacology. Drug Discovery Today, 2018, 23, 141-150.	6.4	35
71	Design, synthesis, and docking of highly hypolipidemic agents: Schizosaccharomyces pombe as a new model for evaluating Î±-asarone-based HMG-CoA reductase inhibitors. Bioorganic and Medicinal Chemistry, 2010, 18, 4238-4248.	3.0	34
72	A Synthetic Combinatorial Strategy for Developing Î±-Conotoxin Analogs as Potent Î±7 Nicotinic Acetylcholine Receptor Antagonists. Journal of Biological Chemistry, 2010, 285, 1809-1821.	3.4	34

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73	Cheminformatics to Characterize Pharmacologically Active Natural Products. Biomolecules, 2020, 10, 1566.	4.0	34
74	Recent progress on cheminformatics approaches to epigenetic drug discovery. Drug Discovery Today, 2020, 25, 2268-2276.	6.4	33
75	Single Nucleotide Polymorphisms in the Promoter Region of the E-cadherin Gene in Gastric Cancer: Case-Control Study in a Young Mexican Population. Annals of Surgical Oncology, 2007, 14, 2246-2249.	1.5	32
76	Identifying Activity Cliff Generators of PPAR Ligands Using SAS Maps. Molecular Informatics, 2012, 31, 837-846.	2.5	32
77	Bicyclic acetals: biological relevance, scaffold analysis, and applications in diversity-oriented synthesis. Organic and Biomolecular Chemistry, 2019, 17, 1037-1052.	2.8	32
78	Interrogating Novel Areas of Chemical Space for Drug Discovery using Chemoinformatics. Drug Development Research, 2012, 73, 430-438.	2.9	31
79	Finding Constellations in Chemical Space Through Core Analysis. Frontiers in Chemistry, 2019, 7, 510.	3.6	31
80	Lessons from Exploring Chemical Space and Chemical Diversity of Propolis Components. International Journal of Molecular Sciences, 2020, 21, 4988.	4.1	31
81	Increased Diversity of Libraries from Libraries: Chemoinformatic Analysis of Bisâ€Diazacyclic Libraries. Chemical Biology and Drug Design, 2011, 77, 328-342.	3.2	30
82	Bioactivity landscape modeling: Chemoinformatic characterization of structureâ€“activity relationships of compounds tested across multiple targets. Bioorganic and Medicinal Chemistry, 2012, 20, 5443-5452.	3.0	30
83	Synthesis of 2-{2-[(Î±/Î²-naphthalen-1-ylsulfonyl)amino]-1,3-thiazol-4-yl} acetamides with 11Î²-hydroxysteroid dehydrogenase inhibition and in combo antidiabetic activities. European Journal of Medicinal Chemistry, 2014, 74, 179-186.	5.5	30
84	Epigenetic relevant chemical space: a chemoinformatic characterization of inhibitors of DNA methyltransferases. RSC Advances, 2015, 5, 87465-87476.	3.6	30
85	Chemoinformatics-based enumeration of chemical libraries: a tutorial. Journal of Cheminformatics, 2020, 12, 64.	6.1	30
86	A chemical space odyssey of inhibitors of histone deacetylases and bromodomains. RSC Advances, 2016, 6, 56225-56239.	3.6	28
87	Systemic QSAR and phenotypic virtual screening: chasing butterflies in drug discovery. Drug Discovery Today, 2017, 22, 994-1007.	6.4	28
88	From flamingo dance to (desirable) drug discovery: a nature-inspired approach. Drug Discovery Today, 2017, 22, 1489-1502.	6.4	28
89	Cheminformatic characterization of natural products from Panama. Molecular Diversity, 2017, 21, 779-789.	3.9	28
90	Inhibitors of DNA Methyltransferases: Insights from Computational Studies. Current Medicinal Chemistry, 2012, 19, 3475-3487.	2.4	27

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91	Antihyperglycemic and sub-chronic antidiabetic actions of morolic and moronic acids, in vitro and in silico inhibition of 11Î²-HSD 1. Phytomedicine, 2013, 20, 571-576.	5.3	27
92	Systematic Mining of Generally Recognized as Safe (GRAS) Flavor Chemicals for Bioactive Compounds. Journal of Agricultural and Food Chemistry, 2013, 61, 7507-7514.	5.2	27
93	Discovery, synthesis and in combo studies of a tetrazole analogue of clofibric acid as a potent hypoglycemic agent. Bioorganic and Medicinal Chemistry Letters, 2013, 23, 3244-3247.	2.2	27
94	Selective Agonists and Antagonists of Formylpeptide Receptors: Duplex Flow Cytometry and Mixture-Based Positional Scanning Libraries. Molecular Pharmacology, 2013, 84, 314-324.	2.3	27
95	Anti-inflammatory and antioxidant properties of a novel resveratrolâ€“salicylate hybrid analog. Bioorganic and Medicinal Chemistry Letters, 2016, 26, 1411-1415.	2.2	27
96	Activity and property landscape modeling is at the interface of chemoinformatics and medicinal chemistry. Future Medicinal Chemistry, 2015, 7, 1197-1211.	2.3	26
97	Getting SMARt in drug discovery: chemoinformatics approaches for mining structureâ€“multiple activity relationships. RSC Advances, 2017, 7, 632-641.	3.6	26
98	In search of AKT kinase inhibitors as anticancer agents: structure-based design, docking, and molecular dynamics studies of 2,4,6-trisubstituted pyridines. Journal of Biomolecular Structure and Dynamics, 2018, 36, 423-442.	3.5	26
99	Proteinâ€“Protein Interaction Modulators for Epigenetic Therapies. Advances in Protein Chemistry and Structural Biology, 2018, 110, 65-84.	2.3	26
100	DiaNat-DB: a molecular database of antidiabetic compounds from medicinal plants. RSC Advances, 2021, 11, 5172-5178.	3.6	26
101	Rationalization of Activity Cliffs of a Sulfonamide Inhibitor of DNA Methyltransferases with Induced-Fit Docking. International Journal of Molecular Sciences, 2014, 15, 3253-3261.	4.1	25
102	Reaching for the bright StARs in chemical space. Drug Discovery Today, 2019, 24, 2162-2169.	6.4	25
103	Progress on open chemoinformatic tools for expanding and exploring the chemical space. Journal of Computer-Aided Molecular Design, 2022, 36, 341-354.	2.9	25
104	ChemMaps: Towards an approach for visualizing the chemical space based on adaptive satellite compounds. F1000Research, 2017, 6, 1134.	1.6	25
105	Characterization of a comprehensive flavor database. Journal of Chemometrics, 2011, 25, 550-560.	1.3	24
106	Comparative molecular field analysis (CoMFA) and comparative molecular similarity indices analysis (CoMSIA) of some benzimidazole derivatives with trichomonicidal activity. European Journal of Medicinal Chemistry, 2011, 46, 3499-3508.	5.5	23
107	A cell-based fascin bioassay identifies compounds with potential anti-metastasis or cognition-enhancing functions. DMM Disease Models and Mechanisms, 2013, 6, 217-35.	2.4	23
108	Data Mining of Protein-Binding Profiling Data Identifies Structural Modifications that Distinguish Selective and Promiscuous Compounds. Journal of Chemical Information and Modeling, 2012, 52, 2454-2461.	5.4	23

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109	Trimethylaurintricarboxylic acid inhibits human DNA methyltransferase 1: insights from enzymatic and molecular modeling studies. Journal of Molecular Modeling, 2012, 18, 1583-1589.	1.8	23
110	The Interplay Between Molecular Modeling and Chemoinformatics to Characterize Proteinâ€“Ligand and Proteinâ€“Protein Interactions Landscapes for Drug Discovery. Advances in Protein Chemistry and Structural Biology, 2014, 96, 1-37.	2.3	23
111	Analyzing Multitarget Activity Landscapes Using Proteinâ€“Ligand Interaction Fingerprints: Interaction Cliffs. Journal of Chemical Information and Modeling, 2015, 55, 251-262.	5.4	23
112	Activity landscape sweeping: insights into the mechanism of inhibition and optimization of DNMT1 inhibitors. RSC Advances, 2015, 5, 63882-63895.	3.6	23
113	Consensus virtual screening of dark chemical matter and food chemicals uncover potential inhibitors of SARS-CoV-2 main protease. RSC Advances, 2020, 10, 25089-25099.	3.6	23
114	Rationality over fashion and hype in drug design. F1000Research, 2021, 10, 397.	1.6	23
115	Yes SIR! On the structureâ€“inactivity relationships in drug discovery. Drug Discovery Today, 2022, 27, 2353-2362.	6.4	23
116	Docking-based CoMFA and CoMSIA studies of non-nucleoside reverse transcriptase inhibitors of the pyridinone derivative type. Journal of Computer-Aided Molecular Design, 2004, 18, 345-360.	2.9	22
117	Synthesis, in vitro and in silico studies of a PPARÎ³ and GLUT-4 modulator with hypoglycemic effect. Bioorganic and Medicinal Chemistry Letters, 2014, 24, 4575-4579.	2.2	22
118	Activity cliffs and activity cliff generators based on chemotype-related activity landscapes. Molecular Diversity, 2015, 19, 1021-1035.	3.9	22
119	Activity Landscape Plotter: A Web-Based Application for the Analysis of Structureâ€“Activity Relationships. Journal of Chemical Information and Modeling, 2017, 57, 397-402.	5.4	22
120	A Fragment Library of Natural Products and its Comparative Chemoinformatic Characterization. Molecular Informatics, 2020, 39, e2000050.	2.5	22
121	Epigenetic Target Fishing with Accurate Machine Learning Models. Journal of Medicinal Chemistry, 2021, 64, 8208-8220.	6.4	22
122	Analysis of a large food chemical database: chemical space, diversity, and complexity. F1000Research, 2018, 7, 993.	1.6	22
123	Diversity and Chemical Library Networks of Large Data Sets. Journal of Chemical Information and Modeling, 2022, 62, 2186-2201.	5.4	22
124	Conformation-opioid activity relationships of bicyclic guanidines from 3D similarity analysis. Bioorganic and Medicinal Chemistry, 2008, 16, 5932-5938.	3.0	21
125	Synthesis and highly potent hypolipidemic activity of alpha-asarone- and fibrate-based 2-acyl and 2-alkyl phenols as HMG-CoA reductase inhibitors. Bioorganic and Medicinal Chemistry, 2014, 22, 5871-5882.	3.0	21
126	Fragment Library of Natural Products and Compound Databases for Drug Discovery. Biomolecules, 2020, 10, 1518.	4.0	21

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127	Synthesis, inÂvitro and in silico screening of ethyl 2-(6-substituted) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 747 Td (benzo[d]th az Journal of Medicinal Chemistry, 2012, 53, 346-355.	5.5	20
128	Docking of a novel DNA methyltransferase inhibitor identified from high-throughput screening: insights to unveil inhibitors in chemical databases. Molecular Diversity, 2013, 17, 337-344.	3.9	20
129	Activity Landscape and Molecular Modeling to Explore the SAR of Dual Epigenetic Inhibitors: A Focus on G9a and DNMT1. Molecules, 2018, 23, 3282.	3.8	20
130	Discovery of a novel protein kinase B inhibitor by structure-based virtual screening. Bioorganic and Medicinal Chemistry Letters, 2009, 19, 4634-4638.	2.2	19
131	Activity landscape of DNA methyltransferase inhibitors bridges chemoinformatics with epigenetic drug discovery. Expert Opinion on Drug Discovery, 2015, 10, 1059-1070.	5.0	19
132	Drug Repurposing for Epigenetic Targets Guided by Computational Methods. , 2016, , 327-357.		19
133	Towards the understanding of the activity of G9a inhibitors: an activity landscape and molecular modeling approach. Journal of Computer-Aided Molecular Design, 2020, 34, 659-669.	2.9	19
134	Conformation-dependent QSAR approach for the prediction of inhibitory activity of bromodomain modulators. SAR and QSAR in Environmental Research, 2017, 28, 41-58.	2.2	18
135	Chemoselective fluorination and chemoinformatic analysis of griseofulvin: Natural vs fluorinated fungal metabolites. Bioorganic and Medicinal Chemistry, 2017, 25, 5238-5246.	3.0	18
136	Flavonoids as Putative Epi-Modulators: Insight into Their Binding Mode with BRD4 Bromodomains Using Molecular Docking and Dynamics. Biomolecules, 2018, 8, 61.	4.0	18
137	Towards a unified Latin American Natural Products Database: LANaPD. Future Science OA, 2020, 6, FSO468.	1.9	18
138	Molecular Modeling and Virtual Screening of DNA Methyltransferase Inhibitors. Current Pharmaceutical Design, 2013, 19, 2138-2147.	1.9	18
139	Chapter 2 Chemoinformaticsâ€"Applications in Food Chemistry. Advances in Food and Nutrition Research, 2009, 58, 33-56.	3.0	17
140	Activity landscape modeling of PPAR ligands with dual-activity difference maps. Bioorganic and Medicinal Chemistry, 2012, 20, 3523-3532.	3.0	17
141	Rapid Scanning Structureâ€"Activity Relationships in Combinatorial Data Sets: Identification of Activity Switches. Journal of Chemical Information and Modeling, 2013, 53, 1475-1485.	5.4	17
142	Tubulin Inhibitors: A Chemoinformatic Analysis Using Cell-Based Data. Molecules, 2021, 26, 2483.	3.8	17
143	Functional group and diversity analysis of BIOFACQUIM: A Mexican natural product database. F1000Research, 2019, 8, 2071.	1.6	17
144	Design and synthesis of Î±â€conotoxin GID analogues as selective Î±4Î²2 nicotinic acetylcholine receptor antagonists. Biopolymers, 2014, 102, 78-87.	2.4	16

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145	Insights into the structure and inhibition ofGiardia intestinalisarginine deiminase: homology modeling, docking, and molecular dynamics studies. Journal of Biomolecular Structure and Dynamics, 2016, 34, 732-748.	3.5	16
146	Chemoinformatics: a perspective from an academic setting in Latin America. Molecular Diversity, 2018, 22, 247-258.	3.9	16
147	Chemical Diversity of Cyanobacterial Compounds: A Chemoinformatics Analysis. ACS Omega, 2019, 4, 6229-6237.	3.5	16
148	Dimeric phenalenones from Talaromyces sp. (IQ-313) inhibit hPTP1B1-400: Insights into mechanistic kinetics from in vitro and in silico studies. Bioorganic Chemistry, 2020, 101, 103893.	4.1	16
149	Epigenetic Target Profiler: A Web Server to Predict Epigenetic Targets of Small Molecules. Journal of Chemical Information and Modeling, 2021, 61, 1550-1554.	5.4	16
150	ChemMaps: Towards an approach for visualizing the chemical space based on adaptive satellite compounds. F1000Research, 2017, 6, 1134.	1.6	16
151	Functional group and diversity analysis of BIOFACQUIM: A Mexican natural product database. F1000Research, 2019, 8, 2071.	1.6	16
152	Bridging informatics and medicinal inorganic chemistry: Toward a database of metallodrugs and metallodrug candidates. Drug Discovery Today, 2022, 27, 1420-1430.	6.4	16
153	Docking of Protein Kinase B Inhibitors: Implications in the Structureâ€Based Optimization of a Novel Scaffold. Chemical Biology and Drug Design, 2010, 76, 269-276.	3.2	15
154	Advances in the development of pyridinone derivatives as non-nucleoside reverse transcriptase inhibitors. RSC Advances, 2016, 6, 2119-2130.	3.6	15
155	Chemical space, diversity and activity landscape analysis of estrogen receptor binders. RSC Advances, 2018, 8, 38229-38237.	3.6	15
156	Transient pockets on XIAP-BIR2: toward the characterization of putative binding sites of small-molecule XIAP inhibitors. Journal of Molecular Modeling, 2012, 18, 2031-2042.	1.8	14
157	Integrating virtual and biochemical screening for protein tyrosine phosphatase inhibitor discovery. Methods, 2014, 65, 219-228.	3.8	14
158	Cheminformatics Explorations of Natural Products. Progress in the Chemistry of Organic Natural Products, 2019, 110, 1-35.	1.1	14
159	Design and synthesis of Nâ€benzoyl amino acid derivatives as <scp>DNA</scp> methylation inhibitors. Chemical Biology and Drug Design, 2016, 88, 664-676.	3.2	13
160	Synthesis and antitubercular activity of new N-[5-(4-chlorophenyl)-1,3,4-oxadiazol-2-yl]-(nitroheteroaryl)carboxamides. Heterocyclic Communications, 2019, 25, 52-59.	1.2	13
161	Conformal prediction of HDAC inhibitors. SAR and QSAR in Environmental Research, 2019, 30, 265-277.	2.2	13
162	Identification, structureâ€“activity relationships and molecular modeling of potent triamine and piperazine opioid ligands. Bioorganic and Medicinal Chemistry, 2009, 17, 5583-5597.	3.0	12

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163	Computational study on the inhibition mechanism of cruzain by nitrile-containing molecules. Journal of Molecular Graphics and Modelling, 2012, 35, 28-35.	2.4	12
164	Benzoic Acid Derivatives with Trypanocidal Activity: Enzymatic Analysis and Molecular Docking Studies toward Trans-Sialidase. Molecules, 2017, 22, 1863.	3.8	12
165	Metronidazole and Secnidazole Carbamates: Synthesis, Antiprotozoal Activity, and Molecular Dynamics Studies. Molecules, 2020, 25, 793.	3.8	12
166	Expanding the Structural Diversity of DNA Methyltransferase Inhibitors. Pharmaceuticals, 2021, 14, 17.	3.8	12
167	CASE Plots for the Chemotypeâ€Based Activity and Selectivity Analysis: A CASE Study of Cyclooxygenase Inhibitors. Chemical Biology and Drug Design, 2012, 80, 752-762.	3.2	11
168	DNA Methyltransferase Inhibitors for Cancer Therapy. , 2015, , 265-290.		11
169	How to Valorize Biodiversity? LetÊ¼s Go Hashing, Extracting, Filtering, Mining, Fishing. Planta Medica, 2015, 81, 436-449.	1.3	11
170	From Qualitative to Quantitative Analysis of Activity and Property Landscapes. Journal of Chemical Information and Modeling, 2020, 60, 5873-5880.	5.4	11
171	Towards the Chemoinformatic-Based Identification of DNA Methyltransferase Inhibitors: 2D- and 3D-Similarity Profile of Screening Libraries. Current Computer-Aided Drug Design, 2012, 8, 317-329.	1.2	10
172	Conditional Probabilistic Analysis for Prediction of the Activity Landscape and Relative Compound Activities. Journal of Chemical Information and Modeling, 2013, 53, 2613-2625.	5.4	10
173	Progress in the Visualization and Mining of Chemical and Target Spaces. Molecular Informatics, 2013, 32, 942-953.	2.5	10
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