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	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
2	Diversity and Chemical Library Networks of Large Data Sets. Journal of Chemical Information and Modeling, 2022, 62, 2186-2201.	5.4	22
3	Natural product drug discovery in the artificial intelligence era. Chemical Science, 2022, 13, 1526-1546.	7.4	75
4	Cheminformatics analysis of molecular datasets of transcription factors associated with quorum sensing inPseudomonas aeruginosa. RSC Advances, 2022, 12, 6783-6790.	3.6	4
5	Bridging informatics and medicinal inorganic chemistry: Toward a database of metallodrugs and metallodrug candidates. Drug Discovery Today, 2022, 27, 1420-1430.	6.4	16
6	The Essence and Transcendence of Scientific Publishing. Frontiers in Research Metrics and Analytics, 2022, 7, 822453.	1.9	5
7	Chemoinformatic Characterization of Synthetic Screening Libraries Focused on Epigenetic Targets. Molecular Informatics, 2022, 41, e2100285.	2.5	10
8	Methyl benzoate and cinnamate analogs as modulators of DNA methylation in hepatocellular carcinoma. Chemical Biology and Drug Design, 2022, 100, 245-255.	3.2	1
9	7-Aminoalkoxy-Quinazolines from Epigenetic Focused Libraries Are Potent and Selective Inhibitors of DNA Methyltransferase 1. Molecules, 2022, 27, 2892.	3.8	5
10	Yes SIR! On the structureâ€“inactivity relationships in drug discovery. Drug Discovery Today, 2022, 27, 2353-2362.	6.4	23
11	Approaches for enhancing the analysis of chemical space for drug discovery. Expert Opinion on Drug Discovery, 2022, 17, 789-798.	5.0	8
12	Discovery and development of lead compounds from natural sources using computational approaches. , 2022, , 539-560.		2
13	Extended connectivity interaction features: improving binding affinity prediction through chemical description. Bioinformatics, 2021, 37, 1376-1382.	4.1	54
14	DiaNat-DB: a molecular database of antidiabetic compounds from medicinal plants. RSC Advances, 2021, 11, 5172-5178.	3.6	26
15	The Acid/Base Characterization of Molecules with Epigenetic Activity. ChemMedChem, 2021, 16, 1745-1754.	3.2	2
16	Epigenetic Target Fishing with Accurate Machine Learning Models. Journal of Medicinal Chemistry, 2021, 64, 8208-8220.	6.4	22
17	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
18	Computational Approaches for the Discovery and Development of Pharmacologically Active Natural Products. Biomolecules, 2021, 11, 630.	4.0	2

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19	Expanding the Chemical Information Science gateway. F1000Research, 2021, 10, 294.	1.6	0
20	Tubulin Inhibitors: A Chemoinformatic Analysis Using Cell-Based Data. Molecules, 2021, 26, 2483.	3.8	17
21	Monosubstituted Coumarins Inhibit Epinephrine-Induced Platelet Aggregation Antiplatelet Effect of Monosubstituted Coumarins. Cardiovascular and Hematological Agents in Medicinal Chemistry, 2021, 19, .	1.0	0
22	Rationality over fashion and hype in drug design. F1000Research, 2021, 10, 397.	1.6	23
23	Advances in the Exploration of the Epigenetic Relevant Chemical Space. ACS Omega, 2021, 6, 22478-22486.	3.5	10
24	Chemoinformatic Analysis of Isothiocyanates: Their Impact in Nature and Medicine. Molecular Informatics, 2021, 40, e2100172.	2.5	4
25	Computational Applications in Secondary Metabolite Discovery (CAiSMD): an online workshop. Journal of Cheminformatics, 2021, 13, 64.	6.1	3
26	An in silico pipeline for the discovery of multitarget ligands: A case study for epi-polypharmacology based on DNMT1/HDAC2 inhibition. Artificial Intelligence in the Life Sciences, 2021, 1, 100008.	2.2	1
27	A critical overview of computational approaches employed for COVID-19 drug discovery. Chemical Society Reviews, 2021, 50, 9121-9151.	38.1	128
28	Latin American databases of natural products: biodiversity and drug discovery against SARS-CoV-2. RSC Advances, 2021, 11, 16051-16064.	3.6	5
29	Synthesis of covalent bonding MWCNT-oligoethylene linezolid conjugates and their antibacterial activity against bacterial strains. RSC Advances, 2021, 11, 28912-28924.	3.6	1
30	Informatics for Chemistry, Biology, and Biomedical Sciences. Journal of Chemical Information and Modeling, 2021, 61, 26-35.	5.4	42
31	Expanding the Structural Diversity of DNA Methyltransferase Inhibitors. Pharmaceuticals, 2021, 14, 17.	3.8	12
32	Glossary of terms used in chemoinformatics of natural products: advanced concepts and applications. , 2021, , 299-318.		0
33	Towards the De Novo Design of HIV-1 Protease Inhibitors Based on Natural Products. Biomolecules, 2021, 11, 1805.	4.0	5
34	Analysis of the Acid/Base Profile of Natural Products from Different Sources. Molecular Informatics, 2020, 39, 1900099.	2.5	5
35	Design, synthesis and evaluation of the antibacterial activity of new Linezolid dipeptide-type analogues. Bioorganic Chemistry, 2020, 95, 103483.	4.1	8
36	Chemoinformatic Approach: The Case of Natural Products of Panama. , 2020, , .		4

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37	Current advances on the development of BET inhibitors: insights from computational methods. Advances in Protein Chemistry and Structural Biology, 2020, 122, 127-180.	2.3	5
38	Novel Linezolid analogues with antiparasitic activity against Hymenolepis nana. Bioorganic Chemistry, 2020, 105, 104359.	4.1	4
39	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
40	In Silico ADME/Tox Profiling of Natural Products: A Focus on BIOFACQUIM. ACS Omega, 2020, 5, 16076-16084.	3.5	88
41	Lessons from Exploring Chemical Space and Chemical Diversity of Propolis Components. International Journal of Molecular Sciences, 2020, 21, 4988.	4.1	31
42	Fragment Library of Natural Products and Compound Databases for Drug Discovery. Biomolecules, 2020, 10, 1518.	4.0	21
43	From Qualitative to Quantitative Analysis of Activity and Property Landscapes. Journal of Chemical Information and Modeling, 2020, 60, 5873-5880.	5.4	11
44	Cheminformatics to Characterize Pharmacologically Active Natural Products. Biomolecules, 2020, 10, 1566.	4.0	34
45	Chemical space and diversity of seaweed metabolite database (SWMD): A cheminformatics study. Journal of Molecular Graphics and Modelling, 2020, 100, 107702.	2.4	8
46	Chemoinformatics-based enumeration of chemical libraries: a tutorial. Journal of Cheminformatics, 2020, 12, 64.	6.1	30
47	Towards a unified Latin American Natural Products Database: LANaPD. Future Science OA, 2020, 6, FSO468.	1.9	18
48	Consistent Cellâ€selective Analog Series as Constellation Luminaries in Chemical Space. Molecular Informatics, 2020, 39, 2000061.	2.5	4
49	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
50	Glossary of terms used in chemoinformatics of natural products: fundamental principles. , 2020, , 417-442.		0
51	Dâ€Peptide Builder: A Web Service to Enumerate, Analyze, and Visualize the Chemical Space of Combinatorial Peptide Libraries. Molecular Informatics, 2020, 39, 2000035.	2.5	7
52	Chemoinformatics approaches to assess chemical diversity and complexity of small molecules. , 2020, , 83-102.		8
53	In silico tools to study molecular targets of neglected diseases: inhibition of TcSir2rp3, an epigenetic enzyme of Trypanosoma cruzi. Advances in Protein Chemistry and Structural Biology, 2020, 122, 203-229.	2.3	10
54	4. Chemical space of naturally occurring compounds. , 2020, , 103-124.		0

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55	Editorial: In silico Methods for Drug Design and Discovery. Frontiers in Chemistry, 2020, 8, 612.	3.6	117
56	Metronidazole and Secnidazole Carbamates: Synthesis, Antiprotozoal Activity, and Molecular Dynamics Studies. Molecules, 2020, 25, 793.	3.8	12
57	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
58	The impact of chemoinformatics on drug discovery in the pharmaceutical industry. Expert Opinion on Drug Discovery, 2020, 15, 293-306.	5.0	67
59	A Fragment Library of Natural Products and its Comparative Chemoinformatic Characterization. Molecular Informatics, 2020, 39, e2000050.	2.5	22
60	Computational-aided design of a library of lactams through a diversity-oriented synthesis strategy. Bioorganic and Medicinal Chemistry, 2020, 28, 115539.	3.0	8
61	Recent progress on cheminformatics approaches to epigenetic drug discovery. Drug Discovery Today, 2020, 25, 2268-2276.	6.4	33
62	Chemoinformatic Resources for Organometallic Drug Discovery. Computational Molecular Bioscience, 2020, 10, 1-11.	0.4	4
63	Finding Constellations in Chemical Space Through Core Analysis. Frontiers in Chemistry, 2019, 7, 510.	3.6	31
64	A general approach for retrosynthetic molecular core analysis. Journal of Cheminformatics, 2019, 11, 61.	6.1	8
65	Exploring the chemical space and the bioactivity profile of lactams: a chemoinformatic study. RSC Advances, 2019, 9, 27105-27116.	3.6	37
66	Reaching for the bright StARs in chemical space. Drug Discovery Today, 2019, 24, 2162-2169.	6.4	25
67	Synthesis of NSC 106084 and NSC 14778 and evaluation of their DNMT inhibitory activity. Bioorganic and Medicinal Chemistry Letters, 2019, 29, 826-831.	2.2	3
68	Quinazolines as inhibitors of chromatin-associated proteins in histones. Medicinal Chemistry Research, 2019, 28, 395-416.	2.4	3
69	Bicyclic acetals: biological relevance, scaffold analysis, and applications in diversity-oriented synthesis. Organic and Biomolecular Chemistry, 2019, 17, 1037-1052.	2.8	32
70	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
71	Exploration of Target Synergy in Cancer Treatment by Cell-Based Screening Assay and Network Propagation Analysis. Journal of Chemical Information and Modeling, 2019, 59, 3072-3079.	5.4	1
72	Conformal prediction of HDAC inhibitors. SAR and QSAR in Environmental Research, 2019, 30, 265-277.	2.2	13

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73	New Approaches for the Discovery of Pharmacologically-Active Natural Compounds. Biomolecules, 2019, 9, 115.	4.0	10
74	Computational Drug Design Methodsâ€"Current and Future Perspectives. , 2019, , 19-44.		60
75	The Acid/Base Profile of a Large Food Chemical Database. Molecular Informatics, 2019, 38, e1800171.	2.5	5
76	Chemical Diversity of Cyanobacterial Compounds: A Chemoinformatics Analysis. ACS Omega, 2019, 4, 6229-6237.	3.5	16
77	DataWarrior: an evaluation of the open-source drug discovery tool. Expert Opinion on Drug Discovery, 2019, 14, 335-341.	5.0	67
78	BIOFACQUIM: A Mexican Compound Database of Natural Products. Biomolecules, 2019, 9, 31.	4.0	58
79	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
80	Chemical Space and Diversity of the NuBBE Database: A Chemoinformatic Characterization. Journal of Chemical Information and Modeling, 2019, 59, 74-85.	5.4	46
81	Chemical space of naturally occurring compounds. Physical Sciences Reviews, 2019, 4, .	0.8	8
82	Cheminformatics Explorations of Natural Products. Progress in the Chemistry of Organic Natural Products, 2019, 110, 1-35.	1.1	14
83	Functional group and diversity analysis of BIOFACQUIM: A Mexican natural product database. F1000Research, 2019, 8, 2071.	1.6	16
84	Functional group and diversity analysis of BIOFACQUIM: A Mexican natural product database. F1000Research, 2019, 8, 2071.	1.6	17
85	Ivermectin as an inhibitor of cancer stemâ€'like cells. Molecular Medicine Reports, 2018, 17, 3397-3403.	2.4	42
86	Exploring the chemical space of peptides for drug discovery: a focus on linear and cyclic penta-peptides. Molecular Diversity, 2018, 22, 259-267.	3.9	10
87	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
88	Insights from pharmacological similarity of epigenetic targets in epipolypharmacology. Drug Discovery Today, 2018, 23, 141-150.	6.4	35
89	Chemoinformatics: a perspective from an academic setting in Latin America. Molecular Diversity, 2018, 22, 247-258.	3.9	16
90	Statistical-based database fingerprint: chemical space dependent representation of compound databases. Journal of Cheminformatics, 2018, 10, 55.	6.1	8

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91	Chemical space, diversity and activity landscape analysis of estrogen receptor binders. RSC Advances, 2018, 8, 38229-38237.	3.6	15
92	QSAR Modeling Using Quantum Chemical Descriptors of Benzimidazole Analogues With Antiparasitic Properties. International Journal of Quantitative Structure-Property Relationships, 2018, 3, 61-79.	0.5	1
93	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
94	Inhibitors of DNA Methyltransferases From Natural Sources: A Computational Perspective. Frontiers in Pharmacology, 2018, 9, 1144.	3.5	36
95	Computational Methods to Discover Compounds for the Treatment of Chagas Disease. Advances in Protein Chemistry and Structural Biology, 2018, 113, 119-142.	2.3	4
96	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
97	Proteinâ€“Protein Interaction Modulators for Epigenetic Therapies. Advances in Protein Chemistry and Structural Biology, 2018, 110, 65-84.	2.3	26
98	Systematic search for benzimidazole compounds and derivatives with antileishmanial effects. Molecular Diversity, 2018, 22, 779-790.	3.9	8
99	Computational Methods for Epigenetic Drug Discovery: A Focus on Activity Landscape Modeling. Advances in Protein Chemistry and Structural Biology, 2018, 113, 65-83.	2.3	7
100	Cheminformatics Approaches to Study Drug Polypharmacology. Methods in Pharmacology and Toxicology, 2018, , 3-25.	0.2	2
101	Analysis of a large food chemical database: chemical space, diversity, and complexity. F1000Research, 2018, 7, 993.	1.6	22
102	Analysis of a large food chemical database: chemical space, diversity, and complexity. F1000Research, 2018, 7, 993.	1.6	43
103	Charting the Bromodomain BRD4: Towards the Identification of Novel Inhibitors with Molecular Similarity and Receptor Mapping. Letters in Drug Design and Discovery, 2018, 15, 1002-1011.	0.7	9
104	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
105	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
106	Systemic QSAR and phenotypic virtual screening: chasing butterflies in drug discovery. Drug Discovery Today, 2017, 22, 994-1007.	6.4	28
107	From flamingo dance to (desirable) drug discovery: a nature-inspired approach. Drug Discovery Today, 2017, 22, 1489-1502.	6.4	28
108	Database fingerprint (DFP): an approach to represent molecular databases. Journal of Cheminformatics, 2017, 9, 9.	6.1	51

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109	Getting SMARt in drug discovery: chemoinformatics approaches for mining structureâ€“multiple activity relationships. RSC Advances, 2017, 7, 632-641.	3.6	26
110	Cheminformatic characterization of natural products from Panama. Molecular Diversity, 2017, 21, 779-789.	3.9	28
111	Platform for Unified Molecular Analysis: PUMA. Journal of Chemical Information and Modeling, 2017, 57, 1735-1740.	5.4	40
112	Chemoselective fluorination and chemoinformatic analysis of griseofulvin: Natural vs fluorinated fungal metabolites. Bioorganic and Medicinal Chemistry, 2017, 25, 5238-5246.	3.0	18
113	The many roles of molecular complexity in drug discovery. Drug Discovery Today, 2017, 22, 120-126.	6.4	107
114	Scaffold Diversity of Fungal Metabolites. Frontiers in Pharmacology, 2017, 8, 180.	3.5	45
115	Benzoic Acid Derivatives with Trypanocidal Activity: Enzymatic Analysis and Molecular Docking Studies toward Trans-Sialidase. Molecules, 2017, 22, 1863.	3.8	12
116	Comparative Cheminformatic Analysis of Inhibitors of DNA Methyltransferases. Chemical Informatics (Wilmington, Del), 2017, 03, .	0.4	0
117	Quantitative Structure-Epigenetic Activity Relationships. Challenges and Advances in Computational Chemistry and Physics, 2017, , 303-338.	0.6	4
118	Open chemoinformatic resources to explore the structure, properties and chemical space of molecules. RSC Advances, 2017, 7, 54153-54163.	3.6	45
119	ChemMaps: Towards an approach for visualizing the chemical space based on adaptive satellite compounds. F1000Research, 2017, 6, 1134.	1.6	16
120	ChemMaps: Towards an approach for visualizing the chemical space based on adaptive satellite compounds. F1000Research, 2017, 6, 1134.	1.6	25
121	Synthesis, Screening and in silico Simulations of Anti-Parasitic Propamidine/Benzimidazole Derivatives. Medicinal Chemistry, 2017, 13, 137-148.	1.5	9
122	Toxicity Assessment of Structurally Relevant Natural Products from Mexican Plants with Antinociceptive Activity. Journal of the Mexican Chemical Society, 2017, 61, .	0.6	6
123	Progress on the Computational Development of Epigenetic Modulators of DNA Methyltransferases 3A and 3B. Journal of the Mexican Chemical Society, 2017, 61, .	0.6	3
124	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
125	Consensus Diversity Plots: a global diversity analysis of chemical libraries. Journal of Cheminformatics, 2016, 8, 63.	6.1	56
126	Drug Repurposing for Epigenetic Targets Guided by Computational Methods. , 2016, , 327-357.		19

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127	The Road Ahead of the Epi-Informatics Field. , 2016, , 399-418.		2
128	Molecular Modeling and Chemoinformatics to Advance the Development of Modulators of Epigenetic Targets. Advances in Protein Chemistry and Structural Biology, 2016, 105, 1-26.	2.3	6
129	Chemoinformatic expedition of the chemical space of fungal products. Future Medicinal Chemistry, 2016, 8, 1399-1412.	2.3	42
130	A chemical space odyssey of inhibitors of histone deacetylases and bromodomains. RSC Advances, 2016, 6, 56225-56239.	3.6	28
131	Statistical correlation of nonconservative substitutions of HIV gp41 variable amino acid residues with the R5X4 HIV-1 phenotype. Virology Journal, 2016, 13, 28.	3.4	4
132	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
133	Activity landscape analysis of novel 5$$upalpha $$-reductase inhibitors. Molecular Diversity, 2016, 20, 771-780.	3.9	10
134	Anti-inflammatory and antioxidant properties of a novel resveratrolâ€“salicylate hybrid analog. Bioorganic and Medicinal Chemistry Letters, 2016, 26, 1411-1415.	2.2	27
135	Advances in the development of pyridinone derivatives as non-nucleoside reverse transcriptase inhibitors. RSC Advances, 2016, 6, 2119-2130.	3.6	15
136	Developmental DNA methyltransferase inhibitors in the treatment of gynecologic cancers. Expert Opinion on Pharmacotherapy, 2016, 17, 323-338.	1.8	10
137	Resveratrol-salicylate derivatives as selective DNMT3 inhibitors and anticancer agents. Journal of Enzyme Inhibition and Medicinal Chemistry, 2016, 31, 695-703.	5.2	40
138	Introduction of Epigenetic Targets in Drug Discovery and Current Status of Epi-Drugs and Epi-Probes. , 2016, , 1-20.		3
139	Probing the Hypothesis of SAR Continuity Restoration by the Removal of Activity Cliffs Generators in QSAR. Current Pharmaceutical Design, 2016, 22, 5043-5056.	1.9	7
140	DNA Methyltransferase Inhibitors for Cancer Therapy. , 2015, , 265-290.		11
141	Ribavirin as a tri-targeted antitumor repositioned drug. Oncology Reports, 2015, 33, 2384-2392.	2.6	37
142	Analyzing Multitarget Activity Landscapes Using Proteinâ€“Ligand Interaction Fingerprints: Interaction Cliffs. Journal of Chemical Information and Modeling, 2015, 55, 251-262.	5.4	23
143	Activity cliffs and activity cliff generators based on chemotype-related activity landscapes. Molecular Diversity, 2015, 19, 1021-1035.	3.9	22
144	How to Valorize Biodiversity? LetÊ¼s Go Hashing, Extracting, Filtering, Mining, Fishing. Planta Medica, 2015, 81, 436-449.	1.3	11

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145	Activity landscape sweeping: insights into the mechanism of inhibition and optimization of DNMT1 inhibitors. RSC Advances, 2015, 5, 63882-63895.	3.6	23
146	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
147	Discovery and Development of Lead Compounds from Natural Sources Using Computational Approaches. , 2015, , 455-475.		10
148	Activity and property landscape modeling is at the interface of chemoinformatics and medicinal chemistry. Future Medicinal Chemistry, 2015, 7, 1197-1211.	2.3	26
149	Epigenetic relevant chemical space: a chemoinformatic characterization of inhibitors of DNA methyltransferases. RSC Advances, 2015, 5, 87465-87476.	3.6	30
150	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
151	Activity landscape of DNA methyltransferase inhibitors bridges chemoinformatics with epigenetic drug discovery. Expert Opinion on Drug Discovery, 2015, 10, 1059-1070.	5.0	19
152	Discovery and development of DNA methyltransferase inhibitors using in silico approaches. Drug Discovery Today, 2015, 20, 569-577.	6.4	53
153	Interaction Fingerprints and Their Applications to Identify Hot Spots. Methods in Molecular Biology, 2015, 1335, 313-324.	0.9	3
154	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
155	Software and Online Resources: Perspectives and Potential Applications. , 2014, , 233-248.		3
156	Toward Drug Repurposing in Epigenetics: Olsalazine as a Hypomethylating Compound Active in a Cellular Context. ChemMedChem, 2014, 9, 560-565.	3.2	67
157	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
158	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
159	Analysis of structure-Caco-2 permeability relationships using a property landscape approach. Molecular Diversity, 2014, 18, 599-610.	3.9	9
160	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
161	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
162	On the validity versus utility of activity landscapes: are all activity cliffs statistically significant?. Journal of Cheminformatics, 2014, 6, 11.	6.1	9

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163	Balancing novelty with confined chemical space in modern drug discovery. Expert Opinion on Drug Discovery, 2014, 9, 151-165.	5.0	47
164	Progress in the Analysis of Multiple Activity Profile of Screening Data Using Computational Approaches. Drug Development Research, 2014, 75, 313-323.	2.9	5
165	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
166	Activity cliffs in drug discovery: Dr Jekyll or Mr Hyde?. Drug Discovery Today, 2014, 19, 1069-1080.	6.4	140
167	Chemoinformatic characterization of activity and selectivity switches of antiprotozoal compounds. Future Medicinal Chemistry, 2014, 6, 281-294.	2.3	10
168	Integrating virtual and biochemical screening for protein tyrosine phosphatase inhibitor discovery. Methods, 2014, 65, 219-228.	3.8	14
169	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
170	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
171	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
172	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
173	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
174	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
175	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
176	Cyclic Systems Distribution Along Similarity Measures: Insights for an Application to Activity Landscape Modeling. Molecular Informatics, 2013, 32, 179-190.	2.5	3
177	Activity Cliffs: Facts or Artifacts?. Chemical Biology and Drug Design, 2013, 81, 553-556.	3.2	49
178	Shifting from the single to the multitarget paradigm in drug discovery. Drug Discovery Today, 2013, 18, 495-501.	6.4	384
179	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
180	Systematic characterization of structureâ€“activity relationships and ADMET compliance: a case study. Drug Discovery Today, 2013, 18, 732-739.	6.4	9

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181	Toward an Efficient Approach to Identify Molecular Scaffolds Possessing Selective or Promiscuous Compounds. Chemical Biology and Drug Design, 2013, 82, 367-375.	3.2	5
182	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
183	Progress in the Visualization and Mining of Chemical and Target Spaces. Molecular Informatics, 2013, 32, 942-953.	2.5	10
184	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
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