Jos L Medina Franco

List of Publications by Citations

249 papers	6,344 citations	41 h-index	66 g-index
290 ext. papers	7,419 ext. citations	4.8 avg, IF	6.54 L-index

#	Paper	IF	Citations
249	Shifting from the single to the multitarget paradigm in drug discovery. *Drug Discovery Today*, **2013**, 18, 495-501	8.8	321
248	Recognizing pitfalls in virtual screening: a critical review. *Journal of Chemical Information and Modeling*, **2012**, 52, 867-81	6.1	295
247	Novel and selective DNA methyltransferase inhibitors: Docking-based virtual screening and experimental evaluation. *Bioorganic and Medicinal Chemistry*, **2010**, 18, 822-9	3.4	138
246	Nanaomycin A selectively inhibits DNMT3B and reactivates silenced tumor suppressor genes in human cancer cells. *Molecular Cancer Therapeutics*, **2010**, 9, 3015-23	6.1	133
245	Synthesis and biochemical evaluation of Δ(2)-isoxazoline derivatives as DNA methyltransferase 1 inhibitors. *Journal of Medicinal Chemistry*, **2011**, 54, 7663-77	8.3	131
244	Characterization of activity landscapes using 2D and 3D similarity methods: consensus activity cliffs. *Journal of Chemical Information and Modeling*, **2009**, 49, 477-91	6.1	131
243	Chemoinformatic analysis of combinatorial libraries, drugs, natural products, and molecular libraries small molecule repository. *Journal of Chemical Information and Modeling*, **2009**, 49, 1010-24	6.1	131
242	Expanding the medicinally relevant chemical space with compound libraries. *Drug Discovery Today*, **2012**, 17, 718-26	8.8	118
241	Natural products as DNA methyltransferase inhibitors: a computer-aided discovery approach. *Molecular Diversity*, **2011**, 15, 293-304	3.1	117
240	Visualization of the Chemical Space in Drug Discovery. *Current Computer-Aided Drug Design*, **2008**, 4, 322-333	1.4	107
239	Activity cliffs in drug discovery: Dr Jekyll or Mr Hyde?. *Drug Discovery Today*, **2014**, 19, 1069-80	8.8	103
238	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		100
237	Molecular modeling and molecular dynamics studies of hydralazine with human DNA methyltransferase 1. *ChemMedChem*, **2009**, 4, 792-9	3.7	94
236	A comparative study of flavonoid analogues on streptozotocin-nicotinamide induced diabetic rats: quercetin as a potential antidiabetic agent acting via 11beta-hydroxysteroid dehydrogenase type 1 inhibition. *European Journal of Medicinal Chemistry*, **2010**, 45, 2606-12	6.8	89
235	Antidiabetic activity of some pentacyclic acid triterpenoids, role of PTP-1B: in vitro, in silico, and in vivo approaches. *European Journal of Medicinal Chemistry*, **2011**, 46, 2243-51	6.8	86
234	Integrating virtual screening and combinatorial chemistry for accelerated drug discovery. *Combinatorial Chemistry and High Throughput Screening*, **2011**, 14, 475-87	1.3	80
233	Activity-difference maps and consensus similarity measure characterize structure-activity relationships. *Journal of Cheminformatics*, **2012**, 4,	8.6	78

232	Computer-guided discovery of epigenetics drugs: molecular modeling and identification of inhibitors of DNMT1. *Journal of Cheminformatics*, **2012**, 4,	8.6	78
231	Advances in the computational development of DNA methyltransferase inhibitors. *Drug Discovery Today*, **2011**, 16, 418-25	8.8	72
230	The many roles of molecular complexity in drug discovery. *Drug Discovery Today*, **2017**, 22, 120-126	8.8	71
229	Molecular dynamics simulations of human DNA methyltransferase 3B with selective inhibitor nanaomycin A. *Journal of Structural Biology*, **2011**, 176, 185-91	3.4	69
228	Structure□ctivity relationships of benzimidazole derivatives as antiparasitic agents: Dual activity-difference (DAD) maps. *MedChemComm*, **2011**, 2, 44-49	5	67
227	A similarity-based data-fusion approach to the visual characterization and comparison of compound databases. *Chemical Biology and Drug Design*, **2007**, 70, 393-412	2.9	65
226	Homology modeling, docking and structure-based pharmacophore of inhibitors of DNA methyltransferase. *Journal of Computer-Aided Molecular Design*, **2011**, 25, 555-67	4.2	64
225	The prince and the pauper. A tale of anticancer targeted agents. *Molecular Cancer*, **2008**, 7, 82	42.1	63
224	Toward drug repurposing in epigenetics: olsalazine as a hypomethylating compound active in a cellular context. *ChemMedChem*, **2014**, 9, 560-5	3.7	60
223	Combinatorial Libraries As a Tool for the Discovery of Novel, Broad-Spectrum Antibacterial Agents Targeting the ESKAPE Pathogens. *Journal of Medicinal Chemistry*, **2015**, 58, 3340-55	8.3	56
222	Molecular scaffold analysis of natural products databases in the public domain. *Chemical Biology and Drug Design*, **2012**, 80, 717-24	2.9	56
221	Consensus models of activity landscapes with multiple chemical, conformer, and property representations. *Journal of Chemical Information and Modeling*, **2011**, 51, 1259-70	6.1	56
220	Towards a systematic characterization of the antiprotozoal activity landscape of benzimidazole derivatives. *Bioorganic and Medicinal Chemistry*, **2010**, 18, 7380-91	3.4	54
219	Scanning structure-activity relationships with structure-activity similarity and related maps: from consensus activity cliffs to selectivity switches. *Journal of Chemical Information and Modeling*, **2012**, 52, 2485-93	6.1	52
218	Multitarget structure-activity relationships characterized by activity-difference maps and consensus similarity measure. *Journal of Chemical Information and Modeling*, **2011**, 51, 2427-39	6.1	50
217	Visualization of molecular fingerprints. *Journal of Chemical Information and Modeling*, **2011**, 51, 1552-63	6.1	50
216	Molecular modeling of inhibitors of human DNA methyltransferase with a crystal structure: discovery of a novel DNMT1 inhibitor. *Advances in Protein Chemistry and Structural Biology*, **2012**, 87, 219-47	5.3	45
215	Effects of cyclic lipodepsipeptide structural modulation on stability, antibacterial activity, and human cell toxicity. *ChemMedChem*, **2012**, 7, 871-82	3.7	44

214	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	3.7	44
213	ADME/Tox Profiling of Natural Products: A Focus on BIOFACQUIM. *ACS Omega*, **2020**, 5, 16076-16084	3.9	43
212	Activity cliffs: facts or artifacts?. *Chemical Biology and Drug Design*, **2013**, 81, 553-6	2.9	42
211	Inhibitors of HMG-CoA Reductase: Current and Future Prospects. *Mini-Reviews in Medicinal Chemistry*, **2009**, 9, 1272-83	3.2	42
210	Discovery and development of DNA methyltransferase inhibitors using in silico approaches. *Drug Discovery Today*, **2015**, 20, 569-77	8.8	41
209	The impact of chemoinformatics on drug discovery in the pharmaceutical industry. *Expert Opinion on Drug Discovery*, **2020**, 15, 293-306	6.2	41
208	Molecular basis for benzimidazole resistance from a novel β-tubulin binding site model. *Journal of Molecular Graphics and Modelling*, **2013**, 45, 26-37	2.8	40
207	Consensus Diversity Plots: a global diversity analysis of chemical libraries. *Journal of Cheminformatics*, **2016**, 8, 63	8.6	40
206	Benzotriazoles and indazoles are scaffolds with biological activity against Entamoeba histolytica. *Journal of Biomolecular Screening*, **2011**, 16, 862-8		38
205	Balancing novelty with confined chemical space in modern drug discovery. *Expert Opinion on Drug Discovery*, **2014**, 9, 151-65	6.2	37
204	Systematic Extraction of Analogue Series from Large Compound Collections Using a New Computational Compound-Core Relationship Method. *ACS Omega*, **2019**, 4, 1027-1032	3.9	36
203	A critical overview of computational approaches employed for COVID-19 drug discovery. *Chemical Society Reviews*, **2021**, 50, 9121-9151	58.5	36
202	DataWarrior: an evaluation of the open-source drug discovery tool. *Expert Opinion on Drug Discovery*, **2019**, 14, 335-341	6.2	34
201	Chemoinformatic analysis of GRAS (Generally Recognized as Safe) flavor chemicals and natural products. *PLoS ONE*, **2012**, 7, e50798	3.7	34
200	Resveratrol-salicylate derivatives as selective DNMT3 inhibitors and anticancer agents. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2016**, 31, 695-703	5.6	33
199	Towards the identification of the binding site of benzimidazoles to β-tubulin of Trichinella spiralis: insights from computational and experimental data. *Journal of Molecular Graphics and Modelling*, **2013**, 41, 12-9	2.8	32
198	Ribavirin as a tri-targeted antitumor repositioned drug. *Oncology Reports*, **2015**, 33, 2384-92	3.5	31
197	BIOFACQUIM: A Mexican Compound Database of Natural Products. *Biomolecules*, **2019**, 9,	5.9	31

196	Ivermectin as an inhibitor of cancer stem-like cells. *Molecular Medicine Reports*, **2018**, 17, 3397-3403	2.9	30
195	Scaffold Diversity of Fungal Metabolites. *Frontiers in Pharmacology*, **2017**, 8, 180	5.6	30
194	A synthetic combinatorial strategy for developing alpha-conotoxin analogs as potent alpha7 nicotinic acetylcholine receptor antagonists. *Journal of Biological Chemistry*, **2010**, 285, 1809-21	5.4	30
193	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, 2246-9	3.1	30
192	Open chemoinformatic resources to explore the structure, properties and chemical space of molecules. *RSC Advances*, **2017**, 7, 54153-54163	3.7	30
191	Chemoinformatic expedition of the chemical space of fungal products. *Future Medicinal Chemistry*, **2016**, 8, 1399-412	4.1	30
190	Computational Drug Design Methods□Current and Future Perspectives **2019**, 19-44		29
189	Design, synthesis, and docking of highly hypolipidemic agents: Schizosaccharomyces pombe as a new model for evaluating alpha-asarone-based HMG-CoA reductase inhibitors. *Bioorganic and Medicinal Chemistry*, **2010**, 18, 4238-48	3.4	29
188	Interrogating Novel Areas of Chemical Space for Drug Discovery using Chemoinformatics. *Drug Development Research*, **2012**, 73, 430-438	5.1	28
187	Vasorelaxant activity of some structurally related triterpenic acids from Phoradendron reichenbachianum (Viscaceae) mainly by NO production: ex vivo and in silico studies. *Fitoterapia*, **2012**, 83, 1023-9	3.2	28
186	Chemical Space and Diversity of the NuBBE Database: A Chemoinformatic Characterization. *Journal of Chemical Information and Modeling*, **2019**, 59, 74-85	6.1	28
185	Density Functional Theory and Electrochemical Studies: Structure-Efficiency Relationship on Corrosion Inhibition. *Journal of Chemical Information and Modeling*, **2015**, 55, 2391-402	6.1	27
184	Insights from pharmacological similarity of epigenetic targets in epipolypharmacology. *Drug Discovery Today*, **2018**, 23, 141-150	8.8	27
183	Database fingerprint (DFP): an approach to represent molecular databases. *Journal of Cheminformatics*, **2017**, 9, 9	8.6	26
182	Systematic mining of generally recognized as safe (GRAS) flavor chemicals for bioactive compounds. *Journal of Agricultural and Food Chemistry*, **2013**, 61, 7507-14	5.7	26
181	Identifying Activity Cliff Generators of PPAR Ligands Using SAS Maps. *Molecular Informatics*, **2012**, 31, 837-46	3.8	26
180	Bioactivity landscape modeling: chemoinformatic characterization of structure-activity relationships of compounds tested across multiple targets. *Bioorganic and Medicinal Chemistry*, **2012**, 20, 5443-52	3.4	26
179	Increased diversity of libraries from libraries: chemoinformatic analysis of bis-diazacyclic libraries. *Chemical Biology and Drug Design*, **2011**, 77, 328-42	2.9	26

178	Systemic QSAR and phenotypic virtual screening: chasing butterflies in drug discovery. *Drug Discovery Today*, **2017**, 22, 994-1007	8.8	25
177	Epigenetic relevant chemical space: a chemoinformatic characterization of inhibitors of DNA methyltransferases. *RSC Advances*, **2015**, 5, 87465-87476	3.7	25
176	Analysis of a large food chemical database: chemical space, diversity, and complexity. *F1000Research*, **2018**, 7, 993	3.6	25
175	Bicyclic acetals: biological relevance, scaffold analysis, and applications in diversity-oriented synthesis. *Organic and Biomolecular Chemistry*, **2019**, 17, 1037-1052	3.9	24
174	Platform for Unified Molecular Analysis: PUMA. *Journal of Chemical Information and Modeling*, **2017**, 57, 1735-1740	6.1	24
173	Getting SMARt in drug discovery: chemoinformatics approaches for mining structure–multiple activity relationships. *RSC Advances*, **2017**, 7, 632-641	3.7	23
172	Activity and property landscape modeling is at the interface of chemoinformatics and medicinal chemistry. *Future Medicinal Chemistry*, **2015**, 7, 1197-211	4.1	23
171	A chemical space odyssey of inhibitors of histone deacetylases and bromodomains. *RSC Advances*, **2016**, 6, 56225-56239	3.7	23
170	Anti-inflammatory and antioxidant properties of a novel resveratrol-salicylate hybrid analog. *Bioorganic and Medicinal Chemistry Letters*, **2016**, 26, 1411-5	2.9	23
169	Data mining of protein-binding profiling data identifies structural modifications that distinguish selective and promiscuous compounds. *Journal of Chemical Information and Modeling*, **2012**, 52, 2454-61	6.1	23
168	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, 3244-7	2.9	23
167	Selective agonists and antagonists of formylpeptide receptors: duplex flow cytometry and mixture-based positional scanning libraries. *Molecular Pharmacology*, **2013**, 84, 314-24	4.3	23
166	Characterization of a comprehensive flavor database. *Journal of Chemometrics*, **2011**, 25, 550-560	1.6	23
165	Inhibitors of DNA methyltransferases: insights from computational studies. *Current Medicinal Chemistry*, **2012**, 19, 3475-87	4.3	23
164	Inhibitors of DNA Methyltransferases From Natural Sources: A Computational Perspective. *Frontiers in Pharmacology*, **2018**, 9, 1144	5.6	23
163	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	3.6	22
162	Analyzing multitarget activity landscapes using protein-ligand interaction fingerprints: interaction cliffs. *Journal of Chemical Information and Modeling*, **2015**, 55, 251-62	6.1	22
161	Rationalization of activity cliffs of a sulfonamide inhibitor of DNA methyltransferases with induced-fit docking. *International Journal of Molecular Sciences*, **2014**, 15, 3253-61	6.3	22

160	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, 3499-508	6.8	22
159	Activity Landscape Plotter: A Web-Based Application for the Analysis of Structure-Activity Relationships. *Journal of Chemical Information and Modeling*, **2017**, 57, 397-402	6.1	20
158	Activity cliffs and activity cliff generators based on chemotype-related activity landscapes. *Molecular Diversity*, **2015**, 19, 1021-35	3.1	20
157	Trimethylaurintricarboxylic acid inhibits human DNA methyltransferase 1: insights from enzymatic and molecular modeling studies. *Journal of Molecular Modeling*, **2012**, 18, 1583-9	2	20
156	Extended connectivity interaction features: improving binding affinity prediction through chemical description. *Bioinformatics*, **2021**, 37, 1376-1382	7.2	20
155	Exploring the chemical space and the bioactivity profile of lactams: a chemoinformatic study.. *RSC Advances*, **2019**, 9, 27105-27116	3.7	19
154	Finding Constellations in Chemical Space Through Core Analysis. *Frontiers in Chemistry*, **2019**, 7, 510	5	19
153	Synthesis, in vitro and in silico studies of a PPAR□and GLUT-4 modulator with hypoglycemic effect. *Bioorganic and Medicinal Chemistry Letters*, **2014**, 24, 4575-4579	2.9	19
152	Conformation-opioid activity relationships of bicyclic guanidines from 3D similarity analysis. *Bioorganic and Medicinal Chemistry*, **2008**, 16, 5932-8	3.4	19
151	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, 345-60	4.2	19
150	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, 5871-82	3.4	18
149	Synthesis, in vitro and in silico screening of ethyl 2-(6-substituted benzo[d]thiazol-2-ylamino)-2-oxoacetates as protein-tyrosine phosphatase 1B inhibitors. *European Journal of Medicinal Chemistry*, **2012**, 53, 346-55	6.8	18
148	Cheminformatic characterization of natural products from Panama. *Molecular Diversity*, **2017**, 21, 779-789	3.1	18
147	A cell-based fascin bioassay identifies compounds with potential anti-metastasis or cognition-enhancing functions. *DMM Disease Models and Mechanisms*, **2013**, 6, 217-35	4.1	18
146	From flamingo dance to (desirable) drug discovery: a nature-inspired approach. *Drug Discovery Today*, **2017**, 22, 1489-1502	8.8	17
145	Reaching for the bright StARs in chemical space. *Drug Discovery Today*, **2019**, 24, 2162-2169	8.8	17
144	Synthesis of 2-{2-[(□naphthalen-1-ylsulfonyl)amino]-1,3-thiazol-4-yl} acetamides with 11□hydroxysteroid dehydrogenase inhibition and in combo antidiabetic activities. *European Journal of Medicinal Chemistry*, **2014**, 74, 179-86	6.8	17
143	The interplay between molecular modeling and chemoinformatics to characterize protein-ligand and protein-protein interactions landscapes for drug discovery. *Advances in Protein Chemistry and Structural Biology*, **2014**, 96, 1-37	5.3	17

142	Activity landscape modeling of PPAR ligands with dual-activity difference maps. *Bioorganic and Medicinal Chemistry*, **2012**, 20, 3523-32	3.4	17
141	Antihyperglycemic and sub-chronic antidiabetic actions of morolic and moronic acids, in vitro and in silico inhibition of 11-HSD 1. *Phytomedicine*, **2013**, 20, 571-6	6.5	17
140	Docking of a novel DNA methyltransferase inhibitor identified from high-throughput screening: insights to unveil inhibitors in chemical databases. *Molecular Diversity*, **2013**, 17, 337-44	3.1	17
139	ChemMaps: Towards an approach for visualizing the chemical space based on adaptive satellite compounds. *F1000Research*, **2017**, 6, 1134	3.6	17
138	Molecular modeling and virtual screening of DNA methyltransferase inhibitors. *Current Pharmaceutical Design*, **2013**, 19, 2138-47	3.3	17
137	Cheminformatics to Characterize Pharmacologically Active Natural Products. *Biomolecules*, **2020**, 10,	5.9	17
136	Activity landscape sweeping: insights into the mechanism of inhibition and optimization of DNMT1 inhibitors. *RSC Advances*, **2015**, 5, 63882-63895	3.7	16
135	Activity landscape of DNA methyltransferase inhibitors bridges chemoinformatics with epigenetic drug discovery. *Expert Opinion on Drug Discovery*, **2015**, 10, 1059-70	6.2	16
134	Protein-Protein Interaction Modulators for Epigenetic Therapies. *Advances in Protein Chemistry and Structural Biology*, **2018**, 110, 65-84	5.3	16
133	Discovery of a novel protein kinase B inhibitor by structure-based virtual screening. *Bioorganic and Medicinal Chemistry Letters*, **2009**, 19, 4634-8	2.9	16
132	ChemMaps: Towards an approach for visualizing the chemical space based on adaptive satellite compounds. *F1000Research*, **2017**, 6,	3.6	16
131	Conformation-dependent QSAR approach for the prediction of inhibitory activity of bromodomain modulators. *SAR and QSAR in Environmental Research*, **2017**, 28, 41-58	3.5	15
130	Rapid scanning structure-activity relationships in combinatorial data sets: identification of activity switches. *Journal of Chemical Information and Modeling*, **2013**, 53, 1475-85	6.1	15
129	Chemoinformatics-applications in food chemistry. *Advances in Food and Nutrition Research*, **2009**, 58, 33-56	6	15
128	Informatics for Chemistry, Biology, and Biomedical Sciences. *Journal of Chemical Information and Modeling*, **2021**, 61, 26-35	6.1	15
127	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	3.7	15
126	Design and synthesis of -conotoxin GID analogues as selective 42 nicotinic acetylcholine receptor antagonists. *Biopolymers*, **2014**, 102, 78-87	2.2	14
125	Consensus Models of Activity Landscapes **2012**, 307-326		14

124	Analysis of a large food chemical database: chemical space, diversity, and complexity. *F1000Research*, **2018**, 7,	3.6	14
123	Recent progress on cheminformatics approaches to epigenetic drug discovery. *Drug Discovery Today*, **2020**, 25, 2268-2276	8.8	14
122	Drug Repurposing for Epigenetic Targets Guided by Computational Methods **2016**, 327-357		14
121	A Fragment Library of Natural Products and its Comparative Chemoinformatic Characterization. *Molecular Informatics*, **2020**, 39, e2000050	3.8	14
120	Flavonoids as Putative Epi-Modulators: Insight into Their Binding Mode with BRD4 Bromodomains Using Molecular Docking and Dynamics. *Biomolecules*, **2018**, 8,	5.9	13
119	Integrating virtual and biochemical screening for protein tyrosine phosphatase inhibitor discovery. *Methods*, **2014**, 65, 219-28	4.6	13
118	Acoplamiento Molecular: Avances Recientes y Retos. *TIP Revista Especializada En Ciencias Químico-Biológicas*,21,		13
117	Chemoinformatics-based enumeration of chemical libraries: a tutorial. *Journal of Cheminformatics*, **2020**, 12, 64	8.6	13
116	Computational study on the inhibition mechanism of cruzain by nitrile-containing molecules. *Journal of Molecular Graphics and Modelling*, **2012**, 35, 28-35	2.8	12
115	Chemoselective fluorination and chemoinformatic analysis of griseofulvin: Natural vs fluorinated fungal metabolites. *Bioorganic and Medicinal Chemistry*, **2017**, 25, 5238-5246	3.4	12
114	Cheminformatics Explorations of Natural Products. *Progress in the Chemistry of Organic Natural Products*, **2019**, 110, 1-35	1.9	12
113	Fragment Library of Natural Products and Compound Databases for Drug Discovery. *Biomolecules*, **2020**, 10,	5.9	12
112	Towards a unified Latin American Natural Products Database: LANaPD. *Future Science OA*, **2020**, 6, FSO468	2.7	12
111	Activity Landscape and Molecular Modeling to Explore the SAR of Dual Epigenetic Inhibitors: A Focus on G9a and DNMT1. *Molecules*, **2018**, 23,	4.8	12
110	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	4.2	11
109	Advances in the development of pyridinone derivatives as non-nucleoside reverse transcriptase inhibitors. *RSC Advances*, **2016**, 6, 2119-2130	3.7	11
108	CASE plots for the chemotype-based activity and selectivity analysis: a CASE study of cyclooxygenase inhibitors. *Chemical Biology and Drug Design*, **2012**, 80, 752-62	2.9	11
107	Docking of protein kinase B inhibitors: implications in the structure-based optimization of a novel scaffold. *Chemical Biology and Drug Design*, **2010**, 76, 269-76	2.9	11

106	Identification, structure-activity relationships and molecular modeling of potent triamine and piperazine opioid ligands. *Bioorganic and Medicinal Chemistry*, **2009**, 17, 5583-97	3.4	11
105	Natural product drug discovery in the artificial intelligence era.. *Chemical Science*, **2022**, 13, 1526-1546	9.4	11
104	Functional group and diversity analysis of BIOFACQUIM: A Mexican natural product database. *F1000Research*, **2019**, 8, 2071	3.6	11
103	Lessons from Exploring Chemical Space and Chemical Diversity of Propolis Components. *International Journal of Molecular Sciences*, **2020**, 21,	6.3	11
102	Design and synthesis of N-benzoyl amino acid derivatives as DNA methylation inhibitors. *Chemical Biology and Drug Design*, **2016**, 88, 664-676	2.9	11
101	Chemoinformatics: a perspective from an academic setting in Latin America. *Molecular Diversity*, **2018**, 22, 247-258	3.1	11
100	Conformal prediction of HDAC inhibitors. *SAR and QSAR in Environmental Research*, **2019**, 30, 265-277	3.5	10
99	How to Valorize Biodiversity? Let's Go Hashing, Extracting, Filtering, Mining, Fishing. *Planta Medica*, **2015**, 81, 436-49	3.1	10
98	Chemoinformatic characterization of activity and selectivity switches of antiprotozoal compounds. *Future Medicinal Chemistry*, **2014**, 6, 281-94	4.1	10
97	DNA Methyltransferase Inhibitors for Cancer Therapy **2015**, 265-290		10
96	Transient pockets on XIAP-BIR2: toward the characterization of putative binding sites of small-molecule XIAP inhibitors. *Journal of Molecular Modeling*, **2012**, 18, 2031-42	2	10
95	Towards the chemoinformatic-based identification of DNA methyltransferase inhibitors: 2D- and 3D-similarity profile of screening libraries. *Current Computer-Aided Drug Design*, **2012**, 8, 317-29	1.4	10
94	Chemical Diversity of Cyanobacterial Compounds: A Chemoinformatics Analysis. *ACS Omega*, **2019**, 4, 6229-6237	3.9	9
93	Analysis of structure-Caco-2 permeability relationships using a property landscape approach. *Molecular Diversity*, **2014**, 18, 599-610	3.1	9
92	On the validity versus utility of activity landscapes: are all activity cliffs statistically significant?. *Journal of Cheminformatics*, **2014**, 6, 11	8.6	9
91	Conditional probabilistic analysis for prediction of the activity landscape and relative compound activities. *Journal of Chemical Information and Modeling*, **2013**, 53, 2613-25	6.1	9
90	Systematic characterization of structure-activity relationships and ADMET compliance: a case study. *Drug Discovery Today*, **2013**, 18, 732-9	8.8	9
89	Progress in the Visualization and Mining of Chemical and Target Spaces. *Molecular Informatics*, **2013** , 32, 942-53	3.8	9

88	MOLECULAR SIMILARITY ANALYSIS343-399		9
87	Discovery and Development of Lead Compounds from Natural Sources Using Computational Approaches **2015**, 455-475		8
86	Chemoinformatics in Food Science **2018**, 501-525		8
85	Insights into the structure and inhibition of Giardia intestinalis arginine deiminase: homology modeling, docking, and molecular dynamics studies. *Journal of Biomolecular Structure and Dynamics* , **2016**, 34, 732-48	3.6	8
84	Functional group and diversity analysis of BIOFACQUIM: A Mexican natural product database. *F1000Research*, **2019**, 8,	3.6	8
83	Synthesis, Screening and in silico Simulations of Anti-Parasitic Propamidine/Benzimidazole Derivatives. *Medicinal Chemistry*, **2017**, 13, 137-148	1.8	8
82	DiaNat-DB: a molecular database of antidiabetic compounds from medicinal plants.. *RSC Advances*, **2021**, 11, 5172-5178	3.7	8
81	Synthesis and antitubercular activity of new N-[5-(4-chlorophenyl)-1,3,4-oxadiazol-2-yl]-(nitroheteroaryl)carboxamides. *Heterocyclic Communications*, **2019**, 25, 52-59	1.7	7
80	Dimeric phenalenones from Talaromyces sp. (IQ-313) inhibit hPTP1B: Insights into mechanistic kinetics from in vitro and in silico studies. *Bioorganic Chemistry*, **2020**, 101, 103893	5.1	7
79	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	5.3	7
78	Metronidazole and Secnidazole Carbamates: Synthesis, Antiprotozoal Activity, and Molecular Dynamics Studies. *Molecules*, **2020**, 25,	4.8	7
77	Activity landscape analysis of novel 5□reductase inhibitors. *Molecular Diversity*, **2016**, 20, 771-80	3.1	7
76	Developmental DNA methyltransferase inhibitors in the treatment of gynecologic cancers. *Expert Opinion on Pharmacotherapy*, **2016**, 17, 323-38	4	7
75	Descubrimiento y desarrollo de f□macos: un enfoque computacional **2017**, 28, 51-58		7
74	Computational methods for the discovery of mood disorder therapies. *Expert Opinion on Drug Discovery*, **2011**, 6, 1227-45	6.2	7
73	Traceless solid-phase synthesis of N-substituted 3,5-bis(substituted-idene)piperidin-4-one derivatives. *Tetrahedron Letters*, **2010**, 51, 5003-5004	2	7
72	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	0.8	7
71	Expanding the Structural Diversity of DNA Methyltransferase Inhibitors. *Pharmaceuticals*, **2020**, 14,	5.2	7

70	Rationality over fashion and hype in drug design. *F1000Research*, **2021**, 10,	3.6	7
69	Chemical space of naturally occurring compounds. *Physical Sciences Reviews*, **2019**, 4,	1.4	7
68	A general approach for retrosynthetic molecular core analysis. *Journal of Cheminformatics*, **2019**, 11, 61	8.6	6
67	Benzoic Acid Derivatives with Trypanocidal Activity: Enzymatic Analysis and Molecular Docking Studies toward Trans-Sialidase. *Molecules*, **2017**, 22,	4.8	6
66	Exploring the chemical space of peptides for drug discovery: a focus on linear and cyclic penta-peptides. *Molecular Diversity*, **2018**, 22, 259-267	3.1	6
65	Parallel synthesis of novel antitumor agents: 1,2,3-triazoles bearing biologically active sulfonamide moiety and their 3D-QSAR. *Molecular Diversity*, **2011**, 15, 927-46	3.1	6
64	Epigenetic Target Fishing with Accurate Machine Learning Models. *Journal of Medicinal Chemistry*, **2021**, 64, 8208-8220	8.3	6
63	Epigenetic Target Profiler: A Web Server to Predict Epigenetic Targets of Small Molecules. *Journal of Chemical Information and Modeling*, **2021**, 61, 1550-1554	6.1	6
62	Progress on open chemoinformatic tools for expanding and exploring the chemical space. *Journal of Computer-Aided Molecular Design*, **2021**, 1	4.2	6
61	Statistical-based database fingerprint: chemical space dependent representation of compound databases. *Journal of Cheminformatics*, **2018**, 10, 55	8.6	6
60	Chemical space, diversity and activity landscape analysis of estrogen receptor binders.. *RSC Advances*, **2018**, 8, 38229-38237	3.7	6
59	The Acid/Base Profile of a Large Food Chemical Database. *Molecular Informatics*, **2019**, 38, e1800171	3.8	5
58	Progress in the analysis of multiple activity profile of screening data using computational approaches. *Drug Development Research*, **2014**, 75, 313-23	5.1	5
57	Integrating computational and mixture-based screening of combinatorial libraries. *Journal of Molecular Modeling*, **2011**, 17, 1473-82	2	5
56	Probing the Hypothesis of SAR Continuity Restoration by the Removal of Activity Cliffs Generators in QSAR. *Current Pharmaceutical Design*, **2016**, 22, 5043-5056	3.3	5
55	Computational-aided design of a library of lactams through a diversity-oriented synthesis strategy. *Bioorganic and Medicinal Chemistry*, **2020**, 28, 115539	3.4	5
54	From Qualitative to Quantitative Analysis of Activity and Property Landscapes. *Journal of Chemical Information and Modeling*, **2020**, 60, 5873-5880	6.1	5
53	Analysis of the Acid/Base Profile of Natural Products from Different Sources. *Molecular Informatics*, **2020**, 39, e1900099	3.8	5

52	Consistent Cell-selective Analog Series as Constellation Luminaries in Chemical Space. *Molecular Informatics*, **2020**, 39, e2000061	3.8	4
51	Statistical correlation of nonconservative substitutions of HIV gp41 variable amino acid residues with the R5X4 HIV-1 phenotype. *Virology Journal*, **2016**, 13, 28	6.1	4
50	Systematic search for benzimidazole compounds and derivatives with antileishmanial effects. *Molecular Diversity*, **2018**, 22, 779-790	3.1	4
49	Drug Discovery with Novel Chemical Libraries. *Drug Designing: Open Access*, **2012**, 1,		4
48	Toward an efficient approach to identify molecular scaffolds possessing selective or promiscuous compounds. *Chemical Biology and Drug Design*, **2013**, 82, 367-75	2.9	4
47	Consensus Virtual Screening of Dark Chemical Matter and Food Chemicals Uncover Potential Inhibitors of SARS-CoV-2 Main Protease		4
46	Toxicity Assessment of Structurally Relevant Natural Products from Mexican Plants with Antinociceptive Activity **2017**, 61,		4
45	Quantitative Structure-Epigenetic Activity Relationships. *Challenges and Advances in Computational Chemistry and Physics*, **2017**, 303-338	0.7	4
44	Design, synthesis and evaluation of the antibacterial activity of new Linezolid dipeptide-type analogues. *Bioorganic Chemistry*, **2020**, 95, 103483	5.1	4
43	Chemical space and diversity of seaweed metabolite database (SWMD): A cheminformatics study. *Journal of Molecular Graphics and Modelling*, **2020**, 100, 107702	2.8	4
42	Tubulin Inhibitors: A Chemoinformatic Analysis Using Cell-Based Data. *Molecules*, **2021**, 26,	4.8	4
41	Molecular Modeling and Chemoinformatics to Advance the Development of Modulators of Epigenetic Targets: A Focus on DNA Methyltransferases. *Advances in Protein Chemistry and Structural Biology*, **2016**, 105, 1-26	5.3	4
40	Computational Methods to Discover Compounds for the Treatment of Chagas Disease. *Advances in Protein Chemistry and Structural Biology*, **2018**, 113, 119-142	5.3	4
39	Synthesis of NSC 106084 and NSC 14778 and evaluation of their DNMT inhibitory activity. *Bioorganic and Medicinal Chemistry Letters*, **2019**, 29, 826-831	2.9	3
38	Avances en el dise□o de f□rmacos asistido por computadora **2015**, 26, 180-186		3
37	D-Peptide Builder: A Web Service to Enumerate, Analyze, and Visualize the Chemical Space of Combinatorial Peptide Libraries. *Molecular Informatics*, **2020**, 39, e2000035	3.8	3
36	Chemoinformatics approaches to assess chemical diversity and complexity of small molecules **2020**, 83-102		3
35	Computational Methods for Epigenetic Drug Discovery: A Focus on Activity Landscape Modeling. *Advances in Protein Chemistry and Structural Biology*, **2018**, 113, 65-83	5.3	3

34	Cyclic Systems Distribution Along Similarity Measures: Insights for an Application to Activity Landscape Modeling. *Molecular Informatics*, **2013**, 32, 179-90	3.8	3
33	Software and Online Resources: Perspectives and Potential Applications **2014**, 233-248		3
32	Progress on the Computational Development of Epigenetic Modulators of DNA Methyltransferases 3A and 3B **2017**, 61,		3
31	Diversity and Chemical Library Networks of Large Data Sets. *Journal of Chemical Information and Modeling*, **2021**,	6.1	3
30	Interaction Fingerprints and Their Applications to Identify Hot Spots. *Methods in Molecular Biology*, **2015**, 1335, 313-24	1.4	3
29	Quinazolines as inhibitors of chromatin-associated proteins in histones. *Medicinal Chemistry Research*, **2019**, 28, 395-416	2.2	2
28	BIOFACQUIM: A Mexican Compound Database of Natural Products		2
27	Chemoinformatics Analysis and Structural Similarity Studies of Food-Related Databases **2014**, 97-110		2
26	Introduction of Epigenetic Targets in Drug Discovery and Current Status of Epi-Drugs and Epi-Probes **2016**, 1-20		2
25	Chemoinformatic Approach: The Case of Natural Products of Panama **2020**,		2
24	Current advances on the development of BET inhibitors: insights from computational methods. *Advances in Protein Chemistry and Structural Biology*, **2020**, 122, 127-180	5.3	2
23	Novel Linezolid analogues with antiparasitic activity against Hymenolepis nana. *Bioorganic Chemistry*, **2020**, 105, 104359	5.1	2
22	The Road Ahead of the Epi-Informatics Field **2016**, 399-418		2
21	Advances in the Exploration of the Epigenetic Relevant Chemical Space. *ACS Omega*, **2021**, 6, 22478-22486	3.9	2
20	Latin American databases of natural products: biodiversity and drug discovery against SARS-CoV-2.. *RSC Advances*, **2021**, 11, 16051-16064	3.7	2
19	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	6.1	1
18	Cheminformatics Approaches to Study Drug Polypharmacology. *Methods in Pharmacology and Toxicology*, **2018**, 3-25	1.1	1
17	A large scale classification of molecular fingerprints for the chemical space representation and SAR analysis. *Journal of Cheminformatics*, **2012**, 4,	8.6	1

16	A cell-based fascin bioassay identifies compounds with potential anti-metastasis or cognition-enhancing functions. *Journal of Cell Science*, **2013**, 126, e1-e1	5.3	1
15	Chemoinformatic Resources for Organometallic Drug Discovery. *Computational Molecular Bioscience*, **2020**, 10, 1-11	1.1	1
14	The Acid/Base Characterization of Molecules with Epigenetic Activity. *ChemMedChem*, **2021**, 16, 1744-1753	3.7	1
13	QSAR Modeling Using Quantum Chemical Descriptors of Benzimidazole Analogues With Antiparasitic Properties. *International Journal of Quantitative Structure-Property Relationships*, **2018** , 3, 61-79	1.2	1
12	Computational Applications in Secondary Metabolite Discovery (CAiSMD): an online workshop. *Journal of Cheminformatics*, **2021**, 13, 64	8.6	1
11	Chemoinformatic Characterization of Synthetic Screening Libraries Focused on Epigenetic Targets.. *Molecular Informatics*, **2021**, e2100285	3.8	1
10	Chemoinformatic Analysis of Isothiocyanates: Their Impact in Nature and Medicine. *Molecular Informatics*, **2021**, 40, e2100172	3.8	0
9	Synthesis of covalent bonding MWCNT-oligoethylene linezolid conjugates and their antibacterial activity against bacterial strains.. *RSC Advances*, **2021**, 11, 28912-28924	3.7	0
8	The Essence and Transcendence of Scientific Publishing.. *Frontiers in Research Metrics and Analytics*, **2022**, 7, 822453	1.3	0
7	Approaches for enhancing the analysis of chemical space for drug discovery. *Expert Opinion on Drug Discovery*,	6.2	0
6	Glossary of terms used in chemoinformatics of natural products: fundamental principles **2020**, 417-442		
5	4. Chemical space of naturally occurring compounds **2020**, 103-124		
4	Polypharmacology in Drug Discovery. *Methods and Principles in Medicinal Chemistry*, **2017**, 1-29	0.4	
3	Cheminformatics analysis of molecular datasets of transcription factors associated with quorum sensing in .. *RSC Advances*, **2022**, 12, 6783-6790	3.7	
2	Progress on Open Chemoinformatic Tools for Drug Discovery **2022**, 227-249		
1	Discovery and development of lead compounds from natural sources using computational approaches **2022**, 539-560		