Jos L Medina Franco

List of Publications by Year in Descending Order

Source: https://exaly.com/author-pdf/9546101/jose-l-medina-franco-publications-by-year.pdf
Version: 2024-04-25

This document has been generated based on the publications and citations recorded by exaly.com. For the latest version of this publication list, visit the link given above.
The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	Natural product drug discovery in the artificial intelligence era.. *Chemical Science*, **2022**, 13, 1526-1546	9.4	11
248	Cheminformatics analysis of molecular datasets of transcription factors associated with quorum sensing in .. *RSC Advances*, **2022**, 12, 6783-6790	3.7	
247	The Essence and Transcendence of Scientific Publishing.. *Frontiers in Research Metrics and Analytics*, **2022**, 7, 822453	1.3	0
246	Progress on Open Chemoinformatic Tools for Drug Discovery **2022**, 227-249		
245	Discovery and development of lead compounds from natural sources using computational approaches **2022**, 539-560		
244	Diversity and Chemical Library Networks of Large Data Sets. *Journal of Chemical Information and Modeling*, **2021**,	6.1	3
243	Informatics for Chemistry, Biology, and Biomedical Sciences. *Journal of Chemical Information and Modeling*, **2021**, 61, 26-35	6.1	15
242	Extended connectivity interaction features: improving binding affinity prediction through chemical description. *Bioinformatics*, **2021**, 37, 1376-1382	7.2	20
241	The Acid/Base Characterization of Molecules with Epigenetic Activity. *ChemMedChem*, **2021**, 16, 1744-1753	3.7	1
240	Epigenetic Target Fishing with Accurate Machine Learning Models. *Journal of Medicinal Chemistry*, **2021**, 64, 8208-8220	8.3	6
239	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
238	Tubulin Inhibitors: A Chemoinformatic Analysis Using Cell-Based Data. *Molecules*, **2021**, 26,	4.8	4
237	Rationality over fashion and hype in drug design. *F1000Research*, **2021**, 10,	3.6	7
236	Progress on open chemoinformatic tools for expanding and exploring the chemical space. *Journal of Computer-Aided Molecular Design*, **2021**, 1	4.2	6
235	DiaNat-DB: a molecular database of antidiabetic compounds from medicinal plants.. *RSC Advances*, **2021**, 11, 5172-5178	3.7	8
234	Advances in the Exploration of the Epigenetic Relevant Chemical Space. *ACS Omega*, **2021**, 6, 22478-22486	3.9	2
233	Chemoinformatic Analysis of Isothiocyanates: Their Impact in Nature and Medicine. *Molecular Informatics*, **2021**, 40, e2100172	3.8	0

232	Computational Applications in Secondary Metabolite Discovery (CAiSMD): an online workshop. *Journal of Cheminformatics*, **2021**, 13, 64	8.6	1
231	A critical overview of computational approaches employed for COVID-19 drug discovery. *Chemical Society Reviews*, **2021**, 50, 9121-9151	58.5	36
230	Latin American databases of natural products: biodiversity and drug discovery against SARS-CoV-2.. *RSC Advances*, **2021**, 11, 16051-16064	3.7	2
229	Synthesis of covalent bonding MWCNT-oligoethylene linezolid conjugates and their antibacterial activity against bacterial strains.. *RSC Advances*, **2021**, 11, 28912-28924	3.7	0
228	Chemoinformatic Characterization of Synthetic Screening Libraries Focused on Epigenetic Targets.. *Molecular Informatics*, **2021**, e2100285	3.8	1
227	Consistent Cell-selective Analog Series as Constellation Luminaries in Chemical Space. *Molecular Informatics*, **2020**, 39, e2000061	3.8	4
226	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
225	Glossary of terms used in chemoinformatics of natural products: fundamental principles **2020**, 417-442		
224	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
223	Chemoinformatics approaches to assess chemical diversity and complexity of small molecules **2020**, 83-102		3
222	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
221	4. Chemical space of naturally occurring compounds **2020**, 103-124		
220	Metronidazole and Secnidazole Carbamates: Synthesis, Antiprotozoal Activity, and Molecular Dynamics Studies. *Molecules*, **2020**, 25,	4.8	7
219	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
218	The impact of chemoinformatics on drug discovery in the pharmaceutical industry. *Expert Opinion on Drug Discovery*, **2020**, 15, 293-306	6.2	41
217	Expanding the Structural Diversity of DNA Methyltransferase Inhibitors. *Pharmaceuticals*, **2020**, 14,	5.2	7
216	Chemoinformatic Resources for Organometallic Drug Discovery. *Computational Molecular Bioscience*, **2020**, 10, 1-11	1.1	1
215	Computational-aided design of a library of lactams through a diversity-oriented synthesis strategy. *Bioorganic and Medicinal Chemistry*, **2020**, 28, 115539	3.4	5

214	Recent progress on cheminformatics approaches to epigenetic drug discovery. *Drug Discovery Today*, **2020**, 25, 2268-2276	8.8	14
213	Design, synthesis and evaluation of the antibacterial activity of new Linezolid dipeptide-type analogues. *Bioorganic Chemistry*, **2020**, 95, 103483	5.1	4
212	Chemoinformatic Approach: The Case of Natural Products of Panama **2020**,		2
211	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
210	Novel Linezolid analogues with antiparasitic activity against Hymenolepis nana. *Bioorganic Chemistry*, **2020**, 105, 104359	5.1	2
209	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
208	ADME/Tox Profiling of Natural Products: A Focus on BIOFACQUIM. *ACS Omega*, **2020**, 5, 16076-16084	3.9	43
207	Lessons from Exploring Chemical Space and Chemical Diversity of Propolis Components. *International Journal of Molecular Sciences*, **2020**, 21,	6.3	11
206	Fragment Library of Natural Products and Compound Databases for Drug Discovery. *Biomolecules*, **2020**, 10,	5.9	12
205	From Qualitative to Quantitative Analysis of Activity and Property Landscapes. *Journal of Chemical Information and Modeling*, **2020**, 60, 5873-5880	6.1	5
204	Cheminformatics to Characterize Pharmacologically Active Natural Products. *Biomolecules*, **2020**, 10,	5.9	17
203	Chemical space and diversity of seaweed metabolite database (SWMD): A cheminformatics study. *Journal of Molecular Graphics and Modelling*, **2020**, 100, 107702	2.8	4
202	Chemoinformatics-based enumeration of chemical libraries: a tutorial. *Journal of Cheminformatics*, **2020**, 12, 64	8.6	13
201	Towards a unified Latin American Natural Products Database: LANaPD. *Future Science OA*, **2020**, 6, FSO468	2.7	12
200	Analysis of the Acid/Base Profile of Natural Products from Different Sources. *Molecular Informatics*, **2020**, 39, e1900099	3.8	5
199	A Fragment Library of Natural Products and its Comparative Chemoinformatic Characterization. *Molecular Informatics*, **2020**, 39, e2000050	3.8	14
198	A general approach for retrosynthetic molecular core analysis. *Journal of Cheminformatics*, **2019**, 11, 61	8.6	6
197	Exploring the chemical space and the bioactivity profile of lactams: a chemoinformatic study.. *RSC Advances*, **2019**, 9, 27105-27116	3.7	19

196	Reaching for the bright StARs in chemical space. *Drug Discovery Today*, **2019**, 24, 2162-2169	8.8	17
195	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
194	Quinazolines as inhibitors of chromatin-associated proteins in histones. *Medicinal Chemistry Research*, **2019**, 28, 395-416	2.2	2
193	Bicyclic acetals: biological relevance, scaffold analysis, and applications in diversity-oriented synthesis. *Organic and Biomolecular Chemistry*, **2019**, 17, 1037-1052	3.9	24
192	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
191	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
190	Conformal prediction of HDAC inhibitors. *SAR and QSAR in Environmental Research*, **2019**, 30, 265-277	3.5	10
189	Computational Drug Design Methods□Current and Future Perspectives **2019**, 19-44		29
188	The Acid/Base Profile of a Large Food Chemical Database. *Molecular Informatics*, **2019**, 38, e1800171	3.8	5
187	Chemical Diversity of Cyanobacterial Compounds: A Chemoinformatics Analysis. *ACS Omega*, **2019**, 4, 6229-6237	3.9	9
186	DataWarrior: an evaluation of the open-source drug discovery tool. *Expert Opinion on Drug Discovery*, **2019**, 14, 335-341	6.2	34
185	Finding Constellations in Chemical Space Through Core Analysis. *Frontiers in Chemistry*, **2019**, 7, 510	5	19
184	Functional group and diversity analysis of BIOFACQUIM: A Mexican natural product database. *F1000Research*, **2019**, 8,	3.6	8
183	Functional group and diversity analysis of BIOFACQUIM: A Mexican natural product database. *F1000Research*, **2019**, 8, 2071	3.6	11
182	Cheminformatics Explorations of Natural Products. *Progress in the Chemistry of Organic Natural Products*, **2019**, 110, 1-35	1.9	12
181	BIOFACQUIM: A Mexican Compound Database of Natural Products. *Biomolecules*, **2019**, 9,	5.9	31
180	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
179	Chemical Space and Diversity of the NuBBE Database: A Chemoinformatic Characterization. *Journal of Chemical Information and Modeling*, **2019**, 59, 74-85	6.1	28

178	Chemical space of naturally occurring compounds. *Physical Sciences Reviews*, **2019**, 4,	1.4	7
177	Ivermectin as an inhibitor of cancer stem-like cells. *Molecular Medicine Reports*, **2018**, 17, 3397-3403	2.9	30
176	Chemoinformatics in Food Science **2018**, 501-525		8
175	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
174	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
173	Insights from pharmacological similarity of epigenetic targets in epipolypharmacology. *Drug Discovery Today*, **2018**, 23, 141-150	8.8	27
172	Flavonoids as Putative Epi-Modulators: Insight into Their Binding Mode with BRD4 Bromodomains Using Molecular Docking and Dynamics. *Biomolecules*, **2018**, 8,	5.9	13
171	Protein-Protein Interaction Modulators for Epigenetic Therapies. *Advances in Protein Chemistry and Structural Biology*, **2018**, 110, 65-84	5.3	16
170	Systematic search for benzimidazole compounds and derivatives with antileishmanial effects. *Molecular Diversity*, **2018**, 22, 779-790	3.1	4
169	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
168	Cheminformatics Approaches to Study Drug Polypharmacology. *Methods in Pharmacology and Toxicology*, **2018**, 3-25	1.1	1
167	Analysis of a large food chemical database: chemical space, diversity, and complexity. *F1000Research*, **2018**, 7,	3.6	14
166	Analysis of a large food chemical database: chemical space, diversity, and complexity. *F1000Research*, **2018**, 7, 993	3.6	25
165	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
164	Chemoinformatics: a perspective from an academic setting in Latin America. *Molecular Diversity*, **2018**, 22, 247-258	3.1	11
163	Statistical-based database fingerprint: chemical space dependent representation of compound databases. *Journal of Cheminformatics*, **2018**, 10, 55	8.6	6
162	Chemical space, diversity and activity landscape analysis of estrogen receptor binders.. *RSC Advances*, **2018**, 8, 38229-38237	3.7	6
161	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

160	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
159	Inhibitors of DNA Methyltransferases From Natural Sources: A Computational Perspective. *Frontiers in Pharmacology*, **2018**, 9, 1144	5.6	23
158	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
157	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
156	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
155	Systemic QSAR and phenotypic virtual screening: chasing butterflies in drug discovery. *Drug Discovery Today*, **2017**, 22, 994-1007	8.8	25
154	From flamingo dance to (desirable) drug discovery: a nature-inspired approach. *Drug Discovery Today*, **2017**, 22, 1489-1502	8.8	17
153	Database fingerprint (DFP): an approach to represent molecular databases. *Journal of Cheminformatics*, **2017**, 9, 9	8.6	26
152	Getting SMARt in drug discovery: chemoinformatics approaches for mining structure□multiple activity relationships. *RSC Advances*, **2017**, 7, 632-641	3.7	23
151	Benzoic Acid Derivatives with Trypanocidal Activity: Enzymatic Analysis and Molecular Docking Studies toward Trans-Sialidase. *Molecules*, **2017**, 22,	4.8	6
150	Cheminformatic characterization of natural products from Panama. *Molecular Diversity*, **2017**, 21, 779-789	3.1	18
149	Platform for Unified Molecular Analysis: PUMA. *Journal of Chemical Information and Modeling*, **2017**, 57, 1735-1740	6.1	24
148	Chemoselective fluorination and chemoinformatic analysis of griseofulvin: Natural vs fluorinated fungal metabolites. *Bioorganic and Medicinal Chemistry*, **2017**, 25, 5238-5246	3.4	12
147	Polypharmacology in Drug Discovery. *Methods and Principles in Medicinal Chemistry*, **2017**, 1-29	0.4	
146	The many roles of molecular complexity in drug discovery. *Drug Discovery Today*, **2017**, 22, 120-126	8.8	71
145	Descubrimiento y desarrollo de f□macos: un enfoque computacional **2017**, 28, 51-58		7
144	Scaffold Diversity of Fungal Metabolites. *Frontiers in Pharmacology*, **2017**, 8, 180	5.6	30
143	ChemMaps: Towards an approach for visualizing the chemical space based on adaptive satellite compounds. *F1000Research*, **2017**, 6,	3.6	16

142	ChemMaps: Towards an approach for visualizing the chemical space based on adaptive satellite compounds. *F1000Research*, **2017**, 6, 1134	3.6	17
141	Synthesis, Screening and in silico Simulations of Anti-Parasitic Propamidine/Benzimidazole Derivatives. *Medicinal Chemistry*, **2017**, 13, 137-148	1.8	8
140	Toxicity Assessment of Structurally Relevant Natural Products from Mexican Plants with Antinociceptive Activity **2017**, 61,		4
139	Progress on the Computational Development of Epigenetic Modulators of DNA Methyltransferases 3A and 3B **2017**, 61,		3
138	Quantitative Structure-Epigenetic Activity Relationships. *Challenges and Advances in Computational Chemistry and Physics*, **2017**, 303-338	0.7	4
137	Open chemoinformatic resources to explore the structure, properties and chemical space of molecules. *RSC Advances*, **2017**, 7, 54153-54163	3.7	30
136	Resveratrol-salicylate derivatives as selective DNMT3 inhibitors and anticancer agents. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2016**, 31, 695-703	5.6	33
135	A chemical space odyssey of inhibitors of histone deacetylases and bromodomains. *RSC Advances*, **2016**, 6, 56225-56239	3.7	23
134	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
133	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
132	Activity landscape analysis of novel 5□reductase inhibitors. *Molecular Diversity*, **2016**, 20, 771-80	3.1	7
131	Anti-inflammatory and antioxidant properties of a novel resveratrol-salicylate hybrid analog. *Bioorganic and Medicinal Chemistry Letters*, **2016**, 26, 1411-5	2.9	23
130	Advances in the development of pyridinone derivatives as non-nucleoside reverse transcriptase inhibitors. *RSC Advances*, **2016**, 6, 2119-2130	3.7	11
129	Developmental DNA methyltransferase inhibitors in the treatment of gynecologic cancers. *Expert Opinion on Pharmacotherapy*, **2016**, 17, 323-38	4	7
128	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
127	Introduction of Epigenetic Targets in Drug Discovery and Current Status of Epi-Drugs and Epi-Probes **2016**, 1-20		2
126	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
125	Consensus Diversity Plots: a global diversity analysis of chemical libraries. *Journal of Cheminformatics*, **2016**, 8, 63	8.6	40

124	Drug Repurposing for Epigenetic Targets Guided by Computational Methods **2016**, 327-357		14
123	The Road Ahead of the Epi-Informatics Field **2016**, 399-418		2
122	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
121	Chemoinformatic expedition of the chemical space of fungal products. *Future Medicinal Chemistry*, **2016**, 8, 1399-412	4.1	30
120	Activity cliffs and activity cliff generators based on chemotype-related activity landscapes. *Molecular Diversity*, **2015**, 19, 1021-35	3.1	20
119	How to Valorize Biodiversity? Let's Go Hashing, Extracting, Filtering, Mining, Fishing. *Planta Medica*, **2015**, 81, 436-49	3.1	10
118	Activity landscape sweeping: insights into the mechanism of inhibition and optimization of DNMT1 inhibitors. *RSC Advances*, **2015**, 5, 63882-63895	3.7	16
117	Avances en el diseño de fármacos asistido por computadora **2015**, 26, 180-186		3
116	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
115	Discovery and Development of Lead Compounds from Natural Sources Using Computational Approaches **2015**, 455-475		8
114	Activity and property landscape modeling is at the interface of chemoinformatics and medicinal chemistry. *Future Medicinal Chemistry*, **2015**, 7, 1197-211	4.1	23
113	Epigenetic relevant chemical space: a chemoinformatic characterization of inhibitors of DNA methyltransferases. *RSC Advances*, **2015**, 5, 87465-87476	3.7	25
112	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
111	Activity landscape of DNA methyltransferase inhibitors bridges chemoinformatics with epigenetic drug discovery. *Expert Opinion on Drug Discovery*, **2015**, 10, 1059-70	6.2	16
110	Discovery and development of DNA methyltransferase inhibitors using in silico approaches. *Drug Discovery Today*, **2015**, 20, 569-77	8.8	41
109	DNA Methyltransferase Inhibitors for Cancer Therapy **2015**, 265-290		10
108	Ribavirin as a tri-targeted antitumor repositioned drug. *Oncology Reports*, **2015**, 33, 2384-92	3.5	31
107	Analyzing multitarget activity landscapes using protein-ligand interaction fingerprints: interaction cliffs. *Journal of Chemical Information and Modeling*, **2015**, 55, 251-62	6.1	22

106	Interaction Fingerprints and Their Applications to Identify Hot Spots. *Methods in Molecular Biology*, **2015**, 1335, 313-24	1.4	3
105	Toward drug repurposing in epigenetics: olsalazine as a hypomethylating compound active in a cellular context. *ChemMedChem*, **2014**, 9, 560-5	3.7	60
104	Design and synthesis of conotoxin GID analogues as selective 42 nicotinic acetylcholine receptor antagonists. *Biopolymers*, **2014**, 102, 78-87	2.2	14
103	Synthesis of 2-{2-[(naphthalen-1-ylsulfonyl)amino]-1,3-thiazol-4-yl} acetamides with 11hydroxysteroid dehydrogenase inhibition and in combo antidiabetic activities. *European Journal of Medicinal Chemistry*, **2014**, 74, 179-86	6.8	17
102	Analysis of structure-Caco-2 permeability relationships using a property landscape approach. *Molecular Diversity*, **2014**, 18, 599-610	3.1	9
101	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
100	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
99	On the validity versus utility of activity landscapes: are all activity cliffs statistically significant?. *Journal of Cheminformatics*, **2014**, 6, 11	8.6	9
98	Balancing novelty with confined chemical space in modern drug discovery. *Expert Opinion on Drug Discovery*, **2014**, 9, 151-65	6.2	37
97	Progress in the analysis of multiple activity profile of screening data using computational approaches. *Drug Development Research*, **2014**, 75, 313-23	5.1	5
96	Synthesis, in vitro and in silico studies of a PPARand GLUT-4 modulator with hypoglycemic effect. *Bioorganic and Medicinal Chemistry Letters*, **2014**, 24, 4575-4579	2.9	19
95	Activity cliffs in drug discovery: Dr Jekyll or Mr Hyde?. *Drug Discovery Today*, **2014**, 19, 1069-80	8.8	103
94	Chemoinformatic characterization of activity and selectivity switches of antiprotozoal compounds. *Future Medicinal Chemistry*, **2014**, 6, 281-94	4.1	10
93	Integrating virtual and biochemical screening for protein tyrosine phosphatase inhibitor discovery. *Methods*, **2014**, 65, 219-28	4.6	13
92	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
91	Software and Online Resources: Perspectives and Potential Applications **2014**, 233-248		3
90	Chemoinformatics Analysis and Structural Similarity Studies of Food-Related Databases **2014**, 97-110		2
89	Antihyperglycemic and sub-chronic antidiabetic actions of morolic and moronic acids, in vitro and in silico inhibition of 11HSD 1. *Phytomedicine*, **2013**, 20, 571-6	6.5	17

88	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
87	Towards the identification of the binding site of benzimidazoles to Etubulin of Trichinella spiralis: insights from computational and experimental data. *Journal of Molecular Graphics and Modelling*, **2013**, 41, 12-9	2.8	32
86	Molecular basis for benzimidazole resistance from a novel Etubulin binding site model. *Journal of Molecular Graphics and Modelling*, **2013**, 45, 26-37	2.8	40
85	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
84	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
83	Cyclic Systems Distribution Along Similarity Measures: Insights for an Application to Activity Landscape Modeling. *Molecular Informatics*, **2013**, 32, 179-90	3.8	3
82	Activity cliffs: facts or artifacts?. *Chemical Biology and Drug Design*, **2013**, 81, 553-6	2.9	42
81	Shifting from the single to the multitarget paradigm in drug discovery. *Drug Discovery Today*, **2013**, 18, 495-501	8.8	321
80	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
79	Systematic characterization of structure-activity relationships and ADMET compliance: a case study. *Drug Discovery Today*, **2013**, 18, 732-9	8.8	9
78	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
77	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
76	Progress in the Visualization and Mining of Chemical and Target Spaces. *Molecular Informatics*, **2013** , 32, 942-53	3.8	9
75	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
74	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
73	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
72	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
71	Molecular modeling and virtual screening of DNA methyltransferase inhibitors. *Current Pharmaceutical Design*, **2013**, 19, 2138-47	3.3	17

70	Expanding the medicinally relevant chemical space with compound libraries. *Drug Discovery Today*, **2012**, 17, 718-26	8.8	118
69	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
68	Activity landscape modeling of PPAR ligands with dual-activity difference maps. *Bioorganic and Medicinal Chemistry*, **2012**, 20, 3523-32	3.4	17
67	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
66	Activity-difference maps and consensus similarity measure characterize structure-activity relationships. *Journal of Cheminformatics*, **2012**, 4,	8.6	78
65	Computer-guided discovery of epigenetics drugs: molecular modeling and identification of inhibitors of DNMT1. *Journal of Cheminformatics*, **2012**, 4,	8.6	78
64	A large scale classification of molecular fingerprints for the chemical space representation and SAR analysis. *Journal of Cheminformatics*, **2012**, 4,	8.6	1
63	Molecular scaffold analysis of natural products databases in the public domain. *Chemical Biology and Drug Design*, **2012**, 80, 717-24	2.9	56
62	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
61	Recognizing pitfalls in virtual screening: a critical review. *Journal of Chemical Information and Modeling*, **2012**, 52, 867-81	6.1	295
60	Interrogating Novel Areas of Chemical Space for Drug Discovery using Chemoinformatics. *Drug Development Research*, **2012**, 73, 430-438	5.1	28
59	Identifying Activity Cliff Generators of PPAR Ligands Using SAS Maps. *Molecular Informatics*, **2012**, 31, 837-46	3.8	26
58	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
57	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
56	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
55	Consensus Models of Activity Landscapes **2012**, 307-326		14
54	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
53	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

52	Chemoinformatic analysis of GRAS (Generally Recognized as Safe) flavor chemicals and natural products. *PLoS ONE*, **2012**, 7, e50798	3.7	34
51	Drug Discovery with Novel Chemical Libraries. *Drug Designing: Open Access*, **2012**, 1,		4
50	Effects of cyclic lipodepsipeptide structural modulation on stability, antibacterial activity, and human cell toxicity. *ChemMedChem*, **2012**, 7, 871-82	3.7	44
49	Trimethylaurintricarboxylic acid inhibits human DNA methyltransferase 1: insights from enzymatic and molecular modeling studies. *Journal of Molecular Modeling*, **2012**, 18, 1583-9	2	20
48	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
47	Inhibitors of DNA methyltransferases: insights from computational studies. *Current Medicinal Chemistry*, **2012**, 19, 3475-87	4.3	23
46	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
45	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
44	Synthesis and biochemical evaluation of (2)-isoxazoline derivatives as DNA methyltransferase 1 inhibitors. *Journal of Medicinal Chemistry*, **2011**, 54, 7663-77	8.3	131
43	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
42	Molecular dynamics simulations of human DNA methyltransferase 3B with selective inhibitor nanaomycin A. *Journal of Structural Biology*, **2011**, 176, 185-91	3.4	69
41	Structure□ctivity relationships of benzimidazole derivatives as antiparasitic agents: Dual activity-difference (DAD) maps. *MedChemComm*, **2011**, 2, 44-49	5	67
40	Integrating virtual screening and combinatorial chemistry for accelerated drug discovery. *Combinatorial Chemistry and High Throughput Screening*, **2011**, 14, 475-87	1.3	80
39	Increased diversity of libraries from libraries: chemoinformatic analysis of bis-diazacyclic libraries. *Chemical Biology and Drug Design*, **2011**, 77, 328-42	2.9	26
38	Advances in the computational development of DNA methyltransferase inhibitors. *Drug Discovery Today*, **2011**, 16, 418-25	8.8	72
37	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
36	Natural products as DNA methyltransferase inhibitors: a computer-aided discovery approach. *Molecular Diversity*, **2011**, 15, 293-304	3.1	117
35	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

34	Integrating computational and mixture-based screening of combinatorial libraries. *Journal of Molecular Modeling*, **2011**, 17, 1473-82	2	5
33	Characterization of a comprehensive flavor database. *Journal of Chemometrics*, **2011**, 25, 550-560	1.6	23
32	Visualization of molecular fingerprints. *Journal of Chemical Information and Modeling*, **2011**, 51, 1552-63	6.1	50
31	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
30	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
29	Computational methods for the discovery of mood disorder therapies. *Expert Opinion on Drug Discovery*, **2011**, 6, 1227-45	6.2	7
28	Benzotriazoles and indazoles are scaffolds with biological activity against Entamoeba histolytica. *Journal of Biomolecular Screening*, **2011**, 16, 862-8		38
27	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
26	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
25	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
24	Traceless solid-phase synthesis of N-substituted 3,5-bis(substituted-idene)piperidin-4-one derivatives. *Tetrahedron Letters*, **2010**, 51, 5003-5004	2	7
23	Novel and selective DNA methyltransferase inhibitors: Docking-based virtual screening and experimental evaluation. *Bioorganic and Medicinal Chemistry*, **2010**, 18, 822-9	3.4	138
22	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
21	Towards a systematic characterization of the antiprotozoal activity landscape of benzimidazole derivatives. *Bioorganic and Medicinal Chemistry*, **2010**, 18, 7380-91	3.4	54
20	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
19	Inhibitors of HMG-CoA Reductase: Current and Future Prospects. *Mini-Reviews in Medicinal Chemistry*, **2009**, 9, 1272-83	3.2	42
18	Molecular modeling and molecular dynamics studies of hydralazine with human DNA methyltransferase 1. *ChemMedChem*, **2009**, 4, 792-9	3.7	94
17	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

16	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
15	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
14	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
13	Chemoinformatics-applications in food chemistry. *Advances in Food and Nutrition Research*, **2009**, 58, 33-56	6	15
12	The prince and the pauper. A tale of anticancer targeted agents. *Molecular Cancer*, **2008**, 7, 82	42.1	63
11	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
10	Visualization of the Chemical Space in Drug Discovery. *Current Computer-Aided Drug Design*, **2008**, 4, 322-333	1.4	107
9	Conformation-opioid activity relationships of bicyclic guanidines from 3D similarity analysis. *Bioorganic and Medicinal Chemistry*, **2008**, 16, 5932-8	3.4	19
8	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
7	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
6	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
5	Acoplamiento Molecular: Avances Recientes y Retos. *TIP Revista Especializada En Ciencias Qu□mico-Biol□gicas*,21,		13
4	Consensus Virtual Screening of Dark Chemical Matter and Food Chemicals Uncover Potential Inhibitors of SARS-CoV-2 Main Protease		4
3	BIOFACQUIM: A Mexican Compound Database of Natural Products		2
2	MOLECULAR SIMILARITY ANALYSIS343-399		9
1	Approaches for enhancing the analysis of chemical space for drug discovery. *Expert Opinion on Drug Discovery*,	6.2	0