

Oscar MÃ©ndez-Lucio

List of Publications by Year in descending order

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Version: 2024-02-01

41
papers

1,436
citations

331670

21
h-index

345221

36
g-index

50
all docs

50
docs citations

50
times ranked

2130
citing authors

#	ARTICLE	IF	CITATIONS
1	De novo generation of hit-like molecules from gene expression signatures using artificial intelligence. <i>Nature Communications</i> , 2020, 11, 10.	12.8	253
2	Polypharmacology modelling using proteochemometrics (PCM): recent methodological developments, applications to target families, and future prospects. <i>MedChemComm</i> , 2015, 6, 24-50.	3.4	109
3	The many roles of molecular complexity in drug discovery. <i>Drug Discovery Today</i> , 2017, 22, 120-126.	6.4	107
4	Lysine harvesting is an antioxidant strategy and triggers underground polyamine metabolism. <i>Nature</i> , 2019, 572, 249-253.	27.8	99
5	Toward Drug Repurposing in Epigenetics: Olsalazine as a Hypomethylating Compound Active in a Cellular Context. <i>ChemMedChem</i> , 2014, 9, 560-565.	3.2	67
6	A geometric deep learning approach to predict binding conformations of bioactive molecules. <i>Nature Machine Intelligence</i> , 2021, 3, 1033-1039.	16.0	64
7	Molecular basis for benzimidazole resistance from a novel β -tubulin binding site model. <i>Journal of Molecular Graphics and Modelling</i> , 2013, 45, 26-37.	2.4	61
8	Towards the identification of the binding site of benzimidazoles to β -tubulin of <i>Trichinella spiralis</i> : Insights from computational and experimental data. <i>Journal of Molecular Graphics and Modelling</i> , 2013, 41, 12-19.	2.4	54
9	Discovery and development of DNA methyltransferase inhibitors using in silico approaches. <i>Drug Discovery Today</i> , 2015, 20, 569-577.	6.4	53
10	Synthesis and antiprotozoal activity of novel 2-[[2-(1H-imidazol-1-yl)ethyl]sulfanyl]-1H-benzimidazole derivatives. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2013, 23, 4221-4224.	2.2	48
11	Cheminformatic expedition of the chemical space of fungal products. <i>Future Medicinal Chemistry</i> , 2016, 8, 1399-1412.	2.3	42
12	Identifying Activity Cliff Generators of PPAR Ligands Using SAS Maps. <i>Molecular Informatics</i> , 2012, 31, 837-846.	2.5	32
13	Design, synthesis and evaluation of semi-synthetic triazole-containing caffeic acid analogues as 5-lipoxygenase inhibitors. <i>European Journal of Medicinal Chemistry</i> , 2015, 101, 573-583.	5.5	30
14	A chemical space odyssey of inhibitors of histone deacetylases and bromodomains. <i>RSC Advances</i> , 2016, 6, 56225-56239.	3.6	28
15	Modelling ligand selectivity of serine proteases using integrative proteochemometric approaches improves model performance and allows the multi-target dependent interpretation of features. <i>Integrative Biology (United Kingdom)</i> , 2014, 6, 1023-1033.	1.3	26
16	Activity and property landscape modeling is at the interface of cheminformatics and medicinal chemistry. <i>Future Medicinal Chemistry</i> , 2015, 7, 1197-1211.	2.3	26
17	Rationalization of Activity Cliffs of a Sulfonamide Inhibitor of DNA Methyltransferases with Induced-Fit Docking. <i>International Journal of Molecular Sciences</i> , 2014, 15, 3253-3261.	4.1	25
18	The Interplay Between Molecular Modeling and Cheminformatics to Characterize Protein-Ligand and Protein-Protein Interactions Landscapes for Drug Discovery. <i>Advances in Protein Chemistry and Structural Biology</i> , 2014, 96, 1-37.	2.3	23

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19	Analyzing Multitarget Activity Landscapes Using Protein-Ligand Interaction Fingerprints: Interaction Cliffs. <i>Journal of Chemical Information and Modeling</i> , 2015, 55, 251-262.	5.4	23
20	Activity cliffs and activity cliff generators based on chemotype-related activity landscapes. <i>Molecular Diversity</i> , 2015, 19, 1021-1035.	3.9	22
21	Activity Landscape Plotter: A Web-Based Application for the Analysis of Structure-Activity Relationships. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 397-402.	5.4	22
22	Homology modeling, docking and molecular dynamics of the <i>Leishmania mexicana</i> arginase: A description of the catalytic site useful for drug design. <i>Journal of Molecular Graphics and Modelling</i> , 2012, 38, 50-59.	2.4	19
23	Activity landscape modeling of PPAR ligands with dual-activity difference maps. <i>Bioorganic and Medicinal Chemistry</i> , 2012, 20, 3523-3532.	3.0	17
24	Data-driven approaches used for compound library design, hit triage and bioactivity modeling in high-throughput screening. <i>Briefings in Bioinformatics</i> , 2018, 19, bbw105.	6.5	17
25	ARWAR: A network approach for predicting Adverse Drug Reactions. <i>Computers in Biology and Medicine</i> , 2016, 68, 101-108.	7.0	17
26	Advances in the development of pyridinone derivatives as non-nucleoside reverse transcriptase inhibitors. <i>RSC Advances</i> , 2016, 6, 2119-2130.	3.6	15
27	Computational study on the inhibition mechanism of cruzain by nitrile-containing molecules. <i>Journal of Molecular Graphics and Modelling</i> , 2012, 35, 28-35.	2.4	12
28	Exploring the Use of Compound-Induced Transcriptomic Data Generated From Cell Lines to Predict Compound Activity Toward Molecular Targets. <i>Frontiers in Chemistry</i> , 2020, 8, 296.	3.6	12
29	CASE Plots for the Chemotype-Based Activity and Selectivity Analysis: A CASE Study of Cyclooxygenase Inhibitors. <i>Chemical Biology and Drug Design</i> , 2012, 80, 752-762.	3.2	11
30	Diversity selection, screening and quantitative structure-activity relationships of osmolyte-like additive effects on the thermal stability of a monoclonal antibody. <i>European Journal of Pharmaceutical Sciences</i> , 2017, 97, 151-157.	4.0	11
31	3D-QSAR studies on purine-carbonitriles as cruzain inhibitors: comparative molecular field analysis (CoMFA) and comparative molecular similarity indices analysis (CoMSIA). <i>MedChemComm</i> , 2011, 2, 1058.	3.4	10
32	Two-step radical reactions that switch low multiplicity channels leading to the carbene and carbyne species detected for Ru(5F) + CH ₄ ⁿ F _n (n = 2-4) interactions under matrix isolation conditions. <i>RSC Advances</i> , 2013, 3, 11607.	3.6	10
33	One Drug for Multiple Targets: A Computational Perspective. <i>Journal of the Mexican Chemical Society</i> , 2017, 60, .	0.6	10
34	Synthesis, Screening and in silico Simulations of Anti-Parasitic Propamidine/Benzimidazole Derivatives. <i>Medicinal Chemistry</i> , 2017, 13, 137-148.	1.5	9
35	Activity landscape analysis, CoMFA and CoMSIA studies of pyrazole CB1 antagonists. <i>Medicinal Chemistry Research</i> , 2013, 22, 4133-4145.	2.4	8
36	Molecular Modeling and Chemoinformatics to Advance the Development of Modulators of Epigenetic Targets. <i>Advances in Protein Chemistry and Structural Biology</i> , 2016, 105, 1-26.	2.3	6

#	ARTICLE	IF	CITATIONS
37	Statistical correlation of nonconservative substitutions of HIV gp41 variable amino acid residues with the R5X4 HIV-1 phenotype. <i>Virology Journal</i> , 2016, 13, 28.	3.4	4
38	Cyclic Systems Distribution Along Similarity Measures: Insights for an Application to Activity Landscape Modeling. <i>Molecular Informatics</i> , 2013, 32, 179-190.	2.5	3
39	Theoretical Study of the Reactions $M^{+} + CH_3F$ (M=Ge, As, Se, Sb). <i>ChemPhysChem</i> , 2010, 11, 1909-1917.	2.1	2
40	Towards understanding polyol additive effects on the pH shift-induced aggregation of a monoclonal antibody using high throughput screening and quantitative structure-activity modeling. <i>International Journal of Pharmaceutics</i> , 2017, 530, 165-172.	5.2	2
41	Computational Structure-Activity Relationship Studies of Epigenetic Target Inhibitors. , 2016, , 359-384.		1