# Oscar MÃ©ndez-Lucio

List of Publications by Year
in descending order



| | | | |
|---|---|---|---|
| 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 | A geometric deep learning approach to predict binding conformations of bioactive molecules. Nature Machine Intelligence, 2021, 3, 1033-1039. | 16.0 | 64 |
| 2 | De novo generation of hit-like molecules from gene expression signatures using artificial intelligence. Nature Communications, 2020, 11, 10. | 12.8 | 253 |
| 3 | Exploring the Use of Compound-Induced Transcriptomic Data Generated From Cell Lines to Predict Compound Activity Toward Molecular Targets. Frontiers in Chemistry, 2020, 8, 296. | 3.6 | 12 |
| 4 | Lysine harvesting is an antioxidant strategy and triggers underground polyamine metabolism. Nature, 2019, 572, 249-253. | 27.8 | 99 |
| 5 | Data-driven approaches used for compound library design, hit triage and bioactivity modeling in high-throughput screening. Briefings in Bioinformatics, 2018, 19, bbw105. | 6.5 | 17 |
| 6 | 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 |
| 7 | Diversity selection, screening and quantitative structureâ€“activity relationships of osmolyte-like additive effects on the thermal stability of a monoclonal antibody. European Journal of Pharmaceutical Sciences, 2017, 97, 151-157. | 4.0 | 11 |
| 8 | Towards understanding polyol additive effects on the pH shift-induced aggregation of a monoclonal antibody using high throughput screening and quantitative structure-activity modeling. International Journal of Pharmaceutics, 2017, 530, 165-172. | 5.2 | 2 |
| 9 | The many roles of molecular complexity in drug discovery. Drug Discovery Today, 2017, 22, 120-126. | 6.4 | 107 |
| 10 | Synthesis, Screening and in silico Simulations of Anti-Parasitic Propamidine/Benzimidazole Derivatives. Medicinal Chemistry, 2017, 13, 137-148. | 1.5 | 9 |
| 11 | One Drug for Multiple Targets: A Computational Perspective. Journal of the Mexican Chemical Society, 2017, 60, . | 0.6 | 10 |
| 12 | Computational Structureâ€“Activity Relationship Studies of Epigenetic Target Inhibitors. , 2016, , 359-384. | | 1 |
| 13 | 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 |
| 14 | Chemoinformatic expedition of the chemical space of fungal products. Future Medicinal Chemistry, 2016, 8, 1399-1412. | 2.3 | 42 |
| 15 | A chemical space odyssey of inhibitors of histone deacetylases and bromodomains. RSC Advances, 2016, 6, 56225-56239. | 3.6 | 28 |
| 16 | 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 |
| 17 | Advances in the development of pyridinone derivatives as non-nucleoside reverse transcriptase inhibitors. RSC Advances, 2016, 6, 2119-2130. | 3.6 | 15 |
| 18 | ARWAR: A network approach for predicting Adverse Drug Reactions. Computers in Biology and Medicine, 2016, 68, 101-108. | 7.0 | 17 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | Analyzing Multitarget Activity Landscapes Using Proteinâ€“Ligand Interaction Fingerprints: Interaction Cliffs. Journal of Chemical Information and Modeling, 2015, 55, 251-262. | 5.4 | 23 |
| 20 | Design, synthesis and evaluation of semi-synthetic triazole-containing caffeic acid analogues as 5-lipoxygenase inhibitors. European Journal of Medicinal Chemistry, 2015, 101, 573-583. | 5.5 | 30 |
| 21 | Activity cliffs and activity cliff generators based on chemotype-related activity landscapes. Molecular Diversity, 2015, 19, 1021-1035. | 3.9 | 22 |
| 22 | Activity and property landscape modeling is at the interface of chemoinformatics and medicinal chemistry. Future Medicinal Chemistry, 2015, 7, 1197-1211. | 2.3 | 26 |
| 23 | Discovery and development of DNA methyltransferase inhibitors using in silico approaches. Drug Discovery Today, 2015, 20, 569-577. | 6.4 | 53 |
| 24 | Polypharmacology modelling using proteochemometrics (PCM): recent methodological developments, applications to target families, and future prospects. MedChemComm, 2015, 6, 24-50. | 3.4 | 109 |
| 25 | 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 |
| 26 | Modelling ligand selectivity of serine proteases using integrative proteochemometric approaches improves model performance and allows the multi-target dependent interpretation of features. Integrative Biology (United Kingdom), 2014, 6, 1023-1033. | 1.3 | 26 |
| 27 | Toward Drug Repurposing in Epigenetics: Olsalazine as a Hypomethylating Compound Active in a Cellular Context. ChemMedChem, 2014, 9, 560-565. | 3.2 | 67 |
| 28 | 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 |
| 29 | Activity landscape analysis, CoMFA and CoMSIA studies of pyrazole CB1 antagonists. Medicinal Chemistry Research, 2013, 22, 4133-4145. | 2.4 | 8 |
| 30 | 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 |
| 31 | 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 |
| 32 | Cyclic Systems Distribution Along Similarity Measures: Insights for an Application to Activity Landscape Modeling. Molecular Informatics, 2013, 32, 179-190. | 2.5 | 3 |
| 33 | Two-step radical reactions that switch low multiplicity channels leading to the carbene and carbyne species detected for Ru(5F) + CH4â^'nFn (n = 2â€“4) interactions under matrix isolation conditions. RSC Advances, 2013, 3, 11607. | 3.6 | 10 |
| 34 | Synthesis and antiprotozoal activity of novel 2-{[2-(1H-imidazol-1-yl)ethyl]sulfanyl}-1H-benzimidazole derivatives. Bioorganic and Medicinal Chemistry Letters, 2013, 23, 4221-4224. | 2.2 | 48 |
| 35 | CASE Plots for the Chemotypeâ€Based Activity and Selectivity Analysis: A CASE Study of Cyclooxygenase Inhibitors. Chemical Biology and Drug Design, 2012, 80, 752-762. | 3.2 | 11 |
| 36 | Identifying Activity Cliff Generators of PPAR Ligands Using SAS Maps. Molecular Informatics, 2012, 31, 837-846. | 2.5 | 32 |

| # | Article | IF | Citations |
|---|---|---|---|
| 37 | Homology modeling, docking and molecular dynamics of the Leishmania mexicana arginase: A description of the catalytic site useful for drug design. Journal of Molecular Graphics and Modelling, 2012, 38, 50-59. | 2.4 | 19 |
| 38 | Activity landscape modeling of PPAR ligands with dual-activity difference maps. Bioorganic and Medicinal Chemistry, 2012, 20, 3523-3532. | 3.0 | 17 |
| 39 | Computational study on the inhibition mechanism of cruzain by nitrile-containing molecules. Journal of Molecular Graphics and Modelling, 2012, 35, 28-35. | 2.4 | 12 |
| 40 | 3D-QSAR studies on purine-carbonitriles as cruzain inhibitors: comparative molecular field analysis (CoMFA) and comparative molecular similarity indices analysis (CoMSIA). MedChemComm, 2011, 2, 1058. | 3.4 | 10 |
| 41 | Theoretical Study of the Reactions M<sup>+</sup>+CH<sub>3</sub>F (M=Ge, As, Se, Sb). ChemPhysChem, 2010, 11, 1909-1917. | 2.1 | 2 |