Alfonso T GarcÃ-a-Sosa

List of Publications by Year
in descending order

55 papers	1,573 citations	236612 25 h-index	315357 38 g-index
60 all docs	60 docs citations	60 times ranked	2151 citing authors

#	Article	IF	Citations
1	A Comprehensive Evaluation of Sdox, a Promising H2S-Releasing Doxorubicin for the Treatment of Chemoresistant Tumors. Frontiers in Pharmacology, 2022, 13, 831791.	1.6	3
2	N-1,2,3-Triazoleâ€“isatin derivatives: anti-proliferation effects and target identification in solid tumour cell lines. RSC Medicinal Chemistry, 2022, 13, 970-977.	1.7	6
3	Impacts of biomedical hashtag-based Twitter campaign: #DHPSP utilization for promotion of open innovation in digital health, patient safety, and personalized medicine. Current Research in Biotechnology, 2021, 3, 146-153.	1.9	15
4	Androgen Receptor Binding Category Prediction with Deep Neural Networks and Structure-, Ligand-, and Statistically Based Features. Molecules, 2021, 26, 1285.	1.7	2
5	Combined NaÃ¯ve Bayesian, Chemical Fingerprints and Molecular Docking Classifiers to Model and Predict Androgen Receptor Binding Data for Environmentally- and Health-Sensitive Substances. International Journal of Molecular Sciences, 2021, 22, 6695.	1.8	4
6	Exploring EZH2-Proteasome Dual-Targeting Drug Discovery through a Computational Strategy to Fight Multiple Myeloma. Molecules, 2021, 26, 5574.	1.7	2
7	Discovery and Validation of Lmj_04_BRCT Domain, a Novel Therapeutic Target: Identification of Candidate Drugs for Leishmaniasis. International Journal of Molecular Sciences, 2021, 22, 10493.	1.8	11
8	IMproving Preclinical Assessment of Cardioprotective Therapies (IMPACT) criteria: guidelines of the EU-CARDIOPROTECTION COST Action. Basic Research in Cardiology, 2021, 116, 52.	2.5	73
9	Machine learning, artificial intelligence, and data science breaking into drug design and neglected diseases. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1513.	6.2	21
10	Breakthroughs in Medicinal Chemistry: New Targets and Mechanisms, New Drugs, New Hopesâ€“6. Molecules, 2020, 25, 119.	1.7	8
11	Activity to Breast Cancer Cell Lines of Different Malignancy and Predicted Interaction with Protein Kinase C Isoforms of Royleanones. International Journal of Molecular Sciences, 2020, 21, 3671.	1.8	7
12	Repurposing old drugs to fight multidrug resistant cancers. Drug Resistance Updates, 2020, 52, 100713.	6.5	60
13	Breakthroughs in Medicinal Chemistry: New Targets and Mechanisms, New Drugs, New Hopesâ€“7. Molecules, 2020, 25, 2968.	1.7	5
14	CoMPARA: Collaborative Modeling Project for Androgen Receptor Activity. Environmental Health Perspectives, 2020, 128, 27002.	2.8	120
15	Structural insights and binding analysis for determining the molecular bases for programmed cell death protein ligand-1 inhibition. MedChemComm, 2019, 10, 1810-1818.	3.5	5
16	The Novel Serine/Threonine Protein Kinase LmjF.22.0810 from Leishmania major may be Involved in the Resistance to Drugs such as Paromomycin. Biomolecules, 2019, 9, 723.	1.8	8
17	Synthesis, In Silico, and In Vitro Evaluation of Anti-Leishmanial Activity of Oxadiazoles and Indolizine Containing Compounds Flagged against Anti-Targets. Molecules, 2019, 24, 1282.	1.7	15
18	Editorial: Multi-Target-Directed Ligands (MTDL) as Challenging Research Tools in Drug Discovery: From Design to Pharmacological Evaluation. Frontiers in Chemistry, 2019, 7, 71.	1.8	34

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19	Benford's law in medicinal chemistry: Implications for drug design. Future Medicinal Chemistry, 2019, 11, 2247-2253.	1.1	5
20	Binding affinities of the farnesoid X receptor in the D3R Grand Challenge 2 estimated by free-energy perturbation and docking. Journal of Computer-Aided Molecular Design, 2018, 32, 211-224.	1.3	10
21	Best Practices for QSAR Model Reporting: Physical and Chemical Properties, Ecotoxicity, Environmental Fate, Human Health, and Toxicokinetics Endpoints. Environmental Health Perspectives, 2018, 126, 126001.	2.8	51
22	Molecular Dynamics Simulations of the Interactions between Glial Cell Line-Derived Neurotrophic Factor Family Receptor GFRÎ±1 and Small-Molecule Ligands. ACS Omega, 2018, 3, 11407-11414.	1.6	69
23	Selenazolyl-hydrazones as Novel Selective MAO Inhibitors With Antiproliferative and Antioxidant Activities: Experimental and In-silico Studies. Frontiers in Chemistry, 2018, 6, 247.	1.8	34
24	Cobalt Complex with Thiazole-Based Ligand as New Pseudomonas aeruginosa Quorum Quencher, Biofilm Inhibitor and Virulence Attenuator. Molecules, 2018, 23, 1385.	1.7	12
25	Data Mining and Machine Learning Models for Predicting Drug Likeness and Their Disease or Organ Category. Frontiers in Chemistry, 2018, 6, 162.	1.8	40
26	Recovering Actives in Multi-Antitarget and Target Design of Analogs of the Myosin II Inhibitor Blebbistatin. Frontiers in Chemistry, 2018, 6, 179.	1.8	1
27	Designing Ligands for Leishmania, Plasmodium, and Aspergillus N-Myristoyl Transferase with Specificity and Anti-Target-Safe Virtual Libraries. Current Computer-Aided Drug Design, 2018, 14, 131-141.	0.8	4
28	Chemical structure and correlation analysis of HIV-1 NNRT and NRT inhibitors and database-curated, published inhibition constants with chemical structure in diverse datasets. Journal of Molecular Graphics and Modelling, 2017, 76, 205-223.	1.3	9
29	Arginase Flavonoid Anti-Leishmanial in Silico Inhibitors Flagged against Anti-Targets. Molecules, 2016, 21, 589.	1.7	24
30	Design, discovery, modelling, synthesis, and biological evaluation of novel and small, low toxicity s-triazine derivatives as HIV-1 non-nucleoside reverse transcriptase inhibitors. Bioorganic and Medicinal Chemistry, 2016, 24, 2519-2529.	1.4	27
31	Optimization of in vivo DNA delivery with NickFect peptide vectors. Journal of Controlled Release, 2016, 241, 135-143.	4.8	56
32	Natural Variation in Arabidopsis Cvi-0 Accession Reveals an Important Role of MPK12 in Guard Cell CO2 Signaling. PLoS Biology, 2016, 14, e2000322.	2.6	69
33	- Molecular Mechanics/Coarse-Grained Simulations as a Structural Prediction Tool for GPCRs/Ligand Complexes. , 2015, , 354-369.		1
34	Virtual Screening for HIV Protease Inhibitors Using a Novel Database Filtering Procedure. Molecular Informatics, 2015, 34, 485-492.	1.4	2
35	Peptide-Ligand Binding Modeling of siRNA with Cell-Penetrating Peptides. BioMed Research International, 2014, 2014, 1-7.	0.9	12
36	Improving the Use of Ranking in Virtual Screening against HIV-1 Integrase with Triangular Numbers and Including Ligand Profiling with Antitargets. Journal of Chemical Information and Modeling, 2014, 54, 3172-3185.	2.5	18

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37	Hydration Properties of Ligands and Drugs in Protein Binding Sites: Tightly-Bound, Bridging Water Molecules and Their Effects and Consequences on Molecular Design Strategies. Journal of Chemical Information and Modeling, 2013, 53, 1388-1405.	2.5	67
38	Drugs, non-drugs, and disease category specificity: organ effects by ligand pharmacology1. SAR and QSAR in Environmental Research, 2013, 24, 319-331.	1.0	9
39	Molecular Property Filters Describing Pharmacokinetics and Drug Binding. Current Medicinal Chemistry, 2012, 19, 1646-1662.	1.2	36
40	DrugLogit: Logistic Discrimination between Drugs and Nondrugs Including Disease-Specificity by Assigning Probabilities Based on Molecular Properties. Journal of Chemical Information and Modeling, 2012, 52, 2165-2180.	2.5	38
41	Diseaseâ€Specific Differentiation Between Drugs and Nonâ€Drugs Using Principal Component Analysis of Their Molecular Descriptor Space. Molecular Informatics, 2012, 31, 369-383.	1.4	11
42	Combined Approach Using Ligand Efficiency, Cross-Docking, and Antitarget Hits for Wild-Type and Drug-Resistant Y181C HIV-1 Reverse Transcriptase. Journal of Chemical Information and Modeling, 2011, 51, 2595-2611.	2.5	27
43	Drug efficiency indices for improvement of molecular docking scoring functions. Journal of Computational Chemistry, 2010, 31, 174-184.	1.5	53
44	Free Energy Calculations of Mutations Involving a Tightly Bound Water Molecule and Ligand Substitutions in a Ligandâ€Protein Complex. Molecular Informatics, 2010, 29, 589-600.	1.4	37
45	Docking and Virtual Screening Using Distributed Grid Technology. QSAR and Combinatorial Science, 2009, 28, 815-821.	1.5	21
46	Design of Multi-Binding-Site Inhibitors, Ligand Efficiency, and Consensus Screening of Avian Influenza H5N1 Wild-Type Neuraminidase and of the Oseltamivir-Resistant H274Y Variant. Journal of Chemical Information and Modeling, 2008, 48, 2074-2080.	2.5	47
47	Structure-based calculation of drug efficiency indices. Bioinformatics, 2007, 23, 2678-2685.	1.8	26
48	Serotype-selective, small-molecule inhibitors of the zinc endopeptidase of botulinum neurotoxin serotype A. Bioorganic and Medicinal Chemistry, 2006, 14, 395-408.	1.4	71
49	The effect of a tightly bound water molecule on scaffold diversity in the computer-aided de novo ligand design of CDK2 inhibitors. Journal of Molecular Modeling, 2006, 12, 422-431.	0.8	37
50	Including Tightly-Bound Water Molecules in de Novo Drug Design. Exemplification Through the in Silico Generation of Poly(ADP-ribose)polymerase Ligands.. ChemInform, 2005, 36, no.	0.1	0
51	Including Tightly-Bound Water Molecules in de Novo Drug Design. Exemplification through the in Silico Generation of Poly(ADP-ribose)polymerase Ligands. Journal of Chemical Information and Modeling, 2005, 45, 624-633.	2.5	51
52	The effect of tightly bound water molecules on the structural interpretation of ligand-derived pharmacophore models. Journal of Computer-Aided Molecular Design, 2004, 18, 89-100.	1.3	34
53	WaterScore: a novel method for distinguishing between bound and displaceable water molecules in the crystal structure of the binding site of protein-ligand complexes. Journal of Molecular Modeling, 2003, 9, 172-182.	0.8	130
54	Density functional study of FeO2, FeO, and FeO. International Journal of Quantum Chemistry, 2000, 80, 307-319.	1.0	33

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55	Synthesis of 6â€²-galactosyllactose, a deviant human milk oligosaccharide, with the aid of Candida antarctica lipase-B. Organic and Biomolecular Chemistry, 0, , .	1.5	0