Jordi JuÃ¡rez-JimÃ©nez

List of Publications by Year
in descending order

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26 papers	976 citations	516215 16 h-index	552369 26 g-index
29 all docs	29 docs citations	29 times ranked	1559 citing authors

#	Article	IF	Citations
1	Synthesis, Biological Evaluation, and Molecular Modeling of Donepezil and N-[(5-(Benzyloxy)-1-methyl-1H-indol-2-yl)methyl]-N-methylprop-2-yn-1-amine Hybrids as New Multipotent Cholinesterase/Monoamine Oxidase Inhibitors for the Treatment of Alzheimerâ€™s Disease. Journal of Medicinal Chemistry, 2011, 54, 8251-8270.	2.9	198
2	Synthesis and Multitarget Biological Profiling of a Novel Family of Rhein Derivatives As Disease-Modifying Anti-Alzheimer Agents. Journal of Medicinal Chemistry, 2014, 57, 2549-2567.	2.9	132
3	Investigating Cryptic Binding Sites by Molecular Dynamics Simulations. Accounts of Chemical Research, 2020, 53, 654-661.	7.6	106
4	Exploring the Size Limit of Templates for Inhibitors of the M2 Ion Channel of Influenza A Virus. Journal of Medicinal Chemistry, 2011, 54, 2646-2657.	2.9	69
5	Tetrahydrobenzo[h][1,6]naphthyridine-6-chlorotacrine hybrids as a new family of anti-Alzheimer agents targeting Î²-amyloid, tau, and cholinesterase pathologies. European Journal of Medicinal Chemistry, 2014, 84, 107-117.	2.6	57
6	Easily Accessible Polycyclic Amines that Inhibit the Wild-Type and Amantadine-Resistant Mutants of the M2 Channel of Influenza A Virus. Journal of Medicinal Chemistry, 2014, 57, 5738-5747.	2.9	51
7	1,2,3,4-Tetrahydrobenzo[h][1,6]naphthyridines as a new family of potent peripheral-to-midgorge-site inhibitors of acetylcholinesterase: Synthesis, pharmacological evaluation and mechanistic studies. European Journal of Medicinal Chemistry, 2014, 73, 141-152.	2.6	39
8	The complex of hypericin with Î²-lactoglobulin has antimicrobial activity with potential applications in dairy industry. Journal of Dairy Science, 2015, 98, 89-94.	1.4	36
9	Blinded predictions of binding modes and energies of HSP90-Î± ligands for the 2015 D3R grand challenge. Bioorganic and Medicinal Chemistry, 2016, 24, 4890-4899.	1.4	32
10	A fluorogenic probe for granzyme B enables in-biopsy evaluation and screening of response to anticancer immunotherapies. Nature Communications, 2022, 13, 2366.	5.8	26
11	Design, synthesis and biological evaluation of N-methyl-N-[(1,2,3-triazol-4-yl)alkyl]propargylamines as novel monoamine oxidase B inhibitors. Bioorganic and Medicinal Chemistry, 2016, 24, 4835-4854.	1.4	23
12	Discovery and In Vivo Proof of Concept of a Highly Potent Dual Inhibitor of Soluble Epoxide Hydrolase and Acetylcholinesterase for the Treatment of Alzheimerâ€™s Disease. Journal of Medicinal Chemistry, 2022, 65, 4909-4925.	2.9	22
13	Mechanism of the Pseudoirreversible Binding of Amantadine to the M2 Proton Channel. Journal of the American Chemical Society, 2016, 138, 15345-15358.	6.6	21
14	Impact of domain knowledge on blinded predictions of binding energies by alchemical free energy calculations. Journal of Computer-Aided Molecular Design, 2018, 32, 199-210.	1.3	19
15	New polycyclic dual inhibitors of the wild type and the V27A mutant M2 channel of the influenza A virus with unexpected binding mode. European Journal of Medicinal Chemistry, 2015, 96, 318-329.	2.6	18
16	A computationally designed binding mode flip leads to a novel class of potent tri-vector cyclophilin inhibitors. Chemical Science, 2019, 10, 542-547.	3.7	17
17	Unveiling a novel transient druggable pocket in BACE-1 through molecular simulations: Conformational analysis and binding mode of multisite inhibitors. PLoS ONE, 2017, 12, e0177683.	1.1	17
18	Exploring the structural basis of the selective inhibition of monoamine oxidase A by dicarbonitrile aminoheterocycles: Role of Asn181 and Ile335 validated by spectroscopic and computational studies. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2014, 1844, 389-397.	1.1	16

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19	Assessing the Suitability of the Multilevel Strategy for the Conformational Analysis of Small Ligands. Journal of Physical Chemistry B, 2015, 119, 1164-1172.	1.2	16
20	Tuning the local solvent composition at a drug carrier surface: the effect of dimethyl sulfoxide/water mixture on the photofunctional properties of hypericinâ€“Î²-lactoglobulin complexes. Journal of Materials Chemistry B, 2017, 5, 1633-1641.	2.9	16
21	Dynamic design: manipulation of millisecond timescale motions on the energy landscape of cyclophilin A. Chemical Science, 2020, 11, 2670-2680.	3.7	16
22	Dual Effect of Prussian Blue Nanoparticles on AÎ²40 Aggregation: Î²-Sheet Fibril Reduction and Copper Dyshomeostasis Regulation. Biomacromolecules, 2021, 22, 430-440.	2.6	11
23	First homology model of Plasmodium falciparum glucose-6-phosphate dehydrogenase: Discovery of selective substrate analog-based inhibitors as novel antimalarial agents. European Journal of Medicinal Chemistry, 2018, 146, 108-122.	2.6	9
24	Combining Virtual Reality Visualization with Ensemble Molecular Dynamics to Study Complex Protein Conformational Changes. Journal of Chemical Information and Modeling, 2020, 60, 6344-6354.	2.5	6
25	Tetrahydrobenzothiophene carboxamides: Beyond the kinase domain and into the fatty acid realm. Bioorganic and Medicinal Chemistry Letters, 2017, 27, 4462-4466.	1.0	1
26	Design of Potential Antimalarial Agents Based on a Homology Model of Plasmodium falciparum Glucose-6-Phosphate Dehydrogenase. Proceedings (mdpi), 2017, 1, 665.	0.2	0