Gustavo M. Seabra

List of Publications by Year
in descending order

35 papers	652 citations	759233 12 h-index	580821 25 g-index
35 all docs	35 docs citations	35 times ranked	945 citing authors

#	Article	IF	Citations
1	Diversity and Chemical Library Networks of Large Data Sets. Journal of Chemical Information and Modeling, 2022, 62, 2186-2201.	5.4	22
2	Biochemical and structural characterization of Haemophilus influenzae nitroreductase in metabolizing nitroimidazoles. RSC Chemical Biology, 2022, 3, 436-446.	4.1	3
3	Effects of pyriproxyfen on zebrafish brain mitochondria and acetylcholinesterase. Chemosphere, 2021, 263, 128029.	8.2	17
4	Ultrasensitive small molecule fluorogenic probe for human heparanase. Chemical Science, 2021, 12, 239-246.	7.4	12
5	Impact on cholinesterase-inhibition and in silico investigations of sesquiterpenoids from Amazonian Siparuna guianensis Aubl.. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 252, 119511.	3.9	7
6	Searching Anti-Zika Virus Activity in 1H-1,2,3-Triazole Based Compounds. Molecules, 2021, 26, 5869.	3.8	5
7	Bifunctional Doscadenamides Activate Quorum Sensing in Gram-Negative Bacteria and Synergize with TRAIL to Induce Apoptosis in Cancer Cells. Journal of Natural Products, 2021, 84, 779-789.	3.0	3
8	Binding Mechanism between Acetylcholinesterase and Drugs Pazopanib and Lapatinib: Biochemical and Biophysical Studies. ACS Chemical Neuroscience, 2021, 12, 4500-4511.	3.5	7
9	Ahp-Cyclodepsipeptides as tunable inhibitors of human neutrophil elastase and kallikrein 7: Total synthesis of tutuilamide A, serine protease selectivity profile and comparison with lyngbyastatin 7. Bioorganic and Medicinal Chemistry, 2020, 28, 115756.	3.0	6
10	Insights on the interaction of furfural derivatives with BSA and HTF by applying multi-spectroscopic and molecular docking approaches. Journal of Molecular Liquids, 2020, 317, 114021.	4.9	16
11	Furan inhibitory activity against tyrosinase and impact on B16F10 cell toxicity. International Journal of Biological Macromolecules, 2019, 136, 1034-1041.	7.5	35
12	Design and Synthesis of Triazole-Phthalimide Hybrids with Anti-inflammatory Activity. Chemical and Pharmaceutical Bulletin, 2019, 67, 96-105.	1.3	17
13	Spiro-acridine inhibiting tyrosinase enzyme: Kinetic, protein-ligand interaction and molecular docking studies. International Journal of Biological Macromolecules, 2019, 122, 289-297.	7.5	14
14	Molecular dynamics simulations reveal the influence of dextran sulfate in nanoparticle formation with calcium alginate to encapsulate insulin. Journal of Biomolecular Structure and Dynamics, 2018, 36, 1255-1260.	3.5	7
15	Response to â€˜On the antiviral activity and developmental toxicity of 6-methylmercaptopurine riboside (6MMPr)â€™ and â€˜Acceleration with the brakes on?â€™. International Journal of Antimicrobial Agents, 2018, 52, 515-516.	2.5	0
16	Reaction mechanism of the dengue virus serine protease: a QM/MM study. Physical Chemistry Chemical Physics, 2016, 18, 30288-30296.	2.8	12
17	QM/MM Simulations of Amyloid-Î² 42 Degradation by IDE in the Presence and Absence of ATP. Journal of Chemical Information and Modeling, 2015, 55, 72-83.	5.4	4
18	PUPIL. Advances in Protein Chemistry and Structural Biology, 2015, 100, 1-31.	2.3	8

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19	Determination of Free Energy Profiles for Polynucleotides Translocation through Mutant Î±-Hemolysin Nanopores. Biophysical Journal, 2014, 106, 71a.	0.5	0
20	Molecular Dynamics of the Dengue Virus NS3/NS2B Protease in Presence of Inhibitor or Substrate. Biophysical Journal, 2014, 106, 262a.	0.5	0
21	Molecular Dynamics Simulations Reveal a Novel Mechanism for ATP Inhibition of Insulin Degrading Enzyme. Journal of Chemical Information and Modeling, 2014, 54, 1380-1390.	5.4	14
22	Molecular Dynamics of the Dengue Virus NS3/NS2b Protease. Biophysical Journal, 2012, 102, 734a.	0.5	0
23	ATP Inhibition of Insulin-Degrading Enzyme: A Computational Study. Biophysical Journal, 2012, 102, 734a.	0.5	0
24	Comment on â€œa minimal implementation of the AMBER-GAUSSIAN interface for Ab Initio QM/MM-MD simulationâ€• Journal of Computational Chemistry, 2012, 33, 1643-1644.	3.3	2
25	A Multiscale Treatment of Angeliâ€™s Salt Decomposition. Journal of Chemical Theory and Computation, 2009, 5, 37-46.	5.3	12
26	Are Current Semiempirical Methods Better Than Force Fields? A Study from the Thermodynamics Perspective. Journal of Physical Chemistry A, 2009, 113, 11938-11948.	2.5	51
27	A versatile AMBERâ€Gaussian QM/MM interface through PUPIL. Journal of Computational Chemistry, 2008, 29, 1564-1573.	3.3	38
28	Chapter 6 Electronic structure and reactivity in double Rydberg anions: characterization of a novel kind of electron pair. Theoretical and Computational Chemistry, 2007, 19, 87-100.	0.4	10
29	Implementation of the SCC-DFTB Method for Hybrid QM/MM Simulations within the Amber Molecular Dynamics Packageâ€. Journal of Physical Chemistry A, 2007, 111, 5655-5664.	2.5	213
30	Molecular photoionization cross sections in electron propagator theory: Angular distributions beyond the dipole approximation. Journal of Chemical Physics, 2005, 123, 114105.	3.0	20
31	Electron propagator theory calculations of molecular photoionization cross sections: The first-row hydrides. Journal of Chemical Physics, 2004, 121, 4143-4155.	3.0	49
32	Application and Testing of Diagonal, Partial Third-Order Electron Propagator Approximations. , 2001, , 131-160.		24
33	Preparation and reactions of 3-[3-(aryl)-1,2,4-oxadiazol-5-yl&#093: propionic acids. Journal of the Brazilian Chemical Society, 1997, 8, 397-405.	0.6	11
34	Anomeric effect enhancement in C-5-substituted 2-methoxytetrahydropyrans. Journal of Molecular Structure, 1997, 412, 51-58.	3.6	6
35	Theoretical study of the O4 molecule. Computational and Theoretical Chemistry, 1995, 335, 59-61.	1.5	7