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	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
2	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
3	Electron propagator theory calculations of molecular photoionization cross sections: The first-row hydrides. Journal of Chemical Physics, 2004, 121, 4143-4155.	3.0	49
4	A versatile AMBERâ€Gaussian QM/MM interface through PUPIL. Journal of Computational Chemistry, 2008, 29, 1564-1573.	3.3	38
5	Furan inhibitory activity against tyrosinase and impact on B16F10 cell toxicity. International Journal of Biological Macromolecules, 2019, 136, 1034-1041.	7.5	35
6	Application and Testing of Diagonal, Partial Third-Order Electron Propagator Approximations. , 2001, , 131-160.		24
7	Diversity and Chemical Library Networks of Large Data Sets. Journal of Chemical Information and Modeling, 2022, 62, 2186-2201.	5.4	22
8	Molecular photoionization cross sections in electron propagator theory: Angular distributions beyond the dipole approximation. Journal of Chemical Physics, 2005, 123, 114105.	3.0	20
9	Design and Synthesis of Triazole-Phthalimide Hybrids with Anti-inflammatory Activity. Chemical and Pharmaceutical Bulletin, 2019, 67, 96-105.	1.3	17
10	Effects of pyriproxyfen on zebrafish brain mitochondria and acetylcholinesterase. Chemosphere, 2021, 263, 128029.	8.2	17
11	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
12	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
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	A Multiscale Treatment of Angeliâ€™s Salt Decomposition. Journal of Chemical Theory and Computation, 2009, 5, 37-46.	5.3	12
15	Reaction mechanism of the dengue virus serine protease: a QM/MM study. Physical Chemistry Chemical Physics, 2016, 18, 30288-30296.	2.8	12
16	Ultrasensitive small molecule fluorogenic probe for human heparanase. Chemical Science, 2021, 12, 239-246.	7.4	12
17	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
18	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

#	Article	IF	Citations
19	PUPIL. Advances in Protein Chemistry and Structural Biology, 2015, 100, 1-31.	2.3	8
20	Theoretical study of the O4 molecule. Computational and Theoretical Chemistry, 1995, 335, 59-61.	1.5	7
21	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
22	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
23	Binding Mechanism between Acetylcholinesterase and Drugs Pazopanib and Lapatinib: Biochemical and Biophysical Studies. ACS Chemical Neuroscience, 2021, 12, 4500-4511.	3.5	7
24	Anomeric effect enhancement in C-5-substituted 2-methoxytetrahydropyrans. Journal of Molecular Structure, 1997, 412, 51-58.	3.6	6
25	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
26	Searching Anti-Zika Virus Activity in 1H-1,2,3-Triazole Based Compounds. Molecules, 2021, 26, 5869.	3.8	5
27	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
28	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
29	Biochemical and structural characterization of Haemophilus influenzae nitroreductase in metabolizing nitroimidazoles. RSC Chemical Biology, 2022, 3, 436-446.	4.1	3
30	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
31	Molecular Dynamics of the Dengue Virus NS3/NS2b Protease. Biophysical Journal, 2012, 102, 734a.	0.5	0
32	ATP Inhibition of Insulin-Degrading Enzyme: A Computational Study. Biophysical Journal, 2012, 102, 734a.	0.5	0
33	Determination of Free Energy Profiles for Polynucleotides Translocation through Mutant Î±-Hemolysin Nanopores. Biophysical Journal, 2014, 106, 71a.	0.5	0
34	Molecular Dynamics of the Dengue Virus NS3/NS2B Protease in Presence of Inhibitor or Substrate. Biophysical Journal, 2014, 106, 262a.	0.5	0
35	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