JosÃ© X Lima Neto

List of Publications by Year
in descending order

25	384	758635 12	794141 19
papers	citations	h-index	g-index

25	25	25	167
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Exploring the Spike-hACE 2 Residueâ€“Residue Interaction in Human Coronaviruses SARS-CoV-2, SARS-CoV, and HCoV-NL63. Journal of Chemical Information and Modeling, 2022, 62, 2857-2868.	2.5	6
2	Blockade of the checkpoint PD-1 by its ligand PD-L1 and the immuno-oncological drugs pembrolizumab and nivolumab. Physical Chemistry Chemical Physics, 2021, 23, 21207-21217.	1.3	9
3	Quantum binding energy features of the drug olmesartan bound to angiotensin type-1 receptors in the therapeutics of stroke. New Journal of Chemistry, 2021, 45, 19487-19496.	1.4	2
4	Exploring human porphobilinogen synthase metalloprotein by quantum biochemistry and evolutionary methods. Metallomics, 2021, 13, .	1.0	5
5	First-principles study of solid-state properties of adrenergic neurotransmitters, orthorhombic noradrenaline, and monoclinic adrenaline. Journal of Applied Physics, 2021, 129, 234702.	1.1	1
6	New ethionamide boosters and EthR2: structural and energetic analysis. Physical Chemistry Chemical Physics, 2021, 23, 23233-23241.	1.3	4
7	Quantum Biochemical Investigation of Lys49-PLA₂ from Bothrops moojeni. Journal of Physical Chemistry B, 2021, 125, 12972-12980.	1.2	6
8	Exploring the Binding Mechanism of GABA_B Receptor Agonists and Antagonists through in Silico Simulations. Journal of Chemical Information and Modeling, 2020, 60, 1005-1018.	2.5	16
9	Insights into solid-state properties of dopamine and L-Dopa hydrochloride crystals through DFT calculations. Chemical Physics Letters, 2020, 761, 138033.	1.2	7
10	A quantum biochemistry investigation of the proteinâ€“protein interactions for the description of allosteric modulation on biomass-degrading chimera. Physical Chemistry Chemical Physics, 2020, 22, 25936-25948.	1.3	3
11	Interaction energies between two antiandrogenic and one androgenic agonist receptor in the presence of a T877A mutation in prostate cancer: a quantum chemistry analysis. New Journal of Chemistry, 2020, 44, 5903-5912.	1.4	14
12	Ribosomal RNAâ€“Aminoglycoside Hygromycin B Interaction Energy Calculation within a Density Functional Theory Framework. Journal of Physical Chemistry B, 2019, 123, 6421-6429.	1.2	19
13	DFT calculations of the structural, electronic, optical and vibrational properties of anhydrous orthorhombic L-threonine crystals. Computational and Theoretical Chemistry, 2019, 1170, 112621.	1.1	13
14	A quantum biochemistry approach to investigate checkpoint inhibitor drugs for cancer. New Journal of Chemistry, 2019, 43, 7185-7189.	1.4	19
15	Inhibition of the checkpoint protein PD-1 by the therapeutic antibody pembrolizumab outlined by quantum chemistry. Scientific Reports, 2018, 8, 1840.	1.6	33
16	Outlining migrainous through dihydroergotamineâ€“serotonin receptor interactions using quantum biochemistry. New Journal of Chemistry, 2018, 42, 2401-2412.	1.4	21
17	Computational biochemical investigation of the binding energy interactions between an estrogen receptor and its agonists. New Journal of Chemistry, 2018, 42, 19801-19810.	1.4	10
18	Computational investigation of the Î±₂Î²₁integrinâ€“collagen triple helix complex interaction. New Journal of Chemistry, 2018, 42, 17115-17125.	1.4	16

#	Article	IF	Citations
19	Quantum binding energy features of the T3-785 collagen-like triple-helical peptide. RSC Advances, 2017, 7, 2817-2828.	1.7	25
20	Energetic description of cilengitide bound to integrin. New Journal of Chemistry, 2017, 41, 11405-11412.	1.4	20
21	A quantum biochemistry model of the interaction between the estrogen receptor and the two antagonists used in breast cancer treatment. Computational and Theoretical Chemistry, 2016, 1089, 21-27.	1.1	25
22	A quantum chemistry investigation of a potential inhibitory drug against the dengue virus. RSC Advances, 2016, 6, 56562-56570.	1.7	28
23	Electronic transport in methylated fragments of DNA. Applied Physics Letters, 2015, 107, 203701.	1.5	9
24	Quantum molecular modelling of ibuprofen bound to human serum albumin. RSC Advances, 2015, 5, 49439-49450.	1.7	42
25	A quantum biochemistry investigation of willardiine partial agonism in AMPA receptors. Physical Chemistry Chemical Physics, 2015, 17, 13092-13103.	1.3	31