

# Josã© X Lima Neto

## List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/683530/publications.pdf>

Version: 2024-02-01

25  
papers

384  
citations

758635

12  
h-index

794141

19  
g-index

25  
all docs

25  
docs citations

25  
times ranked

167  
citing authors

#	ARTICLE	IF	CITATIONS
1	Quantum molecular modelling of ibuprofen bound to human serum albumin. RSC Advances, 2015, 5, 49439-49450.	1.7	42
2	Inhibition of the checkpoint protein PD-1 by the therapeutic antibody pembrolizumab outlined by quantum chemistry. Scientific Reports, 2018, 8, 1840.	1.6	33
3	A quantum biochemistry investigation of willardiine partial agonism in AMPA receptors. Physical Chemistry Chemical Physics, 2015, 17, 13092-13103.	1.3	31
4	A quantum chemistry investigation of a potential inhibitory drug against the dengue virus. RSC Advances, 2016, 6, 56562-56570.	1.7	28
5	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
6	Quantum binding energy features of the T3-785 collagen-like triple-helical peptide. RSC Advances, 2017, 7, 2817-2828.	1.7	25
7	Outlining migrainous through dihydroergotamine's serotonin receptor interactions using quantum biochemistry. New Journal of Chemistry, 2018, 42, 2401-2412.	1.4	21
8	Energetic description of cilengitide bound to integrin. New Journal of Chemistry, 2017, 41, 11405-11412.	1.4	20
9	Ribosomal RNA's Aminoglycoside Hygromycin B Interaction Energy Calculation within a Density Functional Theory Framework. Journal of Physical Chemistry B, 2019, 123, 6421-6429.	1.2	19
10	A quantum biochemistry approach to investigate checkpoint inhibitor drugs for cancer. New Journal of Chemistry, 2019, 43, 7185-7189.	1.4	19
11	Computational investigation of the $\hat{I}^2_{\pm 2} \hat{I}^2_{\pm 1}$ integrin's collagen triple helix complex interaction. New Journal of Chemistry, 2018, 42, 17115-17125.	1.4	16
12	Exploring the Binding Mechanism of GABA <sub>B</sub> Receptor Agonists and Antagonists through in Silico Simulations. Journal of Chemical Information and Modeling, 2020, 60, 1005-1018.	2.5	16
13	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
14	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
15	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
16	Electronic transport in methylated fragments of DNA. Applied Physics Letters, 2015, 107, 203701.	1.5	9
17	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
18	Insights into solid-state properties of dopamine and L-Dopa hydrochloride crystals through DFT calculations. Chemical Physics Letters, 2020, 761, 138033.	1.2	7

#	ARTICLE	IF	CITATIONS
19	Quantum Biochemical Investigation of Lys49-PLA <sub>2</sub> from <i>Bothrops moojeni</i> . Journal of Physical Chemistry B, 2021, 125, 12972-12980.	1.2	6
20	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
21	Exploring human porphobilinogen synthase metalloprotein by quantum biochemistry and evolutionary methods. Metallomics, 2021, 13, .	1.0	5
22	New ethionamide boosters and EthR2: structural and energetic analysis. Physical Chemistry Chemical Physics, 2021, 23, 23233-23241.	1.3	4
23	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
24	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
25	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