

Willian R Rocha

List of Publications by Year in descending order

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106
papers

2,140
citations

172207

29
h-index

288905

40
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108
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108
docs citations

108
times ranked

2506
citing authors

#	ARTICLE	IF	CITATIONS
1	Synthesis, Magnetostructural Correlation, and Catalytic Promiscuity of Unsymmetric Dinuclear Copper(II) Complexes: Models for Catechol Oxidases and Hydrolases. <i>Inorganic Chemistry</i> , 2012, 51, 1569-1589.	1.9	103
2	Pyridine-derived thiosemicarbazones and their tin(IV) complexes with antifungal activity against <i>Candida</i> spp.. <i>European Journal of Medicinal Chemistry</i> , 2011, 46, 1473-1482.	2.6	69
3	The hydrolysis process of the cis-dichloro(ethylenediamine)platinum(II): A theoretical study. <i>Journal of Chemical Physics</i> , 2003, 118, 10584-10592.	1.2	67
4	N4-Phenyl-substituted 2-acetylpyridine thiosemicarbazones: Cytotoxicity against human tumor cells, structure-activity relationship studies and investigation on the mechanism of action. <i>Bioorganic and Medicinal Chemistry</i> , 2012, 20, 3396-3409.	1.4	66
5	Improved quantum mechanical study of the potential energy surface for the bithiophene molecule. <i>Journal of Chemical Physics</i> , 2000, 113, 4206-4215.	1.2	61
6	2-Acetylpyridine- and 2-benzoylpyridine-derived hydrazones and their gallium(III) complexes are highly cytotoxic to glioma cells. <i>European Journal of Medicinal Chemistry</i> , 2012, 50, 163-172.	2.6	58
7	Hydroxylamine as an Oxygen Nucleophile. Structure and Reactivity of Ammonia Oxide. <i>Journal of the American Chemical Society</i> , 2006, 128, 12374-12375.	6.6	57
8	Monte Carlo Simulation of Cisplatin Molecule in Aqueous Solution. <i>Journal of Physical Chemistry B</i> , 2006, 110, 12047-12054.	1.2	55
9	The solvent effect on the aquation processes of the cis-dichloro(ethylenediamine)platinum(II) using continuum solvation models. <i>Chemical Physics Letters</i> , 2004, 387, 182-187.	1.2	43
10	Theoretical Study of the Olefin Insertion Reaction in the Heterobimetallic Pt(H)(PH ₃) ₂ (SnCl ₃)(C ₂ H ₄) Compound. <i>Organometallics</i> , 1998, 17, 1961-1967.	1.1	42
11	A Monte Carlo quantum mechanical study of the solvatochromism of pyrimidine in water and in carbon tetrachloride. <i>Physical Chemistry Chemical Physics</i> , 2001, 3, 1583-1587.	1.3	42
12	An efficient quantum mechanical/molecular mechanics Monte Carlo simulation of liquid water. <i>Chemical Physics Letters</i> , 2001, 335, 127-133.	1.2	42
13	Reaction Mechanism and Tautomeric Equilibrium of 2-Mercaptopyrimidine in the Gas Phase and in Aqueous Solution: A Combined Monte Carlo and Quantum Mechanics Study. <i>Journal of Physical Chemistry A</i> , 2006, 110, 7253-7261.	1.1	42
14	Design, structural and spectroscopic elucidation, and the <i>in vitro</i> biological activities of new diorganotin dithiocarbamates. <i>European Journal of Medicinal Chemistry</i> , 2012, 58, 493-503.	2.6	42
15	HNO Is Produced by the Reaction of NO with Thiols. <i>Journal of the American Chemical Society</i> , 2017, 139, 14483-14487.	6.6	41
16	Rhodium catalyzed hydroformylation of β -pinene and camphene: effect of phosphorous ligands and reaction conditions on diastereoselectivity. <i>Journal of Organometallic Chemistry</i> , 2003, 671, 150-157.	0.8	40
17	A radical rebound mechanism for the methane oxidation reaction promoted by the dicopper center of a pMMO enzyme: a computational perspective. <i>Dalton Transactions</i> , 2016, 45, 2492-2504.	1.6	40
18	Solvent effects on the electronic absorption spectrum of formamide studied by a sequential Monte Carlo/quantum mechanical approach. <i>Theoretical Chemistry Accounts</i> , 2002, 108, 31-37.	0.5	39

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19	Bismuth(III) complexes with 2-acetylpyridine- and 2-benzoylpyridine-derived hydrazones: Antimicrobial and cytotoxic activities and effects on the clonogenic survival of human solid tumor cells. <i>Bioorganic and Medicinal Chemistry</i> , 2016, 24, 2988-2998.	1.4	39
20	Cytotoxic and antimicrobial effects of indium(III) complexes with 2-acetylpyridine-derived thiosemicarbazones. <i>Dalton Transactions</i> , 2017, 46, 918-932.	1.6	37
21	NO/H ₂ S \leftrightarrow Crosstalk Reactions. The Role of Thionitrites (SNO ⁻) and Perthionitrites (SSNO ²⁻). <i>Inorganic Chemistry</i> , 2019, 58, 14981-14997.	1.9	37
22	2-Acetylpyridine- and 2-benzoylpyridine-derived thiosemicarbazones and their antimony(III) complexes exhibit high anti-trypansomal activity. <i>Polyhedron</i> , 2012, 31, 614-621.	1.0	36
23	The electronic spectrum of N-methylacetamide in aqueous solution: a sequential Monte Carlo/quantum mechanical study. <i>Chemical Physics Letters</i> , 2001, 345, 171-178.	1.2	35
24	On the evaluation of thermal corrections to gas phase ab initio relative energies: implications to the conformational analysis study of cyclooctane. <i>Chemical Physics</i> , 2002, 280, 31-42.	0.9	35
25	Kinetics and structural aspects of the cisplatin interactions with guanine: A quantum mechanical description. <i>International Journal of Quantum Chemistry</i> , 2006, 106, 2129-2144.	1.0	35
26	Ab initio conformational analysis of cyclooctane molecule. <i>Journal of Computational Chemistry</i> , 1998, 19, 524-534.	1.5	33
27	Insertion reaction of propene into Rh-H bond in HRh(CO)(PH ₃) ₂ (C ₃ H ₆) compound: A density functional study. <i>International Journal of Quantum Chemistry</i> , 2000, 78, 42-51.	1.0	32
28	Theoretical investigation of the reaction mechanism for the phosphate diester hydrolysis using an asymmetric dinuclear metal complex as a biomimetic model of the purple acid phosphatase enzyme. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 7039.	1.3	30
29	Theoretical study of the potential energy surface for the interaction of cisplatin and their aquated species with water. <i>Journal of Chemical Physics</i> , 2008, 128, 165103.	1.2	30
30	DNA photonuclease activity of four new copper(II) complexes under UV and red light: theoretical/experimental correlations with active species generation. <i>Dalton Transactions</i> , 2010, 39, 2027-2035.	1.6	28
31	Water Solvent Effect on Theoretical Evaluation of ¹ H NMR Chemical Shifts: <i>o</i> -Methyl-Inositol Isomer. <i>Journal of Physical Chemistry A</i> , 2017, 121, 2839-2846.	1.1	27
32	Theoretical analysis of the oxocarbons: structure and spectroscopic properties of croconate ion and its coordination compound with lithium. <i>Physical Chemistry Chemical Physics</i> , 2001, 3, 3499-3505.	1.3	26
33	Theoretical analysis of the oxocarbons: The solvent and counter-ion effects on the structure and spectroscopic properties of the squarate ion. <i>Physical Chemistry Chemical Physics</i> , 2003, 5, 437-445.	1.3	26
34	Reaction path for the insertion reaction of SnCl ₂ into the Pt(SINGLE BOND)Cl bond: An ab initio study. <i>International Journal of Quantum Chemistry</i> , 1997, 65, 643-650.	1.0	25
35	Linear free energy relationship for 4-substituted (o-phenylenediamine)platinum(II) dichloride derivatives using quantum mechanical descriptors. <i>Journal of Inorganic Biochemistry</i> , 2005, 99, 575-583.	1.5	25
36	[Ag(L)NO ₃] Complexes with 2-Benzoylpyridine-Derived Hydrazones: Cytotoxic Activity and Interaction with Biomolecules. <i>ACS Omega</i> , 2018, 3, 7027-7035.	1.6	24

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37	The electronic spectrum of Fe ²⁺ ion in aqueous solution: A sequential Monte Carlo/quantum mechanical study. <i>Chemical Physics Letters</i> , 2007, 449, 144-148.	1.2	22
38	Hydrogen activation and aldehyde elimination promoted by homogeneous Pt-Sn catalyst: a theoretical study. <i>Computational and Theoretical Chemistry</i> , 2004, 677, 133-143.	1.5	21
39	DFT Study of the Homogeneous Hydroformylation of Propene Promoted by a Heterobimetallic Pt-Sn Catalyst. <i>Organometallics</i> , 2011, 30, 4257-4268.	1.1	21
40	Structure and Nature of the Metal-Ligand Interactions in Mixed Iron(II) Phosphametalloenes. <i>Organometallics</i> , 2004, 23, 5308-5313.	1.1	20
41	Quantum-mechanical and molecular mechanics conformational analysis of 1,5-cyclooctadiene. <i>Journal of Computational Chemistry</i> , 1997, 18, 254-259.	1.5	18
42	Design, structural and spectroscopic elucidation, and the in vitro biological activities of new triorganotin dithiocarbamates - Part II. <i>Polyhedron</i> , 2014, 79, 161-169.	1.0	18
43	Carbonyl insertion reaction into the Pt-C bond in heterobimetallic Pt(SnCl ₃)(PH ₃) ₂ (CO)(CH ₃) compound: Theoretical study. <i>Journal of Computational Chemistry</i> , 2000, 21, 668-674.	1.5	17
44	Theoretical analysis of the oxocarbons: The role played by the solvent and counter-ions in the electronic spectrum of the delatate ion. <i>Physical Chemistry Chemical Physics</i> , 2002, 4, 2517-2523.	1.3	17
45	On the isomerization of \hat{I}^2 -pinene: a theoretical study. <i>Computational and Theoretical Chemistry</i> , 2001, 544, 213-220.	1.5	16
46	Phosphorane lifetime and stereo-electronic effects along the alkaline hydrolysis of phosphate esters. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 18255-18267.	1.3	16
47	On the origin of diastereofacial selectivity in the interaction of \hat{I}^2 -pinene with rhodium carbonyl: A density functional study. <i>Computational and Theoretical Chemistry</i> , 2007, 816, 109-117.	1.5	15
48	Quantum Mechanical/Effective Fragment Potential (QM/EFP) Study of Phosphate Monoester Aminolysis in Aqueous Solution. <i>Journal of Physical Chemistry B</i> , 2009, 113, 14831-14836.	1.2	15
49	Formation and Release of NO from Ruthenium Nitrosyl Ammine Complexes [Ru(NH ₃) ₅ (NO)] ^{2+/3+} in Aqueous Solution: A Theoretical Investigation. <i>Journal of Physical Chemistry B</i> , 2016, 120, 11821-11833.	1.2	15
50	Theoretical study of oxocarbons: structure and vibrational spectrum of the D _{6h} and C ₂ forms of the rhodizonate ion. <i>Computational and Theoretical Chemistry</i> , 2004, 684, 141-147.	1.5	13
51	Intramolecular General Acid Catalysis of the Hydrolysis of 2-(2-Imidazolium)phenyl Phosphate, and Bond Length-Reactivity Correlations for Reactions of Phosphate Monoester Monoanions. <i>Journal of Organic Chemistry</i> , 2007, 72, 3800-3807.	1.7	13
52	Insertion reaction of ethylene into the Rh-H bond: A comparative theoretical study. <i>Chemical Physics Letters</i> , 2007, 439, 69-75.	1.2	13
53	DFT study of the full catalytic cycle for the propene hydroformylation catalyzed by a heterobimetallic HPt(SnCl ₃)(PH ₃) ₂ model catalyst. <i>Journal of Computational Chemistry</i> , 2010, 31, 1986-2000.	1.5	13
54	DFT study of the ligand effects on the regioselectivity of the insertion reaction of olefins in the complexes [HRh(CO) ₂ (PR ₃) ₃](L) (R = H, F, Et, Ph, OEt, OPh, and L = propene,) <i>Tj ETQq0 000rgBT /Overlock 10</i>		

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55	Effective targeting of proton transfer at ground and excited states of ortho-(2-imidazolyl)naphthol constitutional isomers. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 2404-2415.	1.3	13
56	C-H Bond Activation of Methane Promoted by (5-Phospholyl)Rh(CO) ₂ : A Theoretical Perspective. <i>Organometallics</i> , 2005, 24, 2262-2268.	1.1	12
57	Theoretical investigation of the structure and nature of the interaction in metal-alkane η^2 -complexes of the type [M(CO) ₅ (C ₂ H ₆)] (M = Cr, Mo, and W). <i>Chemical Physics</i> , 2009, 365, 85-93.	0.9	12
58	An investigation of the BSSE effect on the evaluation of Ab Initio interaction energies for cisplatin-water complexes. <i>Journal of the Brazilian Chemical Society</i> , 2010, 21, 887-896.	0.6	12
59	QUANTUM CHEMICAL STUDY OF CISPLATIN-WATER COMPLEXES: AN INVESTIGATION OF ELECTRON CORRELATION EFFECTS. <i>Journal of Theoretical and Computational Chemistry</i> , 2011, 10, 371-391.	1.8	12
60	Theoretical analysis of the oxocarbons: the electronic spectrum of the rhodizonate ion. <i>Computational and Theoretical Chemistry</i> , 2005, 719, 31-39.	1.5	11
61	Silver(I) complexes with 2-acetylpyridinebenzoylhydrazones exhibit antimicrobial effects against yeast and filamentous fungi. <i>New Journal of Chemistry</i> , 2018, 42, 2125-2132.	1.4	11
62	On the cis \rightarrow trans isomerization of the square-planar [Pt(Cl)(SnCl ₃)(PH ₃) ₂] compound: ab initio gas phase reaction mechanism and solvent effects using continuum models. <i>Journal of the Brazilian Chemical Society</i> , 2000, 11, 112.	0.6	10
63	Solvation and electronic spectrum of Ni ²⁺ ion in aqueous and ammonia solutions: A sequential Monte Carlo/TD-DFT study. <i>Chemical Physics</i> , 2008, 353, 66-72.	0.9	10
64	Solvation and Proton-Coupled Electron Transfer Reduction Potential of 2NO ⁻ to 1HNO in Aqueous Solution: A Theoretical Investigation. <i>Journal of Physical Chemistry B</i> , 2017, 121, 6618-6625.	1.2	10
65	Theoretical studies of metal complexes of anhydrotetracycline: interaction with ZnII. <i>Journal of the Chemical Society Dalton Transactions</i> , 1998, , 2531-2536.	1.1	9
66	Theoretical study of spectroscopic properties of insulated molecular wires formed by substituted oligothiophenes and cross-linked β -cyclodextrin. <i>Journal of Polymer Science, Part B: Polymer Physics</i> , 2011, 49, 1101-1111.	2.4	9
67	C-H bond activation of methane in aqueous solution: A hybrid quantum mechanical/effective fragment potential study. <i>Journal of Computational Chemistry</i> , 2011, 32, 3383-3392.	1.5	9
68	Prediction of conformational population of large cycloalkanes using <i>ab initio</i> correlated methods: Cycloundecane, cyclododecane, and cyclotridecane. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 3188-3197.	1.0	9
69	Propene Hydroformylation Reaction Catalyzed by HRh(CO)(BISBI): A Thermodynamic and Kinetic Analysis of the Full Catalytic Cycle. <i>European Journal of Inorganic Chemistry</i> , 2020, 2020, 3907-3916.	1.0	9
70	Non-structural protein 5 (NS5) as a target for antiviral development against established and emergent flaviviruses. <i>Current Opinion in Virology</i> , 2021, 50, 30-39.	2.6	9
71	Regioselectivity in the interaction of rhodium hydridotricarbonyl with propene: a theoretical study. <i>Computational and Theoretical Chemistry</i> , 2003, 634, 95-106.	1.5	8
72	Crystal Structure and Magnetic Properties of an Oxamato-Bridged Heterobimetallic Tetranuclear [Ni ^{II} Cu ^{II}] ₂ Complex of the Rack Type. <i>European Journal of Inorganic Chemistry</i> , 2018, 2018, 477-484.	1.0	8

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73	Theoretical investigation of the neutral hydrolysis of diethyl 4-nitrophenyl phosphate (paraoxon) in aqueous solution. <i>Journal of Molecular Modeling</i> , 2018, 24, 259.	0.8	8
74	Nitric Oxide Reacts Very Fast with Hydrogen Sulfide, Alcohols, and Thiols to Produce HNO: Revised Rate Constants. <i>Inorganic Chemistry</i> , 2021, 60, 15997-16007.	1.9	8
75	Synthesis, Characterization and Theoretical Calculations of Novel Five Membered Rings Containing Phosphorus and Arsenic Atoms. <i>Journal of the Brazilian Chemical Society</i> , 2002, 13, 597-605.	0.6	7
76	Methanol dehydrogenation promoted by a heterobimetallic Ru(II)-Sn(II) complex as catalyst: A density functional study. <i>Computational and Theoretical Chemistry</i> , 2007, 816, 77-84.	1.5	7
77	Ab initio thermodynamic study of the reaction of CF ₂ Cl ₂ and CHF ₂ Cl CFCs species with OH radical. <i>Chemical Physics Letters</i> , 2007, 448, 164-172.	1.2	7
78	Ligand Exchange Reaction Involving Ru(III) Compounds in Aqueous Solution: A Hybrid Quantum Mechanical/Effective Fragment Potential Study. <i>Journal of Physical Chemistry B</i> , 2011, 115, 2030-2037.	1.2	7
79	Broken symmetry density functional study of biomimetic models for Purple Acid Phosphatases of the type Fe(III)-M(II) (M= Fe, Cu, Ni, Co and Mn). <i>Computational and Theoretical Chemistry</i> , 2012, 979, 89-95.	1.1	7
80	Influence of susceptibility to hydrolysis and hydrophobicity of arylsemicarbazones on their anti-nociceptive and anti-inflammatory activities. <i>European Journal of Medicinal Chemistry</i> , 2012, 50, 140-148.	2.6	7
81	Synthesis and structural characterization of a 8-hydroxyquinoline derivative coordinated to Zn(II). <i>Journal of Molecular Structure</i> , 2018, 1169, 119-129.	1.8	7
82	Reply to the "Comment on "Theoretical analysis of the oxocarbons: structure and spectroscopic properties of croconate ion and its coordination compound with lithium" by M. C. C. Ribeiro and A. O. Cavalcante, <i>Phys. Chem. Chem. Phys.</i> , 2002, 4, 2917. <i>Physical Chemistry Chemical Physics</i> , 2002, 4, 2919-2920.	1.3	6
83	Solvent effects on the metal-to-ligand charge transfer transition of the complex [Ru(NH ₃) ₅ (Pyrazine)] ²⁺ . <i>Chemical Physics Letters</i> , 2014, 612, 78-83.	1.2	6
84	Base Mechanism to the Hydrolysis of Phosphate Triester Promoted by the Cd ²⁺ /Cd ²⁺ Active site of Phosphotriesterase: A Computational Study. <i>Inorganic Chemistry</i> , 2018, 57, 5888-5902.	1.9	6
85	Quantum mechanics/molecular mechanics investigation of the ethene polymerization mechanism catalyzed by a bulky diimine-Ni(II) complex. <i>Journal of the Brazilian Chemical Society</i> , 2011, 22, 428-436.	0.6	5
86	AN EVALUATION OF QUANTUM CHEMICAL CALCULATIONS OF REACTION ENERGIES FOR CATALYTIC ACTIVATION PROCESSES: THE ACTIVATION OF PROPANE BY A RHODIUM CATALYST REVISITED. <i>Journal of Theoretical and Computational Chemistry</i> , 2012, 11, 297-312.	1.8	5
87	ESI-MS, UV-Vis, and Theoretical Investigation of Fe ³⁺ -Amoxicillin Complexation during Coagulation. <i>Journal of Environmental Engineering, ASCE</i> , 2018, 144, .	0.7	5
88	Liquid tin tetrachloride: a Monte Carlo simulation study. <i>Chemical Physics Letters</i> , 2000, 316, 510-516.	1.2	4
89	A theoretical investigation of the activation of propane by a rhodium catalyst. <i>Chemical Physics Letters</i> , 2006, 430, 160-166.	1.2	4
90	Insertion and carbonylation reactions of styrene promoted by [HRh(CO) _x](PMe ₃) _{3-x} (x = 1, 2) compounds: A theoretical investigation. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 2358-2373.	1.0	4

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91	Broken symmetry density functional study of a mixed-valence unsymmetrical dinuclear iron complex. <i>International Journal of Quantum Chemistry</i> , 2010, 110, 1048-1055.	1.0	4
92	Influence of oxidation state of sulfur on the dissociation of $[Tz_2(CH_2)_n]^{m+}(S(O)_m)(CH_2)_n$ adducts generated by electrospray ionization (Tz = tetrazole ring; n = 2, 3; m = 0, 1, 2). <i>Rapid Communications in Mass Spectrometry</i> , 2012, 26, 377-384.	1.2	4
93	Ab initio molecular dynamics simulation of aqueous solution of nitric oxide in different formal oxidation states. <i>Chemical Physics Letters</i> , 2015, 638, 9-14.	1.2	4
94	Theoretical Investigation of the 4,5-Dibromorodamine Methyl Ester (TH9402) Photosensitizer Used in Photodynamic Therapy: Photophysics, Reactions in the Excited State, and Interactions with DNA. <i>Journal of Physical Chemistry B</i> , 2021, 125, 8932-8943.	1.2	4
95	The nature of the M-NO bond in $[M(\text{Imidazole})(\text{PPIX})(L)]_q$ complexes (M=Fe ²⁺ , Ru ²⁺ ; L=NO ⁺ , NO and) <i>J. Phys. Chem. B</i> , 2017, 121, 10784-10793.	1.1	3
96	Quantum mechanical/effective fragment potential (QM/EFP) study of phosphate diester cleavage in aqueous solution. <i>Computational and Theoretical Chemistry</i> , 2014, 1043, 5-12.	1.1	3
97	Insights into the coordination chemistry of alkanes to metal carbonyls from quantum chemical calculations. <i>Journal of Organometallic Chemistry</i> , 2015, 793, 241-247.	0.8	3
98	Reduction Potential of Ru(III)-Based Complexes with Potential Antitumor Activity and Thermodynamics of their Hydrolysis Reactions and Interactions with Possible Biological Targets: a Theoretical Investigation. <i>Journal of the Brazilian Chemical Society</i> , 0, .	0.6	3
99	Revisiting the Tropospheric OH-Initiated Unimolecular Decomposition of Chlorpyrifos and Chlorpyrifos-Methyl: A Theoretical Perspective. <i>Journal of Physical Chemistry A</i> , 2020, 124, 4280-4289.	1.1	3
100	Nature of the bond, reduction potential, and solvation properties of ruthenium nitrosyl complexes of the type $[Ru(NH_3)_4(L)(NO)]^{2+/3+}$ and $[Ru(\text{salen})(L)(NO)]^{2+/3+}$ in different charge and spin states. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26476.	1.0	3
101	Title is missing!. <i>Journal of Computational Chemistry</i> , 1997, 18, 254.	1.5	3
102	Quantum-mechanical vibrational spectrum and conformational analysis for the 1,5-cyclooctadiene. <i>Vibrational Spectroscopy</i> , 1997, 13, 213-219.	1.2	2
103	Theoretical investigation of $[Ru(\text{bpy})_2(\text{HAT})]^{2+}$ (HAT = 1,4,5,8,9,12-hexaazatriphenylene;) <i>J. Phys. Chem. B</i> , 2022, 126, 120817.	2.0	2
104	Dynamics and allostery of Zika virus non-structural protein 5 methyltransferase. <i>Journal of Biomolecular Structure and Dynamics</i> , 2020, 39, 1-13.	2.0	1
105	Electronic structure and mechanism for the uptake of nitric oxide by the Ru(III) antitumor complex NAMI-A. <i>RSC Advances</i> , 2021, 11, 7381-7390.	1.7	0
106	Computational insights into the reactivity of chlorpyrifos and chlorpyrifos-methyl toward singlet oxygen. <i>Journal of Molecular Modeling</i> , 2021, 27, 282.	0.8	0