Adebayo A Adeniyi

List of Publications by Citations

55 papers	484 citations	11 h-index	20 g-index
57 ext. papers	575 ext. citations	3.3 avg, IF	4.48 L-index

#	Paper	IF	Citations
55	One and Multiple Bonds Interatomic Spin-Spin Coupling in -Cymene Ru(II) of 3,5-Dimethyl-, 3,5-Dicarboxylic-, and 5-Phenyl-pyrazole Derivatives. *Journal of Spectroscopy*, **2015**, 2015, 1-11	1.5	80
54	Exploration of chlorinated thienyl chalcones: A new class of monoamine oxidase-B inhibitors. *International Journal of Biological Macromolecules*, **2016**, 91, 680-95	7.9	60
53	Comparing the suitability of autodock, gold and glide for the docking and predicting the possible targets of Ru(II)-based complexes as anticancer agents. *Molecules*, **2013**, 18, 3760-78	4.8	42
52	Pharmacophore-Based 3D-QSAR Analysis of Thienyl Chalcones as a New Class of Human MAO-B Inhibitors: Investigation of Combined Quantum Chemical and Molecular Dynamics Approach. *Journal of Physical Chemistry B*, **2017**, 121, 1186-1203	3.4	37
51	New drug design with covalent modifiers. *Expert Opinion on Drug Discovery*, **2016**, 11, 79-90	6.2	28
50	Anti-oxidant behavior of functionalized chalcone-a combined quantum chemical and crystallographic structural investigation. *Journal of Molecular Structure*, **2017**, 1146, 301-308	3.4	24
49	Implementing QM in docking calculations: is it a waste of computational time?. *Drug Discovery Today*, **2017**, 22, 1216-1223	8.8	23
48	Immunoinformatics prediction of overlapping CD8 T-cell, IFN- and IL-4 inducer CD4 T-cell and linear B-cell epitopes based vaccines against COVID-19 (SARS-CoV-2). *Vaccine*, **2021**, 39, 1111-1121	4.1	15
47	Exploring the Ruthenium-Ligands Bond and Their Relative Properties at Different Computational Methods. *Journal of Chemistry*, **2016**, 2016, 1-15	2.3	13
46	Influence of substituents on the reduction potential and pKa values of diketones tautomers: A theoretical study. *Electrochimica Acta*, **2019**, 297, 947-960	6.7	13
45	Inhibitory activities and possible anticancer targets of Ru(II)-based complexes using computational docking method. *Journal of Molecular Graphics and Modelling*, **2012**, 38, 60-9	2.8	11
44	Probing mechanism of formylketene dithioacetal towards the facile formation of functionalized pyrimidines: A structural approach. *Journal of Molecular Structure*, **2017**, 1127, 498-510	3.4	10
43	Cyclic Voltammetric Study of 2-Hydroxybenzophenone (HBP) Derivatives and the Correspondent Change in the Orbital Energy Levels in Different Solvents. *Electroanalysis*, **2020**, 32, 2659-2668	3	10
42	Computational insight into the contribution of para-substituents on the reduction potential, proton affinity, and electronic properties of nitrobenzene compounds. *Journal of Molecular Modeling*, **2019** , 25, 78	2	10
41	Diabetes mellitus caused by mutations in human insulin: analysis of impaired receptor binding of insulins Wakayama, Los Angeles and Chicago using pharmacoinformatics. *Journal of Biomolecular Structure and Dynamics*, **2017**, 35, 724-737	3.6	9
40	Development of ruthenium-based complexes as anticancer agents: toward a rational design of alternative receptor targets. *Reviews in Inorganic Chemistry*, **2016**, 36,	2.4	9
39	Functionalized Naphthalimide-4-aminoquinoline Conjugates as Promising Antiplasmodials, with Mechanistic Insights. *ACS Medicinal Chemistry Letters*, **2020**, 11, 154-161	4.3	8

38	[2+2] Cycloadditions of Sorbyl Tosylate with Imines/1-Azadienes: A One-Pot Domino Approach for □Alkylidene-□lactams and Their Computational Studies and Antimicrobial Evaluation. *ChemistrySelect*, **2018**, 3, 9484-9492	1.8	7
37	Electronic effect of □diketonato ligands on the redox potential of fac and mer tris(□diketonato) iron(III) complexes: A density functional theory study and molecular electrostatic potential analysis. *International Journal of Quantum Chemistry*, **2019**, 119, e26036	2.1	6
36	Design, synthesis, heme binding and density functional theory studies of isoindoline-dione-4-aminoquinolines as potential antiplasmodials. *Future Medicinal Chemistry*, **2020**, 12, 193-205	4.1	6
35	The Anticancer Activities of Some Nitrogen Donor Ligands Containing bis-Pyrazole, Bipyridine, and Phenanthroline Moiety Using Docking Methods. *Bioinorganic Chemistry and Applications*, **2018**, 2018, 5796287	4.2	6
34	An insight into the anticancer activities of Ru(II)-based metallocompounds using docking methods. *Molecules*, **2013**, 18, 10829-56	4.8	5
33	Theoretical study of the electronic and spectroscopic properties of some Ru(II) anticancer complexes. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2013**, 105, 456-65	4.4	4
32	The stability, kinetics and inter-fragment electron communication of the tautomers of twelve selected □diketone molecules: A computational study. *Journal of Molecular Graphics and Modelling*, **2018**, 85, 25-39	2.8	4
31	Synthesis of pyrazole derivatives and their spectroscopic properties investigated using both experimental and theoretical approaches. *New Journal of Chemistry*, **2014**, 38, 4120	3.6	3
30	Effects of bidentate coordination on the molecular properties rapta-C based complex using theoretical approach. *Journal of Molecular Modeling*, **2013**, 19, 1325-38	2	3
29	The Spectroscopic and Conductive Properties of Ru(II) Complexes with Potential Anticancer Properties. *Journal of Spectroscopy*, **2014**, 2014, 1-14	1.5	3
28	Silver(I) bis(phosphanylamino)naphthalene complexes: Synthesis, structures and density functional theory (DFT) calculations. *Inorganica Chimica Acta*, **2021**, 515, 120041	2.7	3
27	Designing multiepitope-based vaccine against Eimeria from immune mapped protein 1 (IMP-1) antigen using immunoinformatic approach. *Scientific Reports*, **2021**, 11, 18295	4.9	3
26	Computational insight into the anticholinesterase activities and electronic properties of physostigmine analogs. *Future Medicinal Chemistry*, **2019**, 11, 1907-1928	4.1	2
25	The spectroscopic and the QTAIM properties of pyridine and phenanthroline derivatives using experimental and computational methods. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2014**, 128, 540-51	4.4	2
24	Computational properties of □-toluene and □-trifluorotoluene half-sandwich Ru(II) anticancer complexes. *Journal of Biomolecular Structure and Dynamics*, **2014**, 32, 1351-65	3.6	2
23	Experimental and theoretical investigation of the spectroscopic and electronic properties of pyrazolyl ligands. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2014**, 133, 831-45	4.4	2
22	Computational studies of the electronic, conductivities, and spectroscopic properties of hydrolysed Ru(II) anticancer complexes. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2013**, 115, 426-36	4.4	2
21	Theoretical Study of Interatomic Properties of Ruthenium Half-Sandwich Anticancer Complexes Containing Ru-N Bonds. *Asian Journal of Chemistry*, **2015**, 27, 907-918	0.4	2

20	Probing ultrafast reaction mechanisms of photo-excited dithizone through transient absorption spectroscopy and computational CASSCF studies. *Journal of the Optical Society of America B: Optical Physics*, **2020**, 37, A356	1.7	2
19	Exploring substituents and solvent effects on the reduction potential and molecular properties of five derivatives of hydroxybenzophenone (HBP) with their possible conformations and isomers. *Structural Chemistry*, **2021**, 32, 1299-1310	1.8	2
18	Coagulation of organic pollutants by Moringa oleifera protein molecules: in silico approach. *Environmental Science: Water Research and Technology*, **2021**, 7, 1453-1464	4.2	2
17	Intra-molecular electron communication, spectroscopic and conformational stability of the newly developed urethane modified polyetheramide coatings: Computational methods. *Journal of Molecular Graphics and Modelling*, **2017**, 78, 1-13	2.8	1
16	The qualitative and quantitative accuracy of DFT methods in computing 1 J(CF), 1 J(CN) and n J(FF) spin□spin coupling of fluorobenzene and fluoropyridine molecules. *Journal of Quantitative Spectroscopy and Radiative Transfer*, **2015**, 151, 18-25	2.1	1
15	Computational study of the impact of regeneration and unwanted recombination reactions of Ru(II) phenanthroline compounds used as sensitizers in dyes sensitized solar cells. *Computational Materials Science*, **2017**, 139, 301-312	3.2	1
14	Insights into the Intramolecular Properties of□-Arene-Ru-Based Anticancer Complexes Using Quantum Calculations. *Journal of Chemistry*, **2013**, 2013, 1-14	2.3	1
13	The search for a Buruli Ulcer vaccine and the effectiveness of the Bacillus Calmette-Gu□in vaccine.. *Acta Tropica*, **2022**, 106323	3.2	1
12	The conformational search, the stability, fragment interaction and resistance to acidic attack of epoxyl-polyurethanes in different solvent media. *Structural Chemistry*, **2020**, 31, 861-875	1.8	1
11	Cyclic Voltammetric and DFT Analysis of the Reduction of Manganese(III) Complexes with 2-Hydroxybenzophenones. *Electroanalysis*, **2020**, 32, 2913-2925	3	1
10	Immunoinformatics Design of Multiepitope Vaccine Against Enterococcus faecium Infection. *International Journal of Peptide Research and Therapeutics*,1	2.1	1
9	The design of multiepitope vaccines from plasmids of diarrheagenic Escherichia coli against diarrhoea infection: Immunoinformatics approach. *Infection, Genetics and Evolution*, **2021**, 91, 104803	4.5	1
8	Immunoinformatics approach for multi-epitope vaccine design against P. falciparum malaria. *Infection, Genetics and Evolution*, **2021**, 92, 104875	4.5	1
7	Comparative experimental and DFT analysis of novel indole tagged [1,3,4]thiadiazolo[3,2-a]pyrimidin-5-one hybrid. *Journal of Molecular Structure*, **2022**, 1263, 133159	3.4	0
6	Substituente en isomeriese effekte op die reduksieen oksidasiepotensiaal van tris(□diketonato) mangaan(III) komplekse: DFT en MESP analises. *South African Journal of Science and Technology*, **2020**, 119-133	0.1	
5	Unravelling the drugability of MSI2 RNA recognition motif (RRM) protein and the prediction of their effective antileukemia inhibitors from traditional herb concoctions. *Journal of Biomolecular Structure and Dynamics*, **2020**, 1-14	3.6	
4	The conformational change of Plukenetia conophora oil derivatives and their acidic resistance, intra-fragment interactions, stability in different solvent media. *Journal of Molecular Modeling*, **2020**, 26, 312	2	
3	Enhancing the loading and swelling capacity of cellulose crystal through difunctional and multifunctional epoxy crosslinkers and the effects on the elasticity and plasticity: A computational study. *Journal of Molecular Structure*, **2021**, 1228, 129436	3.4	

2	Analysis of the structural, spectroscopic, and molecular electrostatic potential (MESP) of (amino)carbonothionyl (nitro)benzamide derivatives. *Phosphorus, Sulfur and Silicon and the Related Elements*, **2021**, 196, 690-701	1
1	A theoretical investigation of the fragment interaction and nonlinear optical and electronic properties of tris(□diketonato)iron(III) complexes. *Structural Chemistry*, **2020**, 31, 215-232	1.8