# Adebayo A Adeniyi

## List of Publications by Year in Descending Order



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| 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 | The search for a Buruli Ulcer vaccine and the effectiveness of the Bacillus Calmette-Guﬁn vaccine.. *Acta Tropica*, **2022**, 106323 | 3.2 | 1 |
| 54 | 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 |
| 53 | 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 | |
| 52 | 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 | |
| 51 | Silver(I) bis(phosphanylamino)naphthalene complexes: Synthesis, structures and density functional theory (DFT) calculations. *Inorganica Chimica Acta*, **2021**, 515, 120041 | 2.7 | 3 |
| 50 | 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 |
| 49 | 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 |
| 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 | 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 |
| 46 | Immunoinformatics approach for multi-epitope vaccine design against P. falciparum malaria. *Infection, Genetics and Evolution*, **2021**, 92, 104875 | 4.5 | 1 |
| 45 | 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 |
| 44 | 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 | |
| 43 | 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 |
| 42 | Functionalized Naphthalimide-4-aminoquinoline Conjugates as Promising Antiplasmodials, with Mechanistic Insights. *ACS Medicinal Chemistry Letters*, **2020**, 11, 154-161 | 4.3 | 8 |
| 41 | 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 |
| 40 | 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 |
| 39 | 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 |

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| 38 | Cyclic Voltammetric and DFT Analysis of the Reduction of Manganese(III) Complexes with 2-Hydroxybenzophenones. *Electroanalysis*, **2020**, 32, 2913-2925 | 3 | 1 |
| 37 | 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 | |
| 36 | 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 | |
| 35 | 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 | |
| 34 | 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 |
| 33 | Computational insight into the anticholinesterase activities and electronic properties of physostigmine analogs. *Future Medicinal Chemistry*, **2019**, 11, 1907-1928 | 4.1 | 2 |
| 32 | 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 |
| 31 | 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 |
| 30 | [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 |
| 29 | 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 |
| 28 | 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 |
| 27 | 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 |
| 26 | 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 |
| 25 | 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 |
| 24 | 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 |
| 23 | 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 |
| 22 | Implementing QM in docking calculations: is it a waste of computational time?. *Drug Discovery Today*, **2017**, 22, 1216-1223 | 8.8 | 23 |
| 21 | 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 |

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| 20 | 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 |
| 19 | New drug design with covalent modifiers. *Expert Opinion on Drug Discovery*, **2016**, 11, 79-90 | 6.2 | 28 |
| 18 | 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 |
| 17 | Exploring the Ruthenium-Ligands Bond and Their Relative Properties at Different Computational Methods. *Journal of Chemistry*, **2016**, 2016, 1-15 | 2.3 | 13 |
| 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 | 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 |
| 14 | One and Multiple Bonds Interatomic Spin-Spin Coupling in η6-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 |
| 13 | 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 |
| 12 | Computational properties of η6-toluene and η6-trifluorotoluene half-sandwich Ru(II) anticancer complexes. *Journal of Biomolecular Structure and Dynamics*, **2014**, 32, 1351-65 | 3.6 | 2 |
| 11 | 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 |
| 10 | 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 |
| 9 | The Spectroscopic and Conductive Properties of Ru(II) Complexes with Potential Anticancer Properties. *Journal of Spectroscopy*, **2014**, 2014, 1-14 | 1.5 | 3 |
| 8 | 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 |
| 7 | 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 |
| 6 | 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 |
| 5 | Insights into the Intramolecular Properties of η6-Arene-Ru-Based Anticancer Complexes Using Quantum Calculations. *Journal of Chemistry*, **2013**, 2013, 1-14 | 2.3 | 1 |
| 4 | 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 |
| 3 | An insight into the anticancer activities of Ru(II)-based metallocompounds using docking methods. *Molecules*, **2013**, 18, 10829-56 | 4.8 | 5 |

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| 2 | 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 |
| 1 | Immunoinformatics Design of Multiepitope Vaccine Against Enterococcus faecium Infection. *International Journal of Peptide Research and Therapeutics*,1 | 2.1 | 1 |