# Gideon F Tolufashe

List of Publications by Year
in descending order

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|---|---|---|---|
| 34 papers | 658 citations | 623574 14 h-index | 580701 25 g-index |
| 35 all docs | 35 docs citations | 35 times ranked | 694 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Investigating the biological actions of some Schiff bases using density functional theory study. ChemistrySelect, 2023, 8, 535-547. | 0.7 | 0 |
| 2 | Exploring the concerted mechanistic pathway for HIV-1 PRâ€"substrate revealed by umbrella sampling simulation. Journal of Biomolecular Structure and Dynamics, 2022, 40, 1736-1747. | 2.0 | 6 |
| 3 | Mechanistic insight on the inhibition of D, D-carboxypeptidase from Mycobacterium tuberculosis by Î²-lactam antibiotics: an ONIOM acylation study. Journal of Biomolecular Structure and Dynamics, 2022, 40, 7645-7655. | 2.0 | 1 |
| 4 | Crystal, spectroscopic and quantum mechanics studies of Schiff bases derived from 4-nitrocinnamaldehyde. Scientific Reports, 2021, 11, 8151. | 1.6 | 23 |
| 5 | Ag(I) symmetrical N,Nâ€²-diarylformamidine dithiocarbamate PPh3 complexes: Synthesis, structural characterization, quantum chemical calculations and in vitro biological studies. Inorganica Chimica Acta, 2021, 520, 120316. | 1.2 | 20 |
| 6 | Exploring the bioactivity of pentacyclic triterpenoids as potential antimycobacterial nutraceutics: Insights through comparative biomolecular modelling. Journal of Molecular Graphics and Modelling, 2021, 105, 107900. | 1.3 | 4 |
| 7 | Synthesis, crystal structure with free radical scavenging activity and theoretical studies of Schiff bases derived from 1-naphthylamine, 2,6-diisopropylaniline, and substituted benzaldehyde. European Journal of Chemistry, 2021, 12, 204-215. | 0.3 | 8 |
| 8 | Corrosion inhibition potentials of Cucurbita polyesteramide urethane on mild steel in hydrochloric acid medium: Experimental and computational studies. Scientific African, 2021, 12, e00776. | 0.7 | 0 |
| 9 | Solvent-free synthesis of nitrobenzyl Schiff bases: Characterization, antibacterial studies, density functional theory and molecular docking studies. Journal of Molecular Structure, 2020, 1222, 128857. | 1.8 | 24 |
| 10 | Synthesis and structures of divalent Co, Ni, Zn and Cd complexes of mixed dichalcogen and dipnictogen ligands with corrosion inhibition properties: experimental and computational studies. RSC Advances, 2020, 10, 41967-41982. | 1.7 | 25 |
| 11 | Molecular docking and dynamic simulations of some medicinal plants compounds against SARS-CoV-2: an in silico study. Journal of Taibah University for Science, 2020, 14, 1563-1570. | 1.1 | 15 |
| 12 | Biological Activity of Selected Compounds from Annona muricata Seed as Antibreast Cancer Agents: Theoretical Study. Journal of Chemistry, 2020, 2020, 1-10. | 0.9 | 13 |
| 13 | Inhibition study on anti-type 3 of 3Î±-hydroxysteroid dehydrogenase activity against 1,2,3-triazolo[4,5-D]pyrimidine derivatives: Molecular modelling approach. Scientific African, 2020, 8, e00444. | 0.7 | 5 |
| 14 | Density functional theory study of gold(III)-dithiocarbamate complexes with characteristic anticancer potentials. Journal of Inorganic Biochemistry, 2020, 206, 111044. | 1.5 | 11 |
| 15 | Concerted hydrolysis mechanism of HIV-1 natural substrate against subtypes B and C-SA PR: insight through molecular dynamics and hybrid QM/MM studies. Physical Chemistry Chemical Physics, 2020, 22, 2530-2539. | 1.3 | 10 |
| 16 | From Recognition to Reaction Mechanism: An Overview on the Interactions between HIV-1 Protease and its Natural Targets. Current Medicinal Chemistry, 2020, 27, 2514-2549. | 1.2 | 9 |
| 17 | Structure and Function of L,D- and D,D-Transpeptidase Family Enzymes from Mycobacterium tuberculosis. Current Medicinal Chemistry, 2020, 27, 3250-3267. | 1.2 | 13 |
| 18 | Theoretical Model for HIV-1 PR That Accounts for Substrate Recognition and Preferential Cleavage of Natural Substrates. Journal of Physical Chemistry B, 2019, 123, 6389-6400. | 1.2 | 5 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | Identification of potent L,D-transpeptidase 5 inhibitors for Mycobacterium tuberculosis as potential anti-TB leads: virtual screening and molecular dynamics simulations. Journal of Molecular Modeling, 2019, 25, 328. | 0.8 | 13 |
| 20 | The Driving Force for the Acylation of Î² â€Lactam Antibiotics by L,Dâ€Transpeptidase 2: Quantum Mechanics/Molecular Mechanics (QM/MM) Study. ChemPhysChem, 2019, 20, 1126-1134. | 1.0 | 13 |
| 21 | Inhibition mechanism of L,D-transpeptidase 5 in presence of the Î²-lactams using ONIOM method. Journal of Molecular Graphics and Modelling, 2019, 87, 204-210. | 1.3 | 12 |
| 22 | Unraveling the concerted catalytic mechanism of the human immunodeficiency virus type 1 (HIV-1) protease: a hybrid QM/MM study. Structural Chemistry, 2019, 30, 409-417. | 1.0 | 15 |
| 23 | An insight to the molecular interactions of the FDA approved HIVÂPR drugs against L38Lâ†'Nâ†'L PR mutant. Journal of Computer-Aided Molecular Design, 2018, 32, 459-471. | 1.3 | 11 |
| 24 | <scp>DFT</scp> study of the acidâ€catalyzed esterification reaction mechanism of methanol with carboxylic acid and its halide derivatives. International Journal of Quantum Chemistry, 2018, 118, e25497. | 1.0 | 41 |
| 25 | Inhibition of Mycobacterium tuberculosis L,Dâ€Transpeptidase 5â€‰by Carbapenems: MD and QM/MM Mechanistic Studies. ChemistrySelect, 2018, 3, 13603-13612. | 0.7 | 6 |
| 26 | The catalytic role of water in the binding site of l,d-transpeptidase 2 within acylation mechanism: A QM/MM (ONIOM) modelling. Tuberculosis, 2018, 113, 222-230. | 0.8 | 13 |
| 27 | Molecular insight on the non-covalent interactions between carbapenems and l,d-transpeptidase 2 from Mycobacterium tuberculosis: ONIOM study. Journal of Computer-Aided Molecular Design, 2018, 32, 687-701. | 1.3 | 10 |
| 28 | Differential flap dynamics in <scp>l</scp>,<scp>d</scp>-transpeptidase2 from mycobacterium tuberculosis revealed by molecular dynamics. Molecular BioSystems, 2017, 13, 1223-1234. | 2.9 | 36 |
| 29 | Computational model for the acylation step of the Î²-lactam ring: Potential application for l,d-transpeptidase 2 in mycobacterium tuberculosis. Journal of Molecular Structure, 2017, 1128, 94-102. | 1.8 | 41 |
| 30 | Mechanistic investigation of the uncatalyzed esterification reaction of acetic acid and acid halides with methanol: a DFT study. Journal of Molecular Modeling, 2016, 22, 235. | 0.8 | 39 |
| 31 | A comparative modeling and molecular docking study onMycobacterium tuberculosistargets involved in peptidoglycan biosynthesis. Journal of Biomolecular Structure and Dynamics, 2016, 34, 2399-2417. | 2.0 | 23 |
| 32 | The effect of N-methylation of amino acids (Ac-X-OMe) on solubility and conformation: a DFT study. Organic and Biomolecular Chemistry, 2015, 13, 9993-10006. | 1.5 | 55 |
| 33 | Integrated Approach to Structure-Based Enzymatic Drug Design: Molecular Modeling, Spectroscopy, and Experimental Bioactivity. Chemical Reviews, 2014, 114, 493-537. | 23.0 | 100 |
| 34 | Synthesis and structural studies of pentacycloundecane-based HIV-1 PR inhibitors: A hybrid 2D NMR and docking/QM/MM/MD approach. European Journal of Medicinal Chemistry, 2011, 46, 3976-3985. | 2.6 | 38 |