Mwadham M Kabanda

List of Publications by Year
in descending order

53 papers	2,555 citations	201674 27 h-index	189892 50 g-index
53 all docs	53 docs citations	53 times ranked	1664 citing authors

#	Article	IF	Citations
1	A DFT and MP2 mechanistic and kinetic study on hypohalogenation reaction of cysteine and N-acetylcysteine in aqueous solution. Journal of Molecular Liquids, 2022, 349, 118191.	4.9	1
2	Hydrogen bonding between 1-ethyl-3-methyl-imidazolium dicyanamide ionic liquid and selected co-solvents with varying polarity: A DFT study. Journal of Molecular Liquids, 2022, , 119418.	4.9	5
3	Influence of temperature and concentration on the molecular interactions of pyrrolidinium-based ionic liquid with water and alcohols: An experimental and DFT studies. Journal of Molecular Liquids, 2022, 360, 119554.	4.9	3
4	LC-MS based validation and DFT investigation on the antioxidant properties of clovamide: â€¢OH and â€¢OOH scavenging and Cu(II) chelation mechanisms. Journal of Molecular Structure, 2021, 1236, 130349.	3.6	7
5	Proportional coexistence of okanin chalcone glycoside and okanin flavanone glycoside in Bidens pilosa leaves and theoretical investigation on the antioxidant properties of their aglycones. Free Radical Research, 2020, 55, 1-18.	3.3	11
6	A Theoretical Study of the Preferred Reaction Mechanism Between Chloroacetic Acid and Thiourea. Progress in Theoretical Chemistry and Physics, 2020, , 119-142.	0.2	0
7	A DFT mechanistic and kinetic study on the reaction of phloroglucinol with ^{â€¢}OH in different media: Hydrogen atom transfer versus oxidation. Journal of Theoretical and Computational Chemistry, 2019, 18, 1950017.	1.8	6
8	A DFT mechanistic, thermodynamic and kinetic study on the reaction of 1, 3, 5-trihydroxybenzene and 2, 4, 6-trihydroxyacetophenone with ^{â€¢}OOH in different media. Journal of Theoretical and Computational Chemistry, 2019, 18, 1950023.	1.8	5
9	A Theoretical study on the degradation of 2-mercaptobenzothiazole and 2-mercaptobenzimidazole by OH in vacuo and aqueous media. Computational and Theoretical Chemistry, 2018, 1125, 112-127.	2.5	5
10	A DFT study on the addition and abstraction reactions of thiourea with hydroxyl radical. Journal of Sulfur Chemistry, 2018, 39, 23-46.	2.0	13
11	Structural Elucidation of cis/trans Dicaffeoylquinic Acid Photoisomerization Using Ion Mobility Spectrometry-Mass Spectrometry. Journal of Physical Chemistry Letters, 2017, 8, 1381-1388.	4.6	45
12	An appraisal of the hydrogen atom transfer mechanism for the reaction between thiourea derivatives and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.gif" overflow="scroll"><mml:mrow><mml:msup><mml:mrow /><mml:mrow><mml:mtext /></mml:mrow></mml:msup><mml:mtext>OH</mml:mtext></mml:mrow></mml:math> radical: A case-study of dimethylthiourea and diethylthiourea. Computational and Theoretical Chemistry, 2017, 1101, 83-95.	2.5	13
13	The Effect of Geometrical Isomerism of 3,5-Dicaffeoylquinic Acid on Its Binding Affinity to HIV-Integrase Enzyme: A Molecular Docking Study. Evidence-based Complementary and Alternative Medicine, 2016, 2016, 1-9.	1.2	17
14	Preferential alkali metal adduct formation by cis geometrical isomers of dicaffeoylquinic acids allows for efficient discrimination from their trans isomers during ultraâ€highâ€performance liquid chromatography/quadrupole timeâ€ofâ€flight mass spectrometry. Rapid Communications in Mass Spectrometry, 2016, 30, 1011-1018.	1.5	32
15	Experimental and theoretical studies on some selected ionic liquids with different cations/anions as corrosion inhibitors for mild steel in acidic medium. Journal of the Taiwan Institute of Chemical Engineers, 2016, 64, 252-268.	5.3	145
16	Influence of the geometric isomers on the radical scavenging properties of 3,5-dicaffeoylquinic acid: A DFT study in vacuo and in solution. Journal of Theoretical and Computational Chemistry, 2016, 15, 1650052.	1.8	3
17	A theoretical study on the antioxidant properties of methoxy-substituted chalcone derivatives: A case study of kanakugiol and pedicellin through their Fe (II and III) coordination ability. Journal of Theoretical and Computational Chemistry, 2016, 15, 1650048.	1.8	20
18	Synthesis, crystal structure, thermal and theoretical studies of bis(N-ethyl-N-phenyldithiocarbamato) Ni(II) and (N-ethyl-N-phenyldithiocarbamato) (isothiocyanato) (triphenylphosphine) Ni(II). Journal of Chemical Sciences, 2016, 128, 1081-1093.	1.5	13

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19	Investigation of the adsorption characteristics of some selected sulphonamide derivatives as corrosion inhibitors at mild steel/hydrochloric acid interface: Experimental, quantum chemical and QSAR studies. Journal of Molecular Liquids, 2016, 215, 763-779.	4.9	73
20	Antioxidant and antimalarial properties of butein and homobutein based on their ability to chelate iron (II and III) cations: a DFT study in vacuo and in solution. European Food Research and Technology, 2016, 242, 71-90.	3.3	27
21	Quinoxaline derivatives as corrosion inhibitors for mild steel in hydrochloric acid medium: Electrochemical and quantum chemical studies. Physica E: Low-Dimensional Systems and Nanostructures, 2016, 76, 109-126.	2.7	111
22	Adsorption and Corrosion Inhibition Studies of Some Selected Dyes as Corrosion Inhibitors for Mild Steel in Acidic Medium: Gravimetric, Electrochemical, Quantum Chemical Studies and Synergistic Effect with Iodide Ions. Molecules, 2015, 20, 16004-16029.	3.8	109
23	Adsorption, Thermodynamic and Quantum Chemical Studies of 1-hexyl-3-methylimidazolium Based Ionic Liquids as Corrosion Inhibitors for Mild Steel in HCl. Materials, 2015, 8, 3607-3632.	2.9	92
24	Some Phthalocyanine and Naphthalocyanine Derivatives as Corrosion Inhibitors for Aluminium in Acidic Medium: Experimental, Quantum Chemical Calculations, QSAR Studies and Synergistic Effect of Iodide Ions. Molecules, 2015, 20, 15701-15734.	3.8	51
25	Porphyrins as Corrosion Inhibitors for N80 Steel in 3.5% NaCl Solution: Electrochemical, Quantum Chemical, QSAR and Monte Carlo Simulations Studies. Molecules, 2015, 20, 15122-15146.	3.8	76
26	Antioxidant Properties of Kanakugiol Revealed Through the Hydrogen Atom Transfer, Electron Transfer and M2+ (M2+â€‰=â€‰Cu(II) or Co(II) Ion) Coordination Ability Mechanisms. A DFT Study In Vacuo and in Solution. Food Biophysics, 2015, 10, 342-359.	3.0	30
27	A theoretical study of the antioxidant properties of phenolic acid amides investigated through the radical-scavenging and metal chelation mechanisms. European Food Research and Technology, 2015, 241, 553-572.	3.3	14
28	Some Quinoxalin-6-yl Derivatives as Corrosion Inhibitors for Mild Steel in Hydrochloric Acid: Experimental and Theoretical Studies. Journal of Physical Chemistry C, 2015, 119, 16004-16019.	3.1	381
29	Experimental and theoretical studies on the corrosion inhibition of mild steel by some sulphonamides in aqueous HCl. RSC Advances, 2015, 5, 28743-28761.	3.6	92
30	Synthesized photo-cross-linking chalcones as novel corrosion inhibitors for mild steel in acidic medium: experimental, quantum chemical and Monte Carlo simulation studies. RSC Advances, 2015, 5, 76675-76688.	3.6	56
31	Conformational, electronic and antioxidant properties of lucidone, linderone and methyllinderone: DFT, QTAIM and NBO studies. Molecular Physics, 2015, 113, 683-697.	1.7	39
32	Antioxidant Radical Scavenging Properties of Phenolic Pent-4-En-1-Yne Derivatives Isolated FromHypoxis Rooperi. A DFT Studyin vacuoand in Solution. International Journal of Food Properties, 2015, 18, 149-164.	3.0	22
33	A computational study of pyrazinamide: Tautomerism, acidâ€“base properties, micro-solvation effects and acid hydrolysis mechanism. Computational and Theoretical Chemistry, 2014, 1046, 30-41.	2.5	30
34	MP2, DFT and DFT-D study of the dimers of diazanaphthalenes: a comparative study of their structures, stabilisation and binding energies. Molecular Simulation, 2014, 40, 1131-1146.	2.0	9
35	Metronidazole as environmentally safe corrosion inhibitor for mild steel in 0.5M HCl: Experimental and theoretical investigation. Journal of Environmental Chemical Engineering, 2013, 1, 431-439.	6.7	158
36	Isolation, identification and radical scavenging activity of phlorotannin derivatives from brown algae, Ecklonia maxima: An experimental and theoretical study. Free Radicals and Antioxidants, 2013, , .	0.3	6

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37	Weight Loss, Electrochemical, Quantum Chemical Calculation, and Molecular Dynamics Simulation Studies on 2-(Benzylthio)-1,4,5-triphenyl-1H-imidazole as an Inhibitor for Carbon Steel Corrosion in Hydrochloric Acid. Industrial & Engineering Chemistry Research, 2013, 52, 14315-14327.	3.7	71
38	Structures, Stabilization Energies, and Binding Energies of QuinoxalineÂ·Â·Â·(H₂O)_n, Quinoxaline Dimer, and QuinoxalineÂ·Â·Â·Cu Complexes: A Theoretical Study. Journal of Physical Chemistry A, 2013, 117, 1583-1595.	2.5	20
39	DFT STUDY OF THE PROTONATION AND DEPROTONATION ENTHALPIES OF BENZOXAZOLE, 1,2-BENZISOXAZOLE AND 2,1-BENZISOXAZOLE AND IMPLICATIONS FOR THE STRUCTURES AND ENERGIES OF THEIR ADDUCTS WITH EXPLICIT WATER MOLECULES. Journal of Theoretical and Computational Chemistry, 2013, 12, 1350070.	1.8	12
40	Antioxidant Activity of Rooperol Investigated through Cu (I and II) Chelation Ability and the Hydrogen Transfer Mechanism: A DFT Study. Chemical Research in Toxicology, 2012, 25, 2153-2166.	3.3	42
41	Electrochemical and Quantum Chemical Investigation of Some Azine and Thiazine Dyes as Potential Corrosion Inhibitors for Mild Steel in Hydrochloric Acid Solution. Industrial & Engineering Chemistry Research, 2012, 51, 12940-12958.	3.7	132
42	Experimental and Quantum Chemical Studies of Some Bis(trifluoromethyl-sulfonyl) Imide Imidazolium-Based Ionic Liquids as Corrosion Inhibitors for Mild Steel in Hydrochloric Acid Solution. Industrial & Engineering Chemistry Research, 2012, 51, 13282-13299.	3.7	188
43	A comparative study of the dimers of selected hydroxybenzenes. International Journal of Quantum Chemistry, 2012, 112, 519-531.	2.0	18
44	Computational study of the patterns of weaker intramolecular hydrogen bonds stabilizing acylphloroglucinols. International Journal of Quantum Chemistry, 2012, 112, 2650-2658.	2.0	34
45	The conformational preferences of acylphloroglucinolsâ€"a promising class of biologically active compounds. International Journal of Quantum Chemistry, 2012, 112, 3691-3702.	2.0	37
46	Interplay of intramolecular hydrogen bonds, OH orientations, and symmetry factors in the stabilization of polyhydroxybenzenes. International Journal of Quantum Chemistry, 2011, 111, 3701-3716.	2.0	5
47	A computational study of the carboxylic acid of phloroglucinol in vacuo and in water solution. International Journal of Quantum Chemistry, 2010, 110, 595-623.	2.0	35
48	Adducts of acylphloroglucinols with explicit water molecules: Similarities and differences across a sufficiently representative number of structures. International Journal of Quantum Chemistry, 2010, 110, 2378-2390.	2.0	11
49	A study of the intramolecular hydrogen bond in acylphloroglucinols. Computational and Theoretical Chemistry, 2009, 901, 210-219.	1.5	65
50	A Computational Study of the Effects of Different Solvents on the Characteristics of the Intramolecular Hydrogen Bond in Acylphloroglucinols. Journal of Physical Chemistry A, 2009, 113, 15064-15077.	2.5	56
51	A computational study of the interactions of the caespitate molecule with water. International Journal of Quantum Chemistry, 2008, 108, 1772-1791.	2.0	29
52	A computational study of the interactions of the phloroglucinol molecule with water. Computational and Theoretical Chemistry, 2008, 852, 36-45.	1.5	29
53	Model structures for the study of acylated phloroglucinols and computational study of the caespitate molecule. Computational and Theoretical Chemistry, 2007, 805, 39-52.	1.5	51