Tarek EL-Gogary

List of Publications by Year in descending order

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686830 794141 38 399 13 19 citations g-index h-index papers 39 39 39 469 docs citations times ranked citing authors all docs

#	Article	IF	CITATIONS
1	Ab initio-based kinetics of hydrogen atom abstraction from methyl propionate by H and CH3 radicals: a biodiesel model. Structural Chemistry, 2021, 32, 1857-1872.	1.0	12
2	Thermo-kinetic theoretical studies on pyrolysis of dimethoxymethane fuel additive. Fuel, 2021, 290, 119970.	3.4	22
3	First-principle kinetic studies of unimolecular pyrolysis of isopropyl esters as biodiesel surrogates. Theoretical Chemistry Accounts, 2021, 140, 1.	0.5	8
4	Characterization, Hirshfeld surface analysis, DFT study and an in vitro α-glucosidase/α-amylase/radical scavenging profiling of novel 5-styryl-2-(4-tolylsulfonamido) chalcones. Journal of Molecular Structure, 2021, 1245, 131090.	1.8	5
5	Computational Studies on the Thermodynamic and Kinetic Parameters of Oxidation of 2-Methoxyethanol Biofuel via H-Atom Abstraction by Methyl Radical. Scientific Reports, 2019, 9, 15361.	1.6	17
6	Adsorption of Cu ²⁺ and Mg ²⁺ ions on silica gel derived from rice hulls ash: Experimental and theoretical studies. Journal of Theoretical and Computational Chemistry, 2019, 18, 1950026.	1.8	2
7	Oxidation of Methyl Propanoate by the OH Radical. Russian Journal of Physical Chemistry A, 2018, 92, 2476-2484.	0.1	6
8	Umbrella inversion and structure of phosphorus-containing compounds: A quantum chemical study. Journal of Theoretical and Computational Chemistry, 2018, 17, 1850042.	1.8	7
9	Theoretical and experimental studies on anticancer drug mitoxantrone. Journal of Molecular Structure, 2018, 1173, 837-847.	1.8	8
10	A thermochemistry and kinetic study on the thermal decomposition of ethoxyquinoline and ethoxyisoquinoline. International Journal of Chemical Kinetics, 2018, 50, 604-611.	1.0	1
11	Design, Synthesis and Biological Evaluation of Pyrido[2,3-d] Pyrimidine Derivatives as Potential Anticancer Agents. Letters in Drug Design and Discovery, 2018, 15, 1240-1251.	0.4	3
12	Synthesis of novel anthraquinones: Molecular structure, molecular chemical reactivity descriptors and interactions with DNA as antibiotic and anti-cancer drugs. Journal of Molecular Structure, 2017, 1130, 799-809.	1.8	16
13	Interaction of anthraquinone anti-cancer drugs with DNA:Experimental and computational quantum chemical study. Journal of Molecular Structure, 2017, 1127, 751-760.	1.8	39
14	Heteroaromatization with 4-phenyldiazenyl-1-naphthol. Part III: One-pot synthesis and DFT study of 4H-naphthopyran derivatives. European Journal of Chemistry, 2017, 8, 358-366.	0.3	0
15	Structure, stability, energy barrier and ionization energies of chemically modified DNA-bases: Quantum chemical calculations on 37 favored and rare tautomeric forms of tetraphosphoadenine. Computational and Theoretical Chemistry, 2015, 1052, 35-41.	1.1	4
16	Synthesis, spectral and quantum chemical studies on NO-chelating sulfamonomethoxine–cyclophosph(V)azane and its Er(III) complex. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 128, 724-729.	2.0	2
17	Spectral and quantum chemical studies on 1,3-bis(N1-4-amino-6-methoxypyrimidinebenzenesulfonamide-2,2,4,4-ethane-1,2-dithiol)-2,4-dichlorocyclodiphospl and its erbium complex. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 118, 481-487.	h(V)azane	1
18	Utilization of nicotinonitrile-2-thiol in the synthesis of new thiepino [2,3-b] pyridine derivative as an in vitro novel antitumor potent. Medicinal Chemistry Research, 2013, 22, 1674-1678.	1.1	2

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19	Synthesis, spectroscopic, thermal and quantum chemical studies on trivalent erbium NO chelating sulfamonomethoxine–cyclophosph(V)azane complex. Journal of Molecular Structure, 2013, 1048, 202-209.	1.8	2
20	Structure and Stability of Chemically Modified DNA Bases: Quantum Chemical Calculations on 16 Isomers of Diphosphocytosine. , 2013, 2013, 1-10.		3
21	Synthesis, characterization and quantum chemical ab initio calculations of new dimeric aminocyclodiphosph(V)azane and its Co(II), Ni(II) and Cu(II) complexes. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 95, 414-422.	2.0	18
22	Quantum chemical calculations and experimental investigations on 2-aminobenzoic acid-cyclodiphosph(V)azane derivative and its homo-binuclear Cu(II) complex. Journal of Molecular Structure, 2012, 1011, 50-58.	1.8	10
23	Interaction of angelicin with DNA-bases (III) DFT and ab initio second-order Moeller-Plesset study. International Journal of Quantum Chemistry, 2010, 110, 1445-1454.	1.0	1
24	Interaction of psoralens with DNA-bases (II): An ab initio quantum chemical, density functional theory and second-order MÃ-ller-Plesset perturbational study. Computational and Theoretical Chemistry, 2009, 895, 57-64.	1. 5	16
25	Geometry and thermodynamic stabilities of rhodanine tautomers and rotamers: Quantum chemical study. Computational and Theoretical Chemistry, 2009, 907, 66-73.	1.5	15
26	Origin of reverse stability of diphosphouracil tautomers compared to their analogue uracil: DFT and ab initio study. Computational and Theoretical Chemistry, 2008, 851, 54-62.	1.5	9
27	Quantum chemical studies on the potentially important imidates. Computational and Theoretical Chemistry, 2008, 861, 62-67.	1.5	1
28	Synthesis and Chemical Transformation of 2-iodomethyl-1-(phenylmethyl)-1,5,6,7-tetrahydroindol-4-ones. Journal of Chemical Research, 2008, 2008, 227-231.	0.6	3
29	Interaction of psoralens with DNA-bases (I). An ab initio quantum chemical, density functional theory and second-order Møller–Plesset perturbational study. Computational and Theoretical Chemistry, 2007, 808, 97-109.	1.5	32
30	Spectroscopic studies of molecular interactions involving 2,6-diethylaniline and N-ethylaniline donors and iodine as an electron acceptor in different solvents. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2007, 66, 94-101.	2.0	19
31	Spectroscopic and Quantum Mechanical Studies of Substituted Anilines and their Charge-Transfer Complexes with Iodine in Different Solvents. Monatshefte Fýr Chemie, 2006, 137, 1027-1042.	0.9	1
32	Spectroscopic and quantum chemical studies on the structure of 2-arylquinoline-4(1H)-thione derivatives. Journal of Molecular Structure, 2004, 690, 151-157.	1.8	11
33	Molecular complexes of some anthraquinone anti-cancer drugs: experimental and computational study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2003, 59, 1009-1015.	2.0	11
34	Noncovalent attachment of psoralen derivatives with DNA: Hartree–Fock and density functional studies on the probes. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2003, 59, 2635-2644.	2.0	27
35	Molecular mechanics, quantum mechanics, potentiometric, and conductometric studies on the complexes of some rare earth metals with 5-azorhodanine derivatives. International Journal of Quantum Chemistry, 2003, 91, 685-694.	1.0	5
36	Temperature and substituent effects on the dissociation constants of 5-azorhodanine derivatives. Semi-empirical quantum mechanical calculation. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2002, 58, 447-455.	2.0	21

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37	Ab-initio molecular geometry and normal coordinate analysis of tetrahydrothiophene molecule. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2001, 57, 1405-1415.	2.0	14
38	Ab-Initio molecular geometry and normal coordinate analysis of pyrrolidine molecule. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2001, 57, 2647-2657.	2.0	25