

# Tarek EL-Gogary

## List of Publications by Year in descending order

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38  
papers

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times ranked

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#	ARTICLE	IF	CITATIONS
1	Interaction of anthraquinone anti-cancer drugs with DNA: Experimental and computational quantum chemical study. <i>Journal of Molecular Structure</i> , 2017, 1127, 751-760.	1.8	39
2	Interaction of psoralens with DNA-bases (I). An ab initio quantum chemical, density functional theory and second-order Møller-Plesset perturbational study. <i>Computational and Theoretical Chemistry</i> , 2007, 808, 97-109.	1.5	32
3	Noncovalent attachment of psoralen derivatives with DNA: Hartree-Fock and density functional studies on the probes. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2003, 59, 2635-2644.	2.0	27
4	Ab-Initio molecular geometry and normal coordinate analysis of pyrrolidine molecule. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2001, 57, 2647-2657.	2.0	25
5	Thermo-kinetic theoretical studies on pyrolysis of dimethoxymethane fuel additive. <i>Fuel</i> , 2021, 290, 119970.	3.4	22
6	Temperature and substituent effects on the dissociation constants of 5-azorhodanine derivatives. Semi-empirical quantum mechanical calculation. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2002, 58, 447-455.	2.0	21
7	Spectroscopic studies of molecular interactions involving 2,6-diethylaniline and N-ethylaniline donors and iodine as an electron acceptor in different solvents. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2007, 66, 94-101.	2.0	19
8	Synthesis, characterization and quantum chemical ab initio calculations of new dimeric aminocyclodiphosph(V)azane and its Co(II), Ni(II) and Cu(II) complexes. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 95, 414-422.	2.0	18
9	Computational Studies on the Thermodynamic and Kinetic Parameters of Oxidation of 2-Methoxyethanol Biofuel via H-Atom Abstraction by Methyl Radical. <i>Scientific Reports</i> , 2019, 9, 15361.	1.6	17
10	Interaction of psoralens with DNA-bases (II): An ab initio quantum chemical, density functional theory and second-order Møller-Plesset perturbational study. <i>Computational and Theoretical Chemistry</i> , 2009, 895, 57-64.	1.5	16
11	Synthesis of novel anthraquinones: Molecular structure, molecular chemical reactivity descriptors and interactions with DNA as antibiotic and anti-cancer drugs. <i>Journal of Molecular Structure</i> , 2017, 1130, 799-809.	1.8	16
12	Geometry and thermodynamic stabilities of rhodanine tautomers and rotamers: Quantum chemical study. <i>Computational and Theoretical Chemistry</i> , 2009, 907, 66-73.	1.5	15
13	Ab-initio molecular geometry and normal coordinate analysis of tetrahydrothiophene molecule. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2001, 57, 1405-1415.	2.0	14
14	Ab initio-based kinetics of hydrogen atom abstraction from methyl propionate by H and CH <sub>3</sub> radicals: a biodiesel model. <i>Structural Chemistry</i> , 2021, 32, 1857-1872.	1.0	12
15	Molecular complexes of some anthraquinone anti-cancer drugs: experimental and computational study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2003, 59, 1009-1015.	2.0	11
16	Spectroscopic and quantum chemical studies on the structure of 2-arylquinoline-4(1H)-thione derivatives. <i>Journal of Molecular Structure</i> , 2004, 690, 151-157.	1.8	11
17	Quantum chemical calculations and experimental investigations on 2-aminobenzoic acid-cyclodiphosph(V)azane derivative and its homo-binuclear Cu(II) complex. <i>Journal of Molecular Structure</i> , 2012, 1011, 50-58.	1.8	10
18	Origin of reverse stability of diphosphouracil tautomers compared to their analogue uracil: DFT and ab initio study. <i>Computational and Theoretical Chemistry</i> , 2008, 851, 54-62.	1.5	9

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19	Theoretical and experimental studies on anticancer drug mitoxantrone. Journal of Molecular Structure, 2018, 1173, 837-847.	1.8	8
20	First-principle kinetic studies of unimolecular pyrolysis of isopropyl esters as biodiesel surrogates. Theoretical Chemistry Accounts, 2021, 140, 1.	0.5	8
21	Umbrella inversion and structure of phosphorus-containing compounds: A quantum chemical study. Journal of Theoretical and Computational Chemistry, 2018, 17, 1850042.	1.8	7
22	Oxidation of Methyl Propanoate by the OH Radical. Russian Journal of Physical Chemistry A, 2018, 92, 2476-2484.	0.1	6
23	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
24	Characterization, Hirshfeld surface analysis, DFT study and an in vitro $\alpha$ -glucosidase/ $\alpha$ -amylase/radical scavenging profiling of novel 5-styryl-2-(4-tolylsulfonamido) chalcones. Journal of Molecular Structure, 2021, 1245, 131090.	1.8	5
25	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
26	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
27	Structure and Stability of Chemically Modified DNA Bases: Quantum Chemical Calculations on 16 Isomers of Diphosphocytosine. , 2013, 2013, 1-10.		3
28	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
29	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
30	Synthesis, spectroscopic, thermal and quantum chemical studies on trivalent erbium NO chelating sulfamonomethoxine $\alpha$ -cyclophosph(V)azane complex. Journal of Molecular Structure, 2013, 1048, 202-209.	1.8	2
31	Synthesis, spectral and quantum chemical studies on NO-chelating sulfamonomethoxine $\alpha$ -cyclophosph(V)azane and its Er(III) complex. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 128, 724-729.	2.0	2
32	Adsorption of Cu <sup>2+</sup> and Mg <sup>2+</sup> 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
33	Spectroscopic and Quantum Mechanical Studies of Substituted Anilines and their Charge-Transfer Complexes with Iodine in Different Solvents. Monatshefte für Chemie, 2006, 137, 1027-1042.	0.9	1
34	Quantum chemical studies on the potentially important imidates. Computational and Theoretical Chemistry, 2008, 861, 62-67.	1.5	1
35	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
36	Spectral and quantum chemical studies on 1,3-bis(N1-4-amino-6-methoxypyrimidinebenzenesulfonamide-2,2,4,4-ethane-1,2-dithiol)-2,4-dichlorocyclodiphosph(V)azane and its erbium complex. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 118, 481-487.	2.0	1

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37	A thermochemistry and kinetic study on the thermal decomposition of ethoxyquinoline and ethoxyisoquinoline. <i>International Journal of Chemical Kinetics</i> , 2018, 50, 604-611.	1.0	1
38	Heteroaromatization with 4-phenyldiazenyl-1-naphthol. Part III: One-pot synthesis and DFT study of 4H-naphthopyran derivatives. <i>European Journal of Chemistry</i> , 2017, 8, 358-366.	0.3	0