Mohamed K Awad

List of Publications by Year
in descending order

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68 papers	2,219 citations	257450 24 h-index	233421 45 g-index
68 all docs	68 docs citations	68 times ranked	1932 citing authors

#	Article	IF	Citations
1	Design, synthesis and biological evaluation of novel thiohydantoin derivatives as antiproliferative agents: A combined experimental and theoretical assessments. Journal of Molecular Structure, 2022, 1249, 131574.	3.6	13
2	Molecular dynamic simulation studies and surface characterization of carbon steel corrosion with changing green inhibitors concentrations and temperatures. AEJ - Alexandria Engineering Journal, 2022, 61, 2492-2519.	6.4	16
3	Design, synthesis, and computational explorations of novel 2â€thiohydantoin nucleosides with cytotoxic activities. Journal of Heterocyclic Chemistry, 2022, 59, 664-685.	2.6	7
4	Resorcinol Derivative as an Environmentally Friendly Low Carbon Steel Inhibitor in HCl Medium. ACS Omega, 2022, 7, 17609-17619.	3.5	5
5	Design, synthesis, DFT, molecular modelling studies and biological evaluation of novel 3-substituted (E)-5-(arylidene)-1-methyl-2-thioxoimidazolidin-4-ones with potent cytotoxic activities against breast MCF-7, liver HepG2, and lung A549. Journal of Molecular Structure, 2021, 1229, 129805.	3.6	13
6	Chemical, electrochemical, theoretical (DFT & MEP), thermodynamics and surface morphology studies of carbon steel during gas and oil production using three novel di-cationic amphiphiles as corrosion inhibitors in acidic medium. Journal of Molecular Liquids, 2021, 337, 116541.	4.9	14
7	New N-ribosides and N-mannosides of rhodanine derivatives with anticancer activity on leukemia cell line: Design, synthesis, DFT and molecular modelling studies. Carbohydrate Research, 2020, 487, 107894.	2.3	26
8	Synthesis, molecular modeling, TDâ€DFT, antimicrobial, and in vitro therapeutic activity of new spherical nanoâ€sized sulfonamide imine ligands and their zinc (II) and copper (II) complexes. Applied Organometallic Chemistry, 2020, 34, e5953.	3.5	3
9	New Zn (II) and Cd (II) complexes of 2,4â€dihydroxyâ€5â€[(5â€mercaptoâ€1Hâ€1,2,4â€triazoleâ€3â€yl)diazenyl]benzaldehyde: Synthesis, structural characterization, molecular modeling and docking studies, DNA binding and biological activity. Applied Organometallic Chemistry, 2020, 34, e5635.	3.5	12
10	Molecular docking, molecular modeling, vibrational and biological studies of some new heterocyclic Î±-aminophosphonates. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2019, 206, 78-88.	3.9	27
11	High performance corrosion inhibition of novel tricationic surfactants on carbon steel in formation water: Electrochemical and computational evaluations. Journal of Molecular Liquids, 2018, 262, 363-375.	4.9	43
12	Pd (II) complexes of bidentate chalcone ligands: Synthesis, spectral, thermal, antitumor, antioxidant, antimicrobial, DFT and SAR studies. Journal of Molecular Structure, 2018, 1160, 348-359.	3.6	21
13	Factors Influencing the Potency of Alzheimer Inhibitors: Computational and Docking Studies. American Journal of Alzheimer's Disease and Other Dementias, 2018, 33, 166-175.	1.9	8
14	New Ni(II), Pd(II) and Pt(II) complexes coordinated to azo pyrazolone ligand with a potent antiâ€tumor activity: Synthesis, characterization, DFT and DNA cleavage studies. Applied Organometallic Chemistry, 2018, 32, e4104.	3.5	35
15	Design, synthesis, molecular modeling, and biological evaluation of novel Î±-aminophosphonates based quinazolinone moiety as potential anticancer agents: DFT, NBO and vibrational studies. Journal of Molecular Structure, 2018, 1173, 128-141.	3.6	28
16	Design, Synthesis and Docking study of Novel Imidazolyl Pyrazolopyridine Derivatives as Antitumor Agents Targeting MCF7 Cell Line. Current Organic Synthesis, 2018, 15, 275-285.	1.3	10
17	Synthesis of New Î±-Amino Phosphonates Containing 3-Amino-4(3H) Quinazolinone Moiety as Anticancer and Antimicrobial Agents: DFT, NBO, and Vibrational Studies. Current Organic Synthesis, 2018, 15, 286-296.	1.3	6
18	Design of Piperazine Organoiron Macromolecules with Antibacterial and Anticancer Activity. Macromolecular Chemistry and Physics, 2016, 217, 987-996.	2.2	10

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19	Design of blue fluorescence emitter star-shaped macromolecules based on pyrene and anthracene. Polymer, 2016, 98, 210-228.	3.8	16
20	Quantum chemical studies and atomistic simulations of some inhibitors for the corrosion of al surface. Protection of Metals and Physical Chemistry of Surfaces, 2016, 52, 156-168.	1.1	8
21	Photophysics, photochemistry and thermal stability of diarylethene-containing benzothiazolium species. Journal of Photochemistry and Photobiology A: Chemistry, 2015, 301, 20-31.	3.9	5
22	Experimental and quantum chemical studies of the effect of poly ethylene glycol as corrosion inhibitors of aluminum surface. Journal of Industrial and Engineering Chemistry, 2014, 20, 796-808.	5.8	93
23	Molecular structure of amino alcohols on aluminum surface. Journal of Molecular Structure, 2014, 1063, 51-59.	3.6	11
24	Three novel di-quaternary ammonium salts as corrosion inhibitors for API X65 steel pipeline in acidic solution. Part I: Experimental results. Corrosion Science, 2014, 81, 54-64.	6.6	184
25	Dielectrical, conduction mechanism and thermal properties of rhodanine azodyes. Materials Science in Semiconductor Processing, 2014, 19, 150-162.	4.0	62
26	An assessment to evaluate the validity of different methods for the description of some corrosion inhibitors. Journal of Molecular Modeling, 2014, 20, 2422.	1.8	10
27	Computational simulation of the effect of quantum chemical parameters on the molecular docking of HMG-CoA reductase drugs. Journal of Molecular Structure, 2014, 1075, 311-326.	3.6	35
28	QSAR studies for the computational prediction of HMG-CoA reductase inhibitors by genetic function approximation technique. Canadian Journal of Chemistry, 2013, 91, 263-274.	1.1	5
29	Quantum chemical studies and molecular modeling of the effect of polyethylene glycol as corrosion inhibitors of an aluminum surface. Canadian Journal of Chemistry, 2013, 91, 283-291.	1.1	18
30	MP2 and DFT theoretical studies of the geometry, vibrational and electronic absorption spectra of 2-aminopyrimidine. Research on Chemical Intermediates, 2013, 39, 2741-2761.	2.7	14
31	Aromatic ring size effects on the photophysics and photochemistry of styrylbenzothiazole. Photochemical and Photobiological Sciences, 2013, 12, 1220-1231.	2.9	14
32	Modification of the electric properties of molecular devices via gradual increase of number of nitrogen atoms: A computational study. Organic Electronics, 2012, 13, 807-814.	2.6	3
33	Molecular aggregation and photochemical Z/E isomerization of 1-methy-2-[2-(9-phenantheryl)ethenyl] benzothiazolium iodide. Journal of Photochemistry and Photobiology A: Chemistry, 2011, 222, 276-282.	3.9	7
34	The effect of constitutional and conformational isomerization on the electrical properties of diblock molecular diode. Organic Electronics, 2011, 12, 1080-1092.	2.6	11
35	Effect of Applied Voltage on the Geometrical and Electronic Structures of Dipyrimidinylâ"Diphenyl Diblock as a Molecular Diode: A DFT Study. Journal of Physical Chemistry C, 2010, 114, 21728-21735.	3.1	12
36	DFT theoretical studies of antipyrine Schiff bases as corrosion inhibitors. Materials and Corrosion - Werkstoffe Und Korrosion, 2010, 61, 709-714.	1.5	35

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37	Computational simulation of the molecular structure of some triazoles as inhibitors for the corrosion of metal surface. Computational and Theoretical Chemistry, 2010, 959, 66-74.	1.5	243
38	Synthesis, characterization, and biological activity studies of copper(II)â€“metal(II) binuclear complexes of dipyridylglyoxal bis(2-hydroxybenzoyl hydrazone). Journal of Coordination Chemistry, 2010, 63, 330-345.	2.2	35
39	The role of structural chemistry in the inhibitive performance of some aminopyrimidines on the corrosion of steel. Corrosion Science, 2010, 52, 2387-2396.	6.6	165
40	Theoretical investigation of the inhibition of corrosion by some triazole Schiff bases. Materials and Corrosion - Werkstoffe Und Korrosion, 2009, 60, 813-819.	1.5	44
41	Effect of N-methylation on both ground and excited states properties of 1-(9-anthryl)-2-(2-benzothiazolyl) ethene. Journal of Molecular Structure, 2009, 919, 12-20.	3.6	8
42	Solvatochromism, molecular and electronic structures of trans and cis isomers of a typical styryl pyridinium cyanine dye. Journal of Molecular Structure, 2009, 920, 332-341.	3.6	35
43	Photophysical properties and semiempirical calculations of perylene-3,4,9,10-tetracarboxylic tetramethylester (PTME). Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2008, 71, 1063-1069.	3.9	10
44	Quantum chemical studies on the inhibition of corrosion of copper surface by substituted uracils. Applied Surface Science, 2008, 255, 2433-2441.	6.1	206
45	Mechanism of Water Attacking on Brookerâ€™s Merocyanine Dye and Its Effect on the Molecular and Electronic Structures: Theoretical Study. Bulletin of the Chemical Society of Japan, 2006, 79, 838-844.	3.2	8
46	UVâ€“vis, IR and 1H NMR spectroscopic studies of some mono- and bis-azo-compounds based on 2,7-dihydroxynaphthalene and aniline derivatives. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2005, 62, 980-986.	3.9	5
47	Absorption, fluorescence, and semiempirical ASED-MO studies on a typical Brooker's merocyanine dye. Journal of Molecular Structure, 2005, 754, 16-24.	3.6	35
48	Characterization of synthetic and commercial trisiloxane surfactant materials. Applied Organometallic Chemistry, 2004, 18, 28-38.	3.5	24
49	Investigation of regiospecific oxidative heterocyclization of 2-(Nâ€²-benzylidene) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 267 T 129-138.	1.5	4
50	Semiempirical investigation of the inhibition efficiency of thiourea derivatives as corrosion inhibitors. Journal of Electroanalytical Chemistry, 2004, 567, 219-225.	3.8	98
51	Dual emission of chalcone-analogue dyes emitting in the red region. Chemical Physics, 2004, 303, 317-326.	1.9	60
52	Theoretical investigations of [4Ï€S+2Ï€S] cyclodimerization and stereoselectivity of phthalazin derivatives. Computational and Theoretical Chemistry, 2001, 542, 139-147.	1.5	8
53	Theoretical studies of the effect of structural parameters on the inhibition efficiencies of mercapto-1,2,4-triazoline derivatives. Computational and Theoretical Chemistry, 2000, 531, 105-117.	1.5	41
54	FMO treatment of the reactivity and stereochemistry of the cycloaddition processes using ASED-MO method. Computational and Theoretical Chemistry, 2000, 505, 185-197.	1.5	10

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55	Infrared spectra and molecular orbital studies of hydrogen bonded complexes of 2-chloro-4-nitrobenzoic acid. Journal of Molecular Structure, 1996, 378, 103-110.	3.6	24
56	Infrared spectra and molecular orbital studies of hydrogen bonded complexes of 2-chloro-4-nitrobenzoic acid. Computational and Theoretical Chemistry, 1996, 378, 103-110.	1.5	1
57	Nuclear quadrupole resonance and molecular orbital studies of charge distribution in H-bonded complexes of 2-chloro-4-nitrobenzoic acid. Magnetic Resonance in Chemistry, 1995, 33, 476-480.	1.9	19
58	Thermal stabilities, electronic properties and structures of metformin-metal complexes. Journal of Thermal Analysis, 1995, 44, 1493-1498.	0.6	4
59	Spectral, magnetic studies and molecular orbital calculations for (4,5-dimethyl-3-pyrazolyl)aldazine copper(II) complexes. Transition Metal Chemistry, 1995, 20, 448-453.	1.4	12
60	Effect of alkyl substituents on the thermal degradation of poly(alkyl methacrylate): a molecular orbital study using the ASED-MO method. Polymer Degradation and Stability, 1995, 49, 339-346.	5.8	23
61	Theoretical investigations of the stability of degradation products of polystyrene and poly(4-vinylpyridine). Polymer Degradation and Stability, 1994, 46, 165-170.	5.8	13
62	Effect of protonation on the molecular structure and reactivity of a typical merocyanine dye: experimental and theoretical investigation. The Journal of Physical Chemistry, 1993, 97, 3160-3165.	2.9	27
63	Photodimerization of cyclohexene and methane by decatungstate anions: molecular orbital theory. Journal of the American Chemical Society, 1990, 112, 1603-1606.	13.7	49
64	Ethylidyne on the rhodium(100) surface: a theoretical investigation. Langmuir, 1990, 6, 806-816.	3.5	11
65	Photoactivation of water by p-benzoquinone and the role of manganese(III) complexes in oxygen evolution: molecular orbital theory. Journal of the American Chemical Society, 1989, 111, 802-806.	13.7	24
66	Methane activation by hole sites on AlN: A molecular orbital study. Surface Science, 1989, 218, 543-552.	1.9	10
67	Binding of Ru, O, and RuOn (n=1â€“4) to the Ru(001) surface: Structures, stabilities, and diffusion barriers. Surface Science, 1987, 183, 289-301.	1.9	20
68	Factors determining carbon monoxide adsorption sites on palladium and platinum (100) and (111) surfaces: theoretical study. Journal of the American Chemical Society, 1985, 107, 7854-7857.	13.7	103