Mahmoud A A Ibrahim

List of Publications by Citations

90 papers	1,263 citations	20 h-index	32 g-index
96 ext. papers	1,671 ext. citations	3.7 avg, IF	5.76 L-index

#	Paper	IF	Citations
90	Molecular mechanical study of halogen bonding in drug discovery. *Journal of Computational Chemistry*, **2011**, 32, 2564-74	3.5	171
89	In silico drug discovery of major metabolites from spices as SARS-CoV-2 main protease inhibitors. *Computers in Biology and Medicine*, **2020**, 126, 104046	7	64
88	AMBER empirical potential describes the geometry and energy of noncovalent halogen interactions better than advanced semiempirical quantum mechanical method PM6-DH2X. *Journal of Physical Chemistry B*, **2012**, 116, 3659-69	3.4	61
87	Molecular mechanical perspective on halogen bonding. *Journal of Molecular Modeling*, **2012**, 18, 4625-382		60
86	Repurposing of FDA-approved antivirals, antibiotics, anthelmintics, antioxidants, and cell protectives against SARS-CoV-2 papain-like protease. *Journal of Biomolecular Structure and Dynamics*, **2021**, 39, 5129-5136	3.6	47
85	Synthesis, antiproliferative, anti-tubulin activity, and docking study of new 1,2,4-triazoles as potential combretastatin analogues. *European Journal of Medicinal Chemistry*, **2017**, 141, 293-305	6.8	38
84	Natural-like products as potential SARS-CoV-2 M inhibitors: drug discovery. *Journal of Biomolecular Structure and Dynamics*, **2021**, 39, 5722-5734	3.6	37
83	Performance assessment of semiempirical molecular orbital methods in describing halogen bonding: quantum mechanical and quantum mechanical/molecular mechanical-molecular dynamics study. *Journal of Chemical Information and Modeling*, **2011**, 51, 2549-59	6.1	31
82	Comparison of the molecular dynamics and calculated binding free energies for nine FDA-approved HIV-1 PR drugs against subtype B and C-SA HIV PR. *Chemical Biology and Drug Design*, **2013**, 81, 208-18	2.9	30
81	drug repurposing and molecular dynamics puzzled out potential SARS-CoV-2 main protease inhibitors. *Journal of Biomolecular Structure and Dynamics*, **2021**, 39, 5756-5767	3.6	30
80	Structural insights into the South African HIV-1 subtype C protease: impact of hinge region dynamics and flap flexibility in drug resistance. *Journal of Biomolecular Structure and Dynamics*, **2013**, 31, 1370-80	3.6	29
79	Synthesis of novel 1,2-bis-quinolinyl-1,4-naphthoquinones: ERK2 inhibition, cytotoxicity and molecular docking studies. *Bioorganic Chemistry*, **2018**, 81, 700-712	5.1	29
78	In Silico Evaluation of Prospective Anti-COVID-19 Drug Candidates as Potential SARS-CoV-2 Main Protease Inhibitors. *Protein Journal*, **2021**, 40, 296-309	3.9	28
77	Cembrene Diterpenoids with Ether Linkages from Sarcophyton ehrenbergi: An Anti-Proliferation and Molecular-Docking Assessment. *Marine Drugs*, **2017**, 15,	6	26
76	Rutin and flavone analogs as prospective SARS-CoV-2 main protease inhibitors: In silico drug discovery study. *Journal of Molecular Graphics and Modelling*, **2021**, 105, 107904	2.8	26
75	Design, synthesis and biological evaluation of fused naphthofuro[3,2-c] quinoline-6,7,12-triones and pyrano[3,2-c]quinoline-6,7,8,13-tetraones derivatives as ERK inhibitors with efficacy in BRAF-mutant melanoma. *Bioorganic Chemistry*, **2019**, 82, 290-305	5.1	25
74	In Silico Mining of Terpenes from Red-Sea Invertebrates for SARS-CoV-2 Main Protease (M) Inhibitors. *Molecules*, **2021**, 26,	4.8	24

73	Polarization plays the key role in halogen bonding: a point-of-charge-based quantum mechanical study. *Theoretical Chemistry Accounts*, **2019**, 138, 1	1.9	24
72	Role and nature of halogen bonding in inhibitor???receptor complexes for drug discovery: casein kinase-2 (CK2) inhibition as a case study. *Theoretical Chemistry Accounts*, **2018**, 137, 1	1.9	23
71	Graphene and graphene oxide as adsorbents for cadmium and lead heavy metals: A theoretical investigation. *Applied Surface Science*, **2020**, 507, 145038	6.7	22
70	Unconventional Type III Halogen□□Halogen Interactions: A Quantum Mechanical Elucidation of □Hole□□Hole and Di-□Hole Interactions. *ACS Omega*, **2020**, 5, 21824-21835	3.9	20
69	Quantum-mechanical investigation of tetrel bond characteristics based on the point-of-charge (PoC) approach. *Journal of Molecular Modeling*, **2018**, 24, 219	2	19
68	Comparative investigation of interactions of hydrogen, halogen and tetrel bond donors with electron-rich and electron-deficient □systems.. *RSC Advances*, **2019**, 9, 32811-32820	3.7	19
67	Exploring the Linear Optical Properties of Borazine (B3N3) Doped Graphenes. 0D Flakes vs 2D Sheets. *Journal of Physical Chemistry C*, **2017**, 121, 709-722	3.8	18
66	A new insight for chalcogen bonding based on Point-of-Charge approach. *Phosphorus, Sulfur and Silicon and the Related Elements*, **2019**, 194, 444-454	1	18
65	Kaemgalangol A: Unusual seco-isopimarane diterpenoid from aromatic ginger Kaempferia galanga. *F□oterap*□**2018**, 129, 47-53	3.2	17
64	Comparative investigation of □□ole interactions of carbon-containing molecules with Lewis bases, acids and di-halogens. *Chemical Papers*, **2020**, 74, 3569-3580	1.9	15
63	Establishing the pivotal role of local aromaticity in the electronic properties of boron-nitride graphene lateral hybrids. *Physical Chemistry Chemical Physics*, **2016**, 18, 25315-25328	3.6	15
62	□Hole and Lone-Pair Hole Interactions in Chalcogen-Containing Complexes: A Comparative Study. *ACS Omega*, **2020**, 5, 21631-21640	3.9	15
61	A Computational Investigation of Unconventional Lone-Pair Hole Interactions of Group VI□III Elements. *ChemistrySelect*, **2019**, 4, 5489-5495	1.8	14
60	Blue Biotechnology: Computational Screening of Cembranoid Diterpenes for SARS-CoV-2 Main Protease Inhibition. *Marine Drugs*, **2021**, 19,	6	12
59	Non--Lactam Allosteric Inhibitors Target Methicillin-Resistant : An Drug Discovery Study. *Antibiotics*, **2021**, 10,	4.9	12
58	In Silico Targeting Human Multidrug Transporter ABCG2 in Breast Cancer: Database Screening, Molecular Docking, and Molecular Dynamics Study. *Molecular Informatics*, **2021**, e2060039	3.8	12
57	Prospective Drug Candidates as Human Multidrug Transporter ABCG2 Inhibitors: an In Silico Drug Discovery Study. *Cell Biochemistry and Biophysics*, **2021**, 79, 189-200	3.2	11
56	X-ray characterization, Hirshfeld surface analysis, DFT calculations, in vitro and in silico lipoxygenase inhibition (LOX) studies of dichlorophenyl substituted 3-hydroxy-chromenones. *New Journal of Chemistry*,	3.6	11

55	Sarcoehrenbergilides D-F: cytotoxic cembrene diterpenoids from the soft coral .. *RSC Advances*, **2019**, 9, 27183-27189	3.7	10
54	Identification of novel Plasmodium falciparum PI4KB inhibitors as potential anti-malarial drugs: Homology modeling, molecular docking and molecular dynamics simulations. *Computational Biology and Chemistry*, **2019**, 80, 79-89	3.6	10
53	1,3,4-Thiadiazoles and 1,3-thiazoles from one-pot reaction of bisthioureas with 2-(bis(methylthio)methylene)malononitrile and ethyl 2-cyano-3,3-bis(methylthio)acrylate. *Journal of Sulfur Chemistry*, **2017**, 38, 69-75	2.3	10
52	Hole Interactions: A Comparative Investigation Based on Boron-Containing Molecules. *ChemistrySelect*, **2020**, 5, 13223-13231	1.8	10
51	In Vitro and In Silico Evaluation of Anticancer Activity of New Indole-Based 1,3,4-Oxadiazoles as EGFR and COX-2 Inhibitors. *Molecules*, **2020**, 25,	4.8	9
50	Pigmentosins from sp. as antibiofilm agents and a new glycosylated asperfuran from. *Beilstein Journal of Organic Chemistry*, **2019**, 15, 2968-2981	2.5	9
49	Cospatial Hole and Lone Pair Interactions of Square-Pyramidal Pentavalent Halogen Compounds with Systems: A Quantum Mechanical Study. *ACS Omega*, **2021**, 6, 3319-3329	3.9	9
48	On the Potentiality of X-T-X Compounds (T = C, Si, and Ge, and X = F, Cl, and Br) as Tetrel- and Halogen-Bond Donors. *ACS Omega*, **2021**, 6, 19330-19341	3.9	8
47	External electric field effects on the hole and lone-pair hole interactions of group V elements: a comparative investigation.. *RSC Advances*, **2021**, 11, 4022-4034	3.7	8
46	Comparison of hole and R hole interactions formed by tetrel-containing complexes: a computational study.. *RSC Advances*, **2021**, 11, 4011-4021	3.7	8
45	Prospective new amidinothiazoles as leukotriene B4 inhibitors. *Journal of Molecular Structure*, **2019** , 1175, 414-427	3.4	7
44	Design, Synthesis, and Molecular Docking of Paracyclophanyl-Thiazole Hybrids as Novel CDK1 Inhibitors and Apoptosis Inducing Anti-Melanoma Agents. *Molecules*, **2020**, 25,	4.8	7
43	Anti-Viral and Immunomodulatory Properties of Propolis: Chemical Diversity, Pharmacological Properties, Preclinical and Clinical Applications, and In Silico Potential against SARS-CoV-2. *Foods*, **2021**, 10,	4.9	7
42	Azines from one-pot reaction of thiosemicarbazones. *Journal of Sulfur Chemistry*, **2017**, 38, 11-17	2.3	6
41	Exploring Toxins for Hunting SARS-CoV-2 Main Protease Inhibitors: Molecular Docking, Molecular Dynamics, Pharmacokinetic Properties, and Reactome Study.. *Pharmaceuticals*, **2022**, 15,	5.2	6
40	hole interactions of group III VI elements with systems and Lewis bases: a comparative study. *Structural Chemistry*,1	1.8	6
39	Comparative Modeling and Evaluation of Leukotriene B4 Receptors for Selective Drug Discovery Towards the Treatment of Inflammatory Diseases. *Protein Journal*, **2018**, 37, 518-530	3.9	5
38	Euphosantianane A?D: Antiproliferative Premyrsinane Diterpenoids from the Endemic Egyptian Plant. *Molecules*, **2018**, 23,	4.8	5

37	Chemical constituents from coconut waste and their evaluation as potential antiviral agents against SARS-CoV-2. *South African Journal of Botany*, **2021**, 141, 278-289	2.9	5
36	Efficient ab initio quantum mechanical simulations of structural stability and vibrational properties of bulk, monolayer and (n,0) nanotubes: Yttrium sesquioxide Y2O3. *Journal of Raman Spectroscopy*, **2020**, 51, 232-242	2.3	4
35	Carotane sesquiterpenes from : analysis as SARS-CoV-2 binding inhibitors.. *RSC Advances*, **2020**, 10, 34541-34548	3.7	4
34	Elucidating the adsorption and detection of amphetamine drug by pure and doped Al12N12, and Al12P12nano-cages, a DFT study. *Journal of Molecular Liquids*, **2021**, 326, 115297	6	4
33	Synthesis of potentially new schiff bases of -substituted-2-quinolonylacetohydrazides as anti-COVID-19 agents. *Journal of Molecular Structure*, **2021**, 1230, 129649	3.4	4
32	Two novel oxetane containing lignans and a new megastigmane from and analysis of them as prospective SARS-CoV-2 inhibitors.. *RSC Advances*, **2021**, 11, 20151-20163	3.7	4
31	Synthesis, X-ray diffraction analysis, quantum chemical studies and □-amylase inhibition of probenecid derived S-alkylphthalimide-oxadiazole-benzenesulfonamide hybrids. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2022**, 37, 1464-1478	5.6	4
30	Unexpected favourable noncovalent interaction between chlorine oxyanions (ClOx□x = 1□4) and benzene: Benchmarking DFT and SAPT methods with respect to CCSD(T). *Computational and Theoretical Chemistry*, **2021**, 1199, 113214	2	3
29	Repurposing potential of posaconazole and grazoprevir as inhibitors of SARS-CoV-2 helicase. *Scientific Reports*, **2021**, 11, 10290	4.9	3
28	Multi-Subunit SARS-CoV-2 Vaccine Design Using Evolutionarily Conserved T- and B- Cell Epitopes. *Vaccines*, **2021**, 9,	5.3	3
27	Effect of External Electric Field on Tetrel Bonding Interactions in (FTF□□FH) Complexes (T = C, Si, Ge, and Sn). *ACS Omega*, **2021**, 6, 25476-25485	3.9	3
26	Selective SIRT2 inhibitors as promising anticancer therapeutics: An update from 2016 to 2020. *European Journal of Medicinal Chemistry*, **2021**, 224, 113709	6.8	3
25	Naturally occurring plant-based anticancerous candidates as prospective ABCG2 inhibitors: an in silico drug discovery study.. *Molecular Diversity*, **2022**, 1	3.1	3
24	Regio- and stereoselective 1,3-dipolar cycloaddition reactions of C-aryl (or hetaryl)-N-phenylnitrones to monosubstituted ylidene malononitriles and 4-benzylidene-2-phenyloxazol-5(4H)-one. *Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences*, **2017**, 72, 317-326	1	2
23	A Facile Synthesis of Oxoindenothiazine and Dioxospiro(indene-2,4?-thiazine) Derivatives from (Substituted ethylidene)hydrazinecarbothioamides. *Journal of Heterocyclic Chemistry*, **2015**, 52, 1201-1207	1.9	2
22	Unusual chalcogen?chalcogen interactions in like?like and unlike Y?C?Y?Y?C?Y complexes (Y = O, S, and Se).. *Physical Chemistry Chemical Physics*, **2022**,	3.6	2
21	Phenyl-Modified Carbon Nitride Quantum Nanoflakes for Ultra-Highly Selective Sensing of Formic Acid: A Combined Experimental by QCM and Density Functional Theory Study. *ACS Applied Materials & Interfaces*, **2021**, 13, 48595-48610	9.5	2
20	Reaction of N,N-disubstituted hydrazinecarbothioamides with 2-bromo-2-substituted acetophenones. *Arkivoc*, **2019**, 2018, 102-111	0.9	2

19	Synthesis of 3,3Qmethylenebis(4-hydroxyquinolin-2(1H)-ones) of prospective anti-COVID-19 drugs. *Molecular Diversity*, **2021**, 25, 461-471	3.1	2
18	Exploring Natural Product Activity and Species Source Candidates for Hunting ABCB1 Transporter Inhibitors: An In Silico Drug Discovery Study. *Molecules*, **2022**, 27, 3104	4.8	2
17	Hole Interactions of Tetrahedral Group IVVIII Lewis Acid Centers with Lewis Bases: A Comparative Study. *ChemistrySelect*, **2021**, 6, 11856-11864	1.8	1
16	R-hole interactions of group IV-VII radical-containing molecules: A comparative study. *Journal of Molecular Graphics and Modelling*, **2021**, 111, 108097	2.8	1
15	Adsorption of chlorine oxyanions, as water disinfectant by-products, on graphene flakes: A quantum chemical investigation. *Surfaces and Interfaces*, **2021**, 28, 101601	4.1	1
14	Gastroprotection against Rat Ulcers by Sterol Derivative. *Biomolecules*, **2021**, 11,	5.9	1
13	Anti-tumor metabolites from Synadenium grantii Hook F.. *Medicinal Chemistry Research*, **2022**, 31, 666-673	2.2	1
12	Unexplored Hole and Hole Interactions in (X2CY)2 Complexes (X = F, Cl; Y = O, S). *Journal of Molecular Structure*, **2022**, 133232	3.4	1
11	One-pot synthesis, theoretical study and antimicrobial activity of 5,5?-(1,4-phenylenebis-(methanylylidene))Bis(3-Aryl(Alkyl)-2-thioxoimidazolidin-4-one) derivatives. *Phosphorus, Sulfur and Silicon and the Related Elements*, **2019**, 194, 147-155	1	0
10	NS3 helicase inhibitory potential of the marine sponge .. *RSC Advances*, **2022**, 12, 2992-3002	3.7	0
9	Glioma-Targeted Therapeutics: Computer-Aided Drug Design Prospective. *Protein Journal*, **2021**, 40, 601-655	3.9	0
8	Hole and LP-Hole Interactions of PnicogenPnicogen Homodimers under the External Electric Field Effect: A Quantum Mechanical Study.. *ACS Omega*, **2022**, 7, 11264-11275	3.9	0
7	Plant cell cultures: An enzymatic tool for polyphenolic and flavonoid transformations.. *Phytomedicine*, **2022**, 100, 154019	6.5	0
6	Flavonoids of Zinnia elegans: Chemical profile and, in vitro antioxidant and in silico anti-COVID-19 activities. *South African Journal of Botany*, **2022**, 147, 576-585	2.9	0
5	Design, Synthesis, Crystal Structures, Computational Studies, in vitro and in silico Monoamine Oxidase-A&B Inhibitory Activity of Two Novel S-Benzyl Dithiocarbamates. *Journal of Molecular Structure*, **2022**, 133317	3.4	0
4	Prioritizing the Catalytic Gatekeepers through Pan- Inhibitory Mechanism of Entrectinib against ALK, ROS1 and TRKA Tyrosine Kinases.. *Cell Biochemistry and Biophysics*, **2022**, 1	3.2	
3	Computer-based identification of olive oil components as a potential inhibitor of neirisaral adhesion a regulatory protein.. *Journal of Biomolecular Structure and Dynamics*, **2022**, 1-8	3.6	
2	Production of Dual Inhibitory Hydrolysate by Enzymatic Hydrolysis of Squid Processing By-product.. *Marine Biotechnology*, **2022**, 24, 293	3.4	

1	Versisterol, a new endophytic steroid with 3CL protease inhibitory activity from (Forssk.) Vierh.. *RSC Advances*, **2022**, 12, 12583-12589	3.7