

Mahmoud A A Ibrahim

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	NS3 helicase inhibitory potential of the marine sponge .. <i>RSC Advances</i> , 2022 , 12, 2992-3002	3.7	0
89	Prioritizing the Catalytic Gatekeepers through Pan- Inhibitory Mechanism of Entrectinib against ALK, ROS1 and TRKA Tyrosine Kinases.. <i>Cell Biochemistry and Biophysics</i> , 2022 , 1	3.2	
88	Computer-based identification of olive oil components as a potential inhibitor of neirisaral adhesion a regulatory protein.. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022 , 1-8	3.6	
87	Exploring Toxins for Hunting SARS-CoV-2 Main Protease Inhibitors: Molecular Docking, Molecular Dynamics, Pharmacokinetic Properties, and Reactome Study.. <i>Pharmaceuticals</i> , 2022 , 15,	5.2	6
86	Unusual chalcogen?chalcogen interactions in like?like and unlike Y?C?Y?Y?C?Y complexes (Y = O, S, and Se).. <i>Physical Chemistry Chemical Physics</i> , 2022 ,	3.6	2
85	Naturally occurring plant-based anticancerous candidates as prospective ABCG2 inhibitors: an in silico drug discovery study.. <i>Molecular Diversity</i> , 2022 , 1	3.1	3
84	π-Hole and LP-Hole Interactions of Pnicogen□□Pnicogen Homodimers under the External Electric Field Effect: A Quantum Mechanical Study.. <i>ACS Omega</i> , 2022 , 7, 11264-11275	3.9	0
83	Production of Dual Inhibitory Hydrolysate by Enzymatic Hydrolysis of Squid Processing By-product.. <i>Marine Biotechnology</i> , 2022 , 24, 293	3.4	
82	Anti-tumor metabolites from <i>Synadenium grantii</i> Hook F.. <i>Medicinal Chemistry Research</i> , 2022 , 31, 666-673	3.2	1
81	Plant cell cultures: An enzymatic tool for polyphenolic and flavonoid transformations.. <i>Phytomedicine</i> , 2022 , 100, 154019	6.5	0
80	Flavonoids of <i>Zinnia elegans</i> : Chemical profile and, in vitro antioxidant and in silico anti-COVID-19 activities. <i>South African Journal of Botany</i> , 2022 , 147, 576-585	2.9	0
79	Versisterol, a new endophytic steroid with 3CL protease inhibitory activity from (Forssk.) Vierh.. <i>RSC Advances</i> , 2022 , 12, 12583-12589	3.7	
78	Unexplored π-Hole and σ-Hole Interactions in (X2CY)2 Complexes (X = F, Cl; Y = O, S). <i>Journal of Molecular Structure</i> , 2022 , 133232	3.4	1
77	Exploring Natural Product Activity and Species Source Candidates for Hunting ABCB1 Transporter Inhibitors: An In Silico Drug Discovery Study. <i>Molecules</i> , 2022 , 27, 3104	4.8	2
76	Design, Synthesis, Crystal Structures, Computational Studies, in vitro and in silico Monoamine Oxidase-A&B Inhibitory Activity of Two Novel S-Benzyl Dithiocarbamates. <i>Journal of Molecular Structure</i> , 2022 , 133317	3.4	0
75	Synthesis, X-ray diffraction analysis, quantum chemical studies and π-amylase inhibition of probenecid derived S-alkylphthalimide-oxadiazole-benzenesulfonamide hybrids. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2022 , 37, 1464-1478	5.6	4
74	Repurposing of FDA-approved antivirals, antibiotics, anthelmintics, antioxidants, and cell protectives against SARS-CoV-2 papain-like protease. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021 , 39, 5129-5136	3.6	47

73	Natural-like products as potential SARS-CoV-2 M inhibitors: drug discovery. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021 , 39, 5722-5734	3.6	37
72	σ-Hole Interactions of Tetrahedral Group IV/III Lewis Acid Centers with Lewis Bases: A Comparative Study. <i>ChemistrySelect</i> , 2021 , 6, 11856-11864	1.8	1
71	R-hole interactions of group IV-VII radical-containing molecules: A comparative study. <i>Journal of Molecular Graphics and Modelling</i> , 2021 , 111, 108097	2.8	1
70	Adsorption of chlorine oxyanions, as water disinfectant by-products, on graphene flakes: A quantum chemical investigation. <i>Surfaces and Interfaces</i> , 2021 , 28, 101601	4.1	1
69	Phenyl-Modified Carbon Nitride Quantum Nanoflakes for Ultra-Highly Selective Sensing of Formic Acid: A Combined Experimental by QCM and Density Functional Theory Study. <i>ACS Applied Materials & Interfaces</i> , 2021 , 13, 48595-48610	9.5	2
68	drug repurposing and molecular dynamics puzzled out potential SARS-CoV-2 main protease inhibitors. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021 , 39, 5756-5767	3.6	30
67	Elucidating the adsorption and detection of amphetamine drug by pure and doped Al ₁₂ N ₁₂ , and Al ₁₂ P ₁₂ nano-cages, a DFT study. <i>Journal of Molecular Liquids</i> , 2021 , 326, 115297	6	4
66	In Silico Mining of Terpenes from Red-Sea Invertebrates for SARS-CoV-2 Main Protease (M) Inhibitors. <i>Molecules</i> , 2021 , 26,	4.8	24
65	Prospective Drug Candidates as Human Multidrug Transporter ABCG2 Inhibitors: an In Silico Drug Discovery Study. <i>Cell Biochemistry and Biophysics</i> , 2021 , 79, 189-200	3.2	11
64	Unexpected favourable noncovalent interaction between chlorine oxyanions (ClO _x ^{-x} = 1-3) and benzene: Benchmarking DFT and SAPT methods with respect to CCSD(T). <i>Computational and Theoretical Chemistry</i> , 2021 , 1199, 113214	2	3
63	Repurposing potential of posaconazole and grazoprevir as inhibitors of SARS-CoV-2 helicase. <i>Scientific Reports</i> , 2021 , 11, 10290	4.9	3
62	Rutin and flavone analogs as prospective SARS-CoV-2 main protease inhibitors: In silico drug discovery study. <i>Journal of Molecular Graphics and Modelling</i> , 2021 , 105, 107904	2.8	26
61	Multi-Subunit SARS-CoV-2 Vaccine Design Using Evolutionarily Conserved T- and B- Cell Epitopes. <i>Vaccines</i> , 2021 , 9,	5.3	3
60	Anti-Viral and Immunomodulatory Properties of Propolis: Chemical Diversity, Pharmacological Properties, Preclinical and Clinical Applications, and In Silico Potential against SARS-CoV-2. <i>Foods</i> , 2021 , 10,	4.9	7
59	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. <i>ACS Omega</i> , 2021 , 6, 19330-19341	3.9	8
58	Synthesis of potentially new schiff bases of -substituted-2-quinolonylaceto hydrazides as anti-COVID-19 agents. <i>Journal of Molecular Structure</i> , 2021 , 1230, 129649	3.4	4
57	Synthesis of 3,3'-methylenebis(4-hydroxyquinolin-2(1H)-ones) of prospective anti-COVID-19 drugs. <i>Molecular Diversity</i> , 2021 , 25, 461-471	3.1	2
56	In Silico Evaluation of Prospective Anti-COVID-19 Drug Candidates as Potential SARS-CoV-2 Main Protease Inhibitors. <i>Protein Journal</i> , 2021 , 40, 296-309	3.9	28

55	External electric field effects on the σ hole and lone-pair hole interactions of group V elements: a comparative investigation.. <i>RSC Advances</i> , 2021 , 11, 4022-4034	3.7	8
54	Two novel oxetane containing lignans and a new megastigmane from and analysis of them as prospective SARS-CoV-2 inhibitors.. <i>RSC Advances</i> , 2021 , 11, 20151-20163	3.7	4
53	Blue Biotechnology: Computational Screening of Cembranoid Diterpenes for SARS-CoV-2 Main Protease Inhibition. <i>Marine Drugs</i> , 2021 , 19,	6	12
52	Non-Lactam Allosteric Inhibitors Target Methicillin-Resistant : An Drug Discovery Study. <i>Antibiotics</i> , 2021 , 10,	4.9	12
51	Gastroprotection against Rat Ulcers by Sterol Derivative. <i>Biomolecules</i> , 2021 , 11,	5.9	1
50	Effect of External Electric Field on Tetrel Bonding Interactions in (FTF \cdots FH) Complexes (T = C, Si, Ge, and Sn). <i>ACS Omega</i> , 2021 , 6, 25476-25485	3.9	3
49	Chemical constituents from coconut waste and their evaluation as potential antiviral agents against SARS-CoV-2. <i>South African Journal of Botany</i> , 2021 , 141, 278-289	2.9	5
48	In Silico Targeting Human Multidrug Transporter ABCG2 in Breast Cancer: Database Screening, Molecular Docking, and Molecular Dynamics Study. <i>Molecular Informatics</i> , 2021 , e2060039	3.8	12
47	Glioma-Targeted Therapeutics: Computer-Aided Drug Design Prospective. <i>Protein Journal</i> , 2021 , 40, 601-655	3.9	0
46	Selective SIRT2 inhibitors as promising anticancer therapeutics: An update from 2016 to 2020. <i>European Journal of Medicinal Chemistry</i> , 2021 , 224, 113709	6.8	3
45	Comparison of σ hole and π hole interactions formed by tetrel-containing complexes: a computational study.. <i>RSC Advances</i> , 2021 , 11, 4011-4021	3.7	8
44	Cospatial σ Hole and Lone Pair Interactions of Square-Pyramidal Pentavalent Halogen Compounds with π Systems: A Quantum Mechanical Study. <i>ACS Omega</i> , 2021 , 6, 3319-3329	3.9	9
43	Comparative investigation of π σ hole interactions of carbon-containing molecules with Lewis bases, acids and di-halogens. <i>Chemical Papers</i> , 2020 , 74, 3569-3580	1.9	15
42	Efficient ab initio quantum mechanical simulations of structural stability and vibrational properties of bulk, monolayer and (n,0) nanotubes: Yttrium sesquioxide Y ₂ O ₃ . <i>Journal of Raman Spectroscopy</i> , 2020 , 51, 232-242	2.3	4
41	Graphene and graphene oxide as adsorbents for cadmium and lead heavy metals: A theoretical investigation. <i>Applied Surface Science</i> , 2020 , 507, 145038	6.7	22
40	In silico drug discovery of major metabolites from spices as SARS-CoV-2 main protease inhibitors. <i>Computers in Biology and Medicine</i> , 2020 , 126, 104046	7	64
39	π σ Hole Interactions: A Comparative Investigation Based on Boron-Containing Molecules. <i>ChemistrySelect</i> , 2020 , 5, 13223-13231	1.8	10
38	Design, Synthesis, and Molecular Docking of Paracyclophanyl-Thiazole Hybrids as Novel CDK1 Inhibitors and Apoptosis Inducing Anti-Melanoma Agents. <i>Molecules</i> , 2020 , 25,	4.8	7

37	In Vitro and In Silico Evaluation of Anticancer Activity of New Indole-Based 1,3,4-Oxadiazoles as EGFR and COX-2 Inhibitors. <i>Molecules</i> , 2020 , 25,	4.8	9
36	Carotane sesquiterpenes from : analysis as SARS-CoV-2 binding inhibitors.. <i>RSC Advances</i> , 2020 , 10, 34541-34548	3.7	15
35	Hole and Lone-Pair Hole Interactions in Chalcogen-Containing Complexes: A Comparative Study. <i>ACS Omega</i> , 2020 , 5, 21631-21640	3.9	15
34	Unconventional Type III Halogen-Halogen Interactions: A Quantum Mechanical Elucidation of H-Hole-Hole and Di-Hole Interactions. <i>ACS Omega</i> , 2020 , 5, 21824-21835	3.9	20
33	Sarcoehrenbergilides D-F: cytotoxic cembrene diterpenoids from the soft coral .. <i>RSC Advances</i> , 2019 , 9, 27183-27189	3.7	10
32	A Computational Investigation of Unconventional Lone-Pair Hole Interactions of Group V-VIII Elements. <i>ChemistrySelect</i> , 2019 , 4, 5489-5495	1.8	14
31	Identification of novel Plasmodium falciparum PI4KB inhibitors as potential anti-malarial drugs: Homology modeling, molecular docking and molecular dynamics simulations. <i>Computational Biology and Chemistry</i> , 2019 , 80, 79-89	3.6	10
30	One-pot synthesis, theoretical study and antimicrobial activity of 5,5?-(1,4-phenylenebis-(methanylylidene))Bis(3-Aryl(Alkyl)-2-thioxoimidazolidin-4-one) derivatives. <i>Phosphorus, Sulfur and Silicon and the Related Elements</i> , 2019 , 194, 147-155	1	0
29	Prospective new amidinothiazoles as leukotriene B4 inhibitors. <i>Journal of Molecular Structure</i> , 2019 , 1175, 414-427	3.4	7
28	Pigmentosins from sp. as antibiofilm agents and a new glycosylated asperfuran from. <i>Beilstein Journal of Organic Chemistry</i> , 2019 , 15, 2968-2981	2.5	9
27	Comparative investigation of interactions of hydrogen, halogen and tetrel bond donors with electron-rich and electron-deficient E-systems.. <i>RSC Advances</i> , 2019 , 9, 32811-32820	3.7	19
26	A new insight for chalcogen bonding based on Point-of-Charge approach. <i>Phosphorus, Sulfur and Silicon and the Related Elements</i> , 2019 , 194, 444-454	1	18
25	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. <i>Bioorganic Chemistry</i> , 2019 , 82, 290-305	5.1	25
24	Reaction of N,N-disubstituted hydrazinecarbothioamides with 2-bromo-2-substituted acetophenones. <i>Arkivoc</i> , 2019 , 2018, 102-111	0.9	2
23	Polarization plays the key role in halogen bonding: a point-of-charge-based quantum mechanical study. <i>Theoretical Chemistry Accounts</i> , 2019 , 138, 1	1.9	24
22	Role and nature of halogen bonding in inhibitor-receptor complexes for drug discovery: casein kinase-2 (CK2) inhibition as a case study. <i>Theoretical Chemistry Accounts</i> , 2018 , 137, 1	1.9	23
21	Kaemgalangol A: Unusual seco-isopimarane diterpenoid from aromatic ginger Kaempferia galanga. <i>Phytotherapy Research</i> , 2018 , 129, 47-53	3.2	17
20	Quantum-mechanical investigation of tetrel bond characteristics based on the point-of-charge (PoC) approach. <i>Journal of Molecular Modeling</i> , 2018 , 24, 219	2	19

19	Comparative Modeling and Evaluation of Leukotriene B4 Receptors for Selective Drug Discovery Towards the Treatment of Inflammatory Diseases. <i>Protein Journal</i> , 2018 , 37, 518-530	3.9	5
18	Euphosantianane A?D: Antiproliferative Premyrsinane Diterpenoids from the Endemic Egyptian Plant. <i>Molecules</i> , 2018 , 23,	4.8	5
17	Synthesis of novel 1,2-bis-quinolinyl-1,4-naphthoquinones: ERK2 inhibition, cytotoxicity and molecular docking studies. <i>Bioorganic Chemistry</i> , 2018 , 81, 700-712	5.1	29
16	Regio- and stereoselective 1,3-dipolar cycloaddition reactions of C-aryl (or hetaryl)-N-phenylnitrones to monosubstituted yliden malononitriles and 4-benzylidene-2-phenyloxazol-5(4H)-one. <i>Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences</i> , 2017 , 72, 317-326	1	2
15	Exploring the Linear Optical Properties of Borazine (B3N3) Doped Graphenes. 0D Flakes vs 2D Sheets. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 709-722	3.8	18
14	Synthesis, antiproliferative, anti-tubulin activity, and docking study of new 1,2,4-triazoles as potential combretastatin analogues. <i>European Journal of Medicinal Chemistry</i> , 2017 , 141, 293-305	6.8	38
13	Cembrene Diterpenoids with Ether Linkages from <i>Sarcophyton ehrenbergi</i> : An Anti-Proliferation and Molecular-Docking Assessment. <i>Marine Drugs</i> , 2017 , 15,	6	26
12	1,3,4-Thiadiazoles and 1,3-thiazoles from one-pot reaction of bistioureas with 2-(bis(methylthio)methylene)malononitrile and ethyl 2-cyano-3,3-bis(methylthio)acrylate. <i>Journal of Sulfur Chemistry</i> , 2017 , 38, 69-75	2.3	10
11	Azines from one-pot reaction of thiosemicarbazones. <i>Journal of Sulfur Chemistry</i> , 2017 , 38, 11-17	2.3	6
10	Establishing the pivotal role of local aromaticity in the electronic properties of boron-nitride graphene lateral hybrids. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 25315-25328	3.6	15
9	A Facile Synthesis of Oxoindeno[2,3-b]thiazine and Dioxospiro(indene-2,4'-thiazine) Derivatives from (Substituted ethylidene)hydrazinecarbothioamides. <i>Journal of Heterocyclic Chemistry</i> , 2015 , 52, 1201-1207	1.7	2
8	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. <i>Chemical Biology and Drug Design</i> , 2013 , 81, 208-18	2.9	30
7	Structural insights into the South African HIV-1 subtype C protease: impact of hinge region dynamics and flap flexibility in drug resistance. <i>Journal of Biomolecular Structure and Dynamics</i> , 2013 , 31, 1370-80	3.6	29
6	Molecular mechanical perspective on halogen bonding. <i>Journal of Molecular Modeling</i> , 2012 , 18, 4625-38	2	60
5	AMBER empirical potential describes the geometry and energy of noncovalent halogen interactions better than advanced semiempirical quantum mechanical method PM6-DH2X. <i>Journal of Physical Chemistry B</i> , 2012 , 116, 3659-69	3.4	61
4	Performance assessment of semiempirical molecular orbital methods in describing halogen bonding: quantum mechanical and quantum mechanical/molecular mechanical-molecular dynamics study. <i>Journal of Chemical Information and Modeling</i> , 2011 , 51, 2549-59	6.1	31
3	Molecular mechanical study of halogen bonding in drug discovery. <i>Journal of Computational Chemistry</i> , 2011 , 32, 2564-74	3.5	171
2	X-ray characterization, Hirshfeld surface analysis, DFT calculations, in vitro and in silico lipoygenase inhibition (LOX) studies of dichlorophenyl substituted 3-hydroxy-chromenones. <i>New Journal of Chemistry</i> ,	3.6	11

1	Whole interactions of group III-VI elements with π -systems and Lewis bases: a comparative study. <i>Structural Chemistry</i> , 1	1.8	6
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