

Khaled M Elokely

List of Publications by Year in descending order

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papers

756
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687363

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38
times ranked

1417
citing authors

#	ARTICLE	IF	CITATIONS
1	Docking Challenge: Protein Sampling and Molecular Docking Performance. <i>Journal of Chemical Information and Modeling</i> , 2013, 53, 1934-1945.	5.4	194
2	Understanding TRPV1 activation by ligands: Insights from the binding modes of capsaicin and resiniferatoxin. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2016, 113, E137-45.	7.1	127
3	Inhibition of human monoamine oxidase A and B by flavonoids isolated from two Algerian medicinal plants. <i>Phytomedicine</i> , 2018, 40, 27-36.	5.3	58
4	Isolation of Acacetin from <i>Calea urticifolia</i> with Inhibitory Properties against Human Monoamine Oxidase-A and -B. <i>Journal of Natural Products</i> , 2016, 79, 2538-2544.	3.0	32
5	The Resurrection of Phenotypic Drug Discovery. <i>ACS Medicinal Chemistry Letters</i> , 2020, 11, 1820-1828.	2.8	26
6	Targeting SARS-CoV-2 M3CLpro by HCV NS3/4a Inhibitors: <i>In Silico</i> Modeling and <i>In Vitro</i> Screening. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 1020-1032.	5.4	25
7	Molecular mechanisms of the antitumor activity of SB225002: A novel microtubule inhibitor. <i>Biochemical Pharmacology</i> , 2013, 85, 1741-1752.	4.4	23
8	Allosteric inhibitors of the main protease of SARS-CoV-2. <i>Antiviral Research</i> , 2022, 205, 105381.	4.1	23
9	Flavonoids from <i>Perovskia atriplicifolia</i> and Their <i>In Vitro</i> Displacement of the Respective Radioligands for Human Opioid and Cannabinoid Receptors. <i>Journal of Natural Products</i> , 2015, 78, 1461-1465.	3.0	21
10	Clotrimazole-cyclodextrin based approach for the management and treatment of <i>Candidiasis</i> – A formulation and chemistry-based evaluation. <i>Pharmaceutical Development and Technology</i> , 2016, 21, 619-629.	2.4	20
11	Drug activity prediction using multiple-instance learning via joint instance and feature selection. <i>BMC Bioinformatics</i> , 2013, 14, S16.	2.6	18
12	Stress-Based Production, and Characterization of Glutathione Peroxidase and Glutathione S-Transferase Enzymes From <i>Lactobacillus plantarum</i> . <i>Frontiers in Bioengineering and Biotechnology</i> , 2020, 8, 78.	4.1	17
13	A Mitochondrial-targeted purine-based HSP90 antagonist for leukemia therapy. <i>Oncotarget</i> , 2017, 8, 112184-112198.	1.8	17
14	Asphodosides A-E, anti-MRSA metabolites from <i>Asphodelus microcarpus</i> . <i>Phytochemistry</i> , 2014, 105, 79-84.	2.9	13
15	Bioactivity-Guided Isolation of Potential Antidiabetic and Antihyperlipidemic Compounds from <i>Trigonella stellata</i> . <i>Journal of Natural Products</i> , 2018, 81, 1154-1161.	3.0	12
16	Discovery of Novel Small-Molecule Inhibitors of SARS-CoV-2 Main Protease as Potential Leads for COVID-19 Treatment. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 4745-4757.	5.4	12
17	Antiurease activity of plants growing in the Czech Republic. <i>Natural Product Research</i> , 2014, 28, 868-873.	1.8	11
18	Proposed Mechanism for the Antitrypanosomal Activity of Quercetin and Myricetin Isolated from <i>Hypericum afrum</i> Lam.: <i>Phytochemistry, In Vitro Testing and Modeling Studies</i> . <i>Molecules</i> , 2021, 26, 1009.	3.8	11

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19	Isolation and characterization of new secondary metabolites from <i>Asphodelus microcarpus</i> . <i>Medicinal Chemistry Research</i> , 2014, 23, 3510-3515.	2.4	10
20	Design, synthesis and SAR of new-di-substituted pyridopyrimidines as ATP-competitive dual PI3K α /mTOR inhibitors. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2017, 27, 3117-3122.	2.2	10
21	Computationally Assisted Assignment of Kahalalide Y Configuration Using an NMR-Constrained Conformational Search. <i>Journal of Natural Products</i> , 2013, 76, 178-185.	3.0	9
22	Anti-inflammatory of pyrrolizidine alkaloids from <i>Heliotropium digynum</i> . <i>Medicinal Chemistry Research</i> , 2018, 27, 1066-1073.	2.4	9
23	Fluorescence Spectrometric Determination of Drugs Containing -Methylene Sulfone/Sulfonamide Functional Groups Using ¹ N-Methylnicotinamide Chloride as a Fluorogenic Agent. <i>International Journal of Analytical Chemistry</i> , 2011, 2011, 1-9.	1.0	8
24	Discovery and SAR of Novel Disubstituted Quinazolines as Dual PI3K α /mTOR Inhibitors Targeting Breast Cancer. <i>ACS Medicinal Chemistry Letters</i> , 2020, 11, 2156-2164.	2.8	8
25	Bioactive products from singlet oxygen photooxygenation of cannabinoids. <i>European Journal of Medicinal Chemistry</i> , 2018, 143, 983-996.	5.5	7
26	Structure-Activity Relationships of the Antimalarial Agent Artemisinin 10. Synthesis and Antimalarial Activity of Enantiomers of rac-5 ¹ -Hydroxy-d-Secoartemisinin and Analogs: Implications Regarding the Mechanism of Action. <i>Molecules</i> , 2021, 26, 4163.	3.8	6
27	Evaluation and understanding the molecular basis of the antimethicillin-resistant <i>Staphylococcus aureus</i> activity of secondary metabolites isolated from <i>Lamium amplexicaule</i> . <i>Pharmacognosy Magazine</i> , 2018, 14, 3.	0.6	6
28	Microbial Oxidation of the Fusidic Acid Side Chain by <i>Cunninghamella echinulata</i> . <i>Molecules</i> , 2018, 23, 970.	3.8	5
29	Computationally Assisted Lead Optimization of Novel Potent and Selective MAO-B Inhibitors. <i>Biomedicines</i> , 2021, 9, 1304.	3.2	5
30	Discovery of novel class of histone deacetylase inhibitors as potential anticancer agents. <i>Bioorganic and Medicinal Chemistry</i> , 2021, 42, 116251.	3.0	4
31	New Glycosides and Trypanocidal Metabolites from <i>Vangueria edulis</i> . <i>Natural Product Communications</i> , 2015, 10, 1934578X1501001.	0.5	3
32	Ketone Analog of Caffeic Acid Phenethyl Ester Exhibits Antioxidant Activity via Activation of ERK-Dependent Nrf2 Pathway. <i>Applied Sciences (Switzerland)</i> , 2022, 12, 3062.	2.5	2
33	Potential Pro-Inflammatory Effect of Vitamin E Analogs through Mitigation of Tetrahydrocannabinol (THC) Binding to the Cannabinoid 2 Receptor. <i>International Journal of Molecular Sciences</i> , 2022, 23, 4291.	4.1	2
34	Fluorometric Determination of Drugs Containing α -Methylene Sulfoxide Functional Groups Using -Methylnicotinamide Chloride as a Fluorogenic Agent. , 2012, 2012, 1-13.		1
35	Understanding the Molecular Determinants of Capsaicin Mode of Action. <i>Biophysical Journal</i> , 2015, 108, 57a.	0.5	1
36	HCV NS5B RdRp mutations and their effects on ligand binding affinity. <i>International Journal of Modelling and Simulation</i> , 2022, 42, 415-425.	3.3	0

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37	Investigation and Analytical Applications of the Reaction of N1-methylnicotinamide and Active Methylene Containing Drugs. <i>Current Pharmaceutical Analysis</i> , 2021, 17, 1331-1338.	0.6	0
38	Discovery of novel, selective, functionalized 5-(2-(5-arylhexahydropyrrolo[3,4-c]pyrrol-2(1H)-yl)ethyl)- β -butyrolactone sigma-2 ligands. <i>Medicinal Chemistry Research</i> , 0, , .	2.4	0