

# Khaled M Elokely

## List of Publications by Year in descending order

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Version: 2024-02-01

38  
papers

756  
citations

777949

13  
h-index

591227

27  
g-index

38  
all docs

38  
docs citations

38  
times ranked

1566  
citing authors

| #  | ARTICLE   | IF  | CITATIONS |
|----|---|-----|-----------|
| 1  | HCV NS5B RdRp mutations and their effects on ligand binding affinity. <i>International Journal of Modelling and Simulation</i> , 2022, 42, 415-425.   | 2.3 | 0         |
| 2  | 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.   | 1.3 | 2         |
| 3  | 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.   | 1.8 | 2         |
| 4  | Allosteric inhibitors of the main protease of SARS-CoV-2. <i>Antiviral Research</i> , 2022, 205, 105381.  | 1.9 | 23        |
| 5  | 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.  | 2.5 | 25        |
| 6  | Proposed Mechanism for the Antitrypanosomal Activity of Quercetin and Myricetin Isolated from <i>Hypericum afrum</i> Lam.: Phytochemistry, <i>In Vitro</i> Testing and Modeling Studies. <i>Molecules</i> , 2021, 26, 1009.   | 1.7 | 11        |
| 7  | Structure-Activity Relationships of the Antimalarial Agent Artemisinin 10. Synthesis and Antimalarial Activity of Enantiomers of rac-5 <sup>12</sup> -Hydroxy-d-Secoartemisinin and Analogs: Implications Regarding the Mechanism of Action. <i>Molecules</i> , 2021, 26, 4163. | 1.7 | 6         |
| 8  | Discovery of novel class of histone deacetylase inhibitors as potential anticancer agents. <i>Bioorganic and Medicinal Chemistry</i> , 2021, 42, 116251.  | 1.4 | 4         |
| 9  | 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.  | 2.5 | 12        |
| 10 | Computationally Assisted Lead Optimization of Novel Potent and Selective MAO-B Inhibitors. <i>Biomedicines</i> , 2021, 9, 1304.   | 1.4 | 5         |
| 11 | Investigation and Analytical Applications of the Reaction of N1-methylnicotinamide and Active Methylene Containing Drugs. <i>Current Pharmaceutical Analysis</i> , 2021, 17, 1331-1338.   | 0.3 | 0         |
| 12 | Discovery and SAR of Novel Disubstituted Quinazolines as Dual PI3K $\alpha$ /mTOR Inhibitors Targeting Breast Cancer. <i>ACS Medicinal Chemistry Letters</i> , 2020, 11, 2156-2164.   | 1.3 | 8         |
| 13 | 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.   | 2.0 | 17        |
| 14 | The Resurrection of Phenotypic Drug Discovery. <i>ACS Medicinal Chemistry Letters</i> , 2020, 11, 1820-1828.  | 1.3 | 26        |
| 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.   | 1.5 | 12        |
| 16 | Inhibition of human monoamine oxidase A and B by flavonoids isolated from two Algerian medicinal plants. <i>Phytomedicine</i> , 2018, 40, 27-36.  | 2.3 | 58        |
| 17 | Anti-inflammatory of pyrrolizidine alkaloids from <i>Heliotropium digynum</i> . <i>Medicinal Chemistry Research</i> , 2018, 27, 1066-1073.  | 1.1 | 9         |
| 18 | Bioactive products from singlet oxygen photooxygenation of cannabinoids. <i>European Journal of Medicinal Chemistry</i> , 2018, 143, 983-996.   | 2.6 | 7         |

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|----|--|-----|-----------|
| 19 | Microbial Oxidation of the Fusidic Acid Side Chain by <i>Cunninghamella echinulata</i> . <i>Molecules</i> , 2018, 23, 970.   | 1.7 | 5         |
| 20 | 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. | 0.3 | 6         |
| 21 | Design, synthesis and SAR of new-di-substituted pyridopyrimidines as ATP-competitive dual PI3K/mTOR inhibitors. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2017, 27, 3117-3122.   | 1.0 | 10        |
| 22 | A Mitochondrial-targeted purine-based HSP90 antagonist for leukemia therapy. <i>Oncotarget</i> , 2017, 8, 112184-112198.   | 0.8 | 17        |
| 23 | 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.   | 1.5 | 32        |
| 24 | 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.                | 3.3 | 127       |
| 25 | 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.                    | 1.1 | 20        |
| 26 | New Glycosides and Trypanocidal Metabolites from <i>Vangueria edulis</i> . <i>Natural Product Communications</i> , 2015, 10, 1934578X1501001.  | 0.2 | 3         |
| 27 | Flavonoids from <i>Perovskia atriplicifolia</i> and Their in Vitro Displacement of the Respective Radioligands for Human Opioid and Cannabinoid Receptors. <i>Journal of Natural Products</i> , 2015, 78, 1461-1465.                     | 1.5 | 21        |
| 28 | Understanding the Molecular Determinants of Capsaicin Mode of Action. <i>Biophysical Journal</i> , 2015, 108, 57a.   | 0.2 | 1         |
| 29 | Antiurease activity of plants growing in the Czech Republic. <i>Natural Product Research</i> , 2014, 28, 868-873.  | 1.0 | 11        |
| 30 | Asphodolides A-E, anti-MRSA metabolites from <i>Asphodelus microcarpus</i> . <i>Phytochemistry</i> , 2014, 105, 79-84.   | 1.4 | 13        |
| 31 | Isolation and characterization of new secondary metabolites from <i>Asphodelus microcarpus</i> . <i>Medicinal Chemistry Research</i> , 2014, 23, 3510-3515.  | 1.1 | 10        |
| 32 | Drug activity prediction using multiple-instance learning via joint instance and feature selection. <i>BMC Bioinformatics</i> , 2013, 14, S16.   | 1.2 | 18        |
| 33 | Computationally Assisted Assignment of Kahalalide Y Configuration Using an NMR-Constrained Conformational Search. <i>Journal of Natural Products</i> , 2013, 76, 178-185.  | 1.5 | 9         |
| 34 | Molecular mechanisms of the antitumor activity of SB225002: A novel microtubule inhibitor. <i>Biochemical Pharmacology</i> , 2013, 85, 1741-1752.  | 2.0 | 23        |
| 35 | Docking Challenge: Protein Sampling and Molecular Docking Performance. <i>Journal of Chemical Information and Modeling</i> , 2013, 53, 1934-1945.  | 2.5 | 194       |
| 36 | Fluorometric Determination of Drugs Containing $\pm$ -Methylene Sulfoxide Functional Groups Using -Methylnicotinamide Chloride as a Fluorogenic Agent. , 2012, 2012, 1-13.   |     | 1         |

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|----|--|-----|-----------|
| 37 | Fluorescence Spectrometric Determination of Drugs Containing -Methylene Sulfone/Sulfonamide Functional Groups Using <i>N</i> <sup>1</sup> -Methylnicotinamide Chloride as a Fluorogenic Agent. International Journal of Analytical Chemistry, 2011, 2011, 1-9. | 0.4 | 8         |
| 38 | Discovery of novel, selective, functionalized 5-(2-(5-arylhexahydropyrrolo[3,4-c]pyrrol-2(1H)-yl)ethyl)- $\beta$ -butyrolactone sigma-2 ligands. Medicinal Chemistry Research, 0, , .  | 1.1 | 0         |