

Pharmaceutical Chemistry Department

Publication list from Jan 2021- Oct 2022

International publications:

1- New fluorinated diarylureas linked to pyrrolo[2,3-d]pyrimidine scaffold as VEGFR-2 inhibitors: Molecular docking and biological evaluation. **Mai Adel, Khaled A.M. Abouzid., Bioorganic Chemistry, (2022), 127: 106006.**

2- Discovery of EMD37, a 1,2,4-oxadiazole derivative, as a novel endoplasmic reticulum stress inducer with potent anticancer activity. Amal Kamal Abdel-Aziz, **Eman M.E. Dokla, Khaled A.M. Abouzid**, Saverio Minucci., **Biochemical Pharmacology, (2022), 115316**

3- Identification of a promising hit from a new series of pyrazolo[1,5-a]pyrimidine based compounds as a potential anticancer agent with potent CDK1 inhibitory and pro-apoptotic properties through a multistep in vitro assessment. Hossam R. Elgiushy, Sameh H. Mohamed, Heba Taha, Hussein Sawaf, Zeinab Hassan, Nageh A. Abou-Taleb, **Eman M. El-labbad**, Ashraf S. Hassan, **Khaled A.M. Abouzid**, Sherif F. Hammad.. **Bioorganic Chemistry, (2022), 120: 105646.**

4- Molecular design, synthesis and biological evaluation of novel 1,2,5-trisubstituted benzimidazole derivatives as cytotoxic agents endowed with ABCB1 inhibitory action to overcome multidrug resistance in cancer cells. **Abeer H. A. Abdelhafiz, Rabah A. T. Serya, Deena S. Lasheen**, Nessa Wang, Mansour Sobeh, Michael Wink & **Khaled A. M. Abouzid.** **Journal of Enzyme Inhibition and Medicinal Chemistry, (2022), 37, 2710-2724.**

5- Insights into the design of inhibitors of the EGFR family with anticancer activity overcoming resistance: A case of optimizing thieno[2,3-d]pyrimidine-based EGFR inhibitors. **Sandra N. Milik**, Amal Kamal Abdel-Aziz, Morad M. El-Hendawy, Riham I. El-Gogary, Mona Kamal Saadeldin, Saverio Minucci, Christian D. Klein, **Khaled A.M. Abouzid**, **Journal of Molecular Structure, (2022), 1259: 132724.**

6- Tackling Microbial Resistance with Isatin-Decorated Thiazole Derivatives: Design, Synthesis, and in vitro Evaluation of Antimicrobial and Antibiofilm Activity. Refaie M Kassab, Sami A Al-Hussain, Nooran S Elleboudy, Amgad Albohy, Magdi E A Zaki , **Khaled A M Abouzid**, Zeinab A Muhammad. **Drug Design, Development and Therapy, (2022), 25;16:2817-2832**

7- Identification of novel furo [2, 3-d] pyrimidine based chalcones as potent anti-breast cancer agents: synthesis, in vitro and in vivo biological evaluation. Mai A Mansour, Mamdouh A Oraby, Zeinab A Muhammad, **Deena S. Lasheen**, Hatem M Gaber, **Khaled AM Abouzid**, , **RSC Advances, (2022), 12, 8193-8201.**

8- Towards Selective Binding to the GLUT5 Transporter: Synthesis, Molecular Dynamics and In Vitro Evaluation of Novel C-3-Modified 2,5-Anhydro-D-mannitol Analogs. Natasha Rana, **Marwa A Aziz**, Ahmed K Oraby, Melinda Wuest, Jennifer Dufour, **Khaled A M Abouzid**, Frank Wuest, F G West. **Pharmaceutics (2022) 10;14(4):828**

9- Design, synthesis, and biological evaluation of new thieno[2,3-d] pyrimidines derivatives as targeted therapy for PI3K with molecular modelling study. **Fatma M. Elmenier, Deena S.**

Lasheen, Khaled A. M. Abouzeid, Journal of Enzyme Inhibition and Medicinal Chemistry, (2022), 37, 315–332.

10- Induction of apoptosis using ATN as a novel Yes-associated protein inhibitor in human oral squamous cell carcinoma cells. Chu, P. C., **Dokla, E. M. E.**, Hu, J. L. & Weng, J. R. **Environ. Toxicol. 2022, 37, 1404–1412**

11- Discovery of a Benzimidazole-Based Dual FLT3/TrKA Inhibitor Targeting Acute Myeloid Leukemia. **Dokla, E. M. E.**; Abdel-Aziz, A. K.; **Milik, S. N.**; McPhillie, M. J.; Minucci, S.; **Abouzeid, K. A. M. Bioorg. Med. Chem. 2022, 56, 116596.**

12- Structure-based design and synthesis of conformationally constrained derivatives of methyl-piperidinopyrazole (MPP) with estrogen receptor (ER) antagonist activity, Mahmoud A. Ragab, Mohamed Elagawany, Hoda Daabees, Al-Shaimaa F. Ahmed, Eman M. Awad, Cyrielle Billon, Bahaa Elgendy, **Khaled A.M. Abouzeid**, Shaymaa E. Kassab, **Bioorganic Chemistry, (2022) 119: 105554.**

13- Novel 1,3-diaryl pyrazole derivatives bearing methylsulfonyl moiety: Design, synthesis, molecular docking and dynamics, with dual activities as anti-inflammatory and anticancer agents through selectively targeting COX-2, Ahmed M.M. Shaker, **Mai I. Shahin**, Asmaa M. AboulMagd, Seham A. Abdel Aleem, Hamdy M. Abdel-Rahman, **Dalal A. Abou El Ella. Bioorganic Chemistry, (2022) 129: 106143**

14- The natural isoflavone Biochanin-A synergizes 5-fluorouracil anticancer activity in vitro and in vivo in Ehrlich solid-phase carcinoma model. Mohamed Mahmoud, Maha R. A. Abdollah, Mohamed E. Elsesy, **Dalal A. Abou El Ella**, Suher K. Zada, Mai F. Tolba, **phytotherapy research, (2022) 36: 1310-1325.**

15- Recent Advancements in the development of Anti-Breast Cancer Synthetic Small Molecules. Elkaeed, E.B.; Salam, H.A.A.E.; Sabt, A.; **Al-Ansary, G.H.**; Eldehna, W.M.. **Molecules (2021) 26: 7611.**

16- Development of 3-methyl/3-(morpholinomethyl)benzofuran derivatives as novel antitumor agents towards non-small cell lung cancer cells, Mohammad M. Al-Sanea, **Ghada H. Al-Ansary**, Zainab M. Elsayed, Raed M. Maklad, Eslam B. Elkaeed, Mohamed A. Abdelgawad, Syed Nasir Abbas Bukhari, Marwa M. Abdel-Aziz, Howayda Suliman & Wagdy M. Eldehna. **Journal of Enzyme Inhibition and Medicinal Chemistry (2021), 36:1, 987-999.**

17- Biphenylurea/thiourea derivatives tagged with heteroarylsulfonamide motifs as novel VEGFR2 inhibitors; Design, synthesis and anti-angiogenic activity. **Ghada H. Al-Ansary**, Tamer Nasr, Heba Taha, Walid Fayad, Shahenda Mahgoub, **Bioorganic Chemistry, (2021) 107: 104640.**

18- Novel benzene-sulfonamides aryl and arylsulfone conjugates adopting tail/dual tail approaches: Synthesis, carbonic anhydrase inhibitory activity and molecular modelling studies. **Assem H. Eldeeb**, Mahmoud F. Abo-Ashour, Andrea Angeli, Alessandro Bonardi, **Deena S. Lasheen, Eman Z. Elrazaz**, Alessio Nocentini, Paola Gratteri, Hatem A. Abdel-Aziz, Claudiu T. Supuran, **European Journal of Medicinal Chemistry, (2021), 221, 11486.**

19- Indolin-2-One Derivatives as Selective Aurora B Kinase Inhibitors Targeting Breast Cancer. **Dokla, E. M. E.**; Abdel-Aziz, A. K.; **Milik, S. N.**; Mahmoud, A. H.; Saadeldin, M. K.; McPhillie, M. J.; Minucci, S.; **Abouzeid, K. A. M. Bioorg. Chem. 2021, 117, 105451.**

20- Lipid polymer hybrid nanocarriers as a combinatory platform for different anti-SARS-CoV-2 drugs supported by computational studies. Hend Mohamed Abdel-Bar, Inas A. Abdallah, Marwa A. A. Fayed, Yassmin Moatasim, Ahmed Mostafa, Mohammed Farrag El-

Behairy, Hanan Elimam, Yaseen A. M. M. Elshaier and **Khaled A. M. Abouzid**. **RSC Advances**, (2021),11, 28876-28891.

21- Structure- and Ligand-Based in silico Studies towards the Repurposing of Marine Bioactive Compounds to Target SARS-CoV-2. Marwa A.A. Fayed, Mohammed Farrag El-Behairy, Inas A. Abdallah, Hend Mohamed Abdel-Bar, Hanan Elimam, Ahmed Mostafa, Yassmin Moatasim, **Khaled A.M. Abouzid**, and Yaseen A.M.M. Elshaierb. **Arabian Journal of Chemistry**. (2021), 4: 103092.

22- Synthesis, in vitro biological investigation, and molecular dynamics simulations of thiazolopyrimidine based compounds as corticotrophin releasing factor receptor-1 antagonists. Hossam R Elgiushy, Nageh A Abou-Taleb, George G Holz, Oleg G Chepurny, Ioannis Pirmettis, Sotirios Kakabakos, Vlasios Karageorgos, George Liapakis, Amgad Albohy, **Khaled A M Abouzid**, Sherif F Hammad. **Bioorg Chem**. (2021), 114:105079.

23- Discovery of potent thieno[2,3-d]pyrimidine VEGFR-2 inhibitors: Design, synthesis and enzyme inhibitory evaluation supported by molecular dynamics simulations. **Eman Z Elrazaz**, **Rabah A T Serya**, **Nasser S M Ismail**, Amgad Albohy, **Dalal A Abou El Ella**, **Khaled A M Abouzid**. **Bioorg Chem** (2021) 113:105019.

24- Molecular design, synthesis and in vitro biological evaluation of thienopyrimidine-hydroxamic acids as chimeric kinase HDAC inhibitors: a challenging approach to combat cancer. Mona M Abdel-Atty, Nahla A Farag, **Rabah A T Serya**, **Khaled A M Abouzid**, Samar Mowafy. **Journal of Enzyme Inhibition and Medicinal Chemistry** (2021) 36(1):1290-1312.

25- Medicinal Chemistry Strategies Towards SO₂ Donors as Research Tools and Potential Therapeutics. **Eman M El-Labbad**, Xingyue Ji, **Khaled A M Abouzid**, Binghe Wang. **Curr Top Med Chem** (2021);21(32):2870-2881.

26- Green analysis of newly approved binary omeprazole/aspirin mixture in presence of aspirin impurity using ultra-high-performance liquid chromatography and thin-layer chromatography methods. Eglal A Abdelaleem, **Dalal A Abou El Ella**, Alaa M Mahmoud, Nessreen S Abdelhamid. **Biomed Chromatography** (2021) 35(2):e4986

Local publications:

- 1- Synthesis, Biological Evaluation and In-silico ADME Study of Novel Hybridized Benzimidazole- Chalcone Compounds with Potential Antimicrobial Activity. **Mai I. Shahin**, Asmaa I. AbdAlhafiz, **Khaled A. M. Abouzid**, **Wesam E. Mehanna**, **Archives of Pharmaceutical Sciences Ain Shams University**, (2022) 6: 29-36
- 2- Antimicrobial and Cytotoxicity Evaluation of New 3-Allyl-2-iminothiazolidin-4-ones. Shaymaa G. Hammad, Marwa G. El-Gazzar, Mohammad Abdel-Halim **Eman Z. Elrazaz**, Ebaa M. El-Hossary, **Khaled A.M. Abouzid**. **Egyptian Journal of Chemistry** (2021) 64: 4919-4930.
- 3- Synthesis, In Silico and In Vitro Antimicrobial Evaluation of Cyanoketene S,N-Acetals and their Pyrazoles Against Staphylococcus aureus DNA Gyrase Enzyme. Shima Mahmoud Ali; Ahmed H.I. Faraag; Hossam R. Elgiushy; Taghrid S. El-Mahdy; Ahmed A. Askar; Ashraf S. Hassanorcid; **Khaled A. M. Abouzid**; **Sherif F. Hammad**. **Journal of advanced Pharmacy Research** (2021) 5: 341-361.

- 4- Synthesis, Biological Evaluation and In Silico Investigation of Novel Functionalized Imidazole-Based KDM6 Inhibitors. **Amr Mostafa El-Araby, Omar Magdy Qassem Ezzat Ashraf El-Sawy, Eman Zaghlool El-Razaz, Khaled Abouzid, Rabah Ahmed Taha Serya.** Egyptian Journal of Chemistry (2021) 64: 1575-1582.

- 5- Molecular Modeling Studies on Biochanin-A as a Potential Dual Inhibitor for VEGFR-2 and Cyclin D1-CDK-4 Complex. Mohamed Mahmoud Ramadan; Marwa A. Ali; Amgad Albohy; Suher Kamal Zada; Mai Fathy Tolba; **Dalal Abu-ELElla.** Archives of Pharmaceutical Sciences Ain Shams University (2021) 5:16-32