

Ahmed Ali Al-Karmalawy, PhD

➔ Awarded the State Encouragement Award in the field of advanced technological sciences that serve the fields of medical sciences for the year 2022.

➔ Classified from the 2% World's Top Scientists' List (Stanford University - 2023).

Assistant Professor of Pharmaceutical Medicinal Chemistry.

Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Horus University-Egypt, New Damietta 34518, Egypt.

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Academic Qualifications:

Al-Azhar University, Division of Pharmaceutical Chemistry, Cairo, Egypt. November 2017

PhD of Pharmaceutical Chemistry (Medicinal Chemistry),

Advisors: Prof. Abdel-Ghany El-Helby, Prof. Helmy Sakr, Prof. Khaled El-Adl and Ass. Prof. Ibrahim H. Eissa.

Thesis title: Design, synthesis, molecular docking, and anticancer activity of benzoxazole/benzothiazole derivatives as VEGFR-2 inhibitors.

Al-Azhar University, Division of Pharmaceutical Chemistry, Cairo, Egypt. June 2013

MSc of Pharmaceutical Chemistry (Medicinal Chemistry),

Advisors: Prof. Mohammed Kamal and Prof. Khaled El-Adl.

Thesis title: Design, synthesis, molecular docking, and biological evaluation of some novel quinazolin-4(3h)-one derivatives as anti-inflammatory agents and antiepileptic agents.

Cairo University, Faculty of Pharmacy, Cairo, Egypt. May 2006

BSc of Pharmaceutical Sciences.

Work and Teaching Experience:

- **Assistant Prof.** of Medicinal Chemistry (September 2023 till Now): Faculty of Pharmacy, **Horus University-Egypt**, New Damietta, Egypt.
- **Assistant Prof.** of Medicinal Chemistry (October 2022 till August 2023): Faculty of Pharmacy, **Ahram Canadian University**, 6th of October City, Egypt.
- **Assistant Prof.** of Medicinal Chemistry (September 2018 till September 2022): Faculty of Pharmacy, **Horus University in Egypt**, New Damietta, Egypt.

Teaching:

- Teaching lectures on Medicinal Chemistry and Drug Design for undergraduate students at Horus University in Egypt and Ahrum Canadian University.
- Teaching lectures on Organic Chemistry to undergraduate students at Horus University in Egypt and Ahrum Canadian University.
- Supervising practical sessions.
- **Supervisor** for many MSc and PhD students in the Pharmaceutical Chemistry field.
- **Post-PhD student** in Medicinal Chemistry (September 2017 till August 2018): Pharmaceutical Chemistry Lab, Al-Azhar University, Egypt.
- **PhD student** in Medicinal Chemistry (September 2014 till August 2017): Pharmaceutical Chemistry Lab, Al-Azhar University, Egypt.

Research: Design, synthesis, molecular docking, and characterization of new VEGFR-2 inhibitors as anticancer agents.

- **Assistant Lecturer** of Pharmaceutical Chemistry: Faculty of Pharmacy, **Delta University**, Egypt.

Teaching:

- Preparing and teaching laboratory sessions of Organic Chemistry and Analytical Chemistry for undergraduate students at Delta University, Egypt.
- Participating in most student-related activities; correction of quizzes and practical exams.
- **MSc student** Medicinal Chemistry (September 2008 till August 2013): Pharmaceutical Chemistry Lab, Al-Azhar University, Egypt.

Research: Design, synthesis, molecular docking, and characterization of new quinazolin-4(3h)-one derivatives as anti-inflammatory agents and antiepileptic agents.

- **Instructor** of Pharmaceutical Chemistry (September 2006 till August 2007): Faculty of Pharmacy, **Sinai University**, Egypt.

Teaching: Preparing and teaching laboratory sessions of Organic Chemistry, General Chemistry, and Analytical Chemistry for undergraduate students at Sinai University, Egypt.

Professional Skills:

Research skills:

- 1- **Excellent command of drug design programs (Discovery Studio 3.5 and MOE 2019.0102)** for designing different new compounds and examining their expected biological activities and side effects before chemical synthesis.
- 2- **Good command of molecular dynamics programs (Desmond module of the Schrödinger LLC software packages)** for studying the different thermodynamic properties of different docked complexes in comparable physiological conditions.
- 3- **Chemical synthesis** of different types of organic compounds and their identification, isolation, and purification.
- 4- **Creating new schemes for new expected biologically active compounds** depending on their pharmacophoric features and structure-activity relationships.
- 5- **Dealing with different types of reaction pathways** for obtaining the new compounds with the best yield.
- 6- **Extraction of some compounds from natural sources**, examination of their biological activities, and chemical synthesis of simulated similar and superior compounds based on SAR studies.

Language skills: Arabic (Mother tongue), English (good command).

Computer skills: Drug Design Programs (**Discovery Studio 3.5** and **MOE 2019.0102**), Molecular Dynamics Programs (**Desmond module of the Schrödinger LLC software packages**), Chemdraw, and Microsoft Office (Word, Excel, and PowerPoint).

Editorial Positions and Activities:

- 1- **Academic Editor** in **PLOS ONE**.
<https://journals.plos.org/plosone/static/editorial-board>
- 2- **Associate Editor** in **Frontiers in Chemistry**; Section: Medicinal and Pharmaceutical Chemistry.
<https://www.frontiersin.org/journals/chemistry/editors>
- 3- **Topic Editor** in **Frontiers in Chemistry** for a special issue titled (**Recent Advances in the Research and Development of Kinase-inhibitory Anticancer Molecules**).
<https://www.frontiersin.org/research-topics/33242/recent-advances-in-the-research-and-development-of-kinase-inhibitory-anticancer-molecules>
- 4- **Topic Editor** in **Metabolites** for a special issue titled (**Design of Novel Target-Oriented Chemotherapeutic Anti-cancer Agents with ADME Pharmacokinetics**).
https://www.mdpi.com/journal/metabolites/special_issues/Anti-Cancer_Agents_ADME_Pharmacokinetics
- 5- **Topic Editor** in **Separations** for a special issue titled (**Application of Separation and/or Purification Technology in Natural Products, Newly Synthetic Candidates, and Pharmaceuticals**). https://www.mdpi.com/journal/separations/special_issues/5F7733I54I
- 6- **Editor** in **Pharmaceutical Sciences**.
<https://ps.tbzmed.ac.ir/EditorialBoard>
- 7- **Guest Editor** in **Frontiers in Pharmacology**.
<https://www.frontiersin.org/articles/10.3389/fphar.2022.986456/full>
- 8- **Deputy Director of Quality Assurance Unit** at Faculty of Pharmacy, Horus University in Egypt.
- 9- **Deputy Director of the International Students Office** at Horus University in Egypt.
- 10- **Supervisor of EPSF-HUE** from 2018 till 2022.
- 11- **Editor-In-Chief of the Cultural Magazine**, Faculty of Pharmacy, Horus University in Egypt, from 2020 till 2022.
- 12- **Responsible for the Project “Genius Horus”** at Horus University in Egypt, from 2019 till 2022.
- 13- **Creator of a scientific learning YouTube channel for medical career students entitled** (www.youtube.com/MedicinalChemistrywithKarmalawy).
- 14- **Editorial board member for the “International Conference on Cardiology and Cardiovascular Medicine CCM 2021”**.
- 15- **A Reviewer for Different Known and Highly Impacted Scientific Journals**.

Publications:

I published **more than 130 scientific papers**. These articles focused mainly on the design and development of novel effective organic molecules for the treatment of different diseases such as cancer, viruses (especially SARS-CoV-2), bacterial and fungal infections, and Alzheimer’s disease. Also, drug

repurposing of FDA-approved drugs to treat certain urgent diseases such as COVID-19 and cancer using different computational and biological methods. * = Corresponding author.

A) Publications with the peer review process

1. Ashraf K. El-Damasy, Jong Min Oh, Hyun Ji Kim, Seul-Ki Mun, **Ahmed A. Al-Karmalawy**, Radwan Alnajjar, Yu-Jeong Choi, Jong-Jin Kim, Ghilsoo Nam, Hoon Kim, Gyochang Keum: Novel coumarin benzamides as potent and reversible monoamine oxidase-B inhibitors: Design, synthesis, and neuroprotective effects, *Bioorganic Chemistry*, 2023, p 106939.
<https://doi.org/10.1016/j.bioorg.2023.106939>
2. Ahmed A Gaber, Marwa Sharaky, Ayman Abo Elmaaty, Mohamed M Hammouda, Ahmed AE Mourad, Samy Y Elkhawaga, Mahmoud Mohamed Mokhtar, Amr S Abouzied, Mai AE Mourad & **Ahmed A Al-Karmalawy***: Design and synthesis of novel pyrazolopyrimidine candidates as promising EGFR-T790M inhibitors and apoptosis inducers, *Future Medicinal Chemistry*, 2023.
<https://doi.org/10.4155/fmc-2023-0156>
3. Eslam M. Abbass, **Ahmed A. Al-Karmalawy***, Marwa Sharaky, Muhammad Khattab, Abdullah Yahya Abdullah Alzahrani, Aya I. Hassaballah: Rational design and eco-friendly one-pot multicomponent synthesis of novel ethylidenehydrazineylthiazol-4(5H)-ones as potential apoptotic inducers targeting wild and mutant EGFR-TK in triple negative breast cancer, *Bioorganic Chemistry*, 2023, p 106936.
<https://doi.org/10.1016/j.bioorg.2023.106936>
4. Samar A. Antar, Nada A. Ashour, Marwa Sharaky, Muhammad Khattab, Naira A. Ashour, Roaa T. Zaid, Eun Joo Roh, Ahmed Elkamhawy, **Ahmed A. Al-Karmalawy**: Diabetes mellitus: Classification, mediators, and complications; A gate to identify potential targets for the development of new effective treatments, *Biomedicine & Pharmacotherapy*, 2023, p 115734.
<https://doi.org/10.1016/j.biopha.2023.115734>
5. maiy Y. Jaballah, Norhan A. Abdelrahman, **Ahmed A. Al-Karmalawy**, Khaled A. M. Abouzid: Pyridazine Based Compounds with PARP-1 Inhibitory Activity, *Archives of Pharmaceutical Sciences Ain Shams University*, 2023, p 274-285.
<http://dx.doi.org/10.21608/APS.2023.224318.1127>
6. Ahmed Mowafy Tafish, Mohamed El-Sherbiny, **Ahmed A Al-Karmalawy**, Osama Abd El-Azeem Soliman & Noha Mohamed Saleh: Carvacrol-Loaded Phytosomes for Enhanced Wound Healing: Molecular Docking, Formulation, DoE-Aided Optimization, and in vitro/in vivo Evaluation, *International Journal of Nanomedicine*, 2023, p 5749-5780.
<https://doi.org/10.2147/IJN.S421617>
7. Samar A. Antar, Aymen Halouani, Cherry Gad, **Ahmed A. Al-Karmalawy***: An Overview of the Mechanisms of Cadmium-induced Toxicity in the Male Reproductive System, *Pharmaceutical Sciences*, 2023, p 30. <https://doi.org/10.34172/PS.2023.10>
8. Mohamed Y. Zakaria, Marwa Sharaky, Ayman M. Noreddin, Radwan Alnajjar, Rabeh EL-Shesheny, Omnia Kutkat, Mohamed E. El-Beeh, Mohammed A.S. Abourehab, **Ahmed A. Al-Karmalawy***: Investigating the superiority of chitosan/D-alpha-tocopheryl polyethylene glycol succinate binary coated bilosomes in promoting the cellular uptake and anti-SARS-CoV-2 activity of polyphenolic herbal drug candidate, *International Journal of Pharmaceutics*, 2023, p 123385.
<https://doi.org/10.1016/j.ijpharm.2023.123385>
9. Ahmed S. Mohamed, Osama G. Mohamed, Ali M. El Shamy, Fatma S. El Sakhawy, **Ahmed A. Al-Karmalawy**, Ashootosh Tripathi, Rania A. El Gedaily: Anti-Alzheimer Activity and UHPLC-

MS Based Molecular Networking of Pseudobombax ellipticum Cultivars Coupled to Multivariate Data Analysis and In Silico Molecular Docking, *Egyptian Journal of Chemistry*, 2023.

<https://doi.org/10.21608/ejchem.2023.224319.8292>

10. Aya S. Shalaby, Hanaa H. Eid, Riham A. El-Shiekh, Fadia S. Youssef, **Ahmed A. Al-Karmalawy**, Nahla A. Farag, Amany A. Sleem, Fatma Adly Morsy, Khaled M. Ibrahim, Soad H. Tadros: A Comparative GC/MS Analysis of Citrus Essential Oils: Unveiling the Potential Benefits of Herb-Drug Interactions in Preventing Paracetamol-Induced Hepatotoxicity, *Chemistry & Biodiversity*, p 202300778, 2023. <https://doi.org/10.1002/cbdv.202300778>
11. Saad Shaaban, **Ahmed A. Al-Karmalawy***, Abdulrahman G. Alhamzani, Mortaga M. Abou-Krishna, Mahmoud A. Al-Qudah, and Tarek A. Yousef: Synthesis and Molecular Docking Analysis of New Thiazo-Isoindolinedione Hybrids as Potential Inhibitors of the SARS-Cov-2 Main Protease, *Oriental Journal of Chemistry*, 2023. <http://dx.doi.org/10.13005/ojc/390412>
12. Samar El-Kalyoubi, Mohamed M. Khalifa, Mahmoud T. Abo-Elfadl, Ahmed A. El-Sayed, Ahmed Elkamhawy, Kyeong Lee and **Ahmed A. Al-Karmalawy***: Design and synthesis of new spirooxindole candidates and their selenium nanoparticles as potential dual Topo I/II inhibitors, DNA intercalators, and apoptotic inducers, *Journal of Enzyme Inhibition and Medicinal Chemistry*, p 2242714, 2023. <https://doi.org/10.1080/14756366.2023.2242714>
13. Mohamed A. Salem, Osama G. Mohamed, Esraa M. Mosalam, Aya Ibrahim Elberri, Hend Mohamed Abdel-Bar, Mariam Hassan, **Ahmed A. Al-Karmalawy**, Ashootosh Tripathi, Shahira M. Ezzat and Hend E. Abo Mansour: Investigation of the phytochemical composition, antioxidant, antibacterial, anti-osteoarthritis, and wound healing activities of selected vegetable waste, *Scientific Reports*, 2023, p 13034. <https://doi.org/10.1038/s41598-023-38591-y>
14. Saad Shaaban, Yasair S. Al-Faiyz, Ghayah M. Alsulaim, Mohamed Alaasar, Nasser Amri, Hussein Ba-Ghazal, **Ahmed A. Al-Karmalawy** and Aly Abdou: Synthesis of New Organoselenium-Based Succinanic and Malenic Derivatives and *In Silico* Studies as Possible SARS-CoV-2 Main Protease Inhibitors, *Inorganics*, 2023, p 321. <https://doi.org/10.3390/inorganics11080321>
15. **Ahmed A. Al-Karmalawy***, Radwan Alnajjar, Ayman Abo Elmaaty, Faizah A. Binjubair, Sara T. Al-Rashood, Basma S. Mansour, Ahmed Elkamhawy, Wagdy M. Eldehna & Khaled Ahmed Mansour: Investigating the promising SARS-CoV-2 main protease inhibitory activity of secoiridoids isolated from *Jasminum humile*; *in silico* and *in vitro* assessments with structure-activity relationship, *Journal of Enzyme Inhibition and Medicinal Chemistry*, 2023, p 1-13. <https://doi.org/10.1080/07391102.2023.2240419>
16. **Ahmed A. Al-Karmalawy***, Mahmoud Rashed, Marwa Sharaky, Hamada S. Abulkhair, Mohamed M. Hammouda, Haytham O. Tawfik, Moataz A. Shaldam: Novel fused imidazotriazines acting as promising top. II inhibitors and apoptotic inducers with greater selectivity against head and neck tumors: Design, synthesis, and biological assessments, *European Journal of Medicinal Chemistry*, 2023, p 115661. <https://doi.org/10.1016/j.ejmech.2023.115661>
17. Aya S. Shalaby, Hanaa H. Eid, Riham A. El-Shiekh, Osama G. Mohamed, Ashootosh Tripathi, **Ahmed A. Al-Karmalawy**, Amany A. Sleem, Fatma Adly Morsy, Khaled M. Ibrahim, Soad H. Tadros, and Fadia S. Youssef: Taming Food-Drug Interaction Risk: Potential Inhibitory Effects of Citrus Juices on Cytochrome Liver Enzymes Can Safeguard the Liver from Overdose Paracetamol-Induced Hepatotoxicity, *ACS Omega*, 2023, p 26444-26457. <https://doi.org/10.1021/acsomega.3c03100>

18. Samar A. Antar, Ayman M. Mahmoud, Walied Abdo, Cherry Gad, and **Ahmed Ali Al-Karmalawy***: A Comprehensive Overview of Organ Inflammatory Responses: Genesis, Possible Mechanisms, and Mediators of Inflammation, *Pharmaceutical Sciences*, 2023, p 397-416. <http://dx.doi.org/10.34172/PS.2023.9>.
19. Seham S El-Hawary, Abeer S Moawad, Hebatallah S Bahr, Eman Z Attia, Mo`men H El-Katatny, Muhamad Mustafa, **Ahmed A Al-Karmalawy**, Mostafa E Rateb, Jian-ye Zhang, Usama Ramadan Abdelmohsen, Rabab Mohammed: Promising Cytotoxic butenolides from the Soybean endophytic fungus *Aspergillus terreus*: a combined molecular docking and in-vitro studies, *Journal of Applied Microbiology*, 2023, p 129. <https://doi.org/10.1093/jambio/txad129>
20. Samar El-Kalyoubi, Samar S Elbaramawi, Ahmed G Eissa, Essam Al-Ageeli, Yahya Hasan Hobani, Aya Ali El-Sharkawy, Hossam Taha Mohamed, **Ahmed A Al-Karmalawy***, and Hamada S Abulkhair: Design and synthesis of novel uracil-linked Schiff bases as dual histone deacetylase type II/topoisomerase type I inhibitors with apoptotic potential, *Future Medicinal Chemistry*, 2023, p 937-958. <https://doi.org/10.4155/fmc-2023-0112>
21. Ahmed Kandeil, Mounir Abi-Said, Rebecca Badra, Rabeh El-Shesheny, **Ahmed A. Al-Karmalawy**, Radwan Alnajjar, Zumama Khalid, Mina Nabil Kamel, Walid Abi Habib, Jad Abdallah, Vijaykrishna Dhanasekaran, Richard Webby, and Ghazi Kayali: Detection of Coronaviruses in Bats in Lebanon during 2020, *Pathogens*, 2023, p 876. <https://doi.org/10.3390/pathogens12070876>
22. Nader R. Albujuq, Khalid Althumayri, Reem A. K Alharbi, **Ahmed A. Al-Karmalawy**, Mohamed S. Nafie: Design and Synthesis of Benzenesulfonamides Coupled with Piperidine, Morpholine, and N,N-Dimethylethanamine Moieties as Apoptotic Inducers through VEGFR2 and Topoisomerase II Inhibition, *Chemistry Select*, 2023, p 202301315. <https://doi.org/10.1002/slct.202301315>
23. Amany Belal, Mohamed A. Elanany, **Ahmed A. Al-Karmalawy**, Ahmed Elkamhawy, Mohammed A. S. Abourehab, Heba I. Ghamry & Ahmed B. M. Mehany: Design of new captopril mimics as promising ACE inhibitors: ADME, pharmacophore, molecular docking and dynamics simulation with MM-PBSA and PCA calculations, *Journal of Taibah University for Science*, 2023, p 2210348. <https://doi.org/10.1080/16583655.2023.2210348>
24. Mai A. E. Mourad, Ayman Abo Elmaaty, Islam Zaki, Ahmed A. E. Mourad, Amal Hofni, Ahmed E. Khodir, Esam M. Aboubakr, Ahmed Elkamhawy, Eun Joo Roh & **Ahmed A. Al-Karmalawy**: Novel topoisomerase II/EGFR dual inhibitors: design, synthesis and docking studies of naphtho[2',3':4,5]thiazolo[3,2-a]pyrimidine hybrids as potential anticancer agents with apoptosis inducing activity, *Journal of Enzyme Inhibition and Medicinal Chemistry*, 2023, p 2205043. <https://doi.org/10.1080/14756366.2023.2205043>
25. Ahmed A. Hamed, Osama G. Mohamed, Elsayed A. Aboutabl, Fify I. Fathy, Ghada A. Fawzy, Riham A. El-Shiekh, **Ahmed A. Al-Karmalawy***, Areej M. Al-Taweel, Ashootosh Tripathi and Tarek R. Elsayed: Identification of Antimicrobial Metabolites from the Egyptian Soil-Derived *Amycolatopsis keratiniphila* Revealed by Untargeted Metabolomics and Molecular Docking, *Metabolites*, 2023, p 620. <https://doi.org/10.3390/metabo13050620>
26. Ayman Abo Elmaaty, **Ahmed A. Al-Karmalawy***, Mohamed S. Nafie, Marium M. Shamaa, Islam Zaki, Radwan Alnajjar, Mohamed Y. Zakaria: Experimental Design of D- α -tocopherol polyethylene glycol 1000 succinate Stabilized Bile Salt Based Nano-vesicles for Improved Cytotoxicity and Bioavailability of Colchicine Binding Site Inhibitor Candidates: In Vitro, In silico, and Pharmacokinetic Studies, *International Journal of Pharmaceutics*, 2023, p 122980.

<https://doi.org/10.1016/j.ijpharm.2023.122980>

27. Seohyun Son, Ahmed Elkamhawy, Anam Rana Gul, **Ahmed A. Al-Karmalawy**, Radwan Alnajjar, Ahmed Abdeen, Samah F. Ibrahim, Saud O. Alshammari, Qamar A. Alshammari, Won Jun Choi, Tae Jung Park & Kyeong Lee: Development of new TAK-285 derivatives as potent EGFR/HER2 inhibitors possessing antiproliferative effects against 22RV1 and PC3 prostate carcinoma cell lines, *Journal of Enzyme Inhibition and Medicinal Chemistry*, 2023, p 2202358.
<https://doi.org/10.1080/14756366.2023.2202358>
28. **Ahmed A. Al-Karmalawy***, Dalia S. El-Gamil, Rabeh El-Shesheny, Marwa Sharaky, Radwan Alnajjar, Omnia Kutkat, Yassmin Moatasim, Mohamed Elagawany, Sara T. Al-Rashood, Faizah A. Binjubair, Wagdy M. Eldehna, Ayman M. Noreddin & Mohamed Y. Zakaria: Design and statistical optimisation of emulsomal nanoparticles for improved anti-SARS-CoV-2 activity of N-(5-nitrothiazol-2-yl)-carboxamido candidates: *in vitro* and *in silico* studies, *Journal of Enzyme Inhibition and Medicinal Chemistry*, 2023, p 2202357.
<https://doi.org/10.1080/14756366.2023.2202357>
29. Samia M. Al-Muntaser, **Ahmed A. Al-Karmalawy***, Abeer M. El-Naggar, Ali Khalil Ali, Nour E. A. Abd El-Sattar and Eslam M. Abbass: Novel 4-thiophenyl-pyrazole, pyridine, and pyrimidine derivatives as potential antitumor candidates targeting both EGFR and VEGFR-2; design, synthesis, biological evaluations, and *in silico* studies, *RSC Advances*, 2023, p 12184-12203.
<https://doi.org/10.1039/D3RA00416C>
30. Kholoud I. Eissa, Mona M. Kamel, Lamia W. Mohamed, Ahmed S. Doghish, Radwan Alnajjar, **Ahmed A. Al-Karmalawy**, Asmaa E. Kassab: Design, synthesis, and biological evaluation of thienopyrimidine derivatives as multifunctional agents against Alzheimer's disease, *Drug Development Research*, 2023, p 937-961. <https://doi.org/10.1002/ddr.22064>
31. Maan T. Khayat, Hany E. A. Ahmed, Abdelsattar M. Omar, Yosra A. Muhammad, Khadijah A. Mohammad, Azizah M. Malebari, Ahdab N. Khayyat, Ahmed H. Halawa, Hamada S. Abulkhair, **Ahmed A. Al-Karmalawy**, Mohammed Almaghrabi, Majed Alharbi, Anfal S. Aljahdali & Ahmed M. El-Agrody: A novel class of phenylpyrazolone-sulphonamides rigid synthetic anticancer molecules selectively inhibit the isoform IX of carbonic anhydrases guided by molecular docking and orbital analyses, *Journal of Biomolecular Structure and Dynamics*, 2023, p 1-19.
<https://doi.org/10.1080/07391102.2023.2188957>
32. Ahmed A. Hamed, Riham A. El-Shiekh, Osama G. Mohamed, Elsayed A. Aboutabl, Fify I. Fathy, Ghada A. Fawzy, Areej M. Al-Taweel, Tarek R. Elsayed, Ashootosh Tripathi, and **Ahmed A. Al-Karmalawy***: Cholinesterase Inhibitors from an Endophytic Fungus *Aspergillus niveus* Fv-er401: Metabolomics, Isolation and Molecular Docking, *Molecules*, 2023, p 2559.
<https://doi.org/10.3390/molecules28062559>
33. Samar A. Antar, Nada A. Ashour, Mohamed E. Marawan and **Ahmed A. Al-Karmalawy***: Fibrosis: Types, Effects, Markers, Mechanisms for Disease Progression, and Its Relation with Oxidative Stress, Immunity, and Inflammation, *International Journal of Molecular Sciences*, 2023, p 4004. <https://doi.org/10.3390/ijms24044004>
34. Magda Assem, Rady E. El-Araby, **Ahmed A. Al-Karmalawy***, Reem Nabil, Mohamed A. M. Kamal, Amany Belal, Heba I. Ghamry, Mohammed A. S. Abourehab, Mohammed M. Ghoneim, Mohammad Y. Alshahrani and Asmaa A. El Leithy: Promoter methylation might shift the balance of Galectin-3 & 12 expression in de novo adult acute myeloid leukemia patients, *Frontiers in Genetics*, 2023, p 1122864. <https://doi.org/10.3389/fgene.2023.1122864>
35. Yousra T. Eloutify, Riham A. El-Shiekh, Khaled Meselhy Ibrahim, Ahmed R. Hamed, **Ahmed A.**

- Al-Karmalawy**, Aya A. Shokry, Yasmine H. Ahmed, Bharathi Avula, Kumar Katragunta, Ikhlas A. Khan & Meselhy R. Meselhy: Bioactive fraction from *Plumeria obtusa* L. attenuates LPS-induced acute lung injury in mice and inflammation in RAW 264.7 macrophages: LC/QToF-MS and molecular docking, *Inflammopharmacology*, 2023, p 859-875.
<https://doi.org/10.1007/s10787-023-01144-w>
36. Mahmoud A. Ragab, Wagdy M. Eldehna, Alessio Nocentini, Alessandro Bonardi, Hazem E. Okda, Bahaa Elgendy, Tarek S. Ibrahim, Mohammad M. Abd-Alhaseeb, Paola Gratteri, Claudiu T. Supuran, **Ahmed A. Al-Karmalawy**, Mohamed Elagawany: 4-(5-Amino-pyrazol-1-yl)benzenesulfonamide derivatives as novel multi-target anti-inflammatory agents endowed with inhibitory activity against COX-2, 5-LOX and carbonic anhydrase: Design, synthesis, and biological assessments, *European Journal of Medicinal Chemistry*, 2023, p 115180.
<https://doi.org/10.1016/j.ejmech.2023.115180>
37. Faten Farouk, Ayman Abo Elmaaty, Ahmed Elkamhawy, Haytham O. Tawfik, Radwan Alnajjar, Mohammed A. S. Abourehab, Mohamed A. Saleh, Wagdy M. Eldehna & **Ahmed A. Al-Karmalawy***: Investigating the potential anticancer activities of antibiotics as topoisomerase II inhibitors and DNA intercalators: in vitro, molecular docking, molecular dynamics, and SAR studies, *Journal of Enzyme Inhibition and Medicinal Chemistry*, 2023, p 2171029.
<https://doi.org/10.1080/14756366.2023.2171029>
38. Arafa Musa, Saleh K. Ihmaid, David L. Hughes, Musa A. Said, Hamada S. Abulkhair, Ahmed H. El-Ghorab, Mohamed A. Abdelgawad, Khaled Shalaby, Mohamed E. Shaker, Khalid Saad Alharbi, Nasser Hadal Alotaibi, Deborah L. Kays, Laurence J. Taylor, Della Grace Thomas Parambi, Sami I. Alzarea, **Ahmed A. Al-Karmalawy**, Hany E. A. Ahmed & Ahmed M. El-Agrody: The anticancer and EGFR-TK/CDK-9 dual inhibitory potentials of new synthetic pyranopyrazole and pyrazolone derivatives: X-ray crystallography, in vitro, and in silico mechanistic investigations, *Journal of Biomolecular Structure and Dynamics*, 2023, p 1-15.
<https://doi.org/10.1080/07391102.2023.2167000>
39. Ahmed Elkamhawy, Na Kyoung Oh, Noha A. Gouda, Magda H. Abdellattif, Saud O. Alshammari, Mohammed A. S. Abourehab, Qamar A. Alshammari, Amany Belal, Minkyong Kim, **Ahmed A. Al-Karmalawy*** and Kyeong Lee: Novel Hybrid Indole-Based Caffeic Acid Amide Derivatives as Potent Free Radical Scavenging Agents: Rational Design, Synthesis, Spectroscopic Characterization, In Silico and In Vitro Investigations, *Metabolites*, 2023, p 141.
<https://doi.org/10.3390/metabo13020141>
40. Amany A. Alzokaky, **Ahmed A. Al-Karmalawy***, Mohamed A. Saleh, Walied Abdo, Amira E. Farag, Amany Belal, Mohammed A.S. Abourehab, Samar A. Antar: Metformin ameliorates doxorubicin-induced cardiotoxicity targeting HMGB1/TLR4/NLRP3 signaling pathway in mice, *Life Sciences*, 2023, p 121390. <https://doi.org/10.1016/j.lfs.2023.121390>
41. Ahmed Elkamhawy, Seohyun Son, Hwa Young Lee, Mahmoud H. El-Maghrabey, Mohamed A. El Hamd, Saud O. Alshammari, Abeer A. Abdelhameed, Qamar A. Alshammari, Ahmed Abdeen, Samah F. Ibrahim, Wael A. Mahdi, Sultan Alshehri, Radwan Alnajjar, Won Jun Choi, **Ahmed A. Al-Karmalawy**, and Kyeong Lee: Design, Synthesis, Biological Evaluation, and Molecular Dynamics Studies of Novel Lapatinib Derivatives, *Pharmaceuticals*, 2022, p 43.
<https://doi.org/10.3390/ph16010043>
42. **Ahmed A. Al-Karmalawy***, Mohamed S. Nafie, Moataz A. Shaldam, Ayman Abo Elmaaty, Samar A. Antar, Anwar A. El-Hamaky, Mohamed A. Saleh, Ahmed Elkamhawy, and Haytham O. Tawfik: Ligand-Based Design on the Dog-Bone-Shaped BIBR1532 Pharmacophoric Features and

Synthesis of Novel Analogues as Promising Telomerase Inhibitors with In Vitro and In Vivo Evaluations, *Journal of Medicinal Chemistry*, 2022, p 777–792.

<https://doi.org/10.1021/acs.jmedchem.2c01668>

43. Mohammed Farrag El-Behairy, Walaa Hamada Abd-Allah, Mohamed M. Khalifa, Mohamed S. Nafie, Mohamed A. Saleh, Mohammed S. Abdel-Maksoud, Tarfah Al-Warhi, Wagdy M. Eldehna, and **Ahmed A. Al-Karmalawy***: Design and Synthesis of Novel Rigid Dibenzo[b,f]azepines Through Ring Closure Technique as Promising Anticancer Candidates Against Leukemia and Acting as Selective Topoisomerase II Inhibitors and DNA Intercalators, *Journal of Enzyme Inhibition and Medicinal Chemistry*, 2022, p 2157825.
<https://doi.org/10.1080/14756366.2022.2157825>
44. Sanaa A. Ahmed, Moumen S. Kamel, Moustafa O. Aboelez, Xiang Ma, **Ahmed A. Al-Karmalawy**, Sayed A. S. Mousa, Elders Kh. Shokr, H. Abdel-Ghany, Amany Belal, Mohamed A. El Hamd, Zafer S. Al Shehri, and Mahmoud Abd El Aleem Ali El-Remaly: Thieno[2,3-b]thiophene Derivatives as Potential EGFR^{WT} and EGFR^{T790M} Inhibitors with Antioxidant Activities: Microwave Assisted Synthesis and Quantitative In Vitro and In Silico Studies, *ACS Omega*, 2022, p 45535–45544.
<https://doi.org/10.1021/acsomega.2c06219>
45. Mai E. Hussein, Osama G. Mohamed, Ahlam M. El-Fishawy, Hesham I. El-Askary, Ahmed A. Hamed, Marwa M. Abdel-Aziz, Radwan Alnajjar, Amany Belal, Ahmed M. Naglah, Abdulrahman A. Almehezia, **Ahmed A. Al-Karmalawy**, Ashootosh Tripathi and Amira S. El Senousy: Anticholinesterase Activity of Budmunchiamine Alkaloids Revealed by Comparative Chemical Profiling of Two Albizia spp., Molecular Docking and Dynamic Studies, *Plants*, 2022, p 3286.
<https://doi.org/10.3390/plants11233286>
46. Howaida I. Abd-Alla, Omnia Kutkat, Heba-tollah M. Sweelam, Wagdy M. Eldehna, Marwa A. Mostafa, Magda T. Ibrahim, Yassmin Moatasim, Mohamed GabAllah and **Ahmed A. Al-Karmalawy***: Investigating the Potential Anti-SARS-CoV-2 and Anti-MERS-CoV Activities of Yellow Necklacepod among Three Selected Medicinal Plants: Extraction, Isolation, Identification, In Vitro, Modes of Action, and Molecular Docking Studies, *Metabolites*, 2022, p 1109.
<https://doi.org/10.3390/metabo12111109>
47. Mohamed Kh. ElMahdy, Mennatallah O. Zaki, **Ahmed A. Al-Karmalawy***, Walied Abdo, Sulaiman Mohammed Alnasser, Samar A. Antar: Glimepiride ameliorates renal toxicity induced by cadmium in mice: Modulation of Jun N terminal kinase (JNK)/nuclear factor kappa B (NF-κB) and phosphatidylinositol 3-kinases (PI3K)/protein kinase (AKT) pathways, *Life Sciences*, 2022, p 121184. <https://doi.org/10.1016/j.lfs.2022.121184>
48. Tarfah Al-Warhi, Diaeldin M. Elimam, Zainab M. Elsayed, Marwa M. Abdel-Aziz, Raed M. Maklad, **Ahmed A. Al-Karmalawy**, Kamyar Afarinkia, Mohammed A. S. Abourehab, Hatem A. Abdel-Azizj and Wagdy M. Eldehna: Development of novel isatin thiazolyl-pyrazoline hybrids as promising antimicrobials in MDR pathogens, *RSC Advances*, 2022, p 31466-31477.
<https://doi.org/10.1039/D2RA04385H>
49. Tarfah Al-Warhi, **Ahmed A. Al-Karmalawy***, Ayman Abo Elmaaty, Maha A. Alshubramy, Marwa Abdel-Motaal, Taghreed A. Majrashi, Medhat Asem, Ahmed Nabil, Wagdy M. Eldehna & Marwa Sharaky: Biological evaluation, docking studies, and in silico ADME prediction of some pyrimidine and pyridine derivatives as potential EGFR^{WT} and EGFR^{T790M} inhibitors, *Journal of Enzyme Inhibition and Medicinal Chemistry*, 2022, p 176-191.
<https://doi.org/10.1080/14756366.2022.2135512>

50. Ayman Abo Elmaaty, Wagdy M. Eldehna, Muhammad Khattab, Omnia Kutkat, Radwan Alnajjar, Ahmed N. El-Taweel, Sara T. Al-Rashood, Mohammed A. S. Abourehab, Faizah A. Binjubair, Mohamed A. Saleh, Amany Belal and **Ahmed A. Al-Karmalawy***: Anticoagulants as Potential SARS-CoV-2 Mpro Inhibitors for COVID-19 Patients: *In Vitro*, Molecular Docking, Molecular Dynamics, DFT, and SAR Studies, *International Journal of Molecular Sciences*, 2022, p 12235. <https://doi.org/10.3390/ijms232012235>
51. Samar A. Antar, Mohamed A. Saleh, **Ahmed A. Al-Karmalawy***: Investigating the possible mechanisms of pirfenidone to be targeted as a promising anti-inflammatory, anti-fibrotic, anti-oxidant, anti-apoptotic, anti-tumor, and/or anti-SARS-CoV-2, *Life Sciences*, 2022, p 121048. <https://doi.org/10.1016/j.lfs.2022.121048>
52. Eman A. Madbouly, El-Sayed M. Lashine, **Ahmed A. Al-Karmalawy***, Mahmoud M. Sebaiy, Harris Pratsinis, Dimitris Kletsas and Kamel Metwally: Design and synthesis of novel quinazolinone–chalcone hybrids as potential apoptotic candidates targeting caspase-3 and PARP-1: in vitro, molecular docking, and SAR studies, *New Journal of Chemistry*, 2022, p 22013-22029. <https://doi.org/10.1039/D2NJ04053K>
53. Tarfah Al-Warhi, Mostafa M. Elbadawi, Alessandro Bonardi, Alessio Nocentini, **Ahmed A. Al-Karmalawy**, Nada Aljaeed, Ohoud J. Alotaibi, Hatem A. Abdel-Aziz, Claudiu T. Supuran & Wagdy M. Eldehna: Design and synthesis of benzothiazole-based SLC-0111 analogues as new inhibitors for the cancer-associated carbonic anhydrase isoforms IX and XII, *Journal of Enzyme Inhibition and Medicinal Chemistry*, 2022, p 2635-2643. <https://doi.org/10.1080/14756366.2022.2124409>
54. Ateyatallah Aljuhani, Hany E. A. Ahmed, Saleh K. Ihmaid, Abdelsattar M. Omar, Sultan S. Althagfan, Yaser M. Alahmadi, Iqrar Ahmad, Harun Patel, Sahar Ahmed, Mohannad A. Almikhlaifi, Ahmed M. El-Agrody, Mohamed F. Zayed, Safaa Abdulrahman Turkistani, Shorouk H. Abulkhair, Mohammed Almaghrabi, Samir A. Salama, **Ahmed A. Al-Karmalawy** and Hamada S. Abulkhair: *In vitro* and computational investigations of novel synthetic carboxamide-linked pyridopyrrolopyrimidines with potent activity as SARS-CoV-2-MPro inhibitors, *RSC Advances*, 2022, p 26895-26907. <https://doi.org/10.1039/D2RA04015H>
55. Amany Belal, Hazem Elkady, **Ahmed A. Al-Karmalawy**, Ali H. Amin, Mohammed M. Ghoneim, Mohamed El-Sherbiny, Rasha Hamed Al-Serwi, Mohamed Attia Abdou, Mona H. Ibrahim and Ahmed B. M. Mehany: Discovery of Some Heterocyclic Molecules as Bone Morphogenetic Protein 2 (BMP-2)-Inducible Kinase Inhibitors: Virtual Screening, ADME Properties, and Molecular Docking Simulations, *Molecules*, 2022, p 5571. <https://doi.org/10.3390/molecules27175571>
56. Wael H. Roshdy, Mohamed K. Khalifa, James Emmanuel San, Houriiyah Tegally, Eduan Wilkinson, Shymaa Showky, Darren Patrick Martin, Monika Moir, Amel Naguib, Nancy Elguindy, Mokhtar R. Gomaa, Manal Fahim, Hanaa Abu Elsood, Amira Mohsen, Ramy Galal, Mohamed Hassany, Richard J. Lessells, **Ahmed A. Al-Karmalawy**, Rabeh EL-Shesheny, Ahmed M. Kandeil, Mohamed A. Ali and Tulio de Oliveira: SARS-CoV-2 Genetic Diversity and Lineage Dynamics in Egypt during the First 18 Months of the Pandemic, *Viruses*, 2022, p 2283-2303. <https://doi.org/10.3390/v14091878>
57. Ahmed A. Gaber, Mohamed Sobhy, Abdallah Turkey, Hanan Gaber Abdulwahab, **Ahmed A. Al-Karmalawy**, Mostafa. A. Elhendawy, Mohamed. M. Radwan, Eslam B. Elkaeed, Ibrahim M. Ibrahim, Heba S. A. Elzahabi & Ibrahim H. Eissa: Discovery of new 1H-pyrazolo[3,4-d]pyrimidine derivatives as anticancer agents targeting EGFR^{WT} and EGFR^{T790M}, *Journal of Enzyme Inhibition*

and Medicinal Chemistry, 2022, p 2283-2303.

<https://doi.org/10.1080/14756366.2022.2112575>

58. Khaled Ahmed Mansour, Ahmed Elbermawi, **Ahmed A. Al-Karmalawy**, Mohamed-Farid Lahloub & Mona El-Neketi: Cytotoxic effects of extracts obtained from plants of the Oleaceae family: bio-guided isolation and molecular docking of new secoiridoids from *Jasminum humile*, *Pharmaceutical Biology*, 2022, p 1374-1383.
<https://doi.org/10.1080/13880209.2022.2098346>
59. Mohamed A. Salem, Riham A. El-Shiekh, Nora M. Aborehab, **Ahmed A. Al-Karmalawy**, Shahira M. Ezzat, Saleh Alseekh, Alisdair R. Ferni: Metabolomics driven analysis of *Nigella sativa* seeds identifies the impact of roasting on the chemical composition and immunomodulatory activity, *Food Chemistry*, 2022, p 133906. <https://doi.org/10.1016/j.foodchem.2022.133906>
60. Mahmoud M. A. Elsayed, Moustafa O. Aboelez, Mohamed S. Mohamed, Reda A. Mahmoud, Ahmed A. El-Shenawy, Essam A. Mahmoud, **Ahmed A. Al-Karmalawy**, Eman Y. Santali, Sameer Alshehri, Mahmoud Elkot Mostafa Elsadek, Mohamed A. El Hamd, and Abd El hakim Ramadan: Tailoring of Rosuvastatin Calcium and Atenolol Bilayer Tablets for the Management of Hyperlipidemia Associated with Hypertension: A Preclinical Study, *Pharmaceutics*, 2022, p 1629.
<https://doi.org/10.3390/pharmaceutics14081629>
61. Mohamed Elagawany, Ayman Abo Elmaaty, Ahmed Mostafa, Noura M. Abo Shama, Eman Y. Santali, Bahaa Elgendy, and **Ahmed A. Al-Karmalawy***: Ligand-based design, synthesis, computational insights, and in vitro studies of novel N-(5-Nitrothiazol-2-yl)-carboxamido derivatives as potent inhibitors of SARS-CoV-2 main protease, *Journal of Enzyme Inhibition and Medicinal Chemistry*, 2022, p 2112-2132.
<http://dx.doi.org/10.1080/14756366.2022.2105322>
62. Omnia Kutkat, Yassmin Moatasim, **Ahmed A. Al-Karmalawy**, Hamada S. Abulkhair, Mokhtar R. Gomaa, Ahmed N. El-Taweel, Noura M. Abo Shama, Mohamed GabAllah, Dina B. Mahmoud, Ghazi Kayali, Mohamed A. Ali, Ahmed Kandeil & Ahmed Mostafa: Robust antiviral activity of commonly prescribed antidepressants against emerging coronaviruses: in vitro and in silico drug repurposing studies, *Scientific Reports*, 2022, p 12920.
<http://dx.doi.org/10.1038/s41598-022-17082-6>
63. Wael H. Roshdy, Ahmed Kandeil, Rabeh El-Shesheny, Mohamed K. Khalifa, **Ahmed A. Al-Karmalawy**, Shymaa Showky, Amel Naguib, Nancy Elguindy, Manal Fahim, Hanaa Abu Elsood, Ahmed El Taweel, Azza Salamony, Amira Mohsen, Ghazi Kayali, Mohamed A. Ali, and Amr Kandeil: Insight into Genetic Characteristics of Identified SARS-CoV-2 Variants in Egypt from March 2020 to May 2021, *Pathogens*, 2022, p 834.
<https://doi.org/10.3390/pathogens11080834>
64. Amany Belal, Nagwa M. Abdel Gawad, Ahmed B. M. Mehany, Mohammed A. S. Abourehab, Hazem Elkady, **Ahmed A. Al-Karmalawy** & Ahmed S. Ismael: Design, synthesis and molecular docking of new fused 1H-pyrroles, pyrrolo[3,2-d]pyrimidines and pyrrolo[3,2-e][1, 4]diazepine derivatives as potent EGFR/CDK2 inhibitors, *Journal of Enzyme Inhibition and Medicinal Chemistry*, 2022, p 1884–1902. <https://doi.org/10.1080/14756366.2022.2096019>
65. Enas Abdelhameed Mahmoud HUSEEIN, Mohamed SAMIR, **Ahmed A. AL-KARMALAWY**, Shima S. HASSAN, Mona EMBAREK MOHAMED, Fatma Abdel Aziz Mohamed MOSTAFA, Ahmed M. MOHARRAM, Samia S. ALKHALIL, Haiam Mohamed Mahmoud FARRAG: *Ganoderma lucidum* extract inhibits *Schistosoma mansoni* survival in silico and in vitro study, *Annals of Parasitology*, 2022, p 323-330. <https://doi.org/10.17420/ap6802.438>

66. Mohamed M. Hammouda, Ayman Abo Elmaaty, Mohamed S. Nafie, Marwa Abdel-Motaal, Noha S. Mohamed, Mohamed A. Tantawy, Amany Belal, Radwan Alnajjar, Wagdy M. Eldehna, **Ahmed A. Al-Karmalawy***: Design and synthesis of novel benzoazoninone derivatives as potential CBSIs and apoptotic inducers: In Vitro, in Vivo, molecular docking, molecular dynamics, and SAR studies, *Bioorganic Chemistry*, 2022, p 105995.
<https://doi.org/10.1016/j.bioorg.2022.105995>
67. Eman Zekry Attia, Basma Ali Khalifa, Gehan M. Shaban, Mohamed N. Amin, Lina Akil, Ibrahim Khadra, **Ahmed A. Al-Karmalawy**, Radwan Alnajjar, Marco Y. W. Zaki, Omar M. Aly, Mo'men H. El-Katatny, Usama Ramadan Abdelmohsen: Potential topoisomerases inhibitors from *Aspergillus terreus* using virtual screening, *South African Journal of Botany*, 2022, p 632-645.
<https://doi.org/10.1016/j.sajb.2022.06.051>
68. Mohamed M. Hammoud, Muhammad Khattab, Marwa Abdel-Motaal, Johan Van der Eycken, Radwan Alnajjar, Hamada S. Abulkhair & **Ahmed A. Al-Karmalawy***: Synthesis, structural characterization, DFT calculations, molecular docking, and molecular dynamics simulations of a novel ferrocene derivative to unravel its potential antitumor activity, *Journal of Biomolecular Structure and Dynamics*, 2022, p 5199-5216.
<https://doi.org/10.1080/07391102.2022.2082533>
69. Mona F. El-Azab, **Ahmed A. Al-Karmalawy***, Samar A. Antar, Pierre A. Hanna, Karim M. Tawfik, Reem M. Hazem: A novel role of Nano selenium and sildenafil on streptozotocin-induced diabetic nephropathy in rats by modulation of inflammatory, oxidative, and apoptotic pathways, *Life Sciences*, 2022, p 120691. <https://doi.org/10.1016/j.lfs.2022.120691>
70. Amany Belal, Mohamed A. Elanany, Eman Y. Santali, **Ahmed A. Al-Karmalawy**, Moustafa O. Aboelez, Ali H. Amin, Magda H. Abdellattif, Ahmed B. M. Mehany, and Hazem Elkady: Screening a Panel of Topical Ophthalmic Medications against MMP-2 and MMP-9 to Investigate Their Potential in Keratoconus Management, *Molecules*, 2022, p 3584.
<https://doi.org/10.3390/molecules27113584>
71. Mohamed M. Hammoud, Alaa S. Nageeb, M. A. Morsi, Esam Arafa Gomaa, Ayman Abo Elmaaty, and **Ahmed A. Al-Karmalawy***: Design, Synthesis, Biological Evaluation, and SAR Studies of Novel Cyclopentaquinoline Derivatives as DNA Intercalators, Topoisomerase II Inhibitors, and Apoptotic Inducers, *New Journal of Chemistry*, 2022, p 11422-11436.
<https://doi.org/10.1039/D2NJ01646>
72. A. A. El Leithy, **A. A. Al-Karmalawy***, O. M. Youssif, Y. A. Ebrahim, A. S. Khalifa, E. B. Elkaeed, F. S. Abo-Zeid: Spirulina therapeutic potentiality in polycystic ovarian syndrome management using DHEA-induced rat model, *European Review for Medical and Pharmacological Sciences*, 2022, p 2740-2754. http://dx.doi.org/10.26355/eurrev_202204_28604
73. Rogy R. Ezz Eldin, Marwa A. Saleh, Mohammad Hayal Alotaibi, Reem K. Alsuair, Yahya A. Alzahrani, Feras A. Alshehri, Amany F. Mohamed, Shaimaa M. Hafez, Azza Ali Althoqapy, Seham K. Khirala, Mona M. Amin, Yousuf A. F, Azza H. Abdelwahab, Mohamed S. Alesawy, Ayman Abo Elmaaty, and **Ahmed A. Al-Karmalawy***: Ligand-based design and synthesis of N'-Benzylidene-3,4-dimethoxybenzohydrazide derivatives as potential antimicrobial agents; evaluation by in vitro, in vivo, and in silico approaches with SAR studies, *Journal of Enzyme Inhibition and Medicinal Chemistry*, 2022, p 1098-1119.
<https://doi.org/10.1080/14756366.2022.2063282>
74. Rogy R. Ezz Eldin, **Ahmed A. Al-Karmalawy***, Mohammad Hayal Alotaibi, and Marwa A. Saleh: Quinoxaline derivatives as a promising scaffold for breast cancer treatment, *New Journal of*

- Chemistry*, 2022, p 9975-9984. <https://doi.org/10.1039/D2NJ00050D>
75. Abeer M. El-Naggar, A. M. A. Hassan, Eslam B. Elkaeed, Mohamed S. Alesawy, **Ahmed A. Al-Karmalawy***: Design, synthesis, and SAR studies of novel 4-methoxyphenyl pyrazole and pyrimidine derivatives as potential dual tyrosine kinase inhibitors targeting both EGFR and VEGFR-2, *Bioorganic Chemistry*, 2022, p 105770.
<http://dx.doi.org/10.1016/j.bioorg.2022.105770>
76. Nada A Ashour, Ayman Abo Elmaaty, Amany A Sarhan, Eslam B Elkaeed, Ahmed M Moussa, Ibrahim Ali Erfan, **Ahmed A Al-Karmalawy***: A Systematic Review of the Global Intervention for SARS-CoV-2 Combating: From Drugs Repurposing to Molnupiravir Approval, *Drug Design, Development and Therapy*, 2022, p 685–715.
<https://doi.org/10.2147%2FDDDT.S354841>
77. Richie R Bhandare, Chandrashekar S. Munikrishnappa, G.V. Suresh Kumar, Sathish Kumar Konidala, Dilep Kumar Sigalapalli, Yogesh Vaishnav, Sampath Chinnam, Haya Yasin, **Ahmed A. Al-karmalawy**, Afzal B. Shaik: Multistep synthesis and screening of heterocyclic tetrads containing furan, pyrazoline, thiazole and triazole (or oxadiazole) as antimicrobial and anticancer agents, *Journal of Saudi Chemical Society*, 2022, p 101447.
<https://doi.org/10.1016/j.jscs.2022.101447>
78. Mohamed A. Salem, Nora M. Aborehab, **Ahmed A. Al-Karmalawy**, Alisdair R. Fernie, Saleh Alseekh, and S. Hahira M. Ezzat: Potential Valorization of Edible Nuts By-Products: Exploring the Immune-Modulatory and Antioxidants Effects of Selected Nut Shells Extracts in Relation to Their Metabolic Profiles, *Antioxidants*, 2022, p 462.
<https://doi.org/10.3390/antiox11030462>
79. Rana El-Masry, **Ahmed A. Al-Karmalawy***, Radwan A Alnajjar, Sara Mahmoud, Ahmed Mostafa, Hanan Kadry, Sahar Abou-Seri, and Azza Taher: Newly Synthesized Series of Oxindole-Oxadiazole Conjugates as Potential Anti-SARS-CoV-2 Agents: *In Silico* and *In Vitro* Studies, *New Journal of Chemistry*, 2022, p 5078-5090.
<https://doi.org/10.1039/D1NJ04816C>
80. Aml Ghanem, **Ahmed A. Al-Karmalawy***, Ahmed I. Abd El Maksoud, Shaden M. Hanafy, Hamdy A. Emara, Rasha M. Saleh, Mohamed F. Elshal: *Rumex Vesicarius* L. extract improves the efficacy of doxorubicin in triple-negative breast cancer through inhibiting Bcl2, mTOR, JNK1 and augmenting p21 expression, *Informatics in Medicine Unlocked*, 2022, p 100869.
<https://doi.org/10.1016/j.imu.2022.100869>
81. Dina B. Mahmoud, Mohamed Mofreh Bakr, **Ahmed A. Al-Karmalawy**, Yassmin Moatasim, Ahmed El Taweel & Ahmed Mostafa: Scrutinizing the Feasibility of Nonionic Surfactants to Form Isotropic Bicelles of Curcumin: a Potential Antiviral Candidate Against COVID-19, *AAPS PharmSciTech*, 2022, p 44. <http://dx.doi.org/10.1208/s12249-021-02197-2>
82. Ayman Abo Elmaaty, Khaled M. Darwish, Amani Chrouda, Amira A. Boseila, Mohamed A. Tantawy, Sameh S. Elhady, Afzal B. Shaik, Muhamad Mustafa, and **Ahmed A. Al-karmalawy***: *In Silico* and *In Vitro* Studies for Benzimidazole Anthelmintics Repurposing as VEGFR-2 Antagonists: Novel Mebendazole-Loaded Mixed Micelles with Enhanced Dissolution and Anticancer Activity, *ACS OMEGA*, 2021, p 875–899.
<https://doi.org/10.1021/acsomega.1c05519>
83. Dalia Elebeedy, Ingy Badawy, Ayman Abo Elmaaty, Moustafa M. Saleh, Ahmed Kandeil, Aml Ghanem, Omnia Kutkat, Radwan Alnajjar, Ahmed I. Abd El Maksoud, **Ahmed A. Al-karmalawy***: *In vitro* and computational insights revealing the potential inhibitory effect of

- Tanshinone IIA against influenza A virus, *Computers in Biology and Medicine*, 2021, p 105149.
<https://doi.org/10.1016/j.compbiomed.2021.105149>
84. Mohamed M. Khalifa, **Ahmed A. Al-Karmalawy**, Eslam B. Elkaeed, Mohamed S. Nafie, Mohamed A. Tantawy, Ibrahim H. Eissa & Hazem A. Mahdy: Topo II inhibition and DNA intercalation by new phthalazine-based derivatives as potent anticancer agents: design, synthesis, anti-proliferative, docking, and *in vivo* studies, *Journal of Enzyme Inhibition and Medicinal Chemistry*, 2021, p 299-314. <https://doi.org/10.1080/14756366.2021.2007905>
 85. A. A. Mohamed, **A. A. Al-Karmalawy***, A.A. El-Kholy, D.A. El-Damas, H.M. Abostate, S.M. Mostafa, M. Hamada, M.A. Khalik Elkady, Y. Hassan, E. Al-Hussain, M.G. Khalil, I. Badawy, D. Elebeedy, B.A. Alsouk, M.M. Shaheen: Effect of Vitamin D supplementation in patients with liver cirrhosis having spontaneous bacterial peritonitis: a randomized controlled study, *European Review for Medical and Pharmacological Sciences*, 2021, p 6908-6919.
https://doi.org/10.26355/eurrev_202111_27239
 86. Reem M.Hazem, Samar A. Antar, Yossef K. Nafea, **Ahmed A. Al-Karmalawy**, Mohamed A. Salehd, Mona F. El-Azab: Pirfenidone and vitamin D mitigate renal fibrosis induced by doxorubicin in mice with Ehrlich solid tumor, *Life Sciences*, 2021, p 120185.
<https://doi.org/10.1016/j.lfs.2021.120185>
 87. **Ahmed A. Al-Karmalawy***, Raya Soltane, Ayman Abo Elmaaty, Mohamed A. Tantawy, Samar A. Antar, Galal Yahya, Amani Chrouda, Rami Adel Pashameah, Muhamad Mustafa, Mobarak Abu Mraheil, and Ahmed Mostafa: Coronavirus Disease (COVID-19) Control between Drug Repurposing and Vaccination: A Comprehensive Overview, *Vaccines*, 2021, p 1317.
<https://doi.org/10.3390/vaccines9111317>
 88. Mohammed I. A. Hamed, Khaled M. Darwish, Raya Soltane, Amani Chrouda, Ahmed Mostafa, Noura M. Abo Shama, Sameh S. Elhady, Hamada S. Abulhair, Ahmed E. Khodir, Ayman Abo Elmaaty, and **Ahmed A. Al-Karmalawy***: β -Blockers bearing hydroxyethylamine and hydroxyethylene as potential SARS-CoV-2 Mpro inhibitors: rational based design, in silico, in vitro, and SAR studies for lead optimization, *RSC Advances*, 2021, p 35536-35558.
<https://doi.org/10.1039/D1RA04820A>
 89. Shenouda G. Elia, **Ahmed A. Al-Karmalawy**, Mohamed Y. Nasr, Mohamed F. Elshal: Loperamide potentiates doxorubicin sensitivity in triple-negative breast cancer cells by targeting MDR1 and JNK and suppressing mTOR and Bcl-2: In vitro and molecular docking study, *Journal of Biochemical and Molecular Toxicology*, 2021, p 22938.
<https://doi.org/10.1002/jbt.22938>
 90. Mona A. Raslan, Rehab F. Taher, **Ahmed A. Al-Karmalawy**, Dalia El-Ebeedy, Angham G. Metwaly, Nourhan M. Elkateeb, Aml Ghanem, Reem A. Elghaishh, and Ahmed I. Abd El Maksoud: Cordyline fruticosa (L.) A. Chev. leaves: isolation, HPLC/MS profiling and evaluation of nephroprotective and hepatoprotective activities supported by molecular docking, *New Journal of Chemistry*, 2021, p 22216-22233. <https://doi.org/10.1039/D1NJ02663A>
 91. **Ahmed A. Al-Karmalawy***, Mai M. Farid, Ahmed Mostafa, Alia Y. Ragheb, Sara H. Mahmoud, Mahmoud Shehata, Noura M. Abo Shama, Mohamed GabAllah, Gomaa Mostafa-Hedeab, and Mona M. Marzouk: Naturally Available Flavonoid Aglycones as Potential Antiviral Drug Candidates against SARS-CoV-2, *Molecules*, 2021, p 6559.
<https://doi.org/10.3390/molecules26216559>
 92. Rana T. Diab, Zakaria K. Abdel-Sami, Eatedal H. Abdel-Aal, **Ahmed A. Al-Karmalawy***, and Nader E. Abo-Dya: Design and synthesis of a new series of 3,5-disubstituted-1,2,4-oxadiazoles as

potential colchicine binding site inhibitors: antiproliferative activity, molecular docking, and SAR studies, *New Journal of Chemistry*, 2021, p 21657-21669.

<https://doi.org/10.1039/D1NJ02885E>

93. Tahsin Shoala, **Ahmed A. Al-Karmalawy**, Mousa O. Germoush, Salha M. ALshamrani, Mohamed A. Abdein and Nabil S. Awad: Nanobiotechnological Approaches to Enhance Potato Resistance against Potato Leafroll Virus (PLRV) Using Glycyrrhizic Acid Ammonium Salt and Salicylic Acid Nanoparticles, *Horticulturae*, 2021, p 402.

<https://doi.org/10.3390/horticulturae7100402>

94. Mahmoud M. Shehata, Sara H. Mahmoud, Mohammad Tarek, **Ahmed A. Al-Karmalawy**, Amal Mahmoud, Ahmed Mostafa, Mahmoud M. Elhefnawi and Mohamed A. Ali: *In Silico* and *In Vivo* Evaluation of SARS-CoV-2 Predicted Epitopes-Based Candidate Vaccine, *Molecules*, 2021, p 6182. <https://doi.org/10.3390/molecules26206182>

95. Amal Mahmoud, Essam Kotb, Amany I. Alqosaibi, **Ahmed A. Al-Karmalawy**, Ibtesam S. Al-Dhuayan, Hameedah Alabkari: In vitro and in silico characterization of alkaline serine protease from *Bacillus subtilis* D9 recovered from Saudi Arabia, *Heliyon*, 2021, p 08148.

<https://doi.org/10.1016/j.heliyon.2021.e08148>

96. Rehab F. Taher, **Ahmed A. Al-Karmalawy**, Ahmed I. Abd El Maksoud, Hany Khalil, Amr Hassan, Ezzel-Din A. El-Khrisy, Walaa A. El-Kashak: Two new flavonoids and anticancer activity of *Hymenosporem flavum*: in vitro and molecular docking studies, *Journal of Herbmed Pharmacology*, 2021, p 443-458. <http://dx.doi.org/10.34172/jhp.2021.52>

97. Maged A. Aziz, Wesam S. Shehab, **Ahmed A. Al-Karmalawy**, Ahmed F. EL-Farargy and Magda H. Abdellattif: Design, Synthesis, Biological Evaluation, 2D-QSAR Modeling, and Molecular Docking Studies of Novel 1H-3-Indolyl Derivatives as Significant Antioxidants, *International Journal of Molecular Sciences*, 2021, p 10396.

<https://doi.org/10.3390/ijms221910396>

98. Heba A. El Gizawy, Sylvia A. Boshra, Ahmed Mostafa, Sara H. Mahmoud, Muhammad I. Ismail, Aisha A. Alsouk, Azza T. Taher and **Ahmed A. Al-Karmalawy***: *Pimenta dioica* (L.) Merr. Bioactive Constituents Exert Anti-SARS-CoV-2 and Anti-Inflammatory Activities: Molecular Docking and Dynamics, *In Vitro*, and *In Vivo* Studies, *Molecules*, 2021, p 5844.

<http://dx.doi.org/10.3390/molecules26195844>

99. Amr El-Demerdash[‡], **Ahmed A. Al-Karmalawy***, Tarek Mohamed Abdel-Aziz, Sameh S. Elhady, Khaled M. Darwish and Ahmed H. E. Hassan: Investigating the structure–activity relationship of marine natural polyketides as promising SARS-CoV-2 main protease inhibitors, *RSC Advances*, 2021, p 31339-31363. <https://doi.org/10.1039/D1RA05817G>

100.

Ahmed A. Zakia, **Ahmed A. Al-Karmalawy***, Ahmed E. Khodir, Yasser A. El-Amier, Ahmed Ashour: Isolation of cytotoxic active compounds from *Reichardia tingitana* with investigation of apoptosis mechanistic induction: In silico, in vitro, and SAR studies, *South African Journal of Botany*, 2021, p 115-123. <https://doi.org/10.1016/j.sajb.2021.08.006>

101.

Dina B. Mahmoud, Walaa M. Ismail, Yassmin Moatasim, Omnia Kutkat, Aliaa N. ElMeshad, Shahira M. Ezzat, Kadriya S. El Deeb, Ahlam M. El-Fishawy, Mokhtar R. Gomaa, Ahmed Kandeil, **Ahmed A. Al-karmalawy**, Mohamed A. Ali, Ahmed Mostafa: Delineating a potent antiviral activity of *Cuphea ignea* extract loaded nano-formulation against SARS-CoV-2: In silico and in vitro studies, *Journal of Drug Delivery Science and Technology*, 2021, p 102845.

<https://doi.org/10.1016/j.jddst.2021.102845>

102.

Amal Mahmoud, Ahmed Mostafa, **Ahmed A. Al-Karmalawy**, Ahmad Zidan, Hamada S. Abulkhair, Sara H. Mahmoud, Mahmoud Shehata, Mahmoud M. Elhefnawi, Mohamed A. Ali: Telaprevir is a potential drug for repurposing against SARS-CoV-2: computational and *in vitro* studies, *Heliyon*, 2021, p 07962. <https://doi.org/10.1016/j.heliyon.2021.e07962>

103.

Dalia Elebeedy, Walid F. Elkhatib, Ahmed Kandeil, Aml Ghanem, Omnia Kutkat, Radwan Alnajjar, Marwa A. Saleh, Ahmed I. Abd El Maksoud, Ingy Badawy and **Ahmed A. Al-Karmalawy***: Anti-SARS-CoV-2 activities of tanshinone IIA, carnosic acid, rosmarinic acid, salvianolic acid, baicalein, and glycyrrhetic acid between computational and in vitro insights, *RSC Advances*, 2021, p 29267-29286. <https://doi.org/10.1039/d1ra05268c>

104.

Ahmed A. Gaber, Ahmed M. El-Morsy, Farag F. Sherbiny, Ashraf H. Bayoumi, Kamal M. El-Gamal, Khaled El-Adl, **Ahmed A. Al-Karmalawy**, Rogy R. Ezz Eldin, Marwa A. Saleh, Hamada S. Abulkhair: Pharmacophore-linked pyrazolo[3,4-d]pyrimidines as EGFR-TK inhibitors: Synthesis, anticancer evaluation, pharmacokinetics, and in silico mechanistic studies, *Archiv der Pharmazie*, 2021, p 2100258. <https://doi.org/10.1002/ardp.202100258>

105.

Mohamed A. Soltan, Muhammad Alaa Eldeen, Nada Elbassiouny, Ibrahim Mohamed, Dalia A. El-damasy, Eman Fayad, Ola A. Abu Ali, Nermin Raafat, Refaat A. Eid and **Ahmed A. Al-Karmalawy***: Proteome Based Approach Defines Candidates for Designing a Multitope Vaccine against the Nipah Virus, *International Journal of Molecular Sciences*, 2021, p 9330. <https://doi.org/10.3390/ijms22179330>

106.

Abdallah E. Abdallah, Mohamed S. Alesawy, Sally I. Eissa, Esmail M. El-Fakharany, Mohamed H. Kalab, Mohamed H. Sharaf, Noura M. Abo Shama, Sara H. Mahmoud, f Ahmed Mostafa, **Ahmed A. Al-Karmalawy**, and Hazem Elkady: Design and synthesis of new 4-(2-nitrophenoxy)benzamide derivatives as potential antiviral agents: molecular modeling and in vitro antiviral screening, *New Journal of Chemistry*, 2021, p 16557-16571. <https://doi.org/10.1039/D1NJ02710G>

107.

Chao Ma, Mohammed S. Taghour, Amany Belal, Ahmed Mehany, Naglaa Mostafa, Ahmed Nabeeh and Ibrahim Eissa, **Ahmed A. Al-Karmalawy***: Design and Synthesis of New Quinoxaline Derivatives as Potential Histone Deacetylase Inhibitors Targeting Hepatocellular Carcinoma: In Silico, In Vitro, and SAR Studies, *Frontiers in Chemistry*, 2021, p 725135. <https://doi.org/10.3389/fchem.2021.725135>

108.

Mohamed H. El-Shershaby, Kamal M. El-Gamal, Ashraf H. Bayoumi, Khaled El-Adl, Mohamed Alswah, Hany E. A. Ahmed, **Ahmed A. Al-Karmalawy** and Hamada S. Abulkhair: The antimicrobial potential and pharmacokinetic profiles of novel quinoline-based scaffolds: synthesis and in silico mechanistic studies as dual DNA gyrase and DHFR inhibitors, *New Journal of Chemistry*, 2021, p 13986-14004. <https://doi.org/10.1039/D1NJ02838C>

109.

Ayman Abo Elmaaty, Mohammed I. A. Hamed, Muhammad I. Ismail, Eslam B. Elkaeed, Hamada

S. Abulkhair, Muhammad Khattab and **Ahmed A. Al-Karmalawy***: Computational Insights on the Potential of Some NSAIDs for Treating COVID-19: Priority Set and Lead Optimization, *Molecules*, 2021, p 3772. <https://doi.org/10.3390/molecules26123772>

110.

Mohamed A. Soltan, Nada Elbassiouny, Helmy Gamal, Eslam B. Elkaeed, Refaat A. Eid, Muhammad Alaa Eldeen and **Ahmed A. Al-Karmalawy***: *In Silico* Prediction of a Multitope Vaccine against *Moraxella catarrhalis*: Reverse Vaccinology and Immunoinformatics, *Vaccines*, 2021, p 669. <https://doi.org/10.3390/vaccines9060669>

111.

Ahmed Kandeil, Ahmed Mostafa, Omnia Kutkat, Yassmin Moatasim, **Ahmed A. Al-Karmalawy**, Adel A. Rashad, Ahmed E. Kayed, Azza E. Kayed, Rabeh El-Shesheny, Ghazi Kayali and Mohamed A. Ali: Bioactive Polyphenolic Compounds Showing Strong Antiviral Activities against Severe Acute Respiratory Syndrome Coronavirus 2, *Pathogens*, 2021, p 758. <https://doi.org/10.3390/pathogens10060758>

112.

Mohamed H. El-Shershaby, Adel Ghiaty, Ashraf H. Bayoumi, **Ahmed A. Al-Karmalawy**, Ebtehal M. Husseiny, Mona S. El-Zoghbi, Hamada S. Abulkhair: From triazolophthalazines to triazoloquinazolines: A bioisosterism-guided approach toward the identification of novel PCAF inhibitors with potential anticancer activity, *Bioorganic & Medicinal Chemistry*, 2021, p 116266. <https://doi.org/10.1016/j.bmc.2021.116266>

113.

Amany A. Sarhan, Nada A. Ashour, **Ahmed A. Al-Karmalawy***: The journey of antimalarial drugs against SARS-CoV-2: Review article, *Informatics in Medicine Unlocked*, 2021, p 100604. <https://doi.org/10.1016%2Fj.imu.2021.100604>

114.

Raya Soltane, Amani Chrouda, Ahmed Mostafa, **Ahmed A. Al-Karmalawy**, Karim Chouaïb, Abdelwaheb dhahri, Rami Adel Pashameah, Ahlam Alasiri, Omnia Kutkat, Mahmoud Shehata, Hichem Ben Jannet, Jawhar Gharbi and Mohamed A. Ali: Strong Inhibitory Activity and Action Modes of Synthetic Maslinic Acid Derivative on Highly Pathogenic Coronaviruses: COVID-19 Drug Candidate, *Pathogens*, 2021, p 623. <https://doi.org/10.3390/pathogens10050623>

115.

Ahmed A. Zaki, Ahmed Ashour, Sameh S. Elhady, Khaled M. Darwish, **Ahmed A. Al-Karmalawy***: Calendulaglycoside A showing potential activity against SARS-CoV-2 main protease: Molecular docking, molecular dynamics, and SAR studies, *Journal of Traditional and Complementary Medicine*, 2021, p 16-34. <https://doi.org/10.1016/j.jtcme.2021.05.001>

116.

Mohamed F. Elshal, Norhan M. Eid, Ibrahim El-Sayed, Wael El-Sayed, **Ahmed A. Al-Karmalawy***: Concanavalin-A shows synergistic cytotoxicity with tamoxifen via inducing apoptosis in estrogen receptor-positive breast cancer: In vitro and molecular docking studies, *Pharmaceutical Sciences*, 2021, p 76-85. <http://dx.doi.org/10.34172/PS.2021.22>

117.

Ahmed A. Al-Karmalawy, Mohammed A. Dahab, Ahmed M. Metwaly, Sameh S. Elhady, Eslam B. Elkaeed, Ibrahim Eissa, and Khaled M. Darwish: Molecular docking and dynamics simulation revealed the potential inhibitory activity of ACEIs against SARS-CoV-2 targeting hACE2 receptor, *Frontiers in Chemistry*, 2021, p 661230. <https://doi.org/10.3389/fchem.2021.661230>

118. Ayman Abo Elmaaty, Radwan Alnajjar, Mohammed I. A. Hamed, Muhammad Khattab, Mohamed M. Khalifa and **Ahmed A. Al-Karmalawy***: Revisiting activity of some glucocorticoids as a potential inhibitor of SARS-CoV-2 main protease: theoretical study, *RSC Advances*, 2021, p 10027-10042. <https://doi.org/10.1039/D0RA10674G>
119. Reham M. Samra, Amal F. Soliman, Ahmed A. Zakia, Ahmed Ashour, **Ahmed A. Al-Karmalawy**, Madiha A. Hassan, Ahmed M. Zaghoul: Bioassay-guided isolation of a new cytotoxic ceramide from *Cyperus rotundus* L., *South African Journal of Botany*, 2021, p 210-216. <https://doi.org/10.1016/j.sajb.2021.02.007>
120. M Khattab and **Ahmed A. Al-Karmalawy***: Revisiting Activity of Some Nocodazole Analogues as a Potential Anticancer Drugs Using Molecular Docking and DFT Calculations, *Frontiers in Chemistry*, 2021, p 628398. <https://doi.org/10.3389/fchem.2021.628398>
121. **Ahmed A. Al-Karmalawy***, Radwan Alnajjar, Mohammed M. Dahab, Ahmed. M. Metwaly, Ibrahim. H. Eissa: Molecular docking and dynamics simulations reveal the potential of anti-HCV drugs to inhibit COVID-19 main protease, *Pharmaceutical Sciences*, 2021, p 661230. <http://dx.doi.org/10.34172/PS.2021.3>
122. Radwan Alnajjar, Ahmed Mostafa, Ahmed Kandeil, **Ahmed A. Al-Karmalawy***: Molecular docking, molecular dynamics, and in vitro studies reveal the potential of angiotensin II receptor blockers to inhibit the COVID-19 main protease, *Heliyon*, 2020, p 05641. <https://doi.org/10.1016/j.heliyon.2020.e05641>
123. Mohamed S. Alesawy, **Ahmed A. Al-Karmalawy**, Eslam B. Elkaeed, Mohamed Alswah, Ahmed Belal, Mohammed S. Taghour, Ibrahim H. Eissa: Design and discovery of new 1,2,4-triazolo[4,3-c]quinazolines as potential DNA intercalators and topoisomerase II inhibitors, *Archiv der Pharmazie*, 2020, p 2000237. <https://doi.org/10.1002/ardp.202000237>
124. Shenouda G. Eliaa, **Ahmed A. Al-Karmalawy***, Rasha M. Saleh, and Mohamed F. Elshal: Empagliflozin and Doxorubicin Synergistically Inhibit the Survival of Triple-Negative Breast Cancer Cells via Interfering with the mTOR Pathway and Inhibition of Calmodulin: *In Vitro* and Molecular Docking Studies, *ACS Pharmacology & Translational Science*, 2020, p 1330–1338. <https://doi.org/10.1021/acsp.20200144>
125. Aml Ahmed Ghanem, Hamdy Emara, Shaden Hanafy, Ahmed Abd EL-Maksoud, **Ahmed A. Al-Karmalawy*** and Mohamed El Shal: Tanshinone IIA synergistically enhances the antitumor activity of Doxorubicin by interfering with PI3K/AKT/mTOR pathway and inhibition of topoisomerase II: in vitro and molecular docking studies, *New Journal of Chemistry*, 2020, p 17374-17381. <https://doi.org/10.1039/D0NJ04088F>
126. A. Zaki, **Ahmed A. Al-Karmalawy**, Y El-Amier, A. Ashour: Molecular docking reveals the potential of *Cleome amblyocarpa* isolated compounds to inhibit COVID-19 virus main protease,

New Journal of Chemistry, 2020, p 16752-16758.

<https://doi.org/10.1039/D0NJ03611K>

127.

Ahmed A. Al-Karmalawy*, M Khattab: Molecular modelling of mebendazole polymorphs as a potential colchicine binding site inhibitor, *New Journal of Chemistry*, 2020, p 13990-13996.

<https://doi.org/10.1039/D0NJ02844D>

B) The following below mentioned publications have evolved from my doctoral dissertation

128.

Abdel-Ghany A. El-Helby, Helmy Sakr, Ibrahim H. Eissa, **Ahmed A. Al-Karmalawy** and Khaled El-Adl: Benzoxazole/benzothiazole-derived VEGFR-2 inhibitors: Design, synthesis, molecular docking, and anticancer evaluations, *Archiv der Pharmazie*, 2019, p 1900178.

<https://doi.org/10.1002/ardp.201900178>

129.

Abdel-Ghany A. El-Helby, Helmy Sakr, Ibrahim H. Eissa, Hamada Abulkhair, **Ahmed A. Al-Karmalawy** and Khaled El-Adl: Design, synthesis, molecular docking, and anticancer activity of benzoxazole derivatives as VEGFR-2 inhibitors, *Archiv der Pharmazie*, 2019, p 1900113.

<https://doi.org/10.1002/ardp.201900113>

B) The following below mentioned publications have evolved from my master dissertation

130.

M.K. Ibrahim, K. El-Adl, **Ahmed A. Al-Karmalawy**: Design, synthesis, molecular docking and anticonvulsant evaluation of novel 6-iodo-2-phenyl-3-substituted quinazolin-4(3H)-ones, *Bulletin of Faculty of Pharmacy, Cairo University*, 2015, p 101-116.

<https://doi.org/10.1016/j.bfopcu.2015.05.001>

131.

M.K. Ibrahim, K. El-Adl, **Ahmed A. Al-Karmalawy**: Design, synthesis, molecular docking and biological evaluation of some novel quinazolin-4(3H)-one derivatives as anti-inflammatory agents, *Azhar Journal of Pharmaceutical Sciences, Al Azhar University*, 2012.

<https://www.researchgate.net/publication/341194096>.

Conference Presentations:

1- 25th September 2023: Invited speaker in the Second Scientific Forum of the School of Biotechnology, Badr University titled (Future Horizons for Biotechnology).

Oral presentation: The importance of *in silico* studies in the drug discovery process.

2- September 2022: attended and actively participated in the 3rd International Conference of Faculty of Pharmacy, Mansoura University held at Faculty of Pharmacy, Mansoura University.

Oral presentation: Ligand-Based Design and Synthesis of N'-Benzylidene-3,4-dimethoxybenzohydrazide Derivatives as Potential Antimicrobial Agents; Evaluation by In Vitro, In Vivo, and In Silico Approaches with SAR Studies.

3- 7th March 2020: attended and participated in the 8th Scientific Research Conference of the Faculty of Pharmacy, Mansoura University.

Oral presentation: Design, synthesis, and molecular docking of novel benzoxazole derivatives as

antiviral agents.

Poster: Design, synthesis, and molecular docking of novel benzothiazole derivatives as antiviral agents.

- 4- 8-9th December 2019: attended and participated in the poster session of the 2nd International Conference of Faculty of Pharmacy, Suez Canal University “Pharmaceuticals used in Internal Medicine”, Tolip El Forsan Resort, Ismailia, Egypt.

Poster title: Benzoxazole/benzothiazole-derived VEGFR-2 inhibitors: Design, synthesis, molecular docking, and anticancer evaluations.

Ahmed A. Al-Karmalawy, Abdel-Ghany A. El-Helby, Helmy Sakr, Ibrahim H. Eissa, and Khaled El-Adl.

- 5- 7th March 2019: attended and participated in the 7th Scientific Research Conference of the Faculty of Pharmacy, Mansoura University.

Oral presentation: Design, synthesis, molecular docking, and anticancer activity of benzoxazole derivatives as VEGFR-2 inhibitors.

Ahmed A. Al-Karmalawy, Abdel-Ghany A. El-Helby, Helmy Sakr, Ibrahim H. Eissa, Hamada Abulkhair, and Khaled El-Adl.

Courses and Workshops:

- 1- 10th May 2023: attended the online workshop entitled “**Nutritional Therapy and Clinical Nutrition**” at Menoufia University, Menoufia, Egypt.
- 2- 9th May 2023: attended the online workshop entitled “**Drug Design and Discovery Software**” at Menoufia University, Menoufia, Egypt.
- 3- 8-9th May 2023: attended the online workshop related to Bioinformatics entitled “**Biobanking and Clinical Pharmacogenomics PGx**” at Menoufia University, Menoufia, Egypt.
- 4- 24-25th April 2023: “**International Publishing of Scientific Research**”, Faculty and Leadership Development Center (FLDC), Cairo University, Ministry of Higher Education, Egypt.
- 5- 15-16th April 2023: “**Essentials of Integrated Education**”, Faculty and Leadership Development Center (FLDC), Cairo University, Ministry of Higher Education, Egypt.
- 6- 13-15th February 2023: attended the workshop entitled “**Program Course Specifications and Assessment of ILOs: Faculties and Institutes of Higher Education**” from the **National Authority for Quality Assurance and Accreditation of Education (NAQAAE)**, Cairo, Egypt.
- 7- 29-30th January 2023: attended the workshop entitled “**Strategic Planning: Faculties and Institutes of Higher Education**” from the **National Authority for Quality Assurance and Accreditation of Education (NAQAAE)**, Cairo, Egypt.
- 8- 21-22th January 2023: “**Critical Thinking**”, Faculty and Leadership Development Center (FLDC), Cairo University, Ministry of Higher Education, Egypt.
- 9- 19-20th January 2023: attended the course entitled “**Clinical Pharmacy and Drug Discovery Course**” at Ain Shams University, Cairo, Egypt.
- 10- 3-4th December 2022: “**Exams Systems and Students Assessment**”, Faculty and Leadership Development Center (FLDC), Cairo University, Ministry of Higher Education, Egypt.
- 11- 22nd July 2022: attended the workshop entitled “**Analysis of RNA-Seq data**” at Ain Shams University, Cairo, Egypt.
- 12- 22nd July 2022: attended the workshop entitled “**Online Bioinformatics Tools for Bulk NGS and single-cell Tumor Data**” at Ain Shams University, Cairo, Egypt.

- 13- 30-31th July 2022: “**Conference Organization**”, Faculty and Leadership Development Center (FLDC), University Development Center (UDC), Mansoura University, Ministry of Higher Education, Egypt.
- 14- 26-27th July 2022: “**Scientific Research and Methods of Universities Rankings**”, Faculty and Leadership Development Center (FLDC), University Development Center (UDC), Mansoura University, Ministry of Higher Education, Egypt.
- 15- 7-10th April 2021: Organizing the 20th National Symposium hosted by EPSF-HUE for students of the College of Pharmacy all over Egypt, with my team EPSF-HUE, and presented a session entitled “COVID-19 and Mental Health,
<https://www.youtube.com/watch?v=vqlBa8IgfVs>”.
- 16- 13th February 2021: attended the 2nd international JSPS webinar (Preparedness for the next COVID-19 wave Multidisciplinary impacts Health, Education and Environment).
- 17- 12-13th December 2020: attended the international conference (Pharmacists in Front Lines, New Challenges and Innovative Solutions) held at the faculty of pharmacy, MSA University, in co-operation with the University of GREENWICH.
- 18- 10-11th October 2020: attended the virtual scientific conference of the faculty of pharmacy, Tanta University 2020 (New Avenues in Pharmacy & Health Care).
- 19- 10-11th September 2020: attended the Virtual 7th EFMC Young Medicinal Chemists’ Symposium (Registration number: YMCS20/370).
- 20- 9-13th August 2020: attended the 1st International JSPS webinar series (COVID-19 crisis and the sustainable development goals: rule of the science & health challenges).
- 21- 8th August 2020: attended the workshop titled “**Enzyme Kinetics & Basics of Molecular Docking**” from Young Biologist.
- 22- 27-30th January 2020: Organizing the twelfth development conference for students of the College of Pharmacy at Horus University “**Step on The Way 2020 (SOTW 2020)**”, with my team EPSF-HUE, and presented two sessions entitled “**Drug/Drug and Drug/Food interactions**” and “Your Psychological Peace”.
- 23- December 2019: attended the workshop of Prof. Masaharu Sen, (Professor of nanotechnology and Dean of the Graduate School of Natural Science and Technology, Japan), entitled “**Development of Cancer Stem Cells and Drug Delivery System Targeting Cancer**” at The National Research Center, Giza, Egypt.
- 24- September 2019: attended a workshop training “**Measurement of Infection Control, Scientific Writing and Egyptian Knowledge Bank (EKB)**” at Horus University in Egypt, New Damietta, Egypt.
- 25- July 2019: attended and actively participated in the “**University Teacher Support**” Seminar that was held at the Faculty of Engineering, Ain Shams University and was organized by the National Erasmus+ Office-Egypt.
- 26- 19-20th April 2015: attended and actively participated in the “**Molecular Modeling and its Application in Drug Design**” Workshop that was held at the Faculty of Pharmacy, Future University in Egypt.
- 27- 2nd-20th July 2006: completed the didactic and practical requirements of the training course “**Clinical Practice for Pharmacists (Clinical Pharmacology)**” that was held at Cairo University and Bolak El-Dakrour General Hospital.

Honor's, Prizes, and Awards:

- 1- 2023: Awarded the **State Encouragement Award in the field of advanced technological sciences that serve the fields of medical sciences** for the year 2022.
- 2- Classified from the **2% World's Top Scientists' List (Stanford University - 2023)**.
- 3- 2022: Prize of the (highly cited research) from the **International Journal of Molecular Sciences** for the research item: Mohamed A. Soltan, Muhammad Alaa Eldeen, Nada Elbassiouny, Ibrahim Mohamed, Dalia A. El-damasy, Eman Fayad, Ola A. Abu Ali, Nermin Raafat, Refaat A. Eid and **Ahmed A. Al-Karmalawy***: Proteome Based Approach Defines Candidates for Designing a Multitope Vaccine against the Nipah Virus, *International Journal of Molecular Sciences*, 2021.
- 4- 2022: Prize of the (highly cited research) from **WILEY** for the research item: Shenouda G. Elia, **Ahmed A. Al-Karmalawy**, Mohamed Y. Nasr, Mohamed F. Elshal: Loperamide potentiates doxorubicin sensitivity in triple-negative breast cancer cells by targeting MDR1 and JNK and suppressing mTOR and Bcl-2: In vitro and molecular docking study, *Journal of Biochemical and Molecular Toxicology*, 2020.
- 5- 2022: Prize of the (highly cited research) from **WILEY** for the research item: Ahmed A. Gaber, Ahmed M. El-Morsy, Farag F. Sherbiny, Ashraf H. Bayoumi, Kamal M. El-Gamal, Khaled El-Adl, **Ahmed A. Al-Karmalawy**, Rogy R. Ezz Eldin, Marwa A. Saleh, Hamada S. Abulkhair: Pharmacophore-linked pyrazolo[3,4-d]pyrimidines as EGFR-TK inhibitors: Synthesis, anticancer evaluation, pharmacokinetics, and in silico mechanistic studies, *Archiv der Pharmazie*, 2020.
- 6- 2022: Prize of the (highly cited research) from **WILEY** for the research item: Mohamed S. Alesawy, **Ahmed A. Al-Karmalawy**, Eslam B. Elkaeed, Mohamed Alswah, Ahmed Belal, Mohammed S. Taghour, Ibrahim H. Eissa: Design and discovery of new 1,2,4-triazolo[4,3-c]quinazolines as potential DNA intercalators and topoisomerase II inhibitors, *Archiv der Pharmazie*, 2020.
- 7- 2021: Prize of the (highly cited research) from **WILEY** for the research item: Mohamed S. Alesawy, **Ahmed A. Al-Karmalawy**, Eslam B. Elkaeed, Mohamed Alswah, Ahmed Belal, Mohammed S. Taghour, Ibrahim H. Eissa: Design and discovery of new 1,2,4-triazolo[4,3-c]quinazolines as potential DNA intercalators and topoisomerase II inhibitors, *Archiv der Pharmazie*, 2020.
- 8- 2020: The 3rd Best Oral Presentation Award for the practical presentation entitled "Design, synthesis and molecular docking of novel benzoxazole derivatives as antiviral agents" at the 8th Scientific Research Conference of Faculty of Pharmacy, Mansoura University, Mansoura, Egypt.
- 9- 2020: The 3rd Best Poster Award for the poster entitled "Design, synthesis and molecular docking of novel benzothiazole derivatives as antiviral agents" at the 8th Scientific Research Conference of Faculty of Pharmacy, Mansoura University, Mansoura, Egypt.
- 10- 2019: The Best Poster Award for the poster entitled "Benzoxazole/benzothiazole-derived VEGFR-2 inhibitors: Design, synthesis, molecular docking, and anticancer evaluations" at the 2nd International Conference of Faculty of Pharmacy, Suez Canal university "Pharmaceuticals used in Internal Medicine", Tolip El Forsan Resort, Ismailia, Egypt.

References:

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