

# Khaled M. Darwish, Ph.D.

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## Personal Data

Date of birth: Aug. 28, 1983  
Place of birth: Port Said, Egypt  
Marital status: Married  
Languages: Arabic, English  
Address: Department of Medicinal Chemistry  
Faculty of Pharmacy  
Suez Canal University  
Ismailia 41522  
EGYPT

ORCID ID: <https://orcid.org/0000-0002-0597-482X>  
ResearcherID: [M-1052-2019](https://orcid.org/0000-0002-0597-482X)  
WOS *h*-index: **15**  
Scopus *h*-index: **14**  
Voice: (20) 100-5330114  
E-mail: [Khaled\\_darwish@pharm.suez.edu.eg](mailto:Khaled_darwish@pharm.suez.edu.eg)

## Education

03/2013-04/2016

**PhD in Medicinal Chemistry**, Pharmacy, Faculty of Pharmacy, Suez Canal University, Ismailia, Egypt.

- Title: Design and synthesis of novel heterocyclic compounds as potential anti-diabetic agents (**Funded by the Science and Technology Development Fund (STDF), Egypt, Grant #4244, as a Junior Scientist investigator**).
- Projects: Using computational chemistry tools to develop a diverse class of molecules acting as novel PPAR- $\gamma$ /FFAR1 co-agonists tailored for type II diabetes mellitus management acting as insulin sensitizer as well as insulin secretagogue. Our strategy was based on incorporating the structural features of glitazones, keeping the thiazolidindione head as a suitable acid surrogate, with GPCRs' privileged structures through a non-branched linker. The compounds with this pharmacophore were synthesized and using the appropriate analytical techniques including  $^1\text{H-NMR}$ ,  $^{13}\text{C-NMR}$  to determine the accuracy of the synthesized compounds. That is followed by biological assays to evaluate the receptors activation by the synthesized compounds. Several compounds showed balanced dual PPAR- $\gamma$ /FFAR1 agonism with  $\text{EC}_{50}$  down to one-digit micromolar values.

09/2008-01/2013

**MSc in Medicinal Chemistry**, Pharmacy, Faculty of Pharmacy, Suez Canal University, Ismailia, Egypt.

- Title: Spectrophotometric and Chromatographic Analysis of Some Skeletal Muscle Relaxants, Anti-inflammatory and Gastro-intestinal Agents in Different Pharmaceutical Preparations
- Projects: Involving analysis of different medicinal agents both in pure and dosage forms using different analytical techniques together with stability testing and method validation. That involved both straightforward and post-column

derivatization reversed phase HPLC and spectrophotometric analysis including colorimetric analysis through ion-pair complex formation.

## Work Experience

### I. Academic work

- 05/2022-Present Associate Professor in Medicinal Chemistry, Faculty of pharmacy, Suez Canal University, Egypt.
- 05/2016-05/2022 Lecturer (Assistant Professor) in Medicinal Chemistry, Faculty of pharmacy, Suez Canal University, Egypt.
- Performing research in the field of medicinal chemistry
  - Involved with teaching the medicinal chemistry courses to undergraduates
  - Course Titles:
    - Medicinal Chemistry-1 (PMC-301), Regular Pharmacy Program.
    - Medicinal Chemistry-2 (PMC-401), Regular Pharmacy Program.
    - Medicinal Chemistry-3 (PMC-402), Regular Pharmacy Program.
    - Medicinal Chemistry-4 (PMC-501), Regular Pharmacy Program.
    - Drug Design (PMC-502), Regular Pharmacy Program.
    - Drug Synthesis (PMCE), Regular Pharmacy Program.
    - Medicinal Chemistry-I (PC-509), Clinical Pharmacy Program.
    - Medicinal Chemistry-II (PC-610), Clinical Pharmacy Program.
    - Drug Design (PC-E11), Clinical Pharmacy Program.
  - Involved with the supervision of under-graduates in chemistry practical classes.
  - Involved with the supervision of post-graduates in both master and Ph.D. studies within the department of medicinal chemistry.
  - Courses includes:
    - Advanced Topics in Pharmaceutical Medicinal Chemistry.
    - Drug Design and computational tool analysis.
    - Spectroscopic and Chromatographic Studies in Pharmaceutical Chemistry.
    - Advanced Topics in Pharmaceutical Medicinal Chemistry.
    - Biopharmaceutical Reaction Mechanisms.
    - Modern Techniques in Pharmaceutical Analysis.
  - Master degree supervision
    1. *Title:* Design, synthesis, and biological evaluation of novel nitrogen-based rings as potential agents against cancer (ongoing)
    2. *Title:* Analysis of some nitrogenous compounds in different pharmaceutical products and biological fluids (ongoing)
    3. *Title:* Quality control and biological determination for new pharmaceutical compounds (ongoing)
    4. *Title:* Novel analytical techniques for determining certain cardiovascular drugs in their pharmaceutical formulation and biological fluids (ongoing)
    5. *Title:* Design, synthesis, and biological evaluation of heterocyclic compounds as potential anti-tumor agents (finished)
    6. *Title:* Development and assurance through modern analytical techniques to ensure the quality of some drugs in pharmaceutical forms and biological fluids (finished)
  - Ph.D. degree supervision
    1. *Title:* Forensic chromatographic analysis of abused drugs (ongoing)
    2. *Title:* Instrumental analysis for the determination of some cardiovascular drugs in pharmaceutical products and biological fluids (ongoing)

3. *Title:* Analytical techniques regarding the analysis of heterocyclic compounds of therapeutic value (ongoing)
4. *Title:* Design, synthesis and biological evaluation of new fused heterocyclic compounds as kinase modulators (ongoing)
5. *Title:* Design, synthesis, and biological evaluation of heterocyclic compounds as protease inhibitors (finished)
6. *Title:* Design and synthesis of some novel imidazole-based derivatives and their biological evaluation against some chronic diseases (ongoing)

- Involved with establishing assignments, quizzes and exams as required
- Carrying out different administrative works as required

01/2013-04/2016 Assistant Lecturer in medicinal chemistry, Faculty of pharmacy, Suez Canal University, Egypt.

- Contributing to the medicinal chemistry research at the faculty in the area of synthetic medicinal chemistry.
- Teaching the medicinal chemistry practical courses to the undergraduate pharmacy students.

09/2005-01/2013 Demonstrator in medicinal chemistry, Faculty of pharmacy, Suez Canal University, Egypt.

- Involved teaching medicinal chemistry practical courses and with the supervision of undergraduates in chemistry practical classes.
- Contributing to the medicinal chemistry research at the faculty both in the area of synthetic medicinal chemistry and analytical medicinal chemistry.
- Worked as a researcher for the degree of master in medicinal chemistry.

## II. Other relevant work

- Active member of the Development of the environment and community service committee in the CQAAP at the faculty of pharmacy Suez Canal University to meet the overall needs of the surrounding community through what is practiced activities and providing services and measure satisfaction with those services.
- Active member of the Post-graduate and Under-graduate studies and research committee in the CQAAP at the faculty of pharmacy Suez Canal University. Fulfilling the job description as an academic advisor for the post-graduate and PharmD clinical pharmacy program students; **(1)** provide the academic advice regarding the studies within the department of medicinal chemistry, **(2)** Increase student success by helping them make informed decisions about their educational goals, **(3)** arrange and coordinate the time tables for the relevant studies and exams, **(4)** Research and develop resources to assist students in understanding academic regulations, policies, procedures and programs, **(5)** Research and provide input into the development of policies, processes and programs, **(6)** regular check-up and updating the student's logbook through following up the student's educational progress and provide solutions for overdue situations and students perceived as at-risk, **(7)** Refer students to other departments, agencies, institutions and services.

## Teaching Experience

For undergraduate pharmacy students, Faculty of pharmacy, Suez Canal University, Egypt.

- Quality Control and drug purity.
- Spectrophotometric drug analysis.
- Chromatographic drug analysis.
- Titrimetric assay.
- Drug Design and molecular modelling using GOLD, MOE, Autodock and Molegro Virtual docking Programs, GROMACS for molecular dynamics simulations, in addition to ChemDraw Ultra, VMD, and PyMol. Using on-line modelling platforms: SwissModel, BLAST, Charmm-GUI, and Rosetta.
- Modern synthetic protocols, structural activity relationships and drug development techniques within the field of the medicinal chemistry.

### Research Experience

- Synthetic medicinal chemistry including lead development and optimization, combinatorial chemistry especially in the field of heterocyclic chemistry for influencing key targets involved in the pathogenesis of different types of diseases with purification of the synthesized compounds using different chromatographic techniques and characterization using different techniques especially high field NMR, IR, UV and Mass spectrophotometry.
- Experience in the field of computational chemistry such as molecular dynamics, docking, and energy minimization studies using GROMACS, MOE, GOLD and Molegro, VMD software, structure-based and ligand-based rational drug design.
- Spectrophotometric characterization and analysis of medicinal compounds using different techniques including metal chelation, ion pairing and other coupling chemical reactions. Derivative spectrophotometry with good experience in stability testing and method validation.

### Research Interest

- Rational design and *de novo* design, synthesis and testing of new therapeutic agents for the management of cancer, metabolic and cardiovascular diseases which are the main causes of death all over the world.
- Synthesis and biological evaluation of new small molecules with potential antitumor activity with interest in different categories (Cancer growth inhibitors, Protein-protein interactions as cancer drug targets and Selective apoptosis induction in cancer cells).
- The development of metabolic agents focusing mainly in classes such as phosphodiesterase inhibitors and hypoglycemics.
- Development of new antiviral agents especially for HIV, Hepatitis C and B and herpes.
- Development of new ant-infective agents covering antibacterial, antiviral and antifungal agents. Targets include P450 enzymes, reverse transcriptase and DNA polymerase.
- Developments of new analytical methods for the assay of medicinal agents both in single and combined dosage forms and best application within biological fluids.

### Awards and Achievements

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|-----------|--|
| Feb. 2021 | Awarded the certificate of appreciation for international publication from the Vice president of post-graduate and research affairs, Suez Canal University.  |
| Mar. 2016 | Awarded the certificate of appreciation for being an active member of the Development of the environment and community service committee in the CQAAP at the faculty of pharmacy Suez Canal university to Meet the |

overall needs of the surrounding community through what is practiced activities and providing services and measure satisfaction with those services. An increased community satisfaction and participation was recorded compared with the past year. This also warranted the pleasure of the final reviser committee of the National Authority for Quality Assurance and Accreditation of Education (NAQAAE), Egypt on their visit March, 2016.

- Sep. 2016 Awarded the certificate of appreciation for sincere contribution within the medical convey for Saint Katrina village from the Community service and environment development affairs, Suez Canal University.
- Aug. 2005 Awarded a prize from Suez Canal University for graduating from the faculty of pharmacy (Hons).
- Sep. 2005 Awarded the certificate of excellency for graduating from the faculty of pharmacy (Hons) from the Port Said Syndicate of Egyptian Pharmacists.
- Sep. 2005 Offered a permanent academic position from Suez Canal University at the faculty of pharmacy after graduating from the faculty (Hons).
- Oct. 2013 Awarded a prize from Suez Canal University after obtaining MSc in pharmaceutical chemistry at the faculty of pharmacy.

### External Funding

- 09/2012-09/2014 Received a two-year grant as a Junior Scientist investigator from the Science & Technology Development Fund (STDF); The main governmental funding agency in Egypt, (**Grant #4244, Value 418,418 EGP**) under the title: *Design and synthesis of novel antidiabetic agents with dual mode of action*. This helped me to do a PhD in medicinal chemistry in Egypt.
- 10/2015-10/2016 Assigned as a co-Principal investigator for one-year to finish an open-project funded by the Science & Technology Development Fund (STDF) The main governmental funding agency in Egypt, (**Grant #4711, Value 545,916 EGP**) under the title: *Design and synthesis of PDE4 inhibitors for the treatment of COPD and certain cancers*.
- 09/2019-06/2022 Received a two-year grant as Principal investigator from the U.S. - Egypt Science and Technology Joint Fund (Cycle 18); (**Grant #USC18-1086, Value 108,428 USD**) under the title: *Design and Synthesis of novel Kappa Opioid Receptor Ligands for the Treatment of Addiction*. This project is a collaboration between the Medicinal Chemistry departments of both Suez Canal University, Egypt and University of Mississippi, United States.
- 10/2021-Current Received a two-year grant as Principal investigator from the U.S. - Egypt Science and Technology Joint Fund (Cycle 20); (**Grant #USC20-45896, Value 150,716 USD**) under the title: *Targeting the Kv1.3 voltage-gated potassium channel, to design safe and novel immunomodulators*. This project is a collaboration between the Medicinal Chemistry departments of both Suez Canal University, Egypt and University of Temple, United States.

## Membership

- Member of the American Chemical Society (ACS), United States, Membership Badge **201179**
- Member of the Editorial Board of the Scientific Journal, Faculty of Pharmacy - Suez Canal University; **Records of Pharmaceutical and Biomedical Sciences**  
**Print ISSN: 2536-9857 - Online ISSN: 2535-2091**
- Member of the Egyptian Pharmaceutical Association.
- Member of General Syndicate of Egyptian Pharmacists, Egypt.
- Member of the Staff Association of Suez Canal University, Egypt.

## Research and Teaching Related Training

Mar. 2007 – Oct. 2012: Faculty members and Leaders Development Center (FLDC) Suez Canal University, Egypt

Training courses for the preparation of University academic assistant lecturer which involved six different courses including:

- Educational professional preparation for a university teacher (three courses; Effective presentation, Technology employment in teaching, Mini-teaching).
- Ethics in scientific research.
- Skills in efficient communication.
- Quality standards in educational process.

Jun. 2014 – Sep. 2015: Faculty members and Leaders Development Center (FLDC) Suez Canal University, Egypt

Training courses for the preparation of University academic lecturer which involved six different courses including:

- International publication.
- Time management and meetings.
- System of examinations and evaluation of students.
- Credit hours.
- Quality standards in the teaching process.
- Ethics and behavior of the profession.

Sep. 2015 – Sep. 2016: Suez Canal University, Egypt

Attended various courses and workshops run by the university or in joint with the American National Academy of Science.

in developing my competencies in areas such as:

- Excellency in projects design, submissions and execution.
- Working safely and Good laboratory practice.
- Scientific writing and plagiarism.
- Intellectual property rights.
- Digital library professional practice.

Sep. 2016 – Aug. 2021: Suez Canal University, Egypt

Attended various courses and workshops run by the university in developing my competencies in areas such as:

- Endnote.
- E-learning management systems
- Computational research projects.
- Preparing the test item for the medical sector.
- Plagiarism Checker and Avoidance.
- Strategic Planning.

- Academy on Clinical Research Methodology.
- Preparation of the test item for the medical sector.
- Responsible scientific research How to avoid scientific theft.

## Key Skills

- Scientific background
  - Good background in organic chemistry (synthetic organic and medicinal chemistry), analytical chemistry including basic analytical techniques (UV, IR, Mass, NMR, Chromatography) and biological sciences (pharmacology, biochemistry, microbiology).
- Computational and ICT Skills
  - Word, Power Point, Excel (ICDL holder), a range of Chemistry software packages, e.g. ChemDraw, ACD/ChemSketch, ACD/NMR Processor, GOLD, SYBYL, MOE, Autodock, Molegro and PyMOL.
- Teaching and Communication skills
  - Involved with the teaching and supervision of undergraduates in their practical class.
  - Working in laboratories with different research students.
- Languages
  - Speak fluent English and Arabic.

## Peer-reviewer

RCS Advances, Royal Society of Chemistry.  
 Bioorganic Medicinal Chemistry, Elsevier.  
 Letters in Organic Chemistry, Bentham Science.  
 Bioorganic Chemistry, Elsevier.  
 Computational and Structural Biotechnology Journal, Elsevier.  
 Journal of Chemical Information and Modeling, American Chemical Society.  
 All Life, Taylor & Francis.  
 Future Pharmacology, MDPI (Basel).  
 Molecules, MDPI (Basel).  
 Vaccines, MDPI (Basel).  
 Metabolites, MDPI (Basel).  
 Pharmaceuticals, MDPI (Basel).  
 Pharmaceutics, MDPI (Basel).  
 Risk Management and Healthcare Policy, Dovepress.

## Publications

### Papers published in peer reviewed journals

Integration of immunoinformatics and cheminformatics to design and evaluate a multipeptide vaccine against *Klebsiella pneumoniae* and *Pseudomonas aeruginosa* coinfection. Ahmed M. Gouda, Mohamed A. Soltan, Khalid Abd-Elghany, Ashraf E. Sileem, Hanan M. Elnahas, Marwa Abdel-Monem Ateya, Mahmoud H. Elbatreek, **Khaled M. Darwish**, Hanin A. Bogari, Manar O. Lashkar, Mohammed M. Aldurdunji, Sameh S. Elhady, Tarek A. Ahmad, Ahmed Mohamed Said. *Frontiers Molecular Biosciences*. 10(2023).

Molecular and Biological Investigation of Isolated Marine Fungal Metabolites as Anticancer Agents: A Multi-Target Approach. Hanin A. Bogari, Sameh S. Elhady, **Khaled M. Darwish**, Mohamed S. Refaey, Radi A. Mohamed, Reda F. A. Abdelhameed, Ahmad J. Almalki, Mohammed M. Aldurdunji, Manar O. Lashkar, Samah O. Alshehri, Rania T. Malatani, Koji Yamada, Amgad I. M. Khedr. *Metabolites* 13(2023), 162.

- Exploring the Synergistic Effect of Bergamot Essential Oil with Spironolactone Loaded Nano-Phytosomes for Treatment of Acne Vulgaris: In Vitro Optimization, In Silico Studies, and Clinical Evaluation. Rofida Albash, Noha M. Badawi, Mohammed I. A. Hamed, Maha H. Ragaie, Sahar S. Mohammed, Rovan M. Elbesh, **Khaled M. Darwish**, Manar O. Lashkar, Sameh S. Elhady, Shaimaa Mosallam. *Pharmaceuticals* 16(2023), 128.
- Repurposing levocetirizine hydrochloride loaded into cationic ceramide/phospholipid composite (CCPCs) for management of alopecia: central composite design optimization, in-silico and in-vivo studies. Rofida Albash, Rania Moataz El-Dahmy, Mohammed IA Hamed, **Khaled M. Darwish**, Abdulrahman M Alahdal, Amira B Kassem, Abdurrahman M Fahmy. *Drug Delivery*. 29(2022), 2784-2795.
- Quinoline–hydrazone hybrids as dual mutant EGFR inhibitors with promising metallic nanoparticle loading: rationalized design, synthesis, biological investigation and computational studies. Ranza Elrayess, **Khaled M. Darwish**, Mohamed S Nafie, Gharieb S El-Sayyed, Mohamed M Said, Asmaa SA Yassen. *New Journal of Chemistry (RSC)*. First published 13 Sep 2022
- Bio-Guided Isolation of SARS-CoV-2 Main Protease Inhibitors from Medicinal Plants: In Vitro Assay and Molecular Dynamics. Hossam M Abdallah, Ali M El-Halawany, **Khaled M. Darwish**, Mardi M Algandaby, Gamal A Mohamed, Sabrin RM Ibrahim, Abdulrahman E Koshak, Sameh S Elhady, Sana A Fadil, Ali A Alqarni, Ashraf B Abdel-Naim, Mahmoud A Elfaky. *Plants*. 11(2022), 1914.
- Computational analysis of deleterious SNPs in NRAS to assess their potential correlation with carcinogenesis. Mohammed Y Behairy, Mohamed A Soltan, Mohamed Adam, Ahmed M Refaat, Ehab M Ezz, Fayez Althobaiti, Sarah Albogami, Eman Fayad, Ahmed M Gouda, Ashraf E Sileem, Mahmoud Abdelkhalek Elfaky, **Khaled M. Darwish**, Muhammad Alaa Eldeen. *Frontiers in Genetics*. 13(2022), 872845.
- Anti-Quorum Sensing Activities of Gliptins against *Pseudomonas aeruginosa* and *Staphylococcus aureus*. Maan T. Khayat, Hisham A. Abbas, Tarek S. Ibrahim, Ahdab N. Khayyat, Majed Alharbi, **Khaled M. Darwish**, Sameh S. Elhady, El-Sayed Khafagy, Martin K. Safo, Wael A. H. Hegazy. *Biomedicines* 10(2022), 1169.
- Phenolics from *Chrozophora oblongifolia* Aerial Parts as Inhibitors of  $\alpha$ -Glucosidases and Advanced Glycation End Products: In-Vitro Assessment, Molecular Docking and Dynamics Studies. Hossam M. Abdallah, Albraa T. Kashegari, Akram A. Shalabi, **Khaled M. Darwish**, Ali M. El-Halawany, Mardi M. Algandaby, Sabrin R. M. Ibrahim, Gamal A. Mohamed, Ashraf B. Abdel-Naim, Abdulrahman E. Koshak, Peter Proksch, Sameh S. Elhady. *Biology* 11(2022), 762.
- In silico designing and validation of an epitope-based vaccine against common *E. coli* pathotypes. Mohamed A. Soltan, Mohammed Y. Behairy, Mennatallah S. Abdelkader, Sarah Albogami, Eman Fayad, Refaat A. Eid, **Khaled M. Darwish**, Sameh S. Elhady, Ahmed M. Lotfy, Muhammad Alaa Eldeen. *Frontiers in Medicine*. 9(2022), 829467.



- 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. Ayman Abo Elmaaty, **Khaled M. Darwish**, Amani Chrouda, Amira A. Boseila, Mohamed A. Tantawy, Sameh S. Elhady, Afzal B. Shaik, Muhammad Mustafa, Ahmed A. Al-Karmalawy. ACS omega. 7(2022), 875–899.
- Repurposing  $\alpha$ -Adrenoreceptor Blockers as Promising Anti-Virulence Agents in Gram-Negative Bacteria. Ahmad J Almalki, Tarek S. Ibrahim, Sameh S. Elhady, **Khaled M. Darwish**, Wael AH. Hegazy. Antibiotics. 11(2022), 178.
- Computational and Biological Evaluation of  $\beta$ -Adrenoreceptor Blockers as Promising Bacterial Anti-Virulence Agents. Ahmad J. Almalki, Tarek S. Ibrahim, Sameh S. Elhady, Wael AH. Hegazy, **Khaled M. Darwish**. Pharmaceuticals. 15(2022), 110.
- Discovery of tetrahydro- $\beta$ -carboline-and indole-based derivatives as promising phosphodiesterase-4 inhibitors: Synthesis, biological evaluation, and molecular modeling studies. **Khaled M. Darwish**, Ahmad Abdelwaly, Asmaa M. Atta, Mohamed A. Helal. Journal of Molecular Structure. 1248(2022), 131491.
- In silico designing of a multipeptide vaccine against Rhizopus microsporus with potential activity against other mucormycosis causing fungi. Mohamed A. Soltan, Muhammad Alaa Eldeen, Nada Elbassiouny, Hasnaa L. Kamel, Kareem M. Abdelraheem, Hanaa Abd El-Gayyed, Ahmed M. Goda, Mohammed F. Sheha, Eman Fayad, Ola A. Abu Ali, Khalid Abd El Ghany, Dalia A. El-damasy, **Khaled M. Darwish**, Sameh S. Elhady, Ashraf Ibrahim. Cells-Basel. 10(2021), 3014.
- Antioxidant and Anti-inflammatory Activity of *Cynanchum acutum* L. Isolated Flavonoids Using Experimentally Induced Type 2 Diabetes Mellitus: Biological and In Silico Investigation for NF- $\kappa$ B pathway/miR-146a expression Modulation. Reda F. A. Abdelhameed, Sameh S. Elhady, Mahmoud A. Elfaky, Eman S. Habib, Mayada E. Eldin, Eman T. Mehanna, **Khaled M. Darwish**, Dina M. Khodeer, Safwat A. Ahmed and Amany K. Ibrahim. Antioxidants-Basel. 10(2021), 1713.
- VEGFR-Mediated Cytotoxic Activity of Pulicaria undulata Isolated Metabolites: A Biological Evaluation and In Silico Study. Sameh S. Elhady, Reda F. A. Abdelhameed, Salwa H. Zekry, Amany K. Ibrahim, Eman S. Habib, **Khaled M. Darwish**, Reem M. Hazem, Khadijah A. Mohammad, Hashim A. Hassanean, Safwat A. Ahmed. Life-Basel, 11(2021), 759.
- Deciphering the molecular basis of the kappa opioid receptor selectivity: A Molecular Dynamics study. Amr H. Saleh, Amar Chittiboyina, Ahmad Abdelwaly, **Khaled M. Darwish**, Amal A.H.M. Eissa, Mohamed A. Helal Journal of Molecular Graphics & Modelling, 106(2021), 107940.
- Calendulaglycoside A Showing Potential Activity Against SARS-CoV-2 Main Protease: Molecular Docking, Molecular Dynamics, and SAR Studies. Journal of Traditional and Complementary Medicine, Ahmed A. Zaki, Ahmed Ashour, Sameh S. Elhady, **Khaled M. Darwish**, Ahmed A. AlKarmalawy. (2021).

Molecular docking and dynamics simulation revealed the potential inhibitory activity of ACEIs against SARS-CoV-2 targeting hACE2 receptor. Ahmed A. Al-Karmalawy, Mohammed A. Dahab, Ahmed M. Metwaly, Sameh S. Elhady, Eslam B. Elkaeed, Ibrahim H. Eissa, **Khaled M. Darwish**. *Frontiers in Chemistry*, 9(2021), 661230.

In a search for potential drug candidates for combating COVID-19: computational study revealed salvianolic acid B as a potential therapeutic targeting 3CLpro and spike proteins. Ayman Abo Elmaaty, **Khaled M. Darwish**, Muhammad Khattab, Sameh S. Elhady, Mohammed Salah, Mohammed I. A. Hamed, Ahmed A. Al-Karmalawy, Moustafa M. Saleh. *Journal of Biomolecular Structure and Dynamics*, (2021).

Molecular Docking and Dynamics Simulation Study of Hyrtios erectus Isolated Scalarane Sesterterpenes as Potential SARS-CoV-2 Dual Target Inhibitors. Sameh S. Elhady, Reda F. A. Abdelhameed, Rania T. Malatani, Abdulrahman M. Alahdal, Hanin A. Bogari, Ahmad J. Almalki, Khadijah A. Mohammad, Safwat A. Ahmed, Amgad I. M. Khedr, **Khaled M. Darwish**. *Biology-Basel*, 10(2021), 389.

Repurposing of Sitagliptin- Melittin Optimized Nanoformula against SARS-CoV-2; Antiviral Screening and Molecular Docking Studies. Mohammed W Al-Rabia, Nabil A Alhakamy, Osama A A Ahmed, Khalid Eljaaly, Ahmed L Aloafi, Ahmed Mostafa, Hani Z Asfour, Ahmed A Aldarmahi, **Khaled M Darwish**, Tarek S Ibrahim, Usama A Fahmy. *Pharmaceutics*, 13(2021), 307.

Design, Synthesis, Anticancer Activity, and Solid Lipid Nanoparticle Formulation of Indole- and Benzimidazole-Based Compounds as Pro-Apoptotic Agents Targeting Bcl-2 Protein. Manar I Nagy, **Khaled M Darwish**, Safaa M Kishk, Mohamed A Tantawy, Ali M Nasr, Mona Qushawy, Shady A Swidan, Samia M Mostafa, Ismail Salama. *Pharmaceutics (Basel)*, 14(2021),113.

Insights into Novel Drugs Targeting Bcl-2 protein as Potential Anti-cancer Agents. **Khaled Mohamed Darwish**. *Records of Pharmaceutical and Biomedical Sciences*. 5(2021), 33-42.

The Anticancer Activity for the Bumetanide-Based Analogs via Targeting the Tumor-Associated Membrane-Bound Human Carbonic Anhydrase-IX Enzyme. Azizah M Malebari, Tarek S Ibrahim, Ibrahim M Salem, Ismail Salama, Ahdab N Khayyat, Samia M Mostafa, Osama I El-Sabbagh, **Khaled M Darwish**. *Pharmaceutics (Basel)*, 13(2020), 252.

Simultaneous Determination of Losartan and Rosuvastatin in Rat Plasma Using Liquid Chromatography–Tandem Mass Spectrometric Technique for Application into Pharmacokinetic and Drug–Drug Interaction Studies. Magdy Atef Wadie, Safaa M. Kishk, **KM Darwish**, Samia M. Mostafa, MS Elgawish. *Chromatographia*, 83(2020), 1477–1494.

Novel spectrofluorimetric quantification of alogliptin benzoate in biofluids exploiting its interaction with 4-chloro-7-nitrobenzofurazan. HA Aref, SF Hammad, **KM Darwish**, MS Elgawish. *Luminescence*; 35(2020), 284-291

Novel spectrofluorimetric quantification of linagliptin in biological fluids exploiting its interaction with 4-chloro-7-nitrobenzofurazan. HA Aref, SF Hammad, MS Elgawish, **KM Darwish**. *Luminescence*; 35(2020), 626-635.

A:Determination of Novel Promising Combination of Linagliptin and Pioglitazone HCl in Bulk and Laboratory Synthetic Mixture by Earth-Friendly Three Spectrophotometric Methods. HA Aref, SF Haammad, MS Elgawish, **KM Darwish**. Records of Pharmaceutical and Biomedical Sciences; 4(2020), 1-12

Acalypha wilkesiana flowers: Phenolic profiling, cytotoxic activity of their biosynthesized silver nanoparticles and molecular docking study for its constituents as Topoisomerase-I inhibitors. Mohamed A. El Raey, Ali M. El-Hagrassi, Abeer F. Osman, **Khaled M. Darwish**, Mahmoud Emam. Biocatalysis and Agricultural Biotechnology.; 20 (2019), 101243.

Synthesis, biological evaluation, and molecular docking investigation of benzhydrol-and indole-based dual PPAR- $\gamma$ /FFAR1 agonists. **Khaled M. Darwish**, I Salama, S Mostafa, MS Gomaa, ES Khafagy, MA Helal. Bioorganic & medicinal chemistry letters.; 28 (2018), 1595-1602.

Design, synthesis, and biological evaluation of novel thiazolidinediones as PPAR $\gamma$ /FFAR1 dual agonists, **Khaled M. Darwish**, Ismail Salama, Samia Mostafa, Mohamed S. Gomaa. Eur. J. Med. Chem.; 109 (2016) 157-172.

Homology modeling and explicit membrane molecular dynamics simulation to delineate the mode of binding of thiazolidinediones into FFAR1 and the mechanism of receptor activation, M Helal, **Khaled M. Darwish**, M Hammad. Bioorg. Med. Chem. Lett.; 24 (2014) 5330-5336.

RP-HPLC/pre-column derivatization for analysis of omeprazole, tinidazole, doxycycline and clarithromycin, **Khaled M. Darwish**, I Salama, S Mostafa, M El-Sadek. J. Chromatogr. Sci.; 51 (2013) 566-576.

Validated stability-indicating reversed-phase-HPLC method for simultaneous determination of orphenadrine citrate, caffeine and aspirin, **Khaled M. Darwish**, I Salama, S Mostafa, M El-Sadek. Chem Pharm Bull (Tokyo); 60 (2012) 1426-1436.

Extractional spectrophotometric analysis of metronidazole, tinidazole, ornidazole and secnidazole bases through acid-dye complexation using bromothymol blue dye, **Khaled M. Darwish**, I Salama, S Mostafa, M El-Sadek. Pak. J. Pharm. Sci.; 25 (2012) 207-217.

#### Conference proceedings (Posters)

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M. Helal, E. Habib, **K. Darwish**, Rational design and stereoselective synthesis of novel naturally derived PDE4 inhibitors. General Poster Session-MOR Session, 251th ACS National Meeting and Exposition; 2016 Mar 13-17, San Diego, CA, USA.

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## **Referees**

- Prof. Dr. Ashraf H. Abadi  
Professor of Department of Pharmaceutical Chemistry and Vice Dean for Academic Affairs  
Faculty of Pharmacy and Biotechnology, German University in Cairo, Egypt  
E-mail: [ashraf.abadi@guc.edu.eg](mailto:ashraf.abadi@guc.edu.eg)  
Voice: 0202275899908 [extension: 3400]
- Prof. Dr. Mohamed El Hussein El Sadek  
Professor of Medicinal Chemistry  
Faculty of Pharmacy, Zagazig University, Zagazig, Egypt  
E-mail: [m.elhussenysadek@yahoo.com](mailto:m.elhussenysadek@yahoo.com)  
Voice: 0201211652794
- Prof. Dr. Samia Mahmoud Mostafa  
Professor of Medicinal Chemistry  
Faculty of Pharmacy, Suez Canal University, Ismailia, Egypt  
E-mail: [samya\\_ali@pharm.suez.edu.eg](mailto:samya_ali@pharm.suez.edu.eg)  
Voice: 0201004506247
- Prof. Dr. Sherief Khalifa  
Professor of Pharmacognosy and Dean of College of Pharmacy  
Gulf Medical University, Ajman, United Arab Emirates  
E-mail: [jkhalifa\\_99@yahoo.com](mailto:jkhalifa_99@yahoo.com)
- Prof. Ismail Salama  
Professor of Medicinal Chemistry  
Faculty of Pharmacy, Suez Canal University, Ismailia, Egypt  
E-mail: [ismail\\_mohamed@pharm.suez.edu.eg](mailto:ismail_mohamed@pharm.suez.edu.eg)  
Voice: 0201022257643
- Assoc. Prof. Mohamed Helal  
Associate Professor of Medicinal Chemistry  
University of Science and Technology, Biomedical Sciences Program, Zewail City of Science and Technology, October Gardens, 6th of October, Giza, 12578, Egypt

E-mail: [mhelal@zewailcity.edu.eg](mailto:mhelal@zewailcity.edu.eg)  
Voice: 0201201122213