Emadeldin M. Kamel

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EDUCATION

Doctor of Philosophy, Organic chemistry (Medicinal chemistry minor specialization), The Autonomous University of Madrid (UAM) in **Spain** and Beni-Suef University (BSU) in Egypt by joint supervision system, April 2017.

- Thesis title: Phytochemical, Biological and Computational Studies on Plant-derived Phenolic Compounds Isolated from Some Egyptian Folk medicinal Plants.

Master of Science (Master by research), Chemistry of Natural products, Beni-Suef, Egypt, and Bordeaux-1 University in **France**, September 2012.

- Thesis title: Chemistry of Some Phenolic Constituents of Some Egyptian Folk medicinal Plants.

Bachelor of Science, Special Chemistry, Cairo University, Beni-Suef branch, Beni-Suef, Egypt, May 2005.

- Excellent grade with honour

RESEARCH INTERESTS / RESEARCH PROFILE

My research interests are a combination of experimental and computational approaches where I use a variety of computational techniques, theories, and methodologies to investigate applications more mimic the real state.

My research areas include:

- Computational studies on the drug-enzyme interactions and the structure-activity relationship of polyphenols and other natural compounds
- Isolation and identification of bioactive secondary metabolites from medicinal plants and testing their therapeutic activities
- Synthesis and structure modification of pharmaceutical drugs
- Synthesis of organic compounds by radical multicomponent process.

ACADEMIC EMPLOYMENT

- Associate professor Lecturer in organic and medicinal chemistry, Chemistry Department, Beni-Suef University, Beni-Suef, Egypt, from August 2022-up to now.
- Lecturer in organic and medicinal chemistry, Chemistry Department, Beni-Suef University, Beni-Suef, Egypt, from 2017-2022
- Research Scholar, Chemistry Department, Universidad Autónoma de Madrid, Ciudad Universitaria de Cantoblanco, 28049 Madrid, Spain, from 2014 to 2016.
- Assistant Lecturer, Chemistry Department, Beni-Suef University, Beni-Suef, Egypt, from 2012-2016
- Teaching assistant, Chemistry Department, Beni-Suef University, Beni-Suef, Egypt, from 2006-2012

AREAS OF TEACHING EXPERTISE

I am experienced in teaching many organic and medicinal chemistry courses including, principles of chemistry, practical organic and pharmaceutical chemistry, Petroleum and petrochemicals, chemistry of natural products and pharmacognosy, synthetic organic chemistry, in-silico analysis (docking and molecular dynamics simulations), organic chemistry, kinetics, organic reaction mechanism, physical organic chemistry, thermodynamics, chemistry of horocycles, chemistry of

organometallics, Spectroscopy, pharmaceutical chemistry, coordination chemistry and molecular structure, and many other chemistry courses.

GRANTS / AWARDS

- PAROWN (partnership and ownership initiative) scholarship from the European commission and the Egyptian government in October 2010 at University of Bordeaux 1, France
- Erasmus Mundus scholarship (Battuta program) holder in September 2013 at Autonomous university of Madrid, Spain
- Joint Supervision PhD Scholarship from the Egyptian Government (MOHE-CASM) at UAM Spain 2014
- Principal investigator (PI) for the project " A phytochemical and computational study on flavonoids isolated from Trifolium resupinatum L. and their novel hepatoprotective activity" Project ID (6112) funded from the science and technology development fund in Egypt (STDF) 2015

COMMUNITY INVOLVEMENT / ADMINISTRATIVE ACTIVITY / SERVICE

Administrative positions

- Director of the University centre for career development (**UCCD**) at Beni-Suef University belonging to American University in Cairo (from 15 Feb 2019-up to now)
- Manager of the technology transfer office (TTO) at Beni-Suef University (from 2016-October 2019)
- Deputy Manager of Linking Research to Industry Unit at Beni-Suef University (2014-2016)

Career development Expertise

- NCDA Certified career development specialist (120 hours) from the American University in Cairo (AUC) within the framework of university Centre for Career Development Project (UCCD) funded by the United States Agency for International Development (USAID) from 2019-now
- ILO certified Disability equality training (DET) facilitator from the international labour organization (ILO) in Cairo from 2019-now
- Technology transfer expert based on intensive training from the ministry of higher education in Egypt and the US department of Agriculture within the framework of Technology and innovation commercialization office (TICO) project from USAID during the period from 2018-2019
- Certified Entrepreneurship trainer from Endeavor Egypt in 2020
- Attended Employability skills training of trainers from Aspire training solutions in Egypt
- Provided soft and technical skills +16 hrs training for students and graduates from Beni-Suef University during the period from 2019-now (training programs are available upon request)

SUPERVISION

- I have supervised two M.Sc. Theses (master by research) and two PhD theses.

REFERENCES

1. Prof. Dr. Al Mokhtar Lamsabhi, Permanent Professor in Computational Chemistry at the Autonomous University of Madrid, Ciudad Universitaria de Cantoblanco, 28049 Madrid, Spain.
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2. Dr. Ayman M. Mahmoud, Senior Lecturer in Cellular & Molecular Physiology at the Department of Life Sciences, Manchester Metropolitan University, Manchester, UK.
email: a.mahmoud@mmu.ac.uk

LIST OF PUBLICATIONS

1. Emadeldin M Kamel, Sarah I Othman, Faris F Aba Alkhayl, Hassan A Rudayni, Ahmed A Allam, Al Mokhtar Lamsabhi, **Mechanistic insights into alkaloid-based inhibition of squalene epoxidase: A combined in silico and experimental approach for targeting cholesterol biosynthesis**, International Journal of Biological Macromolecules, **2025**, 302, 140609.
2. Emadeldin M. Kamel, Sally Mostafa Khadrawy, Ahmed A. Allam, Sarah I. Othman, Doaa A. Abdelrheem, Faris F. Aba Alkhayl, Al Mokhtar Lamsabhi, **Repurposing dual-C-prenylated flavonoids as potent allosteric inhibitors of PTP1B: Integrated phytochemical, enzymological, and *in silico* evidence**, International Journal of Biological Macromolecules, **2025**, 316, 144808.
3. Emadeldin M Kamel, Doaa A Abdelrheem, Bashir Salah, Al Mokhtar Lamsabhi, **Phytochemical inhibitors of squalene epoxidase: Integrated In silico and In vitro mechanistic insights for targeting cholesterol biosynthesis,** Archives of Biochemistry and Biophysics, **2025**, 768, 110372.
4. Emadeldin M Kamel, Doaa A Abdelrheem, Bashir Salah, Al Mokhtar Lamsabhi, **A Mechanistic Experimental and Computational Exploration of Aldose Reductase Inhibition by Coumarins from Ruta chalepensis,** Biochemical and Biophysical Research Communications, **2025**, 769, 151946.
5. Emadeldin M Kamel, Sarah I Othman, Saleh Alkhedhairi, Faris F Aba Alkhayl, Ahmed A Allam, Al Mokhtar Lamsabhi, **Terpenoid-Based Inhibition of SQLE: Mechanistic Computational and Experimental Insights into Targeting Cholesterol Biosynthesis,** Journal of Computational Biophysics and Chemistry, **2025**.
6. Emadeldin M Kamel, Ahmed A Allam, Hassan A Rudayni, Saleh Alkhedhairi, Faris F Alkhayl, Maha A Alwaili, Al Mokhtar Lamsabhi, **Mechanistic Insights into Polyphenols-mediated Squalene Epoxidase Inhibition: Computational Models and Experimental Validation for Targeting Cholesterol Biosynthesis,** Cell Biochemistry and Biophysics**, 2025**, 1-20.
7. Emadeldin M Kamel, Sarah I Othman, Faris F Alkhayl, Fahad M Alshabrmi, Ahmed A Allam, Noha A Ahmed, Al Mokhtar Lamsabhi, **Multi-pronged approaches to the mechanism-based inactivation of aldose reductase by natural coumarins: molecular insights and experimental validation,** 3 Biotech, **2025**, 15, 1-27.
8. Ahmed A Allam, Hassan A Rudayni, Noha A Ahmed, Faris F Aba Alkhayl, Al Mokhtar Lamsabhi, Emadeldin M Kamel, **Multidimensional insights into squalene epoxidase drug**

development: in vitro mechanisms, in silico modeling, and in vivo implications, Expert Opinion on Therapeutic Targets,**2025**, 1–19.

9. Emadeldin M Kamel, Ahmed A Allam, Hassan A Rudayni, Sarah I Othman, Fahad M Alshabrmi, Faris F Aba Alkhayl, Al Mokhtar Lamsabhi, **Mechanism-Based Inhibition of Aldose Reductase by Natural Xanthones: Computational and Experimental Insights for Diabetic Complications,** Process Biochemistry**, 2025**, 154, 99-118.

10. Maha A Alwaili, Faris F Aba Alkhayl, Hassan A Rudayni, Ahmed A Allam, Al Mokhtar Lamsabhi, Emadeldin M Kamel, **Mechanistic insights into β-glucuronidase inhibition by isoprenylated flavonoids from Centaurea scoparia: Bridging experimental and computational approaches,** Journal of Molecular Structure**, 2025**, 1322, 140354**.**

11. Ahmed A Allam, Hassan A Rudayni, Noha A Ahmed, Faris F Aba Alkhayl, Al Mokhtar Lamsabhi, Emadeldin M Kamel, **Comprehensive Insights into Carbonic Anhydrase Inhibition: A Triad of In vitro, In silico, and In vivo Perspectives,** Enzyme and Microbial Technology, **2025**, 189, 110657.

12. Emadeldin M. Kamel, S.I. Othman, H.A. Rudayni, A.A. Allam, A.M. Lamsabhi, **Multi-pronged molecular insights into flavonoid-mediated inhibition of squalene epoxidase: a pathway to novel therapeutics**, RSC Advances. 15 (2025) 3829-3848.

13. Emadeldin M Kamel, Doaa A Abdelrheem, Fahad M Alshabrmi, Faris F Aba Alkhayl, Sarah I Othman, Ahmed A Allam, Al Mokhtar Lamsabhi, **In vitro and In silico mechanistic insights into PTP1B inhibition by sulfated flavonoids from Flaveria bidentis,** Biocatalysis and Biotransformation, **2025**, 1-17.

14. Rasha H Elsayed, Ayman M Mahmoud, Sayed A El-Toumy, Sayed A Ahmed, Bashir Salah, Al Mokhtar Lamsabhi, Emadeldin M Kamel, **Unveiling the Molecular Mechanisms of Squalene Epoxidase Inhibition by Flavonoids from Erythrina speciosa: Integrative Computational and Experimental Insights, Revista Brasileira de Farmacognosia**, **2025**, 1-20.

15. Reem S Alruhaimi, Omnia E Hussein, Sulaiman M Alnasser, Ibrahim Elbagory, Mohammed A Alzoghaibi, Emadeldin M Kamel, Mohamed El Mohtadi, Ayman M Mahmoud, Haloxylon salicornicum **Phytochemicals Suppress NF-κB, iNOS and Pro-Inflammatory Cytokines in Lipopolysaccharide-Induced Macrophages**, Chemistry & Biodiversity, **2025**, 22, e202401623.

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21. Emadeldin M. Kamel, Doaa A. Abdelrheem, Noha A. Ahmed, Fahad M Alshabrmi, Faris F. Aba Alkhayl, Maha A. Alwaili, Naif G Altoom, Al Mokhtar Lamsabhi, **Mechanism-based allosteric inhibition of PTP1B by prenylated flavonoids from Glycyrrhiza echinata: in vitro experiments and in silico validation,** The protein journal, **2025.**

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28. Reem S Alruhaimi, Emadeldin M Kamel, Sulaiman M Alnasser, Mohammed A Alzoghaibi, Al Mokhtar Lamsabhi, Ayman M Mahmoud, **Mechanistic insights into carbonic anhydrase IX inhibition by coumarins from Calendula officinalis: in vitro and in silico approaches,** 2024, RSC Advances, 14, 33602-33618

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32. Reem S. Alruhaimi, Maisa Siddiq Abduh, Ahmad F. Ahmeda, Albandari Bin-Ammar, Emadeldin M. Kamel, Emad H. M. Hassanein, Chen Li, Ayman M. Mahmoud, **Berberine attenuates inflammation and oxidative stress and modulates lymphocyte E-NTPDase in acute hyperlipidemia, *Drug Development Research*,** 2024, e22166.

33. Maha A. Alwaili, Faris F. Aba Alkhayl, Hassan A. Rudayni, Ahmed A. Allam, Naif G. Altoom, Al Mokhtar Lamsabhi, and Emadeldin M. Kamel**, Unraveling molecular mechanisms of β-**

glucuronidase inhibition by flavonoids from Centaurea scoparia: integrated in silico and in vitro insights, ***New Journal of Chemistry*****,** 2024, 48, 14236-14252.

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35. Nourhan Hamdy Ibrahim, Emadeleldin M. Kamel, Mona Amin Hosny, Ahmed Fouad El-Farargy, Wafaa Abd El badi Mokbel**, Utility of Some New Pyrimidine Thiol Derivatives: Computational study of Molecular Docking and Biological Activity observation,** ***Egyptian Journal of Chemistry,*** **2024**, 10.21608/ejchem.2024.265561.9258.

36. Ayman M. Mahmoud Reem S. Alruhaimi, Omnia E Hussein, Sulaiman M. Alnasser, Ibrahim Elbagory, Mohammed A. Alzoghaibi, Emadeldin M. Kamel, Mohamed El Mohtadi, **Haloxylon salicornicum Phytochemicals Suppress NF-kB, iNOS and Pro-inflammatory Cytokines in Lipopolysaccharide-Induced Macrophages,** ***Chemistry & Biodiversity,*** ***https://doi.org/10.1002/cbdv.202401623***

37. Emadeldin M Kamel, Albandari Bin-Ammar, Ashraf A El-Bassuony, Mohammed M Alanazi, Ali Altharawi, Ahmad F Ahmeda, Ashwag S Alanazi, Al Mokhtar Lamsabhi, Ayman M Mahmoud, **Molecular modeling and DFT studies on the antioxidant activity of Centaurea scoparia flavonoids and molecular dynamics simulation of their interaction with β-lactoglobulin,** ***RSC advances,*** 2023, 13, 12361-12374.

38. R. S. Alruhaimi, E. H. M. Hassanein, M. K. Abd El-Aziz, M. Siddiq Abduh, A. Bin-Ammar, **Emadeleldin M. Kamel,** and A. M. Mahmoud**, The melatonin receptor agonist agomelatine protects against acute pancreatitis induced by cadmium by attenuating inflammation and oxidative stress and modulating Nrf2/HO-1 pathway,** ***International Immunopharmacology***, 2023, 124, 110833.

39. Shaymaa A. Ramadan, Emadeldin M. Kamel, Reem S. Alruhaimi, Albandari Bin-Ammar, Madeha, **An integrated phytochemical, in silico and in vivo approach to identify the protective effect of Caroxylon salicornicum against cisplatin hepatotoxicity,** ***Saudi Pharmaceutical Journal***, 31, 2023, 101766.

40. M. Abdul-Rahman, A. Elwekeel, R. S. Alruhaimi, Emadeldin M. Kamel, A. Bin-Ammar, A. M. Mahmoud, A. S. Moawad and M. A. Zaki, **Multi-Target Action of Garcinia livingstonei Extract and Secondary Metabolites against Fatty Acid Synthase, α-Glucosidase, and Xanthine Oxidase,** ***Saudi Pharmaceutical Journal*****,** 31, 2023, 101762.

41. Maqbool, A. Shahid, Z. Jahan, M. Bilal Khan Niazi, M. Ali Inam, A. M. Tawfeek, Emadeldin M. Kamel, and M. Saeed Akhtar, **Development of ZnO-GO-NiO membrane for removal of lead and cadmium heavy metal ions from wastewater**, ***Chemosphere***, 2023, 338, 139622.

42. D. H. Sami, A. S. Soliman, A. A. Khowailed, R. S. Alruhaimi, E. H. M. Hassanein, Emadeldin M. Kamel, and A. M. Mahmoud, **The protective effect of 7-hydroxycoumarin against cisplatin-induced liver injury is mediated via attenuation of oxidative stress and inflammation and upregulation of Nrf2/HO-1 pathway**, ***Environmental Science and Pollution Research***, 2023, 30, 80181-80191.

43. H. Malik, M. B. K. Niazi, W. Miran, A. M. Tawfeek, Z. Jahan, Emadeldin M. Kamel, N. Ahmed and M. Saeed Akhtar, **Wood as a green and sustainable alternative for environmentally friendly & flexible electronic devices**, ***Chemosphere***, 2023, 336, 139213.

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45. H. A. Mahmoud, Emadeldin M. Kamel, A. M. Mahmoud, R. S. Alruhaimi, A. M. El-Zanaty, H. M. Abd El-Salam and O. F. Abdel-Gawad, **Multitargeted molecular modelling of alginic acid modified with 4-aminophenol dopped with silver nanoparticles as a potent cytotoxic agent, *Heliyon***, 2023, 9, e17106.

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49. Emadeldin M. Kamel, A. M. Tawfeek, A. A. El-Bassuony and A. M. Lamsabhi, **Mechanistic aspects of reactive metabolite formation in clomethiazole catalyzed biotransformation by cytochrome P450 enzymes**, ***Organic & Biomolecular Chemistry***, 21, 2023, 7158-7172.

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