

# Wesam S. Qayed, Ph.D.

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## Education

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- 09/2015      **Ph.D. in Medicinal Chemistry**  
Faculty of Pharmacy, Assiut University  
Joint supervision with the Department of Chemistry, Life Sciences School,  
University of Louisville, Kentucky, USA  
Title of Thesis 'Developmental methods towards total synthesis of natural  
anticancer agent: annonacin'
- 12/2007      **M.Sc.in Medicinal Chemistry**  
Faculty of Pharmacy, Assiut University  
Title of Thesis 'Design, synthesis and antitubercular evaluation of small Schiff  
base combinatorial library'
- 06/2002      **B.Sc. in Pharmaceutical Sciences**  
Faculty of Pharmacy, Assiut University

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## RESEARCH EXPERIENCE

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- 2023 – Present      **Associate Professor**  
Department of Medicinal Chemistry  
Faculty of Pharmacy, Assiut University, Assiut, Egypt.
- 2014 – 2017      **Research Assistant**  
Trainer in MOE (Molecular Operating Environment) program  
Department of Medicinal Chemistry  
Faculty of Pharmacy, Assiut University, Assiut, Egypt.

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## TEACHING EXPERIENCE

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- 2023 – Present      **Associate Professor**  
Department of Medicinal Chemistry  
Faculty of Pharmacy, Assiut University, Assiut, Egypt.  
• Teaching Courses for undergraduate and Postgraduate students.  
• Supervisor for Master and Ph.D students.
- 2016-2022      **Assistant Professor**  
Department of Medicinal Chemistry  
Faculty of Pharmacy, Assiut University, Assiut, Egypt.  
• Teaching Courses for undergraduate and Postgraduate students.  
• Supervisor for Master and Ph.D students.

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## PUBLICATIONS

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- 1) Seung-Heon Shin, Mi-Kyung Ye , Mi-Hyun Chae , Sang-Yen Geum, Ahmed S. Aboraia, Abu-Baker M. Abdel-Aal , **Wesam S. Qayed**, Hend A. A. Abd El-wahab, Ola F. Abou-Ghadir and Tarek Aboul-Fadl. Anti-Allergic and Anti-Inflammatory Effects of Lidocaine-Derived Organic Compounds in a House Dust Mite-Induced Allergic Rhinitis Mouse Model. Biomedicines 12,1965, 2024.
- 2) Bassant S. Moustafa, Mohamed M. Omar, **Wesam S. Qayed**, Hanan F. AbdEl-Halim, Gehad G. Mohamed, Spectral, XRD, morphological, DFT, and molecular modeling investigations of

- newly prepared isatin Schiff base complexes. *Applied Organometallic Chemistry* 38, 7584, 2024.
- 3) **Wesam S. Qayed**, Mostafa A. Hassan, Ahmed Megahed Abouwarda, Yasser Musa Ibrahim and Tarek Aboul-Fadl, Computational Design of Azine-Linked Hybrids of 2-Indolinone-Thiazolodine Scaffold as Novel and Promising Quorum Sensing Inhibitors, *Polycyclic Aromatic Compounds*, 1, 2024.
  - 4) Seung-Heon Shin, Mi-Kyung Ye, Mi-Hyun Chae, Sang-Yen Geum, Ahmed S Aboraia, Abu-Baker M Abdel-Aal, **Wesam S. Qayed**, Hend AA Abd El-wahab, Ola F Abou-Ghadir, Tarek Aboul-Fadl. Effects of Lidocaine-Derived Organic Compounds on Eosinophil Activation and Survival. *Molecules*, 28(15), 5696, 2023.
  - 5) Noha. M. Hosny, Mohamed I GadAllah, **Wesam S. Qayed**, Combined Experimental/Computational Aspects for the Molecular Interaction of Empagliflozin with Bovine Serum Albumin: Quantification, and Application to Human Plasma. *Luminescence* 38(8), 1449, 2023
  - 6) Hanaa. M. Sayed, Amany. S. Ahmed, Iman. SA. Khallaf, **Wesam S. Qayed**, Anber F. Mohammed, Hanan S. M. Farghaly, Ayman Asem. Phytochemical investigation, molecular docking studies and DFT calculations on the antidiabetic and cytotoxic activities of *Gmelina philippensis* CHAM. *Journal of Ethnopharmacology*, 303, 115938, 2023
  - 7) Alessandra M. Balieiro, Eduarda L. S. Anunciação, Clauber H. S. Costa, **Wesam S. Qayed** and José Rogério A. Silva. Computational Analysis of SAM Analogs as Methyltransferase Inhibitors of nsp16/nsp10 complex from SARS-CoV-2. *International Journal of Molecular Sciences*, 23, 13972, 2022
  - 8) **Wesam S. Qayed**, Rafaela S. Ferreira, José Rogério A. Silva. In silico study towards Repositioning of FDA-approved drug candidates for Anticoronaviral Therapy: Molecular Docking, Molecular Dynamics and Binding Free Energy Calculations. *Molecules* 27(18), 5988, 2022
  - 9) **Wesam S Qayed**, Mostafa A Hassan, Wael M El-Sayed, José Rogério A Silva, Tarek Aboul-Fadl. Novel Azine Linked Hybrids of 2-Indolinone and Thiazolodinone Scaffolds as CDK2 Inhibitors with Potential Anticancer Activity: In Silico Design, Synthesis, Biological, Molecular Dynamics and Binding Free Energy Studies. *Bioorganic Chemistry*, 105884, 2022
  - 10) Sara A Hassan, Sheryhan F Gad, Hajjaj HM Abdu-Allah, **Wesam S Qayed**, Sara A AbouElmagd, Elsayed A Ibrahim. Ionic liquid of ketoprofen-piperine modulates the pharmaceutical and therapeutic characters of ketoprofen. *International Journal of Pharmaceutics*, 620, 121724, 2022
  - 11) Noha M. Hosny, Mohammed I. Gadallah, Rosa M. Gomila, **Wesam S. Qayed**. Innovative computationally designed-spectrofluorimetric method for determination of modafinil in tablets and human plasma. *Talanta* 236 122890, 2022
  - 12) Hend A. A. Abd El-Wahab, Ahmed M. Ali, Hamdy M. Abdel-Rahman, **Wesam S. Qayed**. Synthesis, biological evaluation, and molecular modeling studies of acetophenones-tethered 1,2,4-triazoles and their oximes as epidermal growth factor receptor inhibitors. *Chemical*

- biology and Drug Design. 1-13, 2021
- 13) Hend A. A. Abdel El-Wahab, Ahmed K. Hamdy, Carola Schulzke, Tarek Aboul-Fadl, **Wesam S. Qayed**. Crystal structure and Quantum Chemical Calculations of (E)1-benzyl-3-((4-methoxyphenyl)imino)-5-methylindolin-2-one. *Journal of Heterocycle Chemistry*, 1;1–9, 2021
  - 14) Mohamed A. Yousef, Ahmed M. Ali, Wael M. El-Sayed, **Wesam S. Qayed**, Tarek Aboul-Fadl. Design and synthesis of novel isatin-based derivatives targeting cell cycle checkpoint pathways as potential anticancer agents. *Bioorganic Chemistry* 105, 104366, 3, 2020
  - 15) **Wesam S. Qayed**, F A Luzzio. Chiral Pool/Henry/Enzymatic Routes to Acetogenin Synthons. *Letters in Organic Chemistry* 12 (9), 622-630, 2015
  - 16) **Wesam S. Qayed**, AS Aboaraia, HM Abdel-Rahman, AF Youssef. Lipases-catalyzed enantioselective kinetic resolution of alcohols. *J Chem Pharm Res* 7 (5), 311-322, 2015
  - 17) **Wesam S. Qayed**, AS Aboaraia, HM Abdel-Rahman, AF Youssef. Annonaceous Acetogenins as a new anticancer agent. *Der Pharma Chemica* 7 (6), 24-35, 2015
  - 18) **Wesam S. Abdel-Aal**, Hoda Y. Hassan, Tarek Aboul-Fadl, Adel F. Youssef, Pharmacophoric Model Building for Antitubercular Activity of the Individual Schiff Bases of Small Combinatorial Library, *European Journal of Medicinal Chemistry*, vol. 45, pp. 1098 - 1106, 2010
  - 19) **Wesam S. Abdel-Aal**, Hoda Y. Hassan, Tarek Aboul-Fadl, Adel F. Youssef, Solution-Phase Synthesis of Small Schiff Bases Combinatorial Library with Potential Antitubercular Activity, *Der Pharma Chemica*, 1 (2), 1- 13, [www.derpharmachemica.com](http://www.derpharmachemica.com), 2009

### **Poster Presentations**

- 1) Novel Spiro Hybrids of 2-indolinone and Thiazolodinone Scaffolds as Cell Cycle Checkpoints' Pathways Regulators with potential anticancer activity. Tarek Aboul-Fadl, Ahmed K. Hamdy, Hend A.A. AbdElwahab, **Wesam S. Qayed**, Wael M. El-Sayed. 6th Edition of Global Conference on Pharmaceutics and Novel Drug Delivery Systems (Online Event) during June 13-14, 2022.
- 2) Novel Azine linked hybrids of 2-Indolinone and Thiazolodinone scaffolds as CDK2 inhibitors with potential anticancer activity. **Wesam S. Qayed**, Mostafa A. Hassan, Wael M. El-Sayed and Tarek Aboul-Fadl, 5<sup>th</sup> Global Conference on Pharmaceutics and Novel Drug Delivery Systems. 28-30th March 2022 (virtual event)
- 3) "Novel 2-Indolinone Based Derivatives Targeting Cell Cycle Checkpoint's Proteins as Potential Anticancer Agents". Tarek Aboul-Fadl, Mostafa A. Hassan, **Wesam S. Qayed** and Wael M. El-Sayed. 2nd Global Virtual Conference on Pharmaceutical Sciences and Drug Development. August 09-10, 2021
- 4) Ionic liquid of ketoprofen-piperine modulates drugs' solubility, lipophilicity and anti-inflammatory effect. Sara A. Abou Elmagd, Sheryhan F. Gad, **Wesam S. Qayed** and Elsayed A. Ibrahim. Controlled Release Society (CRS) annual meeting (virtual event) July 25-29, 2021
- 5) International Symposium on Drug Design and Development Research (DDDR-2021) December 17-18, 2021
- 6) Utilization of microwave technology for simple, efficient and enhanced synthesis of spiro-thiazolidinones with potential antimycobacterial activity. Ahmed K. Hamdy, Hend A.A. Abd El-wahab, **Wesam S. Qayed**, Tarek Aboul-Fadl. 2nd International Conference of Pharmacy Ain-

Shams University (ICPASU), November 13-15, 2018.

- 7) Modified Lidocaine Derivatives as Potential Inhibitors of Eosinophils. Hend A.A. Abd El-Wahab, Adel F. Youssef Tarek Aboul-Fadl, Ahmed S. M. Aboraia, Abu-Baker M. Abdel-Aal, Mohammed K. Abdel-Hamid, **Wesam S. Abdel-Aal**, Ola M. F. Abou-Ghadir, Mariam E. I. Abdel-Rasoul, Rana M. Ibrahim, Mostafa A. Hassan, Noha G. M. Fekry. 2nd International Congress and Exhibition on Pharmacy (Pharmacy-2018), Paris. August 8-11, 2018
- 8) Novel Synthetic Inhibitors of Eosinophils with Potential Anti-asthmatic Activity Tarek Aboul-Fadl, Ahmed S. M. Aboraia, Abu-Baker M. Abdel-Aal, Mohammed K. Abdel-Hamid, **Wesam S. Qayed**, Ola M. F. Abou-Ghadir, Mariam E. I. Abdel-Rasoul, Rana M. Ibrahim, Mostafa A. Hassan, Noha G. M. Fekry, Hend A.A. Abd El-Wahab and Adel F. Youssef. 4<sup>th</sup> International Congress on Drug Discovery, Designing and Development, Chicago, Illinois, USA, November 2017
- 9) Chiral Pool/Henry/Enzymatic Routes to Acetogenin Synthons. **Wesam S. Qayed**, F A Luzzio. Abstracts of papers of the American Chemical Society 246, Indianapolis, USA. September 13, 2013
- 10) Design, Synthesis, and Antitubercular Evaluation of Small Schiff Base Combinatorial Library. Adel F. Youssef, **Wesam S. Abdel Aal**, Hoda Youssef, Tarek Aboul-Fadl, M.O. Khalid. The 7th International Saudi Pharmaceutical Conference 2008

### **Oral Presentations**

- 1) "Alternative Strategy for Fighting Bacterial Resistance: Quorum Sensing Inhibitions" at 3<sup>rd</sup> International Meet on Medicinal Chemistry, Drug Discovery & Drug Delivery (MEDCHEMMEET2024) June 6, 2024 (Virtual Event)
- 2) Structure-Based Design of Novel Azine Linked Hybrids of 2-Indolinone- Thiazolodine Scaffold as Potential Quorum Sensing Inhibitors for Fighting Antimicrobial Resistance. Wesam S. Qayed, Mostafa A. Hassan, Ahmed Megahed Abouwarda, Yasser Musa Ibrahim, Tarek Aboul-Fadl. International Conference and Expo on Applied Microbiology, June 17-18, 2022 (Virtual Event)
- 3) Keynote speaker "Drug design Resources for Covid-19" two-week workshop "International e-workshop on Exploring resources for COVID-19 Research" (Virtual event) July 26-31, 2021.

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### **GRANT SUPPORT**

2016 – 2018 The Science and Technology Development Funding Authority (Egypt) (STDF)

Scientific researcher in " Novel Synthetic Inhibitors of Eosinophils with Potential anti-asthmatic Activity". PI: Tarek Aboul-Fadl

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### **INVITED LECTURES**

Lecture title "Drug/inhibitor resources for Designing Drugs for Coronavirus". International e-workshop of Exploring resources for COVID-19 Research" July 26- 31, 2021, on a virtual basis.

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### **CURRENT RESEARCH INTERESTS**

Combinatorial libraries synthesis

Computer-Aided Drug Design

Molecular Modeling

Computational Chemistry

Synthetic Organic Chemistry

Design and Synthesis of Novel small molecules that help treat different threatening diseases

Antibiotic resistance fighters ex antiquorum sensing inhibitors