



College of Pharmacy

Research > Drug Design and Action Group

Drug Design and Action Group

Members

- [Dr. Noor Atatreh \(Head\)](#)
- [Prof. Amal Youssef](#)
- [Dr. Mohammad Ghattas](#)
- [Dr. Sawsan Abu Hamdah](#)
- [Dr. Amar Hamrouni](#)
- [Dr. Mohammad Al Sorkhy](#)
- [Ms. Sarah Al Rawashdeh](#)

Contact us

Dr. Mohammad Ghattas
College of Pharmacy, Building P
Al Ain University of Science and Technology
P.O.Box: 64141 Al Ain, UAE
Email: mohammad.ghattas@aau.ac.ae
Phone: +971 3 7024878
Fax: +971 3 7024777

Research areas

- **Studying enzymes *in silico***
Assessing enzymes binding site druggability and analyzing their protein-ligand interactions
- **Computer-aided drug design**
Multidisciplinary drug discovery and optimisation
- **Modelling small molecules**
Predicting dynamics and interactions
- ***in vitro* evaluation of leads**
Screening chemical and phytochemical compounds for their biological/antibacterial activity

Research interest

Our current research is focused on:

- investigating different types of enzyme families in terms of active site druggability and ligand-protein interactions (which should assist medicinal chemist/biochemist in their efforts of finding new inhibitors).
- Using computer-based drug design to inhibit protein-protein interactions and to target different types of enzymes that interfere with the pathogenesis of cancer (*i.e.* MPS1, MCF-7), diabetes mellitus (*i.e.* PTP1B) and bacterial infections (*i.e.* ENRs).
- conducting molecular dynamics simulations to study the molecular details of the aggregation phenomena of different promiscuous inhibitor; which should help researchers in the future in reducing false positive hits usually accompanied with high throughput screening.
- running *in vitro* tests for compounds suggested by computer-based drug design as well as for various plant extracts.

Research facilities

- **Molecular modelling lab includes:**
 - Two advanced workstations
 - Specialised drug design software (e.g. MOE, Maestro, AMBER and ChemAxon)
- **Microbiology lab with state of the art equipment**

Publications

1. AlNeyadi SS, Salem AA, **Ghattas MA**, **Atatreh N**, Abdou IM. Antibacterial activity and

- mechanism of action of the benzazole acrylonitrile-based compounds: In vitro, spectroscopic, and docking studies. *European Journal of Medicinal Chemistry* 2017, 136, 270–282. DOI: <https://doi.org/10.1016/j.ejmech.2017.05.010>
- Malki A, Elbayaa RY, Ali O, Sultan A, **Youssef AM**. Novel quinuclidinone derivatives induced apoptosis in human breast cancer via targeting p53. *Bioorganic Chemistry* 2017, 72: 57-63. DOI: <https://doi.org/10.1016/j.bioorg.2017.03.010>
 - Ghattas MA**, Eissa NA, Bardaweel SK, Abu Mellal A, **Atatreh N**. Computer-aided discovery of antimicrobial agents as potential enoyl acyl carrier protein reductase inhibitors, *Tropical Journal of Pharmaceutical Research* 2017, 16 (2), 397-405. <http://dx.doi.org/10.4314/tjpr.v16i2.19>
 - Hertecant J, Komara M, Nagi A, Al-Zaabi O, Fathallah W, Cui H, Yang Y, Eng CM, Al **Sorkhy M**, **Ghattas MA**, Al-Gazali L, Ali BR. A de novo mutation in the X-linked PAK3 gene is the underlying cause of intellectual disability and macrocephaly in monozygotic twins. *European Journal of Medical Genetics* 2017, 60 (4), 212-216. <http://doi.org/10.1016/j.ejmg.2017.01.004>
 - Basim A, Muhi-Eldeen ZA, Al-Kaissi E, Sauifan G, **Ghattas MA**, Arafat T, Al-Adham I. Design, synthesis and biological screening of aminoacetylenictetrahydrophthalimideanalogues as novel COX inhibitors. *International Journal of Pharmacy and Pharmaceutical Sciences* 2017, 9(2):160. DOI: [10.22159/ijpps.2017v9i2.15511](https://doi.org/10.22159/ijpps.2017v9i2.15511)
 - Ghattas MA**, Raslan N, Sadeq A, **Al Sorkhy M**, **Atatreh N**. Druggability analysis and classification of protein tyrosine phosphatase active sites. *Drug Design, Development and Therapy* 2016, 10:3197-3209. DOI [10.2147/DDDT.S111443](https://doi.org/10.2147/DDDT.S111443)
 - Abduelkarem AR, **Hamrouni AM**. The choice of pharmacy profession as a career: UAE experience. *Asian Journal of Pharmaceutical and Clinical Research*, 2016; 9(4); 1-7.
 - Ghattas MA**, Al Sorkhy M, Atatreh, N. In silico design of new MPS1 inhibitors via a validated structure-based virtual screening approach. *Der Pharma Chemica*, 8(2): [365-374, 2016](https://doi.org/10.31839/2474-3658.201608020365374).
 - Al Sorkhy M.**, Jalili E, Fillfield, B and LA Porter. Direct Interactions with both p27 and Cdk2 Regulate Spy1-Mediated Proliferation in vivo and in vitro. *Cell cycle*. 2016;15(1):128-36. doi: 10.1080/15384101.2015.1121327.
 - Ghattas MA**, Mansour RA, Atatreh N, Bryce RA. Analysis of enoyl acyl carrier protein reductase structure and interactions yield an efficient virtual screening approach and suggest a potential allosteric site. *Chemical Biology and Drug Design*. 87(1): 131–142, 2016. DOI: [10.1111/cbdd.12635](https://doi.org/10.1111/cbdd.12635)
 - Al-jomaily M, Arafat T, Al-kaissi EN, **Ghattas MA**, Muhi-eldeen ZA. Synthesis of 2-[[4-(t-amino-1-yl)but-2-ny-1-yl]oxy]-benzophenone derivatives as H3-antagonists. *International Journal of Pharmaceutical and Pharmaceutical Sciences*. 7(6):174-179, 2015.
 - Qinna NA, Shubbar MH, Matalaka KZ, Al?Jbour N, **Ghattas MA**, Badwan AA. Glucosamine Enhances Paracetamol Bioavailability by Reducing Its Metabolism. *Journal of Pharmaceutical Sciences*. 104:257–265, 2015. DOI: [10.1002/jps.24269](https://doi.org/10.1002/jps.24269)
 - Shkshak K, Afan A, Auzi A, **Hamrouni AM**. The Hypoglycemic Effect of Libyan truffle in Experimental Induced rates. *Tripolitana Medical Journal*. 2014; 3 (1) 1-4.
 - Al-Rahmani R, Al-kaissi E, Arafat T, **Ghattas M**, Muhi-eldeen Z. Synthesis of 2-[[4-(t-amino-1-yl)but-2-yn-1-yl]oxy]-1,3-benzothiazole derivatives as H3-antagonists. *IOSR Journal of Pharmacy*. 2014; 4(9):40-49. DOI: [10.9790/3013-0409040049](https://doi.org/10.9790/3013-0409040049)

15. **Ghattas MA, Atatreh N**, Bichenkova EV, Bryce RA. Protein tyrosine phosphatases: Ligand interaction analysis and optimisation of virtual screening. *Journal of Molecular Graphics and Modelling*. 2014; 52: 114-123. [DOI:10.1016/j.jmgm.2014.06.011](https://doi.org/10.1016/j.jmgm.2014.06.011)
16. Sadek B, **Hamrouni AM**, Adam A. Anti-inflammatory agents of the carbamoylmethyl ester class: synthesis, characterization, and pharmacological evaluation. *Journal of Inflammation Research* 2013;6 1-9.
17. **Hamrouni AM**, Musa F, Alatery A, Aburawi S, Alzatreny A, Auzi A. Phytochemical, Antioxidant, Antibacterial and Anti-Inflammatory Investigation of the Methanolic Extract of Amaranthus Tricolor Seed. *Tripolitana Medical Journal*. 2012; 1 (2), 94-99. [DOI: 10.2147/JIR.S39743](https://doi.org/10.2147/JIR.S39743)
18. Malki A, Elbayaa RY, Ashour HMA, Loffredo CA, **Youssef AM**. Novel thiosemicarbazides induced apoptosis in human MCF-7 breast cancer cells via JNK signaling. *Journal of Enzyme Inhibition and Medicinal Chemistry*. Posted online on November 3 2014. [DOI:10.3109/14756366.2014.971781](https://doi.org/10.3109/14756366.2014.971781)
19. Sadek B, Khanian S, Ashoor A, Prytkova T, **Ghattas MA, Atatreh N**, Nurulain SM, Yang KS, Howarth FC, Oz M. Effects of antihistamines on the function of Human $\alpha 7$ -nicotinic acetylcholine receptors. *European Journal of Pharmacology*. 2015; 746: 308–316. [DOI:10.1016/j.ejphar.2014.10.046](https://doi.org/10.1016/j.ejphar.2014.10.046)

Conferences

1. **Ghattas MA**, Eissa NA, Obaid D, **Atatreh N**. Discovery of Novel Antimicrobial Agents via Structure-Based Drug Design. *Frontiers in Medicinal Chemistry* 12th – 15th Feb 2017, Bern, Switzerland
2. **Atatreh N, Al-Rawashdeh S, Abu Hamdah S, Ghattas MA**. Drug Design Approach for Discovering New Butyrylcholinesterase Inhibitors. *Frontiers in Medicinal Chemistry* 12th – 15th Feb 2017, Bern, Switzerland.
3. **Ghattas MA**, Mansour RA, Atatreh N. A Novel Approach to Improve Enoyl Acyl Carrier Protein Reductases Virtual Screens. *Drug Design 2014 Conference*, 23rd – 26th September 2014, Oxford, United Kingdom.
4. **Youssef AM**, Malki A. Synthesis and Anticancer Activity of Novel Quinuclidinone Derivatives Against Breast Cancer Cells. *DUPHAT Conference*, 10th – 12th March 2013, Dubai, United Arab Emirates.

[View Page](#)