



جامعة العين  
AL AIN UNIVERSITY

## College of Pharmacy

Research Groups > Drug Design and Action Group

## Drug Design and Action Group

### Members

- [Dr. Noor Atatreh \(Head\)](#)
- [Dr. Mohammad Ghattas](#)
- [Dr. Sawsan Abu Hamdah](#)
- [Dr. Mohammad Al Sorkhy](#)
- [Dr. Amar Hamrouni](#)
- [Dr Nizar Al-Bataineh](#)
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## Old Members

- Prof. Amal Yousef
- Ms. Nermin Issa
- Ms. Sarah Al Rawashdeh

## Research areas

- ***in silico* Study of proteins and protein-ligand complexes**  
Assessing enzymes' binding site (e.g. druggability) and analysing their interactions with corresponding ligands so that a novel drug design strategy can be proposed & validated (via pharmacophore & docking).
- **Drug discovery and lead optimization**  
Computer-aided drug design that includes hits discovery and lead optimization of several targets that are involved in Cancer (e.g. MPS1, PTPs, MDM2) and bacterial infections (e.g. ENRs).
- **Studying aggregation-based promiscuity**  
Conducting tens of MD simulation for drug aggregate-protein complexes and extensively analyse them to figure out the driving forces behind such a phenomenon
- ***in vitro* evaluation of leads**  
Screening compounds for their biological activity via different enzymatic assays. When required, this is extended to include antibacterial assay through conventional testing methods.

## Collaborators

- Dr. Richard Bryce – The University of Manchester, UK
- Bassam Ali – UAE University, UAE
- Dr. Basem Sadek – UAE University
- Dr. Sanaa Bardaweel – University of Jordan, Jordan

## Research facilities

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

## Publications

1. Mohamed, F.E., **Al Sorkhy, M., Ghattas, M.A.**, (...), Al-Jasmi, F., Ali, B.R. A Novel Homozygous Missense Variant in the NAGA Gene with Extreme Intrafamilial Phenotypic Heterogeneity. *Journal of Molecular Neuroscience*. 2020, 70(1), pp. 45-55  
<https://doi.org/10.1007/s12031-019-01398-6>
2. Hijazi, A.K., Taha, Z.A., Ababneh, T.S., (...), **Al-Bataineh, N**, Al-Momani, W.M., Ajlouni, A.M. In vitro biological, catalytic, and DFT studies of some iron(III) N-ligated complexes. *Chemical Papers*. Accepted in 2019, In press. *Chemical Papers*.  
<https://doi.org/10.1007/s11696-019-01009-z>
3. Salem, A.A., Lotfy, M., Amin, A., **Ghattas, M.A.**. Characterization of human serum albumin's interactions with safranal and crocin using multi-spectroscopic and molecular docking techniques. *Biochemistry and Biophysics Reports*. 2019, 20,100670.  
<https://doi.org/10.1016/j.bbrep.2019.100670>
4. **Ghemrawi, R.**, Arnold, C., Battaglia-Hsu, S.-F., (...), Guéant, J.-L., Coelho, D. SIRT1 activation rescues the mislocalization of RNA-binding proteins and cognitive defects induced by inherited cobalamin disorders. *Metabolism: Clinical and Experimental*. 2019 101,153992. DOI: <https://doi.org/10.1016/j.metabol.2019.153992>
5. Al Rawashdah S, **Hamrouni A**, Sadek B, Amer R, Metwaly M, **Atatreh N, Ghattas MA**, Molecular modelling studies on alpha 7 nicotinic receptor allosteric modulators yields novel filter-based virtual screening protocol. *Journal of Molecular Graphics and Modelling*. 2019, 44-54. <https://doi.org/10.1016/j.jmgm.2019.07.001>
6. **Atatreh N**, Al Rawashdah S, Al Neyadi Sh, **Abuhamdah S, Ghattas MA**, Discovery of new butyrylcholinesterase inhibitors via structure-based virtual screening. *Journal of Enzyme Inhibition and Medicinal Chemistry*. July 2019, 1373-1379.  
<https://doi.org/10.1080/14756366.2019.1644329>
7. **Atatreh N, Youssef A, Ghattas MA, Al Sorkhy M**, Al Rawashdah S, Al-Harbi Kh, El-Ashmawy I, Almundarij T, Abdelghani A, Abd-El-Aziz A, Anti-inflammatory drug approach: Synthesis and biological evaluation of novel pyrazolo[3,4-d]pyrimidine compounds. *Bioorganic Chemistry*. 2019, 86, 393-400.  
<https://doi.org/10.1016/j.bioorg.2019.02.014>
8. **Atatreh N, Ghattas MA**, Bardaweel SK, Al Rawashdah S, **Al Sorkhy M**. Identification of new inhibitors of Mdm2–p53 interaction via pharmacophore and structure-based virtual screening. *Drug Design, Development and Therapy* 2018, 12, 1-12. DOI <https://doi.org/10.2147/DDDT.S182444>
9. Ben-Mahmoud, A., Ben-Salem, S., **Al-Sorkhy, M.**, John, A., Ali, B.R. and Al-Gazali, L. A B3GALT6 variant in patient originally described as Al-Gazali syndrome and implicating the ER quality control in the mechanism of some ?3GalT6-pathway mutations. *Clin Genet*. 2018 Feb 14. doi: 10.1111/cge.13236.  
**Ghattas MA**, Bryce RA, AlRawashdah S, **Atatreh N**, Zalloum WA. Comparative Molecular Dynamics Simulation of Aggregating and Non-Aggregating Inhibitor Solutions: Understanding the Molecular Basis of Promiscuity. *ChemMedChem* 2018, 13 (6), 500-506. <https://doi.org/10.1002/cmdc.201700654>
10. 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>

11. 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>
12. **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>
13. 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>
14. 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](http://dx.doi.org/10.22159/ijpps.2017v9i2.15511)
15. **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)
16. 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.
17. **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/10.365374.2016).
18. **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.
19. **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)
20. 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.
21. Qinna NA, Shubbar MH, Matalka 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)
22. 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.
23. 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)
24. **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)

25. 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.
26. **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)
27. 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)
28. 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)

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