



Areej Abuhammad

School of Pharmacy, University of Jordan

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Education and Qualifications

- University of Oxford, DPhil in Pharmacology.
Thesis entitled: Arylamine N-Acetyltransferases from Mycobacteria: Investigations of a Potential Target for Anti-Tubercular Therapy. Supervisors: Prof. Edith Sim, Prof. Elspeth Garman.
- University of Jordan, MSc of Pharmaceutical Science. GPA 4/4, Distinction.
Thesis entitled: Combining Docking, Scoring and Molecular Field Analyses to Probe Influenza Neuraminidase-Ligand Interactions. Supervisors: Prof. Mutasem Taha, Prof. Fatma Afifi.
- University of Jordan, BSc in Pharmacy. GPA 3.94/4 Ranked first among 90 students. Distinction.

Employment

- 2018-present University of Jordan, School of Pharmacy, Tenured Associate Professor.
2017-present University of Jordan, School of Pharmacy, Head of Department of Pharmaceutical Sciences.
2017-2018 University of Jordan, School of Pharmacy, Associate Professor.
2013-2017 University of Jordan, School of Pharmacy, Assistant Professor.
2013-2015 University of Oxford, Department of Pharmacology, Visiting Academic.
2013-2014 University of Kingston, Department of Science, Engineering & Computing, Visiting Academic.
2013-2013 University of Oxford, Department of Chemistry and Biochemistry, Postdoctoral Research Assistant.
- University of Jordan, Faculty of Pharmacy, Full Time University Lecturer.
 - University of Jordan, Faculty of Pharmacy, Full-Time Teaching and Research Assistant.
 - University of Jordan, Faculty of Pharmacy, MSc research.
 - University of Jordan, Faculty of Pharmacy, Part-Time Teaching and Research Assistant.
 - Semiramis Pharmacy, Amman, Jordan. Responsible Pharmacist.

Relevant Skills

- General IT skills: Microsoft Office applications, Endnote, GraphPad Prism.
- Graphics production: PYMOL, ChemDraw, Discovery Studio (Accelrys) and Photoshop.
- Computational: Protein Docking (LigandFit, Autodock, GOLD and FRED). Homology modelling (Modeller). Ligand based screening (Catalyst and ROCS).
- Crystallography data processing: CCP4 modules, XDS, PHENIX, PHASER and Coot.
- General lab skills: Performed several applications on different analytical instruments (UV, fluorescence. etc). Cloning, wide range of protein expression, purification and characterisation techniques from prokaryotic systems. A wide range of biochemical and biophysical methods for the analysis of biomolecular interactions: enzymic assays, fragment screening, thermal shift assays, multiangle light scattering.
- X-ray Crystallography of Macromolecules: Protein crystallisation and crystal manipulation, crystallographic data collection in-house and in Diamond Light Source.

Teaching:

Taught several modules in pharmacy including both theoretical and practical sessions including:

- Biotechnology
- Medicinal chemistry
- Drug design
- Pharmaceutical organic chemistry
- Pharmaceutical analytical chemistry
- Pharmacokinetics
- Protein chemistry and characterisation

Schools and Training

Research:

- 26) The AIC School 2019 “Crystallographic Information Fiesta”, 29 August to 3 September 2019, Naples, Italy
- 25) Fragment 2019: The 6th RSC-BMCS Fragment-based Drug Discovery Preconference Workshop, Cambridge 2017
- 24) The 9th WIPO-KIPO-KAIST-KIPA Advanced International Certificate Course (AICC), Seoul, Republic of Korea. October 23-26, 2018.
- 23) Fragment 2017: The 6th RSC-BMCS Fragment-based Drug Discovery Preconference Workshop, Vienna 2017
- 22) The HCST workshop on Proposal Writing for H2020 EU Funding Opportunities, Amman 2016
- 21) The 9th AOFSTR Cheiron School in Synchrotron Radiation 2015 at Spring-8, Hyogo Japan 10-19 September 2015
- 20) IAEA TC Project Design using the Logical Framework Approach (LFA), Amman 2015
- 19) INFO Day for PEER Grants Program, Amman 2014.
- 18) The 6th AONSA Neutron School at BATAN, Tangerang Indonesia 2014
- 17) Training on membrane protein crystallisation at MPL in Diamond Light Source, Didcot 2014
- 16) Training in microscale thermophoresis Monolith NT instrument 2013
- 15) 14th BCA/CCG Intensive Teaching School in X-Ray Structure Analysis, Durham, 2013
- 14) CCP4 Study Weekend, Nottingham.2013
- 13) CCP4 Study Weekend, Warwick.2011
- 12) Computational Biochemistry, Oxford 2011
- 11) Data Analysis GraphPad Prism, Oxford 2011
- 10) Python introduction, Oxford 2011
- 9) Comparative Genomics Course, Oxford 2011
- 8) Workshop on Biomolecular Interactions (ITC, DSF, MS, SPR). Alexandropolis, Greece. 11-14 October 2010
- 7) CCP4 Study Weekend, Nottingham 2010
- 6) BCA/CCP4 Summer School XVII, Oxford 2010
- 5) Linux, Oxford 2010
- 4) Building a Business Course at Said Business School, (9 weeks course), Oxford 2009
- 3) Innovation Plus Programme, Oxford 2009
- 2) Wellcome Trust Programme for Structural Biology: Primer and Advanced NMR Course, Oxford 2009
- 1) The Wellcome Trust Programme for Structural Biology: Crystallography Primer and Advanced, Oxford 2009

Teaching and Learning:

- 3) The University of Jordan workshops for the development of faculty members 2014:
 - Design study plans.
 - Targeted learning outcomes
 - Recent trends in university teaching
 - Evaluation of student learning and preparation of tests
 - Laws, regulations and instructions of the University of Jordan
 - The University of Jordan Charter for Quality Assurance Practices
- 2) Preparation for Learning and Teaching at Oxford, the Scheme for the Development of Teaching and Academic Practice Course Oxford 2013
- 1) Learning and teaching using technology tools, Oxford 2010

Awards and Grants:

- Deanship of Academic Research Grant. Exploring Pyrrole derivatives and bioisosteres as Human Carbonic Anhydrase III Inhibitors. 20000 JOD (2018-2020).
- The L'Oréal-UNESCO For Women in International Rising Talents (15,000 Eur), 2018.
- The L'Oréal-UNESCO For Women in Science Levant and Egypt Regional Fellowship (10,000 Eur), 2017.
- IUCr Travel Grant to attend the First Pan Africa Conference in Crystallography (PCCr1), Dschang, Cameroon.
- Sir Danial Turnberg Travel Fellowship in the University of Bristol. UK: Structural studies on human carbonic anhydrases as potential drug targets.
- IUCr Travel Grant to attend the Chiron School in Spring-8, Hyogo, Japan.
- US-Qatar-MENA Infectious Disease Initiative and CRDF Global (46,000 USD): Discovery of novel coronavirus 3CLprotease inhibitors by combined structure-based and ligand-based virtual screening. In collaboration with Purdue University. *August 2015-August 2017* [Grant Number 61557]
- Jordan Scientific Research Support Fund (148,000 JOD): Structure-based discovery and crystallographic studies of benzoic acid derivatives as novel anti-obesity agents. *August 2015-August 2017* [Grant Number MPH219/2014].

- IAEA Travel grant to attend The 6th AONSA Neutron School at BATAN, Serpong, Indonesia (2014)
- SESAME/Lounsbery Foundation Fellowship for training at MPL in Diamond Light Source (2014).
- Deanship of Academic Research Grant. Enzymic screening for neuraminidase inhibitors of chemical and natural origin as potential antiviral agents 4500 JOD (2014-2016) [Grant Number 1619].
- John Fell OUP Research Fund: The effect of protein homology on microseeding nucleation events in protein crystallography (2013-2014) [Grant Number 122/666].
- University College Old members' Trust Graduate Travel Fund to attend the 4th RSC-BMCS Fragment-based Drug Discovery, which took place in Didcot, Oxford, United Kingdom.
- Keith Prout Crystallography Fund and IUCr Travel Grant to attend the XXII Congress of IUCr, which took place in Madrid, Spain.
- Messel Trust Fund for postgraduate students to attend the 7th SCI-RSC Symposium on Proteinase Inhibitor Design, which took place at Novartis, Basel, Switzerland.
- The University of Jordan Full Scholarship to study PhD in Pharmacology.
- Faculty of Graduate Studies' Award for publishing a paper from MSc thesis – University of Jordan.
- Candidate for The Arabic Honouring Awards/Scientific Fields – Arab Thought Foundation, Lebanon.
- Abdel-Rahim Jardaneh Award for Academic Excellence in Pharmacy – University of Jordan.
- The Hashemite Kingdom of Jordan Ministry of Education Full Scholarship for outstanding students to study Pharmacy at the University of Jordan.

Association Memberships:

- Member of the British Crystallographic Association, UK
- Member of The Royal Society of Chemistry (MRSC), UK
- Member of Biochemical Society, UK

Volunteer Experience and Other Activities

- Master of School of Pharmacy Alumni Day 2019 Ceremony held at University of Jordan in 20th August 2019.
- Jury of the LOREAL UNESCO for Women in Science Fellowship Levant 2019
- Trainer and Mentor in blended learning program in the University of Jordan.
- Chair of the Micorsymposium: “Expression of macromolecular complexes” in the IUCr 2017.
- Member of the scientific committee of the Excellence in Pharmacy Education & Research: A Quality Approach which took place at the University of Jordan, Amman, Jordan 2016.
- Member of Women of Faith, student society to promote interfaith dialogue in Oxford.
- Contributed to the Jordan Scientific Research Support Fund National Project (1,500,000 JOD): Health and Pharmacology Issues in Jordan: Implementation of Structural Biology Laboratory (The Protein Crystallography Beamline in SESAME). 2016- 2019.
- Helper on “The Discover Jordan” garden at RHS Hampton Court Palace Flower Show, London 2012.
- Language helper for the Oxford University Programme in Languages in Arabic, Oxford 2009-2013.
- Helper for the Jordanian Association for Family Planning and Protection, Amman.
- Helper at the Oxford Islamic Centre and the Oxford University Islamic Society, Oxford 2008-2013.
- Completed the Science Innovation Plus, MBA coursework in technology and innovation strategy at Said Business School (One year course), Oxford.
- Completed the Building a Business Course at Said Business School, (9 weeks course), Oxford.
- Attended several courses in communication skills, team working, networking, personal effectiveness and career management, self-development, professional protocol and etiquette, Islamic banking and finance, human rights and public speaking.
- Participation in several free medical days services in rural areas in Jordan.
- Member of the Arab Organization for Human Rights in Jordan, Amman.

Student Supervision.

Ms. Sarmar Melhem, PhD Pharmacy, Kingston University 2018-present
Ms. Lana Reyad, MSc Pharmacy, 2018-present
Mr. Momen Alsamman, MSc Pharmacy, 2018-present
Ms. Dima Ahmad, MSc Pharmacy, 2017-2018
Ms. Aseel Matrouk, MSc Pharmacy, 2017-2018
Mr. Raed Alhoyan, MSc Pharmacy, 2017-2018
Mr. Muhanad Ra'afat, BSc IT, IT graduation project. 2017
Mr. Ahmad Aljakheem, BSc IT, IT graduation project. 2017
Mr. Muath Al-Faraneh, BSc IT, IT graduation project. 2017

Ms. Susan Yasser, BSc IT, IT project, 2016
Ms. Fedaa Saafeen, BSc IT, IT project 2016
Ms. Elham Al-Barghouthi, MSc Pharmacy, 2015-2016
Ms. Saja Al-Assaf, MSc Pharmacy, 2015-2016
Mr. Mohammed Badran, MSc Pharmacy, 2015-2016

Conferences and meetings attended:

- 21) The AIC School 2019 "Crystallographic Information Fiesta", 29 August to 3 September 2019, Naples, Italy
- 20) Fragments 2019: 7th RSC-BMCS Fragment-based Drug Discovery meeting, March 24 to 26, 2019, Cambridge, UK.
- 19) 9th Edition of the WIPO-KIPO-KAIST-KIPA Advanced International Certificate Course (AICC) Face-to-Face Component, October 23 to 26, 2018, Seoul, Republic of Korea.
- 18) FWIS Academy training for International Rising Talents Fellows- CEDEP, Fontainebleau, France 2018.
- 17) The Extraordinary Session at the Académie des sciences, Paris, France 2018
- 16) For Women in Science Scientific Conference, Paris, France 2018.
- 15) WIPO-UNESCO-L'Oréal Course, Geneva, Switzerland 2018.
- 14) The SwedAlex Symposium on Scientific, Social & Cultural Sustainability through Chemical Research, Alexandrina, Egypt 2017.
- 13) The Jordanian Life Sciences for Sustainable Development Conference, Amman 2017.
- 12) The 14th International Conference of the World Forum on Mediation: Muslims and the World: From Impasse to the Way Out, Amman 2017.
- 11) 2nd Scientific Congress of the Association of the Colleges of Pharmacy in the Jordan and 4th International Conference of the Faculty of Pharmacy. Excellence in Pharmacy Education and Research Amman, 2016.
- 10) The 34th Cultural Season of The Jordanian Arabic Language Complex: Arabic Language in Education, Amman, 2016
- 9) The 14th SESAME User's Meeting, Amman, 2016.
- 8) The 13th International Conference of the World Forum on Mediation: The Role of Moderation in the Face of Terrorism, Stability and World Peace, Amman, 2015.
- 7) The Friedrich Naumann Foundation for Freedom Conference: Syrian Students in the Jordanian Educational System-Policies and Challenges, Amman, 2015.
- 6) 5th Jordanian International Pharmaceutical Conference. Alzaytoona Private University of Jordan. Amman 2015.
- 5) The 1st IMAN1-LinkSCEEM User's Meeting, Amman, 2014.
- 4) The 11th SESAME Users' Meeting, Amman, 2013.
- 3) Fragments 2013: 4th RSC-BMCS Fragment-based Drug Discovery, Oxford, 2013.
- 2) ELRIG Drug Discovery 2013, Manchester, 2013.
- 1) RSC's 23rd Symposium on Medicinal Chemistry, Hatfield 2012.

Publications:

Conference presentations and public talks:

- 36) A. Abuhammad**, Structural Studies on carbonic anhydrases: a crystal story from Jordan, Invited speaker in: the advanced crystallography workshop "Hot Topics in Contemporary Crystallography 4". 1-6 October 2019, Mlini, Dubrovnik, Croatia.
- 35) A. Abuhammad**, M. Samman, R. Ahamad, Y.M. Al-Hiari, Structural studies on carbonic anhydrase III complexed with pyrrole carboxylic acid derivatives: a crystal story from Jordan, Poster in: PSB Symposium "Macromolecules in action". 4-5 July 2019, Grenoble, France.
- 34) Abuhammad A**, Structural studies on carbonic anhydrases: the first protein crystallography project in Jordan, Poster in: The 4th Instruct Biennial Structural Biology Conference, 21-24 May 2019, Alcalá de Henares, Spain.
- 33) Abuhammad A**, Structural studies on carbonic anhydrases: the first protein crystallography project in Jordan, Invited Speaker in: The 48th Annual Meeting of the Brazilian Society for Biochemistry and Molecular Biology (SBBq), 14-17 May 2019, São Paulo, Brazil.
- 32) Abuhammad A**, Protein Crystallography and Drug discovery: Exploring carbonic anhydrases, Invited Speaker in: The 5th Middle East Molecular Biology Congress and Exhibition 2018, 3-6 October 2018, Dead Sea, Jordan.
- 31) Abuhammad A**, A crystal for a cure, Poster in: For Women in Science Scientific Conference, 22 March 2018, Paris, France.

- 30) **Abuhammad A**, Protein Crystallography and its Application. Invited Speaker in: The First Conference of Faculty of Pharmacy Yarmouk University: New Trends in Pharmacy between Science and Industry, 22-23 November 2017, Irbid, Jordan.
- 29) **Abuhammad A**, Protein Crystallography in Jordan: a Crystal Story, Invited Speaker In: The SwedAlex Symposium on Scientific, Social & Cultural Sustainability through Chemical Research, 24-26 September 2017, Alexandrina, Egypt.
- 28) **Abuhammad A**, Protein Crystallography Beamline in SESAME. In: 9th Jordanian Workshop of the Applications of the Synchrotron. JAEC May 2017: Amman, Jordan
- 27) **Abuhammad A**, The First Protein Crystallography Project in Jordan. **Invited Speaker** In: The 24th International Congress and General Assembly of the IUCr 21-28 August 2017: Hyderabad, India.
- 26) **Abuhammad A**, Al-Hiari YM, Alzweiri MH, Qaisi AM, Fragment-based design of carbonic anhydrase III inhibitors as potential anti-obesity agents. Abstract in: Fragment 2017-6th RSC-BMCS Fragment-based Drug Discovery. 5-7 March 2017 Vienna, Austria.
- 25) **Abuhammad A**. Protein crystallography in Jordan: the impact of SESAME. **Invited Speaker** in: First Pan African Conference on Crystallography (PCCr1). 6-10 October 2016 Dschang, Cameroon.
- 24) **Abuhammad A**, McDonough M, Brem J, Makena A, Schofield CJ, Garman, EF. "To cross-seed or not to cross-seed": a test case using metallo- β -lactamases as drug targets for antibiotic resistance. **Invited Speaker** in: British Biophysical Society Biennial Meeting. 6-8 July 2016 Liverpool, UK.
- 23) **Abuhammad A**, McDonough M, Brem J, Makena A, Schofield CJ, Garman, EF. Protein structures for drug discovery: homologous proteins as seeds in crystallisation. **Invited Speaker** (Sponsored by Douglas Group) in: BioStruct Workshop "Dilemmas in structural biology: selection and integration of methods". 14-17 February 2016 Athens, Greece.
- 22) **Abuhammad A**. Arylamine N-acetyltransferases drug metabolising enzymes in bacteria: a target for anti-tubercular agents. **Invited Speaker** in: British Pharmacology Society Pharmacology 2015: Microbial Drug Metabolism and Antibiotic Resistance. December 2015 London, UK.
- 21) **Abuhammad A**, McDonough M, Brem J, Schofield CJ, Garman, EF. "From one seed a whole handful": homologous proteins as seeds in crystallisation. **Invited Speaker** in: Instruct Biennial Meeting. 20-22 May 2015 Florence, Italy.
- 20) **Abuhammad A.**, Protein crystallography in Jordan: using a bright light for a bright future. **Invited Speaker** in the Crystallography for the next generation: the legacy of IYCr and the UNESCO Closing" ceremony for the International Year of Crystallography. 22-24 April 2015 Rabat, Morocco.
- 19) **Abuhammad A.**, Seeing Things in a Different Light: The Impact of "The Dream Light" on Drug Design. **Invited Speaker** in: The First Swedish-Jordanian Workshop on Atomic, Molecular and Cluster Physics with Synchrotron Radiation (in celebration of the International Year of Light) 2015 Amman, Jordan.
- 18) **Abuhammad A.**, Utilization Of IMAN1 Supercomputer in Protein Structural Studies. Presentation before His Majesty King Abdullah II during Official Royal visit to the National Project Iman1 Supercomputer 2014 Amman, Jordan.
- 17) **Abuhammad A.**, Fullam E, Bhakta S, Russell A, Westwood I, Finn P, Morris G, Sim E. NAT as a target for anti-tubercular drug therapy: New mechanism of inhibition. Presentation in Recent Trends in Postgraduate Research 2014 Amman, Jordan.
- 16) **Abuhammad A.**, A century of crystallography: impact on drug design. **Invited Speaker** in the 12th SESAME Users' Meeting (in celebration of the International Year of Crystallography) 2014 Amman, Jordan.
- 15) **Abuhammad A.**, Taha MO. And Afifi FA. Screening of plants from Jordanian flora for their antiviral activity for the treatment of Avian Flu: neuraminidase enzyme inhibition. Poster in Influenza Conference 9-11 Sep 2014 Oxford, UK.
- 14) **Abuhammad A**, McDonough M, Brem J, Schofield CJ, Garman, EF. "From one seed a whole handful": homologous proteins as seeds in crystallisation. Presentation in: IUCr 23rd Congress 5-12 August 2014 Montreal, Canada.
- 13) **Abuhammad A**, Lowe ED, McDonough MA, Sim E, Garman EF. Structure of arylamine N-acetyltransferase from *M. tuberculosis*: Triumph over Adversity. Presentation in: British Crystallographic Association Spring Meeting 7-10 April 2014, Loughborough, UK.
- 12) **Abuhammad A**, Lowe ED, McDonough MA, Garman EF, Sim E. Structure of NAT from *Mycobacterium tuberculosis* – a novel method for crystallization of recalcitrant proteins. In: 6th NAT workshop 4-6 October 2013 Toronto, Canada.
- 11) **Abuhammad A**, Fullam E, Bhakta S, Russell A, Westwood I, Finn P, Morris G, Sim E. NAT as a target for anti-tubercular drug therapy – new mechanisms of inhibition. In: 6th NAT workshop 2013 Toronto, Canada.
- 10) **Abuhammad A**, Lowe ED, McDonough MA, Sim E, Garman EF. Structure of arylamine N-acetyltransferase from *M. tuberculosis*: Triumph over Adversity. Invited Speaker in: The 28th European Crystallographic Meeting (ECM28) 25-29 August 2013, Warwick, UK.
- 9) **Abuhammad A**, Fullam E, Garman EF, Sim E. Structural Studies on Novel Antitubercular Targets. In: The

Young Crystallographer Satellite Meeting - British Crystallographic Association Spring Meeting 16-19 April 2012, Warwick, UK.

- 8) **Abuhammad A**, Fullam E, Westwood I, Russell A, Davies S, Sim E. Structural studies on novel antitubercular targets. In: The XXII International Congress and General Assembly of the IUCr 22-30 August 2011: Madrid, Spain.
- 7) **Abuhammad A**, Schweichler J, Lack N, Fullam E, Sim E. NAT in mycobacteria. In: The NAT Symposium 2011: Oxford, UK.
- 6) **Abuhammad A**, Keany S, Ciulli A, Cheng H, Ballet R, Lack N, Abell C, Sim E, Ryan A. Investigation of a novel potential target for anti-tuberculars. In: Proteinase: From Molecules to Medicines, the 7th RSC-SCI Symposium 11-12 April 2011: Basel, Switzerland.
- 5) **Abuhammad A**, Lowe ED, Fullam E, Noble M, Schweichler J, Garman EF, Sim E. Structural studies on the mycobacterial arylamine *N*-acetyltransferases. In: The 5th International *N*-acetyltransferase Workshop 1-3 September 2010: Paris, France.
- 4) **Abuhammad A**, Lowe ED, Fullam E, Noble M, Schweichler J, Garman EF, Sim E. Structural studies on the mycobacterial arylamine *N*-acetyltransferases. In: The 9th International ISSX Meeting: Drug discovery and development 2010: Istanbul, Turkey.
- 3) **Abuhammad AM**, Lowe ED, Fullam E, Noble M, Garman EF, Sim E. Probing the architecture of the *Mycobacterium marinum* arylamine *N*-acetyltransferase active site. In: Young Crystallographers Satellite Meeting of the British Crystallographic Association Spring Meeting 2010: Warwick, UK.
- 2) **Abuhammad A**, Lowe ED, Fullam E, Noble M, Schweichler J, Garman EF, Sim E. Structural studies on the mycobacterial arylamine *N*-acetyltransferases. In: Medical Sciences DPhil Day 2010: Oxford, UK.
- 1) **Abuhammad A**, Fullam E, Talbot J, Kawamura A, Westwood I, Davies SG, Russell A, Sim E. Inhibitors of arylamine *N*-acetyltransferase as potential anti-tuberculars. In: The first RSC/SGC Symposium on Chemical Biology for Drug Discovery 2009: Oxford, UK.

Peer Reviewed Publications:

- 33) Matrook AD, Gupta K, Berger I, **Abuhammad A**. Structural studies on carbonic anhydrases inhibitors. In preparation.
- 32) Dima Ahmad, **Abuhammad A**. Novel drug targets in management of epilepsy. In preparation.
- 31) Dima Ahmad, Gupta K, Berger I, **Abuhammad A**. Dual CA and MMP inhibitor as potential treatment for epilepsy, in preparation.
- 30) Matrook AD, **Abuhammad A**. Carbonic anhydrases in bone and teeth diseases. British Journal of Pharmacology, in preparation.
- 29) Matrook AD, Gupta K, Berger I, **Abuhammad A**. Structural studies on carbonic anhydrases inhibition by rosmarinic acid, in preparation.
- 28) **Abuhammad A**. Alfalah SF, Falah J, Ra'afat M. "MedChemVR": a Virtual Reality Game to Enhance Medicinal Chemistry Education, Virtual Reality, In preparation.
- 27) Alfalah SF, Falah J, Ra'afat M, Aljakheem A, Al-Faraneh M, **Abuhammad A**. Virtual Reality in Medicinal Chemistry Education. Just submitted.
- 26) Al-Assaf SA, **Abuhammad A**, Taha MO. Implementation of docking-based comparative intramolecular contacts analysis (dbCICA) for the discovery of polo-like kinase 1 (PLK1) inhibitors as potential anticancer agents. In preparation.
- 25) **Abuhammad A**, Laurieri, N, Singh, N, Churchill, GC, Structural studies of inhibition of human Impase by Ebselen. In preparation.
- 24) **Abuhammad A**, Taha MO, Abaza I, Afifi FU. Evaluation of the Inhibitory Activities of Traditional Jordanian Flora on Avian Influenza A N9 Neuraminidase. *Phytother Res.* **2019**, just submitted.
- 23) Al-Barghouthy E Y, , **Abuhammad A**, Taha MO. QSAR-guided pharmacophore modeling and subsequent virtual screening identify novel TYK2 inhibitor. *Med Chem Res*, **2019**. 28, 1368-1387.
- 22) **Abuhammad A**, Al-Aqtash, RA, Anson BJ, Mesecar AD, Taha MO. Computational Modeling Studies of the Bat HKU4 Coronavirus 3CL^{pro} Inhibitors for the Development of Antivirals against the Emerging Middle East Respiratory Syndrome Coronavirus. *J. Mol. Recogn*, **2017**; 30:e2644.
- 21) Ryan A, Polycarpou E, Lack N, Evangelopoulos D, Sieg C, Halman A, Bhakta S, Eleftheriadou O, McHugh TD, Keany S, Lowe ED, Ballet R, **Abuhammad A**, Jacobs WR, Ciulli A, Sim E. Investigation of the mycobacterial

enzyme HsaD as a potential novel target for anti-tubercular agents using a fragment-based drug design approach, *Br J Pharmacol*, **2017**, 174 (14), 2209–2224.

- 20) **Abuhammad A**, Fullam, E. Mycobacterial NATs and tuberculosis. Book Chapter in *Arylamine N-acetyltransferases in Health and Disease*, Edited by Sim E and Laurieri N, World Scientific Publishing.
- 19) Afifi FU, Kasabri V, Beltran S, **Abuhammad A**, Abaza IF, Ganado O, Al-Gabbish AH. Comparison of different methods in determination of essential oil composition of origaun syriacum l. From jordan and its modulation of pancreatic enzymes. *Rev Roum Chim*. **2017**, 62(1), 15-21.
- 18) **Abuhammad A**, McDonough MA, Brem J, Makena A, Staunton D, Schofield CJ, Garman EF. "To cross-seed or not to cross-seed": a test case using metallo- β -lactamases as drug targets for antibiotic resistance. *Cryst. Growth Des*. **2017**, 17 (2): 913-924.
- 17) **Abuhammad A**. Cholesterol metabolism: a potential therapeutic target in mycobacteria. Invited review in *Br J Pharmacol*, In press. DOI: 10.1111/bph.13694
- 16) **Abuhammad A**, and Taha MO. Innovative computer-aided methods for the discovery of new kinase ligands. *Future Med. Chem*, **2016**, 8(5):509-26.
- 15) **Abuhammad A**, and Taha MO. QSAR studies in the discovery of novel type-II diabetes therapies. *Expert Opin Drug Discov* **2015**, 11(2):197-214.
- 14) Cocaign A., Kubiak X., Xu X., Garnier G., Sierra-Gallay I. L. d. l., Chi-Bui, L., Dairou, J., Busi, F., **Abuhammad A.**, Haouz, A., Dupret, J.-M., Herrmann, J.-L. & Rodrigues-Lima, F. Structural and functional characterization of the Arylamine N-acetyltransferase from the pathogen *Mycobacterium abscessus*: differences with other mycobacterial isoforms and implications for selective inhibition., *Acta Cryst D* **2014** 70, 3066-3079.
- 13) **Abuhammad A**, Fullam E, Bhakat S, Russell A, Sim E. Exploration of piperidinols as potential antitubercular agents. *Molecules J*, **2014**, 19, 16274-16290.
- 12) Sim E, **Abuhammad A**, Ryan A. Arylamine N-acetyltransferases: From Drug Metabolism and Pharmacogenetics to Drug Discovery. *Br J Pharmacol* **2014**, 171(11), 2705–2725.
- 11) **Abuhammad A**, Lowe ED, McDonough M, P.D.S. Stewart, S.A. Kolek, Sim E, Garman EF. Structure of arylamine N-acetyltransferase from *M. tuberculosis* determined by cross-seeding with homologous protein from *M. marinum*: Triumph over Adversity. *Acta Cryst D*. **2013** (69): 1433-1446.
- 10) Fullam E, Talbot J, **Abuhammed A**, Long H, Westwood IM, Russell AJ, Davies S, Sim E. Design, synthesis and structure-activity relationships of 3,5-diaryl-1H-pyrazoles as inhibitors of arylamine N-acetyltransferase. *Bioorg Med Chem Lett*, **2013** 23 (9), 2759-2764.
- 9) **Abuhammad A**, Fullam E, Lowe ED, Staunton D, Kawamura A, Westwood IM, Bhakta S, Garner AC, Wilson DL, Seden PT, Davies SG, Russell AJ, Garman EF, Sim E. Piperidinols that show anti-tubercular activity as inhibitors of arylamine N-acetyltransferase: an essential enzyme for mycobacterial survival inside macrophages. *PLoS ONE* **2012**, 7(12), e52790.
- 8) **Abuhammad A**, Lack N, Schweichler J, Staunton D, Sim RB, Sim E, Improvement of the expression and purification of *Mycobacterium tuberculosis* arylamine N-acetyltransferase (TBNAT) a potential target for novel anti-tubercular agents. *Protein Expr Purif* **2011**, 80(2), 246-252.
- 7) **Abuhammad A**, Lowe ED, Fullam E, Noble M, Garman EF, Sim E. Probing the architecture of the *Mycobacterium marinum* Arylamine N-Acetyltransferase active site. *Protein Cell* **2010**, 1(4), 384-394.
- 6) Fullam E, **Abuhammad A**, Wilson DL, Anderton MC, Davies SG, Russell AJ, Sim E. Analysis of β -amino alcohols as inhibitors of the potential anti-tubercular target N-acetyltransferase. *Bioorg Med Chem Lett*, **2010**, 21 (4), 1185-1190.
- 5) Wang C, Laurieri N, **Abuhammad A**, Lowe ED, Westwood I, Ryan A, and Sim E. Role of Tyrosine 131 in the active site of paAzoR1, an azoreductase with specificity for the inflammatory bowel disease pro-drug balsalazide. *Acta Cryst F*, **2010**, 66(1), 2-7.
- 4) Fullam E, Kawamura A, Wilkinson H, **Abuhammad A**, Westwood I, Sim E. Comparison of the Arylamine N-Acetyltransferase from *Mycobacterium marinum* and *Mycobacterium tuberculosis*, *Protein J* **2009**, 28, 281-293
- 3) **Abu Hammad A** and Taha MO. Pharmacophore modeling, quantitative structure-activity relationship analysis, and shape-complemented *in silico* screening allow access to novel influenza neuraminidase inhibitors. *J Chem Inf Model*, 2009, 49 (4), 978-996.
- 2) **Abu-Hammad A.**, Zalloum WA, Zalloum H, Abu-Sheikha G and Taha MO. Homology modeling of MCH1 receptor and validation by docking/scoring and protein-aligned CoMFA. *Eur J Med Chem*, **2009**, 44(6), 2583-2596.
- 1) **Abu Hammad A**, Afifi F, Taha MO. Combining Docking, Scoring and Molecular Field Analyses To Probe Influenza Neuraminidase-Ligand Interactions. *J Mol Graphics Modell*, **2007**. 26(2), 443-456.