



Israa H. Isawi

Assistant Professor

Computational Biochemistry and Biomolecular Dynamics

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Profile

Israa Isawi is an Assistant Professor in the Department of Medicinal Chemistry and Pharmacognosy at the Faculty of Pharmacy, Jordan University of Science and Technology. Dr. Isawi earned a PhD in Medicinal Chemistry (Computational Biochemistry) in 2020 from the Department of Chemistry and Biochemistry, The University of North Carolina at Greensboro, NC, USA. She earned a B.Sc. in Pharmacy degree in 2015 from the Faculty of Pharmacy, JUST.

Dr. Isawi conducts research in drug discovery by applying Computer Aided Drug Design (CADD) side by side with the experimental approaches. Her research is focused on constructing molecular models, how ligand interacts at the molecular level, identify active drug candidates, as well optimizing leads.

Education

2016 - 2020

● **Ph.D. in Medicinal Biochemistry: Specialization in Computational Biochemistry and Biomolecular Dynamics laboratory**

GPA: 4.00

Department of Chemistry and Biochemistry, The University of North Carolina at Greensboro (UNCG), NC, USA

Thesis Title: GPR6 Receptor: Model Construction, Docking Studies, Drug Design, and Development.

Advisor: Prof. Patricia H. Reggio, Marie Foscue Rourk Professor

2010 - 2015

● **B.Sc. in Pharmacy**

Cumulative Average 93.4, Distinguished, ranked 1st out of 220 students

Faculty of Pharmacy, Jordan University of Science and Technology (JUST), Irbid, Jordan



Professional Experience

- **Assistant Professor:** Department of Medicinal Chemistry and Pharmacognosy, Faculty of Pharmacy, Jordan University of Science and Technology, Irbid, Jordan
- **Research Assistant:** Department of Chemistry and Biochemistry, The University of North Carolina at Greensboro, NC, USA
Advisor: **Dr. Patricia Reggio** - Computational Biochemistry and Biomolecular Dynamics lab
- **Research Assistant:** Instituto de Química Médica, Consejo Superior de Investigaciones Científicas (CSIC) - Medicinal Chemistry Department, Madrid, Spain
Advisor: **Dr. Nadine Jagerovic** - Organic Synthesis lab
- **Teaching Assistant:** Department of Chemistry and Biochemistry, The University of North Carolina at Greensboro, NC, USA
- **Teaching Assistant:** Department of Medicinal Chemistry and Pharmacognosy, Faculty of Pharmacy, Jordan University of Science and Technology, Irbid, Jordan
- **Research Assistant:** Department of Medicinal Chemistry and Pharmacognosy, Faculty of Pharmacy, Jordan University of Science and Technology, Irbid, Jordan
Advisor: **Dr. Qosay A. Al-Balas** - Computer Aided Drug Design lab



Committee Assignments

- Social Activities Committee, Chair, JUST
- Community Service Committee, Member, JUST
- Department's Quality Control Committee, Member, JUST



Professional Membership

- Member of the Biophysical Society
- Member of the Sociedad Española de Química Quirúrgica (SEQT)
- Member of the International Cannabinoid Research Society
- Member of the American Chemical Society
- Member of the Jordanian Pharmaceutical Association



Research Skills

- Computer Aided Drug Design
- Molecular Docking
- Homology Modeling
- Molecular Dynamics Simulations
- QSAR
- Parametrizing ligands by forcefield tool kit (ffTK)



Computational Chemistry Tools

- Schrödinger Suite (Maestro)
- Discovery Studio (Biovia)
- Spartan (Wavefunction Inc)
- Gaussian and Gaussview
- Moddler
- Visual Molecular Dynamics (VMD)
- CHARMM
- Amber (a molecular dynamic package)
- DataWarrior



Course Instructor

- Pharmaceutical Organic Chemistry
- Medicinal Chemistry II
- Medicinal Chemistry III



Awards

- 2020 ● The American Institute of Chemists Award
- 2019 ● The University of North Carolina at Greensboro Graduate Summer Assistantship
- 2019 ● The Research Assistantship grant from i-Link project (I-LINK1242) - Spain
- 2017/2018/2019 ● International Cannabinoid Research Society - Trainee Travel Award
- 8/2017 - 7/2020 ● Jordan University of Science and Technology Graduate Scholarship
- 8/2016 - 7/2017 ● The University of North Carolina at Greensboro Graduate Teaching Assistantship
- 2015 ● Faculty of Pharmacy honor list for distinguished academic performance
- 2010 - 2015 ● King Abdullah II Fund for Development Scholarship



Publications

- 5 ● **Israa H. Isawi**, Paula Morales, Patricia H. Reggio. Natural and Synthetic Cannabinoids Targeting Non-CB1, Non-CB2 G-protein Coupled Receptors. *New Tools to Interrogate Endocannabinoid Signaling: From Natural Compounds to Synthetic Drugs*. 2020; 168-200
- 4 ● Sonja L. Knowles, Huzefa A. Raja, **Israa H. Isawi**, Laura Flores-Bocanegra, Patricia H. Reggio, Cedric J. Pearce, Joanna E. Burdette, Antonis Rokas, and Nicholas H. Oberlies. Wheldone: Characterization of a Unique Scaffold from the Coculture of *Aspergillus fischeri* and *Xylaria flabelliformis*. *Organic letters*. 2020; 22.5:1878-1882
- 3 ● **Israa H. Isawi**, Paula Morales, Noori Sotudeh, Dow P. Hurst, Diane L. Lynch, Patricia H. Reggio. GPR6 Structural Insights: Homology Model Construction and Docking Studies. *Molecules*. 2020; 25.3: 725
- 2 ● **Israa Isawi**, Paula Morales, Patricia H. Reggio. Towards a Better Understanding of the Cannabinoid-related Orphan Receptors GPR3, GPR6, and GPR12. *Drug Metabolism Reviews*. 2018; 50.1: 74-93
- 1 ● Qosay A. Al-Balas, Mohammad A. Hassan, Nizar A. Al-Shar'i, Nizar M. Mhaidat, Ammar M. Almaaytah, Fatime M. Al-Mahasneh, **Israa H. Isawi**. Novel Glyoxalase-I Inhibitors Possessing a "Zinc Binding Feature" as Potential Anticancer Agents. *Drug Design, Development and Therapy*. 2016; 10: 2623-2629.



Conferences and Workshops

- 20 ● The 9th GDR3545-GPCR international meeting, online, November 6 - 9, 2020.
- 19 ● The 3rd European Research Network on Signal Transduction (ERNEST), Signal transduction: from the genomic to the system level, online, October 12 - 14, 2020.
- 18 ● 2nd COMPARE GPCR ECR Symposium, online, September 29 - October 1, 2020.
- 17 ● Dr. GPCR Summit, online, September 14 - 18, 2020.
- 16 ● European Young Chemists' Network's - EuChemS Chemistry Congress (e-YCN@ECC), online, August 25, 2020.
- 15 ● MedChem Train e-School, online, April 27 - 29, 2020.
- 14 ● Southeast Regional Meeting - American Chemical Society (SERMACS). Savannah, GA, USA, October 20 - 23, 2019.
- 13 ● 29th Annual International Cannabinoid Research Society Meeting (ICRS). Bethesda, MA, USA, June 29 - July 4, 2019.
- 12 ● 2nd Molecules Medicinal Chemistry Symposium: Facing Novel Challenges in Drug Discovery (MMCS 2019). Barcelona, Spain, May 15 - 17, 2019.
- 11 ● 6th European Chemical Biology Symposium / "Chemistry in Life Sciences (6th ECBS/LS-EuChemS). Madrid, Spain, April 3 - 5, 2019.
- 10 ● Carolina Cannabinoid Collaborative (CCC). Raleigh, NC, USA, November 9 - 11, 2018.
- 9 ● 28th Annual International Cannabinoid Research Society Meeting (ICRS). Leiden, Netherland, July 1 - 4, 2018.
- 8 ● Society for Neuroscience 2017 Annual Meeting (SfN). Washington, DC, USA. November 11 - 15, 2017.
- 7 ● Southeast Regional Meeting - American Chemical Society (SERMACS). Charlotte, NC, USA, November 8 - 9, 2017.
- 6 ● Carolina Cannabinoid Collaborative (CCC). Durham, NC, USA. October 27 - 29, 2017.
- 5 ● Phi talk, Phi Science Institute. Amman, Jordan, April 2016.
- 4 ● Career Path. Faculty of Pharmacy, Jordan University of Science and Technology, Irbid, Jordan, October 2016.

- 3 ● The 7th Scientific day of the Faculty of Pharmacy. Jordan University of Science and Technology, Irbid, Jordan, May 2014.
- 2 ● The 4th Pharmaceutical conference. University of Jordan, Amman, Jordan, May 2014.
- 1 ● The 1st Pharmaceutical conference "Pharma Xpress". Jordanian Construction Contractors Association, Amman, Jordan, March 2013.



Oral and Poster Presentation

- 11 ● **Israa H. Isawi**, GPR6 Receptor: Model Construction, Docking Studies, Drug Design, and Development. Faculty of Pharmacy, Jordan University of Science and Technology, Irbid, Jordan, November 23, 2020. (Oral)
- 10 ● **Israa H. Isawi**, Paula Morales, Dow P. Hurst, Aitor Herraiz, Nadine Jagerovic, Patricia H. Reggio. Structure Based Drug Design and Synthesis of Novel GPR6 Modulator. Southeast Regional Meeting - American Chemical Society (SERMACS). Savannah, GA, USA, October 20 - 23, 2019. (Poster)
- 9 ● **Israa H. Isawi**, Paula Morales, Dow P. Hurst, Aitor Herraiz, Nadine Jagerovic, Patricia H. Reggio. GPR6: Model Development, Drug Design and Synthesis. 29th Annual International Cannabinoid Research Society Meeting (ICRS). Bethesda, MA, USA, June 29 - July 4, 2019. (Poster)
- 8 ● **Israa H. Isawi**, Paula Morales, Dow P. Hurst, Nadine Jagerovic, Patricia H. Reggio. Design of Novel GPR6 Inverse Agonists Using a Fragment Replacement Scaffold Hopping Approach. 2nd Molecules Medicinal Chemistry Symposium: Facing Novel Challenges in Drug Discovery (MMCS 2019). Barcelona, Spain, May 15 - 17, 2019. (Poster)
- 7 ● **Israa H. Isawi**, Paula Morales, Dow P. Hurst, Patricia H. Reggio. The Orphan GPCR GPR6: Model Development and Docking Studies. 6th European Chemical Biology Symposium / "Chemistry in Life Sciences (6th ECBS/LS-EuChemS). Madrid, Spain, April 3 - 5, 2019. (Poster)
- 6 ● **Israa H. Isawi**, GPR6 Receptor: Model Development, Drug Design and Synthesis. Instituto de Química Médica, Consejo Superior de Investigaciones Científicas, Madrid, Spain, April 12, 2019. (Oral)
- 5 ● **Israa H. Isawi**, Paula Morales, Dow P. Hurst, Patricia H. Reggio. The Orphan Receptor GPR6: Homology Model Construction and Docking studies. Carolina Cannabinoid Collaborative (CCC). Raleigh, NC, USA, November 9 - 11, 2018. (Oral)

- 4 ● **Israa H. Isawi**, Paula Morales, Dow P. Hurst, Patricia H. Reggio. The Orphan Receptor GPR6: Homology Model Construction. 28th Annual International Cannabinoid Research Society Meeting (ICRS). Leiden, Netherland, July 1 - 4, 2018. (Poster)
- 3 ● **Israa H. Isawi**, Paula Morales, Alyssa Laun, Dow P. Hurst, Zhao-Hui Song, Patricia H. Reggio. Structural Relationship of the Class A Orphan GPCR, GPR6 With the Cannabinoid CB1 and CB2 Receptors. The 27th Annual International Cannabinoid Research Society. Montréal, Canada, June 2017. (Poster)
- 2 ● **Israa H. Isawi**, Paula Morales, Alyssa Laun, Dow P. Hurst, Zhao-Hui Song, Patricia H. Reggio. The Orphan GPCR GPR6: Structural Understanding and Its Relationship with the Cannabinoids. Carolina Cannabinoid Collaborative (CCC). Durham, NC, USA, October 27 - 29, 2017. (Poster)
- 1 ● **Israa H. Isawi**, Paula Morales, Alyssa Laun, Dow P. Hurst, Zhao-Hui Song, Patricia H. Reggio. Towards a Structural Understanding of the Orphan Receptor GPR6: Relationship with the Cannabinoids. Southeast Regional Meeting - American Chemical Society (SERMACS). Charlotte, NC, USA, November 8 - 9, 2017. (Poster)



Languages

- Arabic - mother tongue
- Fluent in English spoken and written



Community Service

- 2018/2019/2020 ● North Carolina Science Olympiad (NCSO), NC, USA
- 2017/2018/2020 ● Lindley Elementary Science Night in Greensboro, USA
- 2018 ● Science Fair at Cornerstone Charter Academy, NC, USA
- 2017 ● Science Everywhere Festival at UNCG, NC, USA
- 2014 ● Pharm.D. Campaign: "I am a pharmacist, and my community are my responsibility", Jordan University of Science and Technology, Irbid, Jordan
- 2013 ● Free medical care day, Irbid villages, Jordan



References

- *Dr. Patricia Reggio*, Marie Foscue Rourk Professor, Department of Chemistry and Biochemistry, The University of North Carolina at Greensboro, United States of America. E-mail: phreggio@uncg.edu
- *Dr. Paula Morales*, Postdoctoral researcher, Instituto de Química Medica, Consejo Superior de Investigaciones Científicas E-28006 Madrid, Spain. E-mail: paulamlcr@gmail.com
- *Dr. Tamam El-Elimat*, Associate Professor, Department of Medicinal Chemistry and Pharmacognosy, Faculty of Pharmacy, Jordan University of Science and Technology, Irbid, Jordan. E-mail: telimat@just.edu.jo