



Israa H. Isawi



Nationality: Jordanian



Date of birth: October 26, 1992



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Work: Department of Medicinal Chemistry and Pharmacognosy
Faculty of Pharmacy, Jordan University of Science and Technology (JUST)
PO Box 3030, Irbid 22110, Jordan



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 experimental approaches. Her research is focused on constructing molecular models, how ligand interacts at the molecular level, identifying active drug candidates, as well as optimizing leads.



Education

Aug 2016 – Aug 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

Sep 2010 – Jan 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



Languages

Arabic - Mother tongue

Fluent in English spoken and written



Professional Experience

Oct. 2020 – Present

Assistant Professor: Department of Medicinal Chemistry and Pharmacognosy, Faculty of Pharmacy, Jordan University of Science and Technology, Irbid, Jordan

Sep. 2021 – Aug. 2022

Assistant Dean of Pharmacy for Postgraduate Students Affairs and Quality Control: Faculty of Pharmacy, Jordan University of Science and Technology, Irbid, Jordan

Aug. 2017 – Aug. 2020

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

Mar. 2019 – Jun. 2019

Research Assistant: Instituto de Química Médica, Consejo Superior de Investigaciones Científicas (CSIC) - Medicinal Chemistry Department, Madrid, Spain

Advisor: **Dr. Nadine Jagerovic** - Organic Synthesis lab

Aug. 2016 – Jul. 2017

Teaching Assistant: Department of Chemistry and Biochemistry, The University of North Carolina at Greensboro, NC, USA

Sep. 2015 – Jun. 2016

Teaching Assistant: Department of Medicinal Chemistry and Pharmacognosy, Faculty of Pharmacy, Jordan University of Science and Technology, Irbid, Jordan

Feb. 2015 – Jun. 2015

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



Teaching

Undergraduate Course Instructor

- Pharmaceutical Organic Chemistry
- Medicinal Chemistry I
- Medicinal Chemistry II
- Medicinal Chemistry III
- Drug Design

Graduate Course Instructor

- Literature Seminar

Online and distance education

- Synchronous Education

- Zoom Video Communications
- Microsoft Teams
- Asynchronous Education
 - E-Learning Moodle
 - Video-based Lectures; YouTube



Awards

The American Institute of Chemists Award	2020
The University of North Carolina at Greensboro Graduate Summer Assistantship	2019
The Research Assistantship grant from i-Link project (I-LINK1242) – Spain	2019
Jordan University of Science and Technology Graduate Scholarship	2017 – 2020
The University of North Carolina at Greensboro Graduate Teaching Assistantship	2016 – 2017
Faculty Of Pharmacy Honor List for Distinguished Academic Performance	2015
King Abdullah II Fund for Development Scholarship	2010 – 2015



Publications

9. Rufaida Al Zoubi, Samah Sokkar, **Israa H. Isawi**, and Qanita Bani Baker. Activation fingerprints and allosteric modulation at the free fatty acid receptor 1 (FFAR1) revealed by molecular dynamics simulation. *Archives of Biochemistry and Biophysics*. 2025; 110473

8. **Israa H. Isawi**, Rayan M. Obeidat, Soraya Alnabulsi, and Rufaida Al Zoubi. Identification of Novel HPK1 Hit Inhibitors: From in Silico Design to In Vitro Validation. *International Journal of Molecular Sciences*. 2025; 26. 9: 4366

7. Oglat, Ammar A., Tala AbuKhalil, Hanan Hasan, **Israa H. Isawi**, Ahmad A. Oqlat, Hamad Yahia Abu Mhanna, and Hanan Fawaz Akhdar. Evaluating the use of breast self-examination (BSE) for recognizing breast Cancer awareness among Jordanian students and workers in Medical Fields. *International Journal of Women's Health*. 2024; 1743-1753

6. Al Sharie, Ahmed H., Yazan O. Al Zu'bi, Tamam El-Elimat, Kinda Al-Kammash, Alma Abu Lil, **Israa H. Isawi**, Sarah Al Sharie, Balqis M. Abu Mousa, Abubaker A. Al Malkawi, and Feras Q. Alali. ANO4 Expression Is a Potential Prognostic Biomarker in Non-Metastasized Clear Cell Renal Cell Carcinoma. *Journal of Personalized Medicine*. 2023; 13. 2: 295

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.



Grants

- Deanship of Research/ Jordan University of Science and Technology Grant No. **35-2025**. Utilizing Machine Learning Models and Molecular Docking for the Identification of MAP4K4 Inhibitors, amount: JD 8,400. (Principal Investigator)
- Deanship of Research/ Jordan University of Science and Technology Grant No. **374-2024**. Development of a Machine Learning Model for Virtual Screening to Identify New HPK1 Inhibitors with Anticancer Activity, amount: JD 6,000. (Principal Investigator)
- Deanship of Research/ Jordan University of Science and Technology Grant No. **396/2023**. Combining Ligand-based and Structure-based Drug Design Strategies to Identify HPK-1 Inhibitors with Anticancer Activity, amount: JD 5,299. (Principal Investigator)
- Deanship of Research/ Jordan University of Science and Technology Grant No. **521/2021**. Computational studies towards the identification of CB2-M1 dual modulators: a novel strategy to tackle Alzheimer's, amount: JD 9,450. (Principal Investigator)
- Deanship of Research/ Jordan University of Science and Technology Grant No. **495/2023**. Molecular Dynamics Simulations Studies on a Virus-encoded G-protein Coupled Receptor. (Co-Principal Investigator)
- Deanship of Research/ Jordan University of Science and Technology Grant No. **419/2022**. Pharmacy Students' Knowledge and Perception of a Newly Developed Course on Drug Design. (Co-Principal Investigator)



Conferences and Workshops

- Multidisciplinary Pharmaceutical Research (MDPR). Irbid, Jordan, Jun.6-8, 2023.
- European Research Network on Signal Transduction (4th ERNEST). Online, Apr.12-14, 2021.
- The 9th GDR3545-GPCR international meeting. Online, Nov.6-9, 2020.
- The 3rd European Research Network on Signal Transduction (ERNEST), Signal transduction: from the genomic to the system level. Online, Oct.12-14, 2020.
- 2nd COMPARE GPCR ECR Symposium. Online, Sep.29 - Oct.1, 2020.
- Dr. GPCR Summit. Online, Sep.14-18, 2020.
- European Young Chemists' Network's - EuChemS Chemistry Congress (e-YCN@ECC). Online, Aug. 25, 2020.
- MedChem Train e-School. Online, Apr.27-29, 2020.
- Southeast Regional Meeting - American Chemical Society (SERMACS). Savannah, GA, USA, Oct.20-23, 2019.
- 29th Annual International Cannabinoid Research Society Meeting (ICRS). Bethesda, MA, USA, Jun.29 – Jul.4, 2019.
- 2nd Molecules Medicinal Chemistry Symposium: Facing Novel Challenges in Drug Discovery (MMCS 2019). Barcelona, Spain, May.15-17, 2019.
- 6th European Chemical Biology Symposium /“Chemistry in Life Sciences” (6th ECBS/LS-EuChemS). Madrid, Spain, Apr.3-5, 2019.
- Carolina Cannabinoid Collaborative (CCC). Raleigh, NC, USA, Nov.9-11, 2018.
- 28th Annual International Cannabinoid Research Society Meeting (ICRS). Leiden, Netherland, Jul.1-4, 2018.
- Society for Neuroscience 2017 Annual Meeting (SfN). Washington, DC, USA. Nov.11-15, 2017.
- Southeast Regional Meeting - American Chemical Society (SERMACS). Charlotte, NC, USA, Nov.8-9, 2017.
- Carolina Cannabinoid Collaborative (CCC). Durham, NC, USA. Oct.27-29, 2017.



Oral and Poster Presentation

- **Israa H. Isawi**, GPR6 Receptor: Model Construction, Docking Studies, Drug Design, and Development. Faculty of Pharmacy, Jordan University of Science and Technology, Irbid, Jordan, Nov.23, 2020. (Oral)
- **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, Oct.20-23, 2019. (Poster)
- **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). Bethseda, MA, USA, Jun.29-Jul.4, 2019. (Poster)
- **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)
- **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, Apr.3-5, 2019. (Poster)
- **Israa H. Isawi**, GPR6 Receptor: Model Development, Drug Design and Synthesis. Instituto de Química Médica, Consejo Superior de Investigaciones Científicas, Madrid, Spain, Apr.12, 2019. (Oral)
- **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, Nov.9-11, 2018. (Oral)
- **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, Jul.1-4, 2018. (Poster)
- **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, Jun. 2017. (Poster)
- **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, Oct.27-29, 2017. (Poster)
- **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, Nov.8-9, 2017. (Poster)



Research Skills

- Homology Modeling
- Molecular Docking
- Virtual Screening
- Rational Drug Designing
- Parametrizing ligands
- Molecular Dynamics Simulations



Computational Chemistry Tools

- Schrödinger Suite (Maestro)
- Discovery Studio (Biovia)
- Spartan (Wavefunction Inc)
- DataWarrior
- Moddler



Academic Supervision and Thesis Committees

Main Advisor

- Rayan Obeidat:
 - M.Sc., Medicinal Chemistry, Department of Medicinal Chemistry and Pharmacognosy, Faculty of Pharmacy, Jordan University of Science and Technology, June 2024.
 - Thesis title: “Computer Aided Drug Design Strategies to Identify HPK-1 Inhibitors with Anticancer Activity”.
- Reema Fuad Anaam
 - M.Sc., Medicinal Chemistry, Department of Medicinal Chemistry and Pharmacognosy, Faculty of Pharmacy, Jordan University of Science and Technology, June 2024.
 - Thesis title: “Discovery of Potential Glyoxalase-I Inhibitors By Investigating Multiple Zinc Coordination Geometries and Interacting Water Molecules”.

- Yazeed Al-Sayeh – 3rd year:
 - M.Sc., Medicinal Chemistry, Department of Medicinal Chemistry and Pharmacognosy, Faculty of Pharmacy, Jordan University of Science and Technology.
 - Thesis title: “Development of a Machine Learning Model for Virtual Screening to Identify New HPK1 Inhibitors with Anticancer Activity”.
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- Mera Ali Aladaileh – 2nd year:
 - M.Sc., Medicinal Chemistry, Department of Medicinal Chemistry and Pharmacognosy, Faculty of Pharmacy, Jordan University of Science and Technology.
 - Thesis title: “Structure-Based Optimization of HPK1 Inhibitors Using Molecular Dynamics Simulations and Free Energy Perturbation”.
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Internal Examiner

- Samah Sokkar:
 - M.Sc., Pharmaceutical Technology, Department of Pharmaceutical Technology, Faculty of Pharmacy, Jordan University of Science and Technology, Dec. 2023.
 - Thesis title: “Computational Studies at the Free Fatty Acid Receptor 1; Endogenous Signaling and The Design of Prospective Allosteric Modulators as Antidiabetics”.
- Roaa Bibars:
 - M.Sc., Pharmaceutical Technology, Department of Pharmaceutical Technology, Faculty of Pharmacy, Jordan University of Science and Technology, Oct. 2023.
 - Thesis title: “Computational Fragment-based Drug Design of Potential Glyoxalase-I Inhibitors”.
- Mohammad Fetian:
 - M.Sc., Pharmaceutical Technology, Department of Pharmaceutical Technology, Faculty of Pharmacy, Jordan University of Science and Technology, Aug. 2023.
 - Thesis title: “Unraveling Potential Glyoxalase-I Inhibitors Utilizing Structure-Based and Ligand-Based Drug Design Techniques”.
- Dalya Mohammed
 - M.Sc., Pharmaceutical Technology, Department of Pharmaceutical Technology, Faculty of Pharmacy, Jordan University of Science and Technology, Aug. 2023.
 - Thesis title: “Structure-Activity Relationship (Sar) Studies of Heteroaryl Amino-Carboxamides as Lsd1 Inhibitors with Potential Anticancer Activity”.
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Editorial Activities

Referee/Reviewer

Journal of Molecular Modeling - Springer



Committee Assignments

Faculty of Pharmacy Board	2023 – 2024	Member
Scientific Research Committee for Undergraduate Students	2021 – 2025	Chair
Faculty Career Paths Committee	2021 – 2025	Member
Departmental Scientific Research Committee	2022 – 2023	Member
Faculty Course Equivalency Committee	2021 – 2023	Member
Faculty Social Activities Committee	2021 – 2022	Member
Faculty Media and Website Committee	2021 – 2022	Member
Departmental Quality Control Committee	2020 – 2021	Member



Professional Membership

	Since
Member of the Sociedad Española de Química Qerapéutica (SEQT)	2019
Member of the International Cannabinoid Research Society	2017
Member of the American Chemical Society	2017
Member of the Jordanian Pharmaceutical Association	2015



References

- *Dr. Paula Morales*, Postdoctoral researcher, Instituto de Química Medica, Consejo Superior de Investigaciones Científicas E-28006 Madrid, Spain. E-mail: paulamlcr@gmail.com
- *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 [Retired]