



## CURRICULUM VITAE

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### 1. Personal Data

Date of Birth: July 07, 1976

Nationality: Jordanian

### 2. Education

- Ph.D. (Computational Chemistry) 2008, Brigham Young University, Provo, UT, USA
- M.Sc. (Physical Chemistry) 2001, Yarmouk University, Irbid, Jordan
- B.Sc. (Chemistry) 1998, Yarmouk University, Irbid, Jordan

### 3. Ph.D. Dissertation

*Ion permeation through membrane channels: molecular dynamics simulations studies, Brigham Young University, Provo, UT, USA.*



#### 4. Employment

##### Academic Positions

- Assistant Professor, Department of Pharmacy, Al-Zaytoonah University of Jordan, Amman, Jordan.  
Feb, 2022 – now
- Assistant Professor (Part Time), Department of Chemistry, The University of Jordan, Amman, Jordan.  
Jul, 2020 – Jan, 2022
- Assistant Professor, Department of Chemistry, King Khalid University, Abha, Saudi Arabia.  
Apr, 2020 – Aug, 2019
- Postdoctoral Fellow, Department of Biochemistry and Molecular Biology, The University of Georgia, Athens, GA, USA.  
Apr, 2009 – Mar, 2010
- Graduate Teaching Assistant, Department of Chemistry and Biochemistry, Brigham Young University, Provo, UT, USA.  
2003–2006
- Teaching Assistant, Department of Chemistry, The University of Jordan, Amman, Jordan.  
2002–2003
- Analyst, Research and Development Department, Dar Al Dawa Veterinary and Agricultural Company, Amman, Jordan.  
2001–2002

##### Administrative Positions

- Director, Unit of Strategic Planning, College of Science, King Khalid University, Abha, Saudi Arabia. One year.
- Web Portal Coordinator, College of Science, King Khalid University, Abha, Saudi Arabia. Two years.
- Academic Planning and Curriculum Developer, New Bachelor of Science Program in Chemistry, Department of Chemistry, King Khalid University, Abha, Saudi Arabia. Five years.
- Director, Committee of Academic Planning and Curriculum, Department of Chemistry, King Khalid University, Abha, Saudi Arabia. Three years.
- Coordinator, Academic Schedules, Department of Chemistry, King Khalid University, Abha, Saudi Arabia. Four years.



- Academic Adviser (undergraduate level), Department of Chemistry, King Khalid University, Abha, Saudi Arabia.

#### 5. **Research Interests**

- Molecular Modeling
- Molecular Dynamics
- Protein Structure-Function Relations
- Computer-Aided Drug Design

#### 6. **Membership in Scientific Societies and Associations**

- Not applicable.

#### 7. **Honors and Awards**

- Travel Award (Biophysical Society in Long Beach, CA, USA).
- Travel Award (Biophysical Society in Baltimore, MD, USA).
- Outstanding Teaching Assistant Award (Department of Chemistry and Biochemistry, Brigham Young University, Provo, UT, USA).

#### 8. **Fellowships and Scholarships**

- Roland K. Robbins Graduate Research Fellowship (Department of Chemistry and Biochemistry, Brigham Young University, Provo, UT, USA).
- Chemistry and Biochemistry Scholarship (Department of Chemistry and Biochemistry, Brigham Young University, Provo, UT, USA).

#### 9. **Teaching Experience**

##### **Graduate Courses**

- Chem 531: Advanced Physical Chemistry
- Chem 532: Quantum Chemistry and Applications.



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**Undergraduate Courses**

- Chem 101: General Chemistry 1
- Chem 102: General Chemistry 2
- Chem 109: General Chemistry Laboratory
- Chem 107: General Chemistry for Engineers
- Chem 231: Physical Chemistry for Chemical Engineering
- Chem 336: Kinetics and Reaction Mechanisms
- Chem 436: Quantum Chemistry

**10. Supervision of Graduate Research**

- Not applicable.

**11. Grants**

- Not applicable.

**12. Patents**

- Not applicable.

**13. Membership of Committees****National and International**

- Not applicable

**University**

- Committee of Academic Planning and Curriculum, Department of Chemistry, King Khalid University, Abha, Saudi Arabia.
- Committee of Strategic Planning, College of Science, King Khalid University, Abha, Saudi Arabia.
- Committee of Academic Planning and Curriculum, College of Science, King Khalid University, Abha, Saudi Arabia.

**14. Professional and Scientific Meetings****Scientific Meetings Organized**

- 2013–2014: Fifth International Chemistry Conference, Department of Chemistry, King Khalid University, Abha, Saudi Arabia.



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**Participation in Scientific meetings**

- Not applicable.

**15. Participation in or organization of curricular and/or extra-curricular activities**

- Not applicable.

**16. Publications****Papers in refereed journals**

1. Al Adem, Kenana; Ferreira, Juliana C.; Fadl, Samar; Mustafa, Morad; and Rabeh, Wael M. Key Allosteric and Active Site Residues of SARS-CoV-2 3CLpro Are Promising Drug Targets. *Biochemical Journal*. 2023; 480(11):791–813.
2. Salman, Haya Ayyal; Yaakop, Amira Suriaty; Aladaileh, Saleem; Mustafa, Morad; Gharaibeh, Mohammed. *Inhibitory effects of Ephedra alte on IL-10, IL-6, hybrid TLR4, TNF- $\alpha$ , IL-1 $\beta$ , and extracted TLR4 receptors: in silico molecular docking*. *Heliyon*. 2021; Submitted to Journal.
3. Jamhour, Rasheed M. A. Q.; Al-Nadaf, Afaf H.; Wedian, Fadel; Al-Mazaideh, Ghassab M.; Mustafa, Morad; Huneif, Mohammed Ayed; Mahmoud, Sabry Younis; Farrag, Eman Saleh; Al-Rimawi, Fuad; Salman, Haya Ayyal; Alqudah, Ali Abdallah; Alakhras, Fadi. *Phytochemicals as a potential inhibitor of COVID-19: An in silico perspective*. *Russian Journal of Physical Chemistry A*. 2022; 96:1589–1597.
4. Mustafa, Morad; Gharaibeh, Mohammad. *Most Probable Druggable Pockets in Mutant p53-Arg175His Clusters Extracted from Gaussian Accelerated Molecular Dynamics Simulations*. *The Protein Journal*. 2022; 41:27–43.
5. Mustafa, Morad; Wedian, Fadel; Aldal'in, Hammad K.; Al-Mazaideh, Ghassab M.; Mahmoud, Sabry Younis; Farrag, Eman Saleh; Gharaibeh, Mohammed; Hijawi, Thameen; Al-Rimawi, Fuad; Abbadi, Jihad; Shalayel, Mohammed Helmy Faris; Siddique, Nadeem A.; Salman, Haya Ayyal; Huneif, Mohammed Ayed. *The efficiency of some active ingredients of Arum Palaestina as inhibitors to 3CL<sup>pro</sup> and Nsp15 proteins*. *Acta Poloniae Pharmaceutica – Drug Research*. 2021;78(5):657–665.
6. Mustafa, Morad; Mirza, Amar; Kannan, Natarajan. *Conformational regulation of the EGFR kinase core by the juxtamembrane and C-terminal tail: a molecular dynamics study*. *Proteins*. 2011;79(1):99–114.
7. Mirza, Amar; Mustafa, Morad; Talevich, Eric; Kannan, Natarajan. *Co-conserved features associated with cis regulation of ErbB tyrosine kinases*. *PLoS One*. 2010;5(12):e14310.



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8. Mustafa, Morad; Henderson, Douglas J.; Busath, David D. *Free-energy profiles for ions in the influenza M<sub>2</sub>-TMD channel*. Proteins. 2009;76(4):794–807.
9. Mustafa, Morad; Henderson, Douglas J.; Busath, David D. *Computational studies of gramicidin permeation: an entryway sulfonate enhances cation occupancy at entry sites*. Biochimica et Biophysica Acta – Biomembranes. 2009;1788(6):1404–1412.
10. Mustafa, Morad; Busath, David D. *The gramicidin channel ion permeation free-energy profile: direct and indirect effects of CHARMM force field improvements*. Interdisciplinary Sciences: Computational Life Sciences. 2009;1(2):113–127.
11. Santos, Andrés; Yuste, Santos B.; López de Haro, Mariano; Alawneh, Morad; Henderson, Douglas. *Contact values for disparate-size hard-sphere mixtures*. Molecular Physics. 2009;107(7):685–691.
12. Alawneh, Morad; Henderson, Douglas; Outhwaite, Christopher W.; Bhuiyan, Lutful Bari. *The effect of dielectric polarization of the electrode on anomalous temperature effects in the electrical double layer*. Molecular Simulation. 2008;34(5):501–507.
13. Alawneh, Morad; Henderson, Douglas J. *Molecular dynamics results for the radial distribution functions of highly asymmetric hard sphere mixtures*. Molecular Physics. 2008;106(5):607–614.
14. Bhuiyan, Lutful Bari; Outhwaite, Christopher W.; Henderson, Douglas; Alawneh, Morad. *A further Monte Carlo and modified poisson-boltzmann analysis of two recent results in the electric double layer theory*. Bangladesh Journal of Physics. 2007;4:93–102.
15. Henderson, Douglas; Alawneh, Morad; Saavedra-Barrera, Rafael; Lozada-Cassou, Marcelo. *Application of a recently proposed test to the hypernetted chain approximation for the electric double layer*. Condensed Matter Physics. 2007;10(3(51)):323–330.
16. Bhuiyan, Lutful Bari; Outhwaite, Christopher W.; Henderson, Douglas; Alawneh, Morad. *A modified poisson-boltzmann theory and Monte Carlo simulation study of surface polarization effects in the planar diffuse double layer*. Molecular Physics. 2007;105(10):1395–1402.
17. Alawneh, Morad; Henderson, Douglas. *Monte Carlo simulation of the double layer at an electrode including the effect of a dielectric boundary*. Molecular Simulation. 2007;33(6):541–547.

#### Books and Book Chapters

- Not applicable.



### Conference Presentations

1. Mustafa, Morad; Mirza, Amar; Kannan, Natarajan. *The structural impact of cancer mutations in EGFR using molecular dynamics simulations*. Georgia Cancer Research Symposium. Nov 5–6, 2008; Athens, GA, USA [Poster].
2. Mustafa, Morad; Busath, David D. *Molecular dynamics simulations of Na<sup>+</sup> transport free-energy profile for gramicidin and two analogs*. Joint Northwest and Rocky Mountain Regional Meeting of the American Chemical Society. Jun 15–18, 2008; Park City, UT, USA [Presentation].
3. Mustafa, Morad; Henderson, Douglas J.; Busath, David D. *CMAP helps solve the gramicidin problem*. Biophysical Society (52nd Annual Meeting). Feb 2–6, 2008. Long Beach, CA, USA [Poster].
4. Mustafa, Morad; Henderson, Douglas J.; Busath, David D. *A comparative study of force fields for tryptophan with experiment using MD simulations*. Telluride Science Research Center (Ion Channel Biophysics). Jul 30–Aug 3, 2007. Telluride, CO, USA [Presentation].
5. Mustafa, Morad; Henderson, Douglas J.; Busath, David D. *Studying the influenza M2 channel occupancy by other ions using MD simulations*. Telluride Science Research Center (Ion Channel Biophysics). Jul 30–Aug 3, 2007. Telluride, CO, USA [Presentation].
6. Mustafa, Morad; Henderson, Douglas J.; Busath, David D. *MD simulations of influenza M2 using different cation sizes in a lipid bilayer*. Biophysical Society (51st Annual Meeting). Mar 3–7, 2007. Baltimore, MD, USA [Presentation].
7. Mustafa, Morad; Henderson, Douglas J.; Busath, David D. *MD simulations of gramicidin A and taurine gramicidin A in a lipid bilayer*. Biophysical Society (51st Annual Meeting). Mar 3–7, 2007. Baltimore, MD, USA [Poster].

### Reports

- Not applicable.