

Curriculum Vitae

1) Personal Information:

Surname: **Mahdiuni**

First name: **Hamid**

Gender: **Male**

Marital Status: **Married**

Nationality: **Iranian**

Date of birth: **21/03/1974**

Place of Birth: **Kermanshah- Iran**

2) Contact details:

Address: **Bioinformatics Lab., Department of Biology, Razi University, Kermanshah, I.R. of Iran**

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3) Education:

Year	Degree	Major	University
Sep 2001- Oct 2008	PhD	Biochemistry	University of Tehran
Sep 1998- Sep 2001	MSc	Biochemistry	University of Tehran
Sep 1994-Sep 1998	BSc	Biology	Razi University

4) Technical Skills and experience:

Computational techniques include:

- Molecular dynamics simulation by GROMACS and NAMD packages
- Protein-ligand docking and protein-protein docking
- AI-based (machine learning and deep learning) drug discovery

Biochemical techniques include:

- Protein extraction and purification
- Enzyme assays
- SDS-PAGE and western blotting
- Chromatography (ion exchange, gel filtration, HPLC)

Biophysical techniques include:

- Construction of artificial lipid bilayer membranes
- Reconstitution of ion channel proteins in artificial membranes
- Patch-clamp and voltage-clamp techniques for determination of ion channel activity

5) Computer Skills:

- Microsoft Office package (Word, Excel, PowerPoint,...)
- Bioinformatics Software, DNA, and protein sequence analysis

6) PhD Research Projects Oct 2002- 2008:

Investigation of interaction between novel anti-TB derivatives of 1, 3, 4- thiadiazoles and artificial membranes. In this investigation, considering the importance of the process of antibacterial drug uptake by Mycobacterium tuberculosis and the way the agents enter the cell, we have studied the effects of novel antituberculosis thiadiazole derivatives on artificial lipid bilayers by voltage clamp technique. In addition, the effect of propyl and ethyl ester derivatives on the well-characterized OmpF (Outer membrane protein F) channel reconstituted in artificial bilayers was studied at the molecular level. Finally, to understand events at the molecular level, we have carried out molecular dynamic simulations of POPC (1-palmitoyl-2-oleoyl-phosphatidylcholine) bilayers containing methyl and propyl ester thiadiazoles.

7) Courses Taught:

1. Advanced topics in protein structure (PhD, Biochemistry)
2. Advanced topics in carbohydrates and lipids (PhD, Biochemistry)
3. Design of enzyme inhibitors (PhD, Biochemistry)
4. Molecular modeling (PhD, Biochemistry)
5. Enzymology (MSc, Biochemistry)
6. Bioinformatics (MSc, Biochemistry)

7. Structure of Macromolecules (MSc, Cellular and molecular biology)
8. Physical Biochemistry (BSc, Cellular and molecular biology)

8) Affiliates:

- American Biophysical Society

9) Research Interests:

- Membrane transporters and ion channels as drug targets
- Design of peptide and peptide-like ligands for disrupting protein-protein interactions
- Structure-based and ligand-based drug discovery

10) Lab Members

- Barhoon, M. (PhD, Biochemistry)
- Ezati, M. (PhD, Biochemistry)
- Veisi-Satri, E. (PhD, Biochemistry)
- Moradi, M.H. (PhD, Biochemistry)
- Mohamadi, N. (MSc, Biochemistry)
- Abdolmaleki, N. (MSc, Biochemistry)
- Shakhani, H. (MSc, Biochemistry)

11) Hobbies:

Reading books and journals, watching scientific documentaries, playing soccer, mountain climbing, and bike riding

12) Publications and presentations (in reverse chronological order):

Published papers:

- 1) M. Barhoon, **H. Mahdiuni**, A. Ebrahimi and R. Khodarahmi. 2026. "Large-scale comparative virtual screening identifies novel molecular targets underlying the multi-target activity of quercetin in psoriasis". Inflammopharmacology, DOI: <https://doi.org/10.1007/s10787-026-02364-6>
- 2) Kh. Pouraghajan, **H. Mahdiuni**, M. Barhoon and M. Ezati. 2025. "Computational biochemistry-guided discovery of novel Glycosidic inhibitors for human sodium-glucose transporter2". Journal of Molecular Liquids, 435, DOI: <https://doi.org/10.1016/j.molliq.2025.128139>

- 3) M. Barhoon and **H. Mahdiuni**. 2025. "Exploring Protein-Protein Docking Tools: Comprehensive Insights into Traditional and Deep-Learning Approaches". *Journal of Chemical Information and Modeling*, 65, 6446-6469.
- 4) A. Amjadi, M. Mohammadpour, Kh. Pouraghajan, **H. Mahdiuni**, L. Nezamabadi Farahani, M. Nadimi, G. A. Mohammadi, M. Bakhtiari, S. Eskandari, and M. R. Masoodi. 2025. "Ameliorating COVID-19-related Acute respiratory distress syndrome (ARDS) with the multi-target strategy utilising natural supplements-from in-silico to a randomised controlled clinical trial". *International Journal of Ayurvedic Medicine*, 15, 935-945,
- 5) M. Afshinpour, P. Parsi, and **H. Mahdiuni**. 2023. "Investigation of molecular details of a bacterial cationic amino acid transporter (GkApcT) during arginine transportation using molecular dynamics simulation and umbrella sampling techniques". *Journal of Molecular Modeling*, 29, 260, DOI: <https://doi.org/10.1007/s00894-023-05670-w>.
- 6) M. Afshinpour and **H. Mahdiuni**. 2023. "Arginine transportation mechanism through cationic amino acid transporter 1: insights from molecular dynamics studies". *Journal of Biomolecular Structure and Dynamics*, 41, DOI: [10.1080/07391102.2023.2175374](https://doi.org/10.1080/07391102.2023.2175374).
- 7) E. Kalehoei, M. Moradi, M. Azadbakht, H. Zhaleh, S. Azizi Lal Abadi, **H. Mahdiuni**, and A. Gharzi. 2023. "Therapeutic effects of L-arginine, L-carnitine, and mesenchymal stem cell-conditioned medium on endometriosis-induced oocyte poor quality in an experimental mouse model". *Journal of Obstetrics and Gynaecology Research*, 49, DOI: [10.1111/jog.15569](https://doi.org/10.1111/jog.15569).
- 8) Kh. Pouraghajan, **H. Mahdiuni**, S. Ghobadi, and R. Khodarahmi. 2022. "LRH-1 (liver receptor homolog-1) derived affinity peptide ligand to inhibit interactions between β -catenin and LRH-1 in pancreatic cancer cells: from computational design to experimental validation". *Journal of Biomolecular Structure and Dynamics*, 40, 3082-3097.
- 9) R. Talandashti, **H. Mahdiuni**, M. Jafari, and F. Mehrnejad. 2019. "Molecular Basis for Membrane Selectivity of Antimicrobial Peptide Pleurocidin in the Presence of Different Eukaryotic and Prokaryotic Model Membranes". *Journal of Chemical Information and Modeling*, 59, 3262-3276.
- 10) A. Nazari, E. Golezar, and **H. Mahdiuni**. 2019. "Antioxidant Activity of the *Ferula gummosa* Boiss.'s Aerial Parts: Measurements Based on Different Assay Methods". *Journal of Reports in Pharmaceutical Sciences*, 8, 61-67.
- 11) M. Mehrabi, **H. Mahdiuni**, H. Rasouli, K. Mansouri, M. Shahlaei, and R. Khodarahmi. 2018. "Comparative experimental/theoretical studies on the EGFR dimerization under the effect of EGF/EGF analogues binding: Highlighting the importance of EGF/EGFR interactions at site III interface". *International Journal of Biological Macromolecules*, 115, 401-417.
- 12) S. Ghobadi, M-R. Ashrafi-Kooshk, **H. Mahdiuni**, and R. Khodarahmi. 2018. "Enhancement of intrinsic fluorescence of human carbonic anhydrase II upon topiramate binding: Some evidence for drug-induced molecular contraction of the protein". *International Journal of Biological Macromolecules*, 108, 240-249.
- 13) E. Golezar, **H. Mahdiuni**, and A. Nazari. 2017. "Different Antioxidant Activity Measurements of the Aerial Parts of *Ferulago angulata*, Traditional Food Additives in Iran". *Indian Journal of Pharmaceutical Sciences*, 79, 900-906.
- 14) B. Akbari, A. Mohammadnia, M. Yaqubi, P. Wee, and **H. Mahdiuni**. 2017. "Comprehensive Dissection of Transcriptome Data and Regulatory Factors in Pancreatic Cancer Cells". *Journal of Cellular Biochemistry*, 118, 3976-3985.
- 15) A. Jangholi, M-R, Ashrafi-Kooshk, S. S. Arab, G. Riaz, F. Mokhtari, M. Poorebrahim, **H. Mahdiuni**, B. I. Kurganov, A. A. Moosavi-Movahedi, and R. Khodarahmi. 2016. "Appraisal of role

of the polyanionic inducer length on amyloid formation by 412-residue 1N4R Tau protein: A comparative study". Archives of Biochemistry and Biophysics, 609, 1-19.

16) N. Bijari, S. Ghobadi, **H. Mahdiuni**, R. Khodarahmi, and S. A. Ghadami. 2015. "Spectroscopic and molecular modeling studies on binding of dorzolamide to bovine and human carbonic anhydrase II". International Journal of Biological Macromolecules, 80, 189-199.

17) M. Haddad-Zahmatkesh, S. J. Hosseini-mehr, and **H. Mahdiuni**. 2014. "Role of CHK2 inhibitors in the cellular responses to ionizing radiation". Mini-Reviews in Medicinal Chemistry, 14, 812-818.

18) S. Heidari, H. Akrami, R. Gharaei, A. Jalili, **H. Mahdiuni**, and E. Golezar. 2014. "Anti-tumor activity of *Ferulago angulata* Boiss. extract in gastric cancer cell line via induction of apoptosis". Iranian Journal of Pharmaceutical Research, 13, 1335-1345.

19) F. Jalali, P. Doraji, and **H. Mahdiuni**. 2014. "Binding of the neuroleptic drug, gabapentin, to bovine serum albumin: Insights from experimental and computational studies". Journal of Luminescence, 148, 347-352.

20) **H. Mahdiuni**, N. Bijari, M. Varzandian, S. A. Ghadami, M. Khazaei, M. R. Nikbakht, and R. Khodarahmi. 2013. "Appraisal of sildenafil binding on the structure and promiscuous esterase activity of native and histidine-modified forms of carbonic anhydrase II". Biophysical Chemistry, 175, 1-16.

21) S. Mirzaaghaei, H. Akrami, H. Asadi, K. Mansouri, and **H. Mahdiuni**. 2012. "*Ferula gummosa* flower and leaf extracts inhibit angiogenesis *in-vitro*". Indian Journal of Cancer, In Press.

22) **H. Mahdiuni**, H. Mobasheri, A., Shafiee, and A. Foroumadi. 2008. "Effects of novel antituberculosis agents on OmpF channel activity". Biochemical and Biophysical Research Communications, 376, 174-179.

Poster and Lecture presentations:

23) N. Abdolmaleki and **H. Mahdiuni**. 2025. "Machine Learning-Driven Discovery of JAK2 Inhibitors from ChEMBL Databank". 4th International Iranian Conference on Bioinformatics, February 4-6, Zanjan-Iran

24) N. Abdolmaleki and **H. Mahdiuni**. 2025. "Leveraging Machine Learning Models for Virtual Screening of ZINC Database to Identify JAK1 Inhibitors". 4th International Iranian Conference on Bioinformatics, February 4-6, Zanjan-Iran

25) **H. Mahdiuni**. 2022. "How can molecular dynamics simulation methods boost drug design and drug discovery projects?". 17th National and 2nd International Conference of Iranian Biophysical Chemistry, September 6-7, Rasht-Guilan.

26) F. Jabari, **H. Mahdiuni**, and S. Sajadimajd. 2022. "Virtual screening, docking, and molecular dynamics simulation studies for the discovery of a novel inhibitor for MCT1 transporter in an open inward conformation". 17th National and 2nd International Conference of Iranian Biophysical Chemistry, September 6-7, Rasht-Guilan.

27) M. Barhoon, **H. Mahdiuni**, and S. Sajadimajd. 2022. "Repurposing of FDA-approved drugs against monocarboxylate transporter 1 (MCT1) in an open-outward conformation by virtual screening and molecular dynamics simulation studies". 17th National and 2nd International Conference of Iranian Biophysical Chemistry, September 6-7, Rasht-Guilan.

- 28) F. Jabari, **H. Mahdiuni**, and S. Sajadimajd. 2022. "Structure-based virtual screening of FDA-approved compounds to find potential inhibitors for human monocarboxylate transporter 1 in an open-inward conformation". The 1st International and 10th National Iranian Conference on Bioinformatics, February 22-24. Kish-Iran.
- 29) M. Barhoon, **H. Mahdiuni**, and S. Sajadimajd. 2022. "Ligand Discovery for the human monocarboxylate transporter 1 (MCT1) in an open- outward conformation by virtual screening on ZINC's FDA-approved drugs". The 1st International and 10th National Iranian Conference on Bioinformatics, February 22-24. Kish-Iran.
- 30) M. Afshinpour and **H. Mahdiuni**. 2019. "Identifying the Hot-Spot Residues of Cationic Amino Acid Transporters During Arginine Transport by the MM-PBSA Approach". The 4th Conference on Protein and Peptide Sciences, May 1st -2nd Isfahan-Iran.
- 31) F. Ghobadi and **H. Mahdiuni**. 2019. "Study of Inhibitory Potential of a Designed Peptide in Complex with β -Catenin Using Steered Molecular Dynamics Simulation". The 4th Conference on Protein and Peptide Sciences, May 1st -2nd Isfahan-Iran.
- 32) P. Parsi and **H. Mahdiuni**. 2019. "Structure Based Virtual Screening on DrugBank Database to Find Ligands Interfering Arginine Transportation Through the Cationic Amino Acid Transporter". The 4th Conference on Protein and Peptide Sciences, May 1st -2nd Isfahan-Iran.
- 33) F. Ghobadi and **H. Mahdiuni**. 2018. "Assessing the stability of a drug-like inhibitory peptide in complex with β -Catenin using umbrella sampling". The 7th Conference on Bioinformatics, January 3rd -5th Tehran, Iran.
- 34) T. Merati and **H. Mahdiuni**. 2018. "Highthroughput structure-based virtual screening to repropose new inhibitory compounds against FoxM1 transcription factor overexpressing in pancreatic cancerous cell lines". The 7th Conference on Bioinformatics, January 3rd -5th Tehran, Iran.
- 35) K. Pouraghajan, S. Ghobadi and **H. Mahdiuni**. 2018. "Designing and screening of a biomimetic peptide library to select blocking peptides interrupting β -catenin/LRH-1 complex in pancreatic cancerous cells". The 7th Conference on Bioinformatics, January 3rd -5th Tehran, Iran.
- 36) K. Pouraghajan and **H. Mahdiuni**. 2017. "MatLab scripting to design peptide libraries with application in deciphering protein assemblies in directing and reprogramming in stem cells". 2nd International Stem Cells & Regenerative Medicine Congress, April 19th-21th Mashhad, Iran.
- 37) K. Pouraghajan, R. Talandashti and **H. Mahdiuni**. 2016. "Phylogenetic analysis of a new *Fasciola gigantica* cathepsin L1 sequence from an Iranian isolate". 6th Conference on Bioinformatics, December 13th -15th Tehran, Iran.
- 38) K. Pouraghajan, S. Ghobadi and **H. Mahdiuni**. 2016. "High-throughput virtual screening of the constructed peptide library to obtain potential disruptive peptide(s) preventing the β -catenin/LRH-1 complex formation in pancreatic cancerous cells". 6th Conference on Bioinformatics, December 13th -15th Tehran, Iran.

(۳۹) خدیجه پورآقاجان، **حمید مهدیونی** و رضا تالاندشتی. ۱۳۹۵. "طراحی یک مدل پیتیدی برای مهار تشکیل کمپلکس β -catenine/LRH-1 در سلول‌های سرطانی پانکراس با استفاده از استراتژی زیست تقلیدی". چهاردهمین کنگره سراسری بیوشیمی ایران، ۲۶-۲۸ آبان ماه، تهران، ایران.

(۴۰) رضا تالاندشتی، **حمید مهدیونی** و خدیجه پورآقاجان. ۱۳۹۵. "طراحی مهارکننده پیتیدی علیه آنتیژن کاتپسین L1 انگل فاسیولا هپاتیکا با استفاده از تئوری جفت‌های Mekler-Idilis". چهاردهمین کنگره سراسری بیوشیمی ایران، ۲۶-۲۸ آبان ماه، تهران، ایران.

(۴۱) مرتضی حیدری، ناصر کاکاوندی، **حمید مهدیونی** و حسین فلاحی. ۱۳۹۵. "ارزیابی مقایسه‌ای قدرت اتصال گروهی از داروهای ضد درد و ضد التهاب با آنزیم‌های COX1 و COX2 با استفاده از روش داکینگ مولکولی". چهاردهمین کنگره سراسری بیوشیمی ایران، ۲۶-۲۸ آبان ماه، تهران، ایران.

(۴۲) ناصر کاکاوندی، مرتضی حیدری، حسین فلاحی و **حمید مهدیونی**. ۱۳۹۵. "مطالعه مقایسه‌ای قدرت اتصال گروهی از داروهای غیر استروئیدی با آنزیم‌های COX1 و COX2 با استفاده از روش‌های مدل‌سازی مولکولی و آنالیز داکینگ". چهاردهمین کنگره سراسری بیوشیمی ایران، ۲۶-۲۸ آبان ماه، تهران، ایران.

43) M. Varzandian and **H. Mahdiuni**. 2012. "Increased distance of His 64 from Trp 5, major reason of increased fluorescence intensity of human carbonic anhydrase II in complex with topiramate: a molecular dynamics simulation study". 17th National & 5th International Iranian Biology Conference, September 4th-6th Kerman, Iran.

44) M. Haddad, M. Varzandian and **H. Mahdiuni**. 2012. "Molecular dynamics simulation of human carbonic anhydrase II in complex with sulfonamide drug of furosemide". 17th National & 5th International Iranian Biology Conference, September 4th-6th Kerman, Iran.

45) M. Amiri, H. Fallahi and **H. Mahdiuni**. 2011 "Isolation of several proteases and α -amylase from *Bacillus subtilis* ATCC1254". 12th Iranian Congress of Biochemistry & 4th International Congress of Biochemistry and Molecular Biology, September 6th-9th Mashhad, Iran.

46) S. Heidari, H. Akrami and **H. Mahdiuni**. 2011 "Study of chemopreventive activity of ethanolic extract of *Ferulago angulata* leaves". 12th Iranian Congress of Biochemistry & 4th International Congress of Biochemistry and Molecular Biology, September 6th-9th Mashhad, Iran.

47) **H. Mahdiuni** and E. Golezar. 2011 "Identification and determination of antioxidant activity of *Ferulago angulata* extract by FRAP, DPPH and CAA assay". 11th Iranian Congress of Biochemistry, February 8th-10th Ghazvin, Iran.

48) **H. Mahdiuni**, A. Foroumadi, H. Mobasheri and A. Shafiee. 2005 "Determination of the incorporation of 2,5-disubstituted-1,3,4-thiadiazole anti tuberculosis agents into artificial bilayer lipid membrane". 15th IUPAB & 5th EBSA International Biophysics Congress, August 27th – September 1st Montpellier, France.

49) **H. Mahdiuni**, H. Hoda, M. Soudi, F. Jalilvand and M. Nemat-Gorgani. 2001. "Optimization of Glucose Oxidase Synthesis in Submerged Cultures of *Aspergillus Niger*". 6th Congress on Biochemistry, October 22th-25th Tehran, Iran.