CV

S. Ahmad Ebadi

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Personal Information

Nationality: Iranian
Date of Birth: 14/04/1984
Place of birth: Tehran
Marital Status: Married

Academic position

Associate Professor, 2021 - Now
Assistant Professor, 2014 – 2021

Education

- Ph.D. in Medicinal Chemistry, Faculty of Pharmacy, Shiraz University of Medical Sciences, 2009-2014
  Dissertation Title: Synthesis and molecular modeling of novel nonpeptidic small molecules as p38MAPK inhibitors and evaluation of TNF-α production in a cell model
  Supervisors: Prof. Miri R. & Prof. Firouzi O., *Advisors*: Prof. Javidnia K. & Prof. Ghahramani M. H.

- M.Sc. in Organic chemistry, Faculty of Chemistry, K. N. Toosi University of Technology, 2007-2009
  Thesis Title: Design and Synthesis of Novel Peptides as Anti-Cancer Agents
  Supervisor: Prof. Balalaie S., *Advisor*: Prof. Davoodi J.

- B.S. in Applied Chemistry, Faculty of Science, K. N. Toosi University of Technology, 2002-2007

Research Experience:

Synthesis of peptide (SPPS)
Synthesis of novel bioactive heterocyclic molecules via multicomponent reaction
Molecular dynamics simulation
Machine learning
Computational chemistry
Virtual screening and molecular modeling

Teaching Experiences

Organic Chemistry Laboratory I and II

- *Pharm. D.* (since 2014)

Organic Synthesis

- *MSc in Medicinal Chemistry* (since 2020)

Computational Chemistry and Molecular Modeling

- *MSc in Medicinal Chemistry* (since 2020)

Medicinal Chemistry I, II and III

- *Pharm. D.* (since 2014)
- *MSc in Medicinal Chemistry* (since 2020)

Leadership experience

Director of medicinal chemistry research lab, 2018 - now

Director of research, 2016 – 2018

Director of graduate studies, 2015 – 2018

Executive secretory of 15th Iranian pharmaceutical sciences congress 2017

Computer Skills

Operating Systems: Windows, Linux

Docking: AutoDock, AutoDock Vina

MD Simulation: GROMACS

***Ab Initio*:** ORCA

Programming Skills: Shell programming, C++, Python

Machine Learning: C++: Malpack

Python: Scikit-learn, Keras, Tensorflow

Ongoing Research Projects

Design, molecular modeling and synthesis of peptidic and heterocyclic molecules as AChE inhibitors

In silico and *in vitro* screening of natural products as anticancer and DNA binding agents

Design, molecular modeling and synthesis of anti-mitotic peptides

Using machine learning approaches in peptide and drug design

Publications

1. Najafi Z, **Ebadi A**, Chehardoli G, et al. Design, synthesis, in vitro, and in silico studies of novel benzylidene 6-methoxy-1-tetralone linked to benzyloxy and benzyl-1, 2, 3-triazole rings as potential tyrosinase inhibitors. *J Mol Struct*. 2023;1271:134018.
2. Esmaili S, **Ebadi A**, Khazaei A, et al. Novel Pyrano [3, 2-c] quinoline-1, 2, 3-triazole Hybrids as Potential Anti-Diabetic Agents: In Vitro α-Glucosidase Inhibition, Kinetic, and Molecular Dynamics Simulation. *ACS Omega*. Published online 2023.
3. Brooshghalan SE, Sabahi M, Ebadi SA, Sadeghian Z, Nayebi AM, Haddadi R. Silibinin chronic treatment in a rat model of Parkinson disease: a comprehensive in-vivo evaluation and in silico molecular modeling. *Eur J Pharmacol*. 2023;941:175517.
4. Bashiri-Nahnjeh M, Sarihi A, **Ebadi A**, Dastan D, Mohammadi M. In silico molecular modeling, neuro-behavioral profile, and toxicity assessment of the essential oil of Ferula gummosa Boiss. as an

anti-seizure agent. *J Ethnopharmacol*. 2023;309:116347.

5. Mahdian M, **Ebadi A**, Bahmani A, Dastan D, Zolfigol MA, Chehardoli G. Synthesis, Molecular Modeling, and Biological Evaluation of New N-(Benzo [d] thiazol-2-yl)-3-amino-but-2-enamide Derivatives as Cytotoxic Agents. *Org Prep Proced Int*. Published online 2023:1-10.
6. Sardari E, **Ebadi A**, Razzaghi-Asl N. In silico repurposing of CNS drugs for multiple sclerosis. *Mult Scler Relat Disord*. 2023;73:104622.
7. Ghorbani H, **Ebadi A**, Faramarzi MA, Mojtabavi S, Mahdavi M, Najafi Z. Synthesis, in vitro α-glucosidase inhibitory activity and molecular dynamics simulation of some new coumarin-fused 4H-pyran derivatives as potential anti-diabetic agents. *J Mol Struct*. 2023;1284:135349.
8. Shahmoradi A, **Ebadi A**, Dastan D. Ferulago bernardii as a New Source of α-Pinene Binds to ctDNA: In Silico and in Vitro Studies. *Chem Biodivers*. Published online 2023. doi:10.1002/cbdv.202301302
9. Babaei F, **Ebadi A**, Dastan D. Ferula haussknechtii Inhibits Acetylcholinesterase: In-Vitro and In-Silico Studies. *ChemistrySelect*. 2023;8(44). doi:10.1002/slct.202302900
10. Eyvari Brooshghalan S, Sabahi M, Ebadi SA, Sadeghian Z, Mohajjel Nayebi A, Haddadi R. Silibinin chronic treatment in a rat model of Parkinson disease: A comprehensive in-vivo evaluation and in silico molecular modeling. *Eur J Pharmacol*. 2023;941. doi:10.1016/j.ejphar.2023.175517
11. Dastan D, **Ebadi A**. Effect of substitution on the binding affinity of 5-bezylidenebarbituric acid derivatives to ctDNA: in silico and in vitro studies. *J Chem Sci*. 2022;134(1):1-11.
12. Dastan D, Zhiyani R, Fasihi K, **Ebadi A**. An arginine-rich peptide inhibits AChE: template-based design, molecular modeling, synthesis, and biological evaluation. *J Mol Model*. 2022;28(4):1-13.
13. **Ebadi A**, Najafi Z, Pakdel-yeganeh H, Dastan D, Chehardoli G. Design, synthesis, molecular modeling and DNA-binding studies of new barbituric acid derivatives. *J Iran Chem Soc*. Published online 2022:1-12.
14. Rezvani S, **Ebadi A**, Razzaghi-Asl N. In silico identification of potential Hsp90 inhibitors via ensemble docking, DFT and molecular dynamics simulations. *J Biomol Struct Dyn*. 2022;40(21):10665-10676. doi:10.1080/07391102.2021.1947383
15. Chehardoli G, Gholamhoseini P, **Ebadi A**, et al. 6-Methoxy-1-tetralone Derivatives Bearing an N-Arylpyridinium Moiety as Cholinesterase Inhibitors: Design, Synthesis, Biological Evaluation, and Molecular Docking Study. *ChemistrySelect*. 2022;7(27). doi:10.1002/slct.202201977
16. Rezvani S, **Ebadi A**, Razzaghi-Asl N. In silico identification of potential Hsp90 inhibitors via ensemble docking, DFT and molecular dynamics simulations. *J Biomol Struct Dyn*. Published online 2021:1-12.
17. Moosavi F, **Ebadi A**, Mohabbati M, et al. Antiproliferative effect, alteration of cancer cell cycle progression and potential MET kinase inhibition induced by 3, 4-dihydropyrimidin-2 (1H)-one C5 amide derivatives. *Eur J Pharmacol*. 2021;894:173850.
18. Razzaghi-Asl N, **Ebadi A**. In silico design of peptide inhibitors of tubulin: amyloid-β as a lead compound. *J Biomol Struct Dyn*. 2021;39(6):2189-2198. doi:10.1080/07391102.2020.1745691
19. Razzaghi-Asl N, **Ebadi A**, Shahabipour S, Gholamin D. Identification of a potential SARS-CoV2 inhibitor via molecular dynamics simulations and amino acid decomposition analysis. *J Biomol Struct Dyn*. 2021;39(17):6633-6648. doi:10.1080/07391102.2020.1797536
20. **Ebadi A**, Olyaie SS, Dastan D. To be ionized or not to be ionized: the vital role of physicochemical properties of galbanic acid derivatives in AChE assay. *J Biomol Struct Dyn*. 2021;39(9):3235-3243. doi:10.1080/07391102.2020.1764391
21. Alikhani R, **Ebadi A**, Karami P, Shahbipour S, Razzaghi-Asl N. Response Surface Study on Molecular Docking Simulations of Citalopram and Donepezil as Potent CNS Drugs. *Iran J Pharm Res*. 2021;20(3):560-576. doi:10.22037/ijpr.2020.113644.14409
22. Khazaei M, Dastan D, **Ebadi A**. Binding of Foeniculum vulgare essential oil and its major compounds to double-stranded DNA: In silico and in vitro studies. *Food Biosci*. 2021;41:100972.
23. Dastan D, Fasihi K, **Ebadi A**. From Venom to AChE Inhibitor: Design, Molecular Modeling, and Synthesis of a Peptidic Inhibitor of AChE. *Int J Pept Res Ther*. 2021;27(1):463-474.
24. Sharifi H, **Ebadi A**, Soleimani M. Biological evaluation and molecular modeling of 3,4-dihydropyrimidine-2(1h)-one derivatives as cytotoxic agents on breast cancer in vitro. *Lett Drug Des Discov*. 2020;17(8):983-992. doi:10.2174/1570180817666200203125010
25. Dastan D, Validi S, **Ebadi A**. Kamonolol acetate from Ferula pseudalliacea as AChE inhibitor: in vitro

and in silico studies. *Struct Chem*. 2020;31(3):965-973. doi:10.1007/s11224-019-01473-z

26. Dastan D, Fasihi K, **Ebadi A**. From Venom to AChE Inhibitor: Design, Molecular Modeling, and Synthesis of a Peptidic Inhibitor of AChE. *Int J Pept Res Ther*. Published online 2020. doi:10.1007/s10989-020-10103-w
27. **Ebadi A**, Olyaie SS, Dastan D. To be ionized or not to be ionized: the vital role of physicochemical properties of galbanic acid derivatives in AChE assay. *J Biomol Struct Dyn*. Published online 2020. doi:10.1080/07391102.2020.1764391
28. Razzaghi-Asl N, **Ebadi A**. In silico design of peptide inhibitors of tubulin: amyloid-β as a lead compound. *J Biomol Struct Dyn*. Published online 2020. doi:10.1080/07391102.2020.1745691
29. Razzaghi-Asl N, **Ebadi A**, Shahabipour S, Gholamin D. Identification of a potential SARS-CoV2 inhibitor via molecular dynamics simulations and amino acid decomposition analysis. *J Biomol Struct Dyn*. Published online 2020. doi:10.1080/07391102.2020.1797536
30. Tahmasebi E, Dastan D, **Ebadi A**. Design, synthesis and biological evaluation of anticholinesterase peptides: Fragment-based vs. template-based peptide design. *Bioorg Chem*. 2020;105:104351.
31. Razzaghi-Asl N, Sepehri S, **Ebadi A**, Karami P, Nejatkhah N, Johari-Ahar M. Insights into the current status of privileged N-heterocycles as antileishmanial agents. *Mol Divers*. 2020;24(2):525-569. doi:10.1007/s11030-019-09953-4
32. Ekhtiyari MS, Moradkhani S, **Ebadi A**, Dastan D. Chemical Composition of the Essential Oils from the Aerial Parts of Eryngium bornmuelleri. *Chem Nat Compd*. 2020;56(6):1154-1155. doi:10.1007/s10600-020-03253-2
33. Miri R, Bohlooli F, Razzaghi-Aslb N, **Ebadi A**. Molecular modeling of indeno [1, 2-b] quinoline-9, 11-diones as cytotoxic agents. *Iran J Pharm Res*. 2018;17(4):1249-1262. https://www.scopus.com/inward/record.uri?eid=2-s2.0-85061360031&partnerID=40&md5=7530575789c751ba51fd97bffc91cbd3
34. Razzaghi-Asl N, Karimi A, **Ebadi A**. The potential of natural product vs neurodegenerative disorders: In silico study of artoflavanocoumarin as BACE-1 inhibitor. *Comput Biol Chem*. 2018;77:307-317. doi:10.1016/j.compbiolchem.2018.10.015
35. Ebrahimi M, Firuzi O, Miri R, Razzaghi-Asl N, **Ebadi A**. Structural Insight into Binding Mode of 9-Hydroxy Aristolochic Acid, Diclofenac and Indomethacin to PLA2. *Interdiscip Sci Comput Life Sci*. 2018;10(2):400-410. doi:10.1007/s12539-016-0197-0
36. **Ebadi A**, Dastan D, Azami M, Karimi A, Razzaghi-Asl N. Molecular Modeling of Human CCR2 Receptor within POPC Lipid Bilayer. *Struct Chem*. 2017;28(3):849-857. doi:10.1007/s11224-016-0891-x
37. **Ebadi A**, Khoshneviszadeh M, Javidnia K, Ghahremani MH, Firuzi O, Miri R. 3,4-Dihydropyrimidin-2(1H)-one C5 amides as inhibitors of T NFα production: Synthesis, biological evaluation and molecular modeling. *Lett Drug Des Discov*. 2017;14(8):885-897. doi:10.2174/1570180814666170306120235
38. Razzaghi-Asl N, Sepehri S, **Ebadi A**, Miri R, Shahabipoura S. Effect of biomolecular conformation on docking simulation: A case study on a potent HIV-1 protease inhibitor. *Iran J Pharm Res*. 2015;14(3):785-802. https://www.scopus.com/inward/record.uri?eid=2-s2.0-84931055558&partnerID=40&md5=e6e3e3f9bb7b3785171d4a62aa54f6a7
39. Razzaghi-Asl N, Sepehri S, **Ebadi A**, Miri R, Shahabipour S. Molecular docking and quantum mechanical studies on biflavonoid structures as BACE-1 inhibitors. *Struct Chem*. 2015;26(2):607-621. doi:10.1007/s11224-014-0523-2
40. Razzaghi-Asl N, Shahabipour S, **Ebadi A**, Bagheri A. Quantum chemical analysis of potential anti-Parkinson agents. *J Chem Sci*. 2015;127(7):1211-1220. doi:10.1007/s12039-015-0889-8
41. Ebadi SA, Razzaghi-Asl N, Khoshneviszadeh M, Miri R. Detailed atomistic molecular modeling of a potent type II p38α inhibitor. *Struct Chem*. 2015;26(4):1125-1137. doi:10.1007/s11224-015-0568-x
42. Nikkhoo AR, Miri R, Arianpour N, Firuzi O, **Ebadi A**, Salarian AA. Cytotoxic activity assessment and c-Src tyrosine kinase docking simulation of thieno[2,3-b] pyridine-based derivatives. *Med Chem Res*. 2014;23(3):1225-1233. doi:10.1007/s00044-013-0729-7
43. Razzaghi-Asl N, Hemmateenejad B, **Ebadi A**, Shahabipour S, Miri R. A new insight into computational molecular design: A case study on BACE-1 inhibitors. *J Comput Methods Sci Eng*.

2014;14(4-5):315-325. doi:10.3233/JCM-140506
44. **Ebadi A**, Razzaghi-Asl N, Shahabipour S, Miri R. Ab-initio and conformational analysis of a potent VEGFR-2 inhibitor: A case study on Motesanib. *Iran J Pharm Res*. 2014;13(2):405-415. https://www.scopus.com/inward/record.uri?eid=2-s2.0-84902104147&partnerID=40&md5=31fb855a3601324d54451c76e0a0a4ac
45. **Ebadi A**, Razzaghi-Asl N, Khoshneviszadeh M, Miri R. Comparative amino acid decomposition analysis of potent type i p38α inhibitors. *DARU, J Pharm Sci*. 2013;21(1). doi:10.1186/2008-2231-21-41
46. Razzaghi-Asl N, **Ebadi A**, Edraki N, Shahabipour S, Miri R. Fragment-based binding effciency indices in bioactive molecular design: A computational approach to BACE-1 inhibitors. *Iran J Pharm Res*. 2013;12(3):423-436. https://www.scopus.com/inward/record.uri?eid=2-s2.0-84883758803&partnerID=40&md5=f21635fe69624f37c35b49be0cd3fddb
47. Razzaghi-Asl N, **Ebadi A**, Edraki N, Shahabipour S, Miri R. Ab initio modeling of a potent isophthalamide-based BACE-1 inhibitor: Amino acid decomposition analysis. *Med Chem Res*. 2013;22(7):3259-3269. doi:10.1007/s00044-012-0277-6
48. Razzaghi-Asl N, **Ebadi A**, Edraki N, Mehdipour A, Shahabipour S, Miri R. Response surface methodology in docking study of small molecule BACE-1 inhibitors. *J Mol Model*. 2012;18(10):4567-4576. doi:10.1007/s00894-012-1424-1
49. Salami M, Moosavi-Movahedi AA, Ehsani MR, et al. Improvement of the antimicrobial and antioxidant activities of camel and bovine whey proteins by limited proteolysis. *J Agric Food Chem*. 2010;58(6):3297-3302. doi:10.1021/jf9033283

Thesis:

- *Supervisor*

1. Synthesis and molecular modeling of novel 3,4-dihydropyrimidin-2-one derivatives as BACE-1 inhibitors, 2017
2. Phytochemical analysis of *Ferula pseudalliacea* essential oils and molecular modeling of Galbanic acid as farensyl transferase inhibitor, 2017
3. Molecular modeling and Synthesis of novel 3,4-dihydropyrimidin-2-one derivatives as anticancer agents, 2018
4. Theoretical design, structure prediction, and molecular dynamic simulation of the p28-apoptin chimeric protein ,2018
5. Biological evaluation and molecular modeling of
6. 3,4-dihydropyrimidine-2(1H)-one derivatives as cytotoxic agents on breast cancer and normal breast cell lines, 2019
7. Biological evaluation and molecular modeling of coumarin compounds in *Ferula pseudalliacea* as acetylcholinesterase inhibitors, 2020
8. Synthesis, biological evaluation and molecular modeling of peptide derivatives as AchE inhibitors, 2020
9. MCSS Based Design, Molecular Modeling, Synthesis and Evaluation of AChE Inhibitory Effect of New Peptidic Compounds, 2020
10. Evaluating the interaction of essential oils and main compounds of *Foeniculum vulgare* with DNA strand: *in vitro* and *in silico* studies, 2020

11. Design, Synthesis and Biological Evaluation of Peptide Compounds as Acetylcholinesterase Inhibitors, 2021
12. Phytochemical and DNA binding evaluation of *Ferulago bernardii* essential oil and extract, 2021
13. Evaluation of *Ferula haussknechtii* essential oil and extract as AChE inhibitor; *in vitro* and *in silico* studies, 2021
14. Synthesis, molecular modeling and binding of the barbituric acid drivatives to DNA, 2021
15. Design, molecular modelling and synthesis of peptidic compounds as G-quadruplex stabilizer, 2022

- ***Advisor***

1. The evaluation of phytochemical, antioxidant and anticholinesterase effects of essential oil and extracts of *Eryngium bornmuelleri*, 2020
2. Investigation of toxicity, anticonvulsant effects, and molecular modeling of *Ferula Gummosa* Boiss. oleo gum resin in male mice, 2022

Research projects

1. Design, Molecular Modeling and Synthesis of Peptidic Compounds as Acetylcholinesterase Inhibitors; 2017
2. Design, synthesis, molecular modeling and binding studies of 2-benzylidenecycloalkane-1,3-dione derivatives to DNA; 2016
3. Biological evaluation and molecular modeling of coumarin compounds from *Ferula pseudalliacea* as AChE inhibitor in the treatment of alzheimer disease; 2015

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References

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