

Curriculum Vitae

Dr. Hajar Sirous-Najafabadi

Date of Birth: 24/8/1983

Nationality: Iranian

Gender: Female

Marital Status: Married

Mobile Number: +989131331258

Author ID: 56415126100

Researcher ID: AAM-3860-2020

ORCID Identifier: 0000-0003-4311-9952

E-mail Address: h_sirous@pharm.mui.ac.ir, h.sirous62@yahoo.com, sirous769@gmail.com

Education and training

- **Dates (from–to):** 2001-2005

Title of qualification awarded: BSc in chemistry

Name and type of organization providing education and training: Department of chemistry, Isfahan University. Iran

- **Dates (from–to):** 2006-2008

Title of qualification awarded: MSc in organic chemistry

Name and type of organization providing education and training: Department of chemistry, Kashan University. Iran

Titles of MSC's thesis: A) chemical constituents evaluation of the essential oil of *Provskia atriplicifolia* Benth. And *Demavendia Pastinacifolia* (Bioss & Hasskn). *Pimonv* from kashan

B) Antioxidant and Antibacterial activity evaluation of the methanolic extracts of *Provskia atriplicifolia* Benth. And *Demavendia Pastinacifolia* (Bioss & Hasskn). *Pimonv* from kashan, supervised by: prof.Abdolhamid Bamoniri, Dr.Abdolrasul H. Ebrahimabadi

- **Dates (from–to):** (2010-2017)

Title of qualification awarded: Ph.D. in medicinal chemistry

Name and type of organization providing education and training: Department of Medicinal Chemistry, Faculty of Pharmacy and Pharmaceutical Sciences, Isfahan University of Medical Sciences. Iran

Titles of PhD's thesis: Design, synthesis and biological evaluation of some potential integrase inhibitors as novel HIV-1 growth inhibitors, supervised by: prof. Afshin Fassihi, Prof. Lotfollah Saghaei. Prof. Hamid Reza Memarian and Mohammad Reza Aghasadeghi

- **Dates (from–to):** October 2015-June 2016

Title of qualification awarded: Ph.D. degree completion as a PhD exchange student

Name and type of organization providing education and training: A) Department of Biotechnology, chemistry and pharmacy of the University of Siena, Italy
B) European research Centre for drug discovery & development, Siena, Italy (<http://www.natsyndrugs.org/>).

Principal subjects/occupational skills covered: computational chemistry, Drug Design, Drug Discovery, Molecular Modeling, Lead Discovery and Lead Optimization, synthesis

of some novel HIV-1 integrase inhibitors as lead compounds identified through computational protocols.

Name of supervisor: Prof. Giuseppe Campiani (campiani@unisi.it)

1) Occupation or current position

● **Dates (from–to):**

1. 2018- present: Researcher and member of Bioinformatics Research Center, School of Pharmacy and Pharmaceutical Sciences, Isfahan University of Medical Sciences, Isfahan, IRAN.
2. 2021-present: Head of Bioinformatic of Bioinformatics Research Center, School of Pharmacy and Pharmaceutical Sciences, Isfahan University of Medical Sciences, Isfahan, IRAN.

2) Teaching Experiences:

1. General Chemistry (2010-)
2. Practical General Chemistry (2010-)

3) Workshops Experiences:

1. Organizing of theoretical and practical training workshop entitled "**essential oil and natural products**" in Ghamsar Essential Oil Research Institute of the university of Kashan and Barij essence pharmaceutical company on May19-20 2008).

4) Training workshop:

1. Attended and successfully completed the theoretical and practical training workshop entitled "**Ultra performance liquid chromatography (UPLC)**" on January 18, 2011.
2. Attended and successfully completed the theoretical training workshop entitled "**Bioinformatics application in pharmaceutical science**" on February 24, 2011.
3. Attended and successfully completed the theoretical and practical training workshop entitled "**Endnote**" on May 16-17, 2012.
4. Attended and successfully completed the theoretical and practical training workshop entitled "**Search skills**" on June 16-17, 2012.
5. Attended and successfully completed the theoretical and practical training workshop entitled "**SPSS**" on July 14-17, 2012.
6. Attended and successfully completed the theoretical and practical training workshop entitled "**Cell Culture**" on September 2, 2012.
7. Attended and successfully completed the theoretical workshop training entitled "**Product commercialization methods**" on December 1, 2019.
8. Attended and successfully completed the theoretical and practical training workshop entitled "**creative thinking tools**" on December 16, 2019.
9. Attended and successfully completed the theoretical and practical training workshop entitled "**Search strategy**" on January 2020.

5) Awards and Honors:

1. Rewarded for nominated project in the *2th scientific festival of Kashan University*.
2. Ph.D. degree completion in the Department of Biotechnology, chemistry and pharmacy of the the University of Siena (Italy).
3. Honored and Rewarded as outstanding oral presenter in *3th International Congress on Pharmacy Updates*. February 5-8, 2020. Tehran, Iran.

6) publications:

1. **Hajar Sirous**, Rezvan Zabihollahi, Mohammad R. Aghasadeghi, Seyed Mehdi Sadat, Lotfollah Saghale, Afshin Fassihi. Docking studies of some 5-hydroxypyridine-4-one derivatives: evaluation of integrase and ribonuclease H domain of reverse transcriptase as possible targets for anti-HIV-1 activity. *Medicinal Chemistry Research*. 2015; 24(5): 2195-2212. DOI: [10.1007/s00044-014-1289-1](https://doi.org/10.1007/s00044-014-1289-1) . (IF: 1.965)
2. Mahboubeh Rostami, **Hajar Sirous**, Rezvan Zabihollahi, Mohammad R. Aghasadeghi, Seyed Mehdi Sadat, Rahele Namazi, Lotfollah Saghale, Hamid R. Memarian, Afshin Fassihi. Design, synthesis and anti-HIV-1 evaluation of a series of 5-hydroxypyridine-4-one derivatives as possible integrase inhibitors. *Medicinal Chemistry Research*, 2015; 24:4113-4127. DOI: [10.1007/s00044-015-1443-4](https://doi.org/10.1007/s00044-015-1443-4) . (IF: 1.965)
3. Azizeh Asadzadeh, **Hajar Sirous**, Morteza Pourfarzam, Parichehreh Yaghmaei, Afshin Fassihi, *In vitro* and *in silico* studies of the inhibitory effects of some novel kojic acid derivatives on tyrosinase enzyme. *Iranian Journal of Basic Medical Sciences*. 2016; 19(2): 132–144. PMID: [27081457](https://pubmed.ncbi.nlm.nih.gov/27081457/) , PMCID: PMC4818360. (IF: 2.699)
4. **Hajar Sirous**, Afshin Fassihi, Simone Brogi, Giuseppe Campiani, Frauke Christ, Zeger Debyser, Sandra Gemma, Stefania Butini, Giulia Chemi, Alessandro Grillo, Rezvan Zabihollahi, Mohammad R. Aghasadeghi, Lotfollah Saghale, Hamid R. Memarian. Synthesis, molecular modelling and biological studies of some 3-hydroxy-pyran-4-one and 3-hydroxy-pyridine-4-one derivatives as HIV-1 integrase inhibitors. *Medicinal Chemistry*, 2019; 15 (7): 755-770. DOI: [10.2174/1573406415666181219113225](https://doi.org/10.2174/1573406415666181219113225) . (IF: 2.745)
5. **Hajar Sirous**, Giulia Chemi, Sandra Gemma, Stefania Butini, Zeger Debyser, Frauke Christ, Lotfollah Saghale, Simone Brogi, Afshin Fassihi, Giuseppe Campiani, Margherita Brindisi. Identification of Novel 3-Hydroxy-pyran-4-One Derivatives as Potent HIV-1 Integrase Inhibitors Using *in silico* Structure-Based Combinatorial Library Design Approach. *Frontiers in Chemistry*, 2019; 7: 574. DOI: [10.3389/fchem.2019.00574](https://doi.org/10.3389/fchem.2019.00574) . (IF: 5.221)

- 6) **Hajar Sirous**, Giulia Chemi, Giuseppe Campiani, Simone Brogi. An integrated *in silico* screening strategy for identifying promising disruptors of p53-MDM2 interaction. *Computational biology and chemistry*, 2019; 83: 107105. DOI: [10.1016/j.compbiolchem.2019.107105](https://doi.org/10.1016/j.compbiolchem.2019.107105) . (IF: 2.877)
- 7) **Hajar Sirous**, Giuseppe Campiani, Simone Brogi, Vincenzo Calderone, Giulia Chemi, Computer-driven development of an *in silico* tool for finding selective histone deacetylase 1 inhibitors. *Molecules*, 2020; 25(8):1952. DOI: [10.3390/molecules25081952](https://doi.org/10.3390/molecules25081952) . (IF: 4.411)
- 8) Zahra Bidram, **Hajar Sirous**, Ghadam Ali Khodarahmi, Farshid Hassanzadeh, Nasim Dana, Amir Ali Hariri, Mahboubeh Rostami. Monastrol s Derivatives; *In-silico* and *In-vitro* Cytotoxicity Assessments. *Research in Pharmaceutical sciences*. 2020; 15 (3):249-262. DOI: [10.4103/1735-5362.288427](https://doi.org/10.4103/1735-5362.288427).
- 9) Simone Brogi, **Hajar Sirous**, Vincenzo Calderone, Giulia Chemi, Amyloid β fibril disruption by oleuropein aglycone: long-time molecular dynamics simulation to gain insight into the mechanism of action of this polyphenol from extra virgin olive oil. *Food & Function*. 2020;11(9):8122-8132. DOI: [10.1039/D0FO01511C](https://doi.org/10.1039/D0FO01511C). (IF: 5.396)
- 10) **Hajar Sirous**, Giuseppe Campiani, Vincenzo Calderone, Simone Brogi, Discovery of novel hit compounds as potential HDAC1 inhibitors: The case of ligand-and structure-based virtual screening. *Computers in Biology and Medicine*. 2021; 137:104808. DOI: [10.1016/j.compbiomed.2021.104808](https://doi.org/10.1016/j.compbiomed.2021.104808). (IF: 4.589)
- 11) **Hajar Sirous**, Behnaz Yazdani B, HIF3A: A Potent Prognostic Biomarker in Different Kinds of Cancer. *Preprints*. DOI: [10.20944/preprints202104.0265.v1](https://doi.org/10.20944/preprints202104.0265.v1)

7) Congresses:

1. **Hajar sirous**, Abdolrasul H. Ebrahimabadi, Abdolhamid Bamoniri, Evaluation of the *In vitro* Antioxidant Activity and Total Phenolic Content of Methanolic extract of *Demavendia Pastinacifolia* (Bioss & Hasskn). *Pimony. 11th Iranian Pharmaceutical Sciences Congress, kerman, Iran.*
2. **Hajar sirous**, Abdolrasul H. Ebrahimabadi, Abdolhamid Bamoniri, In vitro Antioxidant Activity Evaluation of Methanol Extracts From *Astrodaucus orientalis* (L.) Drude. *15th Iranian congress of Organic Chemistry. Kermanshah, Iran*
3. **Hajar sirous**, Abdolrasul H. Ebrahimabadi, Abdolhamid Bamonir, Evaluation of the *in vitro* antioxidant activity of polar and non-polar extracts

from *Perovskia atriplicifolia* Benth. *13th Iranian Pharmaceutical Sciences Congress. Isfahan, Iran.*

4. **Hajar Sirous**, Afshin Fassihi, Simone Brogi, Giuseppe Campiani, Zeger Debyser. Kojic acid-derived integrase inhibitors as novel anti-HIV-1 agents: synthesis, molecular modelling and bioactivity. *2th International Congress on Pharmacy Updates. February 6-8, 2019. Tehran, Iran.*
5. Seyedeh Azin Mirmotahhari, Mahboubeh Rostami, Farshid hassanzadeh, **Hajar Sirous**. Studies of some hybrid derivatives based on dimethyl fumarate-benzothiazole scaffold on NMDA receptor for MS treatment: Molecular docking. *22th Iranian Pharmacy Student Seminar. April 16-19, 2019. Zanjan, Iran.*
6. Niloofar Naghi Ganji, Mahboubeh Rostami, **Hajar Sirous**. Investigation of the molecular docking of a number of hydroxypyridinone-benzothiazole hybrid derivatives as a possible inhibitor of histone deacetylase enzyme. *22th Iranian Pharmacy Student Seminar. April 16-19, 2019. Zanjan, Iran.*
7. Niloofar Naghi Ganji, Mahboubeh Rostami, **Hajar Sirous**. Investigation of the molecular docking of a number of hydroxypyridinone-benzothiazole hybrid derivatives as a possible inhibitor of lactate dehydrogenase enzyme. *22th Iranian Pharmacy Student Seminar. April 16-19, 2019. Zanjan, Iran.*
8. **Hajar Sirous**, Afshin Fassihi, Simone Brogi, Giuseppe Campiani, Zeger Debyser. Structure-based virtual screening, synthesis and biological activity studies for identification of novel HIV-1 integrase inhibitors derived from kojic acid scaffold. *3th International Congress on Pharmacy Updates. February 5-8, 2020. Tehran, Iran.*
9. Mahboubeh Mardanshahi, **Hajar Sirous**. Some new Small Molecules as P53 Re-activators, in-silico study. *3th International Congress on Pharmacy Updates. February 5-8, 2020. Tehran, Iran.*
10. Niloofar Naghi Ganji, Mahboubeh Rostami, **Hajar Sirous**. Some novel pyridone-indoles derivatives as possible LDH inhibitors. *3th International Congress on Pharmacy Updates. February 6-8, 2020. Tehran, Iran.*

9. Other research Projects and activities

- **As a project director**

1. Project Title: "Identification of some novel histone deacetylase inhibitors as anti-Cancer agents using computational drug design approaches" (2018, **accepted project in Bioinformatics Research Center, Isfahan University of Medical Sciences, Grant No. 298025**)
2. Project Title: "Structure-activity relationship studies of some benzamide Analogues as HDAC inhibitors using Pharmacophore-based 3D-QSAR modelling"(2019, **accepted project in Bioinformatics Research Center, Isfahan University of Medical Sciences, Grant No. 298137**)

3. Project Title: "Identification of some direct Hypoxia-inducible factor inhibitors, possessing anti-angiogenic potential as anti-cancer agents using computational structure-based screening approach" (2019, accepted project in Bioinformatics Research Center, Isfahan University of Medical Sciences, Grant No. 299006).
 4. Project Title: "*In silico* design and development of some selective sirtuin2 inhibitors through structural optimization of lead compound". (2020, accepted project in research council of Isfahan University of Medical Sciences, Grant No. 199313).
 5. Project Title: "identification of some selective sirtuin 1 activators using computational structure-based screening approaches" (2020, accepted project in Bioinformatics Research Center, Isfahan University of Medical Sciences, Grant No. 299128)
- **As a project colleague**
 1. Project Title: "Design, Synthesis and initial Cytotoxicity Evaluation of some indole-pyrimidine-oxadiazole derivatives as P53 activators, on Hela Cell line" (2019, accepted project in Pharmaceutical Sciences Research Center)
 - **As a thesis co-supervisor:**
 1. Samane Hatami, Pharm. D. thesis: "Correction of structural defects in PDB files of soluble proteins in cancer signaling pathway" (2019-)
 2. Shahryar Moteshabes, Pharm.D thesis: "Structural search for proposing some new FoxM1 protein inhibitors using virtual screening, molecular docking and 3D-QSAR" (2019-)
 3. Fatemeh mohamadi moghadam, Pharm.D thesis: "Design and selection of anti-EGFR aptamer using in silico SELEX and its evaluation on A431 and HEK293T cells" (2020-)
 4. Behjat nafari, PhD thesis: "Design and selection of anti- vimentin aptamer using in silico SELEX and its evaluation on 2D- and 3D-cultured breast cancer cells" (2021-)
 5. Arman Bigham, Pharm.D thesis: "identification of some selective sirtuin 1 activators using computational structure-based screening approaches" (2021-)
 - **As a thesis Adviser**
 1. Seyedeh Azin Mirmotahari, M.Sc. thesis: "Design, synthesis and *in vivo* evaluation of Anti-inflammatory effects of some amide-fumarate derivatives" (2018-).
 2. Niloofer Naghi Ganji, M.Sc. thesis: "Synthesis, molecular docking and biological evaluation of some pyridone-indole derivatives as possible anti-cancer agents" (2018-)

3. Mahsa zekri, Pharm.D. thesis: “Structural search for proposing some new tyrosine kinase inhibitors using molecular docking- based virtual screening and 3D-QSAR” (2019-)
4. Ali Mehri, M.Sc. thesis: “ Design, synthesis, and cytotoxicity evaluation of new pyrimidine-based derivatives as antitumor agents” (2021-)

- **As reviewer in**

Research in Pharmaceutical Sciences (RPS)

Computational Biology and medicine

Journal of Medical signals and Sensors (JMSS)

8) Scientific skills and competences:

- Knowledge of scientific software:
 - ✓ Molecular Modelling package software: Maestro Suite Molecular Modelling Environment (Schrödinger), Discovery Studio (Accelrys) and Hyperchem.
 - ✓ Molecular Docking software: Autodock (The Scripps Research Institute), Glide (Schrödinger).
 - ✓ Sites of Metabolism prediction software: P450 SOM (Schrödinger)
 - ✓ ADME+T properties prediction software: QikProp (Schrödinger) and web server tools for ADME+T prediction (ChemBio Server, Osiris property explorer, FAF-Drugs2)
 - ✓ quantum mechanical software: Jaguar (Schrödinger)
 - ✓ Phramacophore-based 3D-QSAR:Phase (Schrödinger)
 - ✓ Lead discovery and optimization software: CombiGlide (Schrödinger)
 - ✓ Molecular Dynamics software: GROMACS, Amber (UCSF), Desmond (DESRES).
 - ✓ Homology Modelling software: Prime (Schrödinger).
 - ✓ Molecular Visualization software: PyMOL (Schrödinger), Discovery studio visualizer, Viewer lite, VMD (TCB).
 - ✓ Molecular Editor & Chemical Drawing programs: ChemDraw (CambridgeSoft), Chem Sketch (ACD), Marvin sketch.
 - ✓ Knowledge of bioinformatics databases (PDB, Expasy, UniprotKB)
 - ✓ Knowledge of chemical toolbox: Open Babel

- Knowledge of Linux operating system (Ubuntu, Debian).
- Knowledge of Office packages (Microsoft Office).
- Knowledge of organic chemical synthesis, purification and organic compounds characterization techniques.
- Knowledge of extraction of natural compounds and their antioxidant Activity Evaluation Methods
- Proven ability to make connect and collaborate with European universities and international academic research centers:
 - ✓ European research Centre for drug discovery & development, Siena, Italy.
 - ✓ Department of Biotechnology, chemistry and pharmacy of the University of Siena, Italy.
 - ✓ Department of pharmacy, University of Pisa, Italy
 - ✓ Laboratory of Molecular Virology and Gene Therapy, Department of Pharmaceutical and Pharmacological Sciences, KU Leuven university, Leuven, Belgium
 - ✓ Wellcome Centre for Anti-Infectives Research, Drug Discovery Unit, Division of Biological Chemistry and Drug Discovery, University of Dundee, Dundee, UK.