

Curriculum Vitae

Afshin Fassihi

PharmD, PhD, Rph
Medicinal Chemist



Date of Birth: 16/05/1970

Nationality: Iranian

Education:

PharmD, School of Pharmacy and Pharmaceutical Sciences, Isfahan University of Medical Sciences-Iran (1988-1995)

PhD, School of Pharmacy and Pharmaceutical Sciences, Isfahan University of Medical Sciences-Iran (1996-2002)

Fellowship for PhD Degree Completion, Faculty of Pharmacy, University of Alberta-Canada (2001-2002)

Post-Doctoral Fellowship, Faculty of Pharmacy, University of Alberta-Canada (2003-2004)

Rph, Registered Pharmacist, Iranian Ministry of Health and Medical Education (2005-)

Visiting Associate Professor, Chemistry Department, Wilfrid Laurier University, Waterloo, Canada (May 2012-November 2012)

Visiting Scientist, Bioinformatics and High-Performance Computing Research Group (BIO-HPC), Universidad Católica San Antonio de Murcia, Murcia, Spain (September 2014-January 2015)

Academic positions:

1. Full Professor, Department of Medicinal Chemistry, School of Pharmacy and Pharmaceutical Sciences, Isfahan University of Medical Sciences (April 2016-)
2. Associate Professor, Department of Medicinal Chemistry, School of Pharmacy and Pharmaceutical Sciences, Isfahan University of Medical Sciences (June 2010-April 2016)
3. Assistant Professor, Department of Medicinal Chemistry, School of Pharmacy and Pharmaceutical Sciences, Isfahan University of Medical Sciences (February 2004-June 2010)

Positions held:

1. Head of Library and Information Centre, School of Pharmacy and Pharmaceutical Sciences, Isfahan University of Medical Sciences (2006-2008)
2. Head of Bioinformatic Research Centre Isfahan University of Medical Sciences (2018- 2021)

Membership in Research Centers and Councils:

1. Member of the Research Centers Council, MUI.
2. Member of the Academic Publication Council, MUI.
3. Member of Isfahan School of Pharmacy Academic Publication Council.
4. Member of the Basic Science Research Council, MUI.
5. Member of the Pharmaceutical Sciences Research Centre, MUI.
6. Member of the Bioinformatics Research Centre, MUI
7. Member of the Biosensor Research Centre, MUI
8. Member of the Bioinformatics and High-Performance Computing Research Group (BIO-HPC), Universidad Católica San Antonio de Murcia, Murcia, Spain (2014- 2015)

Awards:

1. Scholarship for PhD degree completion in the University of Alberta. Granted by Iranian Ministry of Health and Medical Education (2001)
2. Distinguished Researcher in Pharmaceutical Sciences, Isfahan University of Medical Sciences (2008)
3. Distinguished Researcher in Pharmaceutical Sciences, nominated by Isfahan Governorship (2010)
4. Distinguished Researcher in Bioinformatics, Isfahan University of Medical Sciences (2012)
5. Distinguished researcher for high h-index, nominated by the Ministry of Health and Medical Education (2016)
6. Distinguished researcher for high h-index, nominated by the Ministry of Health and Medical Education (2017)
7. Distinguished researcher for high h-index, nominated by the Ministry of Health and Medical Education (2018)
8. Distinguished researcher for high h-index, nominated by the Ministry of Health and Medical Education (2019)
9. Distinguished researcher for high h-index, nominated by the Ministry of Health and Medical Education (2020)

Teaching Experiences:

PhD Courses

1. Advanced Medicinal Chemistry (2006-)
2. Application of Computational Soft-Wares in Medicinal Chemistry (2012-)
3. Computational Drug Design (2015-)
4. Advanced Organic Chemistry (2005-)
5. Heterocyclic Chemistry (2006-)
6. Practical Organic Medicinal Synthesis (2006-)
7. Medicinal Chemistry (For the PhD students of Pharmacology, 2005)

MSc Courses:

1. Medicinal Chemistry (2016-)
2. Computational Drug Design (2016-)

PharmD Courses

1. Medicinal Chemistry (2004-2014)
2. General Chemistry (2004-2013)
3. Practical General Chemistry (2004-2013)

Thesis Supervision:

PhD Students

1. Mohammad Hossein Askar Shamsi, PhD Thesis: Synthesis and biological evaluation of benzothiazole and benzyl piperidine derivatives based on 3-hydroxy pyridine-4-one (2017-2021)
2. Mehrdad Mohammad Pour, PhD Thesis: Synthesis and evaluation of acetylcholine esterase, amyloid A β aggregation inhibitory and antioxidant effects of new 3-Hydroxy pyridin-4-one derivatives (2017-2021)
3. Pourya Shirvani, PhD Thesis: Design, synthesis and biological evaluation of some imidazole and indole-2-one derivatives as potential multi-target reverse transcriptase inhibitors and novel anti HIV-1 compounds (2015-2020).
4. Aylar Najafipour, PhD Thesis: Synthesis and evaluation of magnetic nanocomposites carrying methotrexate functionalized with LyP-1 peptide for targeted delivery of chemotherapeutics (2015-2020)
5. Tahereh Mostashari, PhD Thesis: Computer aided design and preparation of some imidazole and pyrroloimidazole compounds as anti-HIV-1 agents, with possible gp41 inhibitory activity (2015-2019)
6. Azizeh Asadzadeh, PhD Thesis: In vitro and in silico studies of the inhibitory effects of some novel Kojic acid derivatives on tyrosinase enzyme (2013-2015).
7. Saghi Sepehri, PhD Thesis: Design, synthesis and biological evaluation of some possible HIV-1 fusion inhibitors as novel anti-AIDS compounds (2012-2016)
8. Hajar Sirous-Najafabadi, PhD Thesis: Design, synthesis and biological evaluation of some potential integrase inhibitors as novel HIV-1 growth inhibitors (2012-2017).

9. Mohsen Shahlaei, PhD Thesis: Modeling of chemokine receptor CCR1 using Homology Modeling, Molecular Dynamic Simulation and Flexible Docking and application of various linear and nonlinear QSAR methods for predicting the activity of CCR1, CCR2 and CCR5 antagonists (2008-2012).
10. Razieh Sabet, PhD Thesis: Application of QSAR methods based on the MOLMAP approach for predicting and proposing synthesis of novel derivatives of 3- hydroxypyridine-4-ones with antibacterial and antifungal activity (2006-2011).

As Co-Supervisor:

11. Fahime Ghasemi, PhD Thesis: Proposing HIV-1 growth inhibitor compounds using nonlinear deep learning modeling and ligand-protein interaction (2015-2017)
12. Mohammad Nazifi, PhD Thesis: Synthesis and determination of K_{part} values of some hydroxypyridinone derivatives coupled with polyamines and the evaluation of their cytotoxic effects (2016-2019)
13. Zohreh Bakherad, PhD Thesis: Design, synthesis and cytotoxic assay of novel 2,3-di(hetero)arylidole derivatives (2015-2019)
14. Neda Fyyazi, PhD Thesis: Molecular modeling and synthesis of some hybrid multi-target Iron chelators as potential antimalarial and anticancer agents by different *in silico* methods (2017-2019)
15. Mahboubeh Mansourian, PhD Thesis: Study of the Human A2B adenosine receptor binding site by Homology Modeling, Molecular Dynamics simulations and Ligand Docking and study of quantitative Structure-Activity-Relationships using various QSAR methods (2009-2013).

MSc. Students:

1. Mansoureh Sattari, MSc Thesis: Preparation and evaluation of micro and nano properties of polyhydroxybutyrate particles and labling them with folic acid for targeted drug delivery to cancer cells (2010-2011)
2. Forough Rezaei, MSc Thesis: Synthesis and biological evaluation of novel leishmanicidal compounds having dual activity on iron absorption and interaction with DNA (2016-2018)
3. Vafa Sheikh Moradi, MSc Thesis: Synthesis and anti-leishmanial evaluation of some NO releasing antimony organometallic derivatives (2016-2017)
4. Ahmad Reza Salehi, MSc Thesis: Search for novel sodium-glucose co-transporter inhibitors using similarity search and structure-based virtual screening (2016-2018)
5. Shokooh Goodarzi, MSc Thesis: Investigation of linezolid analogues with the same antimicrobial activity using computational drug design method: structure- based virtual screening with molecular docking and dynamics (2020-)
6. Hossein Izadi Yazdkhasti, MSc Thesis: Virtual screening based on the molecular structure of proteins involved in cell survival and modulating compounds to find effective agents in the treatment of retinitis pigmentosa (RP) (2021)

Post-doctoral Fellow:

Mahboubeh Rostami (PhD in Organic Chemistry from Chemistry department, Isfahan University), (2010-2011)

PharmD Students

1. Vida Sheibini. Correction of structural defects in PDB files of druggable proteins in pathogenic parasites (2021-).
2. Javad Taherian. Correction of structural defects in PDB files of druggable proteins in pathogenic viruses and bacteria (2021-).
3. Moammadreza Amani. Correction of structural defects in PDB files of druggable proteins in pathogenic fungi (2021-).
4. Shiva sadat Hoseini. Study of the structural features of some benzimidazoles with acetylcholine esterase inhibitory activity using 3D-QSAR method and proposing possible inhibitors using molecular docking-based virtual screening (2020-).
5. Samane Hatami. Correction of structural defects in PDB files of soluble proteins in cancer signaling pathway (2020-2021).
6. Faride Haj akbari. Synthesis of some indane-2-one-hydrazone derivatives as potential anti-HIV agent and evaluation of their possible cytotoxicity (2020-).
7. NiushaAghae. Design, synthesis and cytotoxic effects of some hydrazone derivatives of indole-2-one as potential inhibitors of tyrosine kinases (2019-).
8. Mahsa Zekri. Tyrosine kinase inhibitors, Virtual screening, molecular docking, 3D-QSAR (2019-).
9. Shahryar Moteshabes. Structural search for proposing some new FoxM1 protein inhibitors using virtual screening, molecular docking and 3D-QSAR (2019-).
10. Zeynab Zarrabi. Synthesis, molecular docking and antimetastatic assay of 4-aryl-1,2,3,4-tetrahydropyrimidine-5-carboxamide-2-one as potential Fascin inhibitor (2016-2018)
11. Nahid Tamiz. Molecular docking, synthesis and evaluation of novel compounds as possible anti-HIV-1 agents (2016-2020)
12. Samira Gheisari. PharmD Thesis: Structure-based virtual screening of some 3-hydroxypyridine-4-one and 2,4-pyrimidine dione derivatives as possible inhibitors of hepatitis C virus polymerase by molecular docking method (2014-2018)
13. Parisa Rouhani. PharmD Thesis: Structure-based virtual screening of some 3-hydroxypyridine-4-one and 2,4-pyrimidine dione derivatives as possible inhibitors of endonuclease enzyme in influenza virus by molecular docking method (2014-2015)
14. Narges Riahi. PharmD Thesis: Synthesis, molecular docking and evaluation of cytotoxic effects of some Monastrol derivatives (2015-2018)
15. Alireza Zare. PharmD Thesis: Synthesis, experimental determination of partition coefficients of some novel derivatives of 3-hydroxypyridine-4-one using shake flask method and quantitative study of the relationship between the structure and partition coefficient (QSPR) of these compounds (2011-2013).
16. Sara Rafieepour Alavi. PharmD Thesis: Conformational analysis of novel anti HIV 1,2,3,4-Tetrahydropyrimidones (2011-2013)

17. Mohammad Mahmoudzadeh, PharmD Thesis: Synthesis of a novel chitosan derivative for the preparation of polymeric nanoparticles applicable in targeted drug delivery systems (2009-2012).
18. Maryam Mansouri, PharmD Thesis: Synthesis and antioxidant evaluation of ester derivatives of 4-furyl-3,4-dihydropyrimidine-2-thione-5-carboxylic acid (2009-2012).
19. Kowsar Rezaie, PharmD Thesis: Synthesis and antimicrobial evaluation of novel Schiff base derivatives of 3-amino-2-methylquinazoline-4(3H)-one (2010-2011).
20. Maryam Roozkhosh, PharmD Thesis: Synthesis and antioxidant evaluation of novel amide derivatives of 3,4-dihydropyrimidine-2-one-5-carboxylic acid containing 1-methyl-2-methylthio-imidazole-5-yl-substituent at C-4 position of 3,4-dihydropyrimidine ring (2009-2010).
21. Forough Talebian, PharmD Thesis: Synthesis and conformational analysis of novel potential antitubercular 1,4-dihydropyridine-3,5-dicarboxamides (2009-2010).
22. Amir Sadeghi, PharmD Thesis: Synthesis of novel derivatives of 3-hydroxy-4-pyridinone containing Schiff base moiety at C-5 position of the ring in order to increase antioxidant activity of L1 (2009-2012).
23. Mehrdad Mohammadpour, PharmD Thesis: Synthesis of novel derivatives of 3-hydroxy-4-pyridinone containing hydrazone and oxime moiety at C-5 position of the ring in order to increase antioxidant activity of L1 (2009-2012).
24. Mehdi Azizpour, PharmD Thesis: Synthesis and Antimicrobial Evaluation of Novel Ester and Amide Derivatives of 4-(N1-benzyl-2-thiomethyl-5-imidazolyl)-1,2,3,4-tetrahydropyrimidine-2-one-Carboxylic Acid (2009-2010).
25. Ebrahim Khodadadi, PharmD Thesis: Synthesis and Antioxidant Evaluation of some novel 1, 4 dihydropyridine 3,5-dicarboxamide Compounds Possessing N1-methyl-2-benzylthio-imidazole-5-yl at the C4 Position of the Dihydropyridine Ring (2009-2011).
26. Bitra Sedaghati, PharmD Thesis: Synthesis and Antimicrobial Evaluation of Novel Ester and Amide Derivatives of 1,2,3,4-tetrahydropyrimidine-2-one-5-carboxylic acid Containing N1-anilino-2-methylthio-5-imidazolyl in the 4-Position of the Pyrimidine Ring (2008-2010).
27. Shirin Arbabi, PharmD Thesis: Synthesis and Evaluation of Antimicrobial Activity of Novel Esters of 3,4-dihydropyrimidine-2-thione-5-carboxylates Containing-4-(N1-benzyl-2-methylthio-5-imidazolyl) Substituent at C-4 Position of the Dihydropyrimidine Ring (2008-2010).
28. Behzad Dorkhosh, PharmD Thesis: Synthesis and Antimicrobial Evaluation of Cyclic Hydrazide-Hydrazones (2008-2010).
29. Soheila Rezaie, PharmD Thesis: Synthesis and Antimicrobial Evaluation of Novel Schiff Bases Prepared by the Reaction of 3-amino-2-phenylquinazoline-4(3H)-one with 2-methylthio-imidazole-5-carbaldehyde Derivatives (2008-2010).
30. Alireza Sardari, PharmD Thesis: Synthesis and Antimicrobial Evaluation of Novel Derivatives of 1,2,3,4-tetrahydro pyrimidine thion (2008-2010).
31. Adel Omid, PharmD Thesis: Synthesis and Evaluation of Antimicrobial Effects of Novel Derivatives of 4-(2-thienyl)-6-methyl-1,2,3,4-tetrahydropyrimidine-2-one-5-carboxamide (2008-2010).
32. Sajjad Zarepour, PharmD Thesis: Synthesis of Some Novel Pyrimidine Derivatives Using Biginelli Reaction (2007-2009).
33. Fateme Safari, PharmD Thesis: Synthesis and Quantitative Structure-Activity Relationship (QSAR) Analysis of 4-heteroaryl-2,6-dimethyl-3,5-bis N-phenyl

- (piperidyl)carbamoyl-1,4-dihydropyridine Derivatives with Antimicrobial Effects (2008-2010).
34. Ghassem Bostaki, PharmD Thesis: Evaluation of Antimicrobial and Antifungal activity of Some Novel Iron Chelating Agents with the General Structure of Hydroxypyridinone and Hydroxypyranone (2007-2008).
 35. Zahra Azadpour, PharmD Thesis: Synthesis of Some Novel Derivatives of 4-(2-methylthio-1-benzyl-5-imidazolyl)-2,6-dimethyl-3,5-bis-N-phenyl (pyridyl) carbamoyl-1,4-dihydropyridine as Potentially Active Antitubercular Agents (2006-2008).
 36. Neda Delbari, PharmD Thesis: Synthesis of Some Novel Derivatives of 4-(2-methylthio-1-phenylamino-5-imidazolyl)-2,6-dimethyl-3,5-bis-N-phenyl(pyridyl) carbamoyl-1,4-dihydropyridine as Potentially Active Antitubercular Agents (2006-2008).
 37. Majid Mansouri, PharmD Thesis: Synthesis of Some Novel derivatives of 4-(2-thienyl)-2,6-dimethyl-3,5-bis-N-phenyl (pyridyl) carbamoyl-1,4-dihydropyridine as Potentially Active Antitubercular Agents (2006-2008).
 38. Mehrnaz Ghodratnama, PharmD Thesis: Synthesis of Some Novel Derivatives of 4-(1-methyl-1H-5-imidazolyl)-2,6-dimethyl-3,5-bis-N-phenyl (pyridyl) carbamoyl-1,4-dihydropyridine as Potentially Active Antitubercular Agents (2005-2007).
 39. Ahmad Reza Narouni, PharmD Thesis: Synthesis and Pharmacological Evaluation of Novel Asymmetric Derivatives of 1,4-Dihydropyridine Compounds Containing N1-methyl-5-imidazolyl as C4 Substituent as Calcium Channel Blocking Agents (2004-2005).
 40. Fateme Mohammadian, PharmD Thesis: Synthesis and Pharmacological Evaluation of Novel Symmetric Derivatives of 1,4-Dihydropyridine Compounds Containing N1-methyl-5-imidazolyl as C4 Substituent as Calcium Channel Blocking Agents (2004-2005).

As co-supervisor:

41. Behzad Sartippour, PharmD Thesis: Synthesis and anti-tyrosinase evaluation of some novel derivatives of kojic acid (2011-2012)
42. Vahid Mirmohammadi, PharmD Thesis: Evaluation of cytotoxicity of some derivatives of 2-methyl -4(3H)-quinazolinones against tumor cell lines (Hela and MDA-MB-468) (2010-2012).
43. Azam Aghajani, PharmD Thesis: Cytotoxicity Evaluation of Some Derivatives 1, 2,3, 4-Tetrahydro-pyrimidin on HT-29 and Hela Cell Lines (2008-2010).
44. Mehdi Khorrami, PharmD Thesis: Cytotoxicity Evaluation of Some thienyl- and imidazolyl- 1,4-dihydropyridine-3,5 -dicarboxamides on HT-29 Cell Line (2007-2009).
45. Hoda Mojiri, PharmD Thesis: Pharmacological Evaluation of the Antiinflammatory and Analgesic Effects of Some Novel Derivatives of Hydroxy 4(1H)-Pyridinone (2007-2009).
46. Hamed Shabani, PharmD Thesis: Study on the Synthesis of Zinc Complexes of Bidentate Hydroxypyridinone and Hydroxypyranone Ligands and Determination of Some Physicochemical Properties of the Complexes (2007-2009).
47. Mohammad Reza Bakhshandeh, PharmD Thesis: Evaluation of the IC₅₀ of 10 Novel 1,4 Dihydropyridine Calcium Channel Blocker Compounds with Acetyl

- Group in the C5 Position of the Dihydropyridine Ring instead of the Usual Ester Group (2005-2007).
48. Fereshteh Ahmadi, PharmD Thesis: Synthesis and Determination of Physicochemical Properties of Novel Hydroxypyranones as Iron (III) Bidentate Ligands (2004-2005).
 49. Mohsen Sobhani, PharmD Thesis: Synthesis and Determination of Partition Coefficients of Some Hydroxypyranones as Iron (III) Chelators (2004-2006).
 50. Maryam Amidi, PharmD Thesis: Evaluation of Contraction Inhibiting Effect of 10 Novel Dihydropyridine Calcium Channel Blocker Compounds on Ileum Smooth Muscle of Rat in Comparison with Nifedipine (2005-2006).
 51. Mitra Mohajeri, PharmD Thesis: Synthesis of Derivatives of Phthalimides as Anxiolytic Agents (2004-2006).
 52. Mohsen Shekofteh, PharmD Thesis: A Preliminary Study on Lovastatin Biosynthesis in Iran (2004-2005).
 53. Omid Deilami, PharmD Thesis: Synthesis of Iron (III) Bidentate Ligands of 2-Ethyl-3-Hydroxy Pyridine-4-ones Effective in the Treatment of Malaria (2004-2005).

Articles Published in Peer Reviewed International Journals:

1. Pouria Shirvani, **Afshin Fassihi**. In silico design of novel FAK inhibitors using integrated molecular docking, 3D-QSAR and molecular dynamics simulation studies. *Journal of Biomolecular Structure and Dynamics*. 2021; 21: 1-19.
2. Aylar Najafipour, Ali Gharieh, **Afshin Fassihi**, Hojjat Sadeghi-Aliabadi, Ali Reza Mahdavian. MTX-Loaded Dual Thermoresponsive and pH-Responsive Magnetic Hydrogel Nanocomposite Particles for Combined Controlled Drug Delivery and Hyperthermia Therapy of Cancer. *Molecular Pharmaceutics*. 2021; 18 (1): 275–284.
3. Nahid Tamiz, Tahereh Mostashari-Rad, Aylar Najafipour, Sandra Claes , Dominique Schols , **Afshin Fassihi**. Synthesis, Molecular Docking and Molecular Dynamics Simulation of 2-thioxothiazolidin-4-one derivatives against Gp41. *Current HIV Research*. 2020.
4. Pouria Shirvani, **Afshin Fassihi**, Molecular modelling study on pyrrolo[2,3-b]pyridine derivatives as c-Met kinase inhibitors: a combined approach using molecular docking, 3D-QSAR modelling and molecular dynamics simulation. *Molecular Simulation*. 2020; 46(16).
5. Pouria Shirvani, **Afshin Fassihi**, Lotfollah Saghale, Siska Van Belle, Zeger Debyser, Frauke Christ. Synthesis, anti-HIV-1 and antiproliferative evaluation of novel 4-nitroimidazole derivatives combined with 5-hydroxy-4-pyridinone moiety. *Journal of Molecular Structure*. 2020; 1202 (15): 127344.
6. Aylar Najafipour, Ali Reza Mahdavian, **Afshin Fassihi**, Hojjat Sadeghi-Aliabadi. Alternating Magnetic Field and Ultrasound Waves as Size Controlling Parameters in Preparation of Superparamagnetic Fe₃O₄ Nanoparticles. *Journal of nanoscience and Nanotechnology*. 2020; 20 (2): 871-877.
7. Neda Fayyazi, **Afshin Fassihi**, Somayeh Esmaili, Salman Taheri, Jahan B. Ghasemi, Lotfollah Saghale. Molecular dynamics simulation and 3D-pharmacophore analysis of new quinoline-based analogues with dual potential

- against EGFR and VEGFR-2. *International Journal of Biological Macromolecules*. 2020; 142: 94-113.
8. Zeynab Zarrabi, Lotfollah Saghaie, **Afshin Fassihi**, Nader Pestechian, Sedigheh Saberi. Synthesis and comparison of anti-Leishmania major activity of antimony and iron complexes of 3-hydroxypyran-4-one and 3-hydroxypyridine-4-one as bidentate ligands. *Journal of Reports in Pharmaceutical Sciences*. 2020; 9 (2): 177-182.
 9. Roya Arian, Amirali Hariri, Alireza Mehridehnavi, **Afshin Fassihi**, Fahimeh Ghasemi. Protein kinase inhibitors' classification using K-Nearest neighbor algorithm. *Computational Biology and Chemistry*. 2020; 86: 107269.
 10. Seyed Mohamad Reza Nazifi, Hojjat Sadeghi aliabadi, **Afshin Fassihi**, Mehdi Aliomrani, Lotfollah Saghaie. Synthesis and antiproliferative evaluation of some iron chelators as polyamine transporter targeting agents. *Canadian Journal of Chemistry*. 2019; 97 (8): 629-635.
 11. Narges Riahi, Amirhosein Kefayat, Ahmad Ghasemi, Mohammadhosein Asgarshamsi, Mojtaba Panjehpoor, **Afshin Fassihi**. Design, Synthesis and Molecular Docking Studies of Some Tetrahydropyrimidine Derivatives as Possible Fascin Inhibitors. *Chemistry & Biodiversity*. 2019; 16 (2): e1800339.
 12. Zohreh Bakherad, Maliheh Safavi, **Afshin Fassihi**, Hojjat Sadeghi-Aliabadi, Mohammad Bakherad, Hossein Rastegar, Mina Saeedi, Jahan B Ghasemi, Lotfollah Saghaie, Mohammad Mahdavi. Design and Synthesis of Novel Cytotoxic Indole-Thiosemicarbazone Derivatives: Biological Evaluation and Docking Study. *Chemistry & Biodiversity*. 2019; 16 (4): e1800470.
 13. Zohreh Bakherad, Maliheh Safavi, Saghie Sepehri, **Afshin Fassihi**, Hojjat Sadeghi-Aliabadi, Mohammad Bakherad, Hossein Rastegar, Bagher Larijani, Lotfollah Saghaie, Mohammad Mahdavi. Preparation of some novel imidazopyridine derivatives of indole as anticancer agents: one-pot multicomponent synthesis, biological evaluation and docking studies. *Research on Chemical Intermediates*. 2019; 45 (10): 5261-5290.
 14. Tahereh Mostashari-Rad, Roya Arian, Hourii Sadri, Alireza Mehridehnavi, Marzieh Mokhtari, Fahimeh Ghasemi, **Afshin Fassihi**. Study of CXCR4 chemokine receptor inhibitors using QSPR and molecular docking methodologies. *Journal of Theoretical Computational Chemistry*. 2019; 18 (04): 1950018.
 15. Seyed Mohamad Reza Nazifi, Hojjat Sadeghi-aliabadi, **Afshin Fassihi**, Lotfollah Saghaie. Structure-activity relationship of polyamine conjugates for uptake via polyamine transport system. *Structural Chemistry*. 2019; 30 (1): 175-184.
 16. Tahereh Mostashari-Rad, Lotfollah Saghaie, **Afshin Fassihi**. Gp41 inhibitory activity prediction of theaflavin derivatives using ligand/structure-based virtual screening approaches. *Computational Biology and Chemistry*. 2019; 79: 119-126.
 17. Neda Fayyazi, Somayeh Esmaili, Salman Taheri, Frederico F Ribeiro, Marcus T Scotti, Luciana Scotti, Jahan B Ghasemi, Lotfollah Saghaie, **Afshin Fassihi**. Pharmacophore modeling, synthesis, scaffold hopping and biological β -hematin inhibition interaction studies for anti-malaria compounds. *Current Topics in Medicinal Chemistry*. 2019; 19 (30): 2743-2765.
 18. Aylar Najafipour, Ali Reza Mahdavian, Hojjat Sadeghi-Aliabadi, **Afshin Fassihi**. Dual thermo- and pH-responsive poly (N-isopropylacrylamide-co-(2-dimethylamino) ethyl methacrylate)-g-PEG nanoparticle system and its potential in controlled drug release. *Polymer Bulletin*. 2019; 77: 3129-3142.

19. Pouria Shirvani, **Afshin Fassihi**, Lotfollah Saghaie. Recent Advances in the Design and Development of Non-nucleoside Reverse Transcriptase Inhibitor Scaffolds. *ChemMedChem*. 2019; 14 (1): 52-77.
20. 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 Saghaie, Hamid R Memarian. Synthesis, Molecular Modelling and Biological Studies of 3-hydroxypyrene-4-one and 3-hydroxy-pyridine-4-one Derivatives as HIV-1 Integrase Inhibitors. *Medicinal Chemistry*. 2019; 15 (7): 755-770.
21. Hajar Sirous, Giulia Chemi, Sandra Gemma, Stefania Butini, Zeger Debyser, Frauke Christ, Lotfollah Saghaie, 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.
22. Zohreh Bakherad, Maryam Mohammadi-Khanaposhtani, Hojjat Sadeghi-Aliabadi, Sepideh Rezaei, **Afshin Fassihi**, Mohammad Bakherad, Hossein Rastegar, Mahmood Biglar, Lotfollah Saghaie, Bagher Larijani, Mohammad Mahdavi. New thiosemicarbazide-1, 2, 3-triazole hybrids as potent α -glucosidase inhibitors: Design, synthesis, and biological evaluation. *Journal of Molecular Structure*. 2019; 1192: 192-200.
23. Zohreh Bakherad, Maliheh Safavi, **Afshin Fassihi**, Hojjat Sadeghi-Aliabadi, Mohammad Bakherad, Hossein Rastegar, Jahan B. Ghasemi, Saghi Sepehri, Lotfollah Saghaie, Mohammad Mahdavi. Anti-cancer, anti-oxidant and molecular docking studies of thiosemicarbazone indole-based derivatives. *Research on Chemical Intermediates*. 2019; 45(5): 2827-2854.
24. Razihe Sabet, Afshin Fassihi, Lotfollah Saghaie. Octanol-water partition coefficients determination and QSPR study of some 3-hydroxy pyridine-4-one derivatives. *Journal of Pharmaceutical Research International*. 2018; 22(4); 1-15.
25. Tahere Mostashari Rad, Lotfollah Saghaie, **Afshin Fassihi**. HIV-1 entry inhibitors: A review of experimental and computational studies. *Chemistry Biodiversity*. 2018; 15 (10): e1800159.
26. Forough Rezaei, Lotfollah Saghaie, Razihe Sabet, Afshin Fassihi, a, Gholamreza Hatam. Novel catechol derivatives of arylimidamides as antileishmanial agents. *Chemistry Biodiversity*. 2018; 15 (10): e1800228.
27. Saghi Sepehri, Sepehr Soleymani, Rezvan Zabihollahi, Mohammad R. Aghasadeghi, Mehdi Sadat, Lotfollah Saghaie, **Afshin Fassihi**. Design, synthesis and anti-HIV-1 evaluation of a novel series of 1,2,3,4-tetrahydropyrimidine-5-carboxylic acid derivatives. *Chemistry Biodiversity*. 2018; 15 (4): 1700502.
28. F Ghasemi, A Mehridehnavi, A Fassihi, H Pérez-Sánchez. Deep neural network in QSAR studies using deep belief network. *Appl. Soft. Comput.* 2018; 62; 251-258.
29. Saghi Sepehri, Sepehr Soleymani, Rezvan Zabihollahi, Mohammad R. Aghasadeghi, Mehdi Sadat, Lotfollah Saghaie, **Afshin Fassihi**, Synthesis, Biological Evaluation and molecular docking studies of novel 4-arylpyridin-1(4H)-yl benzoic acid derivatives as anti-HIV-1 agents. *Chemistry Biodiversity*. 2017; 14 (12): e1700295.
30. Mohaddese Behjati, **Afshin Fassihi**, Mehrdad Mohammad Pour, Mahtab Keshvari, Cardioprotection Potential of Some Hydroxypyridine Iron Chelators Against H₂O₂-Induced H9C2 Cell Injury. *Türkiye Klinikleri Cardiovascular Sciences*, 2017; 29(1): 10-6

31. Fahimeh Ghasemi, **Afshin Fassihi**, Horacio Pérez-Sánchez, Alireza Mehri Dehnavi, The role of different sampling methods in improving biological activity prediction using deep belief network. *Journal of Computational Chemistry*, 2017, 38(4), 195–249.
32. Saghi Sepehri, **Afshin Fassihi**, Lotfollah Saghaei, Anti-HIV-1 Activity Prediction of Novel Gp41 Inhibitors Using Structure-Based Virtual Screening and Molecular Dynamics Simulation. *Molecular Informatics*, In Press. DOI: 10.1002/minf.201600060
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Workshops held:

1. **QSAR**, Azad University, Tehran Branch (February 2010)
2. **ChemOffice package and Hyperchem**, Isfahan University of Medical Sciences (September 2017)
3. **Molecular docking simulation**, Isfahan University of Medical Sciences (September 2017)
4. **ChemOffice package and Hyperchem**, Azad University Shahreza Branch (March 2018)
5. **Molecular docking simulation**, Azad University Shahreza Branch (March 2018)
6. **ChemOffice package and Hyperchem**, Azad University Shahreza Branch (June 2018)
7. **Molecular docking simulation**, Azad University Shahreza Branch (June 2018)
8. **ChemOffice package and Hyperchem**, Zist Pardazesh Institute (May 2019)
9. **Molecular docking simulation**, Zist Pardazesh Institute (May 2019)
10. **ChemOffice package and Hyperchem**, Zist Pardazesh Institute (November 2019)
11. **Molecular docking simulation**, Zist Pardazesh Institute (November 2019)
12. **Basic Concepts in Drug Design**, Jaber-ebn-e-Hayyan Institute (September 2020)
13. **ChemOffice package and Hyperchem**, Jaber-ebn-e-Hayyan Institute (December 2020)
14. **Molecular docking simulation**, Jaber-ebn-e-Hayyan Institute (December 2020)
15. **Structure-Based Virtual Screening**, Jaber-ebn-e-Hayyan Institute (December 2020)
16. **Basic Concepts in Drug Design**, Jaber-ebn-e-Hayyan Institute (December 2020)
17. **ChemOffice package and Hyperchem**, Jaber-ebn-e-Hayyan Institute (February 2021)
18. **Molecular docking simulation**, Jaber-ebn-e-Hayyan Institute (February 2021)
19. **Structure-Based Virtual Screening**, Jaber-ebn-e-Hayyan Institute (February 2021)
20. **Basic Concepts in Drug Design**, Iranian Pharmacy Student association (December 2020)
21. **ChemOffice package and Hyperchem**, Iranian Pharmacy Student association (February 2021)
22. **Molecular docking simulation**, Iranian Pharmacy Student association (February 2021)
23. **3D-QSAR**, Jaber-ebn-e-Hayyan Institute (February 2021)
24. **Basic Concepts in Drug Design**, Fartak Daru-Espadana (June 2021)
25. **ChemOffice package and Hyperchem**, Fartak Daru-Espadana (June 2021)
26. **Molecular docking simulation**, Fartak Daru-Espadana (July 2021)

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1. Rezvan Zabihollahi, Roohollah Vahabpour, Christine Hartoonian, **Afshin Fassihi**, Hamid R. Memarian, Mohammad R. Aghasadeghi, Rahele Namazi, S. Sadat, Mansour Salehi, A. Rezaei. Anti-HIV Activity Evaluation of Novel Biginelli Pyrimidines. *12th Iranian Pharmaceutical Sciences Congress. 2010, Zanjan, Iran.*
2. Ghadam A. Khodarahmi, **Afshin Fassihi**, Farshid Hassanzadeh, Mahmoud Etebari, Mehdi Khorrami. Cytotoxicity Evaluation of Some 1, 4-Dihydropyridine-3, 5-Dicarboxamide on HT-29 Cell Line. *12th Iranian Pharmaceutical Sciences Congress. 2010. Zanjan, Iran.*
3. Mohammad Mahmoudzadeh, Farid Dorkoosh, **Afshin Fassihi**, Kamran Ghaedi, Mohammad Nasr-Esfahini. Dexamethason-Chitosan Polymeric Micelles as Novel Non-Viral Gene Carriers: Preparation and Transfection Efficiency Evaluation. *12th Iranian Pharmaceutical Sciences Congress. 2010, Zanjan, Iran.*
4. Amir Sadeghi-Boroujeni, Mehrdad Mohamadpour-Dehkordi, Karim Mahnam, **Afshin Fassihi**. Docking Studies and Molecular Dynamic (MD) Simulation of Novel Antitubercular Dihydropyridines. *12th Iranian Pharmaceutical Sciences Congress. 2010. Zanjan, Iran.*
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7. Raziieh Sabet, Bahram Hemmateenejad, **Afshin Fassihi**, Lotfollah Saghaie, Ramin Miri. Application of QSAR Methods Based on the MOLMAP Approach for Predicting and Proposing Synthesis of Novel Derivatives of 3-hydroxypyridine-4-ones with Antibacterial and Antifungal Activity. *Conferentia Chemometrica, September, 2009, Siofok, Hungary.*
8. Erin Mackenzie, **Afshin Fassihi**, Asghar Davood, Edward E. Knaus, Glen B. Baker. Neurochemical Changes Produced in Rat Brain by Two N-propargyl Analogues of Phenylethylidenehydrazine (PEH). *26th Collegium Internationale Neuro-Psychopharmacologicum Congress (CINP), July, 2008, Munich, Germany.*
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6. Archive der Pharmazie - Chemistry in Life Sciences
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