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. 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 (November 2018-)

Membership in Research Centers and Councils:

1. Isfahan University of Medical Sciences Publication Council
2. School of Pharmacy and Pharmaceutical Sciences Publication Council
3. The Council of Basic Sciences Research Projects, Isfahan University of Medical Sciences
4. Pharmaceutical Sciences Research Centre, Isfahan University of Medical Sciences
5. Bioinformatics Research Centre, Isfahan University of Medical Sciences
6. Biosensor Research Centre, Isfahan University of Medical Sciences

Awards:

1. Scholarship for Ph.D 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)

Teaching Experiences:
PhD Courses

1. Advanced Medicinal Chemistry (2006-)
2. Application of Computational Soft-Wares in Medicinal Chemistry (2012-)
3. Computational Drug Design (20015-)
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)

PharmD Courses

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

Post-doctoral Fellow:

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

Thesis Supervision:

PhD Students

1. 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)
2. 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)
3. Mahboubeh Mansourian, PhD Thesis: Study of the Human A_{2B} adenosine receptor binding site by Homology Modeling, Molecular Dynamics simulations and Ligand Docking and study of quantitative Sutructure-Activity-Relationships using various QSAR methods (2009-2013).
4. Hajar Sirous-Najafabadi, PhD Thesis: Design, synthesis and biological evaluation of some potential integrase inhibitors as novel HIV-1 growth inhibitors (2012-2017)
5. Saghi Sepehri, PhD Thesis: Design, synthesis and biological evaluation of some possible HIV-1 fusion inhibitors as novel anti-AIDS compounds (2012-2016)
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. Aylar Najafipour, PhD Thesis: Synthesis and evaluation of magnetic nanocomposites carrying methotrexate functionalized with LyP-1 peptide for targeted delivery of chemotherapeutics (2015-)
8. 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-)
9. 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-)
10. Mehrdad Mohammad Pour, PhD Thesis: Synthesis and evaluation of acetylcholine esterase, amyloid Aβ aggregation inhibitory and antioxidant effects of new 3-Hydroxy pyridyn-4-one derivatives (2017-)
11. Mohammad Hossein Askar Shamsi, PhD Thesis: Synthesis and biologic evaluation of benzothiazole and benzyl piperidine derivatives based on 3-hydroxy pridine-4-one (2017-)

As Co-Supervisor:

12. Fahime Ghasemi, PhD Thesis: Proposing HIV-1 growth inhibitor compounds using nonlinear deep learning modeling and ligand-protein interaction (2015-2017)
13. 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-)
14. Zohreh Bakherad, PhD Thesis: Design, synthesis and cytotoxic assay of novel 2,3-di(hetero)arylindole derivatives (2015-)
15. Neda Fyyazi, PhD Thesis: Molecular modeling and synthesis of some hybrid multi-target Iron chelators as potential antimalarial and anticancer agents by different *in sillico* methods (2017-)

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)

PharmD Students

1. Zeynab Zarrabi, PharmD Thesis: Synthesis, molecular docking and antimetastatic assay of 4-aryl-1,2,3,4-tetrahydropyrimidine-5-carboxamide-2-one as potential Fascin inhibitor (2016-2018)
2. Nahid Tamiz, Molecular docking, synthesis and evaluation of novel compounds as possible anti-HIV-1 agents (2016-)
3. 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)
4. 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)
5. Narges Riahi, PharmD Thesis: Synthesis, molecular docking and evaluation of cytotoxic effects of some Monastrol derivatives (2015-2018)
6. 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).

7. Sara Rafieepour Alavi, PharmDThesis: Conformational analysis of novel anti HIV 1,2,3,4-Tetrahydropyrimidones (2011-2013)
8. Mohammad Mahmoudzadeh, PharmD Thesis: Synthesis of a novel chitosan derivative for the preparation of polymeric nanoparticles applicable in targeted drug delivery systems (2009-2012).
9. Maryam Mansouri, PharmD Thesis: Synthesis and antioxidant evaluation of ester derivatives of 4-furyl-3,4-dihydropyrimidine-2-thione-5-carboxylic acid (2009-2012).
10. Kowsar Rezaie, PharmD Thesis: Synthesis and antimicrobial evaluation of novel Schiff base derivatives of 3-amino-2-methylquinazoline-4(3H)-one (2010-2011).
11. 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).
12. Forough Talebian, PharmD Thesis: Synthesis and conformational analysis of novel potential antitubercular1,4-dihydropyridine-3,5-dicarboxamides (2009-2010).
13. 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).
14. 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).
15. 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).
16. 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).
17. Bita Sedaghati, PharmD Thesis: Synthesis and Antimicrobial Evaluation of Novel Ester and Amide Derivatives of 1,2,3,4-tetrahyolropyrimidire-2-one-5-carboxylic acid Containing N1-anilino-2- methylthio-5- imidazolyl in the 4-Position of the Pyrimidine Ring (2008-2010).
18. 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) Substitutent at C-4 Position of the Dihydropyrimidine Ring (2008-2010).
19. Behzad Dorkhosh, PharmD Thesis: Synthesis and Antimicrobial Evaluation of Cyclic Hydrazide-Hydrazones (2008-2010).
20. Soheila Rezaie, PharmD Thesis: Synthesis and Antimicrobial Evaluation of Novel Schiff Bases Prepared by the Reaction of 3-amino-2-phenylquinazoline-4(3*H*)-one with 2-methylthio-imidazole-5-carbaldehyde Derivatives (2008-2010).
21. Alireza Sardari, PharmD Thesis: Synthesis and Antimicrobial Evaluation of Novel Derivatives of 1,2,3,4-tetrahydro pyrimidine thion (2008-2010).

22. Adel Omidi, 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).
23. Sajjad Zarepour, PharmD Thesis: Synthesis of Some Novel Pyrimidine Derivatives Using Biginelli Reaction (2007-2009).
24. 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).
25. 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).
26. 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).
27. 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).
28. 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).
29. 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).
30. 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).
31. 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:

32. Behzad Sartippour. PharmD Thesis: Synthesis and anti-tyrosinase evaluation of some novel derivatives of kojic acid (2011-2012)
33. 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).
34. Azam Aghajani, PharmD Thesis: Cytotoxicity Evaluation of Some Derivatives 1, 2,3, 4-Tetraydro-pyrimidin on HT-29 and Hela Cell Lines (2008-2010).
35. Mehdi Khorrami, PharmD Thesis: Cytotoxicity Evaluation of Some thienyl- and imidazolyl- 1,4-dihydropyridine-3,5 -dicarboxamides on HT-29 Cell Line (2007-2009).

36. Hoda Mojiri, PharmD Thesis: Pharmacological Evaluation of the Antiinflammatory and Analgesic Effects of Some Novel Derivatives of Hydroxy 4(1*H*)-Pyridinone (2007-2009).
37. 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).
38. Mohammad Reza Bakhshandeh, PharmD Thesis: Evaluation of the IC_{50} 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).
39. Fereshteh Ahmadi, PharmD Thesis: Synthesis and Determination of Physicochemical Properties of Novel Hydroxypyranones as Iron (III) Bidentate Ligands (2004-2005).
40. Mohsen Sobhani, PharmD Thesis: Synthesis and Determination of Partition Coefficients of Some Hydroxypyranones as Iron (III) Chelators (2004-2006).
41. 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).
42. Mitra Mohajeri, PharmD Thesis: Synthesis of Derivatives of Phthalimides as Anxiolytic Agents (2004-2006).
43. Mohsen Shekofteh, PharmD Thesis: A Preliminary Study on Lovastatin Biosynthesis in Iran (2004-2005).
44. 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***, Lotfollah Saghaie, Recent advances in the design and development of NNRTI scaffolds. ***ChemMedChem***. ***In Press***. doi: 10.1002/cmdc.201800577
2. Tahere Mostashari Rad, Lotfollah Saghaie, **Afshin Fassihi***. HIV-1 entry inhibitors: A review of experimental and computational studies. ***Chemistry and Biodiversity***, ***In Press***. doi: 10.1002/cbdv.201800159
3. Narges Riahi, Amirhosein Kefayat, Ahmad Ghasemi, Mohammadhosein Asgarshamsi, Mojtaba Panjehpour, **Afshin Fassihi***, Design, Synthesis and Molecular Docking Studies of some Tetrahydropyrimidine Derivatives as Possible Fascin Inhibitors. ***Chemistry and Biodiversity***, ***In Press***. doi: 10.1002/cbdv.201800339

4. Foroogh Rezaei, Lotfollah Saghaei, Razieh Sabet, Afshin Fassihi,a, Gholamreza Hatam. Novel catechol derivatives of arylimidamides as antileishmanial agents. ***Chemistry and Biodiversity, In Press***. doi:10.1002/cbdv.201800228
5. Saghi Sepehri, Sepehr Soleymani, Rezvan Zabihollahi, Mohammad R. Aghasadeghi, Mehdi Sadat, Lotfollah Saghai, **Afshin Fassihi**, 'Design, synthesis and anti-HIV-1 evaluation of a novel series of 1,2,3,4-tetrahydropyrimidine-5-carboxylic acid derivatives' ***Chemistry and Biodiversity***, ***In Press***. DOI:10.1002/cbdv.201700502.
6. S. Mohamad Reza Nazifi, Hojjat Sadeghi-aliabadi, Afshin Fassihi, Lotfollah Saghaie. Structure–activity relationship of polyamine conjugates for uptake via polyamine transport system. ***Structural Chemistry***, ***In Press***. doi: 10.1007/s11224-018-1175-4
7. Saghi Sepehri, Sepehr Soleymani, Rezvan Zabihollahi, Mohammad R. Aghasadeghi, Mehdi Sadat, Lotfollah Saghai, **Afshin Fassihi**, Synthesis, Biological Evaluation and molecular docking studies of novel 4-arylpyridin-1(4*H*)-yl) benzoic acid derivatives as antiHIV-1 agents. ***Chemistry and Biodiversity***, ***In Press.*** DOI: 10.1002/cbdv.201700295
8. Mohaddese Behjati, **Afshin Fassihi**, Mehrdad Mohammad Pour, Mahtab Keshvari, Cardioprotection Potential of Some Hydroxypyridine Iron Chelators Against H_2O_2-Induced H9C2 Cell Injury. *Türkiye Klinikleri* ***Cardiovascular Sciences***, 2017;29(1):10-6
9. 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.
10. 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
11. Jesus Carretero, Javier Garcia-Blas, David E. Singh, Florin Isaila, Alexey Lastovetsky, Thomas Fahringer, Radu Prodan, Peter Zangerl, Christi Symeonidou, George Bosilca, **Afshin Fassihi**, Horacio P´erez-S´anchez. Acceleration of MPI Mechanisms for Sustainable HPC Applications. ***Supercomputing Frontiers and Innovations***. 2015, 2(2), 28-45.
12. Saghi Sepehri, Horacio Perez Sanchez, **Afshin Fassihi**. Hantzsch-Type Dihydropyridines and Biginelli-Type Tetrahydropyrimidines: A Review of their Chemotherapeutic Activities. ***Journal of Pharmacy and Pharmaceutical Sciences***, 2015; 18(1): 1-52 (Review Article).
13. Azizeh Asadzadeh, Hajar Sirous, Morteza Pourfarzam, Parichehreh Yaghmaei, **Fassihi**, In vitro and in silico studies of the inhibitory effects of some novel kojic acid derivatives on tyrosinase enzyme. ***Iran J Basic Med Sci.*** 2016; 19(2): 132–144.
14. Azizeh Asadzadeh, **Afshin Fassihi**, Parichehreh Yaghmaei, Morteza Pourfarzam. In Silico Approach for Designing Potent Inhibitors against Tyrosinase. ***Biosciences Biotechnology Research Asia***. 2015; **12** (2), p. 181-187.
15. Azizeh Asadzadeh, Afshin Fassihi,,Parichehreh Yaghmaei, Morteza Pourfarzam. Docking Studies of Some Novel Kojic acid Derivatives as Possible Tyrosinase Inhibitors. ***Biomedical & Pharmacology Journal*** 2015, 8(2), 535-545.
16. Mohammad Mahmoudzadeh, **Afshin Fassihi**, Farid Dorkoosh, Reyhaneh Heshmatnejad, Karim Mahnam, Hassan Sabzyan, Amir Sadeghi. Elucidation

of Molecular Mechanisms Behind the Self-Assembly Behavior of Chitosan Amphiphilic Derivatives through Experiment and Molecular Modeling. ***Pharmaceutical Research.*** 2015; 32(12):3899-915.

17. Dina Morshedi, Farhang Aliakbari, Amir Tayaranian-Marvian, **Afshin Fassihi**, Francisco Pan-Montojo, Horacio Pérez-Sánchez. Cuminaldehyde as the Major Component of Cuminum cyminum, a Natural Aldehyde with Inhibitory Effect on Alpha-Synuclein Fibrillation and Cytotoxicity. ***Journal of Food Science.*** 2015; 80(10): H2336–H2345
18. Mahboubeh Mansourian1, Karim Mahnam, Armin Madadkar-Sobhani, **Afshin Fassihi**, Lotfollah Saghaie. Insights into the human A1 adenosine receptor from molecular dynamics simulation: structural study in the presence of lipid membrane. ***Medicinal Chemistry Research***, 2015; 24:3645-3659
19. Mahboubeh Rostami, Hajar Sirous, Rezvan Zabihollahi, Mohammad R. Aghasadeghi, Seyed Mehdi Sadat, Rahele Namazi, Lotfollah Saghaie, 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.
20. Sepehri S, Sanchez HP, **Fassihi A**. Hantzsch-Type dihydropyridines and biginelli-type tetra-hydropyrimidines: a review of their chemotherapeutic activities. ***Journal of Pharmacy & Pharmaceutical Sciences***, 2015; 18(1): 1-52.
21. Horacio Peréz-Sánchez, **Afshin Fassihi**, José M. Cecilia, Hesham H. Ali, Mario Cannataro. Applications of High Performance Computing in Bioinformatics, Computational Biology and Computational Chemistry. ***Bioinformatics and Biomedical Engineering Lecture Notes in Computer Science***, 2015; 9044: 527-541.
22. K. V. Dileep, C. Remya, J. Cerezo, **A. Fassihi**, H. Pérez-Sánchezc, C. Sadasivan. Comparative studies on the inhibitory activities of selected benzoic acid derivatives against secretory phospholipase A_2, a key enzyme involved in the inflammatory pathway. ***Molecular BioSystems***, 2015; 11(7): 1973-1979.
23. Helena den Haan, **Afshin Fassihi**, Jesús Soto-Iniesta, Josefa Vegara-Meseguer, Silvia Montoro, Horacio Pérez-Sánchez. Application of Modern Drug Discovery Techniques in the Context of Diabetes Mellitus and Atherosclerosis. ***Drug Designing,*** 2015; 4:1.
24. Fahimeh Ghasemi, Alireza Mehri, Jorge Peña-García, Helena den-Haan, Alfonso Pérez-Garrido, **Afshin Fassihi**, Horacio Péréz-Sánchez. Improving Activity Prediction of Adenosine A2B Receptor Antagonists by Nonlinear Models. ***Bioinformatics and Biomedical Engineering Lecture Notes in Computer Science***, 2015; 9044: 635-644.
25. Mahboubeh Mansourian, **Afshin Fassihi**, Lotfollah Saghaie, Armin Madadkar-Sobhani, Karim Mahnam, Maryam Abbasi. QSAR and docking analysis of non-xanthine based A_{2B}AR inhibitors. ***Medicinal Chemistry Research***, 2015; 24(1): 394-407.
26. Saghi Sepehri, Sajjad Gharagani, Lotfollah Saghaie, **Afshin Fassihi**, QSAR and docking studies of some 1,2,3,4-tetrahydropyrimidines: evaluation of gp41 as possible target for anti-HIV-1 activity. ***Medicinal Chemistry Research***, 2015; 24(4): 1707-174.
27. Hajar Sirous-Najafabadi, Rezvan Zabihollahi, Mohammad R. Aghasadeghi, Seyed Mehdi Sadat, Lotfollah Saghaie, **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.
28. Mahnam K, Saffar B, Mobini-Dehkordi M, **Fassihi A**, Mohammadi A. Design of a novel metal binding peptide by molecular dynamics simulation to sequester Cu and Zn ions. ***Research in Pharmaceutical Sciences***, 2014; 9(1): 69-82.
29. Yahya Khazaie, Luis Novo, Ethlinn van Gaal, **Afshin Fassihi**, Seyedeh Zohreh Mirahmadi-Zareh, Mohammad Hossein Nasr Esfahani, Cornelus F. van Nostrum, Wim E. Hennink, Farid Dorkoosh, Poly[N-(2-aminoethyl)ethyleneimine] as a New Non-Viral Gene Delivery Carrier: The Effect of Two Protonatable Nitrogens in the Monomer Unit on Gene Delivery Efficiency. ***Journal of Pharmacy and Pharmaceutical Sciences***, 2014; 17(4): 461-474.
30. Fatemeh Shahmoradi Ghaheh, Sayed Majid Mortazavi, Farzaneh Alihosseini, **Afshin Fassihi**, Ali Shams Nateri, Daryoush Abedi. Assessment of antibacterial activity of wool fabrics dyed with natural dyes. ***Journal of Cleaner Production,*** 2014; 72: 139-145.
31. Mohsen Shahlaei, **Afshin Fassihi**, Elena Papaleo, Morteza Pourfarzam. Molecular dynamics simulation of chemokine receptors in the lipid bilayer: A case study on CCR2. ***Chemical Biology & Drug Design***, 2013; 82: 534–545.
32. Mohammad Mahmoudzadeh, **Afshin Fassihi**, Jaber Emami, Farid A. Dorkoosh. Physicochemical, pharmaceutical and biological approaches toward designing optimized and efficient hydrophobically modified chitosan based polymeric micelles as a nanocarrier system for targeted delivery of anticancer drugs. ***Journal of Drug Targeting***, 2013; 21(8): 693-709 (Review Article).
33. Mohsen Shahlaei, **Afshin Fassihi**, Lotfollah Saghaie, Elham Arkan, Armin Madadkar-Sobhani, Alireza Pourhossein. Computational evaluation of some indenopyrazole derivatives as anticancer compounds; application of QSAR and docking methodologies. ***Journal of Enzyme Inhibition and Medicinal Chemistry,*** 2013; 28 (1): 16-32.
34. Rezvan Zabihollahi, **Afshin Fassihi**, Mohamad Reza Aghasadeghi, Hamid Reza Memarian, Mohammad Soleimani, Keivan Majidzadeh. Inhibitory effect and structure–activity relationship of some Biginelli-type pyrimidines against HSV-1. ***Medicinal Chemistry Research***, 2013; 22(3): 1270-1276.
35. Mahboubeh Mansourian, Lotfollah Saghaie, **Afshin Fassihi**, Armin Madadkar-Sobhani, Karim Mahnam. Linear and nonlinear QSAR modeling of 1,3,8-substituted-9-deazaxanthines as potential selective A_{2B}AR antagonists. ***Medicinal Chemistry Research***, 2013; 22(10): 4549-4567.
36. Mohsen Shahlaei, **Afshin Fassihi**. QSAR analysis of some 1-(3,3-diphenylpropyl)-piperidinyl amides and ureas as CCR5 inhibitors using genetic algorithm-least square support vector machine. ***Medicinal Chemistry Research***, 2013; 22(9): 4384-4400.
37. Mohsen Shahlaei, **Afshin Fassihi**, Armin Madadkar-Sobhani, Lotfollah Saghaie, Elham Arkan. Statistically validated QSAR study of some antagonists of the human CCR5 receptor using least square support vector machine based on the genetic algorithm and factor analysis. ***Medicinal Chemistry Research***, 2013; 22(3): 1399-1414.
38. Mehrdad Mohammadpour, Mohaddeseh Behjati, Amir Sadeghi, **Afshin Fassihi**. Wound healing by topical application of antioxidant iron chelators: kojic acid and deferiprone. ***International wound Journal***, 2013; 10(3): 260-264.
39. Razieh Sabet, Mohaddeseh Behjati, Roohollah Vahhabpour, Arash Memarzadegan, Mahboubeh Rostami, **Afshin Fassihi**, Mohammad R.

Aghasadeghi, Lotfollah Saghaie, Ramin Miri. Iron chelation afforded cardioprotection against H_2O_2-induced H9C2 cell injury: Application of novel 3-hydroxy pyridine-4-one derivatives. ***International Journal of Cardiology***, 2012; 162(1): 60-63.

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