Curriculum Vitae

Mohsen Shahlaei

Medicinal Chemist

Date of Birth: ۲۰/۱۰/۱۹۸۰

Nationality: Iranian

Marital Status: Married

Address: Department of Medicinal Chemistry,
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Education:

BSc.: Department of chemistry, Faculty of Science, Razi University, Kermanshah, IRAN (۲۰۰٤).

MSc.: Department of chemistry, Faculty of Science, Razi University, Kermanshah, IRAN (۲۰۰۷).

Ph.D. Faculty of Pharmacy and Pharmaceutical Sciences, Isfahan University of Medical Sciences, Isfahan, IRAN (۲۰۱۲).

Academic Appointment:

۲۰۱۲- present Assistant Professor, Department of Medicinal Chemistry, Kermanshah University of Medical Sciences

Executive Positions and Appointments

۱. Executive manager of the Journal of Reports in Pharmaceutical Sciences, since ۲۰۱۲.
۲. Information Technology (IT) Manager, Faculty of Pharmacy, Kermanshah University of Medical Sciences, Iran, since ۲۰۱۲.

Honors:

١. Distinguished researcher in pharmaceutical sciences, faculty of pharmacy, Isfahan University of Medical Sciences (٢٠٠٩).
٢. Distinguished researcher in Shamsipur convention in medicinal sciences category (٢٠١٠).
٣. Membership in Talented Assembly of Kermanshah.
٤. Membership in Talented Assembly of Isfahan.
٥. Distinguished researcher in pharmaceutical sciences, faculty of pharmacy, Isfahan University of Medical Sciences (٢٠١٠).
٦. Distinguished Ph. D candidate researcher of Isfahan University of Medical Sciences (٢٠١٠).
٧. Distinguished student researcher of Kermanshah University of medical sciences (٢٠١٠).
٨. Distinguished student researcher of Kermanshah University of Medical Sciences (٢٠١١).
٩. Distinguished Ph. D candidate researcher of Isfahan University of Medical Sciences (٢٠١١).
١٠. Distinguished researcher student in the pharmaceutical sciences part of the ١٧th Razi festival- Tehran (٢٠١١).
١١. Distinguished researcher of Kermanshah University of Medical Sciences (٢٠١٢).
١٢. Distinguished researcher of Kermanshah University of Medical Sciences (٢٠١٣).
١٣. Distinguished teacher of Kermanshah University of Medical Sciences (٢٠١٣).

Published Manuscripts:

١. Pourhossein, A*, Madani, M,. **Shahlaei**, **M.** Evaluation of an ultrasound–assisted digestion method for determination of arsenic and lead in edible citric acid samples by ETAAS. **Canad. J. Anal. Scie. Spec.** ٥٤ (٢٠٠٩) ٣٩-٤٤.

٢. Gholivand, MB., **Shahlaei, M.,** Pourhossein, A. New Zn(II)-Selective Potentiometric Sensor Based on ٣-Hydroxy-٢-Naphthoic Hydrazide. **SENSOR LETTERS** ٧ (٢٠٠٩) ١١٩-١٢٥.

٣. Gholivand, MB.*, Pourhossein, A., **Shahlaei**, **M.,** Determination of Trace amounts of Lead by Adsorptive Cathodic Stripping Voltammetry With L-٣-(٣,٤ Dihydroxyphenyl) Alanine, **Collect. Czech. Chem. Commun.** ٧٤ (٢٠٠٩) ٥٩٩–٦١٠.

٤. Gholivand, MB.*, Pourhossein, A., **Shahlaei**, **M.,** Application of Adsorptive Cathodic Stripping Voltammetry for Determination of Trace Amounts of Zinc Using Nalidixic Acid as a Chelating Agent, **Chem. Anal. (Warsaw),** ٥٤, (٢٠٠٩) ٦٥٥-٦٦٦.

٥. **Shahlaei, M.,** Gholivand, MB.*, Pourhossein, A. Simultaneous Determination of Tyrosine and Histidine by Differential Pulse Cathodic Stripping Voltammetry Using H-point Standard Addition Method in Tap and Seawater, **Electroanalysis** ٢١(٢٠٠٩) ٢٤٩٩ – ٢٥٠٢.

٦. Pourhosseina, A., Madani, M., **Shahlaei**, **M.,** Fakhri, K., Alimohamadi, P., Amiri, M. Ultrasound assisted pseudo-digestion for determination of iron and manganese in citric acid fermentation mediums by electrothermal atomic absorption spectroscopy, **Cent. Eur. J. Chem.** ٧(٢٠٠٩) ٣٨٢-٣٨٧.

٧. **Shahlaei**, **M.,** Gholivand,MB.*, Pourhossein, A. Application of Adsorptive Stripping Voltammetry for Determination of Uranium in the Presence of ٣-Hydroxy-٢-Naphthoic Hydrazide, **Anal. Lett.** ٤٢ (٢٠٠٩) ٣٠٨٥-٣٠٩٥.

٨. Sabet, R, **Shahlaei**, **M.,** Fassihi, A. QSAR study of anthranilic acid sulfonamides as inhibitors of methionine aminopeptidase-٢ using different chemometrics tools, **Recent Advances in Biology, Biophysics, Bioengineering and Computational Chemistry** (٢٠٠٩) ١١٩-١٢٥.

٩. **Shahlaei, M.,** Fassihi, A.*, Nezami, A. QSAR Study of some ٥-methyl/trifluoromethoxy- H-indole-٢,٣-dione-٣-thiosemicarbazone derivatives as antitubercular agents, **Research in Pharmaceutical Sciences** ٤(٢٠٠٩)١٢٣-١٣١.

١٠. Arkan, E., **Shahlaei, M.,** Pourhossein, A., Fakhri, K., Fassihi, A.*, Validated QSAR Analysis of Some Diaryl Substituted Pyrazoles as CCR٢ Inhibitors by Various Linear and Nonlinear Multivariate Chemometrics Methods. **Euro. J. Med. Chem.** ٤٥ (٢٠١٠) ٣٣٩٤-٣٤٠٦.

١١. **Shahlaei, M.,** Fassihi, A.*, Saghaie, L. Application of PC-ANN and PC-LS-SVM in QSAR of CCR١ antagonist compounds:A comparative study. **Euro. J. Med. Chem.** ٤٥ (٢٠١٠) ١٥٧٢–١٥٨٢.

١٢. **Shahlaei**, **M.,** Sabet,R., Bahman Ziari, M., Moeinifard, B., Fassihi, A.*, Karbakhsh, R. QSAR study of anthranilic acid sulfonamides as inhibitors of methionine aminopeptidase-٢ using LS-SVM and GRNN based on principal components, **Euro. J. Med. Chem.** ٤٥ (٢٠١٠) ٤٤٩٩-٤٥٠٨.

١٣. Saghaie, L., **Shahlaei**, **M.,** Madadkar-Sobhani, A., Fassihi, A.* Application of Partial Least Squares and Radial Basis Function Neural Networks in Multivariate Imaging Analysis-Quantitative Structure Activity Relationship: Study of Cyclin Dependent Kinase ٤ Inhibitors, **J. Mol. Graph. Model,** ٢٩ (٢٠١٠) ٥١٨–٥٢٨.

١٤. **Shahlaei, M.,** Fassihi, A,*, Saghaie, L., Shamshirian, D., Sakhi, HR. Comparative Quantitative Structure–Activity Relationship Study of Some ١-Aminocyclopentyl-٣- Carboxyamides as CCR٢ Inhibitors using Stepwise MLR, FA-MLR, GA-PLS, **Med. Chem. Res.** ٢١(٢٠١٢)١٠٠-١١٥.

١٥. Saghaie, L., **Shahlaei, M.*,** Fassihi, A., Madadkar-Sobhani, A., Gholivand, MB., Pourhossein, A. QSAR analysis for some Diaryl Substituted Pyrazoles as CCR٢ Inhibitors by GA-Stepwise MLR, **Chem. Biol. Drug Des.** ٧٧(٢٠١١)٧٥-٨٥.

١٦. Ayatollahi, AM., Ghanadian, M*, Afsharypuor, S., Choudhary, MI., Abdella, OM., **Mohsen Shahlaei**, M., Farzandi, G., Mostafavi, H., Cycloartanes from *Euphorbia aellenii* Rech. f. with their antiproliferative activity, **Iran. J. Pharm. Res.** ١٠ (٢٠١١) ١٠٥-١١٢

١٧. **Shahlaei, M.,** , Madadkar-Sobhani, A.*, Mahnama, K., Fassihi, A.*, Saghaie, L., Mansourian, M. Homology modeling of human CCR٥ and analysis of its binding properties through molecular docking and molecular dynamics simulation. **Biochim. Biophy. Acta-Biomembrane** ١٨٠٨ (٢٠١١) ٨٠٢–٨١٧.

١٨. **Shahlaei, M.**, Fassihi, A*. Saghaie, L., Arkan, E., Pourhossein, A. A modeling study of aldehyde inhibitors of human cathepsin K using partial least squares method. **Research in Pharmaceutical Sciences** ٦ (٢٠١١) ٧١-٨٠.

١٩. Fassihi, A.*, **Shahlaei, M.,** Moeinifard, B., Sabet, R. QSAR study of anthranilic acid sulfonamides as methionine aminopeptidase-٢ inhibitors. In Press, **Monatshefte fur Chemie** ١٤٣ (٢٠١١) ١٨٩-١٩٨.

٢٠. **Shahlaei, M.**, Madadkar-Sobhani, A., Fassihi, A*. Saghaie, L. Exploring a Model of a Chemokine Receptor/Ligand Complex in an Explicit Membrane Environment by Molecular Dynamics Simulation: The Human CCR١ Receptor. **J. Chim. Inform. Model.** ٥١ (٢٠١١) ٢٧١٧-٢٧٣٠.

٢١. Gholivand, MB.*, Pourhossein, A., Shahlaei, **M.,** Simultaneous determination of copper and cadmium in environmental water and tea samples by adsorptive stripping voltammetry. **Turk. J. Chem.** ٣٥ (٢٠١١) ٨٣٩-٨٤٦.

٢٢. **Shahlaei, M.,** Fassihi, A*., Saghaie, L., Arkan, E., Madadkar-Sobhani, A., Pourhossein, A. Computational evaluation of some indenopyrazole derivatives as anticancer compounds; application of QSAR and docking methodologies. **J. Enz. Inhib. Med. Chem.** ٢٨(٢٠١٣) ١٦-٣٢.

٢٣. Moradkhani, S., Ayatollahi, AM., Ghanadian, M., Moin, MR., Razavizadehe, M., **Shahlaei, M.** Phytochemical analysis and metal-chelation activity of Achillea tenuifolia Lam. **Iran. J. Pharm. Res**. ١١ (٢٠١٢) ١٧٧-١٨٣

٢٤. **Shahlaei M.,** Madadkar-Sobhani, A., Fassihi A., Saghaie, L., Arkan, E. QSAR study of some CCR٥ Antagonists as Anti HIV agents using radial basis function neural network and general regression neural network on the basis of Principal Components. In Press, **Med. Chem. Res.** (٢٠١١)

٢٥. **Shahlaei M.,** Fassihi A.*, Saghaie L., Arkan E., Pourhossein A. A QSAR study of some cyclobutenediones as CCR١ antagonists by artificial neural networks based on principal component analysis, Accepted, **DARU** ١٩ (٢٠١١) ٣٧٦-٣٨٤.

٢٦. **Shahlaei M.,** Madadkar-Sobhani, A., Saghaie, L., Fassihi A*. Application of an expert system based on genetic algorithm- adaptive neuro-fuzzy interference System (GA-ANFIS) in QSAR of cathepsin K inhibitors. **Expert systems with applications** ٣٩ (٢٠١٢) ٦١٨٢-٦١٩١.

٢٧. Saghaie, L., Sakhi, H., Hassan Sabzyan,H.*, **Shahlaei,M.,** Shamshirian D., Stepwise MLR and PCR QSAR study of the pharmaceutical activities of antimalarial ٣-hydroxypyridinone agents using B٣LYP/٦-٣١١++G** descriptors. In Press, **Med. Chem. Res. ٢٢ (٢٠١٣) ١٦٧٩-١٦٨٨**

٢٨. **Shahlaie, M.*,** Fassihi, A., Pourhossein, A., Arkan, E., Statistically validated QSAR study of some antagonists of the human CCR٥ receptor using least square support vector machine based on the genetic algorithm and factor analysis. In Press, **Med. Chem. Res. ٢٢ (٢٠١٣) ١٣٩٩-١٤١٤.**

٢٩. **Shahlaei, M.,** Ghanadian, SM.*, Ayatollahi, AM, Mesaik, MA., Abdalla, OM., Afsharypour, S., Rabbani, M., Molecular modeling, structure activity relationship and immunomodulatary properties of lupeol derivatives, **Med. Chem. Res. ٢٢ (٢٠١٣) ١٧٩٥-١٨٠٣**

٣٠. **Shahlaei, M.*,** Pourhossein, A., Direct determination of arsenic in potassium citrate tablet using graphite furnace atomic absorption spectrometry, **J. Rep. Pharm. Sci, ١(٢٠١٢) ١٥-١٨.**

٣١. Saghaie, L., **Shahlaie, M.*,** Fassihi, A. Quantitative structure activities relationships of some ٢-mercaptoimidazoles as CCR٢ inhibitors using genetic algorithm-artificial neural networks, **Research in Pharmaceutical Sciences ٨ (٢٠١٣) ٩٧-١١٢.**

٣٢. Pourhossein, A.*, **Shahlaei, M.** Direct determination of arsenic in beet sugar molasses using nickel as chemical modifier by electrothermal atomic absorption spectrommetry ٦٠ **(٢٠١٣) J. Chinese Chem. Soc. ٢٤١-٢٤٤.**

٣٣. **Shahlaei, M.*,** Pourhossein, A. A ٢D image based method for modeling some c-Src tyrosine kinase inhibitors **Med. Chem. Res ٢٢ (٢٠١٣) ٣٠١٢–٣٠٢٥.**

٣٤. **Shahlaie, M.*,** Fassihi, A. QSAR Analysis of Some ١-(٣, ٣-diphenylpropyl)-piperidinyl Amides and Ureas as CCR٥ Inhibitors Using Genetic Algorithm- Least Square Support Vector Machine, **Accepted (٢٠١٢) Med. Chem. Res**.

٣٥. **Shahlaei, M.*** Pourhossein, A. Modeling of CCR٥ antagonists as anti HIV agents using combined genetic algorithm and adaptive neuro-fuzzy inference system (GA–ANFIS), ٢٢ **(٢٠١٣) Med. Chem. Res. ٤٤٢٣-٤٤٣٦**

٣٦. Maghsoudi, S. Ashrafi, MR.* **Shahlaei, M.** Ghadami, SA. Ghobadi, S. Mostafaie, A. Khodarahmi, R*. Comparative Evaluation of Amphotericin B Binding to the Native and Modified Forms of Rice Lipid-Transfer Protein (LTP١): A Possible Perspective on Improving the Drug Binding Affinity and Specificity, ١٠ **(٢٠١٣) J. Iran. Chem. Soc. ٩٣٧-٩٥٠**

٣٧. **Shahlaei, M.*** Zare, A., Saghaie, L., Fassihi, A. Prediction of partition coefficient for some ٣-hydroxy pyridine-٤-one derivatives using combined partial least square regression and genetic algorithm, ٩ (٢٠١٣) **Res. Pharm. Sci.** ١٤٣-١٥٣

٣٨. **Shahlaei, M.** Pourhossein, A.* Biomass of Aspergillus Niger: Uses and Applications, **J. Rep. Pharm. Sci,** ٢(٢٠١٣) ٦٧-٧٣.

٣٩. **Shahlaei, M.*,** Fassihi, A., Papaleo, E., Pourfarzam, M. Molecular Dynamics Simulation of Chemokine Receptors in the Lipid Bilayer: A Case Study on CCR٢. ٨٢ (٢٠١٣) **Chem. Biol. Drug Des.** ٥٣٤-٥٤٥

٤٠. **Shahlaei, M.*** Descriptor selection methods in QSAR studies: a review study. **Chemical Reviews** ١١٣ (٢٠١٣) ٨٠٩٣–٨١٠٣.

٤١. **Shahlaei, M.*,** Nazari, Z. Computational neural network analysis of the affinity of ٢-pyridyl-٣,٥-diaryl pyrroles analogs for the human glucagon receptor using density functional theory **Accepted, (٢٠١٣) Medicinal Chemistry Research**

٤٢. **Shahlaei, M.,** Pourhossein, A.*, Determination of Arsenic in Drinking Water Samples by Electrothermal Atomic Absorption Spectrometry after Preconcentration Using the Biomass of Aspergillus Niger Loaded on Activated Charcoal, **Accepted, (٢٠١٣) Journal of Chemistry**

٤٣. **Shahlaei, M.*,** Nazari, Z. Prediction of Glucagon Receptor Antagonist Activities of Some Substituted Imidazoles Using Combined Radial Basis Function Neural Network and Density Functional Theory, **Accepted, (٢٠١٣) Medicinal Chemistry Research**

٤٤. **Shahlaei, M*,** Nowroozi, A, Khodarahmi, R. A combined DFT and QSAR calculations to study substituted biphenyl imidazoles as bombesin receptor subtype-٣ agonists, ١١, (٢٠١٤) **Letters in Drug Design & Discovery,** ٦٦٥-٦٧٦

٤٥. **Mohsen Shahlaei**, Ehsan Sohrabi, Jaber Emami, Farshid Hassanzadeh, Lotfollah Saghaie* Simultaneous spectrophotometric determination of Amlodipine and Metoprolol by principal component regression multivariate calibration and comparison with HPLC, ٢ (٢٠١٣) **J. Rep. Pharm. Sci.** ١٧٩-١٨٩

٤٦. **Shahlaei, M*.** Nowroozi, A. Khodarahmi, R. Application of radial basis function neural network and DFT quantum mechanical calculations for the prediction of the activity of ٢-

biarylethylimidazole derivatives as bombesin receptor subtype-٣ (BRS-٣) agonists. **Accepted, (٢٠١٤) Medicinal Chemistry Research**

٤٧. **Shahlaei, M .** Saghaie, L* Prediction of p٣٨ Inhibitory activity of ٣,٤-Dihydropyrido[٣,٢-d] pyrimidone derivatives using an expert system based on principal component analysis and least square support vector machine **Accepted, (٢٠١٤) Research in Pharmaceutical Sciences**

٤٨. **Shahlaei, M *.** Mousavi, A**.** A ٣D Model for Human Melanocortin ٤ Receptor Refined with Molecular Dynamics Simulation. **٣ (٢٠١٤) J. Rep. Pharm. Sci. ٤٢-٥٣**

٤٩. **Shahlaei, M *.** Mousavi, A**.** Refinement of homology□based Melanocortin ٤ receptor structure by multiple molecular dynamics simulation study **Accepted, (٢٠١٤) Chem Biol Drug Des**

٥٠. **Shahlaei, M *.** Andisheh, H. Derakhshandeh, K. Sadrjavadi, K. A novel method for simultaneous determination of codeine and acetaminophen in plasma by combination of UV-Vis spectroscopy and artificial neural network, **٣ (٢٠١٤) J. Rep. Pharm. Sci. ١٤١-١٦٢**

٥١. **Shahlaei, M *.** Rahimi, B. AshrafiKoshk, R. Sadrjavadi, K. Khodarahmi, R Probing of possible olanzapine binding site on Human Serum Albumin: Combination of spectroscopic methods and molecular dynamics simulation, **Accepted, (٢٠١٤) Journal of Luminescence**

٥٢. Moradi, N. AshrafiKoshk, R, Ghobadi, S. **Shahlaei, M.** Khodarahmi, R* Spectroscopic Study of drug-binding characteristics of unmodified and pNPA-based acetylated human serum albumin: Does esterase activity affect microenvironment of drug binding sites on the protein**?** **Accepted, (٢٠١٤) Journal of Luminescence**

٥٣. Sadrjavadi, K. **Shahlaei , M*.** Bahrami, G, Majnooni, MB. Mohebbi , M Comparison of Correlation Ranking and Eigenvalue Ranking Unfolded Principal Component Regression for Direct Determination of Naproxen in Human Serum using Excitation–Emission Matrix Fluorescence Spectroscopy. **Accepted, (٢٠١٤) Journal of Iranian Chemical Society**

Teaching History

١. Teaching of medicinal chemistry I, II and III, Kermanshah University of Medical Sciences, since ٢٠١١.
٢. Teaching of instrumental analysis, Kermanshah University of Medical Sciences Since ٢٠١١.
٣. Teaching of General chemistry, Kermanshah University of Medical Sciences, since ٢٠١٣.
٤. Teaching of Physical chemistry, Kermanshah University of Medical Sciences, since ٢٠١٣.
٥. Several Molecular Modeling workshops

Theses (Supervised or consulted)

١. Alireza Zare, Prediction of partition coefficient for some ٣-hydroxy pyridine-٤-one derivatives using combined partial least square regression and genetic algorithm. **Role:** Supervisor
٢. Ehsan Sohrabi, Simultaneous spectrophotometric determination of Amlodipine andMetoprolol by principal component regression multivariate calibration and comparison with HPLC. **Role:** Supervisor
٣. Sajjad Abdolmaleki, Determination of celecoxib by fluorescence spectroscopy and chemometrics methods and comparison with HPLC method. **Role:** Supervisor
٤. Mehdi Ahmadi, Homology modeling, pharmacophore modeling and molecular docking study of some $P^{٢}X^{٧}$ receptor antagonists. **Role:** Supervisor
٥. Hadi Andisheh, Simultaneous Spectroscopic Determination of Acetaminophen and Codeine in serum using chemometric methods and comparison with HPLC. **Role:** Supervisor
٦. Behnoosh Rahimi, Study of interactions of olanzapine and sertraline with human serum albumin using combination of spectroscopic and molecular modeling methods. **Role:** Supervisor
٧. Elham Esmaili, The study of the interaction of magainin with phospholipid membrane and different solvents (water and methanol) using molecular dynamics simulation. **Role:** Supervisor
٨. Saeid Ghadaki, The effect of curcumine and rosemarinic acid on pre-and postaggregation state of $A\beta_{١٧-٤٢}$ using molecular dynamics simulation studies. **Role:**Supervisor
٩. Shayesteh Gheibi, Effects of dihydropyranocoumarins from Ferulago *macrocarpa*on VEGF, $MMP^{٩}$, $MMP^{٢}$ and study of binding modes using computational methods. **Role:** Consultant
١٠. Hamid Nabiyar, Determination of indomethacin and ibuprofen by fluorescence spectroscopy and chemometrics methods and comparison with HPLC method. **Role:** Supervisor
١١. Zohreh Nazari, Homology modeling, Molecular Dynamics Simulation, Docking and QSAR study of some pyrroles and imidazoles based antagonists of human glucagon receptor. **Role:** Supervisor

١٢. Amin Nowroozi, Homology modeling, Molecular Dynamics Simulation, Docking and QSAR study of some biaryl ethyl imidazole based agonists of human bombesin receptor subtype-٣. **Role:** Supervisor

١٣. Atefeh Mosavai, Homology modeling, Molecular Dynamics Simulation and Docking of some carboxamide agonists of melanocortin subtype ٤ receptor. **Role:** Supervisor

Reviewer of International Journals:

Medicinal Chemistry Research

European Journal of medicinal Chemistry

Research in Pharmaceutical sciences

Current Medicinal Chemistry

Computational and Mathematical Methods in Medicine

Molecular Simulation

Operating System Skills

Windows, Linux

Instrumental Skills:

UV/Visible, Polarogeraph, HPLC, Fluorimeter, Some Skills in Synthesis of organic compounds

Programming Skills

C++, MATLAB, Shell programming

Software Skills:

HyperChem, Dragon, Gaussian, Gaussview, AutoDock, SPSS, Minitab, Chemoffice, web lab viewer, VMD and Gromacs.