Curriculum vitae

Ahmad Mani-Varnosfaderani

Date of Birth: 08 May 1984



Assistant Professor in Analytical Chemistry, Tarbiat Modares University, Tehran, Iran, 2013-present

Assistant Professor in Bioinformatics, Department of Biomedical Engineering, Isfahan University of Medical Sciences, 2012-2013.

International Collaborations

Research stay in Institute of Environmental Assessment and Water Research, Spanish National Research, Council (CSIC), Barcelona, Spain, summer 2018. Investigating error propagation in multivariate curve resolution techniques in collaboration with Prof. Roma Tauler.

PhD Sabbatical Leave, University of Bern, Department of Chemistry and Biochemistry, Berne, Switzerland, Nov 2011- May 2012, Fragmentation analysis of very large molecular databases in the group of Prof. Jean-Louis Reymond.

Educational Background(s)

PhD: Sharif University of Technology, Department of Analytical Chemistry, 2008-2012, Under supervision of Prof. Mehdi Jalali-Heravi

MSc: Sharif University of Technology, Department of Analytical Chemistry, 2006-2008, Under supervision of Prof. Mehdi Jalali-Heravi

BSc: University of Tabriz, Department of Applied Chemistry, 2003-2006.

Thesis Title(s)

PhD Sabbatical Leave: Fragmentation analysis of the GDB-13, using scaffold forest methodology.

PhD: Development and application of chemometrics techniques for classification and similarity analysis of drug activities: Introduction of classical relativity in chemical space.

MSc: Modeling the anti-HIV activities of amides as CCR5 modulators

BSc: Preparation of AuCN for elctroless gold plating in Nickel based plating bathes

Honors

Ranked 2nd among BSc students, Department of Chemistry, University of Tabriz, 2006

Ranked 3rd among Msc students, Department of Chemistry, Sharif University of Technology, 2008.

Ranked 1st, PhD entrance exam, Sharif University of Technology, 2008.

Ranked 1st among analytical chemistry PhD students, Sharif University, 2012.

Ranked 2nd among PhD students, Sharif University, 2012.

Ranked 3rd among more than 9000 students, master entrance exam 2006.

Ranked 4th, National Olympiad of Chemistry students, Tehran, Iran, 2006.

Research Interests

Chemometrics, Metabolomics, Bioinformatics, Drug Discovery, Raman Spectroscopy, Image Analysis, Drug Design, Database Development and Analysis, Clinical Biochemistry, Sample Preparation and Method Development, Analytical Chemistry, Cheminformatics

Peer Reviewed Journal Publications

[38] **A. Mani-Varnosfaderani**, A. Kanginejad, Chemometrics advances on the challenges of the gas chromatography-mass spectrometry metabolomics data: A review, Journal of the Iranian Chemical Society, **2018**, Accepted.

[37] H. Jamalabadi, A. Mani-Varnosfaderani, N. Alizadeh, Detection of alkyl amine vapors using PPy-ZnO hybrid nanocomposite sensor array and artificial neural network, Sensors and Actuators A: Physical, **2018**, In Press.

[36] **A. Mani-Varnosfaderani**, M. S. Neiband, A. Benvidi, Identification of molecular features necessary for selective inhibition of B cell lymphoma proteins using machine learning techniques, Molecular Diversity, **2018**, In Press.

[35] K. Gilany, N. Jafarzadeh, **A. Mani-Varnosfaderani**, A. Minaei-Tehrani, M. Sadeghi, Metabolic fingerprinting of seminal plasma from non-obstructive azoospermia patients: positive versus negative testicular sperm extraction, Journal of Reproduction & Infertility, **2018**, In Press.

[34] **A. Mani-Varnosfaderani**, M. Soleymani, N. Alizadeh, Least absolute shrinkage and selection operator as a multivariate calibration tool for simultaneous determination of diphenylamine and its nitro derivatives in propellants, Propellants, Explosives, Pyrotechnics., **2018**, 43, 379-389.

[33] S. Ahmadi, **A. Mani-Varnosfaderani**, B. Habibi, Motor oil classification using color histograms and pattern recognition techniques, J. AOAC Int., **2018**, In Press.

[32] N. Jafarzadeh, A. Mani-Varnosfaderani, K. Gilany, S. Einaly, H. Ghaznavi, A. Shakeri-Zadeh, The molecular cues for the biological effects of ionizing radiation dose and post-irradiation time on human breast cancer SKBR3 cell line: A Raman spectroscopy study, J. Photochem. Photobiol. B: Biology, **2018**, 180, 1-8.

[31] **A. Mani-Varnosfaderani**, A. Kanginejad, Y. Yamini, Exploring the effects of sparsity constraint on the ranges of feasible solutions for resolution of GC-MS data, Chemom. Intel. Lab. Syst., **2018**, 173, 30-40.

[30] H. Jamalabadi, **A. Mani-Varnosfaderani**, N. Alizadeh, PPy-metal oxide hybrid nanocomposite sensor array for simultaneous determination of volatile organic amines in high humid atmosphere, IEEE Sensors, **2017**, 17, 8282 – 8289.

[29] M. Safari, Y. Yamini, M. M. Yaser, A. Morsali, **A. Mani-Varnosfaderani**, Magnetic metal-organic frameworks for the extraction of trace amounts of heavy metal ions prior to their determination by ICP-AES, Microchimica Acta, **2017**, 184, 1555–1564.

[28] M. S. Neiband, A. Mani-Varnosfaderani, A. Benvidi, Classification of Sphingosine kinase inhibitors using counter-propagation artificial neural networks: A systematic route for designing selective SphK inhibitors, SAR QSAR Environ. Res., 2017, 28, 91-109.

[27] K. Gilany, **A. Mani-Varnosfaderani**, A. Minai-Tehrani, F. Mirzajani, A. Ghassempour, M. Sadeghi, M. Amini, H. Rezadoust, Untargeted metabolomic profiling of seminal plasma in non-obstructive azoospermia men: a non-invasive detection of spermatogenesis, Biomed. Chromatogr., **2017**, In Press.

[26] M. Safari, Y. Yamini, **A. Mani-Varnosfaderani**, H. Asiabi, Synthesis of Fe3O4@PPy–MWCNT nanocomposite and its application for extraction of ultra-trace amounts of PAHs from various samples, J. Iran. Chem. Soc., **2017**, 14, 623–634.

[25] **A. Mani-Varnosfaderani**, A. Kanginejad, K. Gilany, A. Valadkhani, Estimating complicated baselines in analytical signals using the iterative Bayesian regularized artificial neural networks, Anal. Chim. Acta, **2016**, 940, 56–64.

[24] M. Ebrahimi, A. Mani-Varnosfaderani, T. Khayamian, S. Gharaghani, An in silico approach to design peptide mimetics based on docking and molecular dynamics simulation of EGFR-matuzumab complex, J. Iran. Chem. Soc., **2016**, 13, 1805–1817.

[23] **A. Mani-Varnosfaderani**, M. Jamshidi, A. Yeganeh, M. Mahmoudi, Concentration profiling of minerals in iliac crest bone tissue of addicted humans using inductively coupled plasma and discriminant analysis techniques, J. Pharmacut. Biomed. Anal., **2016**, 120, 92–99.

[22] N. Alizadeh, M. Babaei, M. S. Alizadeh, A. Mani-Varnosfaderani, Simultaneous analysis of aliphatic alcohols using an electronic nose based on nano/micro structured conducting polypyrrole film prepared by catalytic electropolymerization on Cu/Au interdigital electrodes using multivariate calibration, IEEE Sensors, **2016**, 16, 418 – 425.

[21] **A. Mani-Varnosfaderani**, M. Ghaemmaghami, Assessment of orthogonality in 2-D separation systems using criteria defined by maximal information coefficient, J. Chromatogr. A, **2015**, 1415, 108-114.

[20] N. Alizadeh, S. Pirsa, **A. Mani-Varnosfaderani**, M. S. Alizadeh, Design and fabrication of opentubular array gas sensors based on conducting polypyrrole modified with crown ethers for simultaneous determination of alkylamines, IEEE Sensors, **2015**, 15, 4130-4136.

[19] M. Asadollahi-Baboli, **A. Mani-Varnosfaderani**, Therapeutic index modeling and predictive QSAR of novel thiazolidin-4-one analogs against Toxoplasma gondii, Eur. J. Pharm. Sci., **2015**, 70, 117-124.

[18] **A. Mani-Varnosfaerani**, A. Valadkhani, M. Jalali-Heravi, CS-MINER: A freely available tool for association mining in Binding-DB, Mol. Inform., **2015**, 34, 185-196. [Hot Paper]

[17] A. Valadkhani, M. Asadollahi-Baboli, **A. Mani-Varnosfaderani**, QSAR study of the inhibitors of the acetyl-CoA carboxylase 1 and 2 using Bayesian regularized genetic neural networks: A comparative study, J. Braz. Chem. Soc. 2015. 26, 619-631.

[16] N. Jafarzadeh, **A. Mani-Varnosfaderani**, K. Gilany, Metabolomics fingerprinting of seminal plasma from unexplained infertile men: A need for novel diagnostic biomarkers, Mol. Rep. Develop, 2015, 82, 150.

[15] F. Fathi, A. Mani-Varnosfaderani, 1H NMR based metabolic profiling in Crohn's disease by random forest methodology, Magnet. Res. Chem., 2014, 52, 370-376.

[14] M. Asadollahi-Baboli, A. Mani-Varnosfaderani, Chemometrics-Assisted GC-MS Analysis of Volatile and Semi-Volatile Constituents of Elettaria cardamomum, Food Anal. Methods, 2014, 7, 1745-1754.

[13] M. Asadollahi-Baboli, **A. Mani-Varnosfaderani**, Rapid and simultaneous determination of tetracycline and cefixime antibiotics by mean of gold nanoparticles-screen printed gold electrode and chemometrics tools, Measurement, 2014, 47, 145-149.

[12] M. Jalali-Heravi, **A. Mani-Varnosfaderani**, A. Valadkhani, Integrated one-against-one classifiers as tools for virtual screening of compound databases: A case study with CNS inhibitors, Molecular Informatics, 2013, 32, 742–753.

[11] M. Asadollahi-Baboli, **A. Mani-Varnosfaderani**, Molecular docking, molecular dynamics simulation, and QSAR model on potent thiazolidine-4-carboxylic acid inhibitors of influenza neuraminidase, Med. Chem. Res. 2013, 22, 1700-1710.

[10] M. Asadollahi-Baboli, **A. Mani-Varnosfaderani**, Application of computational methods to predict absorption maxmia of organic dyes used in solar cells, J. Theor. Comp. Chem., 2013, 12, 1250114.

[9] M. Asadollahi-Baboli, **A. Mani-Varnosfaderani**, Shuffling multivariate adaptive regression splines as a predictive method for modeling of novel pyridylmethylthio derivatives as VEGFR2 inhibitors, Med. Chem. Res., 2013, 22, 2645-2653.

[8] M. Jalali-Heravi, A. Mani. Varnosfaderani, Navigating drug-like chemical space of anti-cancer molecules using genetic algorithms and counterpropagation artificial neural networks, Molecular Informatics, 2012, 31, 63-74.

[7] M. Jalali-Heravi, **A. Mani-Varnosfaderani**, The use of Bayesian nonlinear regression techniques for the modelling of the retention behaviour of volatile components of Artemisia species, SAR QSAR Environ. Res, 23, 2012, 461-483.

[6] H. Parastar, M. Jalali-Heravi, H. Sereshti, A. Mani-Varnosfaderani, Chromatographic fingerprint analysis of secondary metabolites in citrus fruits peels using gas chromatography–mass spectrometry combined with advanced chemometric methods, J. Chromatogr. A., 2012, 1251, 176–187.

[5] R. F. Alamdari, **A. Mani-Varnosfaderani**, M. Asadollahi-Baboli, A. Khalafi-Nezhad, Monte Carlo sampling and multivariate adaptive regression splines as tools for QSAR modelling of HIV-1 reverse transcriptase inhibitors, SAR QSAR Environ. Res. 2012, 23, 665-682.

[4] M. Jalali-Heravi, **A. Mani-Varnosfaderani**, M. M. Mahmoodi, M. Taherinia, P. E. Jahromi, Classification of anti-HIV compounds using counterpropagation artificial neural networks and decision trees, SAR QSAR Environ. Res, 2011, 22, 639-660. [Hot Paper]

[3] M. Jalali-Heravi, **A. Mani-Varnosfaderani**, QSAR modeling of integrin antagonists using enhanced Bayesian regularized genetic neural networks, SAR QSAR Environ. Res, 2011, 22, 293-314.

[2] M. Jalali-Heravi, M. A. Baboli, **A. M. Varnosfaderani**, Shuffling multivariate adaptive regression splines and adaptive neuro-fuzzy inference system as tools for QSAR study of SARS inhibitors, J.Pharm. Biomed. Anal. 2009, 50, 853-860.

[1] M. Jalali-Heravi, **A. M. Varnosfaderani**, QSAR Modeling of 1-(3,3-Diphenylpropyl)-Piperidinyl Amides as CCR5 Modulators Using Multivariate Adaptive Regression Spline and Bayesian Regularized Genetic Neural Networks, QSAR Comb. Sci. 2009, 9, 946-958.

Book(s)

OMICS: New insight to modern biology, Gohar-bar Publication, June 2016.

International Conferences

[7] A. Mani-Varnosfaderani, Investigation of the effects of 'sparsity constraint' on the ranges of feasible solutions in MCR methods, Topics in Chemometrics, May 2017, NewCastle, Australia.

[6] J. Harynuk, L. A. Adutwum, A. Mani-Varnosfaderani, *Comparison of feature selection processes for Chemometric modeling*, PITTCON Conference and Expo 2015, Louisiana, USA.

[5] M. Jalali-Heravi, A. Mani-Varnosfaderani, A. Bigdeli, *Application of robust nonlinear regression techniques for unraveling quantitative structure activity relationships in drug design*, 241st ACS National Meeting, Medicinal Chemistry Division, Anaheim, CA, USA.

[4] M. Jalali-Heravi, A. Mani-Varnosfaderani, A. Bigdeli, M. R. Lotfi, *Classification and similarity* analysis of leads and drug-like molecules using artificial neural networks, decision trees and virtual screening methods, 241st ACS National Meeting, Medicinal Chemistry Division, Anaheim, CA, USA.

[3] M. Jalali-Heravi, A. Mani-Varnosfaderani, M. M. Mahmoodi, M. Taherinia, P. E. Jahromi, *A molecular library for classification and similarity analysis of anti-HIV compounds*, ACS symposium, ACS, March 21-25, Medicinal Chemistry Division, 2010 San Francisco, California, USA.

[2] A. Mani-Varnosfaderani, M. Jalali-Heravi, *Combination of local search methods with Bayesian regularized genetic neural networks: QSAR study of* $\alpha 4\beta 7$ and $\alpha 4\beta 1$ integrin antagonists, 11th conference of chemometrics, Budapest, Hungary, 2009, September.

[1] M. Asadollahi-Baboli, A. Mani-Varnosfaderani, M. Jalali-Heravi, *Application of spline functions for modeling the activity of SARS inhibitors, 11th conference of chemometrics*, Budapest, Hungary, 2009, September.

National Conferences

- [24] A. Mani-Varnosfaderani, A reasonable compromise between the magnitude of L1 and L2 norms in multivariate curve resolution for deconvolution of GC-MS data, 6th Iranian Biannual Conference of Chemometrics, Babolsar, Iran, Oct. 2017.
- [23] M. J. Massror, A. Mani-Varnosfaderani, Discrimination of almonds (amygdalus) with respect to their genotype by using Fourier Transform Infrared Spectroscopy and chemometrics, 6th Iranian Biannual Conference of Chemometrics, Babolsar, Iran, Oct. 2017.
- [22] A. Madani, A. Mani-Varnosfaderani, Classification of different kinds of rice in the north of iran using IR spectroscopy combined with multivariate analysis, 6th Iranian Biannual Conference of Chemometrics, Babolsar, Iran, Oct. 2017.
- [21] M. Neiband, A. Mani-Varnosfaderani, A. Benvidi, QSAR classification models for Bcl-2 and BclxL inhibitors using Supervised Kohonen maps and Linear Discriminant Analysis methods, 6th Iranian Biannual Conference of Chemometrics, Babolsar, Iran, Oct. 2017.

- [20] S. Ehsani, A. Mani-Varnosfaderani, Y. Yamini, H. Amanzadeh, Investigation of the effects of the chemical composition of lubricants on the value of their viscosity index using multivariate calibration methods, 19th Iranian Congers of Chemistry, Shiraz, Jan 2017.
- [19] A. H. Madani, A. Mani-Varnosfaderani, Simultaneous determination and quantification of picoline derivatives using UV-vis spectroscopy and multivariate calibration methods, 19th Iranian Congers of Chemistry, Shiraz, Jan 2017.
- [18] A. Mani-Varnosfaderani, Atefeh Kanginejad, Multivariate curve resolution with lasso regression: a survey on estimation of rotational ambiguity for sparsity constraint, Oral Presentation, 23th seminar of Analytical Chemistry, Sharif University of Technology, Tehran, Iran, August 2016.
- [17] M. Neiband, A. Mani-Varnosfaderani, A. Benvidi, *Classification of Sphingosine kinase inhibitors using genetic algorithm and counter propagation artificial neural network*, Poster Presentation, 23th seminar of Analytical Chemistry, Sharif University of Technology, Tehran, Iran, August 2016.
- [16] A. Mani-Varnosfaderani, K. Gilany, Untargeted metabolomic profiling of seminal plasma of nonobstructive azoospermia men using gas chromatography-mass spectrometry and advanced chemometric techniques, Oral Presentation, 22nd Iranian Seminar of Analytical Chemistry, Tehran, Feb 2016.
- [15] M. Soleimani, A. Mani-Varnosfaderani, N. Alizadeh, Simultaneous determination of diphenylamine derivatives using uv-vis spectroscopy and chemimetrics techniques, Poster Presentation, 22nd Iranian Seminar of Analytical Chemistry, Tehran, Feb 2016.
- [14] A. Mani-Varnosfaderani, A. Kanginejad, Multivariate curve resolution-alternating least squares with sparsity constraint, Poster Presentation, 22nd Iranian Seminar of Analytical Chemistry, Tehran, Feb 2016.
- [13] V. Mohammadrezaei, A. Mani-Varnosfaderani, M. Ebrahimi, QSAR study of tri-substituted 1,2,4triazoles as inhibitors of the annexin A2-S100A10 protein using the multiple linear regression model, Poster Presentation, 5th international Iranian biannual conference of Chemometrics, University of Tehran, October 2015.
- [12] A. Mani-Varnosfaderani, M. Beiband, A. Benvidi, QSAR modeling of Sphingosine kinase inhibitors using multivariate adaptive regression spline and projection based regression techniques, Poster Presentation, 5th international Iranian biannual conference of Chemometrics, University of Tehran, October 2015.
- [11] A. Mani-Varnosfaderani, A. Kanginejad, Estimating complicated baselines in analytical signals by iterative training of bayesian regularized artificial neural networks, Poster Presentation, 5th international Iranian biannual conference of Chemometrics, University of Tehran, October 2015.

- [10] A. Mani-Varnosfaderani, What is in Chemometrics for Chemoinformatics: Validating classical relativity in chemical space, Oral Presentation, 5th international Iranian biannual conference of Chemometrics, University of Tehran, October 2015.
- [9] A. Mani-Varnosfaderani, Learning with Sparsity Constraint: Implementation of a new constraint for multivariate curve resolution-alternating least square algorithm, Oral Presentation, 21th Iranian symposium of Analytical Chemistry, March 2015, Ahvaz, Iran.
- [8] A. Mani-Varnosfaderani, M. Jalali-Heravi, Investigation of Classical Relativity in chemical space by high throughput docking, Oral Presentation, 4th Iranian National Biannual Seminar of Chemometrics, Shiraz, Iran, December 2013.
- [7] A. Mani-Varnosfaderani, A. Valadkhani, M. Jalali-Heravi, Charting the chemical space of the CNS inhibitors: Introduction of "classical relativity" in chemical space, Oral presentation, 19th Iranian symposium of Analytical Chemistry, Mashhad, Iran, February, 2013.
- [6] A. Mani-Varnosfaderani, A. Valadkhani, M. Jalali-Heravi, CS-MINER: A freely available tool for exploring in medicinal-chemical space, Oral presentation, 4th national conference on Bioinformatics, Tehran, Iran, November 2012. Distinguished presentation.
- [5] A. Mani-Varnosfaderani, M. Jalali-Heravi, *Exploring general structure activity relationships*, Oral presentation, 18th Iranian symposium of Analytical Chemistry, Zahedan, Iran, June 2011.
- [4] A. Bigdeli, A. Mani-Varnosfaderani, M. Jalali-Heravi, QSAR study of anti-diabetic inhibitors using artificial neural network modeling assisted with linear and non-linear variable selection methods, Poster Presentation, 18th Symposium of Analytical Chemistry, Zahedan, Iran, June 2011.
- [3] A. Mani-Varnosfaderani, M. Jalali-Heravi, *Classification of glutamate inhibitors using decision trees and counter propagation artificial neural networks*, Oral presentation, 17th Symposium of Analytical Chemistry, Kashan, Iran, September 2010.
- [2] A. Mani-Varnosfaderani, M. Jalali-Heravi, *Application of Bayesian adaptive regression splines* for QSAR modeling of glutamate inhibitors, Oral presentation, Biannual Seminar of Chemometrics, Urumiah, Iran, December 2009.
- [1] A. Mani-Varnosfaderani, M. Jalali-Heravi, *Combination of pattern search optimization and fuzzy inference system as a method for rule extraction from complex systems*, Poster presentation, 16th symposium of Analytical Chemistry, Hamedan, Iran, June 2009.

Courses Taught

- Computer Aided Drug Design (Tarbiat Modares University, 2016- present)
- Analytical Spectroscopy I (Tarbiat Modares University, 2013-present.)
- Statistical Interpretation of Results (Tarbiat Modares University, 2013-present)

- Modeling of Biological Data (Isfahan University of Medical Science, Aug-Nov 2012)
- Bioinformatics (Isfahan University of Medical Science, Aug-Nov 2013)
- Advanced Modeling (Isfahan University of Medical Science, Aug-Nov 2013)
- Analytical. Chem. 2. Lab. Summer 2010.
- Analytical. Chem. 2. Lab. Spring 2010.
- Analytical. Chem. 1. Spring 2010.
- Analytical. Chem. 2. Spring 2010
- Instrumental analysis, Fall 2010.
- Analytical. Chem. 2. Lab, Fall 2010.
- General Chem. Lab. Spring 2009.
- General Chem. Lab. Spring 2009.
- Analytical. Chem. 1. Lab. Fall 2008.
- General Chem. Lab. Fall 2008.
- Analytical. Chem. 1. Lab. Spring 2007.
- General Chem. Lab. Spring 2007.

Journal Reviewer Experiences

Applied Soft Computing (Elsevier Publications) Journal of Chromatography A (Elsevier Publications) Chemometrics and Intelligent Laboratory Systems (Elsevier Publications) Scientific Reports (Nature Publications) SAR and QSAR in Environmental Research (Taylor and Francis Publications) Medicinal Chemistry Research (Springer Publications) Journal of AOAC International Iranian Journal of Mathematical Chemistry Journal of the Iranian Chemical Society (Springer Publications) Iranian Journal of Chemistry and Chemical Engineering

Graduated Students

PhD Degree

Atefeh Kanginejad (June 2018) Hoda Jamalabadi (advisor, 2017)

Master Degree

Amir Hossein Mohammadian (advisor 2018) Alireza Hosseini Madani (2017) Samaneh Ehsani (2017) Maliheh Nazari (advisor 2016) Maryam Sadat Mousavi (advisor 2016) Ziba Abdollahpour (advisor 2016) Masoud Soleymani (advisor 2016) Mahbobeh Jamshidi (2015)

Current Students

PhD Degree

Mohammad Javad Masror Marzieh Sadat Neiband (advisor) Shiva Ahmadi (advisor)

Master Degree

Mojtaba Hasanzadeh Arman Afroz Nastaran Haji Hosseini (advisor)