

دکتر مرتضی عتباتی

مرتبه علمی: دانشیار

وضعیت استخدامی: رسمی قطعی

دانشگاه صنعتی اصفهان ۱۳۸۲

تحصیلات: دکترای شیمی تجزیه

Email: atabati@du.ac.ir

Papers

1. H. Faghihian, A. Mostafavi, M. Atabati, Application of natural zeolite and natrolite obtained from Iranian deposits for adsorption of gases, Research Bulltein of Isfahan University, 11 (1999) 87-100.
2. A.A. Ensafi, M. Atabati, Determination of copper by an adsorption differential pulse stripping method with naphthol derivative, Analytical Letters, 33 (2000) 1591-1601.
3. T. Khayamian, A.A. Ensafi, M. Atabati, Extending the dynamic range of the determination of copper by adsorption differential pulse stripping method using a principal component artificial neural network, Microchemical Journal, 65 (2000) 347-351.
4. A.A. Ensafi, T. Khayamian, M. Atabati, Simultaneous voltammetric determination of molybdenum and copper by adsorption cathodic differential pulse stripping method using a principal component artificial neural network, Talanta, 57 (2002) 785-793.
5. T. Khayamian, A.A. Ensafi, M. Atabati, Simultaneous determination of Os(VIII) and Ru(IV) as catalysts through a single catalytic kinetic run using principal component artificial neural network, Analytical Letters, 35 (2002) 2039-2052.
6. A.A. Ensafi, T. Khayamian, M. Atabati, Differential pulse cathodic stripping adsorption voltammetric determination of trace amounts of lead using factorial design for optimization, Talanta, 59 (2003) 727-733.
7. A.A. Ensafi, T. Khayamian, M. Atabati, M.M. Ardakani, Determination of palladium by adsorption differential pulse stripping method and signal to noise ratio enhancement using the Fourier filtering technique, Canadian Journal of Analytical Sciences and spectroscopy, 49 (2004) 8-14.
8. K. Zarei, M. Atabati, L. Kazemi, Simultaneous determination of Fe(II) and Fe(III) in pharmaceutical formulations with chromogenic mixed reagent by using principal

component artificial neural network and multivariate calibration, *IL Farmaco*, 60 (2005) 37-42.

9. K. Zarei, M. Atabati, Prediction of GC retention indexes for insect-produced methyl-substituted alkanes using an artificial neural network and simple structural descriptors, *Journal of Analytical Chemistry*, 60 (2005) 732-737.

10. K. Zarei, M. Atabati, Z. Malekshabani, Simultaneous spectrophotometric determination of iron, nickel and cobalt in micellar media by using direct signal correction-partial least squares method, *Analytica Chimica Acta*, 556 (2006) 247-254.

11. K. Zarei, M. Atabati, H. Ilkhani, Catalytic adsorptive stripping voltammetry determination of ultra trace amount of molybdenum using factorial design for optimization, *Talanta*, 69 (2006) 816-821.

12. K. Zarei, M. Atabati, Principal component-wavelet neural network as a multivariate calibration method for simultaneous determination of iron, nickel, and cobalt, *Analytical Letters*, 39 (2006) 2085-2094.

13. K. Zarei, M. Atabati, M. Nekoei, Simultaneous spectrophotometric determination of phosphate and silicate by using principal component artificial neural network, *Annali di Chimica*, 97 (2007) 723-731.

14. K. Zarei, M. Atabati, N. Karimian, Simultaneous kinetic spectrophotometric determination of citric and ascorbic acid by H-point standard addition method, *Indian Journal of Chemical Technology*, 14 (2007) 417-422.

15. K. Zarei, M. Atabati, M. Ebrahimi, Quantitative structure-property relationship study of the solvent polarity using wavelet neural networks, *Analytical Sciences*, 23 (2007) 937-942.

16. K. Zarei, M. Atabati, M. Safaei, Simultaneous spectrophotometric determination of aluminum and iron in micellar media by using H-point standard addition method, *Journal of the Chinese Chemical Society*, 54 (2007) 1395-1400.

17. K. Zarei, M. Atabati, N. Karimian, Simultaneous dual wavelength spectrophotometric determination of citric and ascorbic acid using artificial neural network, *Journal of Analytical Chemistry*, 63 (2008) 145-150.

18. M. Atabati, K. Zarei, Prediction of GC retention indexes for insect-produced methyl-substituted alkanes using wavelet neural network, *Journal of the Chinese Chemical Society*, 55 (2008) 732-739.

19. K. Zarei, M. Atabati, QSAR study of anti-HIV activities against HIV-1 and some of their mutant strains for a group of HEPT derivatives, *Journal of the Chinese Chemical Society*, 56 (2009) 206-213.

20. K. Zarei, M. Atabati, M. Karami, Mean centering of ratio kinetic profiles for the simultaneous kinetic determination of binary mixtures in electroanalytical methods, *Analytica Chimica Acta*, 649 (2009) 62-67.

21. M. Atabati, K. Zarei, E. Abdinasab, Classification and regression tree analysis for molecular descriptor selection and binding affinities prediction of imidazobenzodiazepines in quantitative structure-activity relationship studies, *Bulletin of the Korean Chemical Society*, 30 (2009) 2717-2722.
22. K. Zarei, M. Atabati, E. Abdinasab, Spectrophotometric determination of conditional acidity constant of some sulfonephthalein dyes as a function of anionic, neutral and cationic surfactants concentrations using rank annihilation factor analysis, *Eurasian Journal of Analytical Chemistry*, 4 (2009) 314-327.
23. M. Atabati, K. Zarei, M. Mohsennia, Prediction of λ_{\max} of 1,4-naphthoquinone derivatives using ant colony optimization, *Analytica Chimica Acta*, 663 (2010) 7-10.
24. K. Zarei, M. Atabati, R. Shoari, Catalytic adsorptive stripping voltammetry determination of ultra trace amount of tungsten using factorial design for optimization, *Journal of Analytical Chemistry*, 65 (2010) 518-524.
25. K. Zarei, M. Atabati, M. Golmohammadi, Simultaneous kinetic spectrophotometric determination of V(IV) and V(V) by H-point standard addition method, *Asian Journal of Chemistry*, 22 (2010) 3479-3486.
26. M. Atabati, K. Zarei, A. Borhani, Predicting dilution activity coefficients of hydrocarbons in water using ant colony optimization, *Fluid Phase Equilibria*, 293 (2010) 219-224.
27. K. Zarei, M. Atabati, M. Karami, H-point standard addition method applied to simultaneous kinetic determination of antimony(III) and antimony(V) by adsorptive linear sweep voltammetry, *Journal of Hazardous Materials*, 179 (2010) 840-844.
28. K. Zarei, M. Atabati, M. Golmohammadi, Catalytic determination of ultra trace amounts of palladium by linear sweep voltammetry, *Journal of Analytical Chemistry*, 66 (2011) 646-650.
29. M. Atabati, R. Emamalizadeh, The hydrogen perturbation in molecular connectivity indices and their application to QSPR study, *Journal of Solution Chemistry*, 41 (2012) 1922-1936.
30. K. Kor, K. Zarei, M. Atabati, Shuffling multivariate adaptive regression splines for QSPR correlation of the melting point of pyridinium bromides, potential ionic liquids, *Revue Roumaine de Chimie*, 57 (2012) 615-622.
31. M. Atabati, Ant colony optimization as a powerful tool for descriptor selection in QSPR study of infinite dilution activity coefficients of halogenated hydrocarbons in water, *Chinese Journal of Structural Chemistry*, 31 (2012) 953-958.
32. M. Atabati, F. Khandani, Ant colony optimization as a descriptor selection in QSPR modeling for prediction of λ_{\max} of azo dyes, *Chinese Chemical Letters*, 23 (2012) 1209-1212.

33. K. Zarei, M. Atabati, S. Moghaddary, Predicting the heats of combustion of polynitro arene, polynitro heteroarene, acyclic nitramine, nitrate ester and nitroaliphatic compounds using bee algorithm and adaptive neuro-fuzzy inference system, *Chemometrics and Intelligent Laboratory Systems*, 128 (2013) 37-48.
34. K. Zarei, M. Atabati, Prediction of infinite dilution activity coefficients of halogenated hydrocarbons in water using classification and regression tree analysis and adaptive neuro-fuzzy inference systems, *Journal of Solution Chemistry*, 42 (2013) 516-525.
35. M. Atabati, R. Emamalizadeh, A quantitative structure property relationship for prediction of flash point of alkanes using molecular connectivity indices, *Chinese Journal of Chemical Engineering*, 21 (2013) 420-426.
36. K. Zarei, M. Atabati, E. Teymori, Multivariate adaptive regression splines for prediction of rate constants for radical degradation of aromatic pollutants in water, *Journal of Solution Chemistry*, 43 (2014) 445-452.
37. M. Atabati, S. Sharifi, 3D-QSAR study on VEGFR kinase inhibition of aminopyrazolopyridine urea derivatives by CoMFA and CoMSIA, *Medicinal Chemistry Research*, 23 (2014) 3539-3545.
38. K. Zarei, M. Atabati, K. Kor, Bee algorithm and adaptive neuro-fuzzy interference system as tools for QSAR study toxicity of substituted benzenes to *tetrahymena pyriformis*, *Bulletin of Environmental Contamination and Toxicology*, 92 (2014) 642-649.
39. M. Atabati, K. Zarei, A. Borhani, Ant colony optimization as a descriptor selection in QSPR modeling: estimation of the λ_{\max} of anthraquinones-based dyes, *Journal of Saudi Chemical Society*, 20 (2016) S547-S551.
40. K. Kor, A.P.F. Turner, K. Zarei, M. Atabati, V. Beni, W.C. Mak, Structurally responsive oligonucleotide-based single-probe lateral-flow test for detection of miRNA-21 mimics, *Analytical and Bioanalytical Chemistry*, 408 (2016) 1475-1485.
41. B. Bahadori, M. Atabati, K. Zarei, Better prediction of aqueous solubility of chlorinated hydrocarbons using support vector machine modeling, *Environmental Chemistry Letters*, 14 (2016) 541-548.
42. B. Bahadori, M. Atabati, Harmony Search as a Powerful Tool for Feature Selection in QSPR Study of the Drugs Lipophilicity, *Combinatorial Chemistry & High Throughput Screening*, 20 (2017) 321-327.

Conference Proceedings

1. H. Faghihian, A. Mostafavi, M. Atabati, Adsorption of different gases on a natural zeolite, 5th Iranian Seminar of Mineralogy and Crystallography, 4-6 September 1996, Isfahan University.

2. H. Faghihian, A. Mostafavi, M. Atabati, Investigation of molecular sieve property of natrolite for adsorption of gases, 2nd International & 12th National Congress of Chemistry & Chemical Engineering of Iran, 31 August -2 September 1997, Shahid Bahonar University of Kerman.
3. A.A. Ensafi, T. Khayamian, M. Atabati, Determination of copper by adsorption differential pulse voltammetric method using a principal component artificial neural network, 10th Iranian Seminar of Analytical Chemistry, 6-8 February 2001, Sharif University of Technology.
4. T. Khayamian, A.A. Ensafi, M. Atabati, Simultaneous voltammetric determination of molybdenum and copper by adsorption cathodic differential pulse stripping method using a principal component artificial neural network, 11th Iranian Seminar of Analytical Chemistry, 29-31 January 2002, Yazd University.
5. M. Atabati, K. Zarei, L. Kazemi, Simultaneous determination of Fe(II) and Fe(III) in pharmaceutical compounds with chromogenic mixed reagent by using principal component artificial neural network and multivariate calibration, 13th Iran's Seminar of Analytical Chemistry, 18-20 May 2004, Ferdowsi University of Mashhad.
6. M. Atabati, K. Zarei, Prediction of GC retention indices for methyl-substituted alkanes produced by insects using artificial neural network and simple structural descriptors, 13th Iran's Seminar of Analytical Chemistry, 18-20 May 2004, Ferdowsi University of Mashhad.
7. M. Atabati, K. Zarei, M. Nekoei, Simultaneous spectrophotometric determination of iron and cobalt in micellar medium by using a principal component artificial neural network and multivariate calibration, 13th Iran's Seminar of Analytical Chemistry, 18-20 May 2004, Ferdowsi University of Mashhad.
8. M. Atabati, K. Zarei, Use of artificial neural network in a QSAR study of anti-HIV activities for a group of HEPT derivatives, 6th Iranian Biophysical Chemistry Conference, 7-9 September 2004, Damghan University of Basic Sciences.
9. M. Atabati, K. Zarei, M. Ebrahimi, QSPR study of the solvent polarity using wavelet neural network, 14th Iran's Seminar of Analytical Chemistry, 29-31 August 2005, University of Birjand.
10. K. Zarei, M. Atabati, N. Karimian, Simultaneous spectrophotometric determination of citric acid and ascorbic acid using principal component artificial neural network, 14th Iran's Seminar of Analytical Chemistry, 29-31 August 2005, University of Birjand.
11. K. Zarei, M. Atabati, H. Ilkhani, Selective determination of ultra trace concentrations of molybdenum by catalytic adsorptive stripping voltammetry using factorial design for optimization, 6th Biennial Electrochemistry Seminar of Iran, 7-9 September 2005, Bu-Ali Sina University.

12. M. Atabati, K. Zarei, F. Shaeiri, Simultaneous spectrophotometric determination of ampicillin and amoxicillin by rank annihilation factor analysis, 1st Iranian Seminar of Chemometrics, 5-6 September 2006, Arak University.
13. M. Atabati, K. Zarei, Standard addition rank annihilation (SARA) as a new method for simultaneous determination, 12th Asian Chemical Congress, 23-25 August 2007, Malaysia.
14. M. Atabati, K. Zarei, S. Sobhdel, Prediction of pK_a values of benzimidazoles using genetic algorithm, 1st Conference and Workshop on Mathematical Chemistry, 29-31 January 2008, Tarbiat Modares University.
15. M. Atabati, K. Zarei, Ant colony optimization as a powerful tool for descriptor selection in QSPR study of infinite dilution activity coefficients of halogenated hydrocarbons, 17th International Conference on Computing, 3-5 December 2008, Mexico.
16. M. Atabati, K. zarei, R. Emamalizadeh, Prediction of flash point of alkanes using molecular connectivity indices, 2nd Conference and Workshop on Mathematical Chemistry, 14-16 April 2009, Kashan University.
17. K. Zarei, M. Atabati, F. Taheri, Simultaneous determination of vitamin B₂, B₆ and C by differential pulse voltammetry using ANFIS, 10th Asian Conference on Analytical Sciences, 11-13 August 2009, Malaysia.
18. M. Atabati, K. Zarei, M. Golmohammadi, Simultaneous kinetic spectrophotometric determination of V(IV) and V(V) by H-point standard addition method, 10th Asian Conference on Analytical Sciences, 11-13 August 2009, Malaysia.
19. K. Zarei, M. Atabati, M. Karami, H-point standard addition method applied to simultaneous kinetic determination of antimony(III) and antimony(V) by adsorptive linear sweep voltammetry, 2nd Iranian Biannual Seminar of Chemometrics, 28-30 October 2009, Urmia University.
20. M. Atabati, K. Zarei, R. Emamalizadeh, The hydrogen perturbation in molecular connectivity indices and their application to QSPR study, 2nd Iranian Biannual Seminar of Chemometrics, 28-30 October 2009, Urmia University.
21. M. Atabati, K. Zarei, S. Mokhtar, Prediction of aqueous solubility of halogenated hydrocarbons by using support vector machine, 17th Iranian Seminar of Analytical Chemistry, 12-14 September 2010, Kashan University.
22. K. Zarei, M. Atabati, M. Alinejad, R. Alizadeh, Simultaneous voltammetric determination of molybdenum and tungsten using ANFIS, 6th Annual Seminar of Electrochemistry of Iran, 9-11 October 2010, Kish International Convention Center.
23. K. Zarei, M. Atabati, L. Fatemi, β -cyclodextrin incorporated carbon nanotube-modified electrode as an electrochemical sensor for nicaidepine, 9th Biennial Electrochemistry Seminar of Iran, 22-24 January 2011, Yazd University.

24. K. Zarei, M. Atabati, L. Fatemi, Prediction of retention of pesticides in reversed-phase high-performance liquid chromatography using classification and regression tree analysis and adaptive neuro-fuzzy inference systems, 14th Iranian Physical Chemistry Conference, 25-28 February 2011, University of Tehran, Kish.
25. K. Zarei, M. Atabati, K. Kor, QSPR correlation of the melting point for pyridinium bromides ionic liquids using MARS, 15th Iranian Chemistry Congress, 4-6 September 2011, Bu-Ali Sina University.
26. K. Zarei, M. Atabati, Z. Eftekhari, Prediction of solubility of pesticides in water using multivariate adaptive spline (MARS) and adaptive neuro-fuzzy inference system (ANFIS), 15th Iranian Chemistry Congress, 4-6 September 2011, Bu-Ali Sina University.
27. K. Zarei, M. Atabati, Z. Salehabadi, Determination of rate constants for alkaline hydrolysis of dimethyl phthalate in different solvents using MCR-ALS, 15th Iranian Chemistry Congress, 4-6 September 2011, Bu-Ali Sina University.
28. M. Atabati, Z. Nikzad, Prediction of autoignition temperatures for mixtures of flammable liquids with air at elevated pressures using support vector machine, 5th Conference and Workshop on Mathematical Chemistry, 15-17 February 2012, Payam Noor University of Yazd.
29. M. Atabati, E. Rahimi, Genetic algorithm used for modeling of antimicrobial activity of benzylidene hydrazides, 5th Conference and Workshop on Mathematical Chemistry, 15-17 February 2012, Payam Noor University of Yazd.
30. M. Atabati, S. Sharifi, QSAR study of *in vivo* anti-platelet aggregation activities of 4,5,6,7-tetrahydrothieno[3,2-c] pyridine derivatives by genetic algorithm, 5th Conference and Workshop on Mathematical Chemistry, 15-17 February 2012, Payam Noor University of Yazd.
31. M. Atabati, E. Rahimi, QSAR study of *in vitro* antibacterial activity of benzylidene hydrazides, 1st Conference on Computational Science, 6-7 September 2012, Damghan University.
32. M. Atabati, Z. Nikzad, Using group contribution method for prediction of cetane number of alcohol compounds, 1st Conference on Computational Science, 6-7 September 2012, Damghan University.
33. M. Atabati, S. Sharifi, CoMSIA analysis on aminopyrazolopyridine urea derivatives as VEGF receptor inhibitors, 1st Conference on Computational Science, 6-7 September 2012, Damghan University.
34. S.A. Nabavi, M. Atabati, M. Shekari, A theoretical study on corrosion inhibition of carbon steel in petroleum/water mixtures by N-containing compounds, 1st Conference on Computational Science, 6-7 September 2012, Damghan University.
35. M. Atabati, S. Mansory, - Quantitative structure-activity relationship of polysubstituted quinoline derivatives as inhibitors of phosphodiesterase 4, 19th Iranian

Seminar of Analytical Chemistry, 26-28 February 2013, Ferdowsi University of Mashhad.

36. M. Atabati, Z. Nemati, - QSAR study of toxicity of ionic liquids in acetylcholinesterase enzyme - 19th Iranian Seminar of Analytical Chemistry, 26-28 February 2013, Ferdowsi University of Mashhad.

37. M. Atabati, M. Namjomanesh, - Prediction of direct chemiluminescence behavior of organic compounds using support vector machine - 19th Iranian Seminar of Analytical Chemistry, 26-28 February 2013, Ferdowsi University of Mashhad.

38. M. Atabati, B. Bahadori, Quantitative structure-property relationship studies for predicting the lipophilicity of neutral, acidic, basic and amphoteric drugs using support vector machine, 4th Iranian Biennial Chemometrics Seminar, 27-28 November 2013, Shiraz University.

39. M. Atabati, B. Bahadori, Quantitative structure-property relationship (QSPR) prediction of salvation Gibbs energy of bifunctional compounds by support vector machine (SVM), 20th Iranian Analytical Chemistry Conference, 25-27 February 2014, Isfahan University of Technology.

40. M. Atabati, K. Zarei, J. Akhondi, QSAR study of tubulin inhibitors using adaptive neuro-fuzzy inference system (ANFIS), 20th Iranian Analytical Chemistry Conference, 25-27 February 2014, Isfahan University of Technology.

41. M. Atabati, K. Zarei, A. Mahdian, Multivariate adaptive regression splines (MARS) for QSAR study on 5-(2-methylbenzimidazol-1-yl)-N-alkylthiophene-2-carboxamide derivatives as *P. falciparum* dihydroorotate dehydrogenase (PfDHODH) inhibitors, 20th Iranian Analytical Chemistry Conference, 25-27 February 2014, Isfahan University of Technology.

42. M. Atabati, J. Akhondi, 3D-QSAR studies of 2-isopropyl-5-methylcyclohexanol derivatives as antimicrobial by CoMFA and CoMSIA, The 5th Iranian Conference on Bioinformatics, 20-22 May 2014, Tehran University.

43. M. Atabati, B. Bahadori, Modeling of anticancer effects of aryloxazole derivatives using support vector machine, The 5th Iranian Conference on Bioinformatics, 20-22 May 2014, Tehran University.

44. M. Atabati, K. Zarei, H. Kouhestani, QSAR study of 2-benzoxazolyl hydrazone derivatives for anticancer activity using adaptive neuro-fuzzy inference system (ANFIS), The 5th Iranian Conference on Bioinformatics, 20-22 May 2014, Tehran University.

45. M. Atabati, H. Kouhestani, 3D-QSAR study on some benzodiazepine derivatives as anti-alzheimer agents by CoMFA and CoMSIA, 17th Iranian Physical Chemistry Conference, 21-23 October 2014, K. N. Toosi University of Technology.

46. M. Atabati, M. Akbari, QSAR study of antibacterial inhibitors of gram-positive thymidylate kinase using docking descriptors, 17th Iranian Physical Chemistry Conference, 21-23 October 2014, K. N. Toosi University of Technology.
47. K. Kor, K. Zarei, M. Atabati, A novel electrochemical sensor for furosemide based on electropolymerized molecularly poly(o-phenylenediamine), Sweden-Japan Seminar on Nanomaterials and Nanotechnology, 10-11 March 2015, Linköping University, Sweden.
48. K. Kor, A.P.F. Turner, K. Zarei, M. Atabati, V. Beni, W.C. Mak, Combining structure responsive probes and lateral-flow test; a simple and rapid approach miRNA-21 detection, 2nd International Congress on Biosensors, 10-12 June 2015, Gediz University, Izmir, Turkey.
49. M. Atabati, F. Bandari, QSAR studies of anti Alzheimer's compounds using random forest algorithm, 18th Iranian Chemistry Congress, 30 August – 1 September 2015, Semnan University.
50. M. Atabati, M. Teimuori, Tabu search as a descriptor selection in QSAR study of 1,5-diheteroaryl-penta-1,4-dien-3-ones: a class of promising curcumin-based anti-cancer agents, 5th Iranian Biennial Chemometrics Seminar, 25-26 November 2015, University of Tehran.
51. M. Atabati, L. Akhoundi, Bee algorithm as a descriptor selection in QSAR study of β -site amyloid precursor protein cleaving enzyme1 (BACE1) inhibitors, 5th Iranian Biennial Chemometrics Seminar, 25-26 November 2015, University of Tehran.
52. M. Atabati, V. Alizadehfard, QSAR study of pyrazole sulfonamide derivatives, a potent inhibitor of trypanosome brucei N-myristoyltransferase (TbNMT) using bee algorithm, 5th Iranian Biennial Chemometrics Seminar, 25-26 November 2015, University of Tehran.
53. K. Zarei, M. Atabati, M. Ahmadi, QSPR study for retention factor of pesticides in biopartitioning micellar chromatography using bee algorithm, 22nd Iranian Seminar of Analytical Chemistry, 26-28 January 2016, Chemistry & Chemical Engineering Research Center of Iran.
54. M. Atabati, F. Mousavi, QSPR study of activity coefficients at infinite dilution for organic solutes in the ionic liquid 4-(3-hydroxypropyl)-4-methylmorpholinium bis(trifluoromethylsulfonyl)-amide using support vector machine, 13th Chemistry Conference, Payame Noor University, 11-12 May 2016. Hamadan.
55. M. Atabati, Z. Abbasghaei, Classification of 1,4-dihydropyridines as TGF β /Smad inhibitors using genetic algorithm and support vector machine, The 23rd Iranian Seminar of Analytical Chemistry, 30 August – 1 September 2016, Shrarif University of Technology.
56. B. Bahadori, M. Atabati, Giorgetti, Molecular docking descriptors in structure-based QSAR on G protein-coupled receptor three receptor (GPR3) agonists, The 23rd

Iranian Seminar of Analytical Chemistry, 30 August – 1 September 2016, Shrarif University of Technology.

57. K. Zarei, M. Atabati, M. Ahmadi, Prediction of skin sensitization using method classification and regression tree, 2nd National Conference on Computational Science, 28,29 August 2016, Damghan University.

58. M. Atabati, F. Mousavi, Quantitative structure-property relationship studies for predicting flash points of organic compounds using support vector machine, 2nd National Conference on Computational Science, 28,29 August 2016, Damghan University.

59. M. Atabati, Z. Abbasghaei, QSAR study of 1,4 dihydropyridines compounds as inhibitors of tuberculosis using support vector machine classifier, 2nd National Conference on Computational Science, 28,29 August 2016, Damghan University.

پایان نامه های تحصیلات تکمیلی

- ۱- مطالعه QSAR بازدارنده های استیل کولین استراز با استفاده از توصیف کننده های داکینگ مولکولی
- ۲- بکارگیری روش های آنالیز تصویر چند متغیره و رگرسیون اسپلاین وفقی چند متغیره در مطالعات QSAR بازدارنده های گلوکوتایون-S ترنسفرز PI-1 و پلاسمودیوم فالسیپاروم دی هیدروروتیت دهیدروژناز
- ۳- پیشگویی نفتوکینونها با استفاده از الگوریتم مورچه و حلالیت داروهای استاتین با استفاده از شبکه عصبی مصنوعی
- ۴- کاربرد الگوریتم مورچه جهت انتخاب توصیف کننده ها در مطالعات QSPR مربوط به ماکزیمم طول موج مشتقات آنتراکینون و ضریب فعالیت هیدروکربن ها در رقت بی نهایت
- ۵- مطالعات QSPR نقطه اشتعال برای مخلوط های همگن دوتائی ترکیبات آلی با استفاده از روش تاگوچی
- ۶- پیش تغلیظ کافئین با استفاده از اعمال پتانسیل و اندازه گیری به وسیله طیف سنجی تحرک یونی
- ۷- مدل سازی دمای خوداشتعالی ترکیبات آلی و فعالیت مهارکننده های سیکلواکسیژناز با استفاده از شبکه عصبی مصنوعی
- ۸- استفاده از ماشین بردار پشتیبان و روش سهم گروه برای پیشگویی دمای خوداشتعالی و عدد ستان ترکیبات آلی
- ۹- مطالعات 3D-QSAR بر روی مشتقات کوئینولین به عنوان بازدارنده فسفودی استراز ۴
- ۱۰- مطالعات QSPR ضریب فعالیت در رقت بی نهایت ترکیبات آلی در مایع یونی ۴- (۳- هیدروکسی پروپیل)-۴-متیل مرفولینیوم بیس (تری فلوئورومتیل سولفونیل)-آمید و نقطه اشتعال ترکیبات آلی با استفاده از ماشین بردار پشتیبان
- ۱۱- پیشگویی فعالیت پیرازو کوئینولینون ها با استفاده از شبکه عصبی موجک و کاربرد روش RAFA در اندازه گیری همزمان آمپی سیلین و آموکسی سیلین
- ۱۲- مطالعات QSAR مشتقات کوئینولیزیدین با استفاده از الگوریتم جنگل تصادفی

- ۱۳- پیش‌گویی رفتار لومینسانس شیمیایی برخی از ترکیبات آلی
- ۱۴- مطالعات QSAR جهت دسته‌بندی فعالیت مهارکنندگی مشتقات ۱و۴- دی‌هیدروپیریدین با استفاده از ماشین بردار پشتیبان
- ۱۵- مطالعه QSAR بازدارنده‌های ضد باکتریایی تیمیدیلالات کیناز با استفاده از توصیف‌کننده‌های داکینگ مولکولی
- ۱۶- بررسی اثر رزولوشن در بلورنگاری پروتئین‌ها بر روی ناحیه غیر مجاز نمودار رامانچاندرا
- ۱۷- به‌کارگیری پارامتر اختلال هیدروژن در محاسبه اندیس‌های اتصال مولکولی و کاربرد آنها در مطالعات QSPR مربوط به شکست مولی و حجم مولی آلکان‌ها، آلکن‌ها و الکل‌ها و همچنین نقطه اشتعال آلکان‌ها
- ۱۸- پیشگویی ثابت تفکیک اسیدی بنزیمیدازولها با استفاده از الگوریتم ژنتیک و حلالیت آلکیل استات‌ها با استفاده از شبکه عصبی مصنوعی
- ۱۹- اندازه‌گیری همزمان اسید سیتریک و اسید آسکوربیک به روش اسپکتروفتومتری با استفاده از شبکه عصبی مصنوعی و روش افزایش استاندارد نقطه H
- ۲۰- اندازه‌گیری تنگستن به روش ولتامتری عاری سازی جذبی و پیشگویی ثابت اسیدیته سولفونامیدها با استفاده از شبکه عصبی موجک
- ۲۱- مدل‌سازی طول موج ماکزیم جذب رنگهای آزو توسط الگوریتم مورچه و فعالیت دارویی مشتقات کاپسازین با استفاده از ماشین بردار پشتیبان
- ۲۲- پیشگویی قطبیت حلال، فعالیت دارویی (ضد‌ایدز) مشتقات TIBO و ثابت اسیدیته مشتقات فنل با استفاده از روش‌های کموتریکس
- ۲۳- مطالعات QSPR بر روی دمای بحرانی ترکیبات آلی و دمای بحرانی پایین محلول در محلول‌های پلیمری با استفاده از سیستم استنتاج فازی-عصبی تطبیقی (ANFIS)
- ۲۴- مطالعات QSAR و 3D-QSAR بر روی مشتقات ۴و۵و۶و۷- تتراهیدروتینو [۳و۲- C]-پیریدین و آمینوپیرازولوپیریدین اوره
- ۲۵- پیشگویی فعالیت ضد میکروبی بنزیدین هیدرازیدها با استفاده از الگوریتم‌های جستجوی ممنوعه و ژنتیک
- ۲۶- مدل‌سازی سمیت مابعات یونی با استفاده از الگوریتم کرم شب‌تاب
- ۲۷- مطالعات 3D-QSAR مشتقات ۲-ایزوپروپیل-۵-متیل سیکلوهگزانونولو ۴-ان-آریل- [۱،۴]دiazپان اتیل اوره آز
- ۲۸- مطالعات QSPR ضریب فعالیت در رقت بی‌نهایت ترکیبات آلی در مایع یونی ۴- (۳-هیدروکسی پروپیل)-۴-متیل مرفولینیوم بیس (تری فلوئورومتیل سولفونیل)-آمید با استفاده از ماشین بردار پشتیبان
- ۲۹- انتخاب توصیف‌کننده‌ها با استفاده از الگوریتم جستجوی ممنوع در مطالعات QSAR ترکیبات ضد سرطانی مشتقات ۱و۵-دی‌هترو آریل پنتا-۱و۴-دی‌ان-۳-آن
- ۳۰- پیشگویی حلالیت هیدروکربن‌های هالوژن‌دار و ثابت قانون هنری ترکیبات آلی در آب با استفاده از ماشین بردار پشتیبان

۳۱- مطالعات QSP(A)R بازدارنده های TMK و GPR3 ، حلالیت ترکیبات آلی و چربی دوستی دارو ها توسط روش های شبیه سازی دینامیک مولکولی، مدل سازی همسانی، ماشین بردار پشتیبان و الگوریتم جستجوی هارمونی

۳۲- انتخاب توصیف کننده ها با استفاده از الگوریتم جستجوی ممنوع در مطالعات QSAR ترکیبات ضد سرطانی مشتقات ۱و۵-دی هترو آریل پنتا-۱و۴-دی ان-۳-آن و حذف همبستگی بین متغیرهای مشتقات ۳-(۴-آریل-۱ج-۱و۲و۳-تریازول-۱-ایل)-بی فیل با استفاده از عمودسازی گرم-اشمیت

۳۳- مطالعات QSPR نقطه اشتعال برای مخلوطهای همگن دوتائی ترکیبات آلی با استفاده از روش تا کوچی