

Jahan Bakhsh Ghasemi

List of Publications by Citations

Source: <https://exaly.com/author-pdf/2576949/jahan-bakhsh-ghasemi-publications-by-citations.pdf>
Version: 2024-04-10

This document has been generated based on the publications and citations recorded by exaly.com. For the latest version of this publication list, visit the link given above.
The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

321 papers	4,812 citations	35 h-index	47 g-index
342 ext. papers	5,622 ext. citations	3.6 avg, IF	6.27 L-index

#	Paper	IF	Citations
321	Comparative study of BoxBehnken, central composite, and Doehlert matrix for multivariate optimization of Pb (II) adsorption onto Robinia tree leaves. <i>Journal of Chemometrics</i> , 2013 , 27, 12-20	1.6	118
320	Genetic-algorithm-based wavelength selection in multicomponent spectrophotometric determination by PLS: application on copper and zinc mixture. <i>Talanta</i> , 2003 , 59, 311-7	6.2	96
319	Simultaneous spectrophotometric determination of trace amounts of uranium, thorium, and zirconium using the partial least squares method after their preconcentration by alpha-benzoin oxime modified Amberlite XAD-2000 resin. <i>Talanta</i> , 2010 , 80, 1191-7	6.2	80
318	Extraction optimization of pepsin-soluble collagen from eggshell membrane by response surface methodology (RSM). <i>Food Chemistry</i> , 2016 , 190, 186-193	8.5	78
317	Simultaneous determination of copper, nickel, cobalt and zinc using zincon as a metallochromic indicator with partial least squares. <i>Analytica Chimica Acta</i> , 2003 , 487, 181-188	6.6	64
316	Pesticides Removal Using Conventional and Low-Cost Adsorbents: A Review. <i>Clean - Soil, Air, Water</i> , 2011 , 39, 1105-1119	1.6	63
315	Computer Aided Drug Design for Multi-Target Drug Design: SAR /QSAR, Molecular Docking and Pharmacophore Methods. <i>Current Drug Targets</i> , 2017 , 18, 556-575	3	58
314	Vitamin D3 receptor is expressed in the endometrium of cycling mice throughout the estrous cycle. <i>Fertility and Sterility</i> , 2010 , 93, 2738-43	4.8	56
313	QSPR study for estimation of acidity constants of some aromatic acids derivatives using multiple linear regression (MLR) analysis. <i>Computational and Theoretical Chemistry</i> , 2007 , 805, 27-32		55
312	Spectrophotometric determination of acidity constants of 4-(2-pyridylazo)resorcinol in binary methanol-water mixtures. <i>Analytica Chimica Acta</i> , 2002 , 455, 335-342	6.6	55
311	Simultaneous determination of cobalt and nickel. Comparison of prediction ability of PCR and PLS using original, first and second derivative spectra. <i>Microchemical Journal</i> , 2001 , 68, 1-11	4.8	54
310	Methods and applications of structure based pharmacophores in drug discovery. <i>Current Topics in Medicinal Chemistry</i> , 2013 , 13, 1036-47	3	53
309	A new polymerizable fluorescent PET chemosensor of fluoride (F-) based on naphthalimide-thiourea dye. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012 , 90, 85-92	4.4	52
308	3D-QSAR analysis of human immunodeficiency virus entry-1 inhibitors by CoMFA and CoMSIA. <i>European Journal of Medicinal Chemistry</i> , 2010 , 45, 4897-903	6.8	52
307	Quantitative structure-property relationship study of n-octanol-water partition coefficients of some of diverse drugs using multiple linear regression. <i>Analytica Chimica Acta</i> , 2007 , 604, 99-106	6.6	52
306	Spectrophotometric simultaneous determination of nitroaniline isomers by orthogonal signal correction-partial least squares. <i>Talanta</i> , 2005 , 65, 1168-73	6.2	49
305	Spectrophotometric and thermodynamic study on the dimerization equilibrium of ionic dyes in water by chemometrics method. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2006 , 65, 73-8	4.4	49

304	Thrombophilic mutations in Iranian patients with infertility and recurrent spontaneous abortion. <i>Annals of Hematology</i> , 2006 , 85, 268-71	3	47
303	Multivariate statistical analysis methods in QSAR. <i>RSC Advances</i> , 2015 , 5, 104635-104665	3.7	46
302	Two- and three-way chemometrics methods applied for spectrophotometric determination of lorazepam in pharmaceutical formulations and biological fluids. <i>Analytica Chimica Acta</i> , 2005 , 533, 169-177	6.6	46
301	Experimental, computational and chemometrics studies of BSA-vitamin B6 interaction by UV-Vis, FT-IR, fluorescence spectroscopy, molecular dynamics simulation and hard-soft modeling methods. <i>Bioorganic Chemistry</i> , 2016 , 68, 124-36	5.1	46
300	Efficient removal of malachite green from wastewater by using boron-doped mesoporous carbon nitride. <i>Applied Surface Science</i> , 2019 , 469, 236-245	6.7	45
299	Synthesis, experimental, quantum chemical and molecular dynamics study of carbon steel corrosion inhibition effect of two Schiff bases in HCl solution. <i>Journal of Molecular Liquids</i> , 2019 , 285, 626-639	6	44
298	Chemometric analysis of comprehensive two dimensional gas chromatography-mass spectrometry metabolomics data. <i>Journal of Chromatography A</i> , 2017 , 1488, 113-125	4.5	42
297	Simultaneous voltammetric determination of morphine and noscapine by adsorptive differential pulse stripping method and least-squares support vector machines. <i>Talanta</i> , 2007 , 74, 247-54	6.2	41
296	Thermodynamic study of the dimerization equilibrium of methylene blue, methylene green and thiazole orange at various surfactant concentrations and different ionic strengths and in mixed solvents by spectral titration and chemometric analysis. <i>Dyes and Pigments</i> , 2012 , 92, 1031-1041	4.6	40
295	Spectrophotometric Determination of Acidity Constants of Some Recently Synthesized Anthraquinones in Methanol + Water. <i>Journal of Chemical & Engineering Data</i> , 1997 , 42, 1212-1215	2.8	39
294	Thermodynamics study of the adsorption process of methylene blue on activated carbon at different ionic strengths. <i>Journal of Chemical Thermodynamics</i> , 2007 , 39, 967-971	2.9	39
293	Maintaining the stability of nonlinear differential equations by the enhancement of HPM. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2008 , 372, 2855-2861	2.3	39
292	Spectrophotometric simultaneous determination of cobalt, copper and nickel using nitroso-R-salt in alloys by partial least squares. <i>Analytica Chimica Acta</i> , 2004 , 510, 121-126	6.6	39
291	3D-QSAR studies on the toxicity of substituted benzenes to <i>Tetrahymena pyriformis</i> : CoMFA, CoMSIA and VolSurf approaches. <i>Ecotoxicology and Environmental Safety</i> , 2014 , 105, 128-34	7	38
290	Preparation of hierarchical g-C ₃ N ₄ @TiO ₂ hollow spheres for enhanced visible-light induced catalytic CO ₂ reduction. <i>Solar Energy</i> , 2020 , 205, 465-473	6.8	36
289	Prediction of gas chromatography/electron capture detector retention times of chlorinated pesticides, herbicides, and organohalides by multivariate chemometrics methods. <i>Analytica Chimica Acta</i> , 2007 , 588, 200-6	6.6	36
288	Thermodynamics study of the dimerization equilibria of rhodamine B and 6G in different ionic strengths by photometric titration and chemometrics method. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2005 , 62, 649-56	4.4	36
287	QSAR models for CXCR2 receptor antagonists based on the genetic algorithm for data preprocessing prior to application of the PLS linear regression method and design of the new compounds using in silico virtual screening. <i>Molecules</i> , 2011 , 16, 1928-55	4.8	35

- 286 Determination of Acidity Constants of 4-(2-Pyridylazo)resorcinol in Binary Acetonitrile + Water Mixtures. *Journal of Chemical & Engineering Data*, **2003**, 48, 1178-1182 2.8 35
- 285 Spectrophotometric determination of acidity constants of some anthraquinones and anthrones in methanol-water mixtures. *Talanta*, **1993**, 40, 697-9 6.2 35
- 284 In Silico Studies in Drug Research Against Neurodegenerative Diseases. *Current Neuropharmacology*, **2018**, 16, 664-725 7.6 34
- 283 Preparation, optimization and characterization of novel ion exchange membranes by blending of chemically modified PVDF and SPPO. *Separation and Purification Technology*, **2012**, 90, 10-21 8.3 31
- 282 QSRR prediction of the chromatographic retention behavior of painkiller drugs. *Journal of Chromatographic Science*, **2009**, 47, 156-63 1.4 31
- 281 Densities and Viscosities for Binary and Ternary Mixtures of 1, 4-Dioxane + 1-Hexanol + N,N-Dimethylaniline from T = (283.15 to 343.15) K. *Journal of Chemical & Engineering Data*, **2008**, 53, 343-349 2.8 31
- 280 Simultaneous spectrophotometric determination of nitroaniline isomers after cloud point extraction by using least-squares support vector machines. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2007**, 68, 523-30 4.4 30
- 279 Spectrophotometric determination of acidity constants of alizarine red S in water, water-Brij-35 and water-SDS micellar media solutions. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2006**, 64, 660-4 4.4 30
- 278 SPECTROPHOTOMETRIC STUDY OF THE THERMODYNAMICS OF INTERACTION OF SOME METAL IONS WITH MUREXIDE IN BINARY ACETONITRILE-DIMETHYLSULFOXIDE MIXTURES. *Journal of Coordination Chemistry*, **1995**, 36, 183-194 1.6 30
- 277 Investigation and determination of acrylamide in the main group of cereal products using advanced microextraction method coupled with gas chromatography-mass spectrometry. *Journal of Cereal Science*, **2019**, 87, 157-164 3.8 29
- 276 DeepCDA: deep cross-domain compound-protein affinity prediction through LSTM and convolutional neural networks. *Bioinformatics*, **2020**, 36, 4633-4642 7.2 29
- 275 Combined docking, molecular dynamics simulations and spectroscopic studies for the rational design of a dipeptide ligand for affinity chromatography separation of human serum albumin. *Journal of Molecular Modeling*, **2014**, 20, 2446 2 29
- 274 Study of Complex Formation between 4-(2-Pyridylazo) Resorcinol and Al³⁺, Fe³⁺, Zn²⁺, and Cd²⁺ Ions in an Aqueous Solution at 0.1 M Ionic Strength. *Journal of Chemical & Engineering Data*, **2007**, 52, 1171-1178 2.8 29
- 273 QSPR prediction of aqueous solubility of drug-like organic compounds. *Chemical and Pharmaceutical Bulletin*, **2007**, 55, 669-74 1.9 29
- 272 PARAFAC Decomposition of Three-Way Kinetic-Spectrophotometric Spectral Matrices Based on Phosphomolybdenum Blue Complex Chemistry for Nitrite Determination in Water and Meat Samples. *Analytical Letters*, **2005**, 38, 2377-2392 2.2 29
- 271 Thermodynamic characterization of the dimerization equilibrium of an asymmetric dye by spectral titration and chemometric analysis. *Talanta*, **2004**, 62, 835-41 6.2 27
- 270 Photocatalytic degradation of different pollutants by the novel gCN-NS/Black-TiO₂ heterojunction photocatalyst under visible light: Introducing a photodegradation model and optimization by response surface methodology (RSM). *Materials Chemistry and Physics*, **2021**, 258, 123912 4.4 27
- 269 Dynamic structure based pharmacophore modeling of the Acetylcholinesterase reveals several potential inhibitors. *Journal of Biomolecular Structure and Dynamics*, **2019**, 37, 1800-1812 3.6 26

268	Combination of genetic algorithm and partial least squares for cloud point prediction of nonionic surfactants from molecular structures. <i>Annali Di Chimica</i> , 2007 , 97, 69-83		25
267	Kinetic spectrophotometric determination of sulfide using whole kinetic curve and a fixed time method. <i>Microchemical Journal</i> , 2002 , 71, 1-8	4.8	25
266	SIMULTANEOUS CATALYTIC DETERMINATION OF COBALT, NICKEL, AND COPPER USING RESAZURINE SULFIDE REACTION AND PARTIAL LEAST SQUARES CALIBRATION METHOD. <i>Analytical Letters</i> , 2001 , 34, 1389-1399	2.2	25
265	In situ preparation of g-CN nanosheet/FeOCl: Achievement and promoted photocatalytic nitrogen fixation activity. <i>Journal of Colloid and Interface Science</i> , 2021 , 587, 538-549	9.3	25
264	Novel p ⁿ Heterojunction Nanocomposite: TiO ₂ QDs/ZnBi ₂ O ₄ Photocatalyst with Considerably Enhanced Photocatalytic Activity under Visible-Light Irradiation. <i>Journal of Physical Chemistry C</i> , 2020 , 124, 27519-27528	3.8	24
263	QSPR modeling of stability constants of diverse 15-crown-5 ethers complexes using best multiple linear regression. <i>Journal of Inclusion Phenomena and Macrocyclic Chemistry</i> , 2008 , 60, 339-351		24
262	Interaction of some water-soluble metalloporphyrins with human serum albumin. <i>Journal of Molecular Structure</i> , 2004 , 705, 41-47	3.4	24
261	Simultaneous multicomponent spectrophotometric monitoring of methyl and propyl parabens using multivariate statistical methods after their preconcentration by robust ionic liquid-based dispersive liquid-liquid microextraction. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014 , 123, 307-313	4.4	23
260	Simultaneous spectrophotometric determination of trace amount of polycyclic aromatic hydrocarbons in water samples after magnetic solid-phase extraction by using projection pursuit regression. <i>Environmental Monitoring and Assessment</i> , 2013 , 185, 2297-305	3.1	23
259	Application of random forest regression to spectral multivariate calibration. <i>Analytical Methods</i> , 2013 , 5, 1863	3.2	23
258	Spectroscopic characterization of thiazole orange-3 DNA interaction. <i>Applied Biochemistry and Biotechnology</i> , 2008 , 149, 9-22	3.2	23
257	Simultaneous kinetic spectrophotometric determination of periodate and iodate based on their reaction with pyrogallol red in acidic media by chemometrics methods. <i>Analytica Chimica Acta</i> , 2004 , 508, 119-126	6.6	23
256	N-Heterocyclic (4-Phenylpiperazin-1-yl)methanones Derived from Phenoxazine and Phenothiazine as Highly Potent Inhibitors of Tubulin Polymerization. <i>Journal of Medicinal Chemistry</i> , 2017 , 60, 749-766	8.3	22
255	Large-Area Semiconducting Graphene Nanomesh Tailored by Interferometric Lithography. <i>Scientific Reports</i> , 2015 , 5, 11463	4.9	22
254	Application of principal component analysis-multivariate adaptive regression splines for the simultaneous spectrofluorimetric determination of dialkyltins in micellar media. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013 , 115, 357-63	4.4	22
253	Simultaneous spectrophotometric determination of uranium and zirconium using cloud point extraction and multivariate methods. <i>Journal of the Iranian Chemical Society</i> , 2012 , 9, 257-262	2	22
252	Association Equilibrium of Methylene Blue by Spectral Titration and Chemometrics Analysis: A Thermodynamic Study. <i>Journal of the Chinese Chemical Society</i> , 2009 , 56, 459-468	1.5	22
251	KINETIC SIMULTANEOUS DETERMINATION OF Fe(II) AND Fe(III) USING PARTIAL LEAST SQUARES (PLS) AND PRINCIPAL COMPONENT REGRESSION (PCR) CALIBRATION METHODS. <i>Analytical Letters</i> , 2002 , 35, 533-544	2.2	22

- 250 Chlamydia trachomatis prevalence in Iranian women attending obstetrics and gynaecology clinics. *Pakistan Journal of Biological Sciences*, **2007**, 10, 4490-4 0.8 22
- 249 Acrylamide content of collected food products from Tehran's market: a risk assessment study. *Environmental Science and Pollution Research*, **2020**, 27, 30558-30570 5.1 21
- 248 Densities and Viscosities of (1-Propanol + 1,2-Dichloroethane), (1-Propanol + Benzaldehyde), (Benzaldehyde + 1,2-Dichloroethane), and (1-Propanol + 1,2-Dichloroethane + Benzaldehyde) Mixtures from T = 288.15 K to 313.15 K. *Journal of Chemical & Engineering Data*, **2009**, 54, 3284-3290 2.8 21
- 247 Spectrophotometric determination of trace amounts of fluoride using an Al-xylene orange complex as a colored reagent. *Analytical Sciences*, **2009**, 25, 1249-53 1.7 21
- 246 Synthesis, characterization, and photocatalytic performance of Ag/AgFeO₂ decorated on g-C₃N₄-nanosheet under the visible light irradiation. *Journal of the Taiwan Institute of Chemical Engineers*, **2020**, 115, 279-292 5.3 20
- 245 The Influence of Growing Region on Fatty Acids and Sterol Composition of Iranian Olive Oils by Unsupervised Clustering Methods. *JAOCs, Journal of the American Oil Chemists Society*, **2012**, 89, 371-378¹⁸ 20
- 244 Review of the quantitative structure-activity relationship modelling methods on estimation of formation constants of macrocyclic compounds with different guest molecules. *Supramolecular Chemistry*, **2011**, 23, 614-629 1.8 20
- 243 Kinetic spectrophotometric method for simultaneous determination of selenium and tellurium using partial least squares calibration. *Analytica Chimica Acta*, **2004**, 512, 369-373 6.6 20
- 242 Anti-cancer, anti-oxidant and molecular docking studies of thiosemicarbazone indole-based derivatives. *Research on Chemical Intermediates*, **2019**, 45, 2827-2854 2.8 19
- 241 Molecular docking and 3D-QSAR studies of falcipain inhibitors using CoMFA, CoMSIA, and Open3DQSAR. *Medicinal Chemistry Research*, **2012**, 21, 2788-2806 2.2 19
- 240 Evaluation of Authenticity of Iranian Olive Oil by Fatty Acid and Triacylglycerol Profiles. *JAOCs, Journal of the American Oil Chemists Society*, **2009**, 86, 827-833 1.8 19
- 239 A new algorithm for the determination of protolytic constants from spectrophotometric data in multiwavelength mode: Calculations of acidity constants of 4-(2-pyridylazo)resorcinol (PAR) in mixed nonaqueous-water solvents. *Talanta*, **2006**, 68, 1201-14 6.2 19
- 238 Solid phase headspace microextraction of tricyclic antidepressants using a directly prepared nanocomposite consisting of graphene, CTAB and polyaniline. *Mikrochimica Acta*, **2015**, 182, 633-641 5.8 18
- 237 Ultrasound-assisted ionic liquid-based microextraction combined with least squares support vector machines regression for the simultaneous determination of aluminum, gallium, and indium in water and coal samples. *Environmental Monitoring and Assessment*, **2012**, 184, 3971-81 3.1 18
- 236 Alignment Independent 3D-QSAR Modeling of Fullerene (C₆₀) Solubility in Different Organic Solvents. *Fullerenes Nanotubes and Carbon Nanostructures*, **2013**, 21, 367-380 1.8 18
- 235 Simultaneous determination of dopamine and ascorbic acid by linear sweep voltammetry along with chemometrics using a glassy carbon electrode. *Mikrochimica Acta*, **2007**, 157, 139-147 5.8 18
- 234 Spectrophotometric study of the effects of surfactants and ethanol on the acidity constants of fluorescein. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2008**, 71, 1158-65 4.4 18
- 233 Kinetic Spectrophotometric Determination of Nitrite Based on Its Catalytic Effect on the Oxidation of Methyl Red by Bromate. *Analytical Letters*, **2004**, 37, 2205-2214 2.2 18

232	Differential Kinetic Spectrophotometric Determinations of Ascorbic Acid and L-Cysteine by Partial Least Squares Method. <i>Analytical Letters</i> , 2004 , 37, 725-737	2.2	18
231	Simultaneous Spectrophotometric Determination of Benzyl Alcohol and Diclofenac in Pharmaceutical Formulations by Chemometrics Method. <i>Journal of the Chinese Chemical Society</i> , 2005 , 52, 1049-1054	1.5	18
230	Lithium-7 and sodium-23 nmr studies of complexation of Li ⁺ and Na ⁺ ions with 1,10-phenanthroline, 2,2'-bipyridine and 8-hydroxyquinoline in some non-aqueous solutions. <i>Polyhedron</i> , 1996 , 15, 3647-3652	2.7	18
229	SPECTROPHOTOMETRIC STUDY OF THE THERMODYNAMICS OF ALKALINE EARTH CRYPTATES IN DIMETHYLSULFOXIDE. <i>Journal of Coordination Chemistry</i> , 1994 , 31, 265-272	1.6	18
228	An ultrasensitive fluorescence sensor for determination of trace levels of copper in blood samples. <i>Analytical and Bioanalytical Chemistry</i> , 2019 , 411, 5593-5603	4.4	17
227	4D-LQTA-QSAR and docking study on potent Gram-negative specific LpxC inhibitors: a comparison to CoMFA modeling. <i>Molecular Diversity</i> , 2012 , 16, 203-13	3.1	17
226	Spectrophotometric Determination of Acidity Constants of Alizarine Red S in Mixed Aqueous/Organic Solvents. <i>Journal of Chemical & Engineering Data</i> , 2006 , 51, 1530-1535	2.8	17
225	SIMULTANEOUS SPECTROPHOTOMETRIC DETERMINATION OF FOLIC ACID, THIAMIN, RIBOFLAVIN, AND PYRIDOXAL USING PARTIAL LEAST-SQUARES REGRESSION METHOD. <i>Spectroscopy Letters</i> , 2002 , 35, 153-169	1.1	17
224	Computer-aided drug design to explore cyclodextrin therapeutics and biomedical applications. <i>Chemical Biology and Drug Design</i> , 2017 , 89, 257-268	2.9	16
223	Simultaneous spectrophotometric determination of crystal violet and malachite green in water samples using partial least squares regression and central composite design after preconcentration by dispersive solid-phase extraction. <i>Environmental Monitoring and Assessment</i> , 2017 , 189, 196	3.1	16
222	A quantitative structure- property relationship of gas chromatographic/mass spectrometric retention data of 85 volatile organic compounds as air pollutant materials by multivariate methods. <i>Chemistry Central Journal</i> , 2012 , 6 Suppl 2, S4		16
221	Graphene oxide-Elizarin yellow R-magnetic chitosan nanocomposite: a selective and efficient sorbent for sub-trace determination of aluminum in water samples. <i>Analytical Methods</i> , 2017 , 9, 222-231 ^{3.2}		16
220	Docking and 3D-QSAR study of stability constants of benzene derivatives as environmental pollutants with β -cyclodextrin. <i>Journal of Inclusion Phenomena and Macrocyclic Chemistry</i> , 2012 , 73, 405-413		16
219	A quantitative structure property relationship for prediction of solubilization of hazardous compounds using GA-based MLR in CTAB micellar media. <i>Journal of Hazardous Materials</i> , 2009 , 161, 74-80 ^{12.8}		16
218	Simultaneous spectrophotometric determination of minoxidil and tretinoin by the H-point standard addition method and partial least squares. <i>Chemical Papers</i> , 2009 , 63,	1.9	16
217	Improvement of the Prediction Power of the CoMFA and CoMSIA Models on Histamine H3 Antagonists by Different Variable Selection Methods. <i>Scientia Pharmaceutica</i> , 2012 , 80, 547-66	4.3	16
216	Multiwavelength Spectrophotometric Determination of Acidity Constants of Morin in Methanol-Water Mixtures. <i>Collection of Czechoslovak Chemical Communications</i> , 2006 , 71, 1-14		16
215	Conductance study of some transition and heavy metal complexes with 1,10-diaza-18-crown-6 in binary acetonitrile-dimethylsulfoxide mixtures. <i>Journal of Solution Chemistry</i> , 1996 , 25, 485-504	1.8	16

- 214 Dual-acting of Hybrid Compounds - A New Dawn in the Discovery of Multi-target Drugs: Lead Generation Approaches. *Current Topics in Medicinal Chemistry*, **2017**, 17, 1096-1114 3 16
- 213 Spectrophotometric Determination of Acidity Constants of Group B Vitamins in Different Ionic Strengths at 25 \pm 0.1 $^{\circ}$ C. *Journal of the Korean Chemical Society*, **2005**, 49, 269-277 16
- 212 Simultaneous determination of dihydroxybenzene isomers at nitrogen-doped graphene surface using fast Fourier transform square wave voltammetry and multivariate calibration. *Microchemical Journal*, **2019**, 145, 596-605 4.8 16
- 211 A detailed structural study of cytotoxicity effect of ionic liquids on the leukemia rat cell line IPC-81 by three dimensional quantitative structure toxicity relationship. *Ecotoxicology and Environmental Safety*, **2018**, 158, 256-265 7 16
- 210 Experimental and theoretical investigation effect of flavonols antioxidants on DNA damage. *Analytica Chimica Acta*, **2015**, 887, 82-91 6.6 15
- 209 Pharmacophore Identification, Molecular Docking, Virtual Screening, and In Silico ADME Studies of Non-Nucleoside Reverse Transcriptase Inhibitors. *Molecular Informatics*, **2012**, 31, 856-66 3.8 15
- 208 New FRET primers for quantitative real-time PCR. *Analytical and Bioanalytical Chemistry*, **2007**, 387, 2737-2743 4.3 15
- 207 Determination of Trace Amounts of Lorazepam by Adsorptive Cathodic Differential Pulse Stripping Method in Pharmaceutical Formulations and Biological Fluids. *Analytical Letters*, **2006**, 39, 1159-1169 2.2 15
- 206 Simultaneous Spectrophotometric Multicomponent Determination of Folic Acid, Thiamine, Riboflavin, and Pyridoxal by Using Double Divisor Ratio Spectra Derivative Zero Crossing Method. *Analytical Letters*, **2004**, 37, 2609-2623 2.2 15
- 205 g-C₃N₄ nanosheet adorned with Ag₃BiO₃ as a perovskite: An effective photocatalyst for efficient visible-light photocatalytic processes. *Materials Science in Semiconductor Processing*, **2021**, 125, 105651 4.3 15
- 204 A highly selective magnetic solid-phase extraction method for preconcentration of Cd(II) using N,N'-bis(salicylidene)ethylenediamine in water and food samples. *Research on Chemical Intermediates*, **2019**, 45, 3141-3153 2.8 14
- 203 Boron-doped graphitic carbon nitride as a novel fluorescent probe for mercury(II) and iron(III): a circuit logic gate mimic. *New Journal of Chemistry*, **2019**, 43, 12087-12093 3.6 14
- 202 An Alignment Independent 3D-QSAR Modeling of Dispersibility of Single-walled Carbon Nanotubes in Different Organic Solvents. *Fullerenes Nanotubes and Carbon Nanostructures*, **2014**, 22, 605-617 1.8 14
- 201 Toward a continuous wavelet transform-based search method for feature selection for classification of spectroscopic data. *Chemometrics and Intelligent Laboratory Systems*, **2013**, 127, 185-194 3.8 14
- 200 Kinetic spectrophotometric determination of trace amounts of palladium by whole kinetic curve and a fixed time method using resazurine sulfide reaction. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2008**, 71, 841-6 4.4 14
- 199 Determination of Riboflavin in Human Plasma by Excitation-Emission Matrix Fluorescence and Multi-Way Analysis. *Journal of the Chinese Chemical Society*, **2006**, 53, 503-510 1.5 14
- 198 Quantitative Characterization of the Interaction Space of the Mammalian Carbonic Anhydrase Isoforms I, II, VII, IX, XII, and XIV and their Inhibitors, Using the Proteochemometric Approach. *Chemical Biology and Drug Design*, **2016**, 88, 341-53 2.9 14
- 197 High-impressive separation of photoinduced charge carriers on step-scheme ZnO/ZnSnO₃/Carbon dots heterojunction with efficient activity in photocatalytic NH₃ production. *Journal of the Taiwan Institute of Chemical Engineers*, **2021**, 118, 140-151 5.3 14

196	Deep Transferable Compound Representation across Domains and Tasks for Low Data Drug Discovery. <i>Journal of Chemical Information and Modeling</i> , 2019 , 59, 4528-4539	6.1	13
195	Docking and pharmacophore-based alignment comparative molecular field analysis three-dimensional quantitative structure-Activity relationship analysis of dihydrofolate reductase inhibitors by linear and nonlinear calibration methods. <i>Journal of Chemometrics</i> , 2013 , 27, 287-296	1.6	13
194	2D Quantitative structure-property relationship study of mycotoxins by multiple linear regression and support vector machine. <i>International Journal of Molecular Sciences</i> , 2010 , 11, 3052-68	6.3	13
193	Simultaneous spectrophotometric determination of trace amounts of cobalt, nickel, and copper using the partial least-squares method after the preconcentration of their 2-aminocyclopentene-1-dithiocarboxylate complexes on microcrystalline naphthalene. <i>Journal of Analytical Chemistry</i> , 2008 , 63, 232-238	1.1	13
192	Development of a model to predict partition coefficient of organic pollutants in cloud point extraction process. <i>Annali Di Chimica</i> , 2006 , 96, 327-37		13
191	The thermodynamic studies of the molecular interactions of dimethyltin(IV) dichloride with free base meso-tetraarylporphyrins. <i>Polyhedron</i> , 2002 , 21, 683-687	2.7	13
190	A kinetic study of complex formation between calcium ion and cryptand C221 in dimethylsulphoxide solution. <i>Polyhedron</i> , 1996 , 15, 923-927	2.7	13
189	QSPR Modeling of Stability Constants of the Li-Hemispherands Complexes Using MLR: A Theoretical Host-Guest Study. <i>Macrocyclic Chemistry</i> , 2010 , 3, 234-242	2.2	13
188	Voltammetric sensing of oxacillin by using a screen-printed electrode modified with molecularly imprinted polyaniline, gold nanourchins and graphene oxide. <i>Mikrochimica Acta</i> , 2019 , 186, 798	5.8	13
187	Design and synthesis of novel pyrazole-phenyl semicarbazone derivatives as potential β -glucosidase inhibitor: Kinetics and molecular dynamics simulation study. <i>International Journal of Biological Macromolecules</i> , 2021 , 166, 1082-1095	7.9	13
186	Z-scheme g-C ₃ N ₄ nanosheet/MgBi ₂ O ₆ systems with the visible light response for impressive photocatalytic organic contaminants degradation. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2021 , 406, 113023	4.7	13
185	Synthesis of magnetically modified mesoporous nanoparticles and their application in simultaneous determination of Pb(II), Cd(II) and Cu(II). <i>Research on Chemical Intermediates</i> , 2018 , 44, 1689-1709	2.8	13
184	QSPR probing of Na ⁺ complexation with 15-crown-5 ethers derivatives using artificial neural network and multiple linear regression. <i>Journal of Inclusion Phenomena and Macrocyclic Chemistry</i> , 2012 , 72, 423-435		12
183	Multiwavelength spectrophotometric determination of protolytic constants of 4-(2-pyridylazo) resorcinol (PAR) in binary DMF-water mixtures. <i>Talanta</i> , 2005 , 66, 653-8	6.2	12
182	The thermodynamic studies of the molecular interactions of methyltin(IV) tribromide with free base meso-tetraarylporphyrins. <i>Polyhedron</i> , 2002 , 21, 1255-1260	2.7	12
181	Combating Diseases with Computational Strategies Used for Drug Design and Discovery. <i>Current Topics in Medicinal Chemistry</i> , 2018 , 18, 2743-2773	3	12
180	Application of the area correlation constraint in the MCR-ALS quantitative analysis of complex mixture samples. <i>Analytica Chimica Acta</i> , 2020 , 1113, 52-65	6.6	12
179	3D QSAR studies, pharmacophore modeling, and virtual screening of diarylpyrazole-benzenesulfonamide derivatives as a template to obtain new inhibitors, using human carbonic anhydrase II as a model protein. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2017 , 32, 688-700	5.6	11

- 178 Computer-aided scaffold hopping to identify a novel series of casein kinase 1 delta (CK1d) inhibitors for amyotrophic lateral sclerosis. *European Journal of Pharmaceutical Sciences*, **2015**, 78, 151-62^{5.1} 11
- 177 Deposited CuBi₂O₄ and Bi₃ClO₄ nanoparticles on g-C₃N₄ nanosheet: a promising visible light-induced photocatalyst toward the removal of tetracycline hydrochloride and rhodamine B. *Journal of Materials Science*, **2020**, 55, 7775-7791 4.3 11
- 176 Multivariate optimization, preconcentration and determination of mercury ions with (1-(p-acetyl phenyl)-3-(o-methyl benzoate)) triazene in aqueous samples using ICP-AES. *Analytical Methods*, **2016**, 8, 1111-1119 3.2 11
- 175 3D-QSAR, CoMFA, and CoMSIA of new phenyloxazolidinones derivatives as potent HIV-1 protease inhibitors. *Structural Chemistry*, **2013**, 24, 433-444 1.8 11
- 174 3D-QSAR, docking and molecular dynamics for factor Xa inhibitors as anticoagulant agents. *Molecular Simulation*, **2013**, 39, 453-471 2 11
- 173 A quantitative structure-retention relationship study for prediction of chromatographic relative retention time of chlorinated monoterpenes. *Environmental Chemistry Letters*, **2011**, 9, 87-96 13.3 11
- 172 Prediction of Solubility of Nonionic Solutes in Anionic Micelle (SDS) Using a QSPR Model. *QSAR and Combinatorial Science*, **2008**, 27, 338-346 11
- 171 Fluorimetric Study of Complexation of Alkali and Alkaline Earth Cations with 1,10-Phenanthroline, 2,2'-Bipyridine and 8-Hydroxyquinoline in Nonaqueous Solvents. *Journal of Coordination Chemistry*, **1992**, 26, 337-344 1.6 11
- 170 Application of Multivariate Linear and Nonlinear Calibration and Classification Methods in Drug Design. *Combinatorial Chemistry and High Throughput Screening*, **2015**, 18, 795-808 1.3 11
- 169 Synthesis and characterization of novel ZnO/NiCr₂O₄ nanocomposite for water purification by degradation of tetracycline and phenol under visible light irradiation. *Materials Research Bulletin*, **2021**, 139, 111247 5.1 11
- 168 Dispersive solid phase extraction of lead in water samples using embedded 1,5-diphenylcarbazone grafted graphene oxide in microporous magnetic chitosan coupled with flame atomic absorption spectrometry. *Journal of the Iranian Chemical Society*, **2019**, 16, 1411-1421 2 11
- 167 3D-QSAR and virtual screening studies in identification of new Rho kinase inhibitors with different scaffolds. *Journal of the Iranian Chemical Society*, **2015**, 12, 1945-1959 2 10
- 166 Synthesis and cholinesterase inhibitory activity of new 2-benzofuran carboxamide-benzylpyridinium salts. *Bioorganic Chemistry*, **2018**, 80, 180-188 5.1 10
- 165 Quasi 4D-QSAR and 3D-QSAR study of the pan class I phosphoinositide-3-kinase (PI3K) inhibitors. *Medicinal Chemistry Research*, **2013**, 22, 1587-1596 2.2 10
- 164 Optimization of Influential Factors on the Photocatalytic Performance of TiO₂/Graphene Composite in Degradation of an Organic Dye by RSM Methodology. *Journal of Cluster Science*, **2017**, 28, 2979-2995 3 10
- 163 Proteochemometric Modeling of the Interaction Space of Carbonic Anhydrase and its Inhibitors: An Assessment of Structure-based and Sequence-based Descriptors. *Molecular Informatics*, **2017**, 36, 1600102^{3.8} 10
- 162 The same and not the same: heterogeneous functional activation of prostate tumor cells by TLR ligation. *Cancer Cell International*, **2014**, 14, 54 6.4 10
- 161 beta-Correction as a preprocessing method for partial least squares in simultaneous determination of zinc and lead. *Talanta*, **2004**, 63, 751-6 6.2 10

160	Simultaneous Spectrophotometric Determination of Group B Vitamins Using Parallel Factor Analysis: PARAFAC. <i>Journal of the Chinese Chemical Society</i> , 2005 , 52, 1123-1129	1.5	10
159	The Thermodynamic Studies of the Molecular Interactions of Diethyl- and Dibutyltin(IV) Dichloride with Free Basemeso-Tetraarylporphyrins. <i>Bulletin of the Chemical Society of Japan</i> , 2002 , 75, 1137-1141	5.1	10
158	Discovery of new potential antimalarial compounds using virtual screening of ZINC database. <i>Combinatorial Chemistry and High Throughput Screening</i> , 2015 , 18, 227-34	1.3	10
157	Docking of Natural Products against Neurodegenerative Diseases: General Concepts. <i>Combinatorial Chemistry and High Throughput Screening</i> , 2018 , 21, 152-160	1.3	10
156	3D-QSAR Studies of 2-Arylbenzoxazoles as Novel Cholesteryl Ester Transfer Protein Inhibitors. <i>Bulletin of the Korean Chemical Society</i> , 2011 , 32, 645-650	1.2	10
155	g-C ₃ N ₄ -nanosheet/ZnCr ₂ O ₄ S-scheme heterojunction photocatalyst with enhanced visible-light photocatalytic activity for degradation of phenol and tetracycline. <i>Separation and Purification Technology</i> , 2021 , 118511	8.3	10
154	Application of bilinear least squares/residual bilinearization in bulk liquid membrane system for simultaneous multicomponent quantification of two synthetic dyes. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2015 , 144, 48-55	3.8	9
153	A rapid, automated gradient flow injection-spectrophotometric technique for study of metal complexation reactions. <i>Talanta</i> , 2014 , 128, 511-7	6.2	9
152	3D-QSAR and docking studies of the stability constants of different guest molecules with beta-cyclodextrin. <i>Journal of Inclusion Phenomena and Macrocyclic Chemistry</i> , 2014 , 79, 401-413	1.7	9
151	Application of Chemometrics Methods for the Simultaneous Determination of Zinc and Copper after Preconcentration and Separation by Liquid-Liquid Microextraction Based on Solidification of Floating Organic Drop Coupled to Flow Injection Spectrophotometry. <i>Current Analytical Chemistry</i> , 2012 , 8, 373-381	1.7	9
150	SPECTROPHOTOMETRIC INVESTIGATION OF THE ACIDITY CONSTANTS OF FLUORESCIEIN IN VARIOUS WATER-ORGANIC SOLVENT MEDIA. <i>Chemical Engineering Communications</i> , 2008 , 195, 1257-1268	2.2	9
149	Simultaneous kinetic-spectrophotometric determination of sulfide and sulfite by partial least squares and genetic algorithm variable selection. <i>Journal of Analytical Chemistry</i> , 2007 , 62, 348-354	1.1	9
148	Simultaneous square wave voltammetric determination of 2-mercaptobenzothiazole and 2-mercaptobenzoxazole by partial least squares method in water samples. <i>Journal of Hazardous Materials</i> , 2008 , 151, 636-41	12.8	9
147	Conductometric simultaneous determination of acetic acid, monochloroacetic acid and trichloroacetic acid using orthogonal signal correction-partial least squares. <i>Journal of Hazardous Materials</i> , 2006 , 131, 13-8	12.8	9
146	Docking, CoMFA and CoMSIA Studies of a Series of N-Benzoylated Phenoxazines and Phenothiazines Derivatives as Antiproliferative Agents. <i>Bulletin of the Korean Chemical Society</i> , 2013 , 34, 899-906	1.2	9
145	Novel visible-light-responsive Black-TiO ₂ /CoTiO ₃ Z-scheme heterojunction photocatalyst with efficient photocatalytic performance for the degradation of different organic dyes and tetracycline. <i>Journal of the Taiwan Institute of Chemical Engineers</i> , 2021 , 121, 168-183	5.3	9
144	Voltammetric Electronic Tongue for the Simultaneous Determination of Three Benzodiazepines. <i>Sensors</i> , 2019 , 19,	3.8	9
143	Design and synthesis of novel quinazolinone-pyrazole derivatives as potential β -glucosidase inhibitors: Structure-activity relationship, molecular modeling and kinetic study. <i>Bioorganic Chemistry</i> , 2021 , 114, 105127	5.1	9

142	Alignment independent 3D-QSAR, quantum calculations and molecular docking of Mer specific tyrosine kinase inhibitors as anticancer drugs. <i>Saudi Pharmaceutical Journal</i> , 2016 , 24, 197-212	4.4	8
141	Highly selective silica-based fluorescent nanosensor for ferric ion (Fe) detection in aqueous media. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019 , 218, 293-298	4.4	8
140	Application of multivariate optimization procedures for preconcentration and determination of Au(III) and Pt(IV) in aqueous samples with graphene oxide by X-ray fluorescence spectrometry. <i>Environmental Monitoring and Assessment</i> , 2015 , 187, 149	3.1	8
139	Molecular docking, 2D and 3D-QSAR studies of new indole-based derivatives as HCV-NS5B polymerase inhibitors. <i>Journal of the Iranian Chemical Society</i> , 2015 , 12, 1789-1799	2	8
138	Investigation and determination of acrylamide in 24 types of roasted nuts and seeds using microextraction method coupled with gas chromatography-mass spectrometry: central composite design. <i>Journal of Food Measurement and Characterization</i> , 2020 , 14, 1249-1260	2.8	8
137	Simultaneous sensitive determination of benzenediol isomers using multiwall carbon nanotube-ionic liquid modified carbon paste electrode by a combination of artificial neural network and fast Fourier transform admittance voltammetry. <i>New Journal of Chemistry</i> , 2018 , 42, 6479-6487	3.6	8
136	Using Wavelet Analysis To Assist in Identification of Significant Events in Molecular Dynamics Simulations. <i>Journal of Chemical Information and Modeling</i> , 2016 , 56, 1282-91	6.1	8
135	Docking, CoMFA and CoMSIA studies of a series of sulfonamides derivatives as carbonic anhydrase I inhibitors. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2013 , 28, 320-7	5.6	8
134	Chemometric Modeling to Predict Aquatic Toxicity of Benzene Derivatives Using Stepwise-Multi Linear Regression and Partial Least Square. <i>Asian Journal of Chemistry</i> , 2013 , 25, 331-342	0.4	8
133	A quantitative structure-property relationships study of the stability constant of crown ethers by molecular modelling: new descriptors for lariat effect. <i>Journal of Inclusion Phenomena and Macrocyclic Chemistry</i> , 2011 , 70, 37-47		8
132	An alignment independent 3D-QSAR study for predicting the stability constants of structurally diverse compounds with β -cyclodextrin. <i>Journal of Inclusion Phenomena and Macrocyclic Chemistry</i> , 2011 , 71, 195-206		8
131	Simultaneous Kinetic Spectrophotometric Determination of Ascorbic Acid and L-Cysteine by H-Point Standard Addition Method. <i>Mikrochimica Acta</i> , 2004 , 148, 259-265	5.8	8
130	Acenaphtoquinoxaline as a selective fluorescent sensor for Hg (II) detection: experimental and theoretical studies. <i>Heliyon</i> , 2020 , 6, e04986	3.6	8
129	Novel fused 1,2,3-triazolo-benzodiazepine derivatives as potent anticonvulsant agents: design, synthesis, in vivo, and in silico evaluations. <i>Molecular Diversity</i> , 2020 , 24, 179-189	3.1	8
128	Molecular dynamics simulation and 3D-pharmacophore analysis of new quinoline-based analogues with dual potential against EGFR and VEGFR-2. <i>International Journal of Biological Macromolecules</i> , 2020 , 142, 94-113	7.9	8
127	Design and Synthesis of Novel Cytotoxic Indole-Thiosemicarbazone Derivatives: Biological Evaluation and Docking Study. <i>Chemistry and Biodiversity</i> , 2019 , 16, e1800470	2.5	7
126	Synthesis, characterization and magnetic investigations of Fe ₃ O ₄ nanoparticles and zeolite-Y nanocomposites prepared by precipitation method. <i>Journal of Materials Science: Materials in Electronics</i> , 2015 , 26, 5677-5685	2.1	7
125	Mixed 2DBD-LQTA-QSAR study of a series of Plasmodium falciparum dUTPase inhibitors. <i>Medicinal Chemistry Research</i> , 2015 , 24, 1098-1111	2.2	7

124	Developing a highly selective method for preconcentration and determination of cobalt in water and nut samples using 1-(2-pyridylazo)-2-naphthol and UV-visible spectroscopy. <i>Journal of the Science of Food and Agriculture</i> , 2020 , 100, 2272-2279	4.3	7
123	Simultaneous determination of binary solution of triphenylmethane dyes in complex matrices onto magnetic amino-rich SWCNT using second-order calibration method. <i>Environmental Monitoring and Assessment</i> , 2017 , 189, 594	3.1	7
122	Pharmacophore elucidation and 3D-QSAR analysis of a new class of highly potent inhibitors of acid ceramidase based on maximum common substructure and field fit alignment methods. <i>Journal of the Iranian Chemical Society</i> , 2014 , 11, 1329-1336	2	7
121	Docking alignment-3D-QSAR of a new class of potent and non-chiral indole-3-carboxamide-based renin inhibitors. <i>Collection of Czechoslovak Chemical Communications</i> , 2011 , 76, 1447-1469		7
120	Quantitative structure–activity relationship study of nonpeptide antagonists of CXCR2 using stepwise multiple linear regression analysis. <i>Monatshefte für Chemie</i> , 2010 , 141, 111-118	1.4	7
119	Study on economic aspects of goat grubs in Iran. <i>Tropical Animal Health and Production</i> , 1997 , 29, 243-4	1.7	7
118	A potentiometric study of protonation and complex formation of xylenol orange with alkaline earth and aluminum ions. <i>Talanta</i> , 1998 , 46, 875-84	6.2	7
117	Simultaneous spectrophotometric determination of benzyl alcohol and diclofenac in pharmaceuticals using methods based on the first derivative of the optical density ratio. <i>Pharmaceutical Chemistry Journal</i> , 2005 , 39, 671-675	0.9	7
116	SPECTROPHOTOMETRIC STUDY OF COMPLEX FORMATION BETWEEN SOME ALKALI AND ALKALINE EARTH CATIONS AND SEVERAL CONVENTIONAL (N,N), (N,O) AND (O,O) LIGANDS IN 95% ETHANOL. <i>Journal of Coordination Chemistry</i> , 1993 , 28, 231-236	1.6	7
115	Spectrophotometric-chemometrics study of the effect of solvent composition and temperature on the spectral shape and shift of copper and nickel phthalocyanines in different aqueous-nonaqueous mixed solvents. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020 , 227, 117621	4.4	7
114	Facile and green preparation of colorimetric and fluorescent sensors for mercury, silver, and carbonate ions visual detecting: Spectroscopy and theoretical studies. <i>Journal of Molecular Structure</i> , 2021 , 1241, 130626	3.4	7
113	Fluorescence turn off-on probe (β -cyclodextrin-hydroxyquinoline) for monitoring of Cd ions and tetracycline. <i>Methods and Applications in Fluorescence</i> , 2020 , 8, 025009	3.1	6
112	Using chemometric methods for overlap correction of sodium–zinc spectral lines generated by wavelength dispersive X-ray fluorescence in mineral samples. <i>X-Ray Spectrometry</i> , 2014 , 43, 131-137	0.9	6
111	Identification of novel inhibitors of HIV-1 integrase using pharmacophore-based virtual screening combined with molecular docking strategies. <i>Medicinal Chemistry Research</i> , 2013 , 22, 5545-5556	2.2	6
110	Multivariate curve resolution alternating least squares in the quantitative determination of sulfur using overlapped S(K β)/Mo(L β) emission peaks by wavelength dispersive X-ray fluorescence spectrometry. <i>X-Ray Spectrometry</i> , 2015 , 44, 75-80	0.9	6
109	Surfactant-mediated complex formation for determination of traces amounts of zinc, cadmium, and lead with 4-(2-thiazolylazo) resorcinol and chemometric methods. <i>Environmental Monitoring and Assessment</i> , 2011 , 183, 57-63	3.1	6
108	Multi-wavelength spectrophotometric determination of the protolytic constants of tetracycline hydrochloride in some nonaqueous-water mixed solvents: a solvatochromism study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011 , 78, 277-86	4.4	6
107	Kinetic spectrophotometric determination of thiocyanate based on its inhibitory effect on the oxidation of methyl red by bromate. <i>Analytical Sciences</i> , 2001 , 17, 435-7	1.7	6

106	Pharmacophore Modeling, Synthesis, Scaffold Hopping and Biological Hematin Inhibition Interaction Studies for Anti-malaria Compounds. <i>Current Topics in Medicinal Chemistry</i> , 2019 , 19, 2743-2765	2.5	6
105	A dual-emission fluorescence probe for simultaneous quantification of CN ⁻ and CrO ₄ ²⁻ ions based on modified g-C ₃ N ₄ . <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2020 , 389, 112261	4.7	6
104	Chemometrics-spectroscopic study of the effect of temperature and pre-micellar to post-micellar forms of various surfactants on the dimerization of nickel and copper phthalocyanines. <i>Journal of Molecular Liquids</i> , 2020 , 300, 112350	6	6
103	Multi-view self-attention for interpretable drug-target interaction prediction. <i>Journal of Biomedical Informatics</i> , 2020 , 110, 103547	10.2	6
102	SBA-Pr-Imine-Furan as an environmental adsorbent of Pd(II) in aqueous solutions. <i>Environmental Challenges</i> , 2021 , 3, 100032	2.6	6
101	Anthracene modified graphene oxide-silica as an optical sensor for selective detection of Cu ²⁺ and Pb ²⁺ ions. <i>International Journal of Environmental Analytical Chemistry</i> , 2020 , 100, 686-701	1.8	6
100	Characterization of the interaction of glycyrrhizin and glycyrrhetinic acid with bovine serum albumin by spectrophotometric-gradient flow injection titration technique and molecular modeling simulations. <i>International Journal of Biological Macromolecules</i> , 2017 , 102, 92-103	7.9	5
99	A highly selective Ag ⁺ sensor based on 8-hydroxyquinoline functionalized graphene oxide -silica nanosheet and its logic gate behaviour. <i>Journal of Materials Science: Materials in Electronics</i> , 2019 , 30, 17693-17705	2.1	5
98	SBA-Pr-SO ₃ H-catalyzed synthesis of bispyrazole compounds as anti-bacterial agents and inhibitors of phosphorylated RET tyrosine kinase. <i>Journal of the Iranian Chemical Society</i> , 2019 , 16, 1401-1409	2	5
97	Synthesis, antibacterial activity, and CoMFA study of new 1,2,3-triazolyl 7-carboxamidodesacetoxy cephalosporanic acid derivatives. <i>Medicinal Chemistry Research</i> , 2014 , 23, 4531-4541	2.2	5
96	3D-QSAR and Docking Studies of a Series of Carboline Derivatives as Antitumor Agents of PLK1. <i>Journal of Chemistry</i> , 2014 , 2014, 1-10	2.3	5
95	New buffers to improve the quantitative real-time polymerase chain reaction. <i>Bioscience, Biotechnology and Biochemistry</i> , 2007 , 71, 1970-8	2.1	5
94	A QSPR study on the GC retention times of a series of fatty, dicarboxylic and amino acids by MLR and ANN. <i>Annali Di Chimica</i> , 2007 , 97, 925-33		5
93	New unsymmetrical cyanine dyes for real-time thermal cycling. <i>Analytical and Bioanalytical Chemistry</i> , 2007 , 389, 983-8	4.4	5
92	Simultaneous kinetic-spectrophotometric determination of sulfide and sulfite and genetic algorithm variable selection using partial least squares calibration. <i>Journal of Analytical Chemistry</i> , 2006 , 61, 92-98	1.1	5
91	Application and comparison of two-rate and differential kinetic methods in simultaneous spectrophotometric determination of ascorbic acid and L-cysteine in pharmaceutical samples. <i>Pharmaceutical Chemistry Journal</i> , 2006 , 40, 44-51	0.9	5
90	Kinetic Spectrophotometric Determination of Sulfite Using a Full Curve (PLS) and a Fixed Time Method. <i>Analytical Letters</i> , 2003 , 36, 2243-2254	2.2	5
89	A new application of PC-ANN in spectrophotometric determination of acidity constants of PAR. <i>Journal of the Brazilian Chemical Society</i> , 2005 , 16, 1118	1.5	5

88	Comparison of three sensory characterization methods based on consumer perception for the development of a novel functional cereal-based dessert. <i>AIMS Agriculture and Food</i> , 2017 , 2, 258-278	1.2	5
87	A highly sensitive fluorescence measurement of amphetamine using 8-hydroxyquinoline- β -cyclodextrin grafted on graphene oxide. <i>Diamond and Related Materials</i> , 2020 , 109, 108032	3.5	5
86	Simultaneous removal of crystal violet and methyl green in water samples by functionalised SBA-15. <i>International Journal of Environmental Analytical Chemistry</i> , 2020 , 1-17	1.8	5
85	Thermodynamic study of β -cyclodextrin-dye inclusion complexes using gradient flow injection technique and molecular modeling. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2016 , 165, 54-60	4.4	5
84	exploration of novel protease inhibitors against coronavirus 2019 (COVID-19). <i>Informatics in Medicine Unlocked</i> , 2021 , 23, 100516	5.3	5
83	Direct monitoring of diclofenac using a supramolecular fluorescent approach based on β -cyclodextrin nanosponge. <i>Journal of Molecular Liquids</i> , 2021 , 336, 116104	6	5
82	Receptor modeling of environmental aerosol data using MLPCA-MCR-ALS. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2017 , 167, 50-62	3.8	4
81	Formulation and Development of a New Prebiotic Cereal-based Dairy Dessert: Rheological, Sensory and Physical Attributes. <i>Food Science and Technology Research</i> , 2017 , 23, 637-649	0.8	4
80	Second-order data obtained by beta-cyclodextrin complexes: a novel approach for multicomponent analysis with three-way multivariate calibration methods. <i>Talanta</i> , 2014 , 128, 254-62	6.2	4
79	APPLICATION OF MULTIVARIATE IMAGE ANALYSIS IN QSPR STUDY OF pKa OF VARIOUS ACIDS BY PRINCIPAL COMPONENTS-LEAST SQUARES SUPPORT VECTOR MACHINE. <i>Journal of the Chilean Chemical Society</i> , 2015 , 60, 2985-2987	2.5	4
78	Quantitative Structure Activity Relationship Modeling of Environmentally Important Diphenyl Ether Herbicides Using MLR and PLS. <i>Current Analytical Chemistry</i> , 2010 , 6, 3-10	1.7	4
77	Spectrophotometric determination of acidity constants of 4-(2-thiazolylazo)-resorcinol (TAR) in water-organic mixtures. <i>Chinese Chemical Letters</i> , 2010 , 21, 725-729	8.1	4
76	Spectrophotometric studies on the protonation and nickel complexation equilibria of 4-(2-pyridylazo) resorcinol using global analysis in aqueous solution. <i>Journal of the Brazilian Chemical Society</i> , 2007 , 18,	1.5	4
75	A New Variable Selection Method Based on Mutual Information Maximization by Replacing Collinear Variables for Nonlinear Quantitative Structure-Property Relationship Models. <i>Bulletin of the Korean Chemical Society</i> , 2012 , 33, 1527-1535	1.2	4
74	QSPR approaches to elucidate the stability constants between β -cyclodextrin and some organic compounds: Docking based 3D conformer. <i>Journal of Molecular Liquids</i> , 2016 , 219, 1036-1043	6	4
73	Probing the origin of dihydrofolate reductase inhibition via proteochemometric modeling. <i>Journal of Chemometrics</i> , 2019 , 33, e3090	1.6	4
72	Computer-aided molecular design of (E)-N-Aryl-2-ethene-sulfonamide analogues as microtubule targeted agents in prostate cancer. <i>Arabian Journal of Chemistry</i> , 2019 , 12, 2150-2165	5.9	4
71	Application of genetic algorithm and multivariate methods for the detection and measurement of milk-surfactant adulteration by attenuated total reflection and near-infrared spectroscopy. <i>Journal of the Science of Food and Agriculture</i> , 2021 , 101, 2696-2703	4.3	4

70	Sulfidic GO-grafted glass stir-bar as a noble metal ions adsorbent. <i>Microchemical Journal</i> , 2020 , 157, 1048-1057	4.78	3
69	. <i>IEEE Sensors Journal</i> , 2020 , 20, 10138-10144	4	3
68	Inhibition activity prediction for a dataset of candidates' drug by combining fuzzy logic with MLR/ANN QSAR models. <i>Chemical Biology and Drug Design</i> , 2019 , 93, 1139-1157	2.9	3
67	Investigation of different coal types effect on the overall plant recovery. <i>International Journal of Mining Science and Technology</i> , 2014 , 24, 447-450	7.1	3
66	Ultra-Trace Silver Determination in Biological and Water Samples by Electrothermal Atomic Absorption Spectrometry after Electrodeposition on a Graphite Probe. <i>Journal of the Chinese Chemical Society</i> , 2013 , 60, 481-487	1.5	3
65	Selective Spectrophotometric Determination of Aluminium with Xylenol Orange in Acidic Media Using Partial Least Square Method. <i>Asian Journal of Chemistry</i> , 2013 , 25, 2506-2512	0.4	3
64	Identification of Essential 2D and 3D Chemical Features for Discovery of the Novel Tubulin Polymerization Inhibitors. <i>Current Topics in Medicinal Chemistry</i> , 2019 , 19, 1092-1120	3	3
63	Molecular Docking Challenges and Limitations 2017 , 770-794		3
62	Use of Molecular Docking as a Decision-Making Tool in Drug Discovery 2021 , 229-243		3
61	A new Fe ³⁺ colorimetric sensor: Nitrophenyl bispyrazole derivative synthesis using Fe ₃ O ₄ @SiO ₂ @Si-Pr-NH-(CH ₂) ₂ -NH ₂ and its DFT study. <i>Materials Chemistry and Physics</i> , 2022 , 275, 125285	4.4	3
60	An improved ensemble learning machine for biological activity prediction of tyrosine kinase inhibitors. <i>Journal of Chemometrics</i> , 2015 , 29, 213-223	1.6	2
59	Molecular and clinical profile of congenital fibrinogen disorders in Iran, identification of two novel mutations. <i>International Journal of Laboratory Hematology</i> , 2020 , 42, 619-627	2.5	2
58	Enantioseparation and quantitative determination of ibuprofen using vancomycin-mediated capillary electrophoresis combined with molybdenum disulfide-assisted dispersive solid-phase extraction: optimization using experimental design. <i>Journal of the Iranian Chemical Society</i> , 2020 , 17, 1467-1477	2	2
57	High-throughput Docking and Molecular Dynamics Simulations towards the Identification of Novel Peptidomimetic Inhibitors against CDC7. <i>Molecular Informatics</i> , 2018 , 37, e1800022	3.8	2
56	Docking and CoMFA study on novel human CCR5 receptor antagonists. <i>Medicinal Chemistry Research</i> , 2013 , 22, 1356-1364	2.2	2
55	Global and local QSPR models to predict supercooled vapour pressure for organic compounds. <i>SAR and QSAR in Environmental Research</i> , 2015 , 26, 1033-1045	3.5	2
54	Simultaneous spectrophotometric determination of Ga(III) and Tl(III) by using genetic algorithm based on wavelength selection-partial least squares regression. <i>Journal of Analytical Chemistry</i> , 2015 , 70, 148-153	1.1	2
53	Comparative molecular field analysis and comparative molecular similarity index analysis studies on ¹ H NMR chemical shift of NH group of diaryl triazene derivatives. <i>Magnetic Resonance in Chemistry</i> , 2013 , 51, 269-74	2.1	2

52	Artificial Neural Network-Based Quantitative Structural Property Relationship for Predicting Boiling Points of Refrigerants. <i>QSAR and Combinatorial Science</i> , 2009 , 28, 1245-1254		2
51	STUDIES OF DYNAMIC VISCOSITY AND GIBBS ENERGY OF ACTIVATION OF BINARY AND TERNARY MIXTURES OF BENZYLCHLORIDE + NITROBENZENE + ISOBUTANOL FROM T = (288.15 TO 313.15) K. <i>Chemical Engineering Communications</i> , 2011 , 198, 815-836	2.2	2
50	Selection of stabilizable linear part of HPM using a linearization-based technique. <i>Physica Scripta</i> , 2008 , 78, 025002	2.6	2
49	Thermodynamic characterization of the dimerization equilibrium of newly synthesized polymethine cyanine dyes. <i>Journal of the Serbian Chemical Society</i> , 2008 , 73, 1011-1019	0.9	2
48	Enhancing performance and saving energy in CMOS DCVSL gates by using a new transistor sizing algorithm 2005 ,		2
47	A novel Z-scheme oxygen-doped g-C3N4 nanosheet/NaBiS2 nanoribbon for efficient photocatalytic H2O2 production and organic pollutants degradation. <i>Journal of Physics and Chemistry of Solids</i> , 2022 , 163, 110588	3.9	2
46	Pomegranate Punica granatum peel waste as a naked-eye natural colorimetric sensor for the detection and determination of Fe and I ions in water.. <i>Chemosphere</i> , 2022 , 294, 133759	8.4	2
45	Recent Progress in the pKa Estimation of Druglike Molecules by the Nonlinear Regression of Multiwavelength Spectrophotometric pH-Titration Data 2010 , 2010, 1-10		2
44	Molecular Docking Challenges and Limitations. <i>Advances in Medical Technologies and Clinical Practice Book Series</i> , 2016 , 56-80	0.3	2
43	Design, synthesis, biological evaluation, and molecular modeling studies of pyrazole-benzofuran hybrids as new β -glucosidase inhibitor. <i>Scientific Reports</i> , 2021 , 11, 20776	4.9	2
42	Lansoprazole-Based Colorimetric Chemosensor for Efficient Binding and Sensing of Carbonate Ion: Spectroscopy and DFT Studies. <i>Frontiers in Chemistry</i> , 2020 , 8, 626472	5	2
41	Ti3C2 MXene/Ag2ZnGeO4 Schottky heterojunctions with enhanced photocatalytic performances: Efficient charge separation and mechanism studies. <i>Separation and Purification Technology</i> , 2022 , 278, 119560	8.3	2
40	Solvent-free one-pot synthesis of 4-aryl-3,5-dimethyl-1,4,7,8-tetrahydroadipyrzolo[3,4-b:4',3'-e]pyridines using Fe3O4@SiO2@(BuSO3H)3 catalytic Fe3+ system as selective colorimetric. <i>Research on Chemical Intermediates</i> , 2022 , 48, 2111	2.8	2
39	Design and synthesis of g-C3N4/(Cu/TiO2) nanocomposite for the visible light photocatalytic degradation of endosulfan in aqueous solutions. <i>Journal of Molecular Structure</i> , 2022 , 1258, 132650	3.4	2
38	Design of pyrimidine-based scaffolds as potential anticancer agents for human DHFR: three-dimensional quantitative structure-activity relationship by docking derived grid-independent descriptors. <i>Journal of the Iranian Chemical Society</i> , 2019 , 16, 2365-2378	2	1
37	An in silico screening study and design of potent cognition agents. <i>Journal of Computational Science</i> , 2015 , 11, 112-120	3.4	1
36	A chemometric study on the stream sediments of Meshkinshahr, NW Iran, using supervised and unsupervised classification methods. <i>Arabian Journal of Geosciences</i> , 2015 , 8, 2853-2861	1.8	1
35	An intelligent readout integrated circuit (iROIC) with on-chip local gradient operations 2017 ,		1

34	Thermodynamic study of complex formation process of free base meso-tetraphenylporphyrins with dimethyl and dibutyltin(IV) dichloride: a new algorithm for a single thermometric titration. <i>Journal of Inclusion Phenomena and Macrocyclic Chemistry</i> , 2013 , 76, 47-54		1
33	Spectroscopic and molecular modeling studies on the interactions of some benzofuran derivatives with BSA. <i>Monatshefte Für Chemie</i> , 2017 , 148, 1887-1896	1.4	1
32	Predicting Degradation Half-life of Organophosphorus Pesticides in Soil Using Three-Dimensional Molecular Interaction Fields. <i>International Journal of Quantitative Structure-Property Relationships</i> , 2017 , 2, 27-35	1.2	1
31	A new fluorescence probe for detection of Cu in blood samples: Circuit logic gate.. <i>Analytical Biochemistry</i> , 2021 , 639, 114525	3.1	1
30	An On-off Supramolecular Fluorescence Switch for Detection of Pb Ions and Vitamin C. <i>Journal of Fluorescence</i> , 2021 , 1	2.4	1
29	Computational Multi-Target Drug Design. <i>Methods in Pharmacology and Toxicology</i> , 2018 , 51-90	1.1	1
28	Molecular dynamics simulation, 3D-pharmacophore and scaffold hopping analysis in the design of multi-target drugs to inhibit potential targets of COVID-19. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021 , 1-22	3.6	1
27	Orthogonality constrained inverse regression to improve model selectivity and analyte predictions from vibrational spectroscopic measurements. <i>Analytica Chimica Acta</i> , 2021 , 1185, 339073	6.6	1
26	Near-infrared spectroscopy and machine learning-based classification and calibration methods in detection and measurement of anionic surfactant in milk. <i>Journal of Food Composition and Analysis</i> , 2021 , 104, 104170	4.1	1
25	Design, Synthesis, and Nanoengineered Modification of Spherical Graphene Surface by LDH for Removal of As(III) from Aqueous Solutions. <i>Chinese Journal of Chemical Engineering</i> , 2022 ,	3.2	1
24	Determination and degradation of carbamazepine using g-C ₃ N ₄ @CuS nanocomposite as sensitive fluorescence sensor and efficient photocatalyst. <i>Inorganic Chemistry Communication</i> , 2022 , 141, 109512	3.1	1
23	Spectrophotometric Determination of Acidity Constants of 4-(2-Pyridylazo) Resorcinol in Various Micellar Media Solutions. <i>Journal of the Chinese Chemical Society</i> , 2007 , 54, 1093-1097	1.5	0
22	A new fluorescence probe for simultaneous determination of Fe ²⁺ and Fe ³⁺ by orthogonal signal correction-principal component regression. <i>Journal of Molecular Structure</i> , 2021 , 1252, 131978	3.4	0
21	Multicomponent Synthesis and Investigations Fluorescence Activity of Chromenone-Pyrazole Compounds. <i>Journal of Fluorescence</i> , 2021 , 1	2.4	0
20	A theoretical and experimental study of polyaniline/GCE and DNA G-quadruplex conformation as an impedimetric biosensor for the determination of potassium ions.. <i>Chemosphere</i> , 2021 , 133460	8.4	0
19	Synthesis of Ag(I)@FumBrByrBenzimidazole and Its Optical and Catalytic Activities in Click Reactions. <i>ChemistrySelect</i> , 2021 , 6, 6168-6180	1.8	0
18	SBA-ionic liquid as an efficient adsorbent of palladium, silver, and gold ions. <i>Journal of the Iranian Chemical Society</i> , 2022 , 1	2	0
17	A novel fluorescence sensor based on a tripodal carboxylic acid for detection and measurement of Cu in tomato: Experimental and computational studies.. <i>Food and Chemical Toxicology</i> , 2022 , 112964	4.7	0

16	In-situ construction of ZnO/Sb ₂ MoO ₆ nano-heterostructure for efficient visible-light photocatalytic conversion of N ₂ to NH ₃ . <i>Surfaces and Interfaces</i> , 2022 , 30, 101844	4.1	o
15	Multiwavelength spectrophotometric-thermodynamic studies of complexation reactions of newly synthesized triazenes with Hg ²⁺ , Pb ²⁺ , Zn ²⁺ , and Cd ²⁺ in MeOH, EtOH, DMF, and DMSO. <i>Journal of Molecular Liquids</i> , 2022 , 357, 119145	6	o
14	Simultaneous electrochemical determination of morphine and methadone by using CMK-5 mesoporous carbon and multivariate calibration.. <i>Scientific Reports</i> , 2022 , 12, 8270	4.9	o
13	Dihydropyrano quinoline derivatives functionalized nanoporous silica as novel fluorescence sensor for Fe ³⁺ (aq). <i>Journal of Molecular Structure</i> , 2022 , 133408	3.4	o
12	Spectrophotometric determination of the acidity constants of calcon in water and mixed water-organic solvents. <i>Journal of the Serbian Chemical Society</i> , 2009 , 74, 159-169	0.9	
11	SPECTROPHOTOMETRIC INVESTIGATION OF TERNARY COMPLEX FORMATION BETWEEN 1,8-DIHYDROXY-9,10-ANTHRAQUINONE AND IMIDAZOLE WITH Co ²⁺ , Ni ²⁺ , Cu ²⁺ AND Zn ²⁺ IN METHANOL AT 25°C. <i>Spectroscopy Letters</i> , 2002 , 35, 31-42	1.1	
10	Three Dimensional Quantitative Structure Activity Relationship and Pharmacophore Modeling of Tacrine Derivatives as Acetylcholinesterase Inhibitors in Alzheimer's Treatment. <i>Medicinal Chemistry</i> , 2020 , 16, 155-168	1.8	
9	Black Titania; Novel researches in Synthesis and Applications. <i>Inorganic Chemistry Communication</i> , 2021 , 109092	3.1	
8	Effect of Ethanol on the Protolytic Properties of the Vitamins B Group. <i>Journal of the Korean Chemical Society</i> , 2007 , 51, 21-30		
7	The Effect of Single and Double Acetylation of Lysine Residues on Structural and Dynamical Features of Human Splicing Factor TDP-43 - A Statistical Ensemble Analysis. <i>Combinatorial Chemistry and High Throughput Screening</i> , 2018 , 21, 358-373	1.3	
6	Spectrophotometric Study of Acidity and Complex Formation of Anti-Inflammatory Drug Piroxicam with Some Transition Metal Ions in Different Methanol/Water Mixtures by Chemometric Methods. <i>Journal of the Korean Chemical Society</i> , 2009 , 53, 693-703		
5	Exploring 3D-QSPR models of human skin permeability for a diverse dataset of chemical compounds. <i>Journal of Receptor and Signal Transduction Research</i> , 2019 , 39, 442-450	2.6	
4	10-(4-Phenylpiperazine-1-carbonyl)acridin-9(10H)-ones and related compounds: Synthesis, antiproliferative activity and inhibition of tubulin polymerization. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2021 , 32, 127687	2.9	
3	A combined structure-based pharmacophore modeling and 3D-QSAR study on a series of N-heterocyclic scaffolds to screen novel antagonists as human DHFR inhibitors. <i>Structural Chemistry</i> , 2021 , 32, 1571-1588	1.8	
2	Effect of Cold Plasma Treatment, Cross-Linking, and Dual Modification on Corn Starch. <i>Starch/Staerke</i> , 2020 , 008	2.3	
1	Exploratory and machine learning analysis of the stability constants of HgII- triazene ligands complexes. <i>Main Group Chemistry</i> , 2021 , 1-13	0.6	