

Jahan Bakhsh Ghasemi

List of Publications by Year in descending order

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Version: 2024-02-01

330
papers

6,605
citations

81839

39
h-index

155592

55
g-index

342
all docs

342
docs citations

342
times ranked

6747
citing authors

| # | ARTICLE | IF | CITATIONS |
|----|--|-----|-----------|
| 1 | Design, synthesis, and nanoengineered modification of spherical graphene surface by layered double hydroxide (LDH) for removal of As(III) from aqueous solutions. Chinese Journal of Chemical Engineering, 2023, 53, 374-380. | 1.7 | 9 |
| 2 | Using the extract of pomegranate peel as a natural indicator for colorimetric detection and simultaneous determination of Fe ³⁺ and Fe ²⁺ by partial least squares-artificial neural network. Journal of Chemometrics, 2023, 37, . | 0.7 | 1 |
| 3 | Simultaneous removal of crystal violet and methyl green in water samples by functionalised SBA-15. International Journal of Environmental Analytical Chemistry, 2022, 102, 5919-5935. | 1.8 | 9 |
| 4 | SBA-ionic liquid as an efficient adsorbent of palladium, silver, and gold ions. Journal of the Iranian Chemical Society, 2022, 19, 247-255. | 1.2 | 5 |
| 5 | Molecular dynamics simulation, 3D-pharmacophore and scaffold hopping analysis in the design of multi-target drugs to inhibit potential targets of COVID-19. Journal of Biomolecular Structure and Dynamics, 2022, 40, 11787-11808. | 2.0 | 4 |
| 6 | 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. Materials Chemistry and Physics, 2022, 275, 125285. | 2.0 | 11 |
| 7 | An On-off Supramolecular Fluorescence Switch for Detection of Pb ²⁺ Ions and Vitamin C. Journal of Fluorescence, 2022, 32, 165-173. | 1.3 | 1 |
| 8 | A new fluorescence probe for simultaneous determination of Fe ²⁺ and Fe ³⁺ by orthogonal signal correction-principal component regression. Journal of Molecular Structure, 2022, 1252, 131978. | 1.8 | 10 |
| 9 | Black titania; novel researches in synthesis and applications. Inorganic Chemistry Communication, 2022, 135, 109092. | 1.8 | 8 |
| 10 | A new fluorescence probe for detection of Cu ²⁺ in blood samples: Circuit logic gate. Analytical Biochemistry, 2022, 639, 114525. | 1.1 | 9 |
| 11 | A theoretical and experimental study of polyaniline/GCE and DNA G-quadruplex conformation as an impedimetric biosensor for the determination of potassium ions. Chemosphere, 2022, 292, 133460. | 4.2 | 10 |
| 12 | Preparation of a nonenzymatic electrochemical sensor based on a g-C ₃ N ₄ /MWO ₄ (M: Cu, Mn, Co, Ni) composite for the determination of H ₂ O ₂ . New Journal of Chemistry, 2022, 46, 3766-3776. | 1.4 | 10 |
| 13 | A novel Z-scheme oxygen-doped g-C ₃ N ₄ nanosheet/NaBiS ₂ nanoribbon for efficient photocatalytic H ₂ O ₂ production and organic pollutants degradation. Journal of Physics and Chemistry of Solids, 2022, 163, 110588. | 1.9 | 26 |
| 14 | Pomegranate Punica granatum peel waste as a naked-eye natural colorimetric sensor for the detection and determination of Fe ³⁺ and I ⁻ ions in water. Chemosphere, 2022, 294, 133759. | 4.2 | 13 |
| 15 | Solvent-free one-pot synthesis of 4-aryl-3,5-dimethyl-1,4,7,8-tetrahydrodipyrzolo[3,4-b:4'a':3'e']pyridines using Fe ₃ O ₄ @SiO ₂ /(BuSO ₃ H) ₃ catalytic Fe ³⁺ system as selective colorimetric. Research on Chemical Intermediates, 2022, 48, 2111-2133. | 1.3 | 5 |
| 16 | A novel fluorescence sensor based on a tripodal carboxylic acid for detection and measurement of Cu ²⁺ in tomato: Experimental and computational studies. Food and Chemical Toxicology, 2022, 164, 112964. | 1.8 | 4 |
| 17 | Design and synthesis of g-C ₃ N ₄ /(Cu/TiO ₂) nanocomposite for the visible light photocatalytic degradation of endosulfan in aqueous solutions. Journal of Molecular Structure, 2022, 1258, 132650. | 1.8 | 16 |
| 18 | In-situ construction of ZnO/Sb ₂ MoO ₆ nano-heterostructure for efficient visible-light photocatalytic conversion of N ₂ to NH ₃ . Surfaces and Interfaces, 2022, 30, 101844. | 1.5 | 8 |

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|----|--|-----|-----------|
| 19 | 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. | 2.3 | 2 |
| 20 | Simultaneous Determination of Adulterants in Dietary Food Supplements Using Multivariate Data Analysis after Preconcentration with Novel Nanosorbents and Chromatographic Measurement. <i>Journal of AOAC INTERNATIONAL</i> , 2022, 105, 1309-1318. | 0.7 | 1 |
| 21 | Fabrication of S-scheme heterojunction g-C ₃ N ₄ -nanosheet/ZnMoO ₄ nanocomposite with high efficiency in photocatalytic N ₂ fixation and Cr(VI) detoxification. <i>Journal of Materials Science</i> , 2022, 57, 9145-9163. | 1.7 | 17 |
| 22 | 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. | 1.8 | 12 |
| 23 | Simultaneous electrochemical determination of morphine and methadone by using CMK-5 mesoporous carbon and multivariate calibration. <i>Scientific Reports</i> , 2022, 12, 8270. | 1.6 | 11 |
| 24 | Dihydropyrano quinoline derivatives functionalized nanoporous silica as novel fluorescence sensor for Fe ³⁺ in aqueous solutions(aq). <i>Journal of Molecular Structure</i> , 2022, 1265, 133408. | 1.8 | 2 |
| 25 | Enhanced visible-light-driven photocatalysis of in-situ reduced of bismuth on BiOCl nanosheets and montmorillonite loading: Synergistic effect and mechanism insight. <i>Chemosphere</i> , 2022, 304, 135354. | 4.2 | 20 |
| 26 | Graphdiyne-based photocatalysts for solar fuel production. <i>Green Chemistry</i> , 2022, 24, 5739-5754. | 4.6 | 30 |
| 27 | Spiroindeno-pyridineindoles (SIPIs) as new visible colorimetric pH indicators. <i>Chemosphere</i> , 2022, 306, 135630. | 4.2 | 0 |
| 28 | Design and synthesis of novel pyrazole-phenyl semicarbazone derivatives as potential α -glucosidase inhibitor: Kinetics and molecular dynamics simulation study. <i>International Journal of Biological Macromolecules</i> , 2021, 166, 1082-1095. | 3.6 | 33 |
| 29 | In situ preparation of g-C ₃ N ₄ nanosheet/FeOCl: Achievement and promoted photocatalytic nitrogen fixation activity. <i>Journal of Colloid and Interface Science</i> , 2021, 587, 538-549. | 5.0 | 59 |
| 30 | Photocatalytic degradation of different pollutants by the novel gCN-NS/Black-TiO ₂ heterojunction photocatalyst under visible light: Introducing a photodegradation model and optimization by response surface methodology (RSM). <i>Materials Chemistry and Physics</i> , 2021, 258, 123912. | 2.0 | 60 |
| 31 | 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. | 1.7 | 13 |
| 32 | 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. | 1.0 | 2 |
| 33 | Use of Molecular Docking as a Decision-Making Tool in Drug Discovery. , 2021, , 229-243. | | 7 |
| 34 | High-impressive separation of photoinduced charge carriers on step-scheme ZnO/ZnSnO ₃ /Carbon dots heterojunction with efficient activity in photocatalytic NH ₃ production. <i>Journal of the Taiwan Institute of Chemical Engineers</i> , 2021, 118, 140-151. | 2.7 | 32 |
| 35 | In silico exploration of novel protease inhibitors against coronavirus 2019 (COVID-19). <i>Informatics in Medicine Unlocked</i> , 2021, 23, 100516. | 1.9 | 7 |
| 36 | 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. | 1.0 | 1 |

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|----|---|-----|-----------|
| 37 | SBA-Pr-Imine-Furan as an environmental adsorbent of Pd(II) in aqueous solutions. <i>Environmental Challenges</i> , 2021, 3, 100032. | 2.0 | 11 |
| 38 | 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. | 2.7 | 34 |
| 39 | Synthesis of Ag(I)@Fumâ~Prâ~Pyrâ~Benzimidazole and Its Optical and Catalytic Activities in Click Reactions. <i>ChemistrySelect</i> , 2021, 6, 6168-6180. | 0.7 | 4 |
| 40 | Synthesis and characterization of novel ZnO/NiCr ₂ O ₄ nanocomposite for water purification by degradation of tetracycline and phenol under visible light irradiation. <i>Materials Research Bulletin</i> , 2021, 139, 111247. | 2.7 | 30 |
| 41 | In vitro and in silico pharmaceutical activities of the methylated cyclic pentapeptide, persipeptides. <i>Journal of Applied Microbiology</i> , 2021, , . | 1.4 | 0 |
| 42 | Direct monitoring of diclofenac using a supramolecular fluorescent approach based on Î ² -cyclodextrin nanosponge. <i>Journal of Molecular Liquids</i> , 2021, 336, 116104. | 2.3 | 13 |
| 43 | Design and synthesis of novel quinazolinone-pyrazole derivatives as potential Î±-glucosidase inhibitors: Structure-activity relationship, molecular modeling and kinetic study. <i>Bioorganic Chemistry</i> , 2021, 114, 105127. | 2.0 | 28 |
| 44 | 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. | 1.8 | 21 |
| 45 | Orthogonality constrained inverse regression to improve model selectivity and analyte predictions from vibrational spectroscopic measurements. <i>Analytica Chimica Acta</i> , 2021, 1185, 339073. | 2.6 | 1 |
| 46 | 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. | 1.9 | 14 |
| 47 | Ti ₃ C ₂ MXene/Ag ₂ ZnGeO ₄ Schottky heterojunctions with enhanced photocatalytic performances: Efficient charge separation and mechanism studies. <i>Separation and Purification Technology</i> , 2021, 278, 119560. | 3.9 | 20 |
| 48 | Design, synthesis, biological evaluation, and molecular modeling studies of pyrazole-benzofuran hybrids as new Î±-glucosidase inhibitor. <i>Scientific Reports</i> , 2021, 11, 20776. | 1.6 | 15 |
| 49 | Multicomponent Synthesis and Investigations Fluorescence Activity of Chromenoneâ€“Pyrazole Compounds. <i>Journal of Fluorescence</i> , 2021, , 1. | 1.3 | 1 |
| 50 | Exploratory and machine learning analysis of the stability constants of Hg(II)- triazene ligands complexes. <i>Main Group Chemistry</i> , 2021, , 1-13. | 0.4 | 0 |
| 51 | 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. | 2.1 | 19 |
| 52 | 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. | 3.6 | 18 |
| 53 | Anthracene modified graphene oxide-silica as an optical sensor for selective detection of Cu ²⁺ and I ⁻ ions. <i>International Journal of Environmental Analytical Chemistry</i> , 2020, 100, 686-701. | 1.8 | 7 |
| 54 | 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. | 2.0 | 11 |

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|----|--|-----|-----------|
| 55 | A dual-emission fluorescence probe for simultaneous quantification of CN ³⁺ and Cr ₂ O ₇ ²⁻ ions based on modified g-C ₃ N ₄ . <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2020, 389, 112261. | 2.0 | 15 |
| 56 | 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. | 2.3 | 8 |
| 57 | Multi-view self-attention for interpretable drug-target interaction prediction. <i>Journal of Biomedical Informatics</i> , 2020, 110, 103547. | 2.5 | 20 |
| 58 | 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. | 1.8 | 10 |
| 59 | Acenaphthoquinoline as a selective fluorescent sensor for Hg (II) detection: experimental and theoretical studies. <i>Heliyon</i> , 2020, 6, e04986. | 1.4 | 12 |
| 60 | 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. | 1.5 | 54 |
| 61 | Synthesis, characterization, and photocatalytic performance of Ag/AgFeO ₂ decorated on g-C ₃ N ₄ -nanosheet under the visible light irradiation. <i>Journal of the Taiwan Institute of Chemical Engineers</i> , 2020, 115, 279-292. | 2.7 | 35 |
| 62 | Acrylamide content of collected food products from Tehran's market: a risk assessment study. <i>Environmental Science and Pollution Research</i> , 2020, 27, 30558-30570. | 2.7 | 35 |
| 63 | DeepCDA: deep cross-domain compound-protein affinity prediction through LSTM and convolutional neural networks. <i>Bioinformatics</i> , 2020, 36, 4633-4642. | 1.8 | 110 |
| 64 | 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. | 2.9 | 59 |
| 65 | Deposited CuBi ₂ O ₄ and Bi ₃ ClO ₄ nanoparticles on g-C ₃ N ₄ nanosheet: a promising visible light-induced photocatalyst toward the removal of tetracycline hydrochloride and rhodamine B. <i>Journal of Materials Science</i> , 2020, 55, 7775-7791. | 1.7 | 27 |
| 66 | 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. | 0.7 | 6 |
| 67 | Fluorescence turn off-on probe (β -cyclodextrin-hydroxyquinoline) for monitoring of Cd ²⁺ ions and tetracycline. <i>Methods and Applications in Fluorescence</i> , 2020, 8, 025009. | 1.1 | 10 |
| 68 | 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. | 1.6 | 22 |
| 69 | Developing a highly selective method for preconcentration and determination of cobalt in water and nut samples using 1-(2-pyridylazo)-naphthol and UV-visible spectroscopy. <i>Journal of the Science of Food and Agriculture</i> , 2020, 100, 2272-2279. | 1.7 | 9 |
| 70 | Sulfidic GO-grafted glass stir-bar as a noble metal ions adsorbent. <i>Microchemical Journal</i> , 2020, 157, 104878. | 2.3 | 5 |
| 71 | Simultaneous Quantification of Nine Major Water-Soluble Inorganic Ions Using a Potentiometric Electronic Tongue in Cheese Samples. <i>IEEE Sensors Journal</i> , 2020, 20, 10138-10144. | 2.4 | 5 |
| 72 | 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. | 1.2 | 7 |

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|----|---|-----|-----------|
| 73 | 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. | 2.6 | 31 |
| 74 | Lansoprazole-Based Colorimetric Chemosensor for Efficient Binding and Sensing of Carbonate Ion: Spectroscopy and DFT Studies. <i>Frontiers in Chemistry</i> , 2020, 8, 626472. | 1.8 | 12 |
| 75 | Pharmacophore Modeling, Synthesis, Scaffold Hopping and Biological Fe^{2+} -Hematin Inhibition Interaction Studies for Anti-malaria Compounds. <i>Current Topics in Medicinal Chemistry</i> , 2020, 19, 2743-2765. | 1.0 | 9 |
| 76 | Chemometrics as a Powerful and Complementary Tool for Mass Spectrometry Applications in Life Sciences. <i>Applications of Modern Mass Spectrometry</i> , 2020, , 61-97. | 0.2 | 0 |
| 77 | 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. | 0.7 | 0 |
| 78 | An ultrasensitive fluorescence sensor for determination of trace levels of copper in blood samples. <i>Analytical and Bioanalytical Chemistry</i> , 2019, 411, 5593-5603. | 1.9 | 29 |
| 79 | Inhibition activity prediction for a dataset of candidates TM drug by combining fuzzy logic with <sc>MLR</sc>/<sc>ANN QSAR</sc> models. <i>Chemical Biology and Drug Design</i> , 2019, 93, 1139-1157. | 1.5 | 10 |
| 80 | Boron-doped graphitic carbon nitride as a novel fluorescent probe for mercury(<sc>ii</sc>) and iron(<sc>iii</sc>): a circuit logic gate mimic. <i>New Journal of Chemistry</i> , 2019, 43, 12087-12093. | 1.4 | 25 |
| 81 | 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. | 2.5 | 31 |
| 82 | 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. | 1.1 | 9 |
| 83 | 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. | 1.2 | 7 |
| 84 | 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. | 1.2 | 1 |
| 85 | 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. | 2.3 | 69 |
| 86 | Design and Synthesis of Novel Cytotoxic Indole-Thiosemicarbazone Derivatives: Biological Evaluation and Docking Study. <i>Chemistry and Biodiversity</i> , 2019, 16, e1800470. | 1.0 | 14 |
| 87 | Anti-cancer, anti-oxidant and molecular docking studies of thiosemicarbazone indole-based derivatives. <i>Research on Chemical Intermediates</i> , 2019, 45, 2827-2854. | 1.3 | 29 |
| 88 | Investigation and determination of acrylamide in the main group of cereal products using advanced microextraction method coupled with gas chromatography-mass spectrometry. <i>Journal of Cereal Science</i> , 2019, 87, 157-164. | 1.8 | 49 |
| 89 | Highly selective silica-based fluorescent nanosensor for ferric ion (Fe ³⁺) detection in aqueous media. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 218, 293-298. | 2.0 | 13 |
| 90 | A highly selective magnetic solid-phase extraction method for preconcentration of Cd(II) using N,N ² -bis(salicylidene)ethylenediamine in water and food samples. <i>Research on Chemical Intermediates</i> , 2019, 45, 3141-3153. | 1.3 | 18 |

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|-----|--|-----|-----------|
| 91 | 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. <i>Journal of the Iranian Chemical Society</i> , 2019, 16, 1411-1421. | 1.2 | 16 |
| 92 | 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. | 2.5 | 21 |
| 93 | Voltammetric Electronic Tongue for the Simultaneous Determination of Three Benzodiazepines. <i>Sensors</i> , 2019, 19, 5002. | 2.1 | 16 |
| 94 | 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. | 1.3 | 2 |
| 95 | Efficient removal of malachite green from wastewater by using boron-doped mesoporous carbon nitride. <i>Applied Surface Science</i> , 2019, 469, 236-245. | 3.1 | 71 |
| 96 | Simultaneous determination of dihydroxybenzene isomers at nitrogen-doped graphene surface using fast Fourier transform square wave voltammetry and multivariate calibration. <i>Microchemical Journal</i> , 2019, 145, 596-605. | 2.3 | 20 |
| 97 | Probing the origin of dihydrofolate reductase inhibition via proteochemometric modeling. <i>Journal of Chemometrics</i> , 2019, 33, e3090. | 0.7 | 5 |
| 98 | 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. | 2.3 | 4 |
| 99 | Dynamic structure based pharmacophore modeling of the Acetylcholinesterase reveals several potential inhibitors. <i>Journal of Biomolecular Structure and Dynamics</i> , 2019, 37, 1800-1812. | 2.0 | 33 |
| 100 | Combating Diseases with Computational Strategies Used for Drug Design and Discovery. <i>Current Topics in Medicinal Chemistry</i> , 2019, 18, 2743-2773. | 1.0 | 16 |
| 101 | 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. | 1.0 | 5 |
| 102 | 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. | 1.4 | 8 |
| 103 | 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. | 1.3 | 19 |
| 104 | Computational Multi-Target Drug Design. <i>Methods in Pharmacology and Toxicology</i> , 2018, , 51-90. | 0.1 | 1 |
| 105 | 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. <i>Ecotoxicology and Environmental Safety</i> , 2018, 158, 256-265. | 2.9 | 20 |
| 106 | Editorial: In Silico Methodologies Applied to Drug Discovery. <i>Combinatorial Chemistry and High Throughput Screening</i> , 2018, 21, 150-151. | 0.6 | 2 |
| 107 | High-throughput Docking and Molecular Dynamics Simulations towards the Identification of Novel Peptidomimetic Inhibitors against CDC7. <i>Molecular Informatics</i> , 2018, 37, e1800022. | 1.4 | 4 |
| 108 | Synthesis and cholinesterase inhibitory activity of new 2-benzofuran carboxamide-benzylpyridinium salts. <i>Bioorganic Chemistry</i> , 2018, 80, 180-188. | 2.0 | 15 |

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|-----|--|-----|-----------|
| 109 | Docking of Natural Products against Neurodegenerative Diseases: General Concepts. <i>Combinatorial Chemistry and High Throughput Screening</i> , 2018, 21, 152-160. | 0.6 | 15 |
| 110 | In Silico Studies in Drug Research Against Neurodegenerative Diseases. <i>Current Neuropharmacology</i> , 2018, 16, 664-725. | 1.4 | 51 |
| 111 | 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. | 0.6 | 0 |
| 112 | Chemometric analysis of comprehensive two dimensional gas chromatography-mass spectrometry metabolomics data. <i>Journal of Chromatography A</i> , 2017, 1488, 113-125. | 1.8 | 48 |
| 113 | Computer-aided drug design to explore cyclodextrin therapeutics and biomedical applications. <i>Chemical Biology and Drug Design</i> , 2017, 89, 257-268. | 1.5 | 28 |
| 114 | Receptor modeling of environmental aerosol data using MLPCA-MCR-ALS. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2017, 167, 50-62. | 1.8 | 10 |
| 115 | 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. | 1.3 | 23 |
| 116 | Characterization of the interaction of glycyrrhizin and glycyrrhetic 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. | 3.6 | 9 |
| 117 | 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. | 2.5 | 16 |
| 118 | <i>N</i> -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. | 2.9 | 28 |
| 119 | Optimization of Influential Factors on the Photocatalytic Performance of TiO ₂ -Graphene Composite in Degradation of an Organic Dye by RSM Methodology. <i>Journal of Cluster Science</i> , 2017, 28, 2979-2995. | 1.7 | 10 |
| 120 | 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. | 1.3 | 9 |
| 121 | Spectroscopic and molecular modeling studies on the interactions of some benzofuran derivatives with BSA. <i>Monatshefte für Chemie</i> , 2017, 148, 1887-1896. | 0.9 | 2 |
| 122 | Graphene oxide-alizarin yellow-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. | 1.3 | 16 |
| 123 | Proteochemometric Modeling of the Interaction Space of Carbonic Anhydrase and its Inhibitors: An Assessment of Structure-based and Sequence-based Descriptors. <i>Molecular Informatics</i> , 2017, 36, 1600102. | 1.4 | 12 |
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| 125 | An intelligent readout integrated circuit (iROIC) with on-chip local gradient operations. , 2017, , . | | 3 |
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