Raouf K Ghavami

List of Publications by Year
in descending order

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57	678	567144 15	642610 23
papers	citations	h-index	g-index

57	57	57	811
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	High predictive QSAR models for predicting the SARS coronavirus main protease inhibition activity of ketone-based covalent inhibitors. Journal of the Iranian Chemical Society, 2022, 19, 1865-1876.	1.2	6
2	Fading of nanocurcumin-based configured biosensor array for differentiation of carrier proteins in biological fluids. Microchemical Journal, 2022, 175, 107169.	2.3	1
3	Fully united, easy, and economical sensor array for newborn babiesâ€™ amino acids monitoring: Identification of amino acids in healthy and unhealthy with PKU newborn babies. Journal of Pharmaceutical and Biomedical Analysis, 2022, 213, 114683.	1.4	0
4	Robust and predictive QSAR models for predicting the D2, 5-HT1A, and 5-HT2A inhibition activities of fused tricyclic heterocycle piperazine (piperidine) derivatives as atypical antipsychotic drugs. Journal of Molecular Structure, 2022, 1259, 132753.	1.8	2
5	QSAR analysis on a large and diverse set of potent phosphoinositide 3-kinase gamma (PI3KÎ³) inhibitors using MLR and ANN methods. Scientific Reports, 2022, 12, 6090.	1.6	9
6	In-silico Optimization of Frizzled-8 Receptor Inhibition Activity of Carbamazepine: Design New Anti-Cancer Agent. Combinatorial Chemistry and High Throughput Screening, 2022, 25, .	0.6	1
7	Computational study to select the capable anthracycline derivatives through an overview of drug structure-specificity and cancer cell line-specificity. Chemical Papers, 2021, 75, 523-538.	1.0	10
8	Study of interaction of metal ions with methylthymol blue by chemometrics and quantum chemical calculations. Scientific Reports, 2021, 11, 6465.	1.6	2
9	A new approach for simultaneous calculation of pIC50 and logP through QSAR/QSPR modeling on anthracycline derivatives: a comparable study. Journal of the Iranian Chemical Society, 2021, 18, 2785-2800.	1.2	1
10	A 3Ã—3 visible-light cross-reactive sensor array based on the nanoaggregation of curcumin in different pH and buffers for the multivariate identification and quantification of metal ions. Talanta, 2021, 226, 122131.	2.9	10
11	Highly specific fingerprinting of alkaline earth metal ions by a tunable plasmonic nanosensor array based on nanoaggregation of metallochromic dyes-AuNPs. Mikrochimica Acta, 2021, 188, 310.	2.5	1
12	A novel label-free colorimetric aptasensor for sensitive determination of PSA biomarker using gold nanoparticles and a cationic polymer in human serum. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 226, 117644.	2.0	42
13	Facile Approach to Fabricate a Chemical Sensor Array Based on Nanocurcuminâ€“Metal Ions Aggregates: Detection and Identification of DNA Nucleobases. ACS Omega, 2020, 5, 19331-19341.	1.6	8
14	Phytochemicals toward Green (Bio)sensing. ACS Sensors, 2020, 5, 3770-3805.	4.0	30
15	Simultaneous optical detection of human serum albumin and transferrin in body fluids. Mikrochimica Acta, 2020, 187, 208.	2.5	7
16	Two colorimetric ampicillin sensing schemes based on the interaction of aptamers with gold nanoparticles. Mikrochimica Acta, 2019, 186, 485.	2.5	25
17	Spectrophotometric and visual determination of zoledronic acid by using a bacterial cell-derived nanopaper doped with curcumin. Mikrochimica Acta, 2019, 186, 719.	2.5	9
18	Development linear and non-linear QSAR models for predicting AXL kinase inhibitory activity of N-[4-(quinolin-4-yloxy)phenyl]benzenesulfonamides. Journal of Receptor and Signal Transduction Research, 2019, 39, 264-275.	1.3	2

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19	A nanocellulose-based colorimetric assay kit for smartphone sensing of iron and iron-chelating deferoxamine drug in biofluids. Analytica Chimica Acta, 2019, 1087, 104-112.	2.6	39
20	Design of new CD38 inhibitors based on CoMFA modelling and molecular docking analysis of 4â€˘amino-8-quinoline carboxamides and 2,4-diamino-8-quinazoline carboxamides. SAR and QSAR in Environmental Research, 2019, 30, 21-38.	1.0	6
21	In situ synthesis Bismarck brown R reductive products-immobilised AgNPs assisted by catalytic activity of AgNPs as colorimetric probe for Hg2+ detection in water. International Journal of Environmental Analytical Chemistry, 2018, 98, 82-96.	1.8	1
22	Enhanced Sensitivity to Detection Nanomolar Level of Cu2+ Compared to Spectrophotometry Method by Functionalized Gold Nanoparticles: Design of Sensor Assisted by Exploiting First-order Data with Chemometrics. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 191, 336-344.	2.0	7
23	The in silico identification of potent anti-cancer agents by targeting the ATP binding site of the N-domain of HSP90. SAR and QSAR in Environmental Research, 2018, 29, 551-565.	1.0	8
24	A paper-based optical probe for chromium by using gold nanoparticles modified with 2,2â€²-thiodiacetic acid and smartphone camera readout. Mikrochimica Acta, 2018, 185, 374.	2.5	28
25	Predictive and Descriptive CoMFA Models: The Effect of Variable Selection. Combinatorial Chemistry and High Throughput Screening, 2018, 21, 117-124.	0.6	9
26	The Identification of New CD38 Inhibitors by Combined Structure and Ligand Based Virtual Screening Approaches of ZINC Database. Letters in Drug Design and Discovery, 2018, 15, 654-660.	0.4	4
27	Towards the In-silico Design of New HSP90 Inhibitors: Molecular Docking and 3D-QSAR CoMFA Studies of Tetrahydropyrido [4, 3-d] Pyrimidine Derivatives as HSP90 Inhibitors. Medicinal Chemistry, 2018, 14, 439-450.	0.7	6
28	Colorimetric Sensing of Iodide by the Competitive Interactions in the Surface of Gold Nanoparticles with the Simultaneous Aggregation/ Anti-Aggregation Mechanisms in Edible Salts. Current Analytical Chemistry, 2018, 14, 539-547.	0.6	4
29	The identification of new ATAD2 bromodomain inhibitors: the application of combined ligand and structure-based virtual screening. SAR and QSAR in Environmental Research, 2017, 28, 957-971.	1.0	5
30	Design new P-glycoprotein modulators based on molecular docking and CoMFA study of Î±, Î²-unsaturated carbonyl-based compounds and oxime analogs as anticancer agents. Journal of Molecular Structure, 2017, 1130, 922-928.	1.8	4
31	Molecular docking and CoMFA studies of thiazoloquin(az)olin(on)es as CD38 inhibitors: determination of inhibitory mechanism, pharmacophore interactions, and design of new inhibitors. Journal of Biomolecular Structure and Dynamics, 2017, 35, 1890-1898.	2.0	6
32	Application of a new version of GA-RBF neural network for simultaneous spectrophotometric determination of Zn(II), Fe(II), Co(II) and Cu(II) in real samples: An exploratory study of their complexation abilities toward MTB. Talanta, 2016, 160, 86-98.	2.9	15
33	Pharmacophore interactions analysis and prediction of inhibitory activity of 1,7-diazacarbazoles as checkpoint kinase 1 inhibitors: application of molecular docking, 3D-QSAR and RBF neural network. Journal of the Iranian Chemical Society, 2016, 13, 1525-1537.	1.2	3
34	Radial basis function neural networks based on projection pursuit approach and solvatochromic descriptors: single and full column prediction of gas chromatography retention behavior of polychlorinated biphenyls. Journal of Chemometrics, 2016, 30, 589-601.	0.7	3
35	Molecular docking and QSAR analysis of naphthyridone derivatives as ATAD2 bromodomain inhibitors: application of CoMFA, LS-SVM, and RBF neural network. Medicinal Chemistry Research, 2016, 25, 2895-2905.	1.1	10
36	Simultaneously detection of calcium and magnesium in various samples by calmagite and chemometrics data processing. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2016, 169, 72-81.	2.0	6

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37	Investigating the discrimination potential of linear and nonlinear spectral multivariate calibrations for analysis of phenolic compounds in their binary and ternary mixtures and calculation pKa values. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2016, 165, 191-200.	2.0	8
38	QSPR/QSAR solely based on molecular surface electrostatic potentials for benzenoid hydrocarbons. Journal of the Iranian Chemical Society, 2016, 13, 519-529.	1.2	10
39	Radial basis function neural networks based on the projection pursuit and principal component analysis approaches: QSAR analysis of fullerene[C60]-based HIV-1 PR inhibitors. Medicinal Chemistry Research, 2016, 25, 19-29.	1.1	12
40	Combining radial basis function neural network with genetic algorithm to QSPR modeling of adsorption on multi-walled carbonÂnanotubes surface. Journal of Molecular Structure, 2015, 1098, 191-198.	1.8	16
41	Optimization of Auxiliary Solvent Demulsification Microextraction for Determination of Cyanide in Environmental Water and Biological Samples by Microvolume UV-Vis Spectrophotometry. Journal of the Brazilian Chemical Society, 2015, , .	0.6	0
42	Investigation of retention behavior of anthraquinoids in RP-HPLC on 17 different C18 stationary phases by means of quantitative structure retention relationships. Medicinal Chemistry Research, 2013, 22, 2677-2691.	1.1	2
43	Structure-based predictions of 13C-NMR chemical shifts for a series of 2-functionalized 5-(methylsulfonyl)-1-phenyl-1H-indoles derivatives using GA-based MLR method. Journal of Molecular Structure, 2012, 1030, 57-66.	1.8	4
44	Investigation of retention behavior of polychlorinated biphenyl congeners on 18 different HRGC columns using molecular surface average local ionization energy descriptors. Journal of Chromatography A, 2012, 1233, 116-125.	1.8	9
45	Determination of nimesulide in human serum using a glassy carbon electrode modified with SiC nanoparticles. Mikrochimica Acta, 2012, 176, 493-499.	2.5	16
46	SiC nanoparticles-modified glassy carbon electrodes for simultaneous determination of purine and pyrimidine DNA bases. Biosensors and Bioelectronics, 2011, 26, 3864-3869.	5.3	59
47	A novel non-enzymatic hydrogen peroxide sensor based on single walled carbon nanotubesâ€“manganese complex modified glassy carbon electrode. Electrochimica Acta, 2011, 56, 3387-3394.	2.6	49
48	Semi-Empirical Topological Method for Prediction of the Relative Retention Time of Polychlorinated Biphenyl Congeners on 18 Different HR GC Columns. Chromatographia, 2010, 72, 523-533.	0.7	16
49	QSRR Models for KovÃ¡tsâ€™ Retention Indices of a Variety of Volatile Organic Compounds on Polar and Apolar GC Stationary Phases Using Molecular Connectivity Indexes. Chromatographia, 2010, 72, 893-903.	0.7	17
50	QSRR-Based Evaluating and Predicting of the Relative Retention Time of Polychlorinated Biphenyl Congeners on 18 Different High Resolution GC Columns. Chromatographia, 2009, 70, 851-868.	0.7	15
51	QSPR studies on normal boiling points and molar refractivities of organic compounds by correlation-ranking-based PCR and PCâ€“ANN analyses of new topological indices. Canadian Journal of Chemistry, 2009, 87, 1593-1604.	0.6	5
52	Genetic algorithm as a variable selection procedure for the simulation of 13C nuclear magnetic resonance spectra of flavonoid derivatives using multiple linear regression. Journal of Molecular Graphics and Modelling, 2008, 27, 105-115.	1.3	15
53	Highly correlating distance/connectivity-based topological indices. Journal of Molecular Graphics and Modelling, 2008, 27, 506-511.	1.3	17
54	Net analyte signal-based simultaneous determination of antazoline and naphazoline using wavelength region selection by experimental design-neural networks. Talanta, 2006, 68, 1222-1229.	2.9	47

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55	Solvatochromic Linear Solvation Energy Relationships (LSER) for Solubility of Gases in Various Solvents by Target Factor Analysis. Journal of the Chinese Chemical Society, 2005, 52, 11-19.	0.8	2
56	Highly Correlating Distance-Connectivity-Based Topological Indices. 2: Prediction of 15 Properties of a Large Set of Alkanes Using a Stepwise Factor Selection-Based PCR Analysis. QSAR and Combinatorial Science, 2004, 23, 734-753.	1.5	13
57	A facile conversion of epoxides to halohydrins with elemental halogen using isonicotinic hydrazide (isoniazide) as a new catalyst. Journal of Molecular Catalysis A, 2004, 215, 55-62.	4.8	16