

# Avat Arman Taherpour

## List of Publications by Year in descending order

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146  
papers

1,905  
citations

331259

21  
h-index

344852

36  
g-index

149  
all docs

149  
docs citations

149  
times ranked

1974  
citing authors

#	ARTICLE	IF	CITATIONS
1	Photo-induced electron transfer of [C60@Abacavir] nano-complex and feasibility of C60 fullerene application as a chemical shift reagent: a DFT/TD-DFT insights. <i>Journal of the Iranian Chemical Society</i> , 2022, 19, 937-956.	1.2	2
2	N-doped graphene quantum dots from graphene oxide and dendrimer and application in photothermal therapy: An experimental and theoretical study. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2022, 636, 128066.	2.3	10
3	Thermal Rearrangement of Azulenes to Naphthalenes: A Deeper Insight into the Mechanisms. <i>Journal of Organic Chemistry</i> , 2022, 87, 3296-3310.	1.7	5
4	Feasibility of using two benzo-substituted pyrilium-based compounds in dye-sensitized solar cells. <i>Materials Science in Semiconductor Processing</i> , 2021, 123, 105468.	1.9	5
5	Unveiling the mechanistic implications of water oxidation reactions boosted by guanidine proton relays: a chemical-electrochemical-chemical pathway and a non-concerted proton-electron transfer. <i>Journal of Materials Chemistry A</i> , 2021, 9, 2937-2947.	5.2	4
6	Novel donor-acceptor non-fullerene metal-organic solar cells based on open edge Sc@BN: a DFT and TD-DFT study. <i>Journal of the Iranian Chemical Society</i> , 2021, 18, 2271-2282.	1.2	4
7	Mechanism-Based Inactivation of Cytochrome P450 Enzymes: Computational Insights. <i>Chemical Research in Toxicology</i> , 2021, 34, 959-987.	1.7	11
8	When a Dimroth Rearrangement Is Not a Dimroth Rearrangement. <i>Journal of Organic Chemistry</i> , 2021, 86, 8286-8294.	1.7	10
9	Recovered fluorescence of the Cd-nanocluster-Hg(II) system based on experimental results and computational methods. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 255, 119701.	2.0	0
10	Theoretical kinetic and thermodynamic studies of the strain energies and ring size effects of the 1,3-dipolar cycloaddition reactions on ethinamate medicine analogs. <i>Journal of Molecular Structure</i> , 2020, 1204, 127544.	1.8	0
11	Harnessing the enantiomeric recognition ability of hydrophobic polymers of intrinsic microporosity (PIM-1) toward amino acids by converting them into hydrophilic polymer dots. <i>Journal of Materials Chemistry C</i> , 2020, 8, 13827-13835.	2.7	12
12	In Situ Chromophore Doping: A New Mechanism for the Long-Wavelength Emission of Carbon Dots. <i>Journal of Physical Chemistry C</i> , 2020, 124, 10638-10646.	1.5	27
13	Fabrication of Template-Less Self-Propelled Micromotors Based on A Metal-Sandwiched Polytryptophan Body: An Experimental and DFT Study. <i>ChemPlusChem</i> , 2020, 85, 1129-1136.	1.3	4
14	Structural Assessment of Hydrogen Bonds on Methylpentynol Azide Clusters To Achieve Regiochemical Outcome of 1,3-Dipolar Cycloaddition Reactions Using Density Functional Theory. <i>ACS Omega</i> , 2020, 5, 5964-5975.	1.6	5
15	Impedimetric determination of Cs(I) using AuNPs@PoPD-DB24C8: A targeted molecular-scale perturbation. <i>Analytica Chimica Acta</i> , 2020, 1108, 118-128.	2.6	1
16	Ionically Tagged Magnetic Nanoparticles with Urea Linkers: Application for Preparation of 2-Aryl-quinoline-4-carboxylic Acids via an Anomeric-Based Oxidation Mechanism. <i>ACS Omega</i> , 2020, 5, 3207-3217.	1.6	48
17	Regioselective Ortho-C-H sulfenylation of free phenols catalyzed by Co(II)-immobilized on silica-coated magnetic nanoparticles. <i>Molecular Catalysis</i> , 2020, 484, 110772.	1.0	10
18	One-pot synthesis of 2 H-indazolo [2,1-b]phthalazine-triones via nano-Al <sub>2</sub> O <sub>3</sub> / BF <sub>3</sub> / Fe <sub>3</sub> O <sub>4</sub> as an efficient catalyst and theoretical. <i>Journal of Heterocyclic Chemistry</i> , 2020, 57, 2801-2814.	1.4	1

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19	Catalytic application of sulfamic acid-functionalized magnetic Fe <sub>3</sub> O <sub>4</sub> nanoparticles (SA-MNPs) for protection of aromatic carbonyl compounds and alcohols: experimental and theoretical studies. <i>RSC Advances</i> , 2020, 10, 44946-44957.	1.7	4
20	A carbon nanotube-iron (III) oxide nanocomposite as a cathode in dye-sensitized solar cells: Computational modeling and electrochemical investigations. <i>Electrochimica Acta</i> , 2019, 318, 617-624.	2.6	12
21	Proton shuttle efficiency of bicarbonate: A theoretical study on tautomerization and CO <sub>2</sub> hydration. <i>Tetrahedron</i> , 2019, 75, 130693.	1.0	5
22	Aptamer-Based Fluorescent Biosensing of Adenosine Triphosphate and Cytochrome <i>c</i> via Aggregation-Induced Emission Enhancement on Novel Label-Free DNA-Capped Silver Nanoclusters/Graphene Oxide Nanohybrids. <i>ACS Applied Materials &amp; Interfaces</i> , 2019, 11, 46077-46089.	4.0	40
23	Electrochemical sensing of 2-methyl-4, 6-dinitrophenol by nanomagnetic core shell linked to carbon nanotube modified glassy carbon electrode. <i>Materials Science and Engineering C</i> , 2019, 99, 211-221.	3.8	9
24	Human serum albumin binding studies of a new platinum(IV) complex containing the drug pregabalin: experimental and computational methods. <i>Journal of Coordination Chemistry</i> , 2019, 72, 600-618.	0.8	11
25	Molecular interactions between PAMAM dendrimer and some medicines that suppress the growth of hepatitis virus (Adefovir, Entecavir, Telbivudine, Lamivudine, Tenofovir): a theoretical study. <i>International Nano Letters</i> , 2019, 9, 231-244.	2.3	3
26	Efficient ethanol oxidation by hemoglobin-capped gold nanoclusters: The critical role of Fe in the heme group as an oxophilic metal active site. <i>Electrochemistry Communications</i> , 2019, 103, 42-47.	2.3	8
27	Bergman cyclization reactions in fused enediynes: a DFT study. <i>Journal of the Iranian Chemical Society</i> , 2019, 16, 1965-1976.	1.2	2
28	A rhodium-decorated carbon nanotube cathode material in the dye-sensitized solar cell: Conversion efficiency reached to 11%. <i>Electrochimica Acta</i> , 2019, 308, 373-383.	2.6	23
29	Structural distortions of fullerene C <sub>60</sub> n (n = 0 to 6) by first principle density functional theory. <i>Journal of Molecular Structure</i> , 2019, 1184, 546-556.	1.8	3
30	Determination of Hg <sup>2+</sup> and Cu <sup>2+</sup> ions by dual-emissive Ag/Au nanocluster/carbon dots nanohybrids: Switching the selectivity by pH adjustment. <i>Journal of Hazardous Materials</i> , 2019, 367, 437-446.	6.5	70
31	One-step electrochemically driven production of aza macrocycle-based pseudo-cryptand: An accessible route for creating of diverse cryptand-resembles compounds. <i>Electrochimica Acta</i> , 2019, 296, 102-111.	2.6	1
32	Reply to the comment on "A convenient method for preparation of 2-amino-4,6-diphenylnicotinonitrile using HBF <sub>4</sub> as an efficient catalyst via an anomeric based oxidation: A joint experimental and theoretical study" [J. Mol. Struct. 1137 (2017) 674-680], by S. Salehzadeh and F. Maleki, J. Mol. Struct. 1154 (2018) 587-589. <i>Journal of Molecular Structure</i> , 2019, 1179, 719-724.	1.8	1
33	Sub-femtomolar detection of HIV-1 gene using DNA immobilized on composite platform reinforced by a conductive polymer sandwiched between two nanostructured layers: A solid signal-amplification strategy. <i>Analytica Chimica Acta</i> , 2019, 1055, 7-16.	2.6	22
34	A DFT Study of Electronic Structures and Relative Stabilities of Isomeric <i>n,m</i> -Diazaphenanthrenes. <i>Polycyclic Aromatic Compounds</i> , 2019, 39, 462-469.	1.4	6
35	Photoinduced electron transfer process on emission spectrum of N,N'-bis(salicylidene)-1,2-phenylenediamine as a Mg <sup>2+</sup> cation chemosensor: A first principle DFT and TDDFT study. <i>Journal of Molecular Structure</i> , 2018, 1161, 339-344.	1.8	10
36	Separation of anticancer medicines carmustine, lomustine, semustine and melphalan by PAMAM dendrimer: a theoretical study. <i>Journal of the Iranian Chemical Society</i> , 2018, 15, 1223-1234.	1.2	1

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37	Tautomeric preferences of the cis and trans isomers of axitinib. <i>Chemical Physics</i> , 2018, 507, 10-18.	0.9	4
38	A low-overpotential nature-inspired molecular chromium water oxidation catalyst. <i>Electrochimica Acta</i> , 2018, 265, 316-325.	2.6	10
39	Comprehensive facilitating of water oxidation reaction by ultrasonic attenuation of hydrogen-bonded structure of water. <i>Ultrasonics Sonochemistry</i> , 2018, 42, 381-389.	3.8	8
40	Electrochemical sensing of trifluralin in water by fluconazole-immobilized Fe <sub>3</sub> O <sub>4</sub> /SiO <sub>2</sub> nanomagnetic core-shell linked to carbon nanotube modified glassy carbon electrode; an experimental and theoretical modeling. <i>Journal of the Iranian Chemical Society</i> , 2018, 15, 719-732.	1.2	12
41	Adsorption, intercalation and sensing of helium on yttrium functionalized open edge boron nitride: A first principle DFT and TDDFT study. <i>Chemical Physics Letters</i> , 2018, 691, 231-237.	1.2	13
42	Synthesis, characterization, HSA interaction, and antibacterial activity of a new water-soluble Pt(II) complex containing the drug cephalexin. <i>Journal of Coordination Chemistry</i> , 2018, 71, 3708-3730.	0.8	9
43	Transduction of interaction between trace tryptophan and surface-confined chromium salen using impedance spectroscopy. A sensing device that works based on highly selective inhibition of mediator's Faradaic process. <i>Analytica Chimica Acta</i> , 2018, 1030, 70-76.	2.6	5
44	Resolving the Multiple Emission Centers in Carbon Dots: From Fluorophore Molecular States to Aromatic Domain States and Carbon-Core States. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 4189-4198.	2.1	142
45	Novel donor-acceptor non-fullerene metal-organic solar cells: A first DFT and TD-DFT study. <i>Physica B: Condensed Matter</i> , 2018, 542, 37-43.	1.3	15
46	A DFT study of both the hydrolytic degradation and protonation of semustine in variation conditions of pH and interaction of drug with DNA nucleobases. <i>Structural Chemistry</i> , 2018, 29, 1465-1474.	1.0	6
47	Importance of Azo-Hydrazo Tautomerization in the Oxidative Degradation of Procarbazine by Cytochrome P450: Computational Insights. <i>ChemistrySelect</i> , 2018, 3, 6042-6049.	0.7	1
48	Experimental and theoretical studies of interaction of aliphatic chain $\beta$ -aminobisphosphonates with DNA. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2017, 338, 183-191.	2.0	1
49	A convenient method for preparation of 2-amino-4,6-diphenylnicotinonitrile using HBF <sub>4</sub> as an efficient catalyst via an anomeric based oxidation: A joint experimental and theoretical study. <i>Journal of Molecular Structure</i> , 2017, 1137, 674-680.	1.8	29
50	Theoretical and Instrumental Studies of the Competitive Interaction Between Aromatic $\beta$ -Aminobisphosphonates with DNA Using Binding Probes. <i>Applied Biochemistry and Biotechnology</i> , 2017, 182, 925-943.	1.4	4
51	Introduction of a carbon paste electrode based on nickel carbide for investigation of interaction between warfarin and vitamin K <sub>1</sub> . <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 2017, 139, 156-164.	1.4	9
52	Application of novel nanostructured dinitropyrazine molten salt catalyst for the synthesis of sulfanylpyridines via anomeric based oxidation. <i>Journal of the Iranian Chemical Society</i> , 2017, 14, 1839-1852.	1.2	23
53	DFT and TD-DFT theoretical studies on photo-induced electron transfer process on [Cefamandole].C <sub>60</sub> nano-complex. <i>Journal of Molecular Graphics and Modelling</i> , 2017, 75, 42-48.	1.3	27
54	Chemical composition analysis of the essential oil of <i>Mentha piperita</i> L. from Kermanshah, Iran by hydrodistillation and HS/SPME methods. <i>Journal of Analytical Science and Technology</i> , 2017, 8, .	1.0	38

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55	Experimental and Computational Evidence on the Interaction of Cycloalkyl $\pm$ -Aminobisphosphonates with Calf Thymus DNA. <i>DNA and Cell Biology</i> , 2017, 36, 541-551.	0.9	1
56	A first-principle DFT study of solvent effects on metiamide tautomers and imaginary interactions with H <sub>2</sub> -receptors. <i>Journal of the Iranian Chemical Society</i> , 2017, 14, 1613-1632.	1.2	2
57	N <sub>2</sub> elimination thermolysis reactions of 9-(4- and 5-substituted-1,2,3-triazol-1-yl)acridines to produce 1 H-pyrido-[4,3,2-kl] derivatives – A theoretical study. <i>Chemical Physics Letters</i> , 2017, 676, 154-168.	1.2	4
58	Manganese mediated oxidation of progesterone in alkaline medium: Mechanism study and quantitative determination. <i>Electrochimica Acta</i> , 2017, 225, 292-302.	2.6	18
59	The first principle computational study for the competitive mechanisms of oxidative aromatization of 2-substituted imidazolines using KMnO <sub>4</sub> /SiO <sub>2</sub> . <i>Journal of the Iranian Chemical Society</i> , 2017, 14, 2485-2493.	1.2	6
60	Synthesis, structural determination and HSA interaction studies of a new water-soluble Cu(II) complex derived from 1,10-phenanthroline and ranitidine drug. <i>Journal of Coordination Chemistry</i> , 2017, 70, 3186-3198.	0.8	13
61	Synthesis, characterization and <i>in vitro</i> DNA binding studies of a new copper(II) complex containing antioxidant ferulic acid. <i>Journal of Coordination Chemistry</i> , 2017, 70, 2589-2605.	0.8	9
62	Reply to the –Comments on –Experimental and theoretical studies of the nanostructured {Fe <sub>3</sub> O <sub>4</sub> @SiO <sub>2</sub> }(CH <sub>2</sub> ) <sub>3</sub> Im}C(CN) <sub>3</sub> catalyst for 2-amino-3-cyanopyridine preparation via an anomeric based oxidation–, <i>RSC Adv.</i> , 2016, 6, 50100–50111, and –The first computational study for the oxidative aromatization of pyrazolines and 1,4-dihydropyridines using 1,2,4-triazolinediones: an anomeric-based oxidation–, <i>RSC Adv.</i> , 2016, 6, 102, <i>RSC Advances</i> , 2017, 7, 53617-53621.	1.7	6
63	Recognition of switching on or off fluorescence emission spectrum on the Schiff-bases as a Mg <sup>2+</sup> chemosensor: A first principle DFT and TD-DFT study. <i>Journal of Molecular Structure</i> , 2017, 1147, 815-820.	1.8	20
64	Hydrophobic amino acids grafted onto chitosan: a novel amphiphilic chitosan nanocarrier for hydrophobic drugs. <i>Drug Development and Industrial Pharmacy</i> , 2017, 43, 1-11.	0.9	43
65	A DFT study of structures and stabilities of isomeric furo-, thieno-, and selenophenopyridines. <i>Phosphorus, Sulfur and Silicon and the Related Elements</i> , 2017, 192, 422-426.	0.8	0
66	Synthesis, characterization and <i>in vitro</i> DNA binding studies of a new copper(II) complex containing an antiviral drug, valganciclovir. <i>Journal of Coordination Chemistry</i> , 2017, 70, 201-222.	0.8	8
67	Theoretical Calculation of Thermodynamic and Kinetic Quantities for 1,3 Dipolar Cycloaddition Reactions Between Nitrile Sulfides R <sup>2</sup> CNS (R <sup>1</sup> =H, CH <sub>3</sub> , Ph and Ph(CH <sub>3</sub> ) <sub>3</sub> ) with 7-10 Membered Simple Cycloalkynes. <i>Iranian Journal of Science and Technology, Transaction A: Science</i> , 2017, 41, 1139-1148.	0.7	3
68	Theoretical Study of Diffusion Flow of Neurotransmitters Through Single-Wall Armchair(10,10) and Zigzag(18,0) Carbon Nanotubes. <i>Iranian Journal of Science and Technology, Transaction A: Science</i> , 2017, 41, 787-808.	0.7	0
69	Chemical composition analysis of the essential oil of Solanum nigrum L. by HS/SPME method and calculation of the biochemical coefficients of the components. <i>Arabian Journal of Chemistry</i> , 2017, 10, S2372-S2375.	2.3	8
70	Theoretical studies of the free energies of electron transfer and electron transfer kinetics in nanostructure supramolecular complexes of cis-unsaturated thiocrown ethers and Ce and Gd endohedral metallofullerenes [X@C@H](Y)](M=Ce, Gd). <i>Arabian Journal of Chemistry</i> , 2017, 10, S609-S616.	2.3	4
71	Study of electron transfer process between fullerenes and membrane cells of Escherichia coli in the presence of dinitrophenol and dicyclohexylcarbodiimide. <i>Arabian Journal of Chemistry</i> , 2017, 10, S2363-S2371.	2.3	1
72	Theoretical Study of 1,3-Dipolar Reactions of Myrcene and Trimethylsilylazide. <i>Letters in Organic Chemistry</i> , 2017, 14, 159-171.	0.2	1

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73	Interrupting the flux of delocalized electrons on a dibenzo-18-crown-6-embedded graphite sheet and its relative counteraction in the presence of potassium ions. <i>Analyst</i> , 2016, 141, 4227-4234.	1.7	18
74	Study of solvent effects on structural and conformational properties of cimetidine tautomers. <i>Medicinal Chemistry Research</i> , 2016, 25, 2042-2057.	1.1	2
75	Synthesis and characterization of glucose-capped CdSe quantum dots. Electrochemical and computational studies of corresponding carbon-ionic liquid electrode for quantitative determination of minoxidil. <i>Journal of Electroanalytical Chemistry</i> , 2016, 778, 116-125.	1.9	16
76	The first computational study for the oxidative aromatization of pyrazolines and 1,4-dihydropyridines using 1,2,4-triazolinediones: an anomeric-based oxidation. <i>RSC Advances</i> , 2016, 6, 102280-102291.	1.7	30
77	Mechanistic study of allopurinol oxidation using aldehyde oxidase, xanthine oxidase and cytochrome P450 enzymes. <i>RSC Advances</i> , 2016, 6, 109672-109680.	1.7	8
78	The simulation of UV spectroscopy and electronic analysis of temozolomide and dacarbazine chemical decomposition to their metabolites. <i>Journal of Molecular Modeling</i> , 2016, 22, 270.	0.8	12
79	Experimental and theoretical studies of the nanostructured $\{Fe_3O_4@SiO_2@CH_2CN\}_3$ catalyst for 2-amino-3-cyanopyridine preparation via an anomeric based oxidation. <i>RSC Advances</i> , 2016, 6, 50100-50111.	1.7	92
80	Study of complexation between two 1,3-alternate calix[4]crown derivatives and alkali metal ions by electrospray ionization mass spectrometry and density functional theory calculations. <i>Journal of Molecular Structure</i> , 2016, 1108, 16-24.	1.8	2
81	Theoretical study of electron transfer process between fullerenes and neurotransmitters; acetylcholine, dopamine, serotonin and epinephrine in nanostructures [neurotransmitters]. <i>Chemical Biology</i> , 2016, 9, 19-29.	2.2	4
82	First principles studies of electronic and optical properties of helium adsorption on Sc-doped BN monolayer. <i>Journal of the Iranian Chemical Society</i> , 2015, 12, 1983-1990.	1.2	21
83	<sup>1</sup> H-NMR study of the stoichiometry and stability of the Ba <sup>2+</sup> , Sr <sup>2+</sup> , Hg <sup>2+</sup> , Pb <sup>2+</sup> , K <sup>+</sup> , Ag <sup>+</sup> , and Tl <sup>+</sup> complexes with a new macrocyclic diamide in acetonitrile/nitrobenzene solvent mixture. <i>Journal of the Iranian Chemical Society</i> , 2015, 12, 1915-1925.	1.2	0
84	Racemic R,S-venlafaxine hydrochloride-DNA interaction: Experimental and computational evidence. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 145, 540-552.	2.0	26
85	Structural relationships and theoretical study of the free energies of electron transfer, electrochemical properties, and electron transfer kinetic of cephalosporin antibiotics derivatives with fullerenes in nanostructure of [R]C <sub>n</sub> (R=cefadroxil, cefepime, cephalexin, cefotaxime). <i>TJ ETQq1</i> 1 0.784314 rgBT / Osverlock 2015, 5, 153-167.	1.4	0
86	Mechanistic study of the hydrolytic degradation and protonation of temozolomide. <i>RSC Advances</i> , 2015, 5, 41112-41119.	1.7	11
87	Highly selective and sensitive fluorescence optode membrane for uranyl ion based on 5-(9-anthracenylmethyl)-5-aza-2,8-dithia[9],(2,9)-1,10-phenanthroline. <i>RSC Advances</i> , 2015, 5, 92061-92070.	1.7	8
88	Comprehensive insights into the structure and coordination behavior of thiosemicarbazone ligands: a computational assessment of the E-Z interconversion mechanism during coordination. <i>New Journal of Chemistry</i> , 2015, 39, 9313-9324.	1.4	19
89	One-pot Solvent-free Catalytic Dimerization Reaction of Phenylacetylene to 1-Phenyl-naphthalene. <i>Journal of Chemical Sciences</i> , 2015, 127, 1523-1530.	0.7	3
90	DFT study of HOMO structural map of $\beta^2$ -diketones and $\beta^2$ -ketoesters; towards prediction of electrochemical oxidation. <i>Molecular Simulation</i> , 2015, 41, 237-244.	0.9	2

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91	A study of the effects of solvent on structural and conformational properties of ranitidine tautomer forms by DFT method. <i>Structural Chemistry</i> , 2015, 26, 517-529.	1.0	9
92	Conductometric and <sup>1</sup> H NMR studies of thermodynamics of complexation of Zn <sup>2+</sup> , Cd <sup>2+</sup> and Pb <sup>2+</sup> ions with tetrathia-12-crown-4 in dimethylsulfoxide-nitrobenzene mixtures. <i>Journal of Inclusion Phenomena and Macrocyclic Chemistry</i> , 2014, 78, 429-436.	0.9	2
93	Synthesis, Characterization, and DNA Binding Studies of a New Pt(II) Complex Containing the Drug Levetiracetam: Combining Experimental and Computational Methods. <i>Applied Biochemistry and Biotechnology</i> , 2014, 172, 2436-2454.	1.4	25
94	Formation and HERON Reactivity of Cyclic N,N-Dialkoxyamides. <i>Australian Journal of Chemistry</i> , 2014, 67, 507.	0.5	27
95	Development of a novel PVC-membrane fluorescent sensor based on N,N'-bis(dansylamidoethyl)-N,N'-bis(2-pyridylmethyl)propylene-diamine as a new fluoroionophore for highly sensitive and selective monitoring of trace amounts of La <sup>3+</sup> ions in aqueous solutions. <i>Sensors and Actuators B: Chemical</i> , 2014, 192, 378-385.	4.0	22
96	One-pot microwave-assisted solvent-free synthesis, theoretical and experimental studies on barrier rotation of C-N bond of N-alkenyl-1,2,3-triazoles. <i>Structural Chemistry</i> , 2014, 25, 1483-1493.	1.0	4
97	Spectrophotometric study of formation, structure, stability and kinetics of charge-transfer complexation of iodine with 1,4,7,10,13,16-hexamethyl-1,4,7,10,13,16-hexaazacyclooctadecane in chloroform solution. Application of hard-modeling approaches and theoretical calculations. <i>Journal of Molecular Structure</i> , 2013, 1047, 179-185.	1.8	3
98	Theoretical study of 1,3-dipolar cycloaddition reactions between 7-10-membered simple cycloalkynes and triazoles R-N <sub>3</sub> (R=AH, CH <sub>3</sub> , Ph). <i>Structural Chemistry</i> , 2013, 24, 523-534.	1.0	6
99	Theoretical studies on the rotamers and dynamic behaviors of ethyl-5-acetyl-4-(3,4-dimethoxyphenyl)-2,6-dimethyl-1,4-dihydropyridine-3-carboxylate. <i>Structural Chemistry</i> , 2013, 24, 191-200.	1.0	7
100	Free energies, kinetics, and photoelectron-transfer properties, and theoretical and quantitative structural relationship studies of [SWCNT(5,5)-armchair-C <sub>n</sub> H <sub>20</sub> ][R] (R = 1,2-C <sub>60</sub> Pd(dppf), 1,2-C <sub>60</sub> Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5 2,3 1		
101	Free Energies of Electron Transfer, Electron Transfer Kinetic Theoretical and Quantitative Structural Relationships and Electrochemical Properties Studies of Gadolinium Nitride Cluster Fullerenes Gd <sub>3</sub> N@C <sub>n</sub> [X-UT-Y][Gd <sub>3</sub> N@C <sub>n</sub> ] (n = 80, 82, 84, 86 and 88) Supramolecular Complexes. <i>Fullerenes Nanotubes and Carbon Nanostructures</i> , 2013, 21, 485-502.	1.0	10
102	Theoretical Study and Structural Relationships of Free Energies of Electron Transfer, Electrochemical Properties and Electron Transfer Kinetics of Ferrocene Derivatives with Fullerenes in Nanostructures of [(R) <sub>2</sub> Cp <sub>2</sub> -Fe].CnSupramolecular Complexes. <i>Fullerenes Nanotubes and Carbon Nanostructures</i> , 2013, 21, 653-680.	1.0	5
103	Theoretical free energies of electron transfer, electrochemical properties, electron transfer kinetic and quantitative structural relationships studies of alkynyl-dihydrofullerene in [X-UT-Y][R-C <sub>60</sub> -M <sup>+</sup> ] supramolecular complexes. <i>European Journal of Chemistry</i> , 2012, 3, 340-347.	0.3	3
104	Efficient synthesis of 2-hydroxyalkyl alkanedithioates from 1,3-diketones, CS <sub>2</sub> , and epoxides. <i>Journal of Sulfur Chemistry</i> , 2012, 33, 385-390.	1.0	4
105	Chemical composition analysis of the essential oil of <i>Melissa officinalis</i> L. from Kurdistan, Iran by HS/SPME method and calculation of the biophysicochemical coefficients of the components. <i>Natural Product Research</i> , 2012, 26, 152-160.	1.0	22
106	Study of Electrochemical Properties, Free Energies of Electron Transfer and Reduction Potentials of Supramolecular [X-UT-Y] <sub>n</sub> Complexes and Fullerenes C <sub>60</sub> to C <sub>300</sub> . <i>Fullerenes Nanotubes and Carbon Nanostructures</i> , 2012, 20, 17-30.	1.0	1
107	Synthesis of alkyl bis(dimethylamino)methylenecarbamodithioates from 1,1,3,3-tetramethylguanidine, CS <sub>2</sub> and oxiranes. <i>Chinese Chemical Letters</i> , 2012, 23, 699-702.	4.8	3
108	Mechanical buckling of nanocomposite rectangular plate reinforced by aligned and straight single-walled carbon nanotubes. <i>Composites Part B: Engineering</i> , 2012, 43, 2031-2040.	5.9	145

#	ARTICLE	IF	CITATIONS
109	Theoretical and Quantitative Structural Relationship Study on Fullerenes Polarizabilities on the basis of Monopole-Dipole Interactions Theorem. <i>Oriental Journal of Chemistry</i> , 2012, 28, 247-256.	0.1	0
110	Theoretical and Quantitative Structural Relationships of the Electron Transfer and Electrochemical Properties of <i>Cis</i> -Unsaturated Thiocrown Ethers and Supramolecular Complexes [X-UT-Y]@[La <sub>2</sub> @C <sub>72</sub> (Adamantylidene Mono-Adducts) <sub>n</sub> ] (n=0,1). <i>Fullerenes Nanotubes and Carbon Nanostructures</i> , 2011, 19, 166-181.	1.0	7
111	Theoretical and quantitative structural relationships of the electrochemical properties of <i>Cis</i> -unsaturated thiocrown ethers and n-type material bulk-heterojunction polymer solar cells as supramolecular complexes [X-UT-Y]@R (R=PCBM, <i>p</i> -EHO-PCBM, and <i>p</i> -EHO-PCBA). <i>Journal of Information Display</i> , 2011, 12, 145-152.	2.1	0
112	Theoretical and Quantitative Structural Relationships Studies of Free Energies of Electron Transfer, Electron Transfer Kinetic, and Electrochemical Properties of Metal Nitride Cluster Fullerenes Y <sub>3</sub> N@C <sub>80</sub> Methano Mono Adduct Derivatives in [X-UT-V][Y <sub>3</sub> N@C <sub>80</sub> -[6,6]-Methanofullerene-R] (R = DEM,) <i>Tj ETQq0 0 0 rgBT/Overlock</i> 2011, 3, 213-228.	0.0	0
113	Chemical compositions of the essential oil and calculation the biophysicochemical coefficients of the components of <i>Hymenocrater longiflorus</i> Benth. of Iran. <i>Natural Science</i> , 2011, 03, 104-108.	0.2	3
114	Theoretical and Quantitative Structural Relationships of the Electrochemical Properties of [M@C <sub>82</sub> ]@[SWCNT(5,5)-armchair-C <sub>n</sub> H <sub>20</sub> ] (M = La, Y and n =) <i>Tj ETQq0 0 0 rgBT/Overlock 10 T</i> Chemistry, 2010, 1, P97-P109.	1.5	4
115	Microwave-assisted solid phase conversion study of Meldrum's acid to ethylenetetracarboxylic dianhydride (C <sub>6</sub> O <sub>6</sub> ). <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2010, 75, 493-497.	2.0	1
116	9-azidoacridine and 9-acridinyl nitrene. <i>Journal of Physical Organic Chemistry</i> , 2010, 23, 382-389.	0.9	6
117	Theoretical and Quantitative Structural Relationship Studies of Electrochemical Properties of the Nanostructures of <i>Cis</i> -Unsaturated Thiocrown Ethers and Their Supramolecular Complexes [X-UT-Y][M@C <sub>82</sub> ] (M=Ce, Gd). <i>Phosphorus, Sulfur and Silicon and the Related Elements</i> , 2010, 185, 422-432.	0.8	12
118	Topological Relationship Between Wiener, Padmakar-Ivan, and Szeged Indices and Energy and Electric Moments in Armchair Polyhex Nanotubes with the Same Circumference and Varying Lengths. <i>Fullerenes Nanotubes and Carbon Nanostructures</i> , 2010, 18, 72-86.	1.0	11
119	Structural Relationships and Theoretical Study of Electron Transfer Properties of 1,3,2-Dithiazolyl Radicals with Fullerenes in Nanostructure [1,3,2-DTA(s)]@C <sub>n</sub> Supramolecular Complexes. <i>Phosphorus, Sulfur and Silicon and the Related Elements</i> , 2010, 185, 1604-1614.	0.8	6
120	Structural relationship between photophysical data of 1,3,5-trisubstituted oligoaryleneethynylene benzene star-shaped molecules and number of carbon atoms. <i>Physics and Chemistry of Liquids</i> , 2010, 48, 289-297.	0.4	2
121	Chemical composition of the essential oil of <i>Valeriana alliariifolia</i> Adams of Iran. <i>Natural Product Research</i> , 2010, 24, 973-978.	1.0	12
122	Theoretical Study of Structural Relationships and Electrochemical Properties of Supramolecular [14-MR Macrolides]@C <sub>n</sub> Complexes. <i>Analytical Letters</i> , 2010, 43, 658-673.	1.0	8
123	Structural Relationship Study of Electrochemical Properties of the Nano Structures of <i>Cis</i> -Unsaturated Thiocrown Ethers and Their Supramolecular Complexes [X-UT-Y]@[La@C <sub>72</sub> (C <sub>6</sub> H <sub>3</sub> Cl <sub>2</sub> ) Non-IPR Carbon Cage. <i>Fullerenes Nanotubes and Carbon Nanostructures</i> , 2009, 17, 171-186.	1.0	7
124	Structural Relationship Between Degree of Unsaturation with Fermi Energy, Chemical Hardness, and The HOMO-LUMO Gap of (5,5) Armchair Single-Walled Carbon Nanotubes. <i>Fullerenes Nanotubes and Carbon Nanostructures</i> , 2009, 17, 26-37.	1.0	18
125	Design of decoder in quantum computing based on spin field effect. , 2009, , .		1
126	Relationship study of octanol-water partitioning coefficients and total biodegradation of linear simple conjugated polyene and carotene compounds by use of the Randić index and maximum UV wavelength. <i>Physics and Chemistry of Liquids</i> , 2009, 47, 349-359.	0.4	4

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128	Quantitative structural relationship and theoretical study of electrochemical properties of C <sub>60</sub> @[SWCN(5,5)-Armchair-C <sub>n</sub> H <sub>20</sub> ] complexes. <i>Chemical Physics Letters</i> , 2009, 469, 135-139.	1.2	20
129	Theoretical and quantitative structural relationships of the electrochemical and electron transfer properties of [M <sub>x</sub> @C <sub>82</sub> ]@[SWCNT(5,5)-armchair-C <sub>n</sub> H <sub>20</sub> ] (x=0, 1; for x=1: M=Ce & Gd and n=20~300) nanostructure complexes. <i>Chemical Physics Letters</i> , 2009, 483, 233-240.	1.2	12
130	Theoretical and Quantitative Structural Relationship Study of the Electrochemical Properties of [M <sub>2</sub> @C <sub>x</sub> ]@[SWCNT(5,5)-Armchair-C <sub>n</sub> H <sub>20</sub> ] (M = Er and Sc, x = 82 and 84, and n = 20~300) Complexes. <i>Journal of Physical Chemistry C</i> , 2009, 113, 5402-5408.	1.5	20
131	Theoretical Study of Structural Relationships and Electrochemical Properties of Supramolecular [Tetracyclines].C <sub>n</sub> Complexes. <i>Fullerenes Nanotubes and Carbon Nanostructures</i> , 2009, 17, 636-651.	1.0	5
132	Computational note on ab initio studies of 1,3-dipolar cycloaddition reactions between 7~10 membered simple cycloalkynes and nitroxide. <i>Computational and Theoretical Chemistry</i> , 2008, 849, 23-24.	1.5	10
133	Quantitative Relationship Study of Mechanical Structure Properties of Empty Fullerenes. <i>Fullerenes Nanotubes and Carbon Nanostructures</i> , 2008, 16, 196-205.	1.0	21
134	Chemical composition of the essential oil of <i>Thalectrum minus</i> L. of Iran. <i>Natural Product Research</i> , 2008, 22, 97-100.	1.0	5
135	Quantitative Structural Relationship Study of Electrochemical Properties on the Nano Structures of Cis-Unsaturated Thiocrown Ethers and Their Supramolecular Complexes [X@C <sub>84</sub> ] and [X@C <sub>82</sub> ]. <i>Fullerenes Nanotubes and Carbon Nanostructures</i> , 2008, 16, 142-153.	1.0	9
136	One-pot Microwave-Assisted Synthesis of 1H-Phenanthro[9,10-d][1,2,3]triazole. <i>MolBank</i> , 2008, 2008, M577.	0.2	4
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139	Chemical composition of the essential oil of <i>Pelargonium quercetorum</i> Agnew. of Iran. <i>Natural Product Research</i> , 2007, 21, 24-27.	1.0	11
140	Carboxyketenes from 4-Hydroxy-1,3-oxazin-6-ones and Meldrum's Acid Derivatives. <i>Journal of Organic Chemistry</i> , 2007, 72, 1399-1404.	1.7	21
141	The structural relationship between Randić indices, adjacency matrixes, distance matrixes and maximum wave length of linear simple conjugated polyene compounds. <i>Computational and Theoretical Chemistry</i> , 2005, 726, 183-188.	1.5	37
142	AM1 study of conformational properties of cyclohexaketene and expanded cyclohexaketenes. <i>Computational and Theoretical Chemistry</i> , 1999, 488, 141-149.	1.5	4
143	Conformational properties of simple monocyclic conjugated enediynes. <i>Computational and Theoretical Chemistry</i> , 1998, 422, 213-218.	1.5	4
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