Haydar Raissi

List of Publications by Year
in descending order

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Version: 2024-02-01

175	3,516	117625	223800
papers	citations	34	46
		h-index	g-index

176	176	176	2185
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Understanding loading, diffusion and releasing of Doxorubicin and Paclitaxel dual delivery in graphene and graphene oxide carriers as highly efficient drug delivery systems. Applied Surface Science, 2020, 500, 144220.	6.1	88
2	Assessment of the adsorption mechanism of Flutamide anticancer drug on the functionalized single-walled carbon nanotube surface as a drug delivery vehicle: An alternative theoretical approach based on DFT and MD. Applied Surface Science, 2018, 434, 492-503.	6.1	87
3	DFT Calculations and Molecular Dynamics Simulation Study on the Adsorption of 5-Fluorouracil Anticancer Drug on Graphene Oxide Nanosheet as a Drug Delivery Vehicle. Journal of Inorganic and Organometallic Polymers and Materials, 2017, 27, 805-817.	3.7	80
4	The presentation of an approach for estimating the intramolecular hydrogen bond strength in conformational study of β^2-Aminoacrolein. Computational and Theoretical Chemistry, 2005, 730, 161-169.	1.5	79
5	The hybrid of Pd and SWCNT (Pd loaded on SWCNT) as an efficient sensor for the formaldehyde molecule detection: A DFT study. Sensors and Actuators B: Chemical, 2015, 212, 55-62.	7.8	75
6	Covalent organic framework as smart and high efficient carrier for anticancer drug delivery: a DFT calculations and molecular dynamics simulation study. Journal Physics D: Applied Physics, 2018, 51, 345401.	2.8	73
7	On the pseudocapacitive behavior of nanostructured molybdenum oxide. Journal of Solid State Electrochemistry, 2010, 14, 643-650.	2.5	60
8	Theoretical study of solvent and co-solvent effects on the interaction of Flutamide anticancer drug with Carbon nanotube as a drug delivery system. Journal of Molecular Liquids, 2017, 248, 490-500.	4.9	60
9	Screening of the structural, topological, and electronic properties of the functionalized Graphene nanosheets as potential Tegafur anticancer drug carriers using DFT method. Journal of Biomolecular Structure and Dynamics, 2018, 36, 2517-2529.	3.5	60
10	Density functional theory calculations and molecular dynamics simulations of the adsorption of ellipticine anticancer drug on graphene oxide surface in aqueous medium as well as under controlled pH conditions. Journal of Molecular Liquids, 2018, 255, 269-278.	4.9	56
11	Comparative optical and electrochemical studies of nanostructured NiTiO3 and NiTiO3-TiO2 prepared by a low temperature modified Sol-Gel route. Electrochimica Acta, 2014, 132, 512-523.	5.2	55
12	Solvent/co-solvent effects on the electronic properties and adsorption mechanism of anticancer drug Thioguanine on Graphene oxide surface as a nanocarrier: Density functional theory investigation and a molecular dynamics. Applied Surface Science, 2017, 422, 1030-1041.	6.1	55
13	Solvent effects on the stability and the electronic properties of histidine/Pd-doped single-walled carbon nanotube biosensor. Journal of Molecular Liquids, 2016, 214, 313-318.	4.9	53
14	Investigation of the solvent effect, molecular structure, electronic properties and adsorption mechanism of Tegafur anticancer drug on Graphene nanosheet surface as drug delivery system by molecular dynamics simulation and density functional approach. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2017, 88, 159-169.	1.6	53
15	Assessment of solvent effects on the interaction of Carmustine drug with the pristine and COOH-functionalized single-walled carbon nanotubes: A DFT perspective. Journal of Molecular Liquids, 2017, 240, 87-97.	4.9	52
16	The functionalization of carbon nanotubes to enhance the efficacy of the anticancer drug paclitaxel: a molecular dynamics simulation study. Journal of Molecular Modeling, 2017, 23, 222.	1.8	52
17	DFT and MD investigations on the functionalized boron nitride nanotube as an effective drug delivery carrier for Carmustine anticancer drug. Journal of Molecular Liquids, 2019, 276, 577-587.	4.9	49
18	Immunosuppressive agent leflunomide: A SWNTs-immobilized dihydroortate dehydrogenase inhibitory effect and computational study of its adsorption properties on zigzag single walled (6,0) carbon and boron nitride nanotubes as controlled drug delivery devices. European Journal of Pharmaceutical Sciences, 2014, 56, 37-54.	4.0	46

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19	Grafting of a chiral Mn(iii) complex on graphene oxide nanosheets and its catalytic activity for alkene epoxidation. RSC Advances, 2014, 4, 26087.	3.6	45
20	Reinvestigation of intramolecular hydrogen bond in malonaldehyde derivatives: An ab initio, AIM and NBO study. International Journal of Quantum Chemistry, 2011, 111, 3040-3047.	2.0	42
21	Substituent effect on structure, electron density, and intramolecular hydrogen bonding in nitrosoâ€oxime methane. International Journal of Quantum Chemistry, 2011, 111, 3505-3516.	2.0	41
22	Theoretical Description of Substituent Effects in 2,4-Pentanedione: AIM, NBO, and NMR Study. Bulletin of the Chemical Society of Japan, 2012, 85, 87-92.	3.2	41
23	Electronic structures, intramolecular interactions, and aromaticity of substituted 1-(2-iminoethylidene) silan amine: a density functional study. Structural Chemistry, 2013, 24, 123-137.	2.0	41
24	The effects of substitutions on structure, electron density, resonance and intramolecular hydrogen bonding strength in 3-mercapto-propenethial. Computational and Theoretical Chemistry, 2010, 960, 1-9.	1.5	40
25	Investigation of graphene-based nanomaterial as nanocarrier for adsorption of paclitaxel anticancer drug: a molecular dynamics simulation study. Journal of Molecular Modeling, 2017, 23, 36.	1.8	40
26	Strong intramolecular hydrogen bond in triformylmethane ab-initio, AIM and NBO study. Computational and Theoretical Chemistry, 2006, 759, 93-100.	1.5	38
27	The effect of substitution on the intramolecular hydrogen bonding in 3â€hydroxyâ€propenethial. International Journal of Quantum Chemistry, 2008, 108, 1444-1451.	2.0	38
28	Ab initio and DFT computational studies on molecular conformations and strength of the intramolecular hydrogen bond in different conformers of 3-amino-2-iminomethyl acryl aldehyde. Computational and Theoretical Chemistry, 2011, 966, 299-305.	2.5	38
29	Comprehensive study of the interaction between hydrogen halides and methanol derivatives. International Journal of Quantum Chemistry, 2012, 112, 2782-2786.	2.0	37
30	The analysis of electronic structures, adsorption properties, NBO, QTAIM and NMR parameters of the adsorbed hydrogen sulfide on various sites of the outer surface of aluminum phosphide nanotube: a DFT study. Structural Chemistry, 2015, 26, 1059-1075.	2.0	37
31	A theoretical study on the structure of 2-amino-1,3,4-thiadiazole and its 5-substituted derivatives in the gas phase, water, THF and DMSO solutions. Journal of Molecular Liquids, 2015, 203, 137-142.	4.9	37
32	Molecular dynamics simulation and quantum chemical studies on the investigation of aluminum nitride nanotube as phosgene gas sensor. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2016, 86, 305-322.	1.6	37
33	Understanding co-loading of doxorubicin and camptothecin on graphene and folic acid-conjugated graphene for targeting drug delivery: classical MD simulation and DFT calculation. Journal of Biomolecular Structure and Dynamics, 2020, 38, 2737-2745.	3.5	36
34	Conformational study of the (z)-[(2-iminoethylidone)silyl]amine at the MP2, DFT and G2MP2 levels. Computational and Theoretical Chemistry, 2012, 983, 1-6.	2.5	35
35	Ab initio and DFT studies on 1-(thionitrosomethylene) hydrazine: conformers, energies, and intramolecular hydrogen-bond strength. Structural Chemistry, 2013, 24, 1121-1133.	2.0	35
36	Hydrogen bond studies in substituted imino-acetaldehyde oxime. Computational and Theoretical Chemistry, 2012, 996, 68-75.	2.5	34

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37	Investigation of the molecular structure, electronic properties, AIM, NBO, NMR and NQR parameters for the interaction of Sc, Ga and Mg-doped (6,0) aluminum nitride nanotubes with COCl2 gas by DFT study. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2016, 84, 99-114.	1.6	34
38	Molecular structure and vibrational assignment of (trifluoroacetyl) acetone: A density functional study. Journal of Molecular Structure, 2006, 787, 148-162.	3.6	33
39	Assessment of the chitosan-functionalized graphene oxide as a carrier for loading thioguanine, an antitumor drug and effect of urea on adsorption process: Combination of DFT computational and molecular dynamics simulation studies. Journal of Biomolecular Structure and Dynamics, 2019, 37, 2487-2497.	3.5	31
40	Factors affecting the reactivity and selectivity in the oxidation of sulfides with tetra-n-butylammonium peroxomonosulfate catalyzed by Mn(III) porphyrins: Significant nitrogen donor effects. Polyhedron, 2011, 30, 592-598.	2.2	30
41	Payload delivery of anticancer drug Tegafur with the assistance of graphene oxide nanosheet during biomembrane penetration: Molecular dynamics simulation survey. Applied Surface Science, 2020, 517, 146186.	6.1	29
42	Assessment of solvent effects on the inclusion behavior of pyrazinamide drug into cyclic peptide based nanotubes as novel drug delivery vehicles. Journal of Molecular Liquids, 2018, 268, 326-334.	4.9	28
43	The computational study of the Î³-Fe‹sub›2‹/sub›O‹sub›3‹/sub› nanoparticle as Carmustine drug delivery system: DFT approach. Journal of Biomolecular Structure and Dynamics, 2019, 37, 454-464.	3.5	28
44	The pH effects on the capacitive behavior of nanostructured molybdenum oxide. Journal of Solid State Electrochemistry, 2010, 14, 681-686.	2.5	26
45	Economical Oxygenation of Olefins and Sulfides Catalyzed by New Molybdenum(VI) Tridentate Schiff Base Complexes: Synthesis and Crystal Structure. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2012, 638, 1023-1030.	1.2	26
46	Loading and release of anticancer drug from phosphorene as a template material with high efficient carrier: From vacuum to cell membrane. Journal of Molecular Liquids, 2019, 291, 111346.	4.9	26
47	Comparative prediction of binding affinity of Hydroxyurea anti-cancer to boron nitride and carbon nanotubes as smart targeted drug delivery vehicles. Journal of Biomolecular Structure and Dynamics, 2019, 37, 4852-4862.	3.5	26
48	Probing the adsorption and release mechanisms of cytarabine anticancer drug on/from dopamine functionalized graphene oxide as a highly efficient drug delivery system. Journal of Molecular Liquids, 2020, 301, 112458.	4.9	26
49	Synergistic flotation of U(VI)â€“alizarin complex with some diamines followed by spectrophotometric determination of U(VI) using 4,4â€²-diaminophenylmethane. Analytica Chimica Acta, 2006, 559, 181-185.	5.4	25
50	Molecular structure and bonding character of mono and divalent metal cations (Li+, Na+, K+, Be2+,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5 Chemistry, 2014, 25, 1327-1342.	2.0	25
51	Electronic structures, intramolecular hydrogen bond interaction, and aromaticity of substituted 4-amino-3-penten-2-one in ground and electronic excited state. Structural Chemistry, 2015, 26, 491-506.	2.0	25
52	Predicting doxorubicin drug delivery by single-walled carbon nanotube through cell membrane in the absence and presence of nicotine molecules: a molecular dynamics simulation study. Journal of Biomolecular Structure and Dynamics, 2020, 38, 1488-1498.	3.5	25
53	Investigation of the Pristine and Functionalized Carbon Nanotubes as a Delivery System for the Anticancer Drug Dacarbazine: Drug Encapsulation. Journal of Pharmaceutical Sciences, 2021, 110, 2005-2016.	3.3	25
54	Vibrational assignment of 4-amino-3-penten-2-one. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2002, 58, 1681-1695.	3.9	24

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55	Using molecular dynamics simulation to explore the binding of the three potent anticancer drugs sorafenib, streptozotocin, and sunitinib to functionalized carbon nanotubes. Journal of Molecular Modeling, 2019, 25, 159.	1.8	24
56	Stabilization of d-lactate dehydrogenase diagnostic enzyme via immobilization on pristine and carboxyl-functionalized carbon nanotubes, a combined experimental and molecular dynamics simulation study. Archives of Biochemistry and Biophysics, 2019, 661, 178-186.	3.0	24
57	The influence of nicotine on pioglitazone encapsulation into carbon nanotube: the investigation of molecular dynamic and density functional theory. Journal of Biomolecular Structure and Dynamics, 2017, 35, 520-534.	3.5	23
58	A combined molecular dynamics simulation and quantum mechanics study on mercaptopurine interaction with the cucurbit [6,7] urils: Analysis of electronic structure. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 188, 647-658.	3.9	23
59	Vibrational assignment of aluminum(III) Trisâ€“acetylacetone. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2002, 58, 2669-2682.	3.9	22
60	Interactions of the 5-fluorouracil anticancer drug with DNA pyrimidine bases: a detailed computational approach. Structural Chemistry, 2016, 27, 487-504.	2.0	22
61	Theoretical elucidation of the amino acid interaction with graphene and functionalized graphene nanosheets: insights from DFT calculation and MD simulation. Amino Acids, 2020, 52, 1465-1478.	2.7	22
62	Comprehensive theoretical prediction of the dynamics and stability properties of Tegafur pharmaceutical agent on the Graphene based nanostructures in aqueous environment. Applied Surface Science, 2018, 455, 32-36.	6.1	21
63	Probing the effect of polyethene glycol on the adsorption mechanisms of Gem on the hexagonal boron nitride as a highly efficient polymer-based drug delivery system: DFT, classical MD and Well-tempered Metadynamics simulations. Journal of Molecular Graphics and Modelling, 2020, 98, 107613.	2.4	21
64	Modeling the interaction between anti-cancer drug penicillamine and pristine and functionalized carbon nanotubes for medical applications: density functional theory investigation and a molecular dynamics simulation. Journal of Biomolecular Structure and Dynamics, 2020, 38, 1322-1334.	3.5	20
65	An approach to estimate the energy and strength of the intramolecular hydrogen bond in different conformers of 4-methylamino-3-penten-2-one. International Journal of Quantum Chemistry, 2007, 107, 1835-1845.	2.0	19
66	Intramolecular hydrogen bonding in derivatives of 3â€aminoâ€propenethial. International Journal of Quantum Chemistry, 2009, 109, 1497-1504.	2.0	19
67	Intramolecular hydrogen bonding in structural conformers of 2â€amino methylene malonaldehyde: AIM and NBO studies. International Journal of Quantum Chemistry, 2010, 110, 821-830.	2.0	19
68	Hydrogen bonding in acetylacetaldehyde: Theoretical insights from the theory of atoms in molecules. International Journal of Quantum Chemistry, 2009, 109, 1505-1514.	2.0	19
69	DFT and MD study of adsorption sensitivity of aluminium phosphide nanotube towards some air pollutant gas molecules. Molecular Simulation, 2017, 43, 675-690.	2.0	19
70	Understanding the effect of vitamin B6 and PEG functionalization on improving the performance of carbon nanotubes in temozolomide anticancer drug transportation. Journal Physics D: Applied Physics, 2019, 52, 395402.	2.8	19
71	Design of a new drug delivery platform based on surface functionalization 2D covalent organic frameworks. Journal of the Taiwan Institute of Chemical Engineers, 2021, 125, 15-22.	5.3	19
72	Vibrational assignment, structure and intramolecular hydrogen bond study of 3-amino-1-phenyl-2-buten-1-one. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2006, 63, 729-739.	3.9	18

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73	Î²â€Aminoacrolein: An ab initio, AIM and NBO study. International Journal of Quantum Chemistry, 2008, 108, 383-390.	2.0	18
74	Ab initioand DFT computational studies on molecular conformations and intramolecular hydrogen bonding in 3-mercapto-but-2-enethial. Journal of Sulfur Chemistry, 2010, 31, 275-285.	2.0	18
75	Substituent effect on the reaction mechanism of proton transfer in formamide. International Journal of Quantum Chemistry, 2012, 112, 2378-2381.	2.0	18
76	Designing a high-performance smart drug delivery system for the synergetic co-absorption of DOX and EGCG on ZIF-8. RSC Advances, 2020, 10, 44533-44544.	3.6	18
77	Theoretical study of the effects of substitution, solvation, and structure on the interaction between nitriles and methanol. International Journal of Quantum Chemistry, 2012, 112, 1273-1284.	2.0	17
78	Carbon and boron nanotubes as a template material for adsorption of 6-Thioguanine chemotherapeutic: a molecular dynamics and density functional approach. Journal of Biomolecular Structure and Dynamics, 2020, 38, 697-707.	3.5	17
79	DFT study of Ni-doped graphene nanosheet as a drug carrier for multiple sclerosis drugs. Computational and Theoretical Chemistry, 2021, 1196, 113114.	2.5	17
80	ANALYSIS OF THE INTRA-MOLECULAR HYDROGEN BOND STRENGTH IN 3-HYDROXY-PROPENETHIAL (HPT). Journal of Theoretical and Computational Chemistry, 2009, 08, 713-732.	1.8	16
81	Investigation of nanotubes as the smart carriers for targeted delivery of mercaptopurine anticancer drug. Journal of Biomolecular Structure and Dynamics, 2022, 40, 4579-4592.	3.5	16
82	OHâ‹¯S intramolecular hydrogen bond in thiomalonaldehyde derivatives; a quantum chemical study. Computational and Theoretical Chemistry, 2011, 963, 517-524.	2.5	15
83	Enhance the efficiency of 5-fluorouracil targeted delivery by using a prodrug approach as a novel strategy for prolonged circulation time and improved permeation. International Journal of Pharmaceutics, 2019, 568, 118491.	5.2	15
84	DFT computational study towards investigating Cladribine anticancer drug adsorption on the graphene and functionalized graphene. Structural Chemistry, 2020, 31, 1691-1705.	2.0	15
85	Intramolecular hydrogen bond, molecular structure and vibrational assignment of tetra-acetylethane. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2006, 65, 605-615.	3.9	14
86	The effect of formation of second hydrogen bond in adjacent two-ring resonance-assisted hydrogen bonds â€“ Ab initio and QTAIM studies. Computational and Theoretical Chemistry, 2010, 942, 115-120.	1.5	14
87	THE EFFECT OF SUBSTITUTION ON STRUCTURE, INTRAMOLECULAR HYDROGEN BONDING STRENGTH, ELECTRON DENSITY AND RESONANCE IN 3-AMINO 2-IMINOMETHYL ACRYL ALDEHYDE. Journal of Theoretical and Computational Chemistry, 2012, 11, 925-939.	1.8	14
88	A density functional theory-based analysis of the structural, topological and electronic properties of gemcitabine drug adsorption on the pyrrolidine functionalized single-walled carbon nanotube. Journal of Biomolecular Structure and Dynamics, 2019, 37, 2477-2486.	3.5	14
89	Conformational study, molecular structure, and S^{â€¦}Hâ€™N, Sâ€™H^{â€¦}N intramolecular hydrogen bond in thioformyl-3-aminoacrylaldehyde. Journal of Sulfur Chemistry, 2012, 33, 75-85.	2.0	13
90	Solvent effects on the structural, electronic properties and intramolecular Nâ€“H O hydrogen bond strength of 5-aminomethylene-pyrimidine-2,4,6 trion with DFT calculations. Journal of Molecular Liquids, 2016, 215, 77-87.	4.9	13

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91	Assessment of DFT Calculations and Molecular Dynamics Simulation on the Application of Zinc Oxide Nanotube as Hydrogen Cyanide Gas Sensor. Journal of Inorganic and Organometallic Polymers and Materials, 2017, 27, 1878-1885.	3.7	13
92	Adsorption of Ampyra anticancer drug on the graphene and functionalized graphene as template materials with high efficient carrier. Adsorption, 2020, 26, 879-893.	3.0	13
93	Effect of substitution on the intramolecular hydrogen bonding of 4-amino-3-penten-2-one: Ab initio, AIM and NBO studies. Computational and Theoretical Chemistry, 2007, 847, 47-51.	1.5	12
94	Theoretical study on Î²-aminoacroleine; Density functional theory, atoms in molecules theory and natural bond orbitals studies. Journal of Chemical Sciences, 2012, 124, 731-739.	1.5	12
95	Density functional theory study towards investigating the adsorption properties of the Î³-Fe2O3 nanoparticles as a nanocarrier for delivery of Flutamide anticancer drug. Adsorption, 2020, 26, 925-939.	3.0	12
96	Vibrational assignment and structure of 3-(4-methoxyphenyl)pentane-2,4-dione. Journal of Molecular Structure, 2005, 752, 130-143.	3.6	11
97	Evaluation of the origin of conformational and tautomeric preferences inNâ€formylformamide â€“ A quantum chemical study. International Journal of Quantum Chemistry, 2012, 112, 489-497.	2.0	11
98	A Theoretical DFT Study on the Structural Parameters and Intramolecular Hydrogen-Bond Strength in Substituted (Z)-N-(Thionitrosomethylene)thiohydroxylamine Systems. Bulletin of the Chemical Society of Japan, 2013, 86, 1261-1271.	3.2	11
99	The analysis of structural and electronic properties for assessment of intramolecular hydrogen bond (IMHB) interaction: a comprehensive study into the effect of substitution on intramolecular hydrogen bond of 4-nitropyridine-3-thiol in ground and electronic excited state. Structural Chemistry, 2014, 25, 515-538.	2.0	11
100	Evaluation of solvent and ion effects upon leflunomide adsorption characteristics on (6,0) zigzag single-walled carbon nanotube and immobilized dihydroorotate dehydrogenase activity: A computational DFT and experimental study. Journal of Molecular Liquids, 2017, 231, 528-541.	4.9	11
101	Analysis of the structures, energetics, and vibrational frequencies for the hydrogen-bonded interaction of nucleic acid bases with Carmustine pharmaceutical agent: a detailed computational approach. Structural Chemistry, 2018, 29, 1165-1174.	2.0	11
102	Evaluation the synergistic antitumor effect of methotrexateâ€“camptothecin codelivery prodrug from selfâ€assembly process to acidâ€catalyzed both drugs release: A comprehensive theoretical study. Journal of Computational Chemistry, 2020, 41, 1486-1496.	3.3	11
103	Nanotechnology-based approaches for targeting and delivery of drugs via Hexakis (m-PE) macrocycles. Scientific Reports, 2021, 11, 8256.	3.3	11
104	Molecular insights into the loading and dynamics of anticancer drugs on silicene and folic acid-conjugated silicene nanosheets: DFT calculation and MD simulation. Journal of Biomolecular Structure and Dynamics, 2021, 39, 3892-3899.	3.5	11
105	Vibrational assignment, structure and intramolecular hydrogen bond of 4-methylamino-3-penten-2-one. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2005, 62, 1004-1015.	3.9	10
106	Molecular structure, conformational stability, energetic and intramolecular hydrogen bonding in ground, and electronic excited state of 3-mercapto propeneselenal. Structural Chemistry, 2014, 25, 1153-1164.	2.0	10
107	Investigation of adsorption properties of CS2 on interior and exterior surfaces of single-walled silicon-carbide nanotubes and effect of applied electric field: electronic structure, charge density and NMR studies. RSC Advances, 2015, 5, 84022-84037.	3.6	10
108	Theoretical Prediction of Adsorption Properties of Carmustine Drug on Various Sites of the Outer Surface of the Single-Walled Boron Nitride Nanotube and Investigation of Urea Effect on Drug Delivery by DFT and MD. Journal of Cluster Science, 2018, 29, 93-99.	3.3	10

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109	High-performance carbon dioxide capture and storage by multi-functional sphingosine kinase inhibitors through a CO₂-philic membrane. New Journal of Chemistry, 2020, 44, 7771-7779.	2.8	10
110	Conjugation of a smart polymer to doxorubicin through a pH-responsive bond for targeted drug delivery and improving drug loading on graphene oxide. RSC Advances, 2021, 11, 18809-18817.	3.6	10
111	Synthesis of a functionalized tetrahydro-1,4-thiazepine in water as the solvent and theoretical investigation of its tautomeric structures. Monatshefte FÃ¼r Chemie, 2008, 139, 1211-1215.	1.8	9
112	Mild oxidation of alkenes catalyzed by Fe3O4/SiO2 nanoparticles. Reaction Kinetics, Mechanisms and Catalysis, 2014, 112, 397-408.	1.7	9
113	Doped-SiCNT as a promising sensor for detection of CS₂ molecule. Journal of Sulfur Chemistry, 2017, 38, 372-383.	2.0	9
114	Assessment of dynamical properties of mercaptopurine on the peptide-based metalâ€“organic framework in response to experience of external electrical fields: a molecular dynamics simulation. Journal of Molecular Modeling, 2019, 25, 304.	1.8	9
115	Molecular mechanism for the encapsulation of the doxorubicin in the cucurbit[n]urils cavity and the effects of diameter, protonation on loading and releasing of the anticancer drug:Mixed quantum mechanical/ molecular dynamics simulations. Computer Methods and Programs in Biomedicine, 2020, 196, 105563.	4.7	9
116	Design of new drug delivery platform based on surface functionalization of black phosphorus nanosheet with a smart polymer for enhancing the efficiency of doxorubicin in the treatment of cancer. Journal of Biomedical Materials Research - Part A, 2021, 109, 1912-1921.	4.0	9
117	The performance of the single-walled carbon nanotube covalently modified with polyethylene glycol to delivery of Gemcitabine anticancer drug in the aqueous environment. Journal of Biomolecular Structure and Dynamics, 2021, 39, 881-888.	3.5	9
118	Development of the poly(l-histidine) grafted carbon nanotube as a possible smart drug delivery vehicle. Computers in Biology and Medicine, 2022, 143, 105336.	7.0	9
119	Vibrational assignment and structure of 4-amino-3-cyano-3-penten-2-one. Journal of Molecular Structure, 2002, 613, 195-208.	3.6	8
120	Effects of the HCN adsorption on the structural and electronic parameters of the beryllium oxide nanotube. Structural Chemistry, 2016, 27, 557-571.	2.0	8
121	Theoretical investigation insights into the temperature triggered tegafur anticancer drug release from the surface of graphene oxide nanosheet. Journal of Biomolecular Structure and Dynamics, 2020, 38, 2287-2295.	3.5	8
122	Two dimensional porous frameworks of graphyne family as therapeutic delivery vehicles for Idarubicin biomolecule in silico: Density functional theory and molecular dynamics simulation. Journal of Molecular Liquids, 2020, 319, 114334.	4.9	8
123	Understanding dual delivery of doxorubicin and paclitaxel with boron nitride and phosphorene nanosheets as highly efficient drug delivery systems. Journal of Biomolecular Structure and Dynamics, 2021, 39, 5613-5618.	3.5	8
124	Development and evaluation of a pH-responsive and water-soluble drug delivery system based on smart polymer coating of graphene nanosheets: an in silico study. RSC Advances, 2020, 10, 31106-31114.	3.6	8
125	New insights into Hexakis macrocycles as a novel nano-carrier for highly potent anti-cancer treatment: A new challenge in drug delivery. Colloids and Surfaces B: Biointerfaces, 2021, 197, 111402.	5.0	8
126	Molecular interpretation of the carbon nitride performance as a template for the transport of anti-cancer drug into the biological membrane. Scientific Reports, 2021, 11, 18981.	3.3	8

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127	Density functional theory study of the Fourier transform infrared and Raman spectra of Cu(II) bis-acetylacetone. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2005, 62, 343-352.	3.9	7
128	Molecular structure and vibrational assignment of Î±â€chloro acetylacetone: A density functional theory study. International Journal of Quantum Chemistry, 2009, 109, 1481-1496.	2.0	7
129	Nï£¿HÂ·Â·Â·S and Sï£¿HÂ·Â·Â·N intramolecular hydrogen bond in Î²â€thioaminoacrolein: A quantum chemical study. International Journal of Quantum Chemistry, 2011, 111, 3008-3016.	2.0	7
130	A comparative study of openâ€close and related rotamers methods to evaluate the intramolecular hydrogen bond energies in 3â€iminoâ€propenâ€1â€ol and its derivatives. International Journal of Quantum Chemistry, 2012, 112, 1384-1391.	2.0	7
131	CONFORMATIONAL PROPERTIES AND INTRAMOLECULAR HYDROGEN BONDING OF 3-AMINO-PROPENESELENAL: AN AB INITIO AND DENSITY FUNCTIONAL THEORY STUDIES. Journal of Theoretical and Computational Chemistry, 2013, 12, 1350025.	1.8	7
132	Theoretical calculations of intramolecular hydrogen bond of the 2-Amino-2, 4, 6-cycloheptatrien-1-one in the gas phase and solution: Substituent effects and their positions. Journal of Theoretical and Computational Chemistry, 2016, 15, 1650063.	1.8	7
133	Predicting the efficiency of polyethylene glycol-functionalised graphene in delivery of temozolomide anticancer drug and investigating the effect of pH on the drug release process: DFT and free energy calculations. Molecular Simulation, 2020, 46, 1474-1482.	2.0	7
134	The transport of Idarubicin therapeutic agent using a novel graphene sheet as a drug delivery platform through a biomembrane. Journal of Molecular Liquids, 2021, 323, 115050.	4.9	7
135	Investigation into the regioisomeric composition of some fused pyrimidines:¹H NMR and theoretical studies. Journal of Sulfur Chemistry, 2008, 29, 25-30.	2.0	6
136	Synthesis and Theoretical Study of Intramolecular Hydrogen Bond at Two Possible Positions in Pyrazolo[1,2â€b]phthalazine. Chinese Journal of Chemistry, 2012, 30, 779-784.	4.9	6
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