Farzaneh Farzad

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/6412878/publications.pdf

Version: 2024-02-01

37	653	567281	580821
papers	citations	15 h-index	25 g-index

37	37	37	366
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The presentation of an approach for estimating the intramolecular hydrogen bond strength in conformational study of Î²-Aminoacrolein. Computational and Theoretical Chemistry, 2005, 730, 161-169.	1.5	79
2	Assessment of adsorption behavior of 5-fluorouracil and pyrazinamide on carbon nitride and folic acid-conjugated carbon nitride nanosheets for targeting drug delivery. Journal of Molecular Liquids, 2020, 301, 112435.	4.9	42
3	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
4	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
5	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
6	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
7	Molecular structure and vibrational assignment of (trifluoroacetyl) acetone: A density functional study. Journal of Molecular Structure, 2006, 787, 148-162.	3.6	33
8	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
9	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
10	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
11	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
12	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
13	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
14	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
15	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
16	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
17	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
18	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

#	Article	IF	Citations
19	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
20	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
21	Vibrational assignment and structure of 3-(4-methoxyphenyl)pentane-2,4-dione. Journal of Molecular Structure, 2005, 752, 130-143.	3.6	11
22	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
23	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
24	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
25	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
26	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
27	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
28	Molecular dynamics simulation study of Glycine tip-functionalisation of single-walled carbon nanotubes as emerging nanovectors for the delivery of anticancer drugs. Molecular Simulation, 2020, 46, 111-120.	2.0	6
29	Assessment of the effect of external and internal triggers on adsorption and release of paclitaxel from the PEI functionalized silicene nanosheet: A molecular dynamic simulation. Journal of Molecular Graphics and Modelling, 2021, 106, 107930.	2.4	6
30	Cation-pi interaction: A strategy for enhancing the performance of graphene-based drug delivery systems. Inorganic Chemistry Communication, 2022, 141, 109542.	3.9	6
31	Interactions of boron nitride nanosheet with amino acids of differential polarity. Scientific Reports, 2022, 12, .	3.3	5
32	Design of New Materials Based on Functionalization of Cu-BTC for Adsorption and Separation of CH4 and CO2: GCMC and MD Simulations Study. Russian Journal of Physical Chemistry A, 2020, 94, 1415-1421.	0.6	4
33	Surface functionalization of boron nitride nanosheet with folic acid: Toward an enhancement in Doxorubicin anticancer drug loading performance. Journal of Molecular Graphics and Modelling, 2021, 109, 108041.	2.4	4
34	Insights into glyphosate removal efficiency using a new 2D nanomaterial. RSC Advances, 2022, 12, 10154-10161.	3.6	3
35	THEORETICAL INVESTIGATION OF SUBSTITUTION EFFECT ON THE PROTON TRANSFER MECHANISM IN 3-MERCAPTO-PROPENETHIAL. Journal of Theoretical and Computational Chemistry, 2013, 12, 1350045.	1.8	0
36	Quantum chemical studies on molecular conformations, energetic and intramolecular hydrogen bonding in ground and electronic excited state of (thioxosilyl) ethyleneselenol. Journal of Sulfur Chemistry, 2014, 35, 152-163.	2.0	0

#	Article	IF	Citations
37	A strategy toward therapeutic improvement of electric field-sensitive gemcitabine prodrugs in 2D metalâ€“organic frameworks in view of their structure and interactions. Inorganic Chemistry Communication, 2022, , 109281.	3.9	0