Effat Dehghanian

List of Publications by Year
in descending order

18	364	932766 10	887659 17
papers	citations	h-index	g-index

18	18	18	288
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	A novel palladium(II) antitumor agent: Synthesis, characterization, DFT perspective, CT-DNA and BSA interaction studies via in-vitro and in-silico approaches. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 249, 119215.	2.0	52
2	Enhanced ionization of the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi mathvariant="normal">H</mml:mi><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>molecul driven by intense ultrashort laser pulses. Physical Review A, 2010, 81, .	1.0	48
3	Enhanced GROMACS: toward a better numerical simulation framework. Journal of Molecular Modeling, 2019, 25, 355.	0.8	43
4	DNA/BSA binding affinity studies of new Pd(II) complex with S-S and N-N donor mixed ligands via experimental insight and molecular simulation: Preliminary antitumor activity, lipophilicity and DFT perspective. Journal of Molecular Liquids, 2021, 344, 117853.	2.3	35
5	Complex integration steps in decomposition of quantum exponential evolution operators. Chemical Physics Letters, 2006, 419, 346-350.	1.2	33
6	Synthesis and characterization of Pd(II) antitumor complex, DFT calculation and DNA/BSA binding insight through the combined experimental and theoretical aspects. Journal of Molecular Structure, 2021, 1240, 130535.	1.8	31
7	Enhanced ionization of the non-symmetric HeH+ molecule driven by intense ultrashort laser pulses. Journal of Chemical Physics, 2013, 139, 084315.	1.2	23
8	Probing the biomolecular (DNA/BSA) interaction by new Pd(II) complex via in-depth experimental and computational perspectives: synthesis, characterization, cytotoxicity, and DFT approach. Journal of the Iranian Chemical Society, 2022, 19, 3155-3175.	1.2	21
9	Hierarchy cuckoo search algorithm for parameter estimation in biological systems. Chemometrics and Intelligent Laboratory Systems, 2016, 159, 97-107.	1.8	19
10	Biological activity of bis-(morpholineacetato)palladium(II) complex: Preparation, structural elucidation, cytotoxicity, DNA-/serum albumin-interaction, density functional theory, in-silico prediction and molecular modeling. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2022, 281, 121543.	2.0	19
11	A couple of antitumor Pd(II) complexes make DNA-refolding and HSA-unfolding: Experimental and docking studies. Journal of Molecular Liquids, 2022, 349, 118450.	2.3	10
12	Comparison of single best artificial neural network and neural network ensemble in modeling of palladium microextraction. Monatshefte FÃ¼r Chemie, 2015, 146, 1217-1227.	0.9	9
13	Probing the interaction of new and biologically active Pd(II) complex with DNA/BSA via joint experimental and computational studies along with thermodynamic, NLO, FMO and NBO analysis. BioMetals, 2022, 35, 245-266.	1.8	6
14	A multiobjective approach in constructing a predictive model for Fischerâ€Tropsch synthesis. Journal of Chemometrics, 2018, 32, e2969.	0.7	4
15	Cuckoo search algorithm and its application for secondary protein structure prediction. , 2015, , .		3
16	Diverse coordination of dipicolinic acid to Pd(II) ion result antitumor complexes, their interaction with CT-DNA by spectroscopic experiments and computational methods. Journal of Molecular Structure, 2022, 1261, 132937.	1.8	3
17	Synthesis, characterization, cytotoxicity and DNA/BSA binding of two amino acid palladium(II) complexes derived from alanine and valine. Nucleosides, Nucleotides and Nucleic Acids, 2022, 41, 97-122.	0.4	3
18	A modified binary particle swarm optimization with a machine learning algorithm and molecular docking for QSAR modelling of cholinesterase inhibitors. SAR and QSAR in Environmental Research, 2021, 32, 745-767.	1.0	2