Pradeep Kumar Shukla

List of Publications by Year
in descending order

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39	430	840119 11	752256 20
papers	citations	h-index	g-index

40	40	40	567
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Formation of bifunctional cross-linked products due to reaction of NAMI-A with DNA bases â€“ a DFT study. Structural Chemistry, 2022, 33, 807-814.	1.0	0
2	Synthesis of a Pyridone-Based Phthalimide Fleximer and Its Characterization and Supramolecular Property Evaluation. ACS Omega, 2022, 7, 24485-24497.	1.6	4
3	Adsorption of HOOO. radical on pristine and doped grapheneâ€"a first-principles study. Structural Chemistry, 2021, 32, 1171-1179.	1.0	3
4	Effect of N7-methylation on base pairing patterns of guanine: a DFT study. Journal of Molecular Modeling, 2021, 27, 184.	0.8	0
5	Green synthesis, structural analysis and anticancer activity of dihydropyrimidinone derivatives. RSC Advances, 2021, 11, 35737-35753.	1.7	15
6	Effect of axial ligands on the mechanisms of action of Ru(III) complexes structurally similar to NAMI-A: a DFT study. Structural Chemistry, 2020, 31, 679-689.	1.0	7
7	meso-Thiophenium Porphyrins and Their Zn(II) Complexes: A New Category of Cationic Photosensitizers. ACS Medicinal Chemistry Letters, 2020, 11, 2041-2047.	1.3	13
8	Photodynamic activity attained through the ruptured Ï€-conjugation of pyridyl groups with a porphyrin macrocycle: synthesis and the photophysical and photobiological evaluation of 5-mono-(4-nitrophenyl)-10,15,20-tris-[4-(phenoxymethyl)pyridine]-porphyrin and its Zn(ii) complex. Photochemical and Photobiological Sciences, 2020, 19, 1776-1789.	1.6	3
9	A DFT study of reactions of Ru(III) anticancer drug KP1019 with 8-oxoguanine and 8-oxoadenine. Structural Chemistry, 2020, 31, 2087-2092.	1.0	1
10	A theoretical characterization of reactions of HOOO radical with guanine: formation of 8-oxoguanine. Structural Chemistry, 2018, 29, 1109-1118.	1.0	6
11	Does 8-Nitroguanine Form 8-Oxoguanine? An Insight from Its Reaction with ^{â€¢}OH Radical. Journal of Physical Chemistry B, 2018, 122, 1852-1861.	1.2	5
12	Methylation of DNA bases by methyl free radicals: mechanism of formation of C8-methylguanine. Structural Chemistry, 2018, 29, 1333-1340.	1.0	1
13	Mechanism of methylation of 8-oxoguanine due to its reaction with methyldiazonium ion. Molecular Simulation, 2017, 43, 196-204.	0.9	5
14	Mechanisms of reactions of Ru(<scp>iii</scp>)-based drug NAMI-A and its aquated products with DNA purine bases: a DFT study. RSC Advances, 2016, 6, 113620-113629.	1.7	8
15	Ring Substituents Mediate the Morphology of PBDTTPD-PCBM Bulk-Heterojunction Solar Cells. Chemistry of Materials, 2014, 26, 2299-2306.	3.2	119
16	A DFT study of reactions of methyldiazonium ion with DNA/RNA nucleosides: Investigating effect of sugar moiety on methylation pattern of bases. International Journal of Quantum Chemistry, 2014, 114, 1637-1644.	1.0	7
17	Base pairing patterns of DNA base lesion spiroiminodihydantoin: A DFT study. International Journal of Quantum Chemistry, 2013, 113, 2600-2604.	1.0	5
18	A quantum theoretical study of reactions of methyldiazonium ion with DNA base pairs. Chemical Physics, 2011, 388, 31-37.	0.9	8

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19	Hydrogen atom abstraction reactions of the sugar moiety of 2â€²â€deoxyguanosine with an OH radical: A quantum chemical study. International Journal of Quantum Chemistry, 2011, 111, 2160-2169.	1.0	11
20	A quantum chemical study of reactions of DNA bases with sulphur mustard: a chemical warfare agent. Theoretical Chemistry Accounts, 2010, 125, 269-278.	0.5	13
21	Reactions of the OOH radical with guanine: Mechanisms of formation of 8-oxoguanine and other products. Chemical Physics, 2010, 375, 118-129.	0.9	16
22	Effects of diameter, length, chirality and defects on the scavenging action of single-walled carbon nanotubes for OH radicals: A quantum computational study. Chemical Physics, 2010, 369, 101-107.	0.9	13
23	Binding of Urea and Thiourea with a Barbiturate Derivative: Experimental and Theoretical Approach. Journal of Physical Chemistry A, 2010, 114, 97-104.	1.1	16
24	O6-Methylguanine Repair by O6-Alkylguanine-DNA Alkyltransferase. Journal of Physical Chemistry B, 2009, 113, 16285-16290.	1.2	14
25	Repair of O6-methylguanine to guanine by cysteine in the absence and presence of histidine and by cysteine thiolate anion: a quantum chemical study. Physical Chemistry Chemical Physics, 2009, 11, 8191.	1.3	15
26	DNA Lesions Caused by ROS and RNOS: A Review of Interactions and Reactions Involving Guanine. , 2009, , 415-443.		2
27	Improved electrostatic properties using combined Mulliken and hybridization-displaced charges for radicals. Journal of Molecular Modeling, 2008, 14, 631-640.	0.8	9
28	Reactions of NO2Cl with Imidazole: A Model Study for the Corresponding Reactions of Guanine. Journal of Physical Chemistry B, 2008, 112, 7925-7936.	1.2	11
29	Catalytic Involvement of CO₂ in the Mutagenesis Caused by Reactions of ONOO⁻ with Guanine. Journal of Physical Chemistry B, 2008, 112, 4779-4789.	1.2	25
30	H2O3as a Reactive Oxygen Species:Â Formation of 8-Oxoguanine from Its Reaction with Guanine. Journal of Physical Chemistry B, 2007, 111, 4603-4615.	1.2	25
31	Reactions of DNA bases with the anti-cancer nitrogen mustard mechlorethamine: A quantum chemical study. Chemical Physics Letters, 2007, 449, 323-328.	1.2	30
32	Reactions of guanine with methyl chloride and methyl bromide: O6-methylation versus charge transfer complex formation. International Journal of Quantum Chemistry, 2007, 107, 1270-1283.	1.0	14
33	Effect of the earth's conductivity on the radiation characteristics of monopole antenna â€. International Journal of Electronics, 1972, 32, 505-511.	0.9	1
34	Radiation resistance of a cylindrical antenna radiating in weakly ionized plasmaâ€. International Journal of Electronics, 1972, 32, 147-152.	0.9	2
35	Reflection of microwave through laboratory plasmaâ€. International Journal of Electronics, 1972, 33, 91-95.	0.9	1
36	Heating of Electrons in Weakly Ionized Plasma by Magnetic Perturbation. IETE Journal of Research, 1970, 16, 690-695.	1.8	0

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37	Effective Collision Frequency and Radio Frequency Conductivity in the Magnetosphere. IETE Journal of Research, 1970, 16, 616-621.	1.8	1
38	Effect of electron collisions on ÄŒerenkov radiation from magnetoplasmaâ€. International Journal of Electronics, 1970, 28, 421-425.	0.9	0
39	Effect of plasma inhomogeneity and drifting plasma on synchrotron radiation from magnetoplasmaâ€. International Journal of Electronics, 1970, 29, 369-375.	0.9	1