Sadasivam K

List of Publications by Year in descending order

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933447 839539 22 432 10 18 h-index citations g-index papers 22 22 22 511 all docs docs citations times ranked citing authors

#	Article	IF	CITATIONS
1	Antioxidant behavior of mearnsetin and myricetin flavonoid compounds â€" A DFT study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 79, 282-293.	3.9	77
2	Antioxidant potential of orientin: A combined experimental and DFT approach. Journal of Molecular Structure, 2014, 1061, 114-123.	3.6	75
3	A comparative DFT study on the antioxidant activity of apigenin and scutellarein flavonoid compounds. Molecular Physics, 2011, 109, 839-852.	1.7	53
4	Experimental and DFT studies on the antioxidant activity of a C-glycoside from Rhynchosia capitata. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 103, 442-452.	3.9	50
5	Theoretical investigation on the antioxidant behavior of chrysoeriol and hispidulin flavonoid compounds – A DFT study. Computational and Theoretical Chemistry, 2011, 963, 227-235.	2.5	46
6	DFT study of glycosyl group reactivity in quercetin derivatives. Journal of Molecular Structure, 2016, 1120, 15-24.	3.6	26
7	Experimental and theoretical investigations on the antioxidant activity of isoorientin from Crotalaria globosa. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 121, 737-745.	3.9	21
8	A DFT STUDY ON THE ROLE OF DIFFERENT OH GROUPS IN THE RADICAL SCAVENGING PROCESS. Journal of Theoretical and Computational Chemistry, 2012, 11, 871-893.	1.8	20
9	DFT studies on antioxidant mechanisms, electronic properties, spectroscopic (FT-IR and UV) and NBO analysis of C-glycosyl flavone, an isoorientin. Journal of Molecular Structure, 2015, 1082, 131-142.	3.6	20
10	Experimental and theoretical investigation of p–n alkoxy benzoic acid based liquid crystals – A DFT approach. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 123, 511-523.	3.9	18
11	Target prediction and antioxidant analysis on isoflavones of demethyltexasin: a DFT study. Journal of Molecular Modeling, 2019, 25, 169.	1.8	6
12	Theoretical assessment of antioxidant property of polyproponoid and its derivatives. Structural Chemistry, 2020, 31, 1089-1094.	2.0	5
13	TD-DFT, NBO analyses, electronic and NLO properties of hydrogen-bonded undecyloxy benzoic acid with suberic acid mesogen. Molecular Crystals and Liquid Crystals, 2017, 650, 65-79.	0.9	4
14	Theoretical simulations on the antioxidant mechanism of naturally occurring flavonoid: A DFT approach. AIP Conference Proceedings, 2016, , .	0.4	3
15	Comparison of radical scavenging behavior of chromones dihydrogenistein and demethyltexasin—a DFT approach. Structural Chemistry, 2019, 30, 167-173.	2.0	2
16	Density functional theory calculations for interactions of 2-bromo 9H carbazole and 2,7-dibromo 9H carbazole with human serum albumin. Materials Today: Proceedings, 2021, 45, 2540-2543.	1.8	2
17	Radical scavenging behavior of eriodictyol and fustin flavonoid compounds $\hat{a} \in ADFT$ study. AIP Conference Proceedings, 2018, , .	0.4	1
18	Prediction of biological activities of phytoestrogen and its derivative $\hat{a} \in A$ Insilico study. AIP Conference Proceedings, 2019, , .	0.4	1

#	Article	IF	CITATIONS
19	Local orbital locator analysis of isomeric compounds of luteolin and apigenin. AIP Conference Proceedings, 2019, , .	0.4	1
20	Theoretical insight on antioxidant potency of kanzakiflavone-2 and its derivatives. Structural Chemistry, 2021, 32, 1451-1458.	2.0	1
21	Theoretical investigations on the structure and properties of p-n-alkoxy benzoic acid based liquid crystals. AIP Conference Proceedings, 2016, , .	0.4	O

A charge density study to explore the effect of Au and Pt atoms in thiol substituted Oligo (phenylene) Tj ETQq0.0 orgBT /Overlock 10 Td 0.4