

Geradius Deogratis

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/3804320/publications.pdf>

Version: 2024-02-01

11
papers

155
citations

1478505

6
h-index

1281871

11
g-index

11
all docs

11
docs citations

11
times ranked

143
citing authors

#	ARTICLE	IF	CITATIONS
1	Optical and electronic properties of para-functionalized triphenylamine-based dyes: a theoretical study. <i>Structural Chemistry</i> , 2022, 33, 409-419.	2.0	2
2	A Molecular Investigation of the Solvent Influence on Inter- and Intra-Molecular Hydrogen Bond Interaction of Linamarin. <i>Processes</i> , 2022, 10, 352.	2.8	2
3	Influence of heteroatoms on the optoelectronic properties of triphenylamine-based dyes for DSSCs application: A computational approach. <i>Computational and Theoretical Chemistry</i> , 2022, 1210, 113644.	2.5	8
4	Hydrophobic π - π stacking interactions and hydrogen bonds drive self-aggregation of luteolin in water. <i>Journal of Molecular Graphics and Modelling</i> , 2022, 116, 108243.	2.4	6
5	Effect of substituent in the acceptor on optical and electronic properties of triphenylamine based dyes: A density functional theory/time-dependent density functional theory investigation. <i>Materials Science in Semiconductor Processing</i> , 2022, 150, 106935.	4.0	7
6	Ensemble-based screening of natural products and FDA-approved drugs identified potent inhibitors of SARS-CoV-2 that work with two distinct mechanisms. <i>Journal of Molecular Graphics and Modelling</i> , 2021, 105, 107871.	2.4	7
7	Luteolin: a blocker of SARS-CoV-2 cell entry based on relaxed complex scheme, molecular dynamics simulation, and metadynamics. <i>Journal of Molecular Modeling</i> , 2021, 27, 221.	1.8	17
8	Tuning optoelectronic properties of triphenylamine based dyes through variation of pi-conjugated units and anchoring groups: A DFT/TD-DFT investigation. <i>Journal of Molecular Graphics and Modelling</i> , 2020, 94, 107480.	2.4	31
9	Effects of heteroatoms in π -conjugated linkers on the optical and electronic properties of modified triphenylamine based dyes: towards DSSCs TM applications. <i>Journal of Molecular Modeling</i> , 2020, 26, 288.	1.8	23
10	Investigation of optoelectronic properties of triphenylamine-based dyes featuring heterocyclic anchoring groups for DSSCs TM applications: a theoretical study. <i>Structural Chemistry</i> , 2020, 31, 2451-2461.	2.0	13
11	Novel Xanthate Complexes for the Size-Controlled Synthesis of Copper Sulfide Nanorods. <i>Inorganic Chemistry</i> , 2017, 56, 9247-9254.	4.0	39