

Danuta Rusinska-Roszak

List of Publications by Year in descending order

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16
papers

201
citations

1307594

7
h-index

1058476

14
g-index

16
all docs

16
docs citations

16
times ranked

188
citing authors

#	ARTICLE	IF	CITATIONS
1	Intramolecular O-H...C Hydrogen Bond Energy via the Molecular Tailoring Approach to RAHB Structures. <i>Journal of Physical Chemistry A</i> , 2015, 119, 3674-3687.	2.5	52
2	Estimation of the Intramolecular O-H...C Hydrogen Bond Energy via the Molecular Tailoring Approach. Part I: Aliphatic Structures. <i>Journal of Chemical Information and Modeling</i> , 2014, 54, 1963-1977.	5.4	39
3	Energy of Intramolecular Hydrogen Bonding in ortho-Hydroxybenzaldehydes, Phenones and Quinones. Transfer of Aromaticity from ipso-Benzene Ring to the Enol System(s). <i>Molecules</i> , 2017, 22, 481.	3.8	33
4	Estimation of the breakthrough volume of selected steroids for C_{18} solid-phase extraction sorbent using retention data from micro-thin layer chromatography. <i>Journal of Separation Science</i> , 2013, 36, 1104-1111.	2.5	13
5	PM3 conformations of C-13 Taxol [®] side chain methyl ester. <i>Tetrahedron Letters</i> , 1995, 36, 8849-8852.	1.4	12
6	Fragmentation studies of selected drugs utilized in palliative care. <i>European Journal of Mass Spectrometry</i> , 2018, 24, 420-436.	1.0	8
7	De(side chain) model of epothilone: bioconformer interconversions DFT study. <i>Journal of Molecular Modeling</i> , 2009, 15, 859-869.	1.8	7
8	A molecular tailoring approach – a new guide to quantify the energy of push-pull effects: a case study on (E)-3-(1H-pyrrol-2-yl)prop-2-enones. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 22190-22194.	2.8	7
9	Ab initio and PM3 calculated molecular structures and energies of acetoin oxime – the LIX63 progenitor. <i>Computational and Theoretical Chemistry</i> , 1995, 331, 95-107.	1.5	6
10	Extended and Clustered Conformers of Epothilone A. <i>Journal of Physical Chemistry B</i> , 2011, 115, 3698-3707.	2.6	5
11	A computational study of open-chain epothilone analogue. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 967-973.	2.0	4
12	Finding the direct energy-structure correlations in intramolecular aromaticity assisted hydrogen bonding (AAHB). <i>Journal of Molecular Graphics and Modelling</i> , 2021, 105, 107884.	2.4	4
13	Molecular tailoring approach as tool for revealing resonance-assisted hydrogen bond: Case study of Z-pyrrolylenones with the $N\cdots H\cdots O$ intramolecular hydrogen bond. <i>Journal of Computational Chemistry</i> , 2022, 43, 1596-1607.	3.3	4
14	The synthesis of hydrophobic 1-alkyl-1,1,2,2-tetrahydro-2,2-benzo[<i>d</i>]imidazoles. <i>Heterocyclic Communications</i> , 2016, 22, 99-102.	1.2	3
15	Differentiation of stereoisomers with electron impact mass spectrometry: (E)- and (Z)-hydroxyoximes. <i>Organic Mass Spectrometry</i> , 1990, 25, 457-458.	1.3	2
16	Guide to tuning the chalcone molecular properties based on the push-pull effect energy scale created via the molecular tailoring approach. <i>Journal of Computational Chemistry</i> , 2022, 43, 631-643.	3.3	2