Danuta Rusinska-Roszak

List of Publications by Year
in descending order

16	201	1307594 7	1058476 14
papers	citations	h-index	g-index

16	16	16	188
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Guide to tuning the chalcone molecular properties based on the pushâ€pull effect energy scale created via the molecular tailoring approach. Journal of Computational Chemistry, 2022, 43, 631-643.	3.3	2
2	Molecular tailoring approach as tool for revealing resonanceâ€assisted hydrogen bond: Case study of <scp>Z</scp>â€pyrrolylenones with the Nï£¿Hâ‹¯Oï£¾Đ¡ intramolecular hydrogen bond. Journal of Computational Chemistry, 2022, 43, 1596-1607.	3.3	4
3	Finding the direct energy-structure correlations in intramolecular aromaticity assisted hydrogen bonding (AAHB). Journal of Molecular Graphics and Modelling, 2021, 105, 107884.	2.4	4
4	A molecular tailoring approach â€“ a new guide to quantify the energy of pushâ€“pull effects: a case study on (E)-3-(1H-pyrrol-2-yl)prop-2-enones. Physical Chemistry Chemical Physics, 2020, 22, 22190-22194.	2.8	7
5	Fragmentation studies of selected drugs utilized in palliative care. European Journal of Mass Spectrometry, 2018, 24, 420-436.	1.0	8
6	Energy of Intramolecular Hydrogen Bonding in ortho-Hydroxybenzaldehydes, Phenones and Quinones. Transfer of Aromaticity from ipso-Benzene Ring to the Enol System(s). Molecules, 2017, 22, 481.	3.8	33
7	The synthesis of hydrophobic 1-alkyl-1H,1â€²H-2,2â€²-bibenzo[d]imidazoles. Heterocyclic Communications, 2016, 22, 99-102.	1.2	3
8	Intramolecular Oâ€“HÂ·Â·Â·Oâ•C Hydrogen Bond Energy via the Molecular Tailoring Approach to RAHB Structures. Journal of Physical Chemistry A, 2015, 119, 3674-3687.	2.5	52
9	Estimation of the Intramolecular Oâ€“HÂ·Â·Â·Oâ•C Hydrogen Bond Energy via the Molecular Tailoring Approach. Part I: Aliphatic Structures. Journal of Chemical Information and Modeling, 2014, 54, 1963-1977.	5.4	39
10	Estimation of the breakthrough volume of selected steroids for <scp>C</scp>â€18 solidâ€phase extraction sorbent using retention data from microâ€thin layer chromatography. Journal of Separation Science, 2013, 36, 1104-1111.	2.5	13
11	Extended and Clustered Conformers of Epothilone A. Journal of Physical Chemistry B, 2011, 115, 3698-3707.	2.6	5
12	De(side chain) model of epothilone: bioconformer interconversions DFT study. Journal of Molecular Modeling, 2009, 15, 859-869.	1.8	7
13	A computational study of openâ€chain epothilone analogue. International Journal of Quantum Chemistry, 2008, 108, 967-973.	2.0	4
14	PM3 conformations of C-13 TaxolÂ® side chain methyl ester. Tetrahedron Letters, 1995, 36, 8849-8852.	1.4	12
15	Ab initio and PM3 calculated molecular structures and energies of acetoin oxime â€” the LIX63 progenitor. Computational and Theoretical Chemistry, 1995, 331, 95-107.	1.5	6
16	Differentiation of stereoisomers with electron impact mass spectrometry: (E)- and (Z)-Î±-hydroxyoximes. Organic Mass Spectrometry, 1990, 25, 457-458.	1.3	2