

David A Rincón

List of Publications by Year in descending order

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papers

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2258059

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#	ARTICLE	IF	CITATIONS
1	Hydrogen Bonds and n π^* Interactions in the Acetylation of Propranolol Catalyzed by <i>Candida antarctica</i> Lipase B: A QTAIM Study. ACS Omega, 2021, 6, 20992-21004.	3.5	2
2	Concerted double proton-transfer electron-transfer between catechol and superoxide radical anion. Physical Chemistry Chemical Physics, 2017, 19, 26179-26190.	2.8	30
3	On the effects of the basis set superposition error on the change of QTAIM charges in adduct formation. Application to complexes between morphine and cocaine and their main metabolites. RSC Advances, 2016, 6, 110642-110655.	3.6	2
4	Hydration Structure of Cocaine and its Metabolites: A Molecular Dynamics Study. Journal of Solution Chemistry, 2011, 40, 656-679.	1.2	1
5	Theoretical study of morphine and heroin: Conformational study in gas phase and aqueous solution and electron distribution analysis. International Journal of Quantum Chemistry, 2010, 110, 2472-2482.	2.0	3
6	Theoretical study of cocaine and ecgonine methyl ester in gas phase and in aqueous solution. Chemical Physics Letters, 2009, 467, 249-254.	2.6	9
7	On the Electronic Structure of Cocaine and its Metabolites. Journal of Physical Chemistry A, 2009, 113, 13937-13942.	2.5	9
8	Ab initio and density functional study of a caffeic acid amide. Computational and Theoretical Chemistry, 2007, 804, 57-63.	1.5	2