

# Cleber P A Anconi

## List of Publications by Year in descending order

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34  
papers

566  
citations

566801

15  
h-index

642321

23  
g-index

34  
all docs

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docs citations

34  
times ranked

683  
citing authors

#	ARTICLE	IF	CITATIONS
1	<sup>1</sup> H NMR coupling in 2-fluorophenol revisited: Is intramolecular hydrogen bond responsible for this long-range coupling?. <i>Magnetic Resonance in Chemistry</i> , 2011, 49, 763-767.	1.1	49
2	Theoretical Study of the $\beta$ -Cyclodextrin Dimer. <i>Journal of Physical Chemistry A</i> , 2005, 109, 3209-3219.	1.1	43
3	Superstructure based on $\beta$ -CD self-assembly induced by a small guest molecule. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 1934.	1.3	41
4	Ab Initio Calculations on Low-Energy Conformers of $\beta$ -Cyclodextrin. <i>Journal of Physical Chemistry A</i> , 2007, 111, 12127-12135.	1.1	34
5	Theoretical and Experimental Study of Inclusion Complexes Formed by Isoniazid and Modified $\beta$ -Cyclodextrins: <sup>1</sup> H NMR Structural Determination and Antibacterial Activity Evaluation. <i>Journal of Physical Chemistry B</i> , 2014, 118, 81-93.	1.2	34
6	New Insights on Chemical Oxidation of Single-Wall Carbon Nanotubes: A Theoretical Study. <i>Journal of Physical Chemistry C</i> , 2009, 113, 10079-10084.	1.5	31
7	<sup>1</sup> H NMR analysis of <i>o</i> -methylinositol isomers: a joint experimental and theoretical study. <i>Magnetic Resonance in Chemistry</i> , 2012, 50, 608-614.	1.1	31
8	Inclusion complex thermodynamics: The $\beta$ -cyclodextrin and sertraline complex example. <i>Journal of Molecular Graphics and Modelling</i> , 2015, 62, 11-17.	1.3	29
9	Water Solvent Effect on Theoretical Evaluation of <sup>1</sup> H NMR Chemical Shifts: <i>o</i> -Methyl-Inositol Isomer. <i>Journal of Physical Chemistry A</i> , 2017, 121, 2839-2846.	1.1	27
10	Experimental and Theoretical Investigation of Epoxide Quebrachitol Derivatives Through Spectroscopic Analysis. <i>Organic Letters</i> , 2010, 12, 5458-5461.	2.4	25
11	A highly correlated ab initio investigation of the temperature-dependent conformational analysis of cycloheptane. <i>Chemical Physics Letters</i> , 2006, 418, 459-466.	1.2	23
12	Inclusion process of tetracycline in $\beta$ and $\gamma$ -cyclodextrins: A theoretical investigation. <i>Chemical Physics Letters</i> , 2015, 626, 80-84.	1.2	20
13	Inclusion complexes of $\beta$ -cyclodextrin and the cisplatin analogues oxaliplatin, carboplatin and nedaplatin: A theoretical approach. <i>Chemical Physics Letters</i> , 2011, 515, 127-131.	1.2	19
14	Structure and Stability of ( $\beta$ -CD) <sub>3</sub> Aggregate and OEG@( $\beta$ -CD) <sub>3</sub> Pseudorotaxane in Aqueous Solution: A Molecular Dynamics Study. <i>Journal of Physical Chemistry B</i> , 2009, 113, 9762-9769.	1.2	17
15	An efficient methodology to study cyclodextrin clusters: application to $\beta$ -CD hydrated monomer, dimer, trimer and tetramer. <i>Journal of Inclusion Phenomena and Macrocyclic Chemistry</i> , 2007, 59, 265-277.	1.6	16
16	The role played by head-tail configuration on the molecular weight distribution of $\beta$ -cyclodextrin tubes. <i>Journal of Inclusion Phenomena and Macrocyclic Chemistry</i> , 2008, 60, 25-33.	1.6	10
17	Interaction of chemically modified tetracyclines with catalytic Zn(II) ion in matrix metalloproteinase: evidence for metal coordination sites. <i>Theoretical Chemistry Accounts</i> , 2011, 128, 377-388.	0.5	10
18	Synthesis, characterization and phytotoxic activity of hydroxylated isobenzofuran-1(3H)-ones. <i>Journal of Molecular Structure</i> , 2014, 1061, 61-68.	1.8	10

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19	Stability and spatial arrangement of the 2,4-dichlorophenoxyacetic acid and $\beta$ -cyclodextrin inclusion compound: A theoretical study. <i>Chemical Physics Letters</i> , 2015, 633, 158-162.	1.2	10
20	Theoretical study of $\beta$ -CD based [3] pseudorotaxanes: the role played by threadlike polymer on the stability of Cyclodextrin dimers. <i>Journal of the Brazilian Chemical Society</i> , 2008, 19, 1033-1040.	0.6	9
21	Theoretical study of spectroscopic properties of insulated molecular wires formed by substituted oligothiophenes and cross-linked $\beta$ -cyclodextrin. <i>Journal of Polymer Science, Part B: Polymer Physics</i> , 2011, 49, 1101-1111.	2.4	9
22	Prediction of conformational population of large cycloalkanes using <i>ab initio</i> correlated methods: Cycloundecane, cyclododecane, and cyclotridecane. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 3188-3197.	1.0	9
23	Theoretical inclusion of deprotonated 2,4-D and dicamba pesticides in $\beta$ -cyclodextrin. <i>Journal of Inclusion Phenomena and Macrocyclic Chemistry</i> , 2016, 86, 343-349.	0.9	9
24	Theoretical Study of Covalently Bound $\beta$ -Cyclodextrin Associations. <i>Journal of Physical Chemistry C</i> , 2012, 116, 18958-18964.	1.5	8
25	Box-Car design for studying inclusion complexes of triglycerides and $\beta$ -cyclodextrin: application to the heating protocol in molecular-dynamics simulations. <i>Journal of Inclusion Phenomena and Macrocyclic Chemistry</i> , 2011, 71, 103-111.	1.6	7
26	Theoretical study of inclusion of a dinuclear platinum(II) complex in $\alpha$ , $\beta$ , and $\gamma$ -cyclodextrins. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 3403-3408.	1.0	6
27	Inclusion complexes of Schiff bases as phyto-growth inhibitors. <i>Journal of Inclusion Phenomena and Macrocyclic Chemistry</i> , 2013, 75, 197-204.	1.6	6
28	Relative Position and Relative Rotation in Supramolecular Systems through the Analysis of the Principal Axes of Inertia: Ferrocene/Cucurbit[7]uril and Ferrocenyl Azide/ $\beta$ -Cyclodextrin Case Studies. <i>ACS Omega</i> , 2020, 5, 5013-5025.	1.6	6
29	Selective activity of <i>Mucor plumbeus</i> reductase towards ( $\alpha$ )-camphorquinone. <i>Journal of Industrial Microbiology and Biotechnology</i> , 2009, 36, 1023-1027.	1.4	5
30	Estudo teórico e experimental de espectros infravermelho de $\alpha$ -steres de $\beta$ -ácido graxo presentes na composição do biodiesel de soja. <i>Química Nova</i> , 2012, 35, 1752-1757.	0.3	5
31	Formation of $\beta$ -Cyclodextrin inclusion compound with doxycycline: A theoretical approach. <i>Chemical Physics Letters</i> , 2018, 692, 140-145.	1.2	4
32	Host-guest intermolecular hydrogen bonds and stability in aqueous media: the benzaldehyde/ $\beta$ -CD case study. <i>Journal of Inclusion Phenomena and Macrocyclic Chemistry</i> , 2017, 89, 137-142.	0.9	3
33	Condensed-phase relative Gibbs free energy and E/Z descriptors for 2-acetylthiophene and 2-acetylthiophene-N1-phenyl thiosemicarbazones. <i>Journal of Molecular Modeling</i> , 2021, 27, 101.	0.8	1
34	Separation and Qualitative Analysis of Carbonate, Phosphate and Chromate Anions in Qualitative Inorganic Courses. <i>Educacion Química</i> , 2018, 29, 49.	0.1	0