

Clebio Soares Nascimento

List of Publications by Year in descending order

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51
papers

925
citations

394421

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h-index

501196

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52
all docs

52
docs citations

52
times ranked

925
citing authors

#	ARTICLE	IF	CITATIONS
1	Supramolecular Self-Assembly of Cyclodextrin and Higher Water Soluble Guest: Thermodynamics and Topological Studies. <i>Journal of the American Chemical Society</i> , 2008, 130, 8426-8436.	13.7	79
2	Theoretical investigation on functional monomer and solvent selection for molecular imprinting of tramadol. <i>Chemical Physics Letters</i> , 2016, 645, 174-179.	2.6	47
3	Theoretical Study of the $\hat{\alpha}$ -Cyclodextrin Dimer. <i>Journal of Physical Chemistry A</i> , 2005, 109, 3209-3219.	2.5	43
4	Theoretical study of the formation of the $\hat{\alpha}$ -cyclodextrin hexahydrate. <i>Chemical Physics Letters</i> , 2004, 397, 422-428.	2.6	41
5	Molecular modeling study of the recognition mechanism and enantioseparation of 4-hydroxypropranolol by capillary electrophoresis using carboxymethyl- $\hat{\beta}$ -cyclodextrin as the chiral selector. <i>Analyst</i> , 2014, 139, 3901-3910.	3.5	38
6	Efficient molecularly imprinted polymer as a pipette-tip solid-phase sorbent for determination of carvedilol enantiomers in human urine. <i>Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences</i> , 2017, 1061-1062, 399-410.	2.3	38
7	Ab Initio Calculations on Low-Energy Conformers of $\hat{\alpha}$ -Cyclodextrin. <i>Journal of Physical Chemistry A</i> , 2007, 111, 12127-12135.	2.5	34
8	Theoretical and Experimental Study of Inclusion Complexes Formed by Isoniazid and Modified $\hat{\beta}$ -Cyclodextrins: ^1H NMR Structural Determination and Antibacterial Activity Evaluation. <i>Journal of Physical Chemistry B</i> , 2014, 118, 81-93.	2.6	34
9	Molecularly Imprinted Polymer (MIP) for thiamethoxam: A theoretical and experimental study. <i>Journal of Molecular Structure</i> , 2021, 1231, 129980.	3.6	32
10	Inclusion complex thermodynamics: The $\hat{\beta}$ -cyclodextrin and sertraline complex example. <i>Journal of Molecular Graphics and Modelling</i> , 2015, 62, 11-17.	2.4	29
11	Hydrophobic Nanoprecipitates of $\hat{\beta}$ -Cyclodextrin/Avermectins Inclusion Compounds Reveal Insecticide Activity against <i>Aedes aegypti</i> Larvae and Low Toxicity against Fibroblasts. <i>Journal of Agricultural and Food Chemistry</i> , 2018, 66, 7275-7285.	5.2	26
12	Sr ₂ CeO ₄ : Electronic and structural properties. <i>Journal of Alloys and Compounds</i> , 2014, 608, 73-78.	5.5	25
13	A DFT investigation on the host/guest inclusion process of prilocaine into $\hat{\beta}$ -cyclodextrin. <i>Chemical Physics Letters</i> , 2016, 652, 123-129.	2.6	25
14	Carvedilol-Imprinted Polymer: Rational design and selectivity studies. <i>Journal of Molecular Structure</i> , 2019, 1177, 101-106.	3.6	24
15	A highly correlated ab initio investigation of the temperature-dependent conformational analysis of cycloheptane. <i>Chemical Physics Letters</i> , 2006, 418, 459-466.	2.6	23
16	Computational contribution to the electrophoretic enantiomer separation mechanism and migration order using modified $\hat{\beta}$ -cyclodextrins. <i>Electrophoresis</i> , 2017, 38, 1860-1868.	2.4	23
17	Chiral Capillary Electrokinetic Chromatography: Principle and Applications, Detection and Identification, Design of Experiment, and Exploration of Chiral Recognition Using Molecular Modeling. <i>Molecules</i> , 2021, 26, 2841.	3.8	23
18	Inclusion process of tetracycline in $\hat{\beta}$ and $\hat{\gamma}$ -cyclodextrins: A theoretical investigation. <i>Chemical Physics Letters</i> , 2015, 626, 80-84.	2.6	20

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19	Computational study on acetamiprid-molecular imprinted polymer. <i>Journal of Molecular Modeling</i> , 2019, 25, 104.	1.8	20
20	Microextraction by packed molecularly imprinted polymer to selectively determine caffeine in soft and energy drinks. <i>Microchemical Journal</i> , 2020, 158, 105252.	4.5	19
21	Magnetic molecularly imprinted conducting polymer for determination of praziquantel enantiomers in milk. <i>Analyst, The</i> , 2020, 145, 4245-4253.	3.5	19
22	Structure and Stability of (β -CD) ₃ Aggregate and OEG@(β -CD) ₃ Pseudorotaxane in Aqueous Solution: A Molecular Dynamics Study. <i>Journal of Physical Chemistry B</i> , 2009, 113, 9762-9769.	2.6	17
23	An efficient methodology to study cyclodextrin clusters: application to β -CD hydrated monomer, dimer, trimer and tetramer. <i>Journal of Inclusion Phenomena and Macrocyclic Chemistry</i> , 2007, 59, 265-277.	1.6	16
24	Revealing the Binding Process of New 3-Alkylpyridine Marine Alkaloid Analogue Antimalarials and the Heme Group: An Experimental and Theoretical Investigation. <i>Journal of Chemical Information and Modeling</i> , 2016, 56, 571-579.	5.4	16
25	Inclusion vs. micellization in the cetylpyridine chloride / β -cyclodextrin system: A structural and thermodynamic approach. <i>Journal of Molecular Structure</i> , 2019, 1184, 289-297.	3.6	16
26	A theoretical investigation on the encapsulation process of mepivacaine into β -cyclodextrin. <i>Chemical Physics Letters</i> , 2020, 740, 137060.	2.6	15
27	Spherical-shaped Y ₂ O ₃ :Eu ³⁺ nanoparticles with intense photoluminescence emission. <i>Ceramics International</i> , 2015, 41, 1189-1195.	4.8	14
28	Synthesis and evaluation of the mutagenicity of 3-alkylpyridine marine alkaloid analogues with anticancer potential. <i>Mutation Research - Genetic Toxicology and Environmental Mutagenesis</i> , 2018, 825, 31-39.	1.7	14
29	Computational investigation on the host-guest inclusion process of norfloxacin into β -cyclodextrin. <i>Journal of Molecular Modeling</i> , 2016, 22, 220.	1.8	12
30	Theoretical investigation on the molecular inclusion process of prilocaine into p-sulfonic acid calix[6]arene. <i>Chemical Physics Letters</i> , 2016, 646, 52-55.	2.6	12
31	Microextraction by packed molecularly imprinted polymer followed by ultra-high performance liquid chromatography for determination of fipronil and fluzaron residues in drinking water and veterinary clinic wastewater. <i>Microchemical Journal</i> , 2021, 168, 106405.	4.5	12
32	The conformational and tautomeric equilibrium of 5a,6-anhydrotetracycline in aqueous solution at pH 7. <i>Computational and Theoretical Chemistry</i> , 2003, 626, 305-319.	1.5	11
33	Target-Guided Synthesis and Antiplasmodial Evaluation of a New Fluorinated 3-Alkylpyridine Marine Alkaloid Analog. <i>ACS Omega</i> , 2017, 2, 8264-8272.	3.5	11
34	Molecular wires formed from native and push-pull derivatives polypyrroles and β -cyclodextrins: A HOMO-LUMO gap theoretical investigation. <i>Chemical Physics Letters</i> , 2019, 730, 141-146.	2.6	11
35	Stability and spatial arrangement of the 2,4-dichlorophenoxyacetic acid and β -cyclodextrin inclusion compound: A theoretical study. <i>Chemical Physics Letters</i> , 2015, 633, 158-162.	2.6	10
36	Theoretical study of spectroscopic properties of insulated molecular wires formed by substituted oligothiophenes and cross-linked β -cyclodextrin. <i>Journal of Polymer Science, Part B: Polymer Physics</i> , 2011, 49, 1101-1111.	2.1	9

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37	Theoretical Study of Covalently Bound β -Cyclodextrin Associations. <i>Journal of Physical Chemistry C</i> , 2012, 116, 18958-18964.	3.1	8
38	Experimental and theoretical studies of a magnetic mesoporous molecularly imprinted polymer for selective adsorption of estrogens from aqueous solutions. <i>Journal of Molecular Structure</i> , 2022, 1264, 133221.	3.6	8
39	Theoretical study of inclusion of a dinuclear platinum(II) complex in α , β , and γ -cyclodextrins. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 3403-3408.	2.0	6
40	Photoluminescent and structural properties of ZnO containing Eu ³⁺ using PEG as precursor. <i>Journal of Luminescence</i> , 2015, 167, 197-203.	3.1	6
41	Oxybutynin-imprinted polymer: A theoretical investigation. <i>Chemical Physics Letters</i> , 2022, 799, 139640.	2.6	6
42	Elucidation of the chromatographic enantiomer elution order for praziquantel: An experimental and theoretical assessment. <i>Chirality</i> , 2020, 32, 353-358.	2.6	5
43	Molecular inclusion process of urease inhibitors into cyclodextrins: A theoretical study. <i>Chemical Physics Letters</i> , 2017, 675, 69-74.	2.6	4
44	Theoretical study on the formation process of Cross-Linked β -Cyclodextrin molecular tubes. <i>Chemical Physics Letters</i> , 2017, 677, 13-18.	2.6	4
45	Theoretical investigation on the molecular inclusion process of urease inhibitors into p-sulfonic acid calix[4,6]arenes. <i>Chemical Physics Letters</i> , 2018, 692, 117-123.	2.6	4
46	Enantioselective separation of bupropion and its major metabolite hydroxybupropion: An experimental and theoretical study. <i>Chemical Physics Letters</i> , 2019, 730, 1-7.	2.6	4
47	Development and validation of an experimental and theoretical method for the chiral discrimination of dinotefuran. <i>Chirality</i> , 2020, 32, 53-63.	2.6	4
48	Atenolol-imprinted polymer: a DFT study. <i>Journal of Molecular Modeling</i> , 2022, 28, .	1.8	4
49	POLÍMERO DE IMPRESSÃO MOLECULAR PARA O TIACLOPRIDO: UMA INVESTIGAÇÃO TEÓRICA. <i>Química Nova</i> , 2020, 43, .	0.3	2
50	A theoretical study of poly(p-phenylenes) and their cyclodextrin-based insulated molecular wires. <i>Computational and Theoretical Chemistry</i> , 2021, 1197, 113157.	2.5	1
51	Synthesis and Theoretical Study of a Series of 3,5-disubstituted Pyrazoles. <i>Letters in Organic Chemistry</i> , 2020, 17, 932-938.	0.5	1