MÃ¡rio T S Rosado

List of Publications by Year
in descending order

37 papers	1,322 citations	471509 17 h-index	345221 36 g-index
37 all docs	37 docs citations	37 times ranked	1546 citing authors

#	Article	IF	Citations
1	Polymorphic Cocrystals of the Antimalarial Drug Pyrimethamine: Two Case Studies. Crystal Growth and Design, 2021, 21, 3699-3713.	3.0	13
2	Structure and energetics of intermolecular association in two lurasidone co-amorphous drug systems. Journal of Molecular Structure, 2021, 1242, 130709.	3.6	4
3	Dihydrofolate Reductase Inhibitors: The Pharmacophore as a Guide for Co-Crystal Screening. Molecules, 2021, 26, 6721.	3.8	2
4	UV-induced radical formation and isomerization of 4-methoxyindole and 5-methoxyindole. Physical Chemistry Chemical Physics, 2020, 22, 22943-22955.	2.8	5
5	Vibrationally Induced Conformational Isomerization and Tunneling in Pyrrole-2-Carboxylic Acid. Journal of Physical Chemistry A, 2020, 124, 10277-10287.	2.5	1
6	Ordered and Plastic Crystals in the Complex Polymorphism of Pinanediol. Crystal Growth and Design, 2019, 19, 6127-6135.	3.0	12
7	Polymorphism of 1,3-cyclohexanediols: molecular structure and plastic crystal formation of cyclohexanediol isomers. CrystEngComm, 2019, 21, 3395-3408.	2.6	6
8	Photochemistry of matrix-isolated 3-chloro-1,2-benzisoxazole: Generation and characterization of 2-cyanophenoxyl radical and other reactive intermediates. Journal of Molecular Structure, 2018, 1172, 33-41.	3.6	3
9	The Quest for Carbenic Nitrile Imines: Experimental and Computational Characterization of ‹i›C‹/i›â€Amino Nitrile Imine. European Journal of Organic Chemistry, 2015, 2015, 7484-7493.	2.4	34
10	Molecular structure and polymorphism of a cyclohexanediol: trans-1,4-cyclohexanedimethanol. CrystEngComm, 2014, 16, 10977-10986.	2.6	6
11	Polymorphism of cis-1,4-cyclohexanediol, a new plastic crystal former. Considerations on isomeric cyclohexanediols plastic crystal forming abilities. Journal of Molecular Structure, 2014, 1078, 10-19.	3.6	12
12	Rhodium/tris-binaphthyl chiral monophosphite complexes: Efficient catalysts for the hydroformylation of disubstituted aryl olefins. Journal of Organometallic Chemistry, 2012, 698, 28-34.	1.8	31
13	Metalloporphyrin triads: Synthesis and photochemical characterization. Journal of Photochemistry and Photobiology A: Chemistry, 2012, 242, 59-66.	3.9	33
14	Resolved structures of two picolinamide polymorphs. Investigation of the dimorphic system behaviour under conditions relevant to co-crystal synthesis. CrystEngComm, 2012, 14, 8649.	2.6	20
15	Routes to synthesis of porphyrins covalently bound to poly(carbazole)s and poly(fluorene)s: Structural and computational studies on oligomers. Journal of Molecular Structure, 2012, 1029, 199-208.	3.6	11
16	Pyrazinamide-Diflunisal: A New Dual-Drug Co-Crystal. Crystal Growth and Design, 2011, 11, 4780-4788.	3.0	80
17	Synthesis of New Metalloporphyrin Triads: Efficient and Versatile Tripod Optical Sensor for the Detection of Amines. Inorganic Chemistry, 2011, 50, 7916-7918.	4.0	34
18	The structure of mono- and di-amino derivatives of cyclohexane: Energetic and Natural Bond Orbital approaches. Computational and Theoretical Chemistry, 2011, 964, 32-39.	2.5	6

#	Article	IF	Citations
19	Thermal analysis and crystallization from melts. Journal of Thermal Analysis and Calorimetry, 2010, 100, 423-429.	3.6	5
20	Enantioselective ethylation of aromatic aldehydes catalysed by titanium(IV)â€“bis-BINOLate-2â€²,2â€³-propylether complexes: An inside view of the catalytic active species. Journal of Molecular Catalysis A, 2010, 325, 91-97.	4.8	11
21	Conformational Cooling Dynamics in Matrix-Isolated 1,3-Butanediol. Journal of Physical Chemistry A, 2009, 113, 7499-7507.	2.5	64
22	Structure of the 2-isopropylaminoethanol isolated molecule: Conformational analysis and intramolecular interactions. Computational and Theoretical Chemistry, 2008, 863, 73-78.	1.5	4
23	The structure of betaxolol from single crystal X-ray diffraction and natural bond orbital analysis. Journal of Molecular Structure, 2008, 891, 437-442.	3.6	10
24	Structure of Isolated 1,4-Butanediol: Combination of MP2 Calculations, NBO Analysis, and Matrix-Isolation Infrared Spectroscopy. Journal of Physical Chemistry A, 2008, 112, 4669-4678.	2.5	69
25	Hydration of Cyclohexylamines:Â CPCM Calculation of Hydration Gibbs Energy of the Conformers. Journal of Physical Chemistry A, 2007, 111, 3432-3437.	2.5	21
26	Molecular structure of mono- and 1,2-aminoderivatives of cyclohexane: Steric strain effects as determining factors. Computational and Theoretical Chemistry, 2007, 804, 65-74.	1.5	23
27	Conformational study of isolated pindolol by HF, DFT and MP2 calculations. Computational and Theoretical Chemistry, 2007, 806, 231-238.	1.5	9
28	Enthalpy of sublimation/vaporization of trans-cyclohexyl-1,4-diamine and cis-cyclohexyl-1,2-diamine. Journal of Chemical Thermodynamics, 2007, 39, 1354-1356.	2.0	6
29	Stepwise conformational cooling towards a single isomeric state in the four internal rotors system 1,2-butanediol. Physical Chemistry Chemical Physics, 2006, 8, 5339-5349.	2.8	68
30	Conformational Study of Monomeric 2,3-Butanediols by Matrix-Isolation Infrared Spectroscopy and DFT Calculations. Journal of Physical Chemistry A, 2006, 110, 4169-4179.	2.5	72
31	Conformational study of erythritol and threitol in the gas state by density functional theory calculations. Carbohydrate Research, 2005, 340, 283-291.	2.3	14
32	Molecular Structure of Butanediol Isomers in Gas and Liquid States:â€‰ Combination of DFT Calculations and Infrared Spectroscopy Studies. Journal of Physical Chemistry A, 2003, 107, 3891-3897.	2.5	52
33	Synthesis, characterization and biodistribution of bisphosphonates Sm-153 complexes: correlation with molecular modeling interaction studies. Nuclear Medicine and Biology, 2002, 29, 329-338.	0.6	77
34	Vibrational spectra of acid and alkaline glycine salts. Vibrational Spectroscopy, 1998, 16, 35-54.	2.2	154
35	Matrix-Isolation Infrared and Theoretical Studies of the Glycine Conformers. Journal of Physical Chemistry A, 1998, 102, 1041-1054.	2.5	311
36	Vibrational spectra (FT-IR, Raman and MI-IR) of Î±- and Î²-alanine. Journal of Molecular Structure, 1997, 410-411, 343-348.	3.6	36

#	Article	IF	Citations
37	CONFORMATIONAL ISOMERISM IN GLYCINE AND DITHIOGLYCINE: A COMPARATIVE MOLECULAR ORBITAL STUDY. Phosphorus, Sulfur and Silicon and the Related Elements, 1996, 116, 153-173.	1.6	3