

# Mã;rio T S Rosado

## List of Publications by Year in descending order

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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	Matrix-Isolation Infrared and Theoretical Studies of the Glycine Conformers. <i>Journal of Physical Chemistry A</i> , 1998, 102, 1041-1054.	2.5	311
2	Vibrational spectra of acid and alkaline glycine salts. <i>Vibrational Spectroscopy</i> , 1998, 16, 35-54.	2.2	154
3	Pyrazinamide-Diflunisal: A New Dual-Drug Co-Crystal. <i>Crystal Growth and Design</i> , 2011, 11, 4780-4788.	3.0	80
4	Synthesis, characterization and biodistribution of bisphosphonates Sm-153 complexes: correlation with molecular modeling interaction studies. <i>Nuclear Medicine and Biology</i> , 2002, 29, 329-338.	0.6	77
5	Conformational Study of Monomeric 2,3-Butanediols by Matrix-Isolation Infrared Spectroscopy and DFT Calculations. <i>Journal of Physical Chemistry A</i> , 2006, 110, 4169-4179.	2.5	72
6	Structure of Isolated 1,4-Butanediol: Combination of MP2 Calculations, NBO Analysis, and Matrix-Isolation Infrared Spectroscopy. <i>Journal of Physical Chemistry A</i> , 2008, 112, 4669-4678.	2.5	69
7	Stepwise conformational cooling towards a single isomeric state in the four internal rotors system 1,2-butanediol. <i>Physical Chemistry Chemical Physics</i> , 2006, 8, 5339-5349.	2.8	68
8	Conformational Cooling Dynamics in Matrix-Isolated 1,3-Butanediol. <i>Journal of Physical Chemistry A</i> , 2009, 113, 7499-7507.	2.5	64
9	Molecular Structure of Butanediol Isomers in Gas and Liquid States: Combination of DFT Calculations and Infrared Spectroscopy Studies. <i>Journal of Physical Chemistry A</i> , 2003, 107, 3891-3897.	2.5	52
10	Vibrational spectra (FT-IR, Raman and MI-IR) of $\hat{L}$ - and $\hat{D}$ -alanine. <i>Journal of Molecular Structure</i> , 1997, 410-411, 343-348.	3.6	36
11	Synthesis of New Metalloporphyrin Triads: Efficient and Versatile Tripod Optical Sensor for the Detection of Amines. <i>Inorganic Chemistry</i> , 2011, 50, 7916-7918.	4.0	34
12	The Quest for Carbenic Nitrile Imines: Experimental and Computational Characterization of $\hat{C}$ -Amino Nitrile Imine. <i>European Journal of Organic Chemistry</i> , 2015, 2015, 7484-7493.	2.4	34
13	Metalloporphyrin triads: Synthesis and photochemical characterization. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2012, 242, 59-66.	3.9	33
14	Rhodium/tris-binaphthyl chiral monophosphite complexes: Efficient catalysts for the hydroformylation of disubstituted aryl olefins. <i>Journal of Organometallic Chemistry</i> , 2012, 698, 28-34.	1.8	31
15	Molecular structure of mono- and 1,2-aminoderivatives of cyclohexane: Steric strain effects as determining factors. <i>Computational and Theoretical Chemistry</i> , 2007, 804, 65-74.	1.5	23
16	Hydration of Cyclohexylamines: CPCM Calculation of Hydration Gibbs Energy of the Conformers. <i>Journal of Physical Chemistry A</i> , 2007, 111, 3432-3437.	2.5	21
17	Resolved structures of two picolinamide polymorphs. Investigation of the dimorphic system behaviour under conditions relevant to co-crystal synthesis. <i>CrystEngComm</i> , 2012, 14, 8649.	2.6	20
18	Conformational study of erythritol and threitol in the gas state by density functional theory calculations. <i>Carbohydrate Research</i> , 2005, 340, 283-291.	2.3	14

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19	Polymorphic Cocrystals of the Antimalarial Drug Pyrimethamine: Two Case Studies. <i>Crystal Growth and Design</i> , 2021, 21, 3699-3713.	3.0	13
20	Polymorphism of cis-1,4-cyclohexanediol, a new plastic crystal former. Considerations on isomeric cyclohexanediols plastic crystal forming abilities. <i>Journal of Molecular Structure</i> , 2014, 1078, 10-19.	3.6	12
21	Ordered and Plastic Crystals in the Complex Polymorphism of Pinanediol. <i>Crystal Growth and Design</i> , 2019, 19, 6127-6135.	3.0	12
22	Enantioselective ethylation of aromatic aldehydes catalysed by titanium(IV)-bis-BINOLate-2- $\epsilon$ ,2- $\epsilon$ <sup>3</sup> -propylether complexes: An inside view of the catalytic active species. <i>Journal of Molecular Catalysis A</i> , 2010, 325, 91-97.	4.8	11
23	Routes to synthesis of porphyrins covalently bound to poly(carbazole)s and poly(fluorene)s: Structural and computational studies on oligomers. <i>Journal of Molecular Structure</i> , 2012, 1029, 199-208.	3.6	11
24	The structure of betaxolol from single crystal X-ray diffraction and natural bond orbital analysis. <i>Journal of Molecular Structure</i> , 2008, 891, 437-442.	3.6	10
25	Conformational study of isolated pindolol by HF, DFT and MP2 calculations. <i>Computational and Theoretical Chemistry</i> , 2007, 806, 231-238.	1.5	9
26	Enthalpy of sublimation/vaporization of trans-cyclohexyl-1,4-diamine and cis-cyclohexyl-1,2-diamine. <i>Journal of Chemical Thermodynamics</i> , 2007, 39, 1354-1356.	2.0	6
27	The structure of mono- and di-amino derivatives of cyclohexane: Energetic and Natural Bond Orbital approaches. <i>Computational and Theoretical Chemistry</i> , 2011, 964, 32-39.	2.5	6
28	Molecular structure and polymorphism of a cyclohexanediol: trans-1,4-cyclohexanedimethanol. <i>CrystEngComm</i> , 2014, 16, 10977-10986.	2.6	6
29	Polymorphism of 1,3-cyclohexanediols: molecular structure and plastic crystal formation of cyclohexanediol isomers. <i>CrystEngComm</i> , 2019, 21, 3395-3408.	2.6	6
30	Thermal analysis and crystallization from melts. <i>Journal of Thermal Analysis and Calorimetry</i> , 2010, 100, 423-429.	3.6	5
31	UV-induced radical formation and isomerization of 4-methoxyindole and 5-methoxyindole. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 22943-22955.	2.8	5
32	Structure of the 2-isopropylaminoethanol isolated molecule: Conformational analysis and intramolecular interactions. <i>Computational and Theoretical Chemistry</i> , 2008, 863, 73-78.	1.5	4
33	Structure and energetics of intermolecular association in two lurasidone co-amorphous drug systems. <i>Journal of Molecular Structure</i> , 2021, 1242, 130709.	3.6	4
34	CONFORMATIONAL ISOMERISM IN GLYCINE AND DITHIOGLYCINE: A COMPARATIVE MOLECULAR ORBITAL STUDY. <i>Phosphorus, Sulfur and Silicon and the Related Elements</i> , 1996, 116, 153-173.	1.6	3
35	Photochemistry of matrix-isolated 3-chloro-1,2-benzisoxazole: Generation and characterization of 2-cyanophenoxy radical and other reactive intermediates. <i>Journal of Molecular Structure</i> , 2018, 1172, 33-41.	3.6	3
36	Dihydrofolate Reductase Inhibitors: The Pharmacophore as a Guide for Co-Crystal Screening. <i>Molecules</i> , 2021, 26, 6721.	3.8	2

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37	Vibrationally Induced Conformational Isomerization and Tunneling in Pyrrole-2-Carboxylic Acid. Journal of Physical Chemistry A, 2020, 124, 10277-10287.	2.5	1