Dolores Santa MarÃ-a

List of Publications by Year
in descending order

64 papers	1,454 citations	394421 19 h-index	345221 36 g-index
65 all docs	65 docs citations	65 times ranked	1697 citing authors

#	Article	IF	Citations
1	A structural analysis of 2,5â€diarylâ€4 H â€2,4â€dihydroâ€3 H â€1,2,4â€triazolâ€3â€ones: NMR in the solid state, Xâ€ray crystallography, and GIPAW calculations. Magnetic Resonance in Chemistry, 2021, 59, 423-438.	1.9	4
2	Conformational analysis of 2,5â€diarylâ€4â€methylâ€2, 4â€dihydroâ€3 H â€1,2,4â€triazolâ€3â€ones: Multinuclear NMR and DFT calculations. Journal of Heterocyclic Chemistry, 2021, 58, 1130-1140.	2.6	0
3	Weak Intermolecular CHÂ·Â·Â·N Hydrogen Bonding: Determination of ¹³CHâ€“¹⁵N Hydrogen-Bond Mediated J Couplings by Solid-State NMR Spectroscopy and First-Principles Calculations. Journal of Physical Chemistry A, 2020, 124, 560-572.	2.5	22
4	A theoretical and spectroscopic (NMR and IR) study of indirubin in solution and in the solid state. Journal of Physical Organic Chemistry, 2020, 33, e4043.	1.9	5
5	The synergy of different solid-state techniques to elucidate the supramolecular assembly of two 1H-benzotriazole polymorphs. Physical Chemistry Chemical Physics, 2019, 21, 19879-19889.	2.8	4
6	Synthesis of a new 24-membered tetramide macrocycle and X-ray crystal structure determination. Tetrahedron Letters, 2019, 60, 1206-1209.	1.4	2
7	New N,C-Diaryl-1,2,4-triazol-3-ones: Synthesis and Evaluation as Anticancer Agents. Medicinal Chemistry, 2019, 15, 360-372.	1.5	5
8	The Structure of Nâ€phenylâ€pyrazoles and Indazoles: Mononitro, Dinitro, and Trinitro Derivatives. Journal of Heterocyclic Chemistry, 2018, 55, 44-64.	2.6	9
9	The structure of 4,5,6,7-tetrafluoro-1H-benzotriazole in solid state and in solution. Journal of Fluorine Chemistry, 2016, 192, 98-104.	1.7	5
10	The structure and properties of 5,6-dinitro-1H-benzotriazole. Journal of Molecular Structure, 2016, 1113, 153-161.	3.6	8
11	Pyrrole-Pyridine and Pyrrole-Naphthyridine Hosts for Anion Recognition. Molecules, 2015, 20, 9862-9878.	3.8	3
12	New macrocyclic compounds with naphthyridine units for molecular recognition studies of biotin and urea derivatives. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2015, 81, 57-69.	1.6	4
13	The structures of two aldazines: [1,1â€²â€²(1E,1â€²E)â€hydrazineâ€1,2â€diylidenebis(methanâ€1â€ylâ€1â€ylidene)dinaphthalenâ€2â€ol] (Lumogen) and 2,2â€²â€²(1E,1â€²E)â€hydrazineâ€1,2â€diylidenebis(methanâ€1â€ylâ€1â€ylidene)diphenol (salicylaldazine) in the solid state and in solution. Magnetic Resonance in Chemistry, 2013, 51, 530-540.	1.9	9
14	A silver complex of chloroquine: synthesis, characterization and structural properties. New Journal of Chemistry, 2013, 37, 1391.	2.8	6
15	Synthesis and structural study of 2-arylbenzotriazoles related toÂTinuvins. Tetrahedron, 2013, 69, 3027-3038.	1.9	21
16	Structure of NH-benzazoles (1H-benzimidazoles, 1H- and 2H-indazoles, 1H- and 2H-benzotriazoles). Chemistry of Heterocyclic Compounds, 2013, 49, 177-202.	1.2	26
17	Synthetic Hosts for Molecular Recognition of Ureas. Journal of Organic Chemistry, 2011, 76, 6780-6788.	3.2	14
18	High resolution NMR of free radicals: 13C magic angle spinning of two solid organic free radicals derived from 4,5-dihydro-1H-imidazol-3-oxide-1-oxyl and theoretical calculation of their NMR properties. Arkivoc, 2011, 2011, 114-127.	0.5	0

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19	15Nâ€“15N spinâ€“spin coupling constants through intermolecular hydrogen bonds in the solid state. Journal of Magnetic Resonance, 2010, 206, 274-279.	2.1	11
20	Molecular Recognition Studies on Naphthyridine Derivatives. Molecules, 2010, 15, 1213-1222.	3.8	9
21	The behavior of Gliclazide in solution and in the solid state: a case of organic compound presenting a solidâ€solution structure. Magnetic Resonance in Chemistry, 2009, 47, 472-477.	1.9	8
22	A theoretical and experimental NMR study of (+)-biotin methyl ester. Journal of Molecular Structure, 2009, 920, 323-326.	3.6	15
23	Theoretical calculations of a model of NOS indazole inhibitors: Interaction of aromatic compounds with Zn-porphyrins. Bioorganic and Medicinal Chemistry, 2009, 17, 8027-8031.	3.0	16
24	Quantifying Weak Hydrogen Bonding in Uracil and 4-Cyano-4â€˜-ethynylbiphenyl:â€‰ A Combined Computational and Experimental Investigation of NMR Chemical Shifts in the Solid State. Journal of the American Chemical Society, 2008, 130, 945-954.	13.7	112
25	A theoretical and experimental study of the fluxional behaviour of molybdenum dihydrobis- and hydrotris-pyrazolylborates. Dalton Transactions, 2007, , 3995.	3.3	9
26	Synthesis, structure, and isomerism of N-2,4-dinitrophenylbenzotriazoles. Tetrahedron, 2007, 63, 3737-3744.	1.9	10
27	Structure and tautomerism of 4-bromo substituted 1H-pyrazoles. Tetrahedron, 2007, 63, 8104-8111.	1.9	43
28	On the molecular conformation of bisaromatic systems the case of 2-phenyl-2H-benzotriazoles. Chemical Physics, 2007, 340, 32-42.	1.9	5
29	Structural Studies of Two TinuvinÂ® P Analogs: 2-(2,4-Dimethyl-phenyl)-2H-benzotriazole and 2-Phenyl-2H-benzotriazole. Molecules, 2007, 12, 2201-2214.	3.8	11
30	Molecular Recognition:Â Improved Binding of Biotin Derivatives with Synthetic Receptors. Journal of Organic Chemistry, 2006, 71, 2944-2951.	3.2	28
31	Host-Guest Chemistry of Tolbutamide. Molecules, 2006, 11, 478-485.	3.8	7
32	The use of NMR spectroscopy to study tautomerism. Progress in Nuclear Magnetic Resonance Spectroscopy, 2006, 49, 169-206.	7.5	164
33	A new tool for the rational design of methylbiotin hosts. Tetrahedron Letters, 2006, 47, 9017-9020.	1.4	8
34	A1H,13C and15N NMR study in solution and in the solid state of sixN-substituted pyrazoles and indazoles. Magnetic Resonance in Chemistry, 2006, 44, 566-570.	1.9	24
35	The Structure of a Non-Symmetric Disordered Tetramer: A Crystallographic and Solid State Multinuclear NMR Study of the Properties of 3(5)-Ethyl-5(3)-Phenyl-1H-Pyrazole. Supramolecular Chemistry, 2006, 18, 349-356.	1.2	19
36	The structure in the solid state and in solution of 3(5)-trifluoromethyl-4,5(3)-polymethylenepyrazoles. Arkivoc, 2006, 2006, 29-37.	0.5	11

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37	Molecular recognition of biotin, barbital and tolbutamide with new synthetic receptors. Tetrahedron, 2005, 61, 5089-5100.	1.9	24
38	Solid-State NMR Study of the Tautomerism of Acetylacetone Included in a Host Matrix. Helvetica Chimica Acta, 2005, 88, 1931-1942.	1.6	17
39	A non-symmetric disordered tetramer: the unusual structure of 3(5)-ethyl-5(3)-phenyl-1H-pyrazole in the solid state. Acta Crystallographica Section A: Foundations and Advances, 2005, 61, c362-c363.	0.3	0
40	A multinuclear NMR study in the solid state and in solution of thallium(I) tris-(pyrazol-1-yl)borates (thallium scorpionates). Journal of Organometallic Chemistry, 2004, 689, 463-470.	1.8	11
41	Isomer distribution in thallium hydrotris(polymethylenepyrazol-1-yl)borates (thallium scorpionates): a multinuclear NMR study. Polyhedron, 2004, 23, 2985-2991.	2.2	10
42	Towards the design of hostâ€“guest complexes: biotin and urea derivatives versus artificial receptors. Biosensors and Bioelectronics, 2004, 20, 1242-1249.	10.1	20
43	Multiple hydrogen bonds and tautomerism in naphthyridine derivatives. New Journal of Chemistry, 2004, 28, 700-707.	2.8	42
44	Multinuclear NMR solution studies on complexes of hexakis(pyrazol-1-yl)benzene (hpzb) with Ag(I). Inorganica Chimica Acta, 2003, 347, 168-174.	2.4	12
45	The annular tautomerism of 4(5)-phenylimidazole. Perkin Transactions II RSC, 2002, , 564-568.	1.1	20
46	Variety in the Coordination Modes of the Ligand Hexakis(pyrazol-1-yl)benzene (Hpzb) to PdII, PtII and CuI Centres. European Journal of Inorganic Chemistry, 2002, 2002, 3178-3189.	2.0	19
47	1-Benzoylazoles: an experimental (NMR and crystallography) and theoretical study. Journal of Molecular Structure, 2002, 605, 199-212.	3.6	17
48	The molecular structure of 4-tert-butylpyrazoles in the solid state and in solution: an X-ray, NMR and calorimetric study of the buttressing effect of a 4-tert-butyl substituent. New Journal of Chemistry, 2001, 25, 819-823.	2.8	13
49	2,4,6-Tris(azol-1-yl)-1,3,5-triazines: A New Class of Multidentate Ligands. Heterocycles, 2001, 55, 905.	0.7	18
50	The structure at 150 K of a highly disordered pyrazole: 3-trifluoromethyl-5-(2-thienyl)-pyrazole. Journal of Molecular Structure, 2000, 526, 59-64.	3.6	7
51	Rhodium complexes with hydrotris(3-p-anisylpyrazol-1-yl)borate ligand TppAn. Intramolecular Cî—¸H bond activation and dehydro-chlorination processes. Journal of Organometallic Chemistry, 2000, 605, 117-126.	1.8	12
52	Aromatic propellenes. Part 10. Conformational study of hexa(imidazol-1-yl)benzene and hexakis(2-methylimidazol-1-yl)benzene by means of NMR and AM1 calculations. Journal of Molecular Structure, 1999, 478, 285-294.	3.6	3
53	Aromatic propellenes. Part 8.â€ Semiempirical calculations and DNMR studies of hexakis(pyrazol-1-yl)benzenes. Journal of the Chemical Society Perkin Transactions II, 1997, , 2173-2178.	0.9	5
54	Molecular structure and dynamics of C-1-adamantyl substituted N-unsubstituted pyrazoles studied by solid state NMR spectroscopy and X-ray crystallography. Journal of the Chemical Society Perkin Transactions II, 1997, , 1867-1876.	0.9	11

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55	Aromatic propellenes. Synthesis, X-Ray structures and conformational study of polypyrazolylpyridines. Tetrahedron, 1996, 52, 11075-11094.	1.9	12
56	Regular paper. Journal of Organometallic Chemistry, 1996, 526, 341-350.	1.8	27
57	Solidâ€state dye lasers based on modified rhodamine 6G dyes copolymerized with methacrylic monomers. Journal of Applied Physics, 1996, 80, 3167-3173.	2.5	60
58	Toward the Photostability Mechanism of Intramolecular Hydrogen Bond Systems. 4. 3(5)-(1'-Hydroxy-2'-naphthyl)pyrazoles and 3(5)-(2'-Hydroxy-1'-naphthyl)pyrazoles. Journal of Organic Chemistry, 1995, 60, 3427-3439.	3.2	20
59	Imidazole and benzimidazole addition to quinones. Formation of meso and d,l isomers and crystal structure of the d,l isomer of 2,3-Bis(benzimidazol-1'-yl)-1,4-dihydroxybenzene. Tetrahedron, 1994, 50, 12489-12510.	1.9	22
60	Complexes of rhodium and iridium derived from 2,5-bis(pyrazol-1â€²-yl)-1,4-dihydroxybenzene. Journal of Organometallic Chemistry, 1994, 467, 293-301.	1.8	22
61	Reaction of pyrazole addition to quinones. Journal of Organic Chemistry, 1992, 57, 1873-1876.	3.2	26
62	New ultraviolet stabilizers: 3- and 5-(2'-hydroxyphenyl)pyrazoles. Journal of the American Chemical Society, 1992, 114, 5039-5048.	13.7	139
63	Mechanism of photostabilization of polystyrene film by dihydroxyphenyl-pirazoles. Journal of Polymer Science Part A, 1990, 28, 3661-3668.	2.3	14
64	Photoinduced intramolecular proton transfer as the mechanism of ultraviolet stabilizers: a reappraisal. Journal of the American Chemical Society, 1990, 112, 747-759.	13.7	198