Rosa MarÃ-a Claramunt

List of Publications by Year
in descending order

403 papers	8,885 citations	66250 44 h-index	120465 65 g-index
418 all docs	418 docs citations	418 times ranked	6828 citing authors

#	Article	IF	Citations
1	An efficient, one-pot, regioselective synthesis of 2-aryl/hetaryl-4-methyl-5-acylthiazoles under solvent-free conditions. Journal of Sulfur Chemistry, 2022, 43, 12-21.	1.0	5
2	Determination of the tautomerism of albendazole desmotropes using solution and solid state NMR together with DFT theoretical calculations, both energies and chemical shifts. Journal of Molecular Structure, 2022, 1261, 132883.	1.8	3
3	Study of the Addition Mechanism of 1H-Indazole and Its 4-, 5-, 6-, and 7-Nitro Derivatives to Formaldehyde in Aqueous Hydrochloric Acid Solutions. Journal of Organic Chemistry, 2022, 87, 5866-5881.	1.7	2
4	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.	1.1	4
5	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.	1.4	0
6	A 13C chemical shifts study of iodopyrazoles: experimental results and relativistic and non-relativistic calculations. Structural Chemistry, 2021, 32, 925-937.	1.0	1
7	Studies of novel trifluoroacetylated diaryl hydrazone molecular photoswitches in solution and in the solid state. New Journal of Chemistry, 2021, 45, 12471-12478.	1.4	2
8	1,5-Benzodiazepin-2(3H)-ones: In Vitro Evaluation as Antiparkinsonian Agents. Antioxidants, 2021, 10, 1584.	2.2	3
9	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.	1.1	22
10	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.	0.9	5
11	Regiospecific Synthesis and Structural Studies of 3,5-Dihydro-4H-pyrido[2,3-b][1,4]diazepin-4-ones and Comparison with 1,3-Dihydro-2H-benzo[b][1,4]diazepin-2-ones. ACS Omega, 2020, 5, 25408-25422.	1.6	5
12	Perimidines: a unique Ï€-amphoteric heteroaromatic system. Russian Chemical Reviews, 2020, 89, 1204-1260.	2.5	10
13	A GIPAW versus GIAO-ZORA-SO study of 13C and 15N CPMAS NMR chemical shifts of aromatic and heterocyclic bromo derivatives. Solid State Nuclear Magnetic Resonance, 2020, 108, 101676.	1.5	5
14	Theoretical and Spectroscopic Characterization of API-Related Azoles in Solution and in Solid State. Current Pharmaceutical Design, 2020, 26, 4847-4857.	0.9	2
15	A structural study of new tetrakis(1H-pyrazol-1-yl)methanes. Tetrahedron, 2019, 75, 130690.	1.0	2
16	Visible-light mediated regioselective approach towards synthesis of 7-aroyl-6-methyl-[1,2,4]triazolo[3,4-b][1,3,4]thiadiazines. Tetrahedron, 2019, 75, 130728.	1.0	18
17	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.	1.3	4
18	The structure of the anti-aging agent J147 used for treating Alzheimer's disease. Acta Crystallographica Section C, Structural Chemistry, 2019, 75, 271-276.	0.2	3

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19	Multinuclear NMR spectra and GIAO/DFT calculations of N-benzylazoles and N-benzylbenzazoles. Structural Chemistry, 2019, 30, 1729-1735.	1.0	10
20	Synthesis of a new 24-membered tetramide macrocycle and X-ray crystal structure determination. Tetrahedron Letters, 2019, 60, 1206-1209.	0.7	2
21	An Example of Polynomial Expansion: The Reaction of 3(5)-Methyl-1H-Pyrazole with Chloroform and Characterization of the Four Isomers. Molecules, 2019, 24, 568.	1.7	6
22	A theoretical NMR study of polymorphism in crystal structures of azoles and benzazoles. Magnetic Resonance in Chemistry, 2019, 57, 275-284.	1.1	9
23	Synthesis, structure and NMR study of fluorinated isoxazoles derived from hemi-curcuminoids. Journal of Fluorine Chemistry, 2019, 219, 39-49.	0.9	5
24	New N,C-Diaryl-1,2,4-triazol-3-ones: Synthesis and Evaluation as Anticancer Agents. Medicinal Chemistry, 2019, 15, 360-372.	0.7	5
25	The structure of fosfomycin salts in solution and in the solid state by nuclear magnetic resonance spectroscopy and DFT calculations. Tetrahedron, 2018, 74, 3937-3942.	1.0	8
26	Redox Properties and Interchromophoric Electronic Interactions in Isoalloxazineâ^'Anthraquinone Dyads. ChemElectroChem, 2018, 5, 985-990.	1.7	2
27	The structures of 1,4-diaryl-5-trifluoromethyl-1H-1,2,3-triazoles related to J147, a drug for treating Alzheimer's disease. Acta Crystallographica Section C, Structural Chemistry, 2018, 74, 513-522.	0.2	8
28	A vibrational circular dichroism (VCD) methodology for the measurement of enantiomeric excess in chiral compounds in the solid phase and for the complementary use of NMR and VCD techniques in solution: the camphor case. Analyst, The, 2018, 143, 1406-1416.	1.7	19
29	Unusual synthesis of azines and their oxidative degradation to carboxylic acid using iodobenzene diacetate. Synthetic Communications, 2018, 48, 439-446.	1.1	11
30	Molecular structure in the solid state by X-ray crystallography and SSNMR and in solution by NMR of two 1,4-diazepines. Journal of Molecular Structure, 2018, 1155, 205-214.	1.8	7
31	The Structure of Nâ€phenylâ€pyrazoles and Indazoles: Mononitro, Dinitro, and Trinitro Derivatives. Journal of Heterocyclic Chemistry, 2018, 55, 44-64.	1.4	9
32	The structure of four thallium tris(1H-pyrazol-1-yl)hydroborates in the solid state by X-ray crystallography and in solution by NMR and DFT-GIAO calculations. Inorganica Chimica Acta, 2018, 483, 402-410.	1.2	6
33	Libration of phenyl groups detected by <scp>VTâ€SSNMR</scp>: Comparison with Xâ€ray crystallography. Magnetic Resonance in Chemistry, 2018, 56, 1083-1088.	1.1	2
34	Evaluation of the Antioxidant and Neuroprotectant Activities of New Asymmetrical 1,3-Diketones. Molecules, 2018, 23, 1837.	1.7	9
35	Conformational aspects of polymorphs and phases of 2-propyl-1H-benzimidazole. IUCrJ, 2018, 5, 706-715.	1.0	7
36	Curcumin Related 1,4â€Diazepines: Regioselective Synthesis, Structure Analysis, Tautomerism, NMR Spectroscopy, Xâ€ray Crystallography, Density Functional Theory and GIAO Calculations. ChemistrySelect, 2017, 2, 3732-3738.	0.7	6

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37	Supramolecular organization of perfluorinated 1H-indazoles in the solid state using X-ray crystallography, SSNMR and sensitive (VCD) and non sensitive (MIR, FIR and Raman) to chirality vibrational spectroscopies. Physical Chemistry Chemical Physics, 2017, 19, 1632-1643.	1.3	18
38	The organic chemistry of poly(1H-pyrazol-1-yl)methanes. Coordination Chemistry Reviews, 2017, 339, 153-182.	9.5	34
39	The Curious Case of 2-Propyl-1H-benzimidazole in the Solid State: An Experimental and Theoretical Study. Journal of Physical Chemistry A, 2017, 121, 5665-5674.	1.1	14
40	Influence of solvent basicity on DMABN photophysics. Journal of Physical Organic Chemistry, 2017, 30, e3613.	0.9	2
41	19Fâ€NMR Diastereotopic Signals in Two N-CHF2 Derivatives of (4S,7R)-7,8,8-Trimethyl-4,5,6,7-tetrahydro-4,7-methano-2H-indazole. Molecules, 2017, 22, 2003.	1.7	9
42	Crystal structure of (1Z,4Z)-2,4-dimethyl-3H-benzo[b][1,4]diazepine. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 647-650.	0.2	1
43	Effects of Curcuminoid Pyrazoles on Cancer Cells and on the Expression of Telomerase Related Genes. Archiv Der Pharmazie, 2016, 349, 532-538.	2.1	7
44	A theoretical and experimental NMR study of BODIPY 493/503: difluoro{2â€[1â€(3,5â€dimethylâ€2Hâ€pyrrolâ€2â€ylideneâ€N)ethyl]â€3,5â€dimethylâ€1Hâ€pyrrolatoâ€N Magnetic Resonance in Chemistry, 2016, 54, 684-688.	1.1	8
45	NBS mediated one-pot regioselective synthesis of 2,3-disubstituted imidazo[1,2- a]pyridines and their unambiguous characterization through 2D NMR and X-ray crystallography. Tetrahedron, 2016, 72, 3832-3838.	1.0	18
46	¹⁵N NMR Spectroscopy, X-ray and Neutron Diffraction, Quantum-Chemical Calculations, and UV/vis-Spectrophotometric Titrations as Complementary Techniques for the Analysis of Pyridine-Supported Bicyclic Guanidine Superbases. Journal of Organic Chemistry, 2016, 81, 7612-7625.	1.7	29
47	Static and Dynamic Properties of Fluorinated 4-Aryl-1,5-Benzodiazepinones. ChemistrySelect, 2016, 1, 861-870.	0.7	8
48	The structures of two scorpionates: thallium tetrakis(3-phenyl-1H-pyrazol-1-yl)borate and potassium tetrakis(3-cyclopropyl-1H-pyrazol-1-yl)borate. Acta Crystallographica Section C, Structural Chemistry, 2016, 72, 819-825.	0.2	4
49	The structure of 4,5,6,7-tetrafluoro-1H-benzotriazole in solid state and in solution. Journal of Fluorine Chemistry, 2016, 192, 98-104.	0.9	5
50	The structure of Î²-diketones related to curcumin determined by X-ray crystallography, NMR (solution) Tj ETQq0 0 0 rgBT /Overlock 10 T	1.6	18
51	The structure and properties of 5,6-dinitro-1H-benzotriazole. Journal of Molecular Structure, 2016, 1113, 153-161.	1.8	8
52	Photoinduced processes in macrocyclic isoalloxazineâ€“anthracene systems. Journal of Photochemistry and Photobiology A: Chemistry, 2016, 314, 189-197.	2.0	3
53	A theoretical and experimental study of the NMR spectra of 4,5,6,7-tetrafluorobenzazoles with special stress on PCM calculations of chemical shifts. Magnetic Resonance in Chemistry, 2015, 53, 353-362.	1.1	18
54	A multinuclear magnetic resonance study of fluoro derivatives of hydroxybenzaldehydes. Magnetic Resonance in Chemistry, 2015, 53, 624-631.	1.1	3

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55	Pyrrole-Pyridine and Pyrrole-Naphthyridine Hosts for Anion Recognition. Molecules, 2015, 20, 9862-9878.	1.7	3
56	Fluorination Effects on NOS Inhibitory Activity of Pyrazoles Related to Curcumin. Molecules, 2015, 20, 15643-15665.	1.7	20
57	Crystal and molecular structures of two 1H-2-substituted benzimidazoles. Zeitschrift Fur Kristallographie - Crystalline Materials, 2015, 230, .	0.4	7
58	Diazole-based powdered cocrystal featuring a helical hydrogen-bonded network: Structure determination from PXRD, solid-state NMR and computer modeling. Solid State Nuclear Magnetic Resonance, 2015, 65, 49-63.	1.5	28
59	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.	0.9	4
60	Synthesis, structure and biological activity of 3(5)-trifluoromethyl-1H-pyrazoles derived from hemicurcuminoids. Journal of Molecular Structure, 2015, 1100, 518-529.	1.8	15
61	An NMR and Computational Study of Azolo[a]pyrimidines with Special Emphasis on Pyrazolo[1,5â€a]pyrimidines. Journal of Heterocyclic Chemistry, 2015, 52, 336-345.	1.4	14
62	A Spectroscopic Study of Colchicine in the Solid State and in Solution by Multinuclear Magnetic Resonance and Vibrational Circular Dichroism. Helvetica Chimica Acta, 2014, 97, 471-490.	1.0	11
63	An experimental and theoretical NMR study of NH-benzimidazoles in solution and in the solid state: proton transfer and tautomerism. Beilstein Journal of Organic Chemistry, 2014, 10, 1620-1629.	1.3	41
64	Coordination behaviour of new dipyridylpyrazole ligands towards ZnCl₂and PdCl₂fragments. Crystalline structural characterization and multinuclear NMR studies as evidence of linkage and conformational isomers. RSC Advances, 2014, 4, 9383-9394.	1.7	6
65	Mechano Heterocyclic Chemistry: Grinding and Ball Millsâ^—. Advances in Heterocyclic Chemistry, 2014, 112, 117-143.	0.9	22
66	The origin of the splitting of 13C and 15N NMR signals of 3(5)-phenyl-5(3)-methylpyrazolium chloride and bromide in the solid state: Quantum Espresso calculations. Journal of Molecular Structure, 2014, 1075, 551-558.	1.8	8
67	Structural Investigation of Weak Intermolecular Interactions (Hydrogen and Halogen Bonds) in Fluorine-Substituted Benzimidazoles. Crystal Growth and Design, 2014, 14, 3499-3509.	1.4	35
68	Chiral self-assembly of enantiomerically pure (4S,7R)-campho[2,3-c]pyrazole in the solid state: a vibrational circular dichroism (VCD) and computational study. Tetrahedron: Asymmetry, 2014, 25, 507-515.	1.8	13
69	Effect of Substituents on the Regioselectivity of the Reaction of Î±â€Tosyloxyketones with Thioureas in Acidic Medium: Access to 2â€Aminothiazoles and 2â€Iminoâ€2,3â€dihydrothiazoles. Journal of Heterocyclic Chemistry, 2014, 51, 598-603.	1.4	3
70	Structures of Hemiâ€Curcuminoids in the Solid State and in Solution. European Journal of Organic Chemistry, 2013, 2013, 6043-6054.	1.2	17
71	A theoretical study of the conformation and dynamic properties of 1,5-benzodiazepines and their derivatives. Computational and Theoretical Chemistry, 2013, 1019, 108-115.	1.1	17
72	The structures of two aldazines: [1,1â€²â€(1E,1â€²E)â€hydrazineâ€1,2â€diylidenebis(methanâ€1â€ylâ€1â€ylidene)dinaphthalenâ€2â€ol] (Lumogen) and 2,2â€²â€(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.	1.1	9

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73	Structural and thermodynamic properties of new pyrazolo[3,4-d]pyridazinones. Thermochimica Acta, 2013, 574, 63-72.	1.2	16
74	A Facile Method to Determine the Absolute Structure of Achiral Molecules: Supramolecularâ€Tilt Structures. Chemistry - A European Journal, 2013, 19, 6044-6051.	1.7	5
75	Tuning photoinduced processes of covalently bound isoalloxazine and anthraquinone bichromophores. Photochemical and Photobiological Sciences, 2013, 12, 813-822.	1.6	7
76	Intermolecular spinâ€“spin coupling constants between 31P atoms. Comptes Rendus Chimie, 2013, 16, 937-944.	0.2	11
77	A silver complex of chloroquine: synthesis, characterization and structural properties. New Journal of Chemistry, 2013, 37, 1391.	1.4	6
78	The structure of azines derived from Câ€formylâ€1Hâ€imidazoles in solution and in the solid state: tautomerism, configurational and conformational studies. Magnetic Resonance in Chemistry, 2013, 51, 203-221.	1.1	18
79	Synthesis and structural study of 2-arylbenzotriazoles related toÂTinuvins. Tetrahedron, 2013, 69, 3027-3038.	1.0	21
80	Theoretical and Experimental NMR Study of a Series of Five Nitrobenzene-1,2-Diamines. Spectroscopy Letters, 2013, 46, 91-99.	0.5	6
81	Structure of NH-benzazoles (1H-benzimidazoles, 1H- and 2H-indazoles, 1H- and 2H-benzotriazoles). Chemistry of Heterocyclic Compounds, 2013, 49, 177-202.	0.6	26
82	The Structure and Dynamic Properties of 1H-Pyrazole-4-Carboxylic Acids in the Solid State. Zeitschrift Fur Physikalische Chemie, 2013, 227, 841-856.	1.4	3
83	A tris(pyrazol-1-yl)methane bearing carboxylic acid groups at position 4: {1-[bis(4-carboxy-3,5-dimethyl-1H-pyrazol-1-yl)methyl]-3,5-dimethyl-1H-pyrazole-4-carboxylato}sodium dihydrate. Acta Crystallographica Section C: Crystal Structure Communications, 2013, 69, 972-976.	0.4	6
84	Selfâ€Assembly Structures of 1 H â€indazoles in the Solution and Solid Phases: A Vibrational (IR, FIR,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	1.0	14
85	Structure of 1,5-benzodiazepinones in the solid state and in solution: Effect of the fluorination in the six-membered ring. Beilstein Journal of Organic Chemistry, 2013, 9, 2156-2167.	1.3	11
86	The tautomerism of fluorinated indazolinones in the solid state. Journal of Molecular Structure, 2012, 1022, 139-146.	1.8	5
87	The chiral structure of 1H-indazoles in the solid state: a crystallographic, vibrational circular dichroism and computational study. New Journal of Chemistry, 2012, 36, 749.	1.4	32
88	The structure of glibenclamide in the solid state. Magnetic Resonance in Chemistry, 2012, 50, 246-255.	1.1	20
89	Two polymorphs of 8-hydroxycarbostyril: X-ray crystallography, solid-state NMR and DFT calculations. Journal of Molecular Structure, 2012, 1008, 88-94.	1.8	8
90	use of NMR and electronic spectroscopies with DFT calculations. Journal of Molecular Structure, 2012, 1015, 138-146.	1.8	10

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91	Multi-component solvent-free versus stepwise solvent mediated reactions: Regiospecific formation of 6-trifluoromethyl and 4-trifluoromethyl-1H-pyrazolo[3,4-b]pyridines. Journal of Fluorine Chemistry, 2012, 140, 31-37.	0.9	23
92	A theoretical study of the parent NH-benzazoles (benzimidazoles, indazoles and benzotriazoles): geometries, energies, acidity and basicity, NMR properties and molecular electrostatic potentials. Arkivoc, 2012, 2012, 85-107.	0.3	18
93	Pyridyl and pyridiniumyl Î²-diketones as building blocks for palladium(ii) and allylâ€“palladium(ii) isomers. Multinuclear NMR structural elucidation and liquid crystal behaviour. New Journal of Chemistry, 2011, 35, 1020.	1.4	15
94	Synthetic Hosts for Molecular Recognition of Ureas. Journal of Organic Chemistry, 2011, 76, 6780-6788.	1.7	14
95	Improving VEGFR-2 Docking-Based Screening by Pharmacophore Postfiltering and Similarity Search Postprocessing. Journal of Chemical Information and Modeling, 2011, 51, 777-787.	2.5	22
96	Unprecedented 1,3-Diaza[3]ferrocenophane Scaffold as Molecular Probe for Anions. Inorganic Chemistry, 2011, 50, 4212-4220.	1.9	28
97	Crystal and molecular structure of three biologically active nitroindazoles. Journal of Molecular Structure, 2011, 985, 75-81.	1.8	10
98	Synthesis and biological evaluation of indazole derivatives. European Journal of Medicinal Chemistry, 2011, 46, 1439-1447.	2.6	22
99	A 13C and 15N experimental NMR and theoretical study of the structure of linear primary aliphatic amines and ammonium salts: from C1 to C18. Tetrahedron, 2011, 67, 4633-4639.	1.0	14
100	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.	0.3	0
101	Double proton transfer in crystals of 1,3,4,6,7,8â€hexahydroâ€2Hâ€pyrimido[1,2â€a] pyrimidine (hppH):¹³C and¹⁵N CPMAS NMR study of (hppH)₂. Journal of Physical Organic Chemistry, 2010, 23, 526-535.	0.9	11
102	The azido-tetrazole and diazo-1,2,3-triazole tautomerism in six-membered heteroaromatic rings and their relationships with aromaticity: Azines and perimidine. Tetrahedron, 2010, 66, 2863-2868.	1.0	57
103	The structures of chiral and racemate campho[2,3-c]pyrazole: A combined crystallographic, solid-state NMR and computational study. Journal of Molecular Structure, 2010, 965, 74-81.	1.8	13
104	Trifluoroâ€3â€hydroxyâ€1Hâ€indazolecarboxylic Acids and Esters from Perfluorinated Benzenedicarboxylic Acids. European Journal of Organic Chemistry, 2010, 2010, 890-899.	1.2	10
105	Symmetrization of Cationic Hydrogen Bridges of Protonated Sponges Induced by Solvent and Counteranion Interactions as Revealed by NMR Spectroscopy. Chemistry - A European Journal, 2010, 16, 1679-1690.	1.7	49
106	RÃ©action De L'Indazole Avec Le Chlorure De Trityle: Identification Par Rmn Du Proton Des IsomÃ¨res 1-, 2-Et 3-Substitues. Bulletin Des SociÃ©tÃ©s Chimiques Belges, 2010, 94, 421-424.	0.0	3
107	Structural studies of 2â€methylâ€7â€substituted pyrazolo[1,5â€a]pyrimidines. Journal of Heterocyclic Chemistry, 2010, 47, 1259-1268.	1.4	20
108	Energetic studies of urea derivatives: Standard molar enthalpy of formation of 3,4,4â€²-trichlorocarbanilide. Journal of Chemical Thermodynamics, 2010, 42, 536-544.	1.0	9

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109	The solid-state structure of primary fatty amines: True amines or ammonium amides?. Journal of Molecular Structure, 2010, 969, 106-110.	1.8	2
110	15Nâ€“15N spinâ€“spin coupling constants through intermolecular hydrogen bonds in the solid state. Journal of Magnetic Resonance, 2010, 206, 274-279.	1.2	11
111	The interplay of hydrogen bonds and halogen bonds in the structure of NH-pyrazoles bearing C-aryl and C-halogen substituents. Inorganica Chimica Acta, 2010, 363, 1332-1342.	1.2	22
112	Molecular Recognition Studies on Naphthyridine Derivatives. Molecules, 2010, 15, 1213-1222.	1.7	9
113	A theoretical multinuclear NMR study of pyrazolylborates. Heterocyclic Communications, 2010, 16, .	0.6	9
114	Computational Thermochemistry of Six Ureas, Imidazolidin-2-one, N,Nâ€²-Trimethyleneurea, Benzimidazolinone, Parabanic Acid, Barbital (5,5â€²-Diethylbarbituric Acid), and 3,4,4â€²-Trichlorocarbanilide, with an Extension to Related Compounds. Journal of Physical Chemistry A, 2010, 114, 9237-9245.	1.1	18
115	NMR Crystallography of Campho[2,3-c]pyrazole (Zâ€² = 6): Combining High-Resolution ¹H-¹³C Solid-State MAS NMR Spectroscopy and GIPAW Chemical-Shift Calculations. Journal of Physical Chemistry A, 2010, 114, 10435-10442.	1.1	127
116	Fast degenerate double proton transfer in the solid state between two indazolinone tautomers. CrystEngComm, 2010, 12, 4052.	1.3	8
117	The Structures of Indazolinâ€3â€one (=1,2â€Dihydroâ€3Hâ€indazolâ€3â€one) and 7â€Nitroindazolinâ€3â€one. Helvetica Chimica Acta, 2009, 92, 1952-1962.	1.0	11
118	¹³C and ¹⁵N NMR spectra of aminobenzimidazoles in solution and in the solid state. Magnetic Resonance in Chemistry, 2009, 47, 100-104.	1.1	22
119	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.	1.1	8
120	Molecular complexes between Ï€â€excedent heterocycles (indoles and carbazole) and Ï€â€deficient polynitrobenzenes. Magnetic Resonance in Chemistry, 2009, 47, 917-924.	1.1	5
121	Synthesis, reactivity, and NMR spectroscopy of 4,6â€and 6,7â€difluoroâ€3â€methylâ€1Hâ€indazoles. Journal of Heterocyclic Chemistry, 2009, 46, 1408-1412.	1.4	12
122	A theoretical and experimental NMR study of (+)-biotin methyl ester. Journal of Molecular Structure, 2009, 920, 323-326.	1.8	15
123	Structural studies of cyclic ureas: 3. Enthalpy of formation of barbital. Journal of Chemical Thermodynamics, 2009, 41, 1400-1407.	1.0	19
124	Synthesis and structural characterization of pyrazol-1â€²-ylpyrazolo[1,5-a]pyrimidines by multinuclear NMR spectroscopy. Journal of Molecular Structure, 2009, 934, 96-102.	1.8	10
125	Intramolecular interactions and photoinduced electron transfer in isoalloxazine-naphthalene bichromophores. Journal of Photochemistry and Photobiology A: Chemistry, 2009, 203, 166-176.	2.0	8
126	Synthesis and biological evaluation of curcuminoid pyrazoles as new therapeutic agents in inflammatory bowel disease: Effect on matrix metalloproteinases. Bioorganic and Medicinal Chemistry, 2009, 17, 1290-1296.	1.4	50

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127	Fluorinated indazoles as novel selective inhibitors of nitric oxide synthase (NOS): Synthesis and biological evaluation. Bioorganic and Medicinal Chemistry, 2009, 17, 6180-6187.	1.4	46
128	Theoretical calculations of a model of NOS indazole inhibitors: Interaction of aromatic compounds with Zn-porphyrins. Bioorganic and Medicinal Chemistry, 2009, 17, 8027-8031.	1.4	16
129	The annular tautomerism of the curcuminoid NH-pyrazoles. New Journal of Chemistry, 2009, 33, 125-135.	1.4	29
130	Protonation effects on the chemical shifts of Schiff bases derived from 3-hydroxypyridin-4-carboxaldehyde. Arkivoc, 2009, 2010, 102-113.	0.3	1
131	¹³C and ¹⁵N NMR chemical shifts of 1â€(2â€²,4â€²â€dinitrophenyl) and 1â€(2â€²,4â€²,6â€²â€trinitrophenyl) pyrazoles in the solid state and in solution. Magnetic Resonance in Chemistry, 2008, 46, 697-700.	1.1	9
132	NMR studies of novel Schiff bases derived from <scp>L</scp>â€Î±â€amino methyl esters and 3â€hydroxypyridinâ€4â€carboxaldehyde. Magnetic Resonance in Chemistry, 2008, 46, 930-938.	1.1	6
133	Structural studies of cyclic ureas: 1. Enthalpies of formation of imidazolidin-2-one and N,Nâ€²-trimethyleneurea. Journal of Chemical Thermodynamics, 2008, 40, 386-393.	1.0	28
134	Structural studies of cyclic ureas: 2. Enthalpy of formation of parabanic acid. Journal of Chemical Thermodynamics, 2008, 40, 1378-1385.	1.0	17
135	A study in desmotropy. Solid State Nuclear Magnetic Resonance, 2008, 34, 68-76.	1.5	29
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