Angel C De Dios

List of Publications by Year
in descending order

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63 papers	2,795 citations	126907 33 h-index	175258 52 g-index
64 all docs	64 docs citations	64 times ranked	2380 citing authors

#	Article	IF	Citations
1	Ab initio calculations of the NMR chemical shift. Progress in Nuclear Magnetic Resonance Spectroscopy, 1996, 29, 229-278.	7.5	217
2	Solution Structures of Antimalarial Drugâ€'Heme Complexesâ€. Biochemistry, 2002, 41, 10245-10255.	2.5	156
3	4-N-, 4-S-, and 4-O-Chloroquine Analogues: Influence of Side Chain Length and Quinolyl Nitrogen pK_a on Activity vs Chloroquine Resistant Malaria. Journal of Medicinal Chemistry, 2008, 51, 3466-3479.	6.4	120
4	Solid-State15N NMR Chemical Shift Anisotropy of Histidines:Â Experimental and Theoretical Studies of Hydrogen Bondingâ€. Journal of the American Chemical Society, 1999, 121, 10389-10394.	13.7	110
5	Ab initiocalculations of NMR chemical shifts. Journal of Chemical Physics, 2008, 128, 052201.	3.0	106
6	Nuclear magnetic resonance studies of xenon clusters in zeolite NaA. Journal of Chemical Physics, 1992, 96, 1676-1689.	3.0	97
7	Abinitiocalculations of the intermolecular chemical shift in nuclear magnetic resonance in the gas phase and for adsorbed species. Journal of Chemical Physics, 1992, 97, 417-434.	3.0	97
8	Protein Structure Refinement and Prediction via NMR Chemical Shifts and Quantum Chemistry. Journal of the American Chemical Society, 1995, 117, 3800-3807.	13.7	94
9	Ab Initio Study of the Effects of Torsion Angles on Carbon-13 Nuclear Magnetic Resonance Chemical Shielding in N-Formyl-L-alanine Amide, N-Formyl-L-valine Amide, and Some Simple Model Compounds: Applications to Protein NMR Spectroscopy. Journal of the American Chemical Society, 1994, 116, 5307-5314.	13.7	71
10	Synthesis and antimalarial activity of new 4-amino-7-chloroquinolyl amides, sulfonamides, ureas and thioureas. Bioorganic and Medicinal Chemistry, 2009, 17, 270-283.	3.0	70
11	Chemical shifts in proteins: an ab initio study of carbon-13 nuclear magnetic resonance chemical shielding in glycine, alanine, and valine residues. Journal of the American Chemical Society, 1993, 115, 9768-9773.	13.7	69
12	NMR Studies of Chloroquineâ€'Ferriprotoporphyrin IX Complex. Journal of Physical Chemistry A, 2003, 107, 5821-5825.	2.5	69
13	Recent progress in understanding chemical shifts. Solid State Nuclear Magnetic Resonance, 1996, 6, 101-125.	2.3	68
14	Predicting Carbon-13 Nuclear Magnetic Resonance Chemical Shielding Tensors in Zwitterionic L-Threonine and L-Tyrosine via Quantum Chemistry. Journal of the American Chemical Society, 1994, 116, 7784-7786.	13.7	67
15	Xe nuclear magnetic resonance line shapes in nanochannels. Journal of Chemical Physics, 2002, 116, 3805-3821.	3.0	67
16	The31P shielding in phosphine. Journal of Chemical Physics, 1991, 95, 9042-9053.	3.0	65
17	Chemical Shifts of Carbonyl Carbons in Peptides and Proteins. Journal of the American Chemical Society, 1994, 116, 11485-11488.	13.7	62
18	Chemical Shift Tensors in Peptides:â€‰ A Quantum Mechanical Study. Journal of Physical Chemistry A, 1997, 101, 7299-7303.	2.5	61

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19	Progress in C13 and H1 solid-state nuclear magnetic resonance for paramagnetic systems under very fast magic angle spinning. Journal of Chemical Physics, 2008, 128, 052210.	3.0	61
20	Nuclear magnetic shielding of nitrogen in ammonia. Journal of Chemical Physics, 1991, 95, 1069-1079.	3.0	57
21	Overcoming Drug Resistance to Heme-Targeted Antimalarials by Systematic Side Chain Variation of 7-Chloro-4-aminoquinolines. Journal of Medicinal Chemistry, 2008, 51, 1995-1998.	6.4	56
22	Synthesis, structural and larvicidal studies of some triorganotin 2-(p-chlorophenyl)-3-methylbutyrates. Journal of Organometallic Chemistry, 2007, 692, 1398-1404.	1.8	51
23	The NMR Chemical Shift: Insight into Structure and Environment. Annual Reports on NMR Spectroscopy, 1994, 29, 1-69.	1.5	50
24	Ab Initio Study of HOCl, HCl, H2O, and Cl2 Interacting with Four Water Molecules. Journal of Physical Chemistry A, 1998, 102, 1514-1522.	2.5	50
25	The nuclear magnetic shielding as a function of internuclear separation. Journal of Chemical Physics, 1993, 98, 2208-2217.	3.0	48
26	Cytostatic versus Cytocidal Activities of Chloroquine Analogues and Inhibition of Hemozoin Crystal Growth. Antimicrobial Agents and Chemotherapy, 2013, 57, 356-364.	3.2	46
27	Correlations between31P Chemical Shift Anisotropy and Molecular Structure in PolycrystallineO,Oâ€²-Dialkyldithiophosphate Zinc(II) and Nickel(II) Complexes:Â31P CP/MAS NMR and Ab Initio Quantum Mechanical Calculation Studies. Journal of the American Chemical Society, 2005, 127, 2218-2230.	13.7	45
28	Quinine and Chloroquine Differentially Perturb Heme Monomerâ^'Dimer Equilibrium. Inorganic Chemistry, 2008, 47, 6077-6081.	4.0	44
29	NMR chemical shifts and structure refinement in proteins. Journal of Biomolecular NMR, 1993, 3, 607-612.	2.8	38
30	Synthesis and antimalarial activity of new chloroquine analogues carrying a multifunctional linear side chain. Bioorganic and Medicinal Chemistry, 2009, 17, 6560-6566.	3.0	38
31	The hydroxyl functionality and a rigid proximal N are required for forming a novel non-covalent quinine-heme complex. Journal of Inorganic Biochemistry, 2011, 105, 467-475.	3.5	38
32	Structure of the Amodiaquineâ^'FPIX Î¼ Oxo Dimer Solution Complex at Atomic Resolution. Inorganic Chemistry, 2004, 43, 8078-8084.	4.0	35
33	The [sup 129]Xe nuclear shielding tensor surfaces for Xe interacting with rare gas atoms. Journal of Chemical Physics, 2003, 118, 2575.	3.0	34
34	A Basis Size Dependence Study of Carbon-13 Nuclear Magnetic Resonance Spectroscopic Shielding in Alanyl and Valyl Fragments: Toward Protein Shielding Hypersurfaces. Journal of the American Chemical Society, 1995, 117, 9542-9546.	13.7	32
35	The129Xe nuclear shielding surfaces for Xe interacting with linear molecules CO2, N2, and CO. Journal of Chemical Physics, 1997, 107, 4253-4270.	3.0	32
36	129Xe nuclear magnetic resonance studies of xenon in zeolite CaA. Journal of Chemical Physics, 1992, 96, 1690-1697.	3.0	31

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37	Characterization of Polymorphs and Solid-State Reactions for Paramagnetic Systems by13C Solid-State NMR and ab Initio Calculations. Journal of the American Chemical Society, 2007, 129, 10968-10969.	13.7	30
38	129Xe Magic-angle spinning spectra of xenon in zeolite NaA direct observation of mixed clusters of co-adsorbed species. Solid State Nuclear Magnetic Resonance, 1995, 4, 1-12.	2.3	29
39	Evaluating 19F Chemical Shielding in Fluorobenzenes: Implications for Chemical Shifts in Proteins. Journal of the American Chemical Society, 1994, 116, 7453-7454.	13.7	28
40	Solvent Effects on 15N NMR Shielding of 1,2,4,5-Tetrazine and Isomeric Tetrazoles:â€‰ Continuous Set Gauge Transformation Calculation Using the Polarizable Continuum Model. Journal of Physical Chemistry A, 2000, 104, 9600-9604.	2.5	28
41	13C NMR Study of the Self-Association of Chloroquine, Amodiaquine, and Quinine. Journal of Physical Chemistry A, 2004, 108, 8505-8513.	2.5	25
42	Antimalarial drugs and heme in detergent micelles: An NMR study. Journal of Inorganic Biochemistry, 2009, 103, 745-748.	3.5	22
43	Synthesis, larvicidal, QSAR and structural studies of some triorganotin 2,2,3,3-tetramethylcyclopropanecarboxylates. Applied Organometallic Chemistry, 2007, 21, 545-550.	3.5	19
44	Recent Advances in Nuclear Shielding Calculations. Annual Reports on NMR Spectroscopy, 2012, 77, 1-80.	1.5	19
45	Relative to Quinine and Quinidine, Their 9-Epimers Exhibit Decreased Cytostatic Activity and Altered Heme Binding but Similar Cytocidal Activity versus Plasmodium falciparum. Antimicrobial Agents and Chemotherapy, 2013, 57, 365-374.	3.2	19
46	Relationship between NMR Shielding and Heme Binding Strength for a Series of 7-Substituted Quinolines. Journal of Physical Chemistry A, 2006, 110, 7787-7792.	2.5	15
47	Electric Field Effects on 13C and 17O Chemical Shifts and CO Stretching Frequency of Carbon Monoxide Bound to Fe2+. Journal of Physical Chemistry A, 1997, 101, 8132-8134.	2.5	14
48	Ab initioCalculations of119Sn Magnetic Shielding. Magnetic Resonance in Chemistry, 1996, 34, 773-776.	1.9	11
49	Alkali Metal NMR Chemical Shielding as a Probe of Local Structure:â€‰ An Experimental and Theoretical Study of Rb+ in Halide Lattices. Journal of Physical Chemistry A, 2000, 104, 908-914.	2.5	10
50	13C Chemical Shielding Tensors in Ampicillin and Penicillin-V:â€‰ A Theoretical Study. Journal of Physical Chemistry A, 2000, 104, 5837-5842.	2.5	10
51	Anab initio study of solvent polarity and hydrogen bonding effects on the nitrogen NMR shieldings ofN,N-dimethylacetamidine. Magnetic Resonance in Chemistry, 2002, 40, 781-785.	1.9	8
52	NMR studies of peptide T, an inhibitor of HIV infectivity, in an aqueous environment. Journal of Peptide Science, 2004, 10, 622-630.	1.4	8
53	CSGT-DFT calculation of 13C and 15N NMR shielding of the backbone amide group, 13CÎ±, and 13CÎ² in Ï‰-Conotoxin GVIA. Computational and Theoretical Chemistry, 2004, 675, 1-8.	1.5	8
54	Carbon Chemical Shift Tensor Components in Quinolines and Quinoline N-Oxides. Journal of Physical Chemistry A, 2006, 110, 234-240.	2.5	8

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55	Interactions between pairs of antimalarial drugs studied by experimental andab initio13C NMR chemical shifts. Magnetic Resonance in Chemistry, 2006, 44, 276-282.	1.9	6
56	15N Shielding of the Nitrosyl Ligand in Co(NO)(TPP). Journal of Physical Chemistry A, 1999, 103, 3062-3065.	2.5	5
57	Artesunate activation by heme in an aqueous medium. Inorganica Chimica Acta, 2019, 496, 119029.	2.4	5
58	Synthesis, structural and larvicidal studies of a series of triorganotin chrysanthemumates. Applied Organometallic Chemistry, 2011, 25, 777-782.	3.5	4
59	1H and 13C NMR for the Profiling of Natural Product Extracts: Theory and Applications. , 0, , .		4
60	The NMR Chemical Shift: Local Geometry Effects. ACS Symposium Series, 1999, , 220-239.	0.5	3
61	Synthesis and structural determination of two triphenyltin thiosalicylates. Journal of Coordination Chemistry, 2009, 62, 3110-3116.	2.2	3
62	Application of Nuclear Shielding Surfaces to the Fundamental Understanding of Adsorption and Diffusion in Microporous Solids. ACS Symposium Series, 1999, , 335-348.	0.5	1
63	13C chemical shifts in octanethiols adsorbed on gold: a theoretical study. Journal of Molecular Structure, 2002, 602-603, 209-214.	3.6	1