Angel C De Dios

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/10377278/publications.pdf

Version: 2024-02-01

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	Artesunate activation by heme in an aqueous medium. Inorganica Chimica Acta, 2019, 496, 119029.	2.4	5
2	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
3	Cytostatic versus Cytocidal Activities of Chloroquine Analogues and Inhibition of Hemozoin Crystal Growth. Antimicrobial Agents and Chemotherapy, 2013, 57, 356-364.	3.2	46
4	Recent Advances in Nuclear Shielding Calculations. Annual Reports on NMR Spectroscopy, 2012, 77, 1-80.	1.5	19
5	Synthesis, structural and larvicidal studies of a series of triorganotin chrysanthemumates. Applied Organometallic Chemistry, 2011, 25, 777-782.	3.5	4
6	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
7	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
8	Antimalarial drugs and heme in detergent micelles: An NMR study. Journal of Inorganic Biochemistry, 2009, 103, 745-748.	3.5	22
9	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
10	Synthesis and structural determination of two triphenyltin thiosalicylates. Journal of Coordination Chemistry, 2009, 62, 3110-3116.	2.2	3
11	Ab initiocalculations of NMR chemical shifts. Journal of Chemical Physics, 2008, 128, 052201.	3.0	106
12	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
13	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
14	Quinine and Chloroquine Differentially Perturb Heme Monomerâˆ’Dimer Equilibrium. Inorganic Chemistry, 2008, 47, 6077-6081.	4.0	44
15	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
16	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
17	Synthesis, larvicidal, QSAR and structural studies of some triorganotin 2,2,3,3-tetramethylcyclopropanecarboxylates. Applied Organometallic Chemistry, 2007, 21, 545-550.	3.5	19
18	Synthesis, structural and larvicidal studies of some triorganotin 2-(p-chlorophenyl)-3-methylbutyrates. Journal of Organometallic Chemistry, 2007, 692, 1398-1404.	1.8	51

#	Article	IF	Citations
19	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
20	Carbon Chemical Shift Tensor Components in Quinolines and Quinoline N-Oxides. Journal of Physical Chemistry A, 2006, 110, 234-240.	2.5	8
21	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
22	Correlations between31P Chemical Shift Anisotropy and Molecular Structure in PolycrystallineO,Oâ€˜-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
23	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
24	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
25	Structure of the Amodiaquineâ˜FPIX Î¼ Oxo Dimer Solution Complex at Atomic Resolution. Inorganic Chemistry, 2004, 43, 8078-8084.	4.0	35
26	13C NMR Study of the Self-Association of Chloroquine, Amodiaquine, and Quinine. Journal of Physical Chemistry A, 2004, 108, 8505-8513.	2.5	25
27	NMR Studies of Chloroquineâ˜Ferriprotoporphyrin IX Complex. Journal of Physical Chemistry A, 2003, 107, 5821-5825.	2.5	69
28	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
29	Solution Structures of Antimalarial Drugâ˜Heme Complexesâ€. Biochemistry, 2002, 41, 10245-10255.	2.5	156
30	Xe nuclear magnetic resonance line shapes in nanochannels. Journal of Chemical Physics, 2002, 116, 3805-3821.	3.0	67
31	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
32	13C chemical shifts in octanethiols adsorbed on gold: a theoretical study. Journal of Molecular Structure, 2002, 602-603, 209-214.	3.6	1
33	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
34	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
35	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
36	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

#	Article	IF	Citations
37	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
38	15N Shielding of the Nitrosyl Ligand in Co(NO)(TPP). Journal of Physical Chemistry A, 1999, 103, 3062-3065.	2.5	5
39	The NMR Chemical Shift: Local Geometry Effects. ACS Symposium Series, 1999, , 220-239.	0.5	3
40	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
41	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
42	Chemical Shift Tensors in Peptides:â€‰ A Quantum Mechanical Study. Journal of Physical Chemistry A, 1997, 101, 7299-7303.	2.5	61
43	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
44	Ab initioCalculations of119Sn Magnetic Shielding. Magnetic Resonance in Chemistry, 1996, 34, 773-776.	1.9	11
45	Recent progress in understanding chemical shifts. Solid State Nuclear Magnetic Resonance, 1996, 6, 101-125.	2.3	68
46	Ab initio calculations of the NMR chemical shift. Progress in Nuclear Magnetic Resonance Spectroscopy, 1996, 29, 229-278.	7.5	217
47	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
48	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
49	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
50	The NMR Chemical Shift: Insight into Structure and Environment. Annual Reports on NMR Spectroscopy, 1994, 29, 1-69.	1.5	50
51	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
52	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
53	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
54	Chemical Shifts of Carbonyl Carbons in Peptides and Proteins. Journal of the American Chemical Society, 1994, 116, 11485-11488.	13.7	62

#	Article	IF	Citations
55	NMR chemical shifts and structure refinement in proteins. Journal of Biomolecular NMR, 1993, 3, 607-612.	2.8	38
56	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
57	The nuclear magnetic shielding as a function of internuclear separation. Journal of Chemical Physics, 1993, 98, 2208-2217.	3.0	48
58	Nuclear magnetic resonance studies of xenon clusters in zeolite NaA. Journal of Chemical Physics, 1992, 96, 1676-1689.	3.0	97
59	129Xe nuclear magnetic resonance studies of xenon in zeolite CaA. Journal of Chemical Physics, 1992, 96, 1690-1697.	3.0	31
60	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
61	The31P shielding in phosphine. Journal of Chemical Physics, 1991, 95, 9042-9053.	3.0	65
62	Nuclear magnetic shielding of nitrogen in ammonia. Journal of Chemical Physics, 1991, 95, 1069-1079.	3.0	57
63	1H and 13C NMR for the Profiling of Natural Product Extracts: Theory and Applications. , 0, , .		4