Juan A Aguilar

List of Publications by Year
in descending order

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70 papers	3,675 citations	136885 32 h-index	128225 60 g-index
74 all docs	74 docs citations	74 times ranked	3376 citing authors

#	Article	IF	Citations
1	Coherence transfer delay optimisation in PSYCOSY experiments. Magnetic Resonance in Chemistry, 2020, 58, 51-55.	1.1	1
2	Solution-state behaviour of algal mono-uronates evaluated by pure shift and compressive sampling NMR techniques. Carbohydrate Research, 2020, 495, 108087.	1.1	1
3	Hybrid GMPâ€“polyamine hydrogels as new biocompatible materials for drug encapsulation. Soft Matter, 2020, 16, 6514-6522.	1.2	5
4	Impact of Methoxy Substituents on Thermally Activated Delayed Fluorescence and Room-Temperature Phosphorescence in All-Organic Donorâ€“Acceptor Systems. Journal of Organic Chemistry, 2019, 84, 3801-3816.	1.7	43
5	Fluorinated Aromatic Monomers as Building Blocks To Control Î±-Peptoid Conformation and Structure. Journal of the American Chemical Society, 2019, 141, 3430-3434.	6.6	33
6	Reliable, high-quality suppression of NMR signals arising from water and macromolecules: application to bio-fluid analysis. Analyst, The, 2019, 144, 7270-7277.	1.7	10
7	On the Antibacterial Activity of Azacarboxylate Ligands: Lowered Metal Ion Affinities for Bisâ€amide Derivatives of EDTA do not mean Reduced Activity. Chemistry - A European Journal, 2018, 24, 7137-7148.	1.7	3
8	Compressed <scp>NMR</scp>: Combining compressive sampling and pure shift <scp>NMR</scp> techniques. Magnetic Resonance in Chemistry, 2018, 56, 983-992.	1.1	8
9	Separating the coherence transfer from chemical shift evolution in highâ€resolution pure shift <scp>COSY NMR</scp>. Magnetic Resonance in Chemistry, 2018, 56, 969-975.	1.1	8
10	In Situ Molecular-Level Observation of Methanol Catalysis at the Waterâ€“Graphite Interface. ACS Applied Materials & Interfaces, 2018, 10, 34265-34271.	4.0	11
11	Aggregation of Rare Earth Coordination Complexes in Solution Studied by Paramagnetic and DOSY NMR. Chemistry - A European Journal, 2018, 24, 16170-16175.	1.7	15
12	Increased rate of solvent diffusion in a prototypical supramolecular gel measured on the picosecond timescale. Chemical Communications, 2018, 54, 6340-6343.	2.2	4
13	Stabilising Peptoid Helices Using Nonâ€Chiral Fluoroalkyl Monomers. Angewandte Chemie - International Edition, 2018, 57, 10549-10553.	7.2	35
14	Stabilising Peptoid Helices Using Nonâ€Chiral Fluoroalkyl Monomers. Angewandte Chemie, 2018, 130, 10709-10713.	1.6	4
15	Frontispiece: On the Antibacterial Activity of Azacarboxylate Ligands: Lowered Metal Ion Affinities for Bis-amide Derivatives of EDTA do not mean Reduced Activity. Chemistry - A European Journal, 2018, 24, .	1.7	0
16	Guanosineâ€5â€²â€Monophosphate Polyamine Hybrid Hydrogels: Enhanced Gel Strength Probed by zâ€Spectroscopy. Chemistry - A European Journal, 2017, 23, 7755-7760.	1.7	12
17	PARASHIFT Probes: Solution NMR and X-ray Structural Studies of Macrocyclic Ytterbium and Yttrium Complexes. Inorganic Chemistry, 2017, 56, 4028-4038.	1.9	34
18	Excited-State Aromatic Interactions in the Aggregation-Induced Emission of Molecular Rotors. Journal of the American Chemical Society, 2017, 139, 17882-17889.	6.6	141

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19	Conformational study of tylosin A in water and full assignments of ¹H and ¹³C spectra of tylosin A in D₂O and tylosin B in CDCl₃. Magnetic Resonance in Chemistry, 2017, 55, 367-373.	1.1	5
20	Trimeric cyclamers: solution aggregation and high Zâ€² crystals based on guest structure and basicity. Chemical Communications, 2016, 52, 11846-11849.	2.2	4
21	Amorphism and Thermal Decomposition of Salicylsalicylic Acidâ€"AÂCautionary Tale. Journal of Pharmaceutical Sciences, 2016, 105, 3073-3078.	1.6	0
22	HD-2D: routine high-dispersion two-dimensional NMR spectra at no extra cost. RSC Advances, 2016, 6, 83380-83385.	1.7	4
23	Characterization of Two Distinct Amorphous Forms of Valsartan by Solid-State NMR. Molecular Pharmaceutics, 2016, 13, 211-222.	2.3	30
24	Robust NMR water signal suppression for demanding analytical applications. Analyst, The, 2016, 141, 236-242.	1.7	20
25	Ultra-high dispersion NMR reveals new levels of detail. RSC Advances, 2015, 5, 52902-52906.	1.7	5
26	Minimising Research Bottlenecks by Decluttering NMR Spectra. Chemistry - A European Journal, 2015, 21, 6623-6630.	1.7	27
27	Real-time pure shift 15N HSQC of proteins: a real improvement in resolution and sensitivity. Journal of Biomolecular NMR, 2015, 62, 43-52.	1.6	30
28	Supramolecular Gel Control of Cisplatin Crystallization: Identification of a New Solvate Form Using a Cisplatin-Mimetic Gelator. Crystal Growth and Design, 2015, 15, 4591-4599.	1.4	33
29	Bisoprolol and Bisoprolol-Valsartan Compatibility Studied by Differential Scanning Calorimetry, Nuclear Magnetic Resonance and X-Ray Powder Diffractometry. Pharmaceutical Research, 2015, 32, 414-429.	1.7	22
30	Suppressing exchange effects in diffusion-ordered NMR spectroscopy. Journal of Magnetic Resonance, 2014, 238, 16-19.	1.2	33
31	Theoretical and experimental investigation on clarithromycin, erythromycin A and azithromycin and descladinosyl derivatives of clarithromycin and azithromycin with 3-O substitution as anti-bacterial agents. MedChemComm, 2014, 5, 1347-1354.	3.5	16
32	â€œPure shiftâ€•¹H NMR, a robust method for revealing heteronuclear couplings in complex spectra. RSC Advances, 2014, 4, 8278-8282.	1.7	24
33	Simultaneously Enhancing Spectral Resolution and Sensitivity in Heteronuclear Correlation NMR Spectroscopy. Angewandte Chemie - International Edition, 2013, 52, 11616-11619.	7.2	160
34	â€œPerfectingâ€•WATERGATE: clean proton NMR spectra from aqueous solution. Chemical Communications, 2013, 49, 358-360.	2.2	115
35	Left-Handed Helical Preference in an Achiral Peptide Chain Is Induced by an <scp>l</scp>-Amino Acid in an N-Terminal Type II Î²-Turn. Journal of Organic Chemistry, 2013, 78, 2248-2255.	1.7	43
36	Detection of Potential TNA and RNA Nucleoside Precursors in a Prebiotic Mixture by Pure Shift Diffusionâ€Ordered NMR Spectroscopy. Chemistry - A European Journal, 2013, 19, 4586-4595.	1.7	30

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37	Spin echo NMR spectra without J modulation. Chemical Communications, 2012, 48, 811-813.	2.2	218
38	Decoupling Twoâ€Ðimensional NMR Spectroscopy in Both Dimensions: Pure Shift NOESY and COSY. Angewandte Chemie - International Edition, 2012, 51, 6460-6463.	7.2	97
39	Simultaneous enhancement of chemical shift dispersion and diffusion resolution in mixture analysis by diffusion-ordered NMR spectroscopy. Chemical Communications, 2011, 47, 7063.	2.2	55
40	Resolving natural product epimer spectra by matrix-assisted DOSY. Organic and Biomolecular Chemistry, 2011, 9, 7062.	1.5	42
41	Simple Proton Spectra from Complex Spin Systems: Pure Shift NMR Spectroscopy Using BIRD. Angewandte Chemie - International Edition, 2011, 50, 9716-9717.	7.2	113
42	Selective detection of hyperpolarized NMR signals derived from para-hydrogen using the Only Para-hydrogen SpectroscopY (OPSY) approach. Journal of Magnetic Resonance, 2011, 208, 49-57.	1.2	53
43	J-modulation effects in DOSY experiments and their suppression: The Oneshot45 experiment. Journal of Magnetic Resonance, 2011, 208, 270-278.	1.2	60
44	Pure Shift ¹H NMR: A Resolution of the Resolution Problem?. Angewandte Chemie - International Edition, 2010, 49, 3901-3903.	7.2	225
45	True Chemical Shift Correlation Maps: A TOCSY Experiment with Pure Shifts in Both Dimensions. Journal of the American Chemical Society, 2010, 132, 12770-12772.	6.6	107
46	Reversible Interactions with para-Hydrogen Enhance NMR Sensitivity by Polarization Transfer. Science, 2009, 323, 1708-1711.	6.0	761
47	Only para-hydrogen spectroscopy (OPSY), a technique for the selective observation of para-hydrogen enhanced NMR signals. Chemical Communications, 2007, , 1183-1185.	2.2	84
48	A bibracchial lariat aza-crown ether as an abiotic catalyst of malonic acid enolization. New Journal of Chemistry, 2007, 31, 2065.	1.4	0
49	Properties of a Triazolopyridine System as a Molecular Chemosensor for Metal Ions, Anions, and Amino Acids. Journal of Organic Chemistry, 2006, 71, 9030-9034.	1.7	42
50	CO2Fixation by Cu2+and Zn2+Complexes of a Terpyridinophane Aza Receptor. Crystal Structures of Cu2+Complexes, pH-Metric, Spectroscopic, and Electrochemical Studies. Inorganic Chemistry, 2006, 45, 3803-3815.	1.9	46
51	Binuclear Cu2+ complex mediated discrimination between l-glutamate and l-aspartate in water. Chemical Communications, 2005, , 3086.	2.2	40
52	Parahydrogen derived illumination of pyridine based coordination products obtained from reactions involving rhodium phosphine complexes. Dalton Transactions, 2005, , 3773.	1.6	15
53	Shape-Complementarity in the Recognition of Tricarboxylic Acids by a [3+3] Polyazacyclophane Receptor. Journal of Organic Chemistry, 2005, 70, 2042-2047.	1.7	28
54	Dinuclear ZnII Complexes of Polydentate Polyamines as Minimalist Models of Hydrolytic Reactions. European Journal of Inorganic Chemistry, 2004, 2004, 4061-4071.	1.0	14

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55	Stability and kinetics of the acid-promoted decomposition of Cu(ii) complexes with hexaazacyclophanes: kinetic studies as a probe to detect changes in the coordination mode of the macrocycles. Dalton Transactions, 2004, , 94-103.	1.6	23
56	Synthesis and H+, Cu2+, and Zn2+Coordination Behavior of a Bis(fluorophoric) Bibrachial Lariat Aza-Crown. Inorganic Chemistry, 2004, 43, 6114-6122.	1.9	62
57	Potentiometric, NMR, and Fluorescence-Emission Studies on the Binding of Adenosine 5â€²-Triphosphate (ATP) by Open-Chain Polyamine Receptors Containing Naphthylmethyl and/or Anthrylmethyl Groups. Helvetica Chimica Acta, 2003, 86, 3118-3135.	1.0	53
58	Hydrogen-ion driven molecular motions in Cu2+-complexes of a ditopic phenanthrolinophane ligand. Chemical Communications, 2003, , 3032-3033.	2.2	15
59	Interactions of diaryl-polyamines with nucleic acids. Allosteric effects with dinuclear copper complexes. Tetrahedron Letters, 2002, 43, 7801-7803.	0.7	15
60	Cation and anion recognition characteristics of open-chain polyamines containing ethylenic and propylenic chains. Inorganica Chimica Acta, 2002, 339, 307-316.	1.2	36
61	Anion Binding with Two Polyammonium Macrocycles of Different Dimensionality. Inorganic Chemistry, 2001, 40, 4710-4720.	1.9	91
62	Copper complexes of polyaza[n]cyclophanes and their interaction with DNA and RNA. Inorganica Chimica Acta, 2001, 316, 71-78.	1.2	59
63	Fluoride Ion Receptors: A Comparison of a Polyammonium MonocycleVersusits Bicyclic Corollary. Supramolecular Chemistry, 2001, 13, 405-417.	1.5	40
64	Structural characterization in solution of multifunctional nucleotide coordination systems. Perkin Transactions II RSC, 2000, , 1323-1328.	1.1	34
65	New molecular catalysts for ATP cleavage. Criteria of size complementarity. Perkin Transactions II RSC, 2000, , 1187-1192.	1.1	36
66	Synthesis, protonation and Cu2+ co-ordination studies on a new family of thiophenophane receptorsâ€Šâ€. Journal of the Chemical Society Perkin Transactions II, 1999, , 1159-1168.	0.9	9
67	A reinforced polyaza[n.n]paracyclophane containing piperazine rings. Journal of the Chemical Society Dalton Transactions, 1996, , 239-246.	1.1	12
68	Synthesis and protonation behaviour of the macrocycle 2,6,10,13,17,21-hexaaza[22]metacyclophane. Thermodynamic and NMR studies on the interaction of 2,6,10,13,17,21-hexaaza[22]metacyclophane and on the open-chain polyamine 4,8,11,15-tetraazaoctadecane-1,18-diamine with ATP, ADP and AMP. Inorganica Chimica Acta, 1996, 246, 287-294.	1.2	41
69	Multifunctional molecular recognition of ATP, ADP and AMP nucleotides by the novel receptor 2,6,10,13,17,21-hexaaza[22]metacyclophane. Journal of the Chemical Society Chemical Communications, 1995, .	2.0	68
70	Synthesis, protonation and co-ordination abilities of the open-chain polyamine 4,8,11,15-tetraazaoctadecane-1,18-diamine. Journal of the Chemical Society Dalton Transactions, 1994, , 637-644.	1.1	18