

# 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	Reversible Interactions with para-Hydrogen Enhance NMR Sensitivity by Polarization Transfer. <i>Science</i> , 2009, 323, 1708-1711.	6.0	761
2	Pure Shift <sup>1</sup> H NMR: A Resolution of the Resolution Problem?. <i>Angewandte Chemie - International Edition</i> , 2010, 49, 3901-3903.	7.2	225
3	Spin echo NMR spectra without J modulation. <i>Chemical Communications</i> , 2012, 48, 811-813.	2.2	218
4	Simultaneously Enhancing Spectral Resolution and Sensitivity in Heteronuclear Correlation NMR Spectroscopy. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 11616-11619.	7.2	160
5	Excited-State Aromatic Interactions in the Aggregation-Induced Emission of Molecular Rotors. <i>Journal of the American Chemical Society</i> , 2017, 139, 17882-17889.	6.6	141
6	Perfecting WATERGATE: clean proton NMR spectra from aqueous solution. <i>Chemical Communications</i> , 2013, 49, 358-360.	2.2	115
7	Simple Proton Spectra from Complex Spin Systems: Pure Shift NMR Spectroscopy Using BIRD. <i>Angewandte Chemie - International Edition</i> , 2011, 50, 9716-9717.	7.2	113
8	True Chemical Shift Correlation Maps: A TOCSY Experiment with Pure Shifts in Both Dimensions. <i>Journal of the American Chemical Society</i> , 2010, 132, 12770-12772.	6.6	107
9	Decoupling Two-Dimensional NMR Spectroscopy in Both Dimensions: Pure Shift NOESY and COSY. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 6460-6463.	7.2	97
10	Anion Binding with Two Polyammonium Macrocycles of Different Dimensionality. <i>Inorganic Chemistry</i> , 2001, 40, 4710-4720.	1.9	91
11	Only para-hydrogen spectroscopy (OPSY), a technique for the selective observation of para-hydrogen enhanced NMR signals. <i>Chemical Communications</i> , 2007, , 1183-1185.	2.2	84
12	Multifunctional molecular recognition of ATP, ADP and AMP nucleotides by the novel receptor 2,6,10,13,17,21-hexaaza[22]metacyclophane. <i>Journal of the Chemical Society Chemical Communications</i> , 1995, .	2.0	68
13	Synthesis and H <sup>+</sup> , Cu <sup>2+</sup> , and Zn <sup>2+</sup> Coordination Behavior of a Bis(fluorophoric) Bibrachial Lariat Aza-Crown. <i>Inorganic Chemistry</i> , 2004, 43, 6114-6122.	1.9	62
14	J-modulation effects in DOSY experiments and their suppression: The Oneshot45 experiment. <i>Journal of Magnetic Resonance</i> , 2011, 208, 270-278.	1.2	60
15	Copper complexes of polyaza[n]cyclophanes and their interaction with DNA and RNA. <i>Inorganica Chimica Acta</i> , 2001, 316, 71-78.	1.2	59
16	Simultaneous enhancement of chemical shift dispersion and diffusion resolution in mixture analysis by diffusion-ordered NMR spectroscopy. <i>Chemical Communications</i> , 2011, 47, 7063.	2.2	55
17	Potentiometric, NMR, and Fluorescence-Emission Studies on the Binding of Adenosine 5'-Triphosphate (ATP) by Open-Chain Polyamine Receptors Containing Naphthylmethyl and/or Anthrylmethyl Groups. <i>Helvetica Chimica Acta</i> , 2003, 86, 3118-3135.	1.0	53
18	Selective detection of hyperpolarized NMR signals derived from para-hydrogen using the Only Para-hydrogen Spectroscopy (OPSY) approach. <i>Journal of Magnetic Resonance</i> , 2011, 208, 49-57.	1.2	53

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19	CO <sub>2</sub> Fixation by Cu <sup>2+</sup> and Zn <sup>2+</sup> Complexes of a Terpyridinophane Aza Receptor. Crystal Structures of Cu <sup>2+</sup> Complexes, pH-Metric, Spectroscopic, and Electrochemical Studies. <i>Inorganic Chemistry</i> , 2006, 45, 3803-3815.	1.9	46
20	Left-Handed Helical Preference in an Achiral Peptide Chain Is Induced by an $\alpha$ -Amino Acid in an N-Terminal Type II $\beta$ -Turn. <i>Journal of Organic Chemistry</i> , 2013, 78, 2248-2255.	1.7	43
21	Impact of Methoxy Substituents on Thermally Activated Delayed Fluorescence and Room-Temperature Phosphorescence in All-Organic Donor-Acceptor Systems. <i>Journal of Organic Chemistry</i> , 2019, 84, 3801-3816.	1.7	43
22	Properties of a Triazolopyridine System as a Molecular Chemosensor for Metal Ions, Anions, and Amino Acids. <i>Journal of Organic Chemistry</i> , 2006, 71, 9030-9034.	1.7	42
23	Resolving natural product epimer spectra by matrix-assisted DOSY. <i>Organic and Biomolecular Chemistry</i> , 2011, 9, 7062.	1.5	42
24	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-tetrazaoctadecane-1,18-diamine with ATP, ADP and AMP. <i>Inorganica Chimica Acta</i> , 1996, 246, 287-294.	1.2	41
25	Fluoride Ion Receptors: A Comparison of a Polyammonium Monocycle Versus its Bicyclic Corollary. <i>Supramolecular Chemistry</i> , 2001, 13, 405-417.	1.5	40
26	Binuclear Cu <sup>2+</sup> complex mediated discrimination between L-glutamate and L-aspartate in water. <i>Chemical Communications</i> , 2005, , 3086.	2.2	40
27	New molecular catalysts for ATP cleavage. Criteria of size complementarity. <i>Perkin Transactions II RSC</i> , 2000, , 1187-1192.	1.1	36
28	Cation and anion recognition characteristics of open-chain polyamines containing ethylenic and propylenic chains. <i>Inorganica Chimica Acta</i> , 2002, 339, 307-316.	1.2	36
29	Stabilising Peptoid Helices Using Non-Chiral Fluoroalkyl Monomers. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 10549-10553.	7.2	35
30	Structural characterization in solution of multifunctional nucleotide coordination systems. <i>Perkin Transactions II RSC</i> , 2000, , 1323-1328.	1.1	34
31	PARASHIFT Probes: Solution NMR and X-ray Structural Studies of Macrocyclic Ytterbium and Yttrium Complexes. <i>Inorganic Chemistry</i> , 2017, 56, 4028-4038.	1.9	34
32	Suppressing exchange effects in diffusion-ordered NMR spectroscopy. <i>Journal of Magnetic Resonance</i> , 2014, 238, 16-19.	1.2	33
33	Supramolecular Gel Control of Cisplatin Crystallization: Identification of a New Solvate Form Using a Cisplatin-Mimetic Gelator. <i>Crystal Growth and Design</i> , 2015, 15, 4591-4599.	1.4	33
34	Fluorinated Aromatic Monomers as Building Blocks To Control $\beta$ -Peptoid Conformation and Structure. <i>Journal of the American Chemical Society</i> , 2019, 141, 3430-3434.	6.6	33
35	Detection of Potential TNA and RNA Nucleoside Precursors in a Prebiotic Mixture by Pure Shift Diffusion-Ordered NMR Spectroscopy. <i>Chemistry - A European Journal</i> , 2013, 19, 4586-4595.	1.7	30
36	Real-time pure shift 15N HSQC of proteins: a real improvement in resolution and sensitivity. <i>Journal of Biomolecular NMR</i> , 2015, 62, 43-52.	1.6	30

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37	Characterization of Two Distinct Amorphous Forms of Valsartan by Solid-State NMR. <i>Molecular Pharmaceutics</i> , 2016, 13, 211-222.	2.3	30
38	Shape-Complementarity in the Recognition of Tricarboxylic Acids by a [3+3] Polyazacyclophane Receptor. <i>Journal of Organic Chemistry</i> , 2005, 70, 2042-2047.	1.7	28
39	Minimising Research Bottlenecks by Decluttering NMR Spectra. <i>Chemistry - A European Journal</i> , 2015, 21, 6623-6630.	1.7	27
40	“Pure shift” <sup>1</sup> H NMR, a robust method for revealing heteronuclear couplings in complex spectra. <i>RSC Advances</i> , 2014, 4, 8278-8282.	1.7	24
41	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. <i>Dalton Transactions</i> , 2004, , 94-103.	1.6	23
42	Bisoprolol and Bisoprolol-Valsartan Compatibility Studied by Differential Scanning Calorimetry, Nuclear Magnetic Resonance and X-Ray Powder Diffractometry. <i>Pharmaceutical Research</i> , 2015, 32, 414-429.	1.7	22
43	Robust NMR water signal suppression for demanding analytical applications. <i>Analyst</i> , 2016, 141, 236-242.	1.7	20
44	Synthesis, protonation and co-ordination abilities of the open-chain polyamine 4,8,11,15-tetraazaoctadecane-1,18-diamine. <i>Journal of the Chemical Society Dalton Transactions</i> , 1994, , 637-644.	1.1	18
45	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. <i>MedChemComm</i> , 2014, 5, 1347-1354.	3.5	16
46	Interactions of diaryl-polyamines with nucleic acids. Allosteric effects with dinuclear copper complexes. <i>Tetrahedron Letters</i> , 2002, 43, 7801-7803.	0.7	15
47	Hydrogen-ion driven molecular motions in Cu <sup>2+</sup> -complexes of a ditopic phenanthroline ligand. <i>Chemical Communications</i> , 2003, , 3032-3033.	2.2	15
48	Parahydrogen derived illumination of pyridine based coordination products obtained from reactions involving rhodium phosphine complexes. <i>Dalton Transactions</i> , 2005, , 3773.	1.6	15
49	Aggregation of Rare Earth Coordination Complexes in Solution Studied by Paramagnetic and DOSY NMR. <i>Chemistry - A European Journal</i> , 2018, 24, 16170-16175.	1.7	15
50	Dinuclear ZnII Complexes of Polydentate Polyamines as Minimalist Models of Hydrolytic Reactions. <i>European Journal of Inorganic Chemistry</i> , 2004, 2004, 4061-4071.	1.0	14
51	A reinforced polyaza[n.n]paracyclophane containing piperazine rings. <i>Journal of the Chemical Society Dalton Transactions</i> , 1996, , 239-246.	1.1	12
52	Guanosine 5'-Monophosphate Polyamine Hybrid Hydrogels: Enhanced Gel Strength Probed by <sup>31</sup> P Spectroscopy. <i>Chemistry - A European Journal</i> , 2017, 23, 7755-7760.	1.7	12
53	In Situ Molecular-Level Observation of Methanol Catalysis at the Water-Graphite Interface. <i>ACS Applied Materials &amp; Interfaces</i> , 2018, 10, 34265-34271.	4.0	11
54	Reliable, high-quality suppression of NMR signals arising from water and macromolecules: application to bio-fluid analysis. <i>Analyst</i> , 2019, 144, 7270-7277.	1.7	10

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55	Synthesis, protonation and Cu <sup>2+</sup> co-ordination studies on a new family of thiophenophane receptors. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1999, , 1159-1168.	0.9	9
56	Compressed <sup>1</sup> H NMR: Combining compressive sampling and pure shift <sup>1</sup> H NMR techniques. <i>Magnetic Resonance in Chemistry</i> , 2018, 56, 983-992.	1.1	8
57	Separating the coherence transfer from chemical shift evolution in high-resolution pure shift <sup>1</sup> H COSY NMR. <i>Magnetic Resonance in Chemistry</i> , 2018, 56, 969-975.	1.1	8
58	Ultra-high dispersion NMR reveals new levels of detail. <i>RSC Advances</i> , 2015, 5, 52902-52906.	1.7	5
59	Conformational study of tylosin A in water and full assignments of <sup>1</sup> H and <sup>13</sup> C spectra of tylosin A in D <sub>2</sub> O and tylosin B in CDCl <sub>3</sub> . <i>Magnetic Resonance in Chemistry</i> , 2017, 55, 367-373.	1.1	5
60	Hybrid GMP polyamine hydrogels as new biocompatible materials for drug encapsulation. <i>Soft Matter</i> , 2020, 16, 6514-6522.	1.2	5
61	Trimeric cyclamers: solution aggregation and high Zr <sup>2+</sup> crystals based on guest structure and basicity. <i>Chemical Communications</i> , 2016, 52, 11846-11849.	2.2	4
62	HD-2D: routine high-dispersion two-dimensional NMR spectra at no extra cost. <i>RSC Advances</i> , 2016, 6, 83380-83385.	1.7	4
63	Increased rate of solvent diffusion in a prototypical supramolecular gel measured on the picosecond timescale. <i>Chemical Communications</i> , 2018, 54, 6340-6343.	2.2	4
64	Stabilising Peptoid Helices Using Non-Chiral Fluoroalkyl Monomers. <i>Angewandte Chemie</i> , 2018, 130, 10709-10713.	1.6	4
65	On the Antibacterial Activity of Azacarboxylate Ligands: Lowered Metal Ion Affinities for Bis-amide Derivatives of EDTA do not mean Reduced Activity. <i>Chemistry - A European Journal</i> , 2018, 24, 7137-7148.	1.7	3
66	Coherence transfer delay optimisation in PSYCOSY experiments. <i>Magnetic Resonance in Chemistry</i> , 2020, 58, 51-55.	1.1	1
67	Solution-state behaviour of algal mono-uronates evaluated by pure shift and compressive sampling NMR techniques. <i>Carbohydrate Research</i> , 2020, 495, 108087.	1.1	1
68	A bibracchial lariat aza-crown ether as an abiotic catalyst of malonic acid enolization. <i>New Journal of Chemistry</i> , 2007, 31, 2065.	1.4	0
69	Amorphism and Thermal Decomposition of Salicylsalicylic Acid – A Cautionary Tale. <i>Journal of Pharmaceutical Sciences</i> , 2016, 105, 3073-3078.	1.6	0
70	Frontispiece: On the Antibacterial Activity of Azacarboxylate Ligands: Lowered Metal Ion Affinities for Bis-amide Derivatives of EDTA do not mean Reduced Activity. <i>Chemistry - A European Journal</i> , 2018, 24, .	1.7	0