

Federico Rastrelli

List of Publications by Year in descending order

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40
papers

1,298
citations

361413

20
h-index

345221

36
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44
all docs

44
docs citations

44
times ranked

1535
citing authors

#	ARTICLE	IF	CITATIONS
1	Toward the Complete Prediction of the ^1H and ^{13}C NMR Spectra of Complex Organic Molecules by DFT Methods: Application to Natural Substances. <i>Chemistry - A European Journal</i> , 2006, 12, 5514-5525.	3.3	189
2	Predicting ^{13}C NMR Spectra by DFT Calculations. <i>Journal of Physical Chemistry A</i> , 2003, 107, 9964-9973.	2.5	121
3	Prediction of the ^1H and ^{13}C NMR Spectra of $\beta\text{-D-Glucose}$ in Water by DFT Methods and MD Simulations. <i>Journal of Organic Chemistry</i> , 2007, 72, 7373-7381.	3.2	100
4	Predicting the NMR Spectra of Paramagnetic Molecules by DFT: Application to Organic Free Radicals and Transition-Metal Complexes. <i>Chemistry - A European Journal</i> , 2009, 15, 7990-8004.	3.3	97
5	Nanoparticle-Based Receptors Mimic Protein-Ligand Recognition. <i>CheM</i> , 2017, 3, 92-109.	11.7	74
6	Nanoparticle-Assisted NMR Detection of Organic Anions: From Chemosensing to Chromatography. <i>Journal of the American Chemical Society</i> , 2015, 137, 886-892.	13.7	55
7	^{13}C -NMR Chemosensing Using Monolayer-Protected Nanoparticles as Receptors. <i>Journal of the American Chemical Society</i> , 2013, 135, 11768-11771.	13.7	53
8	Lanthanide-Based NMR: A Tool To Investigate Component Distribution in Mixed-Monolayer-Protected Nanoparticles. <i>Journal of the American Chemical Society</i> , 2012, 134, 7200-7203.	13.7	44
9	Predicting the ^1H and ^{13}C NMR spectra of paramagnetic Ru(III) complexes by DFT. <i>Magnetic Resonance in Chemistry</i> , 2010, 48, S132-S141.	1.9	40
10	Seeing through Macromolecules: T_2 -Filtered NMR for the Purity Assay of Functionalized Nanosystems and the Screening of Biofluids. <i>Journal of the American Chemical Society</i> , 2009, 131, 14222-14224.	13.7	36
11	Hydrolytic Nanozymes. <i>European Journal of Organic Chemistry</i> , 2020, 2020, 5044-5055.	2.4	36
12	Nuclear Spin Relaxation Driven by Intermolecular Dipolar Interactions: The Role of Solute-Solvent Pair Correlations in the Modeling of Spectral Density Functions. <i>Journal of Physical Chemistry B</i> , 2006, 110, 5676-5689.	2.6	35
13	Predicting the spin state of paramagnetic iron complexes by DFT calculation of proton NMR spectra. <i>Dalton Transactions</i> , 2014, 43, 9486-9496.	3.3	33
14	Detection and identification of designer drugs by nanoparticle-based NMR chemosensing. <i>Chemical Science</i> , 2018, 9, 4777-4784.	7.4	32
15	Molecular Dynamics Simulation Directed Rational Design of Nanoreceptors with Targeted Affinity. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 7702-7707.	13.8	31
16	Turning Supramolecular Receptors into Chemosensors by Nanoparticle-Assisted ^{13}C -NMR Chemosensing. <i>Journal of the American Chemical Society</i> , 2015, 137, 11399-11406.	13.7	30
17	NMR quantification of trace components in complex matrices by band-selective excitation with adiabatic pulses. <i>Magnetic Resonance in Chemistry</i> , 2009, 47, 868-872.	1.9	29
18	Thermoinduced Lipid Oxidation of a Culinary Oil: A Kinetic Study of the Oxidation Products by Magnetic Resonance Spectroscopies. <i>Journal of Physical Chemistry A</i> , 2010, 114, 10059-10065.	2.5	26

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19	Poly(lipoic acid)-Based Nanoparticles as Self-Organized, Biocompatible, and Corona-Free Nanovectors. <i>Biomacromolecules</i> , 2021, 22, 467-480.	5.4	22
20	Aggregation Behavior of Octyl Viologen Di[bis(trifluoromethanesulfonyl)amide] in Nonpolar Solvents. <i>Journal of Physical Chemistry B</i> , 2008, 112, 16566-16574.	2.6	21
21	Nanoparticle-Assisted NMR Spectroscopy: Enhanced Detection of Analytes by Water-Mediated Saturation Transfer. <i>Journal of the American Chemical Society</i> , 2019, 141, 4870-4877.	13.7	21
22	Nanoparticle-Assisted Affinity NMR Spectroscopy: High Sensitivity Detection and Identification of Organic Molecules. <i>Chemistry - A European Journal</i> , 2016, 22, 16957-16963.	3.3	18
23	Mapping the nanoparticle-coating monolayer with NMR pseudocontact shifts. <i>Chemical Communications</i> , 2012, 48, 1523-1525.	4.1	17
24	Conformational Mobility in Monolayer-Protected Nanoparticles: From Torsional Free Energy Profiles to NMR Relaxation. <i>Journal of Physical Chemistry C</i> , 2015, 119, 20100-20110.	3.1	17
25	Chromatographic NMR Spectroscopy with Hollow Silica Spheres. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 2733-2737.	13.8	17
26	Characterization of Paramagnetic Reactive Intermediates: Predicting the NMR Spectra of Iron(IV)-Oxo Complexes by DFT. <i>Chemistry - A European Journal</i> , 2015, 21, 12960-12970.	3.3	15
27	Nanoparticle-assisted NMR spectroscopy: A chemosensing perspective. <i>Progress in Nuclear Magnetic Resonance Spectroscopy</i> , 2020, 117, 70-88.	7.5	14
28	Dynamic Origin of Chirality Transfer between Chiral Surface and Achiral Ligand in Au ₃₈ Clusters. <i>ACS Nano</i> , 2019, 13, 7127-7134.	14.6	13
29	Ion pairing in 1-butyl-3-methylpyridinium halide ionic liquids studied using NMR and DFT calculations. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 11470-11480.	2.8	12
30	Selective J-resolved spectra: A double pulsed field gradient spin-echo approach. <i>Journal of Magnetic Resonance</i> , 2006, 182, 29-37.	2.1	11
31	Thermo-induced lipid oxidation of a culinary oil: The effect of materials used in common food processing on the evolution of oxidised species. <i>Food Chemistry</i> , 2012, 133, 754-759.	8.2	11
32	Hybrid nanoreceptors for high sensitivity detection of small molecules by NMR chemosensing. <i>Chemical Communications</i> , 2021, 57, 3002-3005.	4.1	7
33	Dynamic covalent capture of hydrazides by a phosphonate-target immobilized on resin. <i>Organic and Biomolecular Chemistry</i> , 2013, 11, 6580.	2.8	5
34	¹ H NMR Chemosensing of Potassium Ions Enabled by Guest-Induced Selectivity Switch of a Gold Nanoparticle/Crown Ether Nanoreceptor. <i>ChemPlusChem</i> , 2019, 84, 1498-1502.	2.8	5
35	Effect of the Sulfonation on the Swollen State Morphology of Styrenic Cross-Linked Polymers. <i>Polymers</i> , 2020, 12, 600.	4.5	5
36	Uniform water-mediated saturation transfer: A sensitivity-improved alternative to WaterLOGSY. <i>Journal of Magnetic Resonance</i> , 2022, 338, 107190.	2.1	3

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37	Chromatographic NMR Spectroscopy with Hollow Silica Spheres. <i>Angewandte Chemie</i> , 2016, 128, 2783-2787.	2.0	2
38	Bioactive Phloroglucinyl Heterodimers: The Tautomeric and Rotameric Equilibria of Arzanol. <i>European Journal of Organic Chemistry</i> , 2016, 2016, 4810-4816.	2.4	0
39	Molecular Dynamics Simulation Directed Rational Design of Nanoreceptors with Targeted Affinity. <i>Angewandte Chemie</i> , 2019, 131, 7784-7789.	2.0	0
40	Chromatographic NMR spectroscopy: the effect of hollow silica microspheres on magnetic field inhomogeneities and resonance lineshapes. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 21383-21392.	2.8	0