JosÃ© A Fernandez

List of Publications by Year
in descending order

129	2,196	279701	330025
papers	citations	23 h-index	37 g-index

135	135	135	2044
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Profiling and Imaging of Lipids on Brain and Liver Tissue by Matrix-Assisted Laser Desorption/Ionization Mass Spectrometry Using 2-Mercaptobenzothiazole as a Matrix. Analytical Chemistry, 2008, 80, 9105-9114.	3.2	126
2	Ribose Found in the Gas Phase. Angewandte Chemie - International Edition, 2012, 51, 3119-3124.	7.2	97
3	Matrix-assisted laser desorption ionization imaging mass spectrometry in lipidomics. Analytical and Bioanalytical Chemistry, 2011, 401, 29-51.	1.9	80
4	Free Fructose Is Conformationally Locked. Journal of the American Chemical Society, 2013, 135, 2845-2852.	6.6	71
5	High conductance values in Ï€-folded molecular junctions. Nature Communications, 2017, 8, 15195.	5.8	54
6	Distribution of lipids in human brain. Analytical and Bioanalytical Chemistry, 2011, 401, 89-101.	1.9	52
7	Six Pyranoside Forms of Free 2â€Deoxyâ€<scp>D</scp>â€ribose. Angewandte Chemie - International Edition, 2013, 52, 11840-11845.	7.2	45
8	Conformational equilibria in vanillin and ethylvanillin. Physical Chemistry Chemical Physics, 2010, 12, 12486.	1.3	44
9	Anatomical Distribution of Lipids in Human Brain Cortex by Imaging Mass Spectrometry. Journal of the American Society for Mass Spectrometry, 2011, 22, 329-338.	1.2	44
10	Binding of S-Methyl-5â€²-Thioadenosine and S-Adenosyl-l-Methionine to Protein MJ0100 Triggers an Open-to-Closed Conformational Change in Its CBS Motif Pair. Journal of Molecular Biology, 2010, 396, 800-820.	2.0	42
11	Domain Organization, Catalysis and Regulation of Eukaryotic Cystathionine Beta-Synthases. PLoS ONE, 2014, 9, e105290.	1.1	42
12	Exploring microsolvation of the anesthetic propofol. Physical Chemistry Chemical Physics, 2012, 14, 4398.	1.3	40
13	Imaging mass spectrometry increased resolution using 2-mercaptobenzothiazole and 2,5-diaminonaphtalene matrices: application to lipid distribution in human colon. Analytical and Bioanalytical Chemistry, 2015, 407, 4697-4708.	1.9	40
14	Unravelling Proteinâ€“DNA Interactions at Molecular Level: A DFT and NCI Study. Journal of Chemical Theory and Computation, 2016, 12, 523-534.	2.3	35
15	Water Sculpts the Distinctive Shapes and Dynamics of the Tumor-Associated Carbohydrate Tn Antigens: Implications for Their Molecular Recognition. Journal of the American Chemical Society, 2018, 140, 9952-9960.	6.6	33
16	IR/UV and UV/UV double-resonance study of guaiacol and eugenol dimers. Journal of Chemical Physics, 2005, 122, 164304.	1.2	32
17	Shaping Micelles: The Interplay Between Hydrogen Bonds and Dispersive Interactions. Angewandte Chemie - International Edition, 2013, 52, 7772-7775.	7.2	31
18	Structural and Vibrational Assignment of p-Methoxyphenethylamine Conformers. Journal of Physical Chemistry A, 2000, 104, 4364-4373.	1.1	30

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19	Structure, binding energy, and intermolecular modes for the aniline/ammonia van der Waals clusters. Journal of Chemical Physics, 1997, 106, 3029-3037.	1.2	29
20	N-Methyl stereochemistry in tropinone: the conformational flexibility of the tropane motif. Physical Chemistry Chemical Physics, 2010, 12, 6076.	1.3	27
21	Deciphering the Lipid Architecture of the Rat Sciatic Nerve Using Imaging Mass Spectrometry. ACS Chemical Neuroscience, 2016, 7, 624-632.	1.7	27
22	Tissue-selective alteration of ethanolamine plasmalogen metabolism in dedifferentiated colon mucosa. Biochimica Et Biophysica Acta - Molecular and Cell Biology of Lipids, 2018, 1863, 928-938.	1.2	27
23	Identification of Biomarkers of Necrosis in Xenografts Using Imaging Mass Spectrometry. Journal of the American Society for Mass Spectrometry, 2016, 27, 244-254.	1.2	26
24	Mimicking anaestheticâ€“receptor interaction: a combined spectroscopic and computational study of propofolâ¯phenol. Physical Chemistry Chemical Physics, 2012, 14, 8956.	1.3	25
25	Lipid fingerprint image accurately conveys human colon cell pathophysiologic state: A solid candidate as biomarker. Biochimica Et Biophysica Acta - Molecular and Cell Biology of Lipids, 2016, 1861, 1942-1950.	1.2	25
26	Mass spectrometry coupled to imaging techniques: the better the view the greater the challenge. Frontiers in Physiology, 2015, 6, 3.	1.3	24
27	A Spectroscopic and Computational Study of Propofol Dimers and Their Hydrated Clusters. ChemPhysChem, 2012, 13, 3819-3826.	1.0	23
28	Modeling the tyrosineâ€“sugar interactions in supersonic expansions: glucopyranoseâ€“phenol clusters. Physical Chemistry Chemical Physics, 2016, 18, 12457-12465.	1.3	23
29	Matrix Sublimation Device for MALDI Mass Spectrometry Imaging. Analytical Chemistry, 2019, 91, 803-807.	3.2	23
30	Isomer structures and vibrational assignment of the methyl-p-aminobenzoate(H2O)1 complex. Journal of Chemical Physics, 2000, 112, 3170-3180.	1.2	22
31	Molecular recognition in the gas phase: benzocaineâ€“phenol as a model of anaestheticâ€“receptor interaction. Physical Chemistry Chemical Physics, 2009, 11, 11608.	1.3	21
32	Neurotransmitter Receptor Localization: From Autoradiography to Imaging Mass Spectrometry. ACS Chemical Neuroscience, 2015, 6, 362-373.	1.7	21
33	Influence of Lipid Fragmentation in the Data Analysis of Imaging Mass Spectrometry Experiments. Journal of the American Society for Mass Spectrometry, 2020, 31, 517-526.	1.2	21
34	Structure of the 4-aminobenzonitrile/water complexes. Chemical Physics Letters, 2002, 353, 195-203.	1.2	20
35	Analysis of the Lipidome of Xenografts Using MALDI-IMS and UHPLC-ESI-QTOF. Journal of the American Society for Mass Spectrometry, 2014, 25, 1237-1246.	1.2	20
36	Microarray and Mass Spectrometry-Based Methodology for Lipid Profiling of Tissues and Cell Cultures. Analytical Chemistry, 2019, 91, 15967-15973.	3.2	20

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37	Mass-Resolved Infrared Spectroscopy of Complexes without Chromophore by Nonresonant Femtosecond Ionization Detection. Journal of Physical Chemistry A, 2012, 116, 6798-6803.	1.1	19
38	Isomerism of the Aniline Trimer. Angewandte Chemie - International Edition, 2018, 57, 15112-15116.	7.2	19
39	S0, S1, and Ion I0 Binding Energies of the p-Methoxyphenethylamine(H2O)1-4 Complexes. Journal of Physical Chemistry A, 2001, 105, 961-968.	1.1	18
40	A combined spectroscopic and theoretical study of propofolÂ·(H2O)3. Journal of Chemical Physics, 2012, 137, 074303.	1.2	18
41	A Spectroscopic Approach to the Solvation of Anesthetics in Jets: Propofol(H2O)n, n = 4â€“6. Journal of Physical Chemistry A, 2012, 116, 8934-8941.	1.1	18
42	Formation of water polyhedrons in propofolâ€“water clusters. Physical Chemistry Chemical Physics, 2013, 15, 568-575.	1.3	16
43	Experimental and theoretical study of the structures and binding energies of eugenol (H[sub 2]O)[sub n], n=0â€“2. Journal of Chemical Physics, 2004, 121, 209.	1.2	15
44	IR mass-resolved spectroscopy of complexes without chromophore: CyclohexanolÂ·(H2O)n, n = 1â€“3 and cyclohexanol dimer. Journal of Chemical Physics, 2013, 139, 174312.	1.2	15
45	Mass resolved IR spectroscopy of anilineâ€“water aggregates. Physical Chemistry Chemical Physics, 2016, 18, 27336-27341.	1.3	15
46	High-Resolution Human Kidney Molecular Histology by Imaging Mass Spectrometry of Lipids. Analytical Chemistry, 2021, 93, 9364-9372.	3.2	15
47	Competing hydrogen bonding in methoxyphenols: The rotational spectrum of o-vanillin. Journal of Molecular Spectroscopy, 2011, 267, 112-117.	0.4	14
48	Water Encapsulation by Nanomicelles. Angewandte Chemie - International Edition, 2014, 53, 12480-12483.	7.2	14
49	Influence of the Anomeric Conformation in the Intermolecular Interactions of Glucose. Journal of Physical Chemistry Letters, 2017, 8, 1147-1151.	2.1	14
50	The Six Isomers of the Cyclohexanol Dimer: A Delicate Test for Dispersion Models. Angewandte Chemie - International Edition, 2020, 59, 14081-14085.	7.2	14
51	Solvation of cyclopentadienyl and substituted cyclopentadienyl radicals in small clusters. I. Nonpolar solvents. Journal of Chemical Physics, 1999, 110, 5159-5173.	1.2	13
52	Structure and ground and first electronic excited state vibrational modes of the ethyl-p-aminobenzoate conformers. Chemical Physics, 2000, 260, 83-93.	0.9	13
53	Conformational behaviour, hydrogen bond competition and intramolecular dynamics in vanillin derivatives: acetovanillone and 6-hydroxy-3-methoxyacetophenone. Physical Chemistry Chemical Physics, 2011, 13, 13310.	1.3	13
54	THE CM-, MM-, AND SUB-MM-WAVE SPECTRUM OF ALLYL ISOCYANIDE AND RADIOASTRONOMICAL OBSERVATIONS IN ORION KL AND THE SgrB2 LINE SURVEYS. Astrophysical Journal, 2013, 777, 120.	1.6	13

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55	Influence of dispersive forces on the final shape of a reverse micelle. Physical Chemistry Chemical Physics, 2015, 17, 2241-2245.	1.3	13
56	Rovibronic signatures of molecular aggregation in the gas phase: subtle homochirality trends in the dimer, trimer and tetramer of benzyl alcohol. Physical Chemistry Chemical Physics, 2021, 23, 23610-23624.	1.3	13
57	Ferrostatinâ€1 modulates dysregulated kidney lipids in acute kidney injury. Journal of Pathology, 2022, 257, 285-299.	2.1	13
58	On the Ãƒ and BÌƒ electronic states of NCO and its clusters with nonpolar solvents. Journal of Chemical Physics, 1997, 107, 8813-8822.	1.2	12
59	A theoretical and experimental study of the ethyl-p-aminobenzoate (H2O)n (n=1â€“4) complexes. Journal of Chemical Physics, 2000, 113, 8531-8540.	1.2	12
60	Discriminating the structure ofexo-2-aminonorbornane using nuclear quadrupole coupling interactions. Journal of Chemical Physics, 2011, 134, 164311.	1.2	12
61	Stepwise Nucleation of Aniline: Emergence of Spectroscopic Fingerprints of the Liquid Phase. Chemistry - A European Journal, 2018, 24, 10291-10295.	1.7	12
62	Exploring Hydrogen Bond in Biological Molecules. Journal of the Indian Institute of Science, 2020, 100, 135-154.	0.9	12
63	Binding energy and structure of the ground, first electronic and ion states of p-methoxyphenethylamine(H2O)1 isomers: a combined experimental and theoretical study. Chemical Physics, 2001, 271, 55-69.	0.9	11
64	Influence of the aliphatic chain on the (hydrogen-bonded) p-aminobenzonitrile complexes with methanol and ethanol. Journal of Chemical Physics, 2003, 119, 9513-9522.	1.2	11
65	Combined Experimental and Theoretical Study of the Benzocaine/Ar van der Waals System in Supersonic Expansions. Journal of Physical Chemistry A, 2009, 113, 982-988.	1.1	11
66	Unraveling the Benzocaineâ€“Receptor Interaction at Molecular Level Using Mass-Resolved Spectroscopy. Journal of Physical Chemistry B, 2013, 117, 13472-13480.	1.2	11
67	Influence of the Cation Adducts in the Analysis of Matrix-Assisted Laser Desorption Ionization Imaging Mass Spectrometry Data from Injury Models of Rat Spinal Cord. Analytical Chemistry, 2017, 89, 8565-8573.	3.2	11
68	Exploring Caffeineâ€“Phenol Interactions by the Inseparable Duet of Experimental and Theoretical Data. Chemistry - A European Journal, 2019, 25, 14230-14236.	1.7	11
69	Exploiting Sphingo- and Glycerophospholipid Impairment to Select Effective Drugs and Biomarkers for CMT1A. Frontiers in Neurology, 2020, 11, 903.	1.1	11
70	Optimization of a MALDI-Imaging protocol for studying adipose tissue-associated disorders. Talanta, 2020, 219, 121184.	2.9	11
71	Molecular Recognition, Transient Chirality and Sulfur Hydrogen Bonding in the Benzyl Mercaptan Dimer. Symmetry, 2021, 13, 2022.	1.1	11
72	Experimental determination of phenol (CH3F)1 complex binding energies in the S0, S1, and I0 states and comparison with ab initio calculations. Journal of Chemical Physics, 2001, 115, 270-276.	1.2	10

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73	The CBS Domain Protein MJ0729 ofMethanocaldococcus jannaschiiIs a Thermostable Protein with a pH-Dependent Self-Oligomerization. Biochemistry, 2009, 48, 2760-2776.	1.2	10
74	Femtosecond Excited State Dynamics of Size Selected Neutral Molecular Clusters. Journal of Physical Chemistry Letters, 2016, 7, 2797-2802.	2.1	10
75	Removal rates for the collisional quenching of various vibronic levels of ground state NCO by simple molecules (N2, O2, NO, CO2, N2O, and SO2). Journal of Chemical Physics, 1997, 106, 7090-7101.	1.2	9
76	ZEKE-PFI Spectroscopy of Benzocaine. Journal of Physical Chemistry A, 2006, 110, 6010-6015.	1.1	9
77	Mimicking anestheticâ€“receptor interactions in jets: the propofolâ€“isopropanol cluster. Physical Chemistry Chemical Physics, 2014, 16, 16968.	1.3	9
78	Optimized Protocol To Analyze Changes in the Lipidome of Xenografts after Treatment with 2-Hydroxyoleic Acid. Analytical Chemistry, 2016, 88, 1022-1029.	3.2	9
79	Competition between stacked and hydrogen bonded structures of cytosine aggregates. Physical Chemistry Chemical Physics, 2017, 19, 8826-8834.	1.3	9
80	Confirmation of sub-cellular resolution using oversampling imaging mass spectrometry. Analytical and Bioanalytical Chemistry, 2019, 411, 7935-7941.	1.9	9
81	Solvation of the methoxy radical in small clusters. Journal of Chemical Physics, 1997, 107, 3363-3375.	1.2	8
82	Solvation of cyclopentadienyl and substituted cyclopentadienyl radicals in small clusters. II. Cyanocyclopentadienyl with polar solvents. Journal of Chemical Physics, 1999, 110, 5174-5182.	1.2	8
83	Structure and identification of the amino-p-phenethylamine conformers. Physical Chemistry Chemical Physics, 2002, 4, 3297-3304.	1.3	8
84	Rotational spectroscopy of antipyretics: Conformation, structure, and internal dynamics of phenazone. Journal of Chemical Physics, 2013, 138, 114304.	1.2	8
85	Magic Numbers in the Solvation of the Propofol Dimer. ChemPhysChem, 2013, 14, 1558-1562.	1.0	8
86	Oï£¿Hâ‹…â‹…â‹…N and Cï£¿Hâ‹…â‹…â‹…O Hydrogen Bonds Control Hydration of Pivotal Tropane Alkaloids: Tropinoneâ‹…â‹…â‹…H₂O Complex. ChemPhysChem, 2014, 15, 918-923.	1.0	8
87	Potential energy surface of fluoroxene: experiment and theory. Physical Chemistry Chemical Physics, 2016, 18, 3966-3974.	1.3	8
88	Phenyl-Î²-D-glucopyranoside and Phenyl-Î²-D-galactopyranoside Dimers: Small Structural Differences but Very Different Interactions. Frontiers in Physics, 2018, 6, .	1.0	8
89	Experimental and theoretical study of methyl-p-aminobenzoate/ammonia complexes. I. MAB(NH3)1. Journal of Chemical Physics, 2000, 113, 8541-8548.	1.2	7
90	The Distorted Tropane of Scopoline. ChemPhysChem, 2013, 14, 1830-1835.	1.0	7

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91	Sugarâ€“peptidic bond interactions: spectroscopic characterization of a model system. Physical Chemistry Chemical Physics, 2017, 19, 12013-12021.	1.3	7
92	Revisiting the spectroscopy of xanthine derivatives: theobromine and theophylline. Physical Chemistry Chemical Physics, 2019, 21, 26430-26437.	1.3	7
93	Revisiting the Spectroscopy of Water Dimer in Jets. Journal of Physical Chemistry Letters, 2021, 12, 1316-1320.	2.1	7
94	Laser mass-resolved spectroscopy and theoretical study of methyl-p-aminobenzoate(H2O)n (n=2,3,4) complexes. Journal of Chemical Physics, 2000, 113, 5804-5811.	1.2	6
95	Structural Studies of Nicotinoids: Cotinine versus Nicotine. Chemistry - A European Journal, 2017, 23, 7238-7244.	1.7	6
96	Isomerism of the Aniline Trimer. Angewandte Chemie, 2018, 130, 15332-15336.	1.6	6
97	Imaging Mass Spectrometryâ€“Based Lipidomic Approach to Classification of Architectural FeaturesÂin Nevi. Journal of Investigative Dermatology, 2019, 139, 2055-2058.e7.	0.3	6
98	Direct Measurements of Removal Rates of CFCl(XÌƒAâ€˜(0,0,0)) and CFCl(XÌƒ1Aâ€˜(0,1,0)) by Simple Alkenes. The Journal of Physical Chemistry, 1996, 100, 12305-12310.	2.9	5
99	Solvation of clyclopentadienyl and substituted clyclopentadienyl radicals in small clusters. III. Pre-reactive clusters. Journal of Chemical Physics, 1999, 110, 5183-5188.	1.2	5
100	Experimental and theoretical study of methyl-p-aminobenzoate/ammonia complexes. II. MAB(NH3)2â€“4. Journal of Chemical Physics, 2000, 113, 8549-8555.	1.2	5
101	Scopine Isolated in the Gas Phase. ChemPhysChem, 2016, 17, 3030-3034.	1.0	5
102	Understanding the role of tyrosine in glycogenin. Molecular BioSystems, 2017, 13, 1709-1712.	2.9	5
103	Mapping Lipid Distribution in Rat Sciatic Nerve Using Imaging Mass Spectrometry. Methods in Molecular Biology, 2018, 1791, 51-65.	0.4	5
104	Excited state dynamics of aniline homoclusters. Physical Chemistry Chemical Physics, 2019, 21, 3098-3105.	1.3	5
105	Improving Spatial Resolution of a LTQ Orbitrap MALDI Source. Journal of the American Society for Mass Spectrometry, 2020, 31, 1755-1758.	1.2	5
106	Solvation of Radicals in Small Clusters. , 1999, , 71-109.		5
107	Polyunsaturated Fatty Acid-Enriched Lipid Fingerprint of Glioblastoma Proliferative Regions Is Differentially Regulated According to Glioblastoma Molecular Subtype. International Journal of Molecular Sciences, 2022, 23, 2949.	1.8	5
108	Direct Measurements of Removal Rates of CHF(XËœ1Aâ€²(0,1,0)) by Simple Alkenes. Laser Chemistry, 1992, 12, 43-52.	0.5	4

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109	Reply to the Comment on â€œStructural and Vibrational Assignment ofp-Methoxyphenethylamine Conformersâ€. Journal of Physical Chemistry A, 2001, 105, 9993-9994.	1.1	4
110	Porous silicon surfaces for metabonomics: Detection and identification of nucleotides without matrix interference. Physica Status Solidi C: Current Topics in Solid State Physics, 2007, 4, 2185-2189.	0.8	4
111	Purification, crystallization and preliminary X-ray diffraction analysis of the CBS-domain pair from theMethanococcus jannaschiiprotein MJ0100. Acta Crystallographica Section F: Structural Biology Communications, 2008, 64, 936-941.	0.7	4
112	Molecular hydration of propofol dimers in supersonic expansions: formation of active centre-like structures. Physical Chemistry Chemical Physics, 2014, 16, 23301-23307.	1.3	4
113	Lyso-Sulfatide Binds Factor Xa and Inhibits Thrombin Generation by the Prothrombinase Complex. PLoS ONE, 2015, 10, e0135025.	1.1	4
114	A Drastic Shift in Lipid Adducts in Colon Cancer Detected by MALDI-IMS Exposes Alterations in Specific K+ Channels. Cancers, 2021, 13, 1350.	1.7	4
115	Transition from Planar to Nonplanar Hydrogen Bond Networks in the Solvation of Aromatic Dimers: Propofol2-(H2O)2â€“4. Journal of Physical Chemistry A, 2013, 117, 3396-3404.	1.1	3
116	Behind the Reactivity of Lactones: A Computational and Spectroscopic Study of PhenolÂ·Î³-Butyrolactone. Journal of Physical Chemistry A, 2014, 118, 2568-2575.	1.1	3
117	Conformational landscape of isolated capped amino acids: on the nature of non-covalent interactions. European Physical Journal D, 2017, 71, 1.	0.6	3
118	Exploration of the theobromineâ€“water dimer: comparison with DNA microhydration. Physical Chemistry Chemical Physics, 2020, 22, 15759-15768.	1.3	3
119	A UHPLC-Mass Spectrometry View of Human Melanocytic Cells Uncovers Potential Lipid Biomarkers of Melanoma. International Journal of Molecular Sciences, 2021, 22, 12061.	1.8	3
120	A Computational Study of the Structures of thep-Methoxyphenethylamine(H2O)2-4Complexes. Journal of Physical Chemistry A, 2001, 105, 11524-11530.	1.1	2
121	Structural Distortion of the Epoxy Groups in Norbornanes: A Rotational Study of exoâ€2,3â€Epoxynorbornane. ChemPhysChem, 2015, 16, 2609-2614.	1.0	2
122	Influence of the solvent in the electronic excitation of aromatic alcohols: Excited state IR-UV of propofol(H2O)8. Journal of Chemical Physics, 2019, 150, 214306.	1.2	2
123	Exploring Epigenetic Marks by Analysis of Noncovalent Interactions. ChemBioChem, 2021, 22, 408-415.	1.3	2
124	Exploring the Influence of Intermolecular Interactions in Prebiotic Chemistry Using Laser Spectroscopy and Calculations. Chemistry - A European Journal, 2021, 28, e202103636.	1.7	2
125	A REMPI and ZEKE-PFI study of 4-amino-3-ethylbenzonitrile. Chemical Physics Letters, 2006, 425, 35-39.	1.2	1
126	Descifrando la anatomÃa molecular de un tejido mediante anÃ¡lisis lipidÃ³mico por espectrometrÃa de masas. Gaceta Medica De Bilbao, 2009, 106, 77-84.	0.0	0

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127	Evaluation of the aggregation process in a mixture of propofol and benzocaine. Physical Chemistry Chemical Physics, 2019, 21, 3537-3544.	1.3	0
128	Noncovalent interactions in isolated molecular aggregates: From single molecules to nanostructures. , 2021, , 143-188.		0
129	The Six Isomers of the Cyclohexanol Dimer: A Delicate Test for Dispersion Models. Angewandte Chemie, 2020, 132, 14185-14189.	1.6	0