JosÃ© A Fernandez

List of Publications by Year
in descending order

129	2,196	279798	330143
papers	citations	23 h-index	37 g-index

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

#	Article	IF	Citations
1	Ferrostatinâ€1 modulates dysregulated kidney lipids in acute kidney injury. Journal of Pathology, 2022, 257, 285-299.	4.5	13
2	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.	4.1	5
3	Exploring Epigenetic Marks by Analysis of Noncovalent Interactions. ChemBioChem, 2021, 22, 408-415.	2.6	2
4	Noncovalent interactions in isolated molecular aggregates: From single molecules to nanostructures. , 2021, , 143-188.		0
5	Revisiting the Spectroscopy of Water Dimer in Jets. Journal of Physical Chemistry Letters, 2021, 12, 1316-1320.	4.6	7
6	A Drastic Shift in Lipid Adducts in Colon Cancer Detected by MALDI-IMS Exposes Alterations in Specific K+ Channels. Cancers, 2021, 13, 1350.	3.7	4
7	High-Resolution Human Kidney Molecular Histology by Imaging Mass Spectrometry of Lipids. Analytical Chemistry, 2021, 93, 9364-9372.	6.5	15
8	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.	2.8	13
9	Molecular Recognition, Transient Chirality and Sulfur Hydrogen Bonding in the Benzyl Mercaptan Dimer. Symmetry, 2021, 13, 2022.	2.2	11
10	A UHPLC-Mass Spectrometry View of Human Melanocytic Cells Uncovers Potential Lipid Biomarkers of Melanoma. International Journal of Molecular Sciences, 2021, 22, 12061.	4.1	3
11	Exploring the Influence of Intermolecular Interactions in Prebiotic Chemistry Using Laser Spectroscopy and Calculations. Chemistry - A European Journal, 2021, 28, e202103636.	3.3	2
12	Exploring Hydrogen Bond in Biological Molecules. Journal of the Indian Institute of Science, 2020, 100, 135-154.	1.9	12
13	Improving Spatial Resolution of a LTQ Orbitrap MALDI Source. Journal of the American Society for Mass Spectrometry, 2020, 31, 1755-1758.	2.8	5
14	Exploiting Sphingo- and Glycerophospholipid Impairment to Select Effective Drugs and Biomarkers for CMT1A. Frontiers in Neurology, 2020, 11, 903.	2.4	11
15	The Six Isomers of the Cyclohexanol Dimer: A Delicate Test for Dispersion Models. Angewandte Chemie - International Edition, 2020, 59, 14081-14085.	13.8	14
16	Optimization of a MALDI-Imaging protocol for studying adipose tissue-associated disorders. Talanta, 2020, 219, 121184.	5.5	11
17	Exploration of the theobromineâ€“water dimer: comparison with DNA microhydration. Physical Chemistry Chemical Physics, 2020, 22, 15759-15768.	2.8	3
18	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.	2.8	21

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19	The Six Isomers of the Cyclohexanol Dimer: A Delicate Test for Dispersion Models. Angewandte Chemie, 2020, 132, 14185-14189.	2.0	0
20	Evaluation of the aggregation process in a mixture of propofol and benzocaine. Physical Chemistry Chemical Physics, 2019, 21, 3537-3544.	2.8	0
21	Exploring Caffeineâ€“Phenol Interactions by the Inseparable Duet of Experimental and Theoretical Data. Chemistry - A European Journal, 2019, 25, 14230-14236.	3.3	11
22	Excited state dynamics of aniline homoclusters. Physical Chemistry Chemical Physics, 2019, 21, 3098-3105.	2.8	5
23	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.	3.0	2
24	Imaging Mass Spectrometryâ€“Based Lipidomic Approach to Classification of Architectural FeaturesÂin Nevi. Journal of Investigative Dermatology, 2019, 139, 2055-2058.e7.	0.7	6
25	Confirmation of sub-cellular resolution using oversampling imaging mass spectrometry. Analytical and Bioanalytical Chemistry, 2019, 411, 7935-7941.	3.7	9
26	Revisiting the spectroscopy of xanthine derivatives: theobromine and theophylline. Physical Chemistry Chemical Physics, 2019, 21, 26430-26437.	2.8	7
27	Microarray and Mass Spectrometry-Based Methodology for Lipid Profiling of Tissues and Cell Cultures. Analytical Chemistry, 2019, 91, 15967-15973.	6.5	20
28	Matrix Sublimation Device for MALDI Mass Spectrometry Imaging. Analytical Chemistry, 2019, 91, 803-807.	6.5	23
29	Isomerism of the Aniline Trimer. Angewandte Chemie, 2018, 130, 15332-15336.	2.0	6
30	Isomerism of the Aniline Trimer. Angewandte Chemie - International Edition, 2018, 57, 15112-15116.	13.8	19
31	Phenyl-Î²-D-glucopyranoside and Phenyl-Î²-D-galactopyranoside Dimers: Small Structural Differences but Very Different Interactions. Frontiers in Physics, 2018, 6, .	2.1	8
32	Mapping Lipid Distribution in Rat Sciatic Nerve Using Imaging Mass Spectrometry. Methods in Molecular Biology, 2018, 1791, 51-65.	0.9	5
33	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.	13.7	33
34	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.	2.4	27
35	Stepwise Nucleation of Aniline: Emergence of Spectroscopic Fingerprints of the Liquid Phase. Chemistry - A European Journal, 2018, 24, 10291-10295.	3.3	12
36	Structural Studies of Nicotinoids: Cotinine versus Nicotine. Chemistry - A European Journal, 2017, 23, 7238-7244.	3.3	6

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37	Influence of the Anomeric Conformation in the Intermolecular Interactions of Glucose. Journal of Physical Chemistry Letters, 2017, 8, 1147-1151.	4.6	14
38	Sugarâ€“peptidic bond interactions: spectroscopic characterization of a model system. Physical Chemistry Chemical Physics, 2017, 19, 12013-12021.	2.8	7
39	High conductance values in Ï€-folded molecular junctions. Nature Communications, 2017, 8, 15195.	12.8	54
40	Competition between stacked and hydrogen bonded structures of cytosine aggregates. Physical Chemistry Chemical Physics, 2017, 19, 8826-8834.	2.8	9
41	Conformational landscape of isolated capped amino acids: on the nature of non-covalent interactions. European Physical Journal D, 2017, 71, 1.	1.3	3
42	Understanding the role of tyrosine in glycogenin. Molecular BioSystems, 2017, 13, 1709-1712.	2.9	5
43	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.	6.5	11
44	Scopine Isolated in the Gas Phase. ChemPhysChem, 2016, 17, 3030-3034.	2.1	5
45	Femtosecond Excited State Dynamics of Size Selected Neutral Molecular Clusters. Journal of Physical Chemistry Letters, 2016, 7, 2797-2802.	4.6	10
46	Modeling the tyrosineâ€“sugar interactions in supersonic expansions: glucopyranoseâ€“phenol clusters. Physical Chemistry Chemical Physics, 2016, 18, 12457-12465.	2.8	23
47	Deciphering the Lipid Architecture of the Rat Sciatic Nerve Using Imaging Mass Spectrometry. ACS Chemical Neuroscience, 2016, 7, 624-632.	3.5	27
48	Mass resolved IR spectroscopy of anilineâ€“water aggregates. Physical Chemistry Chemical Physics, 2016, 18, 27336-27341.	2.8	15
49	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.	2.4	25
50	Unravelling Proteinâ€“DNA Interactions at Molecular Level: A DFT and NCI Study. Journal of Chemical Theory and Computation, 2016, 12, 523-534.	5.3	35
51	Optimized Protocol To Analyze Changes in the Lipidome of Xenografts after Treatment with 2-Hydroxyoleic Acid. Analytical Chemistry, 2016, 88, 1022-1029.	6.5	9
52	Potential energy surface of fluoroxene: experiment and theory. Physical Chemistry Chemical Physics, 2016, 18, 3966-3974.	2.8	8
53	Identification of Biomarkers of Necrosis in Xenografts Using Imaging Mass Spectrometry. Journal of the American Society for Mass Spectrometry, 2016, 27, 244-254.	2.8	26
54	Structural Distortion of the Epoxy Groups in Norbornanes: A Rotational Study of exoâ€2,3â€Epoxynorbornane. ChemPhysChem, 2015, 16, 2609-2614.	2.1	2

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55	Lyso-Sulfatide Binds Factor Xa and Inhibits Thrombin Generation by the Prothrombinase Complex. PLoS ONE, 2015, 10, e0135025.	2.5	4
56	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.	3.7	40
57	Neurotransmitter Receptor Localization: From Autoradiography to Imaging Mass Spectrometry. ACS Chemical Neuroscience, 2015, 6, 362-373.	3.5	21
58	Influence of dispersive forces on the final shape of a reverse micelle. Physical Chemistry Chemical Physics, 2015, 17, 2241-2245.	2.8	13
59	Mass spectrometry coupled to imaging techniques: the better the view the greater the challenge. Frontiers in Physiology, 2015, 6, 3.	2.8	24
60	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.	2.1	8
61	Mimicking anestheticâ€“receptor interactions in jets: the propofolâ€“isopropanol cluster. Physical Chemistry Chemical Physics, 2014, 16, 16968.	2.8	9
62	Molecular hydration of propofol dimers in supersonic expansions: formation of active centre-like structures. Physical Chemistry Chemical Physics, 2014, 16, 23301-23307.	2.8	4
63	Behind the Reactivity of Lactones: A Computational and Spectroscopic Study of PhenolÂ·Î³-Butyrolactone. Journal of Physical Chemistry A, 2014, 118, 2568-2575.	2.5	3
64	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.	2.8	20
65	Water Encapsulation by Nanomicelles. Angewandte Chemie - International Edition, 2014, 53, 12480-12483.	13.8	14
66	Domain Organization, Catalysis and Regulation of Eukaryotic Cystathionine Beta-Synthases. PLoS ONE, 2014, 9, e105290.	2.5	42
67	Free Fructose Is Conformationally Locked. Journal of the American Chemical Society, 2013, 135, 2845-2852.	13.7	71
68	IR mass-resolved spectroscopy of complexes without chromophore: CyclohexanolÂ·(H2O)n, n = 1â€“3 and cyclohexanol dimer. Journal of Chemical Physics, 2013, 139, 174312.	3.0	15
69	Unraveling the Benzocaineâ€“Receptor Interaction at Molecular Level Using Mass-Resolved Spectroscopy. Journal of Physical Chemistry B, 2013, 117, 13472-13480.	2.6	11
70	Formation of water polyhedrons in propofolâ€“water clusters. Physical Chemistry Chemical Physics, 2013, 15, 568-575.	2.8	16
71	Rotational spectroscopy of antipyretics: Conformation, structure, and internal dynamics of phenazone. Journal of Chemical Physics, 2013, 138, 114304.	3.0	8
72	The Distorted Tropane of Scopoline. ChemPhysChem, 2013, 14, 1830-1835.	2.1	7

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73	Magic Numbers in the Solvation of the Propofol Dimer. ChemPhysChem, 2013, 14, 1558-1562.	2.1	8
74	Shaping Micelles: The Interplay Between Hydrogen Bonds and Dispersive Interactions. Angewandte Chemie - International Edition, 2013, 52, 7772-7775.	13.8	31
75	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.	2.5	3
76	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.	4.5	13
77	Six Pyranoside Forms of Free 2â€Deoxyâ€<scp>D</scp>â€ribose. Angewandte Chemie - International Edition, 2013, 52, 11840-11845.	13.8	45
78	A combined spectroscopic and theoretical study of propofolÂ·(H2O)3. Journal of Chemical Physics, 2012, 137, 074303.	3.0	18
79	Mimicking anaestheticâ€“receptor interaction: a combined spectroscopic and computational study of propofolâ€¯phenol. Physical Chemistry Chemical Physics, 2012, 14, 8956.	2.8	25
80	Exploring microsolvation of the anesthetic propofol. Physical Chemistry Chemical Physics, 2012, 14, 4398.	2.8	40
81	Mass-Resolved Infrared Spectroscopy of Complexes without Chromophore by Nonresonant Femtosecond Ionization Detection. Journal of Physical Chemistry A, 2012, 116, 6798-6803.	2.5	19
82	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.	2.5	18
83	A Spectroscopic and Computational Study of Propofol Dimers and Their Hydrated Clusters. ChemPhysChem, 2012, 13, 3819-3826.	2.1	23
84	Ribose Found in the Gas Phase. Angewandte Chemie - International Edition, 2012, 51, 3119-3124.	13.8	97
85	Conformational behaviour, hydrogen bond competition and intramolecular dynamics in vanillin derivatives: acetovanillone and 6-hydroxy-3-methoxyacetophenone. Physical Chemistry Chemical Physics, 2011, 13, 13310.	2.8	13
86	Matrix-assisted laser desorption ionization imaging mass spectrometry in lipidomics. Analytical and Bioanalytical Chemistry, 2011, 401, 29-51.	3.7	80
87	Distribution of lipids in human brain. Analytical and Bioanalytical Chemistry, 2011, 401, 89-101.	3.7	52
88	Anatomical Distribution of Lipids in Human Brain Cortex by Imaging Mass Spectrometry. Journal of the American Society for Mass Spectrometry, 2011, 22, 329-338.	2.8	44
89	Competing hydrogen bonding in methoxyphenols: The rotational spectrum of o-vanillin. Journal of Molecular Spectroscopy, 2011, 267, 112-117.	1.2	14
90	Discriminating the structure ofexo-2-aminonorbornane using nuclear quadrupole coupling interactions. Journal of Chemical Physics, 2011, 134, 164311.	3.0	12

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91	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.	4.2	42
92	Conformational equilibria in vanillin and ethylvanillin. Physical Chemistry Chemical Physics, 2010, 12, 12486.	2.8	44
93	N-Methyl stereochemistry in tropinone: the conformational flexibility of the tropane motif. Physical Chemistry Chemical Physics, 2010, 12, 6076.	2.8	27
94	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.	2.5	11
95	The CBS Domain Protein MJ0729 ofMethanocaldococcus jannaschiiIs a Thermostable Protein with a pH-Dependent Self-Oligomerization. Biochemistry, 2009, 48, 2760-2776.	2.5	10
96	Molecular recognition in the gas phase: benzocaineâ€“phenol as a model of anaestheticâ€“receptor interaction. Physical Chemistry Chemical Physics, 2009, 11, 11608.	2.8	21
97	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
98	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
99	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.	6.5	126
100	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
101	ZEKE-PFI Spectroscopy of Benzocaine. Journal of Physical Chemistry A, 2006, 110, 6010-6015.	2.5	9
102	A REMPI and ZEKE-PFI study of 4-amino-3-ethylbenzonitrile. Chemical Physics Letters, 2006, 425, 35-39.	2.6	1
103	IR/UV and UV/UV double-resonance study of guaiacol and eugenol dimers. Journal of Chemical Physics, 2005, 122, 164304.	3.0	32
104	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.	3.0	15
105	Influence of the aliphatic chain on the (hydrogen-bonded) p-aminobenzonitrile complexes with methanol and ethanol. Journal of Chemical Physics, 2003, 119, 9513-9522.	3.0	11
106	Structure and identification of the amino-p-phenethylamine conformers. Physical Chemistry Chemical Physics, 2002, 4, 3297-3304.	2.8	8
107	Structure of the 4-aminobenzonitrile/water complexes. Chemical Physics Letters, 2002, 353, 195-203.	2.6	20
108	Reply to the Comment on â€œStructural and Vibrational Assignment ofp-Methoxyphenethylamine Conformersâ€• Journal of Physical Chemistry A, 2001, 105, 9993-9994.	2.5	4

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109	S0, S1, and Ion I0 Binding Energies of the p-Methoxyphenethylamine(H2O)1-4 Complexes. Journal of Physical Chemistry A, 2001, 105, 961-968.	2.5	18
110	A Computational Study of the Structures of thep-Methoxyphenethylamine(H2O)2-4Complexes. Journal of Physical Chemistry A, 2001, 105, 11524-11530.	2.5	2
111	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.	1.9	11
112	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.	3.0	10
113	Structure and ground and first electronic excited state vibrational modes of the ethyl-p-aminobenzoate conformers. Chemical Physics, 2000, 260, 83-93.	1.9	13
114	Isomer structures and vibrational assignment of the methyl-p-aminobenzoate(H2O)1 complex. Journal of Chemical Physics, 2000, 112, 3170-3180.	3.0	22
115	Experimental and theoretical study of methyl-p-aminobenzoate/ammonia complexes. II. MAB(NH3)2â€“4. Journal of Chemical Physics, 2000, 113, 8549-8555.	3.0	5
116	A theoretical and experimental study of the ethyl-p-aminobenzoate (H2O)n (n=1â€“4) complexes. Journal of Chemical Physics, 2000, 113, 8531-8540.	3.0	12
117	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.	3.0	6
118	Experimental and theoretical study of methyl-p-aminobenzoate/ammonia complexes. I. MAB(NH3)1. Journal of Chemical Physics, 2000, 113, 8541-8548.	3.0	7
119	Structural and Vibrational Assignment of p-Methoxyphenethylamine Conformers. Journal of Physical Chemistry A, 2000, 104, 4364-4373.	2.5	30
120	Solvation of cyclopentadienyl and substituted cyclopentadienyl radicals in small clusters. II. Cyanocyclopentadienyl with polar solvents. Journal of Chemical Physics, 1999, 110, 5174-5182.	3.0	8
121	Solvation of cyclopentadienyl and substituted cyclopentadienyl radicals in small clusters. I. Nonpolar solvents. Journal of Chemical Physics, 1999, 110, 5159-5173.	3.0	13
122	Solvation of clyclopentadienyl and substituted clyclopentadienyl radicals in small clusters. III. Pre-reactive clusters. Journal of Chemical Physics, 1999, 110, 5183-5188.	3.0	5
123	Solvation of Radicals in Small Clusters. , 1999, , 71-109.		5
124	Structure, binding energy, and intermolecular modes for the aniline/ammonia van der Waals clusters. Journal of Chemical Physics, 1997, 106, 3029-3037.	3.0	29
125	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.	3.0	9
126	On the Ãƒ and BÌƒ electronic states of NCO and its clusters with nonpolar solvents. Journal of Chemical Physics, 1997, 107, 8813-8822.	3.0	12

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127	Solvation of the methoxy radical in small clusters. Journal of Chemical Physics, 1997, 107, 3363-3375.	3.0	8
128	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
129	Direct Measurements of Removal Rates of CHF(XËœ1Aâ€²(0,1,0)) by Simple Alkenes. Laser Chemistry, 1992, 12, 43-52.	0.5	4