Jesus Calvo-Castro

List of Publications by Year
in descending order

23	278	758635 12	887659 17
papers	citations	h-index	g-index

23	23	23	379
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Modifying the Properties of Thermogelling Poloxamer 407 Solutions through Covalent Modification and the Use of Polymer Additives. Macromolecular Chemistry and Physics, 2019, 220, 1900173.	1.1	34
2	Impact of Systematic Structural Variation on the Energetics of Ï€â€“Ï€ Stacking Interactions and Associated Computed Charge Transfer Integrals of Crystalline Diketopyrrolopyrroles. Crystal Growth and Design, 2014, 14, 4849-4858.	1.4	26
3	Detection of nitroaromatic vapours with diketopyrrolopyrrole thin films: exploring the role of structural order and morphology on thin film properties and fluorescence quenching efficiency. Chemical Communications, 2015, 51, 1143-1146.	2.2	22
4	Effects of Fluorine Substitution on the Intermolecular Interactions, Energetics, and Packing Behavior of N-Benzyl Substituted Diketopyrrolopyrroles. Crystal Growth and Design, 2016, 16, 2371-2384.	1.4	22
5	Detection of newly emerging psychoactive substances using Raman spectroscopy and chemometrics. RSC Advances, 2018, 8, 31924-31933.	1.7	21
6	Torsional angle dependence and switching of inner sphere reorganisation energies for electron and hole transfer processes involving phenyl substituted diketopyrrolopyrroles; a density functional study. Dyes and Pigments, 2015, 113, 609-617.	2.0	18
7	Fluorine Directed Two-Dimensional Cruciform Ï€â€“Ï€ Stacking in Diketopyrrolopyrroles. Crystal Growth and Design, 2016, 16, 5385-5393.	1.4	18
8	Intermolecular Interactions and Energetics in the Crystalline Ï€â€“Ï€ Stacks and Associated Model Dimer Systems of Asymmetric Halogenated Diketopyrrolopyrroles. Crystal Growth and Design, 2016, 16, 1531-1542.	1.4	15
9	Development of a Neutral Diketopyrrolopyrrole Phosphine Oxide for the Selective Bioimaging of Mitochondria at the Nanomolar Level. Chemistry - A European Journal, 2020, 26, 3173-3180.	1.7	15
10	Drowning in diversity? A systematic way of clustering and selecting a representative set of new psychoactive substances. RSC Advances, 2017, 7, 53181-53191.	1.7	13
11	Characterisation of the Chemical Composition and Structural Features of Novel Antimicrobial Nanoparticles. Nanomaterials, 2017, 7, 152.	1.9	13
12	Exploring structure based charge transport relationships in phenyl diketopyrrolopyrrole single crystals using a 2D Ï€â€“Ï€ dimer model system. Journal of Materials Chemistry C, 2017, 5, 3993-3998.	2.7	12
13	Twist and shout: a surprising synergy between aryl and N-substituents defines the computed charge transport properties in a series of crystalline diketopyrrolopyrroles. CrystEngComm, 2016, 18, 9382-9390.	1.3	10
14	True absolute determination of photoluminescence quantum yields by coupling multiwavelength thermal lens and photoluminescence spectroscopy. Physical Chemistry Chemical Physics, 2020, 22, 25156-25164.	1.3	8
15	Impact of substituent effects on the Raman spectra of structurally related N-substituted diketopyrrolopyrroles. Vibrational Spectroscopy, 2016, 83, 8-16.	1.2	6
16	Understanding the Contribution of Individual Amino Acid Residues in the Binding of Psychoactive Substances to Monoamine Transporters. ACS Omega, 2020, 5, 17223-17231.	1.6	6
17	A 2-D Ï€â€“Ï€ dimer model system to investigate structure-charge transfer relationships in rubrene. Journal of Materials Chemistry C, 2019, 7, 2029-2036.	2.7	5
18	A Design-of-Experiments approach to developing thermoresponsive gelators from complex polymer mixtures. Molecular Systems Design and Engineering, 2020, 5, 1538-1546.	1.7	5

#	Article	IF	Citations
19	Flipped detection of psychoactive substances in complex mixtures using handheld Raman spectroscopy coupled to chemometrics. Journal of Raman Spectroscopy, 2022, 53, 1428-1444.	1.2	3
20	Role of H-Optimization in the Computed Intermolecular Interactions and Charge-Transfer Integrals in Diketopyrrolopyrroles. Journal of Physical Chemistry A, 2019, 123, 3185-3193.	1.1	2
21	Thermal Lens Spectrometry Reveals Thermo-Optical Property Tuning of Conjugated Polymer Nanoparticles Prepared by Microfluidics. ACS Applied Polymer Materials, 2022, 4, 6219-6228.	2.0	2
22	Investigating structure-charge transport relationships in thiophene substituted naphthyridine crystalline materials by computational model systems. Physical Chemistry Chemical Physics, 2020, 22, 25315-25324.	1.3	1
23	Raman spectroscopy coupled to computational approaches towards understanding self-assembly in thermoreversible poloxamer gels. Journal of Molecular Liquids, 2022, 351, 118660.	2.3	1