Jesus Calvo-Castro

List of Publications by Year
in descending order

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23 papers	278 citations	759055 12 h-index	887953 17 g-index
23 all docs	23 docs citations	23 times ranked	379 citing authors

#	Article	IF	Citations
1	Raman spectroscopy coupled to computational approaches towards understanding self-assembly in thermoreversible poloxamer gels. Journal of Molecular Liquids, 2022, 351, 118660.	2.3	1
2	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
3	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
4	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
5	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
6	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
7	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
8	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
9	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
10	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
11	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
12	Detection of newly emerging psychoactive substances using Raman spectroscopy and chemometrics. RSC Advances, 2018, 8, 31924-31933.	1.7	21
13	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
14	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
15	Characterisation of the Chemical Composition and Structural Features of Novel Antimicrobial Nanoparticles. Nanomaterials, 2017, 7, 152.	1.9	13
16	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
17	Fluorine Directed Two-Dimensional Cruciform Ï€â€“Ï€ Stacking in Diketopyrrolopyrroles. Crystal Growth and Design, 2016, 16, 5385-5393.	1.4	18
18	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

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19	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
20	Impact of substituent effects on the Raman spectra of structurally related N-substituted diketopyrrolopyrroles. Vibrational Spectroscopy, 2016, 83, 8-16.	1.2	6
21	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
22	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
23	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