Ferran Feixas

List of Publications by Year
in descending order

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53 papers	2,641 citations	230014 27 h-index	206121 51 g-index
59 all docs	59 docs citations	59 times ranked	3306 citing authors

#	Article	IF	Citations
1	Discovery and In Vivo Proof of Concept of a Highly Potent Dual Inhibitor of Soluble Epoxide Hydrolase and Acetylcholinesterase for the Treatment of Alzheimerâ€™s Disease. Journal of Medicinal Chemistry, 2022, 65, 4909-4925.	2.9	22
2	Time Evolution of the Millisecond Allosteric Activation of Imidazole Glycerol Phosphate Synthase. Journal of the American Chemical Society, 2022, 144, 7146-7159.	6.6	24
3	Machine Learning Enables Selection of Epistatic Enzyme Mutants for Stability Against Unfolding and Detrimental Aggregation. ChemBioChem, 2021, 22, 904-914.	1.3	22
4	From the Design to the In Vivo Evaluation of Benzohomoadamantane-Derived Soluble Epoxide Hydrolase Inhibitors for the Treatment of Acute Pancreatitis. Journal of Medicinal Chemistry, 2021, 64, 5429-5446.	2.9	12
5	Comprehensive Characterization of the Selfâ€Folding Cavitand Dynamics. Chemistry - A European Journal, 2021, 27, 10099-10106.	1.7	5
6	Protein-directed crystalline 2D fullerene assemblies. Nanoscale, 2020, 12, 3614-3622.	2.8	11
7	2-Oxaadamant-1-yl Ureas as Soluble Epoxide Hydrolase Inhibitors: In Vivo Evaluation in a Murine Model of Acute Pancreatitis. Journal of Medicinal Chemistry, 2020, 63, 9237-9257.	2.9	14
8	Complete Dynamic Reconstruction of C₆₀, C₇₀, and (C₅₉N)₂ Encapsulation into an Adaptable Supramolecular Nanocapsule. Journal of the American Chemical Society, 2020, 142, 16051-16063.	6.6	36
9	Intrinsic enzymatic properties modulate the self-propulsion of micromotors. Nature Communications, 2019, 10, 2826.	5.8	126
10	p38Î³ is essential for cell cycle progression and liver tumorigenesis. Nature, 2019, 568, 557-560.	13.7	72
11	Molecular Dynamics Simulations on Aspergillus niger Monoamine Oxidase: Conformational Dynamics and Interâ€monomer Communication Essential for Its Efficient Catalysis. Advanced Synthesis and Catalysis, 2019, 361, 2718.	2.1	3
12	Hidden Conformations in Aspergillus niger Monoamine Oxidase are Key for Catalytic Efficiency. Angewandte Chemie - International Edition, 2019, 58, 3097-3101.	7.2	18
13	Hidden Conformations in Aspergillus niger Monoamine Oxidase are Key for Catalytic Efficiency. Angewandte Chemie, 2019, 131, 3129-3133.	1.6	0
14	Metal Cluster Electrides: A New Type of Molecular Electride with Delocalised Polyattractor Character. Chemistry - A European Journal, 2018, 24, 9853-9859.	1.7	28
15	Epoxide Hydrolase Conformational Heterogeneity for the Resolution of Bulky Pharmacologically Relevant Epoxide Substrates. Chemistry - A European Journal, 2018, 24, 12254-12258.	1.7	8
16	Toward Bioelectronic Nanomaterials: Photoconductivity in Proteinâ€“Porphyrin Hybrids Wrapped around SWCNT. Advanced Functional Materials, 2018, 28, 1704031.	7.8	25
17	Electron correlation effects in third-order densities. Physical Chemistry Chemical Physics, 2017, 19, 4522-4529.	1.3	13
18	Unraveling factors leading to efficient norbornadieneâ€“quadricyclane molecular solar-thermal energy storage systems. Journal of Materials Chemistry A, 2017, 5, 12369-12378.	5.2	65

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19	Rules of Aromaticity. Challenges and Advances in Computational Chemistry and Physics, 2016, , 321-335.	0.6	7
20	Exploring the validity of the Glidewellâ€“Lloyd extension of Clarâ€™s Ï€-sextet rule: assessment from polycyclic conjugated hydrocarbons. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	24
21	Analysis of a Compound Class with Triplet States Stabilized by Potentially Baird Aromatic [10]Annulenyl Dicationic Rings. Chemistry - A European Journal, 2016, 22, 2793-2800.	1.7	30
22	Octahedral aromaticity in ^{2S+1}A_{1g} X₆^q clusters (X =) Tj ETQq0 0 0 rgBT /Overlock	1.3	12
23	Accelerated Molecular Dynamics Simulations of Protein Folding. Journal of Computational Chemistry, 2016, 37, .	1.5	1
24	Accelerated molecular dynamics simulations of protein folding. Journal of Computational Chemistry, 2015, 36, 1536-1549.	1.5	134
25	Three-center bonding analyzed from correlated and uncorrelated third-order reduced density matrices. Computational and Theoretical Chemistry, 2015, 1053, 173-179.	1.1	8
26	Quantifying aromaticity with electron delocalisation measures. Chemical Society Reviews, 2015, 44, 6434-6451.	18.7	335
27	A Molecular Dynamics Investigation of Mycobacterium tuberculosis Prenyl Synthases: Conformational Flexibility and Implications for Computerâ€aided Drug Discovery. Chemical Biology and Drug Design, 2015, 85, 756-769.	1.5	14
28	Interplay between R513 methylation and S516 phosphorylation of the cardiac voltage-gated sodium channel. Amino Acids, 2015, 47, 429-434.	1.2	23
29	Exploring the role of receptor flexibility in structure-based drug discovery. Biophysical Chemistry, 2014, 186, 31-45.	1.5	129
30	Undecaprenyl Diphosphate Synthase Inhibitors: Antibacterial Drug Leads. Journal of Medicinal Chemistry, 2014, 57, 5693-5701.	2.9	43
31	New Approximation to the Third-Order Density. Application to the Calculation of Correlated Multicenter Indices. Journal of Chemical Theory and Computation, 2014, 10, 3055-3065.	2.3	31
32	Metalloaromaticity. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2013, 3, 105-122.	6.2	105
33	Ultrafast irreversible phototautomerization of o-nitrobenzaldehyde. Chemical Communications, 2011, 47, 6383.	2.2	33
34	Electron Localization Function at the Correlated Level: A Natural Orbital Formulation. Journal of Chemical Theory and Computation, 2011, 7, 1231-1231.	2.3	7
35	All-metal aromatic clusters M42â^’ (M = B, Al, and Ga). Are Ï€-electrons distortive or not?. Physical Chemistry Chemical Physics, 2011, 13, 20673.	1.3	14
36	A non-adiabatic quantum-classical dynamics study of the intramolecular excited state hydrogen transfer in ortho-nitrobenzaldehyde. Physical Chemistry Chemical Physics, 2011, 13, 14685.	1.3	17

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37	Understanding Conjugation and Hyperconjugation from Electronic Delocalization Measures. Journal of Physical Chemistry A, 2011, 115, 13104-13113.	1.1	30
38	Electron delocalization and aromaticity in low-lying excited states of archetypal organic compounds. Physical Chemistry Chemical Physics, 2011, 13, 20690.	1.3	116
39	Aromaticity and electronic delocalization in all-metal clusters with single, double, and triple aromatic character. Theoretical Chemistry Accounts, 2011, 128, 419-431.	0.5	57
40	A dissected ring current model for assessing magnetic aromaticity: A general approach for both organic and inorganic rings. Journal of Computational Chemistry, 2011, 32, 2422-2431.	1.5	61
41	Patterns of Ï€-electron delocalization in aromatic and antiaromatic organic compounds in the light of HÃ¼ckel's 4n + 2 rule. Physical Chemistry Chemical Physics, 2010, 12, 7126.	1.3	38
42	A Critical Assessment of the Performance of Magnetic and Electronic Indices of Aromaticity. Symmetry, 2010, 2, 1156-1179.	1.1	115
43	A Test to Evaluate the Performance of Aromaticity Descriptors in All-Metal and Semimetal Clusters. An Appraisal of Electronic and Magnetic Indicators of Aromaticity. Journal of Chemical Theory and Computation, 2010, 6, 1118-1130.	2.3	84
44	Electron Localization Function at the Correlated Level: A Natural Orbital Formulation. Journal of Chemical Theory and Computation, 2010, 6, 2736-2742.	2.3	115
45	Bonding Analysis of the [C₂O₄]²⁺ Intermediate Formed in the Reaction of CO₂²⁺ with Neutral CO₂. Journal of Physical Chemistry A, 2010, 114, 6681-6688.	1.1	7
46	Domain Averaged Fermi Hole Analysis for Open-Shell Systems. Journal of Physical Chemistry A, 2009, 113, 5773-5779.	1.1	9
47	Peculiarities of Multiple Crâ‹¯Cr Bonding. Insights from the Analysis of Domain-Averaged Fermi Holes. Journal of Physical Chemistry A, 2009, 113, 8394-8400.	1.1	28
48	On the performance of some aromaticity indices: A critical assessment using a test set. Journal of Computational Chemistry, 2008, 29, 1543-1554.	1.5	261
49	Analysis of HÃ¼ckelâ€™s [4n+ 2] Rule through Electronic Delocalization Measures. Journal of Physical Chemistry A, 2008, 112, 13231-13238.	1.1	38
50	Electronic States of o-Nitrobenzaldehyde: A Combined Experimental and Theoretical Study. Journal of Physical Chemistry A, 2008, 112, 5046-5053.	1.1	30
51	Aromaticity of Distorted Benzene Rings:â€‰ Exploring the Validity of Different Indicators of Aromaticity. Journal of Physical Chemistry A, 2007, 111, 4513-4521.	1.1	102
52	Electron delocalization and aromaticity measures within the HÃ¼ckel molecular orbital method. Computational and Theoretical Chemistry, 2007, 811, 3-11.	1.5	46
53	Changes in Protonation States of In-Pathway Residues can Alter Ligand Binding Pathways Obtained From Spontaneous Binding Molecular Dynamics Simulations. Frontiers in Molecular Biosciences, 0, 9, .	1.6	2