JoaquÃ-n Barroso-Flores

List of Publications by Year
in descending order

44 papers	560 citations	759233 12 h-index	677142 22 g-index
48 all docs	48 docs citations	48 times ranked	844 citing authors

#	Article	IF	Citations
1	A Multi-State, Allosterically-Regulated Molecular Receptor With Switchable Selectivity. Journal of the American Chemical Society, 2014, 136, 10340-10348.	13.7	78
2	Effect of the degree of oxidation of graphene oxide on As(III) adsorption. Journal of Hazardous Materials, 2020, 384, 121440.	12.4	53
3	Selective Optical Sensing of Hg(II) in Aqueous Media by H-Acid/SBA-15: A Combined Experimental and Theoretical Study. Journal of Physical Chemistry C, 2013, 117, 9281-9289.	3.1	41
4	Sensitive water-soluble fluorescent chemosensor for chloride based on a bisquinolinium pyridine-dicarboxamide compound. Sensors and Actuators B: Chemical, 2015, 221, 1348-1355.	7.8	33
5	Effect of UV radiation on the structure of graphene oxide in water and its impact on cytotoxicity and As(III) adsorption. Chemosphere, 2020, 249, 126160.	8.2	29
6	In Silico Design of Monomolecular Drug Carriers for the Tyrosine Kinase Inhibitor Drug Imatinib Based on Calix- and Thiacalix[n]arene Host Molecules: A DFT and Molecular Dynamics Study. Journal of Chemical Theory and Computation, 2014, 10, 825-834.	5.3	26
7	Calix[n]arene-based drug carriers: A DFT study of their electronic interactions with a chemotherapeutic agent used against leukemia. Computational and Theoretical Chemistry, 2014, 1035, 84-91.	2.5	24
8	Accurate Estimation of pK_b Values for Amino Groups from Surface Electrostatic Potential (V_{S,min}) Calculations: The Isoelectric Points of Amino Acids as a Case Study. Journal of Chemical Information and Modeling, 2020, 60, 1445-1452.	5.4	23
9	Real-Time Visualization of Cell Membrane Damage Using Gadoliniumâ€“Schiff Base Complex-Doped Quantum Dots. ACS Applied Materials & Interfaces, 2018, 10, 35859-35868.	8.0	19
10	A Redox-Switchable, Allosteric Coordination Complex. Journal of the American Chemical Society, 2018, 140, 14590-14594.	13.7	18
11	Efficient fluorescent chemosensing of iodide based on a cationic meso-tetraarylporphyrin in pure water. Sensors and Actuators B: Chemical, 2019, 281, 462-470.	7.8	16
12	An Allosterically Regulated, Four-State Macrocycle. Inorganic Chemistry, 2018, 57, 3568-3578.	4.0	14
13	Calculation of VS,max and Its Use as a Descriptor for the Theoretical Calculation of pKa Values for Carboxylic Acids. Molecules, 2019, 24, 79.	3.8	13
14	Molecular Heterobimetallic Aluminoxanes and Aluminoxane Sulfides Containing Group 4 Metals. European Journal of Inorganic Chemistry, 2013, 2013, 2849-2857.	2.0	12
15	Theoretical Assessment of the Selective Fluorescence Quenching of 1-Amino-8-naphthol-3,6-disulfonic Acid (H-Acid) Complexes with Zn^{2+}, Cd^{2+}, and Hg^{2+}: A DFT and TD-DFT Study. Journal of Physical Chemistry A, 2014, 118, 12178-12183.	2.5	12
16	Structural and dynamical instability of DNA caused by high occurrence of d5SICS and dNaM unnatural nucleotides. Physical Chemistry Chemical Physics, 2017, 19, 10571-10580.	2.8	11
17	Synthesis of new Î³-lactones from preactivated monosubstituted pyrazines and TMSâ€“ketene acetals. Canadian Journal of Chemistry, 2012, 90, 469-482.	1.1	10
18	A water-stable luminescent Zn-MOF based on a conjugated Ï€-electron ligand as an efficient sensor for atorvastatin and its application in pharmaceutical samples. Journal of Materials Chemistry C, 2022, 10, 5944-5955.	5.5	10

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19	Synthesis of the anisobidentate compound bis(2-amino-cyclopent-1-ene-carbodithioate)diethyltin (IV). Experimental and theoretical study. Journal of Organometallic Chemistry, 2004, 689, 2096-2102.	1.8	9
20	Phosphane-free Câ€“C Heck couplings catalyzed by Pd(II) fluorinated aniline complexes of the type trans-[PdCl2(NH2ArF)2]. Journal of Molecular Catalysis A, 2006, 247, 65-72.	4.8	9
21	Reactivity of electrophilic chlorine atoms due to Ïƒ-holes: a mechanistic assessment of the chemical reduction of a trichloromethyl group by sulfur nucleophiles. Physical Chemistry Chemical Physics, 2016, 18, 27300-27307.	2.8	9
22	A mixed <scp>DFTâ€MD</scp> methodology for the in silico development of drug releasing macrocycles. Calix and thiaâ€calix[N]arenes as carriers for Bosutinib and Sorafenib. Journal of Computational Chemistry, 2016, 37, 940-946.	3.3	9
23	Chemosensing of neurotransmitters with selectivity and naked eye detection of <scp>l</scp>-DOPA based on fluorescent Zn(<scp>ii</scp>)-terpyridine bearing boronic acid complexes. Dalton Transactions, 2021, 50, 4255-4269.	3.3	9
24	Production of few-layer graphene by wet media milling using organic solvents and different types of graphite. Ceramics International, 2020, 46, 2413-2420.	4.8	7
25	Evaluation of Antiproliferative Palladium(II) Complexes of Synthetic Bisdemethoxycurcumin towards In Vitro Cytotoxicity and Molecular Docking on DNA Sequence. Molecules, 2021, 26, 4369.	3.8	7
26	Impact of secondary salts, temperature, and pH on the colloidal stability of graphene oxide in water. Nanoscale Advances, 2022, 4, 2435-2443.	4.6	6
27	Synthesis and Crystal Structures of Stable 4-Aryl-2-(trichloromethyl)-1,3-diaza-1,3-butadienes. Synthesis, 2016, 48, 2205-2212.	2.3	5
28	Evolution of the Fennaâ€“Matthewsâ€“Olson Complex and Its Quantum Coherence Features. Which Led the Way?. ACS Central Science, 2017, 3, 1061-1062.	11.3	5
29	Molecular Group 13 Metallaborates Derived from Mâ€“Oâ€“M Cleavage Promoted by BH₃. Inorganic Chemistry, 2017, 56, 7890-7899.	4.0	5
30	Hydrophobic unnatural base pairs show a Watson-Crick pairing in micro-second molecular dynamics simulations. Journal of Biomolecular Structure and Dynamics, 2020, 38, 4098-4106.	3.5	5
31	Proton to hydride umpolung at a phosphonium center via electron relay: a new strategy for main-group based water reduction. Chemical Science, 2021, 12, 15603-15608.	7.4	4
32	Ab initio calculations of electronic interactions in inclusion complexes of calix- and thiacalix[n]arenes and block s cations. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2013, 75, 39-46.	1.6	3
33	Spectroscopical UVâ€“Vis implications of an intramolecular Î·²â€“Mg coordination in bacteriochlorophyllâ€“a from the Fennaâ€“Matthewsâ€“Olson complex. International Journal of Quantum Chemistry, 2018, 118, e25663.	2.0	3
34	Influence of intramolecular Snâ€“chalcogen interactions on the conformational preferences for three diorganotin(IV) xanthates. Journal of Organometallic Chemistry, 2006, 691, 4937-4944.	1.8	2
35	Synthesis and Crystal Structure of the First Selenonyl Bis(carboxylate) SeO₂(O₂CCH₃)₂. European Journal of Inorganic Chemistry, 2015, 2015, 2923-2927.	2.0	2
36	Aromatization of pyridinylidenes into pyridines is inhibited by exocyclic delocalization. A theoretical mechanistic assessment. Tetrahedron, 2016, 72, 4194-4200.	1.9	2

#	Article	IF	Citations
37	In silico design of calixarene-based arsenic acid removal agents. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2016, 85, 169-174.	1.6	2
38	Fluorescence decay rate of selected compounds from Eysenhardtia polystachya extracts and their viability as biosensors. Materials Science and Engineering C, 2019, 104, 109978.	7.3	2
39	A Digallane Gold Complex with a 12-Electron Auride Center: Synthesis and Computational Studies. Organometallics, 2020, 39, 4372-4379.	2.3	2
40	Electrochemical reactivity of S-phenacyl-O-ethyl-xanthates in hydroalcoholic (MeOH/H2O 4:1) and anhydrous acetonitrile media. Electrochimica Acta, 2021, 380, 138239.	5.2	2
41	A boron, nitrogen-containing heterocyclic carbene (BNC) as a redox active ligand: synthesis and characterization of a lithium BNC-aurate complex. Dalton Transactions, 2022, 51, 7899-7906.	3.3	2
42	Synthesis, Optical Characterization in Solution and Solid-State, and DFT Calculations of 3-Acetyl and 3-(1â€²-(2â€²-Phenylhydrazono)ethyl)-coumarin-(7)-substituted Derivatives. Molecules, 2022, 27, 3677.	3.8	2
43	Electronic Structure Effects Related to the Origin of the Remarkable Near-Infrared Absorption of Blastochloris viridisâ€™ Light Harvesting 1-Reaction Center Complex. Journal of Chemical Theory and Computation, 2022, 18, 4555-4564.	5.3	2
44	Long range 1H19F coupling through multiple bond in thienopyridines, isoquinolines and 2-aza-carbazoles derivatives. Journal of Molecular Structure, 2019, 1176, 562-566.	3.6	1