Ataualpa Ac Braga

List of Publications by Year
in descending order

120 papers	6,320 citations	70961 41 h-index	69108 77 g-index
125 all docs	125 docs citations	125 times ranked	4473 citing authors

#	Article	IF	Citations
1	A facile synthesis and structural elucidation for furfural based chromophores: Prediction of linear and nonlinear optical properties. Journal of Molecular Structure, 2022, 1249, 131543.	1.8	5
2	Palladium-catalyzed sabinene oxidation with hydrogen peroxide: Smart fragrance production and DFT insights. Molecular Catalysis, 2022, 517, 112033.	1.0	1
3	Computational study of the boraformylation of allenes catalyzed by copper complexes. Computational and Theoretical Chemistry, 2022, 1208, 113575.	1.1	1
4	Donor moieties with Dâ€“Ï€â€“a framing modulated electronic and nonlinear optical properties for non-fullerene-based chromophores. RSC Advances, 2022, 12, 4209-4223.	1.7	15
5	Influence of acceptor tethering on the performance of nonlinear optical properties for pyrene-based materials with A-Ï€-D-Ï€-D architecture. Arabian Journal of Chemistry, 2022, 15, 103673.	2.3	29
6	Influence of Peripheral Modification of Electron Acceptors in Nonfullerene (O-IDTBR1)-Based Derivatives on Nonlinear Optical Response: DFT/TDDFT Study. ACS Omega, 2022, 7, 11631-11642.	1.6	14
7	Enriching NLO efficacy via designing non-fullerene molecules with the modification of acceptor moieties into ICIF2F: an emerging theoretical approach. RSC Advances, 2022, 12, 13412-13427.	1.7	38
8	Preparation, QTAIM and Singleâ€Crystal Exploration of the Pyrimethamineâ€Based Coâ€Crystal Salts with Substituted Benzoic Acids. ChemistrySelect, 2022, 7, .	0.7	15
9	Exploration of nonlinear optical enhancement and interesting optical behavior with pyrene moiety as the conjugated donor and efficient modification in acceptor moieties. Optical and Quantum Electronics, 2022, 54, .	1.5	16
10	Enantioselective Synthesis of Î±,Î²â€Unsaturated Aryl Lactams by Heckâ€Matsuda and Heckâ€Mizoroki Arylations of Enelactams. European Journal of Organic Chemistry, 2022, 2022, .	1.2	2
11	Molecular designing of highâ€performance 3D starâ€shaped electron acceptors containing a truxene core for nonfullerene organic solar cells. Journal of Physical Organic Chemistry, 2021, 34, .	0.9	85
12	O-4-Acetylamino-benzenesulfonylated pyrimidine derivatives: synthesis, SC-XRD, DFT analysis and electronic behaviour investigation. Journal of Molecular Structure, 2021, 1224, 129308.	1.8	32
13	DFT study of H₂ adsorption at a Cu-SSZ-13 zeolite: a cluster approach. Physical Chemistry Chemical Physics, 2021, 23, 9980-9990.	1.3	16
14	Electroanalytical profiling of cocaine samples by means of an electropolymerized molecularly imprinted polymer using benzocaine as the template molecule. Analyst, The, 2021, 146, 1747-1759.	1.7	12
15	3,4-Methylenedioxypyrovalerone (MDPV) Sensing Based on Electropolymerized Molecularly Imprinted Polymers on Silver Nanoparticles and Carboxylated Multi-Walled Carbon Nanotubes. Nanomaterials, 2021, 11, 353.	1.9	10
16	A comprehensive study of structural, non-covalent interactions and electronic insights into N-aryl substituted thiosemicarbazones via SC-XRD and first-principles DFT approach. Journal of Molecular Structure, 2021, 1230, 129852.	1.8	14
17	Non-covalent interactions abetted supramolecular arrangements of N-Substituted benzylidene acetohydrazide to direct its solid-state network. Journal of Molecular Structure, 2021, 1230, 129827.	1.8	32
18	An Efficient Synthesis, Spectroscopic Characterization, and Optical Nonlinearity Response of Novel Salicylaldehyde Thiosemicarbazone Derivatives. ACS Omega, 2021, 6, 16058-16065.	1.6	31

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19	Structural modulation of Ï€-conjugated linkers in Dâ€“Ï€â€“A dyes based on triphenylamine dicyanovinylene framework to explore the NLO properties. Royal Society Open Science, 2021, 8, 210570.	1.1	45
20	Palladium-catalyzed synthesis of 5-(arylated) pyrimidines, their characterization, electronic communication, and non-linear optical evaluations. Journal of Molecular Structure, 2021, 1237, 130408.	1.8	27
21	Efficient tuning of small acceptor chromophores with A1-Ï€-A2-Ï€-A1 configuration for high efficacy of organic solar cells via end group manipulation. Journal of Saudi Chemical Society, 2021, 25, 101305.	2.4	53
22	Exploration of second and third order nonlinear optical properties for theoretical framework of organic Dâ€“Ï€â€“Dâ€“Ï€â€“A type compounds. Optical and Quantum Electronics, 2021, 53, 1.	1.5	15
23	Facile Synthesis of Diversely Functionalized Peptoids, Spectroscopic Characterization, and DFT-Based Nonlinear Optical Exploration. ACS Omega, 2021, 6, 26016-26025.	1.6	14
24	Î²-Hydroxy Carbonyl compounds via aldol reaction: Single crystal investigation and quantum chemical exploration for the unveiling of supramolecular behavior. Journal of Molecular Structure, 2021, 1241, 130650.	1.8	14
25	Theoretical investigation of nonlinear optical behavior for rod and T-Shaped phenothiazine based D-Ï€-A organic compounds and their derivatives. Journal of Saudi Chemical Society, 2021, 25, 101339.	2.4	37
26	Synthesis, characterization and DFT calculated properties of electron-rich hydrazinylthiazoles: Experimental and computational synergy. Journal of Molecular Structure, 2021, 1245, 131043.	1.8	19
27	Do Double-Hybrid Exchangeâ€“Correlation Functionals Provide Accurate Chemical Shifts? A Benchmark Assessment for Proton NMR. Journal of Chemical Theory and Computation, 2021, 17, 6876-6885.	2.3	34
28	2-Nitro- and 4-fluorocinnamaldehyde based receptors as naked-eye chemosensors to potential molecular keypad lock. Scientific Reports, 2021, 11, 20847.	1.6	6
29	Molecular engineering of indenoindene-3-ethylrodanine acceptors with A2-A1-D-A1-A2 architecture for promising fullerene-free organic solar cells. Scientific Reports, 2021, 11, 20320.	1.6	39
30	Exploration of promising optical and electronic properties of (non-polymer) small donor molecules for organic solar cells. Scientific Reports, 2021, 11, 21540.	1.6	46
31	Exploration of Photophysical and Nonlinear Properties of Salicylaldehyde-Based Functionalized Materials: A Facile Synthetic and DFT Approach. ACS Omega, 2021, 6, 33914-33922.	1.6	8
32	Molecular salts of terephthalic acids with 2-aminopyridine and 2-aminothiazole derivatives as potential antioxidant agents; Base-Acid-Base type architectures. Journal of Molecular Structure, 2020, 1200, 127126.	1.8	25
33	Cyclization of chalcones into N-propionyl pyrazolines for their single crystal X-ray, computational and antibacterial studies. Journal of Molecular Structure, 2020, 1201, 127186.	1.8	20
34	Molecular structure of 1,4-bis(substituted-carbonyl)benzene: A combined experimental and theoretical approach. Journal of Molecular Structure, 2020, 1205, 127633.	1.8	26
35	A new piperazine: Spectroscopic and theoretical conformational studies. Journal of Molecular Structure, 2020, 1203, 127420.	1.8	1
36	A facile microwave assisted synthesis and structure elucidation of (3R)-3-alkyl-4,1-benzoxazepine-2,5-diones by crystallographic, spectroscopic and DFT studies. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 230, 117995.	2.0	26

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37	Enantioselective Heck Arylation of Acyclic Alkenol Aryl Ethers: Synthetic Applications and DFT Investigation of the Stereoselectivity. Advanced Synthesis and Catalysis, 2020, 362, 884-892.	2.1	8
38	Synthesis and structural analysis of novel indole derivatives by XRD, spectroscopic and DFT studies. Journal of Molecular Structure, 2020, 1203, 127438.	1.8	51
39	2-Amino-3-methylpyridinium, 2-amino-4-methylbenzothiazolium and 2-amino-5-chloropyridinium salts. Experimental and theoretical findings. Journal of Molecular Structure, 2020, 1222, 128914.	1.8	13
40	Exploration of Chromone-Based Thiosemicarbazone Derivatives: SC-XRD/DFT, Spectral (IR, UVâ€“Vis) Characterization, and Quantum Chemical Analysis. ACS Omega, 2020, 5, 30176-30188.	1.6	28
41	An Experimental and Computational Exploration on the Electronic, Spectroscopic, and Reactivity Properties of Novel Halo-Functionalized Hydrazones. ACS Omega, 2020, 5, 18907-18918.	1.6	14
42	Efficient Synthesis, SC-XRD, and Theoretical Studies of O-Benzenesulfonylated Pyrimidines: Role of Noncovalent Interaction Influence in Their Supramolecular Network. ACS Omega, 2020, 5, 15115-15128.	1.6	65
43	Prediction of 15N NMR chemical shifts for nitrogenated aromatic compounds. Arkivoc, 2020, 2020, 113-122.	0.3	1
44	Room temperature synthesis and Raman spectral evidence of carbon bond ranelateâ€“gold nanoparticles. Journal of Raman Spectroscopy, 2020, 51, 1083-1091.	1.2	2
45	Synthesis, characterization, and biological screening of metal complexes of novel sulfonamide derivatives: Experimental and theoretical analysis of sulfonamide crystal. Applied Organometallic Chemistry, 2020, 34, e5623.	1.7	39
46	N,Nâ€²â€bridged binuclear NHC palladium complexes: A combined experimental catalytic and computational study for the Suzuki reaction. Applied Organometallic Chemistry, 2020, 34, e5870.	1.7	11
47	A potent synthesis and supramolecular synthon hierarchy percipience of (E)-NÊ¹-(Napthalen-1-yl-methylene)-benzenesulfonohydrazide and 1-Napthaldehyde: A combined experimental and DFT studies. Journal of Molecular Structure, 2020, 1221, 128797.	1.8	19
48	Probing N-heterocyclic olefin as ancillary ligand in scandium-mediated $$hbox {CO}_2$$ to CO conversion. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	3
49	Heck arylation of acyclic olefins employing arenediazonium salts and chiral N,N ligands: new mechanistic insights from quantum-chemical calculations. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	6
50	Highly efficient one pot palladium-catalyzed synthesis of 3,5-bis (arylated) pyridines: Comparative experimental and DFT studies. Journal of Molecular Structure, 2020, 1213, 128131.	1.8	9
51	Methylone screening with electropolymerized molecularly imprinted polymer on screen-printed electrodes. Sensors and Actuators B: Chemical, 2020, 316, 128133.	4.0	23
52	Nanomolar Detection of Palladium (II) through a Novel Seleno-Rhodamine-based fluorescent and colorimetric chemosensor. Dyes and Pigments, 2020, 179, 108355.	2.0	16
53	Experimental and computational investigations of new indole derivatives: A combined spectroscopic, SC-XRD, DFT/TD-DFT and QTAIM analysis. Journal of Molecular Structure, 2020, 1207, 127803.	1.8	50
54	Computational study on the reaction mechanism of Cp*Rh(III)-catalyzed cross-coupling reactions. , 2020, , .		0

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55	Designing triazatruxene-based donor materials with promising photovoltaic parameters for organic solar cells. RSC Advances, 2019, 9, 26402-26418.	1.7	115
56	Synthesis, XRD, spectral (IR, UVâ€“Vis, NMR) characterization and quantum chemical exploration of benzoimidazoleâ€based hydrazones: A synergistic experimentalâ€computational analysis. Applied Organometallic Chemistry, 2019, 33, e5182.	1.7	42
57	Unveiling the potential of scandium complexes for methane Câ€“H bond activation: a computational study. New Journal of Chemistry, 2019, 43, 12257-12263.	1.4	9
58	DFT perspective on the selectivity and mechanism of ligand-free Heck reaction involving allylic esters and arenediazonium salts. Journal of Organometallic Chemistry, 2019, 896, 5-15.	0.8	10
59	Electrochemical sensing of ecstasy with electropolymerized molecularly imprinted poly(o-phenylenediamine) polymer on the surface of disposable screen-printed carbon electrodes. Sensors and Actuators B: Chemical, 2019, 290, 378-386.	4.0	77
60	On the Amazing Reactivity of the Ranelate Ion: New Applications of an Old Antiosporotic Drug. ChemistrySelect, 2019, 4, 13926-13931.	0.7	5
61	A facile and concise route to (hydroxybenzoyl)pyrido[2,3-d]pyrimidine heterocycle derivatives: synthesis, and structural, spectral and computational exploration. RSC Advances, 2019, 9, 34567-34580.	1.7	16
62	Synthesis, crystal structure analysis, spectral characterization and nonlinear optical exploration of potent thiosemicarbazones based compounds: A DFT refine experimental study. Inorganica Chimica Acta, 2019, 486, 162-171.	1.2	56
63	Prediction of Second-Order Nonlinear Optical Properties of Dâ€“Ïâ€“A Compounds Containing Novel Fluorene Derivatives: A Promising Route to Giant Hyperpolarizabilities. Journal of Cluster Science, 2019, 30, 415-430.	1.7	110
64	Synthesis, crystal structure analysis, spectral IR, UVâ€“Vis, NMR assessments, electronic and nonlinear optical properties of potent quinoline based derivatives: Interplay of experimental and DFT study. Journal of Saudi Chemical Society, 2019, 23, 546-560.	2.4	98
65	Synthesis, single crystal analysis and DFT based computational studies of 2,4-diamino-5-(4-chlorophenyl)-6-ethylpyrim idin-1-ium 3,4,5-trihydroxybenzoate -methanol (DETM). Journal of Molecular Structure, 2019, 1180, 119-126.	1.8	57
66	Synthesis, crystal structure, spectral and DFT studies of potent isatin derived metal complexes. Journal of Molecular Structure, 2018, 1166, 110-120.	1.8	38
67	Unusual Photooxidation of S-Bonded Mercaptopyridine in a Mixed Ligand Ruthenium(II) Complex with Terpyridine and Bipyridine Ligands. Inorganic Chemistry, 2018, 57, 4898-4905.	1.9	14
68	First Theoretical Framework of Triphenylamineâ€“Dicyanovinylene-Based Nonlinear Optical Dyes: Structural Modification of Ï€-Linkers. Journal of Physical Chemistry C, 2018, 122, 4009-4018.	1.5	193
69	Synthetic, XRD, non-covalent interactions and solvent dependent nonlinear optical studies of Sulfadiazine-Ortho-Vanillin Schiff base: (E)-4-((2-hydroxy-3-methoxy- benzylidene)) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 177 Td	1.8	78
70	Synthesis and XRD, FT-IR vibrational, UVâ€“vis, and nonlinear optical exploration of novel tetra substituted imidazole derivatives: A synergistic experimental-computational analysis. Journal of Physics and Chemistry of Solids, 2018, 115, 265-276.	1.9	77
71	Enantioselective, Noncovalent, Substrateâ€Directable Heckâ€“Matsuda and Oxidative Heck Arylations of Unactivated Fiveâ€Membered Carbocyclic Olefins. Chemistry - A European Journal, 2018, 24, 11738-11747.	1.7	29
72	Synthesis, spectral characterization and computed optical analysis of potent triazole based compounds. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 190, 197-207.	2.0	30

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73	Schiff base of isoniazid and ketoprofen: synthesis, X-ray crystallographic, spectroscopic, antioxidant, and computational studies. Turkish Journal of Chemistry, 2018, 42, .	0.5	1
74	Synthesis, spectroscopic, single crystal diffraction and potential nonlinear optical properties of novel pyrazoline derivatives: Interplay of experimental and computational analyses. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 202, 146-158.	2.0	18
75	New insights into the electrophilic aromatic substitution mechanism of tricyanovinylation reaction involving tetracyanoethylene and N,N-dimethylaniline: An interpretation based on density functional theory calculations. Journal of Molecular Structure, 2017, 1142, 58-65.	1.8	1
76	Synthesis, structural, DFT studies, docking and antibacterial activity of a xanthene based hydrazone ligand. Journal of Molecular Structure, 2017, 1143, 235-244.	1.8	80
77	3â€Alkenyltyrosines Accessed by Suzukiâ€“Miyaura Coupling: A Key Intermediate in the Synthesis and Mechanistic Study of Povarov Multicomponent Reactions. Asian Journal of Organic Chemistry, 2017, 6, 913-920.	1.3	7
78	Synthesis, crystal structures, spectroscopic and nonlinear optical properties of chalcone derivatives: A combined experimental and theoretical study. Journal of Molecular Structure, 2017, 1141, 142-156.	1.8	96
79	Nickel-catalysed direct C2-arylation of N-heterocyclic carbenes. Dalton Transactions, 2017, 46, 12027-12031.	1.6	41
80	Theoretical study on selectivity trends in (Nâ€heterocyclic carbene)â€Pd catalyzed mizorokiâ€“heck reactions: Exploring density functionals methods and molecular models. Journal of Computational Chemistry, 2017, 38, 2371-2377.	1.5	13
81	Conformation of some 2,4,6-trisubstitued pyridinium salts. Journal of Molecular Structure, 2017, 1149, 640-644.	1.8	0
82	Stability Study of Hypervalent Tellurium Compounds in Aqueous Solutions. ACS Omega, 2017, 2, 4431-4439.	1.6	16
83	Facile synthesis, single crystal analysis, and computational studies of sulfanilamide derivatives. Journal of Molecular Structure, 2017, 1127, 766-776.	1.8	91
84	Mechanistic Studies on Gold-Catalyzed Direct Arene Câ€“H Bond Functionalization by Carbene Insertion: The Coinage-Metal Effect. Organometallics, 2017, 36, 172-179.	1.1	52
85	Synthesis, X-ray crystallographic, spectroscopic and computational studies of aminothiazole derivatives. Journal of Molecular Structure, 2017, 1131, 136-148.	1.8	45
86	N-Heterocyclic Carbene Based Nickel and Palladium Complexes: A DFT Comparison of the Mizorokiâ€“Heck Catalytic Cycles. Organometallics, 2016, 35, 3170-3181.	1.1	48
87	An experimental and theoretical study into the facile, homogenous (N-heterocyclic) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 187 T and Technology, 2016, 6, 7461-7467.	2.1	20
88	DFT exploration of mechanistic pathways of an aza-Moritaâ€“Baylisâ€“Hillman reaction. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	8
89	Iodine(III)-Mediated Ring Contraction of 1,2-Dihydronaphthalenes: Mechanistic Insight by Computational Investigations. ChemistrySelect, 2016, 1, 2706-2711.	0.7	6
90	Mor-Dalphos-Pd (II) oxidative addition complexes and related NH3 adducts: Insights into bonding and nonbonding interactions. Journal of Molecular Structure, 2016, 1120, 245-249.	1.8	2

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91	Silanol-Assisted Carbinolamine Formation in an Amine-Functionalized Mesoporous Silica Surface: Theoretical Investigation by Fragmentation Methods. Journal of Physical Chemistry B, 2016, 120, 1660-1669.	1.2	20
92	Intermolecular Noncovalent Hydroxy-Directed Enantioselective Heck Desymmetrization of Cyclopentenol: Computationally Driven Synthesis of Highly Functionalized cis-4-Arylcyclopentenol Scaffolds. Journal of Organic Chemistry, 2016, 81, 2010-2018.	1.7	54
93	(N-Heterocyclic Carbene)-Palladate Complexes in Anionic Mizorokiâ€“Heck Coupling Cycles: A Combined Experimental and Computational Study. Organometallics, 2015, 34, 2463-2470.	1.1	55
94	A computational view on the reactions of hydrocarbons with coinage metal complexes. Journal of Organometallic Chemistry, 2015, 784, 2-12.	0.8	39
95	Dispersion-Corrected Density Functional for the Correct Description on Regioselectivity Trends in Heck-Mizoroki Reaction Catalyzed by Anionic (N-Heterocycle Carbene)-Palladium Complexes. Revista Processos QuÃmicos, 2015, 9, 45-49.	0.0	0
96	On the thermal Pummerer rearrangement of substituted sulfoxides. Journal of Sulfur Chemistry, 2014, 35, 248-260.	1.0	0
97	Computational Perspective on Pd-Catalyzed Câ€“C Cross-Coupling Reaction Mechanisms. Accounts of Chemical Research, 2013, 46, 2626-2634.	7.6	306
98	Homogeneous Computational Catalysis: The Mechanism for Cross-Coupling and Other C-C Bond Formation Processes. NATO Science for Peace and Security Series B: Physics and Biophysics, 2012, , 185-206.	0.2	1
99	The role of cyclobutenes in gold(i)-catalysed skeletal rearrangement of 1,6-enynes. Organic and Biomolecular Chemistry, 2012, 10, 6105.	1.5	60
100	Mechanism of Side Reactions in Alkane Cï£¿H Bond Functionalization by Diazo Compounds Catalyzed by Ag and Cu Homoscorpionate Complexesâ€”A DFT Study. ChemCatChem, 2011, 3, 1646-1652.	1.8	47
101	The importance of conformational search: a test case on the catalytic cycle of the Suzukiâ€“Miyaura cross-coupling. Theoretical Chemistry Accounts, 2011, 128, 639-646.	0.5	67
102	A DFT Study of the Effect of the Ligands in the Reductive Elimination from Palladium Bis(allyl) Complexes. Organometallics, 2010, 29, 4983-4991.	1.1	57
103	BrÃ¸nsted Acid Catalyzed Moritaâ€“Baylisâ€“Hillman Reaction: A New Mechanistic View for Thioureas Revealed by ESIâ€MS(/MS) Monitoring and DFT Calculations. Chemistry - A European Journal, 2009, 15, 12460-12469.	1.7	72
104	Vinyl Acetate Synthesis on Homogeneous and Heterogeneous Pd-Based Catalysts: A Theoretical Analysis on the Reaction Mechanisms. Journal of Physical Chemistry A, 2009, 113, 11758-11762.	1.1	13
105	The Mechanism of the Catalytic Functionalization of Haloalkanes by Carbene Insertion: An Experimental and Theoretical Study. Organometallics, 2009, 28, 5968-5981.	1.1	49
106	Câ^'C Reductive Elimination in Palladium Complexes, and the Role of Coupling Additives. A DFT Study Supported by Experiment. Journal of the American Chemical Society, 2009, 131, 3650-3657.	6.6	178
107	Bidentate phosphines as ligands in the palladium-catalyzed intramolecular arylation: the intermolecular base-assisted proton abstraction mechanism. Tetrahedron, 2008, 64, 6021-6029.	1.0	123
108	Mechanistic insights into the transmetalation step of a Suzukiâ€“Miyaura reaction of 2(4)-bromopyridines: characterization of an intermediate. Tetrahedron, 2008, 64, 7437-7443.	1.0	66

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109	Proton-Abstraction Mechanism in the Palladium-Catalyzed Intramolecular Arylation:Â Substituent Effects. Journal of the American Chemical Society, 2007, 129, 6880-6886.	6.6	509
110	DescriÃ§Ãµes estruturais cristalinas de zeÃ³litos. Quimica Nova, 2007, 30, 178-188.	0.3	18
111	A Valuable, Inexpensive CuI/N-Heterocyclic Carbene Catalyst for the Selective Diboration of Styrene. Chemistry - A European Journal, 2007, 13, 2614-2621.	1.7	156
112	Mechanism of Alkane Câ^'H Bond Activation by Copper and Silver Homoscorpionate Complexes. Organometallics, 2006, 25, 5292-5300.	1.1	84
113	A DFT Study of the Full Catalytic Cycle of the Suzukiâ^'Miyaura Cross-Coupling on a Model System. Organometallics, 2006, 25, 3647-3658.	1.1	348
114	Proton Abstraction Mechanism for the Palladium-Catalyzed Intramolecular Arylation. Journal of the American Chemical Society, 2006, 128, 1066-1067.	6.6	698
115	CÃ¡lculos teÃ³ricos de afinidades por prÃ³ton de n-alquilaminas usando o mÃ©todo ONIOM. Quimica Nova, 2006, 29, 187-193.	0.3	1
116	Computational study of the transmetalation process in the Suzukiâ€“Miyaura cross-coupling of aryls. Journal of Organometallic Chemistry, 2006, 691, 4459-4466.	0.8	140
117	Computational Characterization of the Role of the Base in the Suzukiâ^'Miyaura Cross-Coupling Reaction. Journal of the American Chemical Society, 2005, 127, 9298-9307.	6.6	317
118	Spectroscopic evidence for a preferential location of lidocaine inside phospholipid bilayers. Biophysical Chemistry, 2002, 99, 229-243.	1.5	56
119	Mechanism of Palladium-Catalyzed Cross-Coupling Reactions. , 0, , 109-130.		4
120	LDA Conjugate Addition to a Morita-Baylis-Hillman Ester: Experimental and DFT-based Theoretical Observations. , 0, , .		0