Fernanda Duarte

List of Publications by Year
in descending order

66 papers	2,616 citations	159358 30 h-index	205818 48 g-index
103 all docs	103 docs citations	103 times ranked	3581 citing authors

#	Article	IF	Citations
1	Cationâ€“Ï€ interactions in proteinâ€“ligand binding: theory and data-mining reveal different roles for lysine and arginine. Chemical Science, 2018, 9, 2655-2665.	3.7	184
2	Computing organic stereoselectivity â€“ from concepts to quantitative calculations and predictions. Chemical Society Reviews, 2016, 45, 6093-6107.	18.7	175
3	Force Field Independent Metal Parameters Using a Nonbonded Dummy Model. Journal of Physical Chemistry B, 2014, 118, 4351-4362.	1.2	148
4	A General Route to Bicyclo[1.1.1]pentanes through Photoredox Catalysis. ACS Catalysis, 2019, 9, 9568-9574.	5.5	112
5	Resolving Apparent Conflicts between Theoretical and Experimental Models of Phosphate Monoester Hydrolysis. Journal of the American Chemical Society, 2015, 137, 1081-1093.	6.6	92
6	Hostâ€“Guest-Induced Electron Transfer Triggers Radical-Cation Catalysis. Journal of the American Chemical Society, 2020, 142, 2134-2139.	6.6	74
7	Rationalizing the Activity of an â€œArtificial Diels-Alderaseâ€: Establishing Efficient and Accurate Protocols for Calculating Supramolecular Catalysis. Journal of the American Chemical Society, 2020, 142, 1300-1310.	6.6	68
8	The Energetic Significance of Metallophilic Interactions. Angewandte Chemie - International Edition, 2019, 58, 12617-12623.	7.2	65
9	Cooperative Electrostatic Interactions Drive Functional Evolution in the Alkaline Phosphatase Superfamily. Journal of the American Chemical Society, 2015, 137, 9061-9076.	6.6	63
10	Harnessing Sulfinyl Nitrenes: A Unified One-Pot Synthesis of Sulfoximines and Sulfonimidamides. Journal of the American Chemical Society, 2020, 142, 15445-15453.	6.6	59
11	Recent advances in QM/MM free energy calculations using reference potentials. Biochimica Et Biophysica Acta - General Subjects, 2015, 1850, 954-965.	1.1	56
12	Catalytic Asymmetric Synthesis of Cyclohexanes by Hydrogen Borrowing Annulations. Angewandte Chemie - International Edition, 2019, 58, 12558-12562.	7.2	54
13	Highly Active Halogen Bonding and Chalcogen Bonding Chloride Transporters with Nonâ€Protonophoric Activity. Chemistry - A European Journal, 2021, 27, 11738-11745.	1.7	54
14	Discovery of SARS-CoV-2 M^{pro} peptide inhibitors from modelling substrate and ligand binding. Chemical Science, 2021, 12, 13686-13703.	3.7	54
15	Dearomative Photocatalytic Construction of Bridged 1,3â€Diazepanes. Angewandte Chemie - International Edition, 2020, 59, 4121-4130.	7.2	53
16	Synergistic Noncovalent Catalysis Facilitates Base-Free Michael Addition. Journal of the American Chemical Society, 2020, 142, 17743-17750.	6.6	51
17	Empirical valence bond simulations of the hydride transfer step in the monoamine oxidase B catalyzed metabolism of dopamine. Proteins: Structure, Function and Bioinformatics, 2014, 82, 3347-3355.	1.5	50
18	Reverse Polarity Reductive Functionalization of Tertiary Amides via a Dual Iridium-Catalyzed Hydrosilylation and Single Electron Transfer Strategy. ACS Catalysis, 2020, 10, 11438-11447.	5.5	50

#	Article	IF	Citations
19	Catalytic Zinc Complexes for Phosphate Diester Hydrolysis. Angewandte Chemie - International Edition, 2014, 53, 8246-8250.	7.2	49
20	autodE: Automated Calculation of Reaction Energy Profilesâ€" Application to Organic and Organometallic Reactions. Angewandte Chemie - International Edition, 2021, 60, 4266-4274.	7.2	49
21	Molecular Recognition in Asymmetric Counteranion Catalysis: Understanding Chiral Phosphate-Mediated Desymmetrization. Journal of the American Chemical Society, 2017, 139, 8886-8896.	6.6	47
22	Modeling catalytic promiscuity in the alkaline phosphatase superfamily. Physical Chemistry Chemical Physics, 2013, 15, 11160.	1.3	46
23	The Competing Mechanisms of Phosphate Monoester Dianion Hydrolysis. Journal of the American Chemical Society, 2016, 138, 10664-10673.	6.6	46
24	Transmembrane anion transport mediated by halogen bonding and hydrogen bonding triazole anionophores. Chemical Science, 2020, 11, 4722-4729.	3.7	44
25	Tuning the anion binding properties of lanthanide receptors to discriminate nucleoside phosphates in a sensing array. Chemical Science, 2020, 11, 3619-3628.	3.7	43
26	Expanding the Catalytic Triad in Epoxide Hydrolases and Related Enzymes. ACS Catalysis, 2015, 5, 5702-5713.	5.5	42
27	Direct catalytic asymmetric synthesis of Î±-chiral bicyclo[1.1.1]pentanes. Nature Communications, 2021, 12, 1644.	5.8	39
28	The Mechanism of H2Activation by (Amino)Carbenes. Journal of Physical Chemistry A, 2011, 115, 3050-3059.	1.1	38
29	Rationalizing the diverse reactivity of [1.1.1]propellane through Ïƒâ€"Ï€-delocalization. Chemical Science, 2020, 11, 4895-4903.	3.7	36
30	Mass spectrometry reveals potential of Î²-lactams as SARS-CoV-2 M^{pro} inhibitors. Chemical Communications, 2021, 57, 1430-1433.	2.2	35
31	Evolutionary repurposing of a sulfatase: A new Michaelis complex leads to efficient transition state charge offset. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E7293-E7302.	3.3	34
32	Promiscuity in the Enzymatic Catalysis of Phosphate and Sulfate Transfer. Biochemistry, 2016, 55, 3061-3081.	1.2	32
33	Insights on the mechanism of proton transfer reactions in amino acids. Physical Chemistry Chemical Physics, 2011, 13, 7773.	1.3	31
34	Amino-oxetanes as amide isosteres by an alternative defluorosulfonylative coupling of sulfonyl fluorides. Nature Chemistry, 2022, 14, 160-169.	6.6	30
35	Stereospecific 1,3-H Transfer of Indenols Proceeds via Persistent Ion-Pairs Anchored by NHÂ·Â·Â·Ï€ Interactions. Journal of the American Chemical Society, 2018, 140, 16740-16748.	6.6	29
36	Atropisomerism in Diarylamines: Structural Requirements and Mechanisms of Conformational Interconversion. Angewandte Chemie - International Edition, 2020, 59, 18670-18678.	7.2	28

#	Article	IF	Citations
37	How Does Pin1 Catalyze the Cisâ€“Trans Prolyl Peptide Bond Isomerization? A QM/MM and Mean Reaction Force Study. Journal of Physical Chemistry B, 2012, 116, 12972-12979.	1.2	26
38	The Alkaline Hydrolysis of Sulfonate Esters: Challenges in Interpreting Experimental and Theoretical Data. Journal of Organic Chemistry, 2014, 79, 2816-2828.	1.7	26
39	Catalytic Asymmetric Synthesis of Cyclohexanes by Hydrogen Borrowing Annulations. Angewandte Chemie, 2019, 131, 12688-12692.	1.6	26
40	cgbind: A Python Module and Web App for Automated Metallocage Construction and Hostâ€“Guest Characterization. Journal of Chemical Information and Modeling, 2020, 60, 3546-3557.	2.5	26
41	Red-shifted tetra-ortho-halo-azobenzenes for photo-regulated transmembrane anion transport. Organic and Biomolecular Chemistry, 2021, 19, 9058-9067.	1.5	26
42	A transferable active-learning strategy for reactive molecular force fields. Chemical Science, 2021, 12, 10944-10955.	3.7	26
43	Electrophilic Activation of [1.1.1]Propellane for the Synthesis of Nitrogenâ€Substituted Bicyclo[1.1.1]pentanes. Angewandte Chemie - International Edition, 2022, 61, .	7.2	24
44	Computational Modeling of Supramolecular Metallo-organic Cagesâ€“Challenges and Opportunities. ACS Catalysis, 2022, 12, 5806-5826.	5.5	24
45	Concerted or Stepwise: How Much Do Free-Energy Landscapes Tell Us about the Mechanisms of Elimination Reactions?. Journal of Organic Chemistry, 2014, 79, 1280-1288.	1.7	23
46	Deoxydehydration of vicinal diols and polyols catalyzed by pyridinium perrhenate salts. Catalysis Science and Technology, 2017, 7, 5644-5649.	2.1	23
47	Selectivity in organocatalysisâ€”From qualitative to quantitative predictive models. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1518.	6.2	23
48	Characterization of the Zwitterionic Intermediate in 1,1â€Carboboration of Alkynes. Angewandte Chemie - International Edition, 2020, 59, 12731-12735.	7.2	22
49	The catalytic effect of water on the keto-enol tautomerisation reaction of thioformic acid. Molecular Physics, 2010, 108, 1375-1384.	0.8	19
50	Bio-inspired Domino oxa-Michael/Diels-Alder/oxa-Michael Dimerization of para -Quinols. Angewandte Chemie - International Edition, 2018, 57, 6198-6202.	7.2	16
51	Total Synthesis of a Dimeric Thymol Derivative Isolated from Arnica sachalinensis. Angewandte Chemie - International Edition, 2017, 56, 6813-6817.	7.2	13
52	Mechanisms of histone lysine-modifying enzymes: A computational perspective on the role of the protein environment. Journal of Molecular Graphics and Modelling, 2016, 67, 69-84.	1.3	12
53	Atropisomerism in Diarylamines: Structural Requirements and Mechanisms of Conformational Interconversion. Angewandte Chemie, 2020, 132, 18829-18837.	1.6	12
54	The Energetic Significance of Metallophilic Interactions. Angewandte Chemie, 2019, 131, 12747-12753.	1.6	11

#	Article	IF	Citations
55	Dearomative Photocatalytic Construction of Bridged 1,3â€Diazepanes. Angewandte Chemie, 2020, 132, 4150-4159.	1.6	10
56	Collective Synthesis of Illudalane Sesquiterpenes via Cascade Inverse Electron Demand (4 + 2) Cycloadditions of Thiophene S,S-Dioxides. Journal of the American Chemical Society, 2022, 144, 10017-10024.	6.6	7
57	Bio-inspired Domino oxa-Michael/Diels-Alder/oxa-Michael Dimerization of para -Quinols. Angewandte Chemie, 2018, 130, 6306-6310.	1.6	6
58	Relative Binding Energies Predict Crystallographic Binding Modes of Ethionamide Booster Lead Compounds. Journal of Physical Chemistry Letters, 2019, 10, 2244-2249.	2.1	5
59	Characterization of the Zwitterionic Intermediate in 1,1â€Carboboration of Alkynes. Angewandte Chemie, 2020, 132, 12831-12835.	1.6	5
60	autodE: Automated Calculation of Reaction Energy Profilesâ€" Application to Organic and Organometallic Reactions. Angewandte Chemie, 2021, 133, 4312-4320.	1.6	5
61	Hostâ€Guest Chemistry of Selfâ€Assembled Hemiâ€Cage Systems: The Dramatic Effect of Lost Preâ€Organization. Israel Journal of Chemistry, 2019, 59, 257-266.	1.0	4
62	trans-Hydroborationâ€"oxidation products in Î"⁵-steroids via a hydroboration-retro-hydroboration mechanism. Chemical Science, 2020, 11, 12764-12768.	3.7	3
63	Double and Triple Ionisation of Isocyanic Acid. Scientific Reports, 2020, 10, 2288.	1.6	3
64	Single photon double and triple ionization of allene. Physical Chemistry Chemical Physics, 2022, 24, 786-796.	1.3	3
65	Total Synthesis of a Dimeric Thymol Derivative Isolated from Arnica sachalinensis. Angewandte Chemie, 2017, 129, 6917-6921.	1.6	2
66	Electrophilic Activation of [1.1.1]Propellane for the Synthesis of Nitrogenâ€Substituted Bicyclo[1.1.1]pentanes. Angewandte Chemie, 2022, 134, .	1.6	2