

# Paulo J Costa

## List of Publications by Year in descending order

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82  
papers

2,763  
citations

172457

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105  
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105  
docs citations

105  
times ranked

3215  
citing authors

#	ARTICLE	IF	CITATIONS
1	Synthesis and Exploitation of the Biological Profile of Novel Guanidino Xylofuranose Derivatives**. ChemMedChem, 2022, 17, .	3.2	5
2	Halogen Bonding: An Underestimated Player in Membraneâ€“Ligand Interactions. Journal of the American Chemical Society, 2021, 143, 4253-4267.	13.7	34
3	Binding of RuCp complexes with human apo-transferrin: fluorescence spectroscopy and molecular docking methods. BioMetals, 2021, 34, 1029-1042.	4.1	6
4	Optimized Halogen Atomic Radii for PBSA Calculations Using Off-Center Point Charges. Journal of Chemical Information and Modeling, 2021, 61, 3361-3375.	5.4	4
5	Transmembrane Anion Transport Mediated by Halogen Bonds: Using Off-Center Charges. Methods in Molecular Biology, 2021, 2315, 273-284.	0.9	0
6	Alumination of aryl methyl ethers: switching between $sp^{2}$ and $sp^{3}$ C=O bond functionalisation with Pd-catalysis. Chemical Communications, 2021, 57, 11673-11676.	4.1	4
7	Synthesis of Triazoleâ€“Containing Furanosyl Nucleoside Analogues and Their Phosphate, Phosphoramidate or Phoshonate Derivatives as Potential Sugar Diphosphate or Nucleotide Mimetics. ChemPlusChem, 2020, 85, 1676-1691.	2.8	2
8	Catalyst control of selectivity in the C=O bond alumination of biomass derived furans. Chemical Science, 2020, 11, 7850-7857.	7.4	15
9	A New Family of Iron(II)-Cyclopentadienyl Compounds Shows Strong Activity against Colorectal and Triple Negative Breast Cancer Cells. Molecules, 2020, 25, 1592.	3.8	20
10	Halogen bonding in halocarbon-protein complexes and computational tools for rational drug design. Expert Opinion on Drug Discovery, 2019, 14, 805-820.	5.0	36
11	Tackling Halogenated Species with PBSA: Effect of Emulating the Î¶-Hole. Journal of Chemical Theory and Computation, 2019, 15, 4241-4251.	5.3	15
12	Directing self-assembly in solution towards improved cooperativity in Fe( $\eta^{5}$ ) complexes with amphiphilic tridentate ligands. Dalton Transactions, 2019, 48, 4239-4247.	3.3	5
13	Furanosyl Nucleoside Analogues Embodying Triazole or Theobromine Units as Potential Lead Molecules for Alzheimer's Disease. European Journal of Organic Chemistry, 2018, 2018, 2667-2681.	2.4	8
14	Hydrophosphonylation of aldehydes catalyzed by cyclopentadienyl ruthenium(II) complexes. Molecular Catalysis, 2018, 450, 77-86.	2.0	5
15	3. The Halogen bond: Nature and Applications. , 2018, , 81-106.		1
16	Accurate Description of Low-Lying Excited States in a Series of Photoreactive Clusters [Os <sub>3</sub> (CO) <sub>10</sub> (Î±-diimine)] by DFT Calculations. Inorganic Chemistry, 2018, 57, 11704-11716.	4.0	3
17	Biomolecular Simulations of Halogen Bonds with a GROMOS Force Field. Journal of Chemical Theory and Computation, 2018, 14, 5383-5392.	5.3	20
18	Advances in the Computational Modeling of Halogen Bonds in Biochemical Systems. Frontiers in Computational Chemistry, 2018, , 144-183.	0.3	1

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19	New copper(I) and heteronuclear copper(I)–ruthenium(II) complexes: Synthesis, structural characterization and cytotoxicity. <i>Journal of Inorganic Biochemistry</i> , 2017, 169, 68-78.	3.5	39
20	Structure, bonding and reactivity of seven-coordinate allylic Mo(II) and W(II) complexes. <i>Coordination Chemistry Reviews</i> , 2017, 344, 83-100.	18.8	13
21	pH-Switchability and Second-Order Nonlinear Optical Properties of Monocyclopentadienylruthenium(II)/iron(II) Tetrazoles/Tetrazolates: Synthesis, Characterization, and Time-Dependent Density Functional Theory Calculations. <i>Inorganic Chemistry</i> , 2017, 56, 6849-6863.	4.0	10
22	Ion–Pair Halogen Bonds in 2-Halo-Functionalized Imidazolium Chloride Receptors: Substituent and Solvent Effects. <i>Chemistry - an Asian Journal</i> , 2017, 12, 586-594.	3.3	14
23	The halogen bond: Nature and applications. <i>ChemistrySelect</i> , 2017, 2, .	1.5	39
24	New [( $\eta^5$ -C <sub>5</sub> H <sub>5</sub> )Ru(N <sub>3</sub> )(PPh <sub>3</sub> )] [PF <sub>6</sub> ] compounds: colon anticancer activity and GLUT-mediated cellular uptake of carbohydrate-appended complexes. <i>Dalton Transactions</i> , 2016, 45, 11926-11930.	3.3	23
25	Synthesis of glucopyranos-6-yl purine and pyrimidine isonucleosides as potential cholinesterase inhibitors. Access to pyrimidine-linked pseudodisaccharides through Mitsunobu reaction. <i>Pure and Applied Chemistry</i> , 2016, 88, 363-379.	1.9	9
26	Modulating the electron-transfer properties of a mixed-valence system through host–guest chemistry. <i>Chemical Science</i> , 2015, 6, 1334-1340.	7.4	11
27	Tri–thiourea tripod-based molecules as chloride transmembrane transporters: insights from molecular dynamics simulations. <i>Soft Matter</i> , 2014, 10, 3608.	2.7	14
28	Interaction of a calix[4]arene derivative with a DOPC bilayer: Biomolecular simulations towards chloride transport. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2014, 1838, 890-901.	2.6	12
29	CNN Pincer Ruthenium Catalysts for Hydrogenation and Transfer Hydrogenation of Ketones: Experimental and Computational Studies. <i>Chemistry - A European Journal</i> , 2014, 20, 13603-13617.	3.3	47
30	Chloride, carboxylate and carbonate transport by ortho-phenylenediamine-based bisureas. <i>Chemical Science</i> , 2013, 4, 103-117.	7.4	119
31	Gas-phase interaction between nickel (II) and nitrobenzyl azides: An ESI-MSn study. <i>International Journal of Mass Spectrometry</i> , 2013, 351, 27-36.	1.5	3
32	Structural Studies on Dinuclear Ruthenium(II) Complexes That Bind Diastereoselectively to an Antiparallel Folded Human Telomere Sequence. <i>Journal of Medicinal Chemistry</i> , 2013, 56, 8674-8683.	6.4	103
33	Charge Parametrization of the D <sub>v</sub> H <sub>c</sub> <sub>3</sub> Heme Group: Validation Using Constant-(pH, $\epsilon$ ) Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2013, 117, 70-82.	2.6	24
34	A Catenane Assembled through a Single Charge-Assisted Halogen Bond. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 4356-4360.	13.8	83
35	Towards predictable transmembrane transport: QSAR analysis of anion binding and transport. <i>Chemical Science</i> , 2013, 4, 3036.	7.4	104
36	Increased Halide Recognition Strength by Enhanced Intercomponent Preorganisation in Triazolium Containing [2]Rotaxanes. <i>Chemistry - A European Journal</i> , 2013, 19, 17751-17765.	3.3	17

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37	Unveiling the Mechanisms of Catalytic Oxidation Reactions Mediated by Oxo-Molybdenum Complexes: A Computational Overview. <i>Current Organic Chemistry</i> , 2012, 16, 65-72.	1.6	26
38	Ruthenium(II) Thiacrown Complexes Incorporating Noninnocent Redox Active Ligands: Synthesis, Electrochemical Properties, and Theoretical Studies. <i>Inorganic Chemistry</i> , 2012, 51, 10483-10494.	4.0	6
39	Tunable transmembrane chloride transport by bis-indolylureas. <i>Chemical Science</i> , 2012, 3, 1436.	7.4	53
40	Fluorescent Charge-Assisted Halogen-Bonding Macrocyclic Halo-Imidazolium Receptors for Anion Recognition and Sensing in Aqueous Media. <i>Journal of the American Chemical Society</i> , 2012, 134, 11533-11541.	13.7	199
41	A Halogen-Bonding Catenane for Anion Recognition and Sensing. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 1876-1880.	13.8	190
42	Anion templated assembly of [2]catenanes capable of chloride anion recognition in aqueous solvent media. <i>RSC Advances</i> , 2011, 1, 995.	3.6	20
43	Benzene and heterocyclic rings formation in cycloaddition reactions catalyzed by RuCp derivatives: DFT studies. <i>Inorganica Chimica Acta</i> , 2011, 374, 24-35.	2.4	21
44	Investigating the Imidazolium-Anion Interaction through the Anion-Templated Construction of Interpenetrated and Interlocked Assemblies. <i>Chemistry - A European Journal</i> , 2011, 17, 12955-12966.	3.3	30
45	Olefin Epoxidation Catalyzed by $\eta^5$ -Cyclopentadienyl Molybdenum Compounds: A Computational Study. <i>Organometallics</i> , 2010, 29, 303-311.	2.3	84
46	Molecular Dynamics Study of a Heteroditopic-Calix[4]diquinone-Assisted Transfer of KCl and Dopamine Through a Water-Chloroform Liquid-Liquid Interface. <i>Journal of Physical Chemistry B</i> , 2010, 114, 11173-11180.	2.6	10
47	Rotaxanes Capable of Recognising Chloride in Aqueous Media. <i>Chemistry - A European Journal</i> , 2010, 16, 13082-13094.	3.3	61
48	Halogen Bond Anion Templated Assembly of an Imidazolium Pseudorotaxane. <i>Angewandte Chemie - International Edition</i> , 2010, 49, 5322-5326.	13.8	147
49	Rigid ferrocenophane and its metal complexes with transition and alkaline-earth metal ions. <i>Polyhedron</i> , 2010, 29, 1697-1705.	2.2	2
50	Mapping the Mechanism of Nickel-Ferrophite Catalysed Methylation of Baylis-Hillman-Derived $S_N2$ Electrophiles. <i>European Journal of Organic Chemistry</i> , 2009, 2009, 898-903.	2.4	12
51	Synthesis and differentiation of $\Delta^2$ - and $\Delta^1$ -glycopolyporphyrin stereoisomers by electrospray tandem mass spectrometry. <i>Rapid Communications in Mass Spectrometry</i> , 2009, 23, 3478-3483.	1.5	9
52	$MoO_2Cl_2$ as a Novel Catalyst for C-P Bond Formation and for Hydrophosphonylation of Aldehydes. <i>Organometallics</i> , 2009, 28, 6206-6212.	2.3	74
53	Sulfate anion templated synthesis of a triply interlocked capsule. <i>Chemical Communications</i> , 2009, , 7134.	4.1	88
54	Expanding the role of oxo-molybdenum(vi) catalysts: a DFT interpretation of X-H activation leading to reduction or oxidation. <i>Dalton Transactions</i> , 2009, , 8155.	3.3	33

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55	Determination of gas-phase acidities of dimethylphenols: Combined experimental and theoretical study. <i>Journal of the American Society for Mass Spectrometry</i> , 2008, 19, 1590-1599.	2.8	7
56	Hydrogen activation by high-valent oxo-molybdenum(vi) and -rhenium(vii) and -(v) compounds. <i>Dalton Transactions</i> , 2008, , 1727.	3.3	80
57	[Re( $\eta$ -5-C <sub>5</sub> H <sub>5</sub> )(CO) <sub>3</sub> ]+Family of 17-Electron Compounds: Monomer/Dimer Equilibria and Other Reactions. <i>Journal of the American Chemical Society</i> , 2008, 130, 2692-2703.	13.7	69
58	Photoinduced bond cleavage in CH <sub>3</sub> ReO <sub>3</sub> : excited state dynamics. <i>New Journal of Chemistry</i> , 2008, 32, 1904.	2.8	6
59	Mixed Valence Creutz-Taube Ion Analogues Incorporating Thiocrowns: Synthesis, Structure, Physical Properties, and Computational Studies. <i>Inorganic Chemistry</i> , 2008, 47, 11633-11643.	4.0	17
60	Weak $\eta$ -2-Olefin Bonding in Palladium and Platinum Allyl Cationic Complexes Containing Chiral Monodentate Ligands with $\eta$ -Phenyl Methyl Amine Side Chains. <i>Organometallics</i> , 2008, 27, 2949-2958.	2.3	14
61	Catalyzing Aldehyde Hydrosilylation with a Molybdenum(VI) Complex: A Density Functional Theory Study. <i>Chemistry - A European Journal</i> , 2007, 13, 3934-3941.	3.3	72
62	Remote Metal-Arene $\pi$ Bonding in Organometallic Complexes: a DFT Study. <i>Collection of Czechoslovak Chemical Communications</i> , 2007, 72, 703-714.	1.0	3
63	Group 11 complexes with the bis(3,5-dimethylpyrazol-1-yl)methane ligand. How secondary bonds can influence the coordination environment of Ag(i): the role of coordinated water in [Ag <sub>2</sub> ( $\mu$ -L) <sub>2</sub> (OH <sub>2</sub> ) <sub>2</sub> ](OTf) <sub>2</sub> . <i>Dalton Transactions</i> , 2006, , 4104-4113.	3.3	33
64	Photochemistry of Methyltrioxorhenium Revisited: A DFT/TD-DFT and CASSCF/MS-CASPT2 Theoretical Study. <i>Organometallics</i> , 2006, 25, 5235-5241.	2.3	12
65	Olefin epoxidation with tert-butyl hydroperoxide catalyzed by MoO <sub>2</sub> X <sub>2</sub> L complexes: a DFT mechanistic study. <i>Dalton Transactions</i> , 2006, , 1383.	3.3	88
66	Electrochemical Oxidation of CoCp(CO) <sub>2</sub> : Radical-Substrate Reaction of a 17 e-/18 e-Pair and Production of a Unique Dimer Radical. <i>Journal of the American Chemical Society</i> , 2006, 128, 16587-16599.	13.7	57
67	Ring Slippage vs Charge Transfer in the Reductive Chemistry of [IndMo(CO) <sub>2</sub> ( $\eta$ -diimine)] <sup>+</sup> Cations. <i>Organometallics</i> , 2006, 25, 5223-5234.	2.3	11
68	Synthesis, Structural Characterization, and Theoretical Studies of Gold(I) and Gold(I)-Gold(III) Thiolate Complexes: A Quenching of Gold(I) Thiolate Luminescence. <i>Inorganic Chemistry</i> , 2006, 45, 1059-1068.	4.0	61
69	A DFT and MP2 study of luminescence of gold(I) complexes. <i>Inorganica Chimica Acta</i> , 2006, 359, 3617-3624.	2.4	18
70	Formation of pyridine from acetylenes and nitriles catalyzed by RuCpCl, CoCp, and RhCp derivatives - A computational mechanistic study. <i>Journal of Organometallic Chemistry</i> , 2006, 691, 4434-4445.	1.8	62
71	Synthesis and ligand properties towards gold and silver of the ferrocenylamidobenzimidazole ligand. <i>Journal of Organometallic Chemistry</i> , 2006, 691, 4181-4188.	1.8	10
72	New Polynuclear Mo-Fe Complexes with Ferrocenylamidobenzimidazole Ligands. <i>European Journal of Inorganic Chemistry</i> , 2006, 2006, 4096-4103.	2.0	9

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73	A new interpretation of the bonding properties and UV-vis spectra of $[M_3(CO)_6]_2$ clusters (M=Ru, Os): a TD-DFT study. <i>Comptes Rendus Chimie</i> , 2005, 8, 1477-1486.	0.5	9
74	Anodic Preparation of $[Re_2Cp_2(CO)_6]^{2+}$ : A Dimeric Dication that Provides the Powerful One-Electron Oxidant $[ReCp(CO)_3]^+$ . <i>Journal of the American Chemical Society</i> , 2005, 127, 15676-15677.	13.7	34
75	Synthesis and Theoretical Studies of a Double Helical Complex with the Ligand $4,4'$ -Bis(ferrocenyl)-2,2',6,6'-tetrakis(quinquepyridine). <i>European Journal of Inorganic Chemistry</i> , 2004, 3038-3047.	1.6	4
76	Structure, Characterization, and Metal-Complexation Properties of a New Tetraazamacrocyclic Ligand Containing Two Phenolic Pendant Arms. <i>Helvetica Chimica Acta</i> , 2004, 87, 2613-2628.	1.6	4
77	Low-Lying Excited States and Primary Photoproducts of $[Os_3(CO)_{10}(s-cis-L)]$ (L=Cyclohexa-1,3-diene.) <i>Journal of Physical Chemistry B</i> , 2004, 108, 10784-10791.	3.3	8
78	N-Salicylideneamino acidato complexes of oxovanadium(IV). The cysteine and penicillamine complexes. <i>Dalton Transactions</i> , 2004, , 2855.	3.3	24
79	Cyanide-isocyanide isomers in polynuclear complexes. Reactivity and theoretical studies. <i>Inorganica Chimica Acta</i> , 2003, 356, 297-307.	2.4	6
80	The H...H interaction in the solid state structure of $HMn(CO)_5$ . <i>CrystEngComm</i> , 2002, 4, 368-372.	2.6	11
81	T4 Lysozyme/Halobenzene: A Test System for Modeling Biomolecular Halogen Bonds. <i>Journal of Molecular Recognition</i> , 2004, 17, 100-105.	0	0
82	Photomodulation of ultrastable host-guest complexes in water and their application in light-controlled steroid release. <i>Organic Chemistry Frontiers</i> , 2014, 1, 100-105.	4.5	6