David Esteban

List of Publications by Year
in descending order

155 papers	6,646 citations	87843 38 h-index	71651 76 g-index
155 all docs	155 docs citations	155 times ranked	4951 citing authors

#	Article	IF	Citations
1	Nature of Ureaâˆ'Fluoride Interaction:â€‰ Incipient and Definitive Proton Transfer. Journal of the American Chemical Society, 2004, 126, 16507-16514.	6.6	790
2	What Anions Do to Nâˆ'H-Containing Receptors. Accounts of Chemical Research, 2006, 39, 343-353.	7.6	764
3	Why, on Interaction of Urea-Based Receptors with Fluoride, Beautiful Colors Develop. Journal of Organic Chemistry, 2005, 70, 5717-5720.	1.7	478
4	Urea vs. thiourea in anion recognition. Organic and Biomolecular Chemistry, 2005, 3, 1495-1500.	1.5	333
5	Anion-Induced Urea Deprotonation. Chemistry - A European Journal, 2005, 11, 3097-3104.	1.7	251
6	Some guidelines for the design of anion receptors. Coordination Chemistry Reviews, 2006, 250, 1451-1470.	9.5	239
7	Macrocyclic Receptor Exhibiting Unprecedented Selectivity for Light Lanthanides. Journal of the American Chemical Society, 2009, 131, 3331-3341.	6.6	128
8	Chiral receptors for phosphate ions. Organic and Biomolecular Chemistry, 2005, 3, 2632.	1.5	91
9	Lanthanide Complexes Based on a 1,7-Diaza-12-crown-4 Platform Containing Picolinate Pendants: A New Structural Entry for the Design of Magnetic Resonance Imaging Contrast Agents. Inorganic Chemistry, 2008, 47, 7840-7851.	1.9	83
10	Monopicolinate Cyclen and Cyclam Derivatives for Stable Copper(II) Complexation. Inorganic Chemistry, 2012, 51, 6916-6927.	1.9	82
11	Mn(II) compounds as an alternative to Gd-based MRI probes. Future Medicinal Chemistry, 2019, 11, 1461-1483.	1.1	81
12	Hyperfine Coupling Constants on Innerâ€Sphere Water Molecules of Gd^{III}â€Based MRI Contrast Agents. ChemPhysChem, 2012, 13, 3640-3650.	1.0	80
13	Lanthanide dota-like Complexes Containing a Picolinate Pendant: Structural Entry for the Design of Ln^{III}-Based Luminescent Probes. Inorganic Chemistry, 2011, 50, 4125-4141.	1.9	76
14	Lead(II) Thiocyanate Complexes with Bibracchial Lariat Ethers:â€‰ An X-ray and DFT Study. Inorganic Chemistry, 2005, 44, 2224-2233.	1.9	68
15	Understanding Stability Trends along the Lanthanide Series. Chemistry - A European Journal, 2014, 20, 3974-3981.	1.7	68
16	Lanthanide(III) Complexes with Ligands Derived from a Cyclen Framework Containing Pyridinecarboxylate Pendants. The Effect of Steric Hindrance on the Hydration Number. Inorganic Chemistry, 2012, 51, 2509-2521.	1.9	63
17	Metal-Enhanced H-Bond Donor Tendencies of Urea and Thiourea toward Anions:â€‰ Ditopic Receptors for Silver(I) Salts. Inorganic Chemistry, 2005, 44, 8690-8698.	1.9	62
18	Zn(ii), Cd(ii) and Pb(ii) complexation with pyridinecarboxylate containing ligands. Dalton Transactions, 2008, , 5754.	1.6	62

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19	Macrocyclic Receptor Showing Extremely High Sr(II)/Ca(II) and Pb(II)/Ca(II) Selectivities with Potential Application in Chelation Treatment of Metal Intoxication. Inorganic Chemistry, 2011, 50, 3772-3784.	1.9	60
20	Electronic Structure Study of Seven-Coordinate First-Row Transition Metal Complexes Derived from 1,10-Diaza-15-crown-5:Â A Successful Marriage of Theory with Experiment. Inorganic Chemistry, 2005, 44, 9704-9713.	1.9	57
21	Stable Mn²⁺, Cu²⁺ and Ln³⁺ complexes with cyclen-based ligands functionalized with picolinate pendant arms. Dalton Transactions, 2015, 44, 5017-5031.	1.6	55
22	Stability, Water Exchange, and Anion Binding Studies on Lanthanide(III) Complexes with a Macrocyclic Ligand Based on 1,7-Diaza-12-crown-4: Extremely Fast Water Exchange on the Gd³⁺ Complex. Inorganic Chemistry, 2009, 48, 8878-8889.	1.9	54
23	Density functional dependence of molecular geometries in lanthanide(III) complexes relevant to bioanalytical and biomedical applications. Computational and Theoretical Chemistry, 2012, 999, 93-104.	1.1	54
24	Lanthanide(III) Complexes with a Reinforced Cyclam Ligand Show Unprecedented Kinetic Inertness. Journal of the American Chemical Society, 2014, 136, 17954-17957.	6.6	53
25	Lone-Pair Activity in Lead(II) Complexes with Unsymmetrical Lariat Ethers. Inorganic Chemistry, 2006, 45, 5407-5416.	1.9	52
26	Applications of Density Functional Theory (DFT) to Investigate the Structural, Spectroscopic and Magnetic Properties of Lanthanide(III) Complexes. Current Inorganic Chemistry, 2011, 1, 91-116.	0.2	51
27	Characterisation of magnetic resonance imaging (MRI) contrast agents using NMR relaxometry. Molecular Physics, 2019, 117, 898-909.	0.8	50
28	A two-channel chemosensor for the optical detection of carboxylic acids, including cholic acid. Journal of Materials Chemistry, 2005, 15, 2670.	6.7	49
29	17O and 1H relaxometric and DFT study of hyperfine coupling constants in [Mn(H2O)6]2+. RSC Advances, 2014, 4, 7094.	1.7	49
30	Hyperfine Coupling Constants on Inner-Sphere Water Molecules of a Triazacyclononane-based Mn(II) Complex and Related Systems Relevant as MRI Contrast Agents. Inorganic Chemistry, 2013, 52, 11173-11184.	1.9	47
31	Magnetic Anisotropies in Rhombic Lanthanide(III) Complexes Do Not Conform to Bleaneyâ€™s Theory. Inorganic Chemistry, 2016, 55, 3490-3497.	1.9	46
32	Lead(II) Complexes with Macrocyclic Receptors Derived from 4,13-Diaza-18-crown-6. Inorganic Chemistry, 2002, 41, 4337-4347.	1.9	45
33	Seven-Coordination versus Six-Coordination in Divalent First-Row Transition-Metal Complexes Derived from 1,10-Diaza-15-crown-5. Inorganic Chemistry, 2007, 46, 8271-8282.	1.9	43
34	Solution Structure of Ln(III) Complexes with Macrocyclic Ligands Through Theoretical Evaluation of ¹H NMR Contact Shifts. Inorganic Chemistry, 2012, 51, 13419-13429.	1.9	41
35	Developing the family of picolinate ligands for Mn²⁺ complexation. Dalton Transactions, 2017, 46, 1546-1558.	1.6	41
36	Water exchange in lanthanide complexes for MRI applications. Lessons learned over the last 25 years. Dalton Transactions, 2019, 48, 11161-11180.	1.6	41

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37	Mono-, Bi-, and Trinuclear Bis-Hydrated Mn²⁺ Complexes as Potential MRI Contrast Agents. Inorganic Chemistry, 2015, 54, 9576-9587.	1.9	40
38	Definition of an Intramolecular Euâ€toâ€Eu Energy Transfer within a Discrete [Eu₂L] Complex in Solution. Chemistry - A European Journal, 2012, 18, 8163-8173.	1.7	39
39	Stabilizing Divalent Europium in Aqueous Solution Using Size-Discrimination and Electrostatic Effects. Inorganic Chemistry, 2015, 54, 4940-4952.	1.9	39
40	Cadmium(II) and Lead(II) Complexes with Novel Macrocyclic Receptors Derived from 1,10-Diaza-15-crown-5. European Journal of Inorganic Chemistry, 2000, 2000, 1445-1456.	1.0	36
41	Barium Templating Schiff-Base Lateral Macrobicycles. Inorganic Chemistry, 1999, 38, 1937-1944.	1.9	35
42	Reasons behind the Relative Abundances of Heptacoordinate Complexes along the Late First-Row Transition Metal Series. Inorganic Chemistry, 2014, 53, 12859-12869.	1.9	35
43	Eight-Coordinate Zn(II), Cd(II), and Pb(II) Complexes Based on a 1,7-Diaza-12-crown-4 Platform Endowed with a Remarkable Selectivity over Ca(II). Inorganic Chemistry, 2009, 48, 11821-11831.	1.9	34
44	Taking the next step toward inert Mn²⁺ complexes of open-chain ligands: the case of the rigid PhDTA ligand. New Journal of Chemistry, 2018, 42, 8001-8011.	1.4	34
45	Complexation of Mn(II) by Rigid Pyclen Diacetates: Equilibrium, Kinetic, Relaxometric, Density Functional Theory, and Superoxide Dismutase Activity Studies. Inorganic Chemistry, 2021, 60, 1133-1148.	1.9	34
46	Templating Schiff-Base Lateral Macrobicycles:â€‰ An Experimental and Theoretical Structural Study of the Intermediates. Inorganic Chemistry, 2003, 42, 4299-4307.	1.9	33
47	Molecular Recognition of Sialic Acid by Lanthanide(III) Complexes through Cooperative Two-Site Binding. Inorganic Chemistry, 2010, 49, 4212-4223.	1.9	33
48	Lanthanide Complexes Based on a Diazapyridinophane Platform Containing Picolinate Pendants. Inorganic Chemistry, 2012, 51, 10893-10903.	1.9	33
49	Expanding the Family of Pyclen-Based Ligands Bearing Pendant Picolinate Arms for Lanthanide Complexation. Inorganic Chemistry, 2018, 57, 6932-6945.	1.9	33
50	Copper complexes with bibracchial lariat ethers: from mono- to binuclear structures. Inorganica Chimica Acta, 2001, 317, 190-198.	1.2	32
51	Approaching the Kinetic Inertness of Macrocyclic Gadolinium(III)â€Based MRI Contrast Agents with Highly Rigid Openâ€Chain Derivatives. Chemistry - A European Journal, 2016, 22, 896-901.	1.7	31
52	Structure and Dynamics of Lanthanide(III) Complexes with an N-Alkylated do3a Ligand (H3do3a =) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 Journal of Inorganic Chemistry, 2010, 2010, 3586-3595.	1.0	30
53	Metalâ€“Organic Self-Assembled Trefoil Knots for Câ€”Br Bond Activation. ACS Catalysis, 2019, 9, 1907-1914.	5.5	30
54	The effect of ring size variation on the structure and stability of lanthanide(<scp>iii</scp>) complexes with crown ethers containing picolinate pendants. Dalton Transactions, 2011, 40, 384-392.	1.6	29

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55	Cooperative Anion Recognition in Copper(II) and Zinc(II) Complexes with a Ditopic Tripodal Ligand Containing a Urea Group. Inorganic Chemistry, 2014, 53, 2554-2568.	1.9	29
56	Gd3+-Based Magnetic Resonance Imaging Contrast Agent Responsive to Zn2+. Inorganic Chemistry, 2015, 54, 10342-10350.	1.9	29
57	Towards Selective Recognition of Sialic Acid Through Simultaneous Binding to Its <i>cis</i>â€Diol and Carboxylate Functions. European Journal of Organic Chemistry, 2010, 2010, 3237-3248.	1.2	28
58	Highly relaxing gadolinium based MRI contrast agents responsive to Mg2+ sensing. Chemical Communications, 2012, 48, 4085.	2.2	28
59	Optimising the relaxivities of Mn²⁺ complexes by targeting human serum albumin (HSA). Dalton Transactions, 2017, 46, 8494-8504.	1.6	27
60	Complexation of Ln³⁺ Ions with Cyclam Dipicolinates: A Small Bridge that Makes Huge Differences in Structure, Equilibrium, and Kinetic Properties. Inorganic Chemistry, 2016, 55, 2227-2239.	1.9	26
61	Enantiomeric Recognition of <scp>d</scp>- and <scp>l</scp>-Lactate by CEST with the Aid of a Paramagnetic Shift Reagent. Journal of the American Chemical Society, 2017, 139, 17431-17437.	6.6	26
62	The role of ligand to metal charge-transfer states on the luminescence of Europium complexes with 18-membered macrocyclic ligands. Dalton Transactions, 2019, 48, 4035-4045.	1.6	26
63	High Relaxivity Mn²⁺â€Based MRI Contrast Agents. Chemistry - A European Journal, 2014, 20, 17300-17305.	1.7	25
64	Importance of Outerâ€Sphere and Aggregation Phenomena in the Relaxation Properties of Phosphonated Gadolinium Complexes with Potential Applications as MRI Contrast Agents. Chemistry - A European Journal, 2015, 21, 6535-6546.	1.7	25
65	Stable and Inert Yttrium(III) Complexes with Pyclen-Based Ligands Bearing Pendant Picolinate Arms: Toward New Pharmaceuticals for Î²-Radiotherapy. Inorganic Chemistry, 2018, 57, 2051-2063.	1.9	25
66	Lanthanide Complexes with 1H paraCEST and 19F Response for Magnetic Resonance Imaging Applications. Inorganic Chemistry, 2019, 58, 7571-7583.	1.9	25
67	Understanding the Optical and Magnetic Properties of Ytterbium(III) Complexes. Inorganic Chemistry, 2019, 58, 3732-3743.	1.9	25
68	Definition of the Labile Capping Bond Effect in Lanthanide Complexes. Chemistry - A European Journal, 2017, 23, 1110-1117.	1.7	24
69	Lateral Macrobicyclic Architectures:Â Toward New Lead(II) Sequestering Agents. Inorganic Chemistry, 2005, 44, 5428-5436.	1.9	23
70	1,4,7â€Triazacyclononaneâ€Based Bifunctional Picolinate Ligands for Efficient Copper Complexation. European Journal of Inorganic Chemistry, 2017, 2017, 2435-2443.	1.0	23
71	The role of the capping bond effect on pyclen ^{nat}Y³⁺/⁹⁰Y³⁺ chelates: full control of the regiospecific N-functionalization makes the difference. Chemical Communications, 2017, 53, 9534-9537.	2.2	23
72	Metal Ion Complementarity: Effect of Ring-Size Variation on the Conformation and Stability of Lead(II) and Cadmium(II) Complexes with Pendant-Armed Crowns. European Journal of Inorganic Chemistry, 2007, 2007, 2198-2207.	1.0	22

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73	A Coordination Chemistry Approach to Fineâ€Tune the Physicochemical Parameters of Lanthanide Complexes Relevant to Medical Applications. Chemistry - A European Journal, 2018, 24, 3127-3131.	1.7	22
74	Reinforced Ni(<scp>ii</scp>)-cyclam derivatives as dual¹H/¹⁹F MRI probes. Chemical Communications, 2019, 55, 4115-4118.	2.2	22
75	Protonated Macrobicyclic Hosts Containing Pyridine Head Units for Anion Recognition. Chemistry - A European Journal, 2008, 14, 5829-5838.	1.7	21
76	Selective Chelation of Cd(II) and Pb(II) versus Ca(II) and Zn(II) by Using Octadentate Ligands Containing Pyridinecarboxylate and Pyridyl Pendants. Inorganic Chemistry, 2009, 48, 10976-10987.	1.9	21
77	Exceptionally Inert Lanthanide(III) PARACEST MRI Contrast Agents Based on an 18â€Membered Macrocyclic Platform. Chemistry - A European Journal, 2015, 21, 18662-18670.	1.7	21
78	Methylthiazolyl Tacn Ligands for Copper Complexation and Their Bifunctional Chelating Agent Derivatives for Bioconjugation and Copper-64 Radiolabeling: An Example with Bombesin. Inorganic Chemistry, 2019, 58, 2669-2685.	1.9	21
79	Gadolinium(III)â€Based Dual ¹H/¹⁹F Magnetic Resonance Imaging Probes. Chemistry - A European Journal, 2019, 25, 4782-4792.	1.7	21
80	Selfâ€Aggregated Dinuclear Lanthanide(III) Complexes as Potential Bimodal Probes for Magnetic Resonance and Optical Imaging. Chemistry - A European Journal, 2013, 19, 11696-11706.	1.7	19
81	Transient versus Static Electron Spin Relaxation in Mn²⁺ Complexes Relevant as MRI Contrast Agents. Journal of Physical Chemistry A, 2016, 120, 6467-6476.	1.1	19
82	On the consequences of the stereochemical activity of the Bi(<scp>iii</scp>) 6s² lone pair in cyclen-based complexes. The [Bi(DO3A)] case. Dalton Transactions, 2018, 47, 13830-13842.	1.6	19
83	Coordination Properties of GdDO3A-Based Model Compounds of Bioresponsive MRI Contrast Agents. Inorganic Chemistry, 2018, 57, 5973-5986.	1.9	18
84	Accelerating water exchange in Gd^{III}â€“DO3A-derivatives by favouring the dissociative mechanism through hydrogen bonding. Chemical Communications, 2019, 55, 513-516.	2.2	18
85	Controlling water exchange rates in potential Mn2+-based MRI agents derived from NO2A2âˆ. Dalton Transactions, 2019, 48, 3962-3972.	1.6	18
86	Effect of Protonation and Interaction with Anions on a Lead(II) Complex with a Lateral Macrobicycle Containing a Phenol Schiff-Base Spacer. European Journal of Inorganic Chemistry, 2007, 2007, 1635-1643.	1.0	17
87	Spectrally Undiscerned Isomers Might Lead to Erroneous Determination of Water Exchange Rates of paraCEST Eu(III) Agents. Inorganic Chemistry, 2017, 56, 7737-7745.	1.9	17
88	Chapter 2. Gadolinium-based Contrast Agents. New Developments in NMR, 2017, , 121-242.	0.1	17
89	Macrocyclic Receptor Showing Improved Pb^{II}/Zn^{II} and Pb^{II}/Ca^{II} Selectivities. European Journal of Inorganic Chemistry, 2010, 2010, 2495-2503.	1.0	16
90	The Relationship between NMR Chemical Shifts of Thermally Polarized and Hyperpolarized ⁸⁹Y Complexes and Their Solution Structures. Chemistry - A European Journal, 2016, 22, 16657-16667.	1.7	16

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91	Ditopic receptors containing urea groups for solvent extraction of Cu(<scp>ii</scp>) salts. Dalton Transactions, 2017, 46, 3192-3206.	1.6	16
92	Recognition of AMP, ADP and ATP through Cooperative Binding by Cu(II) and Zn(II) Complexes Containing Urea and/or Phenylboronicâ€"Acid Moieties. Molecules, 2018, 23, 479.	1.7	16
93	Combined NMR, DFT and X-ray studies highlight structural and hydration changes of [Ln(AAZTA)]^{â^ˆ’} complexes across the series. Inorganic Chemistry Frontiers, 2020, 7, 795-803.	3.0	16
94	Unexpected Trends in the Stability and Dissociation Kinetics of Lanthanide(III) Complexes with Cyclen-Based Ligands across the Lanthanide Series. Inorganic Chemistry, 2020, 59, 8184-8195.	1.9	15
95	Highly Stable Complexes of Divalent Metal Ions (Mg²⁺, Ca²⁺,) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 Containing a Picolinate Pendant. European Journal of Inorganic Chemistry, 2014, 2014, 6165-6173.	1.0	14
96	Sulphur-rich functionalized calix[4]arenes for selective complexation of Hg²⁺over Cu²⁺, Zn²⁺and Cd²⁺. Dalton Transactions, 2016, 45, 15211-15224.	1.6	14
97	Toward inert paramagnetic Ni(<scp>ii</scp>)-based chemical exchange saturation transfer MRI agents. Dalton Transactions, 2017, 46, 15095-15106.	1.6	14
98	Inert macrocyclic Eu³⁺ complex with affirmative paraCEST features. Inorganic Chemistry Frontiers, 2020, 7, 2274-2286.	3.0	14
99	Paramagnetic chemical exchange saturation transfer agents and their perspectives for application in magnetic resonance imaging. International Reviews in Physical Chemistry, 2021, 40, 51-79.	0.9	14
100	Designing binuclear transition metal complexes: a new example of the versatility of N,Nâ€²-bis(2-aminobenzyl)-4,13-diaza-18-crown-6. Dalton Transactions, 2005, , 2031.	1.6	13
101	Anion Coordination Effect on the Nuclearity of CoII, NiII, CuII, and ZnIIComplexes with a Benzimidazole Pendant-Armed Crown. European Journal of Inorganic Chemistry, 2009, 2009, 400-411.	1.0	13
102	Dimer formation of GdDO3A-arylsulfonamide complexes causes loss of pH-dependency of relaxivity. Dalton Transactions, 2017, 46, 16828-16836.	1.6	13
103	Steric Effects on the Binding of Phosphate and Polyphosphate Anions by Zinc(II) and Copper(II) Dinuclear Complexes of <i>m</i>-Xylyl-bis-cyclen. Inorganic Chemistry, 2018, 57, 6466-6478.	1.9	13
104	Synthesis and structural characterisation of lead(II) isothiocyanate complexes with receptors derived from 1,10-diaza-15-crown-5. Polyhedron, 2003, 22, 2709-2717.	1.0	12
105	Modulating the DNA cleavage ability of copper(<scp>ii</scp>) Schiff bases through ternary complex formation. New Journal of Chemistry, 2018, 42, 15170-15183.	1.4	12
106	Long Wavelength Excitation of Europium Luminescence in Extended, Carboline-Based Cryptates. Inorganic Chemistry, 2018, 57, 7390-7401.	1.9	12
107	Pyclen-Based Ligands Bearing Pendant Picolinate Arms for Gadolinium Complexation. Inorganic Chemistry, 2021, 60, 2390-2405.	1.9	12
108	Receptor versus Counterion: Capability ofN,Nâ€²-Bis(2-aminobenzyl)-diazacrowns for Giving Endo- and/or Exocyclic Coordination of ZnII. European Journal of Inorganic Chemistry, 2007, 2007, 1874-1883.	1.0	11

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109	A pentadentate member of the picolinate family for Mn(ii) complexation and an amphiphilic derivative. Dalton Transactions, 2019, 48, 696-710.	1.6	11
110	PIDAZTA: Structurally Constrained Chelators for the Efficient Formation of Stable Galliumâ€68 Complexes at Physiological pH. Chemistry - A European Journal, 2019, 25, 10698-10709.	1.7	11
111	Understanding the Effect of the Electron Spin Relaxation on the Relaxivities of Mn(II) Complexes with Triazacyclononane Derivatives. Inorganic Chemistry, 2021, 60, 15055-15068.	1.9	11
112	Rigidified Derivative of the Non-macrocyclic Ligand H₄OCTAPA for Stable Lanthanide(III) Complexation. Inorganic Chemistry, 2022, 61, 5157-5171.	1.9	11
113	Barium(II) thiocyanate templating Schiff-base lateral macrobicycles derived from 1,10-diaza-15-crown-5. Polyhedron, 2005, 24, 289-294.	1.0	10
114	Lead(II) Complexes of Lateral Macrobicyclic Receptors That Incorporate a Crown Moiety and a Pyridine Head Unit. European Journal of Inorganic Chemistry, 2010, 2010, 5027-5034.	1.0	10
115	A merged experimental and theoretical conformational study on alkaline-earth complexes with lariat ethers derived from 4,13-diaza-18-crown-6. Inorganica Chimica Acta, 2011, 370, 270-278.	1.2	10
116	Gadolinium Complexes of Highly Rigid, Open-Chain Ligands Containing a Cyclobutane Ring in the Backbone: Decreasing Ligand Denticity Might Enhance Kinetic Inertness. Inorganic Chemistry, 2019, 58, 13170-13183.	1.9	10
117	Mn2+ Complexes Containing Sulfonamide Groups with pH-Responsive Relaxivity. Inorganic Chemistry, 2020, 59, 14306-14317.	1.9	10
118	Complexation of <i>C</i>-Functionalized Cyclams with Copper(II) and Zinc(II): Similarities and Changes When Compared to Parent Cyclam Analogues. Inorganic Chemistry, 2021, 60, 10857-10872.	1.9	10
119	Tuning the copper(<scp>ii</scp>) coordination properties of cyclam by subtle chemical modifications. Dalton Transactions, 2017, 46, 11479-11490.	1.6	9
120	Phosphate and polyphosphate anion recognition by a dinuclear copper(<scp>ii</scp>) complex of an unsymmetrical squaramide. Dalton Transactions, 2019, 48, 10104-10115.	1.6	9
121	Axial Ligation in Ytterbium(III) DOTAM Complexes Rationalized with Multireference and Ligand-Field ab Initio Calculations. Journal of Physical Chemistry A, 2020, 124, 1362-1371.	1.1	9
122	Prediction of Gd(III) complex thermodynamic stability. Coordination Chemistry Reviews, 2022, 467, 214606.	9.5	9
123	Spectroscopic Properties of a Family of Mono- to Trinuclear Lanthanide Complexes. European Journal of Inorganic Chemistry, 2017, 2017, 2122-2129.	1.0	8
124	Effects of the substituents of pyrazole/thiazine ligands on the magnetic properties of chloro-bridged Cu(<scp>ii</scp>) complexes. New Journal of Chemistry, 2017, 41, 8818-8827.	1.4	8
125	Highly Stable and Inert Complexation of Indium(III) by Reinforced Cyclam Dipicolinate and a Bifunctional Derivative for Bead Encoding in Mass Cytometry. Chemistry - A European Journal, 2019, 25, 15387-15400.	1.7	8
126	pHâ€Dependent Hydration Change in a Gdâ€Based MRI Contrast Agent with a Phosphonated Ligand. Chemistry - A European Journal, 2020, 26, 5407-5418.	1.7	8

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127	Binuclear Co(II), Ni(II), Cu(II) and Zn(II) complexes with Schiff-bases derived from crown ether platforms: Rare examples of ether oxygen atoms bridging metal centers. Polyhedron, 2010, 29, 2269-2277.	1.0	7
128	<i>endo</i>- <i>versus exo</i>-Cyclic coordination in copper complexes with methylthiazolylcarboxylate tacn derivatives. Dalton Transactions, 2019, 48, 8740-8755.	1.6	7
129	Expanding the Ligand Classes Used for Mn(II) Complexation: Oxa-aza Macrocycles Make the Difference. Molecules, 2021, 26, 1524.	1.7	7
130	Stable and inert macrocyclic cobalt(<scp>ii</scp>) and nickel(<scp>ii</scp>) complexes with paraCEST response. Dalton Transactions, 2022, 51, 1580-1593.	1.6	7
131	Lead(II) Complexes with Macrocyclic Receptors Derived from 4,13-Diaza-18-crown-6. Inorganic Chemistry, 2002, 41, 7170-7170.	1.9	6
132	Synthesis and crystal structure of manganese(II) complexes with high-denticity ligands derived from azacrowns. Polyhedron, 2007, 26, 4141-4146.	1.0	6
133	Conformational study of lanthanide(III) complexes of N-(2-salicylaldiminatobenzyl)-1-aza-18-crown-6 by using X-ray and ab initio methods. Polyhedron, 2008, 27, 1415-1422.	1.0	6
134	Ditopic binuclear copper(II) complexes for DNA cleavage. Journal of Inorganic Biochemistry, 2020, 205, 110995.	1.5	6
135	Hydrothermal synthesis of six new lanthanides coordination polymers based on 1-H-benzimidazole-5-carboxylic acid: Structure, Hirshfeld analysis, thermal and spectroscopic properties. Inorganica Chimica Acta, 2020, 510, 119740.	1.2	6
136	Versatile Macrocyclic Platform for the Complexation of [^{nat}Y/⁹⁰Y]Yttrium and Lanthanide Ions. Inorganic Chemistry, 2022, 61, 6209-6222.	1.9	6
137	Water exchange rates and mechanisms in tetrahedral [Be(H₂O)₄]²⁺ and [Li(H₂O)₄]⁺ complexes using DFT methods and clusterâ€continuum models. International Journal of Quantum Chemistry, 2016, 116, 1388-1396.	1.0	5
138	Electronic<i>versus</i>steric control in palladium complexes of carboranyl phosphine-iminophosphorane ligands. Dalton Transactions, 2019, 48, 486-503.	1.6	5
139	Lanthanide(III) Complexes Based on an 18-Membered Macrocycle Containing Acetamide Pendants. Structural Characterization and paraCEST Properties. Inorganic Chemistry, 2021, 60, 1902-1914.	1.9	5
140	Scrutinising the role of intramolecular hydrogen bonding in water exchange dynamics of Gd(<scp>iii</scp>) complexes. Dalton Transactions, 2021, 50, 5506-5518.	1.6	5
141	Rigid versions of PDTA^{4âˆ’} incorporating a 1,3-diaminocyclobutyl spacer for Mn²⁺ complexation: stability, water exchange dynamics and relaxivity. Dalton Transactions, 2021, 50, 16290-16303.	1.6	5
142	A Schiff base lateral macrobicycle derived from 4,13-diaza-18-crown-6 in its protonated form. Acta Crystallographica Section C: Crystal Structure Communications, 2005, 61, o92-o94.	0.4	4
143	Solid state and solution structures of alkaline-earth complexes with lariat ethers containing aniline and benzimidazole pendants. Polyhedron, 2012, 31, 402-412.	1.0	4
144	â€œCinderellaâ€•elements: Strategies to increase the stability of group 1 complexes by tailoring crown macrocycles. Inorganica Chimica Acta, 2014, 417, 155-162.	1.2	4

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145	Synthesis and Characterization of Positively Charged <i>tris</i>â€imidazolium Calix[6]arene Hosts for Anion Recognition. ChemistrySelect, 2019, 4, 321-328.	0.7	4
146	Macrocyclic Pyclen-Based Gd3+ Complex with High Relaxivity and pH Response. Inorganic Chemistry, 2020, 59, 7306-7317.	1.9	4
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