## Christopher A Hunter

List of Publications by Year in descending order

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	13827	7931
24,131	67	149
citations	h-index	g-index
250	250	10000
259	259	18233
docs citations	times ranked	citing authors
	citations 259	24,131 67 citations h-index 259 259

#	Article	IF	CITATIONS
1	The nature of .pipi. interactions. Journal of the American Chemical Society, 1990, 112, 5525-5534.	6.6	4,972
2	Aromatic interactions. Perkin Transactions II RSC, 2001, , 651-669.	1.1	1,189
3	Quantifying Intermolecular Interactions: Guidelines for the Molecular Recognition Toolbox. Angewandte Chemie - International Edition, 2004, 43, 5310-5324.	7.2	928
4	Meldola Lecture. The role of aromatic interactions in molecular recognition. Chemical Society Reviews, 1994, 23, 101.	18.7	873
5	What is Cooperativity?. Angewandte Chemie - International Edition, 2009, 48, 7488-7499.	7.2	714
6	Ï€-Ï€ interactions: the geometry and energetics of phenylalanine-phenylalanine interactions in proteins. Journal of Molecular Biology, 1991, 218, 837-846.	2.0	616
7	Sequence-dependent DNA Structure. Journal of Molecular Biology, 1993, 230, 1025-1054.	2.0	438
8	Synthesis and structure elucidation of a new [2]-catenane. Journal of the American Chemical Society, 1992, 114, 5303-5311.	6.6	434
9	Molecular Transformer: A Model for Uncertainty-Calibrated Chemical Reaction Prediction. ACS Central Science, 2019, 5, 1572-1583.	5.3	424
10	Arene—Arene Interactions: Electrostatic or Charge Transfer?. Angewandte Chemie International Edition in English, 1993, 32, 1584-1586.	4.4	368
11	Highly efficient catalysis of the Kemp elimination in the cavity of a cubic coordination cage. Nature Chemistry, 2016, 8, 231-236.	6.6	364
12	Supramolecular topology. Tetrahedron, 1999, 55, 5265-5293.	1.0	290
13	Electrostatic Control of Aromatic Stacking Interactions. Journal of the American Chemical Society, 2005, 127, 8594-8595.	6.6	287
14	Dabco-metalloporphyrin binding: ternary complexes, host-guest chemistry and the measurement of .pipi. interactions. Journal of the American Chemical Society, 1990, 112, 5773-5780.	6.6	281
15	Chemical double-mutant cycles: dissecting non-covalent interactions. Chemical Society Reviews, 2007, 36, 172-188.	18.7	264
16	Virtual cocrystal screening. Chemical Science, 2011, 2, 883.	3.7	245
17	Substituent effects on aromatic stacking interactions. Organic and Biomolecular Chemistry, 2007, 5, 1062.	1.5	221
18	Self-Assembled Porphyrin Polymers. Angewandte Chemie - International Edition, 2000, 39, 764-767.	7.2	210

#	Article	IF	CITATIONS
19	Sequence-dependent DNA structure: tetranucleotide conformational maps. Journal of Molecular Biology, 2000, 295, 85-103.	2.0	199
20	Coordination Cages Based on Bis(pyrazolylpyridine) Ligands: Structures, Dynamic Behavior, Guest Binding, and Catalysis. Accounts of Chemical Research, 2018, 51, 2073-2082.	7.6	194
21	Thermodynamics of induced-fit binding inside polymacrocyclic porphyrin hosts. Journal of the American Chemical Society, 1990, 112, 5780-5789.	6.6	182
22	Solvent Effects on Hydrogen Bonding. Angewandte Chemie - International Edition, 2007, 46, 3706-3709.	7.2	179
23	Hydrogen bonding vs. halogen bonding: the solvent decides. Chemical Science, 2017, 8, 5392-5398.	3.7	176
24	Photoinduced Energy and Electron Transfer in Supramolecular Porphyrin Assemblies. Angewandte Chemie International Edition in English, 1996, 35, 1936-1939.	4.4	172
25	Self-Assembly of a Dimeric Porphyrin Host. Angewandte Chemie International Edition in English, 1994, 33, 2313-2316.	4.4	171
26	Synthesis and Recognition Properties of Aromatic Amide Oligomers:  Molecular Zippers. Journal of the American Chemical Society, 2000, 122, 8856-8868.	6.6	162
27	Chemical Double-Mutant Cycles for the Measurement of Weak Intermolecular Interactions: Edge-to-Face Aromatic Interactions. Angewandte Chemie International Edition in English, 1996, 35, 1542-1544.	4.4	158
28	An AAAA–DDDD quadruple hydrogen-bond array. Nature Chemistry, 2011, 3, 244-248.	6.6	155
29	Non-covalent interactions between iodo-perfluorocarbons and hydrogen bond acceptors. Chemical Communications, 2009, , 2005.	2.2	154
30	Synthesis of a molecular trefoil knot by folding and closing on an octahedral coordination template. Nature Chemistry, 2010, 2, 218-222.	6.6	150
31	Sequence-dependent DNA structure: dinucleotide conformational maps. Journal of Molecular Biology, 2000, 295, 71-83.	2.0	148
32	Cooperative Interactions in a Ternary Mixture. Chemistry - A European Journal, 1998, 4, 845-851.	1.7	143
33	A Binary Quinone Receptor. Angewandte Chemie International Edition in English, 1992, 31, 792-795.	4.4	133
34	Exciton coupling in porphyrin dimers. Chemical Physics, 1989, 133, 395-404.	0.9	125
35	A solvent-resistant halogen bond. Chemical Science, 2014, 5, 4179-4183.	3.7	122
36	Substituent effects on cation-Â interactions: A quantitative study. Proceedings of the National Academy of Sciences of the United States of America, 2002, 99, 4873-4876.	3.3	120

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37	pH-dependent binding of guests in the cavity of a polyhedral coordination cage: reversible uptake and release of drug molecules. Chemical Science, 2015, 6, 625-631.	3.7	120
38	Substituent Effects on Edge-to-Face Aromatic Interactions. Chemistry - A European Journal, 2002, 8, 2847.	1.7	118
39	H-Bond Acceptor Parameters for Anions. Journal of the American Chemical Society, 2017, 139, 6700-6706.	6.6	116
40	DNA base-stacking interactions: a comparison of theoretical calculations with oligonucleotide X-ray crystal structures. Journal of Molecular Biology, 1997, 265, 603-619.	2.0	114
41	Desolvation tips the balance: solvent effects on aromatic interactions. Chemical Communications, 2006, , 3806.	2.2	110
42	Self-Assembly of Oligomeric Porphyrin Rings. Organic Letters, 2000, 2, 2435-2438.	2.4	109
43	Molecular Acrobatics:Â Self-Assembly of Calixarene-Porphyrin Cages. Journal of the American Chemical Society, 2003, 125, 14181-14189.	6.6	109
44	The thermodynamics of self-assembly. Journal of the Chemical Society Chemical Communications, 1995, , 2563.	2.0	102
45	Quantification of solvent effects on molecular recognition in polyhedral coordination cage hosts. Chemical Science, 2013, 4, 2744.	3.7	102
46	Mapping the Internal Recognition Surface of an Octanuclear Coordination Cage Using Guest Libraries. Journal of the American Chemical Society, 2014, 136, 8475-8483.	6.6	101
47	Cooperative Binding at Lipid Bilayer Membrane Surfaces. Journal of the American Chemical Society, 2003, 125, 4593-4599.	6.6	97
48	DABCO-Induced Self-Assembly of a Trisporphyrin Double-Decker Cage:Â Thermodynamic Characterization and Guest Recognition. Journal of the American Chemical Society, 2006, 128, 5560-5569.	6.6	96
49	Validation of a Computational Cocrystal Prediction Tool: Comparison of Virtual and Experimental Cocrystal Screening Results. Crystal Growth and Design, 2014, 14, 165-171.	1.4	96
50	Sequence-dependent DNA structure: the role of the sugar-phosphate backbone 1 1Edited by T. Richmond. Journal of Molecular Biology, 1998, 280, 407-420.	2.0	93
51	Knot tied around an octahedral metal centre. Nature, 2001, 411, 763-763.	13.7	91
52	Self-assembly of macrocyclic porphyrin oligomers. Journal of the Chemical Society Chemical Communications, 1995, , 2567.	2.0	90
53	Quantitative Determination of Intermolecular Interactions with Fluorinated Aromatic Rings. Chemistry - A European Journal, 2001, 7, 3494.	1.7	90
54	DABCO-Directed Self-Assembly of Bisporphyrins (DABCO=1,4-Diazabicyclo[2.2.2]octane). Chemistry - A European Journal, 2005, 11, 2196-2206.	1.7	88

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55	Halogen Bonded Supramolecular Assemblies of [Ru(bipy)(CN) <sub>4</sub> ] <sup>2â^'</sup> Anions and <i>N</i> -Methyl-Halopyridinium Cations in the Solid State and in Solution. Inorganic Chemistry, 2009, 48, 1666-1677.	1.9	86
56	A Supramolecular System for Quantifying Aromatic Stacking Interactions. Chemistry - A European Journal, 2001, 7, 4863-4877.	1.7	83
57	Accurate Length Control of Supramolecular Oligomerization:Â Vernier Assemblies. Journal of the American Chemical Society, 2006, 128, 8975-8979.	6.6	82
58	Molecular recognition of p-benzoquinone by a macrocyclic host. Journal of the Chemical Society Chemical Communications, 1991, , 749.	2.0	81
59	Directed macrocyclisation reactions. Journal of the Chemical Society Chemical Communications, 1994, , 1277.	2.0	78
60	An Evaluation of Force-Field Treatments of Aromatic Interactions. Chemistry - A European Journal, 2002, 8, 2860.	1.7	78
61	Controlled membrane translocation provides a mechanism for signal transduction and amplification. Nature Chemistry, 2017, 9, 426-430.	6.6	78
62	Molecular Zippers. Journal of the American Chemical Society, 1994, 116, 10292-10293.	6.6	76
63	Shape-, Size-, and Functional Group-Selective Binding of Small Organic Guests in a Paramagnetic Coordination Cage. Inorganic Chemistry, 2013, 52, 1122-1132.	1.9	75
64	Complexation-Induced Changes in1H NMR Chemical Shift for Supramolecular Structure Determination. Chemistry - A European Journal, 1999, 5, 1891-1897.	1.7	73
65	Cooperativity, Partially Bound States, and Enthalpy-Entropy Compensation. Chemistry and Biology, 2003, 10, 1023-1032.	6.2	72
66	A 1H NMR study of crystal nucleation in solution. CrystEngComm, 2004, 6, 489.	1.3	70
67	Self-assembly of zinc aminoporphyrins. New Journal of Chemistry, 1999, 23, 309.	1.4	69
68	Influence of Solvent on Aromatic Interactions in Metal Tris-Bipyridine Complexes. Journal of the American Chemical Society, 1998, 120, 3402-3410.	6.6	66
69	Cooperativity in the self-assembly of porphyrin ladders. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 3034-3038.	3.3	65
70	Selective guest recognition by a self-assembled paramagnetic cage complex. Chemical Communications, 2012, 48, 2752.	2.2	65
71	Hydrogen-bond recognition of cyclic dipeptides in water. Chemical Communications, 1998, , 2449-2450.	2.2	63
72	The nucleation of inosine: the impact of solution chemistry on the appearance of polymorphic and hydrated crystal forms. Faraday Discussions, 2007, 136, 179.	1.6	63

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73	Structural consequences of a molecular assembly that is deficient in hydrogen-bond acceptors. Journal of the Chemical Society Chemical Communications, 1992, , 1134.	2.0	62
74	Transmembrane Signalling. Angewandte Chemie - International Edition, 2002, 41, 3878-3881.	7.2	61
75	Noncovalent Functionalâ€Group–Arene Interactions. Angewandte Chemie - International Edition, 2007, 46, 7823-7826.	7.2	61
76	How strong is a ï€-facial hydrogen bond?. Chemical Communications, 1996, , 2531-2532.	2.2	60
77	Structural and Photophysical Properties of Adducts of [Ru(bipy)(CN)4]2-with Different Metal Cations:Â Metallochromism and Its Use in Switching Photoinduced Energy Transfer. Journal of the American Chemical Society, 2007, 129, 4014-4027.	6.6	60
78	Desolvation and substituent effects in edge-to-face aromatic interactions. Chemical Communications, 2009, , 3961.	2.2	60
79	Sequence-dependent DNA Structure: A Database of Octamer Structural Parameters. Journal of Molecular Biology, 2003, 332, 1025-1035.	2.0	59
80	Wechselwirkungen zwischen aromatischen Systemen: Beruhen sie auf elektrostatischen Kräen oder Chargeâ€Transferâ€Ãœbergägen?. Angewandte Chemie, 1993, 105, 1653-1655.	1.6	58
81	Solvent effects of the structures of prenucleation aggregates of carbamazepine. CrystEngComm, 2012, 14, 7115.	1.3	58
82	[2]Catenane or not [2]catenane?. Journal of the Chemical Society Chemical Communications, 1995, , 809.	2.0	57
83	Experimental Measurement of Noncovalent Interactions Between Halogens and Aromatic Rings. ChemBioChem, 2004, 5, 657-665.	1.3	57
84	Relationship between Chemical Structure and Supramolecular Effective Molarity for Formation of Intramolecular H-Bonds. Journal of the American Chemical Society, 2013, 135, 13129-13141.	6.6	57
85	Quantification of the Effect of Conformational Restriction on Supramolecular Effective Molarities. Journal of the American Chemical Society, 2013, 135, 1853-1863.	6.6	57
86	Amide–aromatic hydrogen-bonds in host–guest recognition. Chemical Communications, 1996, , 2529-2530.	2.2	56
87	An Interconverting Family of Coordination Cages and a <i>meso</i> -Helicate; Effects of Temperature, Concentration, and Solvent on the Product Distribution of a Self-Assembly Process. Inorganic Chemistry, 2015, 54, 2626-2637.	1.9	55
88	Chemical Double Mutant Cycles for the Quantification of Cooperativity in H-Bonded Complexes. Journal of the American Chemical Society, 2009, 131, 18518-18524.	6.6	54
89	Triggered Release from Lipid Bilayer Vesicles by an Artificial Transmembrane Signal Transduction System. Journal of the American Chemical Society, 2017, 139, 15768-15773.	6.6	54
90	A new approach to the assembly of electron donor–spacer–acceptor systems. Journal of the Chemical Society Chemical Communications, 1989, .	2.0	53

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91	Cooperativity in the assembly of zipper complexes. Chemical Communications, 1996, , 1723.	2.2	53
92	Quantitative Measurements of Edge-to-Face Aromatic Interactions by Using Chemical Double-Mutant Cycles. Chemistry - A European Journal, 2001, 7, 4854-4862.	1.7	53
93	Preferential Solvation and Hydrogen Bonding in Mixed Solvents. Angewandte Chemie - International Edition, 2008, 47, 6275-6277.	7.2	51
94	Understanding the Influence of Surface Solvation and Structure on Polymorph Stability: A Combined Mechanochemical and Theoretical Approach. Journal of the American Chemical Society, 2018, 140, 17051-17059.	6.6	51
95	Amplification of Bifunctional Ligands for Calmodulin from a Dynamic Combinatorial Library. Chemistry - A European Journal, 2006, 12, 1081-1087.	1.7	50
96	Dissection of Complex Molecular Recognition Interfaces. Journal of the American Chemical Society, 2011, 133, 582-594.	6.6	49
97	Virtual Screening Identifies New Cocrystals of Nalidixic Acid. Crystal Growth and Design, 2014, 14, 1749-1755.	1.4	49
98	Structure–activity relationship for quantifying aromatic interactionsâ€. Chemical Communications, 1998, , 775-776.	2.2	48
99	Molecular Conformation and Crystallization: The Case of Ethenzamide. Crystal Growth and Design, 2012, 12, 6110-6117.	1.4	48
100	Measurement of energy landscape roughness of folded and unfolded proteins. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 19563-19568.	3.3	48
101	Relationship Between Conformational Flexibility and Chelate Cooperativity. Journal of Organic Chemistry, 2011, 76, 2723-2732.	1.7	47
102	Molecular probes of solvation phenomena. Chemical Society Reviews, 2012, 41, 3485.	18.7	47
103	Virtual screening for high affinity guests for synthetic supramolecular receptors. Chemical Science, 2015, 6, 2790-2794.	3.7	46
104	Assembly of a photoactive supramolecule using porphyrin co-ordination chemistry. Journal of the Chemical Society Chemical Communications, 1989, , 226.	2.0	45
105	Chemische Cyclen mit doppelter Strukturvariation zur Bestimmung schwacher intermolekularer Wechselwirkungen: aromatische Kanteâ€aufâ€FlÄcheâ€Wechselwirkungen. Angewandte Chemie, 1996, 108, 1628-1631.	1.6	45
106	Hydrogen bonding properties of non-polar solvents. Organic and Biomolecular Chemistry, 2010, 8, 1455.	1.5	45
107	Allosteric ligand binding to cofacial metalloporphyrin dimers: the mechanism of porphyrin disaggregation. Journal of the Chemical Society Perkin Transactions 1, 1989, , 547.	0.9	44
108	van der Waals interactions in non-polar liquids. Chemical Science, 2013, 4, 834-848.	3.7	44

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109	Evidence for Partially Bound States in Cooperative Molecular Recognition Interfaces. Journal of the American Chemical Society, 2008, 130, 17718-17725.	6.6	43
110	Self-assembly of double-decker cages induced by coordination of perylene bisimide with a trimeric Zn porphyrin: study of the electron transfer dynamics between the two photoactive components. Dalton Transactions, 2009, , 4023.	1.6	43
111	ThX – a next-generation probe for the early detection of amyloid aggregates. Chemical Science, 2020, 11, 4578-4583.	3.7	43
112	Polarisation effects on the solvation properties of alcohols. Chemical Science, 2018, 9, 88-99.	3.7	43
113	Cooperative duplex formation by synthetic H-bonding oligomers. Chemical Science, 2016, 7, 94-101.	3.7	42
114	Azobenzene-porphyrins. Tetrahedron Letters, 1996, 37, 699-702.	0.7	40
115	Self-Assembly, Binding, and Dynamic Properties of Heterodimeric Porphyrin Macrocycles. Journal of Organic Chemistry, 2005, 70, 6616-6622.	1.7	39
116	Cocrystals of spironolactone and griseofulvin based on an in silico screening method. CrystEngComm, 2017, 19, 3592-3599.	1.3	39
117	Photoinduced electron transfer on a supramolecular scaffold. Chemical Communications, 1996, , 1361.	2.2	38
118	Fac and mer isomers of Ru( <scp>ii</scp> ) tris(pyrazolyl-pyridine) complexes as models for the vertices of coordination cages: structural characterisation and hydrogen-bonding characteristics. Dalton Transactions, 2014, 43, 71-84.	1.6	38
119	The role of the counteranion in the cation-Ï $\in$ interaction. Chemical Communications, 2003, , 834-835.	2.2	37
120	From structure to chemical shift and vice-versa. Progress in Nuclear Magnetic Resonance Spectroscopy, 2005, 47, 27-39.	3.9	37
121	Factors Influencing Tetranuclear [2 × 2] Grid vs Dinuclear Side-by-Side Structures for Silver(I) Complexes of Pyridazine-Based Bis-Bidentate Ligands. Inorganic Chemistry, 2008, 47, 10729-10738.	1.9	37
122	Luminescent cyanometallates based on phenylpyridine-Ir(iii) units: solvatochromism, metallochromism, and energy-transfer in Ir/Ln and Ir/Re complexes. Dalton Transactions, 2012, 41, 2408.	1.6	37
123	Footprinting molecular electrostatic potential surfaces for calculation of solvation energies. Physical Chemistry Chemical Physics, 2013, 15, 18262.	1.3	37
124	Sequence-Selective Formation of Synthetic H-Bonded Duplexes. Journal of the American Chemical Society, 2017, 139, 12655-12663.	6.6	37
125	Solvent Effects on Acridine Polymorphism. Crystal Growth and Design, 2010, 10, 1661-1664.	1.4	36
126	H-Bond Self-Assembly: Folding versus Duplex Formation. Journal of the American Chemical Society, 2017, 139, 6654-6662.	6.6	36

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127	A Synthetic Vesicle-to-Vesicle Communication System. Journal of the American Chemical Society, 2019, 141, 17847-17853.	6.6	36
128	Modular assembly of porphyrin sandwiches as potential hosts. Tetrahedron, 2002, 58, 691-697.	1.0	35
129	Metal Hydrides Form Halogen Bonds: Measurement of Energetics of Binding. Journal of the American Chemical Society, 2014, 136, 1288-1291.	6.6	35
130	Homochiral oligomers with highly flexible backbones form stable H-bonded duplexes. Chemical Science, 2017, 8, 206-213.	3.7	35
131	Combined Virtual/Experimental Multicomponent Solid Forms Screening of Sildenafil: New Salts, Cocrystals, and Hybrid Salt–Cocrystals. Crystal Growth and Design, 2018, 18, 7618-7627.	1.4	35
132	Influence of fluorine on aromatic interactions. Journal of the Chemical Society, Faraday Transactions, 1995, 91, 2009.	1.7	34
133	Quantification of Functional Group Interactions in Transition States. Journal of the American Chemical Society, 2003, 125, 9936-9937.	6.6	34
134	Tailbiter: a new amide foldamer. Chemical Communications, 2005, , 3691.	2.2	34
135	Determination of Protein–Ligand Binding Modes Using Complexation-Induced Changes in 1H NMR Chemical Shift. Journal of Medicinal Chemistry, 2008, 51, 2512-2517.	2.9	34
136	Recognition-Controlled Membrane Translocation for Signal Transduction across Lipid Bilayers. Journal of the American Chemical Society, 2017, 139, 6461-6466.	6.6	34
137	Guest Binding and Catalysis in the Cavity of a Cubic Coordination Cage. Chemistry Letters, 2017, 46, 2-9.	0.7	33
138	Sequence-dependent DNA structure. BioEssays, 1996, 18, 157-162.	1.2	32
139	Use of quantitative 1H NMR chemical shift changes for ligand docking into barnase. Journal of Biomolecular NMR, 2009, 43, 11-19.	1.6	32
140	Influence of H-Bond Strength on Chelate Cooperativity. Journal of the American Chemical Society, 2011, 133, 20416-20425.	6.6	32
141	H-Bond donor parameters for cations. Chemical Science, 2019, 10, 5943-5951.	3.7	32
142	Sequence information transfer using covalent template-directed synthesis. Chemical Science, 2019, 10, 5258-5266.	3.7	32
143	Influence of Solvent Polarity on Preferential Solvation of Molecular Recognition Probes in Solvent Mixtures. Journal of Physical Chemistry B, 2012, 116, 14433-14440.	1.2	31
144	Solvent effects on chelate cooperativity. Chemical Science, 2012, 3, 589-601.	3.7	31

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145	The flexibility–complementarity dichotomy in receptor–ligand interactions. Chemical Science, 2015, 6, 1444-1453.	3.7	31
146	An Activatable Cancer-Targeted Hydrogen Peroxide Probe for Photoacoustic and Fluorescence Imaging. Cancer Research, 2019, 79, 5407-5417.	0.4	31
147	Functional group interaction profiles: a general treatment of solvent effects on non-covalent interactions. Chemical Science, 2020, 11, 4456-4466.	3.7	31
148	Contact Mechanics of Nanometer-Scale Molecular Contacts: Correlation between Adhesion, Friction, and Hydrogen Bond Thermodynamics. Journal of the American Chemical Society, 2011, 133, 8625-8632.	6.6	30
149	pH-Controlled selection between one of three guests from a mixture using a coordination cage host. Chemical Science, 2015, 6, 4025-4028.	3.7	30
150	Multivalent recognition of bis- and tris-Zn-porphyrins by N-methylimidazole functionalized gold nanoparticles. Chemical Communications, 2003, , 1004-1005.	2.2	29
151	Transmission of Binding Information across Lipid Bilayers. Chemistry - A European Journal, 2007, 13, 7215-7222.	1.7	29
152	Cooperativity in multiply H-bonded complexes. Chemical Communications, 2009, , 3964.	2.2	29
153	A surface site interaction model for the properties of liquids at equilibrium. Chemical Science, 2013, 4, 1687.	3.7	29
154	The Contrasting Character of Early and Late Transition Metal Fluorides as Hydrogen Bond Acceptors. Journal of the American Chemical Society, 2015, 137, 11820-11831.	6.6	29
155	Mix and match backbones for the formation of H-bonded duplexes. Chemical Science, 2016, 7, 1760-1767.	3.7	29
156	Practicalities and applications of reverse heteronuclear shift correlation: Porphyrin and polysaccharide examples. Magnetic Resonance in Chemistry, 1988, 26, 867-875.	1.1	28
157	Applications of dynamic combinatorial chemistry for the determination of effective molarity. Chemical Science, 2015, 6, 144-151.	3.7	28
158	H-Bonded Duplexes based on a Phenylacetylene Backbone. Journal of the American Chemical Society, 2018, 140, 11526-11536.	6.6	28
159	The roughness of the protein energy landscape results in anomalous diffusion of the polypeptide backbone. Physical Chemistry Chemical Physics, 2015, 17, 762-782.	1.3	27
160	Metal-driven self assembly of C3 symmetry molecular cages. Chemical Communications, 2000, , 1087-1088.	2.2	26
161	Replication of Sequence Information in Synthetic Oligomers. Accounts of Chemical Research, 2021, 54, 1298-1306.	7.6	26
162	Comparative analysis of the influence of H-bond strength and solvent on chelate cooperativity in H-bonded supramolecular complexes. Chemical Science, 2012, 3, 2462.	3.7	25

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163	A Surface Site Interaction Point Method for Dissipative Particle Dynamics Parametrization: Application to Alkyl Ethoxylate Surfactant Self-Assembly. Journal of Physical Chemistry B, 2020, 124, 5047-5055.	1.2	25
164	Sequenceâ ''Structure Relationships in DNA Oligomers:Â A Computational Approach. Journal of the American Chemical Society, 2001, 123, 7399-7406.	6.6	24
165	Chemical Triple-Mutant Boxes for Quantifying Cooperativity in Intermolecular Interactions. Chemistry - A European Journal, 2002, 8, 5435-5446.	1.7	22
166	Dendrimers as scaffolds for the synthesis of spherical porphyrin arrays. Chemical Communications, 2003, , 38-39.	2.2	22
167	Photomodulated molecular recognition of the guanidinium cationElectronic supplementary information (ESI) available: UV/visible absorption spectra of 1, showing changes observed on irradiation at 345 nm and thermal recovery of the original spectrum. See http://www.rsc.org/suppdata/cc/b3/b311060e/. Chemical Communications. 2004 108.	2.2	22
168	A thermodynamic study of selective solvation in solvent mixtures. Organic and Biomolecular Chemistry, 2010, 8, 1943.	1.5	22
169	Substituent effects on aromatic interactions in the solid state. Chemical Communications, 2001, , 1500-1501.	2.2	21
170	The role of functional group concentration in solvation thermodynamics. Chemical Science, 2010, 1, 242.	3.7	21
171	Relationship Between Molecular Contact Thermodynamics and Surface Contact Mechanics. Langmuir, 2012, 28, 17709-17717.	1.6	21
172	Influence of non-covalent preorganization on supramolecular effective molarities. Organic and Biomolecular Chemistry, 2015, 13, 4981-4992.	1.5	21
173	H-bond competition experiments in solution and the solid state. CrystEngComm, 2016, 18, 394-397.	1.3	21
174	Ultrasound-induced gelation of a giant macrocycle. Chemical Communications, 2018, 54, 10874-10877.	2.2	21
175	Building blocks for recognition-encoded oligoesters that form H-bonded duplexes. Chemical Science, 2019, 10, 2444-2451.	3.7	21
176	Structural Mechanics of DNA Wrapping in the Nucleosome. Journal of Molecular Biology, 2010, 396, 264-279.	2.0	20
177	Molecular recognition probes of solvation thermodynamics in solvent mixtures. Organic and Biomolecular Chemistry, 2011, 9, 7571.	1.5	20
178	Supramolecular cage encapsulation as a versatile tool for the experimental quantification of aromatic stacking interactions. Chemical Science, 2019, 10, 1466-1471.	3.7	20
179	Template effects of vesicles in dynamic covalent chemistry. Chemical Science, 2020, 11, 9122-9125.	3.7	20
180	Binding of caffeine by a synthetic co-receptor. Tetrahedron Letters, 2000, 41, 3849-3853.	0.7	19

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181	Alkyltransferase-like protein (Atl1) distinguishes alkylated guanines for DNA repair using cation–i̇́€ interactions. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 18755-18760.	3.3	19
182	Mix and match recognition modules for the formation of H-bonded duplexes. Chemical Science, 2016, 7, 5686-5691.	3.7	19
183	Solid form and solubility. CrystEngComm, 2017, 19, 23-26.	1.3	19
184	Capping Strategies for Covalent Template-Directed Synthesis of Linear Oligomers Using CuAAC. Journal of the American Chemical Society, 2019, 141, 10862-10875.	6.6	19
185	Translation of Chemical Structure into Dissipative Particle Dynamics Parameters for Simulation of Surfactant Self-Assembly. Journal of Physical Chemistry B, 2021, 125, 3942-3952.	1.2	19
186	High-Fidelity Sequence-Selective Duplex Formation by Recognition-Encoded Melamine Oligomers. Journal of the American Chemical Society, 2021, 143, 8669-8678.	6.6	19
187	A peptide cross-linked polyacrylamide hydrogel for the detection of human neutrophil elastase. Electrochimica Acta, 2009, 54, 4985-4990.	2.6	18
188	Versatile Lowâ€Molecularâ€Weight Hydrogelators: Achieving Multiresponsiveness through a Modular Design. Chemistry - A European Journal, 2011, 17, 9753-9761.	1.7	18
189	Water and the Cationâ^ï€ Interaction. Journal of the American Chemical Society, 2021, 143, 12397-12403.	6.6	18
190	Structure-Based Identification of New High-Affinity Nucleosome Binding Sequences. Journal of Molecular Biology, 2012, 420, 8-16.	2.0	17
191	Interplay of Self-Association and Solvation in Polar Liquids. Journal of the American Chemical Society, 2013, 135, 12091-12100.	6.6	17
192	Measurement of supramolecular effective molarities for intramolecular H-bonds in zinc porphyrin–imidazole complexes. Organic and Biomolecular Chemistry, 2014, 12, 1440.	1.5	17
193	Ligand-induced conformational switching and allosteric effects in macrocyclic porphyrin dimers. Journal of the Chemical Society Chemical Communications, 1988, , 694.	2.0	16
194	Enhanced Chelate Cooperativity in Polar Solvents. Journal of the American Chemical Society, 2017, 139, 6675-6681.	6.6	16
195	New building blocks for the assembly of sequence selective molecular zippers. Chemical Communications, 2003, , 1642.	2.2	15
196	Prediction of atomic structure from sequence for double helical DNA oligomers. Biopolymers, 2006, 81, 51-61.	1.2	15
197	The mechanics of nanometre-scale molecular contacts. Faraday Discussions, 2012, 156, 325.	1.6	15
198	Synthesis and conformation of macrocyclic porphyrin dimers with potentially spacious cavities. Journal of the Chemical Society Chemical Communications, 1988, , 692.	2.0	14

#	Article	IF	CITATIONS
199	Construction of Double-helical DNA Structures Based on Dinucleotide Building Blocks. Journal of Biomolecular Structure and Dynamics, 1997, 14, 747-756.	2.0	14
200	Complexation-induced chemical shifts—ab initio parameterization of transferable bond anisotropies. Journal of Magnetic Resonance, 2003, 162, 102-112.	1.2	14
201	A Structural Similarity Analysis of Double-helical DNA. Journal of Molecular Biology, 2004, 343, 879-889.	2.0	14
202	Two-component assembly of recognition-encoded oligomers that form stable H-bonded duplexes. Chemical Science, 2020, 11, 561-566.	3.7	14
203	Solvent similarity index. Physical Chemistry Chemical Physics, 2020, 22, 11967-11975.	1.3	14
204	Dissection of the Polar and Nonâ€Polar Contributions to Aromatic Stacking Interactions in Solution. Angewandte Chemie - International Edition, 2021, 60, 23871-23877.	7.2	14
205	Synthesis and Photochemistry of a New Class of Photocleavable Protein Cross-linking Reagents. Chemistry - A European Journal, 2004, 10, 1705-1710.	1.7	13
206	Steric desolvation enhances the effective molarities of intramolecular H-bonding interactions. Organic and Biomolecular Chemistry, 2012, 10, 6022.	1.5	13
207	Fluorescent and colorimetric molecular recognition probe for hydrogen bond acceptors. Organic and Biomolecular Chemistry, 2017, 15, 9603-9610.	1.5	13
208	Solvatomorphism of Reichardt's dye. CrystEngComm, 2018, 20, 2912-2915.	1.3	13
209	Benchmarking of Halogen Bond Strength in Solution with Nickel Fluorides: Bromine versus Iodine and Perfluoroaryl versus Perfluoroalkyl Donors. Chemistry - A European Journal, 2019, 25, 9237-9241.	1.7	13
210	Molecular replication using covalent base-pairs with traceless linkers. Organic and Biomolecular Chemistry, 2019, 17, 9660-9665.	1.5	13
211	Investigation of porphyrins and metalloporphyrins by fast atom bombardment mass spectrometry. Analytica Chimica Acta, 1990, 241, 281-287.	2.6	12
212	Emergent supramolecular assembly properties of a recognition-encoded oligoester. Chemical Science, 2019, 10, 5397-5404.	3.7	12
213	Structurally-tolerant self-assembly of zinc pyridyl porphyrins. New Journal of Chemistry, 2008, 32, 525.	1.4	11
214	Backbone conformation affects duplex initiation and duplex propagation in hybridisation of synthetic H-bonding oligomers. Organic and Biomolecular Chemistry, 2018, 16, 4183-4190.	1.5	11
215	Cooperative assembly of H-bonded rosettes inside a porphyrin nanoring. Chemical Science, 2021, 12, 1427-1432.	3.7	11
216	Cap control: cyclic <i>versus</i> linear oligomerisation in covalent template-directed synthesis. RSC Advances, 2019, 9, 29566-29569.	1.7	10

#	Article	IF	CITATIONS
217	Influence of Conformational Flexibility on Complexation-Induced Changes in Chemical Shift in a Neocarzinostatin Proteinâ^'Ligand Complex. Journal of Medicinal Chemistry, 2008, 51, 4488-4495.	2.9	9
218	Influence of receptor flexibility on intramolecular H-bonding interactions. Organic and Biomolecular Chemistry, 2015, 13, 8053-8066.	1.5	9
219	Competitor analysis of functional group H-bond donor and acceptor properties using the Cambridge Structural Database. Physical Chemistry Chemical Physics, 2018, 20, 25324-25334.	1.3	9
220	Supramolecular catalysis by recognition-encoded oligomers: discovery of a synthetic imine polymerase. Chemical Science, 2020, 11, 7408-7414.	3.7	9
221	Controlled mutation in the replication of synthetic oligomers. Chemical Science, 2021, 12, 4063-4068.	3.7	9
222	Conformation and electron-transfer chemistry in model photosynthetic reaction centres determined by fast atom bombardment mass spectrometry. Journal of the Chemical Society Perkin Transactions II, 1992, , 411.	0.9	8
223	Enhanced Ligand Affinity for Receptors in which Components of the Binding Site Are Independently Mobile. Chemistry and Biology, 2005, 12, 89-97.	6.2	8
224	Genomic Data Analysis Using DNA Structure:Â An Analysis of Conserved Nongenic Sequences and Ultraconserved Elements. Journal of Chemical Information and Modeling, 2006, 46, 753-761.	2.5	8
225	A Method for the Reversible Trapping of Proteins in Non-Native Conformations. Biochemistry, 2008, 47, 13620-13634.	1.2	8
226	Quantification of cooperativity in the self-assembly of H-bonded rosettes. Organic and Biomolecular Chemistry, 2020, 18, 1602-1606.	1.5	8
227	Folding and duplex formation in mixed sequence recognition-encoded <i>m</i> -phenylene ethynylene polymers. Chemical Science, 2021, 12, 10218-10226.	3.7	8
228	Heteroâ€Coencapsulation within a Supramolecular Cage: Moving away from the Statistical Distribution of Different Guests. Chemistry - A European Journal, 2020, 26, 9454-9458.	1.7	7
229	Redox switching of an artificial transmembrane signal transduction system. Chemical Communications, 2021, 57, 2196-2198.	2.2	7
230	Mapping the binding site topology of amyloid protein aggregates using multivalent ligands. Chemical Science, 2021, 12, 8892-8899.	3.7	6
231	SSIPTools: Software and Methodology for Surface Site Interaction Point (SSIP) Approach and Applications. Journal of Chemical Information and Modeling, 2021, 61, 5331-5335.	2.5	6
232	Transmembrane signal transduction by cofactor transport. Chemical Science, 2021, 12, 12377-12382.	3.7	5
233	Duplex <i>vs.</i> folding: tuning the self-assembly of synthetic recognition-encoded aniline oligomers. Organic and Biomolecular Chemistry, 2021, 19, 8947-8954.	1.5	5
234	Artificial transmembrane signal transduction mediated by dynamic covalent chemistry. Chemical Science, 2021, 12, 14059-14064.	3.7	5

#	Article	IF	CITATIONS
235	Requirements for Quantifications of Weak Intermolecular Interactions from Equilibrium Studies with Supramolecular Complexes. Angewandte Chemie International Edition in English, 1997, 36, 1073-1073.	4.4	4
236	An improved synthesis, crystal structures, and metallochromism of salts of [Ru(tolyl-terpy)(CN)3]â^'. Inorganica Chimica Acta, 2010, 363, 2938-2944.	1.2	4
237	An improved methodology to compute surface site interaction points using high density molecular electrostatic potential surfaces. Journal of Computational Chemistry, 2018, 39, 2371-2377.	1.5	4
238	Stimuliâ€Responsive Selfâ€Sorting Hybrid Hydrogenâ€Bonded/Metalâ€Coordinated Cage. Chemistry - A European Journal, 2021, 27, 3302-3305.	1.7	4
239	Liposome Enhanced Detection of Amyloid Protein Aggregates. Organic Letters, 2021, 23, 647-650.	2.4	4
240	A Neutral DNA Sequenceâ€Selective Vector for Interaction Studies: Fluorescence Binding Experiments Directed Towards a Carbohydrateâ€ÐNA Carrier. European Journal of Organic Chemistry, 2008, 2008, 2220-2231.	1.2	3
241	A pulse-radiolysis approach to fast reductive cleavage of a disulfide bond to uncage enzyme activity. Free Radical Biology and Medicine, 2008, 45, 1271-1278.	1.3	3
242	Triaminopyrimidine derivatives as transmembrane HCl transporters. Organic and Biomolecular Chemistry, 2019, 17, 5633-5638.	1.5	3
243	An empirical model for solvation based on surface site interaction points. Chemical Science, 2021, 12, 13193-13208.	3.7	3
244	Computational screens can speed up the discovery of pharmaceutical cocrystals. ADMET and DMPK, 2018, 6, 284-287.	1.1	3
245	Systematic Parameterization of Ion–Surfactant Interactions in Dissipative Particle Dynamics Using Setschenow Coefficients. Journal of Physical Chemistry B, 2022, 126, 2308-2315.	1.2	3
246	A surface site interaction point methodology for macromolecules and huge molecular databases. Journal of Computational Chemistry, 2017, 38, 419-426.	1.5	2
247	Dissection of the Polar and Nonâ€Polar Contributions to Aromatic Stacking Interactions in Solution. Angewandte Chemie, 2021, 133, 24064.	1.6	2
248	Structural Fingerprints of Transcription Factor Binding Site Regions. Algorithms, 2009, 2, 448-469.	1.2	1
249	Universal Scaling Law for Polypeptide Backbone Dynamics on the Pico- to Millisecond Time Scale. Biophysical Journal, 2009, 96, 322a-323a.	0.2	1
250	Structural DNA Profiles:Â Single Sequence Queries. Journal of Chemical Information and Modeling, 2006, 46, 743-752.	2.5	0
251	Correction to Relationship Between Molecular Contact Thermodynamics and Surface Contact Mechanics. Langmuir, 2014, 30, 9623-9623.	1.6	0
252	Solvent dependence of competitive hydrogen-versushalogen-bonded self-assembly processes in multi-component crystal formation. Acta Crystallographica Section A: Foundations and Advances, 2015, 71, s129-s129.	0.0	0

#	Article	IF	CITATIONS
253	Hydrogen bonds and halogen bonds: solid state, solution phase and theory. Acta Crystallographica Section A: Foundations and Advances, 2017, 73, C597-C597.	0.0	0