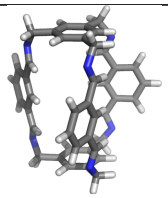
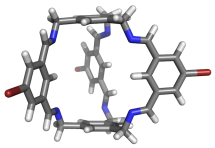
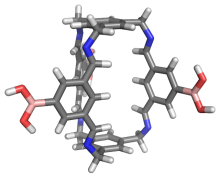
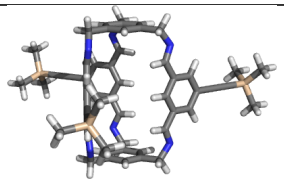
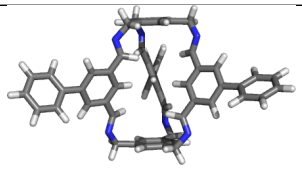
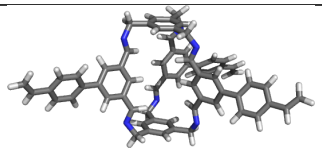
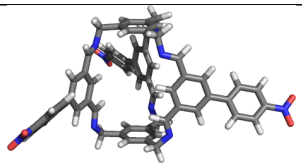
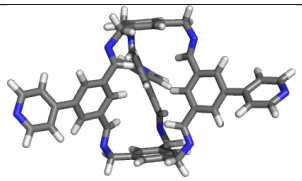
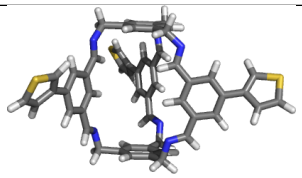
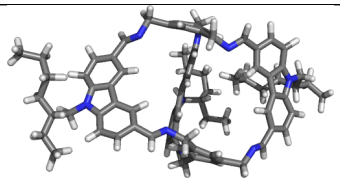
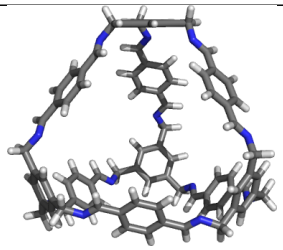
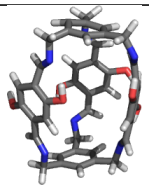
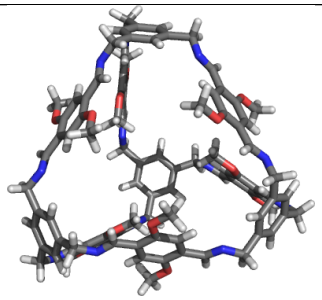
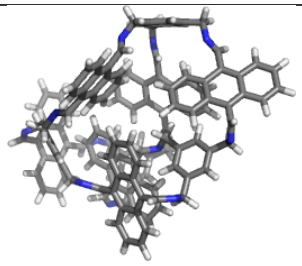
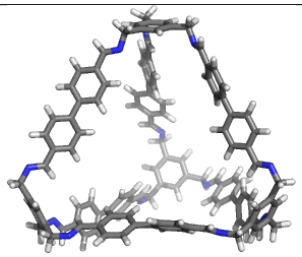
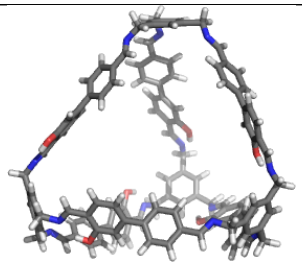
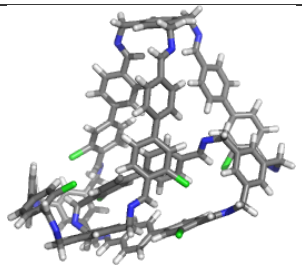
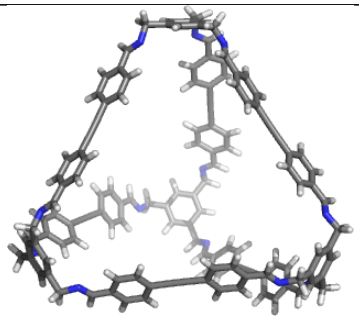
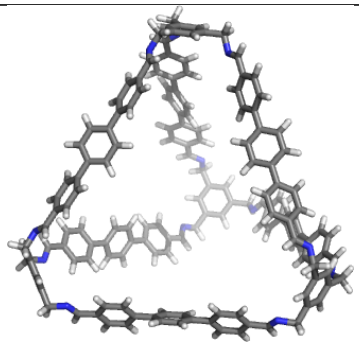
Electronic Supplementary Material (ESI) for Molecular Systems Design & Engineering.

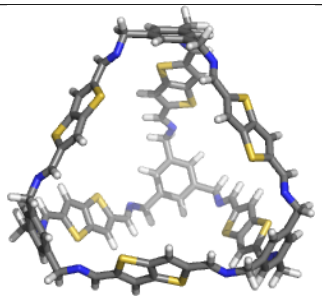
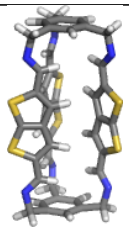
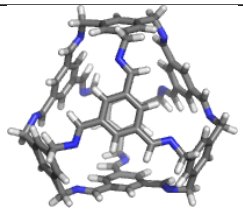
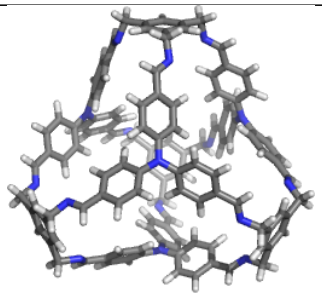
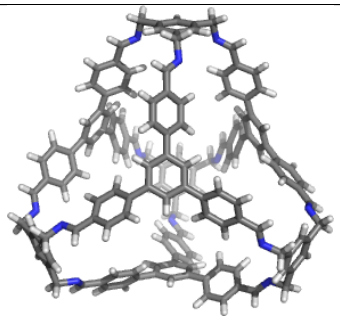
Supporting Information: Computational screening for nested organic cage complexes

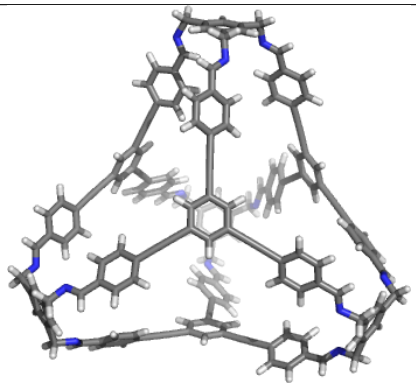
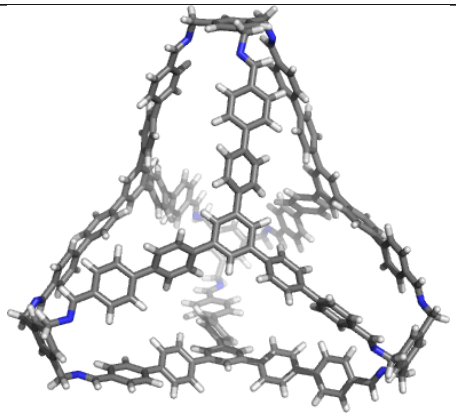
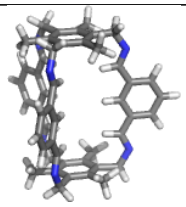
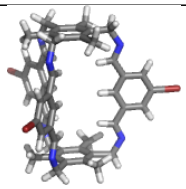
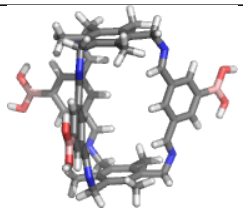
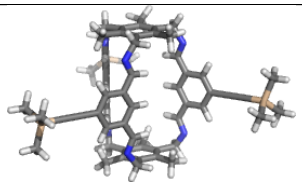
Table S1: A list of all organic cage molecules included in this study, with commonly used literature names and the literature reference where the molecule is reported. Atom colouring is grey (carbon), blue (nitrogen), white (hydrogen), brown (bromine), pink (boron), beige (silicon), yellow (sulfur) and green (fluorine).

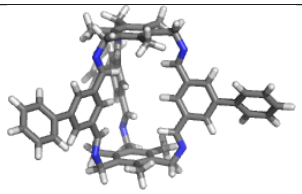
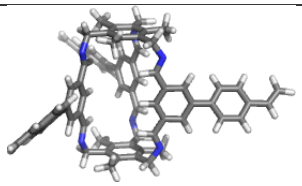
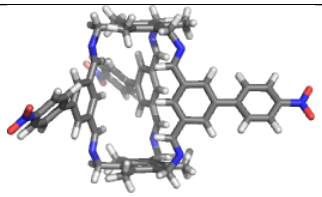
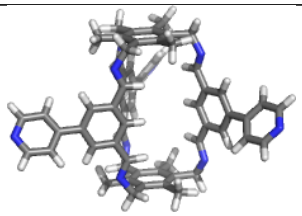
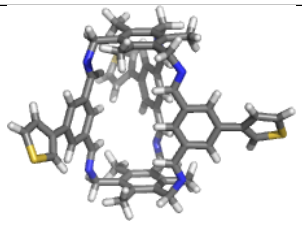
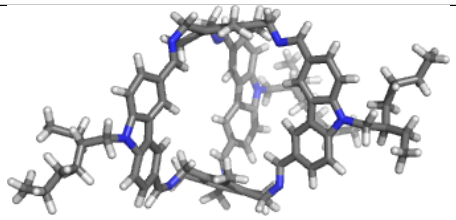
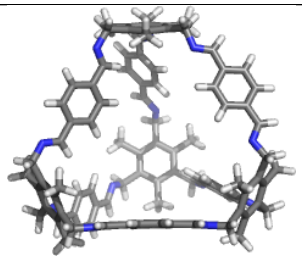
No	Literature name	Image	Reference
1	**A1**		[1]
2	**A2**		[1]
3	**A3**		[1]
4	**A4**		[1]
5	**A5**		[1]
6	**A6**		[1]
7	**A7**		[1]

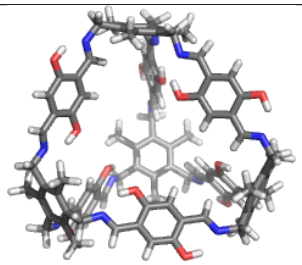
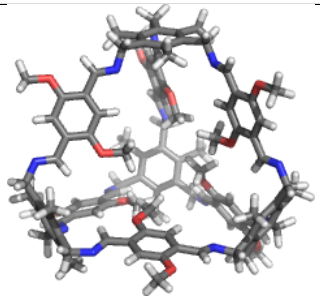
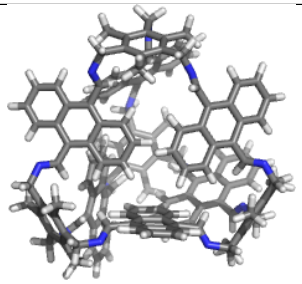
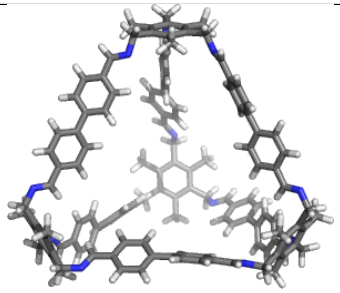
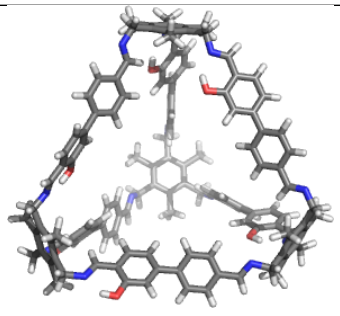
8	**A8**		1
9	**A9**		1
10	**A10**		1
11	**A11**		1
12	**A12**		1
13	**A13**		1
14	**A14**		1

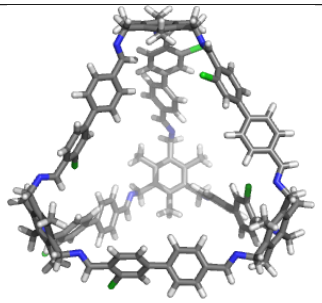
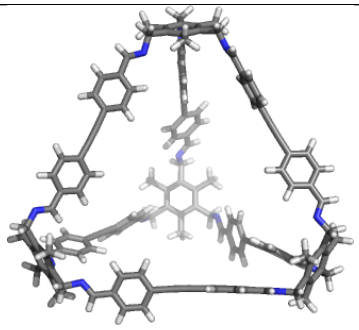
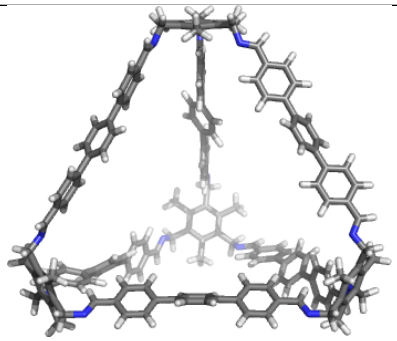
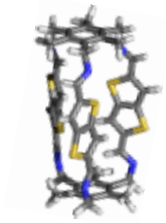
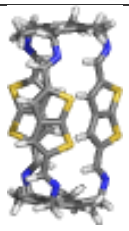
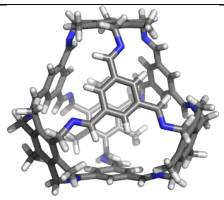
15	**A15**		1
16	**A16**		1
17	**A17**		1
18	**A18**		1
19	**A19**		1

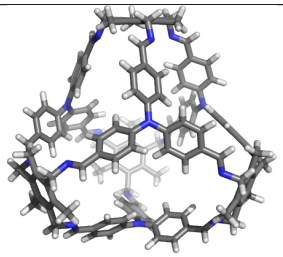
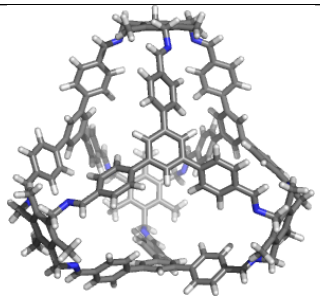
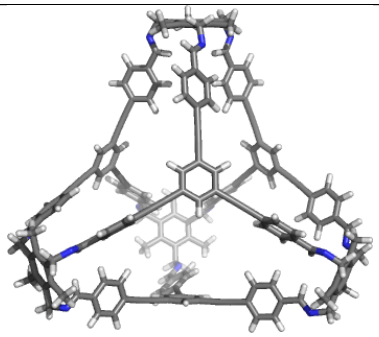
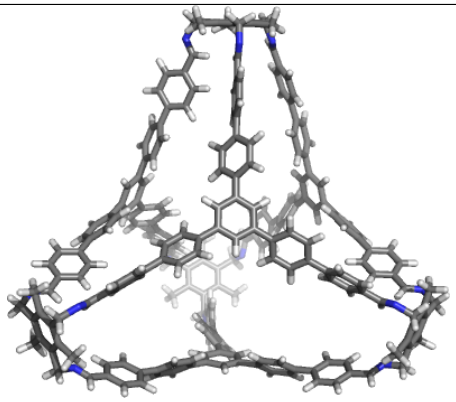
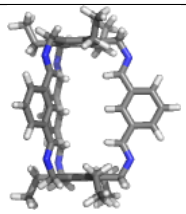
20	**A20**		1
21	**A21**		1
22	**A22**		1
23	**A23**		1
24	**A24**		1

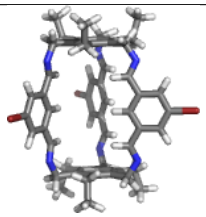
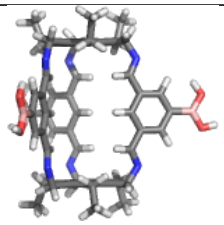
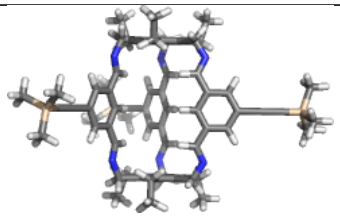
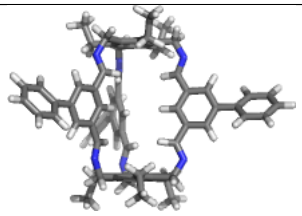
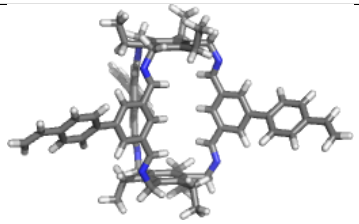
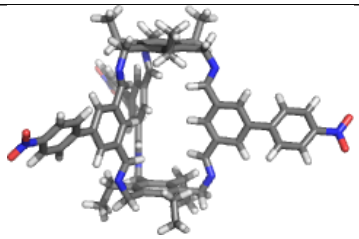
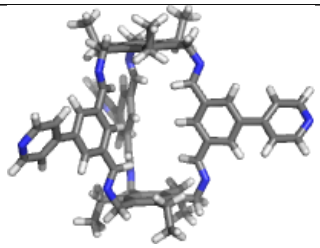
25	**A25**		1
26	**A26**		1
27	**B1**		1
28	**B2**		1
29	**B3**		1
30	**B4**		1

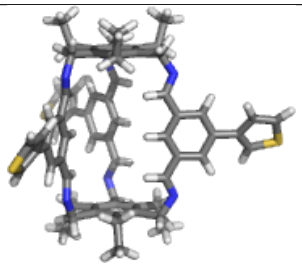
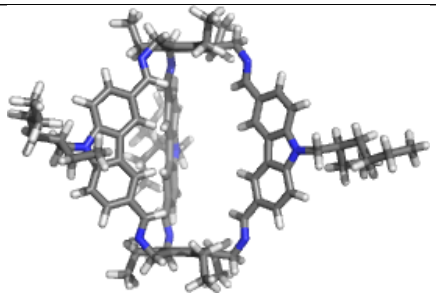
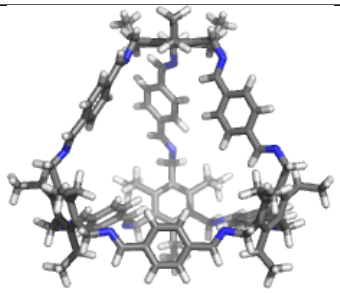
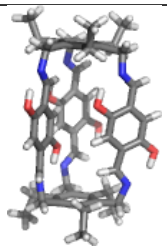
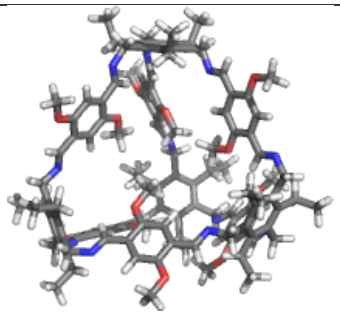
31	**B5**		1
32	**B6**		1
33	**B7**		1
34	**B8**		1
35	**B9**		1
36	**B10**		1
37	**B11**		1

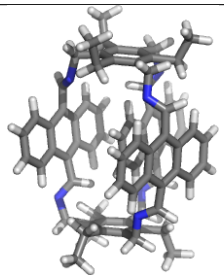
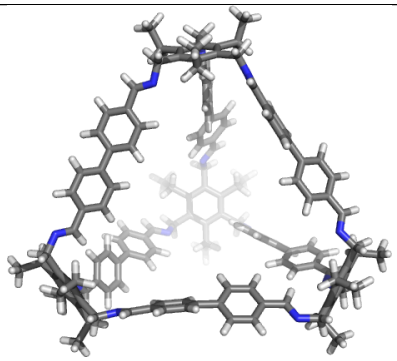
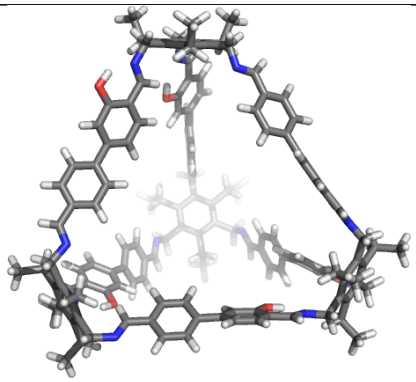
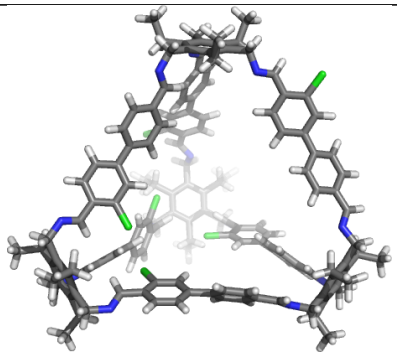
38	**B12**		1
39	**B13**		1
40	**B14**		1
41	**B15**		1
42	**B16**		1

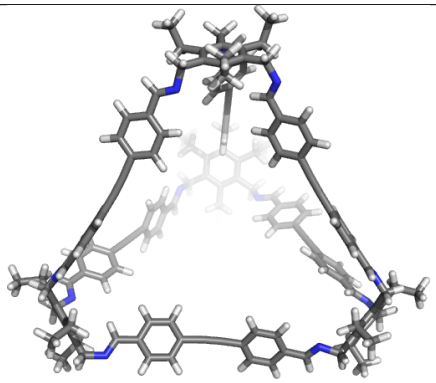
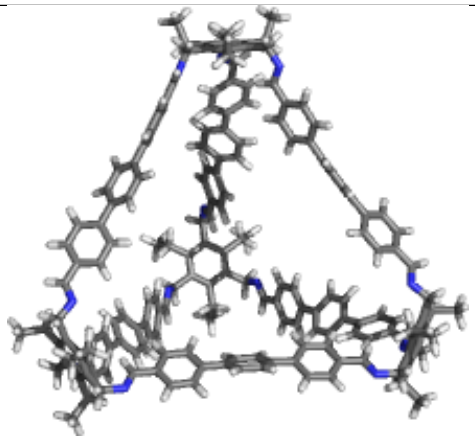
43	**B17**		1
44	**B18**		1
45	**B19**		1
46	**B20**		1
47	**B21**		1
48	**B22**		1

49	**B23**		1
50	**B24**		1
51	**B25**		1
52	**B26**		1
53	**C1**		1

54	**C2**		1
55	**C3**		1
56	**C4**		1
57	**C5**		1
58	**C6**		1
59	**C7**		1
60	**C8**		1

61	**C9**		1
62	**C10**		1
63	**C11**		1
64	**C12**		1
65	**C13**		1

66	**C14**		1
67	**C15**		1
68	**C16**		1
69	**C17**		1

70	**C18**		1
71	**C19**		1
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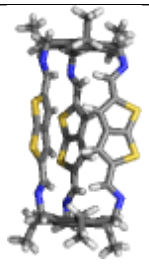
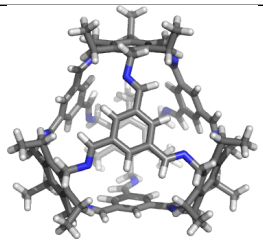
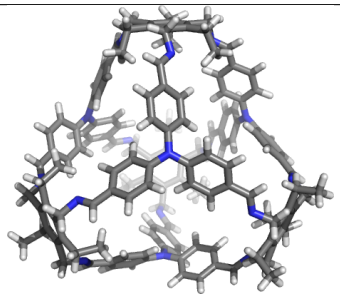
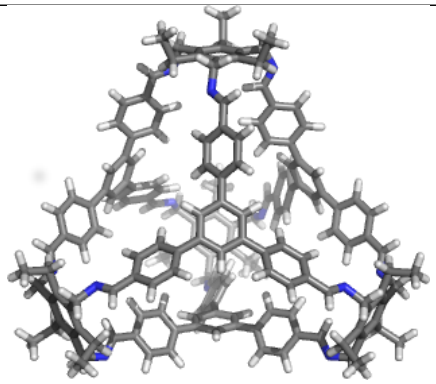
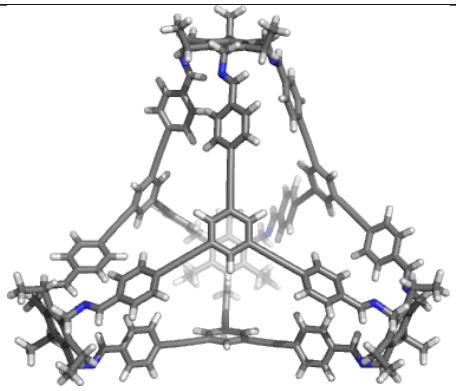
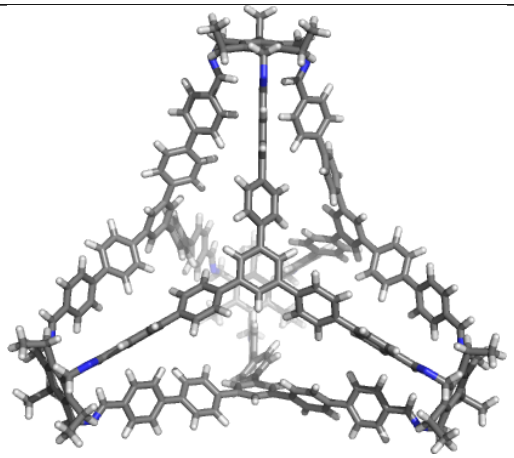
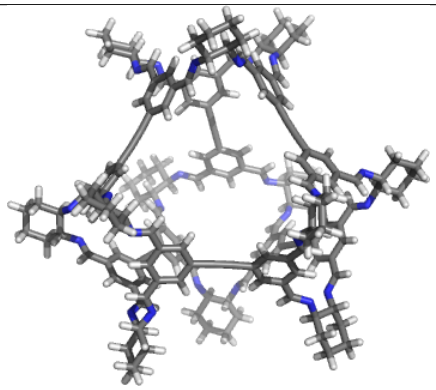
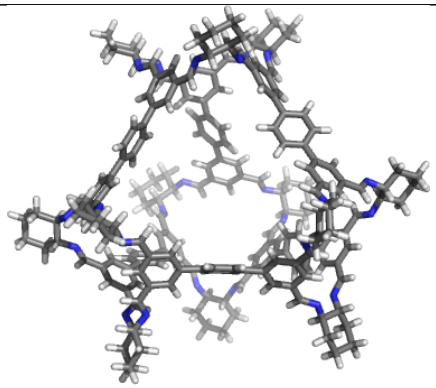
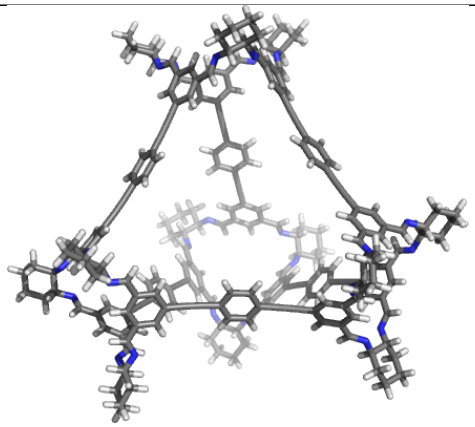
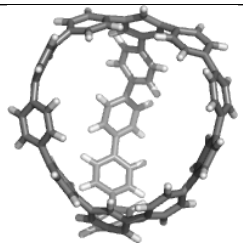
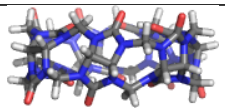
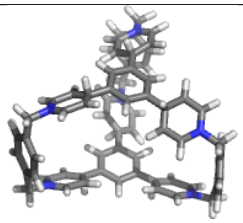
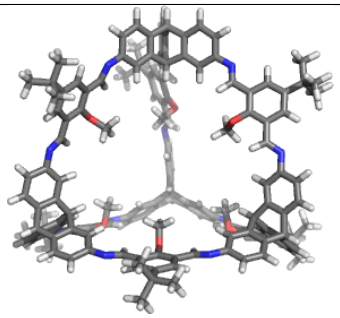
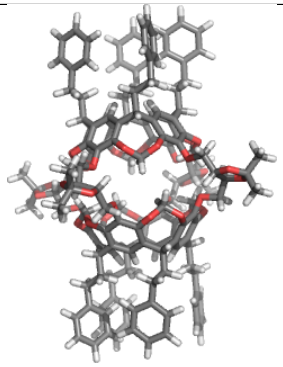
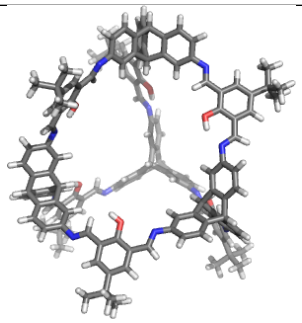
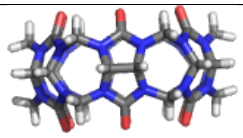
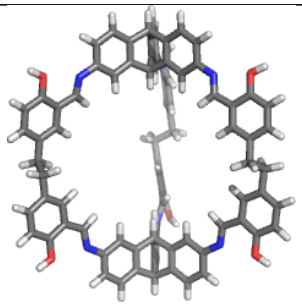
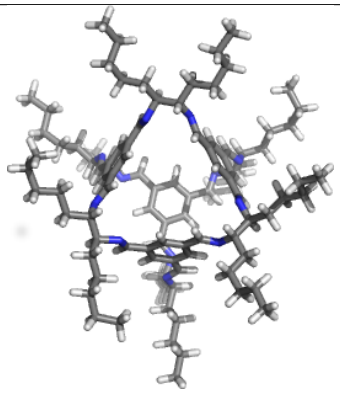
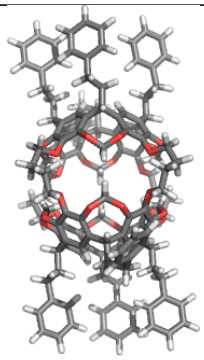
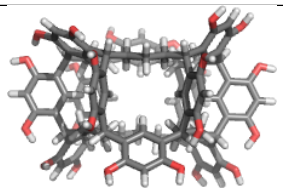
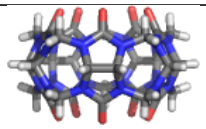
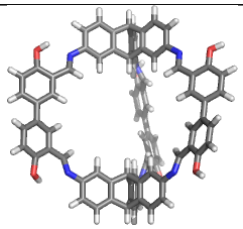
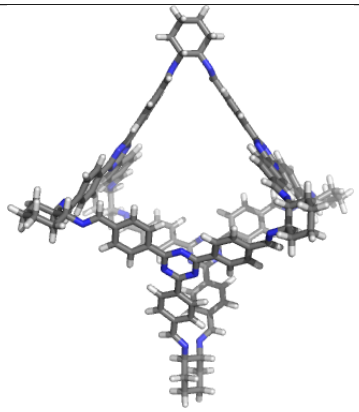
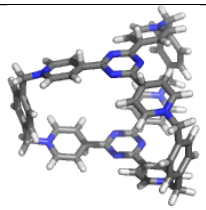
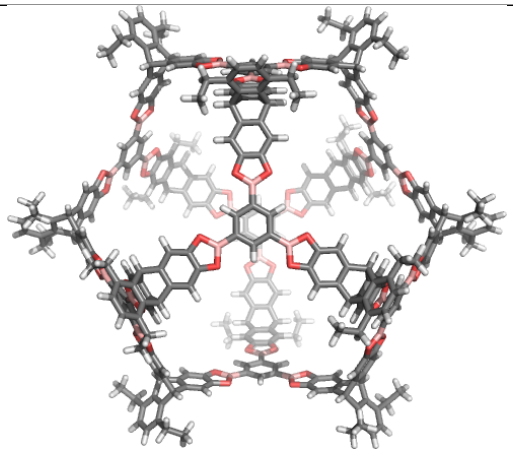
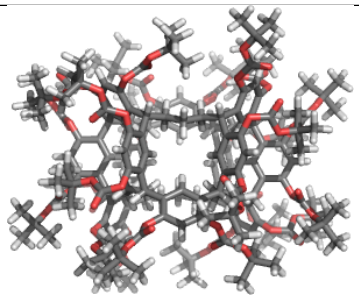
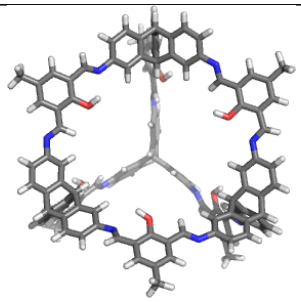
73	**C21**		1
74	**C22**		1,2

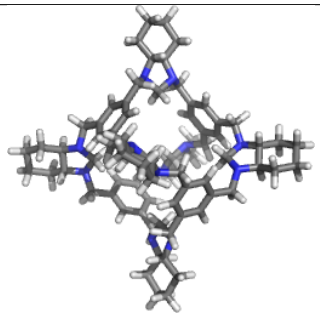
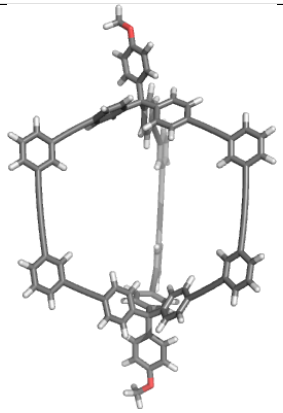
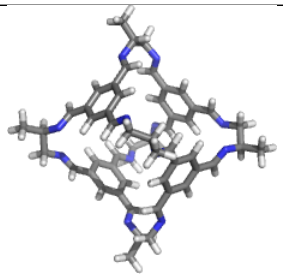
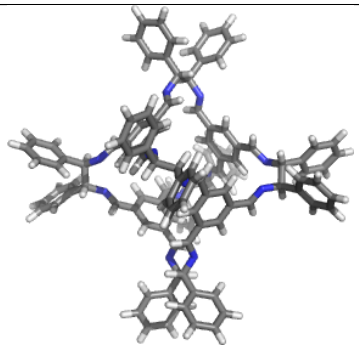
75	**C23**		1
76	**C24**		1
77	**C25**		1
78	**C26**		1

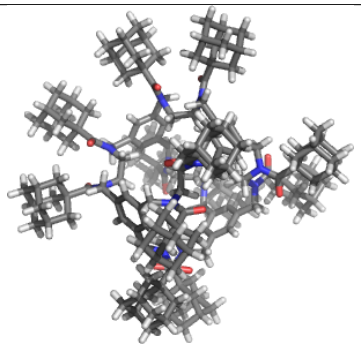
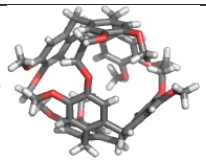
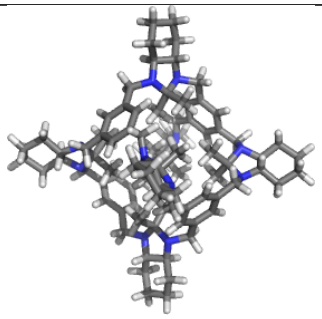
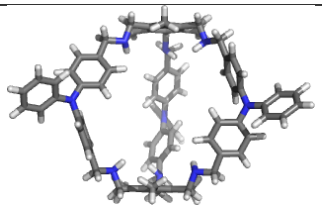
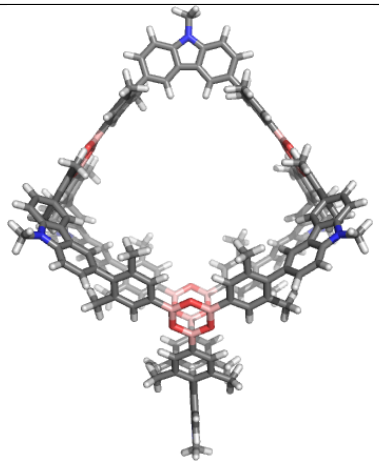
79	**TCC1**$_{[6+12]}$		3
80	**TCC2**$_{[6+12]}$		3
81	**TCC3**$_{[6+12]}$		3
82	Carbon nanocage **1**		4
83	**CB[7]**		5

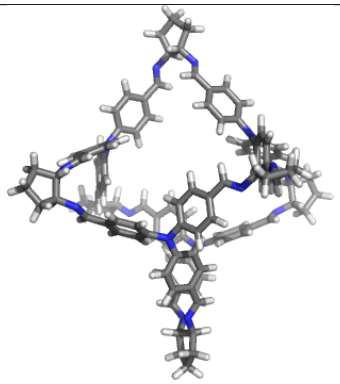
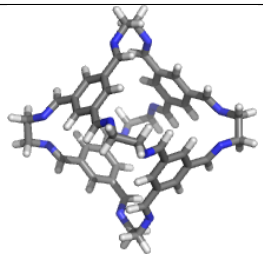
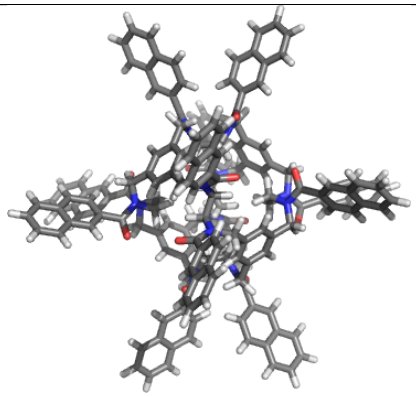
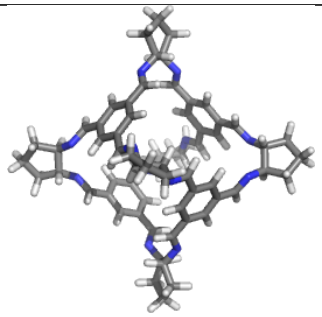
84	ExCage		6
85	Mastalerz cage		7
86	Cram hemicarce-plex		8
87	Mastalerz cage		7
88	**CB[6]**		5
89	Mastalerz cage		9

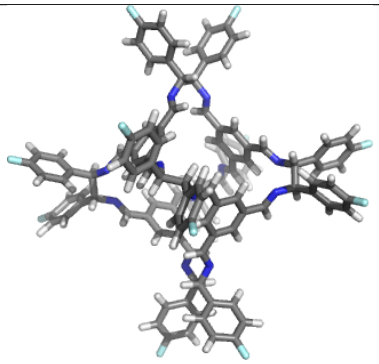
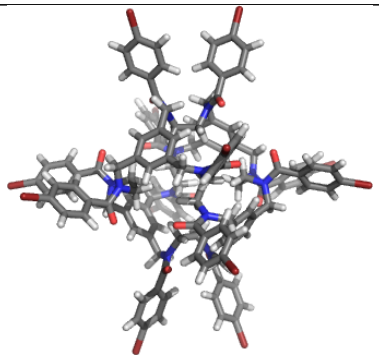
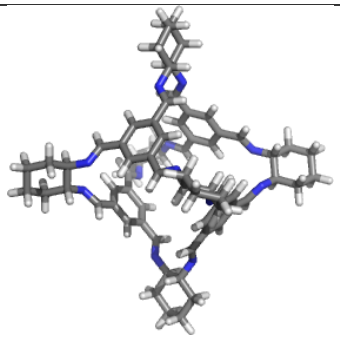
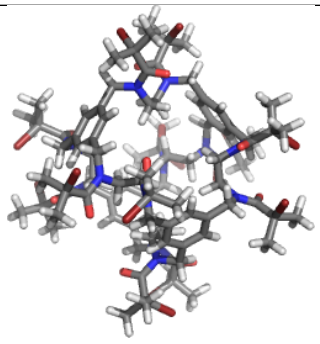
90	Dodecalkyl cage **7**		10
91	Cram hemicarce-plex		8
92	Noria		11
93	**CB[5]**		5
94	Mastalerz cage		9

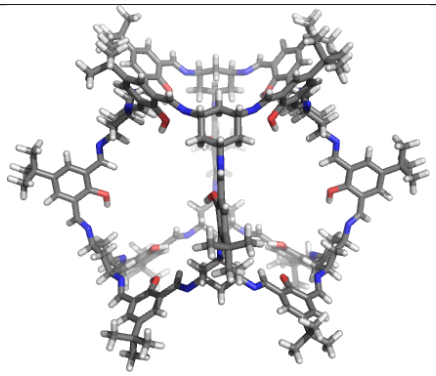
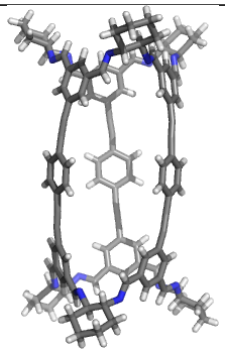
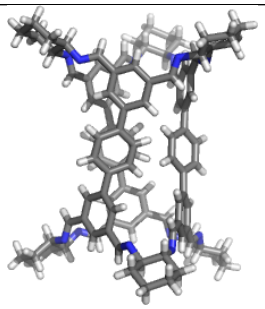
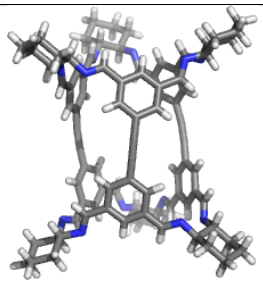
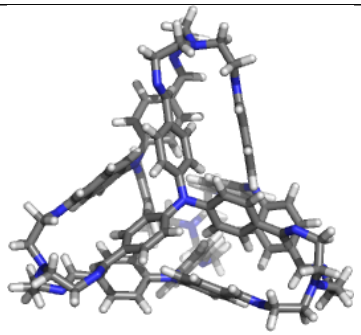
95	Triazine-based cage		12
96	BlueCage		13
97	Mastalerz boronate cage		14
98	Noria		11
99	Mastalerz cage		15

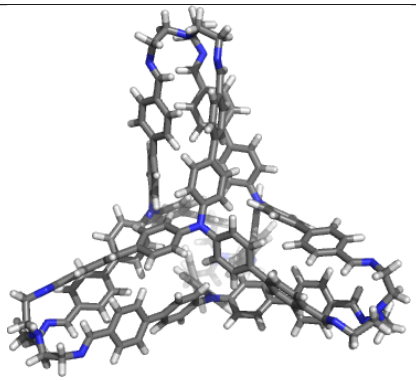
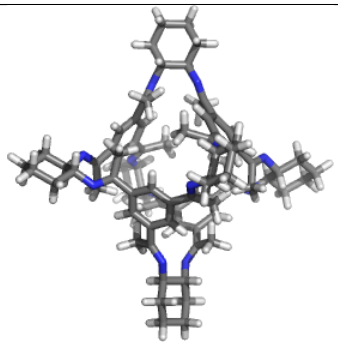
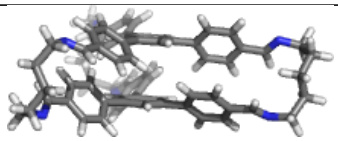
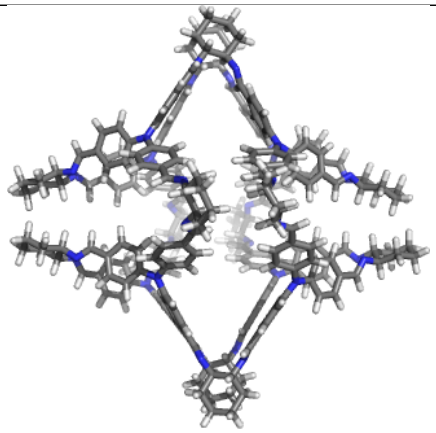
100	**FT-RCC3**		16
101	Doonan cage		17
102	**CC2**		18
103	**CC9**		19

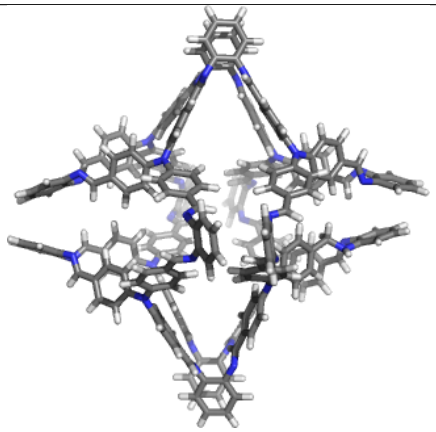
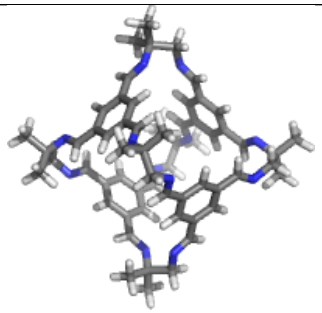
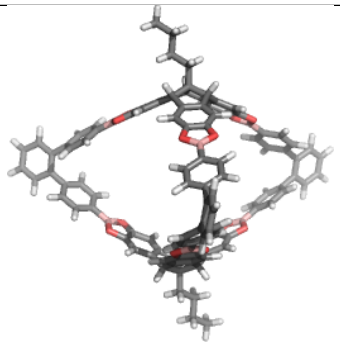
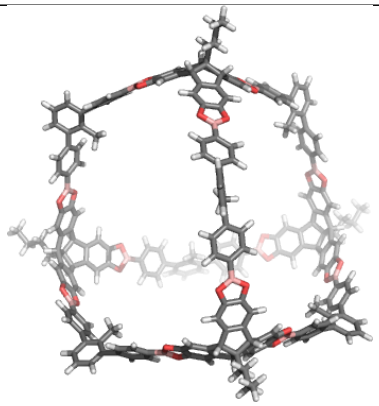
104	**RCC1c**		20
105	Cryptophane		21
106	**AT-RCC3**		16
107	Mukherjee cage		22
108	Iwasawa cage		23

109	**CC9**		24
110	**CC1**		18
111	**RCC1b**		20
112	**CC4**		25

113	**CC10**		19
114	**RCC1a**		20
115	**CC3**		18
116	**RCC1d**		20

117	Gawroński cage		26
118	**TCC3**		27
119	**TCC2**		27
120	**TCC1**		27
121	**CC11**		28

122	**CC12**		28
123	**CC15**		29
124	**CC6**		30
125	**CC7**		31

126	**CC8**		31
127	**CC13**		32
128	Beuerle cage		33
129	Beuerle cage		33

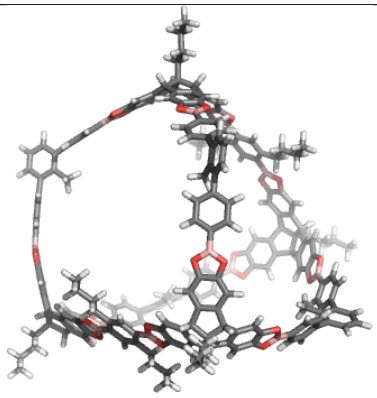
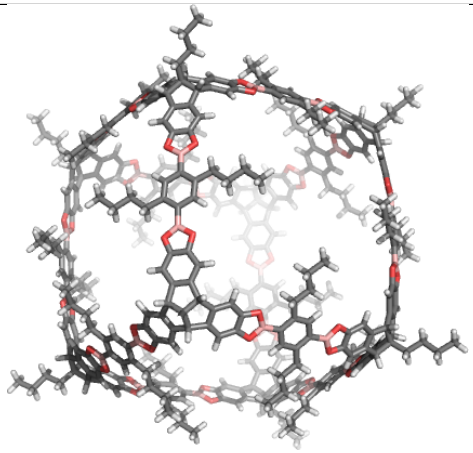
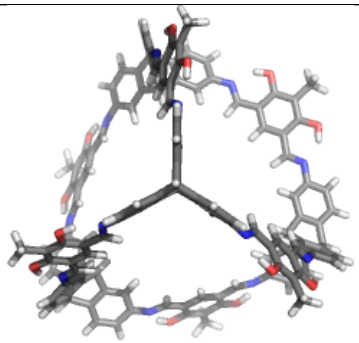
130	Beuerle cage		[33]
131	Beuerle cage		[34]
132	Mastalerz cage		[35]

Table S2: Structural characterisation of the individual cage molecules. The diameters are all given in Ångstrom. D_{max} is the maximum diameter of the molecule, D_{avg} is the average weighted diameter of the molecule, D_{cav} is the diameter of the largest sphere that can be placed inside the molecule's void and the average D_{window} is the average diameter of the molecule's windows.

Cage ID	D_{max}	D_{avg}	D_{cav}	No. of windows	Average D_{window}
1	15.0	11.7	3.2	3	2.5
2	18.5	12.4	4.4	3	3.4
3	16.8	12.2	3.2	3	3.0
4	23.3	12.8	3.3	3	2.7
5	21.8	12.4	1.8	3	2.6
6	28.4	11.7	0.9	3	2.6
7	24.7	12.8	4.2	3	3.0
8	21.5	12.3	1.8	3	2.2
9	21.0	12.7	4.2	3	3.1
10	28.2	15.2	4.6	4	3.9
11	20.2	18.1	10.9	4	6.5
12	16.2	11.7	3.8	4	2.1
13	22.1	17.1	6.5	7	3.9
14	24.7	14.4	0.9	2	2.5
15	24.5	21.6	9.9	4	8.0
16	24.9	21.5	11.9	4	8.5
17	23.6	13.0	0.0	0	0.0
18	27.0	23.7	14.6	4	10.0
19	28.8	25.0	13.5	4	10.6
20	21.9	19.5	11.8	4	7.5
21	16.9	10.3	1.5	3	0.9
22	17.9	14.9	7.2	6	3.6
23	22.4	18.7	9.2	6	4.5
24	25.2	20.4	10.9	6	6.1
25	29.7	23.6	13.0	6	8.3
26	32.7	24.9	13.1	6	8.1
27	15.2	12.4	2.2	3	2.4
28	17.5	12.7	2.2	3	4.0
29	18.6	12.6	3.1	3	2.7
30	23.3	12.9	3.1	3	2.6
31	22.1	13.1	2.2	3	2.3
32	24.9	12.9	3.2	3	2.7
33	23.9	12.8	3.2	3	2.7
34	20.2	12.7	3.2	3	2.5
35	20.0	12.7	3.2	3	2.7
36	29.1	15.9	6.0	3	5.0

37	20.9	18.5	6.3	4	6.8
38	21.6	18.3	7.0	4	5.3
39	24.9	16.5	3.7	5	3.0
40	21.6	16.4	6.0	3	5.4
41	25.5	22.2	9.9	4	8.2
42	25.5	22.2	10.2	4	7.9
43	26.1	22.1	8.9	4	9.1
44	28.1	24.6	12.1	4	10.2
45	29.7	25.9	13.1	4	11.3
46	17.5	11.1	1.7	3	1.1
47	17.7	11.6	2.5	3	1.9
48	17.9	15.3	7.4	6	3.4
49	22.4	19.3	9.7	6	4.8
50	25.2	21.2	11.4	6	6.8
51	29.9	23.5	12.4	6	8.0
52	33.0	24.3	12.2	6	8.4
53	17.3	12.7	2.1	3	2.3
54	17.3	12.9	3.1	3	2.8
55	17.9	12.9	3.0	3	2.7
56	24.8	13.5	3.0	3	2.7
57	22.0	13.5	2.1	3	2.4
58	25.2	13.4	3.1	3	2.7
59	25.3	13.5	2.1	3	2.4
60	21.3	13.4	2.1	3	2.4
61	20.8	13.2	3.1	3	2.8
62	28.6	16.8	5.1	3	4.4
63	23.2	19.0	6.3	4	6.6
64	18.4	11.6	2.1	3	1.5
65	25.2	17.1	4.1	4	5.9
66	18.2	11.9	0.0	0	0.0
67	27.6	22.5	10.0	4	8.3
68	28.1	22.6	10.3	4	8.3
69	27.6	21.7	8.8	4	7.6
70	30.4	24.6	11.7	4	9.9
71	32.3	25.7	13.6	4	10.9
72	19.8	11.5	1.8	3	1.2
73	19.8	11.0	1.6	3	0.9
74	19.8	15.8	7.5	6	3.8
75	24.1	19.5	9.8	6	5.3
76	26.8	20.6	9.0	6	5.7
77	31.3	23.7	12.0	6	7.8
78	34.3	24.1	11.8	6	8.1
79	30.8	21.8	11.2	8	5.6
80	32.8	23.2	11.1	8	6.1
81	37.4	26.3	14.8	8	6.9

82	18.9	16.3	8.2	3	6.9
83	16.6	12.7	3.6	2	2.5
84	18.4	13.8	4.4	3	4.1
85	30.9	23.1	8.1	4	6.1
86	28.8	15.9	4.8	8	1.1
87	31.1	22.8	10.5	4	9.2
88	14.8	12.3	5.0	2	3.5
89	22.2	19.2	7.1	3	7.4
90	28.6	16.2	5.5	4	3.7
91	29.4	15.7	4.1	10	1.9
92	20.6	15.3	5.0	8	1.9
93	12.8	11.0	4.0	2	2.3
94	21.5	17.7	5.2	3	5.9
95	32.9	20.2	10.7	4	8.0
96	18.1	13.9	4.7	3	4.5
97	42.8	32.3	21.9	6	14.4
98	29.6	20.3	4.8	4	2.3
99	29.5	22.5	10.8	4	9.1
100	22.5	14.2	5.7	4	3.2
101	34.4	21.4	10.2	3	9.7
102	20.2	13.6	5.7	4	3.9
103	25.4	15.5	5.4	4	3.6
104	26.4	18.2	4.9	4	3.1
105	15.8	12.1	4.8	5	1.5
106	22.6	13.4	3.4	4	1.4
107	25.3	16.7	8.0	3	6.1
108	34.4	24.6	14.8	4	11.0
109	28.3	17.9	8.4	4	5.1
110	17.6	13.1	5.5	4	3.7
111	29.8	16.5	4.2	4	2.2
112	21.6	14.2	6.1	4	4.3
113	26.7	15.6	5.4	4	3.7
114	28.3	15.7	4.1	4	2.0
115	22.6	14.1	5.5	4	3.7
116	22.2	16.5	4.5	4	2.6
117	34.3	25.4	12.9	6	8.7
118	29.7	16.8	6.4	5	4.4
119	25.8	12.9	1.6	4	1.7
120	24.6	14.6	4.8	5	3.6
121	21.2	13.9	2.9	0	0.0
122	27.9	16.0	5.4	8	2.1
123	22.6	13.4	5.1	5	0.9
124	22.0	10.5	1.3	3	0.8
125	32.3	22.2	11.0	12	3.9
126	32.0	21.3	9.5	12	4.2

127	20.2	13.9	5.7	4	3.9
128	27.5	17.8	8.7	3	7.8
129	38.7	31.1	21.2	4	16.5
130	37.2	28.0	17.6	4	12.9
131	47.2	33.9	25.6	6	8.3
132	28.1	22.8	11.5	4	10.0

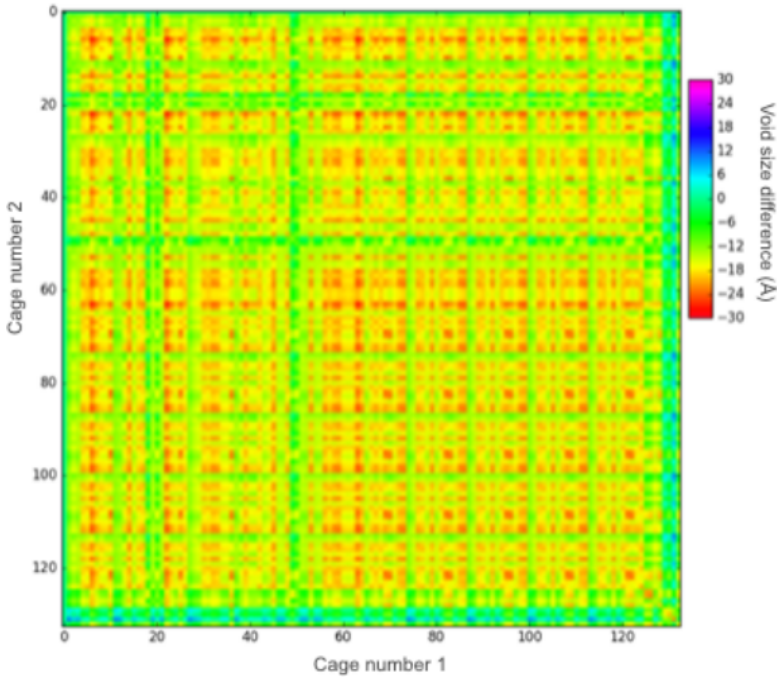


Figure S1: A 2D heat-map plot showing the difference in the match of the void of the larger cage in the pair with the maximum dimension of the smaller cage in the pair. A positive value of the size difference means that the outer cage void is larger than the size of the inner cage. A negative value of the size difference means that the outer cage void is smaller than the size of the inner cage. The plot is symmetric about the diagonal as a pairing of cage x and cage y is equivalent to a pairing of cage y and cage x.

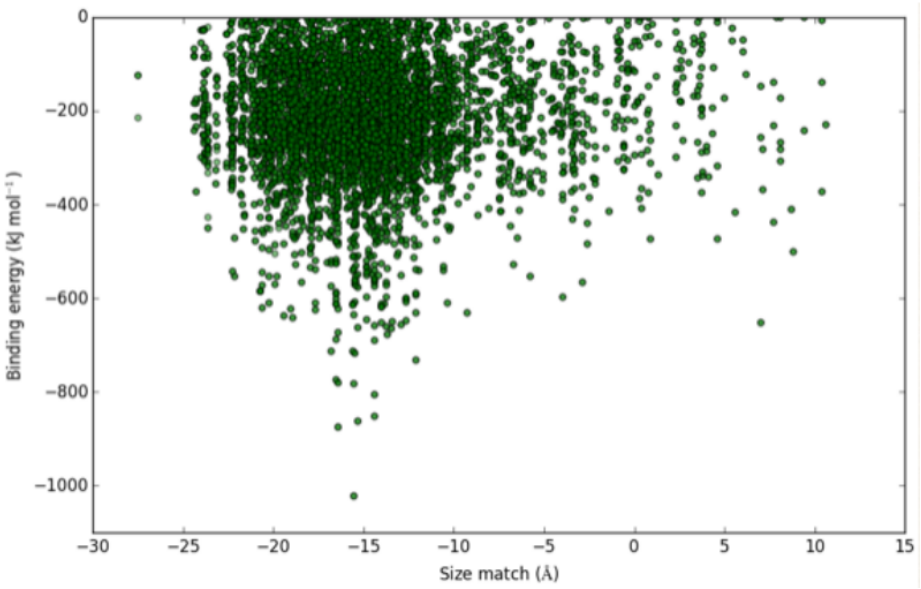


Figure S2: A comparison of binding energy of a pairing to the difference in the match of the void of the larger cage in the pair with the maximum dimension of the smaller cage in the pair. A positive value of the size difference means that the outer cage void is larger than the size of the inner cage. A negative value of the size difference means that the outer cage void is smaller than the size of the inner cage.

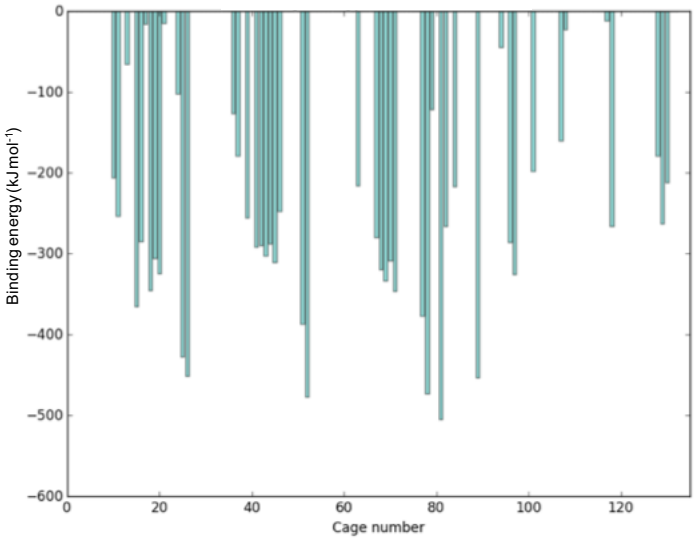


Figure S3: The binding energies of self-catenation in the cage systems, only binding energies that are favourable (negative) are shown.

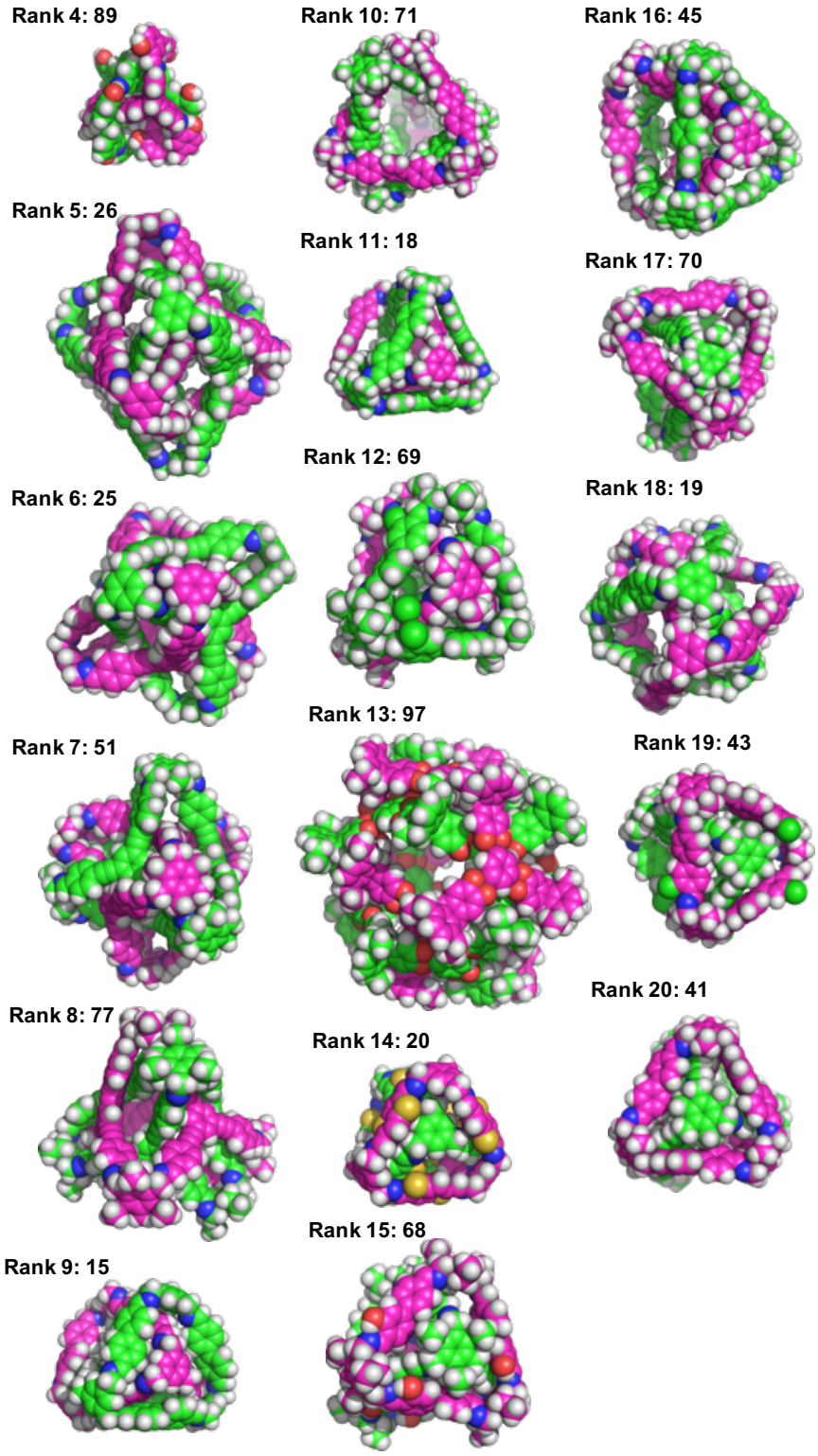


Figure S4: The molecules ranked 4 to 20 that have the most energetically favourable self-catenations. One molecule is shown with green carbons and one with pink carbons.

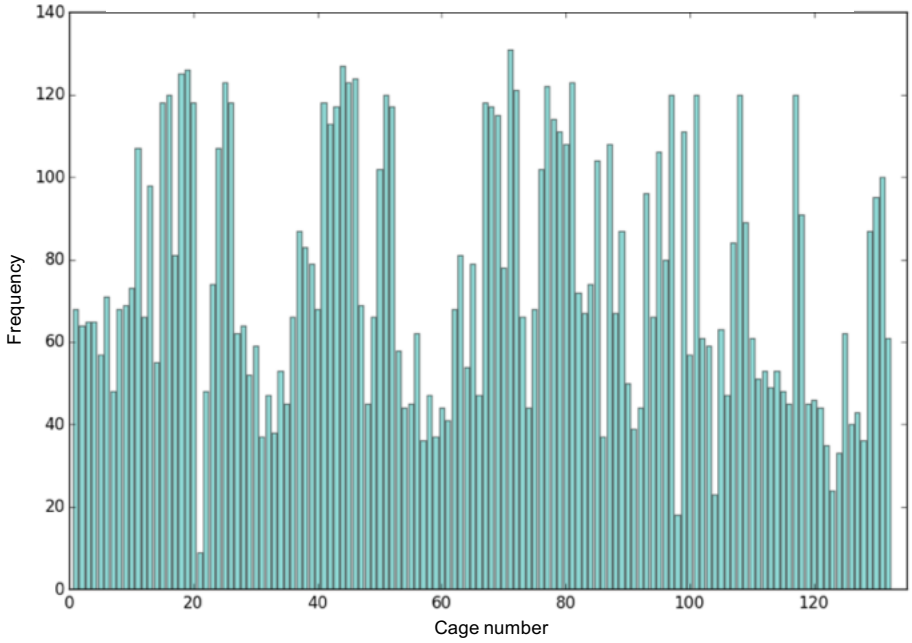


Figure S5: A histogram of the frequency a cage was found in an energetically favourable (E_b <0 kJ mol^{-1}) nested cage pair.

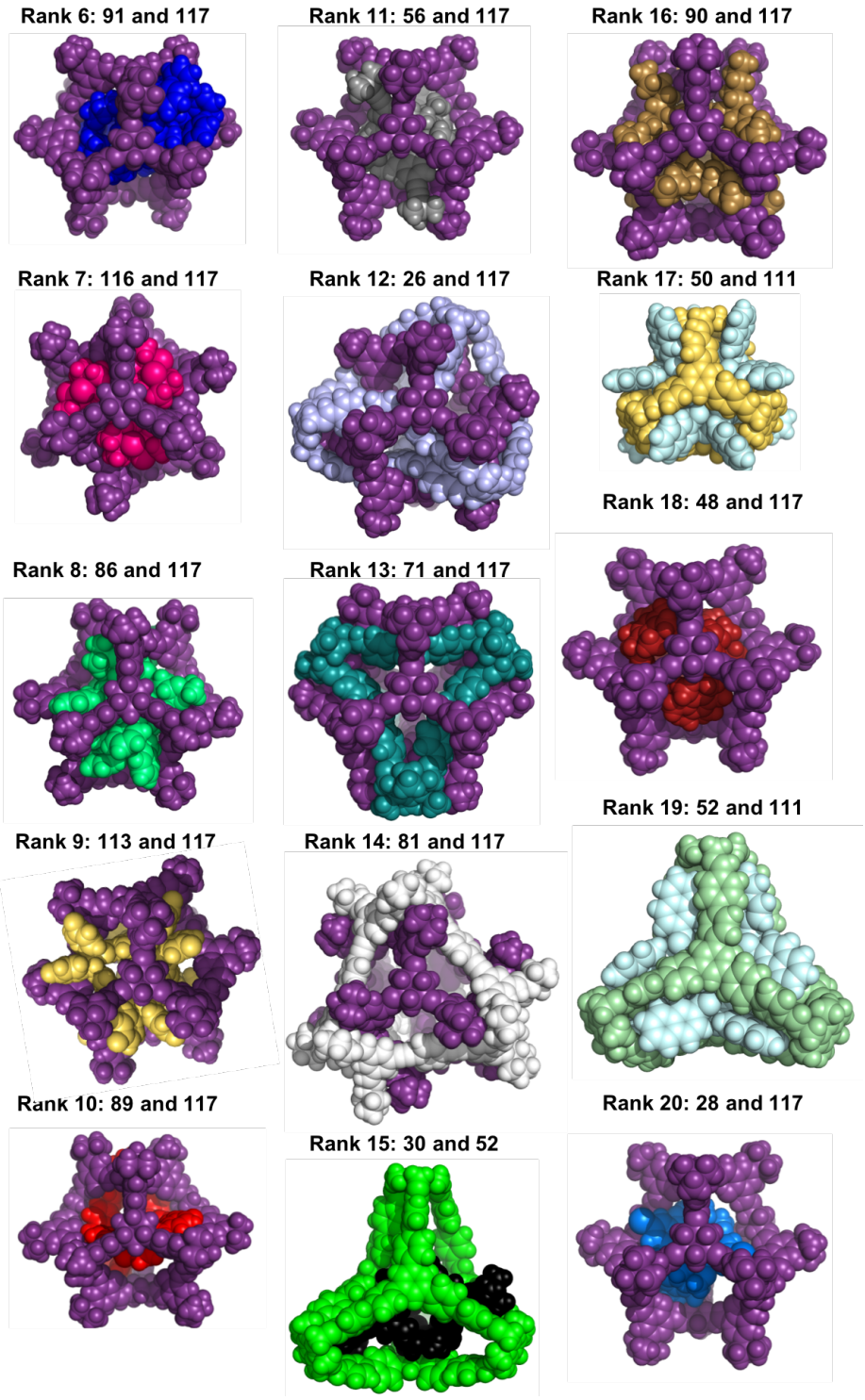


Figure S6: The molecules ranked 6 to 20 that have the most energetically favourable cage-in-a-cage complexes. Cage colouring as follows: **117**, purple; **91**, royal blue; **116**, pink; **86**, mint green; **113**, yellow; **89**, red; **56**, grey; **26**, lilac; **71**, cyan; **81**, white; **30**, bright green; **52**, black; **90**, brown; **50**, pale cyan; **111**, gold; **48**, dark red; **52** pale mint green and **28**, marine blue.

Table S3: A list of which cages meet the criteria for "List 1" and "List 2". "List 1" refers to cages made from precursors that are commercially available or have easily synthesisable precursors and "List 2" refers to cages that meet "List 1" requirements, but are also known to form readily and cleanly, with good yields.

Cage ID	List1	List2
1	✓	
2	✓	
3	✓	
4	✓	
5	✓	
6	✓	
7	✓	
8	✓	
9	✓	
10	✓	
11	✓	✓
12	✓	
13	✓	
14	✓	
15	✓	
16	✓	
17	✓	
18	✓	
19	✓	
20	✓	
21	✓	
22	✓	
23	✓	
24	✓	
25	✓	
26	✓	
27	✓	✓
28	✓	✓
29	✓	
30	✓	✓
31	✓	✓
32	✓	✓
33	✓	
34	✓	✓
35	✓	✓
36	✓	
37	✓	✓

38	✓		
39	✓	✓	
40	✓		
41	✓	✓	
42	✓		
43	✓		
44	✓	✓	
45	✓		
46	✓		
47	✓		
48	✓		
49	✓	✓	
50	✓	✓	
51	✓	✓	
52	✓	✓	
53	✓	✓	
54	✓	✓	
55	✓		
56	✓	✓	
57	✓	✓	
58	✓	✓	
59	✓		
60	✓	✓	
61	✓	✓	
62	✓		
63	✓	✓	
64	✓		
65	✓	✓	
66	✓		
67	✓	✓	
68	✓		
69	✓		
70	✓	✓	
71	✓		
72	✓	✓	
73	✓	✓	
74	✓	✓	
75	✓	✓	
76	✓	✓	
77	✓	✓	
78	✓	✓	
79	✓		
80	✓		
81	✓		
82			

83	✓	✓
84		
85	✓	
86		
87	✓	✓
88	✓	✓
89	✓	
90	✓	✓
91		
92	✓	✓
93	✓	✓
94	✓	✓
95	✓	✓
96		
97	✓	✓
98	✓	✓
99	✓	✓
100	✓	✓
101	✓	✓
102	✓	✓
103	✓	
104	✓	✓
105		
106	✓	✓
107	✓	✓
108	✓	✓
109	✓	✓
110	✓	✓
111	✓	✓
112	✓	✓
113	✓	
114	✓	✓
115	✓	✓
116	✓	✓
117	✓	✓
118	✓	✓
119	✓	✓
120	✓	✓
121	✓	✓
122	✓	✓
123	✓	
124	✓	✓
125	✓	✓
126	✓	✓
127	✓	✓

128	✓	✓
129	✓	✓
130	✓	✓
131	✓	✓
132	✓	✓

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