Supplementary Information

[6+6] Schiff-base Macrocycles With 12 Imines: Giant Analogues of Cyclohexane

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Table of Contents

Experimental

Materials: Deuterated solvents were obtained from Cambridge Isotope Laboratories, Inc.. Chloroform, acetonitrile and ethanol were purged with nitrogen gas before use. 4,6-Diformylresorcinol (**3**),[1] 4,5-diamino-1,2-dialkoxybenzene (**4**)[2] and 3,6-diformyl-2,7-dihydroxynaphthalene (**6**)[3] were prepared according to literature methods.

Equipment: All reactions were carried out under nitrogen unless otherwise noted. The 300MHz ^{1}H and 75.5 MHz ^{13}C NMR spectra were recorded on a Bruker AV-300 spectrometer. IR spectra were obtained from dispersions in potassium bromide using a Bomens MB-series spectrometer. UV-Vis spectra were performed in HPLC grade dichloromethane and distilled THF on a Varian Cary 5000 UV-Vis/near-IR spectrometer using a 1 cm cuvette. Matrix assisted laser desorption/ionization (MALDI) mass spectra were obtained at the UBC Microanalytical Services Laboratory on a Bruker Biflex IV time-of-flight (TOF) mass spectrometer equipped with a MALDI ion source. Samples were analyzed in a dithranol matrix. Electrospray (ESI) mass spectra were obtained at the UBC Microanalytical Services Laboratory on a Micromass LCT time-of-flight (TOF) mass spectrometer equipped with an electrospray ion source. The sample was analyzed in methanol:dichloromethane at 1 μM. Melting points were obtained on a Fisher-John's melting point apparatus and are corrected. Isotope pattern simulations were performed with Isopro 3.0 (MS/MS Software). Fragments were calculated using ChemDraw Ultra 8.0 (CambridgeSoft Corp., Cambridge, MA, USA).

Note about characterization: We have provided characterization of the macrocycles that proves unequivocally that the [6+6] macrocycles have been prepared. We have worked hard to obtain solution ^{1}H NMR spectra of these macrocycles, but this has proven to be very difficult for 2 reasons: (1) solubility – the macrocycles are not very soluble in any solvents; and (2) aggregation – macrocycle **1a** is barely soluble enough to obtain a ^{1}H NMR spectrum, but it is always very broad and ill-defined. We have observed this with other macrocycles and it is attributed to aggregation. Attempts to overcome this by using solvent mixtures or high temperature NMR were unsuccessful. It is not surprising that these macrocycles aggregate strongly in solution.

Synthesis of Macrocycle 1a via Compound 5a. 4,6-Diformylresorcinol (**3**) (0.0334 g, 0.201 mmol) was added to a 100 mL Schlenk flask, which contained a solution mixture of chloroform (25 mL) and acetonitrile (30 mL), under nitrogen. Compound **5a** (0.150 g, 0.201 mmol) was then added to the flask under nitrogen, giving a red solution. The mixture was stirred at 90 ºC for 24 h. A dark red precipitate that formed during the reaction period was isolated by filtration and followed by trituration with hot dichloromethane to yield macrocycle **1a** (0.033 g, 0.013 mmol, 19%).

Synthesis of Macrocycle 1a (one-pot [6+6]). 4,6-Diformylresorcinol (**3**) (0.133 g, 0.803 mmol) and 4,5-diamino-1,2-dihexyloxybenzene (**4a**) (0.248 g, 0.803 mmol) were added to a 100 mL Schlenk flask under nitrogen. Chloroform (25 mL) and acetonitrile (30 mL) were added via syringe into the flask, giving an orange solution. The mixture was stirred under an atmosphere of N_2 at 90 ºC, and the solution turned to deep red after stirring for a

few hours. After 3 d at 90 ºC, the mixture was cooled to room temperature, at which point a red solid slowly precipitated out. The red solid was isolated by filtration, triturated with hot dichloromethane, and dried under vacuum to yield macrocycle **1a** (0.005g, 0.0019 mmol, 1.4%).

Data for 1a. MALDI-TOF-MS: m/z = 2631.1; IR (KBr): υ = 3459 (m), 2929 (m), 2858 (s), 1631 (vs), 1509 (s), 1466 (m), 1333 (m), 1266 (m), 1177 (s), 1154 (s), 1000 (m), 846 (w), 755 (w), 698 (w) cm^{-1}. UV-Vis (THF): λ_{max} (ε) = 256 ($1.30x10^4$), 294 ($1.95x10^4$), 313 ($2.00x10^4$), 376 ($1.79x10^4$), 488 ($9.91x10^5$) nm ($cm^{-1}M^{-1}$); Anal. Calc'd for **1a** · H_2O ($C_{156}H_{206}N_{12}O_{25}$): 70.72% C, 7.84% H, 6.34% N; Found: 70.59% C, 7.85% H, 6.61% N.

Synthesis of Macrocycle 1b. 4,6-Diformylresorcinol (**3**) (0.0721 g, 0.434 mmol) was added to a 100 mL Schlenk flask containing a mixture of chloroform (25 mL) and acetonitrile (30 mL) under nitrogen. Compound **5b** (0.300 g, 0.434 mmol) was then added to flask, giving a red solution. The mixture was stirred at 90 ºC for 24 h. A bright red precipitate formed during the reaction period. The product was isolated by filtration, triturated with hot dichloromethane, and dried under vacuum to yield macrocycle **1b** (0.088 g, 0.036 mmol, 25%).

Data for 1b. MALDI-TOF-MS : m/z = 2463.3; IR (KBr): υ = 3427 (w), 2953 (s), 2932 (s), 2869 (m), 1628 (vs), 1607 (vs), 1579 (vs), 1507 (vs), 1468 (m), 1364 (m), 1321 (w), 1261 (s), 1177 (vs), 1158 (s) 1074 (w), 1048 (w), 989 (m), 929 (w), 890 (w), 848 (m),

729 (w) cm^{-1}. Anal. Calc'd for **1b** · $4H_2O$ ($C_{144}H_{188}N_{12}O_{28}$): 68.22% C, 7.47% H, 6.63% N; Found: 67.88% C, 7.27% H, 6.93% N.

Synthesis of Macrocycle 2a (one-pot [6+6]). 3,6-Diformyl-2,7-dihydroxynaphthalene (**6**) (0.0271 g, 0.125 mmol) and 4,5-diamino-1,2-dihexyloxybenzene (**4a**) (0.0387 g, 0.125 mmol) were added to a 100 mL Schlenk flask under nitrogen. Chloroform (17.5 mL) and acetonitrile (17.5 mL) were added via syringe into the flask, giving an orange solution. The mixture was stirred under an atmosphere of N_2 at 90 ºC for 2 d. An orange precipitate formed after stirring overnight, which was then isolated by filtration. The product was triturated with hot dichloromethane and dried under vacuum to yield macrocycle **2a** (0.048 g, 0.016 mmol, 78 %).

Data for 2a. MALDI-TOF-MS : m/z = 2930.6; IR (KBr): υ = 2954 (s), 2929 (s), 2859 (s), 1638 (vs), 1606 (vs), 1502 (s), 1468 (s), 1408 (w), 1359 (s), 1260 (s), 1203 (m), 1143 (s) 1015 (m), 904 (w), 871 (w), 803 (m) cm^{-1}. Anal. Calc'd for **2a** · $4H_2O$ ($C_{180}H_{224}N_{12}O_{28}$): 71.97% C, 7.52% H, 5.60% N; Found: 71.83% C, 7.43% H, 5.78% N.

Synthesis of Compound 5a. 4,6-Diformylresorcinol (**3**) (0.100 g, 0.602 mmol) and 4,5-diamino-1,2-dihexyloxybenzene (**4a**) (0.371 g, 1.20 mmol) were added to a 100 mL Schlenk flask under nitrogen. Ethanol (40 mL) was added via syringe into the flask, giving an orange solution and orange-red solid. The mixture was stirred at ambient temperature for 2 d, giving a red precipitate with an orange-red supernatant solution. The

red precipitate was isolated by filtration and dried under vacuum to give compound **5a** (0.425 g, 0.569 mmol, 94%).

Data for 5a. ^{1}H NMR (300 MHz, chloroform-d_1) δ 14.01 (s, 2H, O*H*), 8.43 (s, 2H, C*H*=N), 7.36 (s, 1H, aromatic C*H*), 6.71 (s, 2H, aromatic C*H*), 6.51 (s, 1H, aromatic C*H*), 6.32 (s, 2H, aromatic C*H*), 3.94 (t, 8H, OCH_2), 3.86 (broad, 4H, NH_2), 1.76 (m, 8H, CH_2), 1.42 (m, 8H, CH_2), 1.33 (m, 16H, CH_2), 0.89 (t, 12H, CH_3); ^{13}C NMR (75.5 MHz, chloroform-d_1) δ 166.7 (*C*H=N), 158.9, 151.8, 143.7, 137.8, 137.4, 127.8, 115.0, 107.8, 105.5, 103.8 (aromatic *C*H), 72.6, 70.6 (O*C*H_2), 33.1, 33.0, 31.0, 30.6, 27.1, 24.0 (*C*H_2), 15.4 (*C*H_3); ESI-MS: m/z = 747.6 ($(M+H)^+$, 10%), 769.6 ($(M+Na)^+$, 100 %); IR (KBr): υ = 3394 (m), 3292 (w), 3168 (m), 2955 (s), 2928 (s), 2856 (s), 1634 (vs), 1576 (s), 1522 (vs), 1466 (s), 1429 (s), 1388 (m), 1363 (s), 1332 (s), 1289 (vs), 1261 (s), 1241 (s), 1229 (w), 1207 (m), 1178 (vs), 1165 (m), 1137 (m), 1069 (w), 1045 (m), 1014 (w), 997 (m), 951 (m), 930 (w), 906 (w), 872 (w), 838 (s), 787 (w), 758 (w), 721 (w) cm^{-1}; UV-Vis (dichloromethane): λ_{max} (ε) = 262 ($2.91x10^4$), 289 ($3.20x10^4$), 418 ($3.48x10^4$) nm (M^{-1} cm^{-1}); Mp 120-121 ºC.

Synthesis of Compound 5b. 4,6-Diformylresorcinol (**3**) (0.600 g, 3.61 mmol) and 4,5-diamino-1,2-dipentyloxybenzene (**4b**) (2.330 g, 8.31 mmol) were added to a 250 mL Schlenk flask under nitrogen. Ethanol (150 mL) was added via syringe into the flask, giving an orange solution and orange-red solid. The mixture was stirred at ambient temperature for 2 d, giving a red precipitate with an orange-red supernatant solution. The

red precipitate was isolated by filtration and dried under vacuum to give compound **5b** (2.423 g, 3.50 mmol, 97%).

Data for 5b. ^{1}H NMR (300 MHz, chloroform-d_1) δ 13.99 (s, 2H, O*H*), 8.47 (s, 2H, C*H*=N), 7.40 (s, 1H, aromatic C*H*), 6.73 (s, 2H, aromatic C*H*), 6.53 (s, 1H, aromatic C*H*), 6.35 (s, 2H, aromatic C*H*), 3.95 (t, 8H, OCH_2), 3.78 (broad, 4H, NH_2), 1.79 (m, 8H, CH_2), 1.40 (m, 16H, CH_2), 0.92 (t, 12H, CH_3); ^{13}C NMR (75.5 MHz, chloroform-d_1) δ 165.2 (*C*H=N), 157.4, 157.3, 150.4, 142.2, 135.9, 126.4, 113.6, 106.4, 104.0, 102.3 (aromatic *C*H), 71.2, 69.1 (O*C*H_2), 29.3, 28.9, 28.2, 22.5, 22.4 (*C*H_2), 14.0 (*C*H_3); ESI-MS: m/z = 691.4 ($(M+H)^+$, 100%); IR (KBr): υ = 3395 (w), 3177 (w), 2956 (s), 2932 (s), 2860 (m), 1629 (vs), 1521 (vs), 1509 (vs), 1467 (s), 1432 (s), 1389 (m), 1364 (m), 1330 (m), 1287 (s), 1261 (s), 1245 (m), 1205 (m), 1179 (s), 1135 (s), 1074 (w), 1051 (m), 1025 (m), 988 (m), 940 (w), 838 (s), 801 (m), 727 (w) cm^{-1}; Anal. Calc'd for **5b** ($C_{40}H_{58}N_4O_6$): 69.54% C, 8.46% H, 8.11% N; Found: 69.55% C, 8.10% H, 8.50% N.

References

(1) L. R. Worden, K. D. Kaufman, P. J. Smith and G. N. Widiger, *J. Chem. Soc., Chem. Commun.,* 1970, 227-230.

(2) (a) D.-H. Kim, M. J. Choi, and S.-K. Chang, *Bull. Korean Chem. Soc.,* 2000, **21**, 145-147. (b) I. Yilmaz and Ö. Bekâroğlu, *J. Chem. Res.,* 1998, (S) 374-375; (M) 1585-1594.

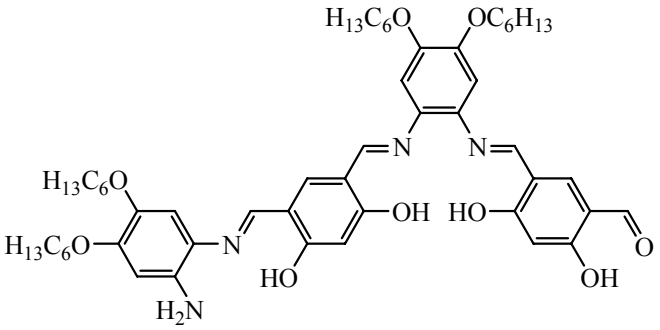
(3) T. J. Katz, L. Liu, N. D. Willmore, J. M. Fox, A. L. Rheingold, S. Shi, C. Nuckolls and B. H. Rickman, *J. Am. Chem. Soc.*, 1997, **119**, 10054-10063.

Table S1. Fragments Observed in MALDI-TOF Spectrum of Crude **1a** (from Figure 1a).

Fragment	Calculated Mass[a]	Observed Mass[a]
A	894.5	894.9
B	1042.5	1042.8
C	1184.8	1185.1
D	1332.8	1332.6
E	1480.8	1481.5
F	1772.0	1772.3
G	1920.0	1918.3
H	2192.3	2191.5
I	2210.3	2209.1
J	2358.3	2357.0
K	2630.5	2631.7
L	2796.5	2794.7

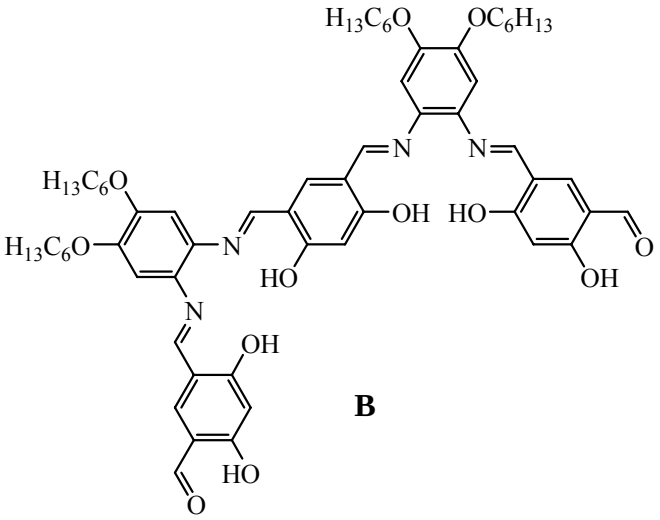
[a] Most intense peak calculated and measured.

Structures of Fragments



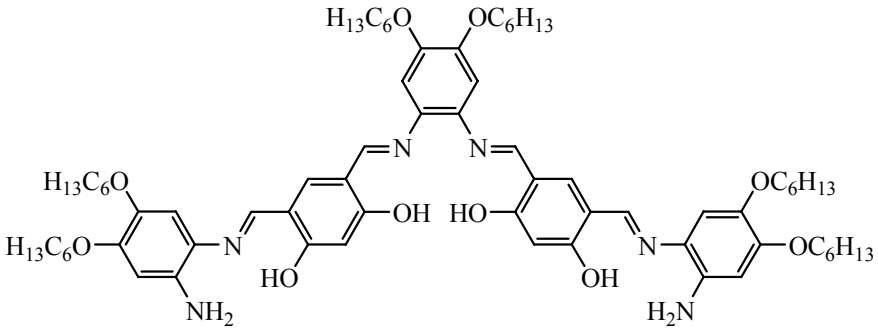
A

$C_{52}H_{70}N_4O_9$
Exact Mass: 894.51
Mol. Wt.: 895.13
m/e: 894.51 (100.0%), 895.52 (57.4%), 896.52 (18.0%),
897.52 (4.1%), 895.51 (1.5%)
C, 69.77; H, 7.88; N, 6.26; O, 16.09



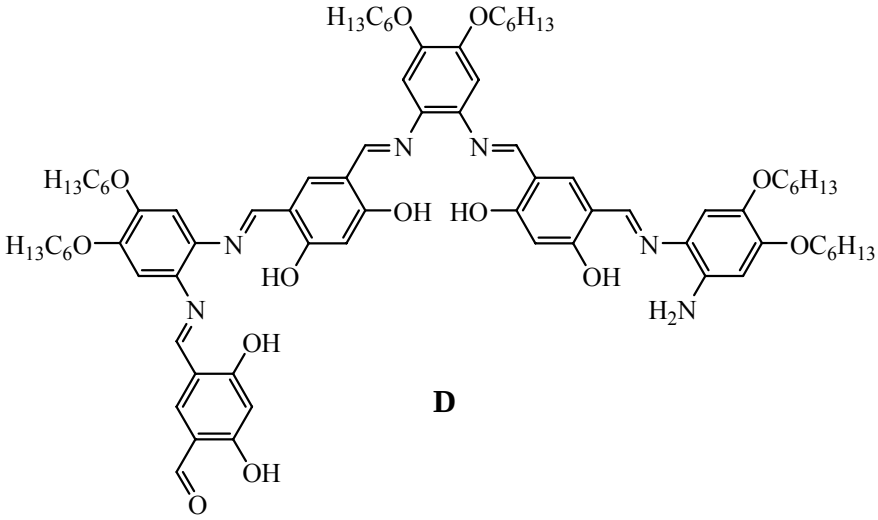
B

$C_{60}H_{74}N_4O_{12}$
Exact Mass: 1042.53
Mol. Wt.: 1043.25
m/e: 1042.53 (100.0%), 1043.53 (66.8%), 1044.54 (21.6%),
1045.54 (6.2%), 1044.53 (3.4%), 1046.54 (1.3%)
C, 69.08; H, 7.15; N, 5.37; O, 18.40



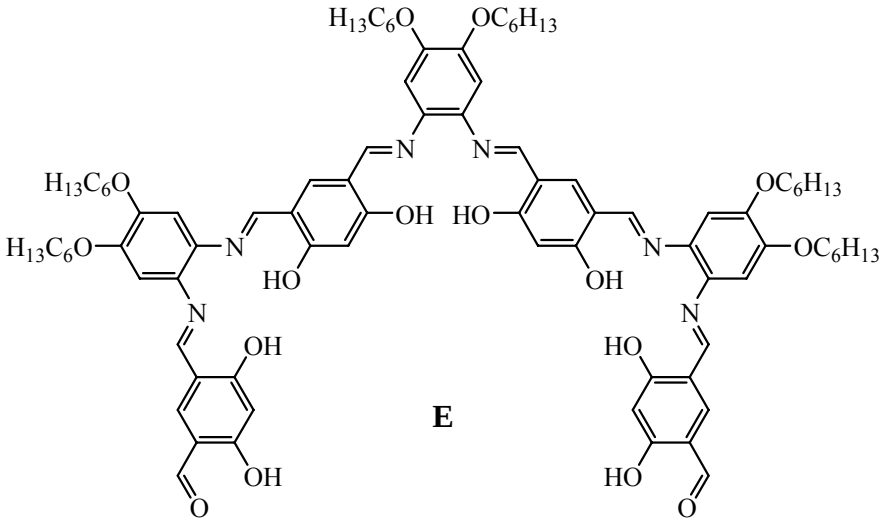
C

$C_{70}H_{100}N_6O_{10}$
Exact Mass: 1184.75
Mol. Wt.: 1185.58
m/e: 1184.75 (100.0%), 1185.75 (78.3%), 1186.76 (29.4%),
1187.76 (9.0%), 1186.75 (3.8%), 1188.76 (2.1%), 1185.76 (1.2%)
C, 70.91; H, 8.50; N, 7.09; O, 13.50



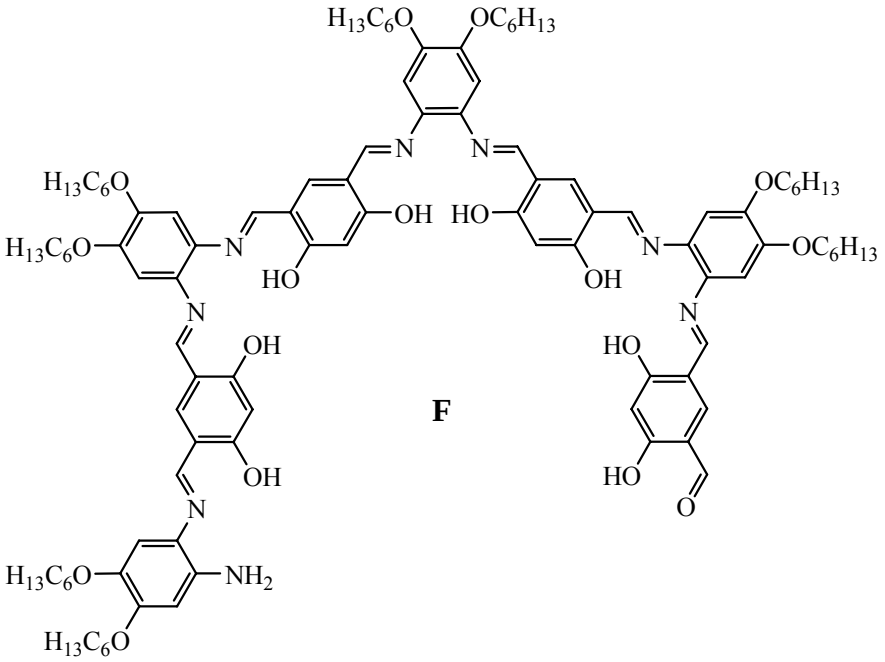
D

$C_{78}H_{104}N_6O_{13}$
Exact Mass: 1332.77
Mol. Wt.: 1333.69
m/e: 1332.77 (100.0%), 1333.77 (86.1%), 1334.77 (40.1%), 1335.78 (10.3%),
1335.77 (3.1%), 1336.78 (3.1%), 1333.76 (2.2%), 1334.78 (1.0%)
C, 70.24; H, 7.86; N, 6.30; O, 15.60



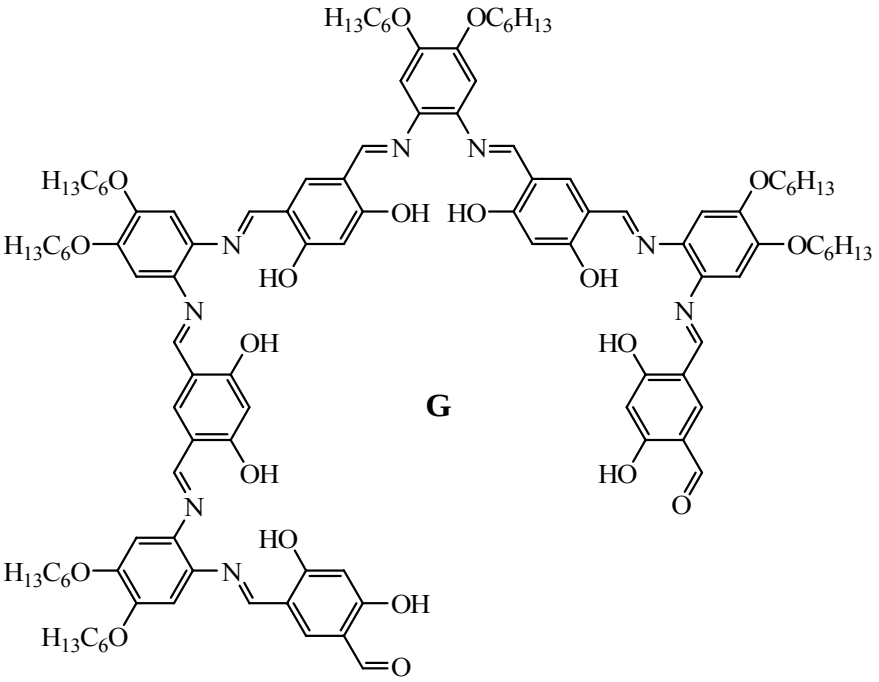
E

$C_{86}H_{108}N_6O_{16}$
Exact Mass: 1480.78
Mol. Wt.: 1481.81
m/e: 1480.78 (100.0%), 1481.79 (94.9%), 1482.79 (47.8%), 1483.79 (17.3%), 1484.80 (3.2%), 1481.78 (2.2%), 1482.78 (2.1%), 1484.79 (1.8%), 1485.80 (1.0%)
C, 69.71; H, 7.35; N, 5.67; O, 17.28



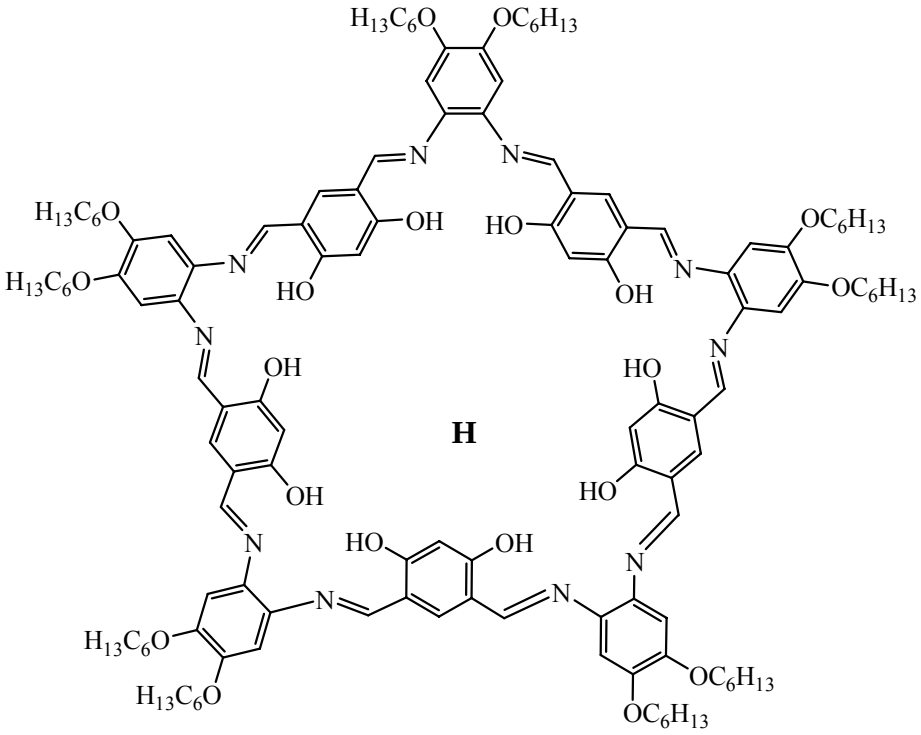
F

$C_{104}H_{138}N_8O_{17}$
Exact Mass: 1771.02
Mol. Wt.: 1772.25
m/e: 1772.02 (100.0%), 1771.02 (85.0%), 1773.02 (59.1%), 1774.03 (24.2%), 1775.03 (8.4%), 1773.03 (2.1%), 1776.03 (2.1%), 1774.02 (1.8%)
C, 70.48; H, 7.85; N, 6.32; O, 15.35



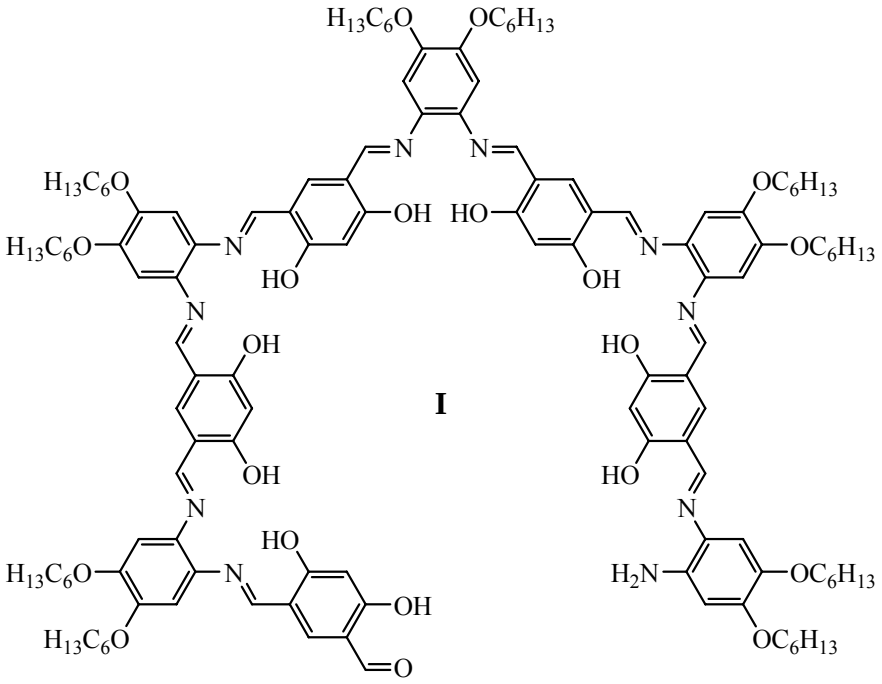
G

$C_{112}H_{142}N_8O_{20}$
Exact Mass: 1919.03
Mol. Wt.: 1920.37
m/e: 1920.04 (100.0%), 1919.03 (81.0%), 1921.04 (64.6%), 1922.04 (29.8%), 1923.05 (7.5%), 1923.04 (3.3%), 1921.03 (2.9%), 1924.05 (2.8%), 1920.03 (2.4%)
C, 70.05; H, 7.45; N, 5.84; O, 16.66



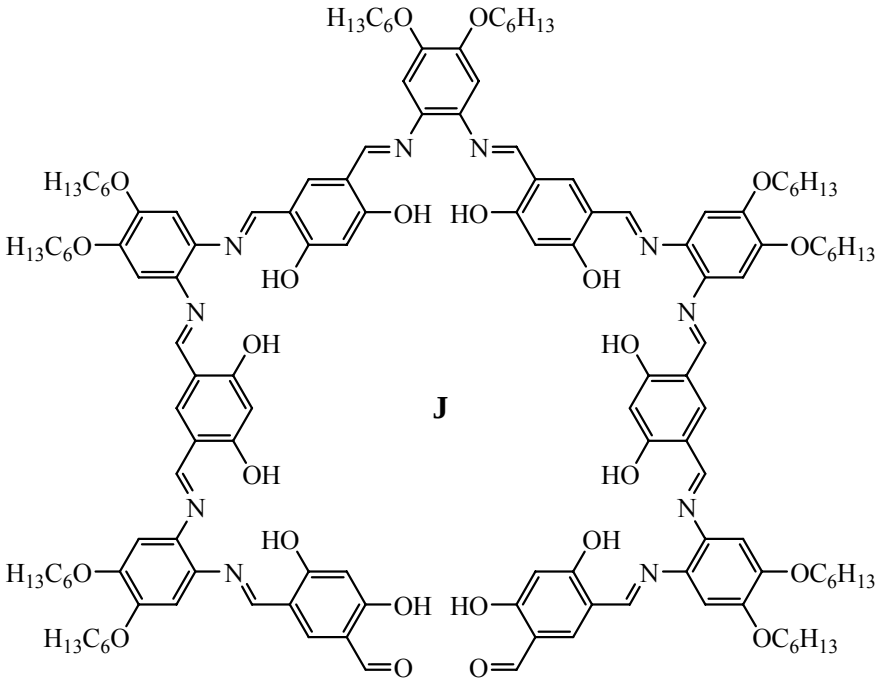
H

$C_{130}H_{170}N_{10}O_{20}$
Exact Mass: 2191.26
Mol. Wt.: 2192.8
m/e: 2192.26 (100.0%), 2193.27 (70.3%), 2191.26 (68.9%), 2194.27 (37.2%), 2195.27 (15.1%), 2193.26 (6.5%), 2196.28 (3.2%), 2194.26 (2.7%), 2196.27 (1.9%), 2192.27 (1.3%), 2197.28 (1.1%)
C, 71.21; H, 7.81; N, 6.39; O, 14.59



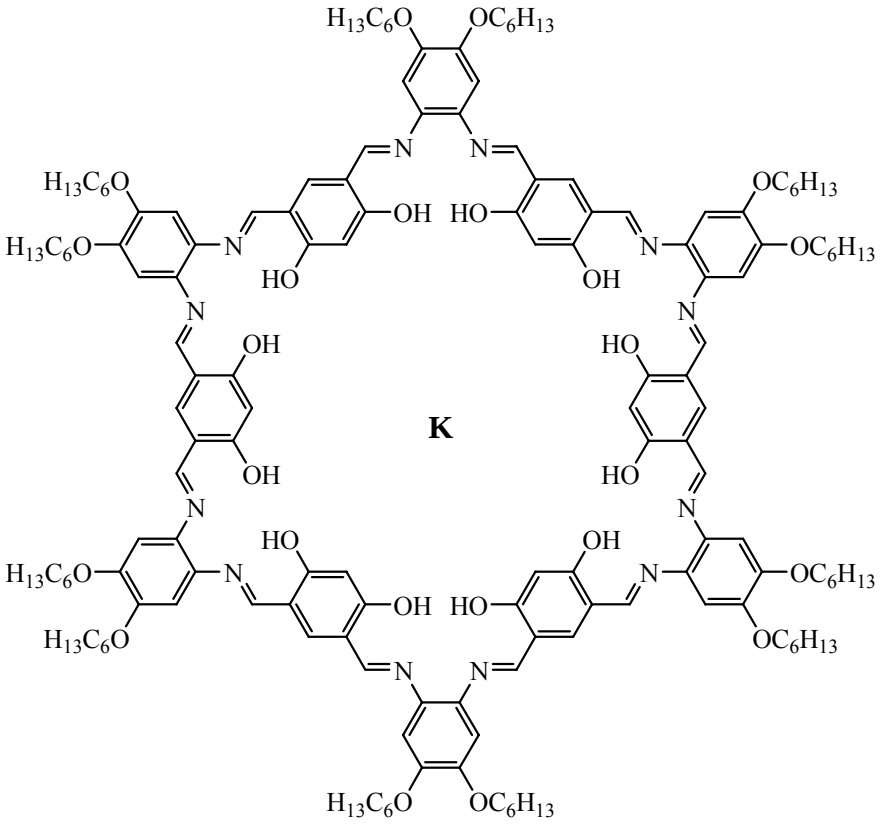
I

$C_{130}H_{172}N_{10}O_{21}$
Exact Mass: 2209.27
Mol. Wt.: 2210.81
m/e: 2210.27 (100.0%), 2211.28 (70.3%), 2209.27 (68.9%), 2212.28 (37.4%), 2213.28 (15.3%), 2211.27 (6.6%), 2214.29 (3.3%), 2212.27 (2.7%), 2214.28 (2.0%), 2210.28 (1.4%), 2215.29 (1.2%)
C, 70.63; H, 7.84; N, 6.34; O, 15.20



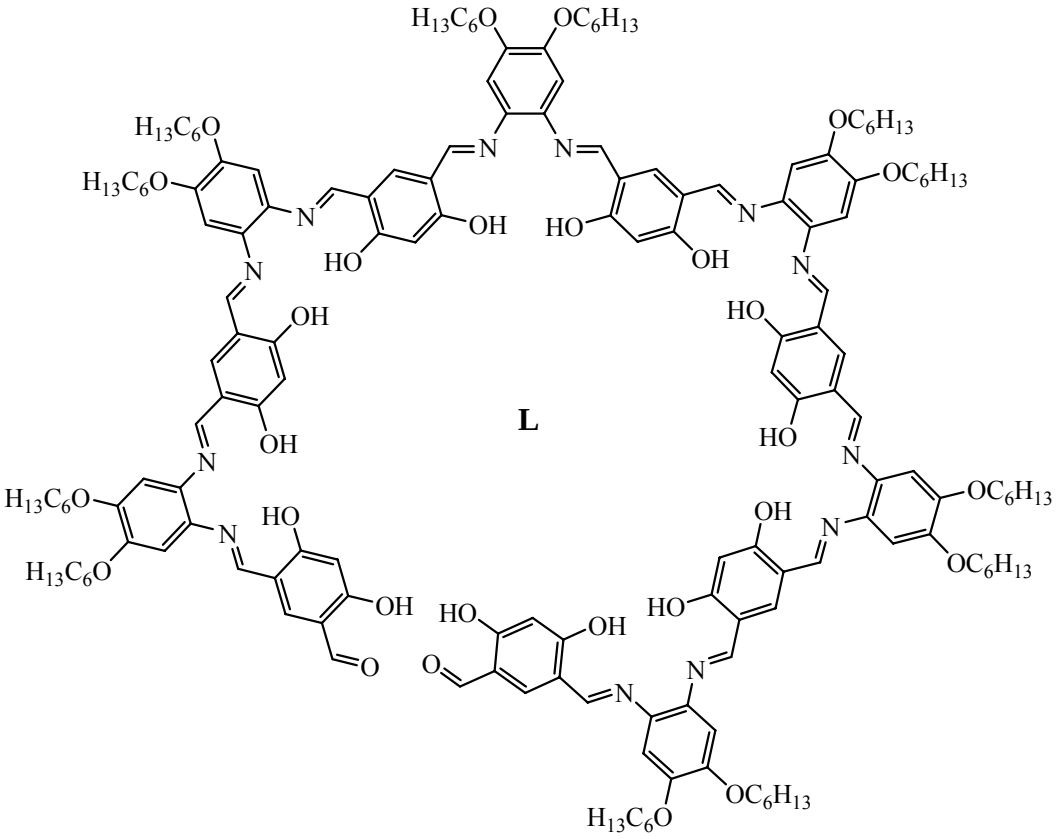
J

$C_{138}H_{176}N_{10}O_{24}$
Exact Mass: 2357.29
Mol. Wt.: 2358.93
m/e: 2358.29 (100.0%), 2359.29 (80.5%), 2357.29 (65.7%), 2360.30 (37.8%), 2361.30 (17.8%), 2360.29 (7.8%), 2362.30 (6.4%), 2358.28 (2.4%), 2359.30 (2.0%), 2361.29 (1.6%), 2363.31 (1.0%)
C, 70.26; H, 7.52; N, 5.94; O, 16.28



K

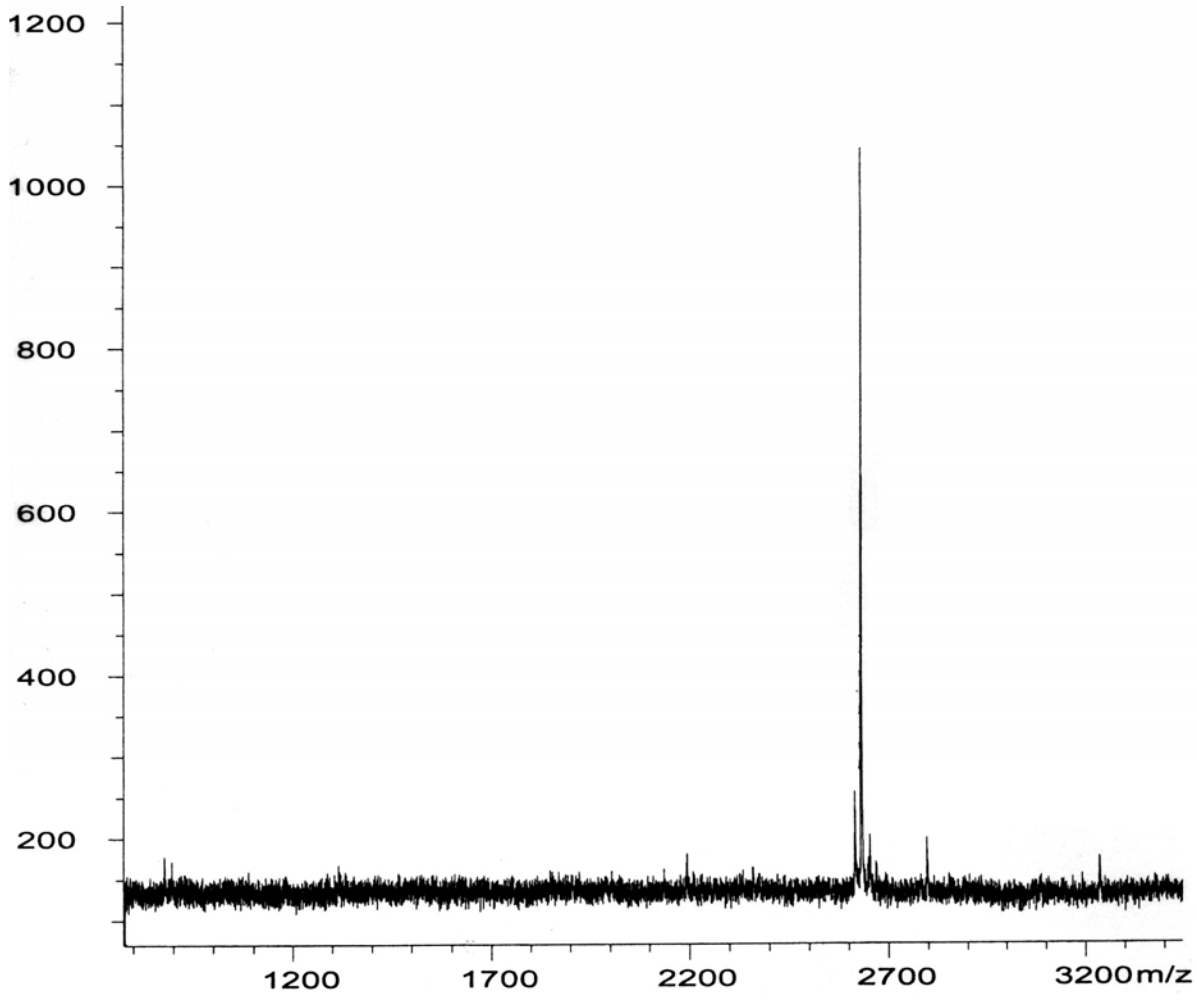
$C_{156}H_{204}N_{12}O_{24}$
Exact Mass: 2629.51
Mol. Wt.: 2631.35
m/e: 2630.51 (100.0%), 2631.52 (87.7%), 2629.51 (57.8%), 2632.52 (53.1%), 2633.52 (25.2%), 2634.53 (9.1%), 2631.51 (4.5%), 2632.51 (3.8%), 2635.53 (2.9%), 2630.52 (1.9%), 2633.53 (1.6%), 2634.52 (1.2%)
C, 71.21; H, 7.81; N, 6.39; O, 14.59



L

$C_{164}H_{210}N_{12}O_{28}$
Exact Mass: 2795.54
Mol. Wt.: 2797.49
m/e: 2796.54 (100.0%), 2797.54 (94.1%), 2798.55 (59.3%), 2795.54 (55.3%),
2799.55 (29.1%), 2800.55 (12.1%), 2798.54 (4.2%), 2801.56 (3.8%),
2797.55 (3.4%), 2799.54 (2.6%), 2796.53 (2.5%), 2802.56 (1.1%)
C, 70.41; H, 7.57; N, 6.01; O, 16.01

Figure S1. MALDI-TOF spectrum of Macrocycle **1a** (another sample).



(we include this figure to show another representative sample of macrocycle **1a**)

Figure S2. MALDI-TOF spectrum of Macrocycle **1b**.

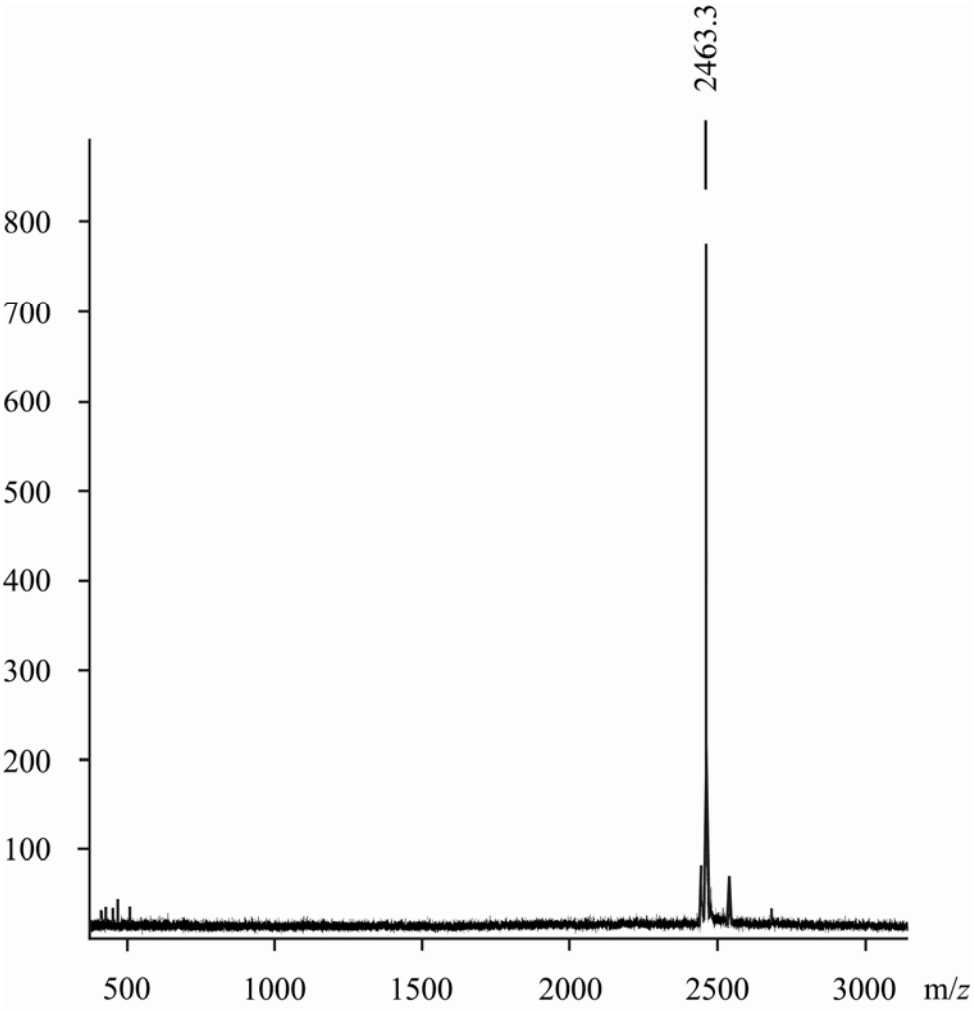
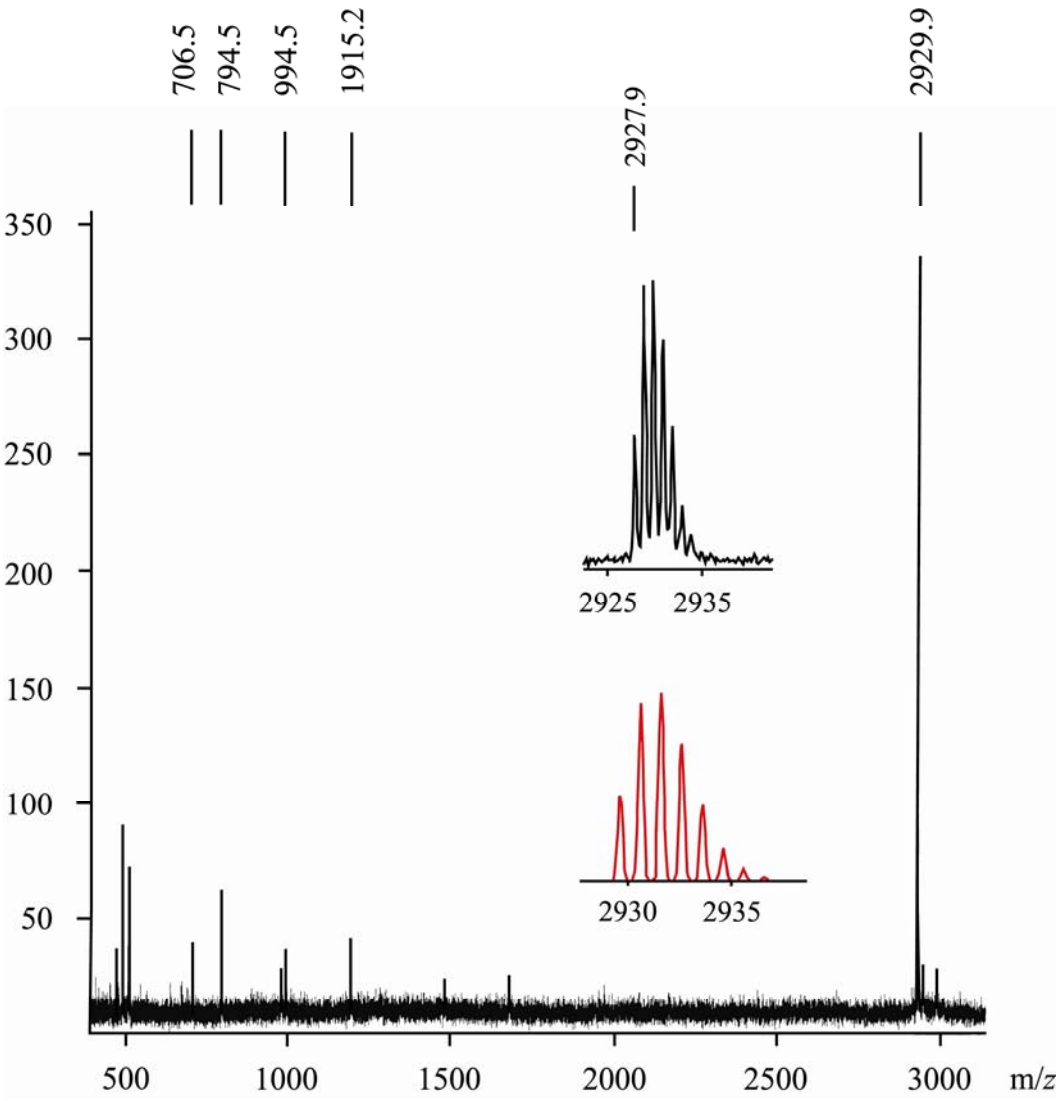


Figure S3. MALDI-TOF spectrum of Macrocycle **2a**. Insets: Experimental (top) and calculated (bottom) isotope distributions for the molecular ion.



Graphics Modification: We used Photoshop to enhance the lines in Figure 1 of the manuscript so that they were easier to see. Attempts to make them visible simply by rescanning and changing the contrast / brightness were not effective as they are really thin. We include below the original scanned figures before any modifications to show that the changes we made were simply to enhance the figures' appearances, not their content.

Figure S4: Original for Figure 1a

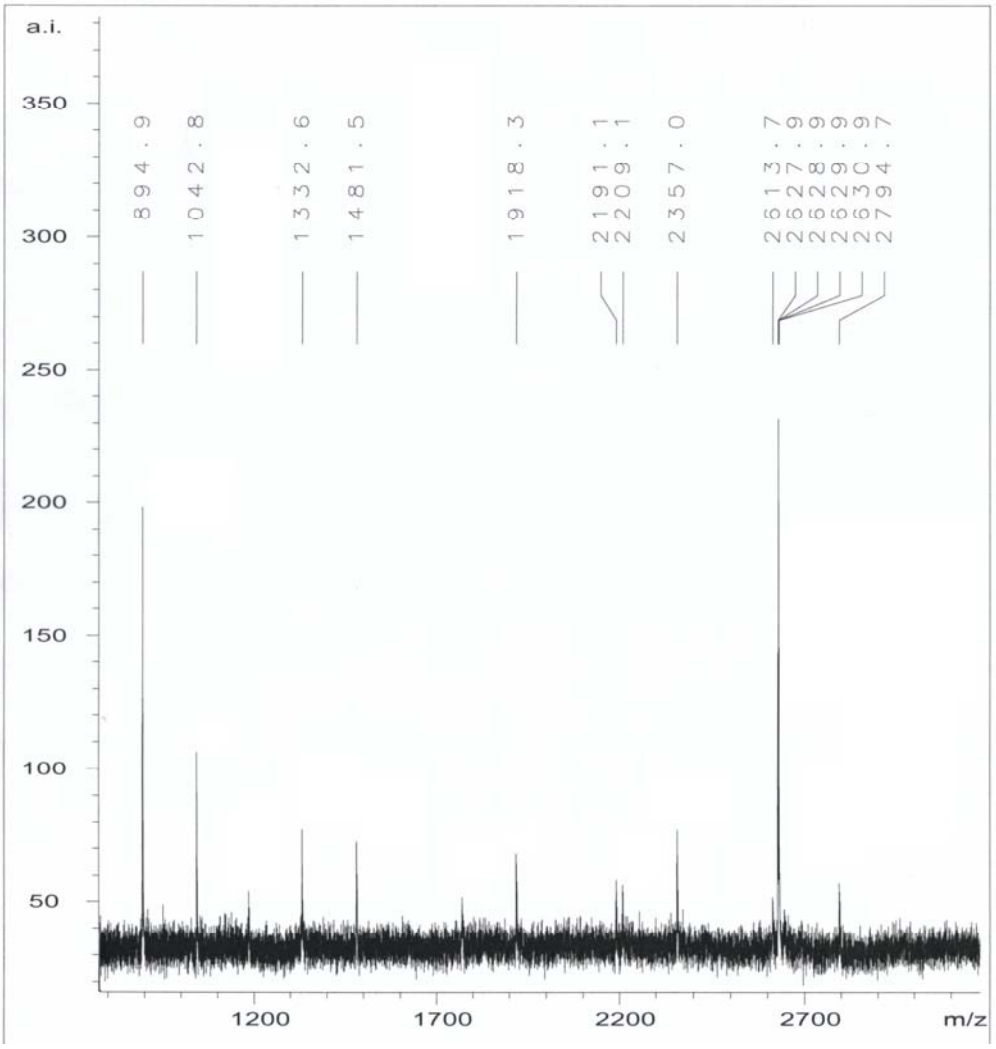


Figure S5: Original for Figure 1b

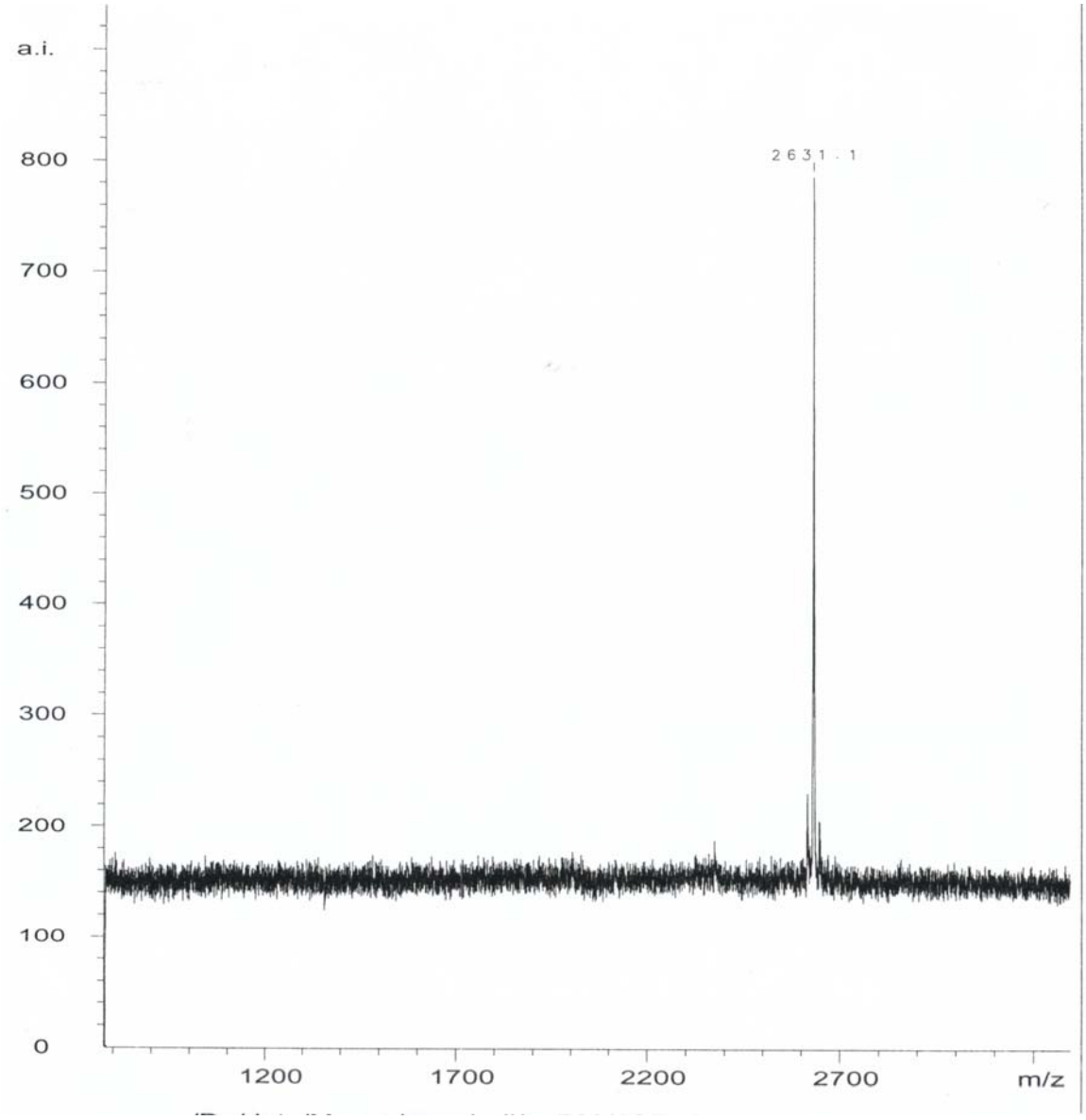
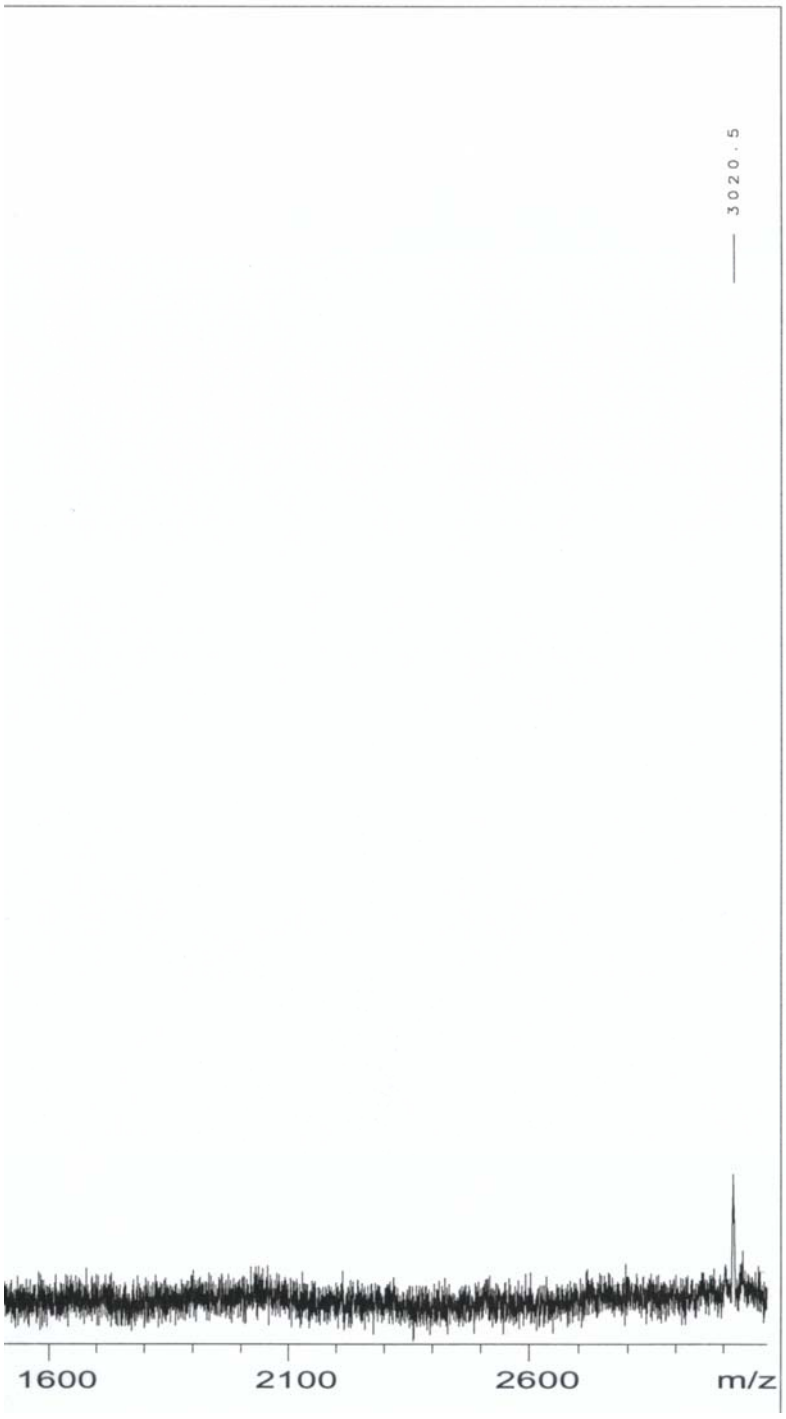


Figure S6: Original for Figure 1c



Computation Details. Semi-empirical calculations were performed on macrocycle **1c** metallated with Ni(II) using PM3 with Spartan '04 for Windows (Wavefunction: Irvine, CA) using a Pentium IV processor. Peripheral substituents on the macrocycle were truncated to H for simplicity. As well, Ni(II) was selected as the metal for calculations to ensure a square planar environment with high symmetry.

Table S2. Energies of Minimized (PM3) Structures

Conformation	**Energy (kcal / mol)**
Flat	-2750.77
Chair	-2774.39
Boat	-2777.66

Figure S7. Picture of Flat Conformation of **1c** metallated with Ni(II).

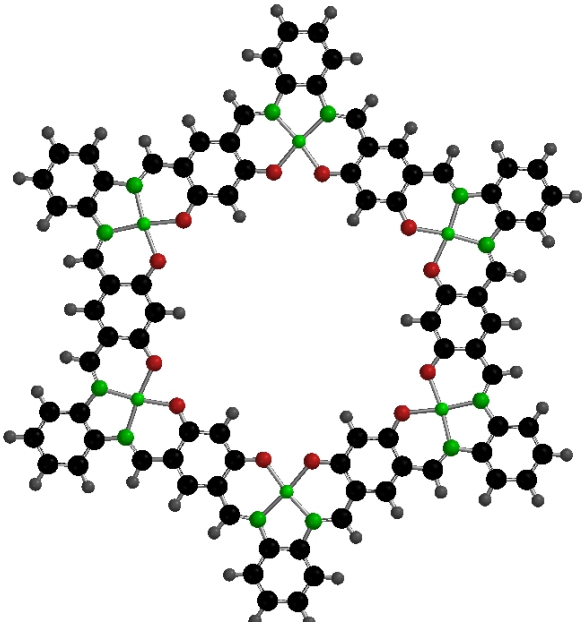


Table S3. Atomic Coordinates for Flat Conformation.

Atom	X (Å)	Y (Å)	Z (Å)
C	5.994	0	3.855
C	8.274	0	2.151
C	7.343	0	4.377
C	5.851	0	2.446
C	6.955	0	1.557
C	8.433	0	3.525
H	4.838	0	2.022
H	9.448	0	3.949
O	6.719	0	0.263
O	4.907	0	4.597
C	9.472	0	1.385
H	10.414	0	1.956
C	7.641	0	5.767
H	8.708	0	6.037
N	6.717	0	6.7
N	9.487	0	0.073
C	10.718	0	-0.665
C	12.932	0	-2.36
C	12.008	0	-0.133
C	10.538	0	-2.064
C	11.652	0	-2.904
C	13.109	0	-0.983
H	12.21	0	0.944
H	11.576	0	-3.998
C	7.056	0	8.094
C	7.406	0	10.861
C	5.935	0	8.949
C	8.342	0	8.639
C	8.51	0	10.019
C	6.119	0	10.333
H	9.25	0	8.026
H	5.287	0	11.046
N	4.68	0	8.252
C	3.536	0	8.896
H	3.513	0	9.996
N	9.161	0	-2.467
C	8.815	0	-3.733
H	9.582	0	-4.523
C	2.274	0	8.24
C	-0.341	0	7.119
C	2.129	0	6.802
C	1.164	0	9.066
C	-0.119	0	8.548
C	0.808	0	6.29
H	1.304	0	10.157
H	0.668	0	5.201
O	3.132	0	5.95

O	-1.527	0	6.548
C	-1.174	0	9.501
H	-0.874	0	10.56
N	-2.444	0	9.167
C	7.462	0	-4.171
C	4.826	0	-5.244
C	7.269	0	-5.541
C	6.336	0	-3.264
C	5.044	0	-3.844
C	5.999	0	-6.09
H	8.144	0	-6.208
H	4.17	0	-3.179
O	6.435	0	-1.951
O	3.587	0	-5.687
C	5.936	0	-7.51
H	6.901	0	-8.04
N	4.807	0	-8.179
C	-3.482	0	10.158
C	-5.703	0	11.844
C	-4.783	0	9.614
C	-3.311	0	11.544
C	-4.422	0	12.38
C	-5.889	0	10.466
H	-2.326	0	12.024
H	-6.923	0	10.102
N	-4.807	0	8.179
C	-5.936	0	7.51
H	-6.901	0	8.04
C	-5.999	0	6.09
C	-6.336	0	3.264
C	-4.826	0	5.244
C	-7.269	0	5.541
C	-7.462	0	4.171
C	-5.044	0	3.844
H	-8.144	0	6.208
H	-4.17	0	3.179
O	-3.587	0	5.687
O	-6.435	0	1.951
C	-8.815	0	3.733
H	-9.582	0	4.523
N	-9.161	0	2.467
C	4.783	0	-9.614
C	4.422	0	-12.38
C	5.889	0	-10.466
C	3.482	0	-10.158
C	3.311	0	-11.544
C	5.703	0	-11.844
H	6.923	0	-10.102
H	2.326	0	-12.024
C	-10.538	0	2.064

C	-13.109	0	0.983
C	-10.718	0	0.665
C	-11.652	0	2.904
C	-12.932	0	2.36
C	-12.008	0	0.133
H	-11.576	0	3.998
H	-12.21	0	-0.944
N	-9.487	0	-0.073
N	2.444	0	-9.167
C	1.174	0	-9.501
H	0.874	0	-10.56
C	-9.472	0	-1.385
H	-10.414	0	-1.956
C	-8.274	0	-2.151
C	-5.994	0	-3.855
C	-6.955	0	-1.557
C	-8.433	0	-3.525
C	-7.343	0	-4.377
C	-5.851	0	-2.446
H	-9.448	0	-3.949
H	-4.838	0	-2.022
O	-6.719	0	-0.263
O	-4.907	0	-4.597
C	-7.641	0	-5.767
H	-8.708	0	-6.037
N	-6.717	0	-6.7
C	0.119	0	-8.548
C	-2.129	0	-6.802
C	-1.164	0	-9.066
C	0.341	0	-7.119
C	-0.808	0	-6.29
C	-2.274	0	-8.24
H	-1.304	0	-10.157
H	-0.668	0	-5.201
C	-7.056	0	-8.094
C	-7.406	0	-10.861
C	-5.935	0	-8.949
C	-8.342	0	-8.639
C	-8.51	0	-10.019
C	-6.119	0	-10.333
H	-9.25	0	-8.026
H	-5.287	0	-11.046
N	-4.68	0	-8.252
C	-3.536	0	-8.896
H	-3.513	0	-9.996
O	-3.132	0	-5.95
O	1.527	0	-6.548
Ni	8.019	0	-1.03
Ni	4.901	0	6.43
Ni	-3.118	0	7.46

Ni	-8.019	0	1.03
Ni	-4.901	0	-6.43
Ni	3.118	0	-7.46
H	-13.805	0	3.023
H	-14.121	0	0.562
H	-6.573	0	12.51
H	-4.285	0	13.467
H	7.547	0	11.948
H	9.52	0	10.444
H	14.121	0	-0.562
H	13.805	0	-3.023
H	6.573	0	-12.51
H	4.285	0	-13.467
H	-7.547	0	-11.948
H	-9.52	0	-10.444

Table S4. Atomic Coordinates for Chair Conformation.

Atom	X (Å)	Y (Å)	Z (Å)
C	-6.646	0.467	-1.681
C	-7.049	-0.306	-4.384
C	-7.943	0.596	-2.315
C	-5.557	0.08	-2.483
C	-5.707	-0.266	-3.839
C	-8.114	0.168	-3.626
H	-4.553	0.047	-2.035
H	-9.116	0.204	-4.075
O	-4.597	-0.532	-4.482
O	-6.371	0.689	-0.419
C	-7.308	-0.841	-5.684
H	-8.364	-0.944	-5.979
C	-9.058	1.163	-1.621
H	-9.973	1.34	-2.208
N	-9.008	1.481	-0.344
N	-6.344	-1.221	-6.497
C	-6.553	-1.827	-7.778
C	-6.67	-3.038	-10.287
C	-7.741	-2.405	-8.218
C	-5.404	-1.861	-8.608
C	-5.471	-2.475	-9.856
C	-7.795	-3.003	-9.474
H	-8.64	-2.42	-7.592
H	-4.595	-2.544	-10.511
C	-10.076	2.098	0.384
C	-11.979	3.301	2.028
C	-9.932	2.051	1.793
C	-11.168	2.753	-0.179
C	-12.119	3.347	0.647

C	-10.886	2.66	2.605
H	-11.295	2.832	-1.265
H	-10.793	2.667	3.698
N	-8.741	1.401	2.251
C	-8.532	1.007	3.49
H	-9.311	1.133	4.258
N	-4.232	-1.279	-8.027
C	-3.147	-0.954	-8.699
H	-3.1	-1.094	-9.79
C	-7.294	0.429	3.912
C	-4.778	-0.428	4.91
C	-6.155	0.354	3.021
C	-7.184	-0.053	5.212
C	-5.977	-0.52	5.718
C	-4.917	-0.035	3.566
H	-8.074	-0.061	5.857
H	-4.027	-0.029	2.92
O	-6.149	0.622	1.739
O	-3.554	-0.69	5.299
C	-5.949	-1.089	7.031
H	-6.919	-1.242	7.529
N	-4.827	-1.435	7.625
C	-1.979	-0.429	-8.062
C	0.477	0.341	-6.861
C	-0.919	0.002	-8.851
C	-1.878	-0.348	-6.619
C	-0.631	-0.006	-6.064
C	0.28	0.43	-8.293
H	-1.032	0.005	-9.944
H	-0.517	-0.009	-4.971
O	-2.838	-0.577	-5.757
O	1.594	0.564	-6.213
C	1.292	0.96	-9.153
H	1.023	1.105	-10.211
N	2.49	1.287	-8.715
C	-4.743	-2.052	8.915
C	-4.298	-3.264	11.386
C	-3.45	-2.035	9.495
C	-5.791	-2.683	9.581
C	-5.565	-3.281	10.817
C	-3.237	-2.649	10.727
H	-6.797	-2.738	9.148
H	-2.244	-2.677	11.191
N	-2.444	-1.407	8.692
C	-1.259	-1.037	9.129
H	-0.983	-1.171	10.186
C	-0.267	-0.469	8.268
C	1.857	0.387	6.589
C	-0.467	-0.394	6.835
C	0.914	0.009	8.823

C	1.956	0.479	8.032
C	0.625	-0.008	6.036
H	1.027	0.016	9.916
H	0.512	-0.014	4.943
O	-1.573	-0.666	6.186
O	2.806	0.649	5.724
C	3.102	1.055	8.664
H	3.049	1.203	9.754
N	4.173	1.417	7.989
C	3.517	1.877	-9.52
C	5.675	3.04	-10.849
C	3.325	2.497	-10.753
C	4.811	1.847	-8.942
C	5.881	2.436	-9.611
C	4.407	3.071	-11.415
H	2.333	2.563	-11.216
H	6.889	2.454	-9.181
C	5.322	2.052	8.561
C	7.663	3.308	9.407
C	6.47	2.058	7.729
C	5.366	2.682	9.802
C	6.539	3.302	10.222
C	7.632	2.693	8.158
H	4.489	2.72	10.46
H	8.529	2.739	7.529
N	6.287	1.425	6.457
N	4.872	1.233	-7.65
C	5.983	0.854	-7.054
H	6.956	0.966	-7.558
C	7.263	1.071	5.648
H	8.315	1.226	5.936
C	7.022	0.493	4.362
C	6.642	-0.392	1.69
C	5.682	0.394	3.819
C	8.1	0.024	3.621
C	7.941	-0.462	2.328
C	5.542	-0.005	2.477
H	9.103	0.037	4.068
H	4.538	-0.016	2.028
O	4.564	0.655	4.451
O	6.373	-0.667	0.438
C	9.068	-1.035	1.66
H	9.989	-1.161	2.252
N	9.021	-1.423	0.402
C	5.998	0.309	-5.732
C	6.16	-0.487	-3.011
C	7.197	-0.164	-5.212
C	4.796	0.256	-4.925
C	4.927	-0.102	-3.57
C	7.3	-0.602	-3.897

H	8.087	-0.189	-5.856
H	4.037	-0.079	-2.926
C	10.097	-2.065	-0.293
C	12.01	-3.34	-1.87
C	9.949	-2.103	-1.702
C	11.199	-2.671	0.303
C	12.155	-3.302	-0.49
C	10.907	-2.749	-2.48
H	11.332	-2.683	1.391
H	10.809	-2.821	-3.57
N	8.751	-1.49	-2.193
C	8.537	-1.165	-3.451
H	9.314	-1.333	-4.213
O	6.149	-0.72	-1.722
O	3.576	0.521	-5.325
Ni	-4.551	-0.93	-6.256
Ni	-7.647	1.079	0.816
Ni	-3.132	-1.078	7.025
Ni	4.505	1.066	6.221
Ni	7.654	-1.105	-0.776
Ni	3.167	0.93	-7.05
H	13.021	-3.778	-0.018
H	12.761	-3.848	-2.485
H	6.519	3.502	-11.373
H	4.253	3.557	-12.384
H	-6.719	-3.52	-11.269
H	-8.732	-3.457	-9.818
H	-12.977	3.862	0.201
H	-12.727	3.779	2.669
H	-6.391	-3.776	11.339
H	-4.127	-3.745	12.355
H	6.57	3.797	11.199
H	8.579	3.807	9.742

Table S5. Atomic Coordinates for Boat Conformation.

Atom	X (Å)	Y (Å)	Z (Å)
C	-6.381	2.128	-1.658
C	-6.665	2.591	-4.448
C	-7.622	2.623	-2.213
C	-5.306	1.895	-2.533
C	-5.411	2.097	-3.92
C	-7.721	2.853	-3.582
H	-4.355	1.527	-2.12
H	-8.666	3.236	-3.992
O	-4.327	1.835	-4.609
O	-6.136	1.891	-0.393
C	-6.852	2.784	-5.855

H	-7.813	3.226	-6.161
C	-8.768	2.851	-1.385
H	-9.646	3.293	-1.879
N	-8.802	2.533	-0.106
N	-5.953	2.437	-6.753
C	-6.117	2.586	-8.17
C	-6.197	2.76	-10.955
C	-7.154	3.27	-8.8
C	-5.097	1.986	-8.953
C	-5.147	2.084	-10.342
C	-7.193	3.351	-10.189
H	-7.951	3.767	-8.234
H	-4.368	1.653	-10.982
C	-9.938	2.718	0.75
C	-12.005	2.966	2.609
C	-9.81	2.143	2.04
C	-11.098	3.416	0.419
C	-12.128	3.533	1.347
C	-10.848	2.277	2.96
H	-11.23	3.895	-0.557
H	-10.78	1.866	3.974
N	-8.555	1.503	2.294
C	-8.289	0.762	3.353
H	-9.071	0.543	4.096
N	-4.049	1.362	-8.202
C	-3.1	0.606	-8.722
H	-3.102	0.361	-9.795
C	-6.986	0.239	3.627
C	-4.362	-0.525	4.399
C	-5.864	0.532	2.761
C	-6.788	-0.534	4.768
C	-5.52	-0.949	5.159
C	-4.577	0.167	3.195
H	-7.655	-0.813	5.382
H	-3.71	0.437	2.575
O	-5.918	1.108	1.587
O	-3.105	-0.736	4.706
C	-5.384	-1.785	6.314
H	-6.313	-2.173	6.759
N	-4.212	-2.092	6.83
C	-2.004	0.1	-7.955
C	0.364	-0.634	-6.569
C	-1.04	-0.686	-8.581
C	-1.858	0.424	-6.552
C	-0.657	0.072	-5.91
C	0.117	-1.087	-7.923
H	-1.192	-0.988	-9.626
H	-0.51	0.364	-4.86
O	-2.747	1.015	-5.795
O	1.452	-0.83	-5.864

C	1.05	-1.935	-8.603
H	0.733	-2.344	-9.575
N	2.233	-2.228	-8.103
C	-4.009	-2.954	7.956
C	-3.34	-4.601	10.105
C	-2.706	-2.905	8.515
C	-4.953	-3.832	8.482
C	-4.616	-4.649	9.558
C	-2.382	-3.736	9.583
H	-5.961	-3.915	8.06
H	-1.377	-3.743	10.023
N	-1.808	-2	7.861
C	-0.648	-1.606	8.344
H	-0.305	-1.948	9.333
C	0.226	-0.728	7.624
C	2.095	0.851	6.184
C	-0.049	-0.356	6.251
C	1.352	-0.22	8.262
C	2.261	0.601	7.6
C	0.922	0.388	5.56
H	1.523	-0.463	9.319
H	0.757	0.622	4.498
O	-1.119	-0.66	5.558
O	2.942	1.468	5.399
C	3.319	1.216	8.341
H	3.335	1.021	9.424
N	4.214	2.011	7.786
C	3.192	-3.099	-8.716
C	5.216	-4.758	-9.68
C	2.926	-3.998	-9.745
C	4.494	-3.035	-8.157
C	5.495	-3.872	-8.642
C	3.941	-4.82	-10.227
H	1.925	-4.092	-10.184
H	6.506	-3.868	-8.217
C	5.215	2.739	8.506
C	7.211	4.3	9.675
C	6.193	3.371	7.694
C	5.257	2.903	9.889
C	6.257	3.678	10.469
C	7.18	4.154	8.291
H	4.508	2.449	10.549
H	7.941	4.679	7.702
N	6.042	3.147	6.286
N	4.636	-2.111	-7.071
C	5.784	-1.704	-6.57
H	6.738	-2.05	-6.997
C	6.917	3.514	5.371
H	7.844	4.034	5.656
C	6.745	3.244	3.976

C	6.499	2.635	1.21
C	5.529	2.642	3.473
C	7.783	3.537	3.097
C	7.703	3.238	1.741
C	5.44	2.369	2.096
H	8.699	4.002	3.488
H	4.518	1.919	1.702
O	4.464	2.339	4.174
O	6.273	2.323	-0.043
C	8.832	3.504	0.901
H	9.677	4.027	1.373
N	8.891	3.129	-0.362
C	5.861	-0.808	-5.455
C	6.1	0.802	-3.129
C	7.098	-0.292	-5.084
C	4.675	-0.427	-4.716
C	4.841	0.333	-3.545
C	7.242	0.544	-3.98
H	7.983	-0.542	-5.685
H	3.957	0.573	-2.937
C	10.013	3.349	-1.226
C	12.065	3.646	-3.096
C	9.928	2.706	-2.487
C	11.123	4.138	-0.93
C	12.146	4.28	-1.863
C	10.957	2.865	-3.413
H	11.22	4.672	0.023
H	10.92	2.403	-4.406
N	8.719	1.972	-2.71
C	8.506	1.165	-3.732
H	9.303	0.964	-4.464
O	6.113	1.433	-1.982
O	3.436	-0.734	-5.012
Ni	-4.318	1.681	-6.419
Ni	-7.443	1.78	0.864
Ni	-2.59	-1.417	6.31
Ni	4.463	2.267	5.989
Ni	7.587	2.24	-1.293
Ni	2.971	-1.522	-6.582
H	3.728	-5.527	-11.037
H	6.006	-5.415	-10.059
H	-6.232	2.833	-12.048
H	-8.012	3.89	-10.678
H	-13.039	4.081	1.081
H	-12.819	3.067	3.336
H	-5.361	-5.34	9.969
H	-3.08	-5.254	10.945
H	6.285	3.802	11.557
H	7.99	4.916	10.137
H	13.017	4.9	-1.624

H	12.871	3.767	-3.827