Supporting Information

Understanding the affinity of bis-exTTF macrocyclic receptors towards fullerene recognition

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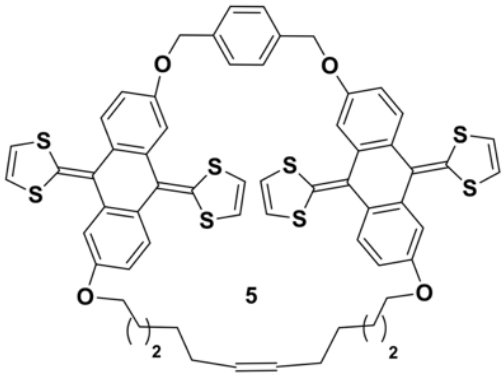
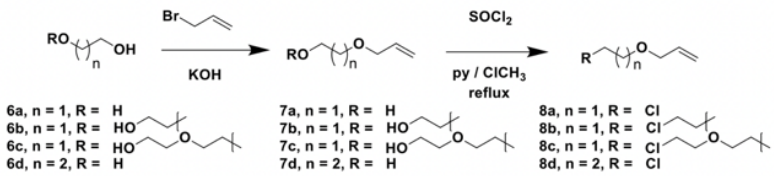
1. Experimental Section

General. All solvents were dried according to standard procedures. Reagents were used as purchased. All air-sensitive reactions were carried out under argon atmosphere. Flash chromatography was performed using silica gel (Merck, Kieselgel 60, 230–240 mesh, or Scharlau 60, 230–240 mesh). Analytical thin layer chromatographies (TLC) were performed using aluminium-coated Merck Kieselgel 60 F254 plates. NMR spectra were recorded on a Bruker Avance 300 (^{1}H: 300 MHz; ^{13}C: 75 MHz), a Bruker Avance 500 (^{1}H: 500 MHz; ^{13}C: 125 MHz) spectrometers at 298 K, unless otherwise stated, using partially deuterated solvents as internal standards. Coupling constants (*J*) are denoted in Hz and chemical shifts (δ) in ppm. Multiplicities are denoted as follows: s = singlet, d = doublet, t = triplet, m = multiplet, b = broad. When necessary, NOESY or bidimensional ^{1}H–^{1}H experiments were executed for the assignation of protons. Electrospray ionization mass spectrometry (ESI-MS) and matrix-assisted laser desorption ionization (coupled to a Time-Of-Flight analyzer) experiments (MALDI-TOF) were recorded on a HP1100MSD spectrometer and a Bruker REFLEX spectrometer, respectively.



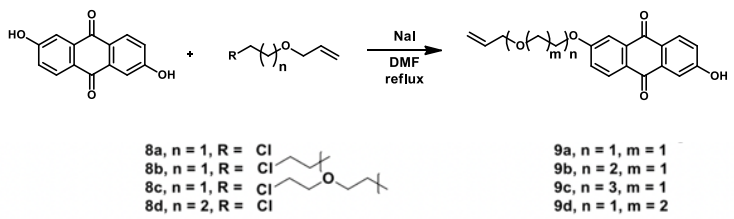
Compound 5 synthesis was previously described in *J. Am. Chem. Soc*., **2011**, *133*, 3184–3190 by some of us.

1.1. Ethylene and propylene glycol derivatives.

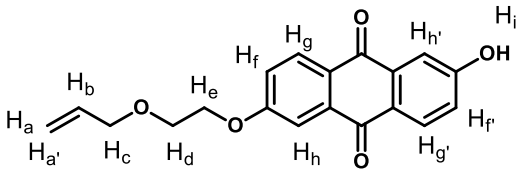


The synthesis and spectroscopic characteristic of compounds **8a-d** have been described previously in the literature.

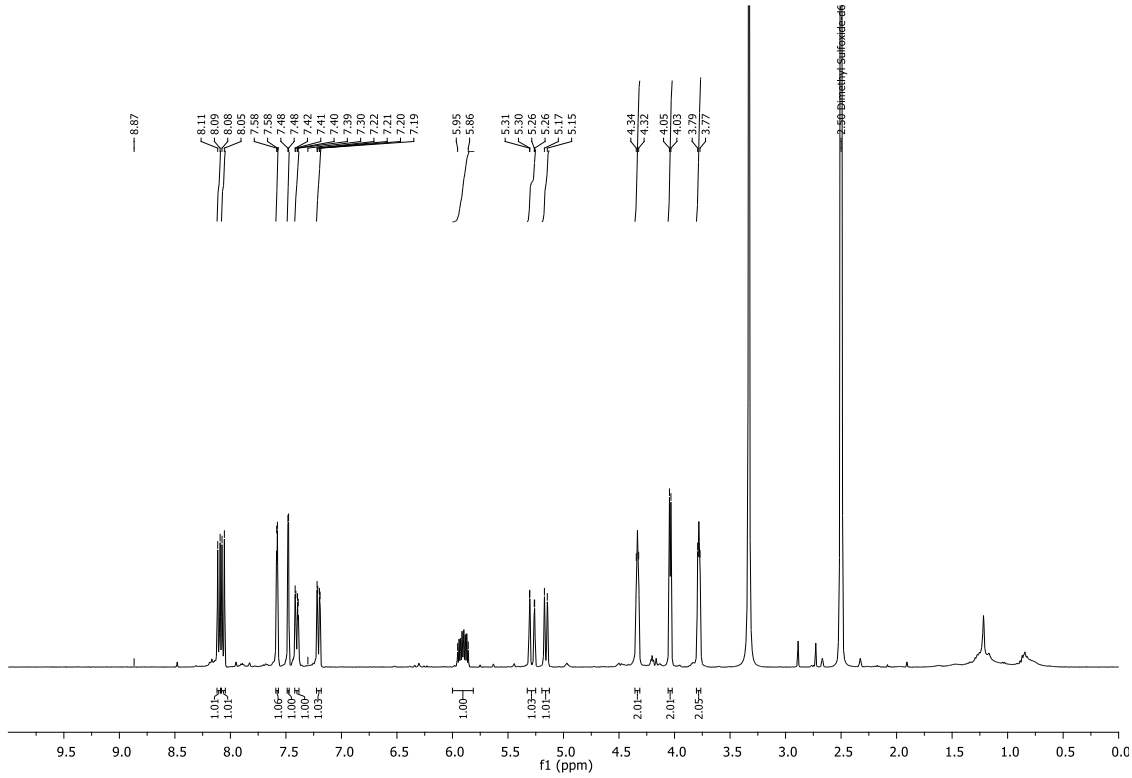
1.2. Mono-substituted anthraflavic acid derivatives.



General procedure. Anthraflavic acid (1 equiv.) was dissolved in dry DMF under inner atmosphere through sonication. K_2CO_3 (1 equiv.) and NaI (catalytic amount) were added. Finally, 1 equivalent of compound **8a**, **8b**, **8c** or **8d** were added and stirred at reflux for 3 hours. The mixture was poured into cold 1 N HCl and filtered off. The solid was re-dissolved in DCM and washed it twice with water. The organic phase was dried with Na_2SO_4 and the solvent removed under vacuum. The crude was purified by column chromatography (silica gel, CH_2Cl_2 to CH_2Cl_2/MeOH 98/2) yielding the compounds **9a** (Y = 15%), **9b** (Y= 18%), **9c** (Y = 20%) and **9d** (Y = 37%).



Compound 9a. ^{1}H NMR (400 MHz, DMSO) δ 11.02 (s, 1H, H_i), 8.10 (d, J = 8.6 Hz, 1H, H_g), 8.06 (d, J = 8.5 Hz, 1H, $H_{g'}$), 7.58 (d, J = 2.5 Hz, 1H, H_h), 7.48 (d, J = 2.3 Hz, 1H, $H_{h'}$), 7.40 (dd, J = 8.7, 2.5 Hz, 1H, H_f), 7.21 (dd, J = 8.5, 2.4 Hz, 1H, $H_{f'}$), 5.95 – 5.85 (m, 1H, H_b), 5.28 (dd, J = 17.3, 1.2 Hz, 1H, H_a), 5.16 (d, J = 10.4 Hz, 1H, $H_{a'}$), 4.34 – 4.32 (m, 2H, H_e), 4.04 (d, J = 5.3 Hz, 2H, H_c), 3.79 – 3.77 (m, 2H, H_d). ^{13}C NMR (101 MHz, DMSO) δ 181.4, 181.0, 163.3, 163.2, 135.4, 135.4, 135.0, 129.9, 129.4, 126.5, 125.2, 121.1, 120.5, 116.6, 112.2, 110.7, 71.1, 68.0, 67.9. MS *m*/*z* calculated for $C_{19}H_{16}O_5$ [M-H$^+$] 323.1; found ESI$^-$ [M-H$^+$] 323.0.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8.11
8.09
8.08
8.05
7.58
7.58
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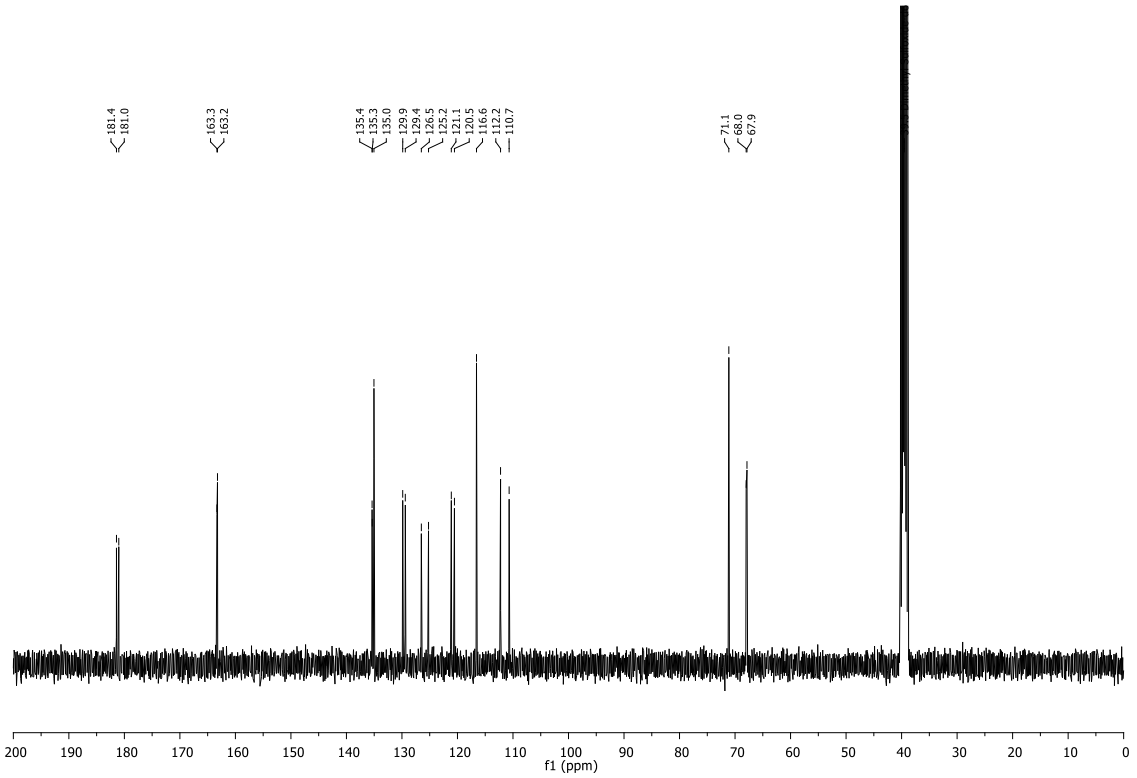
7.39
7.30
7.22
7.21
7.20
7.19
5.95
5.86
5.31
5.30
5.26
5.26
5.17
5.15
4.34
4.32
4.05
4.03
3.79
3.77
2.50 Dimethyl Sulfoxide-d6
1.01
1.01
1.06
1.00
1.00
1.03
1.00
1.03
1.01
2.01
2.01
2.05
f1 (ppm)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181.0
163.3
163.2
135.4
135.3
135.0
129.9
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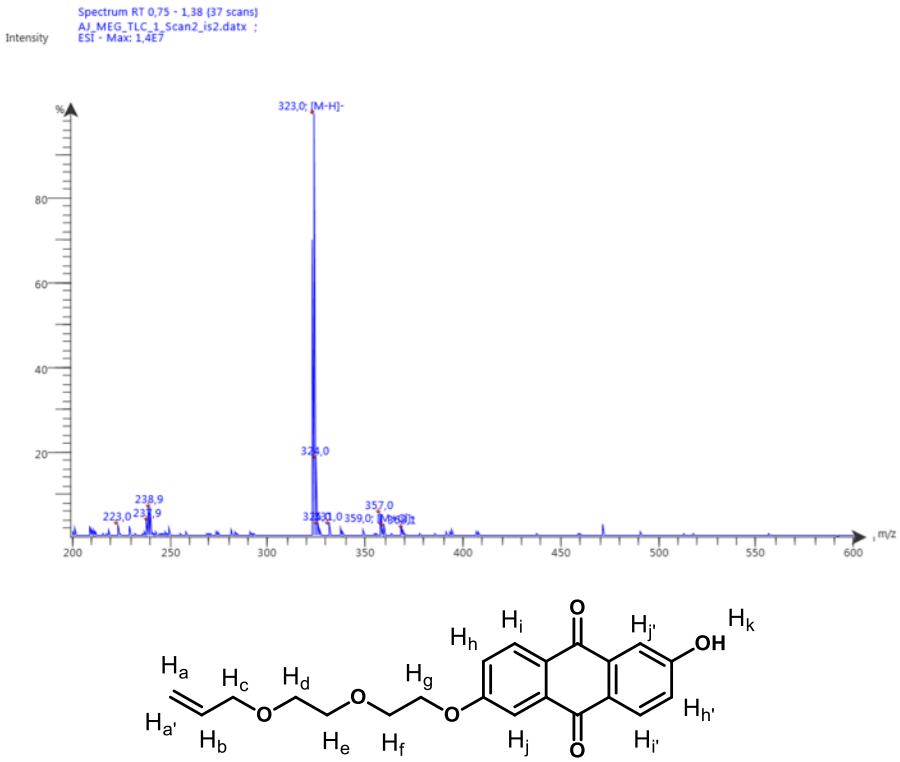
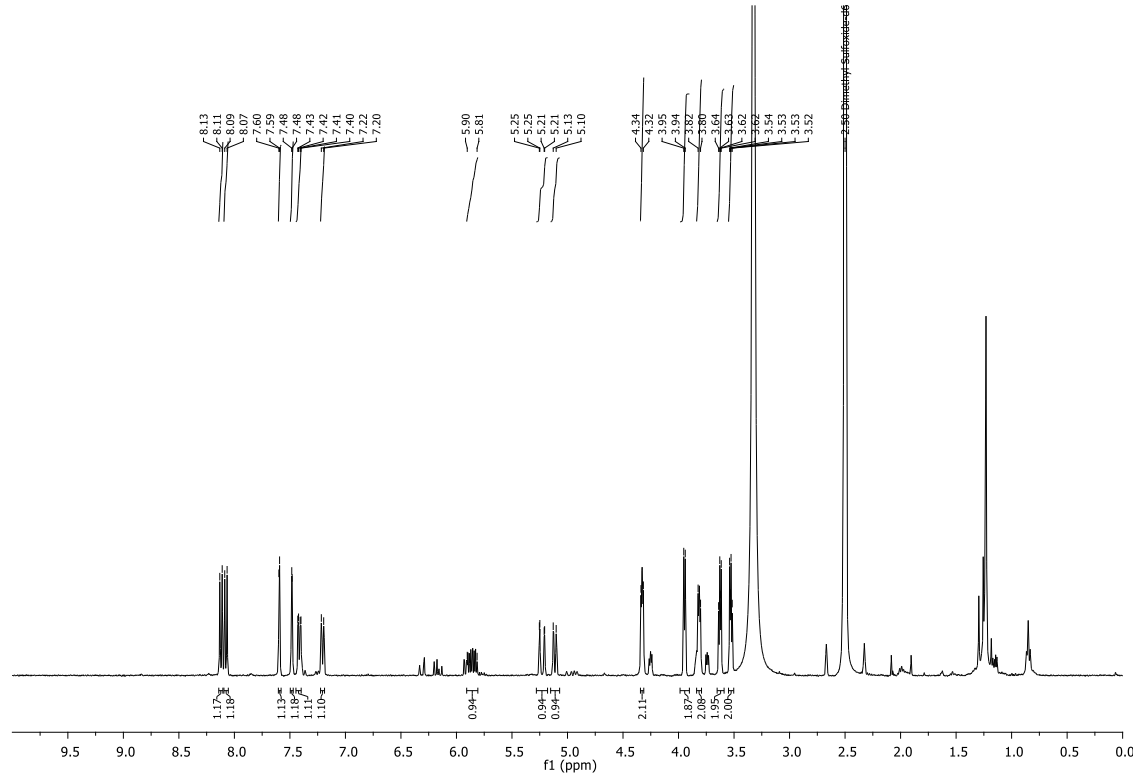
112.2
110.7
71.1
68.0
67.9
f1 (ppm)



Compound 9b. ^{1}H NMR (400 MHz, DMSO) δ 8.12 (d, *J* = 8.7 Hz, 1H, H_i), 8.08 (d, *J* = 8.5 Hz, 1H, $H_{i'}$), 7.60 (d, *J* = 2.5 Hz, 1H, H_j), 7.48 (d, *J* = 1.3 Hz, 1H, $H_{j'}$), 7.41 (dd, *J* = 8.6, 2.7 Hz, 1H, H_h), 7.21 (d, *J* = 8.5 Hz, 1H, $H_{h'}$), 5.90 – 5.81 (m, 1H, H_b), 5.23 (dd, *J* = 17.3, 1.8 Hz, 1H, H_a), 5.12 (d, *J* = 10.6 Hz, 1H, $H_{a'}$), 4.34 – 4.32 (m, 2H, H_g), 3.95 (d, *J* = 5.3 Hz, 2H, H_c), 3.82 – 3.80 (m, 2H, H_f), 3.63 (dd, *J* = 5.7, 3.7 Hz, 2H, H_e), 3.53 (dd, *J* = 5.7, 3.7 Hz, 2H, H_d). ^{13}C NMR (101 MHz, DMSO) δ 181.5, 181.0, 163.4, 163.4, 135.4, 135.3, 129.9, 129.4, 128.2, 126.5, 125.1, 121.2, 120.5, 116.3, 112.3, 110.8, 71.1, 70.0, 69.0, 68.7, 68.1. MS *m/z* calculated for $C_{19}H_{16}O_5$ [M-H$^+$] 367.1; found ESI$^-$ [M-H$^+$] 367.1.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7.42
7.41
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7.20
5.90
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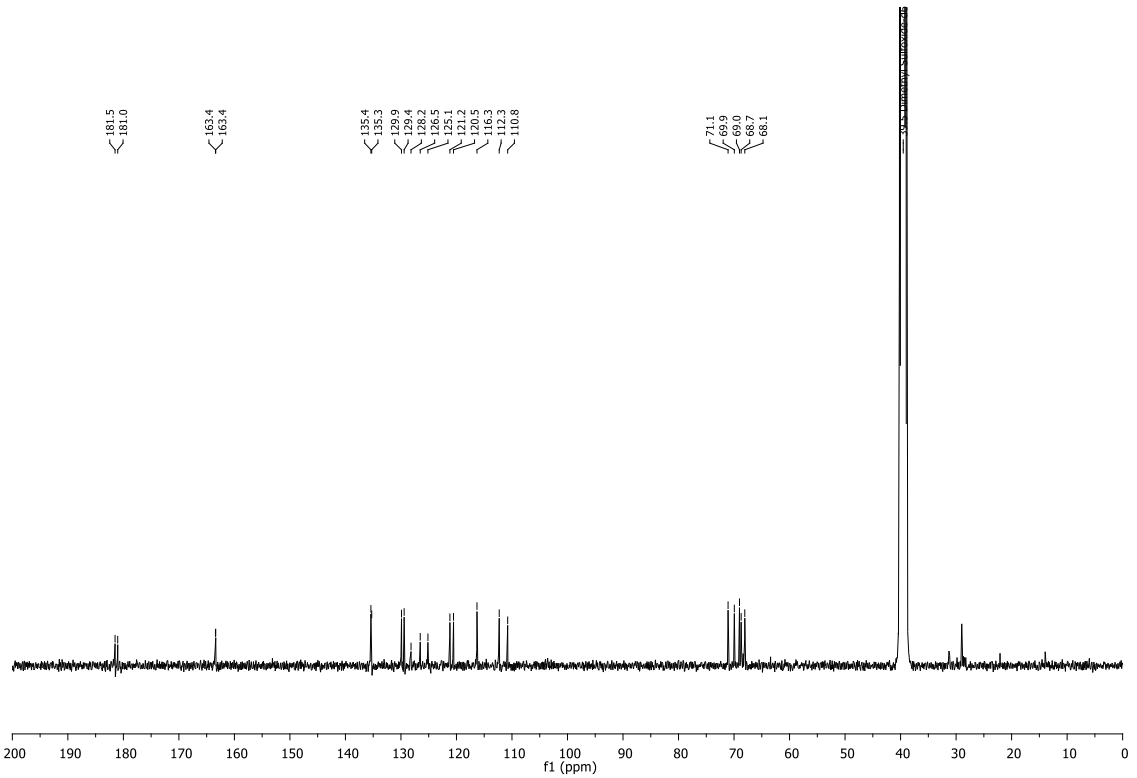
5.21
5.13
5.10
4.34
4.32
3.95
3.94
3.82
3.80
3.64
3.63
3.62
3.62
3.54
3.53
3.53
3.52
2.50 Dimethyl Sulfoxide-d6
1.17
1.94
1.18
1.13
1.18
1.11
1.10
0.94
0.94
0.94
2.11
1.87
2.08
1.95
2.00
f1 (ppm)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181.0
163.4
163.4
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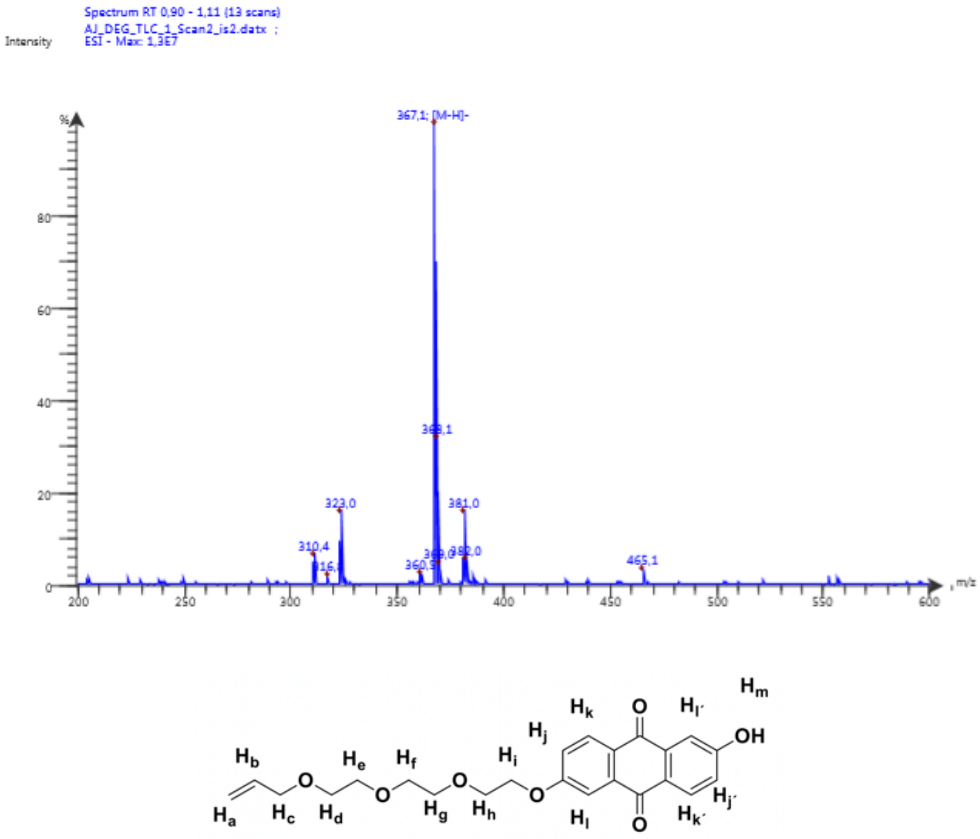
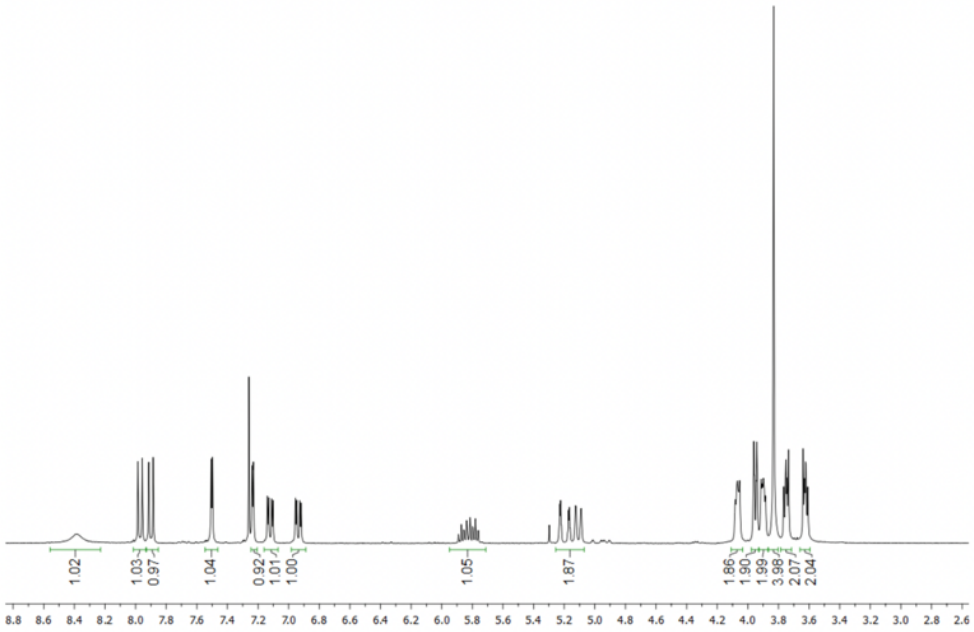
125.1
121.2
120.5
116.3
112.3
110.8
71.1
69.9
69.0
68.7
68.1
39.5 Dimethyl Sulfoxide-d6
f1 (ppm)



Compound 9c. ^{1}H NMR (300 MHz, $CDCl_3$) δ/ppm: 8.38 (s, 1H, H_m), 7.90 (d, J = 8.6 Hz, 1H, H_k), 7.50 (d, J = 2.5 Hz, 1H, $H_{k'}$), 7.50 (d, J = 2.5 Hz, 1H, H_l), 7.24 (d, J = 2.6 Hz, 1H, $H_{l'}$), 7.12 (dd, J = 8.5, 2.6 Hz, 1H, H_j), 6.94 (dd, J = 8.6, 2.7 Hz, 1H, $H_{j'}$), 5.91–5.74 (m, 1H, H_b), 5.24–5.08 (m, 2H, H_a), 4.07 (dd, J = 5.3, 3.1 Hz, 2H, H_i), 3.95 (dt, J = 5.8, 1.2 Hz, 2H, H_c), 3.90 (dd, J = 5.3, 3.1 Hz, 2H, H_h), 3.83 (s, 4H, H_{f+g}), 3.75 (dd, J = 5.7, 3.5 Hz, 2H, H_e), 3.62 (dd, J = 5.8, 3.4 Hz, 2H, H_d). ^{13}C NMR (75 MHz, $CDCl_3$) δ/ppm: 181.9, 181.6, 163.2, 162.2, 135.6, 135.4, 134.5, 130.0, 129.5, 127.0, 126.3, 121.2, 120.7, 117.6, 113.3, 110.0, 72.4, 70.9, 70.9, 69.7, 69.3, 67.9. MS m/z calculated for $C_{23}H_{24}O_7$ [M-H$^+$] 411.15 MALDI-TOF [M-H$^+$] 411.05 (100% I).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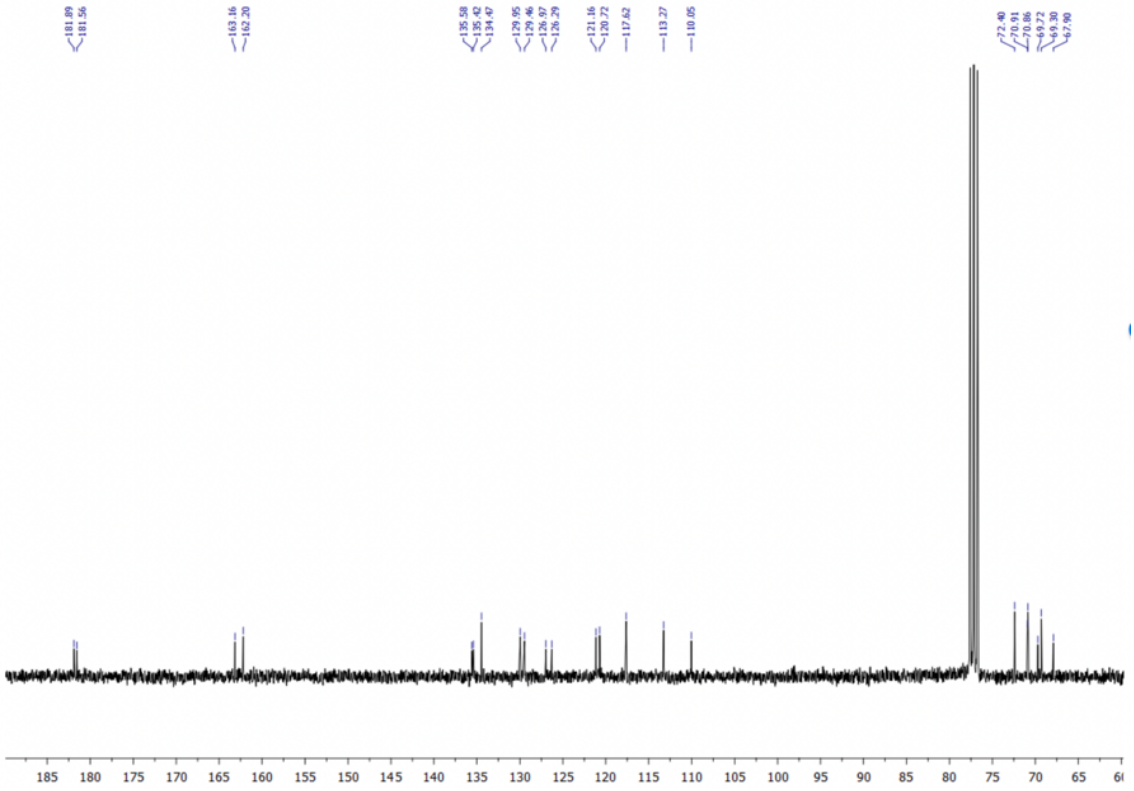
2.04
8.8 8.6 8.4 8.2 8.0 7.8 7.6 7.4 7.2 7.0 6.8 6.6 6.4 6.2 6.0 5.8 5.6 5.4 5.2 5.0 4.8 4.6 4.4 4.2 4.0 3.8 3.6 3.4 3.2 3.0 2.8 2.6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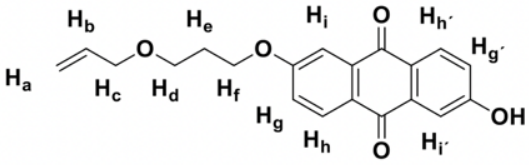
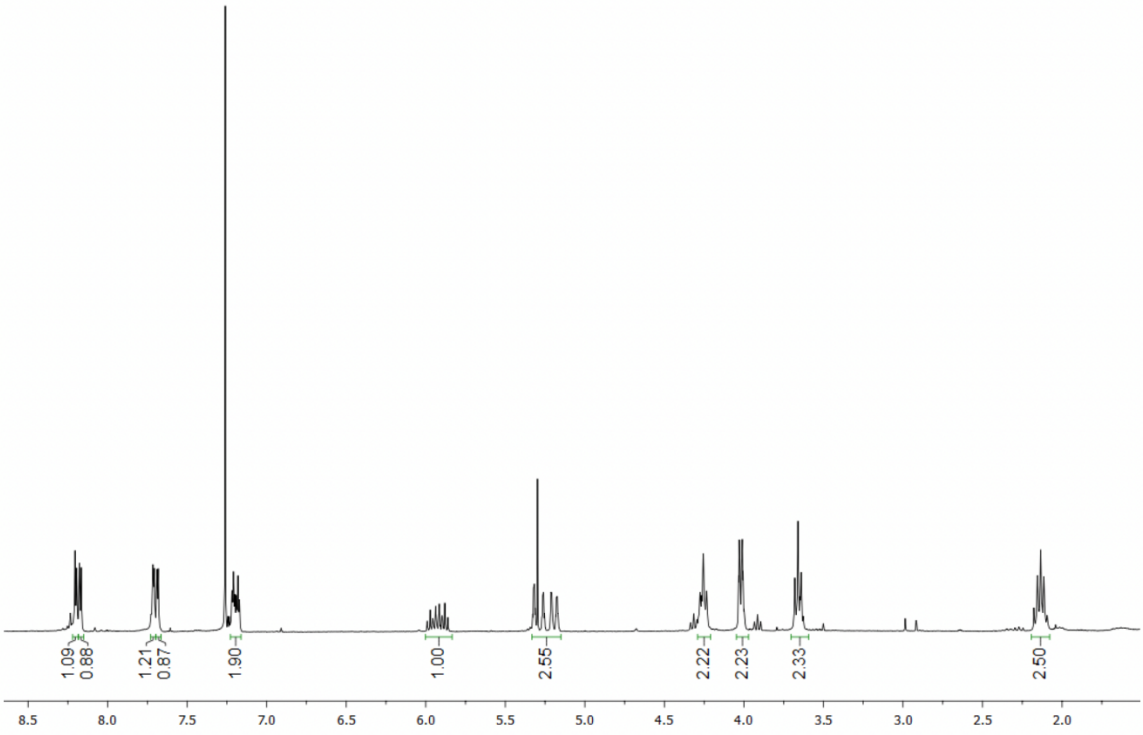
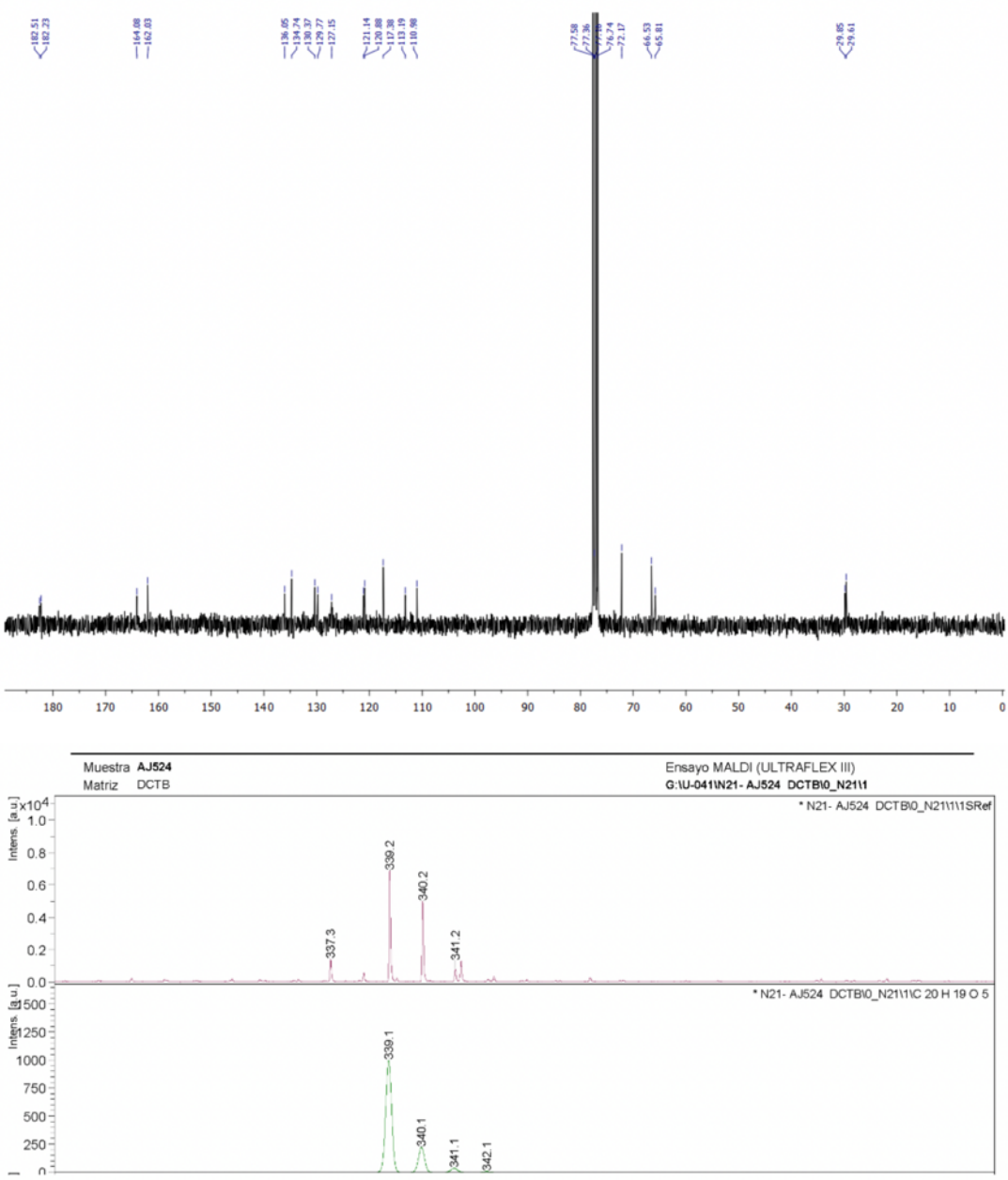
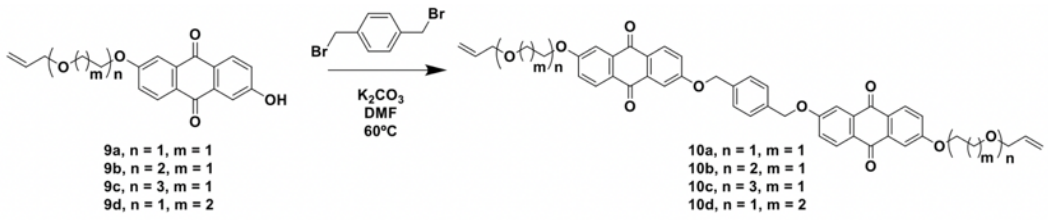


Compound 9d. ^{1}H NMR (300 MHz, $CDCl_3$) δ/ppm: 8.22 (d, J = 3.1 Hz, 1H, H_h), 8.20 (d, J = 3.2 Hz, 1H, $H_{h'}$), 7.73 (d, J = 2.5 Hz, 1H, H_i), 7.71 (d, J = 2.6 Hz, 1H, $H_{i'}$), 7.26–7.17 (m, 2H, $H_{g+g'}$), 6.03–5.85 (m, 1H, H_b), 5.38–5.16 (m, 2H, H_a), 4.32–4.24 (m, 2H, H_f), 4.06–4.01 (m, 2H, H_c), 3.74–3.63 (m, 2H, H_d), 2.23–2.09 (m, 2H, H_e). ^{13}C NMR (75 MHz, $CDCl_3$) δ/ppm: 182.5, 182.2, 164.1, 162.0, 136.0, 134.7, 130.4, 129.8, 127.1, 121.1, 120.9, 117.4, 113.2, 111.0, 72.2, 66.5, 65.8, 29.8, 29.6. MS *m*/*z*: calculated. for C20H18O5 $[M+H]^+$ 339.12 found FAB 339.2.



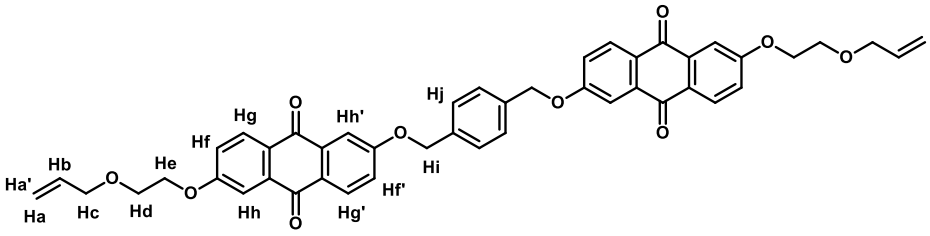


1.3. Bis-substituted of α, α'-dibromoxylene derivatives

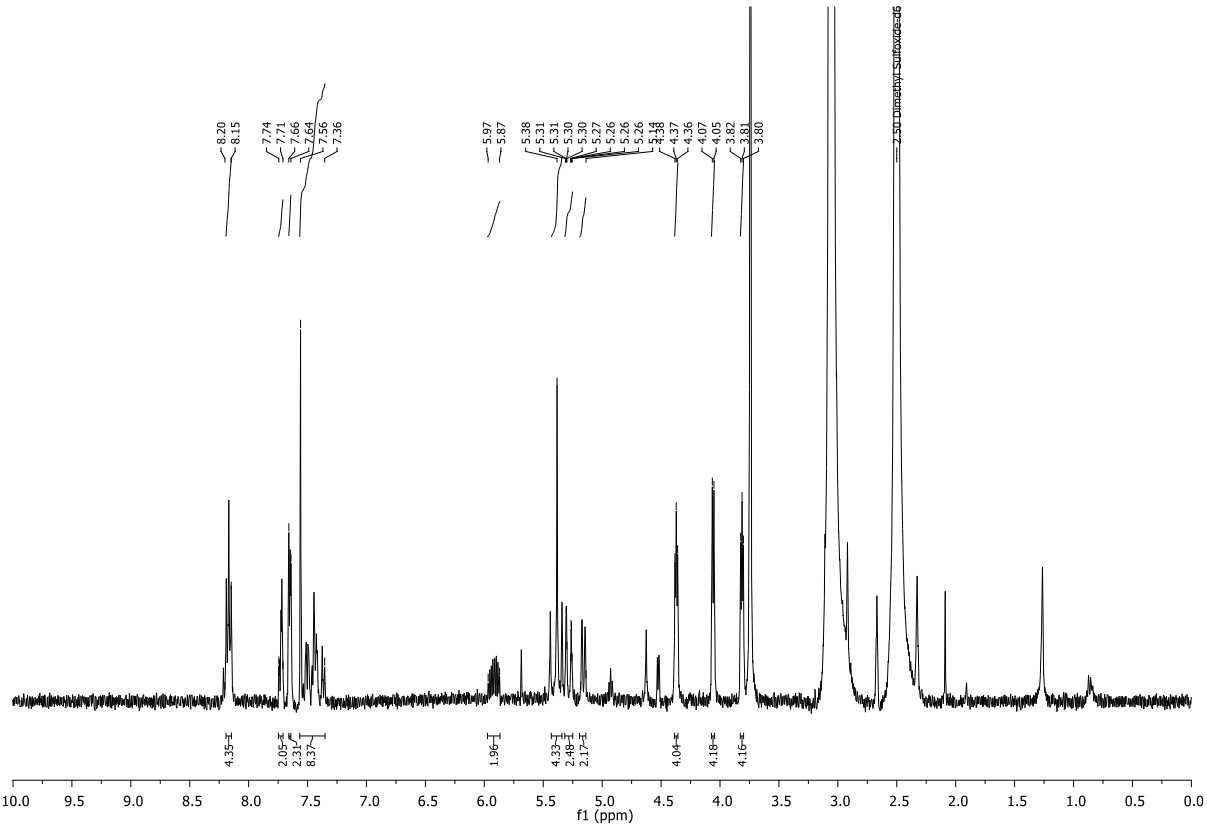


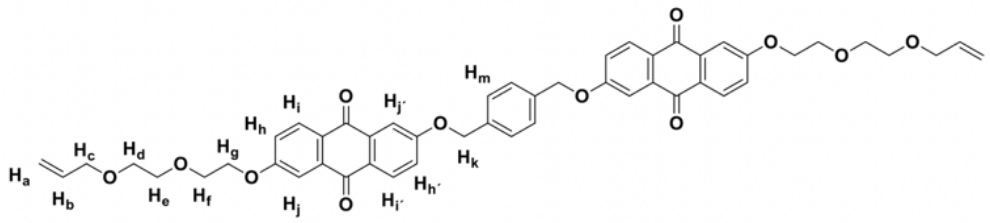
General procedure. Compound **9a**, **9b**, **9c** or **9d** (2.2 eq.) was dissolved in dry DMF under Ar through sonication. K_2CO_3 (2.2 equiv.) and NaI (cat.) were added. Finally, α,α-di-bromo-p-

xylene (1 eq.) was added and heated at 60 ºC for 5h. Then, the mixture was poured in cold 1 N HCl and the solid generated was removed by filtration. The yellow solid was washed with cold MeOH and cold Et_2O yielding the products **10a** (Y = 73%), **10b** (Y = 92%), **10c** (Y = 72%) and **10d** (Y = 90%).

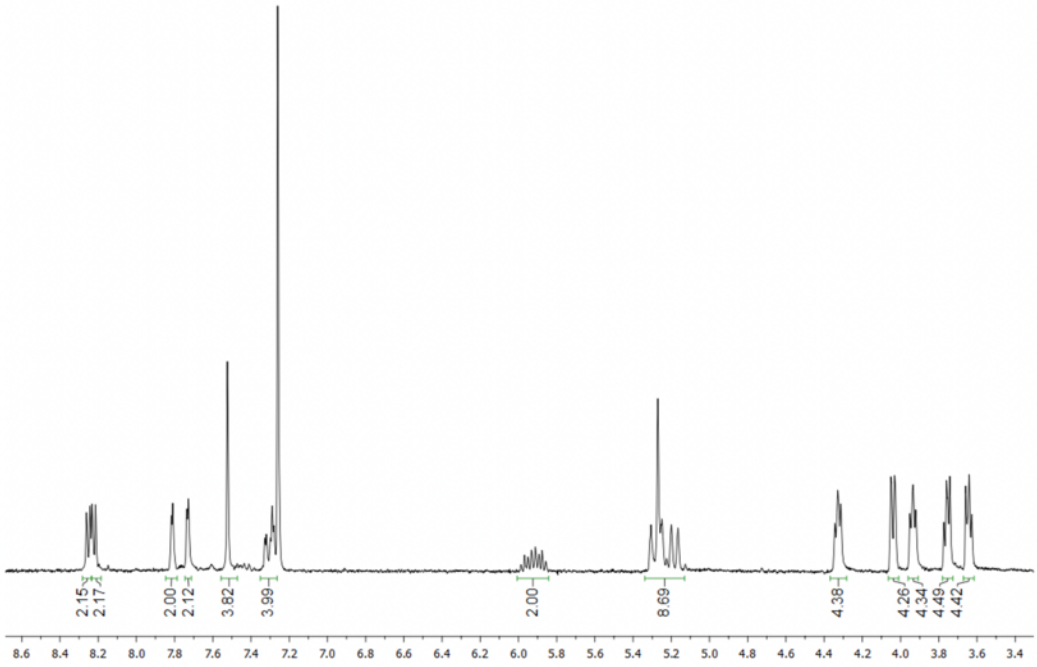


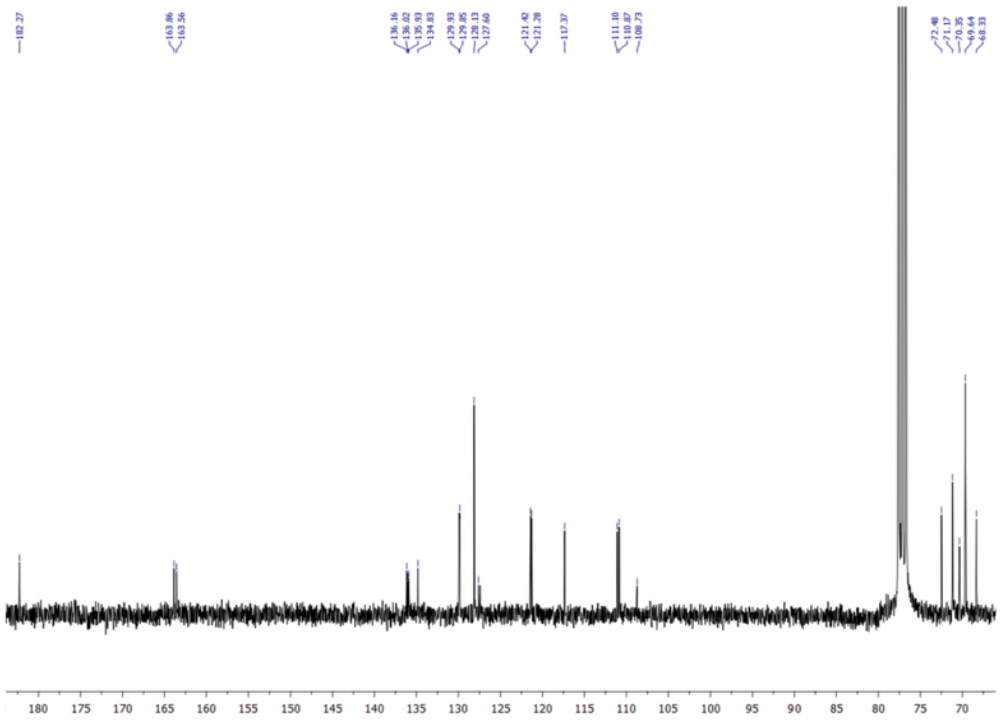
Compound 10a. Due to the insolubility of the product, only ^{1}H NMR could be obtained in dimethyl sulfoxide-d_6 at 80 ºC. ^{1}H NMR (400 MHz, DMSO) δ 8.19 – 8.15 (m, 4H, $H_{g+g'}$), 7.74 – 7.71 (m, 2H, H_h), 7.66 – 7.64 (m, 2H, $H_{h'}$), 7.56 – 7.35 (m, 8H, $H_{f+f'+j}$), 5.97 – 5.87 (m, 2H, H_b), 5.38 (s, 4H, H_h), 5.28 (ddd, J = 4.8, 3.5, 1.9 Hz, 2H, H_a), 5.18 – 5.14 (m, 2H, $H_{a'}$), 4.40 – 4.33 (m, 4H, H_e), 4.06 (d, J = 5.4 Hz, 4H, H_c), 3.83 – 3.79 (m, 4H, H_d).





Compound 10b. ^{1}H NMR (300 MHz, CDCl3) δ/ppm: 8.24 (d, J = 8.7 Hz, 2H, H_i), 8.22 (d, J = 8.7 Hz, 2H, $H_{i'}$), 7.81 (d, J = 2.4 Hz, 2H, H_j), 7.73 (d, J = 2.4 Hz, 2H, $H_{j'}$), 7.52 (s, 4H, H_m), 7.37–7.25 (m, 4H, $H_{h+h'}$), 6.00–5.85 (m, 2H, H_b), 5.35–5.15 (m, 8H, H_{a+k}), 4.40–4.26 (m, 4H, H_g), 4.04 (d, J = 5.6 Hz, 4H, H_c), 3.97–3.90 (m, 4H, H_f), 3.79–3.72 (m, 4H, H_d), 3.67–3.61 (m, 4H, H_e). ^{13}C NMR (75 MHz, $CDCl_3$) δ/ppm: 182.3, 163.9, 163.6, 136.2, 136.0, 135.9, 134.8, 129.9, 129.8, 128.1, 127.6, 121.4, 121.3, 117.4, 111.1, 110.9, 108.7, 72.5, 71.2, 70.4, 69.6, 68.3. MS m/z calculated for $C_{50}H_{46}O_{12}$ [M-Na$^+$] 861.3 found MALDI-TOF [M-Na$^+$] 861.3.

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117.37
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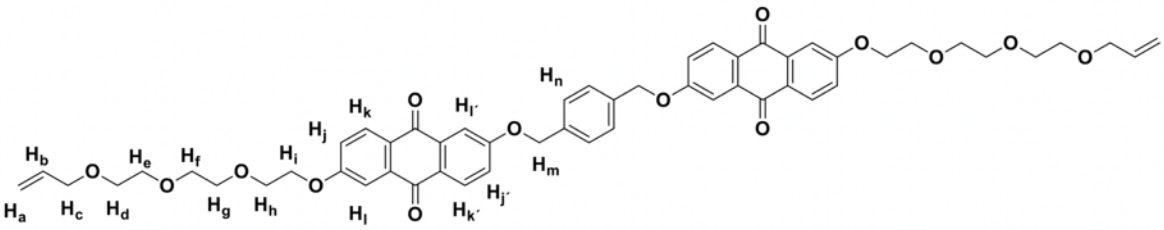
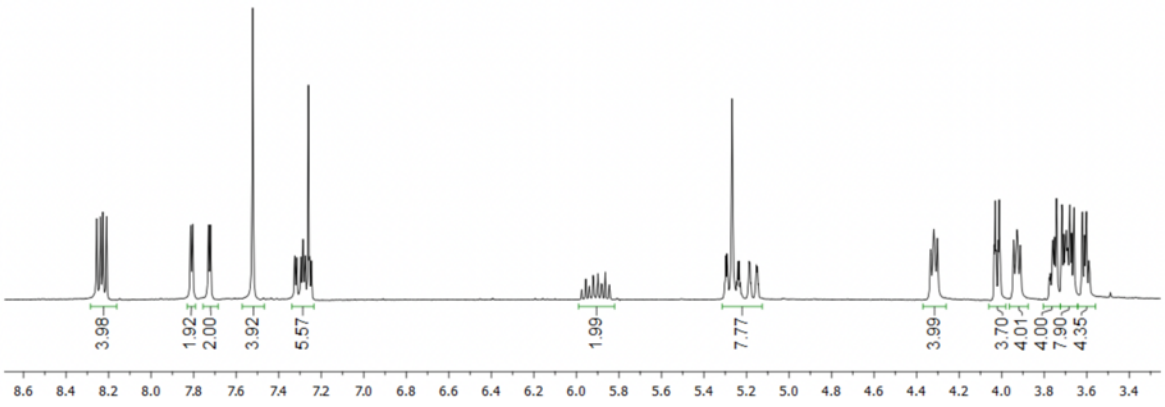
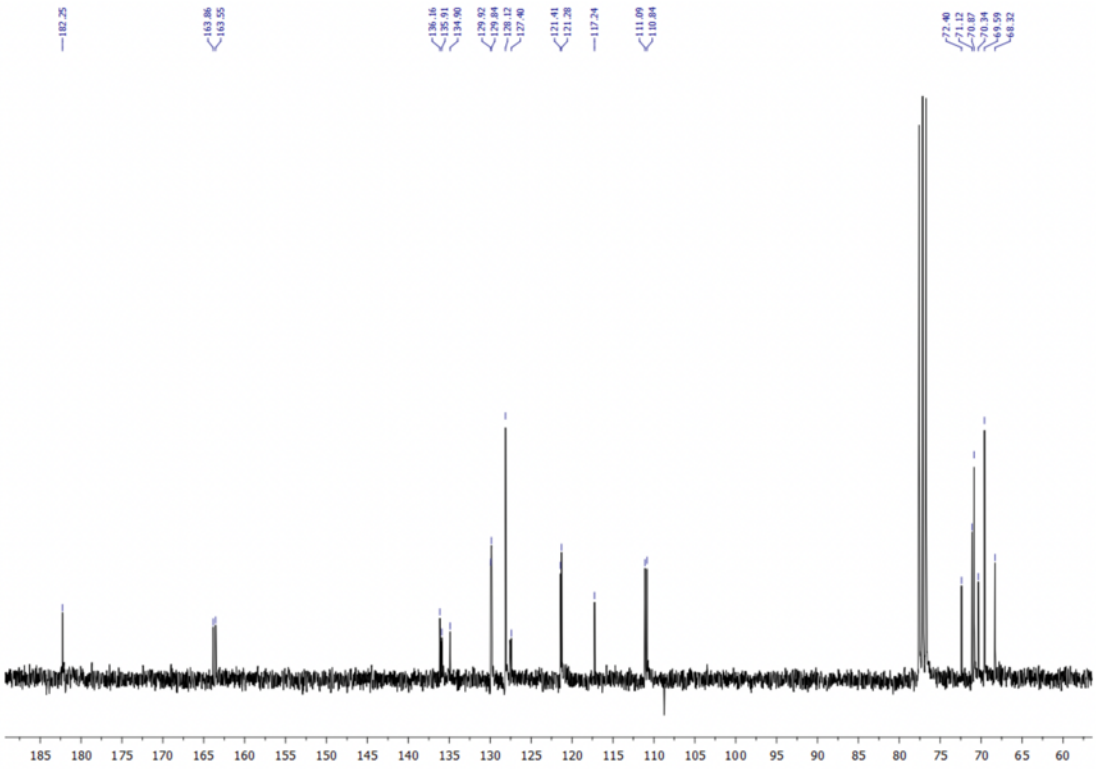
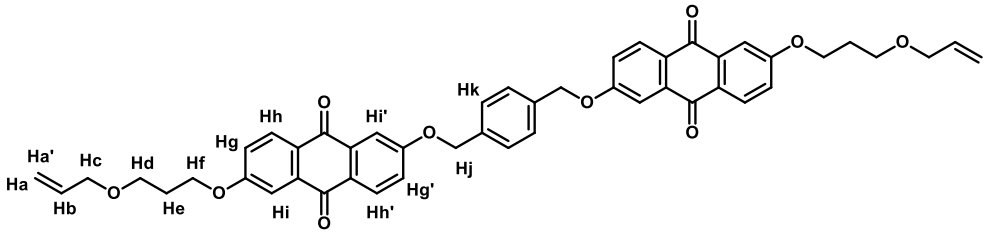


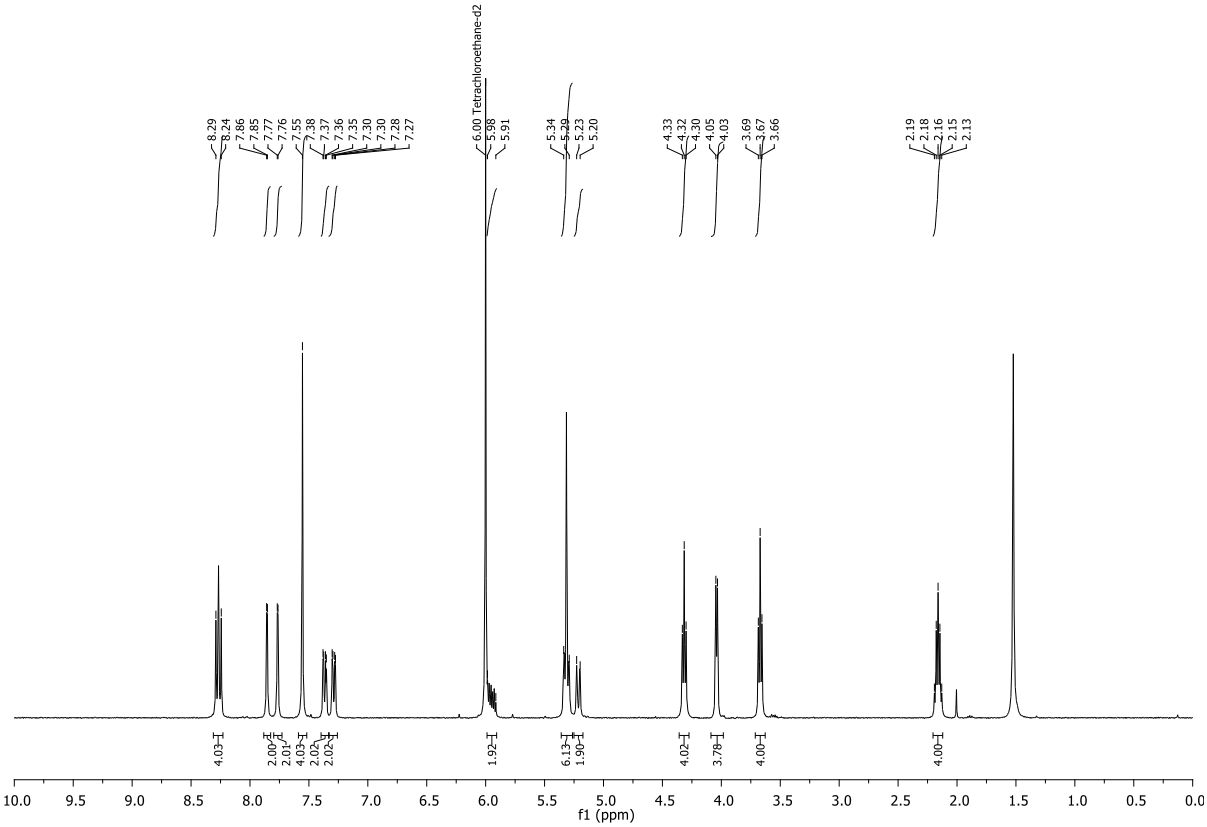
Compound 10c. ^{1}H NMR (300 MHz, $CDCl_3$) δ/ppm: 8.24 (d, J = 8.5 Hz, 2H, H_k), 8.22 (d, J = 8.5 Hz, 2H, $H_{k'}$), 7.81 (d, J = 2.7 Hz, 2H, H_l), 7.73 (d, J = 2.6 Hz, 2H, $H_{l'}$), 7.52 (s, 4H, H_n), 7.34–7.21 (m, 4H, H_j), 5.99–5.82 (m, 2H, H_b), 5.27 (s, 4H, H_n), 5.32–5.13 (m, 4H, H_a), 4.36–4.28 (m, 4H, H_i), 4.02 (dt, J = 5.7, 1.3 Hz, 4H, H_c), 3.95–3.90 (m, 4H, H_h), 3.79–3.72 (m, 4H, H_e), 3.73–3.65 (m, 8H, H_{f+g}), 3.64–3.57 (m, 4H, H_d). ^{13}C NMR (75 MHz, $CDCl_3$) δ/ppm: 189.8, 182.2, 163.9, 163.6, 136.2, 135.9, 134.9, 129.9, 129.8, 128.1, 127.4, 121.4, 121.3, 117.2, 111.1, 110.8, 72.4, 71.1, 70.9, 70.3, 69.6, 68.3.



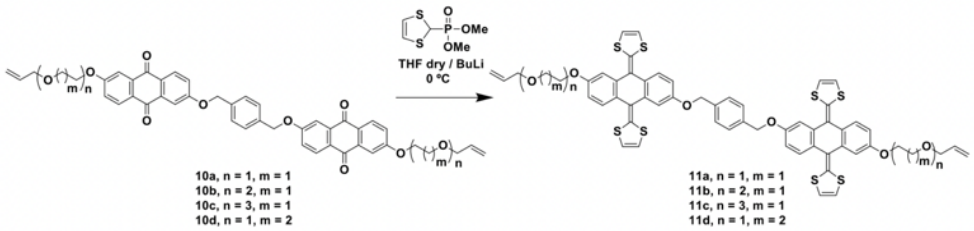




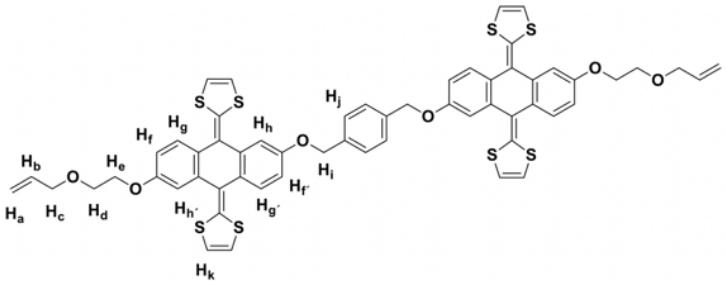
Compound 10d. Due to the insolubility of the product, only ^{1}H NMR could be obtained in tetrachloroethane-d_2 at 80 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29 – 8.24 (m, 4H, $H_{h+h'}$), 7.86 (d, J = 2.6 Hz, 2H, H_i), 7.77 (d, J = 2.6 Hz, 2H, $H_{i'}$), 7.55 (s, 4H, H_n), 7.37 (dd, J = 8.6, 2.6 Hz, 2H, H_g), 7.29 (dd, J = 8.7, 2.6 Hz, 2H, $H_{g'}$), 5.98 – 5.91 (m, 2H, H_b), 5.34 – 5.29 (m, 6H, H_{a+j}), 5.23 – 5.20 (m, 2H, $H_{a'}$), 4.32 (t, J = 6.3 Hz, 4H, H_f), 4.04 (d, J = 5.5 Hz, 4H, H_c), 3.67 (t, J = 6.1 Hz, 4H, H_d), 2.16 (p, J = 6.2 Hz, 4H, H_e).



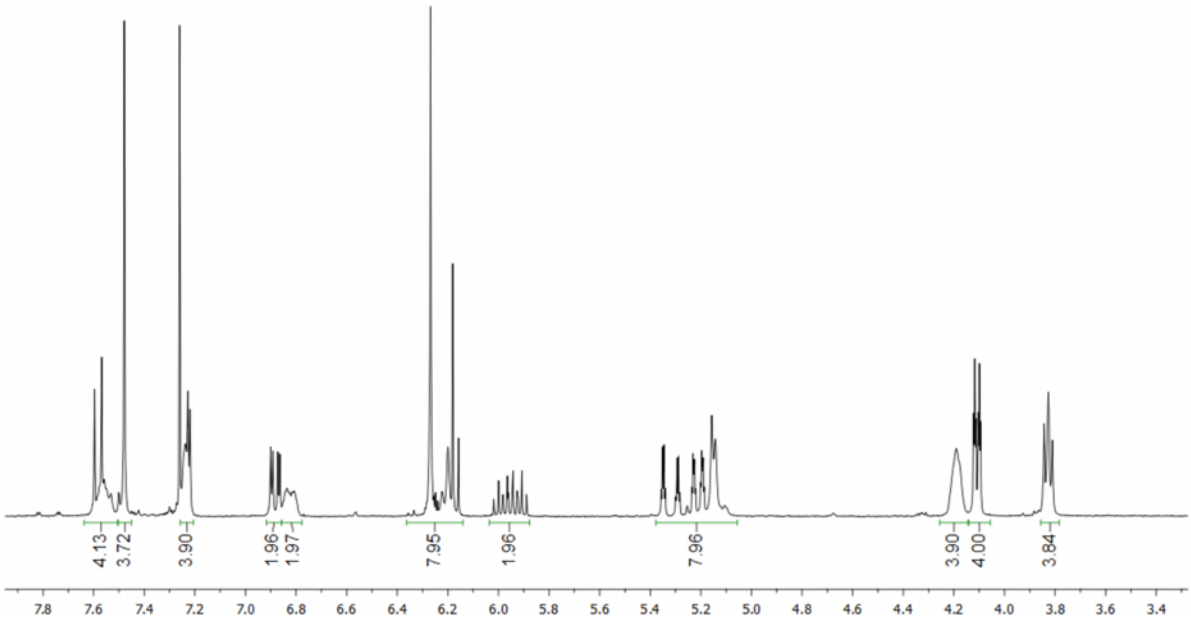
1.4. π-extended tetrathiafulvalene derivatives.

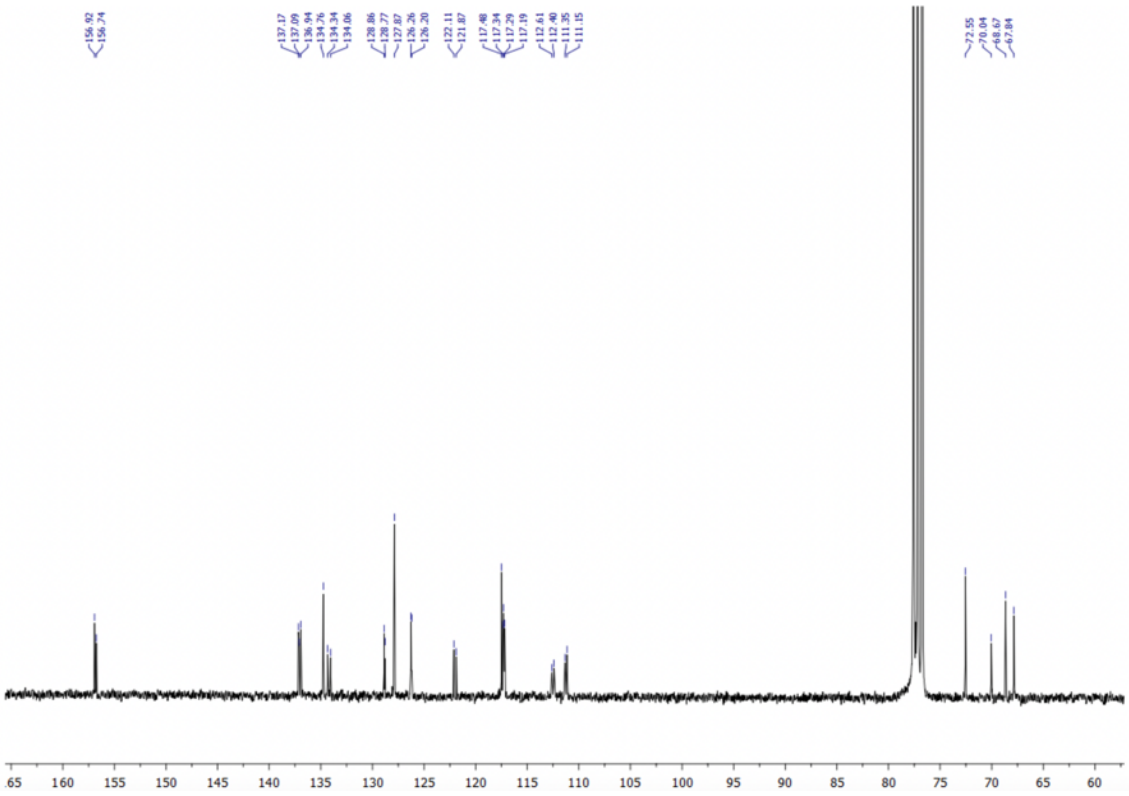


General procedure. Dimethyl (1,3-dithiol-2-yl)phosphonate (12.0 eq.) was dissolved in dry THF, under Ar, and cooled at –78 ºC. Then, a solution of butyllithium 1.6 M in hexanes (12 eq.) was added and stirred for 30 min. In the meantime, 1 equivalent of compound **10a**, **10b**, **10c** or **10d** was dissolved in dry THF, under Ar. Then, this solution was added over the phosphorous ylide solution at –78 ºC. The reaction was allowed to warm to room temperature and stirred for 20 minutes. The reaction was quenched with MeOH and concentrated under vacuum. The crude was purified by column chromatography using deactivate silica gel by treatment with 1% Et_3N in hexane. Column chromatography (silica gel, hexane/DCM, 3:1 to DCM) yielded compounds **11a** (Y = 18%), **11b** (Y =30%), **11c** (Y = 27%) and **11d** (Y = 44%) as yellow solids.



Compound 11a.[1]H NMR (300 MHz, $CDCl_3$) δ/ppm: 7.60–7.52 (m, 4H, H_{g+g}), 7.48 (s, J = 6.5 Hz, 4H, H_j), 7.24–7.19 (m, 4H, $H_{h+h'}$), 6.88 (dd, J = 8.6, 2.6 Hz, 2H, H_f), 6.82 (bd, J = 8.5 Hz, 2H, $H_{f'}$), 6.30–6.13 (m, 8H, H_k), 6.04–5.90 (m, 2H, H_b), 5.38–5.09 (m, 8H, H_{a+i}), 4.19 (bs, 4H, H_d), 4.11 (dt, J = 5.6, 1.4 Hz, 1H, H_c), 3.85–3.80 (m, 4H, H_e). ^{13}C NMR (75 MHz, $CDCl_3$) δ/ppm: 156.9, 156.7, 137.2, 137.1, 136.9, 134.8, 134.3, 134.1, 128.9, 128.8, 127.9, 126.3, 126.2, 122.1, 121.9, 117.5, 117.3, 117.3, 117.2, 112.6, 112.4, 111.4, 111.2, 72.6, 70.0, 68.7, 67.8. MS m/z calculated for $C_{58}H_{46}O_6S_8$ [M^+] 1094.1 found MALDI-TOF [M^+] 1094.1.

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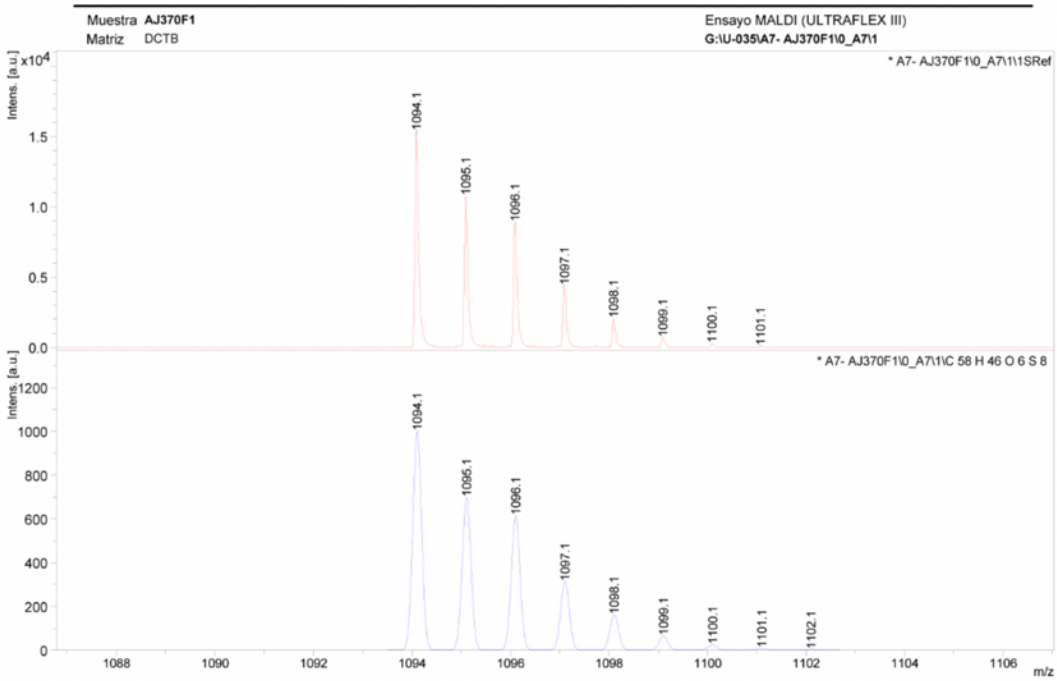
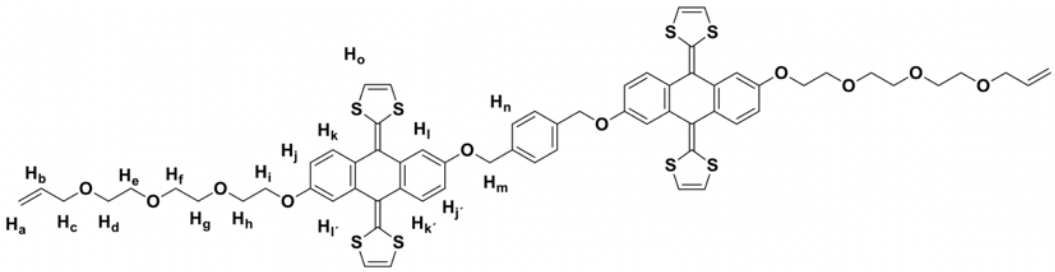
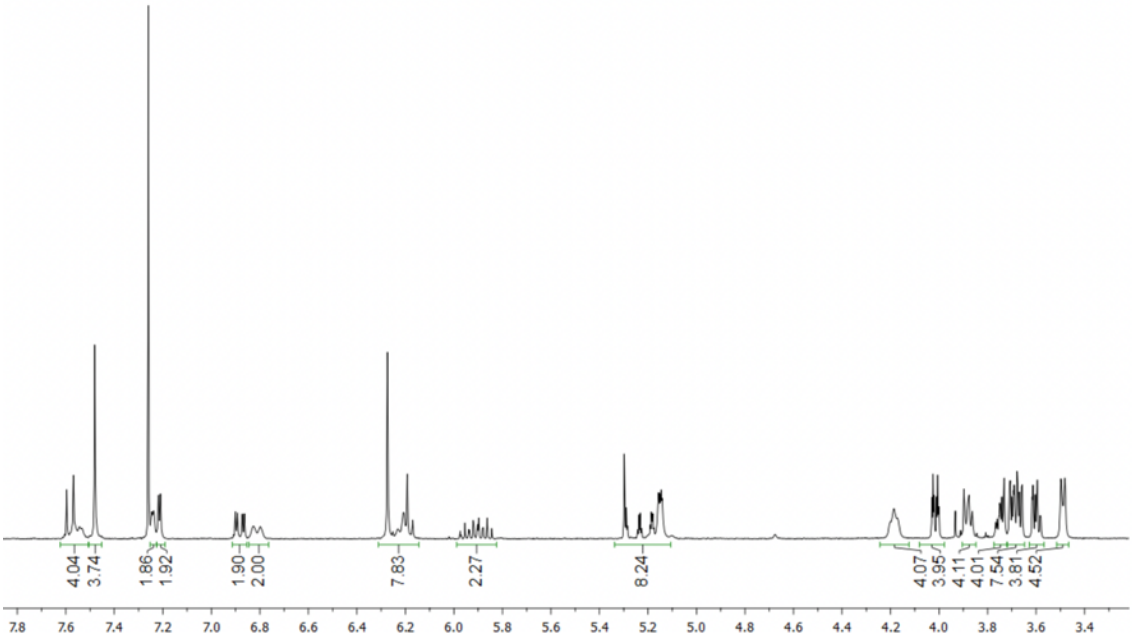
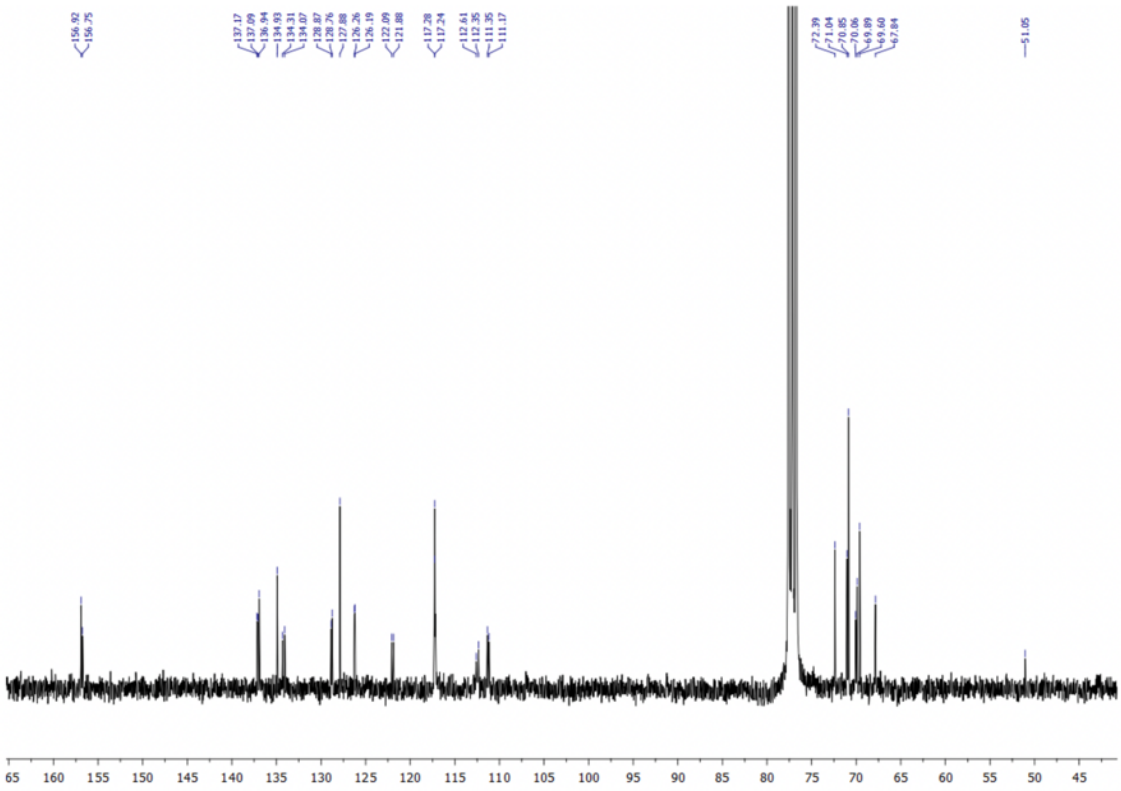
137.09
136.94
134.76
134.34
134.06
128.86
128.77
127.87
126.26
126.20
122.11
121.87
117.48
117.34
117.29
117.19
112.61
112.40
111.35
111.15
72.55
70.04
68.67
67.84

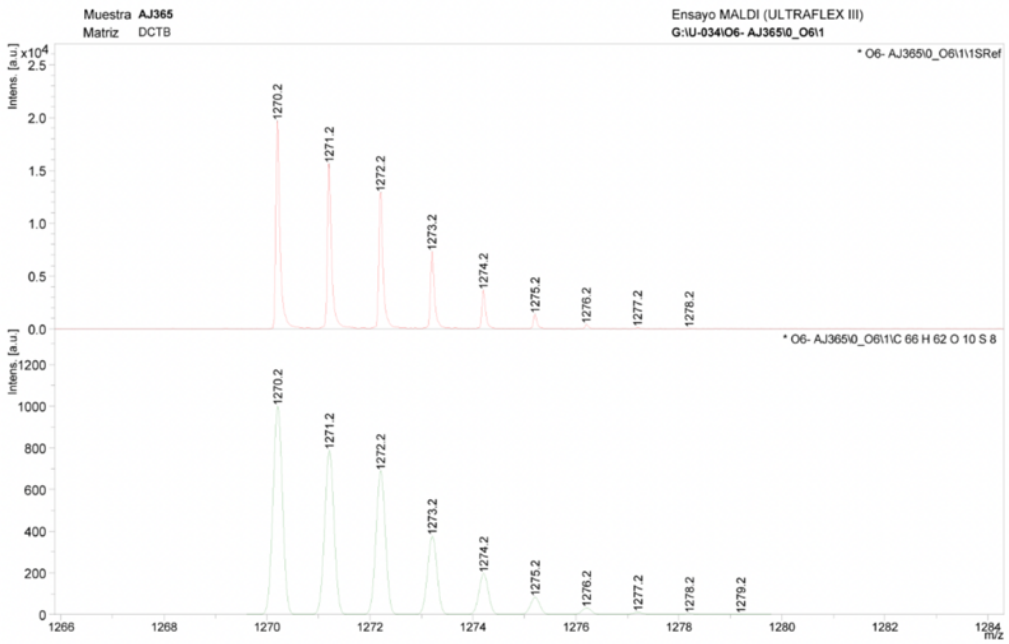

Muestra AJ370F1
Matriz DCTB
Ensayo MALDI (ULTRAFLEX III)
G:\U-035\A7- AJ370F1\0_A7\1
* A7- AJ370F1\0_A7\1\1SRef
Intens. [a.u.]
x10^4
1094.1
1095.1
1096.1
1097.1
1098.1
1099.1
1100.1
1101.1
* A7- AJ370F1\0_A7\1\C 58 H 46 O 6 S 8
1102.1
m/z



Compound 11c. ^{1}H NMR (300 MHz, $CDCl_3$) δ/ppm: 7.62–7.52 (m, 4H, $H_{k+k'}$), 7.48 (s, 4H, H_n), 7.24 (bd, J = 2.3 Hz, 2H, H_l), 7.21 (d, J = 2.5 Hz, 2H, $H_{l'}$), 6.88 (dd, J = 8.6, 2.6 Hz, 2H, H_j), 6.81 (bd, J = 8.9 Hz, 2H, $H_{j'}$), 6.29–6.15 (m, 8H, H_o), 5.99–5.83 (m, 2H, H_b), 5.32 (s, 4H, H_m), 5.31–5.12 (m, 4H, H_a), 4.19 (bt, J = 4.2 Hz, 4H, H_i), 4.02 (dt, J = 5.7, 1.4 Hz, 4H, H_c), 3.91–3.85 (m, 4H, H_h), 3.72–3.65 (m, 8H, H_{f+g}), 3.63–3.57 (m, 4H, H_e), 3.49 (d, J = 4.7 Hz, 4H, H_d).^{13}C NMR (75 MHz, $CDCl_3$) δ/ppm: 156.9, 156.8, 137.2, 137.1, 136.9, 134.9, 134.3, 134.1, 128.9, 128.8, 127.9, 126.3, 126.2, 122.1, 121.9, 117.3, 117.2, 112.6, 112.4, 111.4, 111.2, 72.4, 71.0, 70.8, 70.1, 69.9, 69.6, 67.8, 51.0. MS m/z calculated for $C_{66}H_{62}O_{10}S_8$ [M^+] 1270.2 found MALDI-TOF [M^+] 1270.2.




156.92
156.75
137.17
137.09
136.94
134.93
134.31
134.07
128.87
128.76
127.88
126.26
126.19
122.09
121.88
117.28
117.24
112.61
112.35
111.17
72.39
71.04
70.85
70.06
69.89
69.60
67.84
51.05
65 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45


Muestra AJ365
Matriz DCTB
Ensayo MALDI (ULTRAFLEX III)
G:\U-034\O6- AJ365\0_O6\1
* O6- AJ365\0_O6\1\1SRef
Intens. [a.u.]
x10^4
2.5
2.0
1.5
1.0
0.5
0.0
1270.2
1271.2
1272.2
1273.2
1274.2
1275.2
1276.2
1277.2
1278.2
* O6- AJ365\0_O6\1\C 66 H 62 O 10 S 8
Intens. [a.u.]
1200
1000
800
600
400
200
0
1270.2
1271.2
1272.2
1273.2
1274.2
1275.2
1276.2
1277.2
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1279.2
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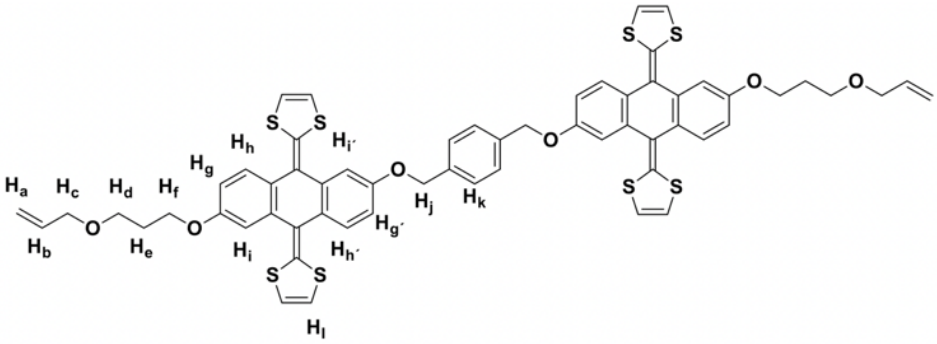
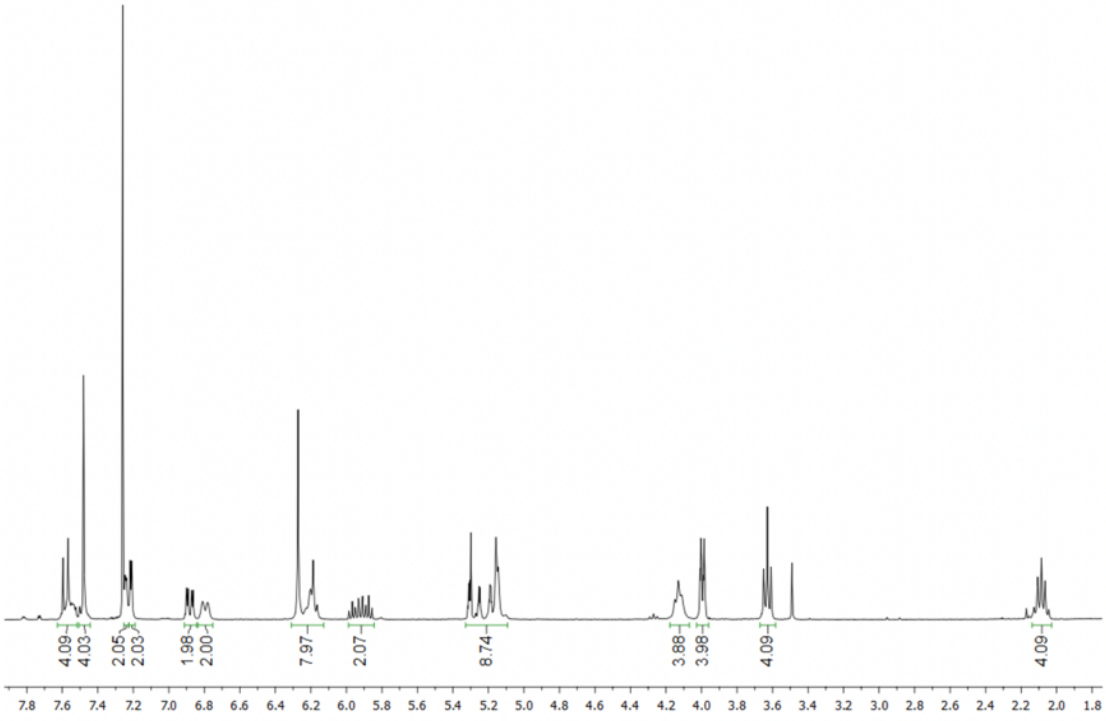
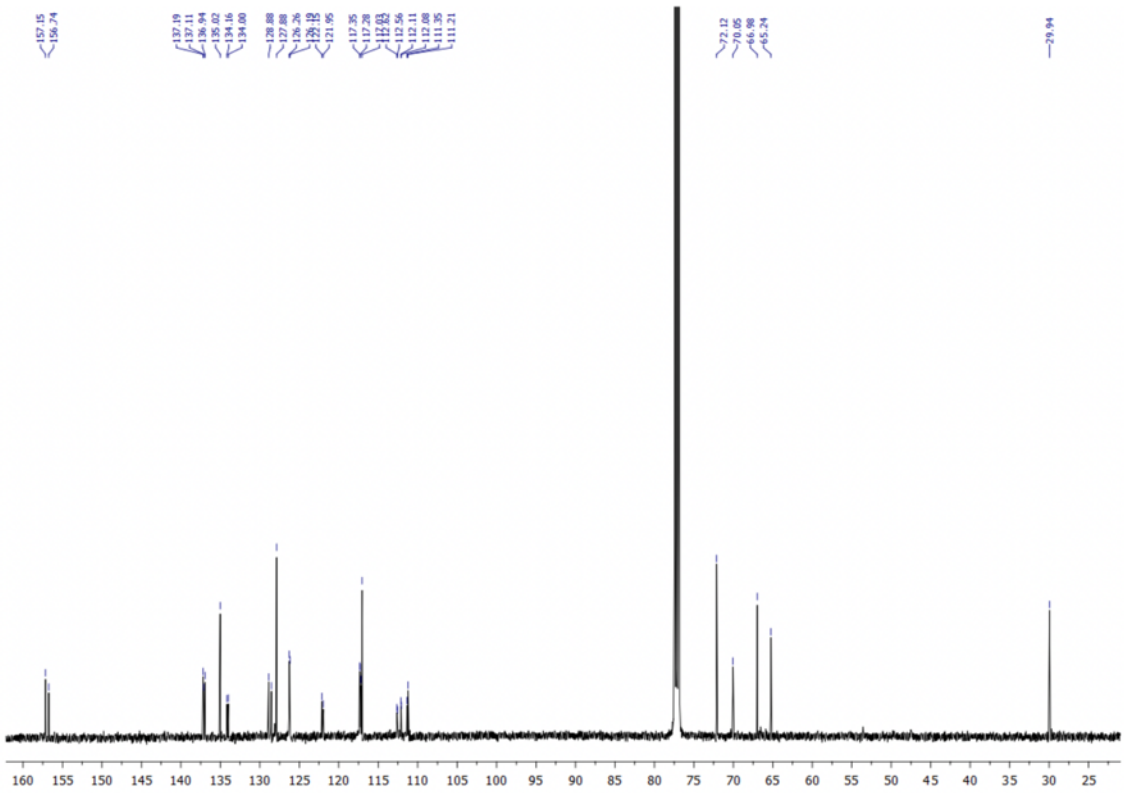
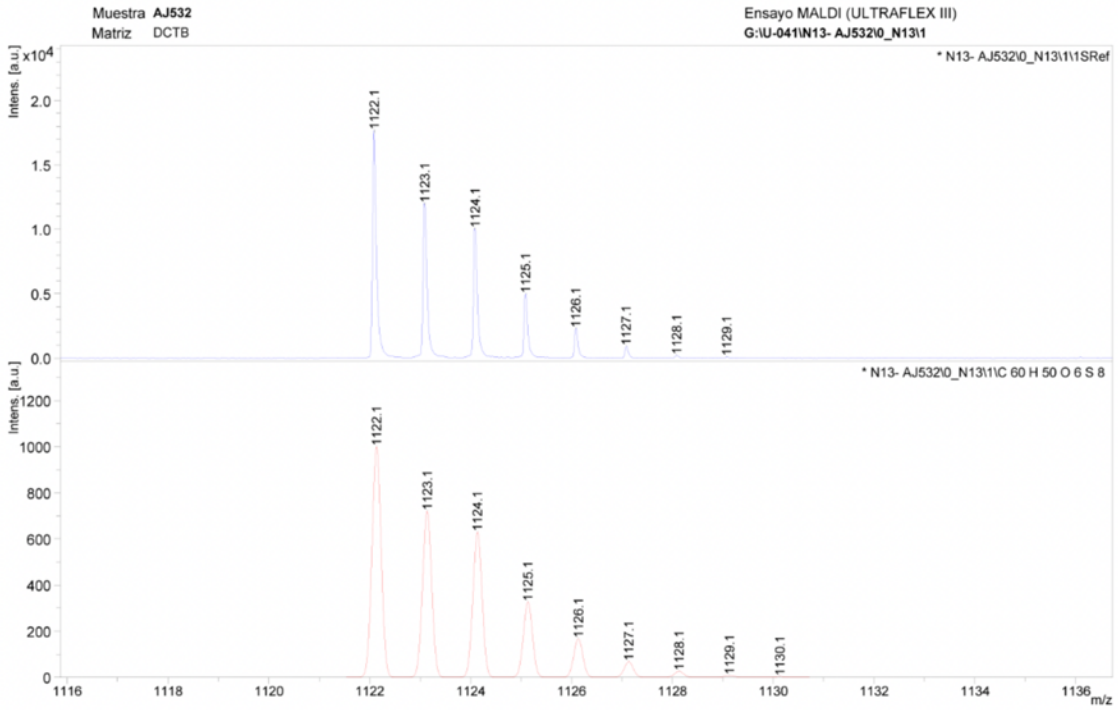
m/z



Compound 11d. ^{1}H NMR (300 MHz, $CDCl_3$) δ/ppm: 7.64–7.50 (m, 4H, $H_{h+h'}$), 7.48 (s, J = 6.5 Hz, 4H, H_k), 7.24 (d, J = 2.2 Hz, 2H, H_i), 7.21 (d, J = 2.5 Hz, 2H, $H_{i'}$), 6.88 (dd, J = 8.6, 2.6 Hz, 2H, H_g), 6.80 (bd, J = 8.6 Hz, 2H, $H_{g'}$), 6.34–6.10 (m, 8H, H_l), 5.99–5.84 (m, 2H, H_b), 5.34–5.08 (m, 8H, H_{a+j}), 4.13 (t, J = 5.8 Hz, 4H, H_f), 3.99 (dt, J = 5.6, 1.4 Hz, 4H, H_c), 3.63 (t, J = 6.2 Hz, 4H, H_d), 2.09 (p, J = 6.2 Hz, 4H, H_e). ^{13}C NMR (126 MHz, $CDCl_3$) δ/ppm: 157.2, 156.7, 137.2, 137.2, 136.9, 135.0, 134.2, 134.0, 128.9, 128.5, 127.9, 126.3, 126.2, 122.2, 122.0, 117.4, 117.3, 117.2, 117.0, 112.6, 112.6, 112.1, 112.1, 111.4, 111.2, 72.1, 70.0, 67.0, 65.2, 29.9. MS m/z calculated for $C_{60}H_{50}O_6S_8$ [M^+] 1122.1 found MALDI-TOF [M^+] 1122.1.




157.15
156.74
137.19
137.11
136.94
135.02
134.16
134.00
128.88
127.88
126.26
122.18
121.95
117.35
117.28
112.56
112.11
112.08
111.35
111.21
72.12
70.05
66.98
65.24
29.94
160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25


Muestra AJ532
Matriz DCTB
Ensayo MALDI (ULTRAFLEX III)
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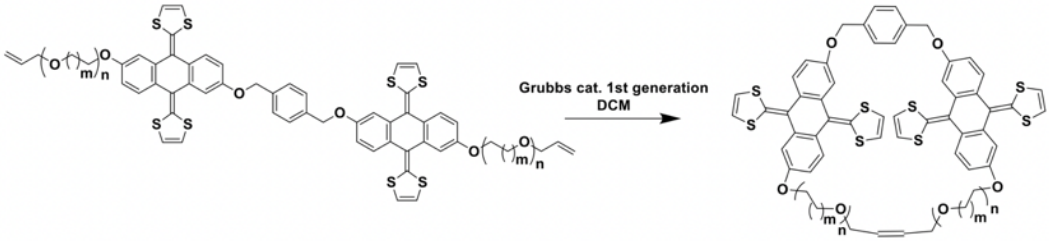
* N13- AJ532\0_N13\1\1SRef
Intens. [a.u.]
x10^4
2.0
1.5
1.0
0.5
0.0
1122.1
1123.1
1124.1
1125.1
1126.1
1127.1
1128.1
1129.1
* N13- AJ532\0_N13\1\1C 60 H 50 O 6 S 8
Intens. [a.u.]
1200
1000
800
600
400
200
0
1122.1
1123.1
1124.1
1125.1
1126.1
1127.1
1128.1
1129.1
1130.1
1116 1118 1120 1122 1124 1126 1128 1130 1132 1134 1136
m/z

1.5. π-extended tetrathiafulvalene macrocyclic derivatives.

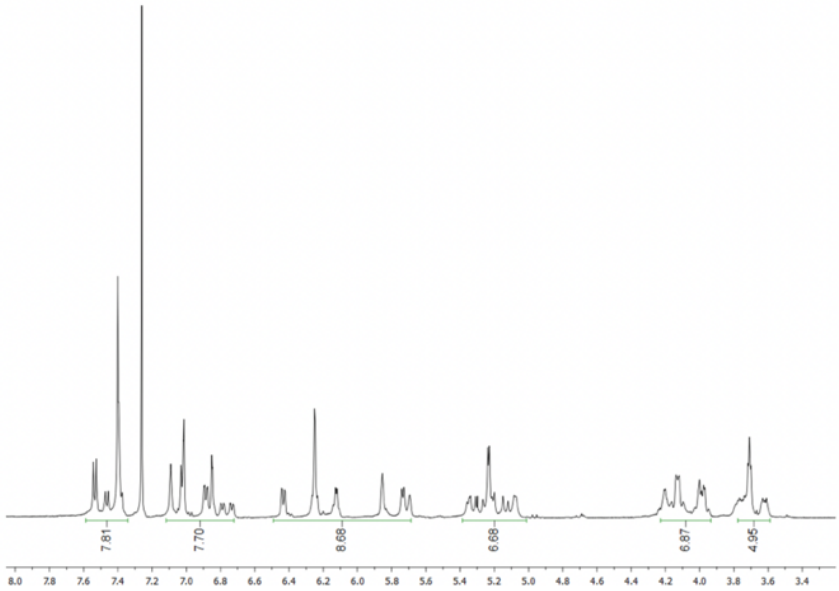


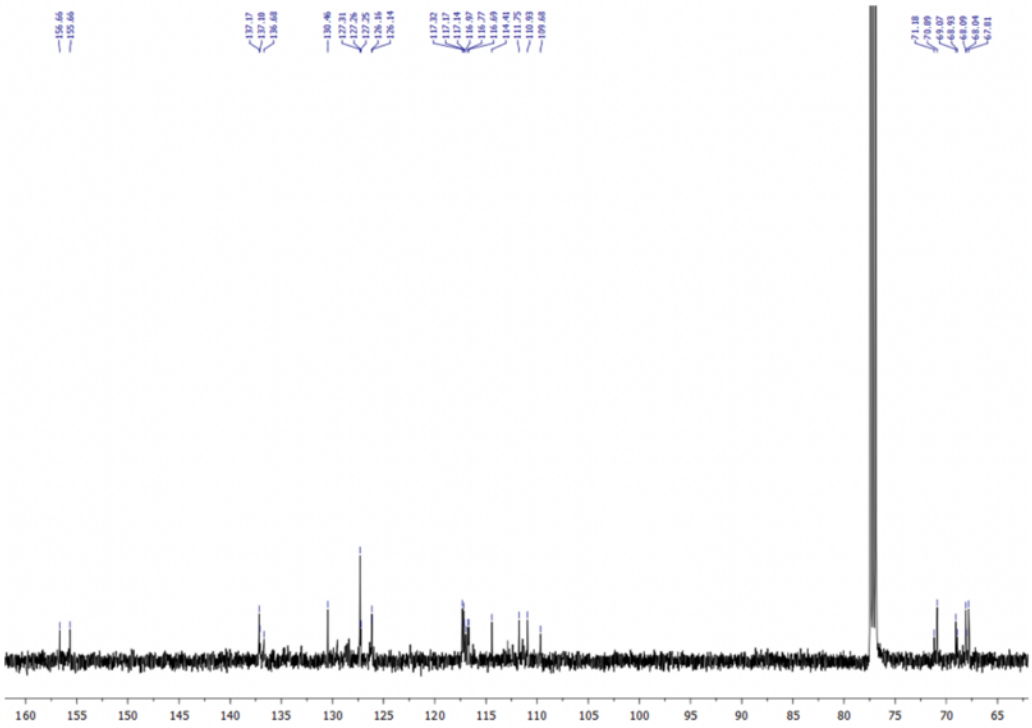
11a, n = 1, m = 1
11b, n = 2, m = 1
11c, n = 3, m = 1
11d, n = 1, m = 2

1, n = 1, m = 1
2, n = 2, m = 1
3, n = 3, m = 1
4, n = 1, m = 2

General procedure. A solution 10^{-4} M of compound **11** in DCM was degassed by nitrogen bubbling during 30 min. Then, catalytic amount of Grubbs catalyst 1st generation was added and stirred at room temperature for 3 h. The solution was filtered on celite and concentrated under vacuum. The solid was then purified by chromatography column using deactivate silica gel. Chromatography column (silica gel, hexane/ DCM , 3:1 to DCM) yielded compounds **1** (Y = 50%), **2** (Y = 60%), **3** (Y = 55%) and **4** (Y = 81%) as yellow solids.

Compound 1.^{1}H NMR (500 MHz, $CDCl_3$) δ/ppm: 7.59–7.34 (m, 8H), 7.12–6.69 (m, 8H), 6.48–5.66 (m, 8H), 5.39–5.03 (m, 6H), 4.24–3.92 (m, 7H), 3.83–3.55 (m, 5H). ^{13}C NMR (126 MHz, $CDCl_3$) δ/ppm: 156.7, 155.7, 137.2, 137.1, 136.7, 130.5, 127.3, 127.3, 127.2, 126.2, 126.1, 117.3, 117.2, 117.1, 117.0, 116.8, 116.7, 114.4, 111.8, 110.9, 109.7, 71.2, 70.9, 69.1, 68.9, 68.1, 68.0, 67.8. MS *m*/*z*: calculated for $C_{56}H_{42}O_6S_8$[M+] 1066.1 found MALDI-TOF 1066.1.


7.81
7.70
8.68
6.68
6.87
4.95
8.0 7.8 7.6 7.4 7.2 7.0 6.8 6.6 6.4 6.2 6.0 5.8 5.6 5.4 5.2 5.0 4.8 4.6 4.4 4.2 4.0 3.8 3.6 3.4


156.66
155.66
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137.10
136.68
130.46
127.31
127.26
127.25
126.16
126.14
117.32
117.17
117.14
116.97
116.77
116.69
114.41
111.75
110.93
109.68
71.18
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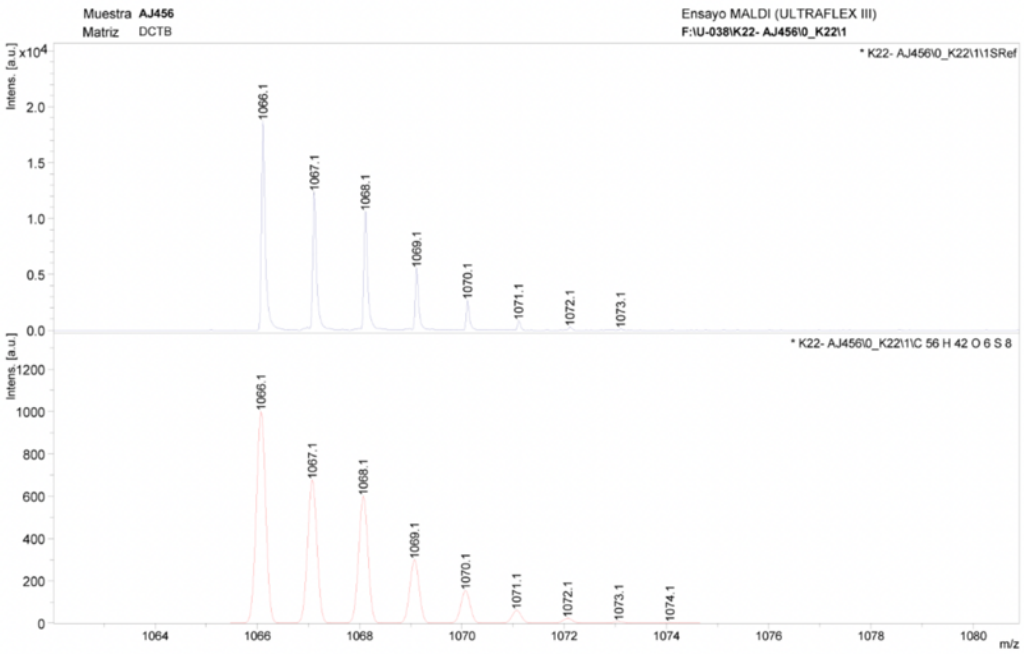
69.07
68.93
68.09
67.64
67.81
160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65


Muestra AJ456
Matriz DCTB
Ensayo MALDI (ULTRAFLEX III)
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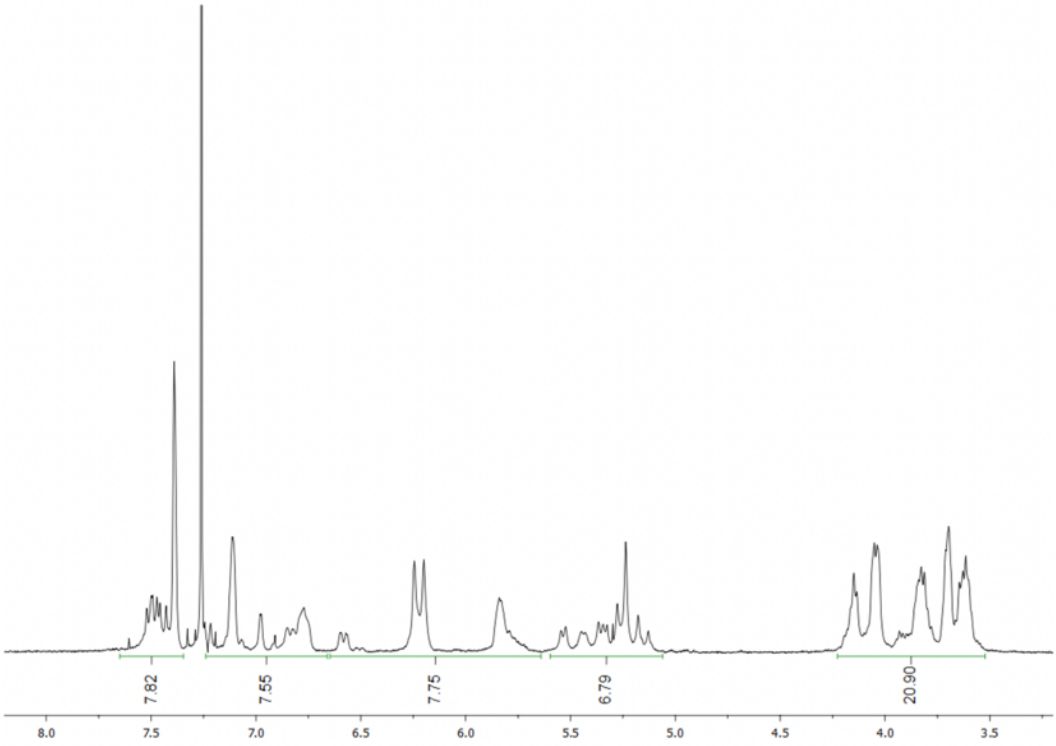
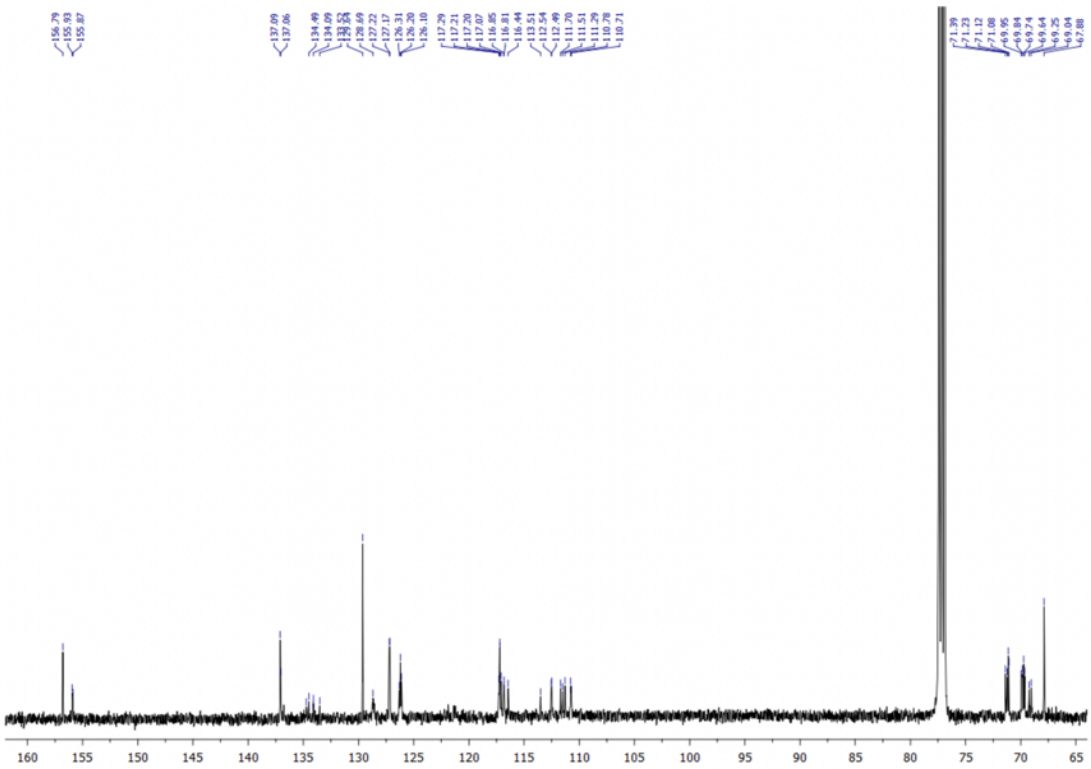
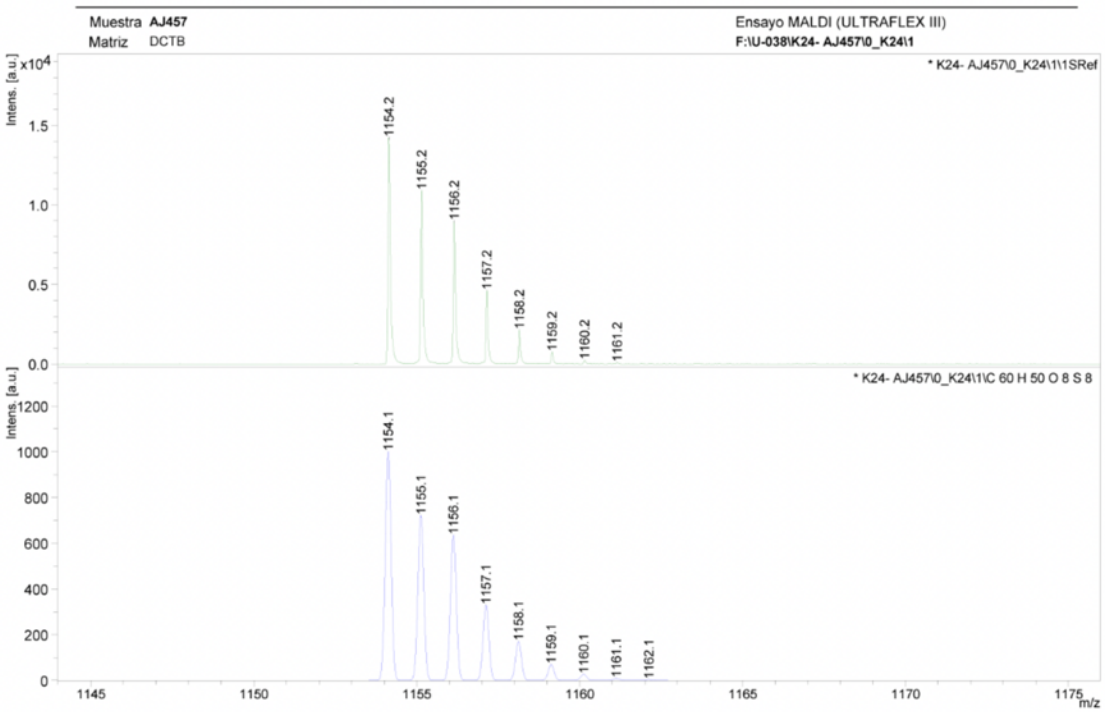
* K22- AJ456\0_K22\1\1SRef
Intens. [a.u.]
x10^4
2.0
1.5
1.0
0.5
0.0
1066.1
1067.1
1068.1
1069.1
1070.1
1071.1
1072.1
1073.1
* K22- AJ456\0_K22\1\C 56 H 42 O 6 S 8
Intens. [a.u.]
1200
1000
800
600
400
200
0
1066.1
1067.1
1068.1
1069.1
1070.1
1071.1
1072.1
1073.1
1074.1
1064
1066
1068
1070
1072
1074
1076
1078
1080
m/z

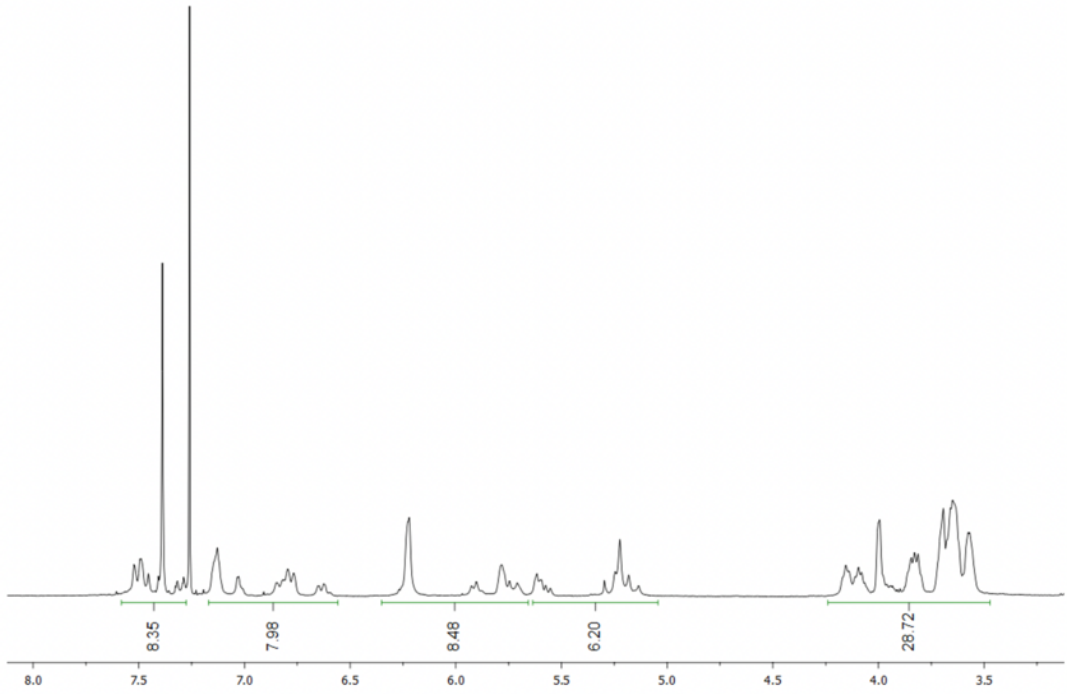
Compound 2. ^{1}H NMR (300 MHz, $CDCl_3$) δ/ppm: 7.63–7.34 (m, 8H), 7.19–6.65 (m, 8H), 6.62–5.64 (m, 8H), 5.57–5.06 (m, 6H), 4.09 (m, 20H). ^{13}C NMR (126 MHz, $CDCl_3$) δ/ppm: 156.8, 155.9, 155.9, 137.1, 137.1, 134.7, 134.5, 134.1, 134.1, 133.5, 129.6, 128.7, 127.2, 127.2, 126.3, 126.2, 126.1, 117.3, 117.2, 117.2, 117.1, 116.8, 116.8, 116.4, 113.5, 112.5, 112.5, 111.7, 111.5, 111.3, 110.8, 110.7, 71.4, 71.3, 71.1, 71.1, 70.0, 69.8, 69.7, 69.6, 69.2, 69.0, 67.9. MS *m*/*z*: calculated for $C_{60}H_{50}O_8S_8$ [M+] 1154.1 found MALDI-TOF 1154.2.

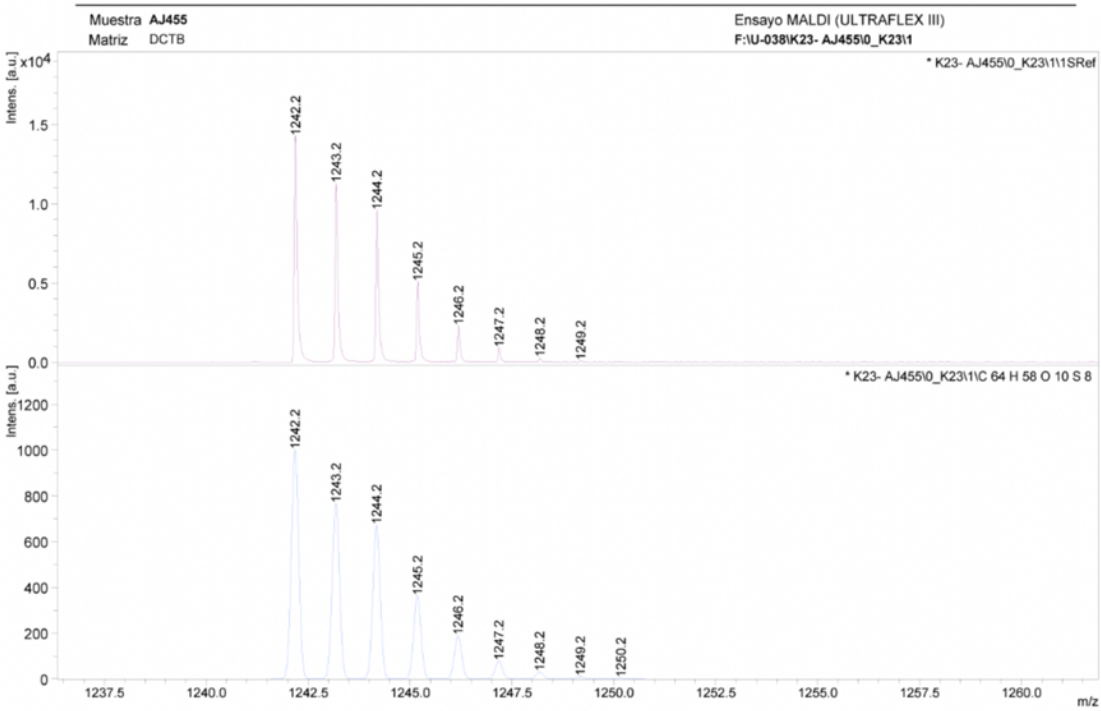




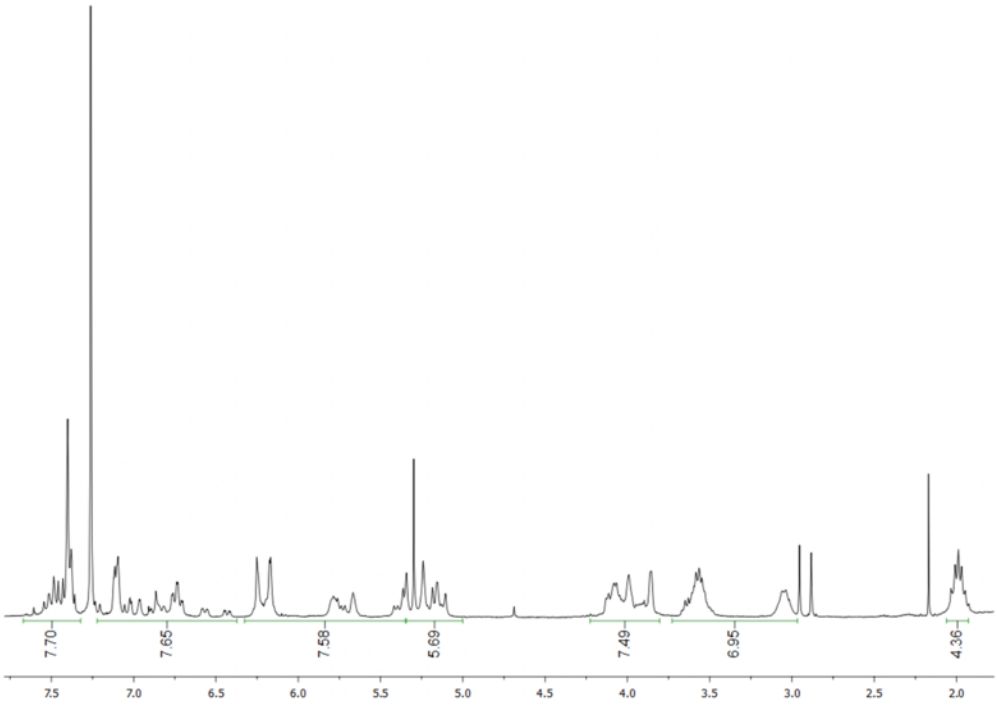

Muestra AJ457
Matriz DCTB
Ensayo MALDI (ULTRAFLEX III)
F:\U-038\K24- AJ457\0_K24\1
* K24- AJ457\0_K24\1\1SRef
* K24- AJ457\0_K24\1\C 60 H 50 O 8 S 8
Intens. [a.u.]
m/z

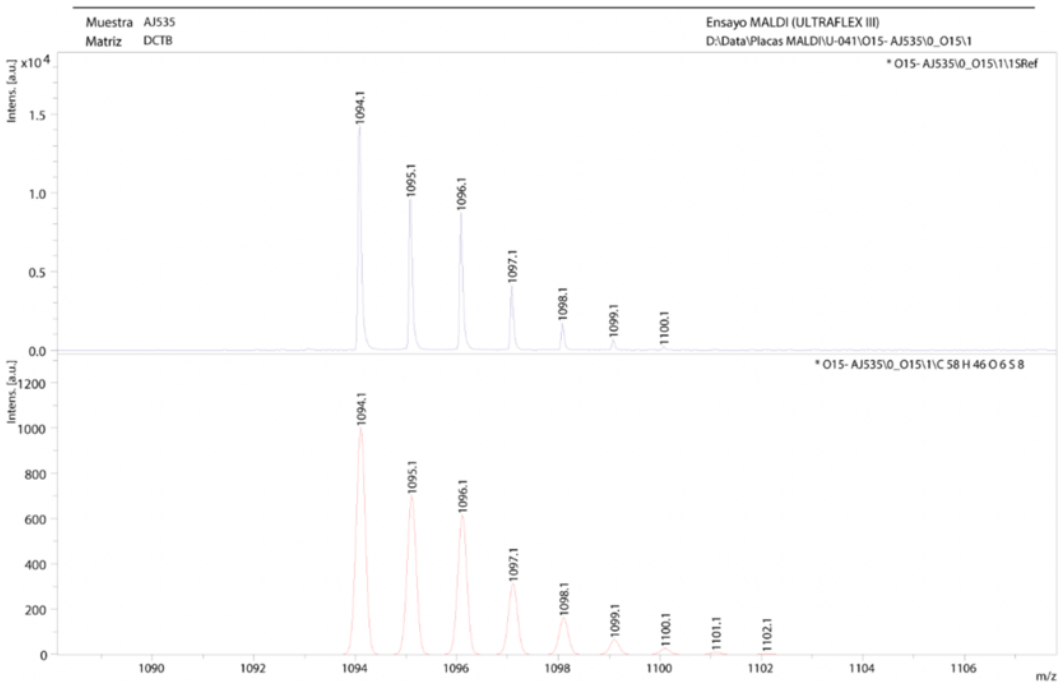
Compound 3. ^{1}H NMR (300 MHz, $CDCl_3$) δ/ppm: 7.56–7.28 (m, 8H), 7.18–6.56 (m, 8H), 6.32–5.68 (m, 8H), 5.64–5.07 (m, 6H), 4.22–3.49 (m, 28H). MS *m*/*z*: calculated for $C_{64}H_{58}O_{10}S_8$ [M+] 1242.2 found MALDI-TOF 1242.2.





Compound 4. ^{1}H NMR (300 MHz, $CDCl_3$) δ/ppm: 7.66–7.34 (m, 8H), 7.21–6.39 (m, 8H), 6.32–5.35 (m, 8H), 5.33–5.02 (m, 6H), 4.21–3.81 (m, 7H), 3.74–2.97 (m, 7H), 2.06–1.87 (m, 4H). MS *m*/*z*: calculated for $C_{58}H_{46}O_6S_8$ [M+] 1094.1 found MALDI-TOF 1094.1.





2. Theoretical Calculations

2.1. Semiempirical calculations

Minimum-energy geometry optimizations at the semiempirical PM7 level of theory[1] were performed for the different exTTF-based hosts accommodating inside a carbon nanotube of increasing size. The MOPAC2012 (version 15.229L) software was employed for this purpose.[2] The nanotubes selected were zig–zag (*n*,0) single-walled carbon nanotubes (SWNTs) with *n* = 8–18. The length of the nanotube was selected large enough (ca. 17 Å) to avoid terminal effects between the receptor and the nanotube edges (for *n* = 8, $C_{144}H_{16}$). See Figure S1 for the representative minimum-energy structure of **1**·SWNT(8,0) at the PM7 level.

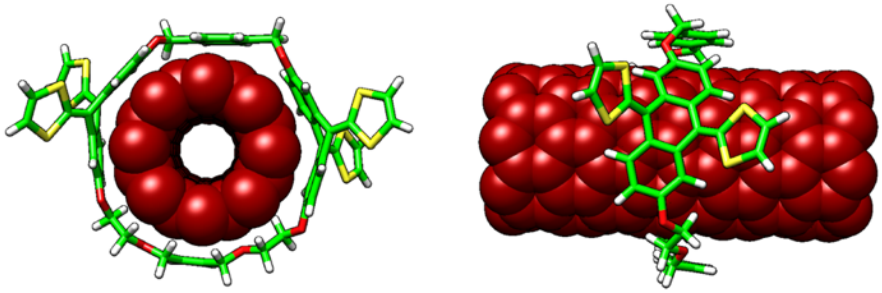


Figure S1. Minimum-energy geometry calculated at the PM7 level for the representative **1**·SWNT(8,0) supramolecular complex.

The binding energy of the host–guest formation was calculated upon increasing the nanotube size to determine the thickest nanotube that each exTTF-based ring can host (Figure S2). The binding energy (ΔE_{bind}) was estimated as the energy difference between the host–guest complex and the isolated monomers at their respective minimum-energy geometry. Note that we are not interested here in absolute ΔE_{bind} values but rather in the size of the nanotube at which ΔE_{bind} starts to increase dramatically. The host–guest geometry with a nanotube diameter prior to that at which ΔE_{bind} increases significantly was taken to measure the diameter of the macrocyclic host. This takes place for SWNT(*n*,0) with *n* = 8, 9, 9, 10 and 13 for **1**, **4**, **5**, **2** and **3**, respectively (see Figure S2).

[1] J. J. P. Stewart, *J. Mol. Model.* **2013**, *19*, 1–32.

[2] a) MOPAC2012, James J. P. Stewart, Stewart Computational Chemistry, Version 15.229L, web: HTTP://OpenMOPAC.net. b) J. D. C. Maia, G. A. Urquiza Carvalho, C. P. Mangueira, S. R. Santana, L. A. F. Cabral, G. B. Rocha, *J. Chem. Theory Comput.* **2012**, *8*, 3072–3081.

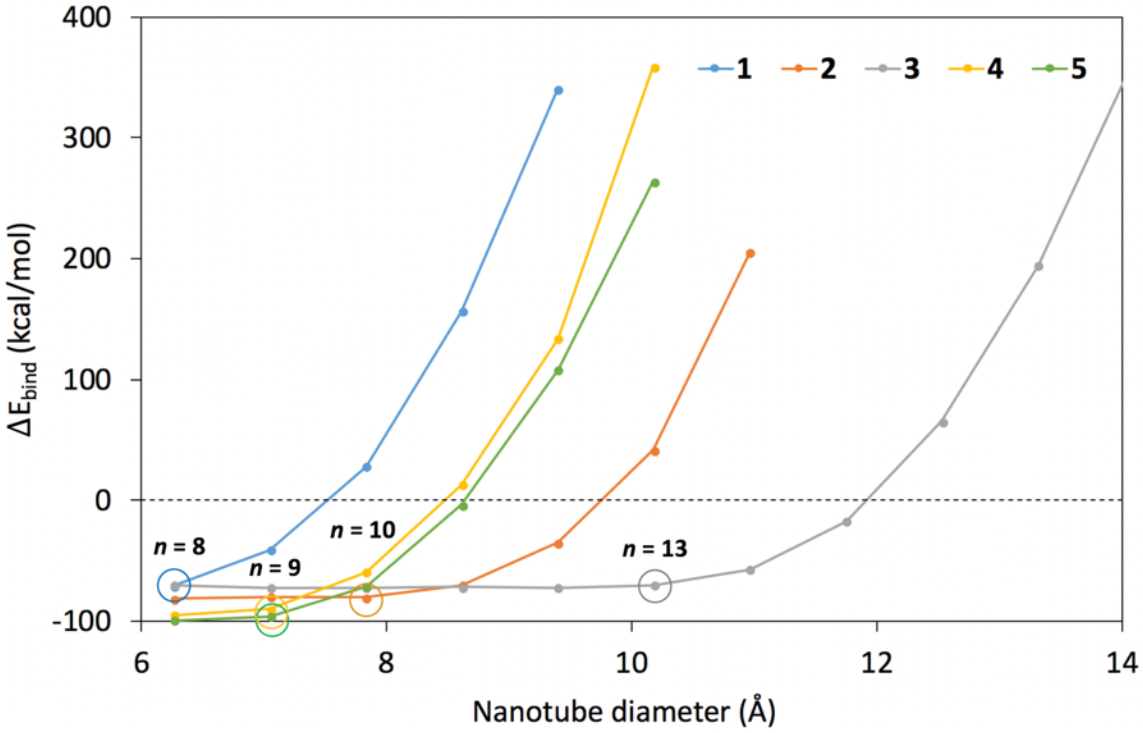


Figure S2. Evolution of the binding energy of the host·SWNT(*n*,0) complexes as a function of the nanotube size diameter. The largest nanotube able to be accommodated inside the macrocycle in each host without penalizing ΔE_{bind} is marked with a cycle.

The diameter of the nanotubes was calculated directly by measuring the distance between two opposing carbon atoms at the same cross section using the minimum-energy geometry of the isolated system. The diameter of macrocycles **1**–**5** was calculated by using the above-mentioned host–guest structures **1**·SWNT(8,0), **2**·SWNT(10,0), **3**·SWNT(13,0), **4**·SWNT(9,0) and **5**·SWNT(9,0), as the perimeter of the macrocycle through the sum of the distances between different atoms positioned in the perimeter path divided by π (Figure S3). The effective diameters (Table S1 and S2) of the host macrocycles and the guest (nanotube or fullerene) used to assess the host–guest matching in the macrocycle cavity were calculated by subtracting (host) and adding (guest) twice the van der Waals radius of carbon atom (r_C = 1.7 Å).

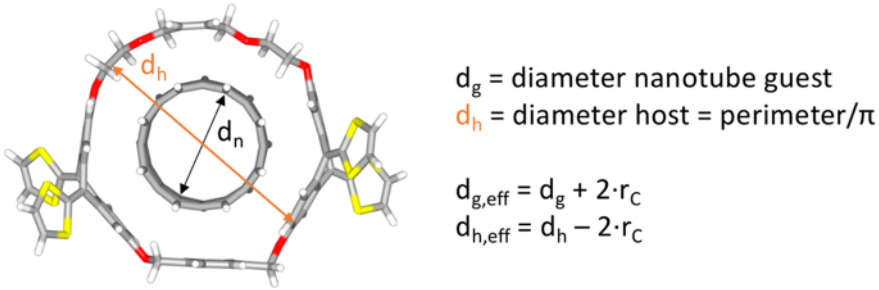
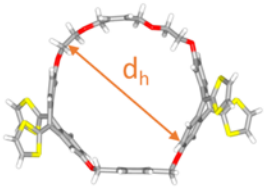


Figure S3. Definition of the diameter and effective diameter of the host macrocycles and nanotube guest.

Table S1. Diameters and effective diameters (in Å) for the exTTF-based macrocyclic host derivatives.



Host	perimeter (Å)	d_h	$d_{h,eff}$
1	41.6	13.2	9.8
2	47.1	15.0	11.6
3	54.2	17.3	13.9
4	43.8	13.9	10.5
5	44.6	14.2	10.8

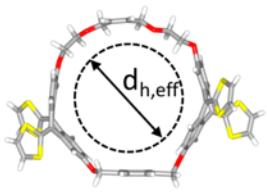
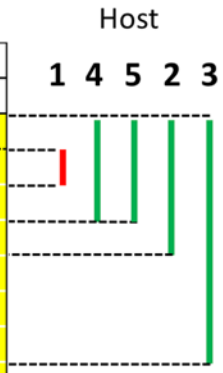


Table S2. Diameters and effective diameters (in Å) for the SWNTs and C_{60} guests. The range of SWNTs (and C_{60}) able to be accommodated inside the macrocycle cavity for each host is sketched on the right side of the Table as vertical green bars.

SWNT (*n*,0)	hypothetical	calculated	
n	d_g	d_g	$d_{g,eff}$
C_{60}	7.0	7.1	10.5
8	6.3	6.3	9.7
9	7.0	7.0	10.4
10	7.8	7.8	11.2
11	8.6	8.6	12.0
12	9.4	9.4	12.8
13	10.2	10.1	13.5
14	11.0	10.9	14.3
15	11.7	11.7	15.1
16	12.5	12.5	15.9
17	13.3	13.3	16.7
18	14.1	14.1	17.5



The theoretical diameters calculated for the minimum-energy geometries of zig–zag SWNTs(*n*,0) with *n* = 8–18 at the PM7 level are in very good accord with the hypothetical values extracted from the corresponding formula of an ideal nanotube

$$d = \frac{\sqrt{3}\, a_{C\text{–}C}}{\pi}\sqrt{n^2 + n \cdot m + m^2}$$

with $a_{C\text{–}C}$ = 1.421 Å and *m* = 0 (Table S2). The diameter of the fullerene C_{60} is calculated to be 7.1 Å (d_{eff} = 10.5 Å), which is approximately the diameter of the nanotube with *n* = 9 (7.0 Å). The ring that can host the SWNT of *n* = 9 will therefore be able to bear the C_{60} molecule. Host system **4** is therefore predicted as the smallest ring that can host C_{60}.

2.2. Molecular mechanics/molecular dynamics simulations

The potential mean force (PMF) profile was calculated at the molecular mechanics level of theory using the general MM3 force-field and the Weighted Histogram Analysis Method (WHAM).[3] For that purpose, we developed a modified version of TINKER-5.1[4] containing the adapted files from Petr Bouř to perform WHAM by scanning centroids between two groups of atoms.[5] The host and guest centroids were used to define a constraint distance for the WHAM method with 40 windows and 1000 integration points without periodic boundary conditions and at a constant T = 298 K via default thermostat. The interval of the constraint distance was set from 0 to 25 Å. As the MM3 force-field is not able to reproduce the typical butterfly shape of the exTTF moiety, all the torsions that belong to the exTTF unit were restrained along the simulations. A minimization was first performed on each point, followed by 0.5 ps of equilibration and 500 ps of production regime. The force constant of the constraint was set to 2 kcal/Å^2. Two opposite directions were considered for the PMF profile generation: the extraction of the C_{60} embraced in the host cavity (decomplexation), and the inclusion of the C_{60} from the outside of the ring (complexation). The decomplexation process was used for obtaining the final profiles as the PMF converges with less computational effort. See Figure 2 in the main text for the PMF profiles in the macrocyclic host·fullerene guest self-assembly.

2.3. Density functional theory calculations

Density functional theory calculations were performed to quantify the affinity of our novel macrocyclic receptors towards fullerene recognition by using the Gaussian-09.D01 suite of packages.[6] First, we optimized the structure of the two self-assembling modes found in the host–guest complexes: the inside-ring and the outside-ring adsorption modes. For that purpose, we used the Grimme's dispersion-corrected B97D3 functional,[7] which has demonstrated a great accuracy-computational cost trade-off.[8] The popular and cost-effective Pople's 6-31G** basis set was used throughout.[9] Note that we do not include the

[3] a) B. Roux, *Comput. Phys. Commun.* **1995**, *91*, 275–282. b) S. Kumar, J. M. Rosenberg, D. Bouzida, R. H. Swendsen and P. A. Kollman, *J. Comput. Chem.* **1992**, *13*, 1011–1021.

[4] https://dasher.wustl.edu/tinker/

[5] http://hanicka.uochb.cas.cz/~bour/programs/F/docs/WHAM.doc

[6] Gaussian 09, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman and D. J. Fox, Gaussian, Inc., Wallingford CT, **2016**.

[7] a) S. Grimme, *J. Comput. Chem.* **2006**, *27*, 1787–1799. b) S. Grimme, S. Ehrlich and L. Goerigk, *J. Comput. Chem.* **2011**, *32*, 1456–1465.

[8] L. Goerigk, H. Kruse and S. Grimme, *ChemPhysChem* **2011**, *12*, 3421–3433.

[9] R. Ditchfield, W. J. Hehre and J. A. Pople, *J. Chem. Phys.* **1971**, *54*, 724–728.

counterpoise correction to the basis set superposition error as there is still debate on its usefulness.[10]

Minimum-energy geometries were also obtained for the constituting monomers at the B97D3/6-31G** level. Due to the large conformational space of the flexible macrocycles, several conformers were optimized. However, we found that the structures provided by the MM/MD simulations at large host-guest distances (ca. 25 Å) lead to the most stable conformers, with the two exTTF moieties interacting in a saddle-to-saddle arrangement and the long alkyl ether chains accommodated in a knot-like shape to maximize the intramolecular noncovalent interactions (Figure 3a in the main text).

Frequency calculations were performed at the B97D3/6-31G** level for the minimum-energy host–guest structures and constituting monomers to i) confirm that local minima are found, and ii) incorporate the zero-point energy, thermal corrections, enthalpic and entropic terms in order to obtain the free energy of the system. The solvation effect was accounted by performing single-point calculations with the popular SMD solvent model based on the solute's density,[11] which is the recommended choice for computing free energies of solvation ($\Delta\Delta G_{\text{solv}}$), and using chlorobenzene as the solvent. Note that the binding free energy for the host–guest complexation ($\Delta G_{\text{bind,theor}}$) can be calculated according to:

$$\Delta G_{\text{bind,theor}} = \Delta G_{\text{bind,gas}} + \Delta\Delta G_{\text{solv}}$$

where

$$\Delta G_{\text{bind,gas}} = \Delta H_{\text{bind}} - T\Delta S_{\text{bind}}$$

and

$$\Delta\Delta G_{\text{solv}} = \Delta G_{\text{solv,complex}} - \Delta G_{\text{solv,host}} - \Delta G_{\text{solv,guest}}$$

ΔH_{bind} and ΔS_{bind} are the enthalpic and entropic binding contributions, respectively, calculated as the magnitude difference between the complex and the constituting monomers at their respective minimum-energy geometries, and $\Delta G_{\text{solv,X}}$ is the solvation energy of system X.

In order to compute the entropic term, we used the rigid-rotor harmonic oscillator (RRHO) approach popularized by Grimme,[12] and recently set as a default procedure in some quantum chemistry packages.[13] In this approach, the entropic terms for frequencies below a certain cut-off are obtained from the free-rotor approximation, whereas for those above, the typical harmonic oscillator expression is used. A damping function is employed to interpolate between these two expressions close to the cut-off frequency. A temperature T = 298.15 K, an average molecular moment of inertia $B_{\text{av}} = 10^{-44}$ kg m^2, and a frequency cutoff ω_0 = 100 cm^{-1} was used as recommended. Residual imaginary low-energy frequencies calculated for the inside-ring adsorption mode of our host–guest complexes were treated as real.

Note that the internal energy contribution (ΔE_{bind}) in the ΔH_{bind} term, can be decomposed according to

[10] X. W. Sheng, L. Mentel, O. V. Gritsenko and E. J. Baerends, *J. Comput. Chem.* **2011**, *32*, 2896–2901.
[11] A. V. Marenich, C. J. Cramer and D. G. Truhlar, *J. Phys. Chem. B* **2009**, *113*, 6378–6396.
[12] S. Grimme, *Chem. Eur. J.* **2012**, *18*, 9955–9964.
[13] https://orcaforum.kofo.mpg.de/app.php/dlext/?view=detail&df_id=15

$$\Delta E_{\text{bind}} = \Delta E_{\text{int}} + E_{\text{def}}$$

where ΔE_{int} and E_{def} are the interaction and deformation energy, respectively. The deformation energy in the host–guest complexes mainly arises from the macrocyclic receptor, which has a large conformational space, whereas fullerene barely contributes due to its rigid structure. Moreover, the ΔE_{def} of the macrocycle can be further split into two contributions:

$$E_{\text{def}} \approx E_{\text{def,host}} = E_{\text{def,intra}} + E_{\text{def,complex}}$$

accounting for the energy loss due to the rupture of the intramolecular noncovalent interactions in the relaxed entangled receptor ($E_{\text{def,intra}}$), and the deformation coming from the disposition of the macrocycle upon complexation ($E_{\text{def,complex}}$) (see Figure 3 in the main text). Inside-ring and outside-ring adsorption modes for one receptor are considered to have the same $E_{\text{def,intra}}$, as it is the energy difference between the open-ring (Figure 3b) and the most stable (Figure 3a) conformation. Otherwise, $E_{\text{def,complex}}$ accounts for the different stability of the macrocycle between the two modes in the complex formation, and it is calculated as the energy difference between the geometry at the complex (Figure 3c-d) and the open-ring configuration (Figure 3b). A positive value of $E_{\text{def,complex}}$ indicates an energetically unfavourable strained macrocycle disposition in the complex (Figure 3c), whereas a negative value of $E_{\text{def,complex}}$ indicates that the macrocycle in the host–guest complex adopts a favourable conformation, stabilized by intermolecular interactions (Figure 3d), compared to the system in the relaxed open-ring conformation (Figure 3b).

Finally, the noncovalent index (NCI) was calculated for the **4**·C_{60} complex by using the NCIPLOT-3.0 software.[14] The PROMOLECULAR densities were employed, along with density and reduced density gradient thresholds of 0.2 and 1.0 a.u., respectively, and a discarding density parameter of 0.95 a.u. for the intermolecular NCI selection.

The computational protocol used herein therefore consists of four steps: i) semiempirical approaches for initial exploration of cavity matching, ii) molecular mechanics/molecular dynamics calculations for the conformational sampling and understanding the complexation/decomplexation process, iii) high-level DFT free energies for accurate binding quantification, and iv) NCI plots to visualize and categorize the noncovalent interactions governing the supramolecular assembly. This protocol allows us to quantify the binding energy of the host-guest assemblies in a high accuracy/computational cost ratio. We are aware that other methodologies can be used to determine the complexation strength and understand the nature of the forces governing the self-assembling process. Techniques such as the symmetry-adapted perturbation theory (SAPT)[15] could complement the NCI analysis and help in establishing a more precise description of the weak noncovalent forces present in our systems. However, the main goal of our work is devoted to quantifying the host-guest binding strength upon increasing the host size.

[14] a) E. R. Johnson, S. Keinan, P. Mori-Sánchez, J. Contreras-García, A. J. Cohen and W. Yang, *J. Am. Chem. Soc.* **2010**, *132*, 6498–6506. b) J. Contreras-García, E. R. Johnson, S. Keinan, R. Chaudret, J.-P. Piquemal, D. N. Beratan and W. Yang, *J. Chem. Theory Comput.* **2011**, *7*, 625–632.

[15] E. G. Hohenstein, R. M. Parrish, C. D. Sherrill, J. M. Turney and H. F. Schaefer, *J. Chem. Phys.* **2011**, *135*, 174107.

Geometry structures were represented using the Chimera-1.12 software,[16] whereas the NCI surfaces were plotted by using the VMD-1.9.3 program.[17]

Table S3. Deformation energy contributions obtained at the B97D3/6-31G** level of theory for the self-assembly of **1**–**5** receptors with fullerene C_{60}.

Complex	E_{def}	$E_{def,intra}$	$E_{def,complex}$	$E_{def,host}$	$E_{def,guest}$
inside-ring mode					
1·C_{60}[a]	-	-	-	-	-
2·C_{60}	37.5	31.6	5.3	36.9	0.6
3·C_{60}	42.7	43.6	–1.3	42.3	0.4
4·C_{60}	34.2	31.0	2.6	33.6	0.6
5·C_{60}	34.1	26.3	7.2	33.5	0.6
outside-ring mode					
1·C_{60}	14.6	28.5	–14.0	14.5	0.1
2·C_{60}	17.6	31.6	–14.4	17.2	0.4
3·C_{60}	22.7	43.6	–21.0	22.7	0.0
4·C_{60}	14.1	31.0	–16.9	14.1	0.0
5·C_{60}	14.0	26.3	–12.2	14.0	0.0

[a] An outside-ring mode with an opened ring macrocycle resembling the inside-ring mode is found for **1**·C_{60}. This adsorption mode offers the following thermodynamic parameters: E_{def} = –34.7 kcal/mol, $E_{def,intra}$ = 28.5 kcal/mol, $E_{def,complex}$ = 6.2, $E_{def,host}$ = 34.6 kcal/mol and $E_{def,guest}$ = 0.1 kcal/mol.

Table S4. Thermodynamic parameters obtained at the B97D3/6-31G**+SMD level of theory for the self-assembly of **1**–**5** receptors with fullerene C_{60}.

Complex	ΔH_{bind}	$-T\cdot\Delta S_{bind}$	$\Delta G_{bind,gas}$	$\Delta\Delta G_{solv}$
inside-ring mode				
1·C_{60}[a]	-	-	-	-
2·C_{60}	–21.2	11.5	–9.7	12.5
3·C_{60}	–19.9	14.7	–5.1	10.3
4·C_{60}	–24.8	15.5	–9.3	10.5
5·C_{60}	–25.8	14.5	–11.3	11.3
outside-ring mode				
1·C_{60}	–32.6	16.0	–16.6	13.4
2·C_{60}	–32.0	13.8	–18.3	14.0
3·C_{60}	–35.7	17.2	–18.5	13.7
4·C_{60}	–34.9	16.6	–18.4	12.3
5·C_{60}	–34.6	16.0	–18.6	12.3

[a] An outside-ring mode with an opened ring macrocycle resembling the inside-ring mode is found for **1**·C_{60}. This adsorption mode offers the following thermodynamic parameters: ΔH_{bind} = –19.3 kcal/mol, $-T\cdot\Delta S_{bind}$ = 14.6 kcal/mol, $\Delta G_{bind,gas}$ = –4.7 kcal/mol and $\Delta\Delta G_{solv}$ = 11.1 kcal/mol.

[16] E. F. Pettersen, T. D. Goddard, C. C. Huang, G. S. Couch, D. M. Greenblatt, E. C. Meng and T. E. Ferrin, *J. Comput. Chem.* **2004**, *25*, 1605–1612.

[17] W. Humphrey, A. Dalke and K. Schulten, *J. Mol. Graph.* **1996**, *14*, 33–38.

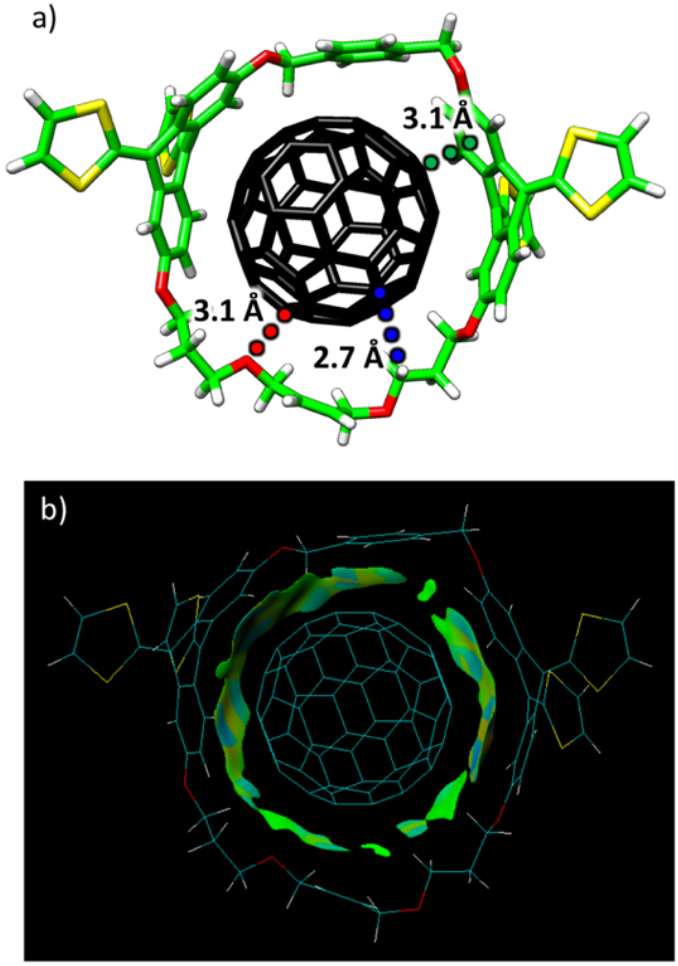


Figure S4. Noncovalent interactions participating in the stabilization of the inside-ring self-assembling mode of **4**·C_{60}: a) characteristic intermolecular contacts (π–π in green, *n*···π in red and CH···π in blue), and b) intermolecular NCI surface.

XYZ B97D3/6-31G**-optimized geometries

172
1-C60-inside-ring

O	-3.159473	-5.077551	-0.480978
C	-5.897307	-1.893335	-0.319923
C	-5.423010	-2.469349	0.890707
C	-6.630170	-0.610108	-0.236719
C	-6.145905	0.282943	0.842806
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C	-9.812287	-0.449986	-2.601204
S	-8.374555	-1.402922	-2.269767
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H	-4.578973	2.436695	3.710753
H	-7.784804	-3.028597	6.524880
H	-7.438030	-5.280091	5.281287
H	-10.747034	1.438837	-2.118778
H	-10.533545	-0.865778	-3.299357
O	-5.203352	3.777096	1.402623
C	-2.319015	-5.277296	0.660036
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H	-2.782438	-6.003612	1.348809
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C	1.830793	-6.097840	-0.214920
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H	3.524304	-6.986285	-1.219813
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186
2-C60-inside-ring
O      -2.885032      -5.676213       0.027116
C      -5.923951      -2.834306      -0.514797
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3-C60-inside-ring
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C	-6.988868	-4.170217	5.091428
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S	-8.564353	-3.090362	-2.500429
H	-5.935967	-3.350398	-2.666407
H	-4.155930	-4.256272	1.875512
H	-4.346308	-5.221554	-2.314131
H	-5.298327	0.145206	3.209315
H	-6.961665	1.066199	-1.357781
H	-5.487589	2.468280	2.423940
H	-7.828881	-2.662442	6.393250
H	-7.187400	-5.071749	5.664618
H	-11.379298	-0.695033	-2.773071
H	-10.818834	-3.135429	-3.464253
O	-6.402794	3.142663	-0.087239
C	-2.323524	-5.902931	0.968341
H	-2.222014	-4.889301	1.387280
H	-2.698595	-6.563023	1.767354
C	-0.961444	-6.342408	0.479289
C	-0.561535	-6.109728	-0.846526
C	-0.032532	-6.874816	1.385089
C	0.755963	-6.347860	-1.242259
C	1.284089	-7.125372	0.982182
C	1.699857	-6.842608	-0.328400
H	-1.285871	-5.721289	-1.555651
H	-0.331496	-7.076080	2.414948
H	1.065499	-6.124535	-2.262568
H	1.998684	-7.535060	1.698317
C	3.131785	-7.068991	-0.765883
H	3.742342	-7.442090	0.070872
H	3.172946	-7.807893	-1.576738
O	3.755755	-5.901880	-1.344080
C	5.419831	-2.919017	1.094411
C	5.685112	-2.972237	-0.308516
C	6.029360	-1.834040	1.881578
C	6.141664	-0.559029	1.151798
C	6.440136	-0.606557	-0.238365
C	6.570584	-1.932309	-0.877591
C	4.539157	-3.860161	1.647361
C	5.078468	-3.974963	-1.079829
C	4.249459	-4.947369	-0.490797
C	3.966479	-4.879851	0.882572
C	6.532407	0.618239	-0.935868
C	5.899546	0.675782	1.775955
C	6.347436	1.845807	-0.301854
C	6.002610	1.877794	1.059650
C	7.509529	-2.204347	-1.845674
C	6.522257	-2.011104	3.151598
S	8.708618	-1.007502	-2.424078
C	9.719169	-2.160385	-3.281216
C	9.294359	-3.435286	-3.341772
S	7.769553	-3.824255	-2.561004
S	7.357303	-0.732141	4.089621
C	8.012773	-1.810198	5.314366
C	7.637895	-3.101318	5.273008
S	6.526970	-3.588098	4.000852
H	4.248390	-3.770851	2.692294
H	5.195961	-3.999134	-2.160245
H	3.266729	-5.563032	1.348363
H	6.687389	0.609892	-2.012647
H	5.561431	0.677689	2.806251
H	6.386105	2.778346	-0.860726
H	10.628354	-1.779592	-3.738421
H	9.808465	-4.243035	-3.855533
H	8.673432	-1.373195	6.058211
H	7.949378	-3.865933	5.979553
O	5.737325	3.108437	1.598275
C	5.206078	3.135294	2.931382
H	5.948679	2.731437	3.641944
H	4.294191	2.520644	2.985285

C	4.871227	4.571140	3.306753
H	4.660090	4.586928	4.386932
H	5.748174	5.216660	3.118631
C	-6.473570	4.327582	0.718226
H	-6.895574	4.110012	1.709967
H	-7.173796	4.981086	0.179397
C	-5.147906	5.068296	0.860840
H	-4.566532	4.962842	-0.073770
H	-5.375597	6.144841	0.991728
O	3.712450	5.082125	2.669761
C	3.923641	5.641412	1.367632
H	3.960963	4.851550	0.602714
H	4.875936	6.198817	1.330182
C	2.759930	6.610584	1.142831
H	2.734574	7.302663	1.995201
H	1.804961	6.063185	1.113447
O	-4.409651	4.600625	1.981294
C	-3.326273	5.487553	2.279775
H	-3.716035	6.498761	2.504696
H	-2.638295	5.573410	1.426556
C	-2.590634	4.972975	3.518964
H	-1.984047	4.086505	3.273908
H	-3.338868	4.679383	4.269090
O	2.918063	7.421105	-0.017583
C	2.581899	6.766846	-1.239195
H	1.644632	6.202351	-1.133797
H	3.370984	6.053328	-1.546882
C	2.439143	7.833091	-2.316979
H	3.332800	8.474192	-2.295617
H	2.390774	7.340055	-3.304236
O	1.318527	8.701759	-2.132555
C	0.163588	8.353930	-2.891992
H	0.460488	8.087289	-3.923504
H	-0.421819	9.285938	-2.965876
C	-0.727513	7.255391	-2.344068
H	-1.208170	6.642313	-3.111462
O	-1.797598	5.987891	4.129778
C	-0.489090	6.203037	3.599601
H	-0.053034	5.269215	3.206753
H	0.120708	6.526787	4.455965
C	-0.404117	7.290591	2.524414
H	0.590309	7.769760	2.567940
H	-1.160365	8.068991	2.737533
O	-0.612314	6.720315	1.236041
C	-0.602441	7.695490	0.180619
H	0.394010	8.147108	0.066942
H	-1.314538	8.509559	0.431307
C	-1.057438	6.997502	-1.068114
H	-1.765780	6.189914	-0.881248
C	-2.946897	1.944448	0.153604
C	-3.300884	1.823658	-1.257488
C	-2.631755	2.597665	-2.217447
C	-1.581289	3.522050	-1.802314
C	-1.241502	3.634411	-0.444193
C	-1.940945	2.834189	0.553367
C	-3.023441	0.618105	0.753442
C	-3.425868	-0.323233	-0.284886
C	-3.598772	0.420300	-1.528624
C	-3.217556	-0.156357	-2.749689
C	-2.229664	1.997942	-3.486873
C	-0.530500	3.496649	-2.815361
C	0.817542	3.586333	-2.430955
C	1.166012	3.702561	-1.017841
C	0.157145	3.732028	-0.044279
C	0.325293	2.991243	1.201652
C	-0.973069	2.434827	1.572323
C	-1.051167	1.158001	2.151718
C	-2.101504	0.232168	1.737009
C	-2.881007	-1.612183	-0.307544
C	-1.916620	-2.015911	0.710209
C	-1.533741	-1.112595	1.714600
C	-0.132140	-1.017888	2.112599
C	0.165631	0.386033	2.383835
C	1.415199	0.921088	2.027678
C	1.497360	2.250950	1.426689
C	2.546158	2.220520	0.410717
C	2.386980	2.937708	-0.786262

C	-0.931041	2.552493	-3.854854
C	2.930455	0.101257	-3.121333
C	2.001533	0.488666	-4.099061
C	0.951902	-0.438281	-4.513783
C	0.874234	-1.715107	-3.934343
C	1.843567	-2.120881	-2.918869
C	3.188916	-1.100913	-1.106795
C	3.486634	0.298952	-0.836153
C	3.327326	1.044187	-2.079200
C	2.789095	2.339844	-2.057248
C	1.819074	2.740697	-3.072757
C	1.433745	1.833474	-4.074083
C	-0.264937	0.334292	-4.742226
C	-1.514502	-0.198821	-4.386266
C	-1.595749	-1.526122	-3.784140
C	-0.423878	-2.268018	-3.562413
C	-0.255746	-3.010180	-2.317583
C	1.145786	-2.924354	-1.919841
C	1.481961	-2.806656	-0.560099
C	2.522373	-1.873751	-0.147934
C	3.110754	0.875704	0.385275
C	2.413639	0.072169	1.384860
C	2.127159	-1.277018	1.123816
C	0.830999	-1.834241	1.495458
C	0.431269	-2.779784	0.454780
C	-0.915242	-2.862152	0.068671
C	-1.265890	-2.981006	-1.344528
C	-2.482706	-2.212930	-1.575594
C	-2.647976	-1.500381	-2.773857
C	0.032785	1.737287	-4.470845
C	-2.516049	0.648286	-3.746756
C	2.850172	-1.227608	-2.519423

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O	-3.197229	-5.213787	-0.077671
C	-6.060641	-2.153780	-0.395154
C	-5.547329	-2.489871	0.888098
C	-6.907709	-0.948695	-0.511571
C	-6.511169	0.148625	0.397742
C	-6.029916	-0.208452	1.693989
C	-5.943378	-1.642691	2.031322
C	-5.642973	-2.923517	-1.498905
C	-4.617825	-3.538502	1.022403
C	-4.182060	-4.256699	-0.100277
C	-4.729611	-3.968310	-1.362283
C	-5.583847	0.813714	2.548733
C	-6.494665	1.494515	0.007420
C	-5.599581	2.158729	2.168591
C	-6.031706	2.501395	0.876349
C	-6.249804	-2.151291	3.267996
C	-7.998170	-0.870030	-1.341983
S	-6.840385	-1.152442	4.632078
C	-7.334389	-2.503816	5.641668
C	-7.056650	-3.745086	5.203689
S	-6.227991	-3.899701	3.661342
S	-9.070729	0.558916	-1.447080
C	-10.336319	-0.236052	-2.371297
C	-10.113282	-1.498498	-2.779297
S	-8.577431	-2.233881	-2.346392
H	-5.971382	-2.649514	-2.499322
H	-4.184294	-3.726723	1.999356
H	-4.369512	-4.515570	-2.230655
H	-5.157740	0.553781	3.515842
H	-6.747414	1.783566	-1.009679
H	-5.230888	2.912659	2.858027
H	-7.824749	-2.267771	6.582193
H	-7.289115	-4.663200	5.736366
H	-11.231152	0.341805	-2.586048
H	-10.799493	-2.095399	-3.373838
O	-5.987824	3.764293	0.352602
C	-2.366904	-5.312220	1.082778
H	-2.306354	-4.333289	1.581900
H	-2.807659	-6.027412	1.797615
C	-0.955963	-5.708668	0.703556
C	-0.500027	-5.700847	-0.622891
C	-0.040901	-5.977564	1.734226

C	0.854450	-5.904725	-0.906689
C	1.309743	-6.192106	1.445424
C	1.780398	-6.136549	0.123372
H	-1.206444	-5.500295	-1.423251
H	-0.381307	-5.995554	2.770941
H	1.202000	-5.858228	-1.938398
H	2.006691	-6.400628	2.258835
C	3.244960	-6.354346	-0.196627
H	3.809557	-6.612702	0.712027
H	3.355642	-7.178553	-0.913335
O	3.877060	-5.241115	-0.867607
C	5.547865	-2.024137	1.253061
C	5.812727	-2.227313	-0.135464
C	6.115956	-0.828514	1.903872
C	6.167669	0.358139	1.027848
C	6.464275	0.154210	-0.349512
C	6.664027	-1.231501	-0.822214
C	4.683066	-2.916285	1.905854
C	5.217957	-3.313481	-0.794380
C	4.386528	-4.218908	-0.108620
C	4.109491	-4.010862	1.251529
C	6.478006	1.280660	-1.200458
C	5.849908	1.645887	1.495671
C	6.188724	2.558041	-0.730731
C	5.835968	2.743802	0.620575
C	7.609262	-1.577891	-1.757378
C	6.611540	-0.831255	3.184160
S	8.747392	-0.408908	-2.495147
C	9.799815	-1.613586	-3.221191
C	9.432135	-2.903638	-3.120204
S	7.934490	-3.261051	-2.273827
S	7.386868	0.586308	3.959819
C	8.069608	-0.304609	5.313072
C	7.749486	-1.606020	5.428621
S	6.677416	-2.292893	4.216544
H	4.391737	-2.719767	2.935925
H	5.336952	-3.449788	-1.866232
H	3.406762	-4.640500	1.784862
H	6.638749	1.143464	-2.267504
H	5.516902	1.759125	2.521768
H	6.148429	3.409853	-1.405732
H	10.686745	-1.252890	-3.734953
H	9.977248	-3.744633	-3.540164
H	8.702885	0.247803	6.001973
H	8.084776	-2.264281	6.225532
O	5.431995	4.003844	0.967984
C	5.021941	4.225802	2.330535
H	5.875931	4.036161	3.001076
H	4.217209	3.519600	2.592608
C	4.539416	5.666138	2.469482
H	4.503210	5.910867	3.541132
H	5.272687	6.342926	2.009918
C	-5.188519	4.748646	1.038728
H	-4.302097	4.272767	1.472397
H	-5.777712	5.205127	1.852313
C	-4.742913	5.790856	0.015696
H	-4.286296	5.265048	-0.832657
H	-5.606057	6.354806	-0.365193
C	3.150967	5.921224	1.879871
H	2.415435	5.241785	2.349012
H	3.132580	5.715327	0.797495
C	-3.720764	6.764693	0.602328
O	-2.620111	6.000836	1.091339
O	2.811848	7.283912	2.152917
C	1.410895	7.541229	2.174517
H	1.321592	8.555946	2.595956
H	0.904575	6.853995	2.881685
C	0.747431	7.492202	0.819358
H	1.388335	7.782581	-0.016225
C	-1.551411	6.775726	1.635903
H	-1.075634	6.137662	2.395591
H	-1.957957	7.659415	2.165663
C	-0.541388	7.186187	0.588640
H	-0.922983	7.225611	-0.433488
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H	-4.164393	7.356414	1.428007
C	-2.161254	0.355851	1.564406

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C      -3.110981       0.221520       0.464131
C      -3.426887       1.332816      -0.330941
C      -2.805112       2.621511      -0.059317
C      -1.893682       2.754697       0.999095
C      -1.565426       1.598773       1.829849
C      -1.361524      -0.865626       1.622296
C      -1.817023      -1.750612       0.553939
C      -2.896994      -1.077042      -0.160337
C      -3.016147      -1.219341      -1.548846
C      -3.553268       1.187679      -1.777314
C      -2.546811       3.278219      -1.336643
C      -1.379678       4.038601      -1.510408
C      -0.428088       4.168632      -0.413459
C      -0.680995       3.541157       0.816680
C       0.400055       2.871791       1.533472
C      -0.145011       1.669976       2.159287
C       0.625427       0.495511       2.213344
C       0.005111      -0.798290       1.939370
C      -0.890891      -2.532919      -0.151552
C       0.526993      -2.469751       0.179810
C       0.967702      -1.616802       1.205449
C       2.179073      -0.826586       1.020902
C       1.969626       0.476757       1.645690
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C       1.692062       2.852346       0.985417
C       1.954099       3.504803      -0.296411
C       0.914976       4.151378      -0.980795
C      -3.007743       2.389691      -2.400281
C       1.263846       2.331507      -4.196472
C      -0.102537       2.261754      -4.510421
C      -0.724068       0.969786      -4.783491
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C       1.465930      -0.132336      -4.402870
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C      -0.500912      -1.405827      -4.108050
C       0.581353      -2.078718      -3.397203
C       1.797570      -1.290624      -3.578570
C       2.712148      -1.160127      -2.521559
C       3.331134       0.133330      -2.249689
C       2.911155       2.686587      -1.029935
C       3.235425       1.530047      -0.206831
C       3.445010       0.280221      -0.801494
C       2.897431      -0.917940      -0.179445
C       2.446751      -1.811094      -1.239892
C       1.282376      -2.571968      -1.064925
C       0.328788      -2.700943      -2.164166
C      -1.014305      -2.678672      -1.598857
C      -2.055870      -2.035872      -2.283006
C      -2.279758       2.292334      -3.596893
C      -3.353047      -0.065777      -2.375707
C       2.064202       1.111414      -4.141336

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O      -3.266977      -5.213393      -0.231983
C      -6.040766      -2.112554      -0.822067
C      -5.767979      -2.562486       0.502732
C      -6.860666      -0.894563      -0.985311
C      -6.659551       0.110449       0.081892
C      -6.437369      -0.370688       1.408124
C      -6.394363      -1.829566       1.619045
C      -5.447003      -2.810596      -1.891075
C      -4.874660      -3.627382       0.716995
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C      -4.571288      -3.875324      -1.676360
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C	-6.938143	-2.455806	2.712319
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C	-8.492634	-3.032458	4.756849
C	-8.106130	-4.226537	4.272572
S	-6.965198	-4.233706	2.935301
S	-8.839085	0.706445	-2.144086
C	-9.903518	0.015512	-3.358889
C	-9.591861	-1.199418	-3.845491
S	-8.148439	-1.979637	-3.217486
H	-5.587825	-2.456222	-2.909712
H	-4.625387	-3.901644	1.737229
H	-4.064393	-4.358849	-2.508758
H	-5.964769	0.207618	3.432875
H	-6.633507	1.872530	-1.185948
H	-5.941381	2.618844	2.996511
H	-9.175945	-2.886730	5.589092
H	-8.430022	-5.191090	4.653929
H	-10.752653	0.616156	-3.673425
H	-10.149581	-1.730134	-4.612216
O	-6.163325	3.710210	0.488689
C	-2.572648	-5.284550	1.018650
H	-2.601886	-4.302396	1.514712
H	-3.073124	-6.009392	1.682593
C	-1.118677	-5.648998	0.810163
C	-0.523732	-5.688756	-0.459934
C	-0.315941	-5.846001	1.944613
C	0.850103	-5.910423	-0.589186
C	1.058576	-6.067080	1.812180
C	1.658166	-6.101160	0.544230
H	-1.140662	-5.520553	-1.338245
H	-0.763480	-5.805347	2.939147
H	1.307508	-5.918051	-1.578008
H	1.670124	-6.216448	2.703634
C	3.133510	-6.399333	0.389125
H	3.623452	-6.487297	1.370306
H	3.269735	-7.350788	-0.142791
O	3.837613	-5.448784	-0.434458
C	5.627137	-1.995791	1.155207
C	5.899872	-2.454042	-0.169774
C	6.277017	-0.748495	1.610373
C	6.457673	0.263382	0.546602
C	6.732118	-0.206934	-0.769855
C	6.834355	-1.661336	-0.988683
C	4.699740	-2.719699	1.925847
C	5.248286	-3.593921	-0.654435
C	4.362259	-4.328335	0.154148
C	4.073510	-3.878653	1.452281
C	6.834696	0.731995	-1.813525
C	6.319354	1.648313	0.774771
C	6.709820	2.098781	-1.580494
C	6.450695	2.566286	-0.279185
C	7.779136	-2.230048	-1.807854
C	6.745101	-0.578590	2.891871
S	9.024157	-1.285059	-2.681573
C	10.022332	-2.664736	-3.115468
C	9.558467	-3.890414	-2.811795
S	7.996972	-3.995746	-2.011244
S	7.640357	0.869730	3.448885
C	8.197355	0.168220	4.960504
C	7.751337	-1.059898	5.279979
S	6.652384	-1.844493	4.155630
H	4.399714	-2.335753	2.898487
H	5.384143	-3.921457	-1.682103
H	3.325215	-4.370876	2.065612
H	6.958842	0.382520	-2.836814
H	6.039627	1.999188	1.763467
H	6.759656	2.818886	-2.394397
H	10.957384	-2.458897	-3.629338
H	10.061573	-4.825453	-3.042752
H	8.861359	0.772570	5.572558
H	7.999729	-1.599500	6.189842
O	6.314561	3.920316	-0.158450
C	5.532324	4.463113	0.925306
H	6.199052	4.740986	1.757841
H	4.822452	3.708918	1.290887
C	4.765044	5.659741	0.368671

H	5.468368	6.454035	0.077855
H	4.273670	5.319871	-0.553589
C	-5.422047	4.561500	1.386297
H	-4.654857	3.958919	1.894373
H	-6.097712	4.973389	2.154615
C	-4.731356	5.663760	0.589283
H	-2.272084	6.711334	-0.185284
H	-3.270001	8.107245	0.228881
H	3.330691	8.052166	0.254752
H	2.306740	6.706187	-0.242323
H	-4.266395	5.199139	-0.290625
H	-5.462338	6.396706	0.218167
C	3.700296	6.204139	1.331006
H	4.177158	6.684789	2.200920
H	3.108244	5.365704	1.729569
C	-3.648439	6.341750	1.444157
C	-2.706235	7.264732	0.661225
C	2.753370	7.194433	0.637732
C	1.622042	7.704197	1.548640
H	2.073090	8.188141	2.434042
H	1.048954	6.846324	1.928311
C	0.722436	8.688047	0.844727
H	1.250293	9.462090	0.277610
C	-1.568014	7.797380	1.553533
H	-1.025542	6.944660	1.985763
H	-2.020235	8.334094	2.407633
C	-0.621982	8.723499	0.837935
H	-1.104681	9.523016	0.266177
H	-4.114798	6.904582	2.269863
H	-3.038012	5.556538	1.918969
C	-3.179253	1.289581	0.777165
C	-3.546545	0.441579	-0.350783
C	-3.495982	0.948599	-1.658398
C	-3.067681	2.322736	-1.889029
C	-2.711316	3.140094	-0.803561
C	-2.768753	2.612132	0.554672
C	-2.483997	0.462253	1.758287
C	-2.421618	-0.899565	1.233252
C	-3.079961	-0.910020	-0.069732
C	-2.560200	-1.696693	-1.107195
C	-2.964242	0.122973	-2.740137
C	-2.269186	2.347995	-3.112127
C	-1.148181	3.188062	-3.203360
C	-0.779096	4.038312	-2.074801
C	-1.545117	4.013331	-0.898322
C	-0.884486	4.027997	0.404232
C	-1.641471	3.161182	1.303038
C	-0.969992	2.365745	2.245359
C	-1.399571	0.988376	2.477689
C	-1.275064	-1.681431	1.448238
C	-0.146276	-1.133503	2.195437
C	-0.208016	0.175592	2.702097
C	0.956874	1.049302	2.604950
C	0.486101	2.402787	2.323804
C	1.214306	3.235660	1.458466
C	0.516560	4.066050	0.480658
C	1.312856	4.088532	-0.744129
C	0.677174	4.076207	-1.996620
C	-2.206178	0.987772	-3.638357
C	2.420080	1.103807	-3.387760
C	1.334697	0.577998	-4.105594
C	0.906613	-0.797728	-3.874535
C	1.580252	-1.594612	-2.934504
C	2.710546	-1.049046	-2.188451
C	3.484930	1.125442	-1.282715
C	3.013664	2.476524	-1.561198
C	2.355044	2.465774	-2.863164
C	1.208816	3.248406	-3.075579
C	0.080599	2.700621	-3.821787
C	0.142485	1.391648	-4.325777
C	-0.550766	-0.833519	-3.954135
C	-1.279122	-1.664565	-3.089012
C	-0.579099	-2.493308	-2.110195
C	0.822512	-2.461457	-2.034411
C	1.482014	-2.448919	-0.731966
C	2.647813	-1.576900	-0.827943
C	2.994344	-0.755252	0.253988

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C       3.422477       0.618173       0.022362
C       2.500749       3.271619      -0.524188
C       2.439990       2.744385       0.835889
C       2.891891       1.443676       1.103464
C       2.137098       0.579958       2.005295
C       2.197915      -0.778568       1.477545
C       1.082511      -1.622285       1.575294
C       0.715350      -2.471176       0.444492
C      -0.737742      -2.500503       0.363922
C      -1.372626      -2.509056      -0.886956
C      -1.022908       0.518850      -4.233070
C      -2.504809      -1.173809      -2.468392
C       3.121522       0.275477      -2.411341

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O       0.047624      -4.434986      -4.475052
C      -0.921317      -4.810609      -0.411976
C       0.367623      -4.297519      -0.760598
C      -1.263491      -4.950905       1.013908
C      -0.711631      -3.888091       1.870504
C       0.582853      -3.378773       1.547198
C       1.266839      -3.903917       0.344687
C      -1.830790      -5.123874      -1.438234
C       0.704394      -4.166785      -2.123044
C      -0.203888      -4.543899      -3.125540
C      -1.484530      -5.004314      -2.781452
C       1.107796      -2.351530       2.353867
C      -1.424812      -3.339531       2.942456
C       0.418888      -1.847531       3.463062
C      -0.864550      -2.337358       3.750078
C       2.631996      -4.083069       0.312670
C      -1.953892      -6.028380       1.515923
S       3.670852      -3.873666       1.753603
C       5.137285      -4.484764       1.016676
C       5.087402      -4.834460      -0.281625
S       3.554550      -4.632545      -1.114840
S      -2.285717      -6.277523       3.257796
C      -2.781025      -7.957064       3.106309
C      -2.875966      -8.470084       1.866451
S      -2.495321      -7.411593       0.516150
H      -2.844314      -5.423821      -1.179723
H       1.629080      -3.678996      -2.413163
H      -2.190552      -5.242758      -3.573802
H       2.051015      -1.879684       2.087898
H      -2.448699      -3.643314       3.145320
H       0.869801      -1.055021       4.052417
H       6.024130      -4.526861       1.642561
H       5.924394      -5.209861      -0.863987
H      -3.009477      -8.491547       4.024413
H      -3.193260      -9.482012       1.629650
O      -1.674504      -1.891242       4.759991
C       1.380342      -4.732171      -4.928880
H       1.773952      -5.598107      -4.373970
H       1.241557      -5.032125      -5.977762
C       2.351447      -3.574502      -4.839991
C       1.930692      -2.252785      -5.058757
C       3.701212      -3.820149      -4.546469
C       2.835063      -1.194023      -4.943734
C       4.606497      -2.760650      -4.434127
C       4.177258      -1.436938      -4.611820
H       0.884330      -2.056760      -5.281494
H       4.037504      -4.842867      -4.371264
H       2.493092      -0.168951      -5.068863
H       5.644211      -2.960046      -4.161914
C       5.147964      -0.290319      -4.418223
H       6.046902      -0.642132      -3.886536
H       5.462182       0.118616      -5.388474
O       4.595336       0.845988      -3.733170
C       4.064752       0.820063       0.429747
C       4.180356       2.037763      -0.304123
C       3.804112       0.893933       1.878709
C       2.961645       2.034993       2.283558
C       3.153919       3.270021       1.586512
C       4.107312       3.300360       0.459492
C       4.118590      -0.397247      -0.269695
C       4.332507       1.984261      -1.696611
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C	4.429625	0.754523	-2.370072
C	4.321685	-0.448425	-1.651704
C	2.373391	4.373553	1.966971
C	1.979153	1.952322	3.276745
C	1.420919	4.298050	2.989603
C	1.199270	3.067588	3.625242
C	4.930439	4.370095	0.198419
C	4.404079	0.042962	2.775090
S	4.989197	5.846613	1.209373
C	6.468451	6.486230	0.509232
C	6.998364	5.826135	-0.536269
S	6.160998	4.388789	-1.102320
S	4.049524	0.006541	4.526974
C	5.379350	-1.058736	4.959437
C	6.145348	-1.533701	3.959622
S	5.753070	-1.045356	2.321925
H	3.960185	-1.331581	0.265306
H	4.343772	2.892110	-2.294325
H	4.333483	-1.411061	-2.151156
H	2.453971	5.303484	1.408134
H	1.733417	1.000522	3.738052
H	0.823801	5.172164	3.233853
H	6.868898	7.398545	0.942868
H	7.892956	6.124095	-1.076382
H	5.509818	-1.289526	6.013068
H	6.987466	-2.208617	4.089259
O	0.225809	2.836281	4.556200
C	-0.844091	3.791102	4.686549
H	-1.143901	4.171999	3.700906
H	-0.531571	4.636991	5.318405
C	-1.985450	3.005865	5.313063
H	-2.240390	2.171020	4.644038
H	-1.656032	2.570035	6.273209
C	-1.190119	-0.860011	5.634570
H	-0.935218	0.048785	5.067717
H	-0.282849	-1.214519	6.153229
C	-2.286692	-0.560822	6.659733
H	-2.752534	-1.515551	6.965454
H	-1.818126	-0.107995	7.543762
O	-3.089471	3.877216	5.499418
C	-4.254117	3.158147	5.964192
H	-4.930548	3.940058	6.335965
H	-3.983687	2.495495	6.796195
O	-3.261313	0.384542	6.241034
C	-4.934412	2.395246	4.851717
H	-5.507162	3.018369	4.160345
C	-4.144682	-0.055292	5.210982
H	-4.862026	-0.798950	5.617368
H	-3.588258	-0.575364	4.413822
C	-4.889329	1.080149	4.570198
H	-5.456340	0.740029	3.698680
C	-3.005408	-1.760745	-2.877622
C	-2.828529	-1.021657	-4.123986
C	-3.806404	-0.105408	-4.540012
C	-4.999875	0.106231	-3.726676
C	-5.169729	-0.607475	-2.528684
C	-4.155479	-1.563152	-2.097215
C	-1.701359	-1.879201	-2.237878
C	-0.717749	-1.216839	-3.083987
C	-1.412268	-0.686942	-4.252078
C	-1.026885	0.549134	-4.795371
C	-3.406679	1.181814	-5.101429
C	-5.337799	1.524252	-3.785042
C	-5.834414	2.175656	-2.645202
C	-6.011096	1.434755	-1.400035
C	-5.685082	0.070329	-1.342516
C	-4.989313	-0.465954	-0.176820
C	-4.042395	-1.475478	-0.642677
C	-2.785938	-1.592481	-0.029181
C	-1.591507	-1.801354	-0.843145
C	0.341725	-0.501796	-2.506608
C	0.458183	-0.417345	-1.053352
C	-0.496655	-1.047879	-0.241799
C	-1.014925	-0.370280	0.941148
C	-2.427879	-0.708489	1.077094
C	-3.339821	0.258368	1.529939
C	-4.646120	0.383523	0.888428

C	-4.983729	1.803421	0.827414
C	-5.654027	2.318084	-0.294633
C	-4.353738	2.188689	-4.634814
C	-3.216783	4.991493	-1.126457
C	-3.324794	4.907647	-2.523722
C	-2.131313	4.695571	-3.336586
C	-0.875136	4.574617	-2.721307
C	-0.762923	4.662401	-1.269001
C	-2.089479	4.127245	0.757907
C	-3.505014	3.793282	0.889526
C	-4.201264	4.327203	-0.276517
C	-5.255772	3.604558	-0.856540
C	-5.366947	3.516601	-2.309275
C	-4.420518	4.155123	-3.125843
C	-2.489270	3.812416	-4.441666
C	-1.577398	2.843225	-4.889375
C	-0.270112	2.718574	-4.251061
C	0.073961	3.566791	-3.186564
C	0.773868	3.032892	-2.021937
C	0.255277	3.708963	-0.838762
C	0.077214	2.991049	0.352301
C	-1.113832	3.206033	1.166855
C	-3.887509	2.555477	1.430285
C	-2.871412	1.601128	1.863167
C	-1.511510	1.920092	1.734046
C	-0.563557	0.914338	1.266838
C	0.421601	1.577536	0.417222
C	0.924725	0.925397	-0.718246
C	1.101360	1.667942	-1.962833
C	0.738536	0.786079	-3.067440
C	0.069943	1.300583	-4.191401
C	-3.903946	3.478133	-4.311239
C	-2.045354	1.502542	-5.226388
C	-1.911327	4.868674	-0.486980

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O	-4.525555	3.849836	-3.389222
C	-2.440827	4.447756	0.209530
C	-3.452624	3.443812	0.159526
C	-1.696121	4.626641	1.469599
C	-1.462927	3.369841	2.205204
C	-2.481476	2.376607	2.176963
C	-3.696141	2.648127	1.380558
C	-2.158572	5.174718	-0.962058
C	-4.152909	3.223647	-1.041358
C	-3.885172	4.000082	-2.179705
C	-2.876214	4.974523	-2.139886
C	-2.236602	1.157969	2.842445
C	-0.242508	3.104963	2.851789
C	-1.032854	0.902902	3.495085
C	-0.015682	1.873988	3.481804
C	-4.953959	2.266215	1.783340
C	-1.314793	5.855528	1.952150
S	-5.283666	1.471722	3.353033
C	-7.027790	1.658952	3.289112
C	-7.559659	2.178226	2.167585
S	-6.456372	2.614612	0.871906
S	-0.501203	6.101197	3.529246
C	-0.707254	7.845495	3.568799
C	-1.250160	8.434298	2.488001
S	-1.699792	7.402959	1.138575
H	-1.331328	5.880794	-0.967778
H	-4.844381	2.391264	-1.111517
H	-2.647623	5.536522	-3.042914
H	-2.977309	0.364424	2.813815
H	0.554560	3.836090	2.779280
H	-0.856610	-0.053327	3.981025
H	-7.595124	1.325802	4.153996
H	-8.620924	2.329695	1.989411
H	-0.363709	8.365194	4.459044
H	-1.412342	9.502441	2.371879
O	1.179942	1.514342	4.043275
C	-5.859738	3.320036	-3.373135
H	-6.446053	3.820562	-2.585782
H	-6.273099	3.616280	-4.347978
C	-5.940563	1.817195	-3.199861

C	-4.930349	0.973627	-3.687317
C	-7.034982	1.252518	-2.527518
C	-5.001096	-0.407652	-3.487523
C	-7.109252	-0.129382	-2.331764
C	-6.090443	-0.970776	-2.804651
H	-4.068267	1.410561	-4.186289
H	-7.813942	1.899865	-2.123539
H	-4.193254	-1.051596	-3.829456
H	-7.948136	-0.553978	-1.778155
C	-6.185150	-2.463940	-2.570943
H	-6.829382	-2.670754	-1.700741
H	-6.629662	-2.959633	-3.446157
O	-4.924076	-3.128020	-2.405441
C	-2.853803	-2.961883	1.251194
C	-2.670164	-4.031702	0.322093
C	-2.046967	-2.967491	2.489335
C	-0.700401	-3.554563	2.338945
C	-0.552150	-4.652751	1.439684
C	-1.734686	-5.110000	0.690155
C	-3.761710	-1.942682	0.913197
C	-3.366799	-4.016963	-0.893687
C	-4.298174	-3.008472	-1.186421
C	-4.503285	-1.963042	-0.272707
C	0.727558	-5.216171	1.270898
C	0.425440	-3.060821	3.024692
C	1.829754	-4.747851	1.976858
C	1.682353	-3.658748	2.856169
C	-2.001769	-6.438073	0.449295
C	-2.545016	-2.565452	3.707157
S	-0.972538	-7.778784	1.039961
C	-2.134308	-9.056221	0.715324
C	-3.272319	-8.716345	0.083834
S	-3.487546	-7.028918	-0.356635
S	-1.619284	-2.612506	5.240902
C	-2.981675	-2.253419	6.289838
C	-4.166448	-2.000110	5.705542
S	-4.240416	-2.055060	3.953948
H	-3.873536	-1.078427	1.562050
H	-3.180752	-4.772069	-1.653098
H	-5.175448	-1.140334	-0.495851
H	0.876277	-5.995072	0.525937
H	0.331955	-2.157827	3.618308
H	2.820807	-5.168089	1.821347
H	-1.863081	-10.063124	1.020927
H	-4.062051	-9.407149	-0.198796
H	-2.792549	-2.234477	7.359572
H	-5.081647	-1.744496	6.232683
O	2.829131	-3.238695	3.468238
C	2.789201	-2.045062	4.264855
H	2.099124	-2.173015	5.117151
H	2.440891	-1.197771	3.656472
C	4.201871	-1.790575	4.775288
H	4.167538	-0.931923	5.461049
H	4.552590	-2.665411	5.347148
C	2.248303	2.472740	3.984136
H	2.025856	3.341099	4.621030
H	2.396976	2.820881	2.950291
C	3.510364	1.765780	4.448626
H	3.341373	1.304097	5.444600
H	3.758469	0.958576	3.742851
O	5.103372	-1.469255	3.720818
C	5.912316	-2.573392	3.296017
H	5.287714	-3.463920	3.126792
H	6.664384	-2.811018	4.069998
C	6.600348	-2.221544	1.993888
H	5.845709	-1.908819	1.257317
H	7.087815	-3.141275	1.593958
O	4.525804	2.752357	4.514071
C	5.834916	2.197569	4.667978
H	5.820751	1.384591	5.420721
H	6.459119	3.014128	5.052787
C	6.440848	1.662084	3.381310
H	5.769336	0.948515	2.883470
H	7.358618	1.096600	3.626861
O	7.564640	-1.199138	2.206124
C	8.025064	-0.641583	0.967055
H	7.163603	-0.297731	0.370303

H	8.537901	-1.424003	0.372795
C	8.973847	0.489964	1.273721
H	10.010093	0.203442	1.454341
O	6.732143	2.771970	2.526259
C	7.230617	2.354938	1.248008
H	7.233054	3.263061	0.629803
H	6.541824	1.630954	0.786888
C	8.625284	1.785958	1.356236
H	9.398521	2.512739	1.636601
C	-0.078972	-2.772865	-1.552361
C	0.287614	-2.159366	-0.279940
C	1.623856	-2.169660	0.141279
C	2.645516	-2.801096	-0.683100
C	2.294673	-3.399186	-1.903515
C	0.901879	-3.384793	-2.347160
C	-1.115332	-1.949156	-2.168298
C	-1.387798	-0.824666	-1.276247
C	-0.521668	-0.955616	-0.108469
C	0.037378	0.187160	0.483234
C	2.206614	-0.984700	0.759343
C	3.862255	-2.001818	-0.581951
C	4.680729	-1.826573	-1.706212
C	4.316273	-2.440561	-2.978887
C	3.143508	-3.209160	-3.074214
C	2.277634	-3.077776	-4.242593
C	0.892778	-3.186290	-3.793433
C	-0.101538	-2.391623	-4.387690
C	-1.127122	-1.763508	-3.559671
C	-1.661996	0.444385	-1.808596
C	-1.663122	0.638801	-3.255726
C	-1.406119	-0.441261	-4.114526
C	-0.554491	-0.253907	-5.285219
C	0.251740	-1.459068	-5.453401
C	1.583461	-1.357002	-5.887369
C	2.616112	-2.181868	-5.269089
C	3.832937	-1.381914	-5.168608
C	4.666003	-1.508219	-4.045619
C	3.590983	-0.875725	0.313282
C	4.706736	2.076053	-3.076595
C	4.716636	1.888066	-1.685766
C	3.695310	2.519308	-0.854437
C	2.698845	3.310441	-1.448679
C	2.689283	3.505668	-2.895478
C	3.306555	2.287646	-4.966143
C	4.112295	1.082221	-5.134761
C	4.978954	0.951982	-3.966118
C	5.246562	-0.319681	-3.433725
C	5.262109	-0.513357	-1.986408
C	4.996584	0.567237	-1.130836
C	3.344379	1.588250	0.216349
C	2.009060	1.481861	0.641718
C	0.975092	2.305252	0.022210
C	1.312777	3.205507	-0.999282
C	0.449107	3.332736	-2.168492
C	1.297742	3.519376	-3.339270
C	0.945106	2.931949	-4.565259
C	1.969093	2.301759	-5.392397
C	3.551441	-0.061684	-5.723393
C	2.160961	-0.046640	-6.167858
C	1.385430	1.112146	-6.005286
C	0.000870	1.006783	-5.556561
C	-0.271024	2.131268	-4.666153
C	-1.085682	1.949917	-3.537369
C	-0.718282	2.560763	-2.265420
C	-1.074964	1.633269	-1.197689
C	-0.241394	1.505269	-0.077304
C	4.147195	0.382906	0.042457
C	1.431030	0.172475	0.926422
C	3.673351	2.900972	-3.693404

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O	3.819844	5.902873	-0.511021
C	0.056436	4.370365	0.575570
C	0.200818	5.751944	0.242650
C	-1.319585	3.870068	0.784980
C	-2.315537	4.493407	-0.118992

C	-2.178400	5.881777	-0.393452
C	-1.020448	6.583373	0.192178
C	1.205817	3.558736	0.602410
C	1.469080	6.251991	-0.089852
C	2.592104	5.413894	-0.097668
C	2.465229	4.066550	0.266141
C	-3.100908	6.488439	-1.269791
C	-3.337425	3.751846	-0.741254
C	-4.133033	5.761556	-1.857314
C	-4.247184	4.382417	-1.604088
C	-1.080219	7.854087	0.704888
C	-1.688637	3.015344	1.794533
S	-2.583084	8.824636	0.770063
C	-1.944182	10.070892	1.831841
C	-0.641861	10.001920	2.162230
S	0.299119	8.672627	1.501491
S	-3.391814	2.577302	2.123607
C	-3.062552	1.632165	3.556988
C	-1.778506	1.492124	3.937253
S	-0.555174	2.314103	2.983192
H	1.109277	2.497222	0.816153
H	1.580403	7.287491	-0.405315
H	3.332155	3.415707	0.220568
H	-2.980206	7.537288	-1.534552
H	-3.385701	2.681143	-0.575457
H	-4.832982	6.230022	-2.546365
H	-2.631428	10.847966	2.155149
H	-0.118220	10.715005	2.793125
H	-3.916701	1.167930	4.037425
H	-1.444157	0.877748	4.768339
O	-5.258594	3.736258	-2.265664
C	3.871147	6.237601	-1.930654
H	3.017222	6.882785	-2.186632
H	4.794593	6.817041	-2.045948
C	3.895741	4.995008	-2.785498
C	5.107792	4.503384	-3.299402
C	2.724447	4.241245	-2.981762
C	5.162377	3.274538	-3.961289
C	2.782846	2.994153	-3.611609
C	4.003393	2.492608	-4.090396
H	6.022292	5.081314	-3.156781
H	1.772690	4.609355	-2.602183
H	6.112342	2.881761	-4.321207
H	1.877543	2.394311	-3.706438
C	4.064184	1.112497	-4.708999
H	3.160294	0.543026	-4.450838
H	4.118387	1.184219	-5.804551
O	5.233362	0.342430	-4.365947
C	5.734449	-1.400938	-0.564985
C	5.279688	-0.051564	-0.651417
C	5.910343	-1.993492	0.774729
C	4.940710	-1.517871	1.781166
C	4.515058	-0.155481	1.703217
C	5.056865	0.678093	0.614231
C	5.958706	-2.107711	-1.763012
C	5.053922	0.529911	-1.913169
C	5.336789	-0.180732	-3.091877
C	5.792065	-1.505722	-3.010225
C	3.552733	0.301896	2.618140
C	4.371068	-2.361222	2.743321
C	3.005909	-0.536548	3.593999
C	3.404716	-1.882469	3.641241
C	5.439962	1.985782	0.805235
C	6.944812	-2.843792	1.091647
S	5.330671	2.826091	2.381372
C	6.164827	4.282887	1.870149
C	6.560259	4.354892	0.587108
S	6.209463	2.988871	-0.452794
S	7.235066	-3.488532	2.735652
C	8.852130	-4.092423	2.409301
C	9.304269	-4.012390	1.144774
S	8.233853	-3.310262	-0.058314
H	6.219876	-3.163301	-1.721929
H	4.639906	1.529287	-1.969816
H	5.962695	-2.060862	-3.930234
H	3.169235	1.316617	2.532610
H	4.584208	-3.427156	2.751467

H	2.239760	-0.151445	4.260992
H	6.285472	5.070622	2.608265
H	7.043521	5.213616	0.130688
H	9.398902	-4.522350	3.244122
H	10.271850	-4.367817	0.801056
O	2.856509	-2.820972	4.476303
C	1.578304	-2.514370	5.047813
H	0.917001	-2.066465	4.292237
H	1.700749	-1.799884	5.877674
C	0.957654	-3.843896	5.503205
H	1.224658	-4.608771	4.764524
H	1.356030	-4.152274	6.487351
C	-5.302715	2.310579	-2.162998
H	-5.457187	1.993823	-1.120554
H	-4.361423	1.868879	-2.518569
C	-6.465047	1.834991	-3.024333
H	-7.398045	2.343384	-2.718321
H	-6.277982	2.082811	-4.084991
O	-0.461981	-3.792824	5.511626
C	-1.010244	-2.920135	6.491145
H	-0.573029	-1.908307	6.430509
H	-0.827962	-3.308747	7.512523
C	-2.502897	-2.812843	6.243713
H	-2.975508	-2.284905	7.094280
H	-2.931321	-3.827621	6.191046
O	-6.558293	0.430882	-2.832166
C	-7.527176	-0.186696	-3.676902
H	-7.214720	-0.101775	-4.736385
H	-8.509764	0.308605	-3.569582
C	-7.658212	-1.660002	-3.301859
H	-6.651384	-2.107231	-3.247675
H	-8.213791	-2.166976	-4.103920
O	-2.704686	-2.090583	5.031668
C	-4.052397	-1.677983	4.818802
H	-4.007011	-0.979464	3.976542
H	-4.441471	-1.139310	5.704206
C	-5.016595	-2.830782	4.482266
H	-4.735300	-3.275625	3.512369
H	-4.948777	-3.617261	5.245136
O	-6.381841	-2.423462	4.490713
C	-6.781898	-1.603799	3.388065
H	-7.861332	-1.771272	3.268842
H	-6.301857	-1.938215	2.451006
C	-6.528858	-0.132032	3.627226
H	-6.427924	0.147280	4.678645
O	-8.397626	-1.912376	-2.114089
C	-7.739990	-1.588761	-0.880946
H	-6.666533	-1.429603	-1.036086
H	-7.871146	-2.440409	-0.195560
C	-8.397400	-0.346690	-0.262025
H	-9.483547	-0.506439	-0.230178
H	-8.193151	0.535109	-0.891640
O	-7.992212	-0.115858	1.086817
C	-6.731903	0.555137	1.216269
H	-6.751228	1.506055	0.654216
H	-5.913287	-0.054752	0.791332
C	-6.491063	0.821643	2.681000
H	-6.351769	1.862024	2.979751
C	-2.962950	0.015895	-0.783606
C	-2.137775	0.049151	0.416722
C	-2.272651	-0.951169	1.392138
C	-3.240787	-2.026695	1.200300
C	-4.038749	-2.058572	0.044391
C	-3.896091	-1.015969	-0.968811
C	-2.146008	0.474014	-1.907042
C	-0.816047	0.794249	-1.397556
C	-0.811100	0.526987	0.033793
C	0.327578	-0.021493	0.642779
C	-1.087983	-1.519732	2.027094
C	-2.651412	-3.260920	1.716106
C	-2.883353	-4.477686	1.054004
C	-3.710297	-4.508364	-0.149047
C	-4.278836	-3.324088	-0.643308
C	-4.281101	-3.061319	-2.080012
C	-4.043883	-1.635194	-2.279880
C	-3.263717	-1.195397	-3.360834
C	-2.294371	-0.120151	-3.169798

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C       0.321129       0.503405      -2.171530
C       0.166351      -0.121042      -3.483137
C      -1.114518      -0.424351      -3.974725
C      -1.353249      -1.689952      -4.659744
C      -2.681060      -2.166044      -4.280381
C      -2.906365      -3.538721      -4.088231
C      -3.722283      -3.994771      -2.967028
C      -3.134615      -5.227757      -2.452552
C      -3.128170      -5.478903      -1.071491
C      -1.322179      -2.946941       2.227132
C       0.524132      -6.027747      -0.701806
C       0.669982      -5.431595       0.560433
C       1.640206      -4.357268       0.754431
C       2.427018      -3.918471      -0.325336
C       2.272059      -4.538291      -1.638443
C       0.513528      -5.603266      -3.025117
C      -0.813969      -6.077577      -2.646324
C      -0.807277      -6.340196      -1.210866
C      -1.942363      -6.047273      -0.438013
C      -1.791812      -5.429962       0.875427
C      -0.510928      -5.126164       1.364307
C       1.055194      -3.387671       1.671612
C       1.276733      -2.016058       1.472287
C       2.091268      -1.560352       0.352992
C       2.652906      -2.492501      -0.529092
C       2.645587      -2.229918      -1.962957
C       2.410907      -3.493637      -2.651048
C       1.617488      -3.525876      -3.808554
C       0.648964      -4.601168      -3.999002
C      -1.955095      -5.533189      -3.255915
C      -1.814227      -4.489769      -4.266490
C      -0.537622      -4.032713      -4.630418
C      -0.302691      -2.606052      -4.830083
C       1.028963      -2.292791      -4.322534
C       1.257998      -1.076198      -3.659176
C       2.086163      -1.042844      -2.457100
C       1.506972      -0.066375      -1.538522
C       1.508328      -0.324949      -0.159351
C      -0.272747      -3.861163       2.050943
C       0.185862      -1.064156       1.655145
C       1.341082      -5.572601      -1.823275

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O      -2.750203       4.261447      -4.140628
C      -0.892382       4.770118      -0.410098
C      -2.137573       4.080376      -0.468787
C      -0.228143       4.901806       0.899855
C      -0.417268       3.737036       1.784720
C      -1.664193       3.053730       1.738143
C      -2.688241       3.540233       0.791294
C      -0.317746       5.224939      -1.614587
C      -2.766462       3.888997      -1.712834
C      -2.195018       4.397186      -2.890543
C      -0.956214       5.057340      -2.840142
C      -1.821499       1.906337       2.541630
C       0.616472       3.252659       2.606991
C      -0.806534       1.445688       3.378421
C       0.426231       2.120735       3.413627
C      -4.029206       3.569931       1.091754
C       0.447308       6.033489       1.290170
S      -4.691648       3.090968       2.683891
C      -6.294350       3.757672       2.420875
C      -6.567666       4.267583       1.206141
S      -5.292825       4.215084      -0.001939
S       1.175261       6.256339       2.912388
C       1.461670       7.982293       2.745661
C       1.190456       8.547341       1.555502
S       0.576262       7.506187       0.280661
H       0.674046       5.671254      -1.598563
H      -3.655544       3.270830      -1.772940
H      -0.502162       5.402223      -3.766373
H      -2.743014       1.332528       2.495103
H       1.594412       3.715392       2.537839
H      -0.949619       0.557283       3.988851
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H      -7.522139       4.690407       0.904416
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H	1.865557	8.503969	3.609058
H	1.342069	9.595062	1.310518
O	1.392651	1.593348	4.228458
C	-4.174611	4.084698	-4.221568
H	-4.673817	4.796365	-3.544723
H	-4.415493	4.368956	-5.255646
C	-4.653257	2.675832	-3.937942
C	-3.893456	1.559279	-4.320817
C	-5.876967	2.474826	-3.281023
C	-4.342154	0.266324	-4.038173
C	-6.322771	1.181303	-2.993268
C	-5.555763	0.065480	-3.361818
H	-2.932338	1.709765	-4.808723
H	-6.465709	3.334391	-2.960062
H	-3.732540	-0.594413	-4.304085
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C       0.046938       0.389191       0.268248
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5-C60-outside-ring
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monomer-1
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C       2.637093       2.499984       0.100928
C       3.223170       1.606512      -2.077675
C       3.606301       2.132460      -0.837299
C      -1.156893       0.713544      -2.436637
C       0.310170       2.488812       2.140546
S      -0.246417      -0.679505      -3.068271
C      -1.648452      -1.665533      -3.436563
C      -2.860140      -1.105223      -3.267815
S      -2.917992       0.545682      -2.680067
S       1.730051       1.732276       2.919078
C       0.973948       1.481480       4.480700
C      -0.267224       1.965486       4.656917
S      -1.013757       2.804404       3.306183
H      -1.391353       4.801907       1.670512
H      -2.706700       3.160451      -2.815587
H      -3.330582       5.797649       0.513902
H       1.573719       1.131766      -3.362145
H       2.974512       2.968337       1.022212
H       3.976346       1.327930      -2.812531
H      -1.468057      -2.681740      -3.774271
H      -3.810673      -1.595724      -3.455443
H       1.533769       0.916626       5.219417
H      -0.853131       1.868945       5.566080
O       4.939327       2.312259      -0.498030
C       5.636291       3.274285      -1.305811
H       5.177157       4.269704      -1.176565
H       5.586470       3.007065      -2.372938
C       7.084566       3.316817      -0.859389
H       7.572415       4.210494      -1.296559
H       7.124651       3.416276       0.241575
C       4.949023      -1.623676      -1.647971
H       4.509247      -1.287127      -2.602319
H       5.145298      -2.706280      -1.711731
C       6.239589      -0.876727      -1.383408
H       6.843360      -0.854766      -2.309198
H       6.017928       0.163201      -1.104603
O       7.727664       2.124558      -1.285642
C       9.042239       1.981583      -0.735187
H       8.993806       2.079985       0.366121
H       9.698982       2.793193      -1.099535
O       6.936679      -1.549691      -0.332073
C       9.599176       0.634206      -1.134218
H      10.429103       0.638417      -1.843537
C       7.966063      -0.744835       0.251128
H       8.298449      -1.310022       1.135168
H       7.551782       0.218409       0.587282
C       9.125325      -0.543491      -0.694237
H       9.576147      -1.467685      -1.066216

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monomer-2
O       6.901810       1.428081      -0.127382
C       2.840994       1.496714       0.930576
C       3.384705       2.408674      -0.025433
C       1.403802       1.608637       1.229687
C       0.570313       1.943069       0.061332
C       1.096352       2.871658      -0.878084
C       2.464318       3.382774      -0.652237
C       3.689463       0.552850       1.525440
C       4.747804       2.327558      -0.339901
C       5.587462       1.391248       0.286574
C       5.057348       0.502100       1.233187
C       0.286221       3.223869      -1.977328
C      -0.703305       1.380382      -0.123853
C      -0.999213       2.709772      -2.134953
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C	-1.504025	1.780444	-1.205668
C	2.823697	4.687265	-0.894622
C	0.896786	1.600997	2.503454
S	1.681950	5.934748	-1.489414
C	2.723806	7.309425	-1.153496
C	3.969167	7.054782	-0.713727
S	4.437355	5.372242	-0.517739
S	-0.802270	2.024214	2.892022
C	-0.529931	2.250140	4.612220
C	0.690378	1.957220	5.099416
S	1.900998	1.372993	3.966746
H	3.268827	-0.196556	2.194392
H	5.182957	2.957547	-1.112122
H	5.667733	-0.261121	1.700807
H	0.679527	3.887021	-2.745879
H	-1.033125	0.602381	0.558453
H	-1.617438	2.987744	-2.986347
H	2.314509	8.298996	-1.338116
H	4.719902	7.807575	-0.488698
H	-1.369395	2.601919	5.206451
H	0.983030	2.040074	6.142883
O	-2.763193	1.314401	-1.441983
C	7.799116	0.419978	0.369528
H	8.776917	0.731406	-0.020899
H	7.845404	0.457243	1.470129
C	7.435623	-0.974872	-0.096837
C	7.353543	-2.037714	0.816973
C	7.100644	-1.207484	-1.438665
C	6.892902	-3.291380	0.412598
C	6.636063	-2.462840	-1.844963
C	6.502726	-3.507485	-0.919094
H	7.612918	-1.867952	1.863505
H	7.146710	-0.384582	-2.151412
H	6.781261	-4.096194	1.137365
H	6.329992	-2.616285	-2.880062
C	5.914740	-4.845199	-1.316231
H	5.406710	-4.777129	-2.291396
H	6.695416	-5.613014	-1.403495
O	5.037487	-5.370888	-0.307802
C	1.390196	-3.535369	0.664378
C	2.029728	-3.173654	-0.554679
C	0.055720	-2.963482	0.938942
C	-0.800227	-2.863114	-0.259879
C	-0.161068	-2.487391	-1.482018
C	1.298662	-2.256824	-1.456293
C	2.015821	-4.473182	1.506904
C	3.271048	-3.752927	-0.887315
C	3.872537	-4.686610	-0.030679
C	3.246769	-5.037872	1.177261
C	-0.944898	-2.415196	-2.644003
C	-2.170440	-3.153064	-0.253432
C	-2.320530	-2.682764	-2.633361
C	-2.937260	-3.055047	-1.428809
C	1.908810	-1.233131	-2.141041
C	-0.310450	-2.482760	2.167981
S	1.029935	-0.054454	-3.149370
C	2.392839	1.020072	-3.398729
C	3.578726	0.652314	-2.881686
S	3.644660	-0.855321	-1.990558
S	-1.897986	-1.733657	2.520449
C	-1.445623	-1.104196	4.097719
C	-0.226919	-1.417253	4.569454
S	0.805747	-2.422042	3.566355
H	1.513178	-4.792819	2.418308
H	3.729211	-3.507186	-1.840344
H	3.721730	-5.775350	1.821453
H	-0.470495	-2.183825	-3.595724
H	-2.665993	-3.499069	0.650726
H	-2.880401	-2.623621	-3.562546
H	2.207411	1.935831	-3.950828
H	4.497889	1.224409	-2.949015
H	-2.173145	-0.486468	4.614604
H	0.175793	-1.082372	5.520002
O	-4.269110	-3.347974	-1.283817
C	-5.085483	-3.385731	-2.458525
H	-4.773683	-4.218765	-3.111011
H	-5.000523	-2.444795	-3.024038

C	-6.525704	-3.566286	-2.015959
H	-7.142034	-3.837566	-2.896073
H	-6.589996	-4.398587	-1.290491
C	-3.301594	0.373286	-0.500126
H	-3.236361	0.783821	0.519898
H	-2.723886	-0.561396	-0.519886
C	-4.743289	0.083802	-0.887213
H	-4.778912	-0.282593	-1.919104
H	-5.125809	-0.720484	-0.235583
O	-6.962290	-2.349049	-1.441103
C	-8.252523	-2.428685	-0.846309
H	-8.277581	-3.205537	-0.059673
H	-9.023397	-2.686488	-1.596658
C	-8.538880	-1.062053	-0.236798
H	-8.573885	-0.289701	-1.019688
H	-7.717233	-0.788176	0.447926
O	-5.603578	1.219850	-0.864822
C	-5.781584	1.795614	0.418823
H	-4.873864	2.329436	0.758431
H	-6.021083	1.022683	1.174232
C	-6.919095	2.799225	0.336067
H	-6.738202	3.472749	-0.521687
H	-6.938670	3.417621	1.254970
O	-9.772167	-1.166459	0.470237
C	-10.200468	0.095884	1.009170
H	-9.360207	0.620174	1.483926
H	-10.939370	-0.164339	1.782292
C	-10.866026	0.956788	-0.036158
H	-11.792351	0.536199	-0.437274
O	-8.143569	2.096823	0.170555
C	-9.222862	2.935895	-0.210878
H	-8.941036	3.526054	-1.105183
H	-9.442041	3.678318	0.586976
C	-10.461103	2.138304	-0.533278
H	-11.104216	2.621890	-1.273973

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monomer-3

O	-0.922441	5.339526	1.879401
C	0.318710	1.361474	2.404375
C	0.092499	1.832037	1.080917
C	0.946059	0.033823	2.578685
C	1.987571	-0.246988	1.566916
C	1.778688	0.229906	0.235634
C	0.540064	0.984303	-0.047601
C	0.064351	2.234877	3.481895
C	-0.392746	3.145360	0.885538
C	-0.601253	4.004452	1.972239
C	-0.392805	3.533949	3.281566
C	2.794613	0.016461	-0.716485
C	3.194220	-0.890308	1.888198
C	3.984966	-0.636855	-0.392939
C	4.182951	-1.075176	0.918303
C	-0.128579	0.929013	-1.249517
C	0.595985	-0.837513	3.580993
S	0.441182	0.029796	-2.679870
C	-1.049149	0.173961	-3.593110
C	-2.026392	0.933766	-3.065851
S	-1.725995	1.677648	-1.510763
S	1.332514	-2.454336	3.815882
C	0.289493	-2.942748	5.139955
C	-0.636857	-2.064539	5.564325
S	-0.725385	-0.516686	4.748303
H	0.284131	1.908848	4.496426
H	-0.532734	3.506408	-0.126643
H	-0.545172	4.214413	4.117118
H	2.707280	0.442724	-1.712599
H	3.392408	-1.195686	2.912216
H	4.797823	-0.728981	-1.108086
H	-1.108720	-0.354908	-4.539880
H	-2.999401	1.108894	-3.513040
H	0.444219	-3.937030	5.549988
H	-1.355516	-2.244602	6.357937
O	5.375721	-1.725303	1.209874
C	-1.204644	5.901831	0.584899
H	-1.163991	6.984729	0.761736
H	-0.411656	5.649460	-0.136082

C	-2.565431	5.483093	0.075077
C	-3.674707	5.580459	0.931959
C	-2.743839	4.955518	-1.211313
C	-4.920275	5.099285	0.528823
C	-3.993442	4.471468	-1.613777
C	-5.084743	4.507420	-0.734480
H	-3.539935	5.983493	1.934958
H	-1.891684	4.874574	-1.886233
H	-5.764157	5.133225	1.220206
H	-4.107041	3.999636	-2.589107
C	-6.381573	3.810932	-1.094413
H	-7.033666	3.740169	-0.208230
H	-6.931985	4.351550	-1.875630
O	-6.174705	2.507802	-1.668791
C	-3.918801	-0.424559	0.328814
C	-4.323931	-0.581380	-1.032287
C	-3.068100	-1.470786	0.920400
C	-2.110893	-2.079608	-0.022172
C	-2.527346	-2.258864	-1.376171
C	-3.874698	-1.789899	-1.754516
C	-4.320205	0.730311	1.016458
C	-5.074935	0.433311	-1.643429
C	-5.470383	1.577910	-0.932784
C	-5.111393	1.715027	0.416477
C	-1.618835	-2.839612	-2.275038
C	-0.823841	-2.468258	0.366781
C	-0.352707	-3.279783	-1.872941
C	0.044568	-3.100881	-0.537851
C	-4.685957	-2.470062	-2.630939
C	-3.229281	-1.946605	2.198310
S	-4.228393	-4.019317	-3.407994
C	-5.845385	-4.422914	-3.967728
C	-6.812893	-3.505110	-3.792257
S	-6.369113	-1.989580	-3.019830
S	-2.358489	-3.375663	2.831880
C	-3.323327	-3.538729	4.286269
C	-4.260114	-2.603197	4.529953
S	-4.428231	-1.303533	3.359469
H	-3.959434	0.903644	2.028404
H	-5.326238	0.382748	-2.700494
H	-5.380468	2.594535	0.988862
H	-1.879390	-2.910028	-3.329160
H	-0.453403	-2.255070	1.365160
H	0.319416	-3.711637	-2.608870
H	-5.978115	-5.388597	-4.448111
H	-7.846352	-3.616066	-4.109417
H	-3.100578	-4.381346	4.935178
H	-4.912550	-2.578626	5.398684
O	1.248090	-3.492097	-0.020290
C	2.241714	-3.983937	-0.924674
H	2.549145	-3.175170	-1.604252
H	1.853488	-4.822455	-1.524776
C	3.410009	-4.478959	-0.067693
H	3.801789	-3.658058	0.546623
H	3.036633	-5.263013	0.607598
C	6.230797	-1.110160	2.184175
H	7.050852	-1.825159	2.327085
H	5.708318	-0.976174	3.144878
C	6.795477	0.231363	1.731334
H	7.661249	0.485167	2.377506
H	7.149477	0.157761	0.687353
O	4.431334	-5.065628	-0.877119
C	5.552683	-4.221944	-1.149642
H	6.418763	-4.885761	-1.281583
H	5.758104	-3.541754	-0.310527
C	5.355639	-3.387235	-2.419630
H	5.265177	-4.044639	-3.305019
H	4.427308	-2.795351	-2.342281
O	5.773014	1.210764	1.852741
C	6.217519	2.532251	1.593750
H	6.889066	2.883413	2.403088
H	6.783681	2.588385	0.645683
C	5.003249	3.441516	1.513050
H	5.320142	4.496294	1.633791
H	4.318457	3.196960	2.345470
O	6.474868	-2.513201	-2.524273
C	6.383383	-1.603161	-3.610206

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H       6.790933      -2.049699      -4.539401
H       5.328940      -1.335486      -3.801568
C       7.163044      -0.343241      -3.250920
H       8.194421      -0.619731      -2.978940
H       7.207690       0.319953      -4.130712
O       6.564757       0.312804      -2.130759
C       6.092978       1.640136      -2.369065
H       5.801434       2.019654      -1.382141
H       6.922594       2.269631      -2.745769
C       4.901358       1.712281      -3.302912
H       4.702458       0.820012      -3.899503
O       4.358124       3.253959       0.261116
C       3.080134       3.893021       0.211474
H       3.178975       4.973122       0.431965
H       2.408501       3.448296       0.967026
C       2.458655       3.714757      -1.167551
H       1.398430       3.987017      -1.099050
H       2.515919       2.656267      -1.456930
O       3.003726       4.562800      -2.180939
C       4.245402       4.093094      -2.726029
H       5.015532       4.034539      -1.943543
H       4.544117       4.876632      -3.440399
C       4.095234       2.777367      -3.446589
H       3.250655       2.721873      -4.138079

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monomer-4
O       3.295701      -5.658347      -1.505947
C       0.380375      -3.367084       0.474281
C       0.768203      -3.074539      -0.864056
C      -0.776779      -2.623821       1.019287
C      -1.839343      -2.367696       0.018382
C      -1.418457      -2.027564      -1.305070
C       0.033122      -2.008848      -1.572770
C       1.053251      -4.394876       1.160447
C       1.771048      -3.840314      -1.477769
C       2.412503      -4.871627      -0.783177
C       2.073118      -5.135960       0.552621
C      -2.401274      -1.817680      -2.285347
C      -3.207828      -2.499620       0.296123
C      -3.767247      -1.940435      -2.002302
C      -4.175188      -2.290511      -0.704716
C       0.672085      -1.055094      -2.323678
C      -0.820947      -2.136430       2.298460
S      -0.169533       0.283121      -3.143324
C       1.282325       1.173764      -3.566969
C       2.466912       0.617886      -3.256664
S       2.453032      -0.938579      -2.448578
S      -2.184533      -1.181326       2.957152
C      -1.366727      -0.704862       4.437697
C      -0.140770      -1.206219       4.663605
S       0.536489      -2.285371       3.455823
H       0.739082      -4.661082       2.168326
H       2.031470      -3.676637      -2.520536
H       2.550814      -5.949837       1.094867
H      -2.097804      -1.600508      -3.308003
H      -3.550285      -2.821302       1.277202
H      -4.492922      -1.787462      -2.796276
H       1.150629       2.134931      -4.053056
H       3.436768       1.063849      -3.452091
H      -1.890173      -0.020460       5.097607
H       0.472694      -0.980068       5.529557
O      -5.482422      -2.449247      -0.317561
C       4.599674      -5.851945      -0.930125
H       4.537162      -6.350708       0.050522
H       5.094715      -6.546051      -1.623463
C       5.364035      -4.551261      -0.809966
C       5.281818      -3.591474      -1.833666
C       6.126968      -4.263717       0.329840
C       5.918689      -2.357274      -1.702828
C       6.775347      -3.029731       0.456588
C       6.657736      -2.057535      -0.547373
H       4.679099      -3.804366      -2.714478
H       6.188008      -4.993969       1.138173
H       5.808768      -1.599160      -2.476684
H       7.333226      -2.801394       1.366452
C       7.256624      -0.678094      -0.357323
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H	7.475596	-0.502855	0.709089
H	8.195516	-0.571830	-0.917585
O	6.433455	0.380148	-0.870871
C	2.701062	1.275828	0.821204
C	3.253230	2.065333	-0.233629
C	1.383871	1.664646	1.346588
C	0.462273	2.184376	0.321881
C	1.003365	3.019175	-0.694187
C	2.466737	3.225679	-0.711188
C	3.422723	0.170683	1.292677
C	4.498427	1.703982	-0.767106
C	5.223308	0.614397	-0.254113
C	4.685284	-0.155937	0.788016
C	0.108408	3.564276	-1.638089
C	-0.905413	1.871130	0.337107
C	-1.259897	3.301790	-1.591548
C	-1.773697	2.433702	-0.610733
C	3.049946	4.428478	-1.032730
C	1.085979	1.706553	2.684240
S	2.117730	5.903765	-1.443090
C	3.470719	7.017139	-1.311365
C	4.689078	6.492822	-1.088336
S	4.812806	4.745174	-0.951263
S	-0.431975	2.401916	3.338186
C	0.120078	2.482709	5.003078
C	1.330420	1.967831	5.289995
S	2.248775	1.258643	3.969927
H	2.971668	-0.483142	2.037507
H	4.922896	2.238656	-1.613560
H	5.196307	-1.032243	1.168841
H	0.492659	4.168216	-2.457796
H	-1.262810	1.151637	1.066819
H	-1.937500	3.714031	-2.336831
H	3.256967	8.075107	-1.437237
H	5.610574	7.062916	-1.006220
H	-0.550966	2.936755	5.727707
H	1.781752	1.946399	6.278534
O	-3.112530	2.167310	-0.665088
C	-3.593169	1.144974	0.229779
H	-3.451115	1.469691	1.274830
H	-3.014607	0.224573	0.079105
C	-5.057053	0.887828	-0.064647
H	-5.169218	0.599721	-1.118322
H	-5.371483	0.022565	0.532917
C	-6.456489	-2.731572	-1.345784
H	-6.146339	-3.643395	-1.880710
H	-6.511712	-1.907014	-2.072678
C	-7.815400	-2.895855	-0.668224
H	-8.451796	-3.539025	-1.292585
H	-7.673978	-3.408297	0.293934
O	-7.309501	1.570238	0.068000
C	-8.330698	2.544921	0.214052
H	-8.123322	3.420231	-0.436934
H	-8.345670	2.932252	1.252278
O	-9.006371	-1.141547	-1.758486
C	-9.681556	1.954876	-0.116053
H	-10.506207	2.390385	0.454471
C	-9.027890	0.282612	-1.945876
H	-9.381006	0.412733	-2.980705
H	-8.016460	0.698656	-1.862396
C	-9.974967	0.995202	-1.012197
H	-11.018441	0.676699	-1.091710
C	-8.536244	-1.562454	-0.467411
H	-9.387984	-1.679759	0.225076
H	-7.858620	-0.812809	-0.034722
C	-5.982868	2.058158	0.247263
H	-5.836403	2.409378	1.288205
H	-5.783898	2.913757	-0.422296

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O	5.624527	-4.245083	-2.087195
C	2.094804	-3.122941	-0.089725
C	2.486294	-2.475890	-1.301991
C	0.800118	-2.754135	0.514400
C	-0.242091	-2.415292	-0.475897
C	0.158169	-1.719702	-1.659942

C	1.593860	-1.441569	-1.865065
C	2.915485	-4.142339	0.429011
C	3.674246	-2.884897	-1.933353
C	4.485721	-3.881859	-1.382665
C	4.111289	-4.514887	-0.190392
C	-0.832072	-1.413769	-2.607714
C	-1.580203	-2.801137	-0.320575
C	-2.175993	-1.756484	-2.426957
C	-2.550080	-2.475463	-1.282246
C	2.066118	-0.317349	-2.506868
C	0.585447	-2.697845	1.870371
S	1.018083	0.982099	-3.138037
C	2.301897	2.134747	-3.439728
C	3.566175	1.715451	-3.246292
S	3.800060	0.066078	-2.703358
S	-0.971410	-2.234863	2.619930
C	-0.334410	-2.005617	4.238135
C	0.949087	-2.340262	4.454901
S	1.867569	-2.969920	3.095127
H	2.586631	-4.697447	1.305466
H	3.972968	-2.466927	-2.890725
H	4.718546	-5.318200	0.223012
H	-0.550175	-0.944346	-3.547225
H	-1.889488	-3.418884	0.519144
H	-2.897989	-1.493852	-3.194194
H	2.010923	3.132782	-3.755065
H	4.456841	2.322338	-3.382660
H	-1.003205	-1.580144	4.980105
H	1.468859	-2.243474	5.403663
O	-3.818070	-2.935094	-1.025461
C	6.864294	-4.084854	-1.352316
H	6.931751	-4.817520	-0.532154
H	7.642608	-4.321182	-2.089019
C	6.989064	-2.677957	-0.820607
C	7.012032	-1.595050	-1.717733
C	6.918534	-2.417889	0.554389
C	6.922957	-0.285218	-1.248664
C	6.836147	-1.102076	1.024625
C	6.804188	-0.025805	0.127814
H	7.049859	-1.790407	-2.789290
H	6.884192	-3.249713	1.258209
H	6.904153	0.548002	-1.950450
H	6.753780	-0.914390	2.096479
C	6.595928	1.394223	0.608952
H	6.469864	1.422840	1.702547
H	7.456405	2.024405	0.347043
O	5.486882	2.048675	-0.035571
C	1.529358	1.411767	1.192570
C	1.856705	2.388372	0.203893
C	0.132184	1.328806	1.652667
C	-0.869502	1.546581	0.596278
C	-0.550783	2.482330	-0.428406
C	0.749468	3.186060	-0.365330
C	2.542945	0.578706	1.685122
C	3.198413	2.537823	-0.172527
C	4.212704	1.748508	0.394580
C	3.880507	0.736270	1.306052
C	-1.493808	2.673824	-1.458627
C	-2.106773	0.879312	0.583997
C	-2.739883	2.049984	-1.444343
C	-3.065060	1.171034	-0.397341
C	0.884192	4.509924	-0.717002
C	-0.184501	1.239602	2.984611
S	-0.484041	5.536215	-1.261099
C	0.356578	7.069424	-1.088064
C	1.662069	7.031429	-0.767397
S	2.401774	5.451668	-0.552206
S	-1.857985	1.244558	3.626280
C	-1.401878	1.443588	5.313131
C	-0.087676	1.452395	5.606268
S	1.050366	1.266349	4.284720
H	2.283632	-0.235936	2.357136
H	3.487078	3.228356	-0.956899
H	4.623323	0.046785	1.689159
H	-1.239526	3.303851	-2.308530
H	-2.284628	0.094990	1.311063
H	-3.467683	2.226233	-2.234131

H	-0.217923	7.973562	-1.271033
H	2.304839	7.899843	-0.650352
H	-2.205843	1.544203	6.037498
H	0.325280	1.556123	6.606419
O	-4.327722	0.638294	-0.417416
C	-4.755599	-0.102386	0.743272
H	-4.436031	0.426498	1.655641
H	-4.285682	-1.097016	0.731213
C	-6.273582	-0.215301	0.697104
H	-6.561367	-0.598212	-0.289235
H	-6.571592	-0.983676	1.428360
C	-4.848549	-2.564151	-1.953688
H	-4.616254	-2.961915	-2.956309
H	-4.888904	-1.464946	-2.021071
C	-6.177717	-3.108879	-1.441202
H	-6.179547	-4.207170	-1.480437
H	-6.267088	-2.833683	-0.381402
C	-8.560989	0.885402	0.950357
C	-9.136173	0.809786	-0.487288
H	-8.420827	0.300426	-1.144621
H	-9.228810	1.837385	-0.878194
C	-8.679969	-2.489487	-1.448929
C	-10.471509	0.111753	-0.535362
H	-11.249031	0.532735	0.109737
C	-9.786778	-1.684747	-2.183965
H	-10.330385	-2.343140	-2.875876
H	-9.296672	-0.927792	-2.816101
C	-10.759920	-0.989335	-1.253885
H	-11.759270	-1.421854	-1.162595
C	-7.359386	-2.518020	-2.232463
H	-7.114279	-1.476871	-2.503685
H	-7.489078	-3.050220	-3.187777
C	-7.033676	1.085331	0.997606
H	-6.739460	1.443642	1.996867
H	-6.726921	1.864512	0.283825
H	-9.026855	-3.511180	-1.232170
H	-8.493649	-2.020504	-0.473115
H	-8.812298	-0.043651	1.486880
H	-9.067196	1.696440	1.494938

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C60

C	2.546482	-2.196229	-1.187708
C	1.372021	-3.062420	-1.209432
C	0.785360	-3.479644	-0.004663
C	1.350216	-3.047633	1.269914
C	2.479740	-2.214914	1.290551
C	3.089942	-1.781195	0.037689
C	2.429739	-1.249600	-2.292070
C	1.182264	-1.529780	-2.995816
C	0.528583	-2.649907	-2.326845
C	-0.868635	-2.671635	-2.197518
C	-0.667809	-3.500895	0.130387
C	0.246147	-2.801897	2.192249
C	0.314420	-1.733992	3.099998
C	1.489116	-0.868360	3.121653
C	2.550791	-1.104174	2.234711
C	3.204679	0.015863	1.565420
C	3.537705	-0.402463	0.207506
C	3.425991	0.508019	-0.854671
C	2.860798	0.076161	-2.129131
C	0.413833	-0.474229	-3.510031
C	0.861792	0.904188	-3.340199
C	2.061366	1.174003	-2.663551
C	2.131998	2.284369	-1.719030
C	2.975292	1.872811	-0.601308
C	2.654823	2.275084	0.704490
C	2.771623	1.328300	1.808944
C	1.668142	1.573555	2.731997
C	1.039193	0.496580	3.375461
C	-1.000902	-3.082417	1.488166
C	-2.429739	1.249600	2.292072
C	-2.860797	-0.076163	2.129131
C	-3.425991	-0.508020	0.854671
C	-3.537703	0.402462	-0.207506
C	-3.089941	1.781194	-0.037690
C	-1.372024	3.062420	1.209432

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C      -0.528584       2.649908       2.326845
C      -1.182267       1.529778       2.995814
C      -0.413834       0.474230       3.510032
C      -0.861792      -0.904188       3.340200
C      -2.061366      -1.174002       2.663551
C      -2.975291      -1.872812       0.601309
C      -2.654824      -2.275084      -0.704490
C      -2.771624      -1.328301      -1.808943
C      -3.204678      -0.015863      -1.565421
C      -2.550789       1.104174      -2.234711
C      -2.479739       2.214915      -1.290551
C      -1.350215       3.047633      -1.269913
C      -0.785358       3.479644       0.004664
C       0.868633       2.671633       2.197516
C       1.478608       3.105088       0.944573
C       0.667807       3.500894      -0.130386
C       1.000903       3.082419      -1.488166
C      -0.246147       2.801899      -2.192249
C      -0.314420       1.733994      -3.099997
C      -1.489117       0.868362      -3.121656
C      -1.039193      -0.496580      -3.375461
C      -1.668142      -1.573556      -2.731997
C      -2.131997      -2.284369       1.719032
C      -1.478606      -3.105087      -0.944572
C      -2.546484       2.196230       1.187707

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monomer-1-open
O      -2.156820      -4.667406      -0.719890
C      -4.978889      -1.631244      -1.384065
C      -4.787174      -2.117978      -0.060841
C      -5.864420      -0.462854      -1.566828
C      -5.770841       0.523048      -0.468212
C      -5.614367       0.017056       0.858322
C      -5.528410      -1.447847       1.028693
C      -4.251735      -2.232503      -2.430539
C      -3.863514      -3.151302       0.180060
C      -3.130229      -3.711695      -0.876404
C      -3.348131      -3.266554      -2.191954
C      -5.463322       0.931436       1.912411
C      -5.743897       1.906990      -0.686180
C      -5.458630       2.314008       1.694823
C      -5.578614       2.801943       0.383902
C      -6.127804      -2.128356       2.056428
C      -6.741853      -0.332450      -2.612678
S      -7.127550      -1.339045       3.315662
C      -7.795697      -2.827539       3.969970
C      -7.334005      -3.990286       3.475436
S      -6.106465      -3.913366       2.219105
S      -7.875709       1.041224      -2.797205
C      -8.834929       0.307393      -4.074361
C      -8.425180      -0.877591      -4.562096
S      -6.968807      -1.581891      -3.874927
H      -4.346618      -1.843090      -3.442547
H      -3.691044      -3.473472       1.202615
H      -2.761278      -3.700540      -2.999174
H      -5.295493       0.562607       2.922836
H      -5.771516       2.315148      -1.693942
H      -5.331306       2.990233       2.536415
H      -8.538616      -2.734384       4.757477
H      -7.647982      -4.977722       3.802779
H      -9.704366       0.859217      -4.421277
H      -8.912919      -1.427519      -5.362344
O      -5.502416       4.131452       0.048242
C      -1.590458      -4.845368       0.584128
H      -1.631291      -3.891049       1.134755
H      -2.176369      -5.583266       1.157093
C      -0.143365      -5.266456       0.465416
C       0.645882      -4.853854      -0.619840
C       0.462344      -5.972312       1.516473
C       2.016759      -5.123401      -0.643024
C       1.839163      -6.220477       1.503429
C       2.631296      -5.790668       0.427746
H       0.177695      -4.313432      -1.439767
H      -0.139270      -6.304583       2.364102
H       2.626852      -4.782106      -1.477380
H       2.302264      -6.742259       2.342852
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C       4.128173      -6.039688       0.435203
H       4.501518      -6.088075       1.472037
H       4.367858      -6.996763      -0.048243
O       4.878858      -5.081122      -0.320226
C       5.012128      -1.025357       0.770473
C       5.639367      -1.511393      -0.417706
C       5.061419       0.427297       1.034201
C       4.980289       1.260204      -0.183637
C       5.627554       0.778874      -1.356937
C       6.315859      -0.525379      -1.285211
C       4.340142      -1.943920       1.592310
C       5.554889      -2.873847      -0.732664
C       4.895974      -3.776575       0.118581
C       4.287878      -3.310933       1.294420
C       5.536680       1.546522      -2.534918
C       4.267635       2.473960      -0.225291
C       4.862081       2.765003      -2.564133
C       4.221778       3.233895      -1.403610
C       7.526432      -0.769202      -1.885431
C       5.263262       0.956069       2.285410
S       8.441373       0.466239      -2.805263
C       9.944636      -0.441620      -2.876895
C       9.940240      -1.694367      -2.386764
S       8.432299      -2.306087      -1.722397
S       5.444707       2.708751       2.616509
C       6.045625       2.518915       4.257554
C       6.077577       1.275922       4.770606
S       5.513967      -0.041262       3.752419
H       3.795982      -1.584981       2.464033
H       5.955572      -3.257116      -1.668291
H       3.727115      -3.976082       1.943368
H       5.968241       1.164173      -3.458157
H       3.712633       2.790411       0.652459
H       4.789652       3.349258      -3.479327
H      10.799622       0.048938      -3.334209
H      10.791696      -2.369549      -2.387881
H       6.343145       3.421571       4.784338
H       6.404941       1.021890       5.775160
O       3.551666       4.422928      -1.532690
C       2.836597       4.922410      -0.399513
H       3.521820       5.134777       0.436823
H       2.083932       4.195416      -0.055679
C       2.140410       6.196147      -0.867032
H       2.886917       6.935513      -1.213418
H       1.488003       5.955194      -1.727186
C      -4.812246       4.995896       0.959893
H      -3.967214       4.469758       1.427573
H      -5.487531       5.348743       1.755373
C      -4.258748       6.161738       0.144484
H      -3.718149       5.751402      -0.728407
H      -5.071082       6.807780      -0.237991
O       1.385769       6.691736       0.228915
C       0.537100       7.776536      -0.156141
H      -0.159066       7.451094      -0.949381
H       1.147513       8.597611      -0.585008
O      -3.379504       6.872289       1.004360
C      -0.186243       8.266788       1.065066
H       0.468024       8.619961       1.865358
C      -2.580878       7.833953       0.308878
H      -3.211292       8.684026      -0.022938
H      -2.148074       7.381020      -0.599753
C      -1.514865       8.302880       1.257909
H      -1.896330       8.687017       2.206799

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monomer-2-open
O      -1.203245      -5.071586      -0.558243
C      -4.932768      -3.186387      -0.967090
C      -4.265546      -3.130532       0.288212
C      -6.198444      -2.438220      -1.111660
C      -6.215916      -1.155168      -0.377966
C      -5.556468      -1.111551       0.889309
C      -4.900211      -2.345483       1.367131
C      -4.319518      -3.895849      -2.019209
C      -3.018437      -3.762057       0.449697
C      -2.430838      -4.463407      -0.613881
C      -3.095342      -4.539493      -1.851292
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C	-5.508997	0.109530	1.578519
C	-6.787954	0.013764	-0.896253
C	-6.101069	1.271651	1.068766
C	-6.738419	1.222094	-0.180566
C	-4.943396	-2.764721	2.672530
C	-7.287826	-2.925614	-1.789332
S	-5.819569	-1.887044	3.965262
C	-5.739769	-3.185403	5.147604
C	-5.029046	-4.280948	4.825058
S	-4.247698	-4.312826	3.250363
S	-8.861551	-2.077666	-1.895322
C	-9.757794	-3.446869	-2.536882
C	-9.066462	-4.561835	-2.834733
S	-7.331976	-4.544885	-2.552723
H	-4.784132	-3.902760	-3.003556
H	-2.495765	-3.654157	1.394705
H	-2.616385	-5.066270	-2.674276
H	-4.959683	0.174647	2.516135
H	-7.226085	0.029138	-1.891498
H	-6.034910	2.197261	1.634203
H	-6.254683	-3.029625	6.091736
H	-4.883306	-5.144092	5.468903
H	-10.826991	-3.316592	-2.680481
H	-9.492199	-5.468637	-3.255676
O	-7.306970	2.304921	-0.805275
C	-0.403815	-4.860598	0.615478
H	-0.431999	-3.791283	0.886702
H	-0.812830	-5.431588	1.465342
C	1.020312	-5.260210	0.319230
C	1.639432	-4.838062	-0.870528
C	1.775320	-5.971192	1.262370
C	2.988118	-5.108993	-1.102424
C	3.134197	-6.226039	1.037271
C	3.753963	-5.793514	-0.143156
H	1.053651	-4.294736	-1.610205
H	1.306350	-6.308423	2.187743
H	3.468422	-4.760178	-2.015116
H	3.717407	-6.757218	1.791505
C	5.228791	-6.048274	-0.386541
H	5.748186	-6.257263	0.563328
H	5.375074	-6.917740	-1.041625
O	5.874343	-4.979677	-1.094860
C	6.040248	-1.105025	0.521057
C	6.340780	-1.363530	-0.851481
C	6.079485	0.296208	0.985766
C	5.604698	1.271236	-0.017020
C	5.910875	1.016311	-1.383635
C	6.673731	-0.206345	-1.707630
C	5.670691	-2.184193	1.339114
C	6.259389	-2.675842	-1.336758
C	5.915718	-3.742731	-0.490741
C	5.617594	-3.497321	0.858051
C	5.430610	1.917007	-2.355305
C	4.841113	2.401020	0.331202
C	4.703513	3.053062	-2.005481
C	4.406808	3.301467	-0.653425
C	7.672086	-0.239084	-2.649756
C	6.597677	0.667770	2.201632
S	8.197162	1.196693	-3.583575
C	9.670272	0.472352	-4.211343
C	9.891238	-0.826582	-3.940025
S	8.685936	-1.677414	-2.984690
S	6.766308	2.368622	2.743090
C	7.818712	2.017279	4.106770
C	8.064352	0.725311	4.389356
S	7.309087	-0.490541	3.368991
H	5.368113	-1.996870	2.367917
H	6.406592	-2.892083	-2.392362
H	5.297830	-4.294422	1.521731
H	5.596457	1.705456	-3.410148
H	4.548888	2.540060	1.367262
H	4.331714	3.741138	-2.762139
H	10.320887	1.107058	-4.806863
H	10.747842	-1.400576	-4.282950
H	8.203379	2.864836	4.667585
H	8.677811	0.370750	5.213248
O	3.662688	4.422880	-0.398161

C	3.352776	4.720966	0.966510
H	4.273744	4.853405	1.556754
H	2.765087	3.907695	1.422036
C	2.532339	6.005445	0.960124
H	3.113278	6.825680	0.500008
H	1.616037	5.869772	0.368258
C	-7.001370	3.598265	-0.281113
H	-5.914896	3.710112	-0.135790
H	-7.498967	3.762633	0.688314
C	-7.477244	4.620299	-1.308087
H	-7.049798	4.371362	-2.296228
H	-8.578521	4.596981	-1.401624
O	2.241553	6.292570	2.327786
C	1.479270	7.476601	2.532946
H	1.864692	8.311250	1.919486
H	1.617256	7.736016	3.592448
C	-0.014896	7.306795	2.270985
H	-0.574637	8.116420	2.782571
H	-0.345949	6.344725	2.706252
O	-7.020127	5.887402	-0.855525
C	-7.313150	6.949482	-1.763248
H	-8.394558	7.189875	-1.734440
H	-7.057989	6.657053	-2.797897
C	-6.496602	8.184249	-1.386424
H	-6.580252	8.358789	-0.297734
H	-6.928658	9.052616	-1.904435
O	-0.265678	7.343113	0.870837
C	-1.607371	6.981349	0.549744
H	-2.325185	7.643585	1.074541
H	-1.811784	5.951475	0.911854
C	-1.778804	7.067468	-0.940411
H	-0.857413	6.938445	-1.511094
O	-5.137072	8.127160	-1.800344
C	-4.297450	7.336000	-0.949101
H	-4.732932	6.331450	-0.816040
H	-4.240426	7.791379	0.059910
C	-2.942812	7.234467	-1.587219
H	-2.953080	7.241890	-2.678701

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O	0.507591	-5.813742	-0.482198
C	-3.559685	-5.231736	-1.349052
C	-3.152820	-5.348853	0.009533
C	-4.983507	-4.950698	-1.623122
C	-5.615508	-4.056296	-0.630296
C	-5.218168	-4.200390	0.735032
C	-4.192040	-5.214379	1.051007
C	-2.574985	-5.330689	-2.352574
C	-1.793789	-5.539091	0.321260
C	-0.836274	-5.647040	-0.698336
C	-1.234443	-5.551691	-2.043448
C	-5.773372	-3.333885	1.688836
C	-6.528458	-3.052724	-0.978906
C	-6.707924	-2.350426	1.342438
C	-7.077502	-2.202539	-0.003553
C	-4.242446	-6.017010	2.162872
C	-5.683082	-5.536786	-2.648623
S	-5.570165	-5.961014	3.364075
C	-5.140303	-7.460116	4.175117
C	-4.009280	-8.077153	3.788648
S	-3.067564	-7.327246	2.507113
S	-7.433045	-5.286559	-2.935330
C	-7.613740	-6.600833	-4.088204
C	-6.502597	-7.259257	-4.464423
S	-4.974632	-6.743692	-3.765929
H	-2.854436	-5.184625	-3.394349
H	-1.493219	-5.554266	1.364000
H	-0.477365	-5.610411	-2.822961
H	-5.440466	-3.391396	2.723668
H	-6.784759	-2.865856	-2.019138
H	-7.110917	-1.700419	2.114387
H	-5.802273	-7.804752	4.964947
H	-3.619377	-8.995912	4.218364
H	-8.615794	-6.803140	-4.456650
H	-6.470278	-8.073825	-5.182867
O	-7.932829	-1.237282	-0.472444

C	0.980295	-5.716294	0.864035
H	0.576504	-4.798065	1.327187
H	0.618286	-6.571017	1.460857
C	2.490067	-5.662751	0.867809
C	3.211268	-5.156870	-0.224929
C	3.188512	-6.046293	2.023780
C	4.602846	-5.035288	-0.161619
C	4.577603	-5.901974	2.094647
C	5.298700	-5.395352	1.001981
H	2.674541	-4.862705	-1.124148
H	2.641675	-6.444022	2.880279
H	5.155983	-4.634250	-1.009011
H	5.104646	-6.184773	3.007623
C	6.808203	-5.264782	1.086303
H	7.117613	-5.068282	2.126644
H	7.292875	-6.197896	0.766992
O	7.359921	-4.276949	0.209763
C	6.712522	-0.171961	0.823241
C	7.510132	-0.659648	-0.257544
C	6.509553	1.287038	0.929384
C	6.405078	1.974300	-0.374158
C	7.215858	1.494595	-1.441613
C	8.092462	0.335467	-1.180986
C	6.128590	-1.104797	1.694683
C	7.679398	-2.040812	-0.418103
C	7.110734	-2.952331	0.487175
C	6.328595	-2.483510	1.553705
C	7.106697	2.120836	-2.699131
C	5.521002	3.047526	-0.594682
C	6.258836	3.206963	-2.904969
C	5.460739	3.676473	-1.847102
C	9.373780	0.240746	-1.666120
C	6.518353	1.960010	2.126640
S	10.155612	1.517261	-2.650326
C	11.785399	0.873301	-2.516420
C	11.939267	-0.308799	-1.893103
S	10.496687	-1.098459	-1.272949
S	6.397273	3.742672	2.276643
C	6.880394	3.812691	3.965419
C	7.060406	2.646921	4.611791
S	6.793908	1.163486	3.707528
H	5.458165	-0.758275	2.479144
H	8.220112	-2.442724	-1.271794
H	5.829747	-3.167372	2.233295
H	7.668106	1.726777	-3.544319
H	4.851158	3.351054	0.203864
H	6.176180	3.682907	-3.880062
H	12.587091	1.454338	-2.964157
H	12.884661	-0.827934	-1.760545
H	6.989925	4.798391	4.409504
H	7.337460	2.547775	5.657854
O	4.633377	4.728241	-2.144751
C	3.784375	5.229601	-1.109726
H	4.377439	5.593594	-0.255424
H	3.098874	4.446761	-0.747623
C	2.982290	6.367539	-1.731600
H	3.663485	7.162583	-2.087494
H	2.426510	5.987217	-2.608615
C	-8.263216	-0.163272	0.412221
H	-7.361929	0.215919	0.918018
H	-8.981186	-0.491221	1.181185
C	-8.853400	0.953991	-0.442685
H	-8.136868	1.204507	-1.245928
H	-9.795670	0.630851	-0.921836
O	2.096957	6.852065	-0.733404
C	1.208575	7.841973	-1.235652
H	0.610126	7.447505	-2.077700
H	1.760948	8.726185	-1.604107
C	0.273476	8.240597	-0.098595
H	0.847221	8.705685	0.724510
H	-0.216213	7.335309	0.306009
O	-9.057499	2.059467	0.425314
C	-9.296185	3.279413	-0.265794
H	-10.278327	3.272195	-0.772956
H	-8.522147	3.455573	-1.035003
C	-9.221444	4.400115	0.767564
H	-8.280289	4.287635	1.336896

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H     -10.057353       4.326917       1.487799
O      -0.682691       9.142154      -0.638037
C      -1.663562       9.532380       0.314031
H      -1.217371      10.133213       1.128074
H      -2.144047       8.649969       0.775161
C      -2.719807      10.344750      -0.428275
H      -2.266892      11.251137      -0.873059
H      -3.124214       9.734874      -1.258070
O      -3.735695      10.676051       0.507974
C      -4.870677      11.275801      -0.120458
H      -5.271409      10.605766      -0.901637
H      -4.568779      12.214303      -0.629530
C      -5.889075      11.574741       0.942255
H      -5.537669      12.249218       1.726460
O      -9.245816       5.634891       0.065481
C      -8.939964       6.741565       0.904529
H      -8.007151       6.562194       1.469807
H      -9.745451       6.926216       1.639031
C      -8.734459       7.959006       0.008152
H      -9.680248       8.250446      -0.486649
H      -8.011267       7.693872      -0.785930
O      -8.231214       9.001986       0.830987
C      -7.804621      10.136321       0.073376
H      -8.677382      10.617820      -0.414097
H      -7.122487       9.818749      -0.734613
C      -7.140510      11.093740       1.021402
H      -7.765044      11.395005       1.865646

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O      -0.398056      -5.319664      -0.599184
C      -3.808250      -2.980704      -1.345813
C      -3.450639      -3.276187      -0.001076
C      -4.941128      -2.057563      -1.572126
C      -5.015980      -0.958637      -0.584731
C      -4.649346      -1.262172       0.762684
C      -4.245409      -2.647844       1.072840
C      -3.021488      -3.527293      -2.379498
C      -2.328048      -4.078568       0.269202
C      -1.548871      -4.591600      -0.777659
C      -1.913671      -4.330164      -2.110255
C      -4.617912      -0.221398       1.701573
C      -5.359819       0.357357      -0.922128
C      -4.966312       1.090810       1.362681
C      -5.353132       1.380147       0.043538
C      -4.625756      -3.305593       2.213650
C      -5.881502      -2.250403      -2.552618
S      -5.682772      -2.581532       3.465924
C      -6.000066      -4.085450       4.319381
C      -5.344348      -5.186723       3.910876
S      -4.232253      -5.020258       2.559066
S      -7.314601      -1.202722      -2.785085
C      -8.143428      -2.280165      -3.899129
C      -7.494195      -3.390095      -4.294673
S      -5.878379      -3.659010      -3.658330
H      -3.244332      -3.273138      -3.414270
H      -2.046295      -4.249308       1.303419
H      -1.290788      -4.718616      -2.913665
H      -4.271045      -0.424218       2.713565
H      -5.579321       0.633492      -1.950833
H      -4.909355       1.866212       2.120924
H      -6.699367      -4.047006       5.150246
H      -5.434181      -6.171507       4.361335
H      -9.135253      -1.984112      -4.229895
H      -7.881648      -4.126524      -4.993432
O      -5.708725       2.627316      -0.406068
C       0.194325      -5.329809       0.704160
H      -0.013840      -4.373367       1.210844
H      -0.249370      -6.131755       1.317659
C       1.694170      -5.480233       0.597932
C       2.395073      -5.011901      -0.524455
C       2.417370      -5.960185       1.700918
C       3.791691      -4.993430      -0.528470
C       3.815659      -5.916594       1.704736
C       4.516496      -5.418996       0.596240
H       1.836408      -4.647749      -1.383880
H       1.884998      -6.333705       2.577226
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H 4.328532 -4.599350 -1.389706
H 4.364929 -6.253413 2.585752
C 6.027650 -5.300165 0.625257
H 6.392237 -5.293709 1.666101
H 6.507218 -6.145128 0.112770
O 6.514204 -4.152932 -0.090360
C 5.142079 -0.293879 0.851921
C 5.771040 -0.589372 -0.395839
C 4.628518 1.076728 1.059484
C 4.063846 1.694946 -0.158334
C 4.692730 1.396330 -1.400397
C 5.865318 0.499377 -1.388484
C 4.993734 -1.332219 1.785763
C 6.209083 -1.895040 -0.654630
C 6.064006 -2.911873 0.301836
C 5.457722 -2.628761 1.535268
C 4.136367 1.928348 -2.580199
C 2.922644 2.520258 -0.133068
C 3.024181 2.765758 -2.549850
C 2.416183 3.072191 -1.319428
C 6.979615 0.710246 -2.161950
C 4.749208 1.748172 2.250632
S 7.170716 2.113207 -3.259118
C 8.891394 1.888048 -3.537950
C 9.471355 0.796093 -3.007823
S 8.454535 -0.303326 -2.087646
S 4.243946 3.451156 2.499896
C 5.069454 3.657752 4.038771
C 5.663422 2.577997 4.577877
S 5.557925 1.061985 3.694830
H 4.456353 -1.145460 2.713908
H 6.613045 -2.166258 -1.627287
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H 4.562190 1.654568 -3.543840
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H 2.597230 3.173796 -3.463793
H 9.397945 2.633957 -4.144415
H 10.517908 0.526333 -3.120954
H 5.042727 4.646928 4.487845
H 6.188694 2.562987 5.529061
O 1.316728 3.885412 -1.390186
C 0.771368 4.417259 -0.175352
H 1.571427 4.899286 0.413056
H 0.339079 3.609681 0.439864
C -0.293928 5.422785 -0.601189
H 0.151072 6.112980 -1.330182
H -1.110909 4.896265 -1.112920
C -5.377195 3.738138 0.434419
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H -5.842530 3.625198 1.427601
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C -0.869831 6.246568 0.548138
H -0.069102 6.817137 1.058128
H -1.349846 5.602356 1.311389
C -5.215655 6.219366 0.486894
O -6.061158 7.362899 0.383010
O -1.821157 7.133566 -0.033907
C -2.318109 8.139425 0.857113
H -1.469406 8.696166 1.301221
H -2.885245 7.684256 1.687303
C -3.165236 9.051466 0.014060
H -2.607419 9.575364 -0.766047
C -5.470093 8.520647 0.995570
H -4.995125 8.242493 1.952927
H -6.308818 9.191985 1.223823
C -4.498692 9.210138 0.066300
H -4.960425 9.862242 -0.678893
H -5.054484 5.988893 1.561996
H -4.224223 6.408550 0.043396

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O -1.779738 -5.097864 -0.418102
C -4.702800 -2.236907 -1.360611
C -4.572206 -2.671206 -0.011435

C	-5.640239	-1.131079	-1.641920
C	-5.687982	-0.111753	-0.571717
C	-5.602718	-0.570774	0.778820
C	-5.429511	-2.020559	1.002409
C	-3.877371	-2.827567	-2.337722
C	-3.609164	-3.641072	0.322494
C	-2.783886	-4.195290	-0.667200
C	-2.938940	-3.803693	-2.008011
C	-5.609520	0.380716	1.810079
C	-5.740134	1.263208	-0.830949
C	-5.692742	1.754145	1.550047
C	-5.733512	2.199360	0.218434
C	-6.056648	-2.713328	2.005657
C	-6.449332	-1.086412	-2.748835
S	-7.199220	-1.962255	3.163115
C	-7.818965	-3.475921	3.807667
C	-7.244543	-4.616607	3.385179
S	-5.928725	-4.487923	2.226263
S	-7.648501	0.207678	-3.055454
C	-8.475070	-0.624518	-4.364511
C	-7.962729	-1.795881	-4.783243
S	-6.514770	-2.385091	-3.979922
H	-3.925205	-2.473509	-3.365838
H	-3.482901	-3.921918	1.364087
H	-2.279946	-4.230523	-2.761588
H	-5.499769	0.053386	2.842602
H	-5.714756	1.641646	-1.850302
H	-5.694895	2.455860	2.379914
H	-8.626353	-3.413677	4.532270
H	-7.518137	-5.614670	3.716561
H	-9.351163	-0.139114	-4.785998
H	-8.361497	-2.399784	-5.593799
O	-5.724027	3.515134	-0.163233
C	-1.251687	-5.171860	0.911200
H	-1.363842	-4.192460	1.405391
H	-1.816582	-5.908943	1.506162
C	0.218806	-5.522726	0.858177
C	1.006844	-5.178557	-0.251161
C	0.837813	-6.098123	1.979000
C	2.387572	-5.391646	-0.233981
C	2.223742	-6.288281	2.004345
C	3.013074	-5.931654	0.900080
H	0.529020	-4.738744	-1.123684
H	0.237820	-6.375124	2.847470
H	2.994813	-5.106177	-1.091050
H	2.695383	-6.709653	2.893959
C	4.517070	-6.127807	0.935639
H	4.886393	-6.081441	1.973942
H	4.793339	-7.111050	0.530657
O	5.234826	-5.206098	0.105413
C	5.164307	-1.071438	0.846092
C	5.745055	-1.617711	-0.339580
C	5.147744	0.398230	0.993910
C	4.935424	1.125469	-0.274428
C	5.519552	0.581932	-1.453238
C	6.292903	-0.670274	-1.331688
C	4.596917	-1.953807	1.778913
C	5.731331	-3.005040	-0.534894
C	5.183990	-3.868932	0.427994
C	4.610466	-3.341569	1.594938
C	5.292095	1.241657	-2.677590
C	4.158673	2.296815	-0.353575
C	4.550825	2.419011	-2.748252
C	3.981926	2.957085	-1.579638
C	7.469934	-0.891899	-2.003313
C	5.403525	1.033283	2.183973
S	8.231394	0.314036	-3.087392
C	9.781818	-0.505227	-3.204718
C	9.896398	-1.710227	-2.617758
S	8.485045	-2.352485	-1.790108
S	5.511353	2.814111	2.369252
C	6.239956	2.782013	3.969227
C	6.373549	1.586127	4.570309
S	5.806119	0.167886	3.700578
H	4.084253	-1.553127	2.651687
H	6.097207	-3.443117	-1.460623
H	4.128164	-3.980870	2.327757

H	5.671952	0.805330	-3.599672
H	3.654148	2.654678	0.538330
H	4.376665	2.920983	-3.697965
H	10.566543	-0.004875	-3.765662
H	10.788074	-2.331152	-2.632310
H	6.529392	3.735837	4.402040
H	6.786933	1.427554	5.562708
O	3.249134	4.101879	-1.743436
C	2.694600	4.721845	-0.574619
H	3.500540	4.957298	0.142012
H	1.993183	4.030818	-0.075912
C	1.969839	5.986381	-1.020342
H	2.674692	6.622651	-1.575770
H	1.172710	5.706316	-1.725252
C	-5.345759	4.494746	0.816211
H	-4.529453	4.097739	1.441776
H	-6.200375	4.717997	1.478302
C	-4.868207	5.740982	0.079814
H	-2.766681	7.530614	-0.201212
H	-4.261382	8.434554	-0.417656
H	1.172376	8.640581	-0.909732
H	-0.284533	7.651708	-0.907665
H	-4.045235	5.444025	-0.587645
H	-5.674087	6.124818	-0.562556
C	1.377514	6.764922	0.162941
H	2.189650	7.091609	0.833282
H	0.736846	6.096512	0.762376
C	-4.384618	6.831200	1.048217
C	-3.621519	7.960331	0.343278
C	0.554379	7.983844	-0.276391
C	-0.002966	8.793756	0.914523
H	0.846972	9.175976	1.505322
H	-0.560399	8.114244	1.574581
C	-0.873358	9.940600	0.472498
H	-0.357051	10.736812	-0.072621
C	-3.091472	9.032334	1.321091
H	-2.545124	8.525315	2.130539
H	-3.944558	9.539547	1.797876
C	-2.203737	10.047655	0.642658
H	-2.707245	10.921573	0.220371
H	-5.239777	7.245731	1.606407
H	-3.718653	6.378681	1.802721