Electronic Supplementary Material (ESI) for Chemical Science.

Supporting Information

Cyclic Tris-[5]Helicenes with Möbius Geometries and Möbius Aromaticity.

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Synthetic procedure

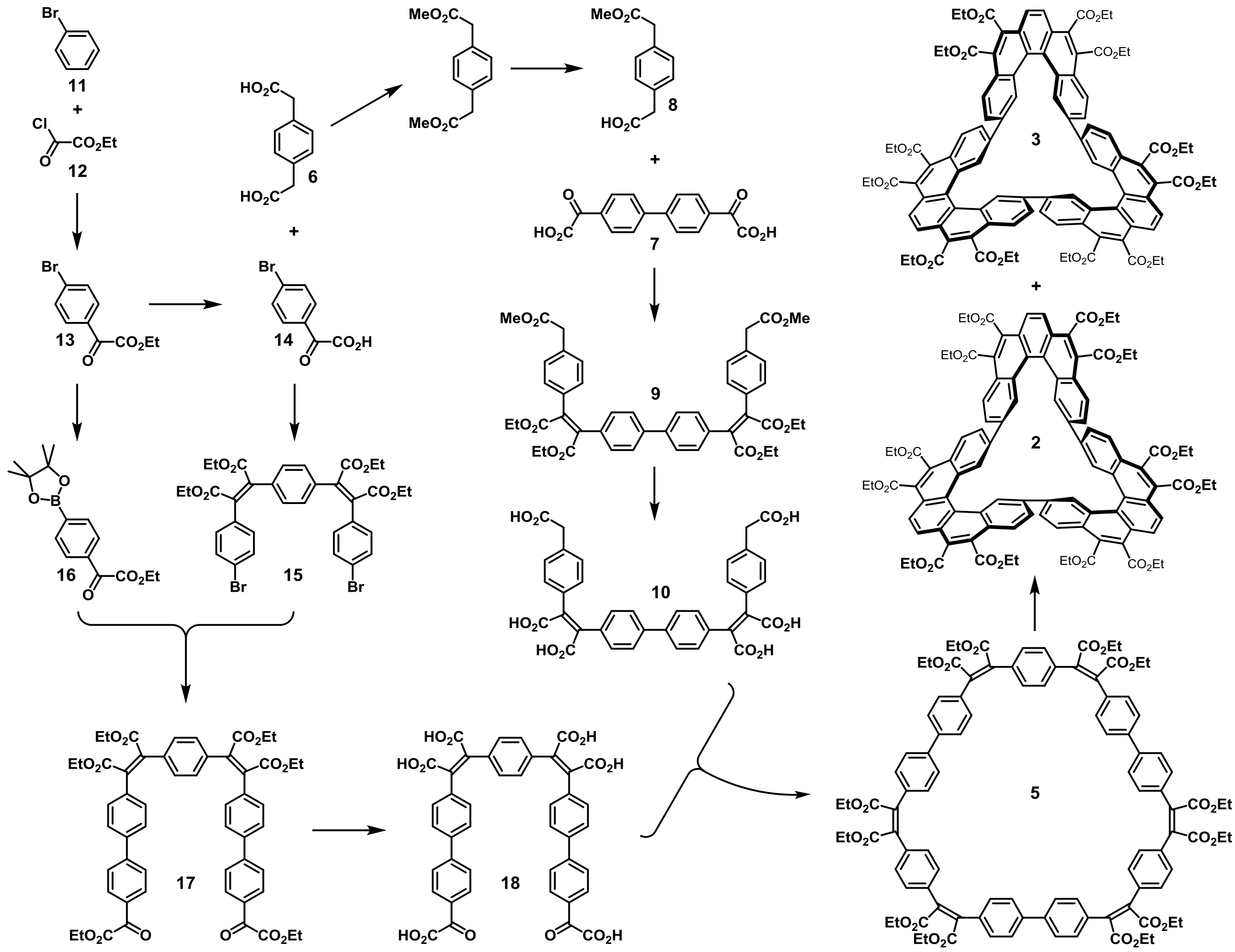


Figure S1: Global strategy for the synthesis of cyclo-tris-helicenes **2** and **3**.

Dimethyl phenylene-1,4-diacetate:[S1]

To a stirred dispersion of phenylene-1,4-diacetic acid **6** (20.0 g, 194.2 g/mol, 0.1 mol) in 500 mL of methanol, thionyl chloride (87.0 mL, 119.0 g/mol, d = 1.64, 1.1 mol) was slowly added with caution through a reflux condenser. The reaction mixture was heated at reflux with stirring for 4 hours. After cooling room temperature, the solution was concentrated and the residue was recrystallized from methanol at room temperature. Yield: 18.9 g (222.2 g/mol, 85.0 mmol, 85 %) of white powder.

^{1}H NMR (400 MHz, CD_2Cl_2): δ = 7.21 (s, 4H), 3.66 (s, 6H), 3.55 (s, 4H).

4-(Methoxycarbonylmethyl)phenylacetic acid **8**:

Dimethyl phenylene-1,4-diacetate (10.0 g, 222.2 g/mol, 45.0 mmol) was dissolved by heating to reflux with stirring in 1,4-dioxane (75 mL). A solution of potassium hydroxide (2.5 g, 56.1 g/mol, 45.0 mmol) in methanol (25 mL) was added through the condenser at reflux. The reflux was maintained for 75 min. After cooling to room temperature, the solution was concentrated and the solid obtained was triturated in DCM. Insoluble materials were filtered off and washed with DCM. The mother liquor was dried with sodium sulfate and the solvent was evaporated to recover dimethyl phenylene-1,4-diacetate **(**3.00 g, 222.2 g/mol, 13.5 mmol, 30%). The solid was then triturated with 1M aqueous HCl, DCM was added and the remaining solid, almost pure phenylene-1,4-diacetic acid **6** (1.60 g, 194.2 g/mol, 8.2 mmol, 18%), was filtered off. The aqueous phase was extracted with DCM. The combined organic phases were dried over sodium sulphate and concentrated to obtain the phenylenediacetic monoester as a white solid. Yield: 4.4 g (208.2 g/mol, 21.3 mmol, 47%).

^{1}H NMR (400 MHz, CD_2Cl_2) : δ = 7.22 (s, 4H), 3.65 (s, 3H), 3.63 (s, 2H), 3.59 (s, 2H).

^{13}C NMR (100 MHz, CD_2Cl_2) : δ = 176.7, 172.4, 133.9, 132.9, 130.12, 130.10, 52.5, 41.1, 40.8.

ESI-HRMS: m/z calcd for $C_{11}H_{12}O_4Na$ $[M+Na]^+$: 231.0627, found 231.0624.

Mp : 90-91 °C

Tetraethyl 4,4’-biphenylylenebis(4-(methoxycarbonylmethyl)phenyl)maleate **9**:

A solution of 4-(methoxycarbonylmethyl)phenylacetic acid **8** (2.80 g, 208.2 g/mol, 13.4 mmol), biphenylylene-4,4'-diglyoxylic acid **7** (2.00 g, 298.3 g/mol, 6.7 mmol), triethylamine (5.6 mL, 101.19 g/mol, 0.726 g/mL, 40.2 mmol), and acetic anhydride (5.7 mL, 102.09g/mol, 1.08 g/mL, 60.3 mmol) in dry THF (120 mL) was heated at reflux with stirring under argon overnight. The mixture was cooled to room temperature and a solution of bromoethane (10 mL, 108.97 g/mol, 1.47 g/mL, 135 mmol), DBU (10 mL, 152.24 g/mol, 1.02 g/mL, 67 mmol) and ethanol (11.7 mL, 46.1 g/mol, 0.789 g/mL, 201 mmol) in THF (20 mL) was added. The mixture was then heated to reflux for 24 hours. After cooling to room temperature, excess 1M aqueous hydrochloric acid was poured into the mixture. After extraction with DCM, the combined organic phases were dried over sodium sulfate and the solvent was evaporated. The crude product was purified by column chromatography on silica with petroleum ether:ethylacetate 3:2 and recrystallization from methanol. Yield: 3.4 g (790.9 g/mol, 4.3 mmol, 65%) of pale yellow solid.

^{1}H NMR (400 MHz, $CDCl_2CDCl_2$): δ = 7.42 (d, 8 Hz, 4H), 7.13 (d, 8 Hz, 4H), 7.12 (d, 8 Hz, 4H), 7.08 (d, 8 Hz, 4H), 4.29 (q, 7 Hz, 8H), 3.67 (s, 6H), 3.57 (s, 4H), 1.32 (t, 7 Hz, 6H), 1.31 (t, 7 Hz, 6H).

^{13}C NMR (100 MHz, $CDCl_2CDCl_2$): δ = 171.7, 167.9, 167.8, 139.4, 138.0, 137.7, 134.0, 133.8, 133.2, 130.2, 129.8, 129.1, 126.4, 61.8, 52.1, 40.6, 14.0.

ESI-HRMS: m/z calcd for $C_{46}H_{46}O_{12}Na$ $[M+Na]^+$: 813.2881, found 813.2885.

Mp : 103-108°C

4,4’-Biphenylylenebis(4-(hydroxycarbonylmethyl)phenyl)maleic acid **10**:

To a suspension of the hexa-ester **9** (2.70 g, 790.9 g/mol, 3.4 mmol) in ethanol (200mL), a solution of potassium hydroxide (21.5 g, 56.11 g/mol, 383 mmol) in water (200 mL) was added. The mixture was heated with stirring at reflux overnight. After cooling to room temperature, excess 2M aqueous hydrochloric acid was added and the mixture was extracted with ethylacetate:THF 1:1. The combined organic phases were dried over sodium sulfate and the solvent was evaporated. The solid obtained was dissolved in THF, salts were removed by filtration and the solvent was evaporated. The obtained yellow solid was used without further purification. Yield: 2.20 g (650.6 g/mol, 3.4 mmol, quantitative yield) of a yellow solid.

^{1}H NMR (400 MHz, CD_3SOCD_3): δ = 7.87 (d, 8 Hz, 4H), 7.58 (d, 8 Hz, 4H), 7.45 (d, 8 Hz, 4H), 7.37 (d, 8 Hz, 4H), 3.64 (s, 4H).

^{13}C NMR (100 MHz, CD_3SOCD_3): δ = 172.2, 165.2, 165.1, 140.7, 138.1, 137.9, 137.4, 130.2, 130.0, 129.4, 127.4, 127.0, 125.39, 40.5

FD-HRMS : m/z calcd for $C_{36}H_{22}O_{10}Na$ [M(dianhydride)]$^+$: 614.1213, found 614.1221

Mp : 286-292°C

4-Bromophenylglyoxylic ester **13**:[S2]

A solution of bromobenzene **11** (10 mL, 157.0 g/mol, 1.5 g/mL, 95.5 mmol) and ethyl oxalyl chloride **12** (15 mL, 136.5 g/mol, 1.22g/mL, 133.8 mmol) in dichloromethane (150 mL) was immersed in a 0°C bath then aluminium chloride (24.2 g, 133.3 g/mol, 181.5 mmol) was added by portion. The final mixture was stirred at 0°C for 30 minutes and at room temperature for 10 minutes. The mixture was poured in 300 mL of an aqueous cold solution of HCl 1M, and stirred for 5 more minutes. The mixture was neutralized by adding 300 mL of an aqueous solution of NaOH 1M. After extraction of the aqueous phase with chloroform, the combined organic phases were washed with water, dried with sodium sulfate and concentrated. The resulting oil was then purified by column chromatography on silica (petroleum ether:ethylacetate 95:5). Yield: 15.47 g (257.1 g/mol, 60.2 mmol, 63%).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.90 (d, 2H, J = 8 Hz), 7.66 (d, 2H, J =8 Hz), 4.45(q, 2H, J = 7 Hz), 1.42 (t, 3H, J = 7 Hz).

4-bromophenylglyoxylic acid **14**:

To a suspension of ethyl 4-bromophenylglyoxylate **13** (3.00 g, 257.1 g/mol, 11.7 mmol) in ethanol (25 mL) was added solution of sodium hydrogen carbonate (10.0 g, 84.0 g/mol, 119.0 mmol) in water (100 mL). The mixture was heated at reflux with stirring for 16 hours, let cool to room temperature, and poured into 1M aqueous hydrochloric acid (200 mL). The white precipitate was filtered off, air-dried and used without further purification. Yield 2.50 g (229.0 g/mol, 10.9 mmol, 93%).[S3]

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.23 (d, 9 Hz, 2H), 7.68 (d, 9 Hz, 2H), 6.04 (broad s, 1H).

Tetraethyl 1,4-phenylenebis(4-bromophenyl)maleate **15**:

Phenylene-1,4-diacetic acid **6** (2.00 g, 194.2 g/mol, 10.3 mmol) and 4-bromophenylglyoxylic acid **14** (5.20 g, 229.0 g/mol, 22.7 mmol) were dissolved in dry THF (250 mL) under argon. Triethylamine (8.5 mL, 0.7 g/mL, 101.2 g/mol, 61.3 mmol) and acetic anhydride (8.5 mL, 1.1 g/mL, 102.9 g/mol, 89.4 mmol) were added and the mixture was heated at reflux with stirring for 16 h. A solution of ethanol (15.2 mL, 0.8 g/mL, 46.1 g/mol, 293 mmol), 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU, 15.4 mL, 1.02 g/mL, 152.2 g/mol, 102.5 mmol) and bromoethane (15.3 mL, 1.47 g/mL, 109.0 g/mol, 205.6 g/mol) in THF (50 mL) was added and the mixture was heated with stirring at reflux for 24 h. The solution was cooled to room temperature, 1M aqueous hydrochloric acid (200 mL) was added, the product was extracted with DCM, the organic phase was dried with sodium sulfate and concentrated, and the residue was recrystallized from ethanol. Yield 6.22 g (728.4 g/mol, 8.5 mmol, 83%) of a yellow powder.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.29 (d, 9 Hz, 4H), 6.92 (s, 4H), 6.89 (d, 9 Hz, 4H), 4.26 (q, 7 Hz, 8H), 1.27 (t, 7 Hz, 6H), 1.26 (t, 7 Hz, 6H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 167.4, 167.3, 138.8, 137.8, 134.6, 133.4, 131.5, 129.7, 122.9, 62.1, 62.0, 14.11, 14.08.

ESI-HRMS: m/z calcd for $C_{34}H_{32}O_8NaBr_2$ $[M+Na]^+$: 749.0356 , found 749.0383

Mp : 149-152°C

Ethyl 4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenylglyoxylate **16**:

4-Bromophenylglyoxylic ester **13** (5.28 g, 257.1 g/mol, 20.5 mmol) was dissolved in 80 mL of anhydrous 1,4-dioxane. [1,1'-Bis(diphenylphosphino)ferrocene]palladium(II) dichloride (0.9 g, 731.7 g/mol, 1.2 mmol), bispinacolatodiboron (6.1 g, 253.94 g/mol, 24 mmol), and potassium acetate (5.9 g, 98.2 g/mol, 60 mmol) were added and the mixture was stirred at 90°C under argon for 2.5 hours. After cooling to room temperature, DCM and water were added, the phases were separated and the aqueous phase was extracted with DCM. The combined organic phases were dried with anhydrous sodium sulfate and concentrated. Column chromatography on silica in 9:1 petroleum ether:acetone yielded the product (5.47 g, 304.2 g/mol, 18.0 mmol, 87 %) as a colourless oil (which solidified on standing) containing traces of pinacol that we could not remove.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.97 (d, 8 Hz, 2H), 7.92 (d, 8 Hz, 2H), 4.45 (q, 7 Hz, 2 H), 1.41 (t, 7 Hz, 3H), 1.35 (s, 12 H).

^{13}C NMR (100 MHz, $CDCl_3$) : δ = 186.8, 163.9, 135.2, 134.4, 129.1, 84.5, 62.5, 25.1, 14.3, 14.2.

ESI-HRMS: m/z calcd for $C_{16}H_{21}BO_5Na$ $[M+Na]^+$: 327.1374, found: 327.1372.

Mp : 36-40 °C

Tetraethyl 1,4-phenylenebis(4'-ethoxyoxalylbiphenyl-4-yl)maleate **17**:

Tetraethyl 1,4-phenylenebis(4-bromophenyl)maleate **15** (2.91 g, 728.4 g/mol, 4.0 mmol), ethyl 4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenylglyoxylate **16** (2.93 g, 304.2 g/mol, 9.7 mmol), tetrakis(triphenylphosphine)palladium (462 mg, 1155.6 g/mol, 0.4 mmol) and potassium phosphate (2.55 g, 212.3 g/mol, 12.0 mmol) were dispersed in toluene (150 mL). The mixture was heated at reflux with stirring under argon for 20 h. After cooling to room temperature, the mixture was diluted with DCM and water, the phases were separated, the aqueous phase was extracted with DCM and the combined organic phases were dried over sodium sulphate and concentrated. The residue was purified by column chromatography on silica in petroleum ether:acetone 4:1 until the product started to elute, then 3:1 to complete its elution. Yield: 1.63 g (923.0 g/mol, 1.8 mmol, 45%) of yellow solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.03 (d, 8 Hz, 4 H), 7.60 (d, 8 Hz, 4 H), 7.40 (d, 8 Hz, 4 H), 7.14 (d, 8 Hz, 4 H), 6.98 (s, 4H), 4.46 (q, 7 Hz, 4H), 4.28 (q, 7 Hz, 4H), 4.25 (q, 7 Hz, 4H), 1.43 (t, 7 Hz, 6 H), 1.29 (t, 7 Hz, 6 H), 1.23 (t, 7 Hz, 6 H).

^{13}C NMR (100 MHz, $CDCl_3$) : δ = 185.8, 167.7, 167.6, 163.8, 146.5, 139.4, 138.44, 138.40, 135.0, 134.8, 131.7, 130.8, 130.6, 129.8, 127.4, 127.1, 62.6, 62.1, 62.0, 14.3, 14.2, 14.1.

ESI-HRMS: m/z calcd for $C_{54}H_{50}O_{14}Na$ $[M+Na]^+$: 945.3092, found 945.3105.

Mp : 162-165°C

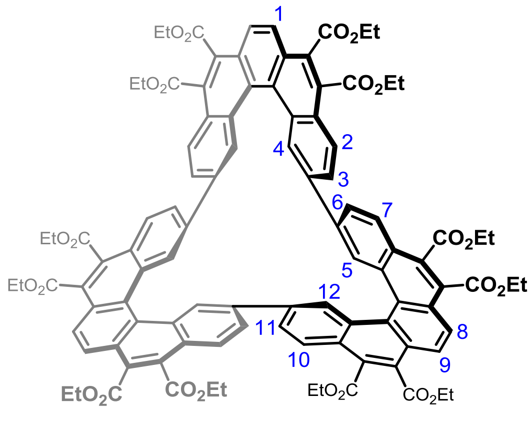
1,4-Phenylenebis(4'-hydroxyoxalylbiphenyl-4-yl)maleic acid **18**:

To a stirred suspension of the hexa-ester **17** (1.30 g, 923.0 g/mol, 1.4 mmol) in ethanol (200 mL) was added a solution of sodium hydrogen carbonate (8.5 g, 84.0 g/mol, 101.2 mmol) in water (200 mL). The mixture was heated at reflux with stirring for 24 h. After cooling to room temperature, the solution was carefully poured

into 1M aqueous hydrochloric acid (150 mL). The mixture was extracted three times with ethyl acetate and the combined organic phases were dried over sodium sulphate and concentrated. The resulting orange solid, which contains besides the hexaacid also some corresponding anhydride, was used without further purification. Yield 1.06 g (754.6 g/mol, 1.4 mmol, quantitative).
^{1}H NMR (400 MHz, CD_3COCD_3): δ = 8.56 (d, 8 Hz, 4H), 8.37 (d, 8 Hz, 4H), 8.36 (d, 8 Hz, 4H), 8.19 (d, 8 Hz, 4H), 8.17 (s, 4H).
^{13}C NMR (100 MHz, CD_3COCD_3) : δ = 187.9, 166.1, 166.0, 165.7, 146.7, 142.7, 140.3, 139.0, 133.1, 131.8, 131.7, 131.5, 131.3, 129.1, 128.8, 128.7, 128.6, 128.2.
ESI-MS: m/z calcd for $[M-H]^-$: found 717.25.
Mp > 300°C

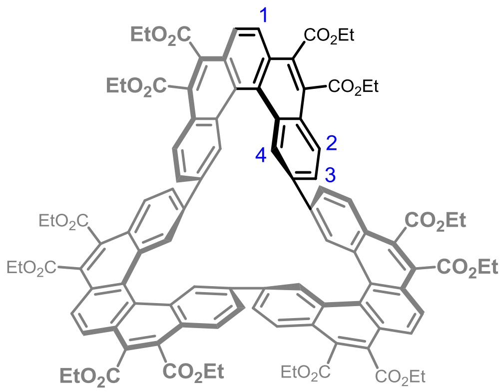
Six-block macrocycle **5** :
Triethylamine (4.4 mL, 101.2 g/mol, 0.726 g/mL, 31.6 mmol) and acetic anhydride (3.7 mL, 102.1 g/mol, 1.08 g./mL, 39.3 mmol) were added to a solution of hexa-acid **18** (570 mg, 754.7 g/mol, 0.76 mmol) and hexa-acid **10** (494 mg, 650.6 g/mol, 0.76 mmol) in dry THF (1L). The mixture was stirred with heating at reflux under argon for 72 hours. Then, ethanol (9.3 mL, 46.1 g/mol, 0.789 g/mL, 159.6 mmol), DBU (10.2 mL, 152.2 g/mol, 1.02 g./mL, 68.4 mmol) and bromoethane (8.5 mL, 109.0 g/mol, 1.47 g/mL, 114 mmol) were added in THF (30 mL) and the solution was stirred with heating at reflux for 24 hours. The solution is concentrated to 200 mL, and after cooling to room temperature, 1M aqueous hydrochloric acid (500 mL) was added. The yellow solution was extracted with DCM, dried over sodium sulphate and concentrated. The crude product was purified column chromatography on silica in DCM:Ethanol 100:1 followed by maceration first in acetone, then in methanol, to precipitate remaining acetone- and methanol-insoluble polymeric side products, and by further column chromatography on silica in DCM:acetone 20:1. Yield: 368 mg (1705.9 g/mol, 0.22 mmol, 29%) of a yellow solid.
^{1}H NMR (400 MHz, CD_3COCD_3): δ = 7.13 (d, 8Hz, 12H), 7.07 (d, 8 Hz, 12H), 6.99 (s, 12H), 4.27 (q, 7 Hz, 12H), 4.23 (q, 7 Hz, 12H), 1.29 (t, 7 Hz, 18H), 1.22 (t, 7 Hz, 18H).
^{13}C NMR (100 MHz, CD_3COCD_3): δ = 168.1, 167.9, 140.8, 139.9, 139.2, 136.0, 135.5, 131.3, 130.5, 127.5, 62.4, 62.3, 14.5, 14.4 ppm.
FD-HRMS: m/z calcd for $C_{102}H_{96}O_{24}$ $[M]^+$: 1704.6292, found: 1704.6338.
Mp : 118-121°C

Cyclo-tris-(5,6,9,10-tetrakis(ethoxycarbonyl)-[5]helicen-2,13-ylene) **2** and **3**:
A solution of macrocycle **5** (109 mg, 1705.9 g/mol, 0.064 mmol) and iodine (131 mg) in ethylacetate (900 mL) was stirred for 2 days at room temperature under air in a Peschl photoreactor with irradiation from a medium-pressure 150 W mercury immersion lamp inside a borosilicate immersion tube in which cooling water circulated. The solvent was evaporated, a 0.4 M aqueous solution of sodium thiosulphate (100mL) was added and the product was extracted with DCM (2×100mL). The organic phases were concentrated and the crude product was purified by column chromatography on silica in DCM:ethanol 100:1, followed by recrystallization from ethanol. The filtrated solid was the less symmetric isomer **2**. Yield: 20 mg (1693.7g/mol, 0.012 mmol, 18%) of yellow solid.
The mother liquor recovered from the crystallization was concentrated and purified by column chromatography on silica in DCM to yield the other, more symmetric, isomer **3**. Yield: 20 mg (1693.7g/mol, 0.012 mmol, 18%) of yellow solid.
2: ^{1}H NMR (400MHz, CD_3COCD_3): δ = 8.95 (broad s, 2H), 8.34 (d, 9 Hz, 2H), 8.26 (d, 9 Hz, 2H), 8.16 (d, 9 Hz, 2H), 8.05-7.99 (m, 6H), 7.89 (d, 9 Hz, 2H), 7.88 (s, 2H), 7.66 (d, 9 Hz, 2H), 7.57 (s, 2H), 6.93 (broad peak, 2H), 4.91 (q, 7 Hz, 4H), 4.72 (q, 7 Hz, 4H), 4.65-4.55 (m, 4H), 4.52-4.39 (m, 8H), 4.38-4.31 (m, 4H), 1.78 (t, 7 Hz, 6H), 1.65 (t, 7 Hz, 6H), 1.51 (t, 7 Hz, 6H), 1.36 (t, 7 Hz, 6H), 1.35 (t, 7 Hz, 6H), 1.27 (t, 7 Hz, 6H) ppm.
^{13}C NMR (100MHz, CD_3COCD_3): 169.0, 168.7, 168.4, 168.2, 168.0, 167.8, 139.4, 139.3, 133.7, 133.4, 132.9, 132.0, 131.6, 131.3, 130.82, 130.77, 130.7, 130.6, 130.4, 130.1, 129.8, 129.5, 129.21, 129.17, 128.9, 128.7, 128.6, 128.3, 127.93, 127.87, 127.3, 126.8, 126.2, 126.0, 125.9, 124.5, 63.8, 63.6, 63.5, 63.4, 63.13, 63.10, 15.4, 15.15, 15.07, 14.9, 14.7 ppm.
Mp : 212-215°C



C_2-symmetric

Concentrated tube for 2D NMR (COSY and NOESY) and assignment of aromatic protons:
^{1}H NMR (400MHz, CD_3COCD_3): δ = 9.26 (broad s, 2H, H12), 8.39 (d, 9 Hz, 2H, H8 or H9), 8.36 (d, 9 Hz, 2H, H7), 8.26 (d, 9 Hz, 2H, H10), 8.19 (d, 9 Hz, 2H, H8 or H9), 8.07 (dd, 9 Hz, 2Hz, 2H, H3), 8.04 (s, 2H, H1), 8.00 (d, 2 Hz, 2H, H5), 7.94 (d, 9 Hz, 2H, H2), 7.73 (dd, 9 Hz, 2 Hz, 2H, H6), 7.66 (d, 2 Hz, 2H, H4), 7.35 (broad doublet, 9 Hz, 2H, H11), 4.881 (q, 7 Hz, 4H), 4.73 (q, 7 Hz, 4H), 4.59-4.45 (m, 12H), 4.39-4.33 (m, 4H), 1.74 (t, 7 Hz, 6H), 1.66 (t, 7 Hz, 6H), 1.47 (t, 7 Hz, 6H), 1.40 (t, 7 Hz, 6H), 1.38 (t, 7 Hz, 6H), 1.29 (t, 7 Hz, 6H) ppm.

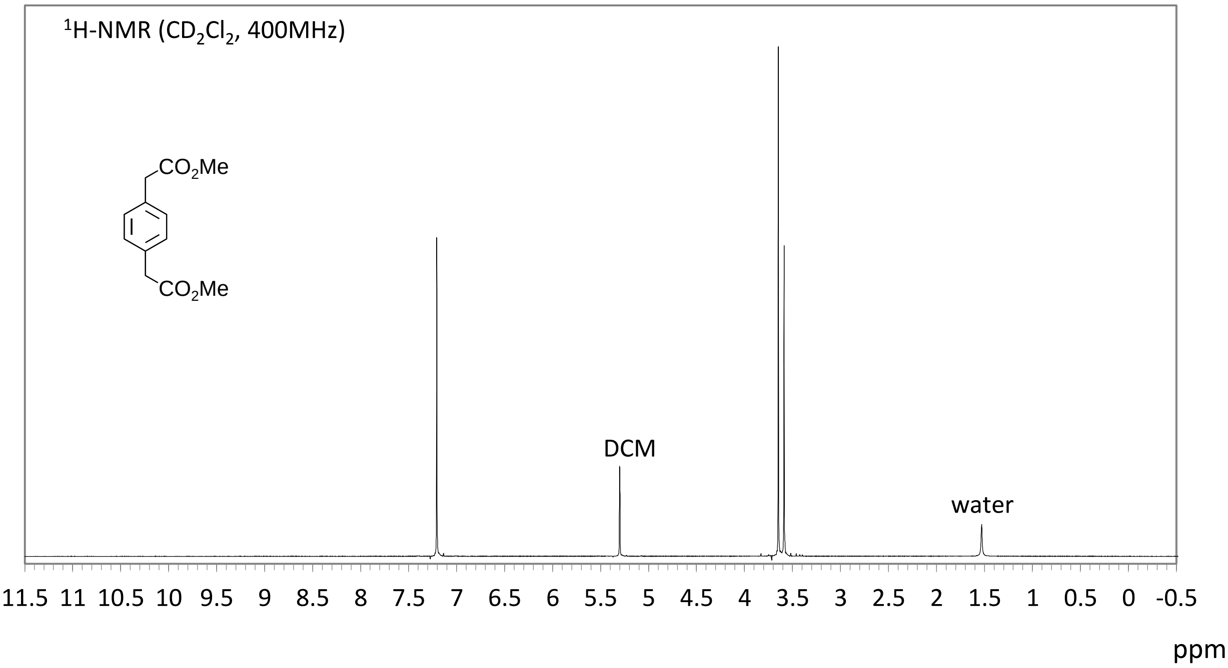


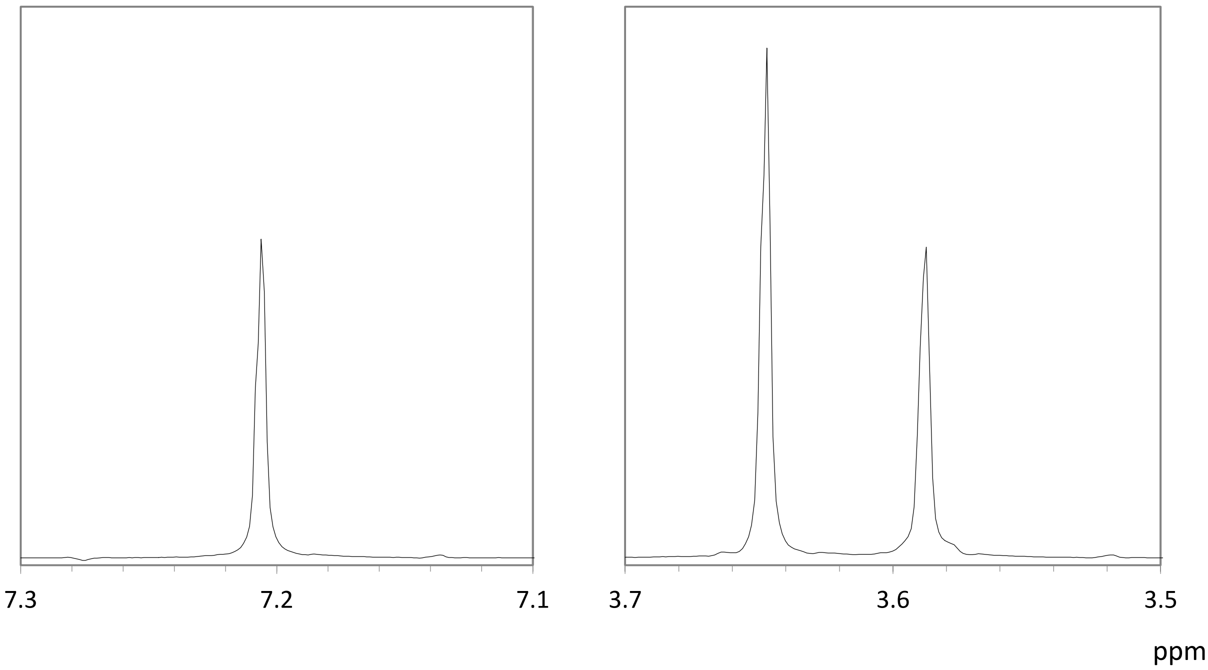
D_3-symmetric

3: ^{1}H NMR (400 MHz, CD_3COCD_3): 8.88 (d, 2 Hz, 6H, H4), 8.27 (s, 6H, H1), 8.09 (d, 9 Hz, 6H, H2), 7.51 (dd, 9 Hz, 2 Hz, 6H, H3), 4.59-4.45 (m, 12H), 4.53 (q, 7 Hz, 12H), 1.44 (t, 7 Hz, 18H), 1.43 (t, 7 Hz, 18H) ppm.
^{13}C NMR (100 MHz, CD_3COCD_3): 168.3, 168.2, 139.5, 134.6, 132.0, 130.5, 130.1, 129.6, 129.4, 128.5, 128.2, 127.9, 126.4, 63.4, 63.3, 15.0, 14.9 ppm.
FD-HRMS: m/z calcd for $C_{102}H_{84}O_{24}$ $[M]^+$: 1692.5353, found: 1692.5288.
Mp : 135-140°C

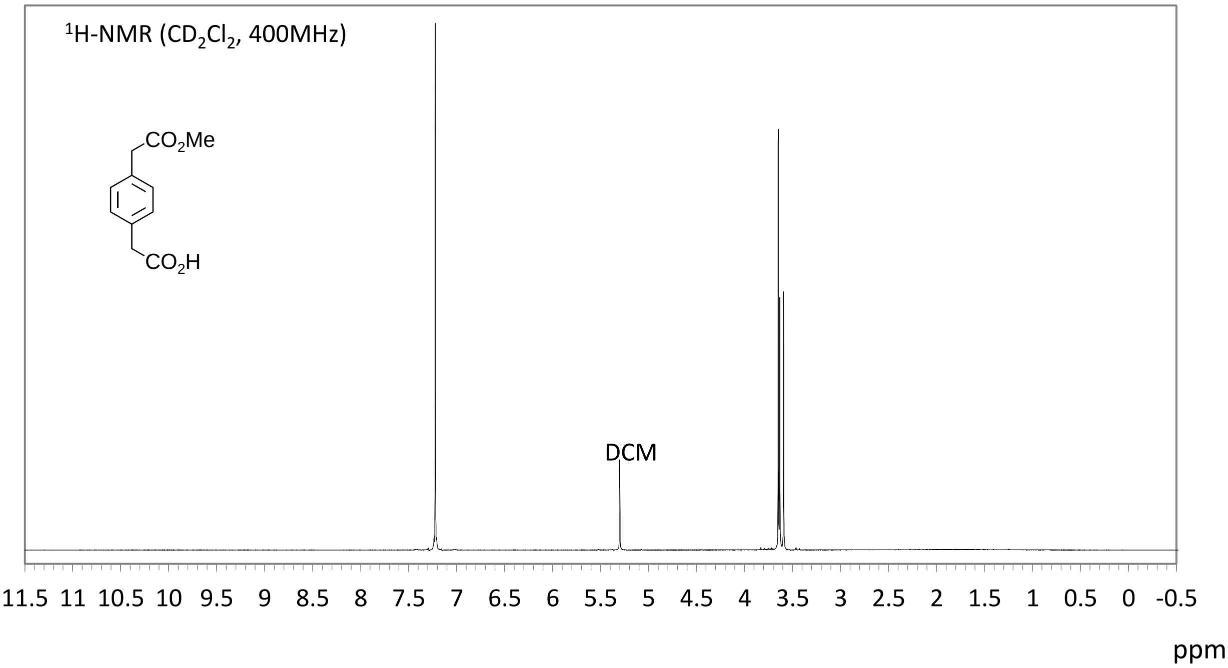
NMR spectra

Dimethyl phénylène-1,4-diacetate[S1]

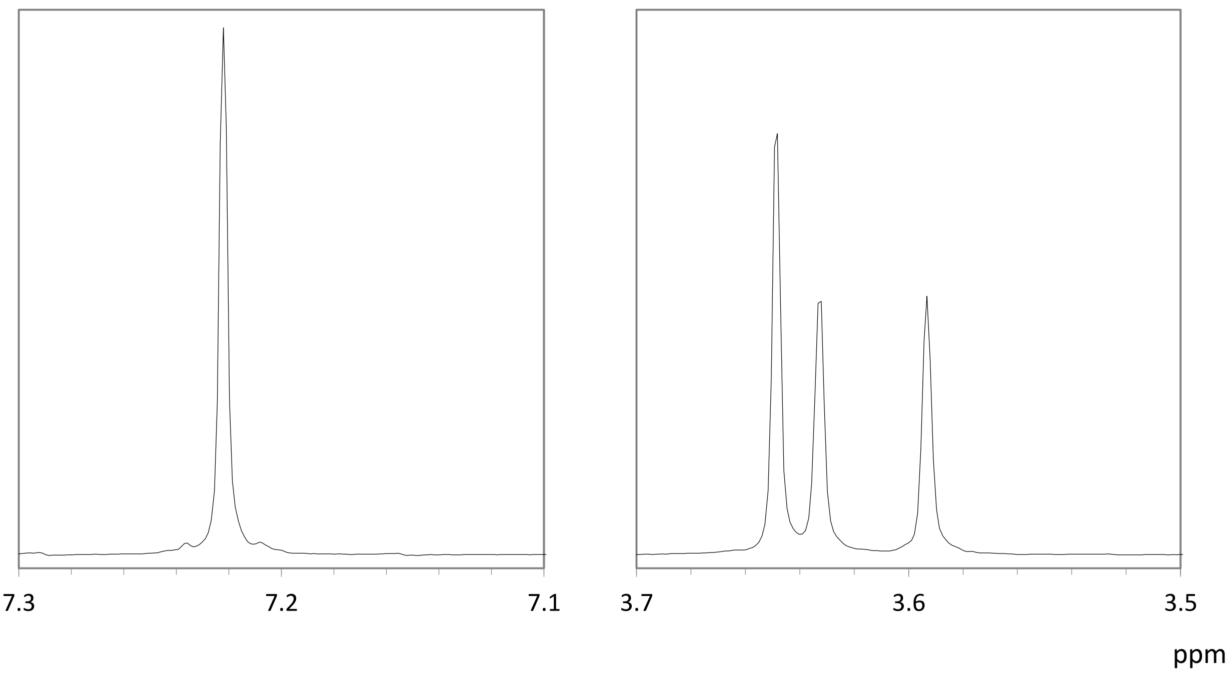




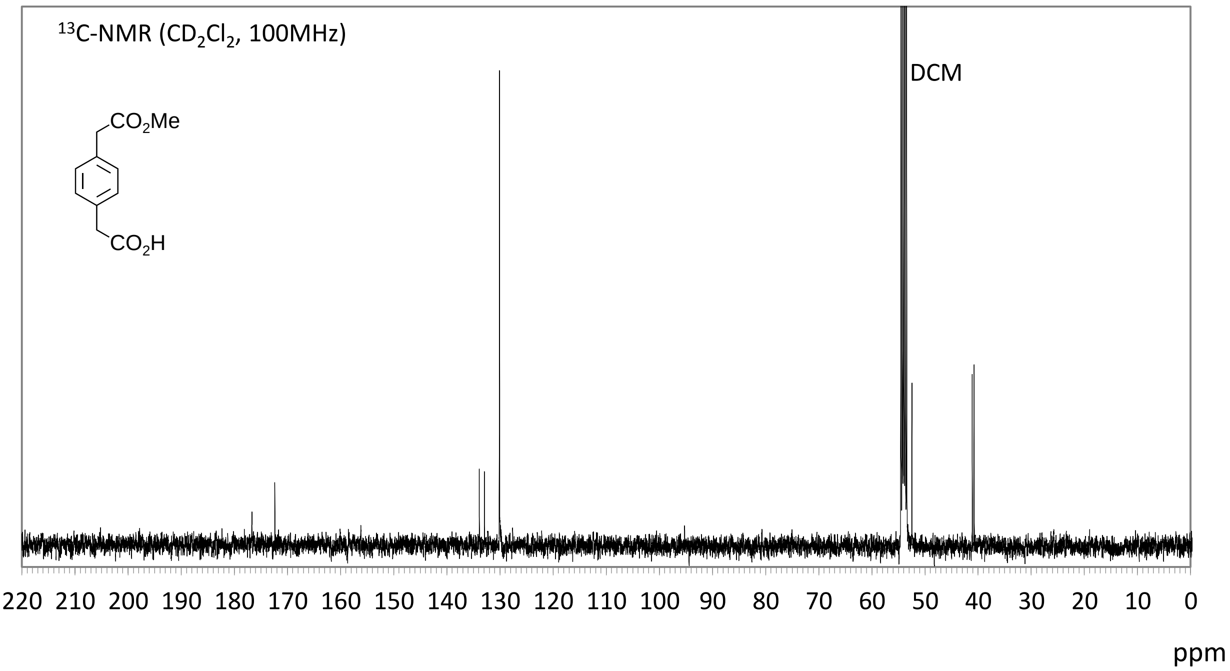
Compound **8**



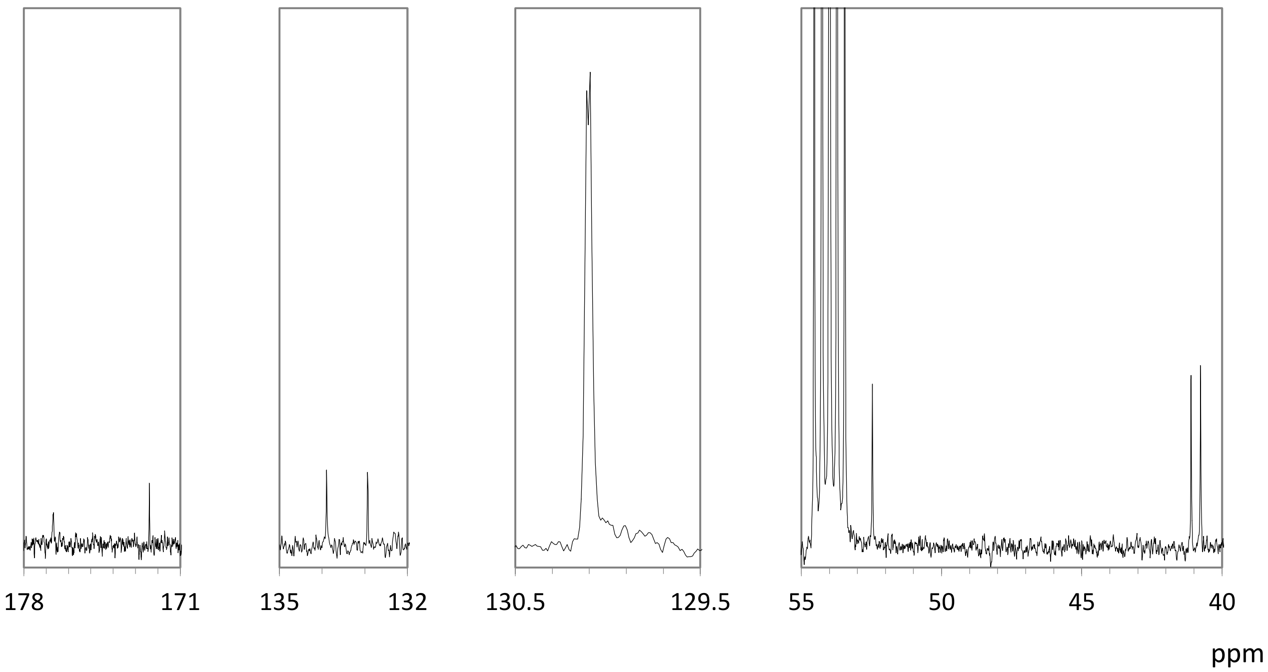
^{1}H-NMR (CD_2Cl_2, 400MHz)
CO2Me
CO2H
DCM
11.5 11 10.5 10 9.5 9 8.5 8 7.5 7 6.5 6 5.5 5 4.5 4 3.5 3 2.5 2 1.5 1 0.5 0 -0.5
ppm



7.3
7.2
7.1
3.7
3.6
3.5
ppm

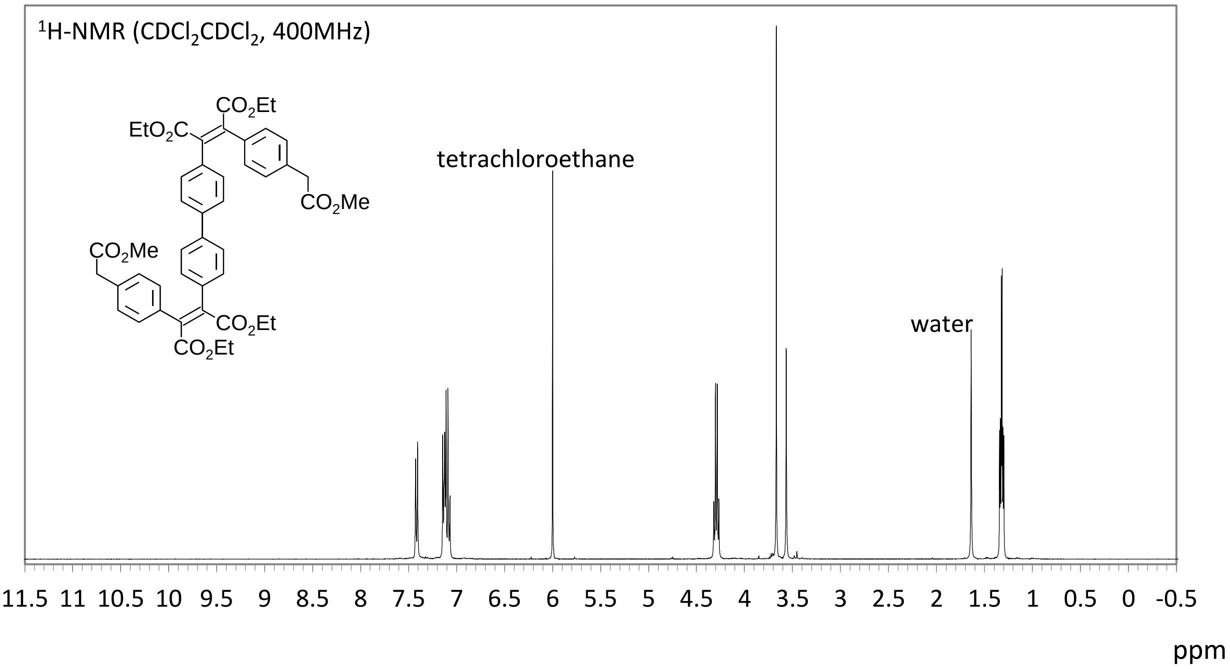


^{13}C-NMR (CD_2Cl_2, 100MHz)
CO2Me
CO2H
DCM
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm

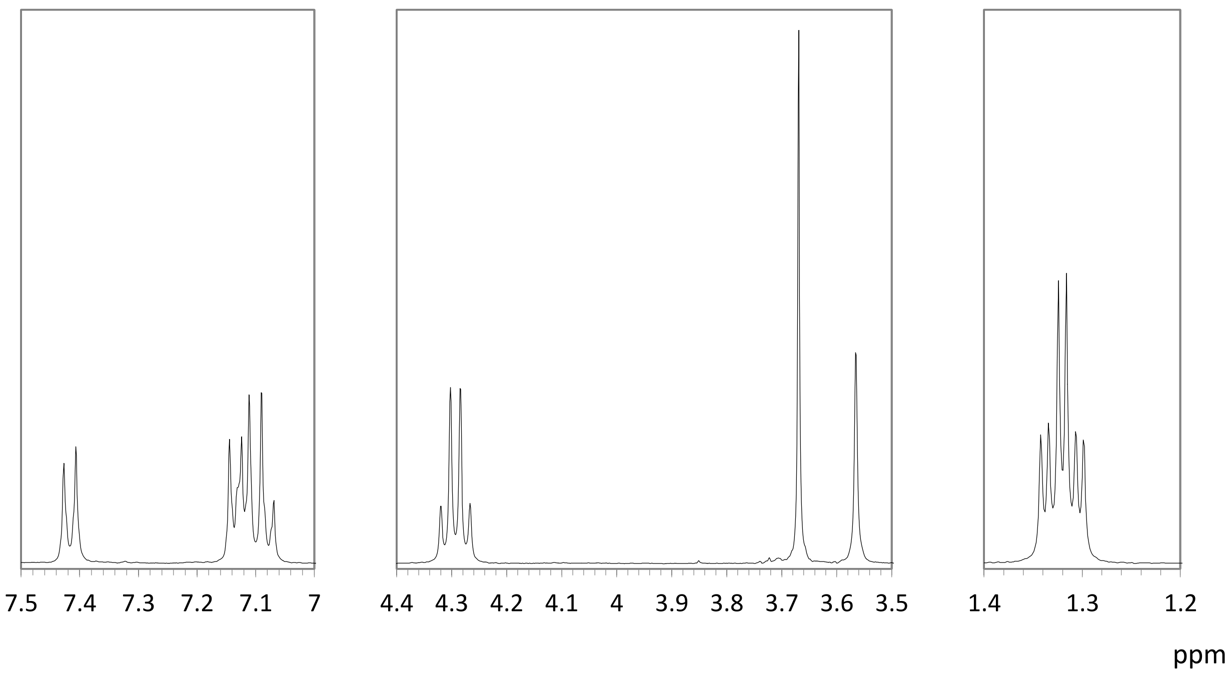


178
171
135
132
130.5
129.5
55
50
45
40
ppm

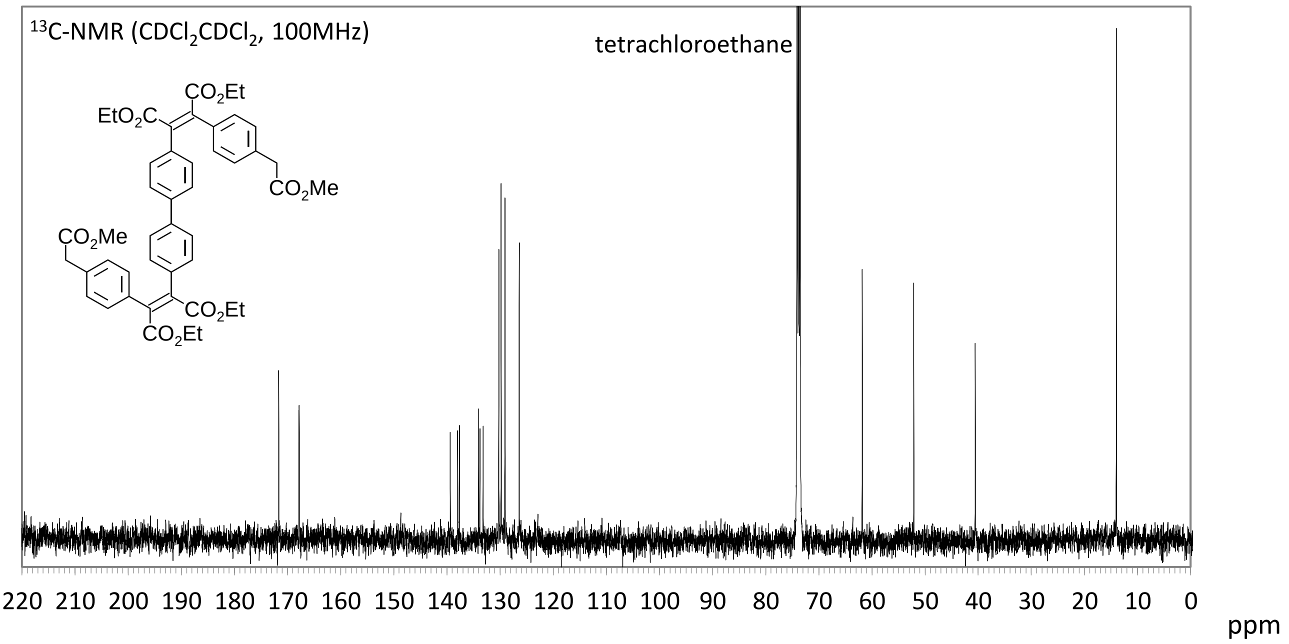
Compound **9**

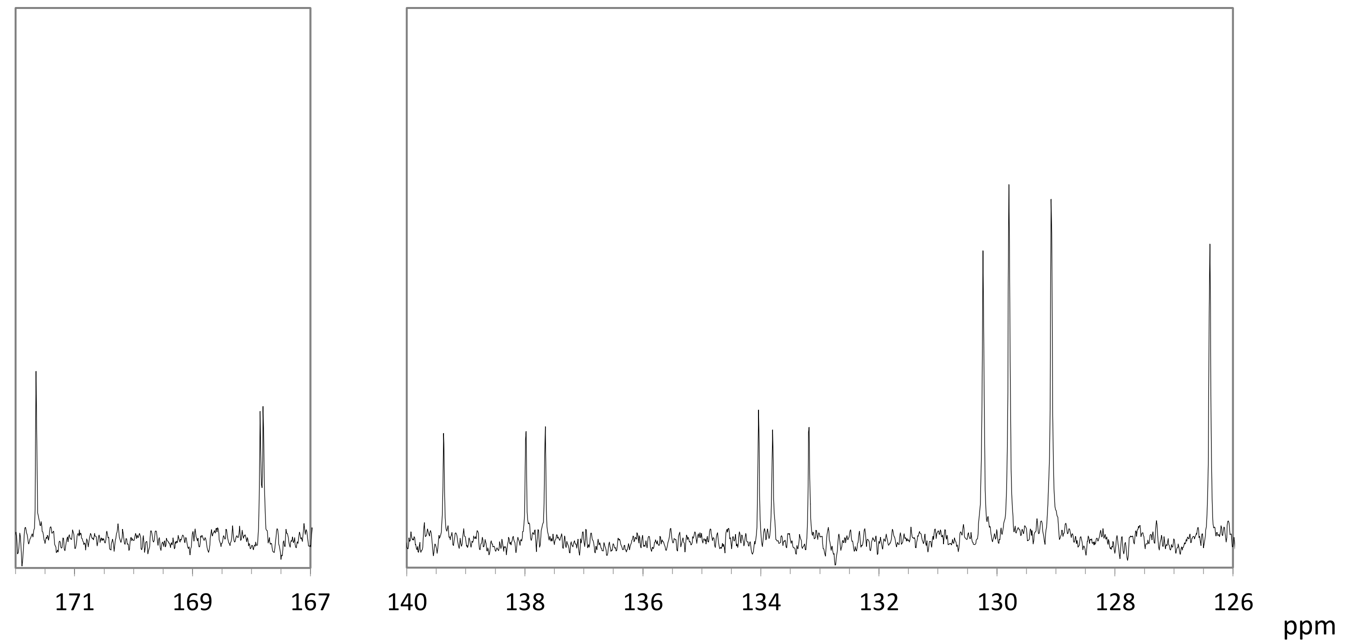


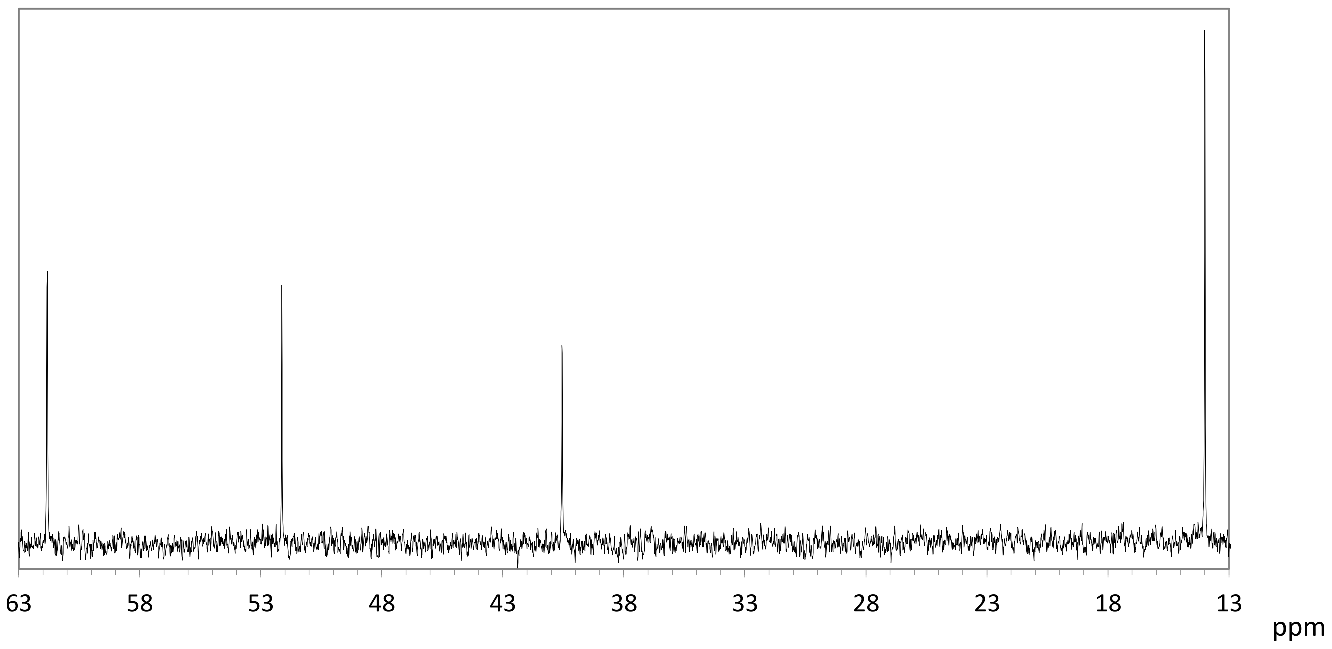
¹H-NMR (CDCl2CDCl2, 400MHz)
CO2Et
EtO2C
CO2Me
CO2Me
CO2Et
CO2Et
tetrachloroethane
water
11.5 11 10.5 10 9.5 9 8.5 8 7.5 7 6.5 6 5.5 5 4.5 4 3.5 3 2.5 2 1.5 1 0.5 0 -0.5
ppm



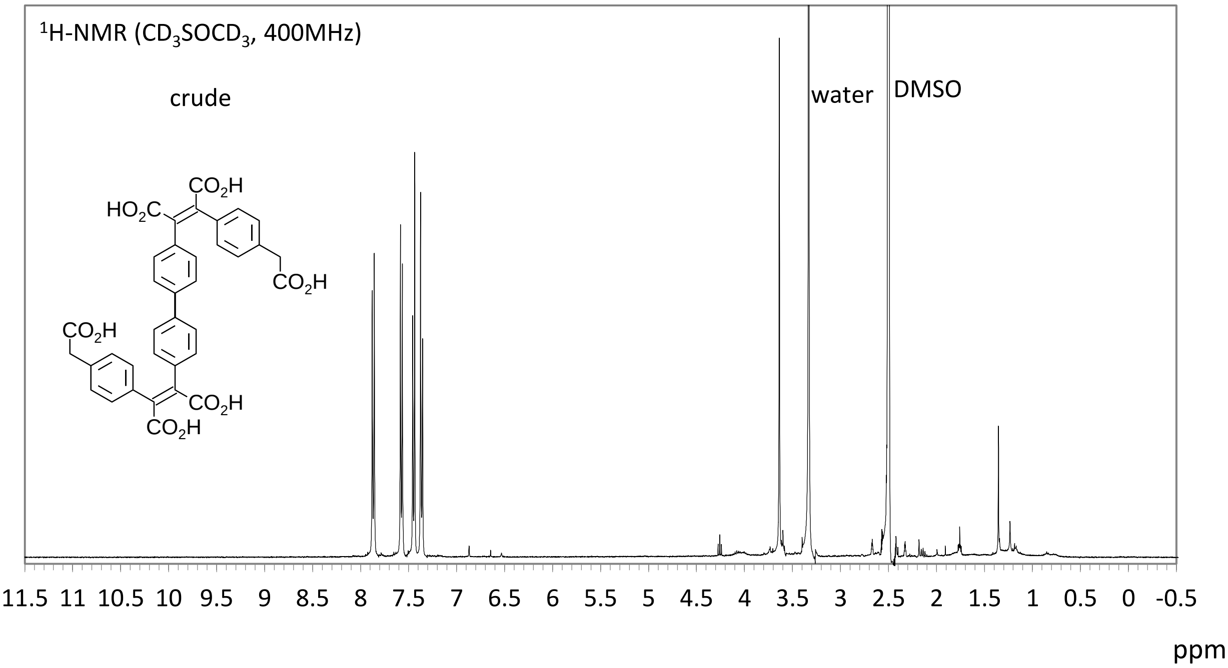
7.5 7.4 7.3 7.2 7.1 7
4.4 4.3 4.2 4.1 4 3.9 3.8 3.7 3.6 3.5
1.4 1.3 1.2
ppm


13C-NMR (CDCl2CDCl2, 100MHz)
tetrachloroethane
CO2Et
EtO2C
CO2Me
CO2Me
CO2Et
CO2Et
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm

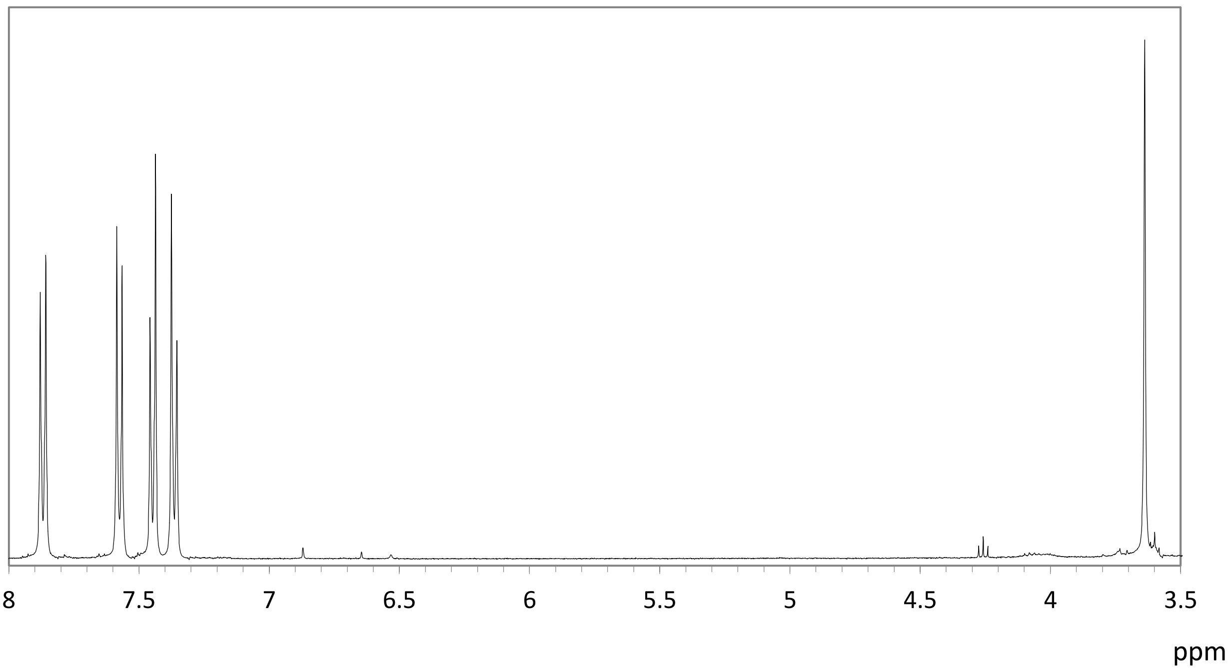

171 169 167
140 138 136 134 132 130 128 126
ppm


63 58 53 48 43 38 33 28 23 18 13
ppm

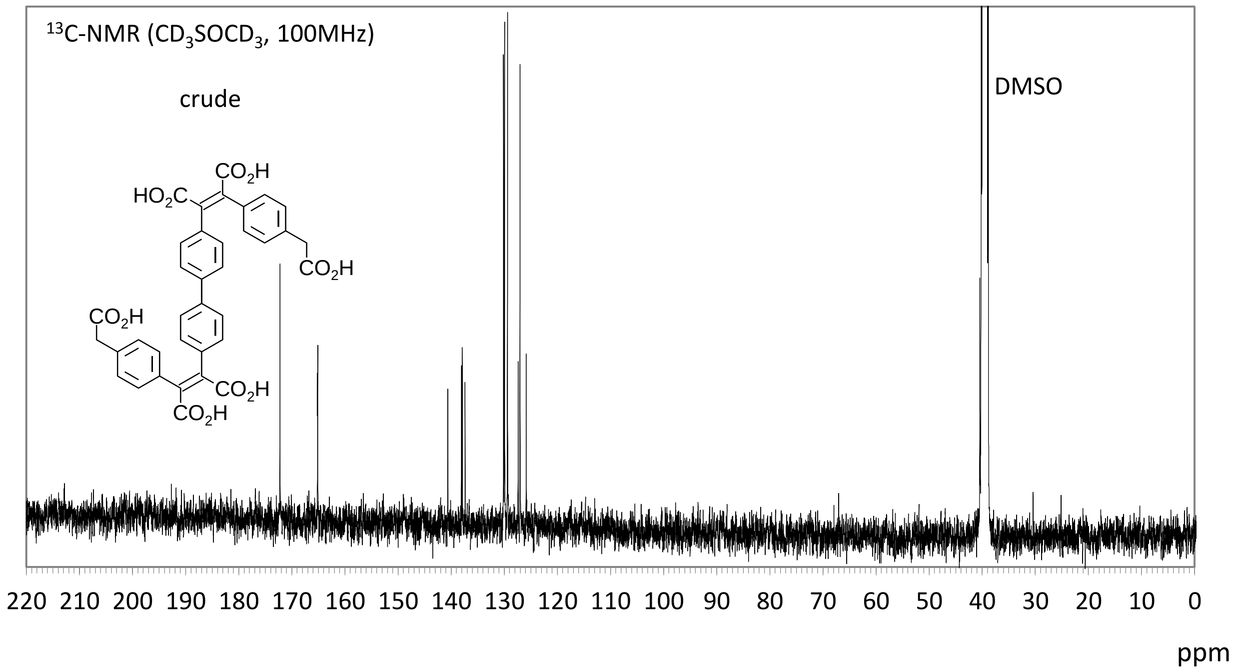
Compound **10**



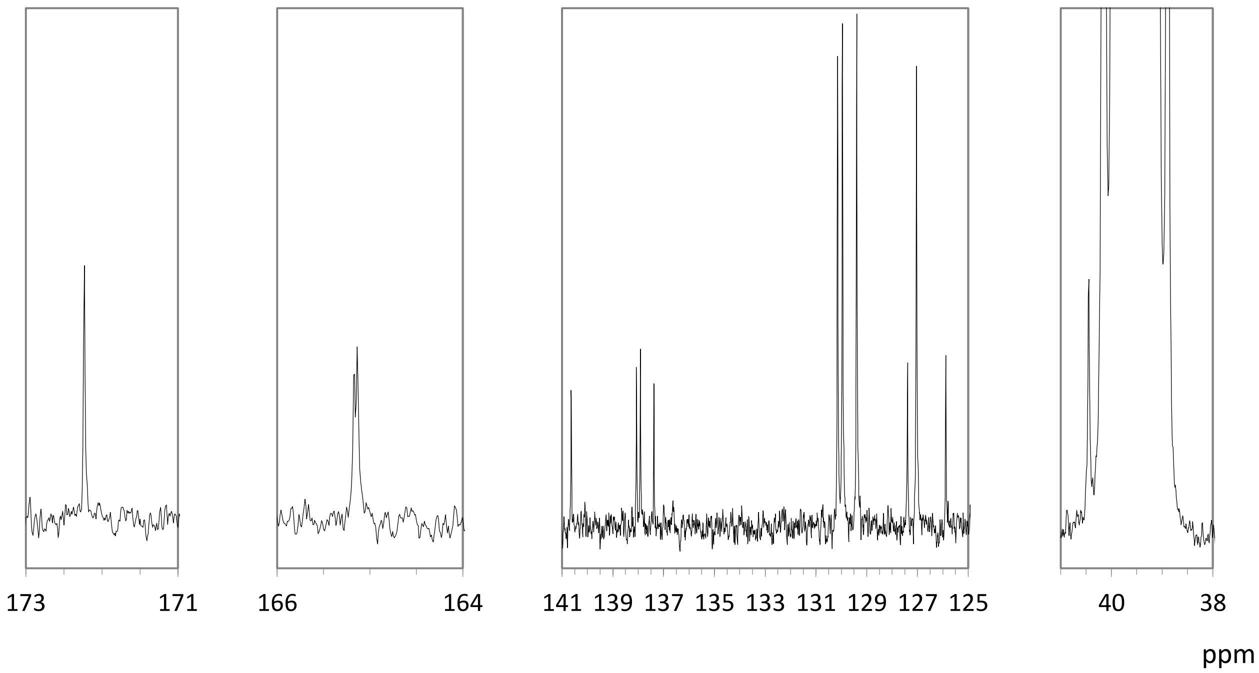
1H-NMR (CD3SOCD3, 400MHz)
crude
HO2C
CO2H
CO2H
CO2H
CO2H
CO2H
water
DMSO
11.5 11 10.5 10 9.5 9 8.5 8 7.5 7 6.5 6 5.5 5 4.5 4 3.5 3 2.5 2 1.5 1 0.5 0 -0.5
ppm



8 7.5 7 6.5 6 5.5 5 4.5 4 3.5
ppm

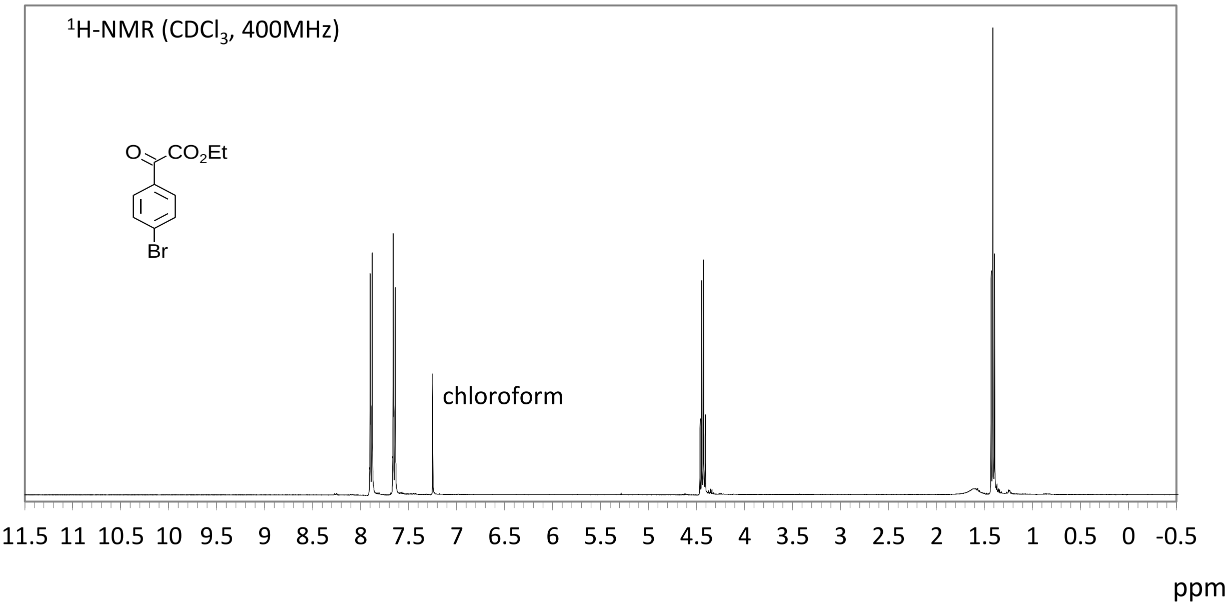


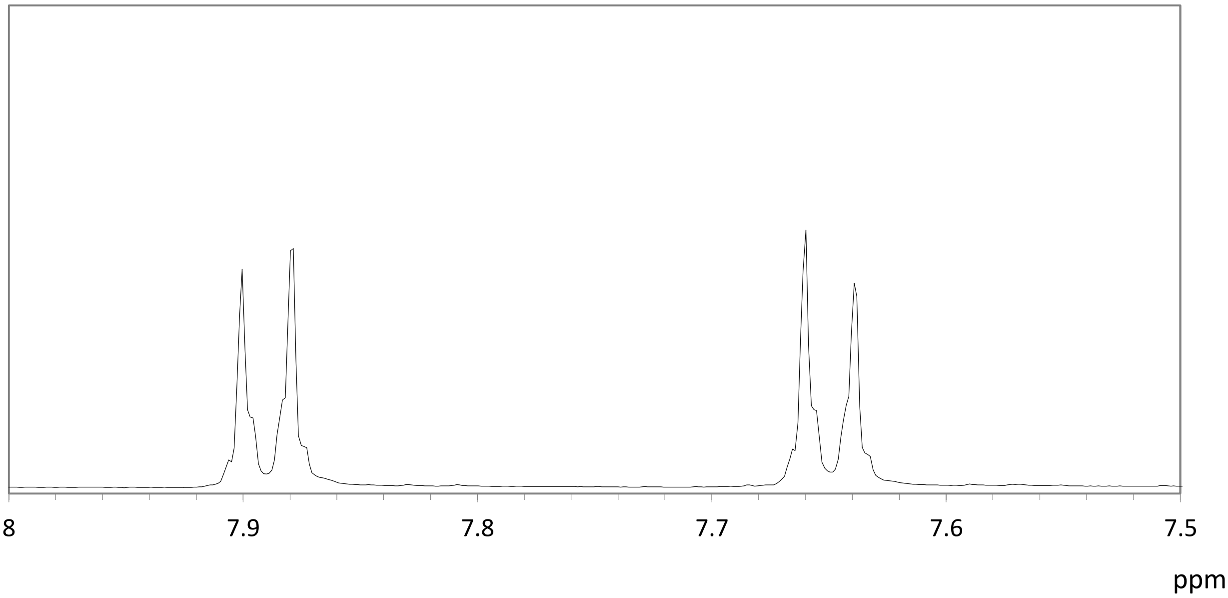
^{13}C-NMR (CD_3SOCD_3, 100MHz)
crude
DMSO
HO_2C
CO_2H
CO_2H
CO_2H
CO_2H
CO_2H
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm

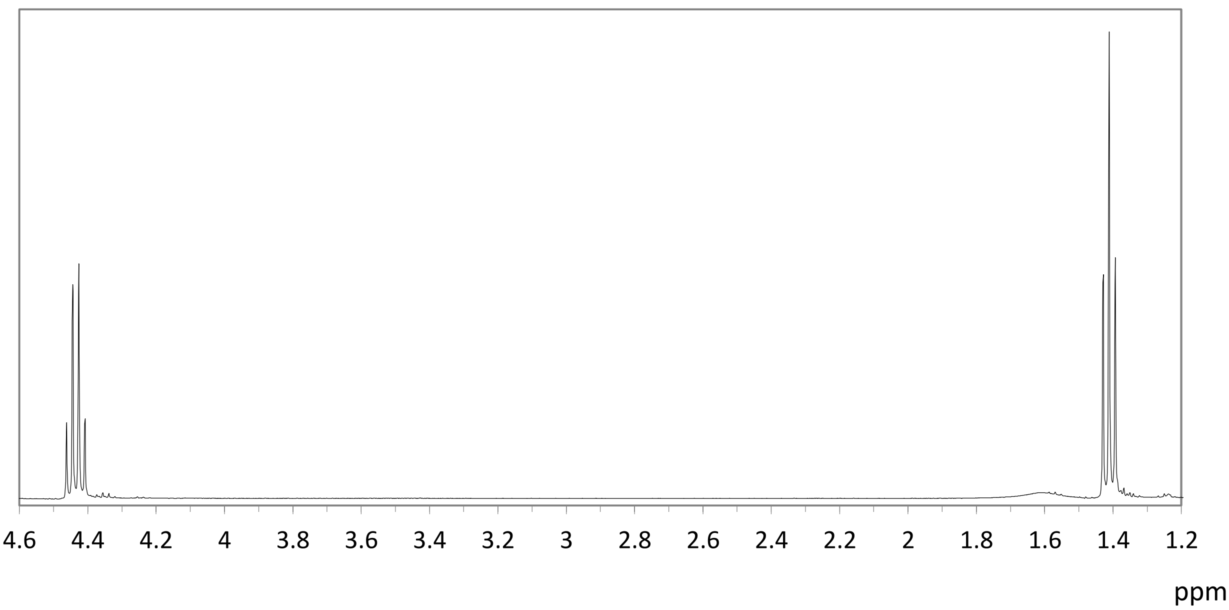


173 171
166 164
141 139 137 135 133 131 129 127 125
40 38
ppm

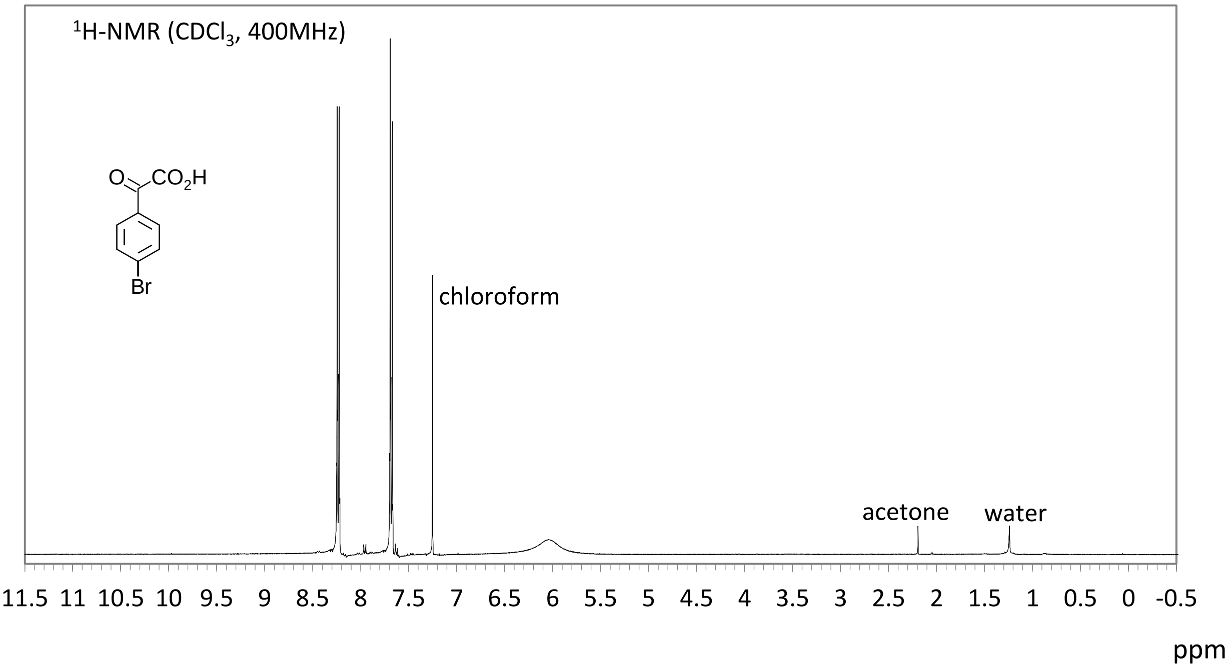
Compound **13**[S2]

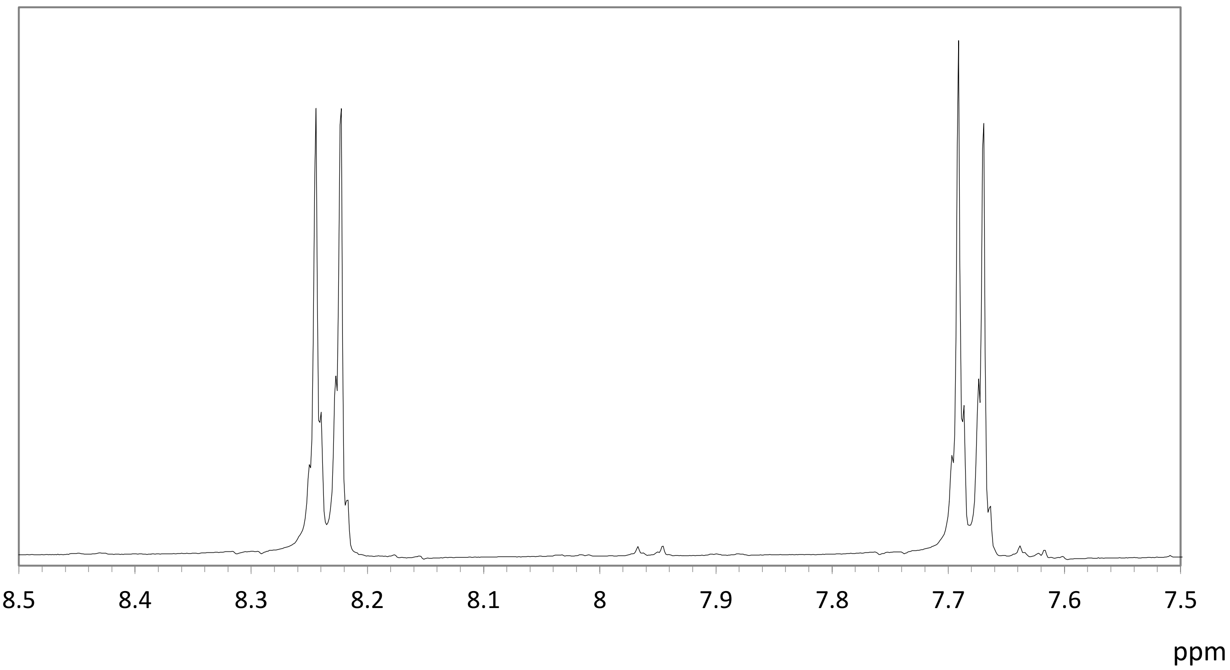




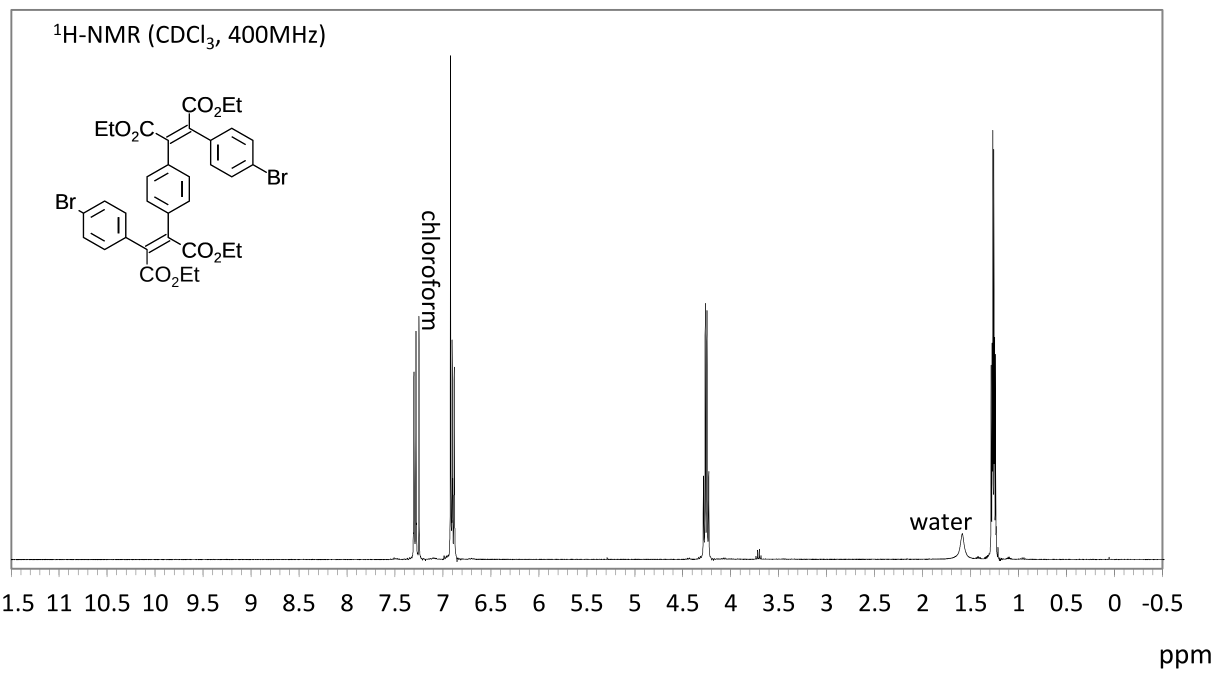


Compound **14**[S3]

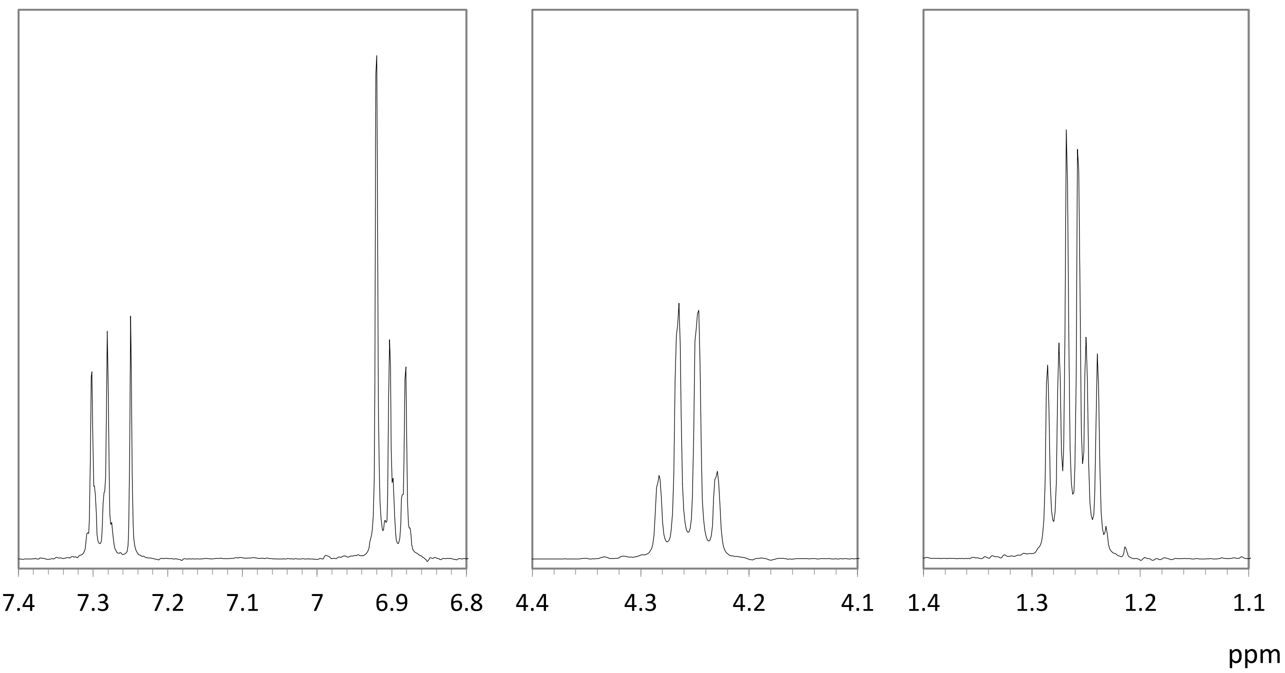




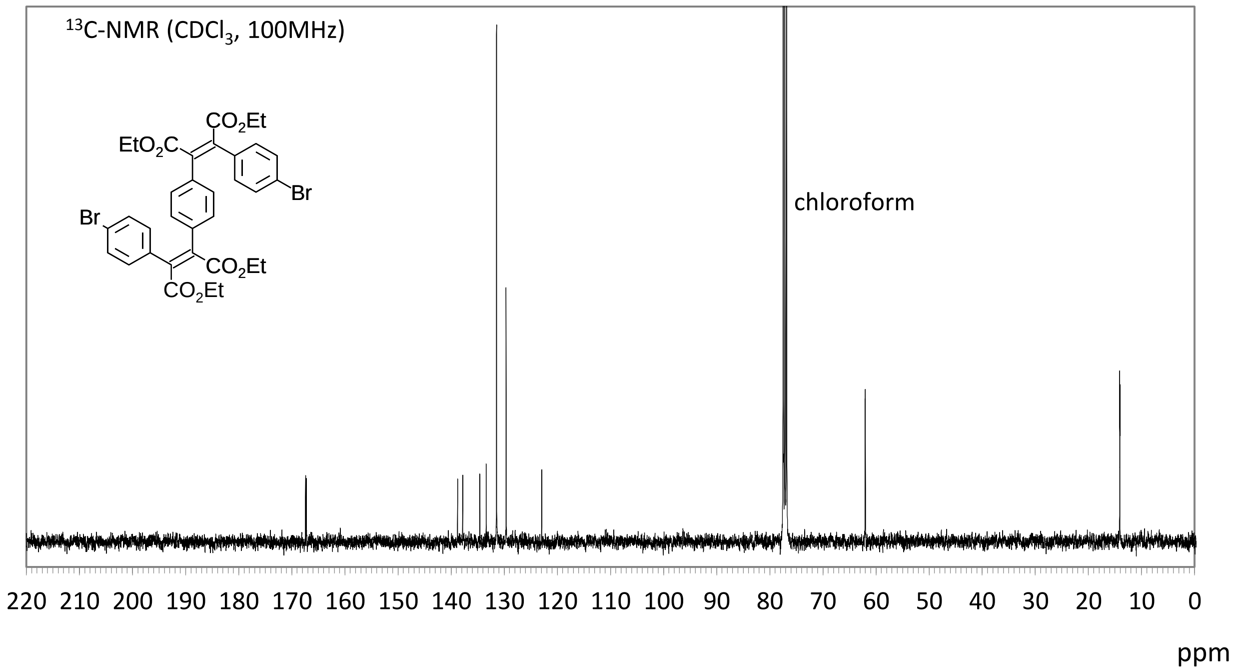
Compound **15**



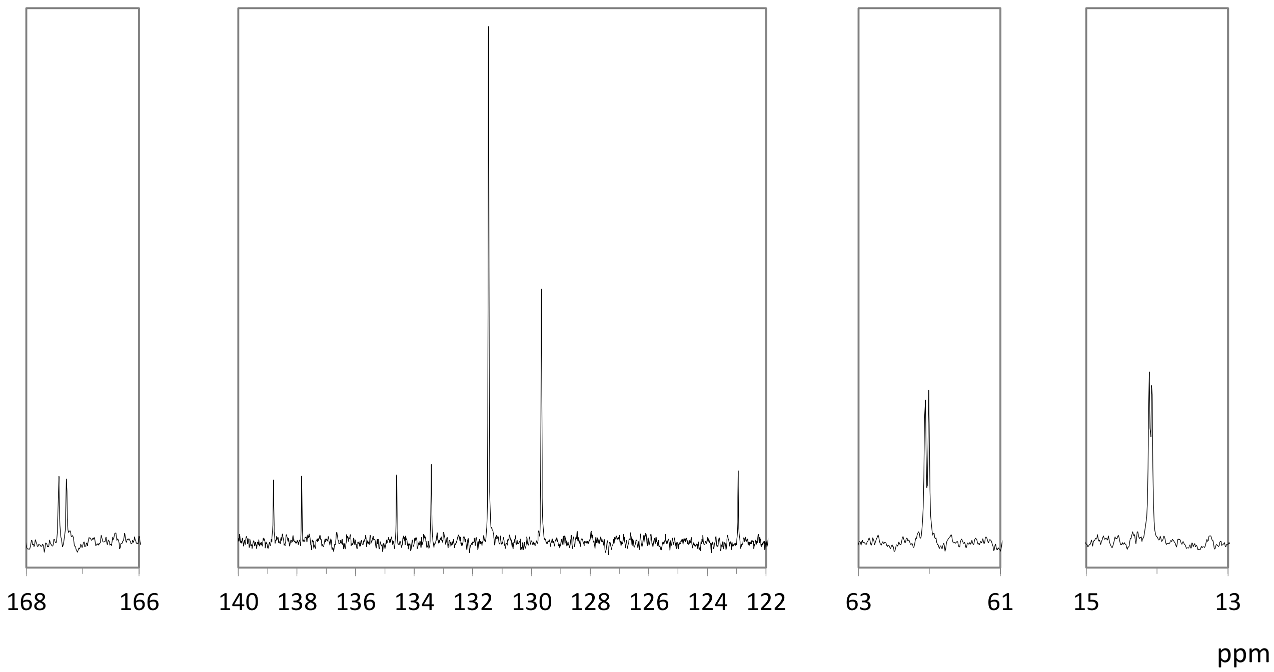
^{1}H-NMR ($CDCl_3$, 400MHz)
CO_2Et
EtO_2C
Br
Br
CO_2Et
CO_2Et
chloroform
water
11.5 11 10.5 10 9.5 9 8.5 8 7.5 7 6.5 6 5.5 5 4.5 4 3.5 3 2.5 2 1.5 1 0.5 0 -0.5
ppm



7.4 7.3 7.2 7.1 7 6.9 6.8
4.4 4.3 4.2 4.1
1.4 1.3 1.2 1.1
ppm

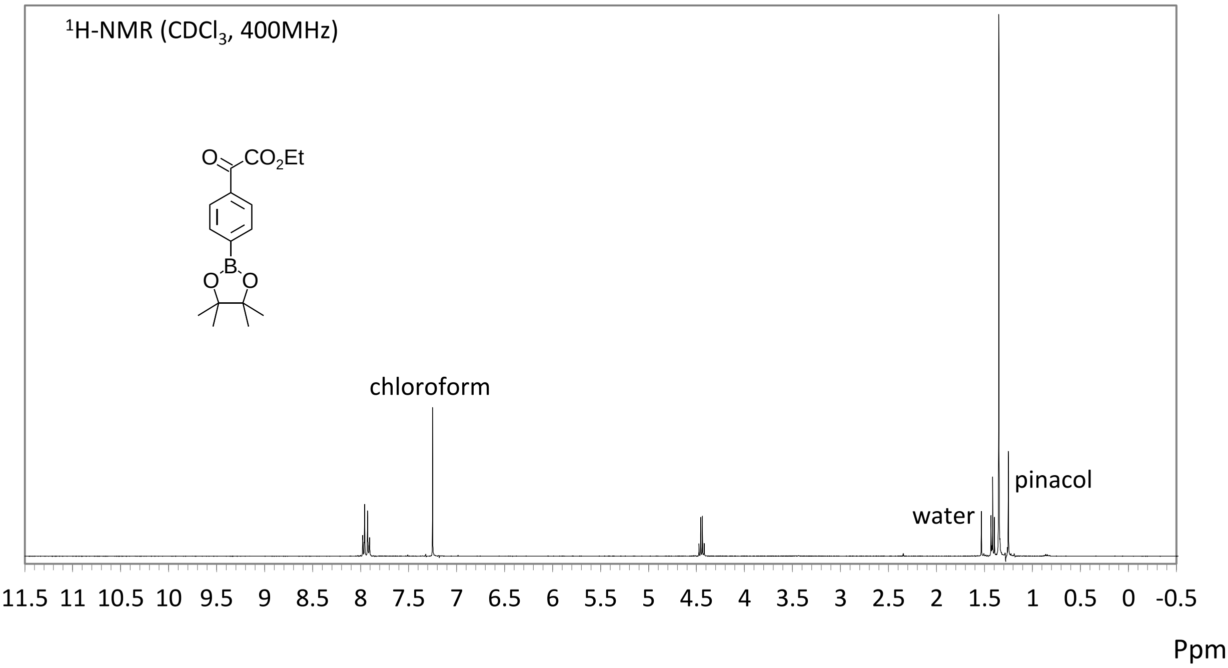


^{13}C-NMR (CDCl$_3$, 100MHz)
EtO$_2$C
CO$_2$Et
Br
Br
CO$_2$Et
CO$_2$Et
chloroform
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm

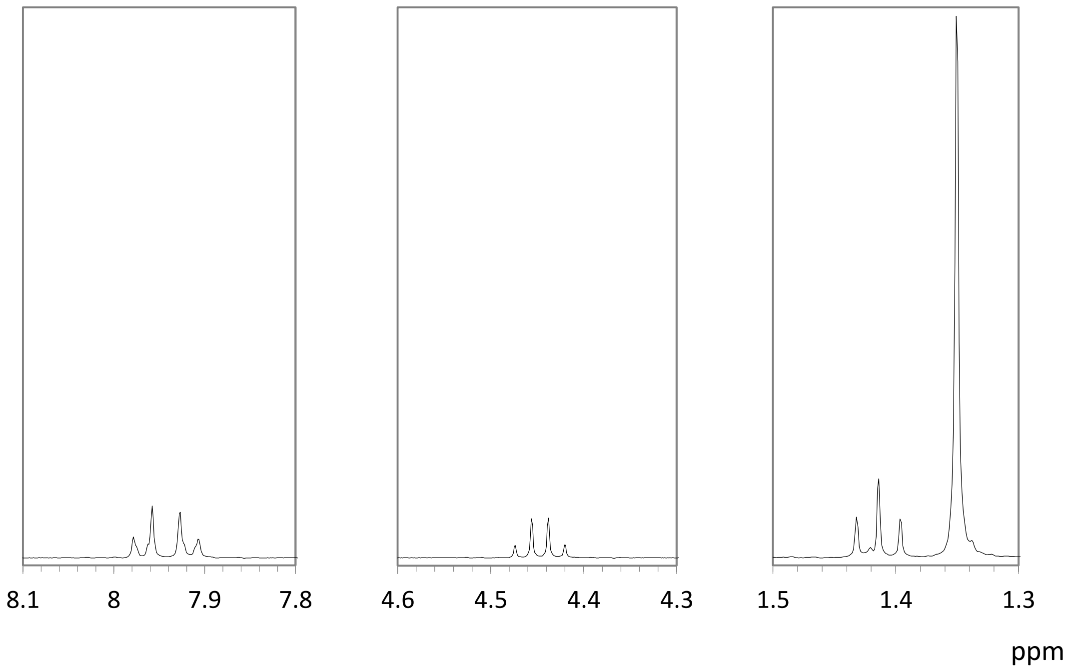


168 166
140 138 136 134 132 130 128 126 124 122
63 61
15 13
ppm

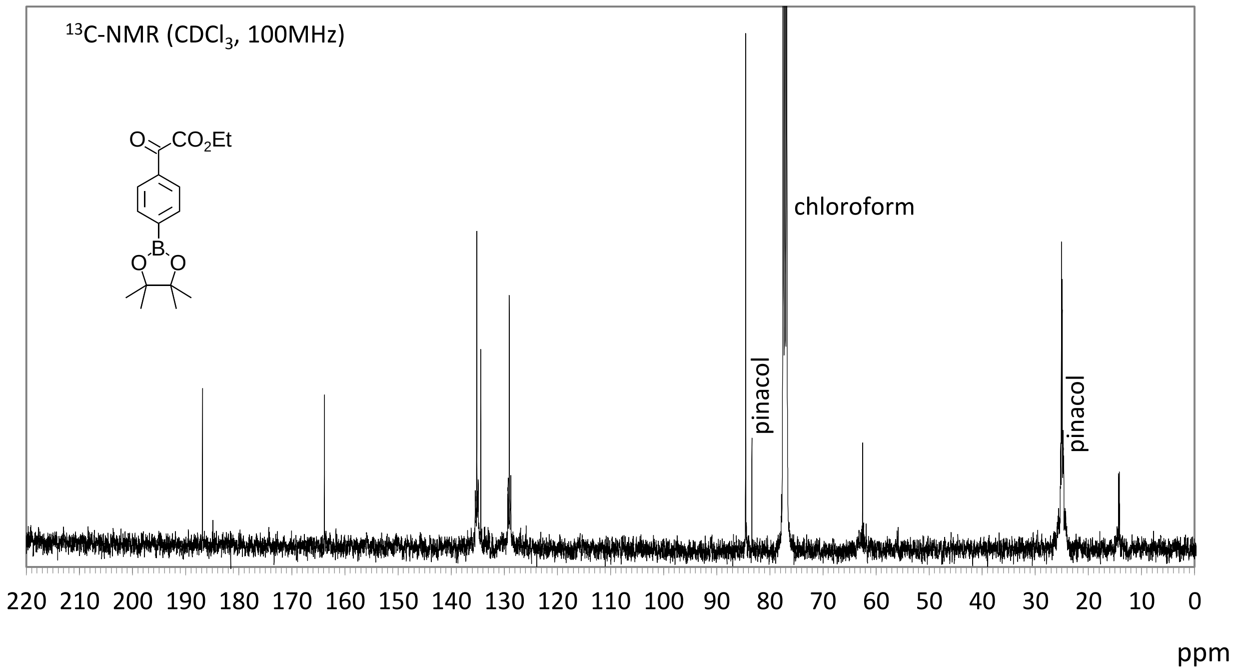
Compound **16**



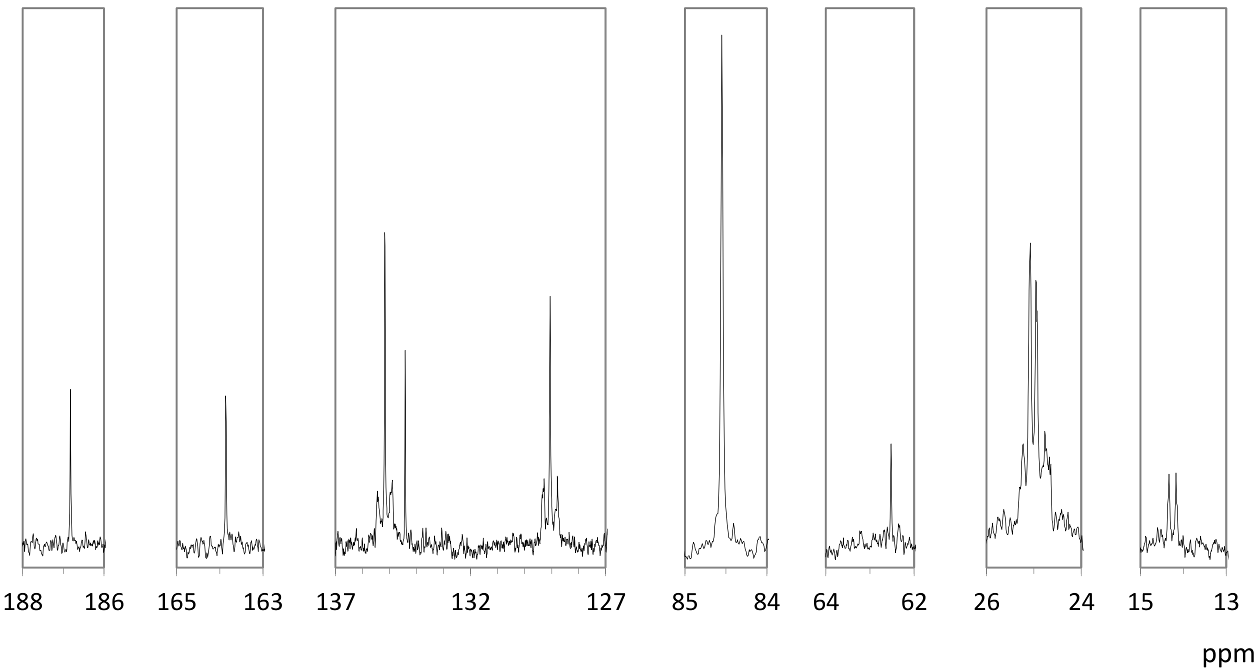
1H-NMR (CDCl3, 400MHz)
O
CO2Et
B
O
O
chloroform
water
pinacol
11.5 11 10.5 10 9.5 9 8.5 8 7.5 7 6.5 6 5.5 5 4.5 4 3.5 3 2.5 2 1.5 1 0.5 0 -0.5
Ppm



8.1 8 7.9 7.8
4.6 4.5 4.4 4.3
1.5 1.4 1.3
ppm

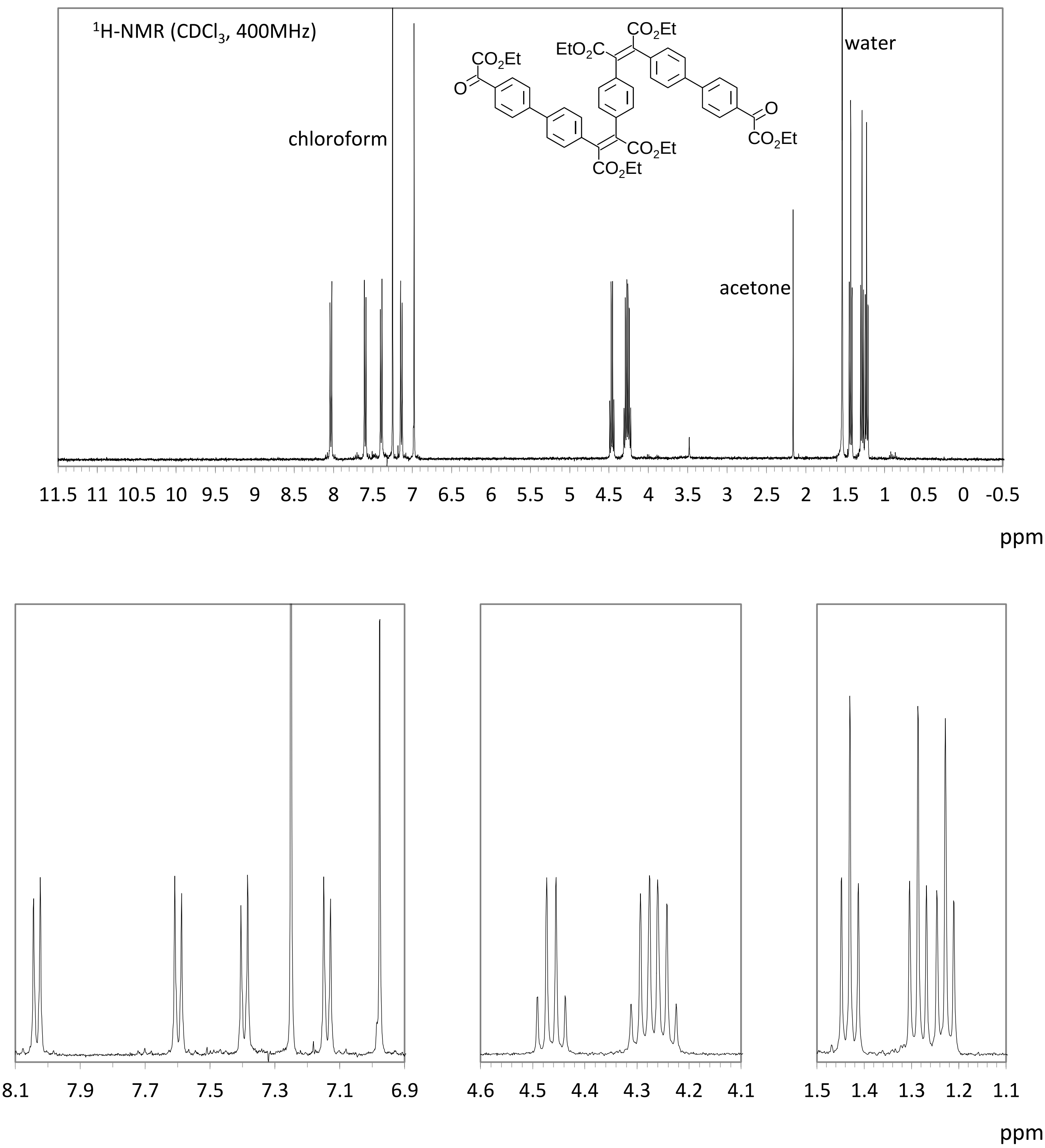


^{13}C-NMR (CDCl$_3$, 100MHz)
CO$_2$Et
chloroform
pinacol
pinacol
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm

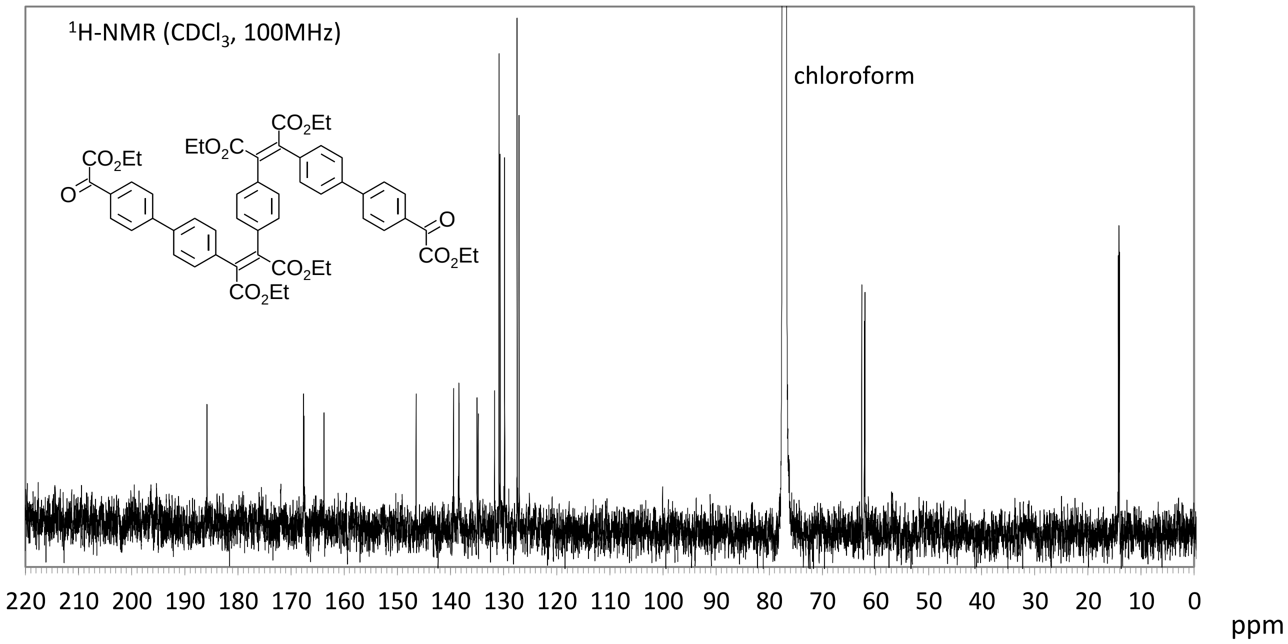


188 186 165 163 137 132 127 85 84 64 62 26 24 15 13
ppm

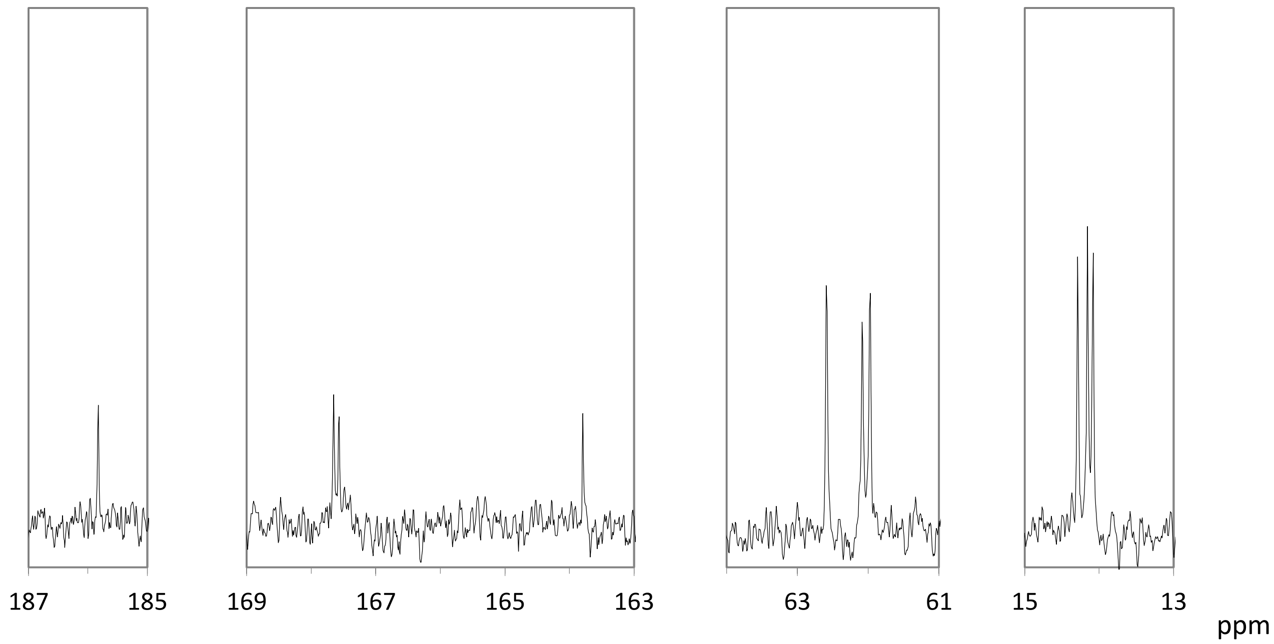
Compound **17**



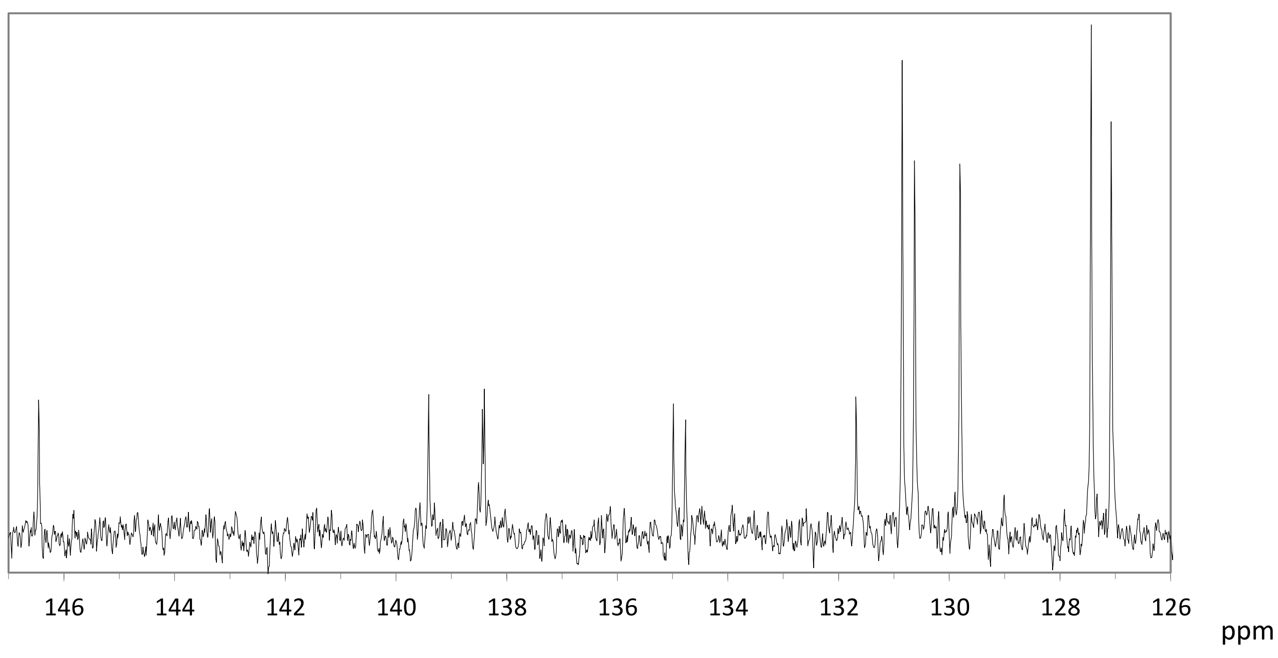
^{1}H-NMR ($CDCl_3$, 400MHz)
chloroform
water
acetone
CO_2Et
EtO_2C
O
11.5 11 10.5 10 9.5 9 8.5 8 7.5 7 6.5 6 5.5 5 4.5 4 3.5 3 2.5 2 1.5 1 0.5 0 -0.5
ppm
8.1 7.9 7.7 7.5 7.3 7.1 6.9
4.6 4.5 4.4 4.3 4.2 4.1
1.5 1.4 1.3 1.2 1.1
ppm



^{1}H-NMR ($CDCl_3$, 100MHz)
chloroform
CO_2Et
EtO_2C
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm

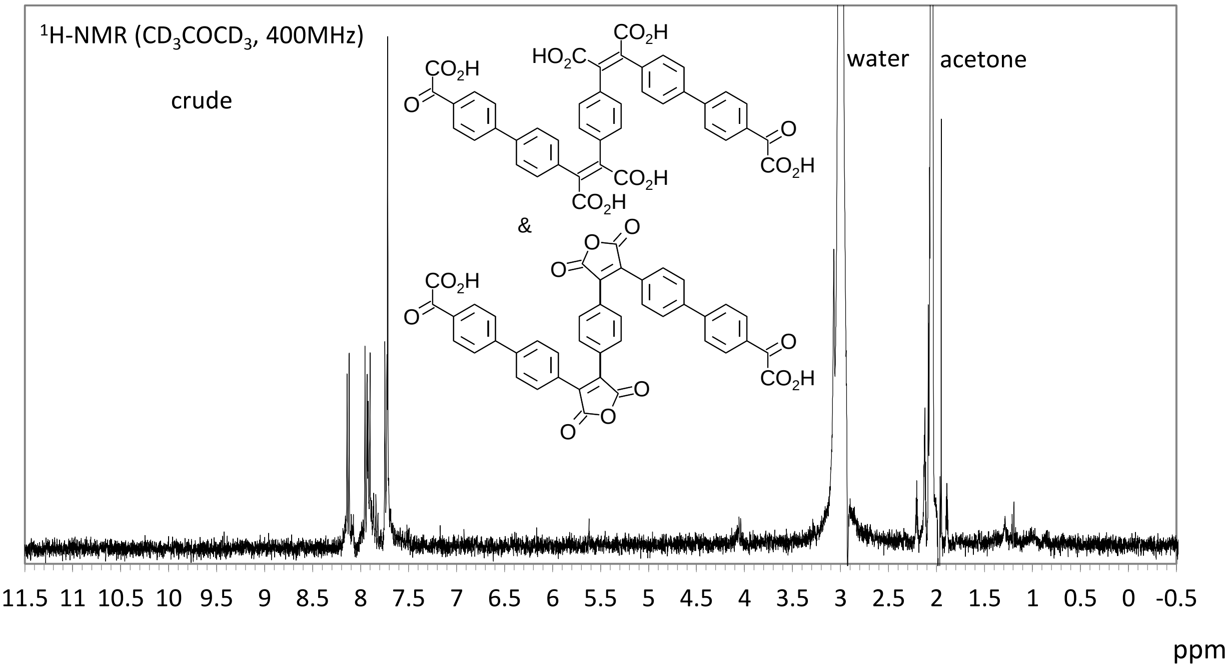


187 185
169 167 165 163
63 61
15 13
ppm

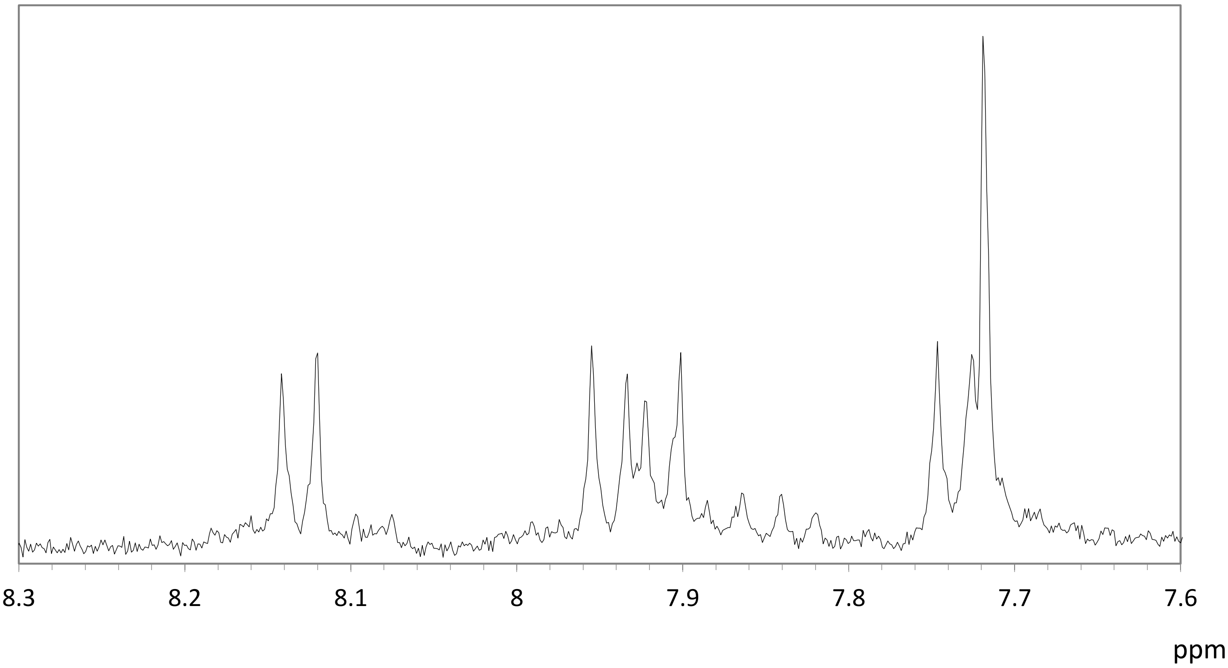


146 144 142 140 138 136 134 132 130 128 126
ppm

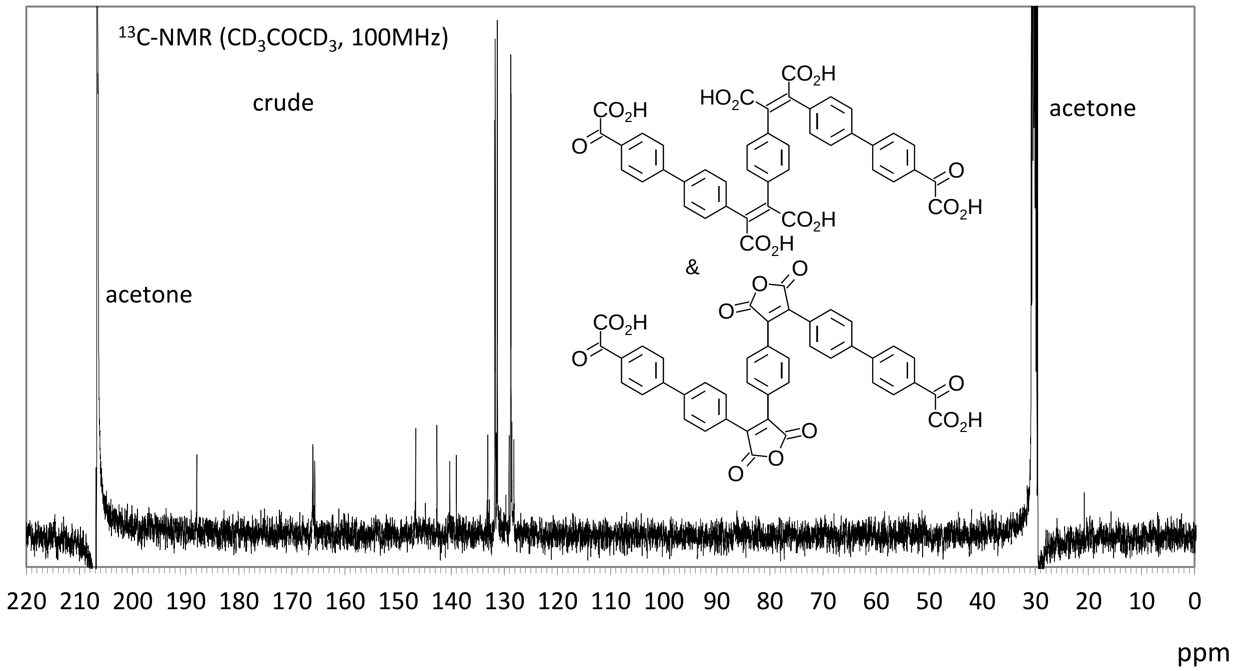
Compound **18**



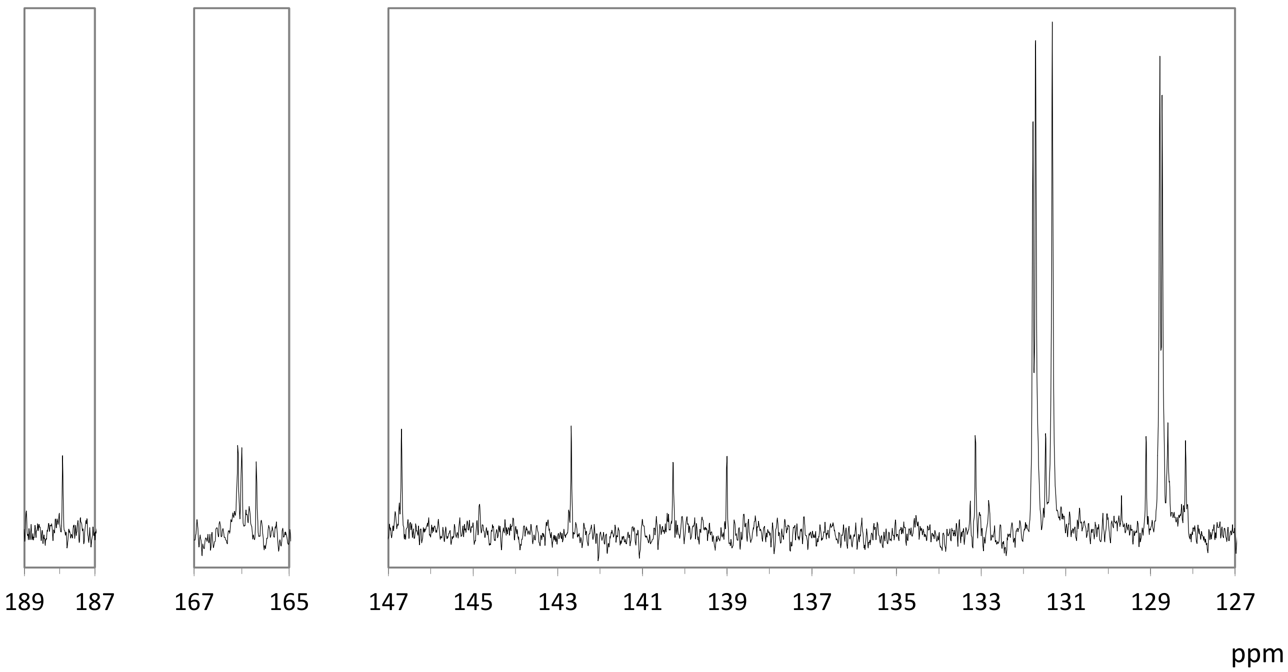
¹H-NMR (CD₃COCD₃, 400MHz)
crude
water
acetone
&
CO₂H
HO₂C
O
11.5 11 10.5 10 9.5 9 8.5 8 7.5 7 6.5 6 5.5 5 4.5 4 3.5 3 2.5 2 1.5 1 0.5 0 -0.5
ppm



8.3 8.2 8.1 8 7.9 7.8 7.7 7.6
ppm

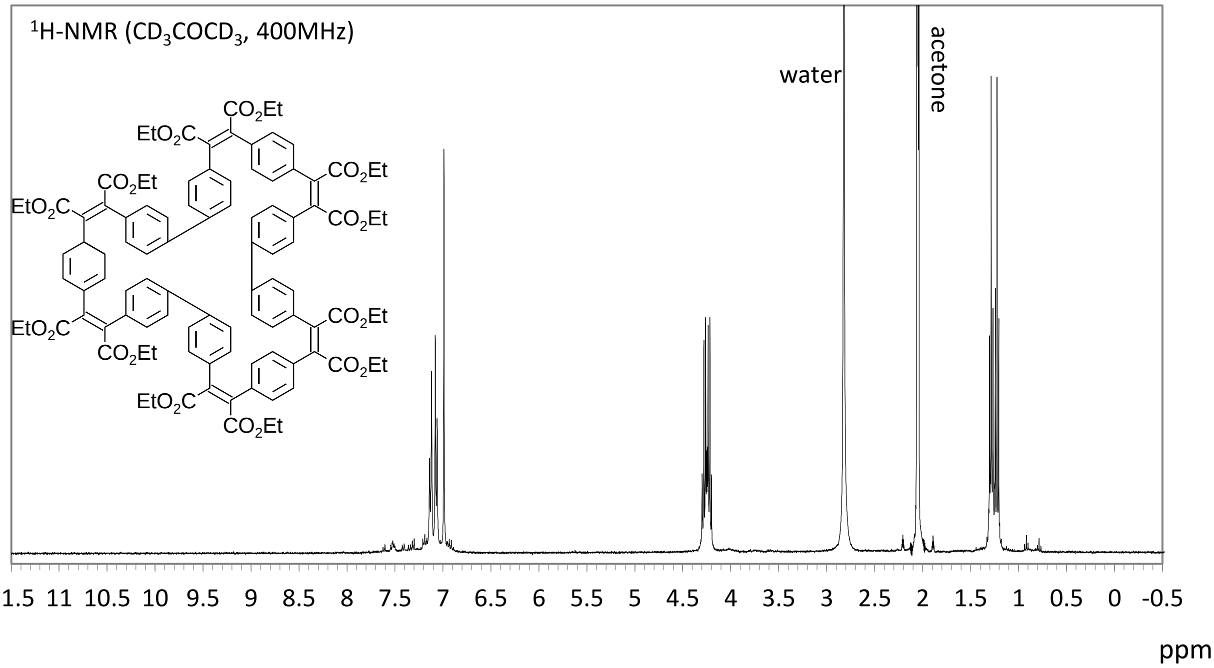


^{13}C-NMR (CD$_3$COCD$_3$, 100MHz)
crude
acetone
acetone
&
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm

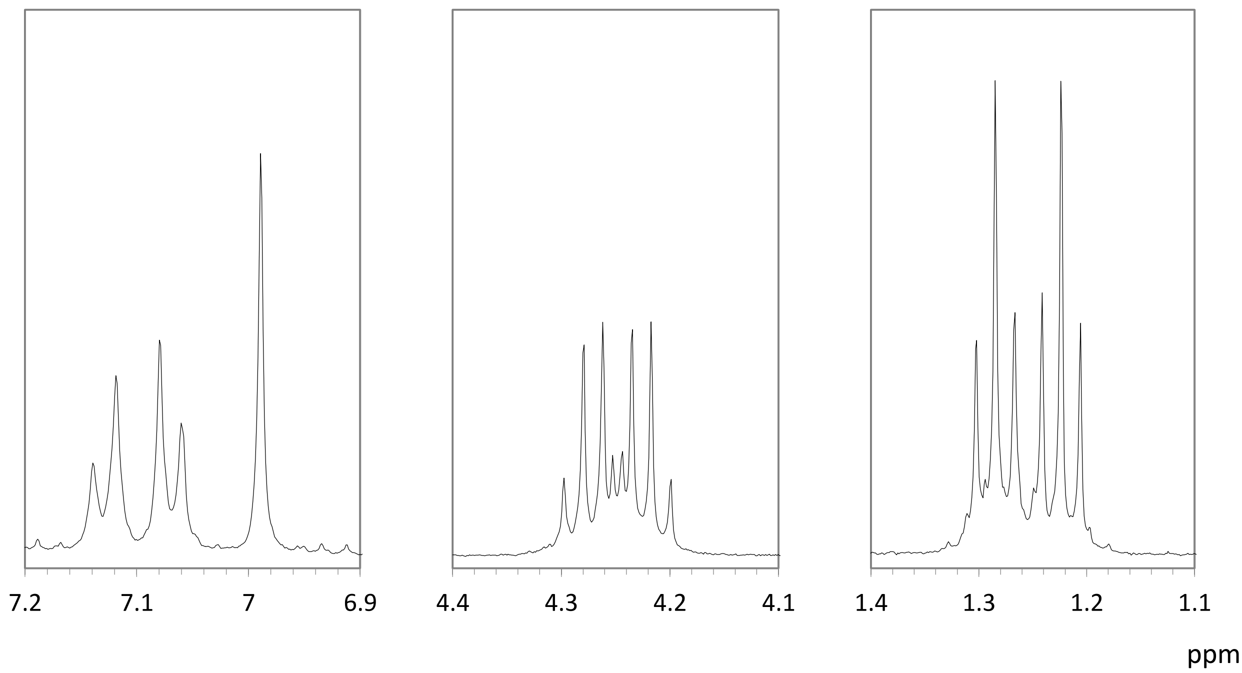


189 187
167 165
147 145 143 141 139 137 135 133 131 129 127
ppm

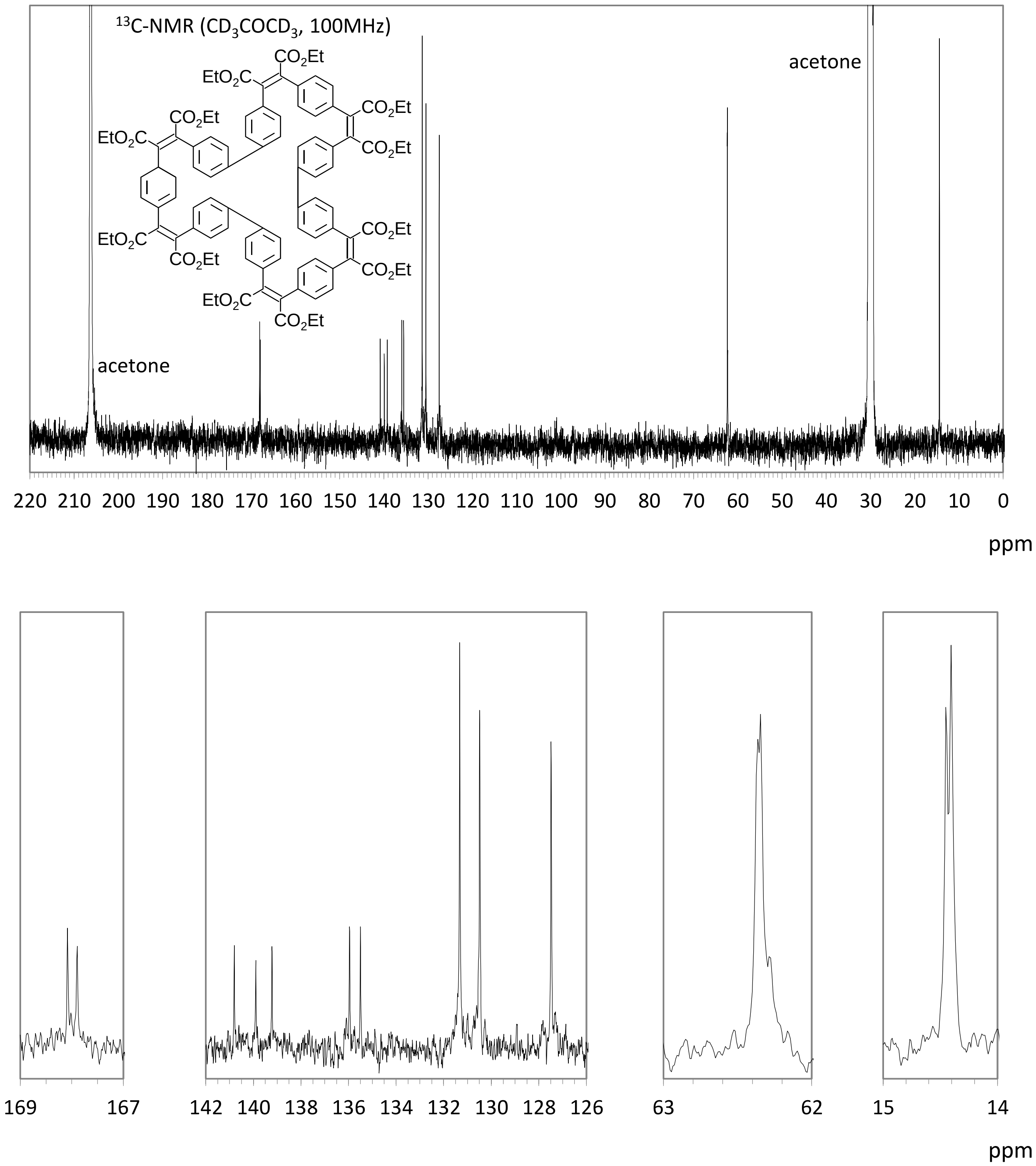
Compound **5**



1H-NMR (CD3COCD3, 400MHz)
water
acetone
CO2Et
EtO2C
11.5 11 10.5 10 9.5 9 8.5 8 7.5 7 6.5 6 5.5 5 4.5 4 3.5 3 2.5 2 1.5 1 0.5 0 -0.5
ppm

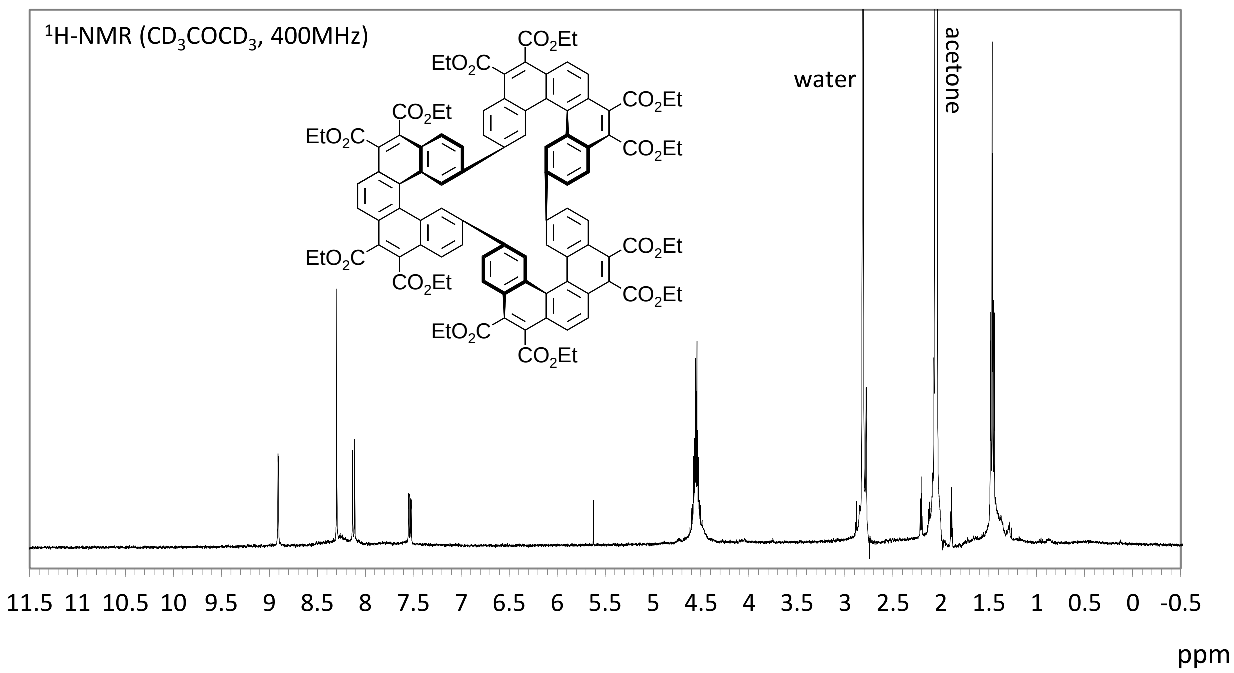


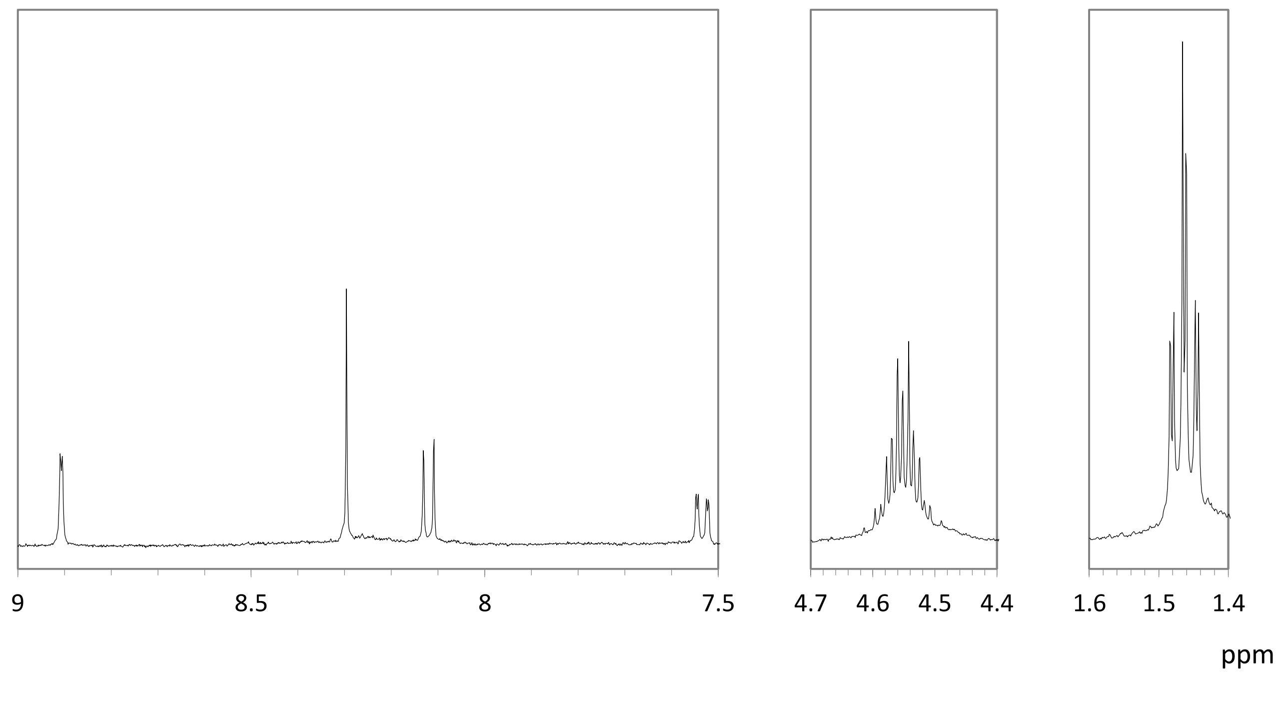
7.2 7.1 7 6.9
4.4 4.3 4.2 4.1
1.4 1.3 1.2 1.1
ppm

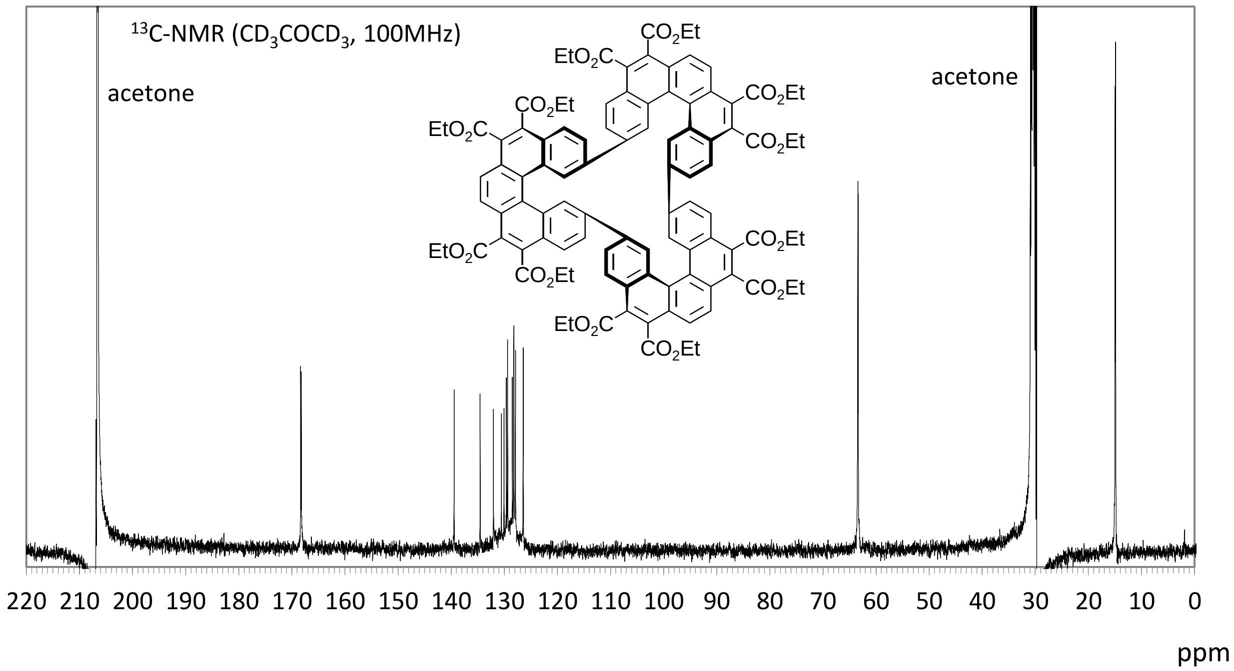


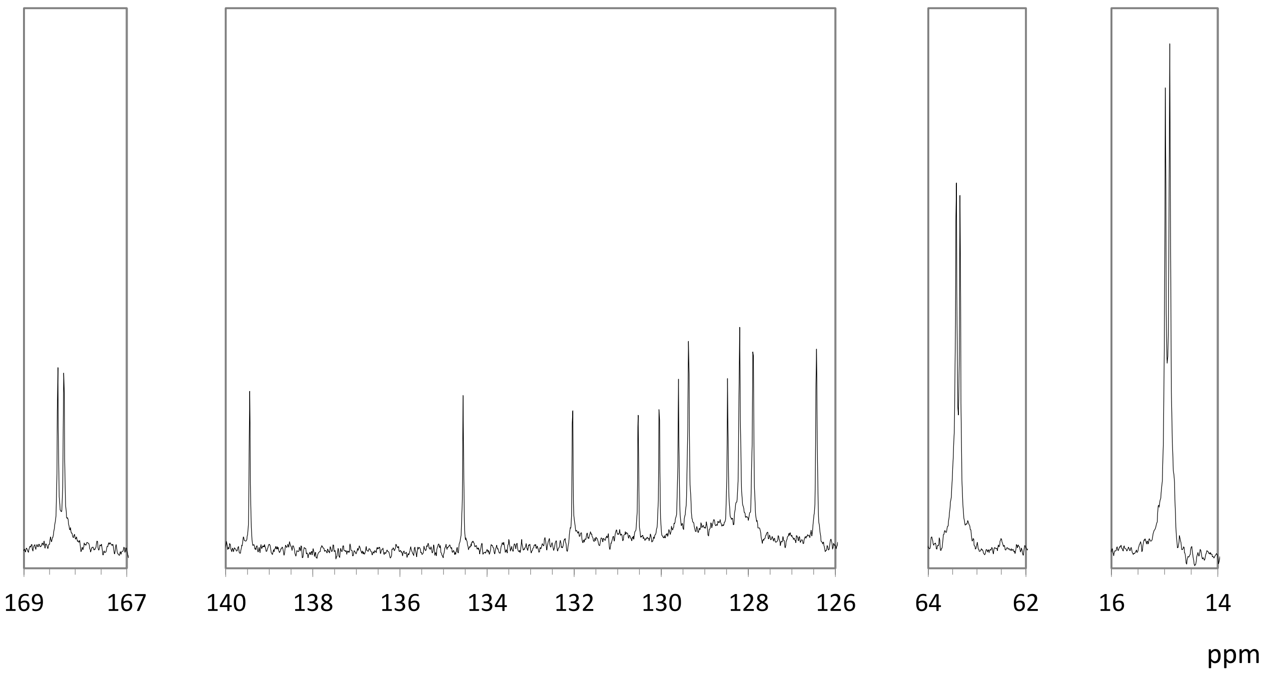
^{13}C-NMR (CD_3COCD_3, 100MHz)
CO_2Et
EtO_2C
acetone
acetone
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm
169 167
142 140 138 136 134 132 130 128 126
63 62
15 14
ppm

Compound **3** (C_3-symmetric)

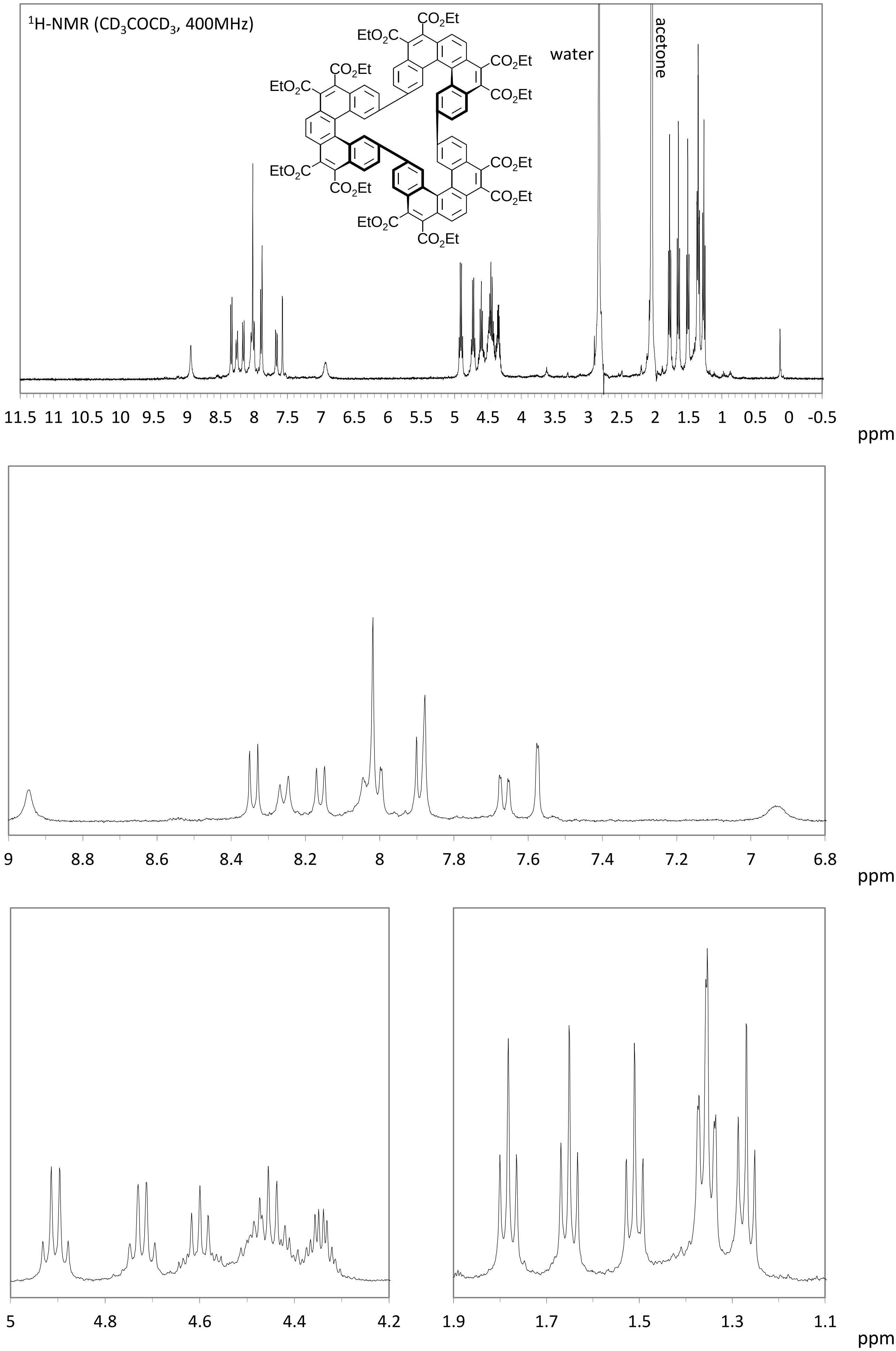


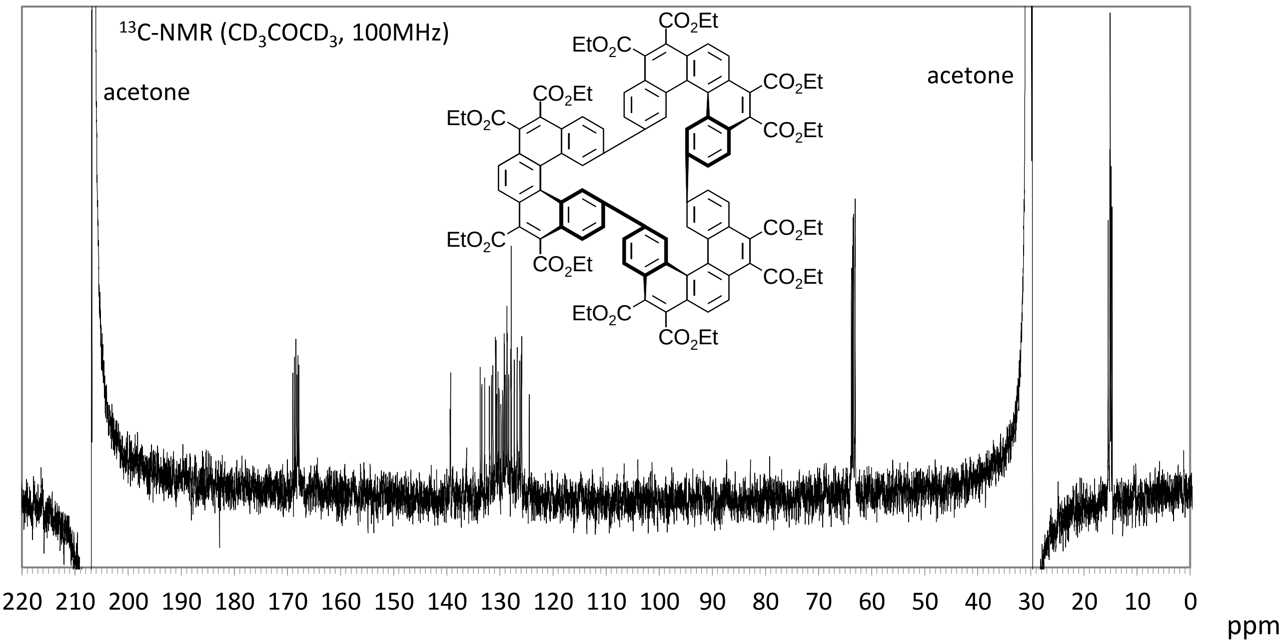



13C-NMR (CD3COCD3, 100MHz)
acetone
acetone
CO2Et
EtO2C
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm

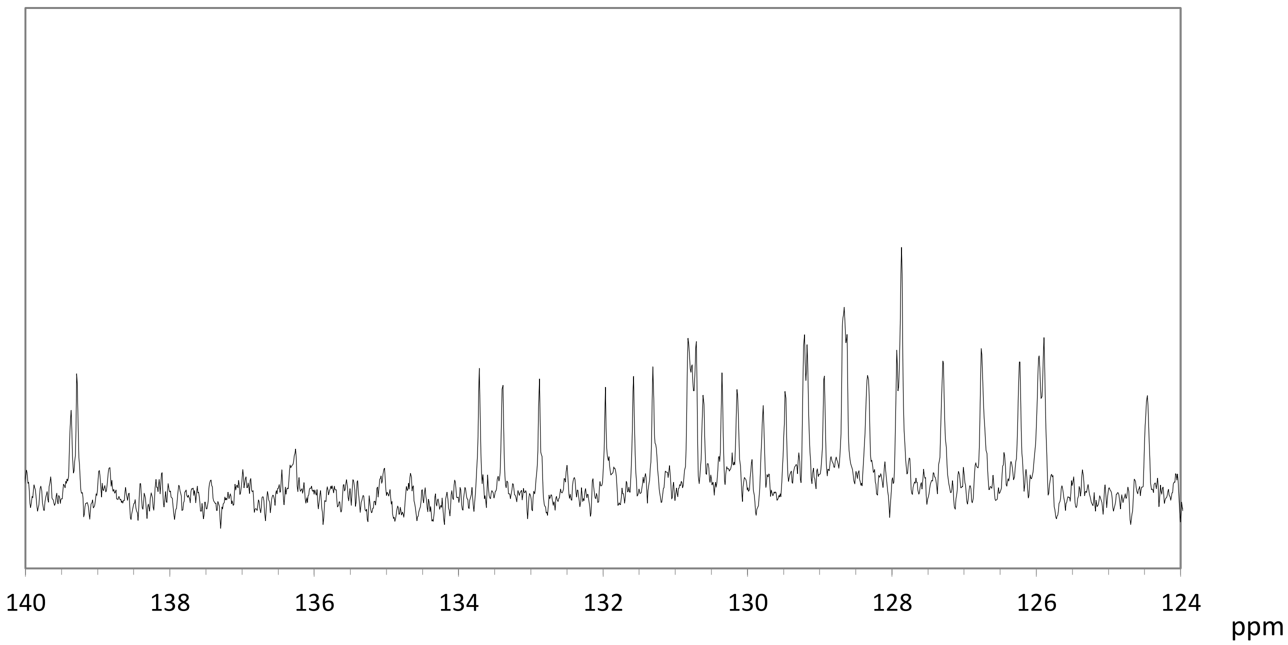

169 167 140 138 136 134 132 130 128 126 64 62 16 14
ppm

Compound **2** (C_2-symmetric)

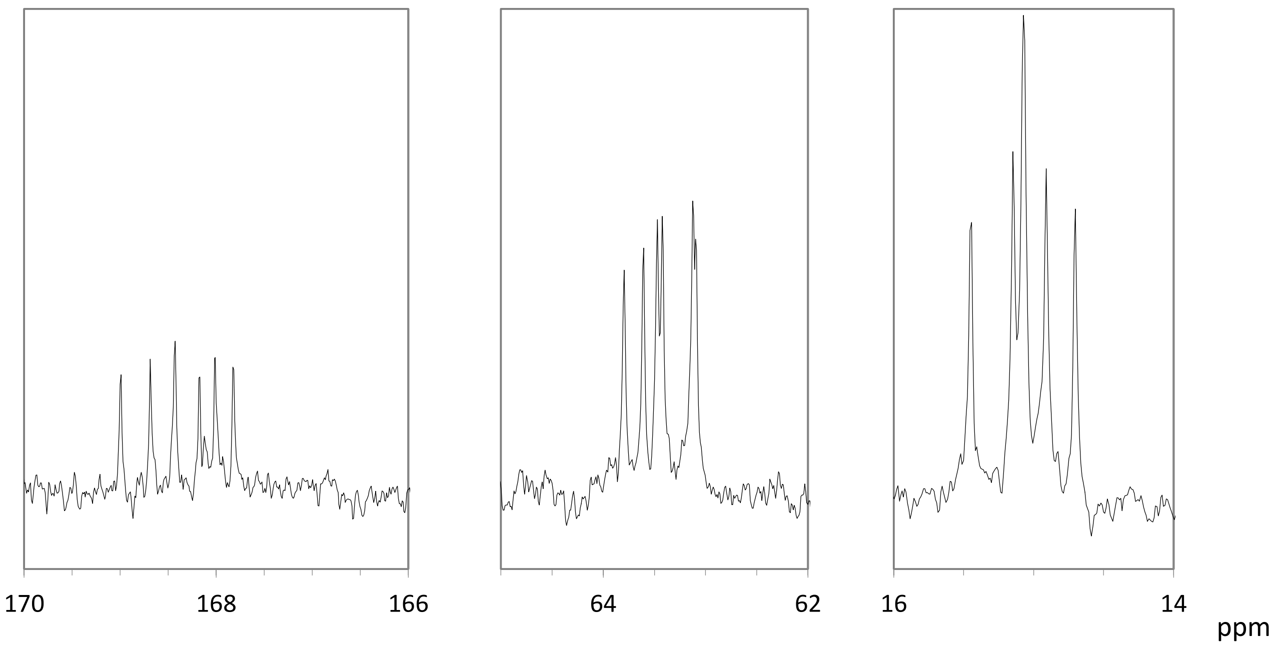




^{13}C-NMR (CD_3COCD_3, 100MHz)
acetone
acetone
CO_2Et
EtO_2C
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm



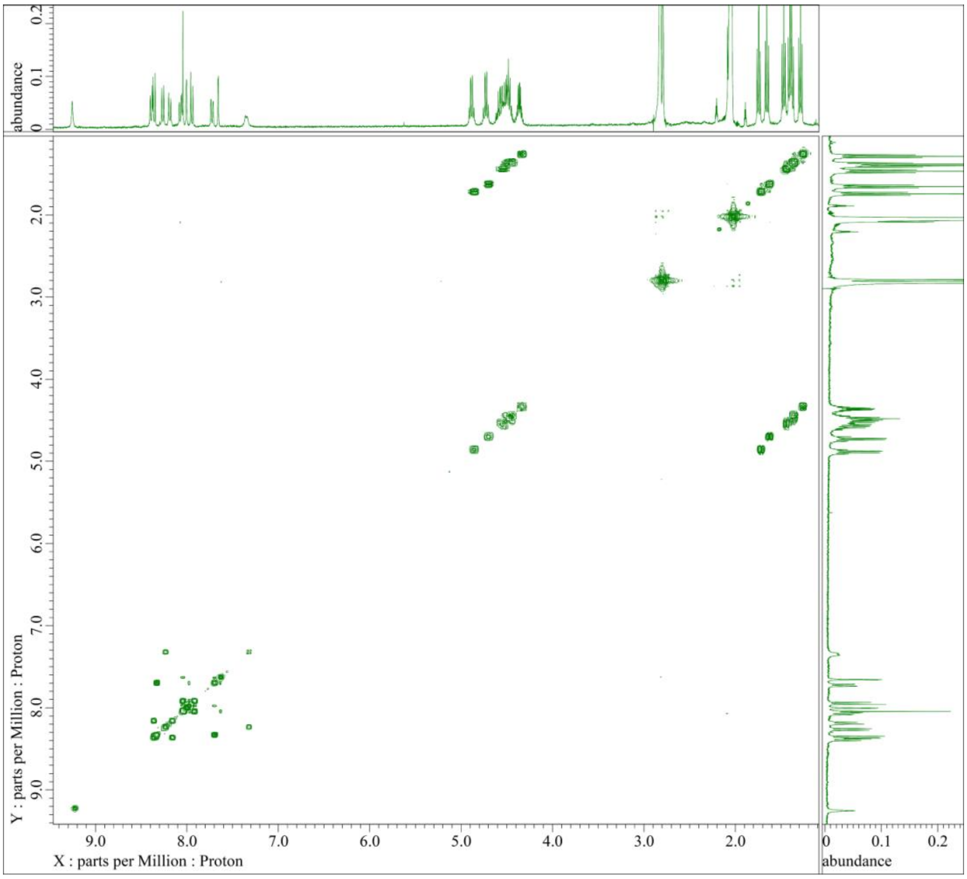
140 138 136 134 132 130 128 126 124
ppm

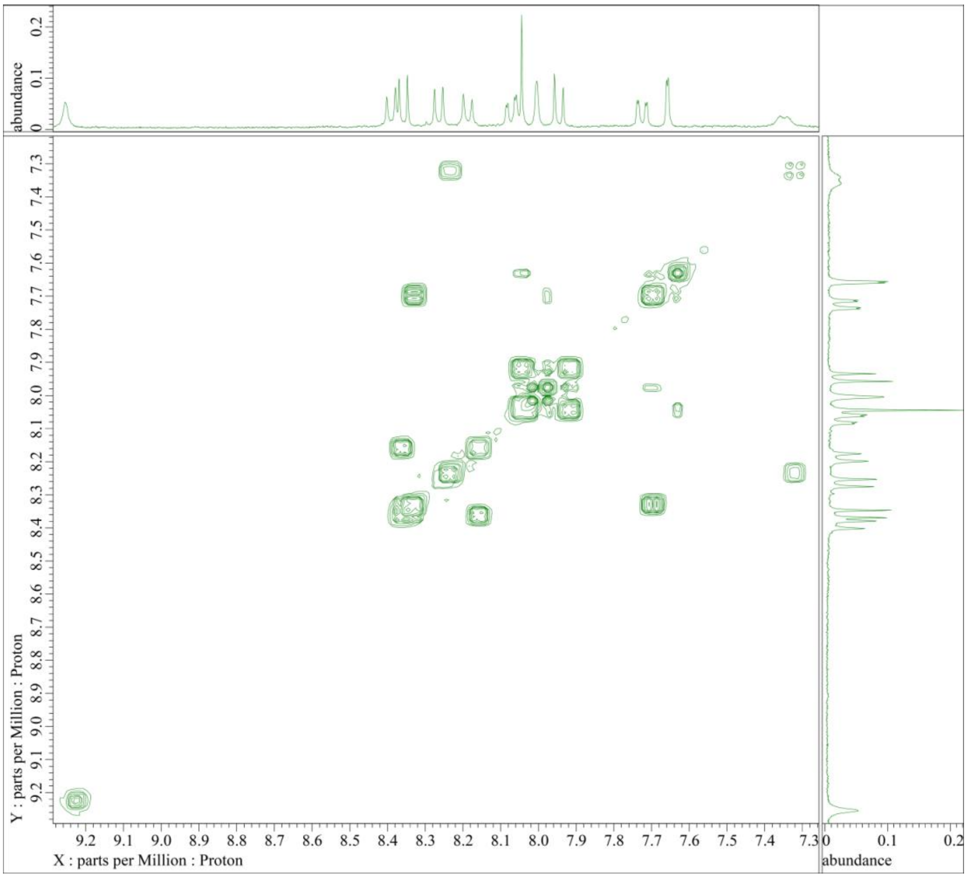


170 168 166
64 62
16 14
ppm

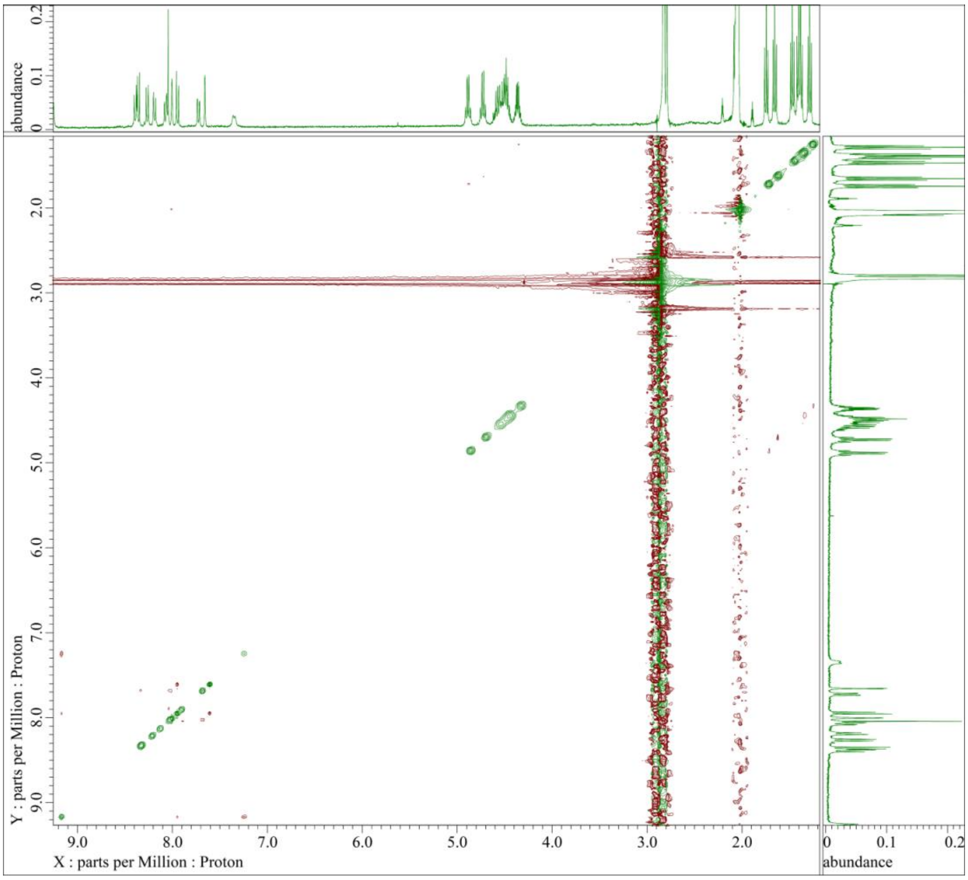
2D-NMR spectra of compound **2**

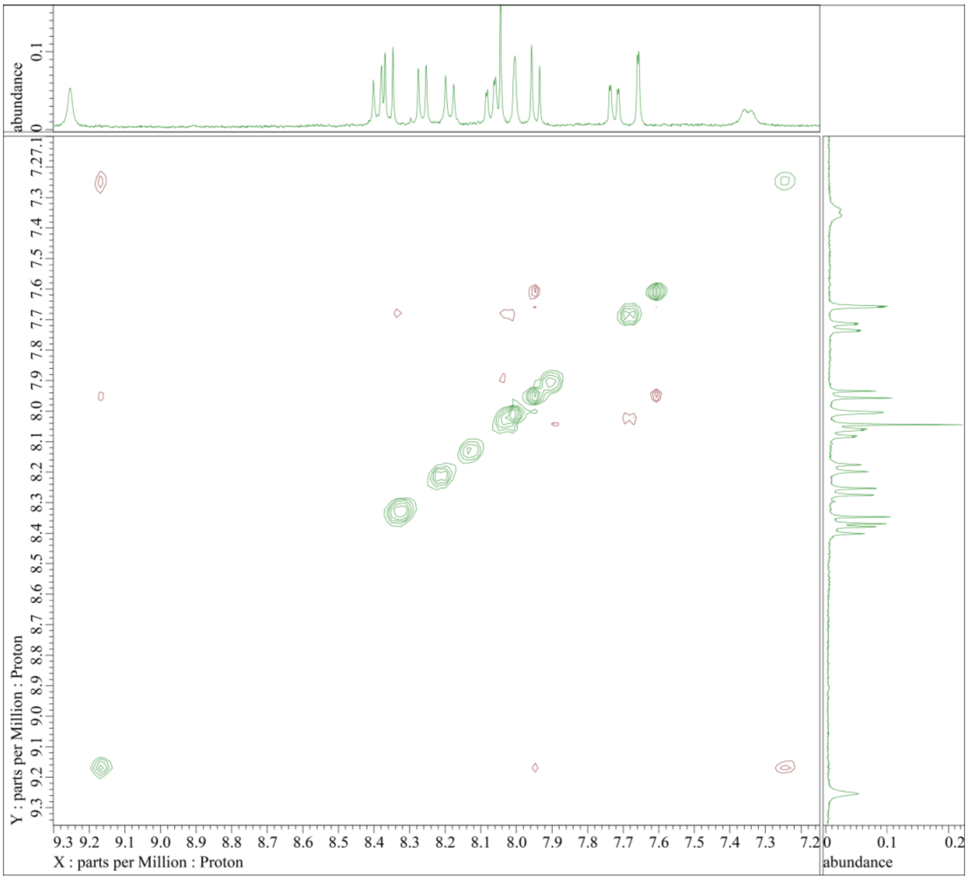
COSY





NOESY


abundance
X : parts per Million : Proton
Y : parts per Million : Proton


abundance
X : parts per Million : Proton
Y : parts per Million : Proton

Single crystal X-ray diffraction

The crystallographic data were collected with a Bruker APEX II Quasar diffractometer, equipped with a graphite monochromator centred on the path of MoK_{α} radiation. Single crystals of **2** and **3** were coated with Cargille™ NHV immersion oil and mounted on a fiber loop. The program SAINT was used to integrate the data, which was thereafter corrected using SADABS [1]. The structure was solved using direct methods and refined by a full-matrix least-squares method on F^2 using SHELXL-2014 [2]. All non-hydrogen atoms were refined with anisotropic displacement parameters. Hydrogen atoms were assigned to ideal positions and refined isotropically using a riding model.

For compound **3**, in spite of the decent size of the crystals, they were not diffracting at high resolution. Therefore, the data were cut at 1.10 angstrom as there is no diffraction above and R_{int} becomes larger. The result is a low θ_{max} value as well as a quite poor resolution and data/parameters ratio. In addition, in spite of a very long data collection strategy, the completeness cannot go higher than 94 % for the crystal we tested, unless decreasing significantly the resolution and loosing useful data. The reason for that is not only coming from the fact that the crystal is very weakly diffracting (as a consequence of the absence of any heavy atom and a large unit cell with several disordered groups), but also because of the anisotropic shape of the crystal (a thin plate) for which the diffracting power is strongly dependent of the orientation, so that several reflections at high angles were not present.
For the refinement of the crystal structure, several ethyl groups in the macrocycles were found to be disordered over two positions, and were refined using DFIX, SADI, EADP, EXYZ and SIMU constraints/restraints. Several lattice cyclohexane molecules were also found to be disordered and were refined using DFIX, DANG, EADP, EXYZ, SADI and SIMU constraints/restraints. Additional disordered cyclohexane molecules are also present in the unit cell, but cannot be modelized reliably without using an unappropriate number of constraints. Therefore, those were treated as a diffuse contribution to the overall scattering without specific atom positions by SQUEEZE/PLATON. Based on the electronic density, we can estimate about 4 molecules of cyclohexane per macrocycle. However, this exact number must be taken with care.

For compound **2**, several ethyl chains were found to be disordered over two positions and were refined using EADP, DFIX and SADI constraints/restraints. The crystal structure contains several lattice chloroform molecules. Four of them were introduced but one last cannot be modelized properly without using an inappropriate number of constraints. Therefore this one was treated as a diffuse contribution to the overall scattering without specific atom positions by the SQUEEZE procedure in PLATON.

Additional information about the refinement can be found in the _refine_special_details in the CIF files.
The CIF files have been deposited at the Cambridge Crystallographic Data Centre as supplementary publication no. CCDC 1826374 (**2**) and 1826373 (**3**).

Table : crystallographic data

Compound	3	2
Formula	$2(C_{102}H_{84}O_{24})\cdot 8(C_6H_{12})$	$C_{102}H_{84}O_{24}\cdot 2.5(CHCl_3)$
FW ($g\cdot mol^{-1}$)	4060.62	1992.11
Crystal color	yellow	yellow
Crystal size (mm)	0.58 x 0.16 x 0.03	0.55 x 0.23 x 0.04
Crystal system	triclinic	triclinic
Space group	$P2_1/n$	P-1
Temperature	125 K	120 K
a (Å)	19.450(2)	15.6031(9)
b (Å)	33.881(4)	23.6859(13)
c (Å)	34.509(4)	26.9809(15)
a (º)	90	84.266(2)
β (º)	103.592(5)	75.642(3)
γ (º)	90	75.481(3)
V ($Å^3$)	22104(4)	9343.9(9)
d_{calc}	1.356	1.416
μ (mm^{-1})	0.084	0.305
θ_{min} - θ_{max}	2.17° - 18.17°	2.31° - 24.90°
Refl. coll. / unique	723389 / 17552	559003 / 34349
Completeness to 2θ	0.938	0.987
R_{int}	0.1274	0.0722
Refined param./restr.	2560 / 470	2441 / 21
$^aR_1$ ($I > 2\sigma(I)$)	0.1449	0.1155
$^bwR_2$ (all data)	0.3592	0.3148
Goodness of fit	1.136	1.070

$^aR_1 = \Sigma||F_0| - |F_C||/\Sigma|F_0|$ and $^bwR_2 = [\Sigma w(F_0^2 - F_C^2)^2/\Sigma w(F_o^2)^2]^{1/2}$

Anisotropy of the induced current density (ACID) Plots[S6,S7]

The geometries were optimized at the B3LYP/6-31G* level of density functional theory (DFT) using Gaussian 09 Rev D.01.[S8] The anisotropy of the current density was calculated using our ACID method implemented in the Gaussian program with NMR=CSGT (6-31G*) IOp(10/93). The orientation of the magnetic field is orthogonal to the peripheral ring current and pointing towards the viewer. The ester groups are omitted, for the sake of clarity.

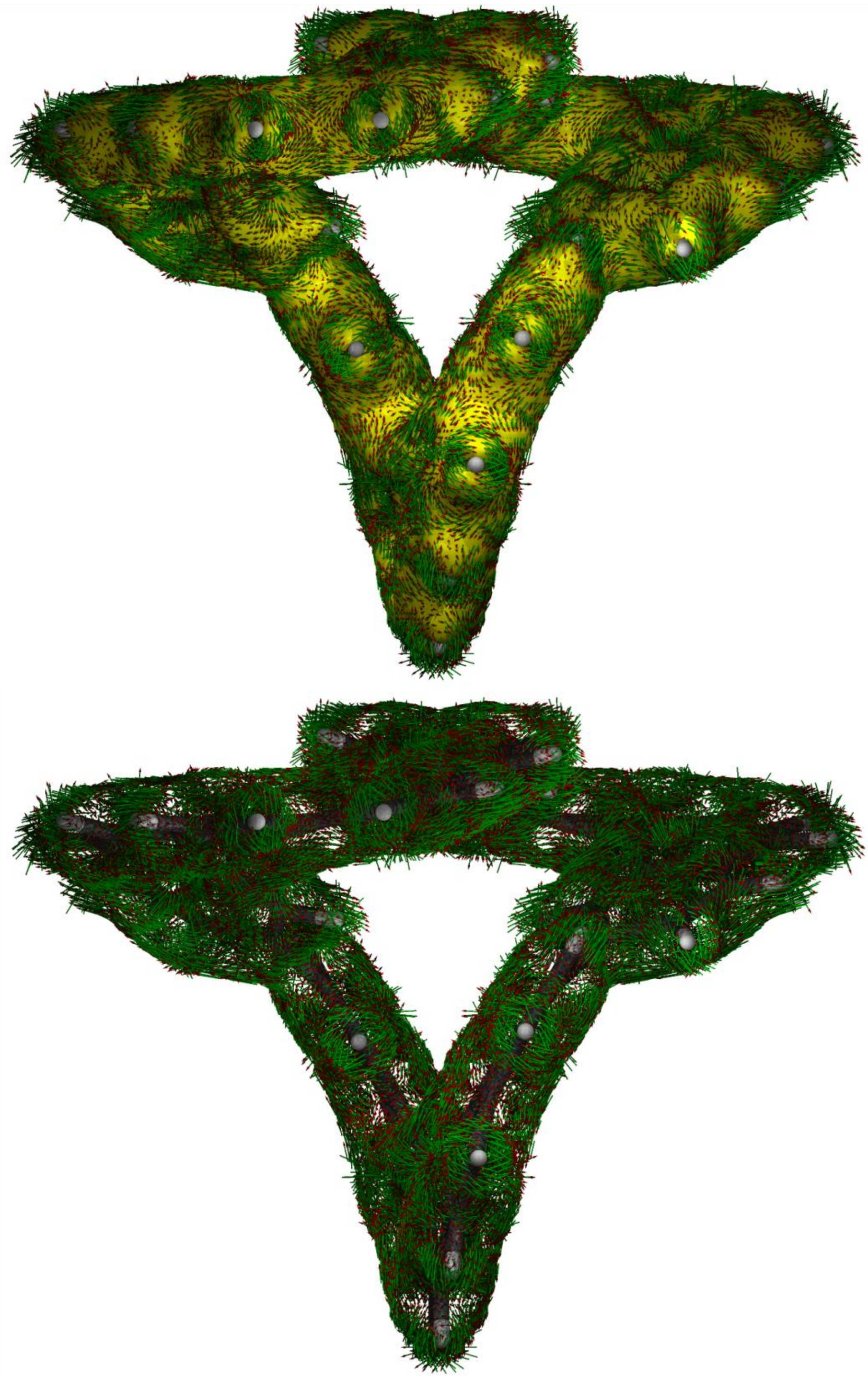


Figure S2: Top: ACID plot of single twisted Möbius compound **2** at an isosurface value (IV) of 0.032: current density vectors (green arrows with red arrowheads) are plotted onto surface. The length of the arrows is proportional to the absolute value of the current. Bottom: the current density vectors are represented without the ACID isosurface for clarity. There is a paratropic current (counter clockwise) following the inner periphery and a diatropic current (clockwise) in the outer periphery of the π system.

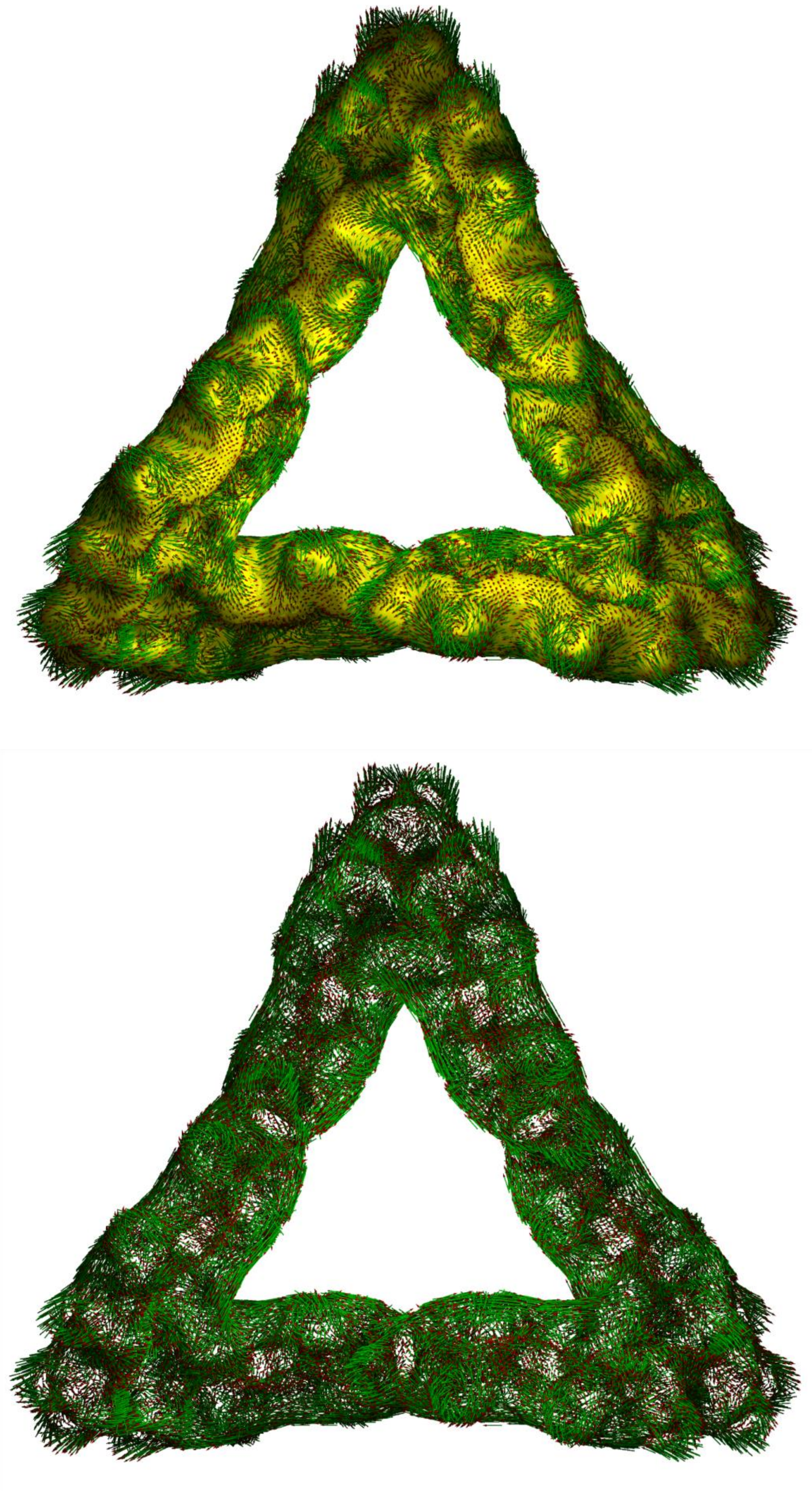


Figure S3: Top: ACID plot of triple twisted Möbius compound **3** at an isosurface value (IV) of 0.032. Current density vectors (green arrows with red arrowheads) are plotted onto surface. The length of the arrows is proportional to the absolute value of the current. Bottom: the current density vectors are represented without the ACID isosurface. There is a paratropic current (counter clockwise) following the inner periphery and a diatropic current (clockwise) in the outer periphery of the π system.

Orbital plots

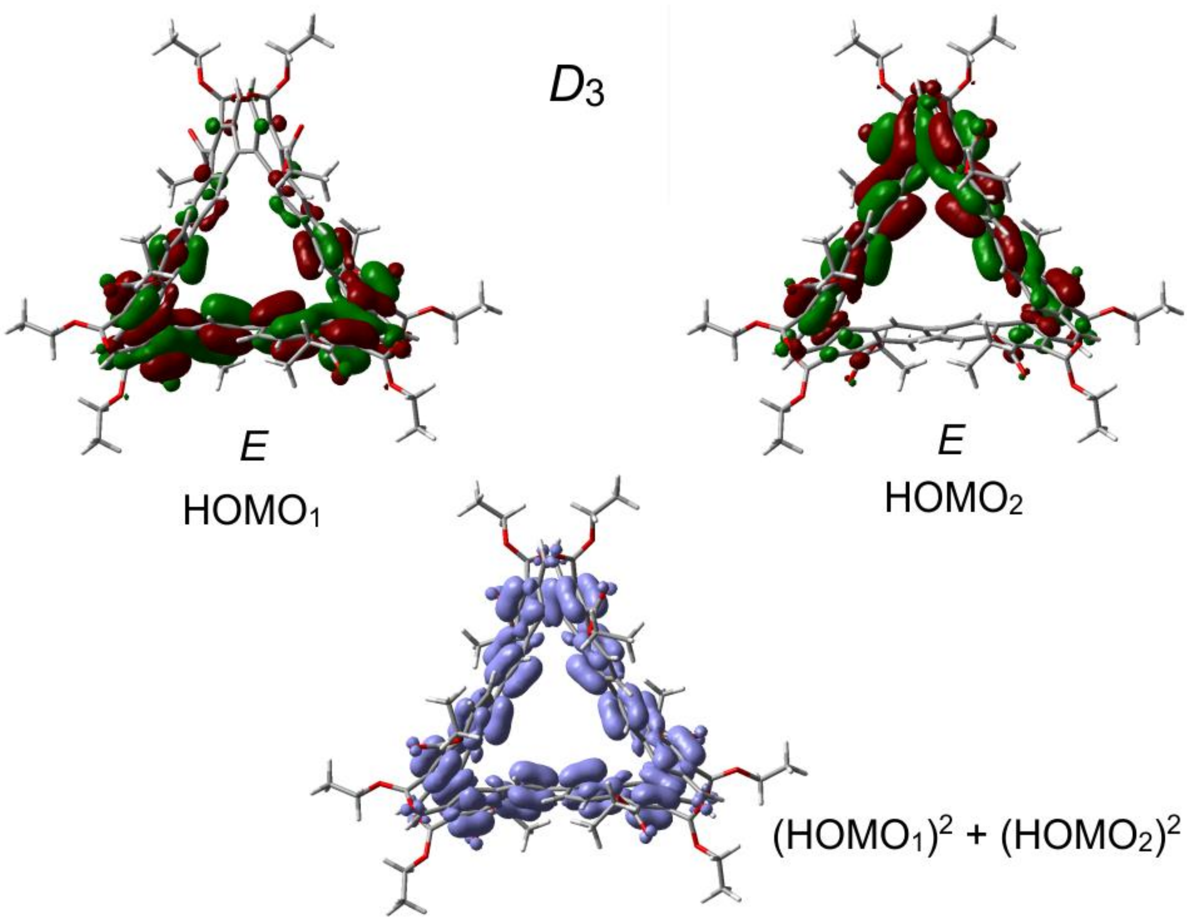


Figure S4: Top: Orbital plot (IV=0.02) of degenerated HOMOs of triple twisted Möbius compound 3 (D3 symmetry). Bottom: Sum of the squared HOMO orbitals. The MO representations prove the triply twisted topology of the π system.

Cartesian Coordinates of B3LYP/6-31G* optimized structures

For the determination of thermodynamic data Grimmes dispersion correction D3 (Stefan Grimme, Jens Antony, Stephan Ehrlich, Helge Krieg, J. Chem. Phys. **132**, 154104, **2010**) was included in ground state optimizations. Frequency analyses were performed with a vibrational scaling factor of 0.9613 (Merrick et al., *J. Phys. Chem. A*, Vol. **111**, No. 45, **2007**). Standard conditions (T=298K, p=1atm) for the calculation of entropies were employed.

Table 1: Relative energies and free enthalpy with and without dispersion correction of compound **2** and **3**.

Compound	E_{rel}	$\Delta G°$ (298K)	E_{rel} (D3)	$\Delta G°$ (298K, D3)
2	5.79	7.09	-13.03	-9.73
3	0.00	0.00	0.00	0.00

B3LYP/6-31G* optimized structures

Compound **2**

$E_{RB3LYP/6\text{-}31G*}$ = -5743.0765975 Hartree

NImag = 0

C	-3.03098	-6.12300	-2.10114
H	-3.35520	-6.44205	-3.09339
H	-1.95568	-6.29158	-1.99667
C	-2.84827	8.27179	-3.90583
H	-2.89831	9.34022	-4.14238
H	-1.89112	8.07321	-3.41299
H	-2.87620	7.70864	-4.84399
C	-4.01156	7.89056	-3.01033
H	-4.97861	8.08146	-3.48646
H	-3.99894	8.43255	-2.05945
C	-3.81272	-6.82076	-0.99984
H	-3.49931	-6.46662	-0.01257
H	-3.64077	-7.90205	-1.04903
H	-4.88548	-6.63706	-1.11038
C	10.03629	-4.18349	-2.25448
H	10.98171	-4.72419	-2.37911
H	9.74856	-3.76913	-3.22469
H	10.20494	-3.36264	-1.54898
C	2.45065	-8.00611	-4.52559
H	2.50445	-9.03061	-4.90948
H	1.52300	-7.90251	-3.95316
O	-2.61377	-2.48379	7.56276
O	4.83738	2.56403	2.96009
O	4.90972	4.77977	-2.81796
O	2.76316	2.29660	7.42884
O	-4.32381	-1.44617	6.50760
O	4.49205	3.47384	5.00452
O	4.33560	0.91010	6.57557
C	5.34409	1.99906	-1.84263
O	3.32572	4.76121	-1.20498
O	7.61370	2.54993	-2.31766
O	-4.97220	-2.48131	3.12420
C	1.79740	-0.14107	-2.75224
H	1.78936	-1.21741	-2.75218
C	2.96879	0.52096	-2.32493
C	2.02911	-2.03313	-0.49988
H	2.00489	-0.98731	-0.21422
C	-1.10105	-1.00046	5.32952
O	7.13732	-4.59475	-3.65725

C	1.20337	0.66090	5.30688
O	5.50833	-6.61477	-2.09905
C	4.56740	-5.91744	-2.41990
C	-3.32953	2.48970	-1.13376
O	6.58807	3.65863	-0.63717
C	0.62537	0.52245	-3.09221
C	-1.83088	0.33197	-2.78699
H	-1.84114	1.39564	-2.62343
C	0.75511	1.24807	2.95947
C	-0.81992	-1.41227	2.92399
C	-0.10686	-2.45046	0.81813
O	3.55146	-6.35239	-3.19295
C	4.16137	2.67117	-2.04605
C	-0.25117	1.47590	1.98460
H	-1.21241	0.99149	2.10845
C	2.96867	1.94824	-2.37738
C	1.94793	2.02805	2.91817
C	-2.96622	-1.81077	-2.77227
O	7.71734	-4.44442	-1.46872
C	3.12707	-2.50045	-1.27223
C	-0.49043	-0.63929	4.10499
C	4.16969	-0.19610	-1.90469
C	-1.39706	-3.03819	0.71091
H	-1.65439	-3.62450	-0.16539
C	-0.63510	-0.25449	-3.18261
C	2.81890	2.03065	4.06952
O	-4.45465	-3.82129	4.87601
C	0.65497	1.93721	-3.15284
H	-0.22301	2.49110	-3.46917
C	2.11076	-4.72757	-1.18629
H	2.14787	-5.78366	-1.41955
C	1.03295	-4.22560	-0.49960
H	0.23997	-4.89814	-0.18916
C	4.23145	-1.63490	-1.69439
C	-0.63733	-1.63872	-3.47831
H	0.25547	-2.11982	-3.86408
C	-2.22424	2.00296	-0.38116
H	-2.15187	0.93672	-0.19555
C	0.13046	-1.60349	1.88958

H	1.11209	-1.15925	2.00335
C	-3.00556	-0.40463	-2.51017
C	-5.43209	-0.57511	-2.12635
C	5.56307	-3.69317	-2.08117
O	-3.90568	6.47096	-2.74119
O	-4.75702	-4.69161	-3.63956
C	6.67811	-1.49218	-1.87077
H	7.63858	-1.99143	-1.91317
C	1.16722	3.05076	0.84977
H	1.36445	3.72286	0.02215
C	-2.33127	-1.75312	5.28519
C	4.12242	2.77699	4.07949
C	5.38240	0.55381	-1.83182
O	-3.19063	-4.68413	-1.99846
C	2.40448	1.45096	5.24920
C	3.20494	-3.90332	-1.54694
C	-2.83512	-2.22302	4.08943
C	-0.48176	-0.58426	6.54716
H	-0.90535	-0.90582	7.49021
C	4.43148	-4.46938	-2.04732
O	-7.11439	4.93351	-3.38655
C	1.79953	2.62081	-2.82071
H	1.80385	3.70279	-2.87970
C	-4.24705	0.21930	-2.05017
C	4.08400	4.17077	-1.94772
C	-4.38082	1.62413	-1.68052
C	-1.22787	2.84315	0.11292
O	-8.13634	4.09809	-1.55004
C	-1.77533	-2.38235	-3.29107
H	-1.75941	-3.43635	-3.53986
C	0.99007	-2.86758	-0.09541
C	2.15084	2.87178	1.79501
H	3.07990	3.41671	1.69079
C	-2.03370	-2.15511	2.89218
C	-3.46523	3.90864	-1.27270
C	-0.09143	2.40230	0.96601
C	5.49030	-2.27261	-1.87037
C	-5.79345	3.65775	-1.90780
C	-4.08970	-4.09584	-2.82187
C	-3.08191	-1.96242	6.57266
C	-4.14562	-2.60885	-2.59768
O	-6.56175	-3.84722	-1.47428
C	0.50886	0.39123	4.10380
C	0.68597	0.13074	6.52663
H	1.18712	0.36438	7.45873
O	-7.59499	-2.56236	-3.02090
C	3.29335	1.51775	6.46886
C	6.87899	-4.30224	-2.51061
C	-2.32489	-2.89987	1.71897
H	-3.28238	-3.39801	1.62761
C	3.58855	2.48690	8.60512
H	4.54687	2.90493	8.28318
H	3.78334	1.51162	9.06268
C	-5.16868	-1.69755	7.65683
H	-4.67596	-1.29804	8.54846
H	-5.26398	-2.78075	7.78029
C	-1.32985	4.23129	-0.15681
H	-0.56946	4.90479	0.22391
C	6.56363	2.82269	-1.52058
C	6.62612	-0.13584	-1.75251
H	7.54519	0.42809	-1.69138
C	-5.35192	-2.00113	-2.34597
C	-4.69836	4.47083	-1.75463
C	-2.42133	4.74551	-0.80917
H	-2.50459	5.81694	-0.93951
C	-5.66434	2.22426	-1.83055
C	-4.15354	-2.94417	4.09249
C	4.93856	6.22947	-2.76122
H	5.48595	6.51807	-1.85755
H	3.91346	6.59600	-2.66491
C	-6.81752	1.40144	-1.95308
H	-7.79561	1.86423	-1.96176
C	2.84015	3.42011	9.53745
H	2.64940	4.38265	9.05285
H	3.43576	3.59859	10.43952
H	1.87987	2.98907	9.83901
C	6.13711	3.21079	2.87895
H	6.06827	4.19087	3.35662
H	6.30651	3.33405	1.80776
C	-6.70740	0.04551	-2.00453
H	-7.60164	-0.55900	-2.05454
C	-4.86422	5.95299	-1.94558
C	8.85165	3.25951	-2.04259
H	8.94983	3.38754	-0.96220
H	9.62974	2.58231	-2.40269
O	-5.76199	6.61071	-1.46183
C	-7.14207	4.24926	-2.22711
C	-6.62058	-2.81532	-2.34433
C	5.60895	6.72882	-4.02680
H	6.62840	6.34163	-4.11597
H	5.65655	7.82317	-4.01058
H	5.04530	6.42175	-4.91354
C	-6.30096	-3.05789	3.07037
H	-6.64128	-3.24344	4.09176
H	-6.91230	-2.27368	2.61797
C	-8.32992	5.64834	-3.71959
H	-8.53718	6.36111	-2.91561
H	-9.15726	4.93336	-3.75943
C	7.20498	2.34876	3.53498
H	7.00282	2.22638	4.60280
H	8.18609	2.82450	3.41953
H	7.24507	1.35816	3.07030
C	-6.50472	-1.03005	7.39327
H	-6.38375	0.04881	7.25262
H	-7.17511	-1.19443	8.24395
H	-6.97830	-1.44373	6.49713
C	-6.32579	-4.33285	2.24099
H	-5.98379	-4.14057	1.21876
H	-7.35167	-4.71777	2.19401
H	-5.69580	-5.10177	2.69747
C	8.89839	4.59506	-2.76594
H	8.74222	4.46012	-3.84096
H	9.87846	5.06198	-2.61508
H	8.13180	5.26961	-2.37621
C	-8.10291	6.33523	-5.05241
H	-9.00481	6.88420	-5.34439
H	-7.87418	5.60581	-5.83603
H	-7.27299	7.04672	-4.98975
C	-7.72984	-4.71487	-1.43876
H	-8.62313	-4.08532	-1.43984
H	-7.64544	-5.21996	-0.47418
C	-7.75435	-5.70591	-2.59224
H	-8.60816	-6.38221	-2.46645
H	-7.85820	-5.18767	-3.54787
H	-6.83807	-6.30197	-2.62267
H	2.40882	-7.32055	-5.37772
C	3.66254	-7.72099	-3.65961
H	3.71849	-8.38577	-2.79178
H	4.59999	-7.82040	-4.21480
C	8.96676	-5.13332	-1.73694
H	8.76914	-5.93936	-2.44682
H	9.24309	-5.56116	-0.77067

Compound **3**

$E_{RB3LYP/6-31G*}$ = -5743.0858303 Hartree
NImag = 0

O	3.44986	-2.43077	5.50117
O	4.95744	-4.11861	5.43148
O	-2.52882	-6.80578	-4.40623
O	-4.52316	-1.21868	5.40449
O	-6.66991	-1.69790	4.86144
C	2.02827	-3.12990	2.97362
H	1.85949	-3.42914	4.00015
C	4.33686	-3.23372	4.87751
C	2.24187	-3.74397	7.19581
H	2.08688	-3.84200	8.27650
H	1.27788	-3.50418	6.73499
H	2.59350	-4.70582	6.81230
C	1.18554	-2.90503	0.70179
C	3.26323	-2.65008	6.92300
H	2.92311	-1.68144	7.29626
H	4.23135	-2.89355	7.36703
C	0.99290	-3.21824	2.07214
H	0.03736	-3.60757	2.40770
C	2.42731	-2.41277	0.32135
H	2.59430	-2.15157	-0.71541
O	-0.46721	9.03687	2.42390
O	-1.25672	7.64153	4.02431
C	-7.11197	-1.24856	6.16714
H	-8.05079	-1.78377	6.32864
H	-6.37824	-1.56093	6.91432
C	-2.19394	-7.35541	-5.70582
H	-2.83612	-8.23478	-5.79683
H	-2.45867	-6.62607	-6.47515
C	-0.65840	7.91450	2.84411
C	-7.32030	0.25792	6.19242
H	-7.74219	0.55670	7.15898
H	-6.37036	0.78205	6.05677
H	-8.01375	0.56706	5.40384
C	-5.80521	-5.46317	7.01757
H	-6.37340	-6.04001	7.75547
H	-4.89490	-6.01901	6.77188
H	-5.51325	-4.51116	7.47241
C	-6.65235	-5.23795	5.77976
H	-7.56825	-4.67947	5.99938
H	-6.94473	-6.17782	5.30147
C	-2.15206	7.87779	-6.12454
H	-3.20710	7.93751	-6.41139
H	-1.88532	8.82512	-5.64597
C	-1.25238	7.55632	-7.30270
H	-1.34304	8.33995	-8.06284
H	-0.20517	7.49854	-6.98981
H	-1.52718	6.59914	-7.75720
O	-1.87569	-4.74722	-5.09134
C	2.75687	8.64417	5.55771
H	3.15304	8.89706	6.54726
H	3.58871	8.62638	4.84668
H	2.06194	9.43226	5.25065
O	7.06064	-2.28744	4.75184
C	8.12190	-2.57044	5.69598
H	9.07404	-2.59761	5.15749
H	7.94376	-3.56387	6.11910
C	8.09188	-1.48265	6.75236
H	8.88156	-1.66074	7.49051
H	8.25396	-0.49663	6.30508
H	7.12957	-1.47067	7.27411
O	7.76931	-4.00852	3.46625
C	6.95804	-3.14277	3.71709
C	-2.98956	9.31999	4.46718
H	-3.27553	10.12224	5.15718
H	-2.97546	9.72851	3.45309
H	-3.74753	8.53207	4.52235
C	-1.61996	8.77856	4.84737
H	-0.84784	9.54561	4.74892
H	-1.61534	8.38237	5.86572
C	-0.72228	-7.73162	-5.78237
H	-0.51484	-8.22113	-6.74090
H	-0.09116	-6.84166	-5.70950
H	-0.45580	-8.42393	-4.97740
C	-4.77395	4.85516	-6.61881
H	-3.94389	4.68779	-7.30961
H	-5.23369	5.82463	-6.82549
C	-5.79408	3.72962	-6.69560
H	-6.24409	3.70605	-7.69481
H	-5.31768	2.76291	-6.51175
H	-6.59265	3.87902	-5.96184
C	10.59159	-2.79588	-3.07422
H	11.52069	-3.04326	-3.60073
H	10.82333	-2.68925	-2.00920
H	9.89215	-3.62578	-3.20671
O	4.64836	0.02600	-5.34875
C	2.65047	1.59774	-0.63884
C	-3.58432	-3.93566	-0.37524
O	6.86591	0.28851	-4.98817
O	-5.20937	-5.73505	-4.27666
C	-3.10694	0.38050	0.41813
C	-2.57010	3.36464	-2.65550
C	-2.76985	1.34591	-0.66066
C	2.74587	1.92529	-2.01610
H	2.19203	2.77136	-2.40965
C	5.52237	-0.34102	-3.14290
C	-1.81261	-4.26262	-2.09213
C	3.51392	-2.30416	1.22250
C	-3.17235	1.09818	-1.99918
H	-3.63702	0.15263	-2.25792
C	-4.15318	-3.24328	0.75641
C	0.80254	4.47900	1.99277
C	4.43102	0.20086	-2.36876
C	-0.84712	6.45800	0.78090
C	3.37024	0.49925	-0.18755
H	3.29683	0.21246	0.85325
C	0.84443	3.26571	-0.12565
H	0.48106	3.15491	-1.13896
C	0.13225	-3.21847	-0.29852
C	-2.03117	3.58857	-1.35428
C	3.32844	-2.73111	2.57083
C	-3.82248	-1.87093	1.10844
C	-0.45925	-4.10108	-2.48754
H	-0.15470	-4.42400	-3.47512
C	-1.21132	-3.25918	0.05077
H	-1.50611	-2.94717	1.04408
C	0.48311	-3.60066	-1.61959
H	1.52107	-3.57023	-1.93391
C	0.25771	4.26188	0.69289
C	-1.54015	4.91137	-1.00022
C	-0.74434	5.18005	0.17405
C	-3.28979	-0.97091	0.15350
H	-3.06806	-1.34789	-0.83629
C	-4.21148	-1.35851	2.38103
C	-2.21097	-3.75701	-0.81973
C	3.60219	1.24650	-2.85251
H	3.68331	1.54782	-3.88869
C	2.33952	2.62318	1.64372
H	3.15877	2.01691	2.01565
C	4.25442	-0.22772	-1.02052
O	0.86177	4.98716	4.99824
C	1.90612	2.47735	0.29978
C	-1.90585	7.32166	-1.22851
H	-2.28570	8.15727	-1.80171
C	4.48135	-2.88095	3.42354
C	-3.37312	0.83566	1.73613

H	-3.22917	1.88156	1.98608	O	-3.39647	7.90740	-3.76127
O	1.55505	7.01734	4.28538	O	7.55046	-2.48537	-4.18165
O	-5.39711	-7.32044	-2.67679	O	-7.54380	-4.60087	3.34487
C	6.48717	-1.10630	-2.52371	O	8.82004	-1.09048	-2.92315
C	-5.01145	-2.17963	3.25300	O	-2.72740	3.36341	-5.69228
C	1.80248	3.58846	2.46273	C	-5.34101	-1.65872	4.62316
H	2.18334	3.70504	3.46981	C	-2.34721	-5.47718	-4.24453
C	-1.97883	6.00919	-1.78346	C	5.60664	-0.00475	-4.60318
C	-3.90286	-0.00709	2.68539	O	-1.99690	6.81175	-5.15734
H	-4.13566	0.38003	3.66958	C	7.37151	-2.21039	-0.45069
C	-2.16207	2.56437	-0.38491	H	8.32124	-2.38081	-0.94128
H	-1.82056	2.76632	0.62187	C	7.65540	-1.64303	-3.31664
C	-3.95431	-5.41426	-2.31375	C	-4.91045	-6.28563	-3.08191
C	-4.35811	-4.93958	-1.01096	C	0.93897	5.82726	4.12639
C	0.41917	5.65644	2.72696	C	5.94852	-2.45916	1.49978
C	4.84880	-1.96209	0.75599	C	-6.44718	-4.19114	3.66282
C	-5.18359	-3.88339	1.49106	C	7.22045	-2.56170	0.86194
C	-1.46123	7.51804	0.04946	H	8.04800	-2.99939	1.40555
H	-1.49525	8.50738	0.48642	C	-2.71172	6.93999	-4.02034
C	-3.07077	2.07317	-2.96383	C	-6.32826	-5.70111	-6.38776
H	-3.42490	1.86847	-3.96641	H	-6.99794	-6.25028	-7.05862
C	-2.75375	-5.02763	-2.86937	H	-6.78474	-4.73243	-6.16143
C	-2.48994	5.76199	-3.11120	H	-5.38421	-5.52079	-6.91180
C	-5.53940	-3.36645	2.79156	C	-3.19228	4.20882	-4.95647
C	5.11181	-1.27153	-0.48263	C	7.06570	0.54671	-6.40285
C	-6.10208	-6.50207	-5.11973	H	6.25430	1.18920	-6.75390
H	-7.03201	-6.68185	-4.57150	H	8.00624	1.10177	-6.43450
H	-5.64225	-7.47549	-5.31975	C	7.14275	-0.74031	-7.21052
C	-5.50675	-5.45148	-0.33664	H	7.39204	-0.50344	-8.25148
H	-6.07068	-6.25420	-0.79346	H	7.90841	-1.41025	-6.80901
C	6.33322	-1.53076	-1.15383	H	6.18325	-1.26291	-7.19506
O	-5.85758	-4.47058	4.84417	C	2.06306	7.29632	5.61164
C	-2.70711	4.47712	-3.55994	H	1.22401	7.28841	6.31527
C	-0.32039	6.64422	2.11283	H	2.74498	6.49099	5.90152
C	5.74553	-2.83940	2.87643	C	10.01186	-1.50739	-3.63796
C	-5.83638	-5.01448	0.91636	H	10.70063	-0.66881	-3.51177
H	-6.65693	-5.47589	1.45003	H	9.76329	-1.61615	-4.69616
O	-4.24217	4.99615	-5.27724				

B3LYP-D3/6-31G* optimized structures

Compound **2**

$E_{\text{RB3LYP-D3/6-31G*}}$ = -5743.393149 Hartree

NImag = 0

$E_{\text{RB3LYP-D3/6-31G*}} + E_{\text{zero-point}}$ = -5741.792953 Hartree

$E_{\text{RB3LYP-D3/6-31G*}} + H_{\text{corr}}$ = -5741.673997 Hartree

$E_{\text{RB3LYP-D3/6-31G*}} + G_{\text{corr}}$ = -5741.961009 Hartree

C	-3.43918	-5.64597	-2.51270	H	2.70340	-7.46534	-7.03058
H	-3.42949	-5.78728	-3.59616	H	1.67568	-6.60958	-5.86100
H	-2.45272	-5.88146	-2.10408	O	-2.48363	-3.83894	6.81696
C	-2.77833	8.80096	-2.38396	O	5.19731	0.85311	2.60139
H	-2.74994	9.89582	-2.39957	O	4.65827	5.38101	-1.65005
H	-1.77530	8.43102	-2.14808	O	3.41624	0.06400	7.21429
H	-3.05082	8.44530	-3.38259	O	-4.20960	-2.66296	5.94840
C	-3.78278	8.32419	-1.35310	O	5.12469	1.97112	4.57666
H	-4.79778	8.67446	-1.56857	O	4.94434	-0.75976	5.76754
H	-3.52947	8.65244	-0.33959	C	4.92922	2.53476	-1.24016
C	-4.52802	-6.46912	-1.84501	O	2.69832	5.15359	-0.54900
H	-4.56155	-6.26223	-0.77102	O	7.20681	3.20935	-0.91953
H	-4.33163	-7.53733	-1.98958	O	-4.96151	-2.92150	2.52820
H	-5.50363	-6.23461	-2.27719	C	1.57532	0.49132	-2.85819
C	9.92351	-3.07117	-2.88764	H	1.61796	-0.56410	-3.05483
H	10.92437	-3.47564	-3.07696	C	2.70644	1.11768	-2.29088
H	9.61350	-2.49119	-3.76109	C	1.86112	-1.79081	-1.09090
H	9.98049	-2.40776	-2.01768	H	1.81298	-0.85459	-0.54565
C	2.61865	-6.56295	-6.41564	C	-0.94771	-2.07519	4.83336

O	7.18060	-3.34810	-4.49130
C	1.52085	-0.64721	4.97465
O	5.55468	-5.72446	-3.61140
C	4.60103	-4.99629	-3.79800
C	-3.23395	2.66140	-0.52062
O	5.67531	3.82000	0.62378
C	0.36716	1.14227	-3.05797
C	-2.04725	0.86490	-2.65295
H	-2.06709	1.90968	-2.39784
C	0.98007	0.44365	2.83255
C	-0.79936	-1.99073	2.38323
C	-0.22798	-2.54560	0.06924
O	3.63222	-5.25426	-4.69907
C	3.75754	3.20843	-1.50360
C	-0.05238	0.95264	2.00967
H	-1.05398	0.55644	2.12491
C	2.64324	2.53152	-2.09616
C	2.25715	1.06609	2.80655
C	-3.17767	-1.27456	-2.77976
O	7.62733	-3.69717	-2.29317
C	2.98010	-2.02844	-1.92357
C	-0.37021	-1.50877	3.67695
C	3.91635	0.38421	-1.93623
C	-1.53698	-3.06334	-0.10028
H	-1.85161	-3.43821	-1.06498
C	-0.87353	0.33560	-3.16973
C	3.20829	0.71545	3.82487
O	-4.43813	-4.63212	3.91834
C	0.34552	2.55238	-2.90951
H	-0.55551	3.11546	-3.12885
C	2.00647	-4.20099	-2.47103
H	2.06530	-5.15388	-2.98080
C	0.89612	-3.90527	-1.71424
H	0.09650	-4.63531	-1.63100
C	4.05506	-1.05476	-2.06241
C	-0.87838	-1.02778	-3.56352
H	0.00316	-1.47669	-4.00899
C	-2.09759	1.99668	0.01042
H	-2.09312	0.91209	0.03351
C	0.09616	-1.98727	1.29177
H	1.10446	-1.63086	1.45405
C	-3.18383	0.08597	-2.35283
C	-5.57116	-0.10007	-1.78550
C	5.48318	-2.90436	-2.85177
O	-3.77641	6.87679	-1.39227
O	-4.81585	-3.91692	-4.12425
C	6.48868	-0.78283	-2.01223
H	7.47880	-1.21205	-2.11103
C	1.46657	2.56389	1.06411
H	1.66246	3.38769	0.39112
C	-2.22615	-2.73014	4.69274
C	4.60650	1.26119	3.74233
C	5.06931	1.13491	-1.56534
O	-3.61975	-4.23738	-2.22175
C	2.82226	-0.02106	4.92413
C	3.10690	-3.30781	-2.54453
C	-2.79813	-2.92876	3.45017
C	-0.22858	-1.96019	6.06314
H	-0.63025	-2.42682	6.95367
C	4.38371	-3.69335	-3.08951
O	-6.99785	5.73383	-1.77058
C	1.46199	3.22351	-2.47544
H	1.41650	4.29865	-2.35971
C	-4.35741	0.64059	-1.69051
C	3.63006	4.66513	-1.15877
C	-4.38741	1.95671	-1.07879
C	-0.98721	2.68917	0.48437
O	-7.95729	4.49457	-0.13961
C	-2.00845	-1.79273	-3.39806
H	-2.00106	-2.82255	-3.73932
C	0.83319	-2.71425	-0.94844
C	2.49053	2.09303	1.85511

H	3.47075	2.55238	1.77672
C	-2.04921	-2.65348	2.24989
C	-3.27750	4.08662	-0.42946
C	0.15570	2.02559	1.15894
C	5.34873	-1.58431	-2.29857
C	-5.68175	4.04666	-0.79939
C	-4.32845	-3.49501	-3.09983
C	-2.95779	-3.15851	5.93115
C	-4.36837	-2.05868	-2.64714
O	-6.65452	-3.52316	-1.85048
C	0.71983	-0.58968	3.81166
C	1.00720	-1.36346	6.10037
H	1.57855	-1.37694	7.01987
O	-7.87722	-1.84198	-2.73204
C	3.84930	-0.28667	5.98868
C	6.84359	-3.34832	-3.32810
C	-2.41784	-3.12037	0.95773
H	-3.39582	-3.55735	0.79914
C	4.37003	-0.12097	8.29031
H	5.27324	0.44893	8.05088
H	4.64624	-1.17956	8.33865
C	-5.08798	-3.20663	6.96140
H	-4.70770	-2.92469	7.94873
H	-5.06237	-4.29814	6.88547
C	-0.98877	4.10534	0.39647
H	-0.12076	4.66499	0.72852
C	5.96057	3.25808	-0.41774
C	6.34540	0.49517	-1.55443
H	7.22162	1.06769	-1.28767
C	-5.54458	-1.47423	-2.23567
C	-4.52364	4.76940	-0.64139
C	-2.10984	4.77981	-0.01984
H	-2.11374	5.86258	-0.00297
C	-5.64150	2.61949	-0.99136
C	-4.13687	-3.60196	3.35014
C	4.69473	6.78240	-1.27933
H	4.98914	6.83895	-0.22529
H	3.68833	7.19950	-1.37157
C	-6.83877	1.86574	-1.14590
H	-7.79170	2.35177	-0.98224
C	3.70309	0.36130	9.56363
H	3.42358	1.41590	9.47744
H	4.39099	0.25127	10.40898
H	2.79908	-0.21905	9.77553
C	6.58429	1.23210	2.42716
H	6.69643	2.28636	2.69262
H	6.75676	1.11021	1.35478
C	-6.79971	0.53432	-1.44108
H	-7.72335	-0.02247	-1.50257
C	-4.60385	6.26588	-0.52113
C	8.25334	3.82147	-0.11696
H	8.08168	3.57394	0.93378
H	9.16782	3.33329	-0.46134
O	-5.31931	6.85866	0.25869
C	-7.00271	4.76036	-0.83869
C	-6.81951	-2.26217	-2.30984
C	5.68544	7.46902	-2.19887
H	6.67970	7.02362	-2.10766
H	5.75581	8.53114	-1.94052
H	5.36430	7.38603	-3.24197
C	-6.26821	-3.50404	2.30164
H	-6.67062	-3.85023	3.25792
H	-6.86988	-2.67027	1.93299
C	-8.12429	6.64198	-1.73275
H	-8.16899	7.08487	-0.73268
H	-9.04471	6.07225	-1.89498
C	7.49417	0.33133	3.24833
H	7.27363	0.43692	4.31321
H	8.54291	0.60013	3.07418
H	7.34962	-0.71631	2.96677
C	-6.47065	-2.64581	6.69179
H	-6.46425	-1.55219	6.73862

H	-7.18000	-3.02249	7.43664
H	-6.81741	-2.94726	5.69795
C	-6.19598	-4.63598	1.28704
H	-5.79911	-4.27518	0.33409
H	-7.20058	-5.03766	1.10991
H	-5.56522	-5.44383	1.66800
C	8.30166	5.32456	-0.33186
H	8.43676	5.55515	-1.39313
H	9.14064	5.75358	0.22719
H	7.37598	5.78546	0.02086
C	-7.89144	7.68168	-2.81136
H	-8.72014	8.39769	-2.82585
H	-7.82005	7.21136	-3.79728
H	-6.96288	8.23035	-2.62246
C	-7.78132	-4.42427	-2.02504
H	-8.68567	-3.91936	-1.67446
H	-7.54987	-5.25468	-1.35532
C	-7.92042	-4.87928	-3.47020
H	-8.70628	-5.64003	-3.53957
H	-8.19152	-4.03634	-4.10956
H	-6.98125	-5.29969	-3.83912
H	2.58612	-5.69264	-7.07838
C	3.79919	-6.47152	-5.46844
H	3.84854	-7.32097	-4.77917
H	4.75550	-6.41783	-5.99819
C	8.94312	-4.20617	-2.63288
H	8.84823	-4.85872	-3.50444
H	9.22860	-4.80203	-1.76316

Compound **3**

$E_{\text{RB3LYP-D3/6-31G*}}$ = -5743.372385 Hartree

NImag = 0

$E_{\text{RB3LYP-D3/6-31G*}} + E_{\text{zero-point}}$ = -5741.773588 Hartree

$E_{\text{RB3LYP-D3/6-31G*}} + H_{\text{corr}}$ = -5741.654061 Hartree

$E_{\text{RB3LYP-D3/6-31G*}} + G_{\text{corr}}$ = -5741.945510 Hartree

O	3.83046	-1.71818	5.53282
O	5.40640	-3.34230	5.40959
O	-1.18241	-7.09421	-4.40580
O	-4.19282	-2.02804	5.39178
O	-6.25130	-2.77790	4.81090
C	2.51222	-2.68881	2.98703
H	2.38532	-3.00856	4.01414
C	4.75939	-2.45506	4.89234
C	2.67310	-3.23098	7.07583
H	2.46914	-3.41862	8.13604
H	1.71990	-3.04130	6.57125
H	3.13428	-4.12568	6.64884
C	1.67105	-2.61255	0.70488
C	3.60456	-2.03708	6.92908
H	3.16504	-1.12613	7.34132
H	4.56939	-2.22604	7.40807
C	1.51637	-2.94993	2.07597
H	0.63530	-3.49067	2.40460
C	2.81562	-1.92018	0.33451
H	2.94531	-1.63380	-0.70059
O	-2.04459	8.80893	2.38445
O	-2.62675	7.29538	3.96686
C	-6.75587	-2.42435	6.12247
H	-7.65656	-3.03296	6.23290
H	-6.02079	-2.72137	6.87609
C	-0.78416	-7.56121	-5.71884
H	-1.12420	-8.59926	-5.74464
H	-1.32119	-6.98282	-6.47619
C	-2.06261	7.66803	2.79734
C	-7.06580	-0.93785	6.20808
H	-7.52287	-0.70594	7.17676
H	-6.14706	-0.35410	6.10903
H	-7.76267	-0.64514	5.41625
C	-4.98302	-5.97898	7.15073
H	-5.50293	-6.52807	7.94315
H	-3.97971	-6.40073	7.03545
H	-4.87996	-4.93336	7.45872
C	-5.76051	-6.08042	5.85279
H	-6.76745	-5.65720	5.93583
H	-5.86216	-7.11369	5.50553
C	-3.63325	7.12813	-6.30141
H	-4.70414	6.96513	-6.46423
H	-3.50209	8.16049	-5.96129
C	-2.80725	6.81401	-7.53376
H	-3.11380	7.45803	-8.36504
H	-1.74297	6.97895	-7.33936
H	-2.94088	5.76908	-7.83202
O	-1.05427	-4.94731	-5.12172
C	0.83292	9.05681	5.58073
H	1.07798	9.41648	6.58588
H	1.68541	9.25199	4.92286
H	-0.02383	9.62496	5.20431
O	7.17107	-1.14880	4.93862
C	8.15345	-1.37163	5.97770
H	9.13791	-1.07012	5.60569
H	8.18375	-2.44453	6.19231
C	7.71521	-0.55832	7.17992
H	8.42767	-0.69019	8.00135
H	7.66263	0.50665	6.93203
H	6.72689	-0.88211	7.52224
O	8.34308	-2.49343	3.54849
C	7.33781	-1.86724	3.81112
C	-4.54003	8.77616	4.35103
H	-4.94585	9.52765	5.03777
H	-4.50113	9.20706	3.34735
H	-5.21361	7.91326	4.34289
C	-3.14707	8.36146	4.79898
H	-2.45175	9.20523	4.76804
H	-3.15493	7.93344	5.80433
C	0.72142	-7.45597	-5.90640
H	1.00935	-7.89066	-6.87030
H	1.03184	-6.40821	-5.89148
H	1.24571	-7.99606	-5.11157
C	-5.48480	3.84572	-6.66928
H	-4.64292	3.94524	-7.36051
H	-6.19510	4.65800	-6.84135
C	-6.14586	2.48202	-6.79669
H	-6.57123	2.36512	-7.79990
H	-5.41066	1.68926	-6.63689
H	-6.95172	2.37619	-6.06334
C	10.90640	-0.81206	-2.96735
H	11.88194	-0.88932	-3.46072
H	11.07401	-0.72510	-1.88852
H	10.34245	-1.72632	-3.16931
O	4.67546	0.84972	-5.32414
C	2.30823	2.01491	-0.62737
C	-2.81294	-4.50291	-0.38957
O	6.77398	1.56871	-4.87000
O	-3.96624	-6.59293	-4.33599
C	-3.08389	-0.17953	0.39259
C	-3.07069	2.83126	-2.69696
C	-2.91776	0.82267	-0.69042
C	2.34682	2.34381	-2.00805
H	1.64335	3.06400	-2.41263

C	5.52521	0.66268	-3.08538
C	-1.01542	-4.47814	-2.10720
C	3.85875	-1.63040	1.24610
C	-3.24329	0.49575	-2.03406
H	-3.51561	-0.52161	-2.29383
C	-3.49622	-3.92415	0.73915
C	-0.03738	4.52885	1.97878
C	4.33711	0.97906	-2.33364
C	-1.98388	6.20001	0.73590
C	3.21988	1.07739	-0.16351
H	3.19357	0.78727	0.87836
C	0.24023	3.34512	-0.13813
H	-0.08645	3.17517	-1.15534
C	0.69844	-3.10136	-0.30462
C	-2.60758	3.15886	-1.39008
C	3.73211	-2.08248	2.59132
C	-3.40789	-2.51583	1.08639
C	0.28041	-4.05637	-2.50439
H	0.63939	-4.30507	-3.49571
C	-0.61119	-3.40005	0.04412
H	-0.96003	-3.15883	1.03934
C	1.11184	-3.39343	-1.63183
H	2.12317	-3.16082	-1.94824
C	-0.51605	4.22621	0.67110
C	-2.37314	4.54993	-1.04149
C	-1.65244	4.95837	0.13765
C	-3.03553	-1.54157	0.13013
H	-2.75169	-1.87780	-0.85784
C	-3.87405	-2.07570	2.35850
C	-1.49817	-4.07004	-0.83081
C	3.32479	1.83885	-2.83388
H	3.35549	2.14520	-3.87158
C	1.79471	2.96028	1.65458
H	2.69907	2.50090	2.03932
C	4.23332	0.52995	-0.98516
O	-0.11464	5.05155	4.98228
C	1.41238	2.74713	0.30317
C	-3.15639	6.85561	-1.28972
H	-3.66983	7.60933	-1.87202
C	4.88161	-2.03754	3.45301
C	-3.42139	0.22708	1.71131
H	-3.45728	1.28229	1.96041
O	0.18753	7.17661	4.27150
O	-3.95844	-8.15598	-2.70288
C	6.60786	0.09569	-2.45084
C	-4.52160	-3.02066	3.22686
C	1.09053	3.81865	2.46590
H	1.43184	3.99689	3.47810
C	-2.99070	5.54782	-1.83638
C	-3.79887	-0.69132	2.66276
H	-4.09380	-0.34772	3.64674
C	-2.55865	2.13479	-0.41445
H	-2.27785	2.40370	0.59507
C	-2.90189	-6.01365	-2.32794
C	-3.39013	-5.62947	-1.02622
C	-0.62656	5.62452	2.69945
C	5.11840	-1.05861	0.80010
C	-4.39797	-4.73499	1.47285
C	-2.76643	7.13310	-0.00841

H	-2.98083	8.10308	0.42065
C	-3.31274	1.46714	-3.00471
H	-3.60608	1.19418	-4.01093
C	-1.79729	-5.40259	-2.88203
C	-3.43064	5.20092	-3.16513
C	-4.83949	-4.28151	2.76877
C	5.26550	-0.33109	-0.43421
C	-4.55226	-7.55558	-5.24240
H	-5.49987	-7.90671	-4.82121
H	-3.88052	-8.41784	-5.31417
C	-4.42890	-6.33976	-0.35290
H	-4.84018	-7.23060	-0.80912
C	6.52221	-0.35650	-1.08704
O	-5.02685	-5.32420	4.86224
C	-3.40020	3.89506	-3.60576
C	-1.51296	6.47289	2.07126
C	6.12636	-1.76461	2.93020
C	-4.83546	-5.96640	0.89892
H	-5.55964	-6.56907	1.43105
O	-5.01089	4.07387	-5.31887
O	-4.70692	7.13800	-3.84956
O	7.94498	-1.02617	-4.10143
O	-6.60419	-5.83750	3.32655
O	8.88883	0.57935	-2.80733
O	-3.17034	2.82184	-5.74518
C	-4.93566	-2.56305	4.59534
C	-1.32094	-5.75905	-4.26067
C	5.58720	1.01818	-4.54003
O	-3.18847	6.23149	-5.25760
C	7.66027	-0.83228	-0.37075
H	8.63176	-0.82236	-0.84901
C	7.86722	-0.19043	-3.22667
C	-3.64987	-7.05514	-3.10866
C	-0.17735	5.88842	4.10622
C	6.28083	-1.34638	1.55937
C	-5.60868	-5.22373	3.64867
C	7.55909	-1.20882	0.93996
H	8.44591	-1.48422	1.49561
C	-3.87180	6.29322	-4.09608
C	-4.73421	-6.85327	-6.57408
H	-5.16668	-7.54368	-7.30623
H	-5.40210	-5.99258	-6.46995
H	-3.77297	-6.49433	-6.95604
C	-3.81203	3.53699	-5.00474
C	7.00610	1.80918	-6.28179
H	6.11563	2.28027	-6.70721
H	7.83292	2.52336	-6.29124
C	7.35871	0.52112	-7.01086
H	7.62246	0.74582	-8.05068
H	8.20173	0.02021	-6.52717
H	6.50611	-0.16238	-7.00616
C	0.51635	7.57430	5.62219
H	-0.33772	7.34740	6.26971
H	1.36416	6.97527	5.97027
C	10.15349	0.40050	-3.49402
H	10.69347	1.32965	-3.29822
H	9.96076	0.31369	-4.56695

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