Electronic Supporting Information

Foldamers with Unusual Structural Architecture from Spirobi(indane) Building Blocks

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General Methods.

Unless otherwise stated, all the chemicals and reagents were obtained commercially. All solvents were dried according to procedures given in the literature procedure; Chromatography was done on pre-coated silica gel plates. Column chromatographic purifications were done with 100-200 Mesh Silica gel. NMR spectra were recorded in

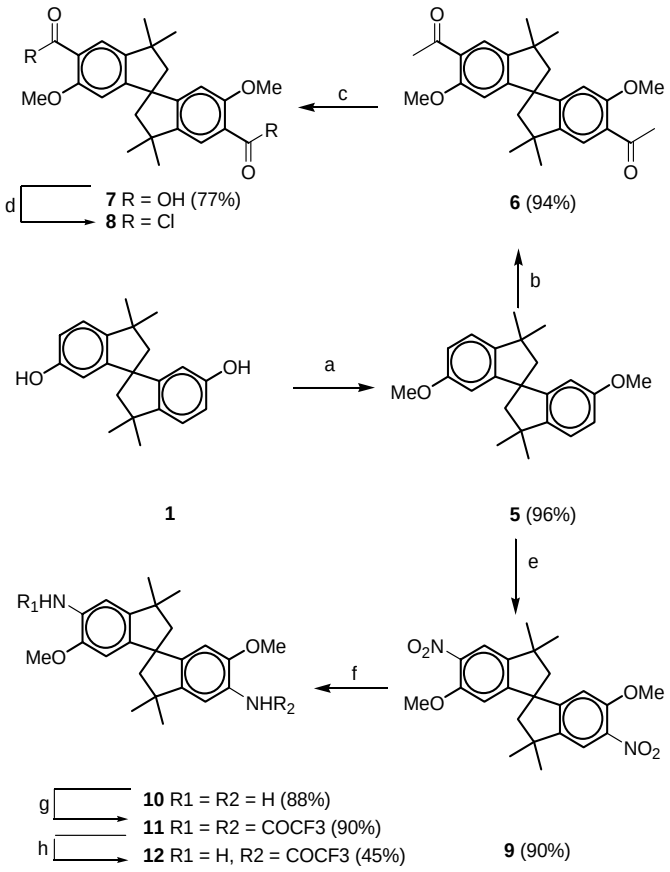
$CDCl_3$ on 200 / 300 / 400 / 500 MHz NMR spectrometers. All chemical shifts are reported in δ ppm downfield to TMS and peak multiplicities are reported as singlet (s), doublet (d), triplet (t), quartet (q), broad (br), broad singlet (bs) and multiplet (m). Elemental analyses were performed on a Elmentar-Vario- EL (Heraeus Company Ltd., Germany). IR spectra were recorded in nujol or $CHCl_3$ using Shimadzu FTIR-8400 spectrophotometer. Melting points were determined on a Buchi Melting Point B-540. MALDI-TOF Mass spectra were obtained from Voyager-PE, Voyager DEPRO and Voyager-DE STR Models. Single crystal X-ray data were collected on a *Bruker SMART APEX* CCD Area diffractometer with graphite monochromatized (Mo K_α = 0.71073Å) radiation at room temperature. All the data were corrected for Lorentzian, polarization and absorption effects using Bruker's SAINT and SADABS programs. SHELX-97 was used for structure solution and full matrix least squares refinement on F^2. Hydrogen atoms were included in the refinement as per the riding model.

Experimental Procedures:

The foldamer building blocks were synthesized starting from the precursor **1**, which is easily available in multi-gram quantities by the one-step acid-mediated rearrangement of bisphenol A (Scheme-1). To get the bis-acid building block **7**, the bis-alkoxy derivative **5** was first subjected to a bis-Friedel-Craft's acylation to deliver bis-acylated building block **6**, followed by the haloform reaction. This two-stage procedure for the installation of the carboxy group in *ortho* position to the alkoxy groups of the aryl rings was preferred over a possible metal-directed (lithiation) one-step carboxylation procedure, due to the anticipated difficulties associated with subsequent procedures, particularly when working on a larger scale. It should be noted that the bis-acid derivative **7** could be made in

excellent yield according to this two-step procedure. The bis-amine **10** was obtained by controlled nitration of **5** followed by reduction of the nitro groups. All efforts to make the mono-trifluro acetyl derivative **12** by direct trifluoro acetylation under controlled conditions were not encouraging as the reaction mixture was always contaminated with **10** and **11**, which made the separation of the three components tedious. Therefore, the bis-amine **10** was first bis-acylated to afford **11**, which was subjected to mono-deacylation under controlled conditions to afford **12** in moderate yield along with the bis-acyl starting material **11**.

Scheme 1. Synthetic route to the 1,1'-spirobi(indane) building blocks[a].

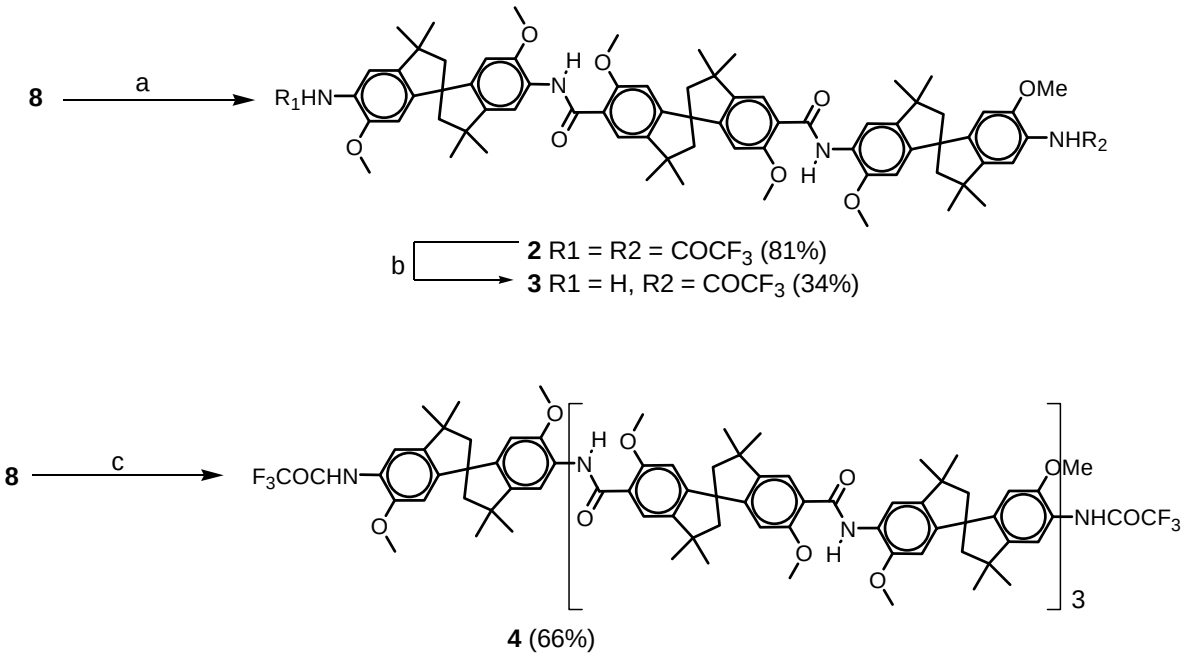


[a] Reagents and Conditions: (a) Me_2SO_4, K_2CO_3, acetone, reflux, 8h; (b) $SnCl_4$, AcCl, DCM, RT, 24h; (c) (i) NaOCl, KOH, dioxane, 70°C, 24h; (ii) H^+ ; (d) $(COCl)_2$, DCM, DMF (cat.), RT, 3h; (e) AcOH, HNO_3, H_2SO_4 (cat.), RT, 30min; (f) ammonium formate, MeOH, Pd-C, RT, 12h; (g) TFA, DCC, CH3CN, RT, 12 h; (h) K_2CO_3, MeOH, RT, 12 h.

This method was found to be more productive, since the bis- and mono-acylated derivatives **11** and **12**, respectively, could easily be separated. Furthermore, unreacted **11** could be recycled to afford **12**. Trifluoro acetyl protection was selected as the method of choice in our case, due to the relatively easy procedures available for deblocking it. Although the selective deprotection of the t-BOC group has been implemented in segment doubling strategies in foldamer synthesis, we could not apply it in our case, since the building blocks contain other alkoxy groups that would have interfered in the deprotection reaction when using the established TMSI/CH_3CN or BBr_3/DCM protocols.

Synthesis of the oligomers was attempted by segment doubling strategy with the building blocks **8** and **12**.

Scheme 2. Synthesis of 1,1'-spirobi(indane) oligomers 2 - 4[a].



[a] Reagents and Conditions: (a) **11** (2.5eq.), DCM, Et_3N, RT, 12h; (b) K_2CO_3, MeOH, RT 24h; (c) **3** (2.5 eq.), Et_3N, DCM, RT, 12h.

On the basis of this strategy, the oligomer **2** containing three 1,1'-spirobi(indane) building blocks was first assembled by reacting excess mono-amine **12** with the acid chloride **8**, obtained by reacting the bis-acid **7** with oxalyl chloride (Scheme 1). The oligomer **2**, obtained in 81% yield, was then subjected to mono-deacylation by using the standard K_2CO_3/MeOH conditions affording the mono-amine **3** in moderate yield. A second course of segment doubling involving **3** and **8** furnished the oligomer **4** composed of seven 1,1'-spirobi(indane) building blocks (Scheme- 2).

Experimental Section:

3,3,3',3'-Tetramethyl-1,1'-spirobi(indan)-6,6'-diol (1): A mixture of bisphenol-A (100 g) and methane sulphonic acid (5 g) was heated at 135 °C for 3 h leading to a molten reaction mixture, which was poured into 2 l of water under constant stirring. The precipitate was filtered and extensively washed with water. The dried crude material was crystallized from aq. ethanol to afford the known 1,1'-spirobi(indanol) **1** (20.2 g, 14 %); Mp: 216-218 °C.

6,6'-Dimethoxy-3,3,3',3'-tetramethyl-1,1'-spirobi(indane) (5): To a cooled solution of **1** (10g, 32.46 mmol) in acetone (80 ml), powdered potassium carbonate (22.43g, 162.33 mmol) was added and the reaction mixture was stirred at room temperature for 15 min. To this pre-cooled mixture (ice bath), dimethyl sulphate (Me_2SO_4) (20.47g, 15.36 ml, 162.33 mmol) was added drop wise. The ice bath was removed and the reaction mixture stirred at room temperature for 8 h. The reaction was poured over ice water with constant stirring. The white precipitate was filtered and washed several times with chilled water and dried in decicator over P_2O_5 provides **5** as white solid. Yield 10.5 g (96.25 %); (R_f =

0.7, 15 % EtOAc/Pet.ether); Mp: 120-121 °C; IR ($CHCl_3$) ν(cm^{-1}) = 3018, 2956, 2862, 2358, 1608, 1558, 1488, 1456, 1313, 1271, 1215, 1118, 1031, 929, 757, 669; ^{1}H NMR (300 MHz, $CDCl_3$) : δ 7.10-7.06 (d, *J* = 8.34 Hz, 2 H), 6.81-6.76 (dd, *J* = 2.41, 8.3 Hz, 2 H), 6.34-6.33 (d, *J* = 2.4 Hz, 2 H), 3.7 (s, 6 H), 2.38-2.20 (q, *J* = 8.84 Hz, 4 H), 1.38 (s, 6 H), 1.32 (s, 6 H); ^{13}C NMR (50 MHz, $CDCl_3$) : δ 159.2, 151.8, 144.5, 122.4, 113.2, 109.0, 59.5, 57.8, 55.3, 42.7, 31.7, 30.5, LCMS : 375.1 (M + K); Anal. Calcd. (%) for $C_{23}H_{28}O_2$: C = 82.10, H = 8.39; found: C = 81.93, H = 8.67.

5,5'-Diacetyl-6,6'-dimethoxy-3,3,3',3'-tetramethyl-1,1'-spirobi(indane) (6): To a solution of **5** (7g, 20.8 mmol) in dry DCM (60 ml) containing acetyl chloride (9g, 8.15 ml, 125 mmol) $SnCl_4$ (29.89g, 13.42 ml, 125 mmol) was added drop wise at 0 °C. The reaction mixture was stirred at 0 °C for another 15 min. The ice bath was removed and the reaction mixture stirred at room temperature for 24 h. The reaction mixture was cooled in ice bath and diluted with DCM (50 ml). The reaction was quenched by drop wise addition of water (10 ml) and then with 1N HCl (80 ml). The product was extracted with DCM (3 x 250ml). Further purification by column chromatography provided **6** as white crystalline solid. Yield 7.531 g (86.06 %); (R_f = 0.5, 15 % EtOAc/Pet.ether); Mp: 194-196 °C; IR ($CHCl_3$) ν(cm^{-1}): 3018, 2999, 2956, 2947, 2864, 2333, 1666, 1600, 1566, 1481, 1465, 1404, 1359, 1282, 1244, 1224, 1182, 1153, 1136, 1043, 1008, 916, 846, 754, 667; ^{1}H NMR (200 MHz, $CDCl_3$) : δ 7.57 (s, 2 H), 6.32 (s, 2 H), 3.74 (s, 3 H), 2.6 (s, 3 H), 2.40-2.34 (d, *J* = 13.14 Hz, 2 H), 2.26-2.19 (d, *J* = 13.14 Hz, 2 H), 1.4 (s, 6 H), 1.33 (s, 6 H); ^{13}C NMR (50 MHz, $CDCl_3$) : δ 199.9, 159.2, 155.9, 144.4, 127.9, 123.8, 106.8, 59.0, 58.3, 55.6, 42.9, 31.7, 31.4, 30.2; LCMS : 421.2 (M + 1), 443.2 (M + Na); Anal. Calcd. (%) for $C_{27}H_{32}O_4$: C = 77.11, H = 7.67; found: C = 77.31, H = 7.42.

6,6'-Dimethoxy-3,3,3',3'-tetramethyl-1,1'-spirobi(indan)-5,5'-dicarboxylic acid (7): To a 1000 ml round bottom flask containing sodium hypochlorite (NaOCl) solution (500 ml, 4% w/v) and dioxane (80 ml), **6** (8.5g, 20.23 mmol) was added. Then, powdered sodium hydroxide (31g) was added slowly at 0 °C with vigorous stirring. The ice bath was removed and the reaction mixture was heated at 70 °C for 24 h. The reaction mixture was washed with DCM (200 ml) to remove any unreacted starting material. The aqueous layer was acidified with conc. HCl to precipitate the bis-acid which was filtered, dried and recrystallized from DCM:MeOH (4:1) to furnish **7** as a colorless crystalline solid. Yield 6.57 g (76.57 %); Decomposed at 272-278 °C; IR ($CHCl_3$) ν(cm^{-1}): 3244, 3012, 2962, 1731, 1610, 1481, 1471, 1419, 1215, 1047, 759, 667; ^{1}H NMR (200 MHz, DMSO-d_6) : δ 7.6 (s, 2 H), 6.46 (br, 2 H), 6.29 (s, 2 H), 3.69 (s, 6 H), 2.35-2.28 (d, *J* = 13.13 Hz, 2 H), 2.19-2.13 (d, *J* = 13.13 Hz, 2 H), 1.34 (s, 6 H), 1.26 (s, 6 H); ^{13}C NMR (50 MHz, $CDCl_3$ + DMSO-d_6) : δ 166.4, 157.7, 154.5, 143.2, 124.5, 118.4, 106.1, 57.8, 57.2, 55.2, 41.8, 30.4, 29.1; LCMS : 425.1 (M + 1); Anal. Calcd. (%) for $C_{25}H_{28}O_6$, C = 70.74, H = 6.65; found: C = 70.80, H = 6.57.

6,6'-Dimethoxy-3,3,3',3'-tetramethyl-5,5'-dinitro-1,1'-spirobi(indane) (9): To a chilled mixture (0 °C) of glacial acetic acid (70 ml), concentrated nitric acid (20 ml), and conc. sulphuric acid (8 ml, 99 %) 5g (14.88 mmol) of **5** were slowly added. The reaction mixture was stirred for 5 min at 0 °C and then at room temperature for 30 min. The reaction was poured into ice water and the precipitate was filtered off, dried, and purified by column chromatography furnished **9** as yellow solid. Yield 5.73 g (89.85 %); (R_f = 0.4, 12.5 % EtOAc/Pet.ether); Mp: 246-247 °C; IR ($CHCl_3$) ν(cm^{-1}): 3020, 2962, 2399, 1618, 1581, 1521, 1487, 1458, 1350, 1292, 1215, 1155, 1058, 929, 757, 669.5; ^{1}H NMR (300 MHz,

$CDCl_3$) : δ 7.64 (s, 2 H), 6.41 (s, 2 H), 3.8 (s, 6 H), 2.47-2.40 (d, *J* = 13.26 Hz, 2 H), 2.77-2.21 (d, *J* = 13.26 Hz, 2 H), 1.42 (s, 6 H), 1.36 (s, 6 H); ^{13}C NMR (50 MHz, $CDCl_3$) : δ 155.6, 153.1, 144.3, 139.6, 119.4, 108.7, 58.7, 58.6, 56.6, 43.2, 31.3, 30.0; LCMS : 427.1 (M + 1), 449.14 (M + Na); Anal. Calcd. (%) for $C_{23}H_{26}N_2O_6$: C = 64.78, H = 6.15, N = 6.57; found: C = 64.78, H = 6.65, N = 6.33.

5,5'-Diamino-6,6'-dimethoxy-3,3,3',3'-tetramethyl-1,1'-spirobi(indane) (10): **9** (5g, 11.737 mmol) was subjected to transfer hydrogenation in a 500 ml flask containing methanol (120 ml), ammonium formate (7.40g, 117.37 mmol), and 10% Pd/c (0.5g, 10 mol %). The crude bis-amine **10** was purified by column chromatography. Yield 3.78 g (88 %); (R_f = 0.25, 20 % EtOAc/Pet.ether); Mp: 235-238 °C; IR ($CHCl_3$) ν(cm^{-1}): 3461, 3382, 3018, 2954, 2399, 1618, 1596, 1500, 1458, 1446, 1317, 1215, 1080, 1018, 908, 862, 757, 669; ^{1}H NMR (300 MHz, $CDCl_3$) : δ 6.58 (s, 2 H), 6.25 (s, 2 H), 3.86 (br, 2 H), 3.7 (s, 6 H), 2.31-2.24 (d, *J* = 13.01 Hz, 2 H), 2.16-2.10 (d, *J* = 12.88 Hz, 2 H), 1.33 (s, 6 H), 1.29 (s, 6 H); ^{13}C NMR (75 MHz, $CDCl_3$) : δ 147.2, 144.4, 140.4, 135.2, 108.0, 106.1, 59.7, 57.5, 55.6, 42.7, 31.5, 30.4; LCMS : 367.2 (M + 1); Anal. Calcd. (%) for $C_{23}H_{30}N_2O_2$: C = 75.37, H = 8.25, N = 7.64; found: C = 75.13, H = 8.48, N = 7.43.

5,5'-Bis(2,2,2-trifluroacetamido)-6,6'-dimethoxy-3,3,3',3'-tetramethyl-1,1'-spirobi(indane) (11): To a solution of the bis-amine **10** (6g, 16.39 mmol) in dry acetonitrile (40 ml) maintained at 0 °C, trifluoroacetic acid (5.6g, 3.8ml, 49.18 mmol) and N,N'-dicyclohexylcarbodiimide (DCC) (10.14g, 49.2 mmol) were added under argon atmosphere. The reaction mixture was stirred at room temperature over night and then filtered. The filtrate was concentrated to afford the crude product, which was purified by column chromatography to furnish **11** as white solid. Yield 8.32 g (89.76 %); (R_f = 0.7,

10 % EtOAc/Pet.ether); Mp: 202-204 °C; IR ($CHCl_3$) ν(cm^{-1}): 3404, 3020, 2958, 2862, 2434, 2401, 1733, 1608, 1537, 1488, 1465, 1421, 1317, 1217, 1151, 1080, 1060, 1014, 908, 891, 848, 769, 669; ^{1}H NMR (200 MHz, $CDCl_3$) : δ 8.59 (s, 2 H), 8.16 (s, 2 H), 6.31 (s, 2 H), 3.77 (s, 6 H), 2.40-2.34 (d, *J* = 13.14 Hz, 2 H), 2.22-2.16 (d, *J* = 13.01 Hz, 2 H), 1.41 (s, 6 H), 1.34 (s, 6 H), 1.34 (s, 6 H); ^{13}C NMR (50 MHz, $CDCl_3$) : δ 154.6, 153.9, 148.3, 147.2, 144.8, 124.4, 113.8, 105.6, 59.2, 58.2, 56.1, 43.4, 31.4, 30.2; LCMS : 581.1 (M + Na); Anal. Calcd. (%) for $C_{27}H_{28}F_6N_2O_4$: C = 58.06, H = 5.05, N = 5.02; found: C = 57.79, H = 5.31, N = 5.26.

5-Amino-5'-(2,2,2-trifluroacetamido)-6,6'-dimethoxy-3,3,3',3'-tetramethyl-1,1' spirobi(indane) (12): To a solution of **11** (2g, 3.533 mmol) in methanol (25 ml) containing water (2 ml), powdered potassium carbonate (0.73g, 5.3 mmol) was added. The reaction mixture was stirred at room temperature for 12 h. The volatiles were removed under reduced pressure and the residue was extracted with DCM. The organic layer was washed with water followed by brine and dried over anhydrous Na_2SO_4, concentrated and purified by column chromatography affording **12** as white solid. Yield 0.73 g (44.85 %); (R_f = 0.25, 7.5 % EtOAc/Pet.ether); Mp: 87 °C; IR ($CHCl_3$) ν(cm^{-1}): 3442, 3365, 3018, 2948, 2856, 2837, 2661, 2401, 2343, 1721, 1619, 1502, 1488, 1463, 1450, 1379, 1317, 1276, 1253, 1191, 1168, 1147, 1118, 1087, 1060, 1029, 1008, 970, 927, 891, 810, 775, 757, 667; ^{1}H NMR (200 MHz, $CDCl_3$) : δ 8.6 (s, 1 H), 8.14 (s, 1 H), 6.77 (s, 1 H), 6.36 (s, 1 H), 6.23 (s, 1 H), 4.92 (bs, 2 H), 3.78 (s, 3 H), 3.72 (s, 3 H), 2.37-2.12 (m, 4 H), 1.4 (s, 3 H), 1.35 (s, 3 H), 1.33 (s, 3 H), 1.31 (s, 3 H); ^{13}C NMR (125 MHz, $CDCl_3$) : δ 30.2, 30.4, 31.4, 31.5, 43.1, 43.2, 55.8, 56.2, 57.9, 59.3, 59.5, 105.8, 106.2, 110.4, 113.7, 124.2, 131.6, 142.4, 144.6, 144.7, 147.9, 148.2, 148.6, 153.7, 154.0,

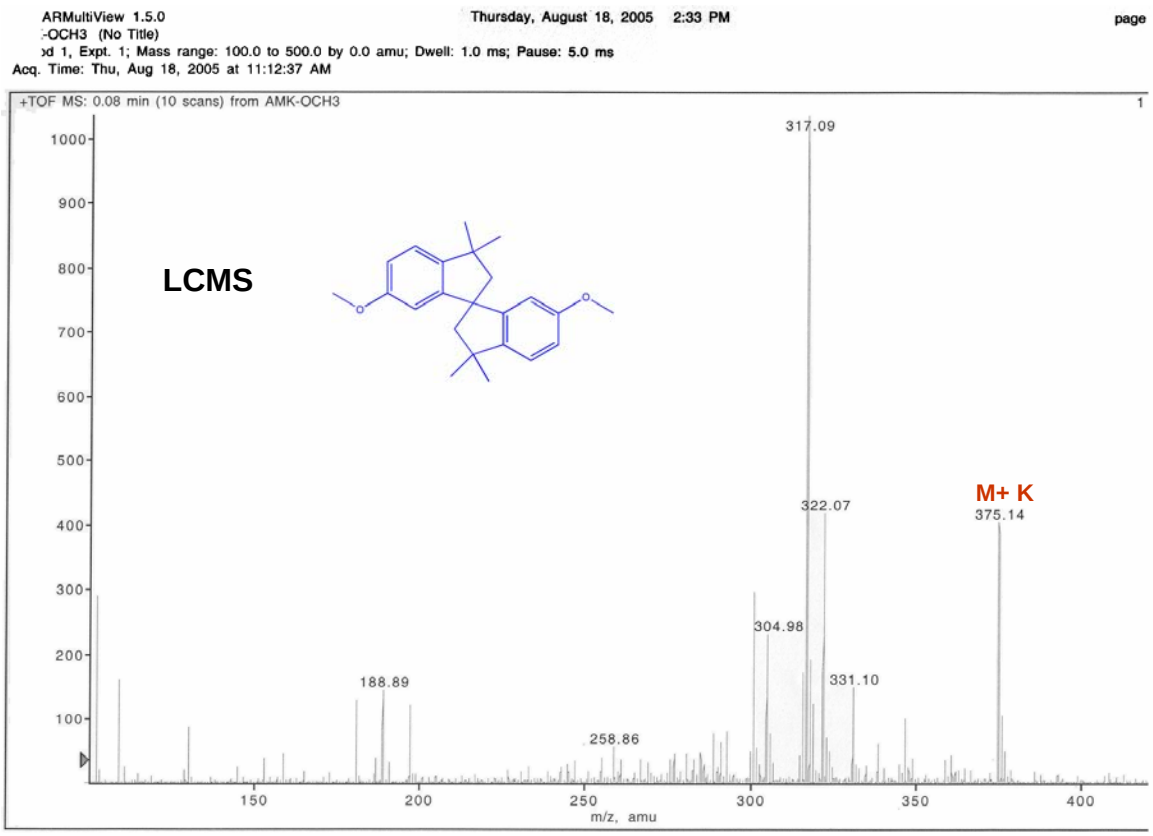
154.3; LCMS : 463.2 (M + 1), 485.1 (M + Na), 501.1 (M + K); Anal. Calcd. (%) for $C_{25}H_{29}F_3N_2O_3$: C = 64.92, H = 6.32, N = 6.06; found: C = 64.69, H = 6.08, N = 6.24.

Trimer (2): To a solution of bis-acid **7** (1.1g, 2.521 mmol) in DCM (10 ml) containing DMF (cat.), oxalyl chloride was added (1.92g, 1.31ml, 15.127 mmol) drop wise at 0 °C under argon atmosphere. The ice bath was removed and the reaction mixture was stirred at room temperature for 3 h. The volatiles were removed under reduced pressure. The crude acid chloride was dissolved in DCM (10 ml). To this mixture, the mono-amine **12** (2.91g, 6.30 mmol) and triethylamine (1.02g, 1.42 ml, 10.08 mmol) were added and the reaction mixture was stirred at room temperature over night. The reaction mixture was stripped off the solvent under reduced pressure and the crude product was purified by column chromatography to give **2** as a white solid. Yield 2.51 g (81.22 %); (R_f = 0.35, 15% EtOAc/Pet.ether); Mp: > 275 °C; IR ($CHCl_3$) ν(cm^{-1}): 3404, 3336, 3018, 2958, 2866, 2401, 1728, 1652, 1602, 1537, 1485, 1417, 1315, 1215, 1149, 1060, 1014, 757, 667; ^{1}H NMR (400 MHz, $CDCl_3$) : δ 10.66 (s, 2 H), 8.59 (s, 2 H), 8.54 (s, 2 H), 8.20 (s, 2 H), 8.15 (s, 2 H), 6.44 (s, 2 H), 6.38 (s, 2 H), 6.31 (s, 2 H), 3.9 (s, 6 H), 3.79 (s, 6 H), 3.78 (s, 6 H), 2.45-2.20 (m, 12 H), 1.47 (s, 6 H), 1.45 (s, 6 H), 1.41 (s, 6 H), 1.39 (s, 6 H), 1.38 (s, 6 H), 1.34 (s, 6 H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 30.2, 30.3, 30.3, 31.4, 31.5, 43.1, 43.2, 43.3, 43.4, 56.2, 56.2, 56.3, 57.0, 58.1, 59.4, 58.5, 59.0, 59.3, 59.5, 105.4, 105.8, 106.9, 107.0, 107.2, 113.7, 113.8, 114.3, 117.1, 121.8, 124.2, 125.9, 126.1, 127.5, 128.1, 144.4, 144.8, 144.8, 145.4, 147.8, 148.2, 148.4, 153.6, 154.0, 154.4, 154.5, 155.2, 157.6, 158.2, 163.2, 165.5; LCMS: 1313.6 (M + 1); Anal. Calcd. (%) for $C_{75}H_{82}F_6N_4O_{10}$: C = 68.58, H = 6.29, N = 4.27; found: C = 68.72, H = 6.08, N = 4.33.

Mono-trifluoroacetamide trimer (3): To a solution of the trimer **2** (1g, 0.762 mmol) in methanol (50 ml) containing water (2 ml) and dioxane (30 ml), powdered potassium carbonate (0.158g, 5eq, 1.143 mmol) was added. The reaction mixture was stirred at room temperature for 24 h. The volatiles were removed under reduced pressure and the product was purified by column chromatography. Yield 0.31 g (34.23 %); (R_f = 0.3, 20 % EtOAc/Pet.ether); Mp: > 275 °C; IR ($CHCl_3$) ν(cm^{-1}): 3402, 3336, 3018, 2956, 2862, 2434, 2399, 1724, 1654, 1602, 1537, 1483, 1465, 1417, 1315, 1247, 1149, 1060, 1014, 929, 908, 892, 848, 669; ^{1}H NMR (400 MHz, $CDCl_3$) : δ 10.70 (b, 1 H), 10.67 (b, 1 H), 8.63 (b, 1 H), 8.57 (s, 1 H), 8.55-8.54 (d, *J* = 3.7 Hz, 1 H), 8.23-8.22 (d, *J* = 2 Hz, 2H), 8.18 (s, 1 H), 6.71 (s, 1 H), 6.47-6.45 (d, *J* = 4.2 Hz, 2 H), 6.40-6.39 (d, *J* = 6.5 Hz, 2 H), 6.33-6.30 (d, *J* = 12 Hz, 2 H), 3.93 (s, 6 H), 3.81 (s, 6 H), 3.8 (s, 3 H), 3.74 (s, 3 H), 2.47-2.19 (m, 12 H), 1.49-1.29 (m, 36 H); ^{13}C NMR (100 MHz, $CDCl_3$) : δ 163.2, 163.1, 157.5, 155.2, 155.1, 154.3, 154.0, 148.4, 148.3, 148.2, 148.0, 147.8, 145.4, 145.4, 145.3, 145.2, 144.8, 144.7, 144.6, 144.6, 144.6, 144.5, 144.3, 128.1, 127.7, 127.7, 125.9, 124.2, 121.8, 121.8, 121.7, 117.1, 114.2, 113.8, 113.7, 113.6, 107.0, 106.2, 105.8, 105.5, 105.3, 59.5, 59.4, 59.2, 58.4, 58.0, 57.8, 56.3, 56.2, 56.2, 56.1, 56.1, 55.8, 43.4, 43.2, 43.2, 43.1, 42.9, 31.5, 31.4, 31.4, 30.4, 30.3, 30.3, 30.2, 30.2; LCMS : 1217.5 (M + 1), 1239.5 (M + Na); Anal. Calcd. (%) for $C_{73}H_{83}F_3N_4O_9$: C = 72.02, H = 6.87, N = 4.60; found: C = 72.24, H = 6.67, N = 4.77.

Heptamer (4): To a solution of bis-acid **7** (0.045g, 0.106 mmol) in DCM (5 ml) containing dry DMF (cat.), oxalyl chloride (0.08g, 0.05 ml, 0.636 mmol) was added at 0 °C under argon atmosphere. The ice bath was removed and the reaction mixture stirred at room temperature for 3 h. The volatiles were stripped off and a mixture of mono-amine **3**

(0.322g, 0.265 mmol) dissolved in DCM (10 ml) and triethyl amine (0.054g, 0.07 ml, 0.530 mmol) were added to this crude bis-acid chloride at 0 °C. The ice bath was removed after the addition and the reaction mixture was stirred at room temperature for 12 h. Purification of the crude material by column chromatography furnished **4** as white solid. Yield 0.197 g (65.88 %); (R_f = 0.35, 35 % EtOAc/Pet.ether); Mp: > 275 °C; IR ($CHCl_3$) ν(cm^{-1}): 3404, 3338, 3010, 2958, 2864, 2399, 1733, 1654, 1600, 1533, 1481, 1481, 1465, 1417, 1315, 1286, 1215, 1149, 1070, 1016, 929, 848, 769, 669; ^{1}H NMR (400 MHZ, CDCl3) : δ 10.66 (s, 3 H), 10.62 (s, 3 H), 8.58 (bs, 2 H), 8.53 (s, 2 H), 8.52 (s, 4 H), 8.20 (s, 2 H), 8.19 (s, 4 H), 8.15 (s,2 H), 6.43 (s, 6 H), 6.37 (s, 6 H), 6.29 (s, 2 H), 3.89 (s, 18 H), 3.78 (s, 12 H), 3.77 (s, 12 H), 2.44-2.19 (m, 28 H), 1.46 (s, 18 H), 1.45 (s, 18 H), 1.41 (s, 6 H), 1.38 (s, 36 H), 1.34 (s, 6 H); ^{13}C NMR(100 MHz, CDCl3) : δ 163.2, 157.6, 155.2, 155.1, 155.1, 148.4, 148.2, 147.8, 145.5, 145.4, 145.1, 145.0, 144.8, 144.8, 144.4, 128.1, 128.1, 127.9, 127.8, 125.9, 124.2, 121.9, 121.8, 117.1, 113.9, 113.8, 113.7, 107.0, 105.9, 105.6, 105.4, 59.6, 59.5, 59.3, 58.4, 58.1, 59.0, 56.3, 56.2, 56.2, 43.4, 43.3, 43.3, 43.23, 31.5, 31.4, 30.4, 30.3, 30.3; MALDI-TOF MS : 2843.84 (M + Na); Anal. Calcd. (%) for $C_{171}H_{190}F_6N_8O_{22}$: C = 72.74, H = 6.78, N = 3.97; found : C = 72.54, H = 6.54, N = 4.21.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Thursday, August 18, 2005 2:33 PM
page
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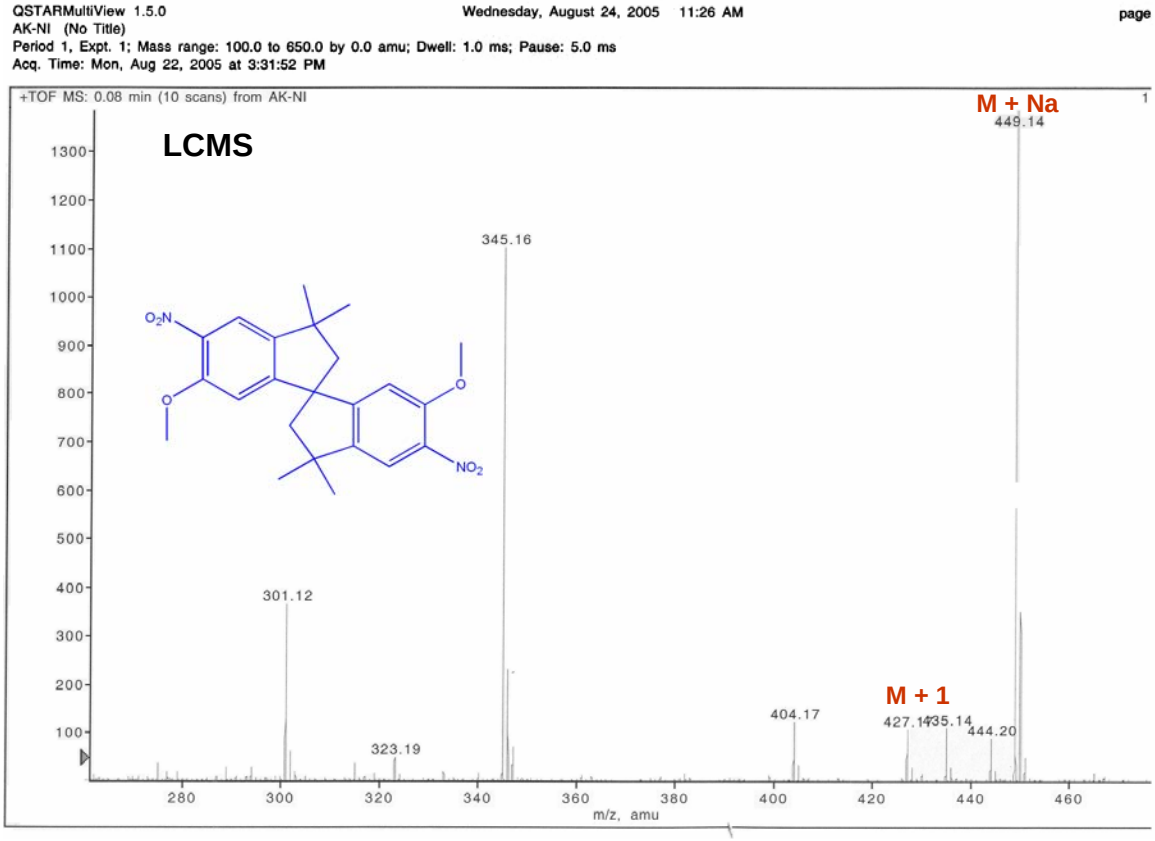
LCMS
317.09
322.07
M+ K
375.14
304.98
331.10
188.89
258.86
m/z, amu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page
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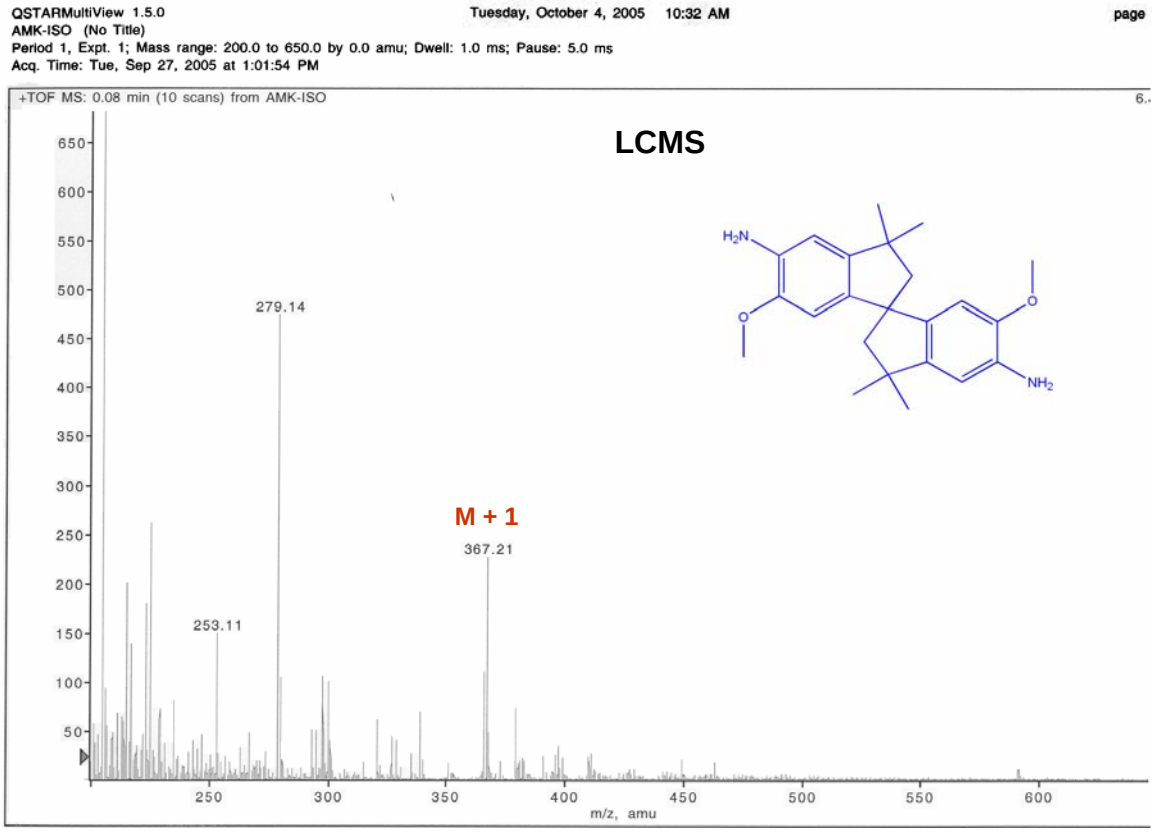
LCMS
M + Na
449.14
345.16
301.12
323.19
404.17
M + 1
427.14
435.14
444.20
m/z, amu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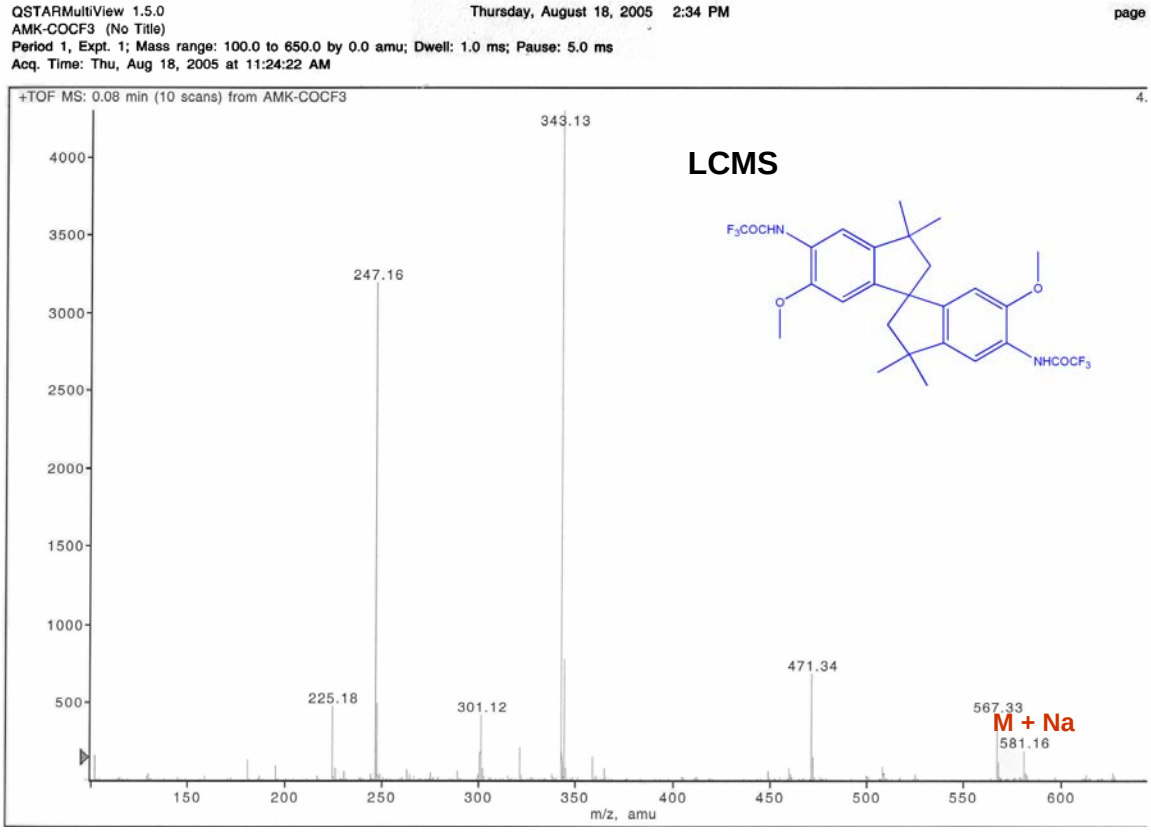
LCMS
279.14
M + 1
367.21
253.11
m/z, amu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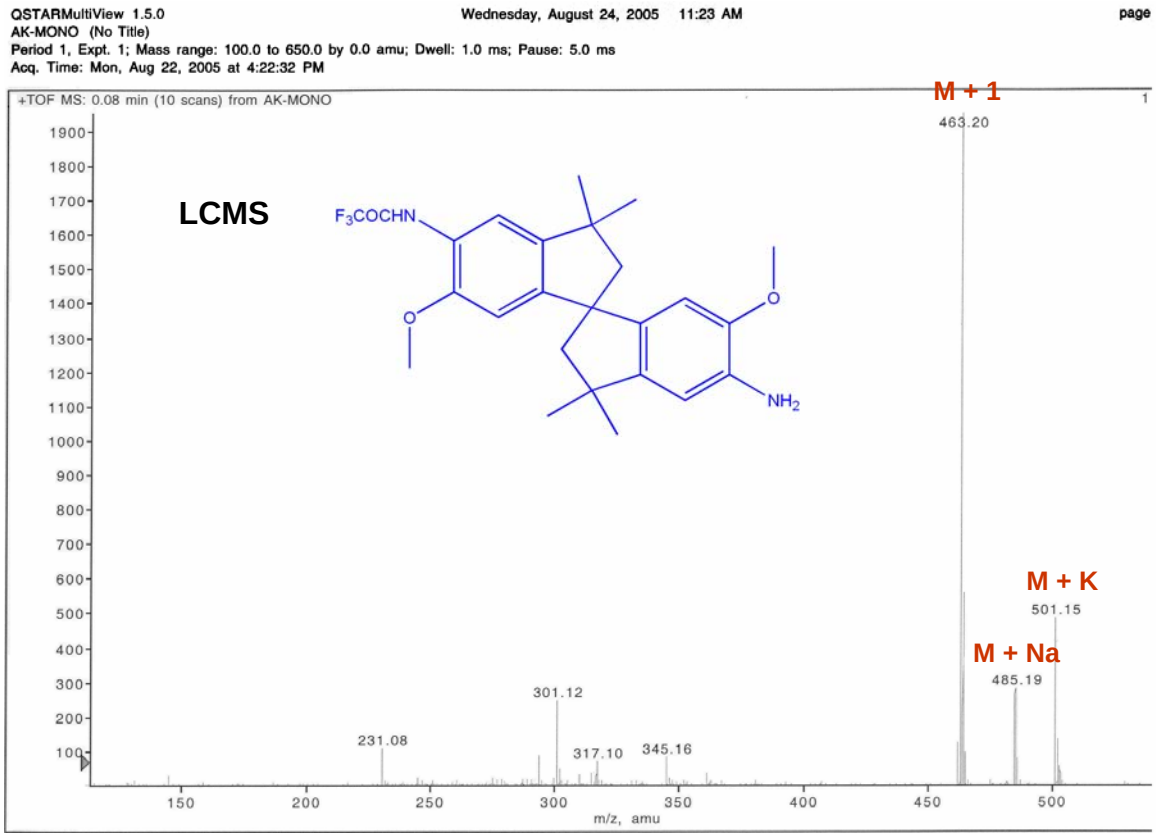
LCMS
343.13
247.16
471.34
225.18
301.12
567.33
M + Na
581.16
m/z, amu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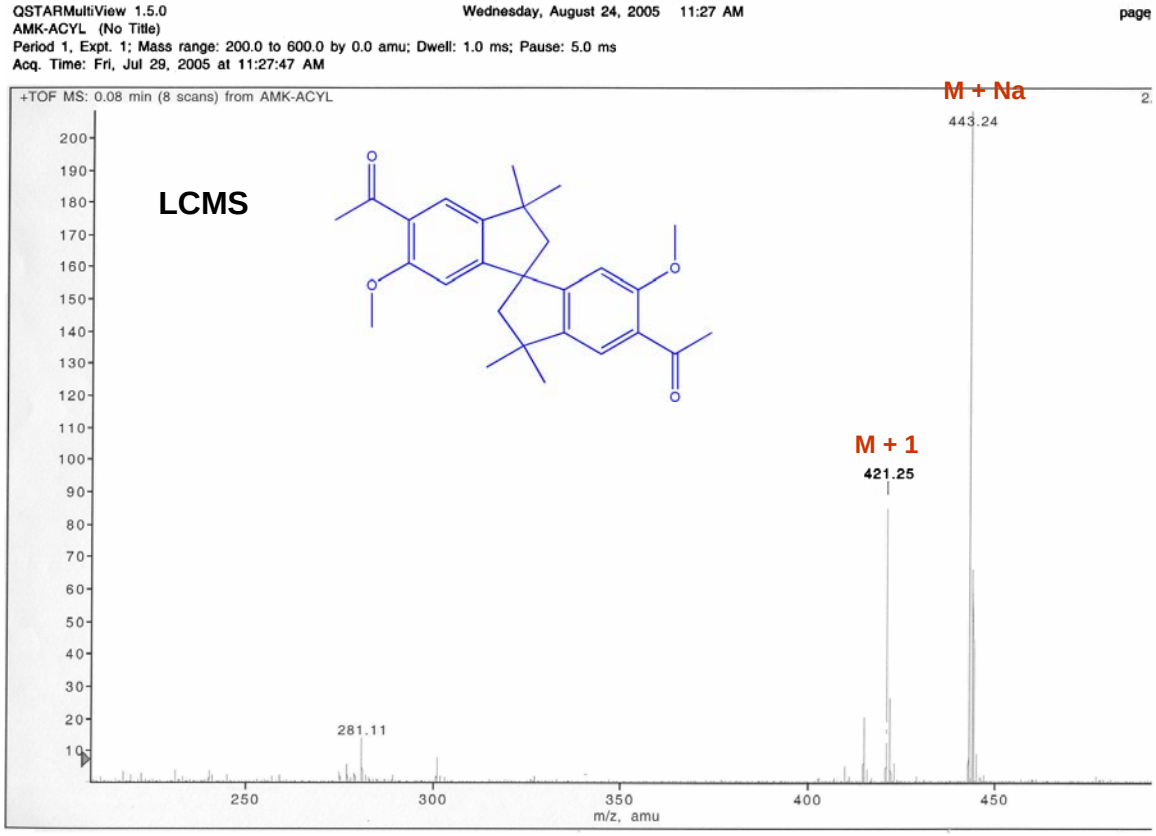
LCMS
F3COCHN
NH2
M + 1
463.20
M + K
501.15
M + Na
485.19
301.12
231.08
317.10
345.16
m/z, amu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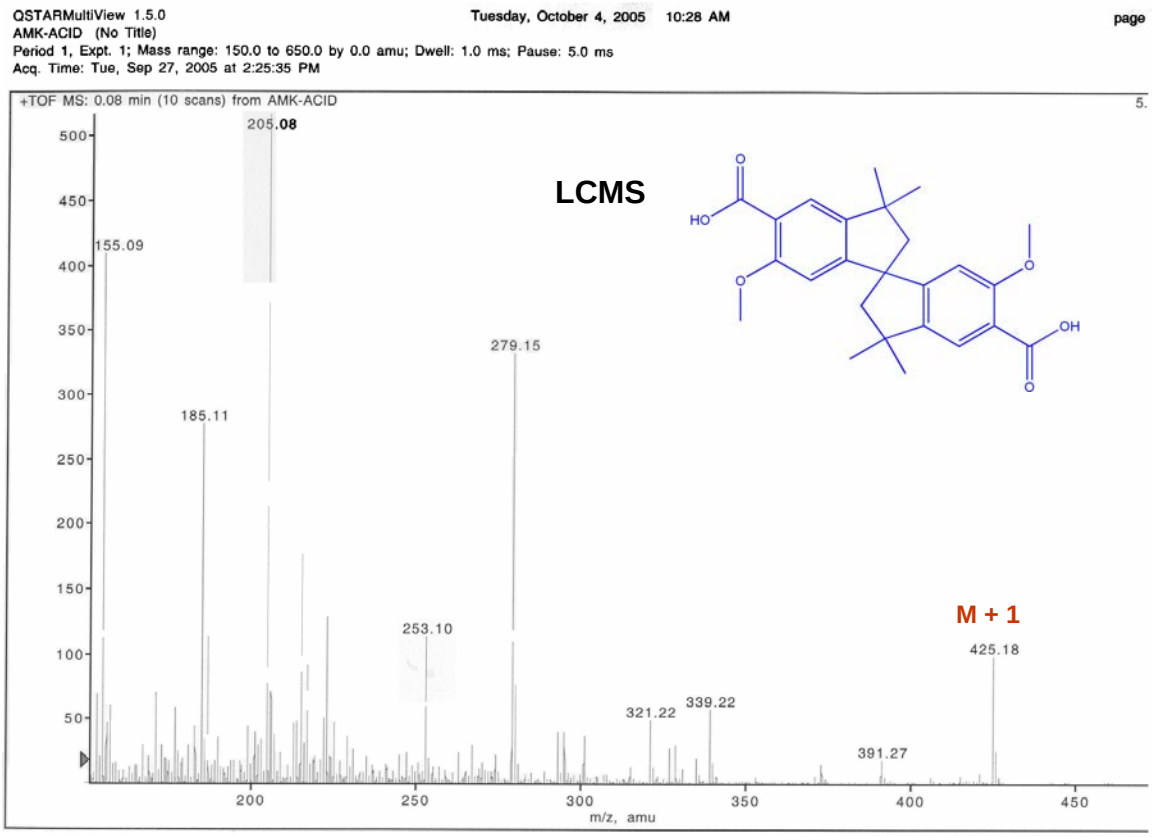
LCMS
M + Na
443.24
M + 1
421.25
281.11
m/z, amu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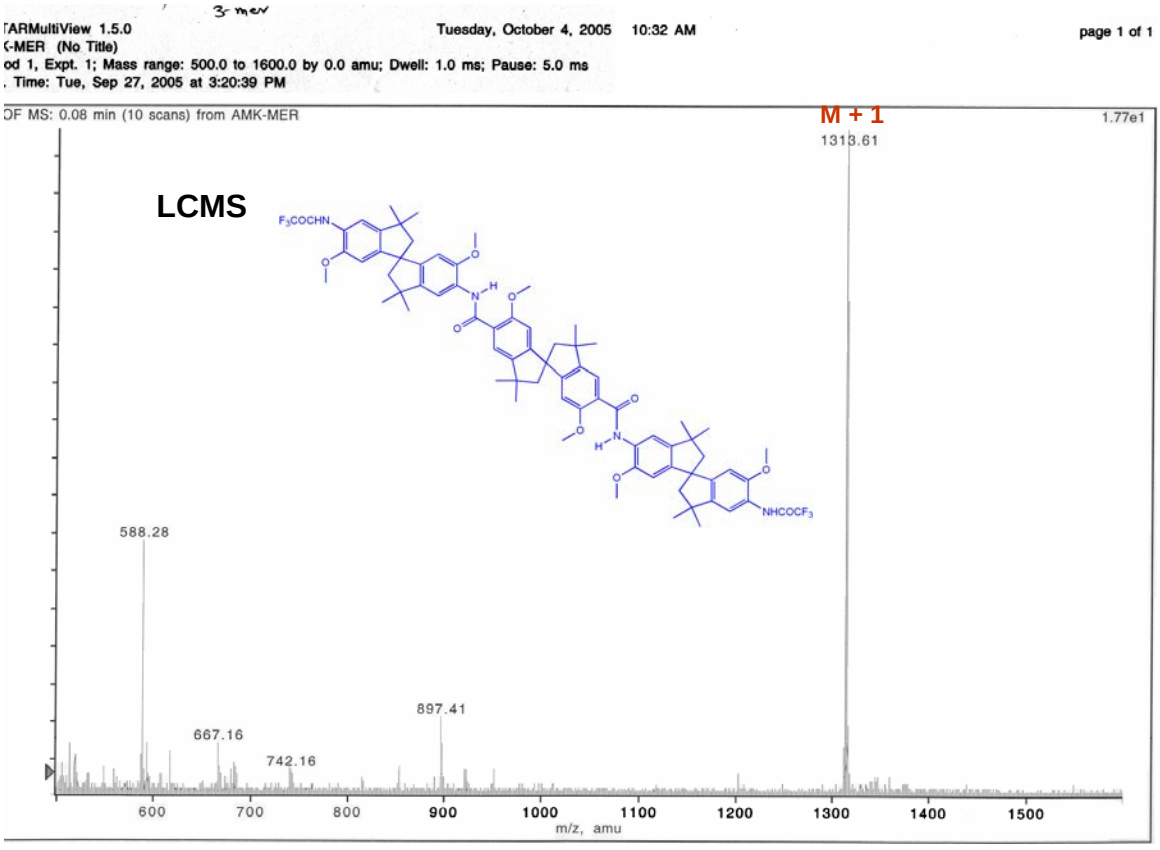
LCMS
205.08
155.09
279.15
185.11
253.10
425.18
321.22
339.22
391.27
M + 1
m/z, amu


3- mer
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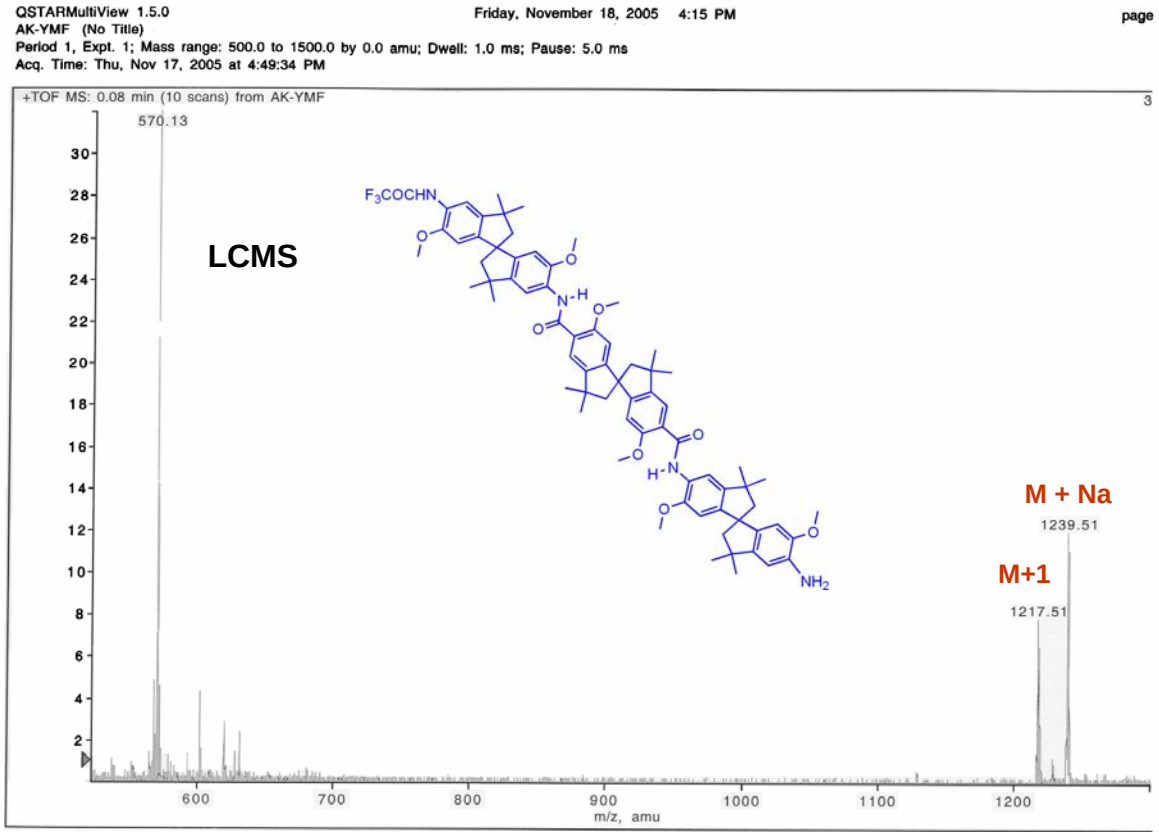
Tuesday, October 4, 2005 10:32 AM
page 1 of 1
(-MER (No Title)
od 1, Expt. 1; Mass range: 500.0 to 1600.0 by 0.0 amu; Dwell: 1.0 ms; Pause: 5.0 ms
. Time: Tue, Sep 27, 2005 at 3:20:39 PM
OF MS: 0.08 min (10 scans) from AMK-MER
LCMS
M + 1
1313.61
588.28
897.41
667.16
742.16
m/z, amu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Friday, November 18, 2005 4:15 PM
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+TOF MS: 0.08 min (10 scans) from AK-YMF
LCMS
M + Na
1239.51
M+1
1217.51
m/z, amu
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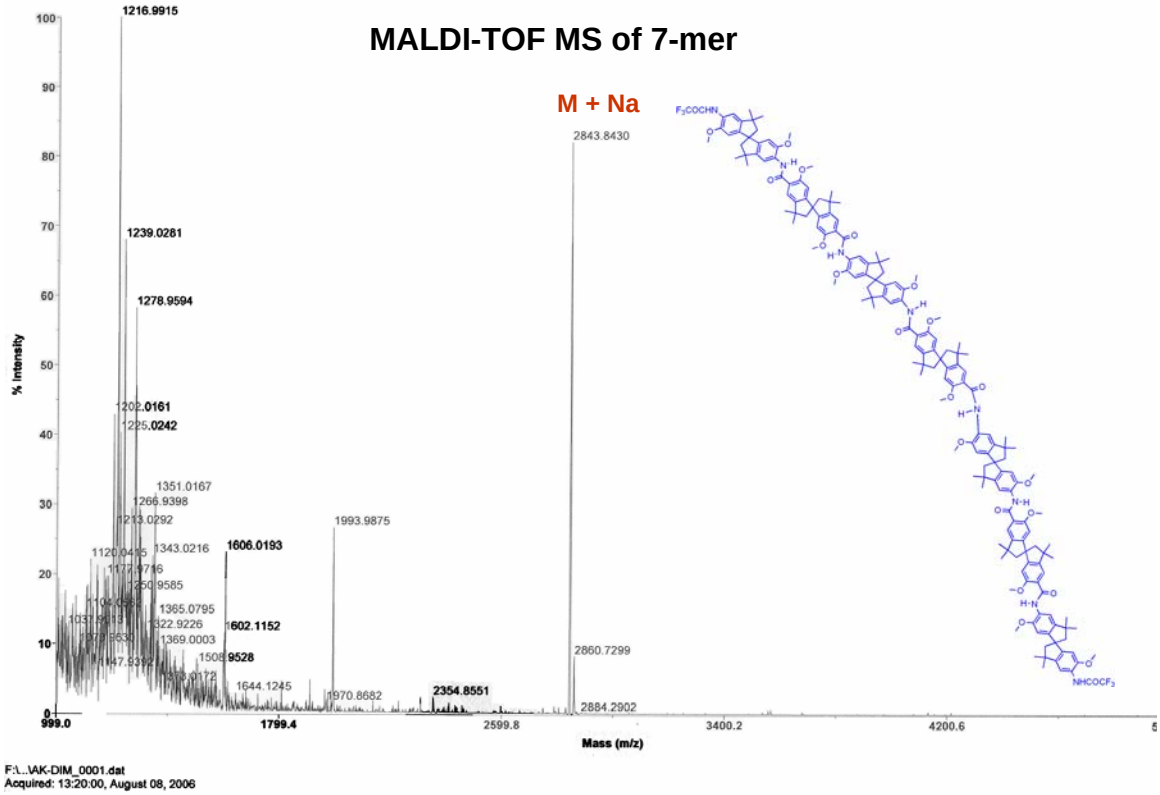
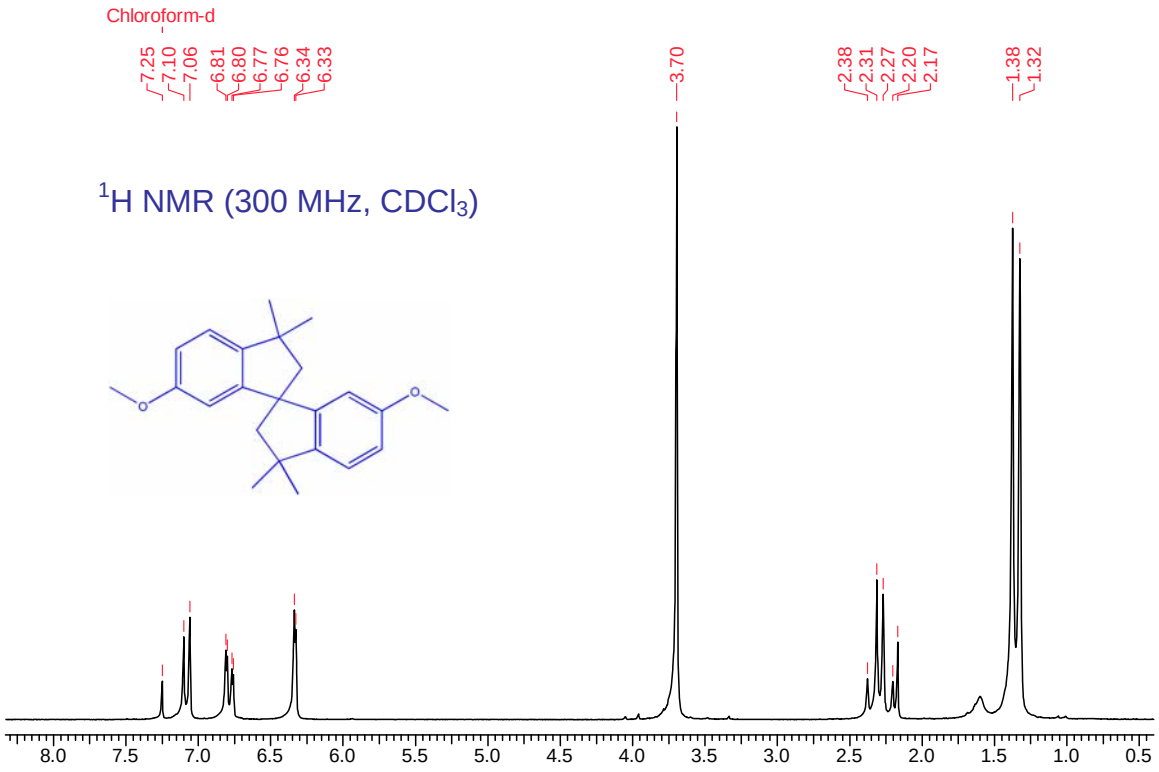
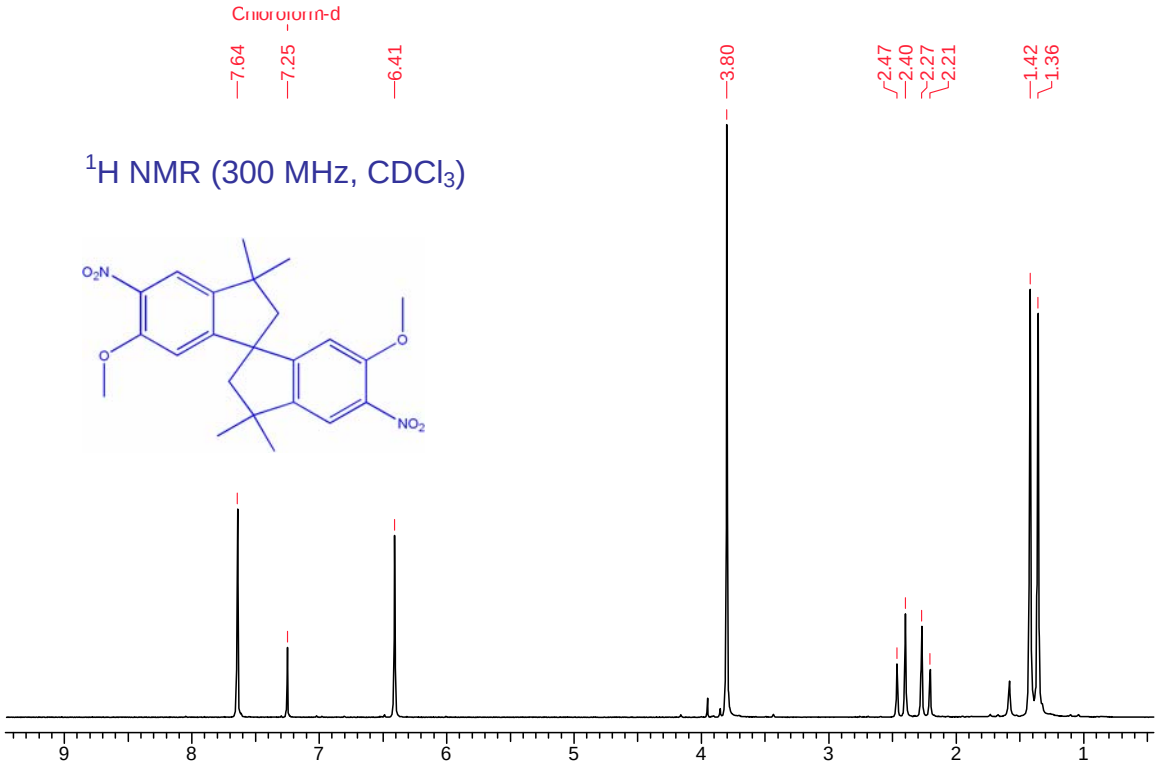
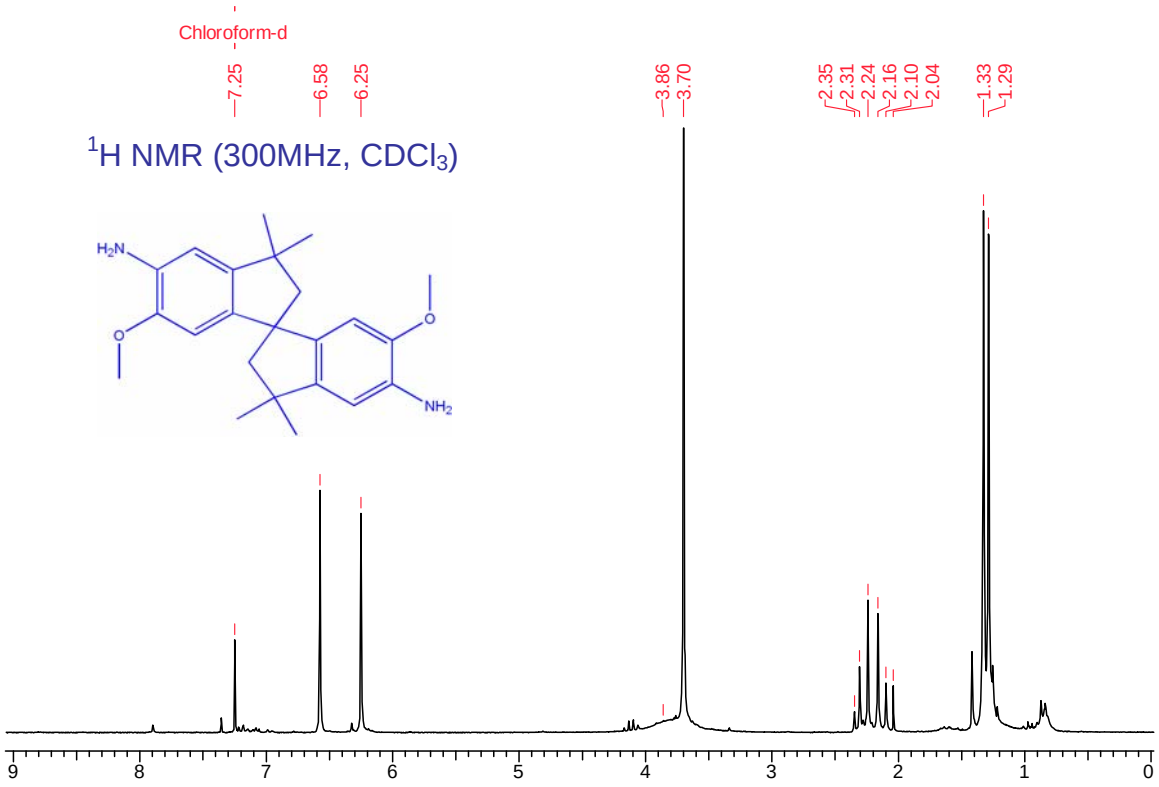
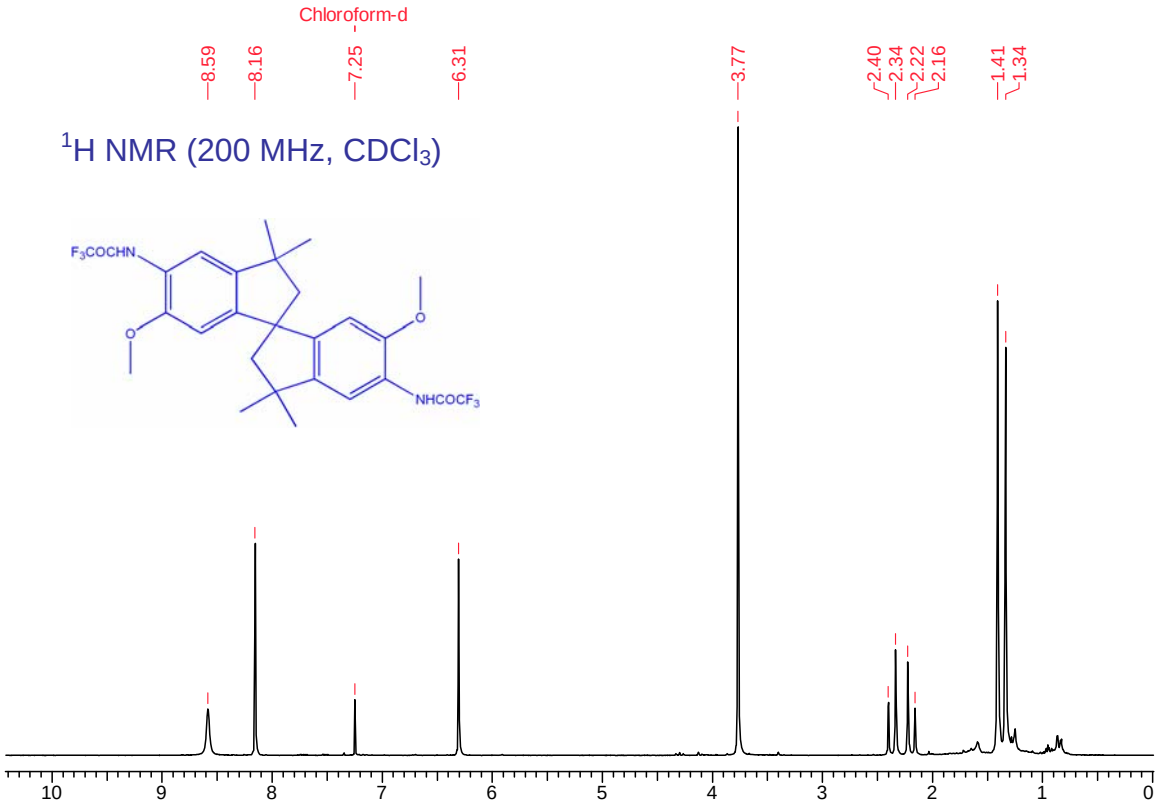
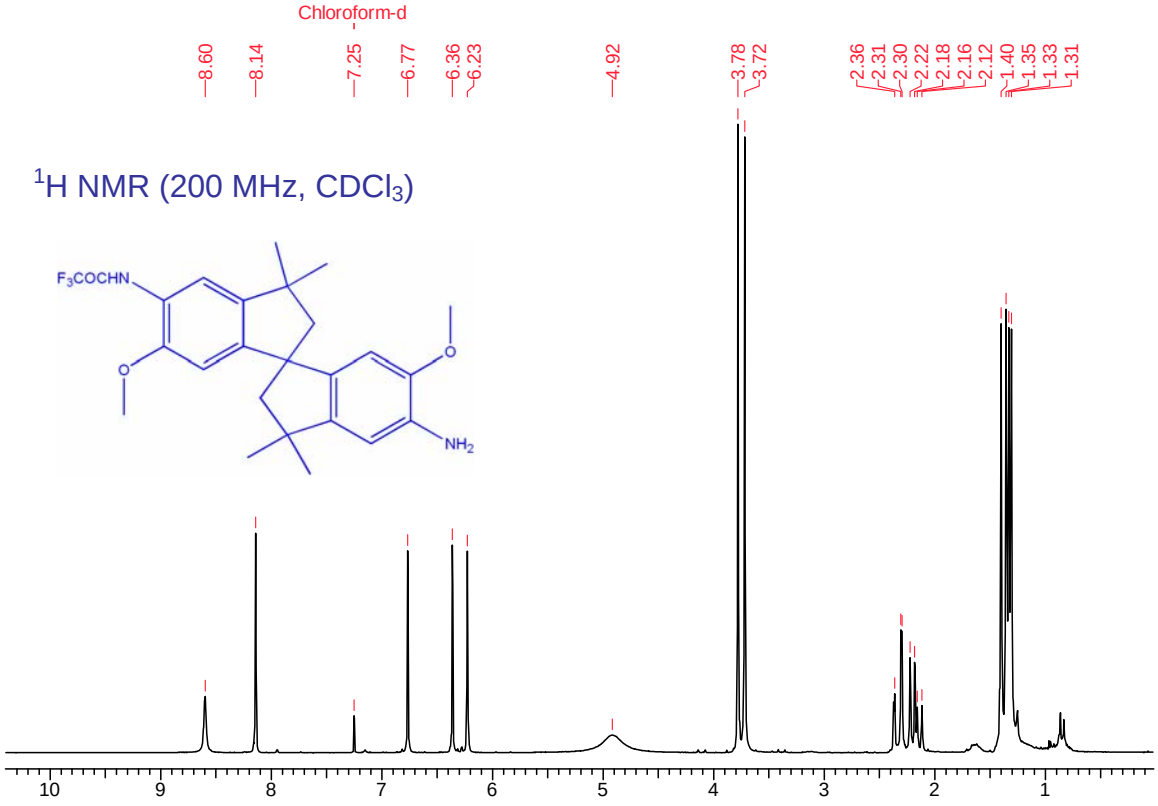

MALDI-TOF MS of 7-mer
M + Na
2843.8430
1216.9915
1239.0281
1278.9594
1993.9875
1606.0193
2860.7299
2884.2902
2354.8551
% Intensity
Mass (m/z)
F:\..\AK-DIM_0001.dat
Acquired: 13:20:00, August 08, 2006

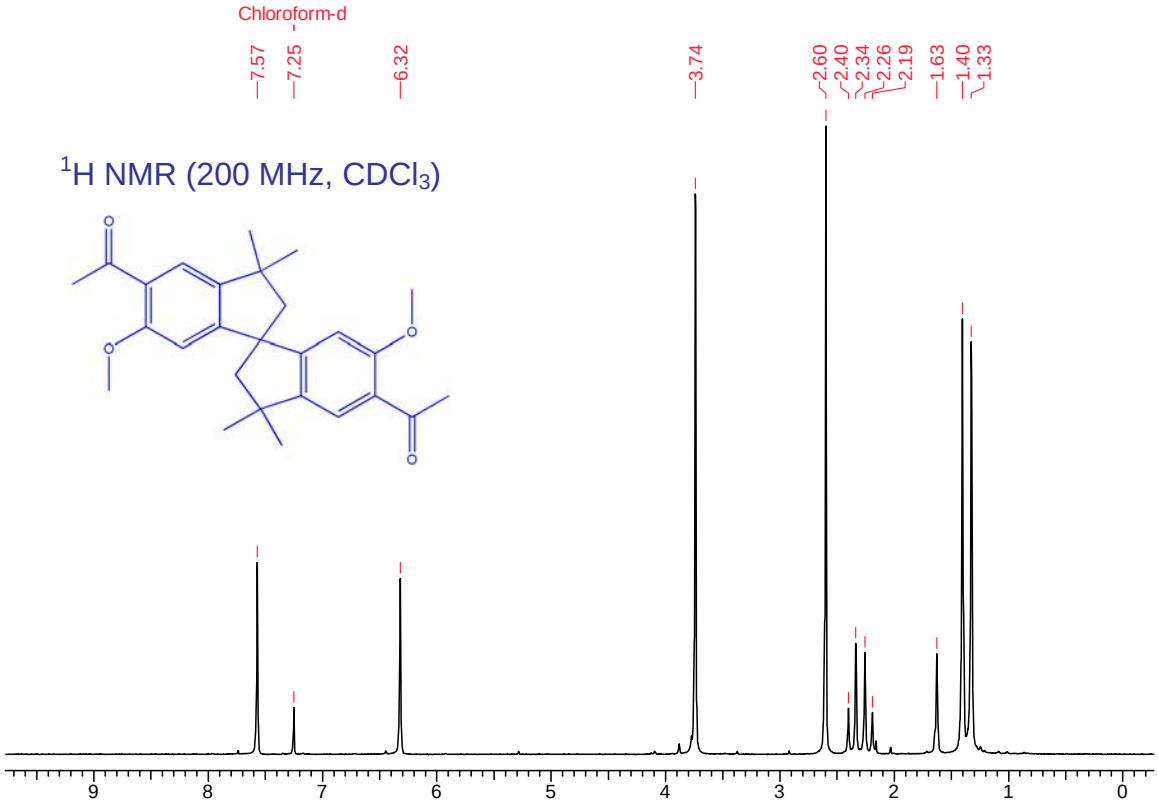

Chloroform-d
7.25
7.10
7.06
6.81
6.80
6.77
6.76
6.34
6.33
3.70
2.38
2.31
2.27
2.20
2.17
1.38
1.32
1H NMR (300 MHz, CDCl3)
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5

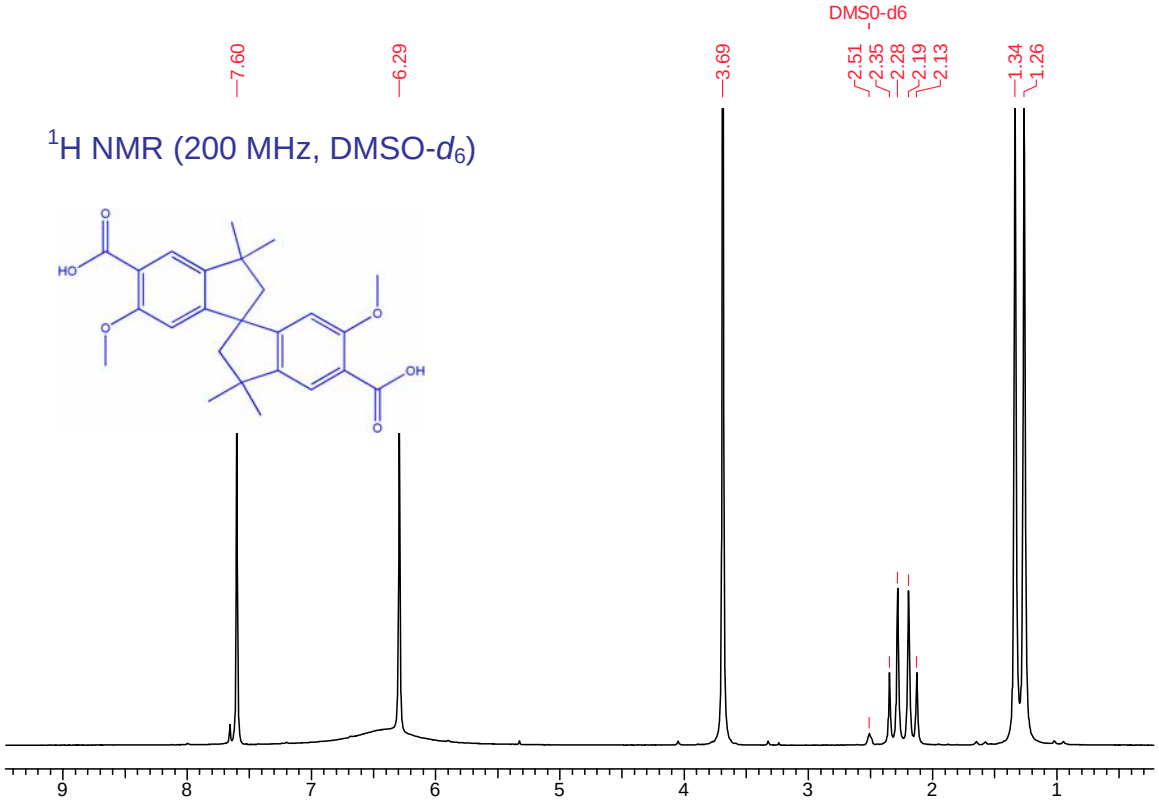

Chloroform-d
7.64
7.25
6.41
3.80
2.47
2.40
2.27
2.21
1.42
1.36
1H NMR (300 MHz, CDCl3)
O2N
NO2
9
8
7
6
5
4
3
2
1

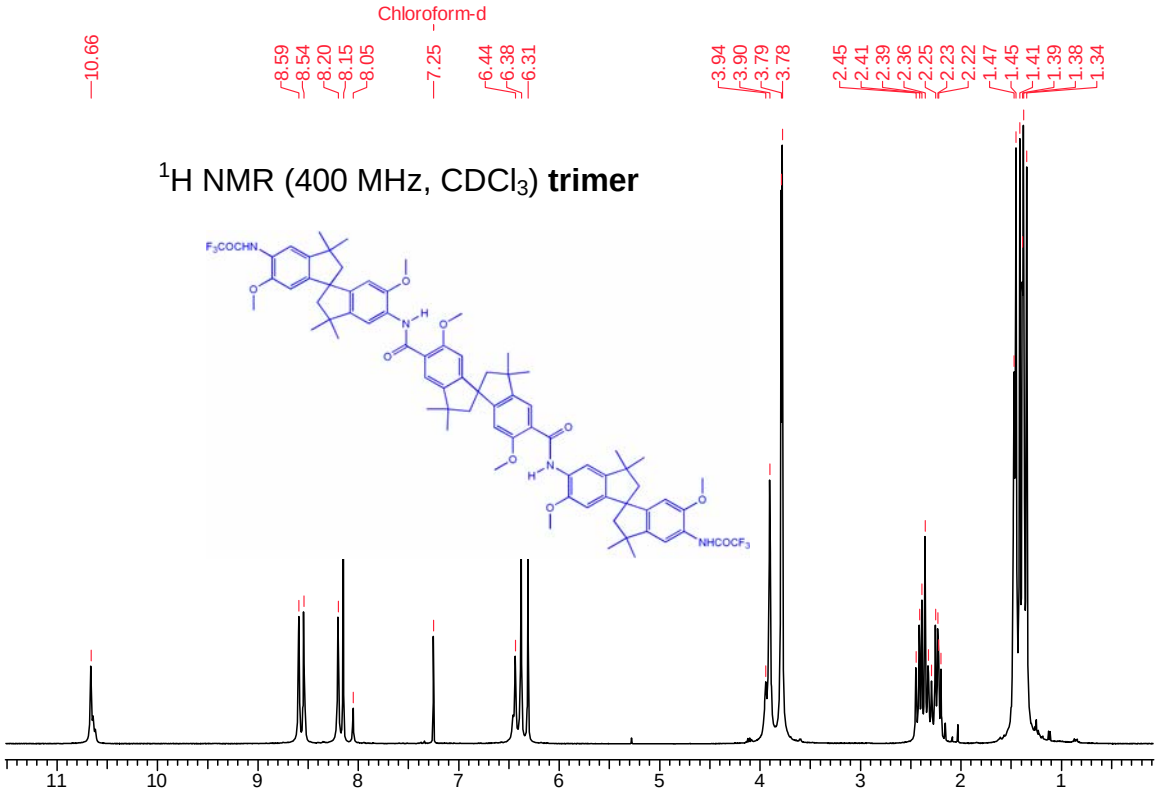

Chloroform-d
7.25
6.58
6.25
3.86
3.70
2.35
2.31
2.24
2.16
2.10
2.04
1.33
1.29
1H NMR (300MHz, CDCl3)
H2N
O
O
NH2
9
8
7
6
5
4
3
2
1
0

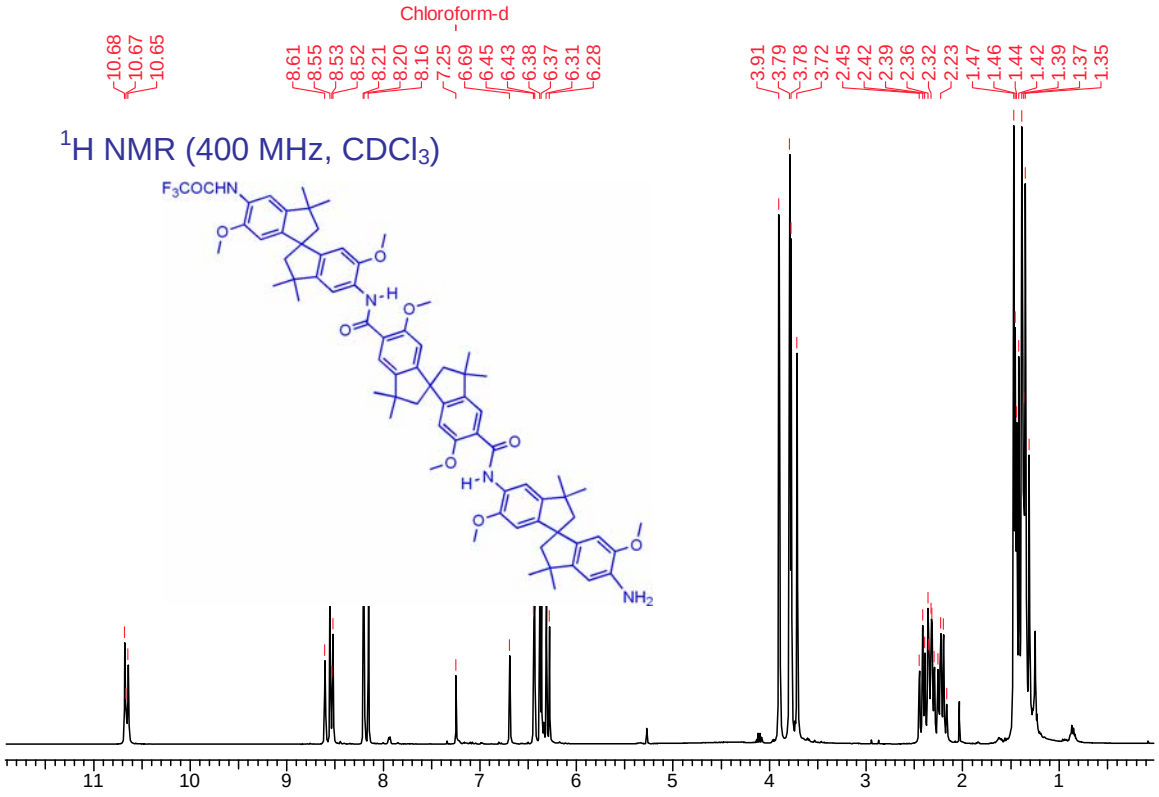

Chloroform-d
8.59
8.16
7.25
6.31
3.77
2.40
2.34
2.22
2.16
1.41
1.34
1H NMR (200 MHz, CDCl3)
F3COCHN
O
O
NHCOCF3
10
9
8
7
6
5
4
3
2
1
0


Chloroform-d
8.60
8.14
7.25
6.77
6.36
6.23
4.92
3.78
3.72
2.36
2.31
2.30
2.22
2.18
2.16
2.12
1.40
1.35
1.33
1.31
1H NMR (200 MHz, CDCl3)
F3COCHN
O
O
O
NH2
10
9
8
7
6
5
4
3
2
1

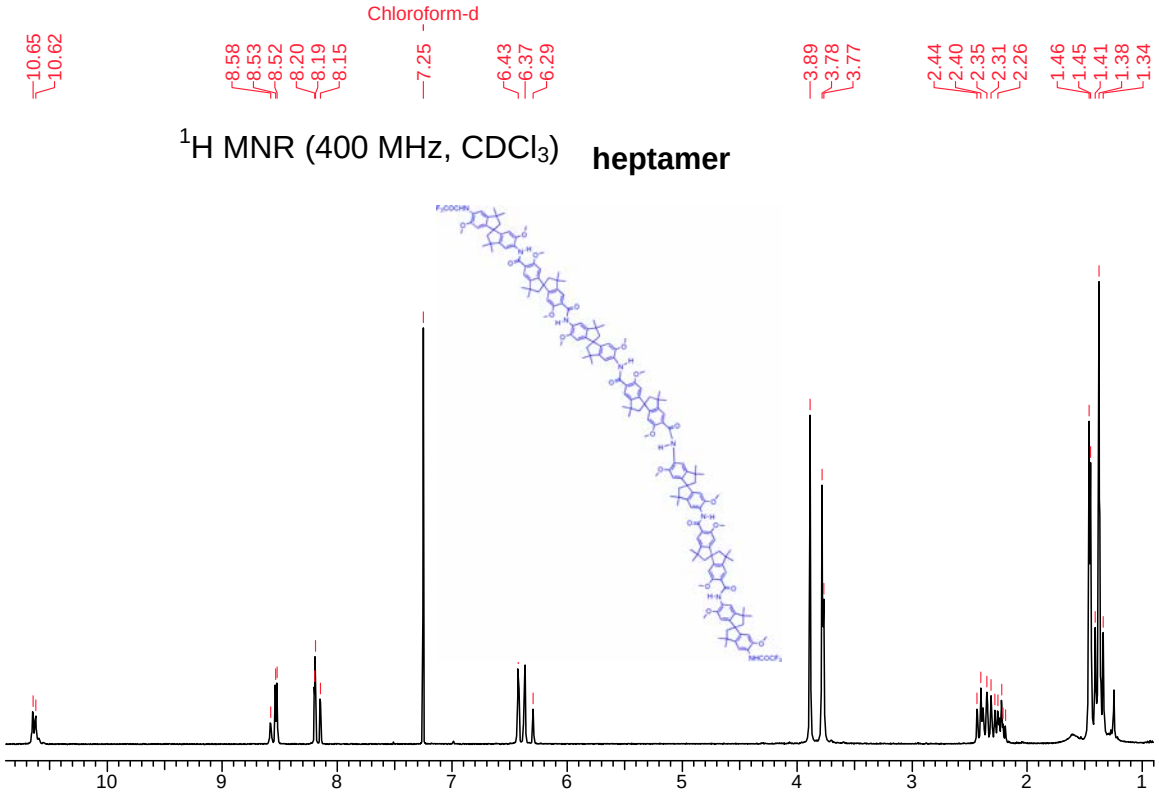

Chloroform-d
7.57
7.25
6.32
3.74
2.60
2.40
2.34
2.26
2.19
1.63
1.40
1.33
1H NMR (200 MHz, CDCl3)
O
O
O
O
O
9
8
7
6
5
4
3
2
1
0


DMSO-d6
7.60
6.29
3.69
2.51
2.35
2.28
2.19
2.13
1.34
1.26
^{1}H NMR (200 MHz, DMSO-d_6)
HO
OH
O
9
8
7
6
5
4
3
2
1

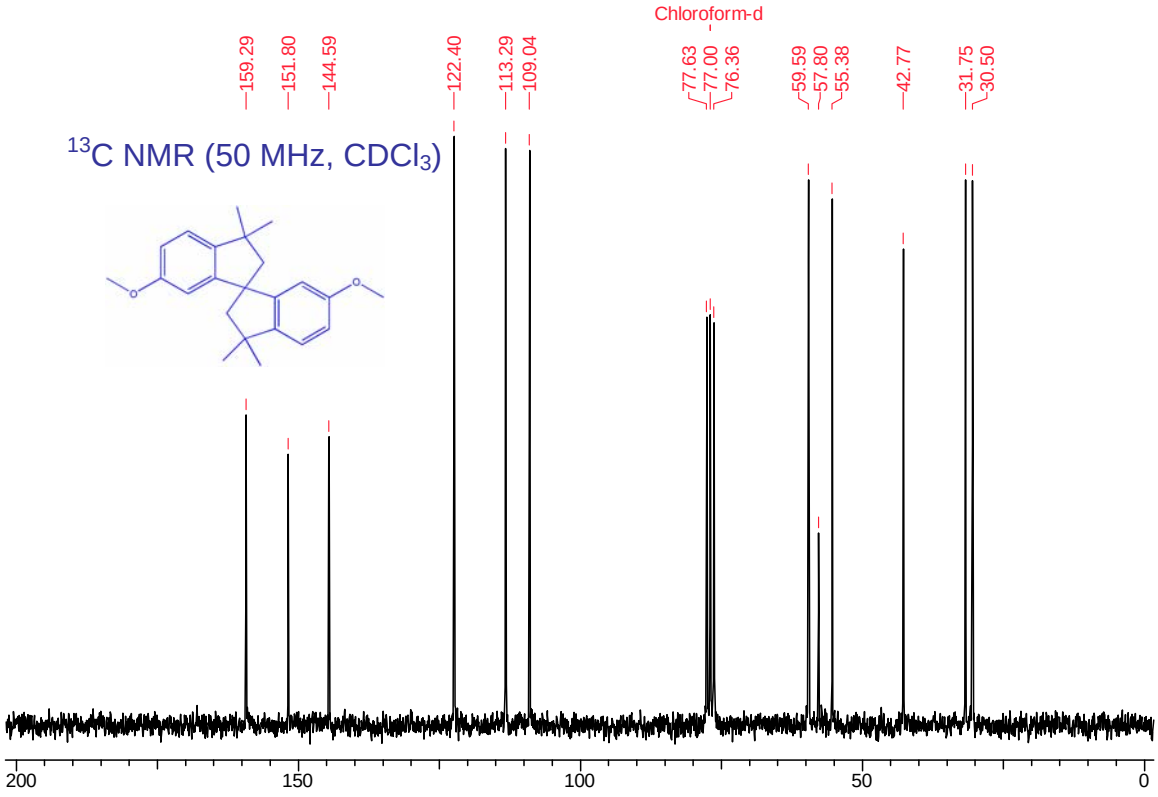

Chloroform-d
10.66
8.59
8.54
8.20
8.15
8.05
7.25
6.44
6.38
6.31
3.94
3.90
3.79
3.78
2.45
2.41
2.39
2.36
2.25
2.23
2.22
1.47
1.45
1.41
1.39
1.38
1.34
^{1}H NMR (400 MHz, $CDCl_3$) **trimer**
F_3COCHN
$NHCOCF_3$
11
10
9
8
7
6
5
4
3
2
1

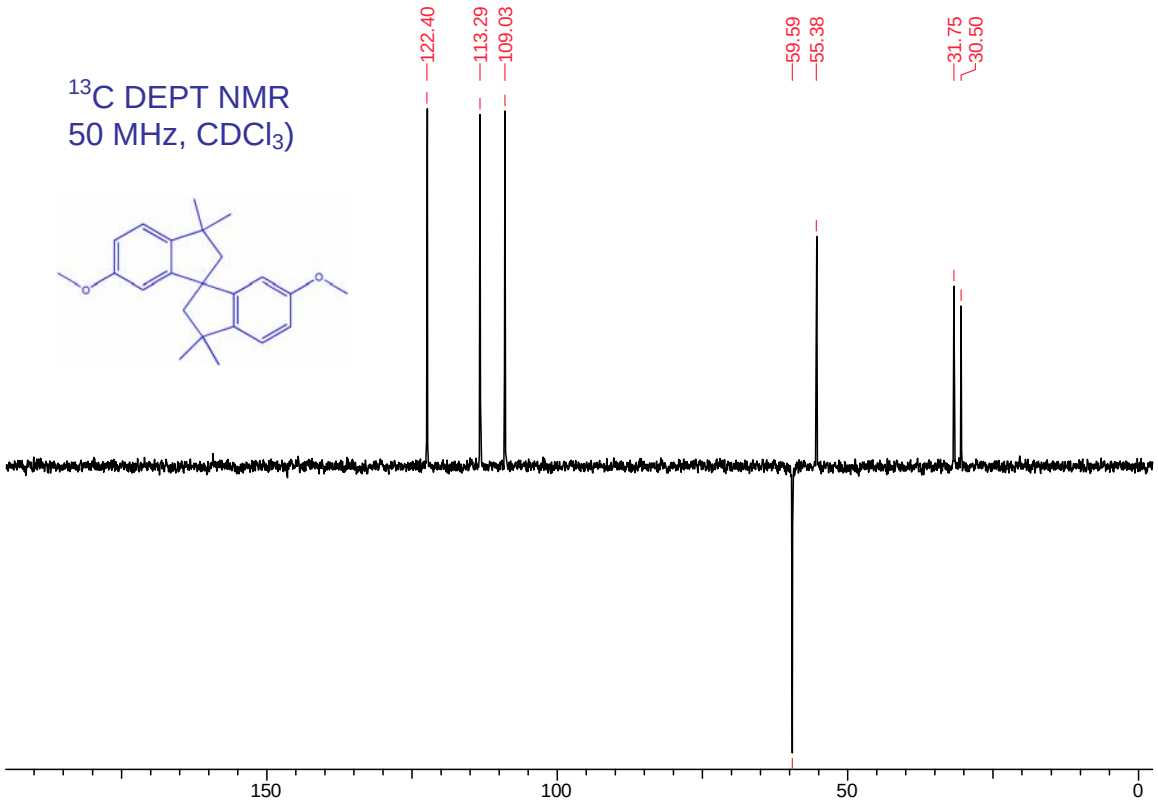


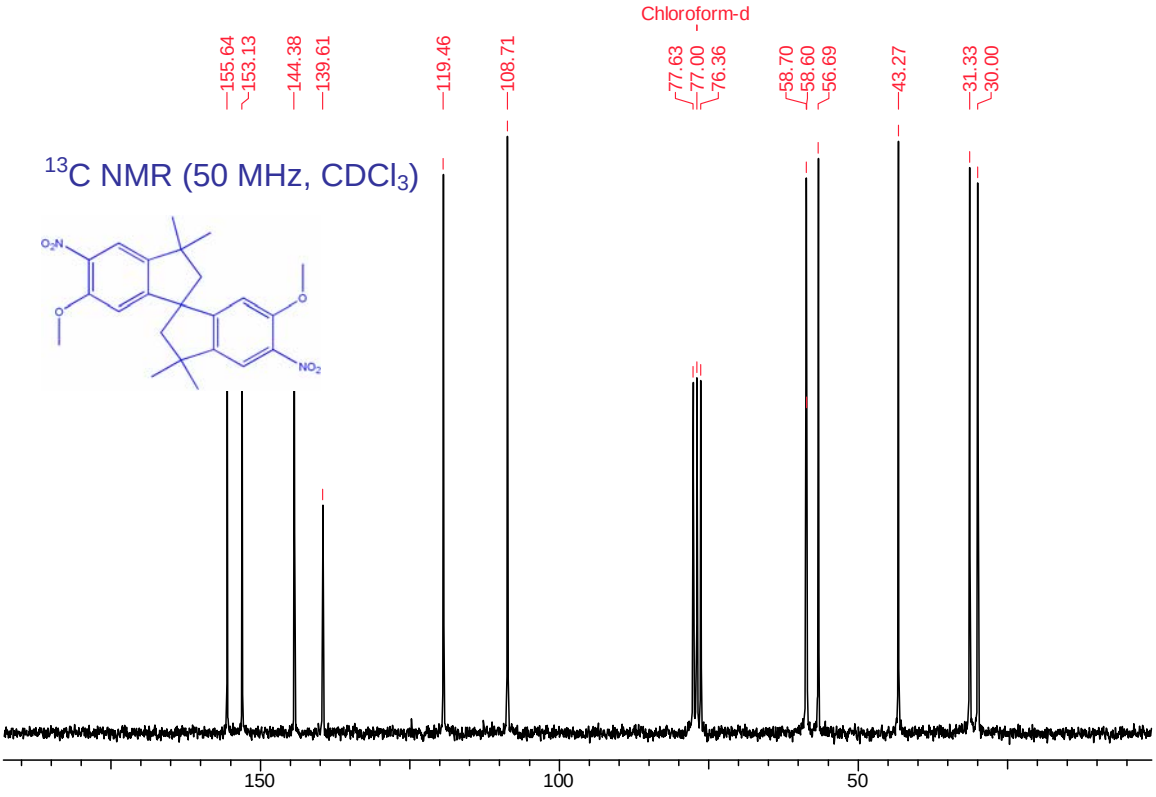
^{1}H NMR (400 MHz, $CDCl_3$)



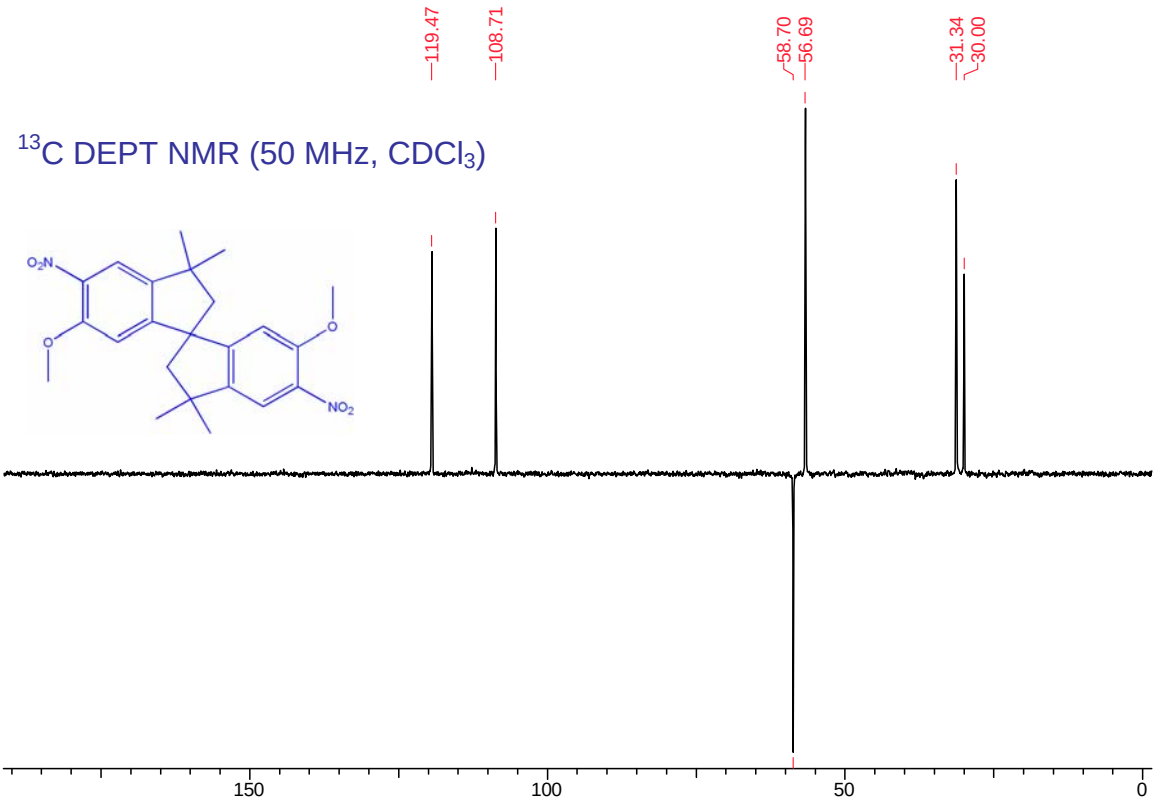
^{1}H MNR (400 MHz, $CDCl_3$) **heptamer**


Chloroform-d
159.29
151.80
144.59
122.40
113.29
109.04
77.63
77.00
76.36
59.59
57.80
55.38
42.77
31.75
30.50
13C NMR (50 MHz, CDCl3)
200
150
100
50
0

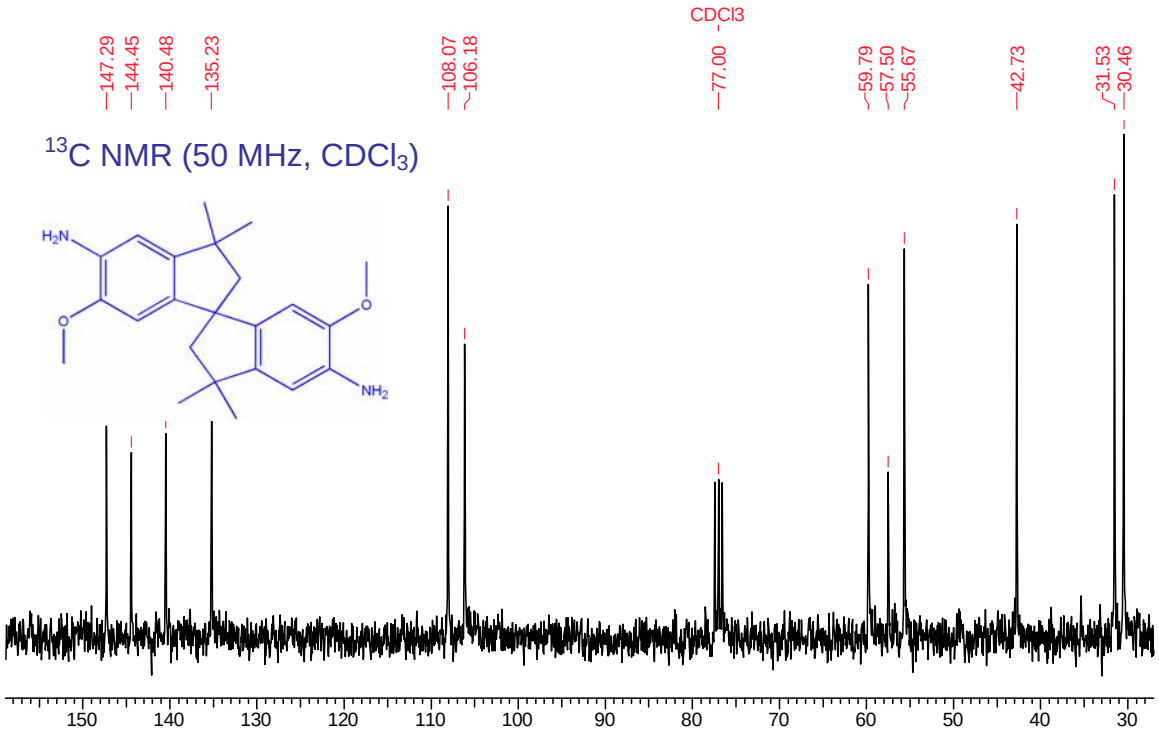

122.40
113.29
109.03
59.59
55.38
31.75
30.50
13C DEPT NMR
50 MHz, CDCl3)
150
100
50
0

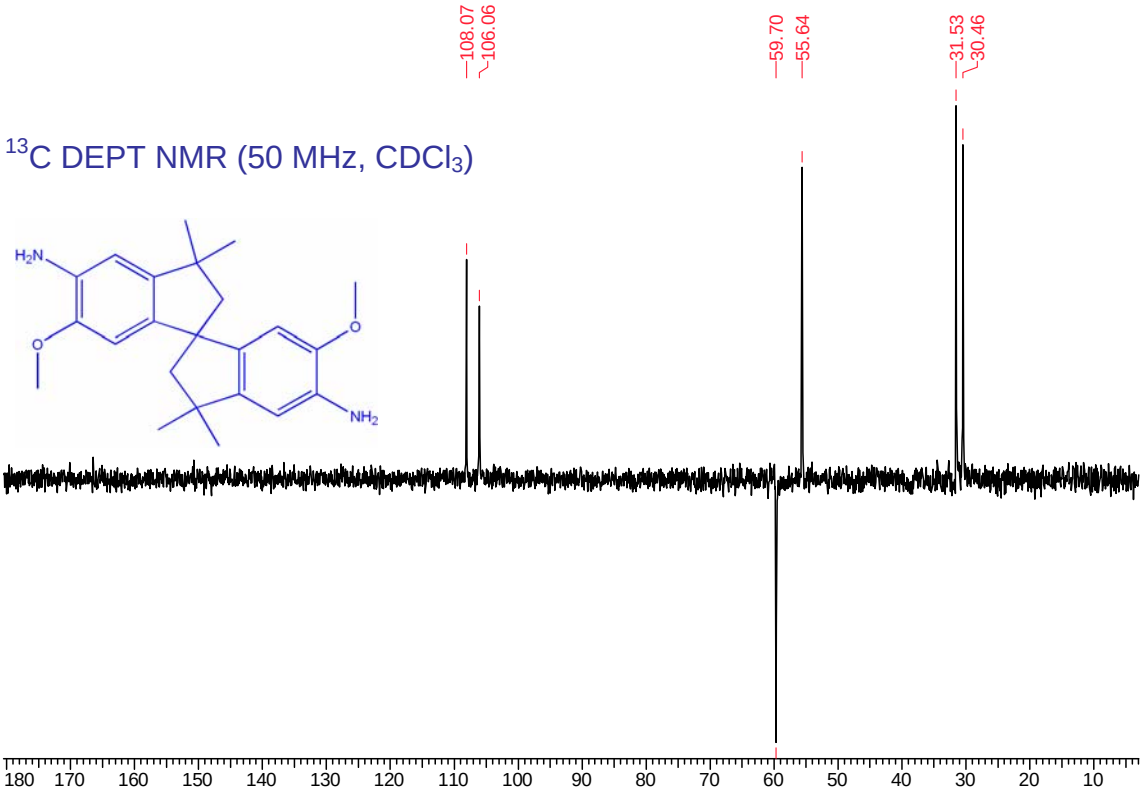


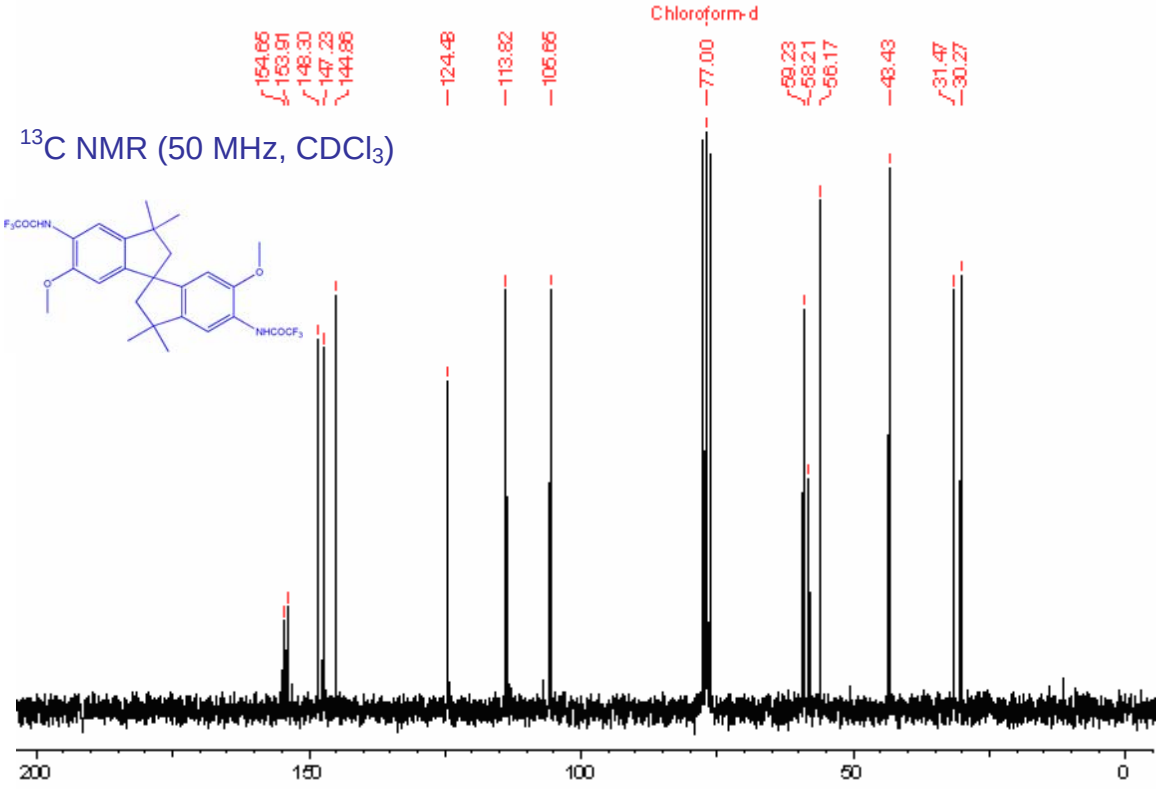
^{13}C NMR (50 MHz, $CDCl_3$)

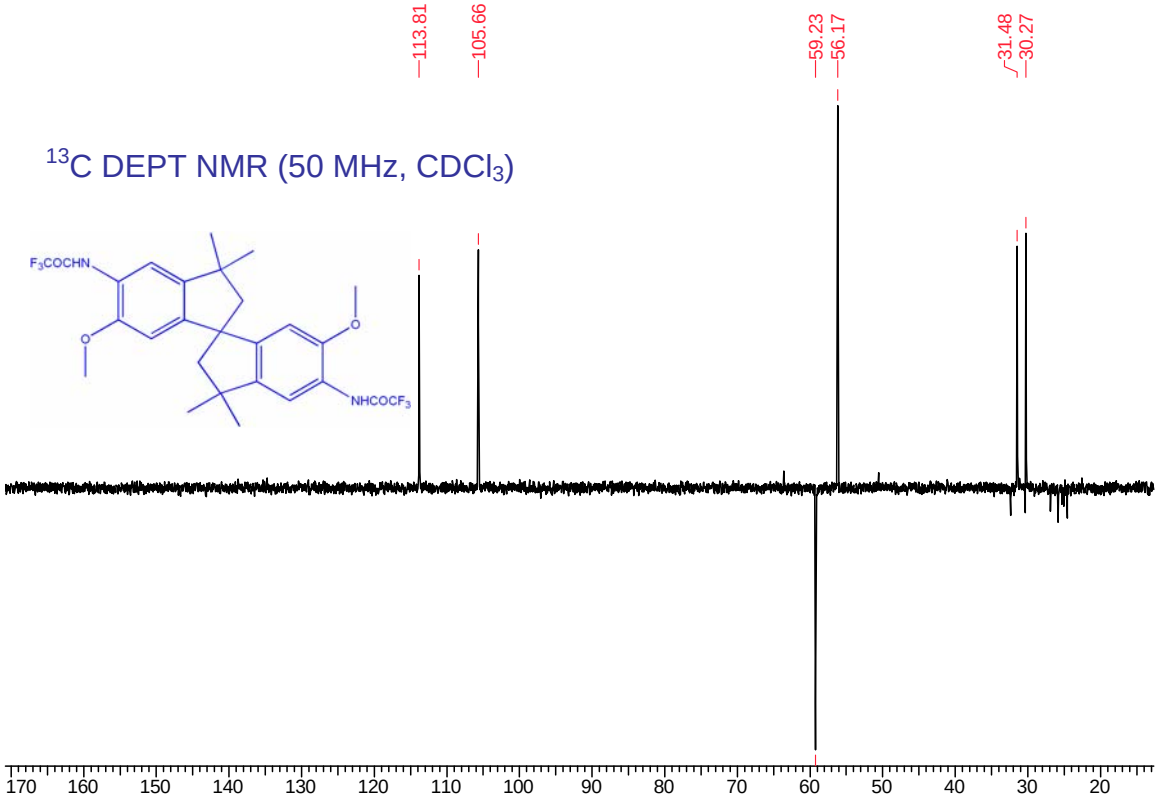


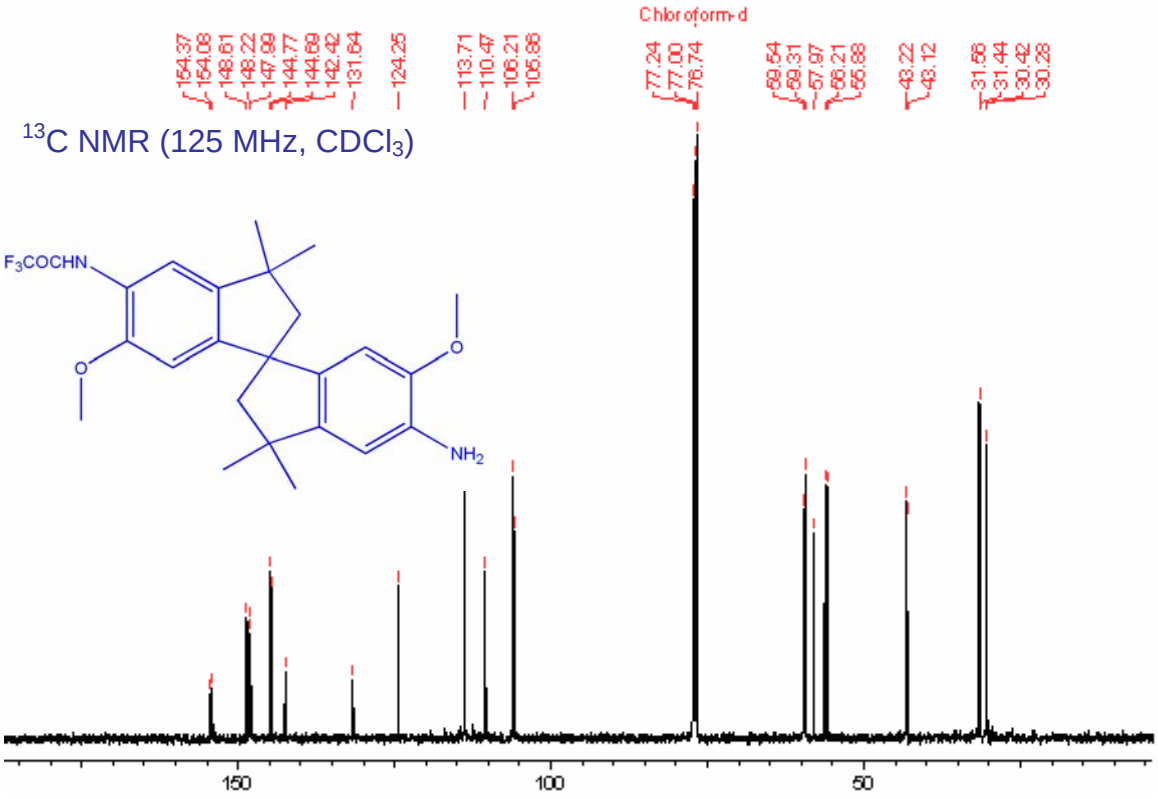
^{13}C DEPT NMR (50 MHz, $CDCl_3$)

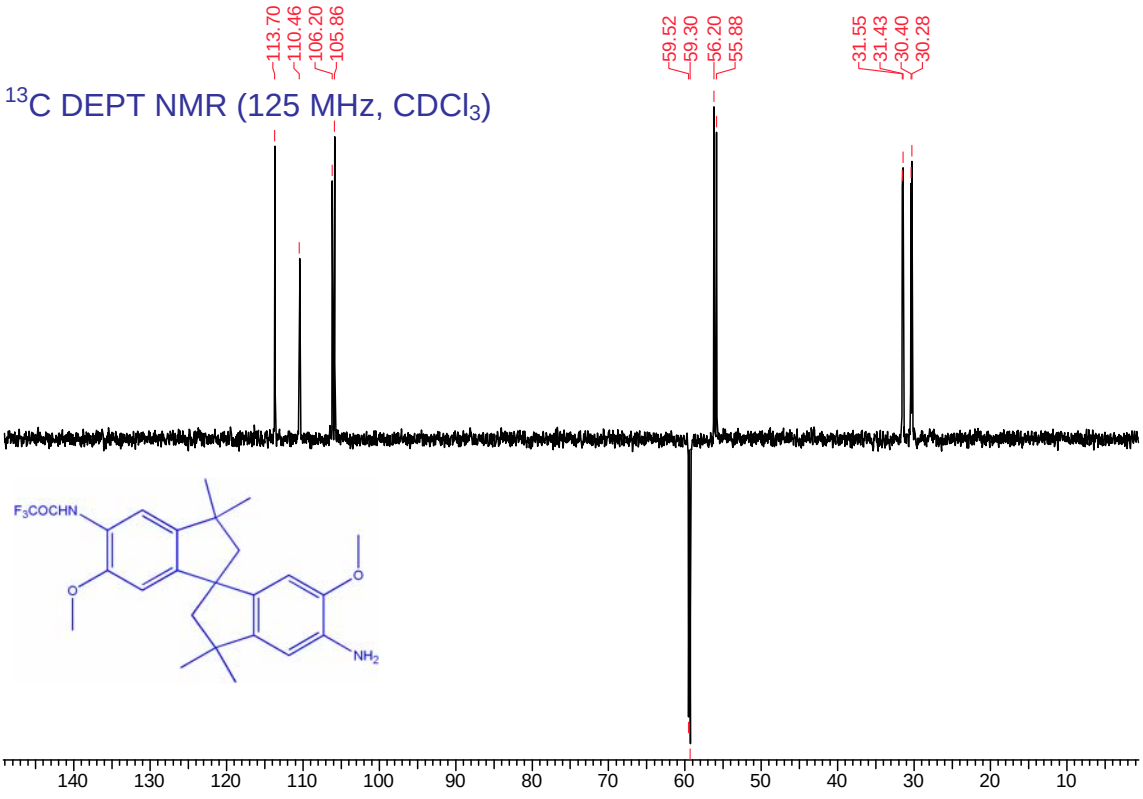

CDCl3
147.29
144.45
140.48
135.23
108.07
106.18
77.00
59.79
57.50
55.67
42.73
31.53
30.46
13C NMR (50 MHz, CDCl3)
H2N
O
O
NH2
150
140
130
120
110
100
90
80
70
60
50
40
30

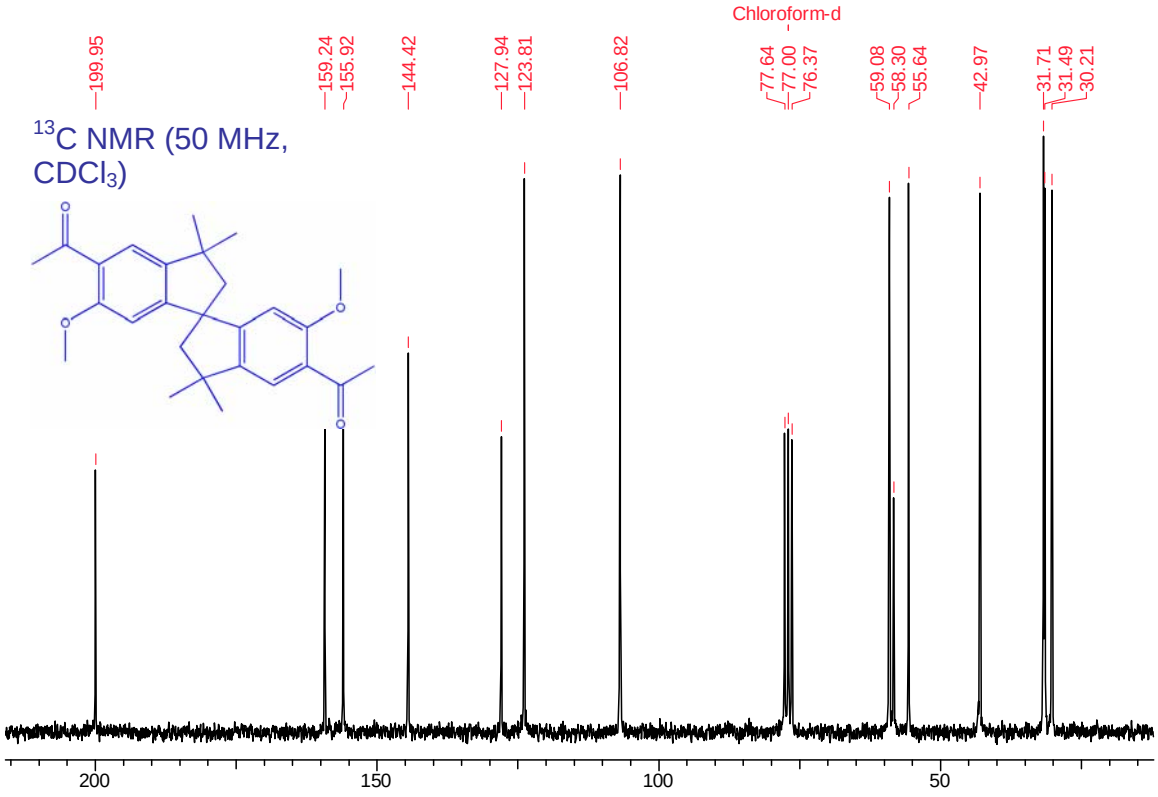

108.07
106.06
59.70
55.64
31.53
30.46
13C DEPT NMR (50 MHz, CDCl3)
H2N
O
O
NH2
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10

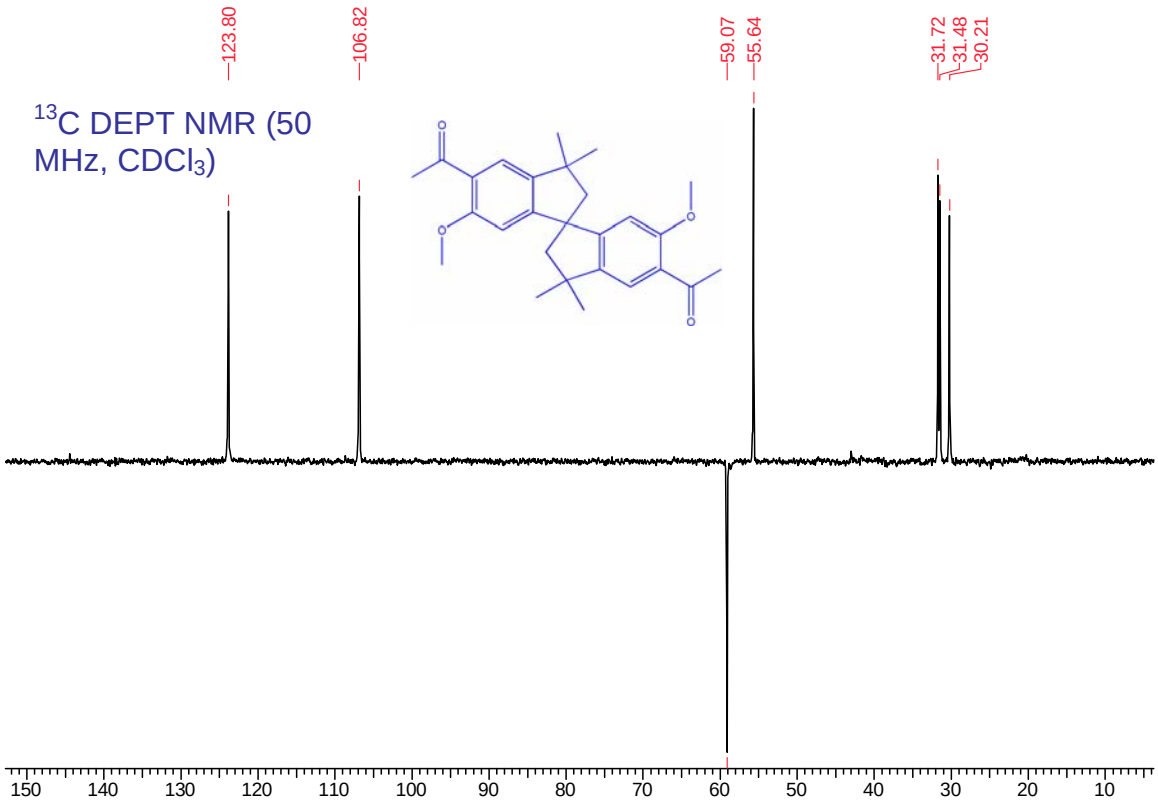

Chloroform-d
154.86
153.91
148.30
147.23
144.86
124.48
113.82
105.65
77.00
59.23
58.21
56.17
43.43
31.47
30.27
13C NMR (50 MHz, CDCl3)
F3COCHN
NHCOCF3
200
150
100
50
0

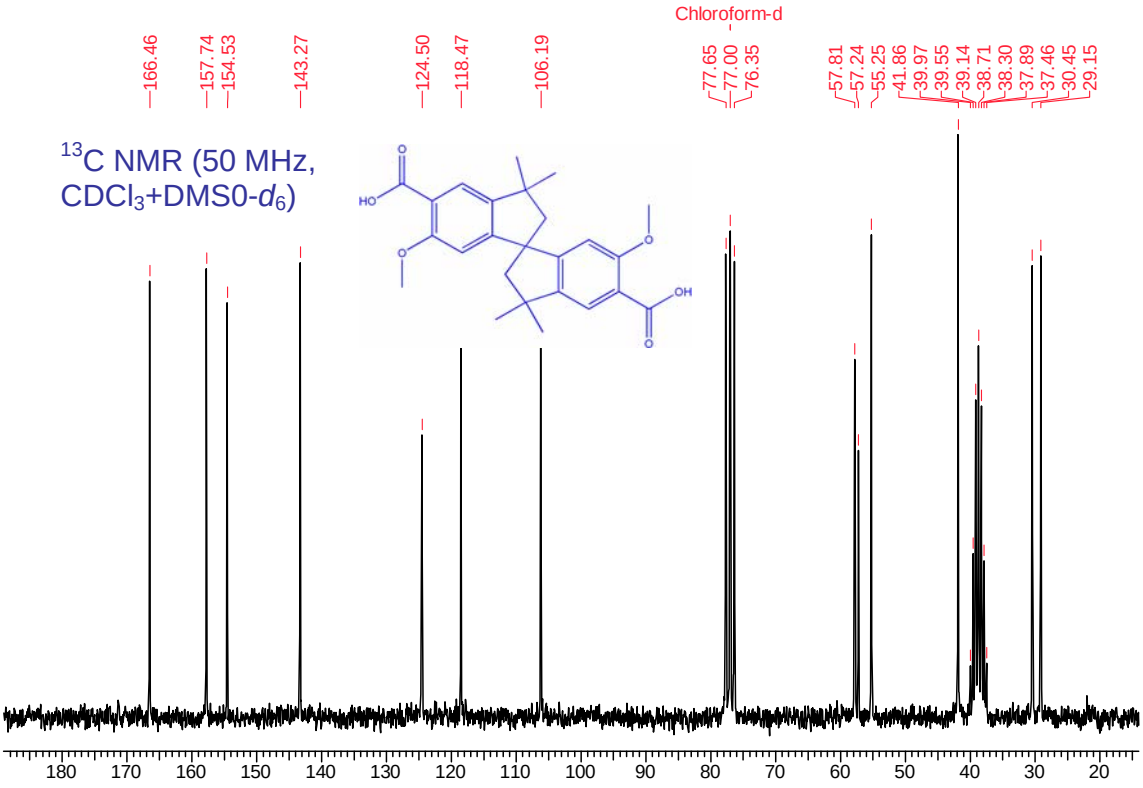

113.81
105.66
59.23
56.17
31.48
30.27
13C DEPT NMR (50 MHz, CDCl3)
F3COCHN
NHCOCF3
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20


Chloroform-d
154.37
154.08
148.61
148.22
147.98
144.77
144.69
142.42
131.64
124.25
113.71
110.47
106.21
105.86
77.24
77.00
76.74
69.54
69.31
57.97
56.21
55.88
43.22
43.12
31.56
31.44
30.42
30.28
13C NMR (125 MHz, CDCl3)
F3COCHN
O
O
NH2
150
100
50


113.70
110.46
106.20
105.86
59.52
59.30
56.20
55.88
31.55
31.43
30.40
30.28
13C DEPT NMR (125 MHz, CDCl3)
F3COCHN
O
O
NH2
140
130
120
110
100
90
80
70
60
50
40
30
20
10


Chloroform-d
199.95
159.24
155.92
144.42
127.94
123.81
106.82
77.64
77.00
76.37
59.08
58.30
55.64
42.97
31.71
31.49
30.21
13C NMR (50 MHz, CDCl3)
200
150
100
50


123.80
106.82
59.07
55.64
31.72
31.48
30.21
13C DEPT NMR (50 MHz, CDCl3)
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10


Chloroform-d
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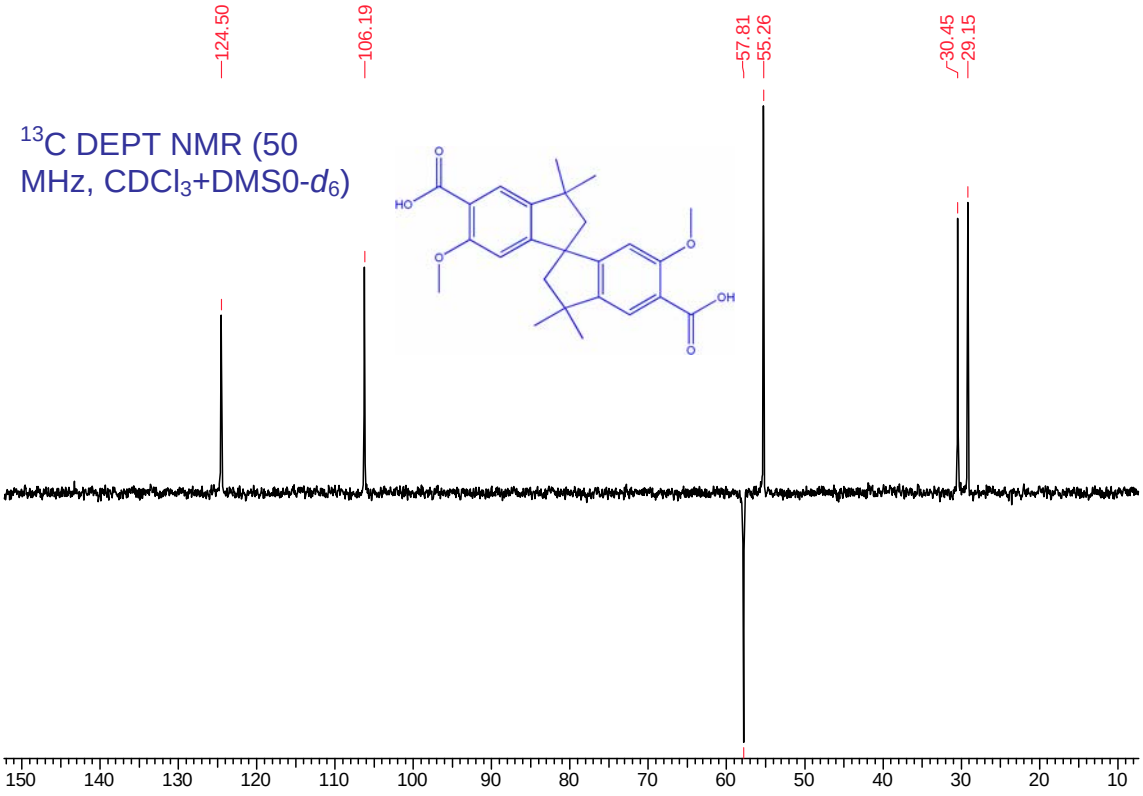
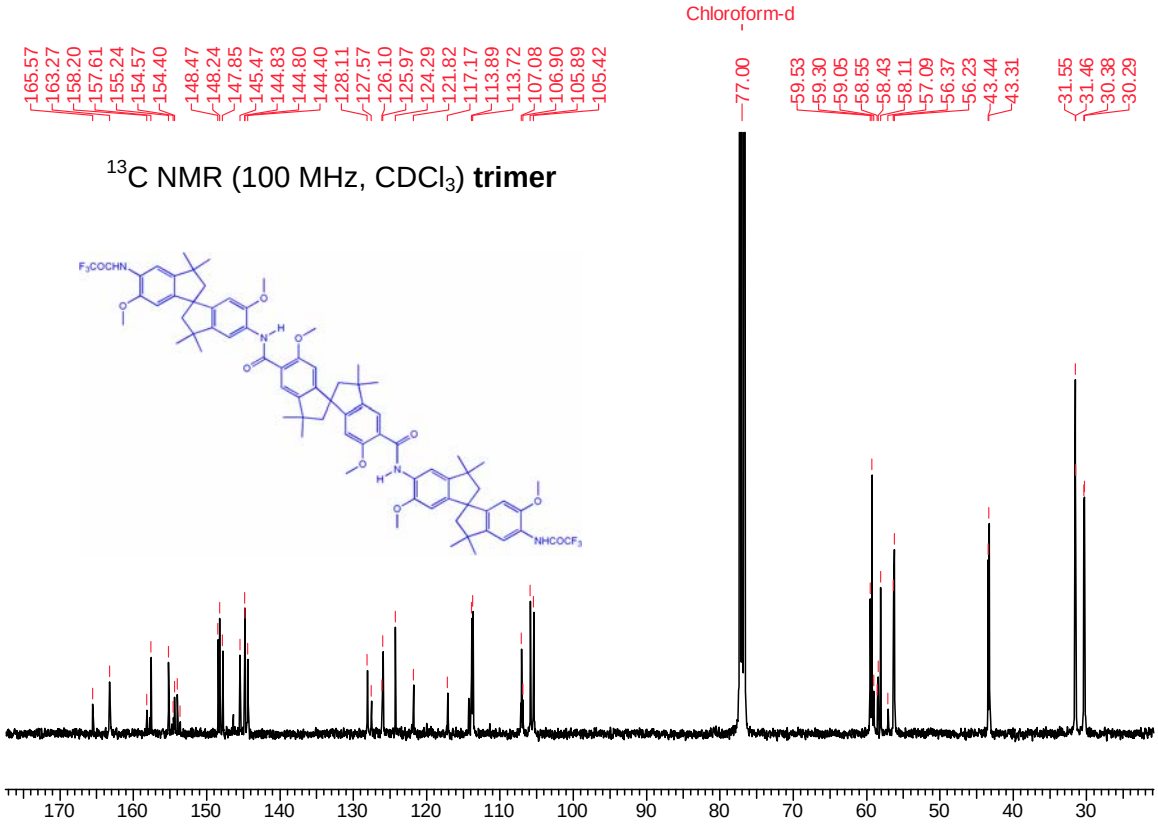
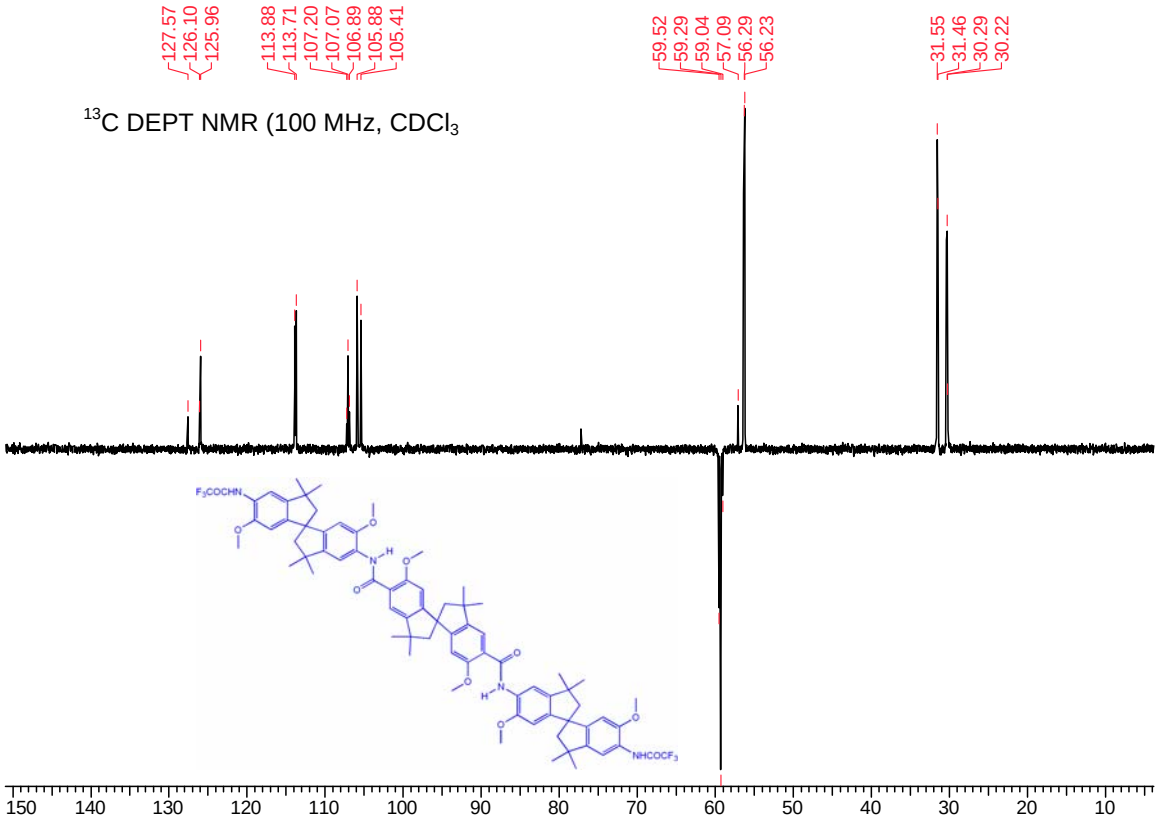
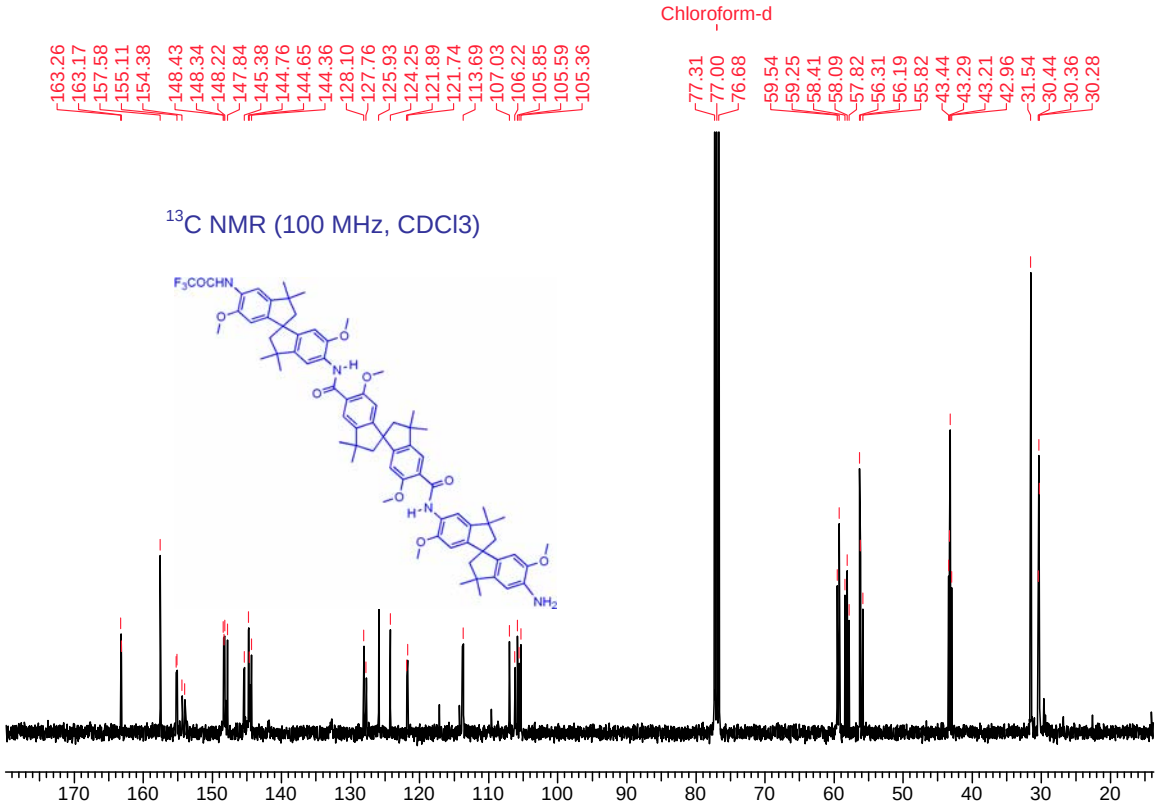
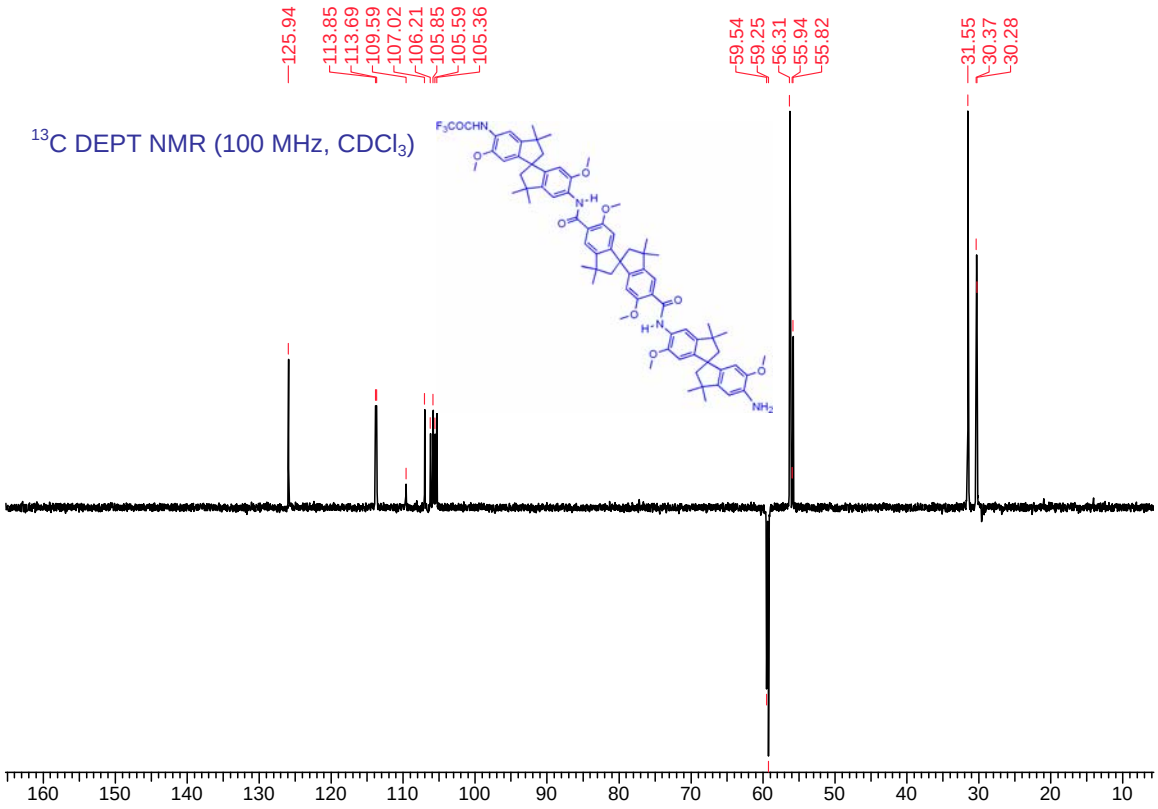
157.74
154.53
143.27
124.50
118.47
106.19
77.65
77.00
76.35
57.81
57.24
55.25
41.86
39.97
39.55
39.14
38.71
38.30
37.89
37.46
30.45
29.15
13C NMR (50 MHz, CDCl3+DMS0-d6)
HO
OH
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20

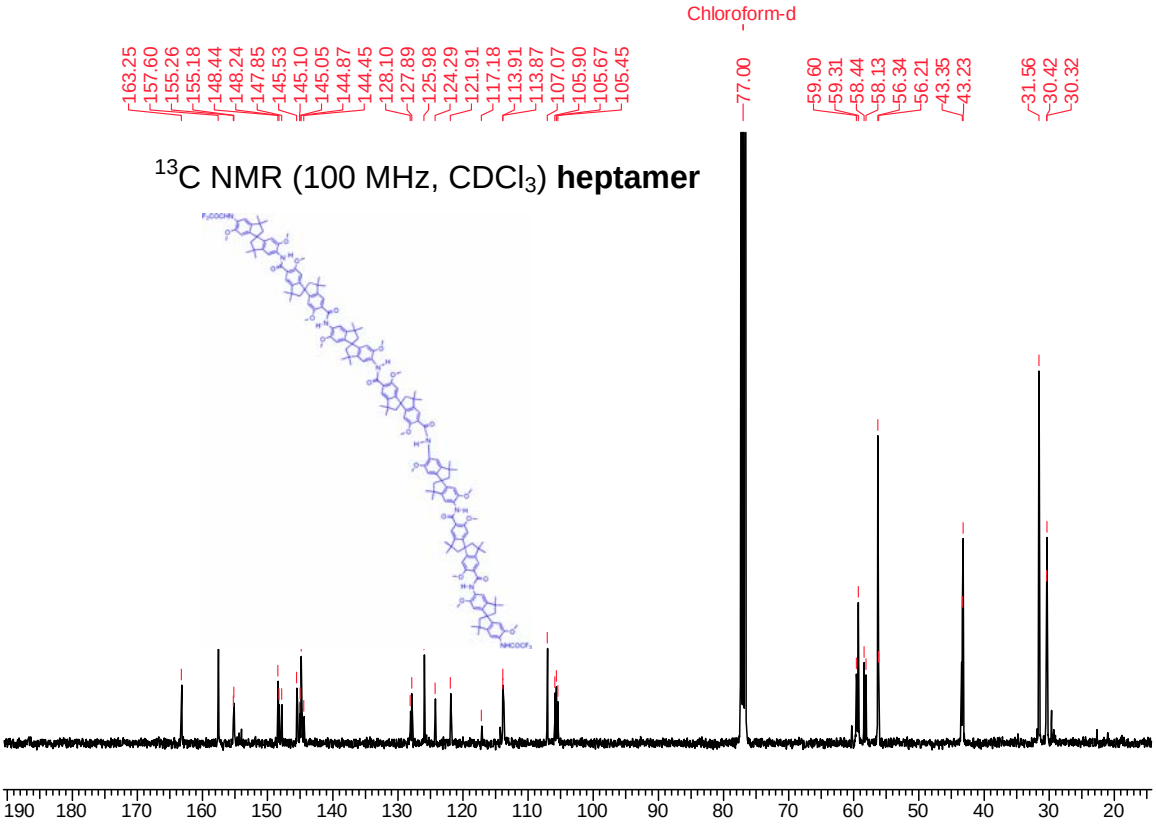

124.50
106.19
57.81
55.26
30.45
29.15
13C DEPT NMR (50 MHz, CDCl3+DMS0-d6)
HO
OH
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10


Chloroform-d
165.57
163.27
158.20
157.61
155.24
154.57
154.40
148.47
148.24
147.85
145.47
144.83
144.80
144.40
128.11
127.57
126.10
125.97
124.29
121.82
117.17
113.89
113.72
107.08
106.90
105.89
105.42
77.00
59.53
59.30
59.05
58.55
58.43
58.11
57.09
56.37
56.23
43.44
43.31
31.55
31.46
30.38
30.29
13C NMR (100 MHz, CDCl3) trimer
F3COCHN
NHCOCF3
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30

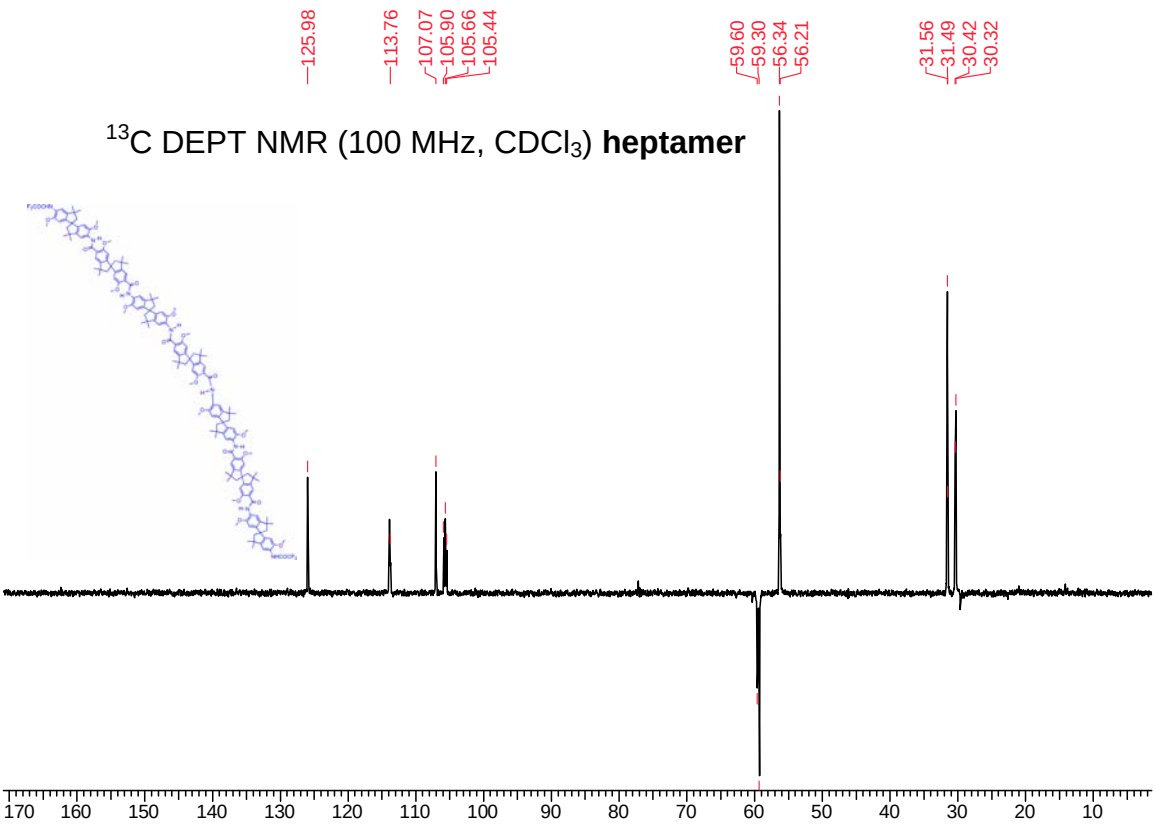

127.57
126.10
125.96
113.88
113.71
107.20
107.07
106.89
105.88
105.41
59.52
59.29
59.04
57.09
56.29
56.23
31.55
31.46
30.29
30.22
13C DEPT NMR (100 MHz, CDCl3
F3COCHN
NHCOCF3
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10


Chloroform-d
163.26
163.17
157.58
155.11
154.38
148.43
148.34
148.22
147.84
145.38
144.76
144.65
144.36
128.10
127.76
125.93
124.25
121.89
121.74
113.69
107.03
106.22
105.85
105.59
105.36
77.31
77.00
76.68
59.54
59.25
58.41
58.09
57.82
56.31
56.19
55.82
43.44
43.29
43.21
42.96
31.54
30.44
30.36
30.28
13C NMR (100 MHz, CDCl3)
F3COCHN
NH2
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20


125.94
113.85
113.69
109.59
107.02
106.21
105.85
105.59
105.36
59.54
59.25
56.31
55.94
55.82
31.55
30.37
30.28
13C DEPT NMR (100 MHz, CDCl3)
F3COCHN
NH2
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10



^{13}C NMR (100 MHz, $CDCl_3$) **heptamer**



^{13}C DEPT NMR (100 MHz, $CDCl_3$) **heptamer**

Details of the quantum chemical calculations: The starting geometries for the complete geometry optimization of the various oligomers (trimer, pentamer, heptamer) were built on the basis of the X-ray structure of the trimer. The highly restricted spiro structure and the extended intramoleculer hydrogen bonding system exclude conformational alternatives. Nevertheless, deviations from this structure, e.g. by distortions of the hydrogen bonds, were additionally examined, but such structures could not be kept as minimum structures.

The trimer (figure 1) and the pentamer structures were determined at the HF/6-31F* level of ab initio MO theory, the heptamer structure was optimized at the HF/3-21G level because of its huge size. It could be shown that the optimum oligomer structures of the pentamer at the HF/6-31G* and HF/3-21G levels are in close correspondence. The pdb-files for the trimer, pentamer and heptamer are given on the following pages. The calculations were performed employing the GAUSSIAN03 program package.[1]

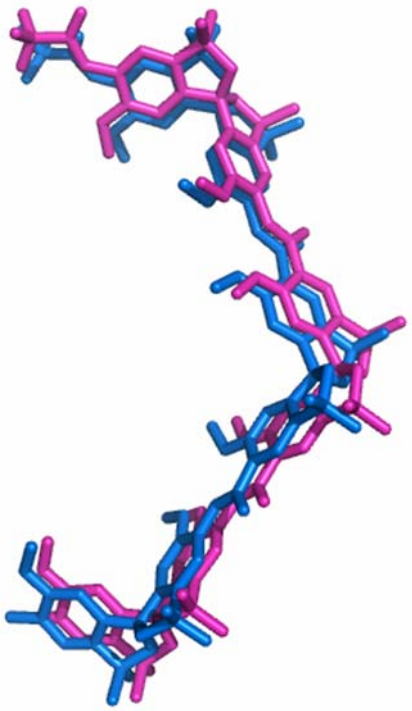


Figure 1. Overlay of the crystal structure (blue) and the optimised structure obtained from the theoretical calculations (pink) for 3 (RMSD = 0.138).

The total energies are:

Trimer (**3**) (HF/6-31G*): -4002.664136 a.u.

Pentamer (HF/6-31G*): -6858.277784 a.u.

Heptamer (**4**) (HF(3-21G): -9214.397450 a.u.

Reference

[1] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. Montgomery, T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, B.; W. Chen, M. W. Wong, C. Gonzalez, J. A. Pople, Revision B.04 ed.; Gaussian Inc.: Pittsburgh PA, 2003.

pdb-file trimer (HF/6-31G*)

```
HEADER
REMARK Spartan exported Wed Jun  7 15:47:46 2006
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HETATM    2  F   UNK  0001      12.095   7.544   2.132
HETATM    3  F   UNK  0001      13.318   7.497   0.385
HETATM    4  N   UNK  0001      11.149   4.994   0.248
HETATM    5  H   UNK  0001      10.514   5.612  -0.207
HETATM    6  N   UNK  0001       4.502  -2.444  -0.057
HETATM    7  H   UNK  0001       4.006  -2.053   0.710
HETATM    8  N   UNK  0001      -6.686  -1.085   0.083
HETATM    9  H   UNK  0001      -6.128  -0.929  -0.725
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HETATM   12  H   UNK  0001     -10.891   8.173  -0.967
HETATM   13  O   UNK  0001      13.026   4.981   1.541
HETATM   14  O   UNK  0001       9.043   4.433  -1.144
HETATM   15  O   UNK  0001       5.355  -0.774   1.740
HETATM   16  O   UNK  0001       4.331  -3.858  -1.802
HETATM   17  O   UNK  0001       2.139  -2.000   1.174
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HETATM   19  O   UNK  0001      -6.818  -2.256   2.002
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HETATM   24  C   UNK  0001      10.850   3.624   0.083
HETATM   25  C   UNK  0001      11.197   1.276   0.387
HETATM   26  C   UNK  0001      10.077   1.005  -0.361
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HETATM   28  H   UNK  0001       8.436   1.815  -1.473
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HETATM   31  H   UNK  0001       8.136   3.723  -2.850
HETATM   32  H   UNK  0001       7.569   5.263  -2.200
HETATM   33  H   UNK  0001       7.116   3.755  -1.403
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HETATM   35  C   UNK  0001      13.176  -0.236   0.042
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HETATM   44  H   UNK  0001      10.244  -1.257   1.465
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HETATM   72  C   UNK  0001       2.429  -3.705  -0.434
HETATM   73  C   UNK  0001       1.621  -3.067   0.528
HETATM   74  C   UNK  0001      11.597   2.592   0.613
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HETATM   80  C   UNK  0001       0.337  -3.523   0.779
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HETATM   86  C   UNK  0001      -0.101  -6.440  -1.491
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HETATM   88  H   UNK  0001       1.504  -7.884  -1.234
HETATM   89  H   UNK  0001      -0.091  -8.610  -1.344
HETATM   90  H   UNK  0001       0.416  -7.806   0.135
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HETATM  102  C   UNK  0001      -3.138  -5.840   2.080
HETATM  103  C   UNK  0001      -4.010  -7.051   1.702
HETATM  104  H   UNK  0001      -5.044  -6.882   1.986
HETATM  105  H   UNK  0001      -3.666  -7.947   2.211
HETATM  106  H   UNK  0001      -3.992  -7.240   0.634
HETATM  107  C   UNK  0001      -3.200  -5.635   3.599
HETATM  108  H   UNK  0001      -2.636  -4.758   3.900
HETATM  109  H   UNK  0001      -2.787  -6.496   4.118
HETATM  110  H   UNK  0001      -4.222  -5.506   3.939
HETATM  111  C   UNK  0001      -3.568  -4.607   1.301
HETATM  112  C   UNK  0001      -2.683  -4.297   0.290
HETATM  113  C   UNK  0001      -2.910  -3.218  -0.551
HETATM  114  H   UNK  0001      -2.200  -2.986  -1.321
HETATM  115  C   UNK  0001      -4.044  -2.441  -0.378
HETATM  116  C   UNK  0001      -3.428  -1.001  -2.191
HETATM  117  H   UNK  0001      -2.448  -0.753  -1.799
HETATM  118  H   UNK  0001      -3.863  -0.125  -2.646
HETATM  119  H   UNK  0001      -3.335  -1.784  -2.934
HETATM  120  C   UNK  0001      -4.964  -2.740   0.647
HETATM  121  C   UNK  0001      -4.698  -3.827   1.470
HETATM  122  H   UNK  0001      -5.405  -4.035   2.250
HETATM  123  C   UNK  0001      -6.239  -1.994   0.977
HETATM  124  C   UNK  0001      -7.853  -0.304   0.155
HETATM  125  C   UNK  0001      -8.744  -0.297   1.212
HETATM  126  H   UNK  0001      -8.558  -0.929   2.052
HETATM  127  C   UNK  0001      -9.864   0.531   1.165
HETATM  128  C   UNK  0001     -10.099   1.336   0.078
HETATM  129  C   UNK  0001      -9.210   1.343  -0.995
HETATM  130  H   UNK  0001      -9.392   1.985  -1.835
HETATM  131  C   UNK  0001      -8.099   0.531  -0.955
HETATM  132  C   UNK  0001      -7.358   1.201  -3.119
HETATM  133  H   UNK  0001      -8.281   0.919  -3.613
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HETATM  134  H   UNK  0001       -6.524   0.964  -3.764
HETATM  135  H   UNK  0001       -7.366   2.268  -2.924
HETATM  136  C   UNK  0001      -10.963   0.654   2.209
HETATM  137  C   UNK  0001      -11.867  -0.591   2.191
HETATM  138  H   UNK  0001      -11.306  -1.478   2.470
HETATM  139  H   UNK  0001      -12.287  -0.766   1.207
HETATM  140  H   UNK  0001      -12.689  -0.481   2.895
HETATM  141  C   UNK  0001      -10.415   0.851   3.629
HETATM  142  H   UNK  0001      -11.225   1.042   4.328
HETATM  143  H   UNK  0001       -9.729   1.692   3.670
HETATM  144  H   UNK  0001       -9.883  -0.030   3.974
HETATM  145  C   UNK  0001      -11.713   1.924   1.720
HETATM  146  H   UNK  0001      -11.345   2.782   2.272
HETATM  147  H   UNK  0001      -12.780   1.864   1.907
HETATM  148  C   UNK  0001      -11.388   2.131   0.210
HETATM  149  C   UNK  0001      -12.501   1.639  -0.766
HETATM  150  H   UNK  0001      -13.135   0.883  -0.318
HETATM  151  H   UNK  0001      -12.027   1.181  -1.627
HETATM  152  C   UNK  0001      -13.313   2.876  -1.239
HETATM  153  C   UNK  0001      -13.691   2.751  -2.721
HETATM  154  H   UNK  0001      -14.260   3.611  -3.060
HETATM  155  H   UNK  0001      -14.303   1.868  -2.886
HETATM  156  H   UNK  0001      -12.807   2.669  -3.345
HETATM  157  C   UNK  0001      -14.595   3.072  -0.410
HETATM  158  H   UNK  0001      -14.376   3.157   0.648
HETATM  159  H   UNK  0001      -15.275   2.236  -0.550
HETATM  160  H   UNK  0001      -15.114   3.977  -0.711
HETATM  161  C   UNK  0001      -12.328   4.004  -0.974
HETATM  162  C   UNK  0001      -11.283   3.596  -0.182
HETATM  163  C   UNK  0001      -10.290   4.501   0.194
HETATM  164  H   UNK  0001       -9.474   4.170   0.808
HETATM  165  C   UNK  0001      -10.363   5.807  -0.235
HETATM  166  C   UNK  0001       -8.360   6.460   0.875
HETATM  167  H   UNK  0001       -8.671   6.118   1.857
HETATM  168  H   UNK  0001       -7.789   7.370   0.980
HETATM  169  H   UNK  0001       -7.738   5.700   0.413
HETATM  170  C   UNK  0001      -11.430   6.237  -1.048
HETATM  171  C   UNK  0001      -12.404   5.326  -1.406
HETATM  172  H   UNK  0001      -13.215   5.655  -2.035
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CONECT    2   22
CONECT    3   22
CONECT    4    5   23   24
CONECT    5    4
CONECT    6    7   68   71
CONECT    7    6
CONECT    8    9  123  124
CONECT    9    8
CONECT   10   11   12  170
CONECT   11   10
CONECT   12   10
CONECT   13   23
CONECT   14   29   30
CONECT   15   63   64
CONECT   16   71
CONECT   17   73   76
CONECT   18  115  116
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CONECT   19  123
CONECT   20  131  132
CONECT   21  165  166
CONECT   22    1    2    3   23
CONECT   23    4   13   22
CONECT   24    4   29   74
CONECT   25   26   34   74
CONECT   26   25   27   46
CONECT   27   26   28   29
CONECT   28   27
CONECT   29   14   24   27
CONECT   30   14   31   32   33
CONECT   31   30
CONECT   32   30
CONECT   33   30
CONECT   34   25   35   39   43
CONECT   35   34   36   37   38
CONECT   36   35
CONECT   37   35
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CONECT   40   39
CONECT   41   39
CONECT   42   39
CONECT   43   34   44   45   46
CONECT   44   43
CONECT   45   43
CONECT   46   26   43   47   60
CONECT   47   46   48   49   50
CONECT   48   47
CONECT   49   47
CONECT   50   47   51   55   59
CONECT   51   50   52   53   54
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CONECT   56   55
CONECT   57   55
CONECT   58   55
CONECT   59   50   60   69
CONECT   60   46   59   61
CONECT   61   60   62   63
CONECT   62   61
CONECT   63   15   61   68
CONECT   64   15   65   66   67
CONECT   65   64
CONECT   66   64
CONECT   67   64
CONECT   68    6   63   69
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CONECT   70   69
CONECT   71    6   16   72
CONECT   72   71   73   84
CONECT   73   17   72   80
CONECT   74   24   25   75
CONECT   75   74
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CONECT   77   76
CONECT   78   76
CONECT   79   76
CONECT   80   73   81   82
CONECT   81   80
CONECT   82   80   83   98
CONECT   83   82   84   86
CONECT   84   72   83   85
CONECT   85   84
CONECT   86   83   87   91   95
CONECT   87   86   88   89   90
CONECT   88   87
CONECT   89   87
CONECT   90   87
CONECT   91   86   92   93   94
CONECT   92   91
CONECT   93   91
CONECT   94   91
CONECT   95   86   96   97   98
CONECT   96   95
CONECT   97   95
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CONECT  100   99
CONECT  101   99
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CONECT  110  107
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CONECT  113  112  114  115
CONECT  114  113
CONECT  115   18  113  120
CONECT  116   18  117  118  119
CONECT  117  116
CONECT  118  116
CONECT  119  116
CONECT  120  115  121  123
CONECT  121  111  120  122
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CONECT  124    8  125  131
CONECT  125  124  126  127
CONECT  126  125
CONECT  127  125  128  136
CONECT  128  127  129  148
CONECT  129  128  130  131
CONECT  130  129
CONECT  131   20  124  129
CONECT  132   20  133  134  135
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CONECT  145  136  146  147  148
CONECT  146  145
CONECT  147  145
CONECT  148  128  145  149  162
CONECT  149  148  150  151  152
CONECT  150  149
CONECT  151  149
CONECT  152  149  153  157  161
CONECT  153  152  154  155  156
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CONECT  156  153
CONECT  157  152  158  159  160
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CONECT  159  157
CONECT  160  157
CONECT  161  152  162  171
CONECT  162  148  161  163
CONECT  163  162  164  165
CONECT  164  163
CONECT  165   21  163  170
CONECT  166   21  167  168  169
CONECT  167  166
CONECT  168  166
CONECT  169  166
CONECT  170   10  165  171
CONECT  171  161  170  172
CONECT  172  171
END
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pdb-file pentamer (HF/6-31G*)

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HEADER
REMARK Spartan exported Mon Jul 31 08:39:23 2006
HETATM    1  F   UNK  0001      -9.825  -1.226   1.716
HETATM    2  F   UNK  0001      -9.202  -1.217   3.755
HETATM    3  F   UNK  0001     -11.275  -1.055   3.270
HETATM    4  N   UNK  0001      -9.150   1.302   1.923
HETATM    5  H   UNK  0001      -8.777   0.645   1.276
HETATM    6  N   UNK  0001      -2.009   8.071   0.386
HETATM    7  H   UNK  0001      -1.430   7.622   1.057
HETATM    8  N   UNK  0001       8.190   4.792  -0.834
HETATM    9  H   UNK  0001       7.417   4.664  -1.446
HETATM   10  N   UNK  0001       8.191  -4.791   0.834
HETATM   11  C   UNK  0001       1.974 -10.394   1.171
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HETATM   12  H   UNK  0001       7.418  -4.663   1.446
HETATM   13  O   UNK  0001     -10.484   1.452   3.765
HETATM   14  O   UNK  0001      -7.326   1.686   0.117
HETATM   15  O   UNK  0001      -2.693   6.463   2.306
HETATM   16  O   UNK  0001      -1.999   9.493  -1.360
HETATM   17  O   UNK  0001       0.454   7.404   1.245
HETATM   18  O   UNK  0001       6.091   5.817  -2.179
HETATM   19  O   UNK  0001       9.237   6.293   0.478
HETATM   20  O   UNK  0001       7.451   2.654  -2.104
HETATM   21  O   UNK  0001       7.452  -2.653   2.104
HETATM   22  C   UNK  0001     -10.071  -0.697   2.907
HETATM   23  C   UNK  0001      -9.935   0.835   2.905
HETATM   24  C   UNK  0001      -8.760   2.640   1.690
HETATM   25  C   UNK  0001      -8.824   5.006   2.041
HETATM   26  C   UNK  0001      -7.857   5.184   1.080
HETATM   27  C   UNK  0001      -7.325   4.092   0.399
HETATM   28  H   UNK  0001      -6.566   4.241  -0.344
HETATM   29  C   UNK  0001      -7.776   2.827   0.703
HETATM   30  C   UNK  0001      -6.478   1.769  -0.999
HETATM   31  H   UNK  0001      -6.943   2.333  -1.799
HETATM   32  H   UNK  0001      -6.311   0.753  -1.322
HETATM   33  H   UNK  0001      -5.529   2.222  -0.737
HETATM   34  C   UNK  0001      -9.296   6.329   2.625
HETATM   35  C   UNK  0001     -10.687   6.692   2.073
HETATM   36  H   UNK  0001     -10.691   6.723   0.989
HETATM   37  H   UNK  0001     -11.002   7.665   2.441
HETATM   38  H   UNK  0001     -11.428   5.963   2.384
HETATM   39  C   UNK  0001      -9.352   6.317   4.158
HETATM   40  H   UNK  0001     -10.115   5.636   4.523
HETATM   41  H   UNK  0001      -9.589   7.308   4.537
HETATM   42  H   UNK  0001      -8.401   6.012   4.583
HETATM   43  C   UNK  0001      -8.199   7.302   2.113
HETATM   44  H   UNK  0001      -7.460   7.440   2.894
HETATM   45  H   UNK  0001      -8.600   8.282   1.883
HETATM   46  C   UNK  0001      -7.502   6.649   0.880
HETATM   47  C   UNK  0001      -7.967   7.201  -0.502
HETATM   48  H   UNK  0001      -8.027   6.376  -1.203
HETATM   49  H   UNK  0001      -8.956   7.644  -0.454
HETATM   50  C   UNK  0001      -6.898   8.211  -1.004
HETATM   51  C   UNK  0001      -7.283   9.665  -0.677
HETATM   52  H   UNK  0001      -7.454   9.803   0.385
HETATM   53  H   UNK  0001      -8.188   9.951  -1.206
HETATM   54  H   UNK  0001      -6.493  10.348  -0.973
HETATM   55  C   UNK  0001      -6.685   8.079  -2.518
HETATM   56  H   UNK  0001      -5.935   8.778  -2.875
HETATM   57  H   UNK  0001      -7.609   8.286  -3.053
HETATM   58  H   UNK  0001      -6.361   7.078  -2.783
HETATM   59  C   UNK  0001      -5.678   7.789  -0.199
HETATM   60  C   UNK  0001      -6.011   6.940   0.826
HETATM   61  C   UNK  0001      -5.030   6.470   1.697
HETATM   62  H   UNK  0001      -5.296   5.799   2.491
HETATM   63  C   UNK  0001      -3.726   6.868   1.519
HETATM   64  C   UNK  0001      -2.955   5.696   3.445
HETATM   65  H   UNK  0001      -3.634   6.208   4.118
HETATM   66  H   UNK  0001      -2.006   5.553   3.941
HETATM   67  H   UNK  0001      -3.369   4.728   3.185
HETATM   68  C   UNK  0001      -3.372   7.742   0.468
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HETATM   69  C   UNK  0001      -4.358   8.199  -0.386
HETATM   70  H   UNK  0001      -4.092   8.863  -1.179
HETATM   71  C   UNK  0001      -1.404   8.901  -0.495
HETATM   72  C   UNK  0001       0.091   9.101  -0.360
HETATM   73  C   UNK  0001       0.973   8.383   0.471
HETATM   74  C   UNK  0001      -9.287   3.730   2.353
HETATM   75  H   UNK  0001     -10.038   3.580   3.100
HETATM   76  C   UNK  0001       1.275   6.634   2.082
HETATM   77  H   UNK  0001       2.020   6.094   1.510
HETATM   78  H   UNK  0001       0.618   5.930   2.569
HETATM   79  H   UNK  0001       1.763   7.248   2.829
HETATM   80  C   UNK  0001       2.327   8.672   0.472
HETATM   81  H   UNK  0001       3.005   8.118   1.092
HETATM   82  C   UNK  0001       2.815   9.676  -0.350
HETATM   83  C   UNK  0001       1.972  10.394  -1.171
HETATM   84  C   UNK  0001       0.619  10.102  -1.169
HETATM   85  H   UNK  0001      -0.067  10.634  -1.798
HETATM   86  C   UNK  0001       2.717  11.460  -1.960
HETATM   87  C   UNK  0001       2.447  12.856  -1.371
HETATM   88  H   UNK  0001       1.397  13.115  -1.464
HETATM   89  H   UNK  0001       3.026  13.613  -1.894
HETATM   90  H   UNK  0001       2.703  12.902  -0.318
HETATM   91  C   UNK  0001       2.349  11.465  -3.449
HETATM   92  H   UNK  0001       2.479  10.481  -3.889
HETATM   93  H   UNK  0001       2.976  12.165  -3.995
HETATM   94  H   UNK  0001       1.317  11.764  -3.600
HETATM   95  C   UNK  0001       4.195  11.021  -1.752
HETATM   96  H   UNK  0001       4.868  11.868  -1.694
HETATM   97  H   UNK  0001       4.508  10.428  -2.604
HETATM   98  C   UNK  0001       4.260  10.132  -0.473
HETATM   99  C   UNK  0001       4.770  10.859   0.811
HETATM  100  H   UNK  0001       4.169  10.538   1.654
HETATM  101  H   UNK  0001       4.661  11.935   0.738
HETATM  102  C   UNK  0001       6.246  10.438   1.054
HETATM  103  C   UNK  0001       7.234  11.467   0.477
HETATM  104  H   UNK  0001       8.257  11.122   0.588
HETATM  105  H   UNK  0001       7.144  12.419   0.994
HETATM  106  H   UNK  0001       7.060  11.639  -0.580
HETATM  107  C   UNK  0001       6.528  10.255   2.550
HETATM  108  H   UNK  0001       5.882   9.497   2.982
HETATM  109  H   UNK  0001       6.361  11.185   3.087
HETATM  110  H   UNK  0001       7.557   9.956   2.725
HETATM  111  C   UNK  0001       6.321   9.136   0.272
HETATM  112  C   UNK  0001       5.254   8.987  -0.587
HETATM  113  C   UNK  0001       5.160   7.886  -1.425
HETATM  114  H   UNK  0001       4.321   7.791  -2.085
HETATM  115  C   UNK  0001       6.139   6.907  -1.382
HETATM  116  C   UNK  0001       5.095   5.682  -3.158
HETATM  117  H   UNK  0001       4.111   5.606  -2.711
HETATM  118  H   UNK  0001       5.322   4.767  -3.683
HETATM  119  H   UNK  0001       5.116   6.511  -3.854
HETATM  120  C   UNK  0001       7.221   7.019  -0.486
HETATM  121  C   UNK  0001       7.295   8.152   0.315
HETATM  122  H   UNK  0001       8.132   8.227   0.980
HETATM  123  C   UNK  0001       8.320   6.004  -0.249
HETATM  124  C   UNK  0001       8.981   3.647  -0.638
HETATM  125  C   UNK  0001      10.095   3.572   0.177
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HETATM  126  H   UNK  0001      10.424   4.451   0.688
HETATM  127  C   UNK  0001      10.756   2.354   0.333
HETATM  128  C   UNK  0001      10.320   1.231  -0.323
HETATM  129  C   UNK  0001       9.213   1.293  -1.168
HETATM  130  H   UNK  0001       8.874   0.408  -1.671
HETATM  131  C   UNK  0001       8.552   2.489  -1.323
HETATM  132  C   UNK  0001       6.958   1.569  -2.835
HETATM  133  H   UNK  0001       7.696   1.197  -3.537
HETATM  134  H   UNK  0001       6.101   1.934  -3.381
HETATM  135  H   UNK  0001       6.645   0.761  -2.182
HETATM  136  C   UNK  0001      11.992   2.070   1.172
HETATM  137  C   UNK  0001      13.250   2.624   0.479
HETATM  138  H   UNK  0001      13.198   3.705   0.395
HETATM  139  H   UNK  0001      13.362   2.223  -0.523
HETATM  140  H   UNK  0001      14.143   2.375   1.045
HETATM  141  C   UNK  0001      11.902   2.655   2.587
HETATM  142  H   UNK  0001      12.752   2.339   3.186
HETATM  143  H   UNK  0001      10.997   2.328   3.089
HETATM  144  H   UNK  0001      11.900   3.740   2.569
HETATM  145  C   UNK  0001      11.992   0.516   1.209
HETATM  146  H   UNK  0001      11.515   0.188   2.126
HETATM  147  H   UNK  0001      12.996   0.108   1.215
HETATM  148  C   UNK  0001      11.153   0.001  -0.000
HETATM  149  C   UNK  0001      11.992  -0.514  -1.209
HETATM  150  H   UNK  0001      12.996  -0.106  -1.215
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HETATM  154  H   UNK  0001      11.900  -3.738  -2.569
HETATM  155  H   UNK  0001      12.753  -2.337  -3.186
HETATM  156  H   UNK  0001      10.997  -2.326  -3.089
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HETATM  158  H   UNK  0001      13.362  -2.221   0.522
HETATM  159  H   UNK  0001      14.144  -2.373  -1.046
HETATM  160  H   UNK  0001      13.198  -3.703  -0.396
HETATM  161  C   UNK  0001      10.756  -2.352  -0.333
HETATM  162  C   UNK  0001      10.320  -1.229   0.323
HETATM  163  C   UNK  0001       9.214  -1.292   1.168
HETATM  164  H   UNK  0001       8.875  -0.407   1.671
HETATM  165  C   UNK  0001       8.553  -2.488   1.323
HETATM  166  C   UNK  0001       6.958  -1.568   2.835
HETATM  167  H   UNK  0001       7.697  -1.196   3.537
HETATM  168  H   UNK  0001       6.101  -1.933   3.382
HETATM  169  H   UNK  0001       6.646  -0.760   2.182
HETATM  170  C   UNK  0001       8.982  -3.645   0.639
HETATM  171  C   UNK  0001      10.095  -3.571  -0.177
HETATM  172  H   UNK  0001      10.424  -4.449  -0.688
HETATM  173  H   UNK  0001     -10.037  -3.581  -3.100
HETATM  174  C   UNK  0001      -8.759  -2.642  -1.690
HETATM  175  C   UNK  0001      -9.286  -3.731  -2.353
HETATM  176  C   UNK  0001      -6.478  -1.770   1.000
HETATM  177  H   UNK  0001      -6.943  -2.335   1.799
HETATM  178  C   UNK  0001       2.329  -8.672  -0.472
HETATM  179  H   UNK  0001       3.006  -8.118  -1.092
HETATM  180  N   UNK  0001      -2.007  -8.072  -0.386
HETATM  181  H   UNK  0001      -1.429  -7.622  -1.057
HETATM  182  H   UNK  0001       2.978 -12.164   3.995
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HETATM  187  C   UNK  0001       0.092  -9.101   0.360
HETATM  188  O   UNK  0001       9.238  -6.292  -0.478
HETATM  189  O   UNK  0001       6.092  -5.816   2.179
HETATM  190  O   UNK  0001       0.455  -7.405  -1.246
HETATM  191  O   UNK  0001      -1.997  -9.494   1.360
HETATM  192  O   UNK  0001      -2.692  -6.463  -2.306
HETATM  193  O   UNK  0001      -7.326  -1.688  -0.116
HETATM  194  H   UNK  0001      -5.529  -2.223   0.738
HETATM  195  H   UNK  0001     -11.427  -5.964  -2.385
HETATM  196  C   UNK  0001      -8.823  -5.007  -2.041
HETATM  197  H   UNK  0001     -10.113  -5.637  -4.524
HETATM  198  C   UNK  0001      -6.684  -8.081   2.518
HETATM  199  H   UNK  0001      -9.587  -7.308  -4.538
HETATM  200  H   UNK  0001      -8.400  -6.013  -4.583
HETATM  201  H   UNK  0001     -10.690  -6.724  -0.990
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HETATM  203  H   UNK  0001      -6.565  -4.242   0.344
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HETATM  216  C   UNK  0001      -9.351  -6.318  -4.159
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HETATM  220  H   UNK  0001      -8.186  -9.953   1.205
HETATM  221  H   UNK  0001      -2.005  -5.552  -3.941
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HETATM  225  C   UNK  0001      -3.725  -6.868  -1.519
HETATM  226  C   UNK  0001      -2.954  -5.696  -3.445
HETATM  227  H   UNK  0001      -3.368  -4.728  -3.184
HETATM  228  C   UNK  0001      -6.896  -8.212   1.004
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HETATM  230  H   UNK  0001      -3.633  -6.208  -4.118
HETATM  231  C   UNK  0001      -6.010  -6.941  -0.827
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HETATM  233  C   UNK  0001      -1.403  -8.901   0.494
HETATM  234  C   UNK  0001      -3.371  -7.743  -0.469
HETATM  235  C   UNK  0001       0.620 -10.102   1.168
HETATM  236  C   UNK  0001       0.974  -8.383  -0.471
HETATM  237  C   UNK  0001       1.276  -6.634  -2.082
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HETATM  239  H   UNK  0001       0.619  -5.930  -2.570
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pdb-file heptamer (HF/3-21G)

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HETATM    5  H   UNK  0001       5.436  -5.596  -2.279
HETATM    6  N   UNK  0001       6.901   4.031  -3.247
HETATM    7  H   UNK  0001       6.011   4.241  -3.662
HETATM    8  N   UNK  0001      -1.549  10.009  -0.133
HETATM    9  H   UNK  0001      -1.134   9.247   0.373
HETATM   10  N   UNK  0001     -10.291   5.428  -0.034
HETATM   11  C   UNK  0001     -13.712  -2.142  -1.003
HETATM   12  H   UNK  0001      -9.974   4.805  -0.754
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HETATM   14  O   UNK  0001       6.000  -3.857  -1.459
HETATM   15  O   UNK  0001       5.297   2.403  -4.465
HETATM   16  O   UNK  0001       8.531   4.801  -1.870
HETATM   17  O   UNK  0001       4.939   5.703  -3.748
HETATM   18  O   UNK  0001       0.524   8.553   0.541
HETATM   19  O   UNK  0001      -1.114  11.787  -1.477
HETATM   20  O   UNK  0001      -2.697   8.220   1.352
HETATM   21  O   UNK  0001      -8.354   5.739  -1.729
HETATM   22  C   UNK  0001       4.499  -7.686  -3.216
HETATM   23  C   UNK  0001       5.451  -6.746  -3.951
HETATM   24  C   UNK  0001       6.554  -4.576  -3.610
HETATM   25  C   UNK  0001       7.911  -3.278  -5.075
HETATM   26  C   UNK  0001       8.022  -2.305  -4.110
HETATM   27  C   UNK  0001       7.411  -2.453  -2.875
HETATM   28  H   UNK  0001       7.503  -1.686  -2.135
HETATM   29  C   UNK  0001       6.678  -3.586  -2.626
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HETATM   31  H   UNK  0001       7.378  -3.362   0.033
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HETATM   34  C   UNK  0001       8.714  -2.931  -6.321
HETATM   35  C   UNK  0001      10.009  -3.769  -6.350
HETATM   36  H   UNK  0001      10.588  -3.614  -5.448
HETATM   37  H   UNK  0001      10.617  -3.494  -7.206
HETATM   38  H   UNK  0001       9.773  -4.825  -6.423
HETATM   39  C   UNK  0001       7.919  -3.156  -7.618
HETATM   40  H   UNK  0001       7.695  -4.208  -7.756
HETATM   41  H   UNK  0001       8.495  -2.820  -8.474
HETATM   42  H   UNK  0001       6.984  -2.607  -7.594
HETATM   43  C   UNK  0001       9.020  -1.415  -6.095
HETATM   44  H   UNK  0001       8.278  -0.826  -6.620
HETATM   45  H   UNK  0001       9.998  -1.140  -6.468
HETATM   46  C   UNK  0001       8.878  -1.135  -4.561
HETATM   47  C   UNK  0001      10.227  -1.049  -3.766
HETATM   48  H   UNK  0001      10.102  -1.565  -2.823
HETATM   49  H   UNK  0001      11.042  -1.515  -4.303
HETATM   50  C   UNK  0001      10.505   0.462  -3.483
HETATM   51  C   UNK  0001      11.452   1.064  -4.543
HETATM   52  H   UNK  0001      11.059   0.911  -5.540
HETATM   53  H   UNK  0001      12.433   0.601  -4.480
HETATM   54  H   UNK  0001      11.566   2.130  -4.383
HETATM   55  C   UNK  0001      11.095   0.671  -2.079
HETATM   56  H   UNK  0001      11.263   1.725  -1.885
HETATM   57  H   UNK  0001      12.046   0.156  -1.989
HETATM   58  H   UNK  0001      10.422   0.286  -1.321
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HETATM   59  C   UNK  0001       9.121   1.075  -3.639
HETATM   60  C   UNK  0001       8.250   0.215  -4.261
HETATM   61  C   UNK  0001       6.957   0.621  -4.556
HETATM   62  H   UNK  0001       6.282  -0.058  -5.035
HETATM   63  C   UNK  0001       6.555   1.889  -4.214
HETATM   64  C   UNK  0001       4.307   1.602  -5.127
HETATM   65  H   UNK  0001       4.632   1.319  -6.120
HETATM   66  H   UNK  0001       3.427   2.222  -5.196
HETATM   67  H   UNK  0001       4.078   0.711  -4.557
HETATM   68  C   UNK  0001       7.430   2.768  -3.555
HETATM   69  C   UNK  0001       8.718   2.352  -3.273
HETATM   70  H   UNK  0001       9.372   3.022  -2.767
HETATM   71  C   UNK  0001       7.459   4.967  -2.454
HETATM   72  C   UNK  0001       6.699   6.244  -2.246
HETATM   73  C   UNK  0001       5.494   6.595  -2.862
HETATM   74  C   UNK  0001       7.171  -4.428  -4.834
HETATM   75  H   UNK  0001       7.069  -5.198  -5.565
HETATM   76  C   UNK  0001       3.748   6.010  -4.498
HETATM   77  H   UNK  0001       2.901   6.150  -3.840
HETATM   78  H   UNK  0001       3.589   5.152  -5.128
HETATM   79  H   UNK  0001       3.891   6.894  -5.104
HETATM   80  C   UNK  0001       4.889   7.804  -2.564
HETATM   81  H   UNK  0001       3.962   8.077  -3.021
HETATM   82  C   UNK  0001       5.477   8.654  -1.650
HETATM   83  C   UNK  0001       6.665   8.319  -1.031
HETATM   84  C   UNK  0001       7.272   7.123  -1.337
HETATM   85  H   UNK  0001       8.194   6.825  -0.885
HETATM   86  C   UNK  0001       7.125   9.401  -0.065
HETATM   87  C   UNK  0001       8.287  10.206  -0.682
HETATM   88  H   UNK  0001       9.148   9.563  -0.831
HETATM   89  H   UNK  0001       8.578  11.017  -0.021
HETATM   90  H   UNK  0001       8.011  10.623  -1.641
HETATM   91  C   UNK  0001       7.569   8.818   1.287
HETATM   92  H   UNK  0001       6.795   8.184   1.694
HETATM   93  H   UNK  0001       7.773   9.614   1.995
HETATM   94  H   UNK  0001       8.471   8.227   1.173
HETATM   95  C   UNK  0001       5.827  10.262   0.083
HETATM   96  H   UNK  0001       6.049  11.310   0.233
HETATM   97  H   UNK  0001       5.270   9.902   0.938
HETATM   98  C   UNK  0001       4.979  10.022  -1.211
HETATM   99  C   UNK  0001       5.180  11.092  -2.341
HETATM  100  H   UNK  0001       5.204  10.581  -3.296
HETATM  101  H   UNK  0001       6.105  11.637  -2.222
HETATM  102  C   UNK  0001       3.941  12.040  -2.308
HETATM  103  C   UNK  0001       4.219  13.300  -1.462
HETATM  104  H   UNK  0001       3.321  13.904  -1.383
HETATM  105  H   UNK  0001       4.996  13.902  -1.923
HETATM  106  H   UNK  0001       4.533  13.033  -0.461
HETATM  107  C   UNK  0001       3.513  12.450  -3.727
HETATM  108  H   UNK  0001       3.271  11.576  -4.321
HETATM  109  H   UNK  0001       4.313  12.994  -4.219
HETATM  110  H   UNK  0001       2.640  13.093  -3.695
HETATM  111  C   UNK  0001       2.905  11.175  -1.609
HETATM  112  C   UNK  0001       3.478  10.088  -0.979
HETATM  113  C   UNK  0001       2.706   9.207  -0.247
HETATM  114  H   UNK  0001       3.168   8.385   0.253
HETATM  115  C   UNK  0001       1.339   9.406  -0.160
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HETATM  116  C   UNK  0001       1.010   7.345   1.157
HETATM  117  H   UNK  0001       1.480   6.702   0.423
HETATM  118  H   UNK  0001       0.129   6.869   1.553
HETATM  119  H   UNK  0001       1.703   7.562   1.952
HETATM  120  C   UNK  0001       0.743  10.493  -0.807
HETATM  121  C   UNK  0001       1.545  11.371  -1.519
HETATM  122  H   UNK  0001       1.058  12.195  -1.997
HETATM  123  C   UNK  0001      -0.727  10.817  -0.829
HETATM  124  C   UNK  0001      -2.945  10.099  -0.039
HETATM  125  C   UNK  0001      -3.730  11.044  -0.673
HETATM  126  H   UNK  0001      -3.251  11.781  -1.274
HETATM  127  C   UNK  0001      -5.108  11.008  -0.514
HETATM  128  C   UNK  0001      -5.701  10.050   0.271
HETATM  129  C   UNK  0001      -4.926   9.099   0.918
HETATM  130  H   UNK  0001      -5.398   8.347   1.516
HETATM  131  C   UNK  0001      -3.562   9.125   0.764
HETATM  132  C   UNK  0001      -3.189   7.282   2.321
HETATM  133  H   UNK  0001      -3.680   7.789   3.142
HETATM  134  H   UNK  0001      -2.322   6.756   2.688
HETATM  135  H   UNK  0001      -3.878   6.578   1.872
HETATM  136  C   UNK  0001      -6.133  11.968  -1.102
HETATM  137  C   UNK  0001      -6.089  13.307  -0.337
HETATM  138  H   UNK  0001      -5.120  13.779  -0.463
HETATM  139  H   UNK  0001      -6.253  13.152   0.722
HETATM  140  H   UNK  0001      -6.851  13.983  -0.712
HETATM  141  C   UNK  0001      -5.910  12.221  -2.602
HETATM  142  H   UNK  0001      -6.706  12.842  -3.001
HETATM  143  H   UNK  0001      -5.895  11.285  -3.149
HETATM  144  H   UNK  0001      -4.967  12.731  -2.771
HETATM  145  C   UNK  0001      -7.471  11.203  -0.847
HETATM  146  H   UNK  0001      -7.723  10.637  -1.735
HETATM  147  H   UNK  0001      -8.288  11.878  -0.629
HETATM  148  C   UNK  0001      -7.212  10.193   0.322
HETATM  149  C   UNK  0001      -7.732  10.661   1.723
HETATM  150  H   UNK  0001      -7.829  11.737   1.783
HETATM  151  H   UNK  0001      -7.020  10.340   2.473
HETATM  152  C   UNK  0001      -9.092   9.935   1.977
HETATM  153  C   UNK  0001      -9.239   9.524   3.452
HETATM  154  H   UNK  0001     -10.175   9.000   3.613
HETATM  155  H   UNK  0001      -9.230  10.403   4.090
HETATM  156  H   UNK  0001      -8.426   8.872   3.749
HETATM  157  C   UNK  0001     -10.291  10.811   1.560
HETATM  158  H   UNK  0001     -10.203  11.119   0.526
HETATM  159  H   UNK  0001     -10.347  11.698   2.184
HETATM  160  H   UNK  0001     -11.216  10.256   1.669
HETATM  161  C   UNK  0001      -8.984   8.735   1.046
HETATM  162  C   UNK  0001      -7.962   8.885   0.142
HETATM  163  C   UNK  0001      -7.720   7.903  -0.808
HETATM  164  H   UNK  0001      -6.912   8.022  -1.499
HETATM  165  C   UNK  0001      -8.513   6.783  -0.834
HETATM  166  C   UNK  0001      -7.371   5.830  -2.770
HETATM  167  H   UNK  0001      -7.549   6.690  -3.403
HETATM  168  H   UNK  0001      -7.472   4.928  -3.351
HETATM  169  H   UNK  0001      -6.370   5.888  -2.361
HETATM  170  C   UNK  0001      -9.563   6.620   0.086
HETATM  171  C   UNK  0001      -9.793   7.609   1.025
HETATM  172  H   UNK  0001     -10.594   7.476   1.715
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HETATM  173  H   UNK  0001      -3.272 -11.777   1.273
HETATM  174  C   UNK  0001      -2.963 -10.094   0.038
HETATM  175  C   UNK  0001      -3.750 -11.039   0.672
HETATM  176  C   UNK  0001      -3.203  -7.276  -2.321
HETATM  177  H   UNK  0001      -3.694  -7.782  -3.142
HETATM  178  C   UNK  0001     -12.165  -1.568   0.742
HETATM  179  H   UNK  0001     -11.819  -0.862   1.467
HETATM  180  N   UNK  0001     -10.302  -5.412   0.035
HETATM  181  H   UNK  0001      -9.985  -4.790   0.755
HETATM  182  N   UNK  0001      -1.568 -10.006   0.132
HETATM  183  C   UNK  0001       6.649  -8.330   1.031
HETATM  184  H   UNK  0001       7.755  -9.627  -1.995
HETATM  185  H   UNK  0001      -2.335  -6.751  -2.687
HETATM  186  C   UNK  0001      -5.719 -10.041  -0.271
HETATM  187  C   UNK  0001     -11.967  -3.685  -0.395
HETATM  188  O   UNK  0001     -11.828   5.721   1.613
HETATM  189  O   UNK  0001     -10.424   3.148  -1.330
HETATM  190  O   UNK  0001     -10.431  -3.133   1.332
HETATM  191  O   UNK  0001     -11.839  -5.702  -1.613
HETATM  192  O   UNK  0001      -8.366  -5.728   1.730
HETATM  193  O   UNK  0001      -2.712  -8.215  -1.352
HETATM  194  H   UNK  0001      -3.890  -6.571  -1.872
HETATM  195  H   UNK  0001      -5.144 -13.771   0.460
HETATM  196  C   UNK  0001      -5.128 -11.000   0.513
HETATM  197  H   UNK  0001      -4.990 -12.724   2.768
HETATM  198  C   UNK  0001      -9.256  -9.508  -3.453
HETATM  199  H   UNK  0001      -6.728 -12.834   2.999
HETATM  200  H   UNK  0001      -5.915 -11.277   3.147
HETATM  201  H   UNK  0001      -6.275 -13.142  -0.725
HETATM  202  C   UNK  0001      -4.943  -9.091  -0.918
HETATM  203  H   UNK  0001      -5.413  -8.338  -1.516
HETATM  204  C   UNK  0001      -3.579  -9.119  -0.764
HETATM  205  C   UNK  0001      -6.112 -13.298   0.334
HETATM  206  H   UNK  0001      -9.248 -10.386  -4.091
HETATM  207  H   UNK  0001      -7.850 -11.724  -1.785
HETATM  208  C   UNK  0001      -7.231 -10.182  -0.323
HETATM  209  C   UNK  0001      -7.491 -11.193   0.845
HETATM  210  H   UNK  0001      -8.309 -11.866   0.627
HETATM  211  H   UNK  0001      -8.442  -8.857  -3.749
HETATM  212  H   UNK  0001     -10.191  -8.982  -3.614
HETATM  213  C   UNK  0001      -7.751 -10.648  -1.725
HETATM  214  H   UNK  0001      -7.038 -10.328  -2.475
HETATM  215  C   UNK  0001      -6.154 -11.959   1.100
HETATM  216  C   UNK  0001      -5.932 -12.213   2.600
HETATM  217  H   UNK  0001      -7.743 -10.626   1.734
HETATM  218  H   UNK  0001     -11.235 -10.238  -1.671
HETATM  219  H   UNK  0001     -10.223 -11.103  -0.528
HETATM  220  H   UNK  0001     -10.368 -11.681  -2.186
HETATM  221  H   UNK  0001      -7.482  -4.918   3.352
HETATM  222  C   UNK  0001      -9.000  -8.721  -1.047
HETATM  223  C   UNK  0001      -7.735  -7.892   0.808
HETATM  224  H   UNK  0001      -6.927  -8.012   1.499
HETATM  225  C   UNK  0001      -8.526  -6.770   0.834
HETATM  226  C   UNK  0001      -7.382  -5.820   2.770
HETATM  227  H   UNK  0001      -6.382  -5.879   2.361
HETATM  228  C   UNK  0001      -9.110  -9.920  -1.978
HETATM  229  C   UNK  0001     -10.310 -10.794  -1.562
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HETATM  230  H   UNK  0001       -7.561  -6.680   3.403
HETATM  231  C   UNK  0001       -7.978  -8.872  -0.142
HETATM  232  C   UNK  0001       -9.808  -7.593  -1.025
HETATM  233  C   UNK  0001      -11.358  -5.025  -0.707
HETATM  234  C   UNK  0001       -9.576  -6.605  -0.085
HETATM  235  C   UNK  0001      -13.067  -3.348  -1.170
HETATM  236  C   UNK  0001      -11.520  -2.780   0.574
HETATM  237  C   UNK  0001       -9.909  -2.284   2.370
HETATM  238  H   UNK  0001       -9.566  -1.341   1.966
HETATM  239  H   UNK  0001       -9.080  -2.832   2.783
HETATM  240  C   UNK  0001      -13.253  -1.258  -0.048
HETATM  241  H   UNK  0001      -10.608  -7.459  -1.715
HETATM  242  H   UNK  0001      -13.382  -4.063  -1.901
HETATM  243  C   UNK  0001      -11.348   5.043   0.708
HETATM  244  C   UNK  0001      -11.959   3.704   0.396
HETATM  245  C   UNK  0001      -11.514   2.798  -0.573
HETATM  246  H   UNK  0001       -6.875 -13.973   0.709
HETATM  247  H   UNK  0001      -10.653  -2.105   3.135
HETATM  248  C   UNK  0001       -9.903   2.298  -2.367
HETATM  249  H   UNK  0001       -9.562   1.354  -1.961
HETATM  250  H   UNK  0001       -9.072   2.844  -2.779
HETATM  251  H   UNK  0001      -10.646   2.120  -3.132
HETATM  252  C   UNK  0001      -12.161   1.587  -0.740
HETATM  253  H   UNK  0001      -11.816   0.881  -1.465
HETATM  254  C   UNK  0001      -13.251   1.280   0.049
HETATM  255  C   UNK  0001      -13.707   2.165   1.004
HETATM  256  C   UNK  0001      -13.060   3.370   1.171
HETATM  257  H   UNK  0001      -13.374   4.086   1.901
HETATM  258  C   UNK  0001      -14.939   1.636   1.724
HETATM  259  C   UNK  0001      -16.199   2.353   1.196
HETATM  260  H   UNK  0001      -16.148   3.413   1.421
HETATM  261  H   UNK  0001      -17.090   1.946   1.664
HETATM  262  H   UNK  0001      -16.288   2.241   0.123
HETATM  263  C   UNK  0001      -14.847   1.804   3.250
HETATM  264  H   UNK  0001      -13.944   1.342   3.632
HETATM  265  H   UNK  0001      -15.703   1.341   3.731
HETATM  266  H   UNK  0001      -14.836   2.854   3.522
HETATM  267  C   UNK  0001      -14.925   0.128   1.317
HETATM  268  H   UNK  0001      -15.924  -0.268   1.195
HETATM  269  H   UNK  0001      -14.425  -0.439   2.093
HETATM  270  C   UNK  0001      -14.085   0.012   0.000
HETATM  271  C   UNK  0001      -14.925  -0.102  -1.317
HETATM  272  H   UNK  0001      -14.423   0.463  -2.092
HETATM  273  H   UNK  0001      -15.923   0.295  -1.195
HETATM  274  C   UNK  0001      -14.942  -1.611  -1.724
HETATM  275  C   UNK  0001      -16.203  -2.325  -1.196
HETATM  276  H   UNK  0001      -16.155  -3.385  -1.421
HETATM  277  H   UNK  0001      -17.093  -1.916  -1.664
HETATM  278  H   UNK  0001      -16.292  -2.212  -0.123
HETATM  279  C   UNK  0001      -14.849  -1.778  -3.250
HETATM  280  H   UNK  0001      -13.945  -1.318  -3.631
HETATM  281  H   UNK  0001      -15.704  -1.314  -3.731
HETATM  282  H   UNK  0001      -14.841  -2.828  -3.522
HETATM  283  H   UNK  0001        7.079   5.187   5.565
HETATM  284  C   UNK  0001        6.563   4.565   3.610
HETATM  285  C   UNK  0001        7.180   4.417   4.834
HETATM  286  C   UNK  0001        6.354   3.165   0.230
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HETATM  287  H   UNK  0001       7.385   3.351  -0.033
HETATM  288  C   UNK  0001       4.875  -7.811   2.564
HETATM  289  H   UNK  0001       3.947  -8.082   3.021
HETATM  290  N   UNK  0001       6.893  -4.042   3.247
HETATM  291  H   UNK  0001       6.003  -4.251   3.662
HETATM  292  H   UNK  0001      -1.151  -9.245  -0.373
HETATM  293  C   UNK  0001      -0.747 -10.816   0.829
HETATM  294  N   UNK  0001       5.775   5.669   3.223
HETATM  295  H   UNK  0001       5.709   3.582  -0.524
HETATM  296  C   UNK  0001       8.027   2.292   4.110
HETATM  297  C   UNK  0001       6.687  -6.254   2.246
HETATM  298  H   UNK  0001       8.456  -8.241  -1.173
HETATM  299  O   UNK  0001       0.508  -8.554  -0.542
HETATM  300  O   UNK  0001       4.928  -5.711   3.748
HETATM  301  O   UNK  0001       8.522  -4.815   1.870
HETATM  302  O   UNK  0001       5.293  -2.411   4.465
HETATM  303  O   UNK  0001       6.008   3.847   1.459
HETATM  304  H   UNK  0001       6.170   2.103   0.315
HETATM  305  H   UNK  0001       9.782   4.808   6.424
HETATM  306  C   UNK  0001       7.917   3.265   5.075
HETATM  307  H   UNK  0001       7.703   4.196   7.756
HETATM  308  C   UNK  0001      11.094  -0.690   2.079
HETATM  309  H   UNK  0001       8.501   2.806   8.475
HETATM  310  H   UNK  0001       6.989   2.596   7.594
HETATM  311  H   UNK  0001      10.595   3.596   5.448
HETATM  312  C   UNK  0001       7.416   2.441   2.875
HETATM  313  H   UNK  0001       7.507   1.673   2.136
HETATM  314  C   UNK  0001       6.685   3.576   2.626
HETATM  315  C   UNK  0001      10.016   3.752   6.350
HETATM  316  H   UNK  0001      12.046  -0.177   1.989
HETATM  317  H   UNK  0001      11.045   1.496   4.303
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NMR Studies.

DMSO-d_6 titration studies of foldamer 2 (trimer) and 4 (heptamer):

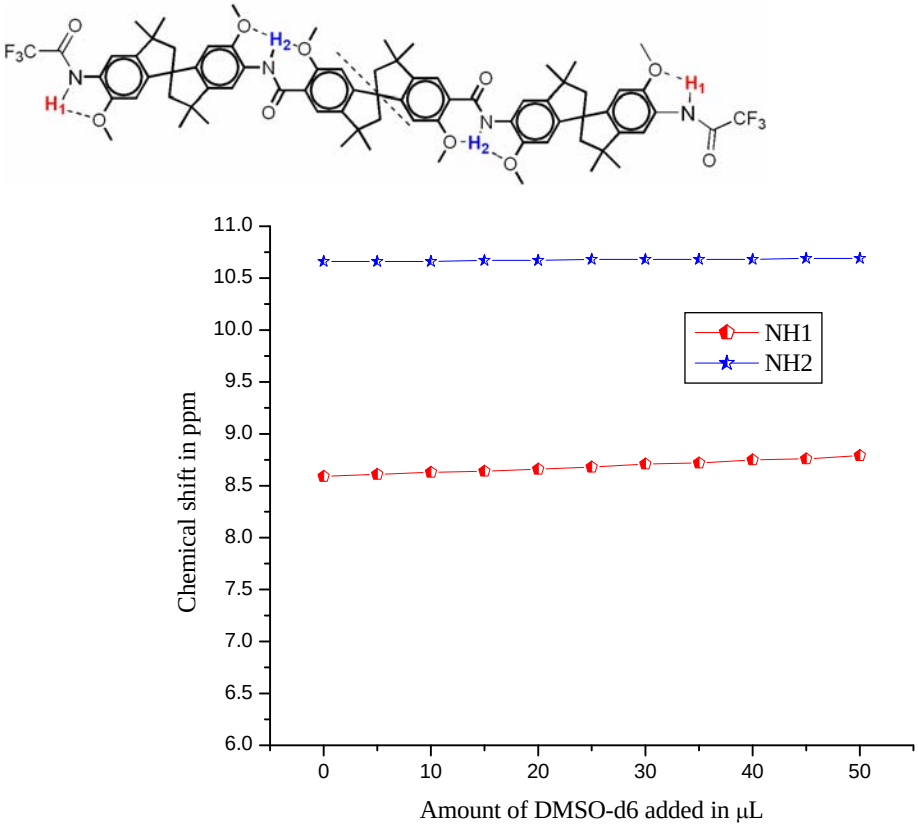

Figure 1. Molecular structure of foldamer **2** (*top*) and its DMSO-d_6 titration graph (bottom). The initial concentration of the sample in $CDCl_3$ was 5 mmol, and the total amount of [D6]DMSO used was 11 % of the total volume.

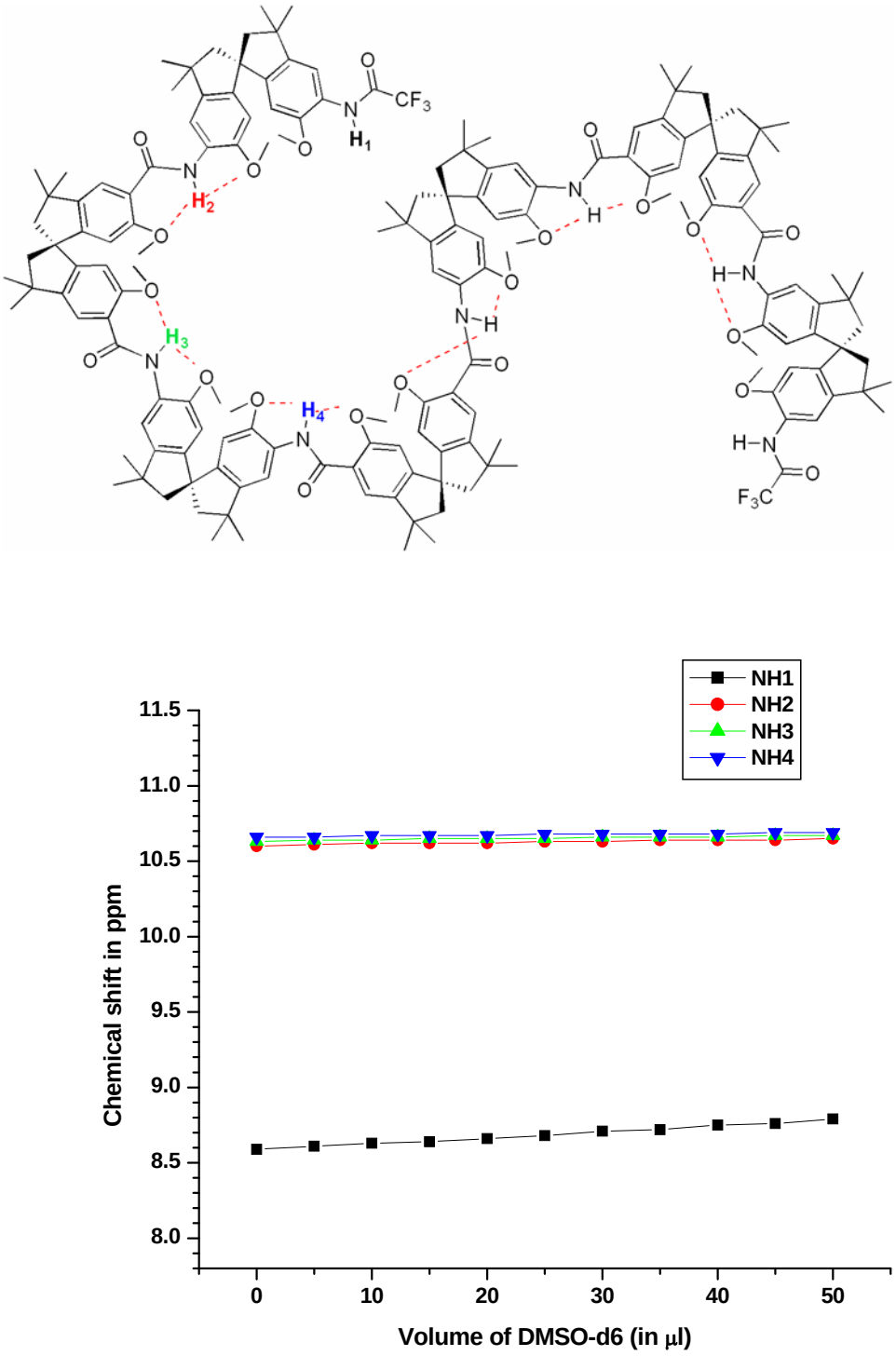

Figure 2. Molecular structure of heptamer **4** (*top*) and its DMSO-d_6 titration graph (bottom). The initial concentration of the sample in $CDCl_3$ was 5 mmol, and the total amount of [D6]DMSO used was 11 % of the total volume. *Note:* The chemical shifts of the amide NHs (NH2, NH3, and NH4) were poorly dispersed and their assignments could not be verified unambiguously.

Amount of DMSO-*d6* in μL	Chemical shift in ppm (NH_1)	Chemical shift in ppm (NH_2)
0	8.59	10.66
5	8.61	10.66
10	8.63	10.66
15	8.64	10.67
20	8.66	10.67
25	8.68	10.68
30	8.71	10.68
35	8.72	10.68
40	8.75	10.68
45	8.76	10.69
50	8.79	10.69

Table -1. DMSO-d_6 titration table for **2** (trimer)

Amount of DMSO-*d6* in μL	Chemical shift in ppm (NH_1)	Chemical shift in ppm (NH_2)	Chemical shift in ppm (NH_3)	Chemical shift in ppm (NH_4)
0	8.59	10.60 (2H)	10.63 (3H)	10.66 (1H)
5	8.61	10.61	10.64	10.66
10	8.63	10.62	10.64	10.67
15	8.64	10.62	10.65	10.67
20	8.66	10..62	10.65	10.67
25	8.68	10.63	10.65	10.68
30	8.71	10.63	10.66	10.68
35	8.72	10.64	10.66	10.68
40	8.75	10.64	10.66	10.68
45	8.76	10.64	10.67	10.69
50	8.79	10.65	10.67	10.69

Table -2. DMSO-d_6 titration table for **4** (heptamer).

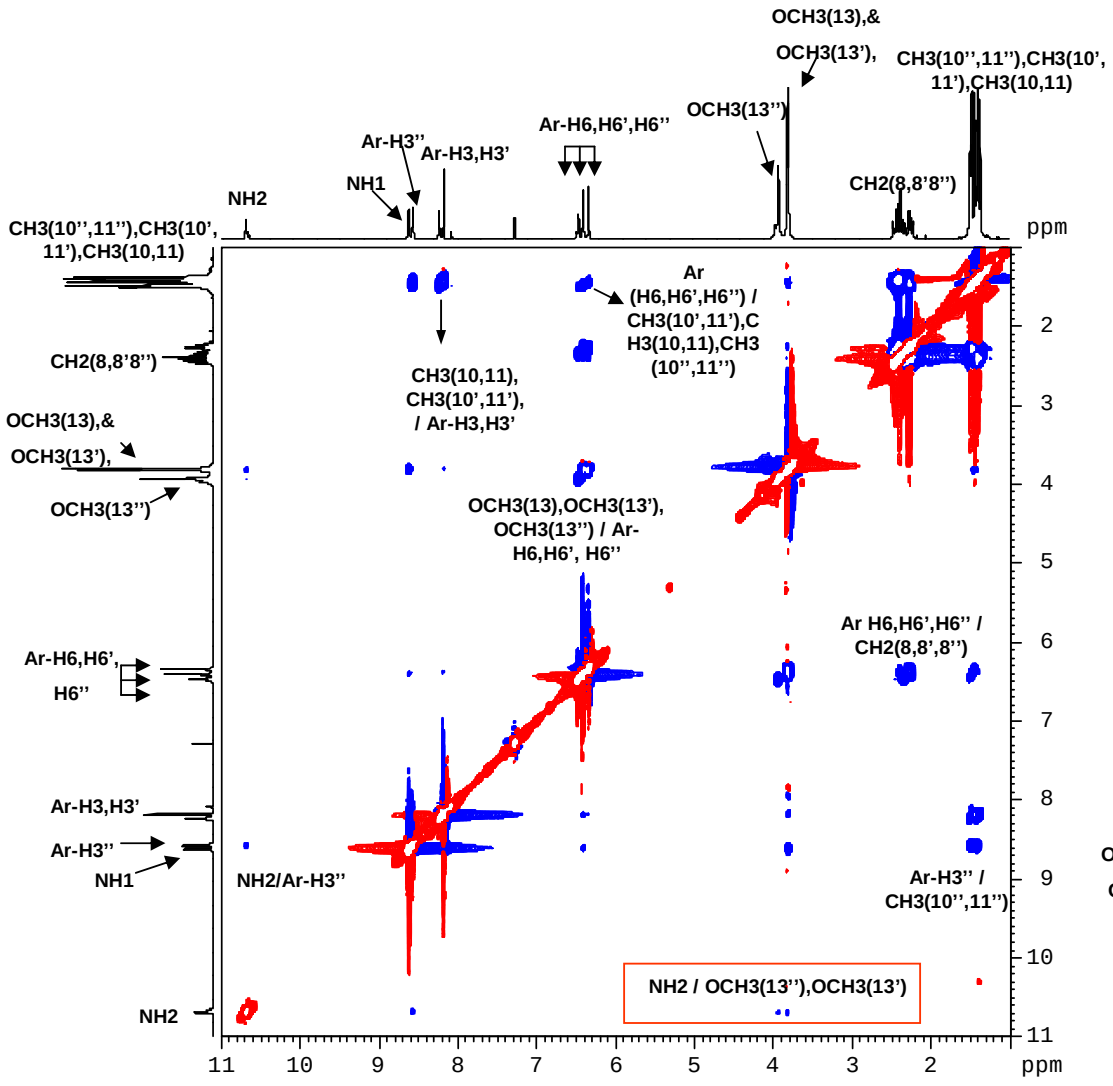

Figure 3. 2D ROESY spectrum of the oligomer **2** ($CDCl_3$, 400 MHz). *Note: The bifurcated H-bonding interaction (NH vs OMe) has been highlighted with red border.*

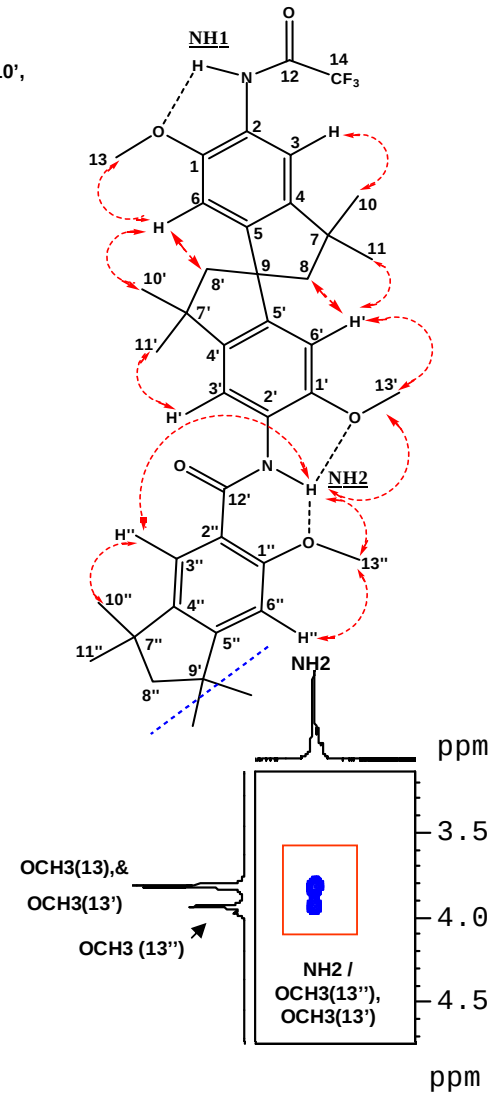

Figure 4. Molecular structure (symmetrical half) of **2** with atom labeling (top) and expanded 2D ROESY spectra showing characteristic bifurcated H-bonding interactions (bottom).

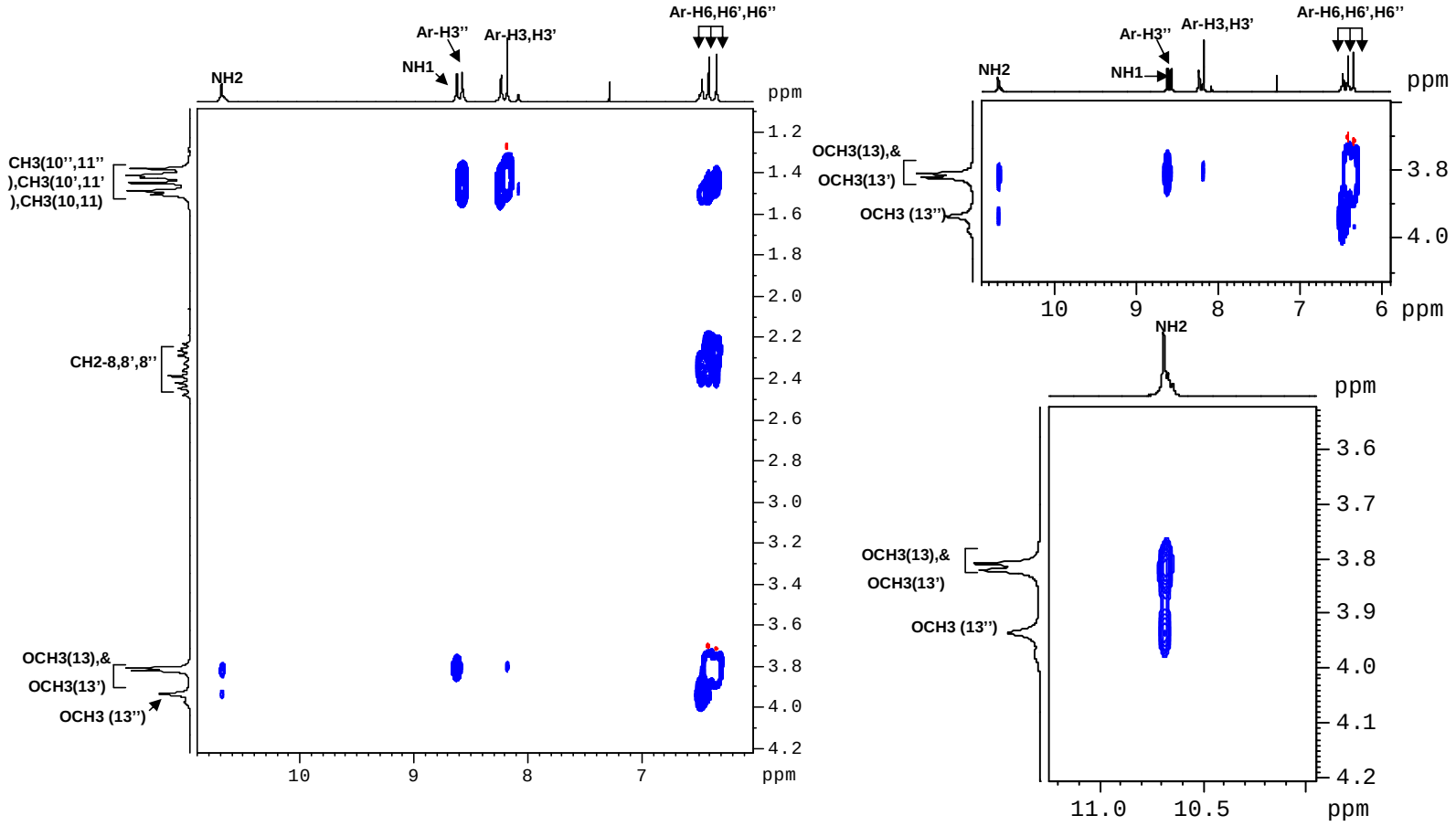

Figure 5. Partial 2D ROESY spectra of **2** showing various expanded regions.

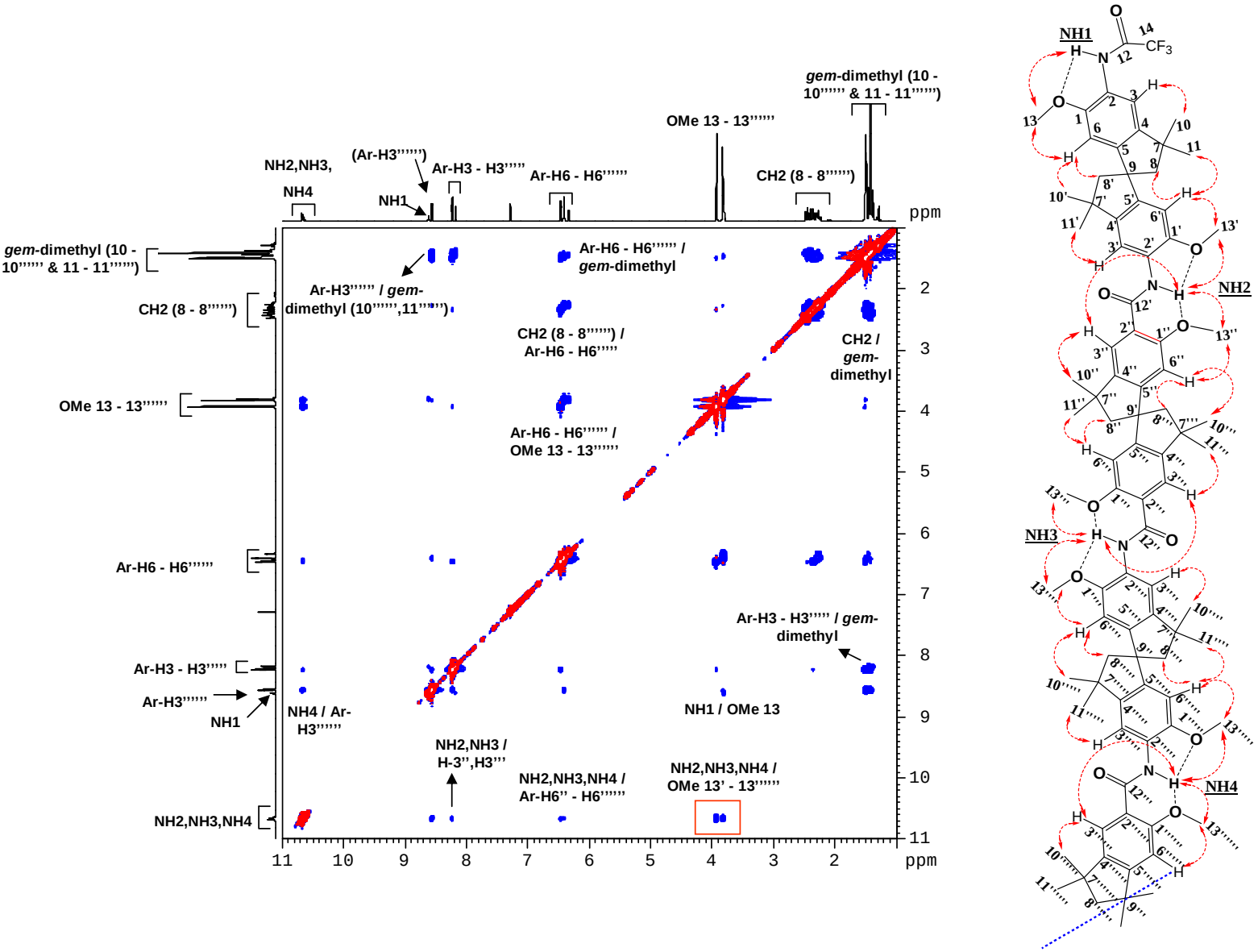

Figure 6. Molecular structure (symmetrical half) of **4** with atom labeling (right) and 2D ROESY spectra (left) [$CDCl_3$, 400 MHz]. *Note: The bifurcated H-bonding interaction (NH vs OMe) has been highlighted with red border.*

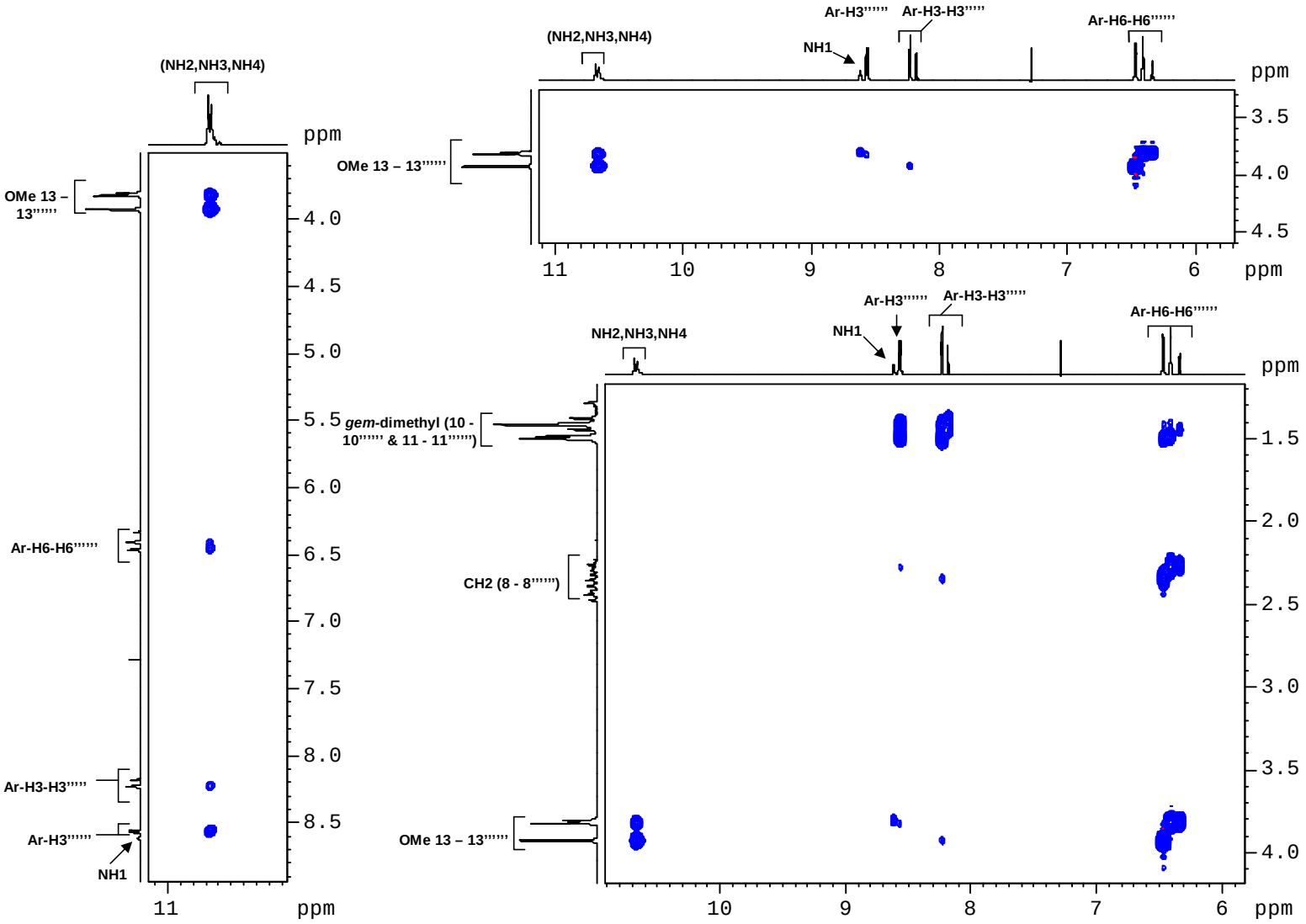

Figure 7. Partial 2D ROESY spectra of **4** showing various expanded regions.

Crystal data for 3. ($C_{80.52}H_{98.04}F_3N_4O_{10}$: M = 1338.78, Crystal dimensions 0.62 x 0.57 x 0.37 mm^3, triclinic, space group P-1, a = 10.861(4), b = 18.959(7), c = 23.398(9) Å, α = 85.319(7), β = 80.280(7), γ = 84.741(7)°; V = 4718(3) $Å^3$; Z = 2; T = 100(2) K, ρ_{calcd} = 0.927 gcm^{-3}, μ (Mo-K_α) = 0.065 mm^{-1}, F(000) = 1396, $2\theta_{max}$ = 50.00°, 45149 reflections collected, 16471 unique, 6779 observed ($I > 2\sigma(I)$) reflections, 904 refined parameters, R value 0.1546, wR2 = 0.3704 (all data R = 0.2679, wR2 = 0.4358), S = 1.206, minimum and maximum transmission 0.9609 and 0.9764 respectively, maximum and minimum residual electron densities +0.603 and –0.345 e $Å^{-3}$. Crystallographic data for of **3** has been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. CCDC- 656837.

Crystals of **3** were highly unstable in open atmosphere. Crystals were stabilized by sacking them in paraffin oil and immediately taken into the liquid nitrogen stream maintained at 100 K for X-ray data collection. All data were corrected for Lorentzian, polarization and absorption effects using SAINT and SADABS programs (Bruker, 2003). Restrained refinement was carried out for the solvent molecules cyclohexane and methyl propionate to keep their geometry fixed. Crystallographic data for of **3** has been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. CCDC- 656837. Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB2 1EZ, UK.