Supporting information for

Soluble and stable alternating main chain merocyanine copolymers through quantitative spiropyran-merocyanine conversion

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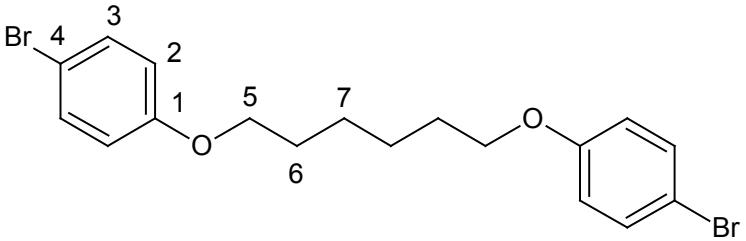
*Synthesis of **1**.* $SPBr_2$ **1** was synthesized according to Komber *et al.* in 63% yield.[1] ^1H and ^{13}C NMR data are identical to those given in ref [1].

MS (EI, 70 V); *m/z* = 449.98 (100) [M^+], 450 (50) [MH^+], 214 (5).

EA (%): calcd (found) for $C_{20}H_{19}Br_2NO$: C 53.48 (53.47), H 4.26 (4.37), N 3.12 (2.94)

*General synthesis of **2a,b,c**[2] and bis-phenyl model compound 7.* A mixture of dibromohexane (8.723 g, 35.75 mmol, 1eq), 4-bromophenol (13.695 g, 79.16 mmol, 2.2 eq), K_2CO_3 (20.1681 g, 144.95 mmol, 4.0 eq) and dry DMF (100 ml) was stirred at 60 °C under argon. After 40 h, the mixture was cooled to room temperature and HCl (180 ml, 1M) was added and stirred for 30 min, whereby a white solid formed which was filtered off. The product was obtained as white crystals after recrystallization from ethanol (3x). Yields were 83 %, 84 % and 95 % for **2a**, **2b** and **2c**, respectively. The yield for **7** was 69 %.

1,6-Bis(4-bromophenoxy)hexane **2a**



^1H NMR (300 MHz, $CDCl_3$): δ 7.36 (d, 4H, H_3), 6.77 (d, 4H, H_2), 3.93 (t, 4H, H_5), 1.81 (m, 4H, H_6), 1.53 ppm (m, 4H, H_7).

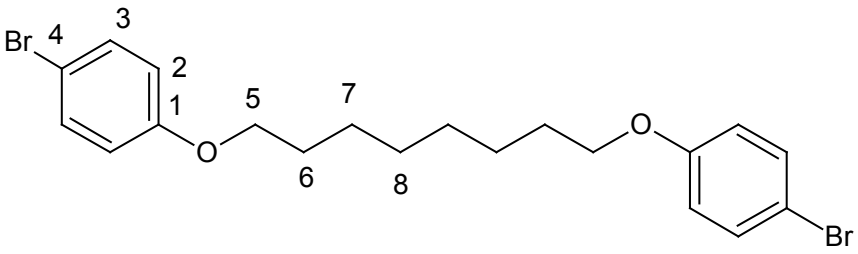
^{13}C NMR (75 MHz, $CDCl_3$): δ 158.38 (C_1), 132.36 (C_3), 116.50 (C_2), 112.83 (C_4), 68.25 (C_5), 29.25 (C_6), 25.94 ppm (C_7).

MS (EI, 70 V); m/z = 463 (100), 465 (70).

EA (%): calcd (found) for $C_{18}H_{20}Br_2O_2$: C 50.49 (50.18), H4.71 (7.86).

[1] Sommer, M.; Komber, H. *Macromol. Rapid Commun*. **2013**, *34*, 57-62.
[2] Neigenfink, J.; Martin, A.; Wendel, V.; Abraham, W. *J. prakt. Chem.* **1998**, *340*, 632.

1,6-Bis(4-bromophenoxy)octane **2b**



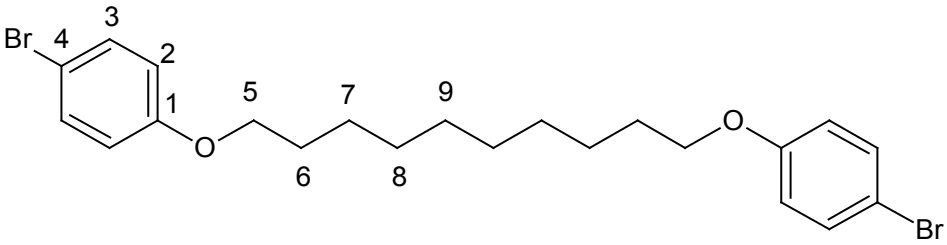
^{1}H NMR (300 MHz, $CDCl_3$): δ 7.35 (d, 4H, H_3), 6.77 (d, 4H, H_2),3.91 (t, 4H, H_5), 1.77 (m, 4H, H_6),1.51-1.35 ppm (m, 8H, H_7, H_8).

^{13}C NMR (75 MHz, $CDCl_3$):δ 158.44 (C_1), 132.35 (C_3), 116.51 (C_2), 112.78 (C_4), 68.40 (C_5), 29.39 and 29.30 (C_6, C_8), 26.08 ppm (C_7).

MS (EI, 70 V); m/z = 214 (100), 282 (51), 457 (45) [MH^+]

EA (%): calcd (found) for $C_{20}H_{24}Br_2O_2$: C 52.04 (52.65), H 5.30 (5.43).

1,6-Bis(4-bromophenoxy)decane **2c**



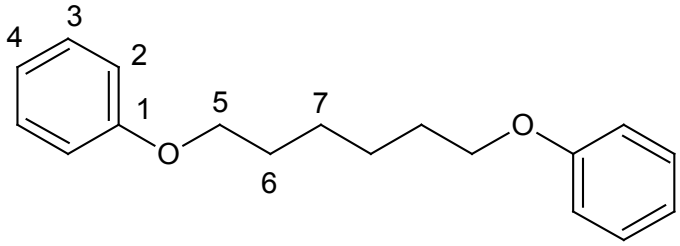
^{1}H NMR (300 MHz, $CDCl_3$): δ 7.35 (d, 4H, H_3), 6.79 (d, 4H, H_2), 3.91 (t, 4H, H_5), 1.76 (m, 4H, H_6), 1.46-1.32 ppm (12H, H_7, H_8, H_9).

^{13}C NMR (75 MHz, $CDCl_3$): δ 158.38 (C_1), 132.31 (C_3), 116.44 (C_2), 112.69 (C_4), 68.37 (C_5), 29.58, 29.46 and 29.29 (C_6, C_8, C_9), 26.11 ppm (C_7).

MS (EI, 70 V); m/z = 519 (100), 521 (70).

EA (%): calcd (found) for $C_{22}H_{28}Br_2O_2$: C54.56 (54.40), H 5.83 (5.87).

1,6-Bis(phenoxy)hexane **7**



^{1}H NMR (500 MHz, $CDCl_3$): δ 7.24 (t, 4H, H_3), 6.90 (t, 2H, H_4), 6.87 (d, 4H, H_2), 3.94 (t, 4H, H_5), 1.79 (m, 4H, H_6), 1.52 ppm (m, 4H, H_7).

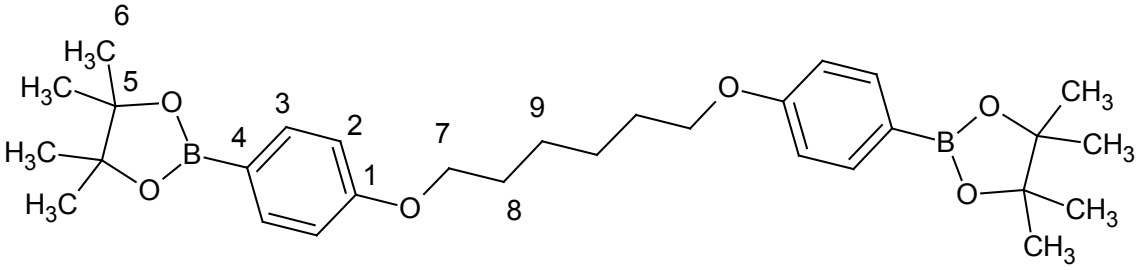
^{13}C NMR (125 MHz, $CDCl_3$): δ 159.10 (C_1), 129.39 (C_3), 120.50 (C_4), 114.52 (C_2), 67.72 (C_5), 29.25 (C_6), 25.89 ppm (C_7).

MS (EI, 70 V); m/z = 271 (100) [MH^+], 288 (65), 214 (65)

EA (%): calcd (found) for $C_{18}H_{22}O_2$: C 79.96 (79.27, H 8.20 (8.39).

General synthesis of ***3a,b,c***. **2a** (5.992g, 14.0 mmol) was dissolved in anhydrous THF (200 ml) under argon and cooled down to -78 °C. n-BuLi (14.0 ml, 28.0 mmol) was added at -78°C, stirred for 2h, when isopropoxy-4,4,5,5-tetramethyl-1,3,2-dioxaborolan (7.5 ml, 36.7 mmol) was added. The mixture was warmed to room temperature and stirred for 70 h. A mixture of ice and water (200 ml) was added, the whole extracted with diethyl ether (3x 200 ml), and the organic phase was washed with brine (50 ml). Finally, the solvents were removed under reduced pressure. The raw products were recrystallized from ethanol (3x) to give yields of **3a,b,c** of 84 %, 90 % and 75 %, respectively.

1,6-Bis(4-[4,4,5,5-tetramethyl-1,3,2-dioxaborolan]phenoxy)hexane **3a**



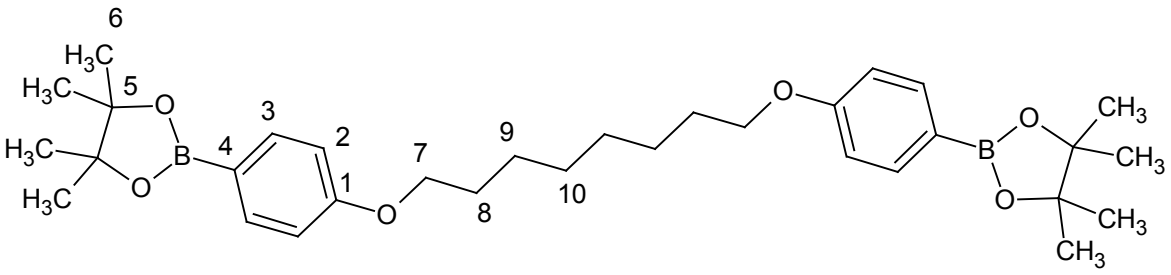
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.74 (d, 4H, H_3), 6.88 (d, 4H, H_2), 3.99 (t, 4H, H_7), 1.82 (m, 4H, H_8), 1.54 (m, 4H, H_9), 1.33 ppm (s, 24H, H_6).

^{13}C NMR (125 MHz, $CDCl_3$): δ 161.70 (C_1), 136.50 (C_3), 120.51 (br, C_4), 113.87 (C_2), 83.50 (C_5), 67.60 (C_7), 29.14 (C_8), 25.84 (C_9), 24.85 ppm (C_6).

MS (EI, 70 V); m/z = 177 (100), 523 (90) [MH^+], 540 (60).

EA (%): calcd (found) for $C_{30}H_{44}B_2O_6$: C68.99 (68.94), H 8.49 (8.82).

1,6-Bis(4-[4,4,5,5-tetramethyl-1,3,2-dioxaborolan]phenoxy)octane **3b**



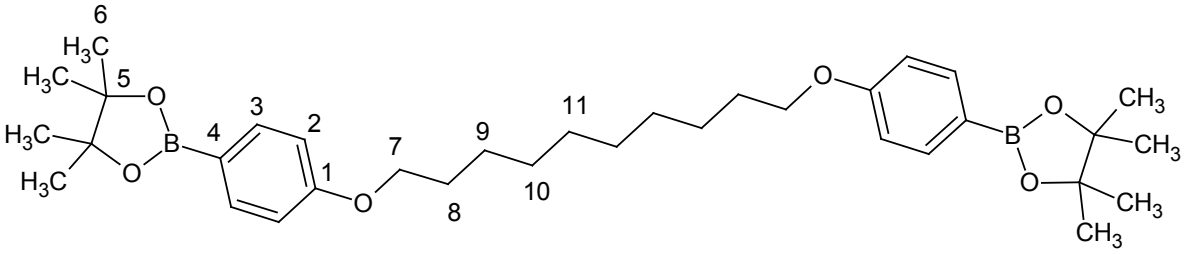
^{1}H NMR (300 MHz, $CDCl_3$): δ 7.73 (d, 4H, H_3), 6.88 (d, 4H, H_2), 3.97 (t, 4H, H_7), 1.78 (m, 4H, H_8), 1.52-1.30 (8H, H_9, H_{10}), 1.33 ppm (s, 24H, H_6).

^{13}C NMR (75 MHz, $CDCl_3$): δ 161.93 (C_1), 136.64 (C_3), 120.5 (br, C_4), 114.07 (C_2), 83.63 (C_5), 67.92 (C_7), 29.43 and 29.36 (C_8, C_{10}), 26.11 (C_9), 25.01 ppm (C_6).

MS (EI, 70 V); m/z = 551(100) [MH^+], 205 (56), 425 (35).

EA (%): calcd (found) for $C_{32}H_{48}B_2O_6$: 69.84 (69.79), H 8.79 (9.15)

1,6-Bis(4-[4,4,5,5-tetramethyl-1,3,2-dioxaborolan]phenoxy)decane **3c**



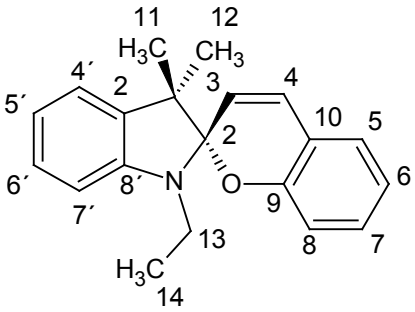
^{1}H NMR (300 MHz, $CDCl_3$): δ 7.74 (d, 4H, H_3), 6.88 (d, 4H, H_2), 3.97 (t, 4H, H_7), 1.77 (m, 4H, H_8), 1.50-1.33 (12H, H_9, H_{10}, H_{11}), 1.33 ppm (s, 24H, H_6).

^{13}C NMR (75 MHz, $CDCl_3$): δ 161.93 (C_1), 136.61 (C_3), 120.5 (br, C_4), 114.00 (C_2), 83.62 (C_5), 67.90 (C_7), 29,61, 29.49 and 29.34 (C_8, C_{10}, C_{11}), 26.14 (C_9), 24.99 ppm (C_6).

MS (EI, 70 V); m/z = 579 (100) [MH^+], 233 (60), 596 (45)

EA (%): calcd (found) for $C_{34}H_{52}B_2O_6$: C70.60 (70.60), H 9.06 (9.47)

Synthesis of model compound spiropyran ***8***. **8** was synthesized starting from 1-ethyl-2,3,3-trimethyl-3*H*-indolium iodide[3] and salicylaldehyde. A mixture of 1-ethyl-2,3,3-trimethyl-3*H*-indolium iodide (0.401 g, 1.27 mmol) and salicylaldehyde (0.160 g, 1.31 mmol) was dissolved in ethanol (6.6 ml) under an argon atmosphere. Piperidine (0.15 ml, 1.15 mmol) was added and the mixture was refluxed for 9h. The solvent was removed under reduced pressure and the product was obtained as beige crystals in 43 % yield after recrystallization from ethanol (3x).



^{1}H NMR (500 MHz, $CDCl_3$): δ 7.15 (dt, 1H, $H_{6'}$), 7.08 (dt, 1H, H_7), 7.06 (dd, 1H, $H_{4'}$), 7.03 (dd, 1H, H_5), 6.82 (d, 1H, H_4), 6.81 (2 t, 2H, H_6,$H_{5'}$), 6.68 (d, 1H, H_8), 6.54 (d, 1H, $H_{7'}$), 5.67 (d, 1H, H_3), 3.34 and 3.20 (2 m, 2H, H_{13}), 1.30 (s, 3H, H_{12}), 1.17 (t, 3H, H_{14}), 1.15 ppm (s, 3H, H_{11}; NOESY to H_3).

^{13}C NMR (125 MHz, $CDCl_3$): δ 154.26 (C_9), 147.19 ($C_{8'}$), 136.61 ($C_{9'}$), 129.61 (C_7), 129.17 (C_4), 127.42 ($C_{6'}$), 126.63 (C_5), 121.62 ($C_{4'}$), 119.86 (C_3,C_6), 118.63 (C_{10}), 118.43 ($C_{5'}$), 115.13 (C_8), 106.14 ($C_{7'}$), 104.44 (C_2), 52.13 ($C_{3'}$), 37.81 (C_{13}), 26.04 (C_{11}), 20.08 (C_{12}), 14.36 ppm (C_{14}).

MS(EI, 70 V); m/z = 292 (100) [MH^+].

[3] M. V. Reddington, *Bioconjugate Chem.* **2007,** *18,* 2178.

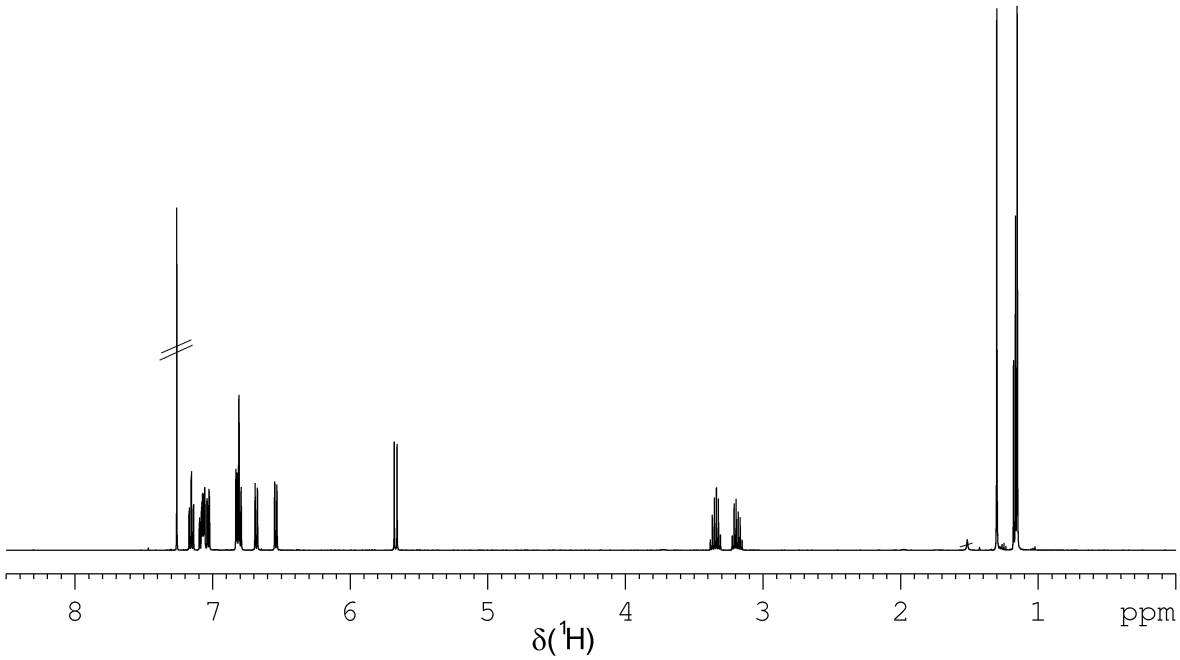
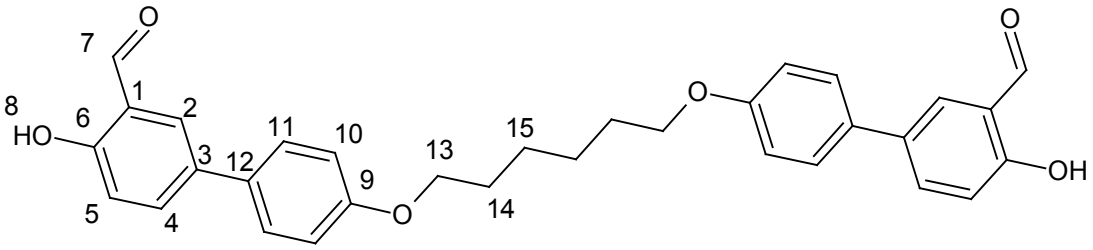


*Figure SI-1. ^{1}H NMR spectrum of **8**; solvent: $CDCl_3$.*

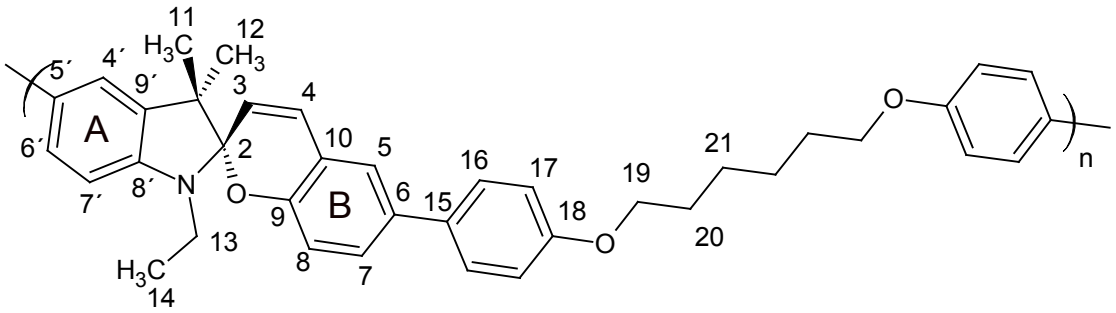
*Synthesis of model compound **9**.* **3a** (100 mg, 0.191 mmol), 5-bromosalicylaldehyde (0.478 mmol, 96.2 mg), potassium carbonate (260 mg), tris(dibenzylideneacetone) dipalladium (1 mol%) and 2-dicyclohexylphosphino-2′,6′-dimethoxybiphenyl (6 mol%) were dissolved in 5 ml of a degassed THF/water mixture (2:1) and stirred at 80°C for 36 h. The reaction mixture was cooled to room temperature. The formed solid was filtered off, washed with 3x20 ml water and 5x20 ml THF. The solid was recrystallized from chloroform to give the product as a white powder in 52 % (51 mg) yield.



^{1}H NMR (500 MHz, $CDCl_3$): δ 10.94 (s, 2H, H_8), 9.96 (s, 2H, H_7), 7.72 (dd, 2H, H_4), 7.70 (d, 2H, H_2), 7.47 (d, 4H, H_{11}), 7.05 (d, 2H, H_5), 6.98 (d, 4H, H_{10}), 4.03 (t, 4H, H_{13}), 1.87 (m, 4H, H_{14}), 1.59 ppm (m, 4H, H_{15}).

^{13}C NMR (125 MHz, $CDCl_3$): δ 196.65 (C_7), 160.55 (C_6), 158.75 (C_9), 135.41 (C_4), 133.12 (C_3), 131.83 (C_{12}), 131.30 (C_2), 127.64 (C_{11}), 120.74 (C_1), 118.05 (C_5), 115.02 (C_{10}), 67.99 (C_{13}), 29.23 (C_{14}), 25.89 ppm (C_{15}).

P(SP-*alt*-C_6) **4a**



^{1}H NMR (500 MHz, $CDCl_3$): δ 7.49 (d, H_{16} next to A), 7.44 (d, H_{16} next to B), 7.35 (d, $H_{6'}$), 7.28 (d, H_7), 7.26 (s, $H_{4'}$), 7.22 (s, H_5), 6.95 (H_{17}), 6.88 (d, H_4), 6.76 (d, H_8), 6.59 (d, $H_{7'}$), 5.73 (d, H_3), 4.02 (H_{19}), 3.39 and 3.24 (H_{13}), 1.86 (H_{20}), 1.58 (H_{21}), 1.37 (s, H_{12}), 1.21 (s, H_{11}), 1.20 ppm (t, H_{14}).

^{13}C NMR (125 MHz, $CDCl_3$): δ 158.21 (C_{18} next to B), 157.81 (C_{18} next to A), 153.34 (C_9), 146.26 ($C_{8'}$), 137.25 ($C_{9'}$), 134.56 (C_{15} next to A), 133.22 (C_{15} next to B), 132.92 (C_6), 131.77 ($C_{5'}$), 129.32 (C_4), 127.97 (C_7), 127.54 (C_{16}), 126.01 ($C_{6'}$), 124.83 (C_5), 120.40 ($C_{4'}$), 120.09 (C_3), 118.70 (C_{10}), 115.38 (C_8), 114.76 and 114.71 (C_{17}), 106.30 ($C_{7'}$), 104.80 (C_2), 67.93 (C_{19}), 52.26 ($C_{3'}$), 37.94 (C_{13}), 29.30 (C_{20}), 26.22 (C_{11}), 25.92 (C_{21}), 20.16 (C_{12}), 14.44 ppm (C_{14}).

EA (%): calcd (found) for C38H41NO3: C 81.54 (81.75), H 7.38 (7.62), N 2.50 (2.34)

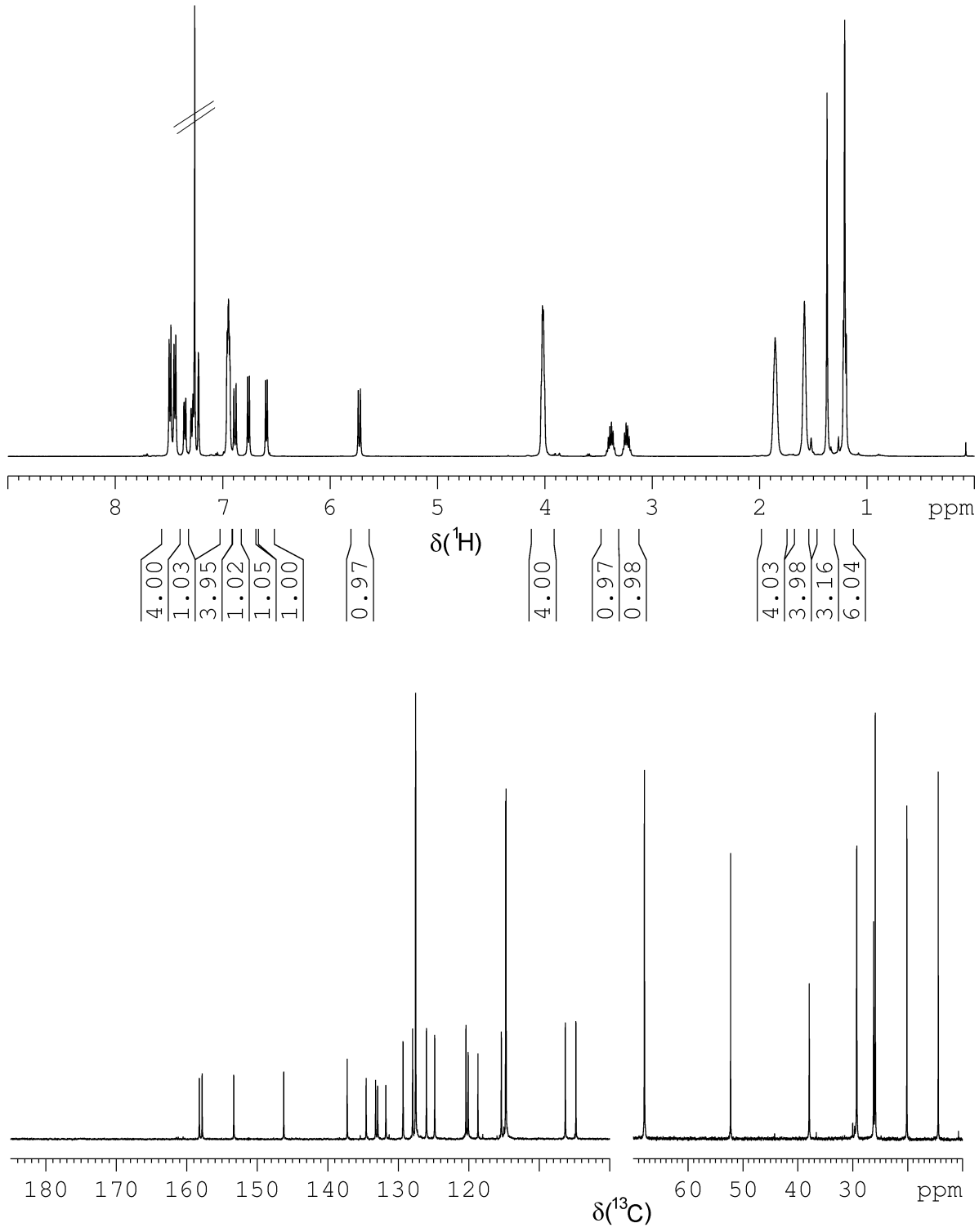


*Figure SI-2. ^{1}H (top) and ^{13}C NMR spectrum (bottom) of P(SP-alt-C_6) (**4a**); solvent: $CDCl_3$.*

P(SP-*alt*-C_8) **4b**

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.49 (d, H_{16} next to A), 7.44 (d, H_{16} next to B), 7.35 (d, $H_{6'}$), 7.28 (d, H_7), 7.26 (s, $H_{4'}$), 7.22 (s, H_5), 6.95 (H_{17}), 6.88 (d, H_4), 6.76 (d, H_8), 6.59 (d, $H_{7'}$), 5.73 (d, H_3), 4.00 (H_{19}), 3.39 and 3.24 (H_{13}), 1.82 (H_{20}), 1.51 (H_{21}), 1.42 (H_{22}), 1.37 (s, H_{12}), 1.21 (s, H_{11}), 1.20 ppm (t, H_{14}).
^{13}C NMR (125 MHz, $CDCl_3$): δ 158.25 (C_{18} next to B), 157.85 (C_{18} next to A), 153.34 (C_9), 146.25 ($C_{8'}$), 137.25 ($C_{9'}$), 134.52 (C_{15} next to A), 133.18 (C_{15} next to B), 132.94 (C_6), 131.77 ($C_{5'}$), 129.32 (C_4), 127.97 (C_7), 127.54 (C_{16}), 126.01 ($C_{6'}$), 124.83 (C_5), 120.40 ($C_{4'}$), 120.09 (C_3), 118.70 (C_{10}), 115.38 (C_8), 114.76 and 114.71 (C_{17}), 106.30 ($C_{7'}$), 104.80 (C_2), 68.06 (C_{19}), 52.26 ($C_{3'}$), 37.94 (C_{13}), 29.3 (C_{20}, C_{22}), 26.22 (C_{11}), 26.02 (C_{21}), 20.16 (C_{12}), 14.44 ppm (C_{14}).

P(SP-*alt*-C_{10}) **4c**

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.48 (d, H_{16} next to A), 7.44 (d, H_{16} next to B), 7.34 (d, $H_{6'}$), 7.28 (d, H_7), 7.26 (s, $H_{4'}$), 7.23 (s, H_5), 6.94 (H_{17}), 6.87 (d, H_4), 6.75 (d, H_8), 6.58 (d, $H_{7'}$), 5.72 (d, H_3), 3.99 (m, H_{19}), 3.38 and 3.23 (m, H_{13}), 1.80 (m, H_{20}), 1.48 (m, H_{21}), 1.37 (H_{22}, H_{23}), 1.36 (s, H_{12}), 1.21 (s, H_{11}), 1.20 ppm (t, H_{14}).
^{13}C NMR (125 MHz, $CDCl_3$): δ 158.26 (C_{18} next to B), 157.85 (C_{18} next to A), 153.32 (C_9), 146.24 ($C_{8'}$), 137.24 ($C_{9'}$), 134.49 (C_{15} next to A), 133.15 (C_{15} next to B), 132.93 (C_6), 131.78 ($C_{5'}$), 129.31 (C_4), 127.95 (C_7), 127.52 (C_{16}), 125.99 ($C_{6'}$), 124.82 (C_5), 120.38 ($C_{4'}$), 120.07 (C_3), 118.68 (C_{10}), 115.36 (C_8), 114.75 and 114.70 (C_{17}), 106.28 ($C_{7'}$), 104.78 (C_2), 68.09 (C_{19}), 52.24 ($C_{3'}$), 37.93 (C_{13}), 29.48, 29.36 and 29.32(C_{20}, C_{22}, C_{23}), 26.20 (C_{11}), 26.06 (C_{21}), 20.15 (C_{12}), 14.43 ppm (C_{14}).

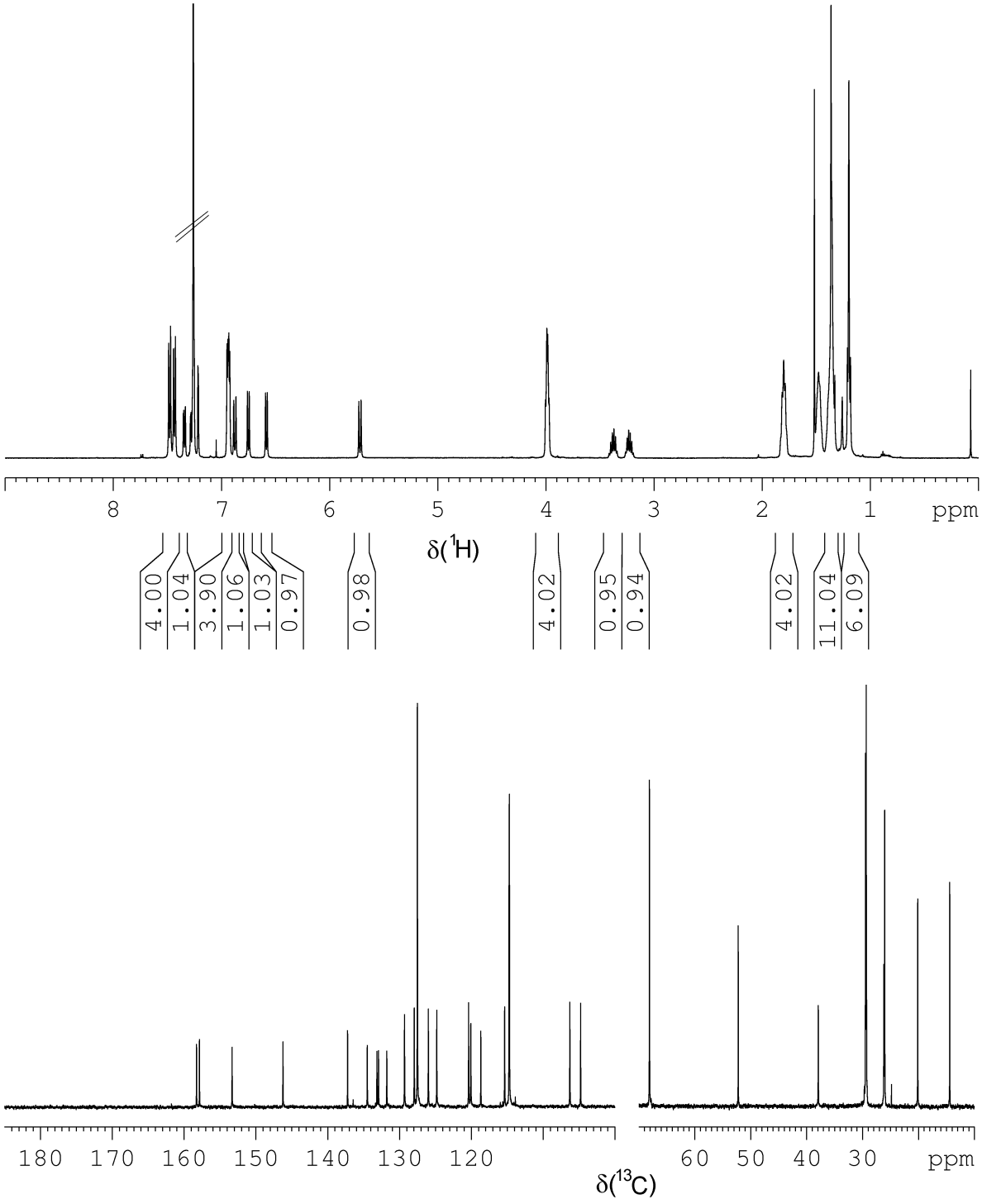


*Figure SI-3. ^{1}H (top) and ^{13}C NMR spectrum (bottom) of P(SP-alt-C_{10}) (**4c**); solvent: $CDCl_3$.*

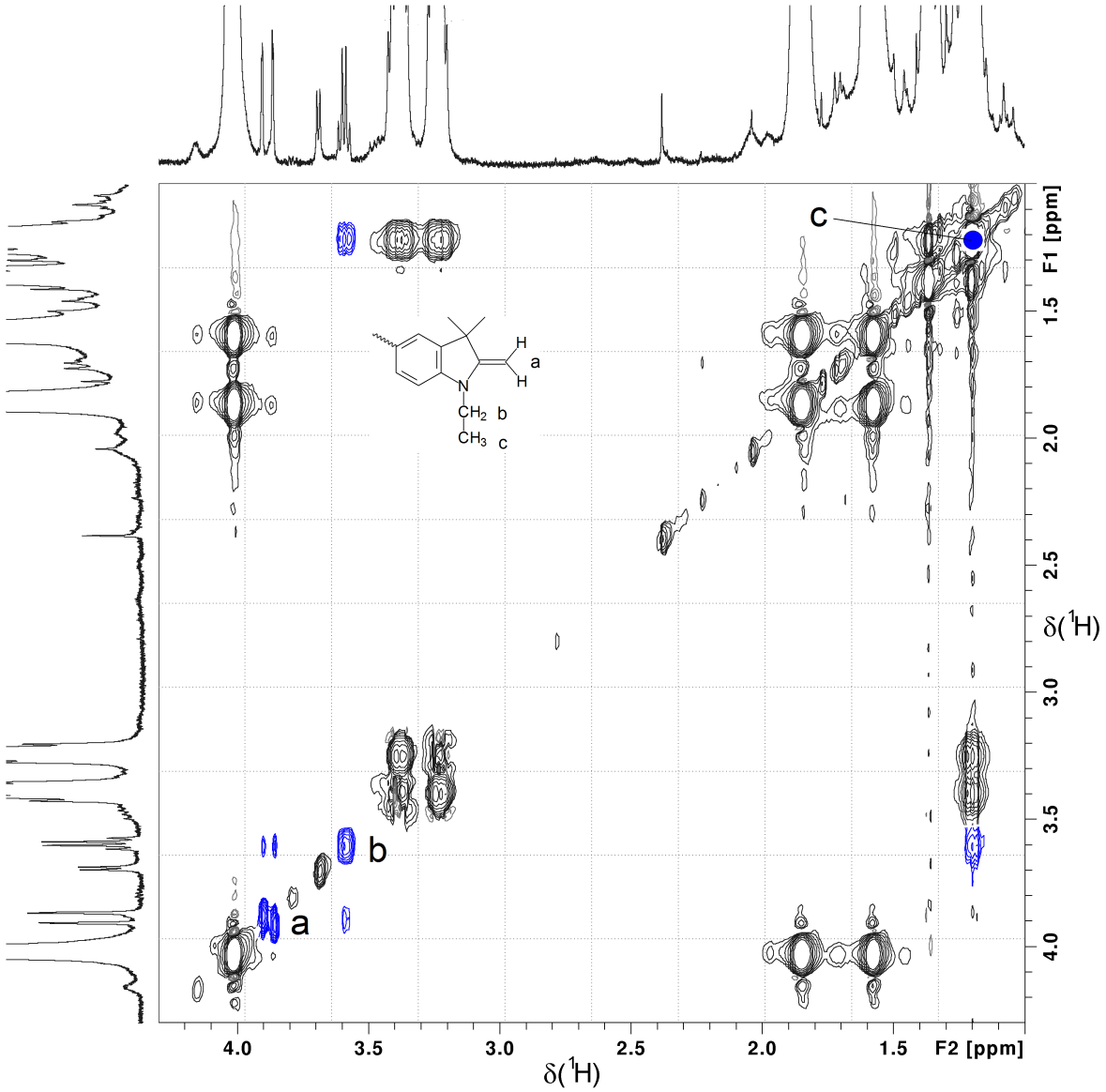
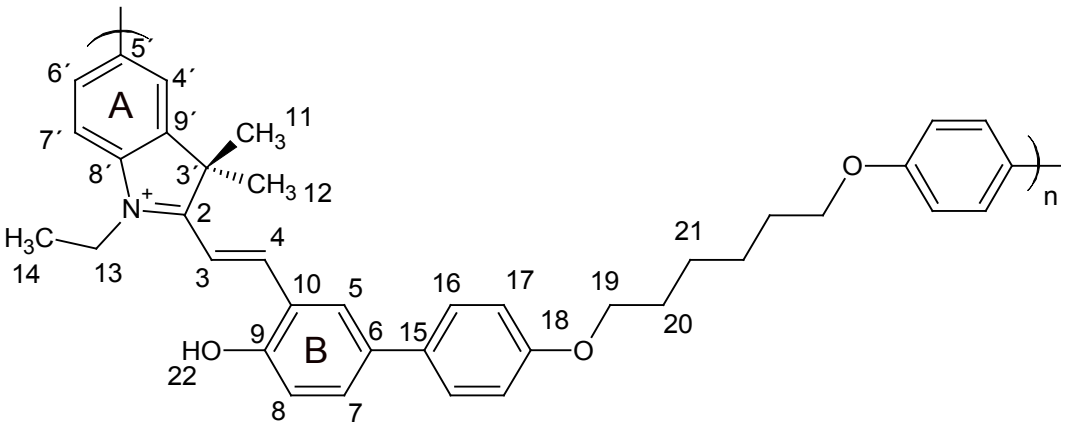


Figure SI-4. ^{1}H-^{1}H *TOCSY spectrum of P(SP-alt-*C_6*) (entry P2 in Table 1) with highligted signals and correlations of the indoline endgroup (solvent:* $CDCl_3$*)*

P(MCH$^+$-*alt*-C$_6$) **5a**



^{1}H NMR (500 MHz, DMSO-d$_6$): δ 11.4 (br, H$_{22}$), 8.61 (d, H$_4$), 8.32 (s, H$_5$), 8.19 (s, H$_{4'}$), 7.94 (d, H$_{7'}$), 7.89 (d, H$_{6'}$), 7.87 (d, H$_3$), 7.77 (d, H$_{16}$ next to A), 7.74 (d, H$_7$), 7.66 (d, H$_{16}$ next to B), 7.23 (d, H$_8$), 7.09 (d, H$_{17}$ next to A), 7.04 (d, H$_{17}$ next to B), 4.69 (m, H$_{13}$), 4.07 (m, H$_{19}$ next to A), 4.05 (m, H$_{19}$ next to B), 1.86 (s, H$_{11/12}$), 1.79 (m, H$_{20}$), 1.53 (m, H$_{21}$), 1.50 ppm (t, H$_{14}$).

^{13}C NMR (125 MHz, DMSO-d$_6$): δ 181.03 (C$_2$), 159.12 (C$_{18}$ next to A), 158.79 (C$_9$), 158.18 (C$_{18}$ next to B), 149.63 (C$_4$), 144.63 (C$_{9'}$), 141.20 (C$_5$), 139.34 (C$_{8'}$), 133.50 (C$_7$), 131.88 (C$_6$), 131.46 (C$_{15}$ next to B), 131.13 (C$_{15}$ next to A), 128.45 (C$_{16}$ next to A), 127.89 (C$_5$), 127.60 (C$_{16}$ next to B), 126.98 (C$_{6'}$), 121.60 (C$_{10}$), 120.85 (C$_{4'}$), 117.56 (C$_8$), 115.38 (C$_{7'}$), 115.15 (C$_{17}$ next to A), 114.92 (C$_{17}$ next to B), 111.96 (C$_3$), 67.71 (C$_{19}$ next to A), 67.64 (C$_{19}$ next to B), 52.17 (C$_{3'}$), 42.29 (C$_{13}$), 28.79 (C$_{20}$), 26.43 (C$_{11/12}$), 25.45 (C$_{21}$), 13.63 ppm (C$_{14}$).

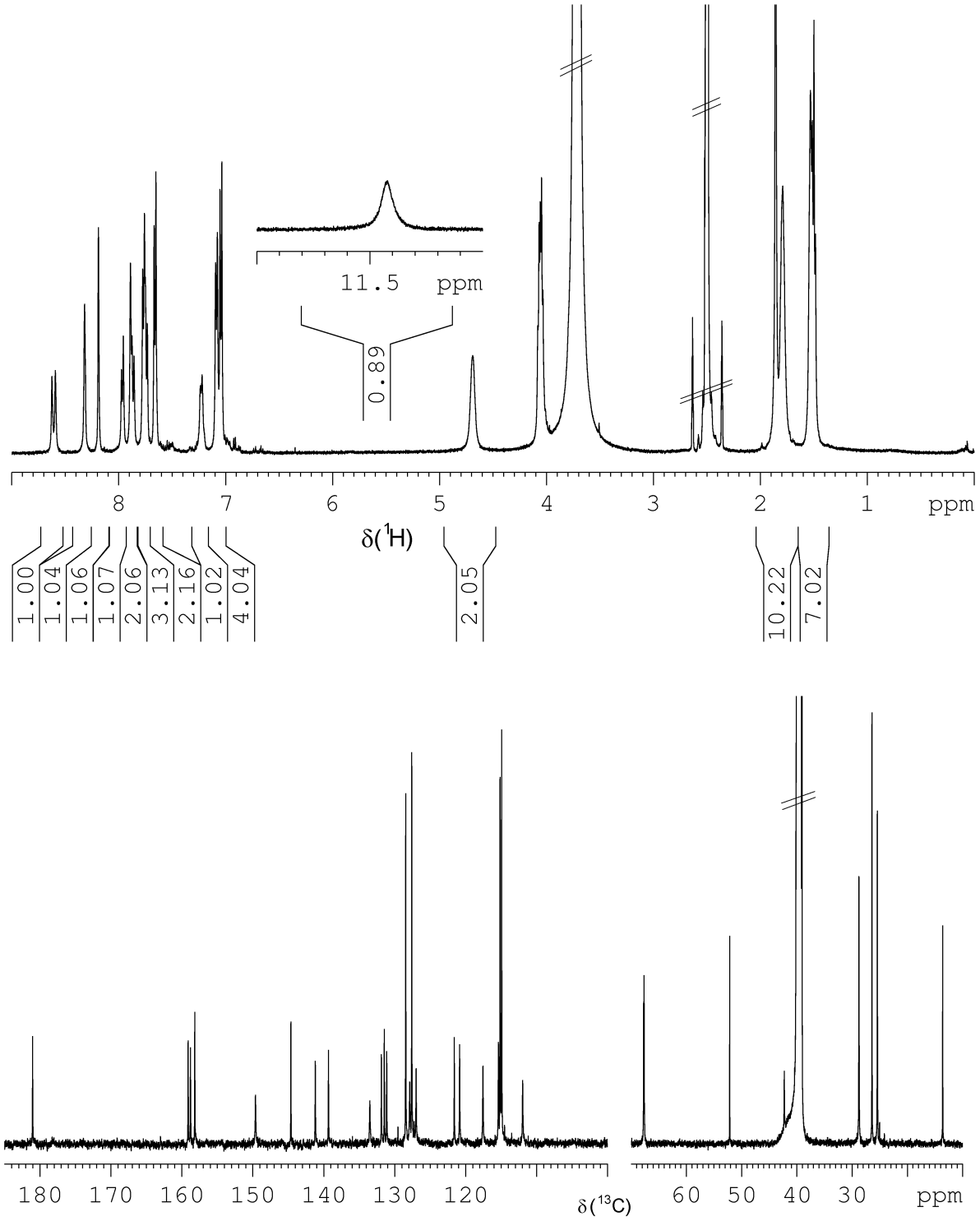


Figure SI-5. ^{1}H *(top) and* ^{13}C *NMR spectrum (bottom) of P(MCH*$^{+}$*-alt-C*$_6$*) (**5a**); solvent: CDCl*$_3$.

5b P(MCH^+-*alt*-C_8)

^{1}H NMR (500 MHz, DMSO-d_6): δ 11.4 (br, H_{22}), 8.60 (d, H_4), 8.31 (s, H_5), 8.18 (s, $H_{4'}$), 7.96 (d, $H_{7'}$), 7.88 (d, $H_{6'}$), 7.86 (d, H_3), 7.76 (d, H_{16} next to A), 7.73 (d, H_7), 7.65 (d, H_{16} next to B), 7.23 (d, H_8), 7.07 (d, H_{17} next to A), 7.03 (d, H_{17} next to B), 4.69 (m, H_{13}), 4.04 (m, H_{19} next to A), 4.02 (m, H_{19} next to B), 1.85 (s, $H_{11/12}$), 1.76 (m, H_{20}), 1.50 (t, H_{14}), 1.46 (m, H_{21}), 1.39 ppm (m, H_{22}),.

^{13}C NMR (125 MHz, DMSO-d_6): δ 181.05 (C_2), 159.16 (C_{18} next to A), 158.75 (C_9), 158.23 (C_{18} next to B), 149.65 (C_4), 144.64 ($C_{9'}$), 141.26 (C_5), 139.33 ($C_{8'}$), 133.55 (C_7), 131.97 (C_6), 131.46 (C_{15} next to B), 131.13 (C_{15} next to A), 128.47 (C_{16} next to A), 127.90 (C_5), 127.62 (C_{16} next to B), 127.02 ($C_{6'}$), 121.63 (C_{10}), 120.85 ($C_{4'}$), 117.55 (C_8), 115.40 ($C_{7'}$), 115.16 (C_{17} next to A), 114.94 (C_{17} next to B), 111.96 (C_3), 67.78 (C_{19} next to A), 67.72 (C_{19} next to B), 52.20 ($C_{3'}$), 42.32 (C_{13}), 28.89 and 28.84 (C_{20}, C_{22}), 26.46 ($C_{11/12}$), 25.62 (C_{21}), 13.65 ppm (C_{14}).

5c P(MCH^+-*alt*-C_{10})

^{1}H NMR (500 MHz, DMSO-d_6): δ 11.4 (br, H_{22}), 8.60 (d, H_4), 8.31 (s, H_5), 8.17 (s, $H_{4'}$), 7.95 (d, $H_{7'}$), 7.86 ($H_{6'}$, H_3), 7.75 (d, H_{16} next to A), 7.72 (d, H_7), 7.65 (d, H_{16} next to B), 7.24 (d, H_8), 7.06 (d, H_{17} next to A), 7.02 (d, H_{17} next to B), 4.69 (m, H_{13}), 4.03 (m, H_{19} next to A), 4.01 (m, H_{19} next to B), 1.85 (s, $H_{11/12}$), 1.74 (m, H_{20}), 1.49 (t, H_{14}), 1.44 (m, H_{21}), 1.34 ppm (H_{22}, H_{23}).

^{13}C NMR (125 MHz, DMSO-d_6): δ 180.92 (C_2), 159.10 (C_{18} next to A), 158.79 (C_9), 158.15 (C_{18} next to B), 149.85 (C_4), 144.44 ($C_{9'}$), 141.32 (C_5), 139.16 ($C_{8'}$), 133.52 (C_7), 131.94 (C_6), 131.43 (C_{15} next to B), 131.05 (C_{15} next to A), 128.31 (C_{16} next to A), 127.78 (C_5), 127.502 (C_{16} next to B), 126.97 ($C_{6'}$), 121.51 (C_{10}), 120.75 ($C_{4'}$), 117.46 (C_8), 115.19 ($C_{7'}$), 114.98 (C_{17} next to A), 114.75 (C_{17} next to B), 111.63 (C_3), 67.69 (C_{19} next to A), 67.62 (C_{19} next to B), 52.09 ($C_{3'}$), 42.21 (C_{13}), 29.02, 28.87 and 28.82 (C_{20}, C_{22}, C_{23}), 26.48 ($C_{11/12}$), 25.60 (C_{21}),
13.65 ppm (C_{14}).

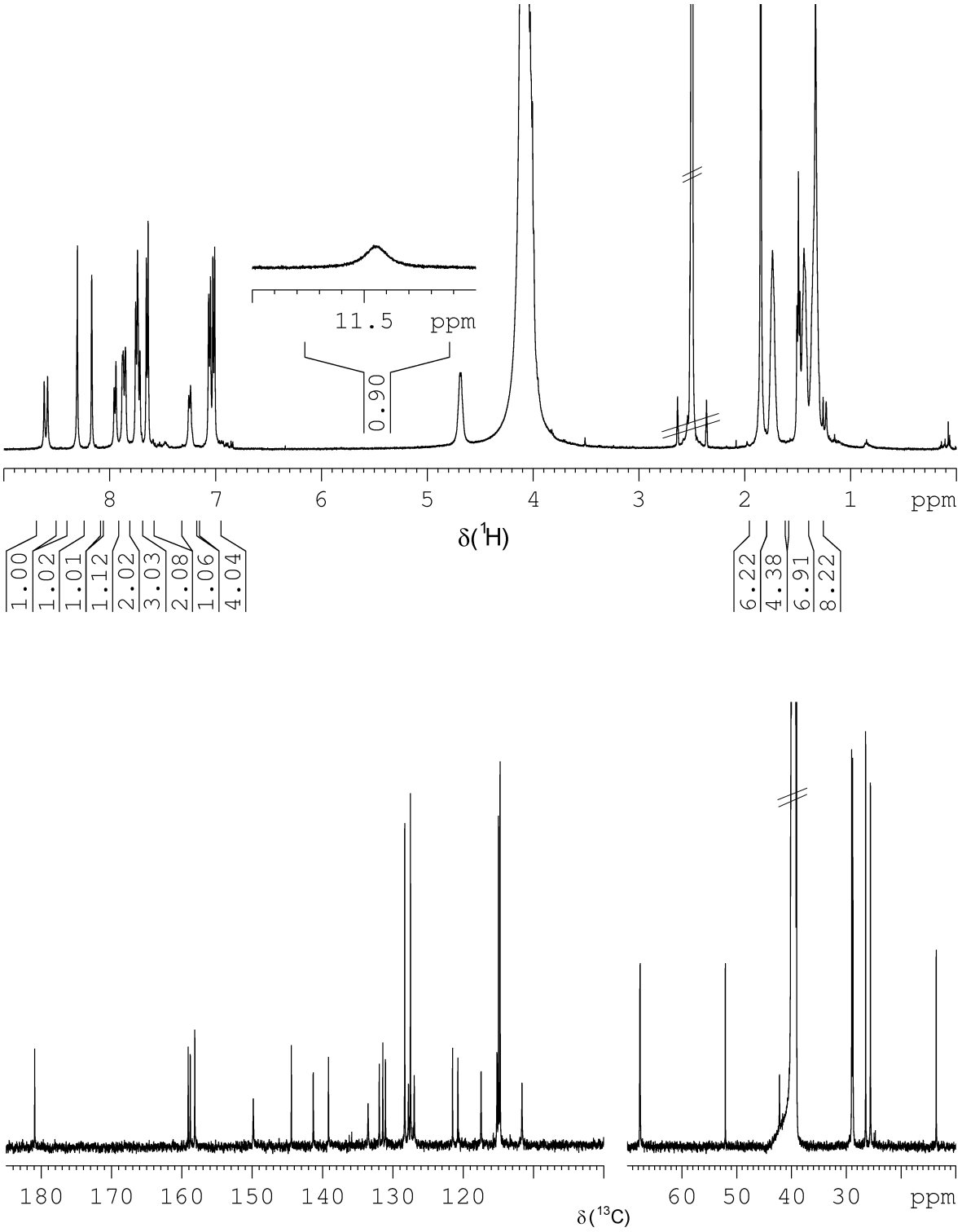


*Figure SI-6. ^{1}H (top) and ^{13}C NMR spectrum (bottom) of P(MCH^{+}-alt-C_{10}) (**5c**); solvent: $CDCl_3$.*

COSY, HMBC and HSQC spectra for ^{1}H and ^{13}C signal assignment of P(MCH^{+}-alt-C_8)

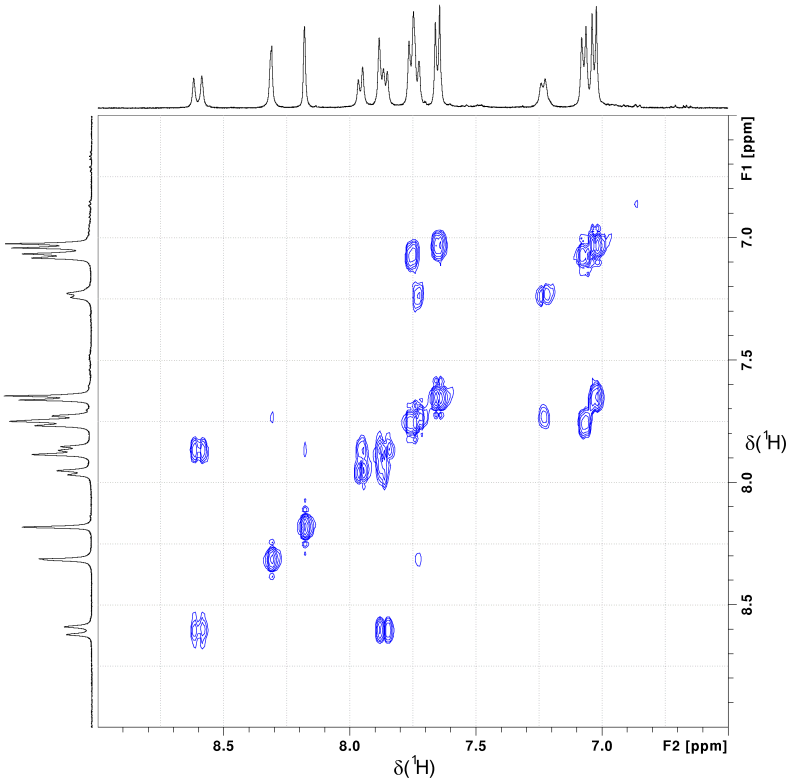


*Figure SI-7. ^{1}H-^{1}H COSY spectrum of P(MCH^{+}-alt-C8) (**5b**); solvent: DMSO-d_6.*

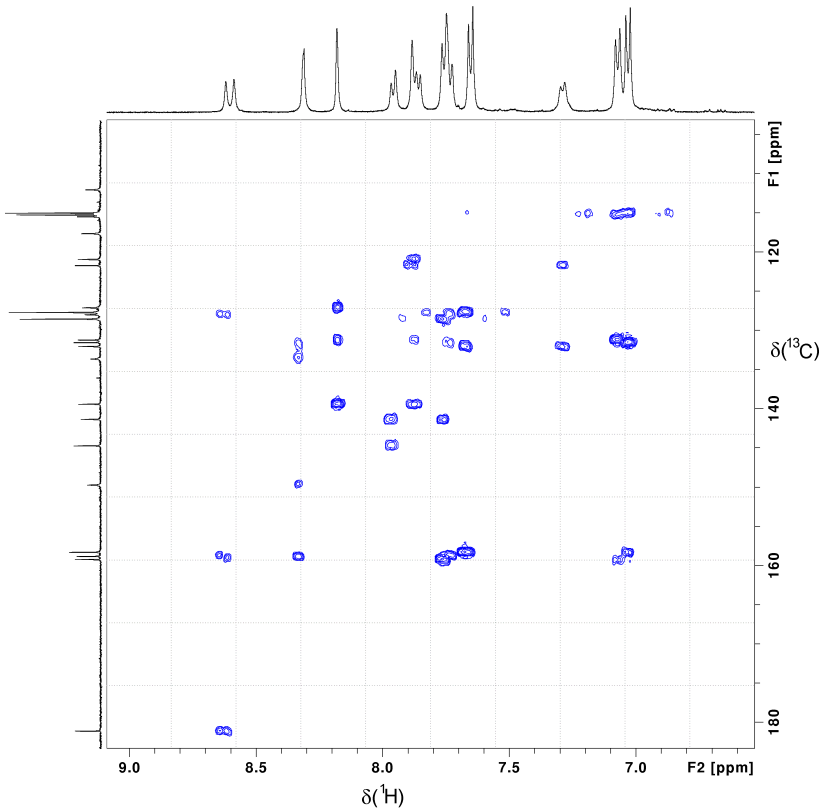


*Figure SI-8. ^{1}H-^{13}C HMBC spectrum of P(MCH^{+}-alt-C_8) (**5b**); solvent: DMSO-d_6.*

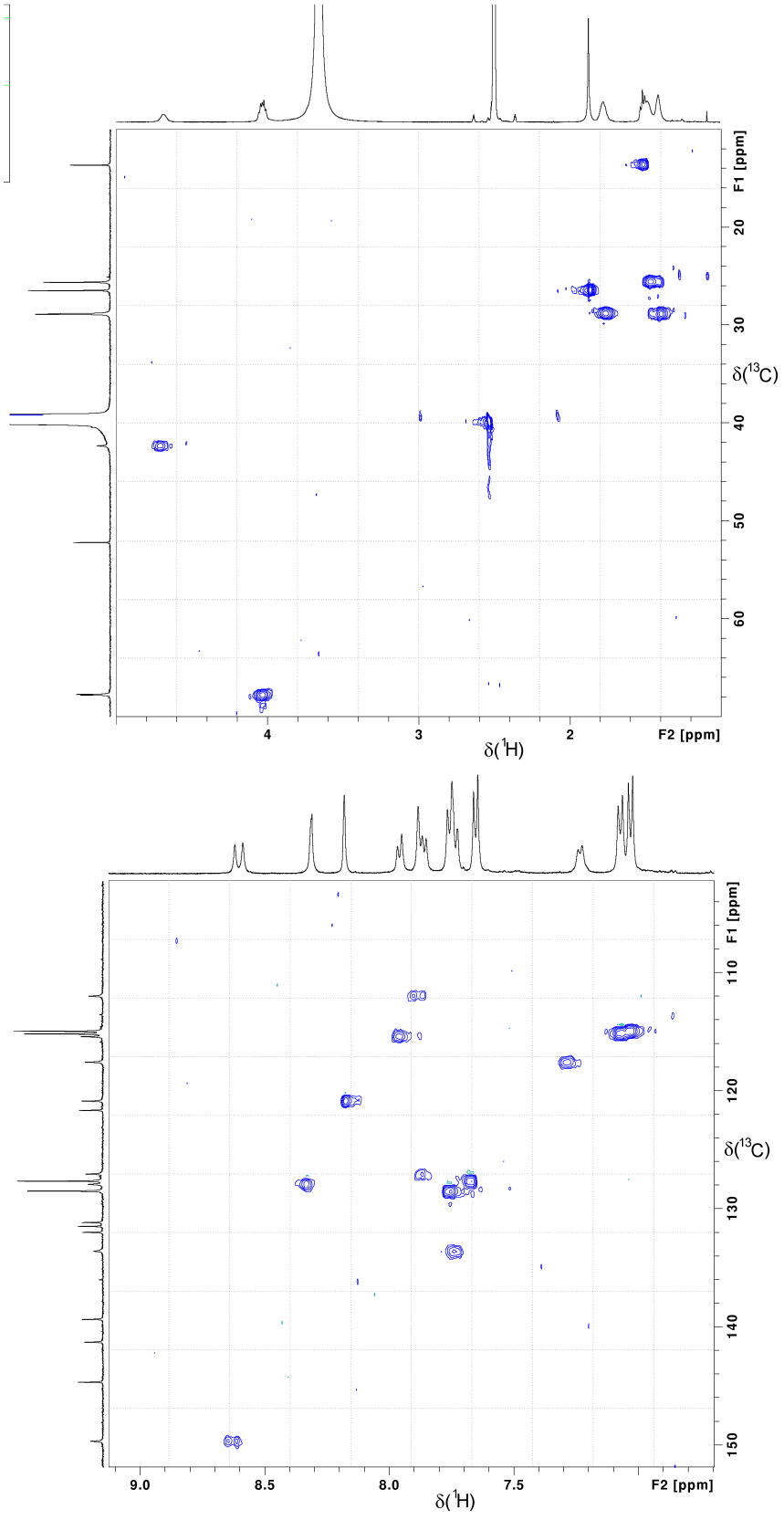


Figure SI-9. ^{1}H-^{13}C *HSQC spectra (different regions) of P(MCH*$^{+}$*-alt-C*$_8$*) (**5b**); solvent: DMSO-d*$_6$.

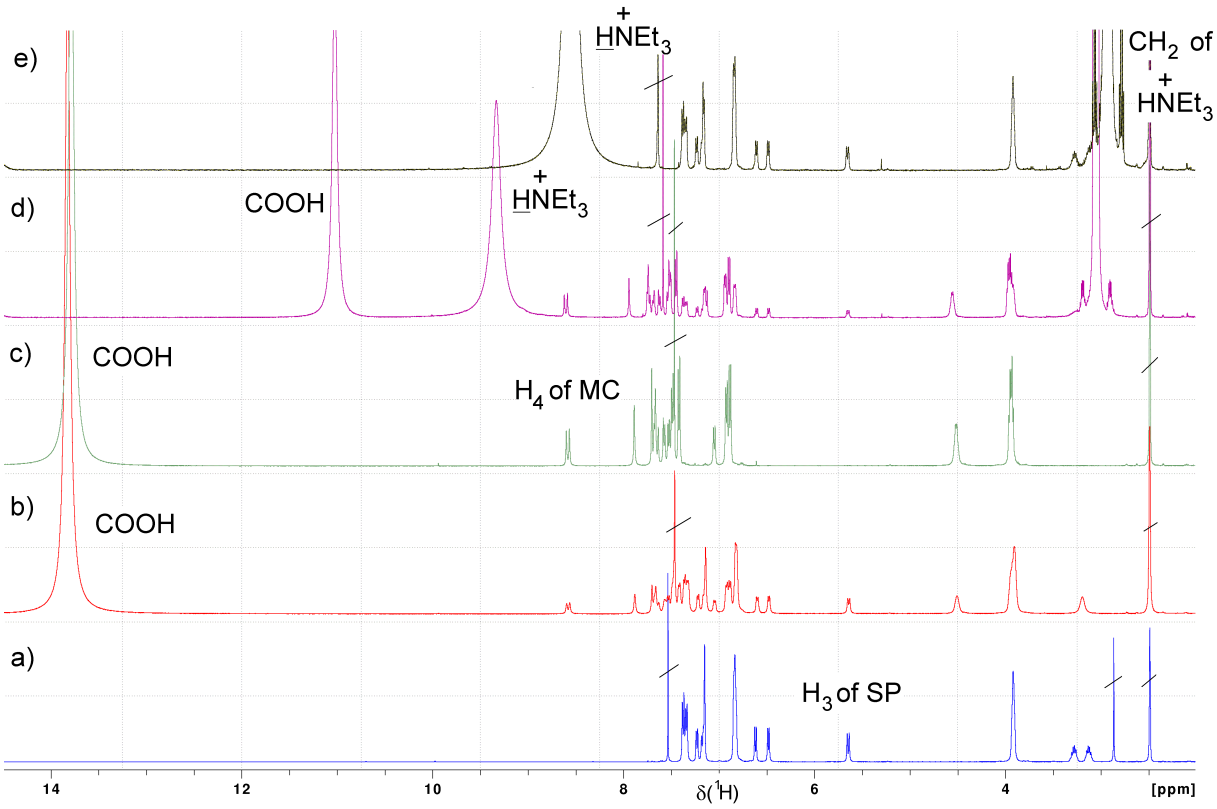


Figure SI-10. ^{1}H *NMR spectra of (a) P(SP-alt-*C_6*) (**4b**), (b) after addition of 50 eq trifluoroacetic acid and 1.5 h reaction time and (c) after 8 h reaction time (complete isomerization to P(*MCH^{+}*-alt-*C_6*) (**5b**). Spectrum (d) was obtained after addition of 30 eq triethylamine and (e) after addition of further 50 eq (complete re-isomerization to P(SP-alt-C6) (**4b**). The spectra d) and e) were recorded immediately after mixing. Solvent:* $CDCl_3$*/DMSO-*d_6 *(4:1 v/v).*

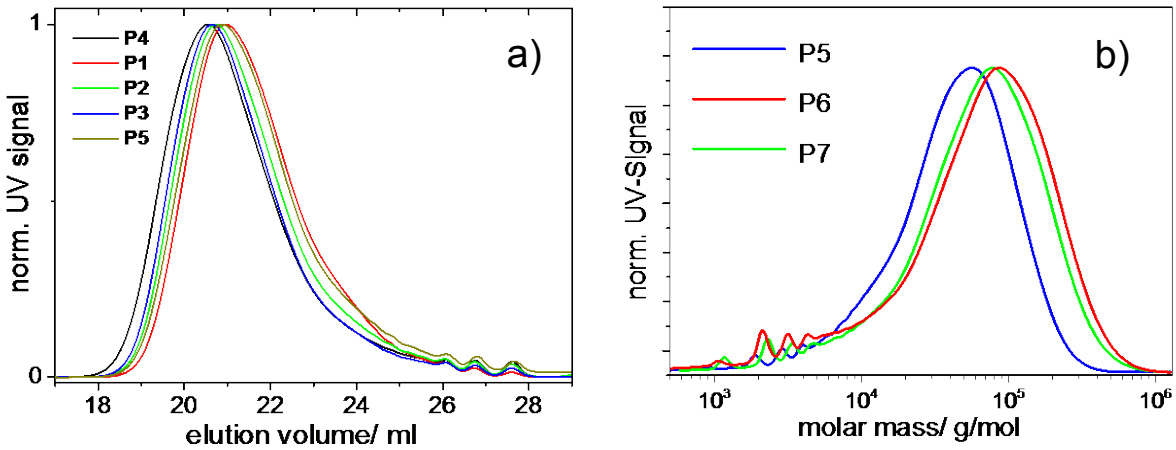


*Figure SI-11. a) SEC curves of entries P1-5 (**4a**), b) SEC curves of entries P5-7 (**4a,b,c**). Curves were taken in THF at 1.0 ml/min.*

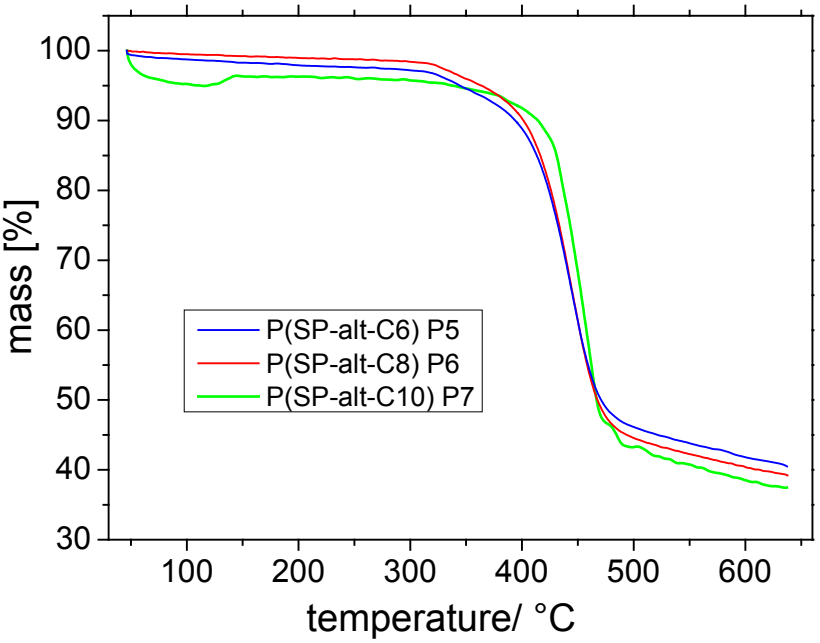


*Figure SI-12. Thermogravimetric analysis of **4a,b,c**. Curves were taken at 10 K/min under nitrogen. The dip at ~100 °C represents noise from the instrument.*

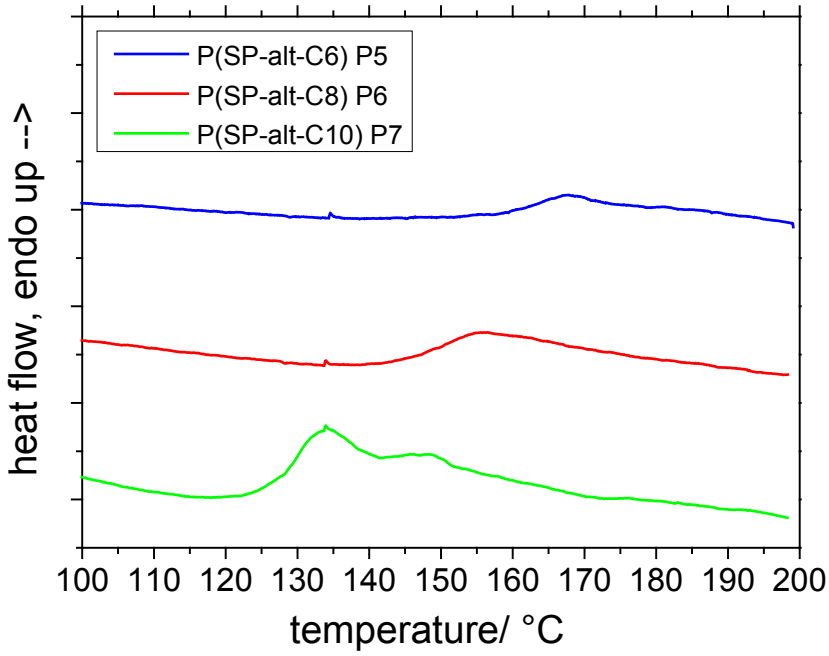


*Figure SI-13. DSC curves of **4a,b,c**. Curves were taken at 10 K/min, second heating is shown.*

Description of the Polarizable Continuum Model (PCM)

We have implemented a quantum mechanical continuum solvent model as described by Sanchez et al.[4] In this model, the electrostatic interaction of the solute with the solvent is obtained by solving Poisson's equation in presence of a dielectric medium, which is given by a smoothed step function that is unity inside the solvation cavity and reaches the experimental static dielectric constant ε of the solvent outside the cavity. The shape of the solvation cavity is calculated from the positions of the nuclei of the solute and their van der Waals radii. We have used the set of van der Waals radii given by Bondi et al[5], except for the radius of hydrogen where we have used 1.09 Å as suggested in ref[6].

The model has one additional parameter β that controls the slope of the step function. We have chosen the value $\beta = 6.4$ minimizing the mean absolute error between our calculations and experimental solvation free energies[7] of Ag^+ and Cl^- in water.

The contribution of the cavity formation energy was calculated by scaling the quantum surface area with the experimental macroscopic surface tension of the solvent. Dispersion and repulsion interactions were neglected for the DMSO solvent. This is justified, since the solute molecules we compare to each other in this study all have approximately the same quantum surface area. We have used a static dielectric constant of $\varepsilon = 47.2$[8] and a surface tension of $\gamma = 43.5$ dyn/cm for DMSO[9]. In order to judge the importance of the energetic contributions proportional to the quantum surface area in this work, we compared the calculated energies to a calculation with zero surface tension and found the energy differences to be within 0.1 eV to the presented values. Similarly, structure relaxation of the gas-phase structures in presence of DMSO had only a minor effect, i.e. the SP/MC/MCH+ energy differences changed less than 0.05 e.

[4] Sanchez, V. M.; Sued, M.; Scherlis, D. A. *J. Chem. Phys*. **2009**, *131*, 174108.
[5] Bondi, A. *J. Phys. Chem.* **1964**, *68*, 441-451.
[6] Tomasi, J.; Mennucci, B.; Cammi, R. *Chem. Rev.* **2005**, 105, 2999–3094.
[7] Scherlis, D. A.; Fattebert, J.-L.; Gygi, F.; Cococcioni, M.; Marzari, N. *J. Chem. Phys*. **2006**, *124*, 074103.
[8] McLain, S. E.; Soper, A. K.; Luzar, A. *J. Chem. Phys*. **2006**, *124*, 074502.
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Relaxed structures

Here we present the coordinates of the relaxed structures considered in this work. The length unit is Å.

SP R=PhOMe gasphase	MC R=PhOMe gasphase	MCH^+ R=PhOMe gasphase
57	57	58
C 13.9020 17.1133 9.7954	C 13.9020 17.1133 9.7954	C 13.8561 13.1240 7.1555
C 14.2314 16.2259 8.7598	C 14.2314 16.2259 8.7598	N 14.7110 14.1692 7.1696
C 14.8941 17.7008 10.5655	C 14.8941 17.7008 10.5655	C 14.2158 15.5612 7.1059
C 15.5635 15.8736 8.5190	C 15.5635 15.8736 8.5190	C 15.2185 16.7007 7.0769
C 16.2380 17.3792 10.3155	C 16.2380 17.3792 10.3155	H 13.5440 15.6865 7.9696
C 16.5579 16.4678 9.3082	C 16.5579 16.4678 9.3082	H 13.5920 15.6172 6.2004
N 13.0756 15.7983 8.0876	N 13.0756 15.7983 8.0876	H 15.8117 16.7693 7.9953
C 12.4012 17.3084 9.8096	C 12.4012 17.3084 9.8096	H 14.6398 17.6300 6.9937
C 11.9212 16.0552 8.9517	C 11.9212 16.0552 8.9517	H 15.8827 16.6536 6.2062
C 12.0889 18.6345 9.0842	C 12.0889 18.6345 9.0842	C 12.4397 13.1110 7.1224
C 11.7837 17.3394 11.2101	C 11.7837 17.3394 11.2101	C 11.4999 14.1220 7.0457
C 13.2361 14.6594 7.1749	C 13.2361 14.6594 7.1749	H 12.0512 12.0919 7.1753
C 12.0822 14.3126 6.2425	C 12.0822 14.3126 6.2425	C 10.0729 13.9528 7.0567
C 10.6276 16.2864 8.2233	C 10.6276 16.2864 8.2233	H 11.8147 15.1590 6.9805
O 11.7776 14.9428 9.9176	O 11.7776 14.9428 9.9176	C 9.2446 15.1148 7.0368
C 9.6430 15.3704 8.1855	C 9.6430 15.3704 8.1855	C 9.4289 12.6968 7.1553
C 10.9507 13.9010 9.6245	C 10.9507 13.9010 9.6245	C 7.8537 14.9889 7.1186
C 9.8273 14.0664 8.7858	C 9.8273 14.0664 8.7858	O 9.8505 16.3280 6.9500
C 11.2132 12.6566 10.2047	C 11.2132 12.6566 10.2047	C 8.0468 12.5523 7.2491
C 10.4182 11.5625 9.8741	C 10.4182 11.5625 9.8741	H 10.0412 11.7965 7.2047
C 9.0335 12.9497 8.4813	C 9.0335 12.9497 8.4813	C 7.2676 13.7354 7.2254
C 9.3345 11.6754 8.9786	C 9.3345 11.6754 8.9786	H 7.2284 15.8851 7.0973
C 8.5955 10.4722 8.5356	C 8.5955 10.4722 8.5356	H 9.1764 17.0311 6.9888
H 17.0287 17.8322 10.9140	H 17.0287 17.8322 10.9140	C 7.4457 11.2183 7.4381
C 8.6348 8.1289 7.8268	C 8.6348 8.1289 7.8268	H 6.1795 13.6645 7.2791
C 7.2392 8.1288 7.7056	C 7.2392 8.1288 7.7056	C 8.0149 10.0775 6.8509
C 9.2911 9.2897 8.2387	C 9.2911 9.2897 8.2387	C 6.3444 11.0301 8.2985
C 6.5259 9.3102 7.9681	C 6.5259 9.3102 7.9681	C 7.5672 8.7935 7.1550
C 7.1972 10.4587 8.3721	C 7.1972 10.4587 8.3721	H 8.8234 10.1924 6.1257
O 6.4949 7.0387 7.3432	O 6.4949 7.0387 7.3432	C 5.8861 9.7596 8.6133
C 7.1779 5.7938 7.2160	C 7.1779 5.7938 7.2160	H 5.8711 11.8909 8.7750
H 14.6381 18.4038 11.3615	H 14.6381 18.4038 11.3615	C 6.5169 8.6256 8.0712
H 15.8382 15.1434 7.7586	H 15.8382 15.1434 7.7586	H 8.0343 7.9348 6.6752
H 17.6006 16.1965 9.1368	H 17.6006 16.1965 9.1368	H 5.0581 9.6151 9.3076
H 12.4444 18.6250 8.0451	H 12.4444 18.6250 8.0451	O 6.0499 7.4226 8.4948
H 12.6051 19.4517 9.6058	H 12.6051 19.4517 9.6058	C 6.7668 6.2526 8.0915
H 11.0126 18.8571 9.0924	H 11.0126 18.8571 9.0924	H 6.3042 5.4189 8.6287
H 12.0612 16.4591 11.8000	H 12.0612 16.4591 11.8000	H 7.8301 6.3260 8.3706
H 10.6874 17.3925 11.1539	H 10.6874 17.3925 11.1539	H 6.6806 6.0815 7.0073
H 12.1325 18.2367 11.7405	H 12.1325 18.2367 11.7405	C 16.0643 12.3163 7.1822
H 13.5273 13.7592 7.7502	H 13.5273 13.7592 7.7502	C 16.0690 13.7174 7.2042
H 14.1020 14.9191 6.5485	H 14.1020 14.9191 6.5485	C 17.2676 14.4358 7.2530
H 11.2634 13.8023 6.7597	H 11.2634 13.8023 6.7597	C 17.2580 11.6064 7.1680
H 12.4615 13.6246 5.4745	H 12.4615 13.6246 5.4745	C 14.6426 11.8151 7.1880
H 11.6783 15.1991 5.7375	H 11.6783 15.1991 5.7375	C 18.4609 13.7090 7.2426
H 10.5243 17.2360 7.7025	H 10.5243 17.2360 7.7025	H 17.3087 15.5164 7.3003
H 8.7225 15.5708 7.6346	H 8.7225 15.5708 7.6346	C 18.4654 12.3127 7.1887

H 12.0543 12.5550 10.8914	H 12.0543 12.5550 10.8914	H 17.2594 10.5159 7.1368
H 10.6403 10.5913 10.3178	H 10.6403 10.5913 10.3178	C 14.3355 10.9449 5.9492
H 8.2074 13.0777 7.7778	H 8.2074 13.0777 7.7778	C 14.3458 11.0242 8.4853
H 9.2180 7.2402 7.5886	H 9.2180 7.2402 7.5886	H 19.4049 14.2532 7.2735
H 10.3798 9.2797 8.3027	H 10.3798 9.2797 8.3027	H 19.4124 11.7735 7.1668
H 5.4396 9.2994 7.8711	H 5.4396 9.2994 7.8711	H 14.5163 11.4924 5.0154
H 6.6206 11.3579 8.5970	H 6.6206 11.3579 8.5970	H 13.2944 10.5961 5.9563
H 6.4034 5.0366 7.0543	H 6.4034 5.0366 7.0543	H 14.9864 10.0608 5.9585
H 7.7430 5.5497 8.1313	H 7.7430 5.5497 8.1313	H 14.5193 11.6356 9.3806
H 7.8674 5.7982 6.3555	H 7.8674 5.7982 6.3555	H 15.0112 10.1522 8.5357
		H 13.3095 10.6606 8.5023

SP R=NO_2 gasphase	MC R= NO_2 gasphase	MCH^+ R= NO_2 gasphase
45	45	46
C 8.6605 10.4460 7.4827	C 8.9529 10.8973 7.3707	C 8.9924 10.9561 7.2896
C 8.6744 9.2552 8.2249	C 8.8861 9.4969 7.3210	C 8.8826 9.5591 7.2393
C 7.4732 10.9199 6.9458	C 7.8019 11.6641 7.4848	C 7.8582 11.7496 7.4040
C 7.4989 8.5307 8.4505	C 7.6491 8.8465 7.3837	C 7.6373 8.9248 7.2915
C 6.2832 10.2073 7.1647	C 6.5598 11.0235 7.5574	C 6.6065 11.1290 7.4674
C 6.3051 9.0292 7.9134	C 6.4968 9.6303 7.5051	C 6.5057 9.7358 7.4076
N 9.9563 8.9802 8.6845	N 10.2083 8.9809 7.2124	N 10.2046 9.0150 7.1373
C 10.0515 11.0512 7.4427	C 10.3915 11.3418 7.2891	C 10.4422 11.3533 7.2070
C 10.9254 9.9442 8.2086	C 10.8291 12.1620 8.5425	C 10.8932 12.1450 8.4594
C 10.5304 11.2759 5.9979	C 10.6290 12.1628 5.9996	C 10.7230 12.1675 5.9186
C 10.0668 12.4059 8.1742	C 11.1214 9.9986 7.2048	C 11.1271 9.9962 7.1258
C 10.3327 7.7236 9.3158	C 10.6465 7.5734 7.1735	C 10.5939 7.5896 7.0556
C 10.3488 6.5213 8.3636	C 9.6004 6.4708 7.1614	C 9.5266 6.5090 7.0585
C 11.7538 10.4563 9.3517	C 12.5145 9.9507 7.1279	C 12.5446 9.9180 7.0295
O 11.7785 9.2840 7.1865	C 13.3907 8.8656 7.0425	C 13.3944 8.8387 6.9437
C 13.0412 10.1232 9.5513	C 14.7865 8.8890 6.9055	C 14.8264 8.8482 6.8150
C 13.0429 8.8903 7.4371	C 15.5701 10.0642 6.8535	C 15.5889 10.0386 6.7386
C 13.7459 9.2933 8.5993	C 16.9292 9.9843 6.6607	C 16.9555 9.9817 6.5680
C 13.6594 8.0791 6.4708	C 17.5927 8.7278 6.5028	C 17.6390 8.7611 6.4466
C 14.9777 7.6836 6.6419	C 15.4412 7.5501 6.7786	C 15.5370 7.6048 6.7266
C 15.0745 8.8922 8.7561	C 16.8824 7.5661 6.5588	C 16.9253 7.5809 6.5245
C 15.6768 8.1032 7.7793	O 14.7919 6.4876 6.8469	O 14.9518 6.3907 6.8153
H 7.4573 11.8435 6.3634	H 12.9664 10.9470 7.1218	H 13.0047 10.9083 7.0189
H 7.5004 7.6077 9.0305	H 13.0210 7.8421 7.0632	H 12.9378 7.8524 6.9562
H 5.3430 10.5771 6.7560	H 7.8645 12.7532 7.5232	H 7.9368 12.8366 7.4481
H 5.3778 8.4801 8.0836	H 7.5485 7.7689 7.3428	H 7.5129 7.8504 7.2454
H 9.8786 12.0238 5.5257	H 5.6462 11.6101 7.6541	H 5.7045 11.7331 7.5640
H 11.5595 11.6598 5.9717	H 5.5303 9.1284 7.5578	H 5.5242 9.2639 7.4523
H 10.4861 10.3590 5.4005	H 11.0533 13.2009 8.2683	H 10.5069 13.1702 8.3954
H 9.4471 13.1196 7.6146	H 10.0345 12.1756 9.2983	H 10.5095 11.6898 9.3809
H 9.6545 12.3397 9.1893	H 11.7265 11.7372 9.0085	H 11.9871 12.2042 8.5288
H 11.0859 12.8159 8.2317	H 10.3448 11.5965 5.1030	H 10.4502 11.6020 5.0183
H 11.3231 7.8645 9.7717	H 10.0211 13.0773 6.0359	H 10.1210 13.0850 5.9416
H 9.6377 7.5301 10.1499	H 11.6836 12.4556 5.9088	H 11.7795 12.4578 5.8495
H 11.1120 6.6389 7.5840	H 11.2795 7.4655 6.2795	H 11.1870 7.4962 6.1316
H 10.5666 5.6007 8.9230	H 11.3079 7.4258 8.0426	H 11.2698 7.4184 7.9087
H 9.3770 6.3960 7.8682	H 8.9460 6.5153 6.2824	H 8.8590 6.5668 6.1918
H 11.2199 11.0672 10.0778	H 10.1469 5.5193 7.1150	H 10.0568 5.5488 6.9933
H 13.5736 10.4728 10.4387	H 8.9922 6.4509 8.0731	H 8.9411 6.4903 7.9840
H 13.0911 7.7830 5.5893	H 15.1270 11.0536 6.9678	H 15.1246 11.0216 6.8066
H 15.4852 7.0608 5.9078	N 17.7167 11.2066 6.6170	N 17.7324 11.2440 6.5096

H 15.6518 9.1943 9.6296	H 18.6694 8.7358 6.3371	H 18.7173 8.7665 6.2962
N 17.0824 7.7220 7.9340	H 17.3718 6.5991 6.4425	H 17.4191 6.6134 6.4403
O 17.7011 8.1770 8.9033	O 17.1271 12.2946 6.7158	O 17.1013 12.2994 6.5831
O 17.5719 6.9732 7.0801	O 18.9451 11.0933 6.4832	O 18.9519 11.1431 6.4002
		H 14.0057 6.4658 7.0270

SP R=PhOMe DMSO	MC R=PhOMe DMSO	MCH^+ R=PhOMe DMSO
57	57	58
C 13.9008 17.1131 9.7960	C 13.8450 13.1145 7.1565	C 13.8590 13.1246 7.1556
C 14.2299 16.2261 8.7589	N 14.7063 14.1713 7.1731	N 14.7100 14.1691 7.1693
C 14.8927 17.7009 10.5666	C 14.2060 15.5574 7.1064	C 14.2145 15.5630 7.1062
C 15.5629 15.8732 8.5185	C 15.2135 16.6944 7.0749	C 15.2191 16.7004 7.0771
C 16.2383 17.3796 10.3163	H 13.5337 15.6912 7.9692	H 13.5444 15.6867 7.9710
C 16.5587 16.4680 9.3078	H 13.5836 15.6141 6.1999	H 13.5930 15.6168 6.1995
N 13.0759 15.7983 8.0885	H 15.8083 16.7628 7.9937	H 15.8119 16.7694 7.9964
C 12.4005 17.3083 9.8098	H 14.6368 17.6256 6.9883	H 14.6383 17.6297 6.9941
C 11.9209 16.0569 8.9514	H 15.8794 16.6419 6.2047	H 15.8829 16.6537 6.2055
C 12.0890 18.6349 9.0846	C 12.4442 13.0949 7.1184	C 12.4389 13.1108 7.1230
C 11.7837 17.3398 11.2098	C 11.4838 14.1086 7.0466	C 11.5032 14.1212 7.0461
C 13.2364 14.6590 7.1743	H 12.0572 12.0735 7.1571	H 12.0514 12.0914 7.1746
C 12.0823 14.3135 6.2423	C 10.0798 13.9498 7.0539	C 10.0729 13.9511 7.0574
C 10.6282 16.2861 8.2236	H 11.7773 15.1545 6.9837	H 11.8157 15.1585 6.9810
O 11.7788 14.9429 9.9180	C 9.2682 15.1841 7.0265	C 9.2461 15.1137 7.0367
C 9.6425 15.3712 8.1855	C 9.4268 12.6914 7.1509	C 9.4306 12.6958 7.1564
C 10.9505 13.9003 9.6241	C 7.8355 14.9967 7.1200	C 7.8534 14.9879 7.1182
C 9.8276 14.0666 8.7858	O 9.7816 16.3413 6.9398	O 9.8490 16.3250 6.9496
C 11.2135 12.6566 10.2046	C 8.0534 12.5563 7.2457	C 8.0483 12.5546 7.2485
C 10.4182 11.5617 9.8744	H 10.0362 11.7868 7.1963	H 10.0428 11.7961 7.2055
C 9.0333 12.9504 8.4806	C 7.2658 13.7540 7.2300	C 7.2677 13.7349 7.2250
C 9.3347 11.6759 8.9789	H 7.2123 15.8943 7.0993	H 7.2285 15.8849 7.0971
C 8.5958 10.4722 8.5360	C 7.4441 11.2257 7.4336	H 9.1773 17.0345 6.9880
H 17.0297 17.8327 10.9153	H 6.1772 13.6697 7.2888	C 7.4468 11.2185 7.4391
C 8.6350 8.1279 7.8268	C 8.0075 10.0802 6.8456	H 6.1798 13.6648 7.2792
C 7.2395 8.1299 7.7057	C 6.3416 11.0369 8.2931	C 8.0143 10.0780 6.8498
C 9.2913 9.2893 8.2391	C 7.5603 8.7944 7.1545	C 6.3458 11.0312 8.2991
C 6.5261 9.3108 7.9684	H 8.8199 10.1927 6.1244	C 7.5667 8.7925 7.1545
C 7.1971 10.4597 8.3728	C 5.8816 9.7640 8.6093	H 8.8246 10.1918 6.1265
O 6.4937 7.0417 7.3434	H 5.8663 11.8997 8.7655	C 5.8865 9.7595 8.6128
C 7.1804 5.7898 7.2148	C 6.5110 8.6297 8.0703	H 5.8716 11.8920 8.7752
H 14.6375 18.4042 11.3627	H 8.0345 7.9365 6.6790	C 6.5173 8.6278 8.0704
H 15.8385 15.1441 7.7569	H 5.0539 9.6261 9.3083	H 8.0351 7.9341 6.6752
H 17.6024 16.1966 9.1359	O 6.0391 7.4183 8.4979	H 5.0574 9.6162 9.3086
H 12.4441 18.6248 8.0445	C 6.7705 6.2517 8.0937	O 6.0452 7.4208 8.4971
H 12.6049 19.4521 9.6066	H 6.3172 5.4118 8.6317	C 6.7676 6.2498 8.0907
H 11.0124 18.8571 9.0920	H 7.8327 6.3381 8.3717	H 6.3037 5.4169 8.6288
H 12.0610 16.4590 11.8000	H 6.6870 6.0818 7.0088	H 7.8301 6.3259 8.3704
H 10.6869 17.3920 11.1535	C 16.0620 12.3172 7.1828	H 6.6806 6.0817 7.0062
H 12.1325 18.2370 11.7408	C 16.0571 13.7199 7.2057	C 16.0633 12.3163 7.1824
H 13.5268 13.7589 7.7502	C 17.2594 14.4358 7.2542	C 16.0677 13.7173 7.2041
H 14.1028 14.9182 6.5486	C 17.2581 11.6103 7.1651	C 17.2666 14.4361 7.2527
H 11.2627 13.8037 6.7590	C 14.6421 11.8068 7.1894	C 17.2568 11.6054 7.1681
H 12.4627 13.6248 5.4743	C 18.4572 13.7130 7.2422	C 14.6428 11.8157 7.1877
H 11.6794 15.2001 5.7365	H 17.3002 15.5167 7.3027	C 18.4604 13.7093 7.2424
H 10.5238 17.2356 7.7022	C 18.4678 12.3170 7.1847	H 17.3090 15.5170 7.2997
H 8.7212 15.5713 7.6336	H 17.2615 10.5186 7.1324	C 18.4646 12.3121 7.1888

H 12.0555 12.5542 10.8914	C 14.3400 10.9359 5.9510	H 17.2589 10.5147 7.1374
H 10.6418 10.5902 10.3186	C 14.3526 11.0144 8.4859	C 14.3352 10.9452 5.9483
H 8.2063 13.0782 7.7776	H 19.3985 14.2650 7.2766	C 14.3456 11.0246 8.4860
H 9.2187 7.2396 7.5896	H 19.4173 11.7798 7.1591	H 19.4056 14.2538 7.2735
H 10.3810 9.2790 8.3039	H 14.5176 11.4916 5.0202	H 19.4128 11.7724 7.1674
H 5.4389 9.3004 7.8711	H 13.2972 10.5900 5.9596	H 14.5164 11.4938 5.0148
H 6.6196 11.3589 8.5972	H 14.9895 10.0490 5.9542	H 13.2938 10.5966 5.9567
H 6.4025 5.0359 7.0532	H 14.5215 11.6321 9.3787	H 14.9866 10.0606 5.9593
H 7.7419 5.5498 8.1313	H 15.0187 10.1415 8.5409	H 14.5192 11.6371 9.3808
H 7.8680 5.7984 6.3550	H 13.3153 10.6519 8.5010	H 15.0113 10.1519 8.5345
		H 13.3089 10.6615 8.5015

SP R=NO_2 DMSO	MC R= NO_2 DMSO	MCH^+ R= NO_2 DMSO
45	45	46
C 8.6616 10.4469 7.4815	C 8.9524 10.8989 7.3701	C 8.9952 10.9562 7.2875
C 8.6761 9.2551 8.2236	C 8.8812 9.4999 7.3217	C 8.8878 9.5592 7.2391
C 7.4742 10.9215 6.9445	C 7.8026 11.6680 7.4841	C 7.8620 11.7513 7.4005
C 7.5000 8.5298 8.4510	C 7.6488 8.8421 7.3821	C 7.6433 8.9231 7.2917
C 6.2830 10.2076 7.1637	C 6.5633 11.0221 7.5554	C 6.6106 11.1290 7.4643
C 6.3050 9.0285 7.9136	C 6.4969 9.6268 7.5022	C 6.5112 9.7345 7.4068
N 9.9568 8.9798 8.6808	N 10.2116 8.9857 7.2215	N 10.2087 9.0161 7.1410
C 10.0524 11.0523 7.4425	C 10.3893 11.3389 7.2905	C 10.4430 11.3530 7.2061
C 10.9241 9.9460 8.2102	C 10.8318 12.1584 8.5443	C 10.8928 12.1441 8.4585
C 10.5305 11.2764 5.9975	C 10.6318 12.1578 5.9977	C 10.7250 12.1665 5.9177
C 10.0653 12.4063 8.1753	C 11.1093 9.9959 7.2093	C 11.1250 9.9970 7.1280
C 10.3324 7.7231 9.3166	C 10.6450 7.5717 7.1734	C 10.5950 7.5874 7.0572
C 10.3493 6.5217 8.3641	C 9.5971 6.4728 7.1614	C 9.5224 6.5137 7.0595
C 11.7545 10.4555 9.3512	C 12.5181 9.9455 7.1271	C 12.5466 9.9199 7.0309
O 11.7826 9.2784 7.1857	C 13.3793 8.8683 7.0424	C 13.3857 8.8393 6.9449
C 13.0423 10.1246 9.5517	C 14.7951 8.8915 6.9020	C 14.8249 8.8532 6.8148
C 13.0439 8.8901 7.4355	C 15.5675 10.0596 6.8513	C 15.5830 10.0393 6.7386
C 13.7482 9.2951 8.5994	C 16.9412 9.9876 6.6609	C 16.9572 9.9860 6.5680
C 13.6618 8.0770 6.4684	C 17.5986 8.7344 6.5052	C 17.6456 8.7660 6.4486
C 14.9784 7.6825 6.6391	C 15.4484 7.5661 6.7777	C 15.5375 7.6125 6.7260
C 15.0749 8.8955 8.7572	C 16.8810 7.5733 6.5608	C 16.9294 7.5904 6.5264
C 15.6805 8.1036 7.7787	O 14.7957 6.4908 6.8490	O 14.9645 6.3980 6.8084
H 7.4570 11.8459 6.3624	H 12.9661 10.9428 7.1205	H 13.0057 10.9103 7.0200
H 7.5007 7.6062 9.0309	H 13.0072 7.8477 7.0638	H 12.9314 7.8536 6.9555
H 5.3419 10.5777 6.7540	H 7.8640 12.7575 7.5254	H 7.9426 12.8387 7.4461
H 5.3769 8.4785 8.0842	H 7.5497 7.7642 7.3430	H 7.5201 7.8483 7.2475
H 9.8785 12.0251 5.5257	H 5.6487 11.6092 7.6526	H 5.7073 11.7339 7.5611
H 11.5599 11.6604 5.9723	H 5.5284 9.1271 7.5576	H 5.5300 9.2596 7.4527
H 10.4861 10.3587 5.4001	H 11.0482 13.1974 8.2641	H 10.4917 13.1647 8.3991
H 9.4462 13.1200 7.6143	H 10.0394 12.1678 9.3026	H 10.5228 11.6754 9.3796
H 9.6541 12.3389 9.1912	H 11.7338 11.7403 9.0082	H 11.9869 12.2150 8.5165
H 11.0848 12.8156 8.2328	H 10.3459 11.5917 5.1008	H 10.4538 11.5987 5.0177
H 11.3220 7.8655 9.7732	H 10.0244 13.0730 6.0385	H 10.1235 13.0851 5.9442
H 9.6362 7.5320 10.1498	H 11.6860 12.4540 5.9109	H 11.7830 12.4537 5.8522
H 11.1125 6.6394 7.5840	H 11.2698 7.4730 6.2721	H 11.1809 7.4952 6.1288
H 10.5674 5.6014 8.9245	H 11.3035 7.4278 8.0450	H 11.2655 7.4145 7.9135
H 9.3768 6.3946 7.8693	H 8.9448 6.5169 6.2804	H 8.8554 6.5749 6.1914
H 11.2216 11.0658 10.0794	H 10.1476 5.5225 7.1133	H 10.0557 5.5548 6.9919
H 13.5746 10.4737 10.4393	H 8.9931 6.4507 8.0761	H 8.9404 6.4952 7.9881
H 13.0925 7.7799 5.5869	H 15.1133 11.0439 6.9648	H 15.1046 11.0150 6.8090
H 15.4805 7.0597 5.9012	N 17.7118 11.1929 6.6187	N 17.7196 11.2321 6.5078

H 15.6468 9.1994 9.6336	H 18.6744 8.7249 6.3379	H 18.7241 8.7545 6.2989
N 17.0701 7.7249 7.9325	H 17.3744 6.6063 6.4426	H 17.4257 6.6229 6.4426
O 17.7050 8.1722 8.9039	O 17.1310 12.2957 6.7215	O 17.1025 12.3030 6.5762
O 17.5769 6.9691 7.0843	O 18.9516 11.1049 6.4811	O 18.9499 11.1523 6.3955
		H 14.0153 6.4351 7.0276