Electronic Supplementary Information

Anion receptors based on ureidocalix[4]arenes immobilised in the *partial cone* conformation

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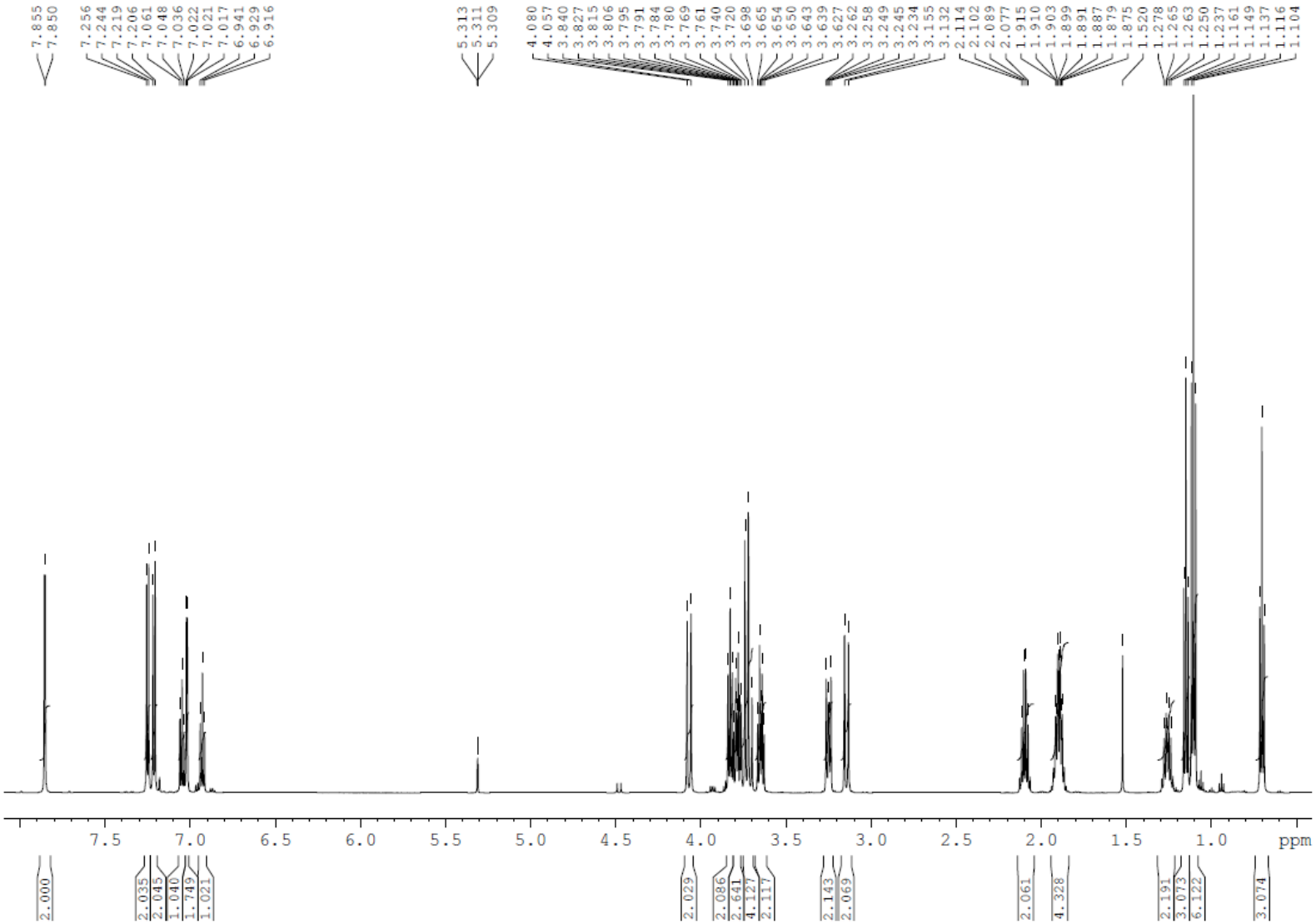
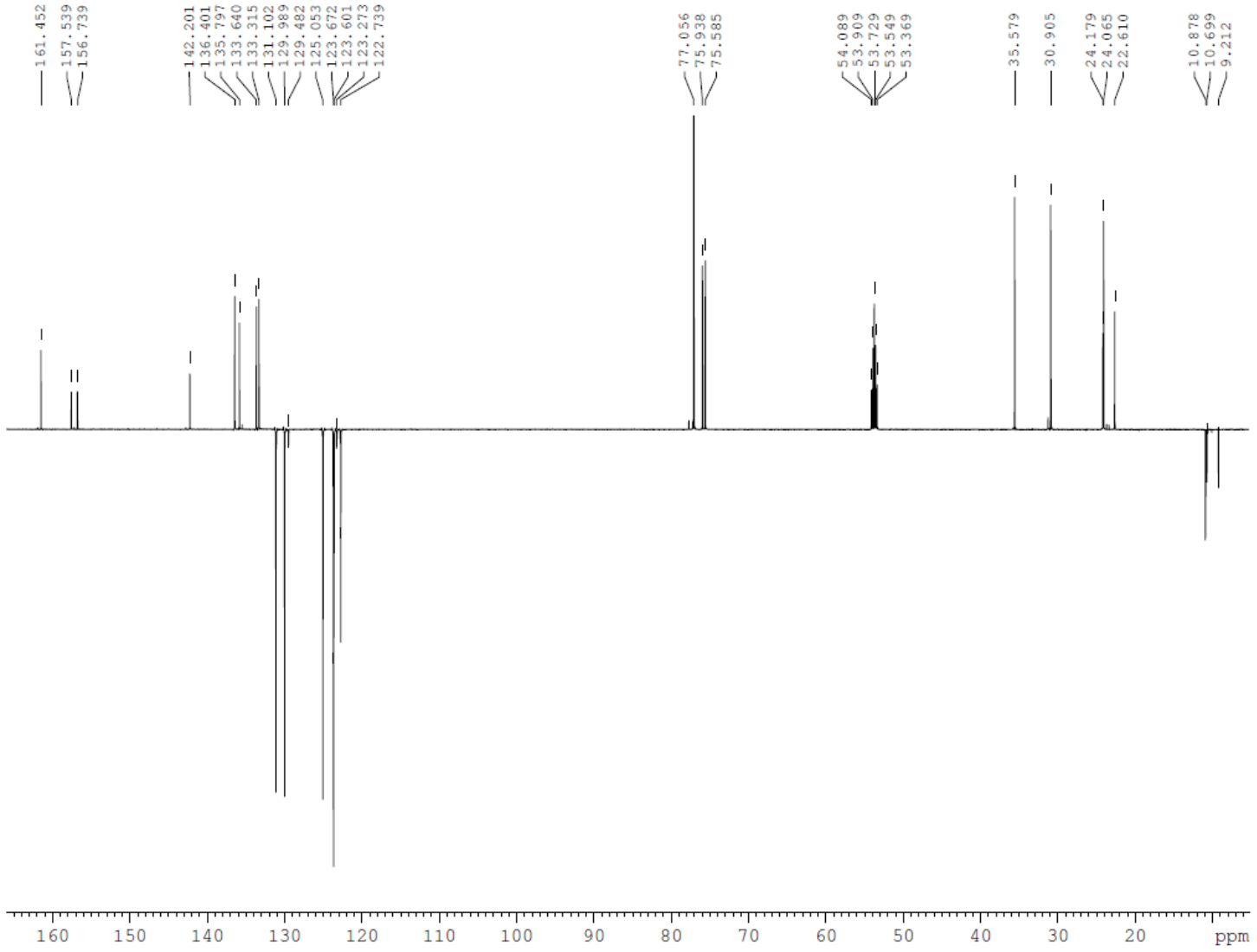
Content:

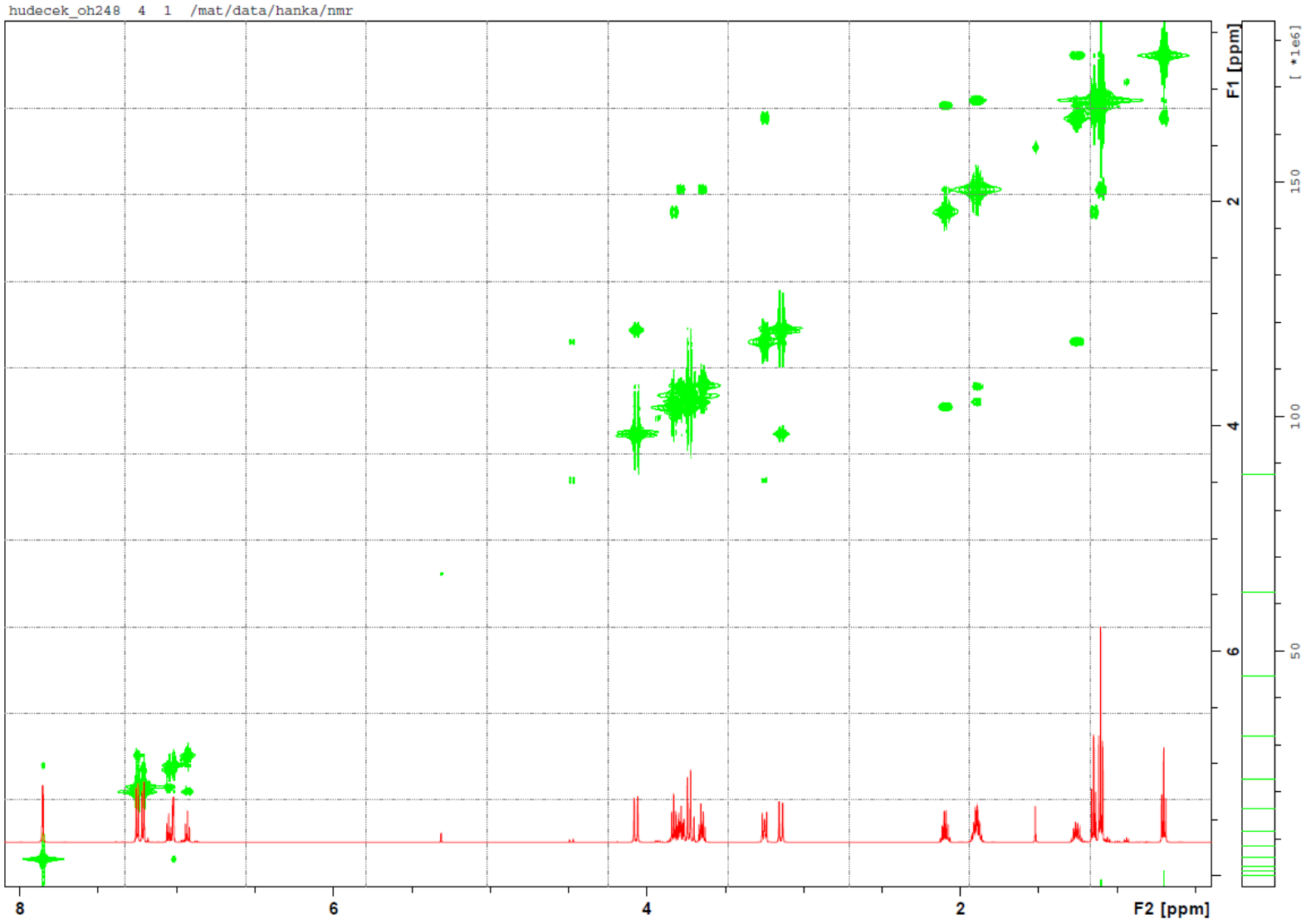
^{1}H NMR spectrum of compound **4** (CD_2Cl_2, 298 K, 600 MHz)



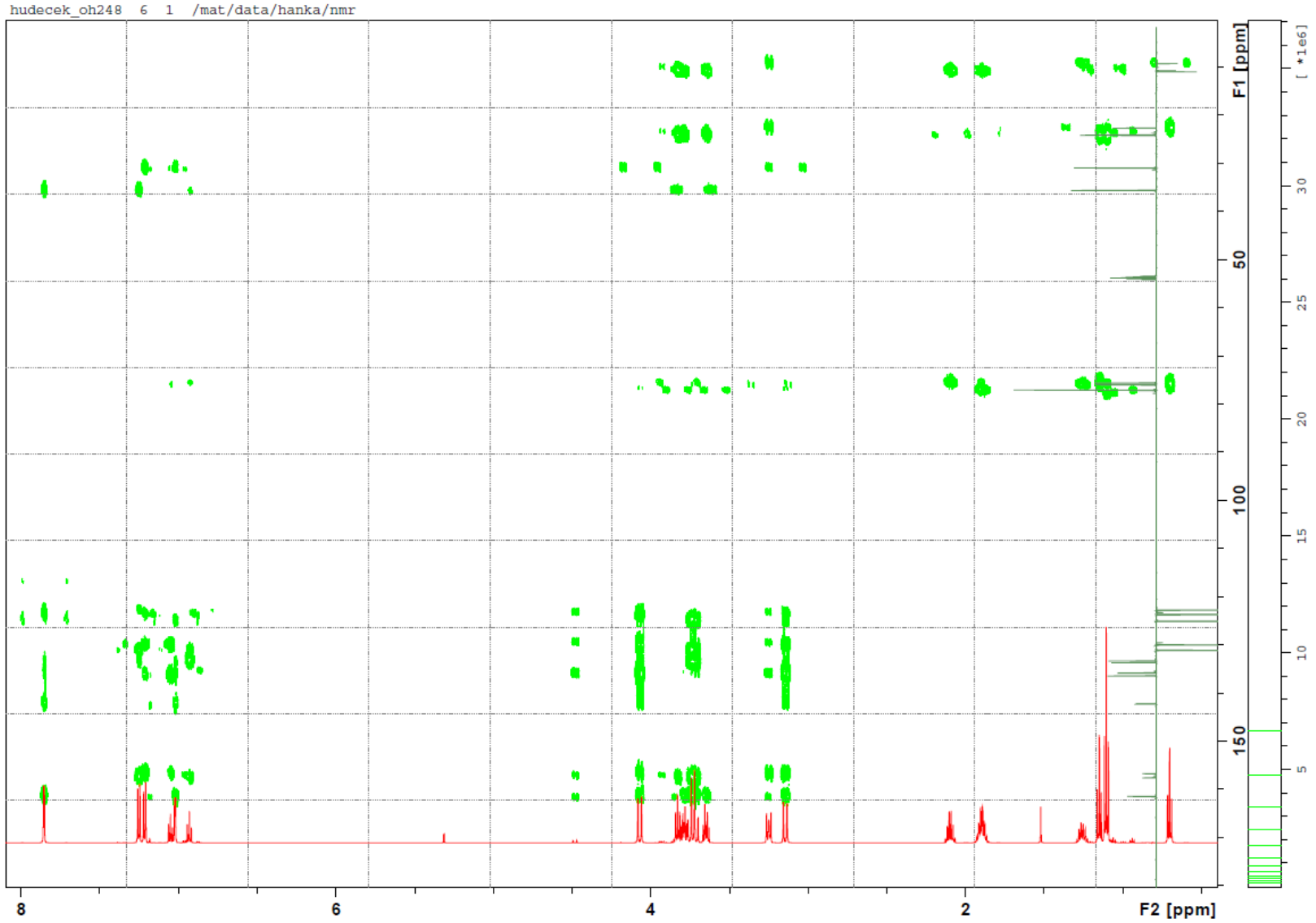
^{13}C NMR spectrum of compound **4** (CD_2Cl_2, 298 K, 150 MHz)



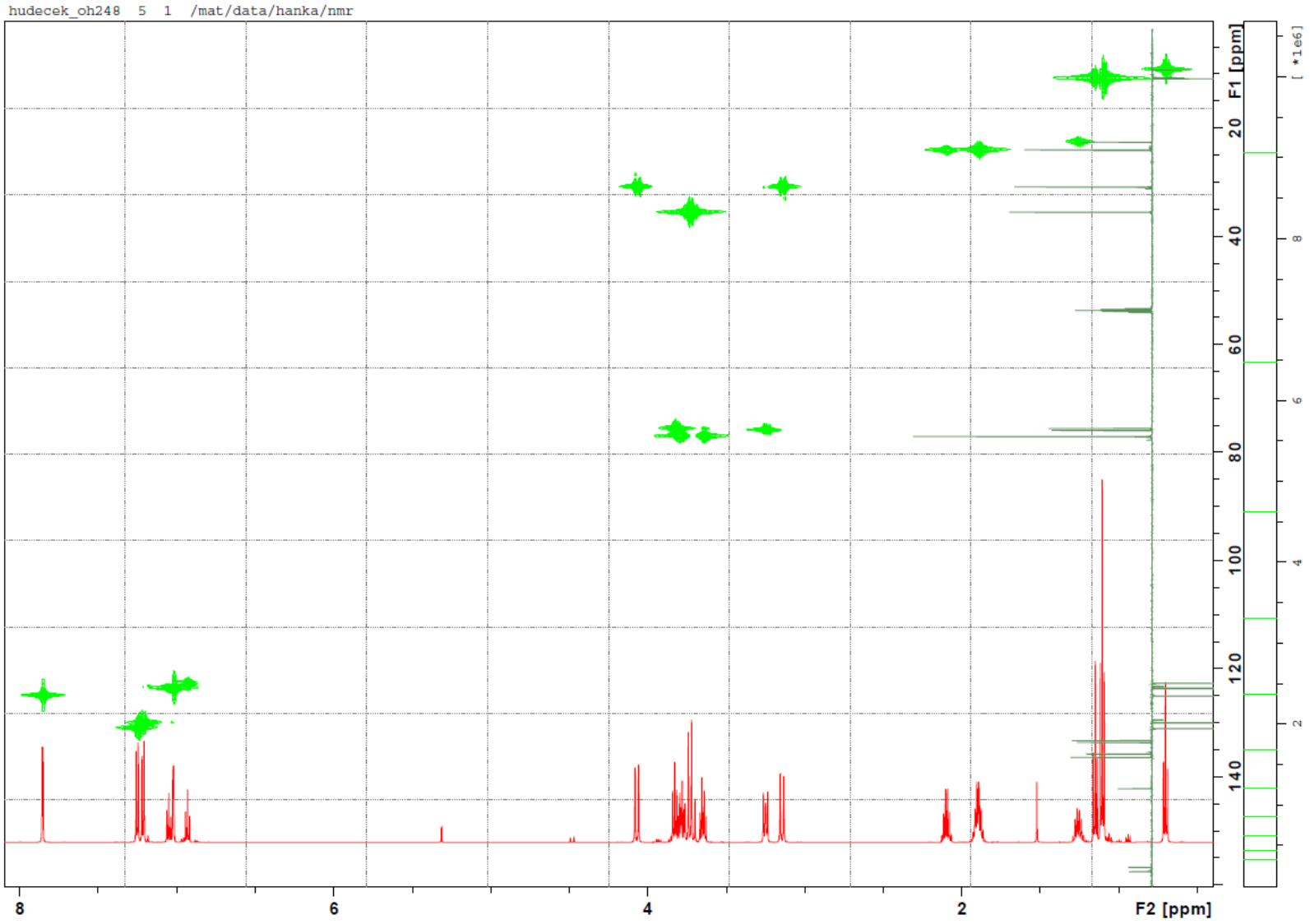
COSY spectrum of compound **4** (CD_2Cl_2, 298 K)



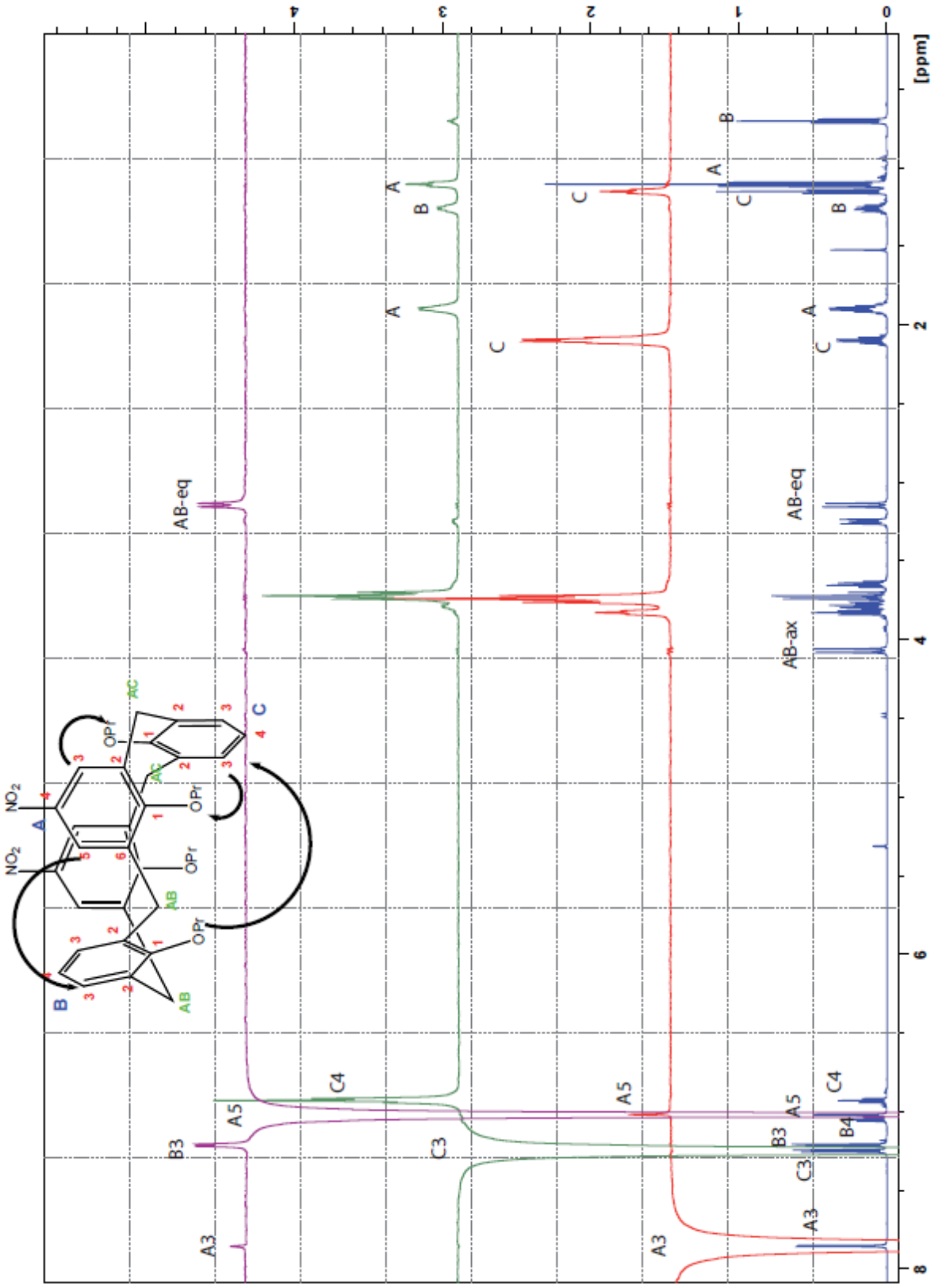
HMBC spectrum of compound **4** (CD_2Cl_2, 298 K)



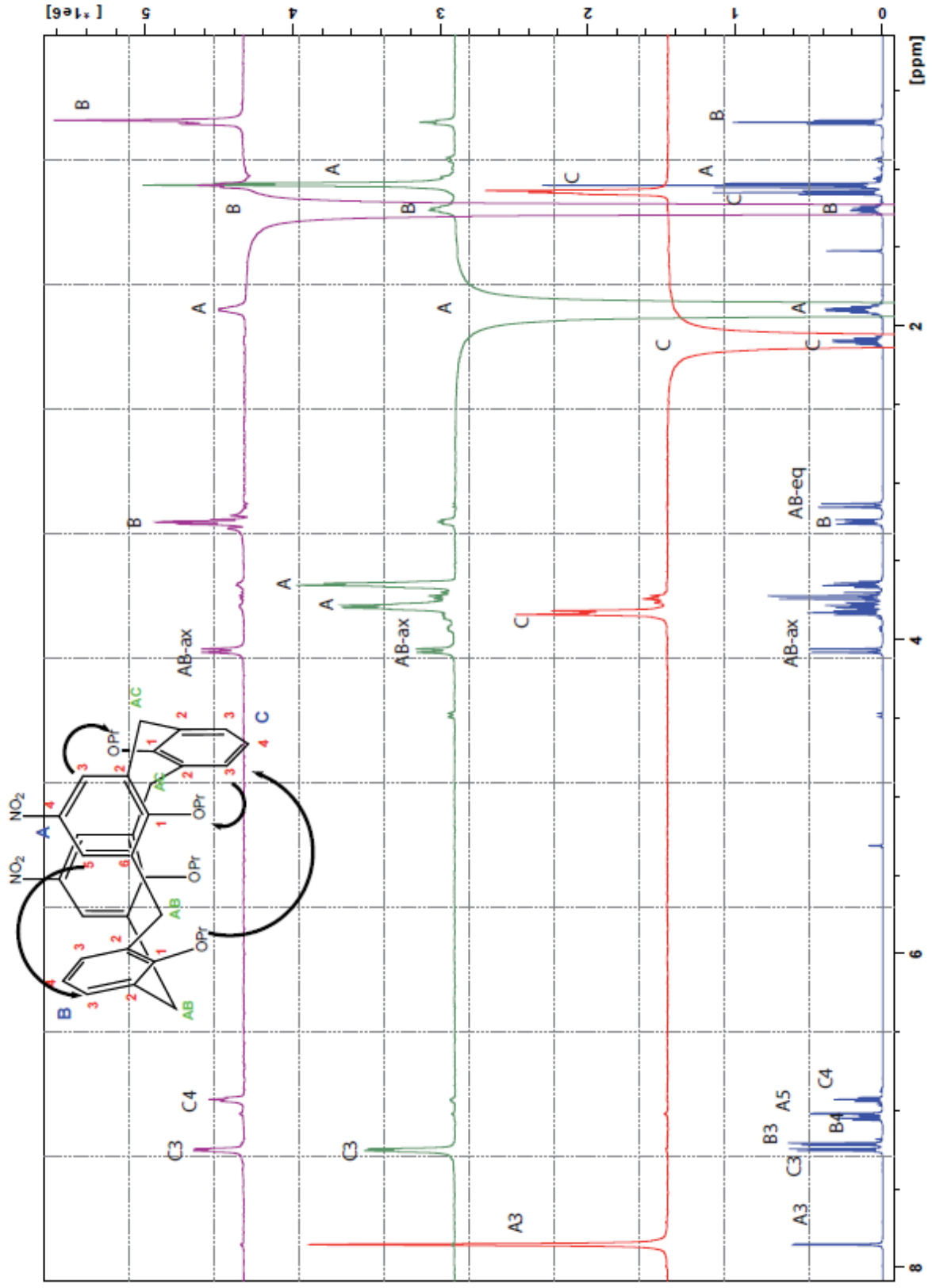
HMQC spectrum of compound **4** (CD_2Cl_2, 298 K)



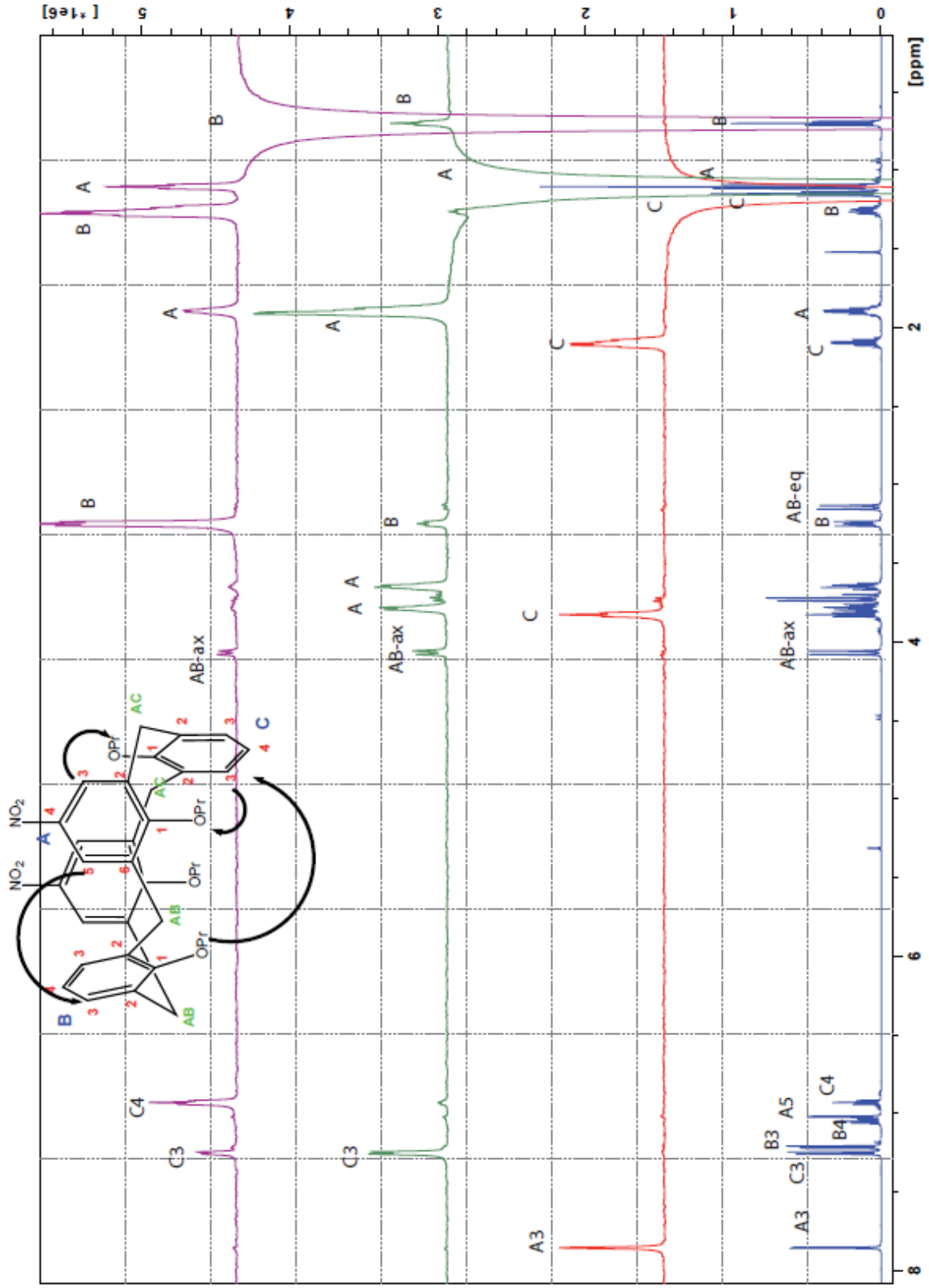
NOE (1) spectrum of compound **4** (CD_2Cl_2, 298 K)



NOE (2) spectrum of compound **4** (CD_2Cl_2, 298 K)



NOE (3) spectrum of compound **4** (CD_2Cl_2, 298 K)

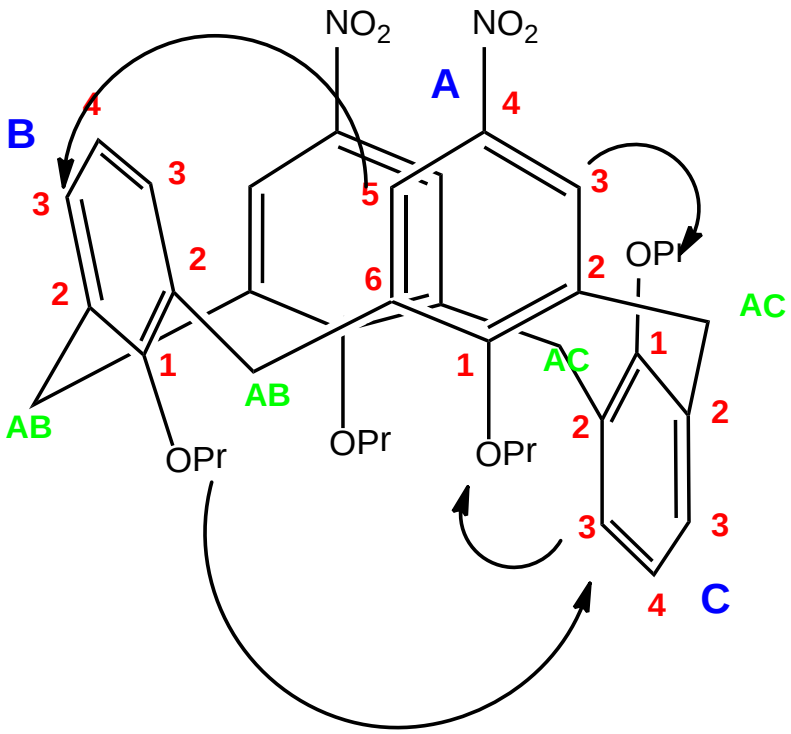


1H NMR assignment of compound **4** in CD_2Cl_2:

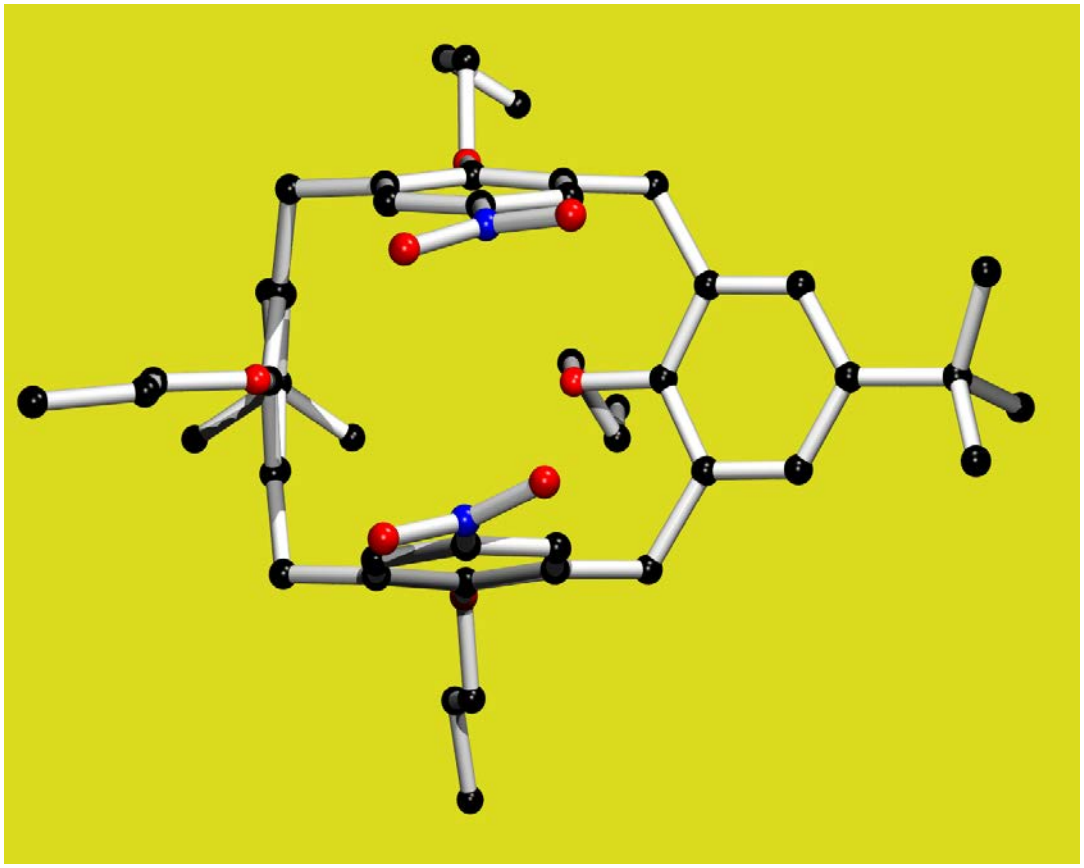
^{1}H NMR (600.1 MHz, CD_2Cl_2, 298K) δ 7.85 (d, 2H, *J* = 2.8 Hz , H-3 –*A*), 7.25 (d, 2H, *J* = 7.5 Hz, H-3 –*C*), 7.22 (d, 2H, *J* = 7.5 Hz, H-3 –*B*), 7.06 (dd, 1H, *J* = 7.5 Hz, H-4 –*B*), 7.02 (d, 2H, *J* = 2.8 Hz , H-5 –*A*), 6.93 (dd, 1H, *J* = 7.5 Hz, H-4 –*C*), 4.08 (d, 2H, *J* = 13.9 Hz, CH_2 –*AB* - *ax*), 3.83 (t, 2H, *J* = 7.4 Hz, OCH_2 –*C*), 3.75 – 3.80 (m, 2H, OCH_2 –*A*), 3.75 and 3.71 (2 x d, 2 x 2H, *J* = 13.1, 13.1 Hz, CH_2 –*AC)*, 3.62 – 3.68 (m, 2H, OCH_2 –*A*), 3.22 – 3.28 (m, 2H, OCH_2 –*C*), 3.15 (d, 2H, *J* = 13.9 Hz, CH_2 –*AB* - *eq*), 2.05 – 2.14 (m, 2H, OCH_2CH_2 –*C*), 1.85 – 1.94 (m, 4H, OCH_2CH_2 –*A*), 1.20 – 1.30 (m, 2H, OCH_2CH_2 –*B*), 1.15 (t, 3H, *J* = 7.5 Hz, CH_3-*C*), 1.10 (t, 6H, *J* = 7.4 Hz, CH_3-*A*), 0.70 (t, 3H, *J* = 7.6 Hz, CH_3-*B*).

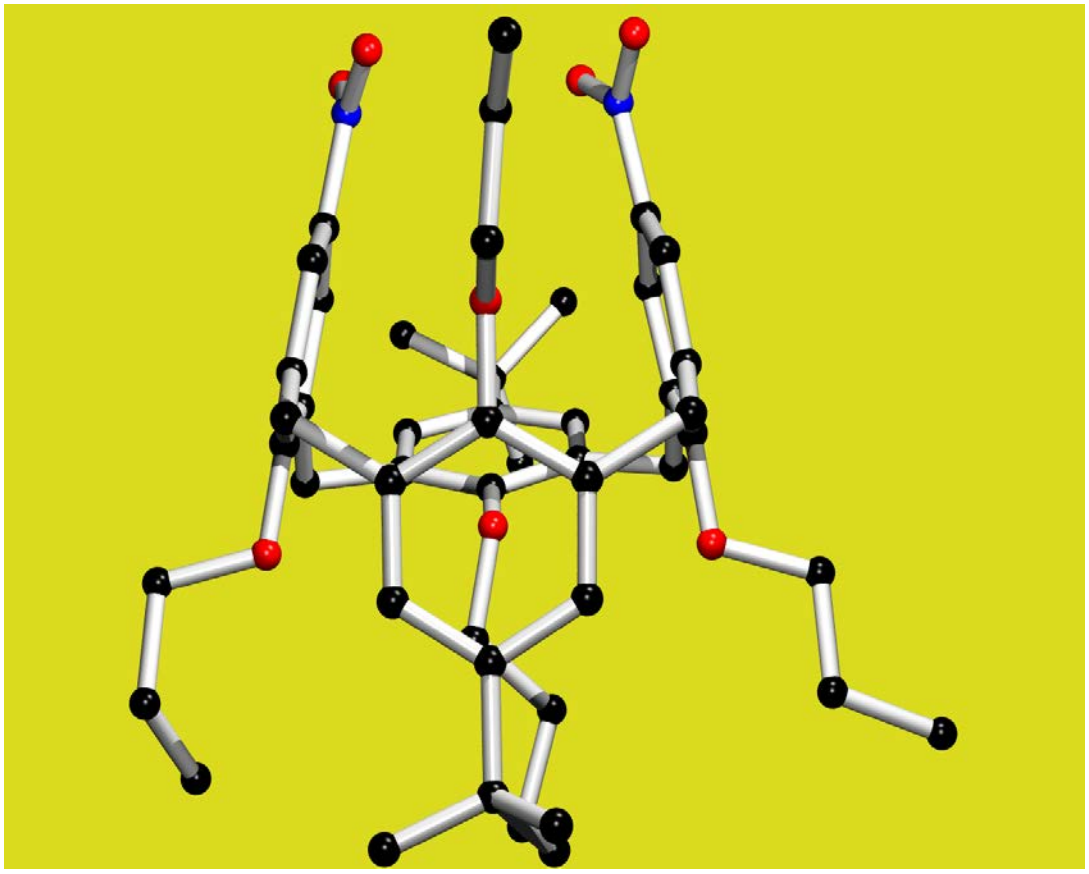
^{13}C NMR (150.9 MHz, CD_2Cl_2, 298K) δ 161.5 (quart. C-1 –*A*), 157.5 (quart. C-1 –*C*), 156.7 (quart. C-1 –*B*), 142.2 (quart. C-4 –*A*), 136.4 (quart. C-2-*B*), 135.8 (quart. C-6-*A*), 133.6 (quart. C-2-*A*), 133.3 (quart. C-2-*C*), 131.1.1 (CH-3–*C*), 130.0 (CH-3-*B)*, 125.1 (CH-3-*A)*, 123.7 (CH-5-*A* and CH-4-*B)*, 122.7 (CH-4-*C)*, 77.1 (OCH_2-*A*), 75.9 and 75.6 (OCH_2-*B*, *C*), 35.6 (CH_2-*A*,*C*), 30.9 (CH_2-*A*,*B*), 24.2 and 24.1 (O*C*$H_2$$CH_3$ - *A*, *C*), 24.1 (O*C*$H_2$$CH_3$ - *B*), 10.9 and 10.7 (CH_3 - *A*, *C*), 9.2 (CH_3 - *B*).

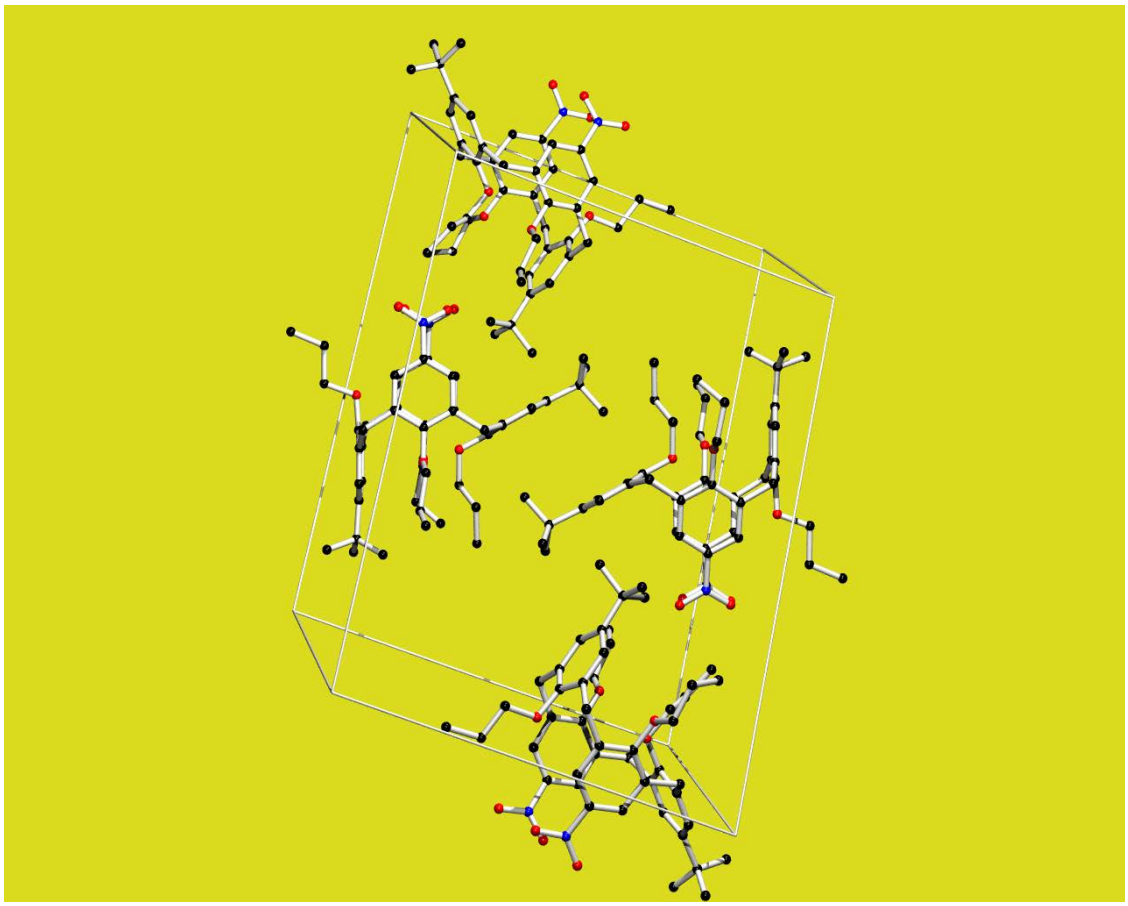
NOE contacts observed

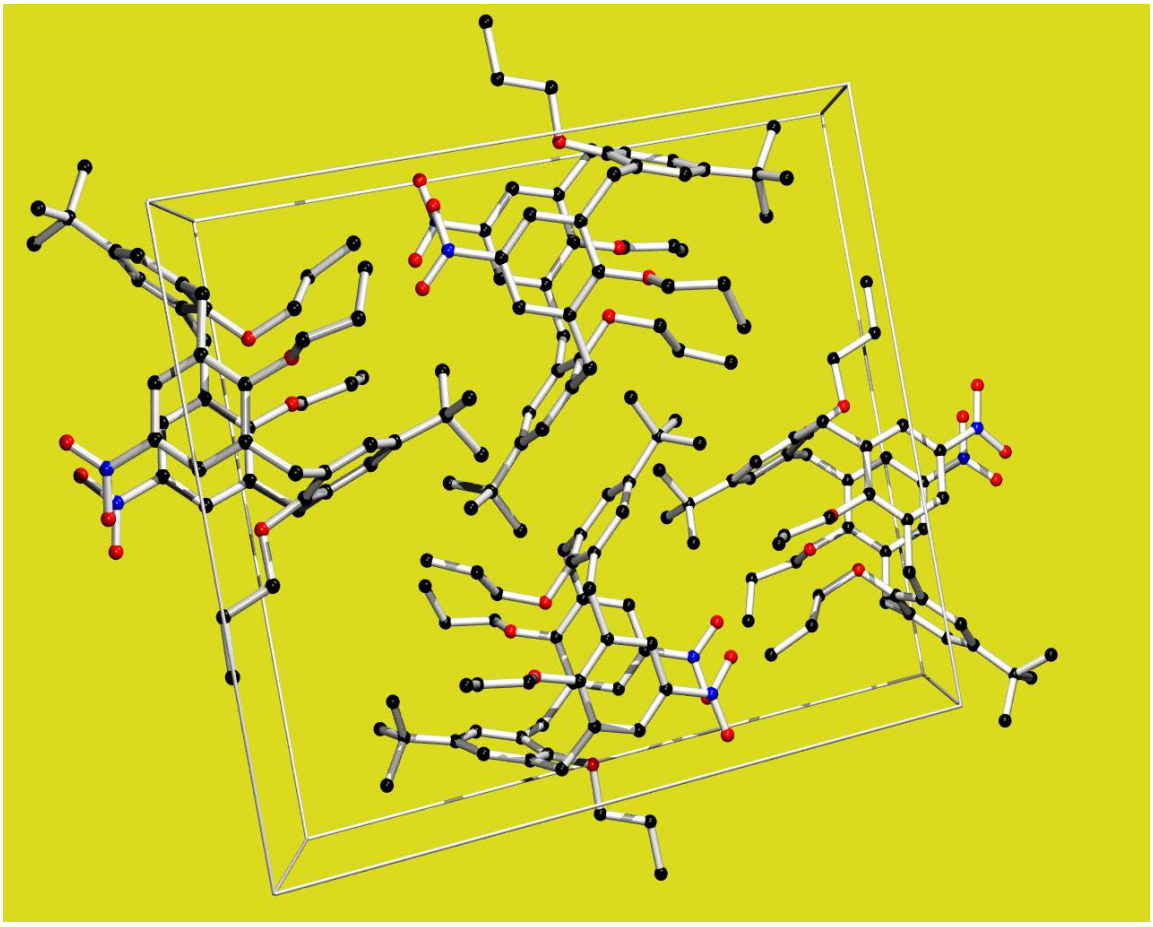


Crystallographic measurements (compound **5**):

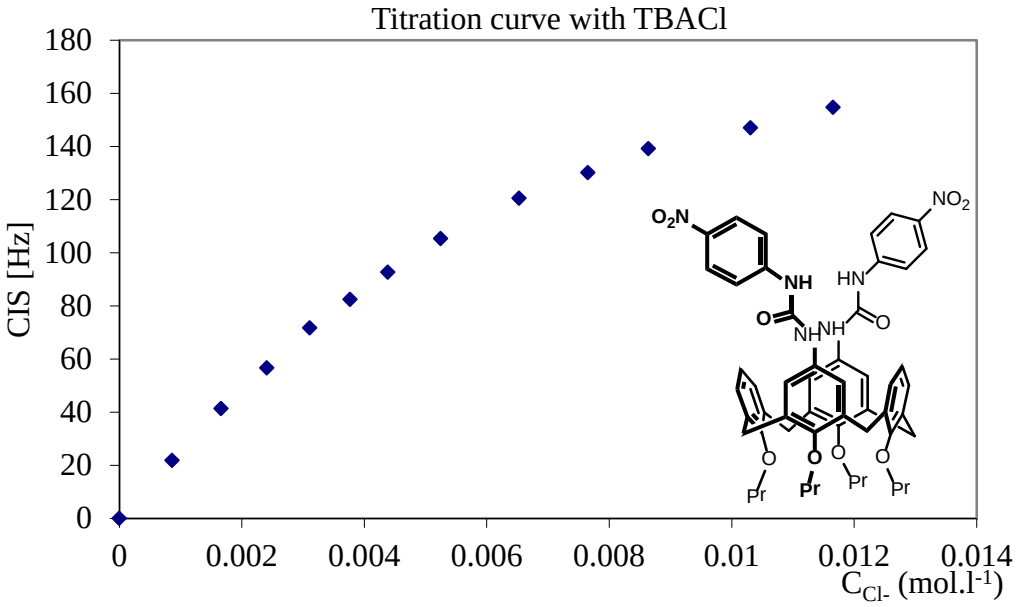




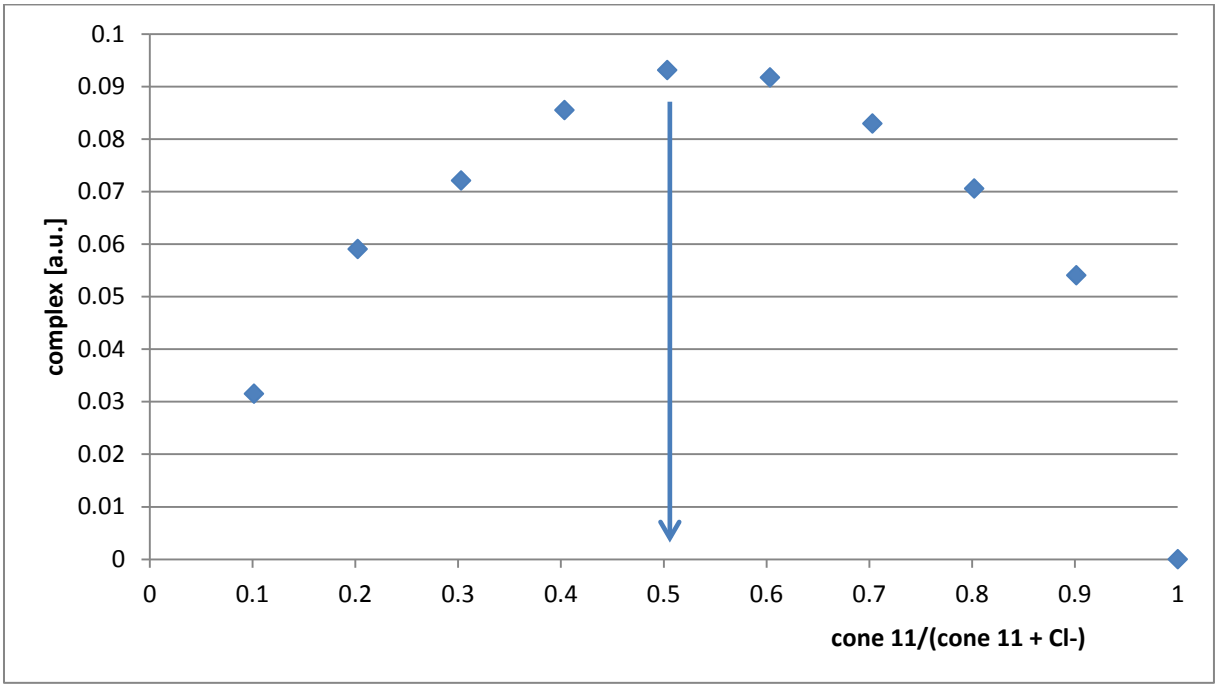




Titration of model compound: the *cone* analogue of receptor **11**.



$K_{Cl-} = 173 \pm 24\ M^{-1}$



Job plot for system *cone* **11**/Cl^- in DMSO-d_6 (1H NMR titration, 300 MHz, 298 K)