Supporting information

Effects on Rotational Dynamics of Azo and Hidrazodicarboxamide-based Rotaxanes

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1. Variable-Temperature NMR Experiments

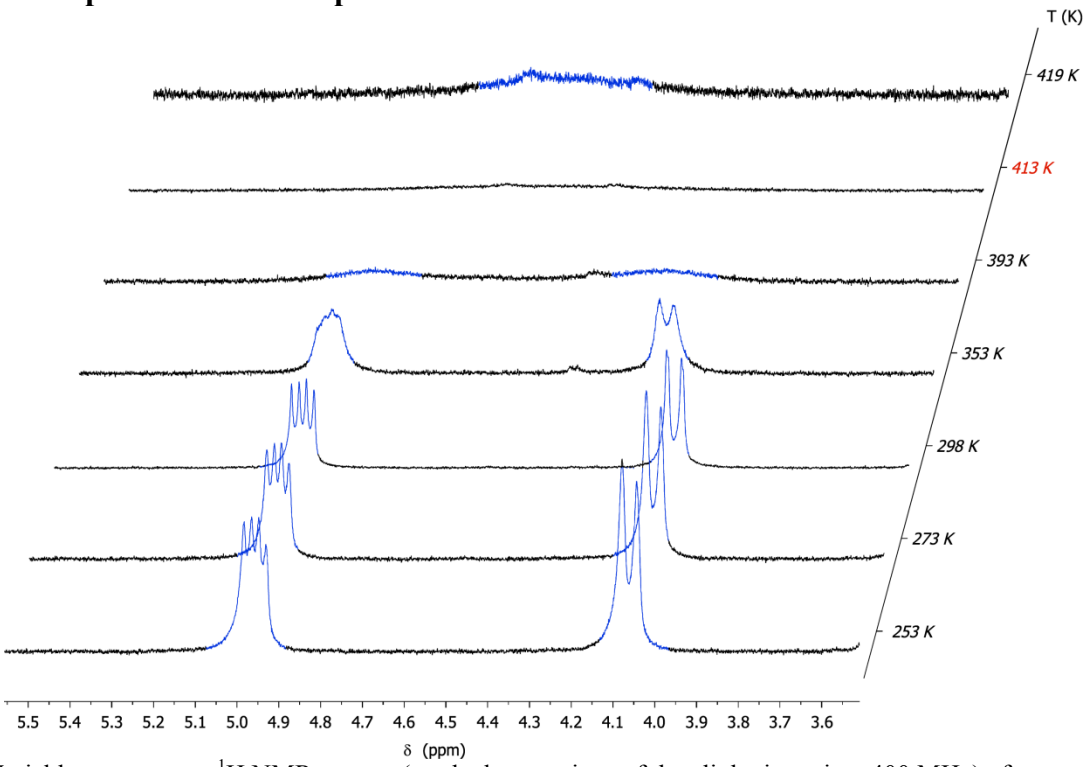


Figure S1. Variable temperature ^{1}H NMR spectra (stacked expansions of the aliphatic region, 400 MHz) of rotaxane **3**.

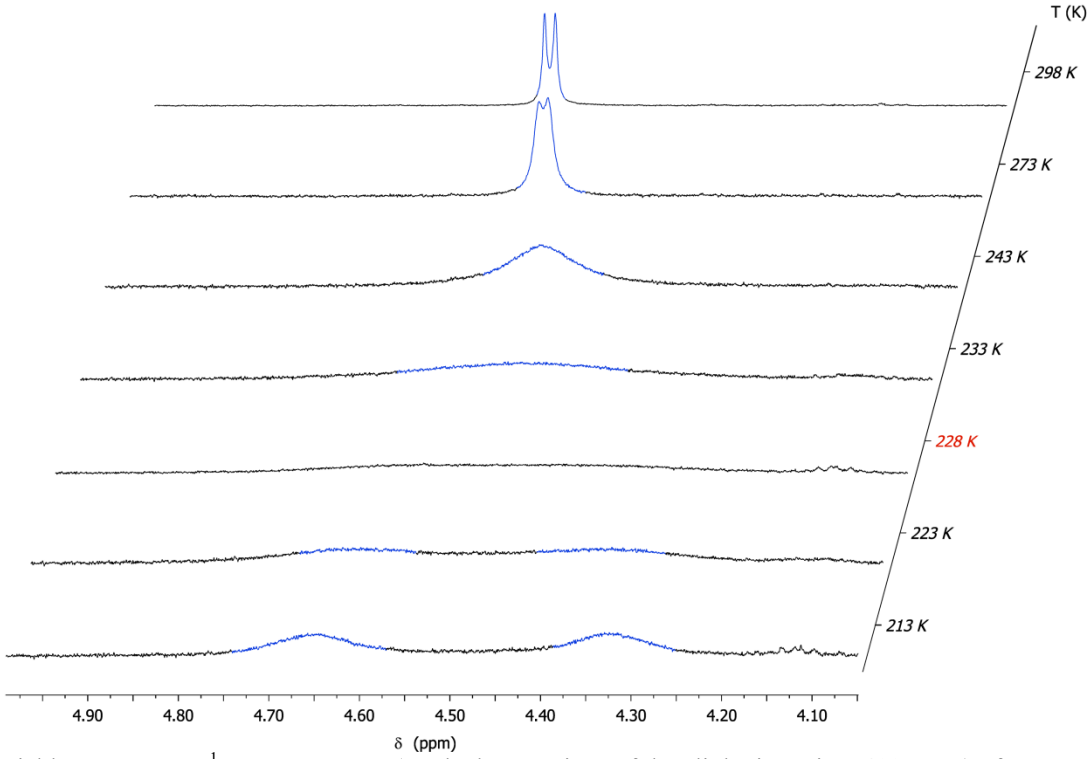


Figure S2. Variable temperature ^{1}H NMR spectra (stacked expansions of the aliphatic region, 400 MHz) of rotaxane [2H]-**3**.

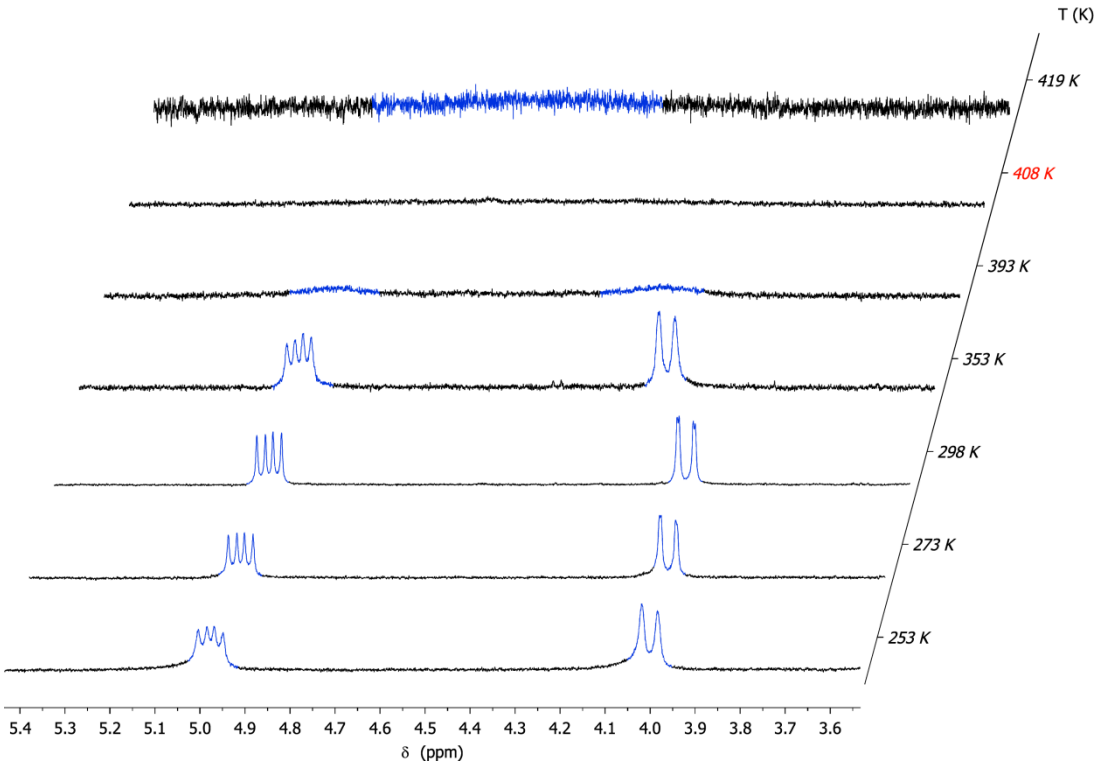


Figure S3. Variable temperature ^{1}H NMR spectra (stacked expansions of the aliphatic region, 400 MHz) of *N*-oxide-based rotaxane **4**.

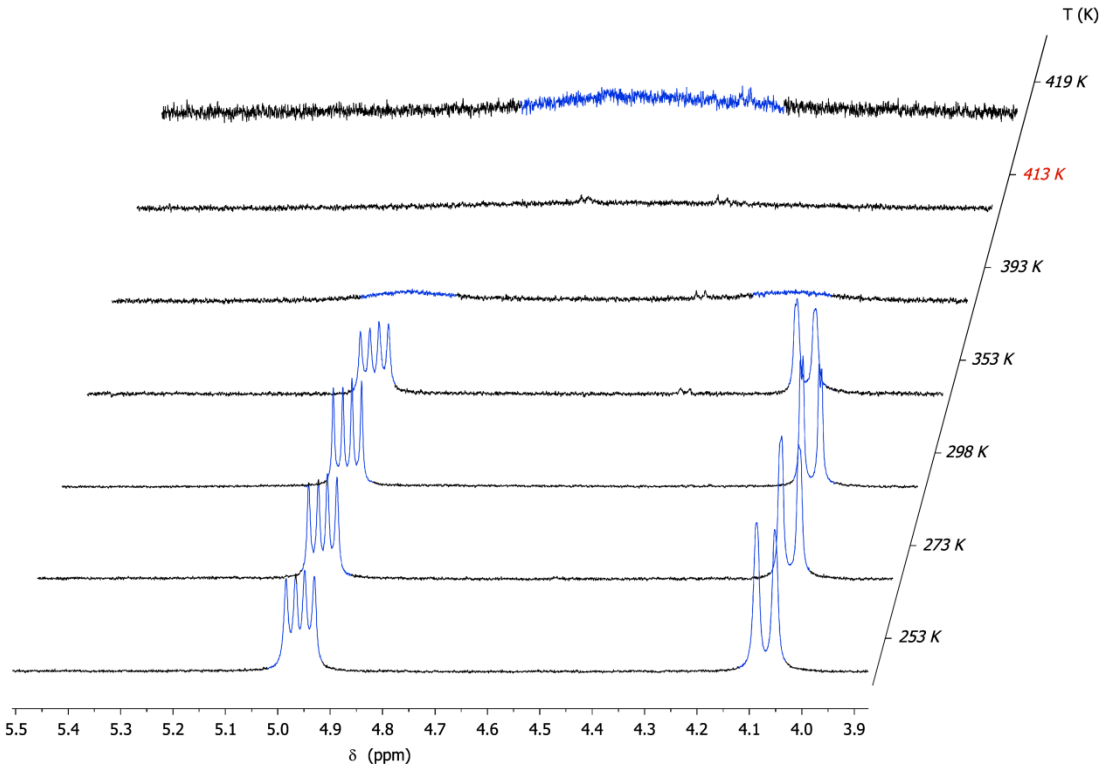
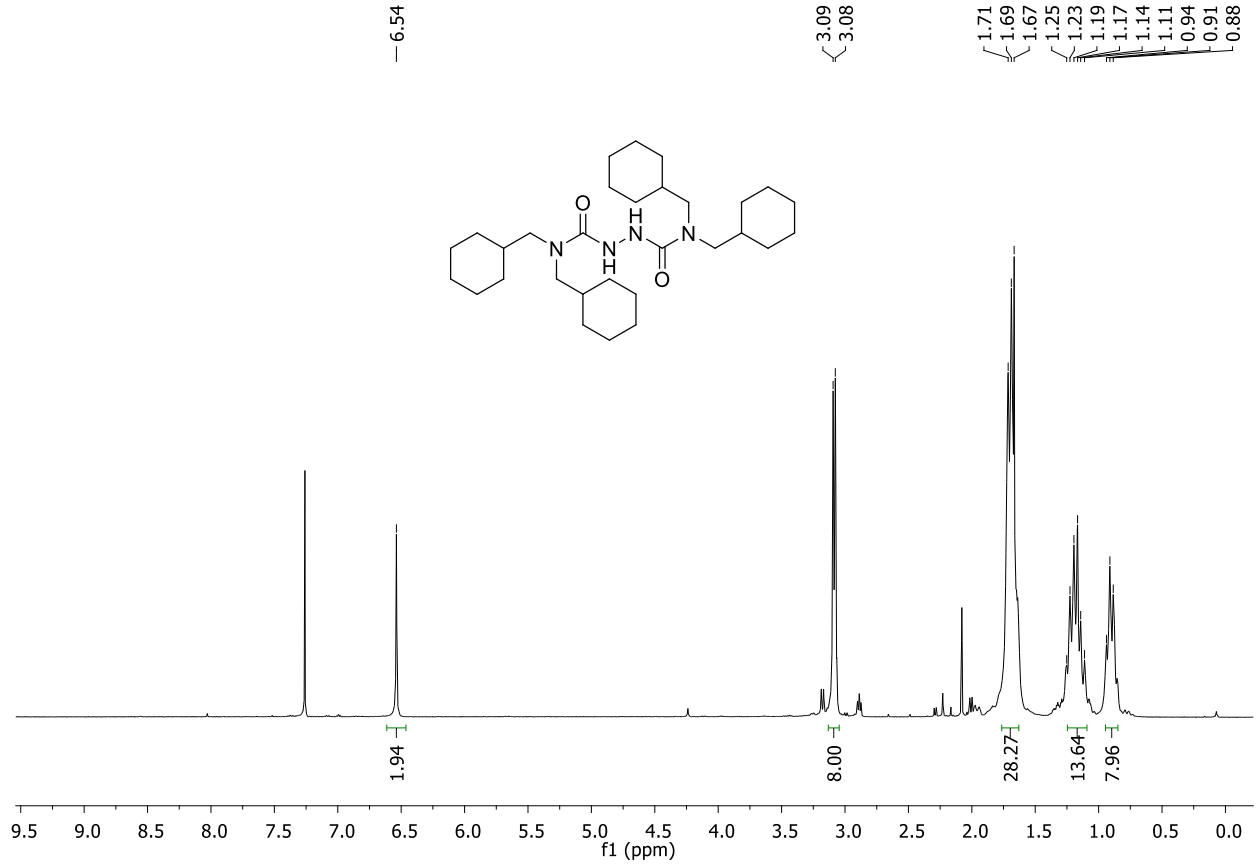


Figure S4. Variable temperature ^{1}H NMR spectra (stacked expansions of the aliphatic region, 400 MHz) of salt **5**.

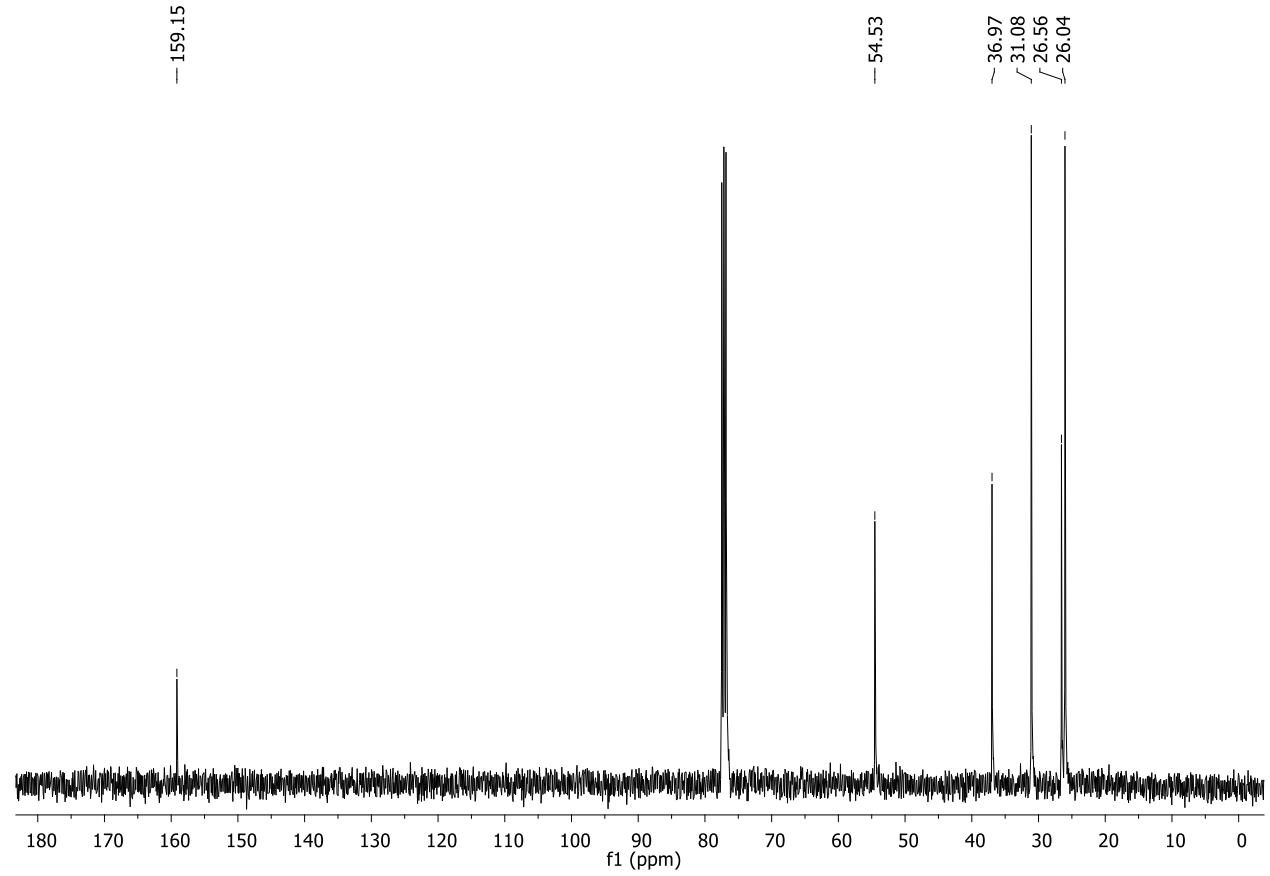
Free energies of activation were calculated using the Eyring equation, $\Delta G_c^{\neq} = -RT_c \cdot \ln(k_c h/k_b T_c)$, where $k_c = (\pi\Delta\upsilon)/\sqrt{2}$ or $kc = \pi\sqrt{(\Delta\upsilon^2 + 6J^2)}/\sqrt{2}$ and *R*, *h* and *kb* are the gas, Planck and Boltzmann constants, respectively.

2. ^{1}H and ^{13}C NMR Spectra of synthesized compounds

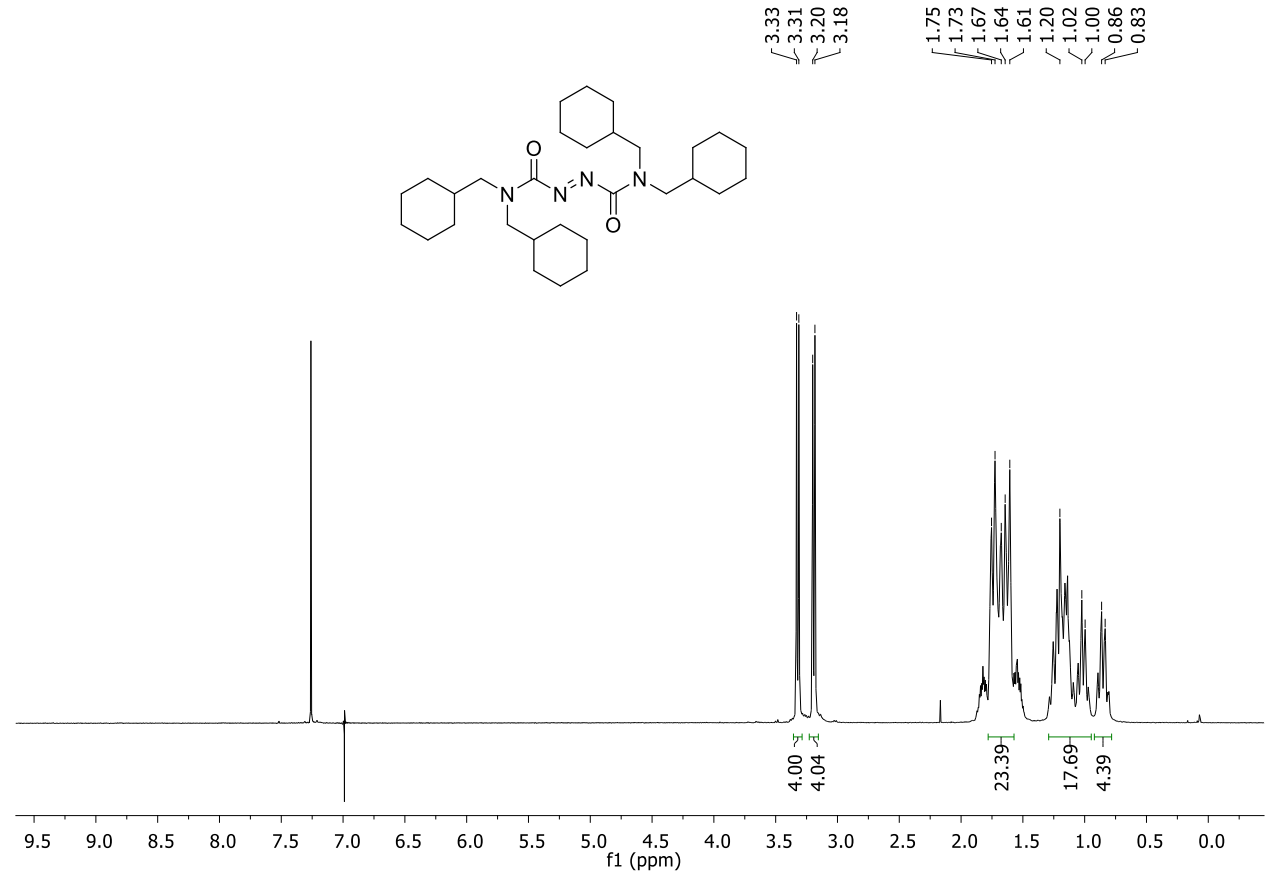
[2H]-**2** (^{1}H NMR, 400 MHz, $CDCl_3$, 298K)



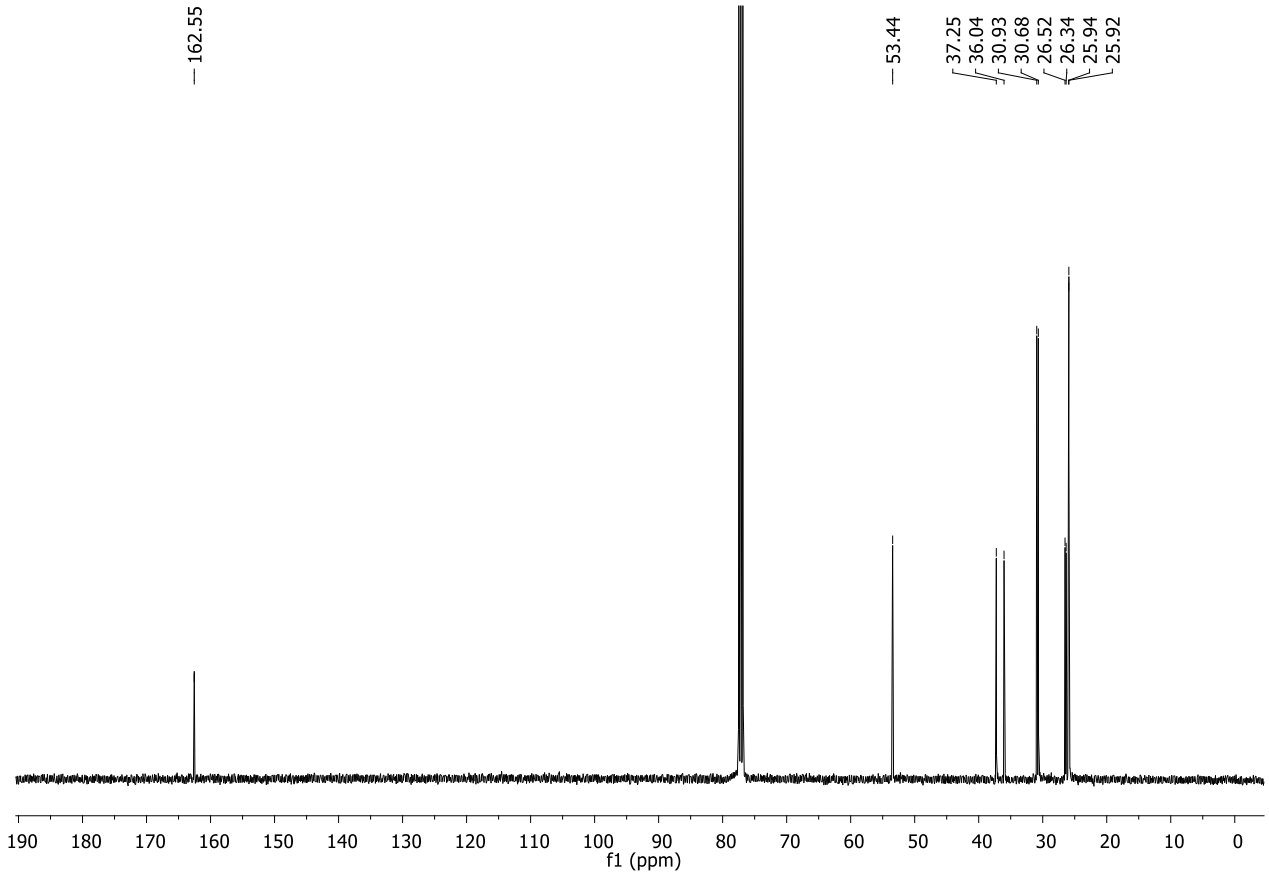
[2H]-**2** (^{13}C NMR, 100 MHz, $CDCl_3$, 298K)



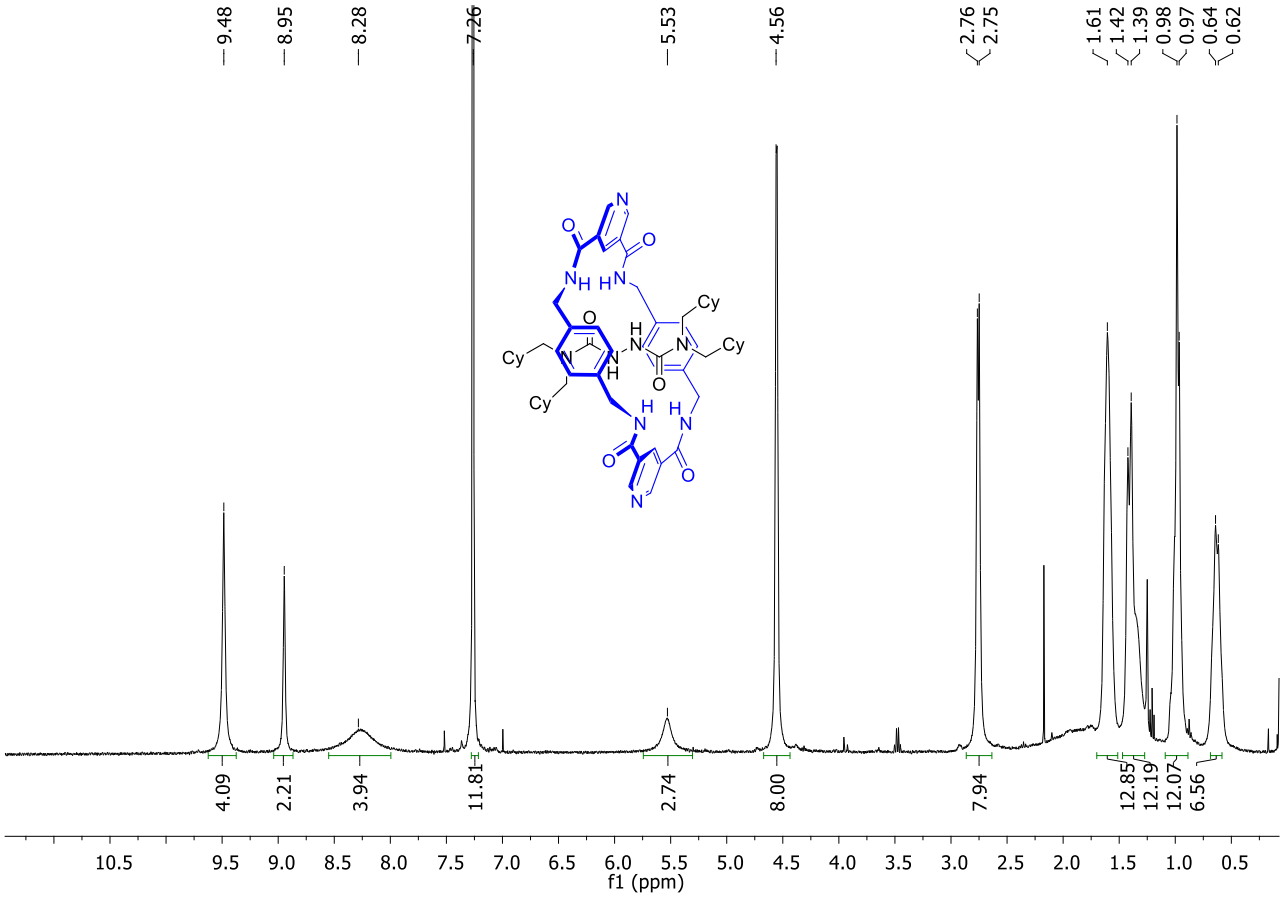
2 (^{1}H NMR, 400 MHz, $CDCl_3$, 298K)



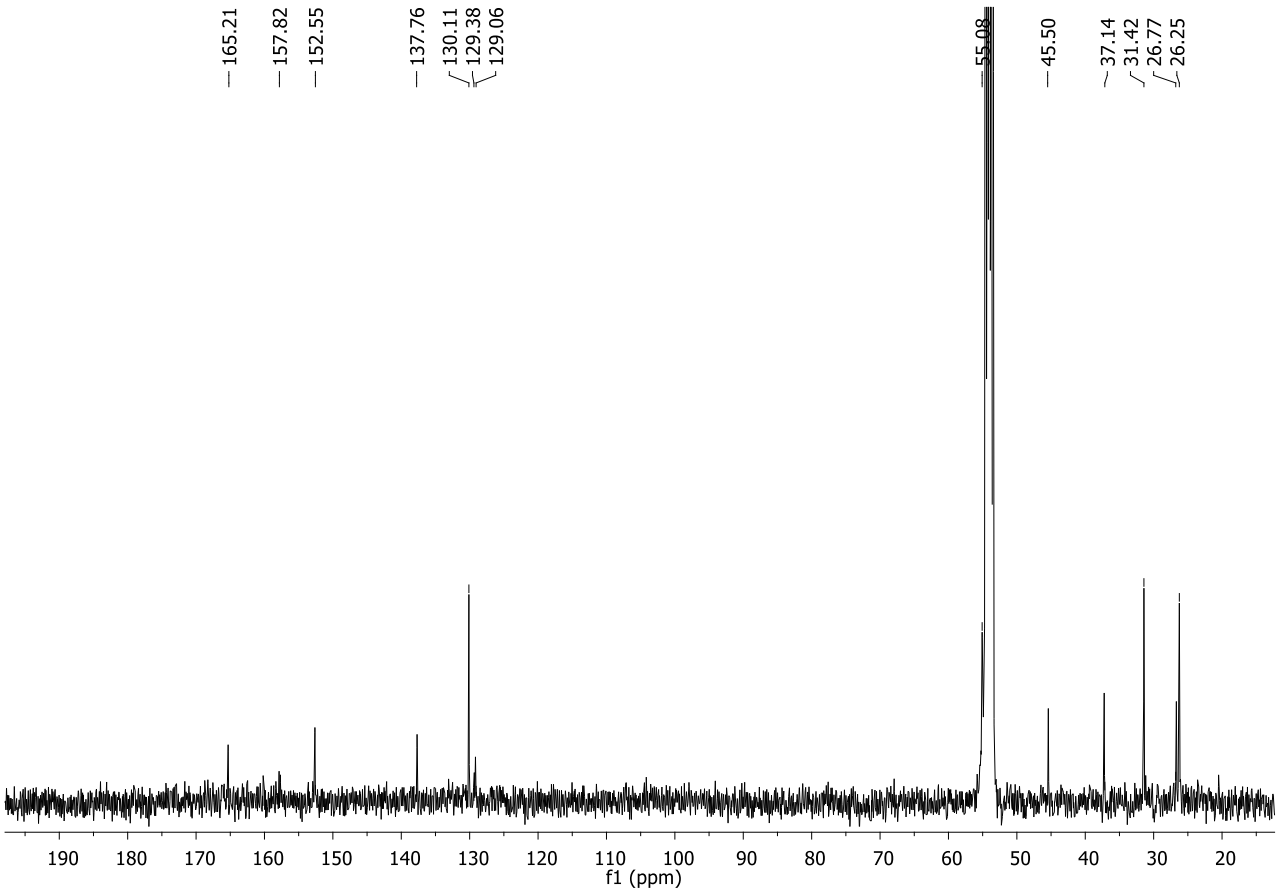
2 (^{13}C NMR, 100 MHz, $CDCl_3$, 298K)



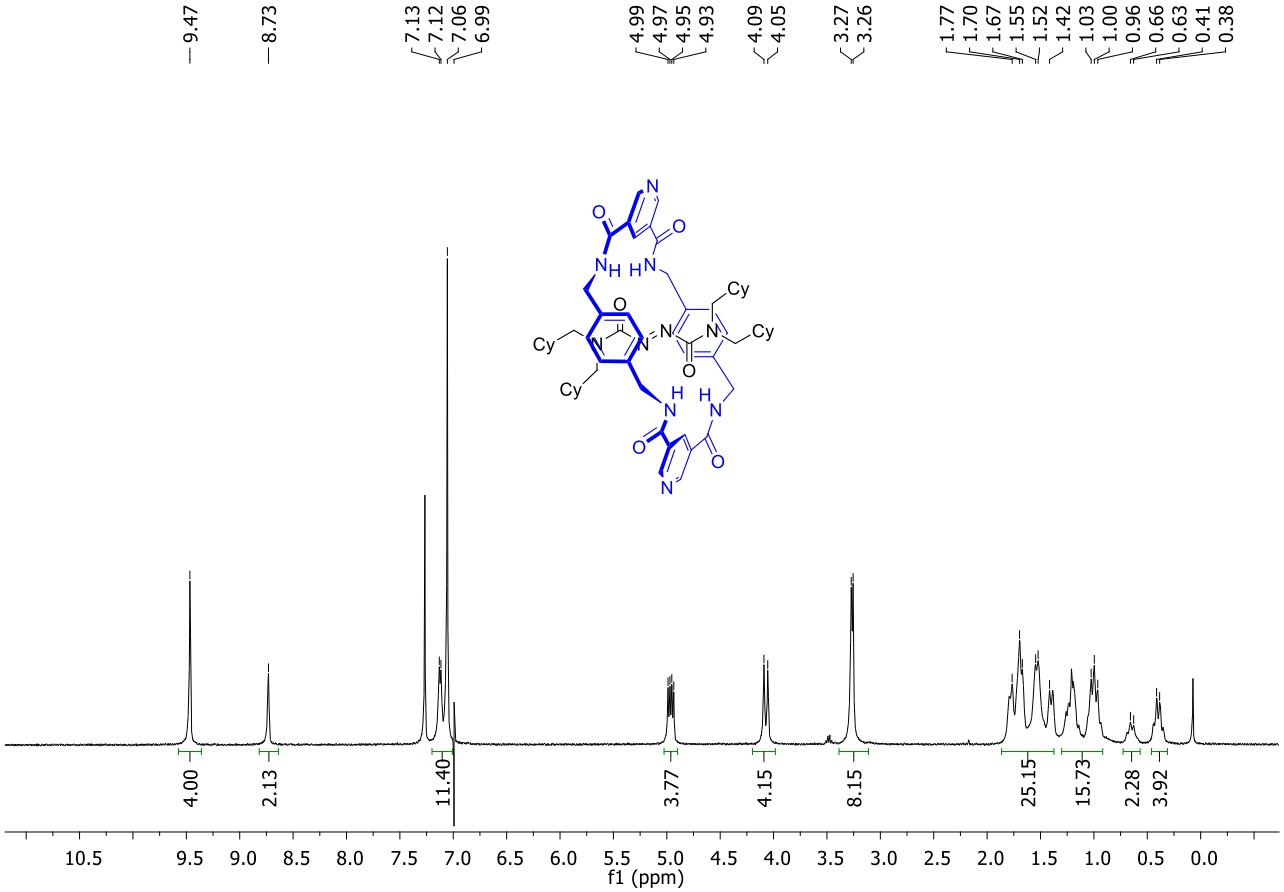
[2H]-**3** (^{1}H NMR, 400 MHz, $CDCl_3$, 298K)



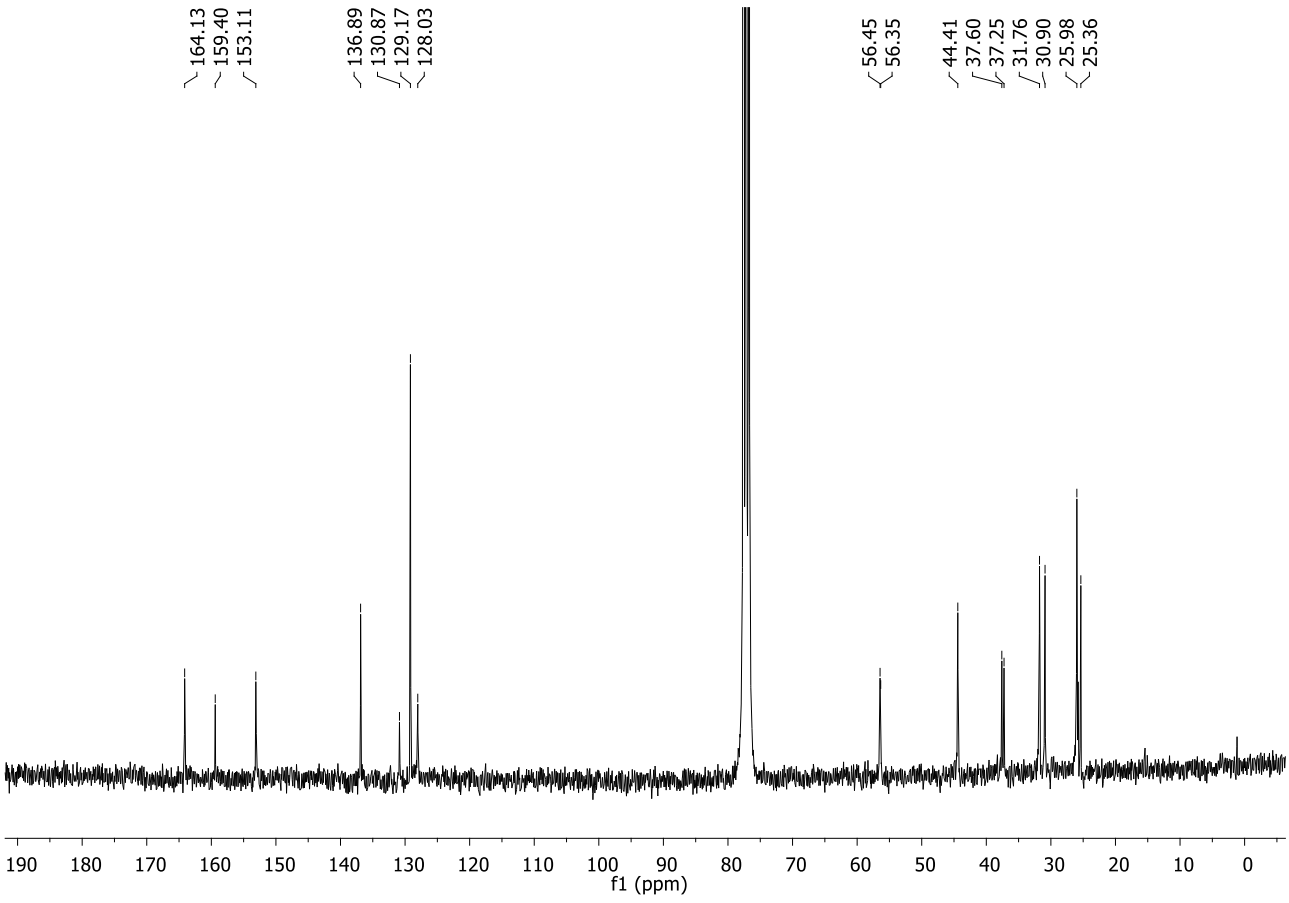
[2H]-**3** (^{13}C NMR, 100 MHz, CD_2Cl_2, 298K)



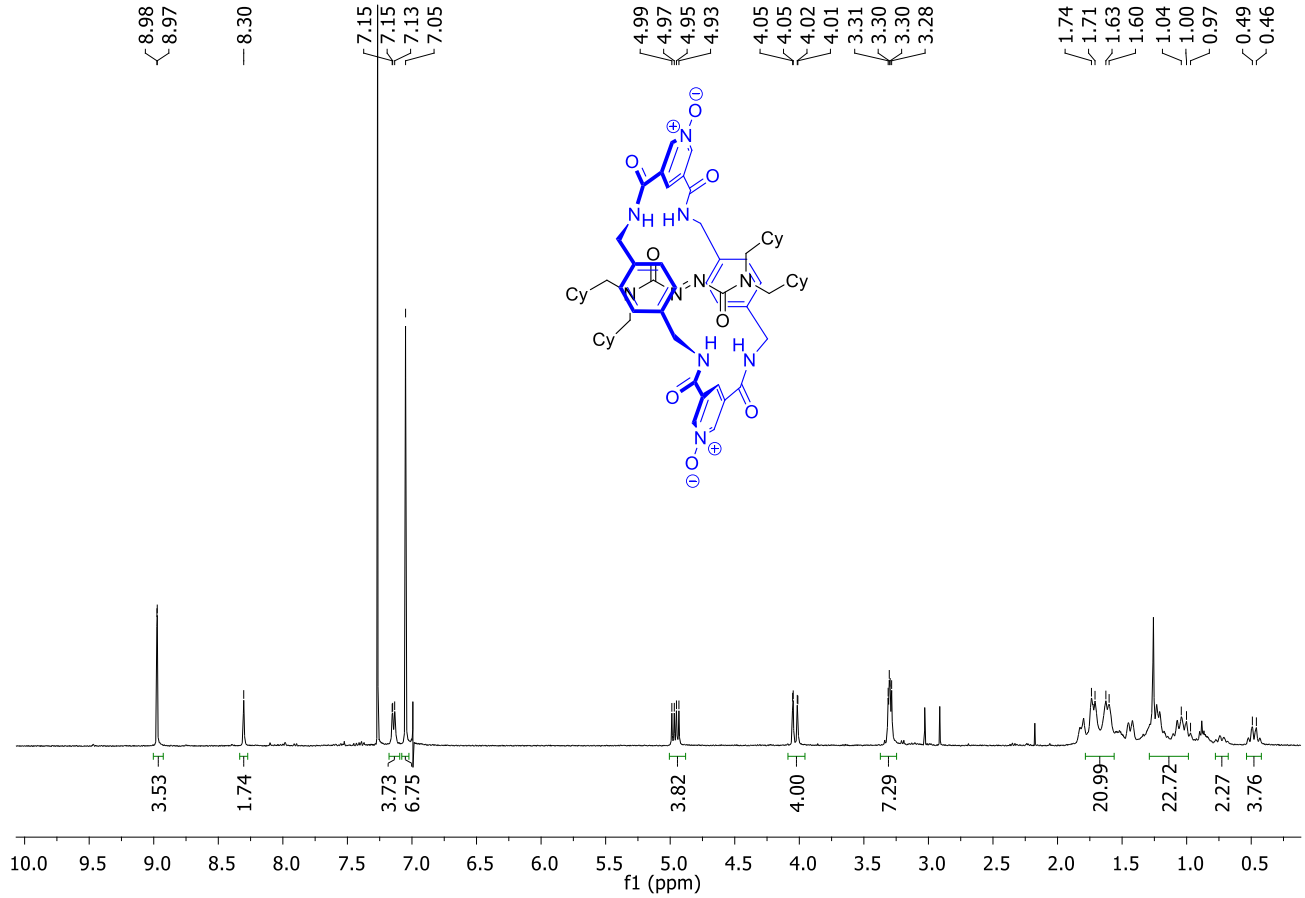
3 (^{1}H NMR, 400 MHz, $CDCl_3$, 298K)



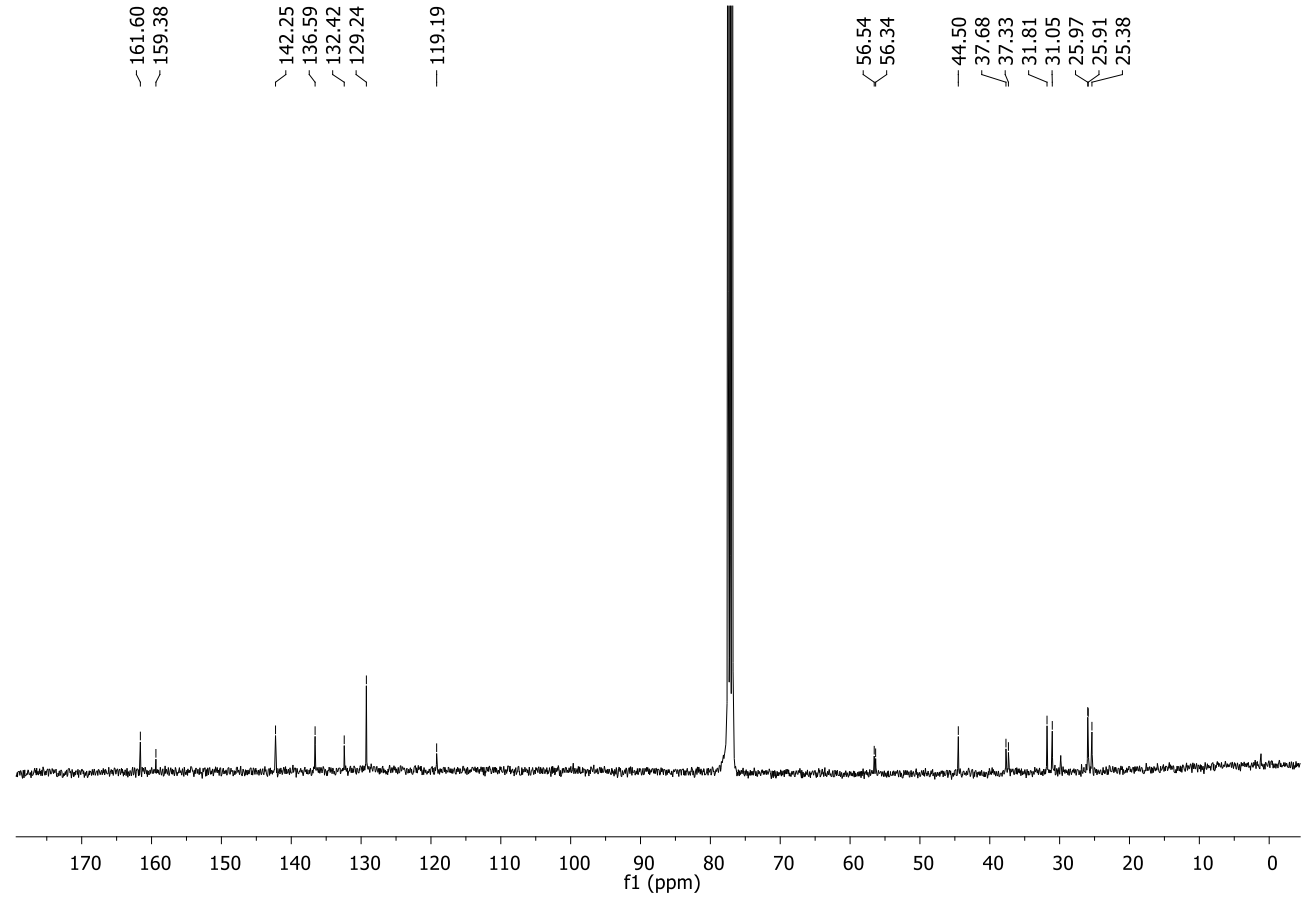
3 (^{13}C NMR, 75 MHz, $CDCl_3$, 298K)



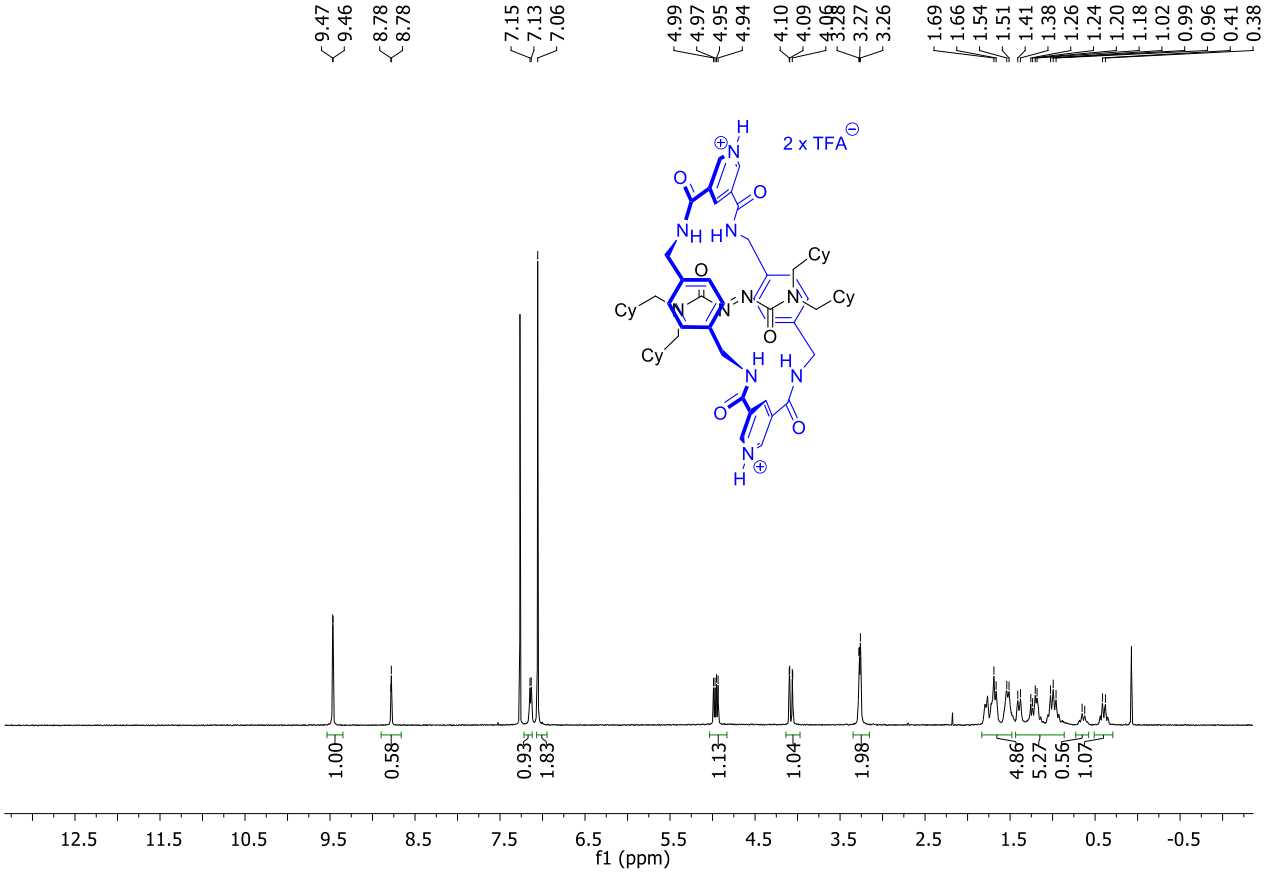
4 (^{1}H NMR, 400 MHz, $CDCl_3$, 298K)



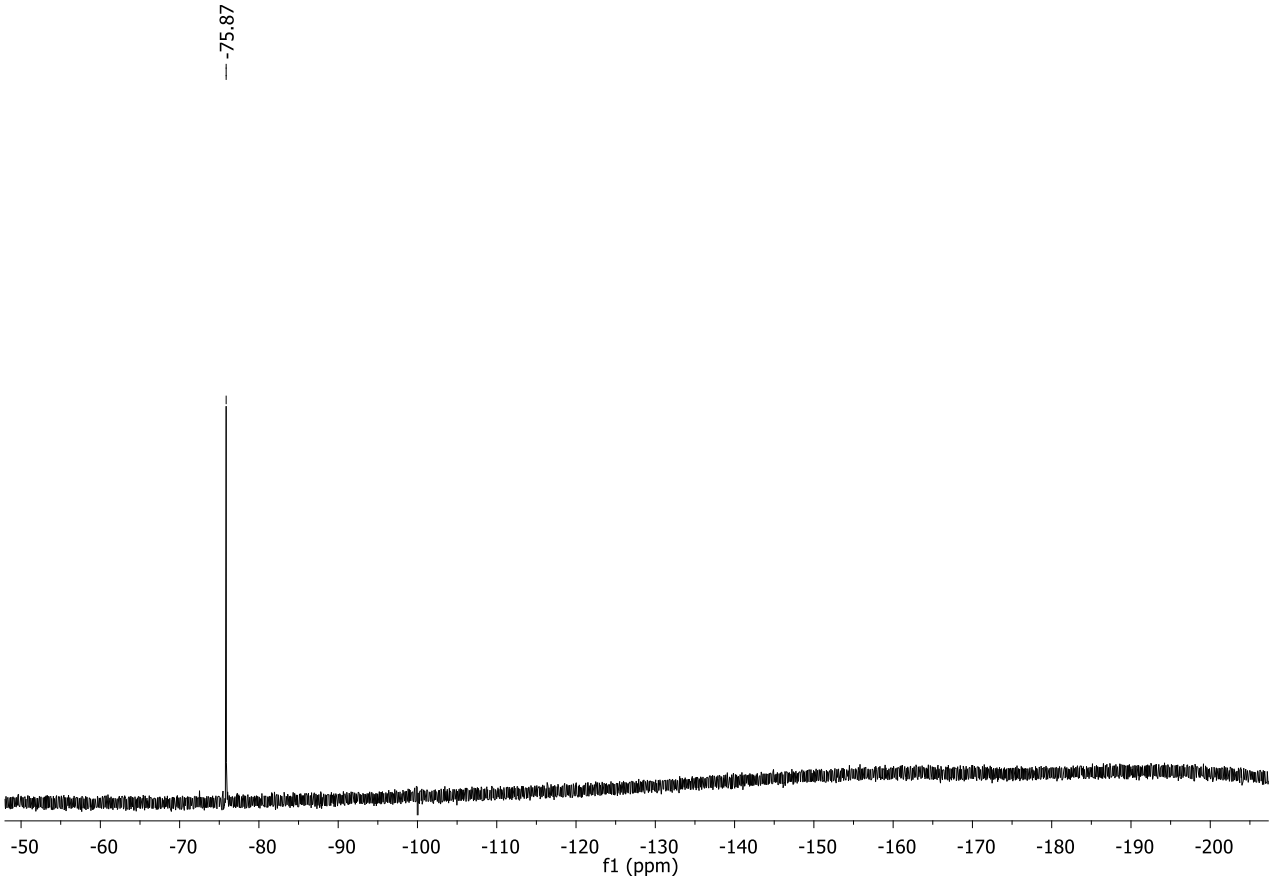
4 (^{13}C NMR, 100 MHz, $CDCl_3$, 298K)



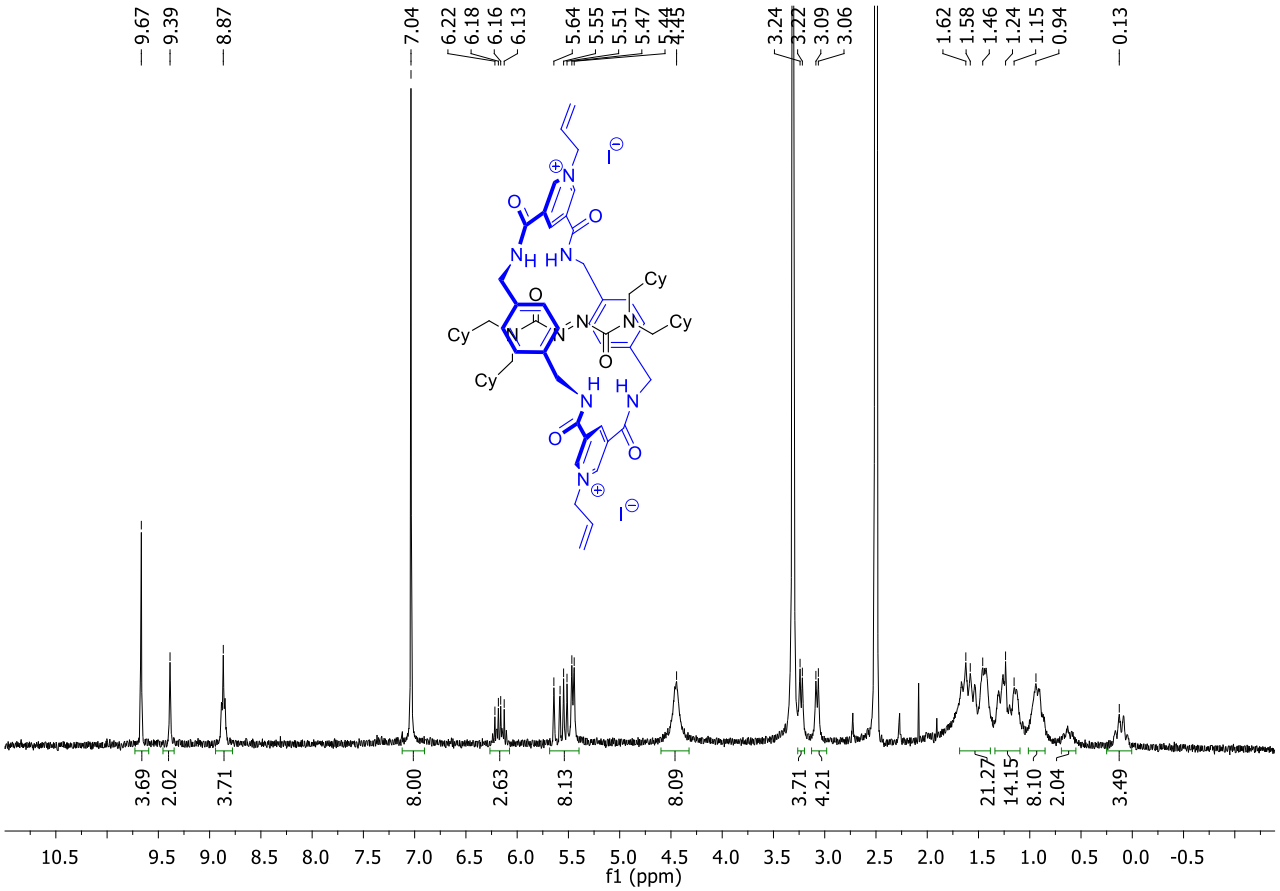
5 (^{1}H NMR, 400 MHz, $CDCl_3$, 298K)



5 (^{19}F NMR, 282 MHz, CHCl3, 298K)



6 (^{1}H NMR, 300 MHz, DMSO-*d6*, 298K)



6 (^{13}C NMR, 75 MHz, DMSO-*d6*, 298K)