

Supporting Information

to the article

Nitro-derivatives of Benzoazacrown Ethers: Synthesis, Structure, and Complexation with Metal and Ammonium Cations and Fluoride Anion

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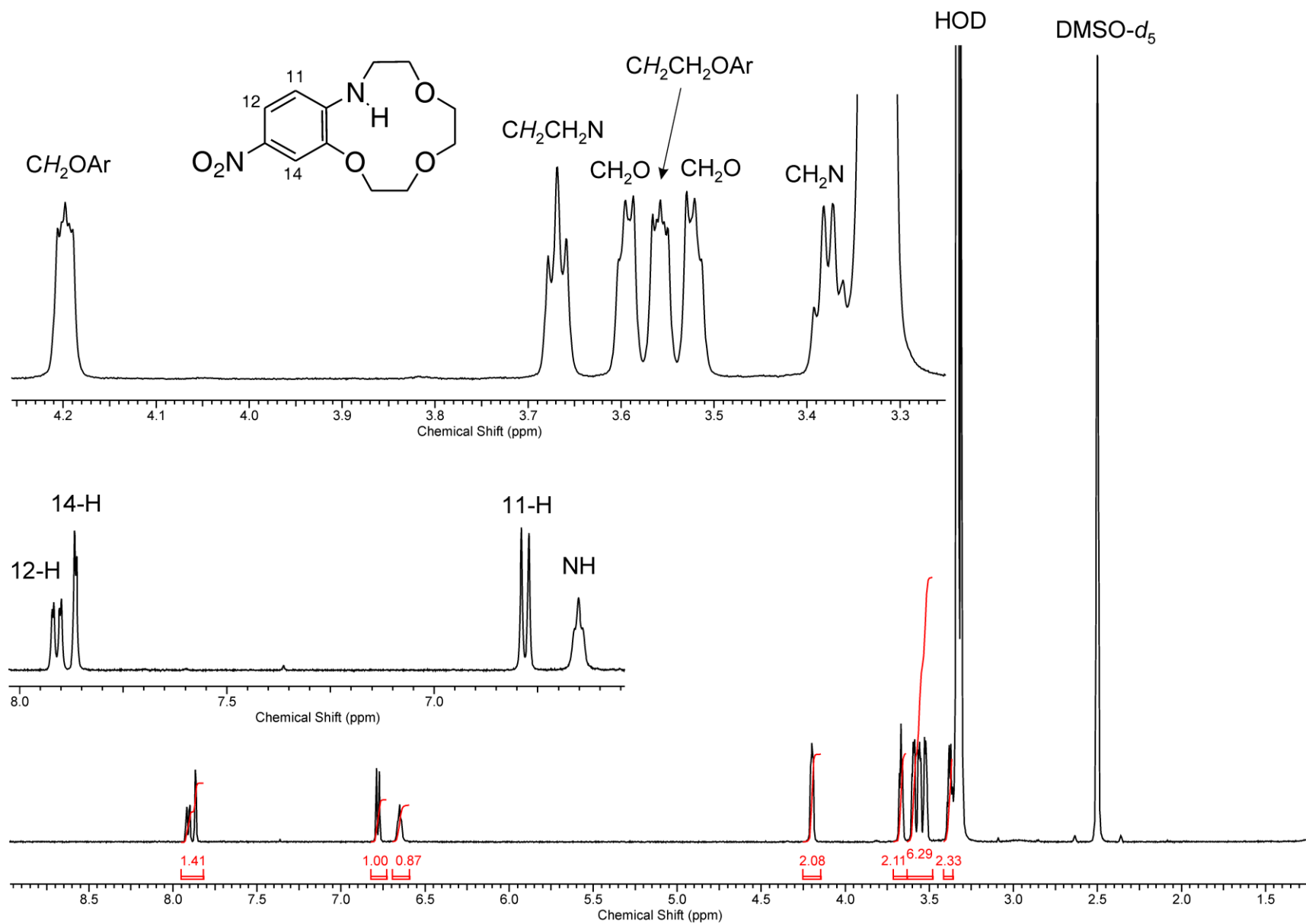


Figure S1. ^1H NMR spectrum of compound **1a** (500.13 MHz, $\text{DMSO-}d_6$, 25 $^\circ\text{C}$).

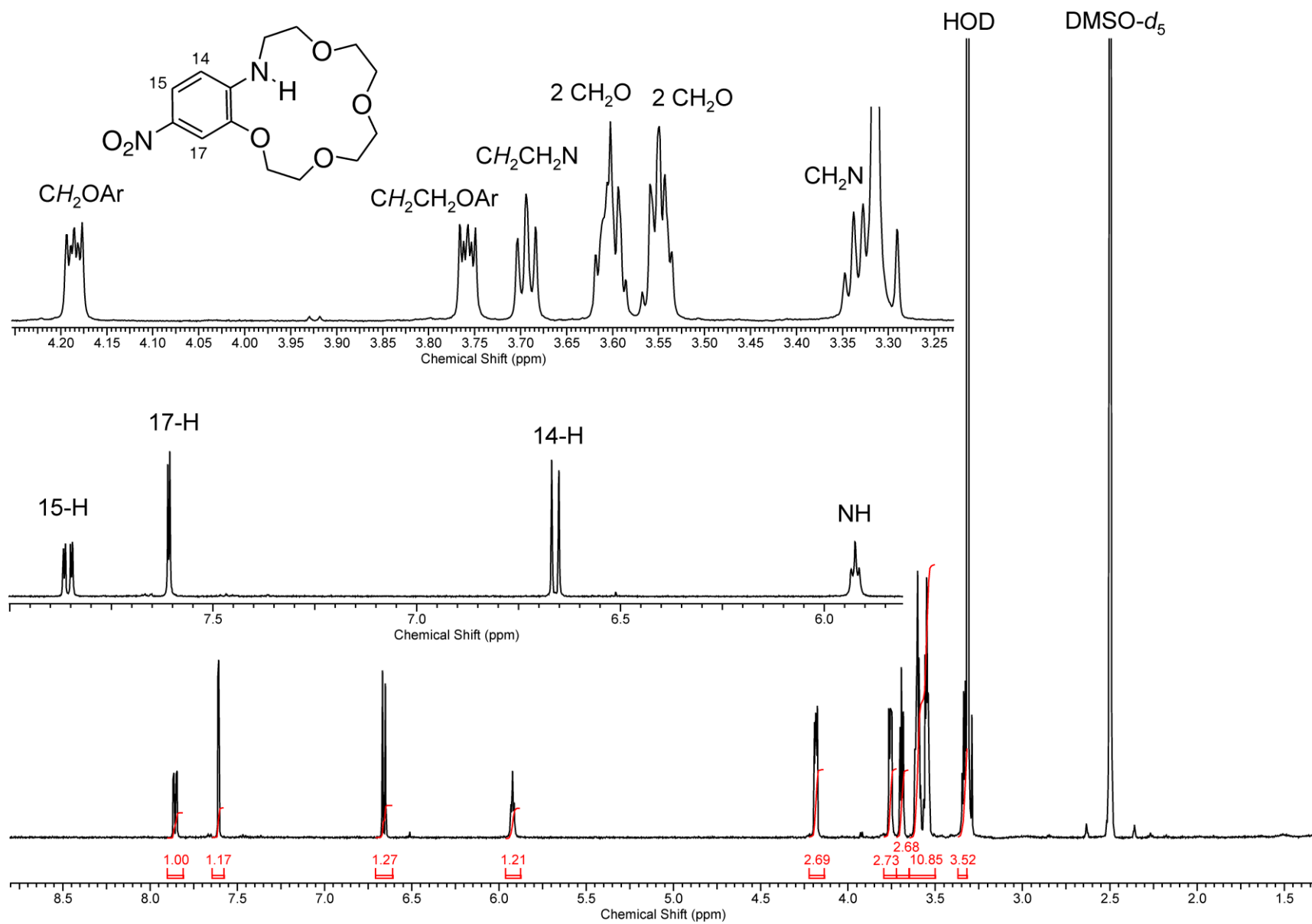


Figure S2. ^1H NMR spectrum of compound **1b** (500.13 MHz, $\text{DMSO-}d_6$, $25\text{ }^\circ\text{C}$).

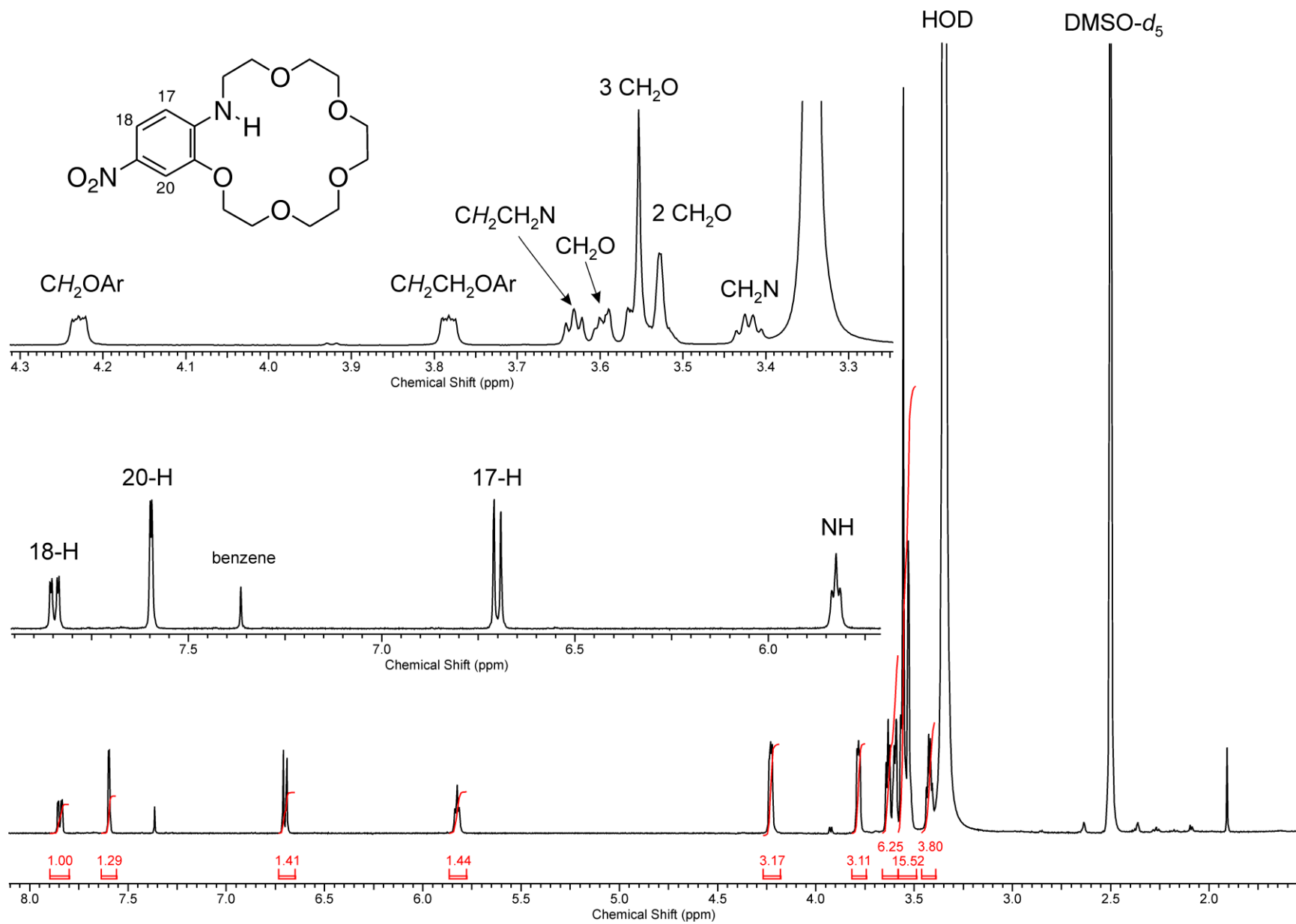


Figure S3. ^1H NMR spectrum of compound **1c** (500.13 MHz, $\text{DMSO}-d_6$, 25 °C).

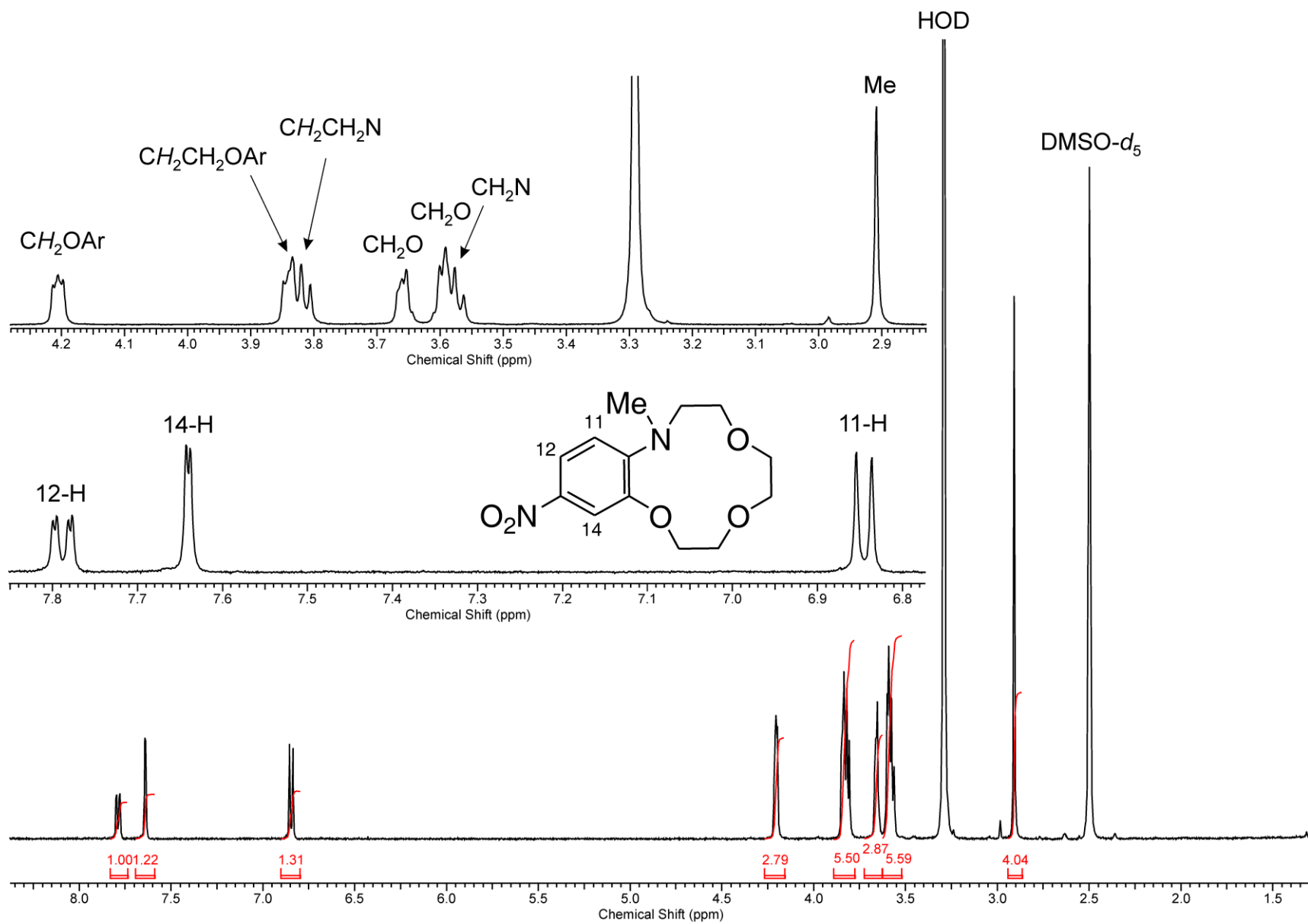


Figure S4. ^1H NMR spectrum of compound **2a** (500.13 MHz, $\text{DMSO-}d_6$, 25 $^\circ\text{C}$).

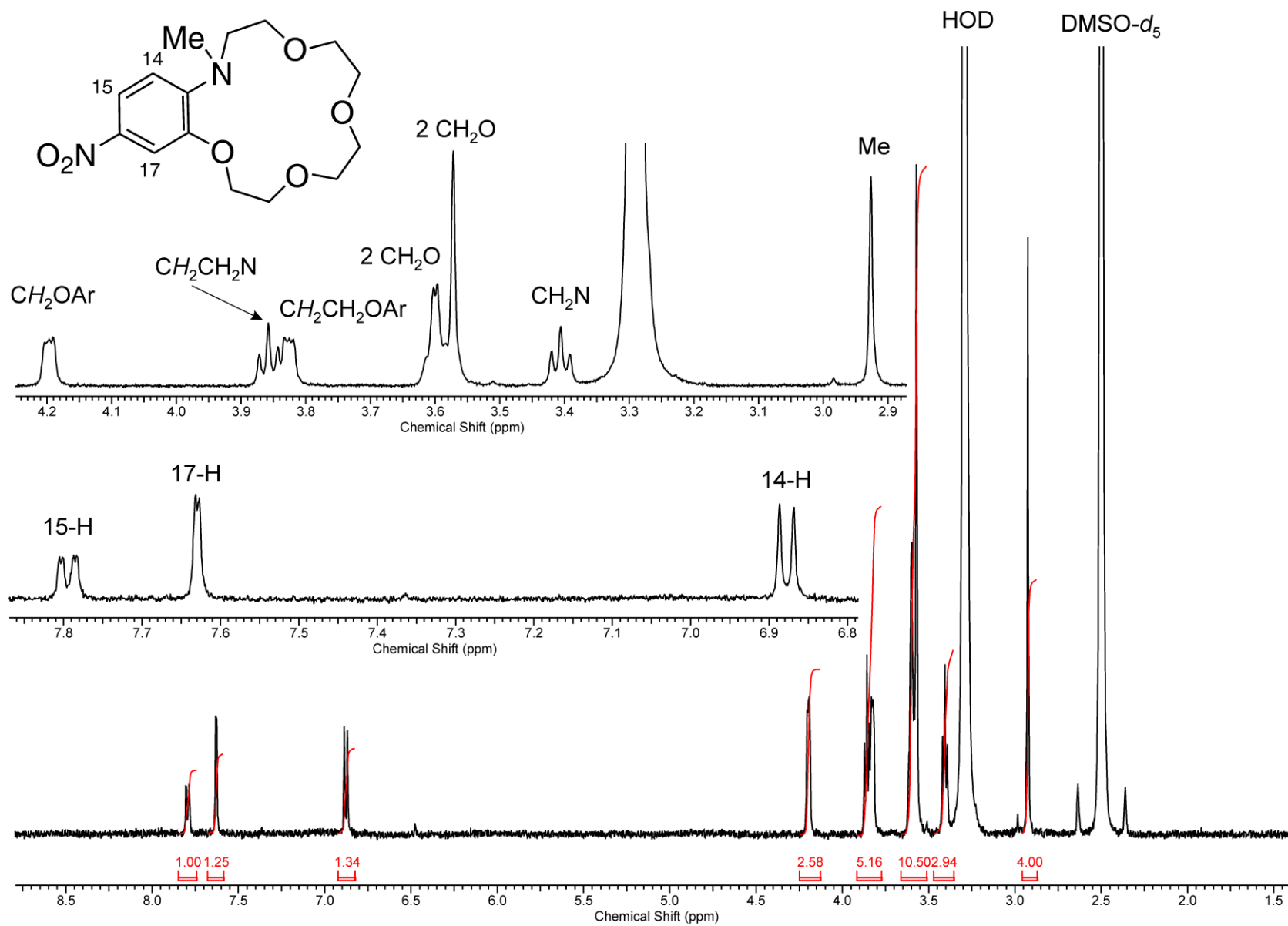


Figure S5. ^1H NMR spectrum of compound **2b** (500.13 MHz, $\text{DMSO-}d_6$, 25 °C).

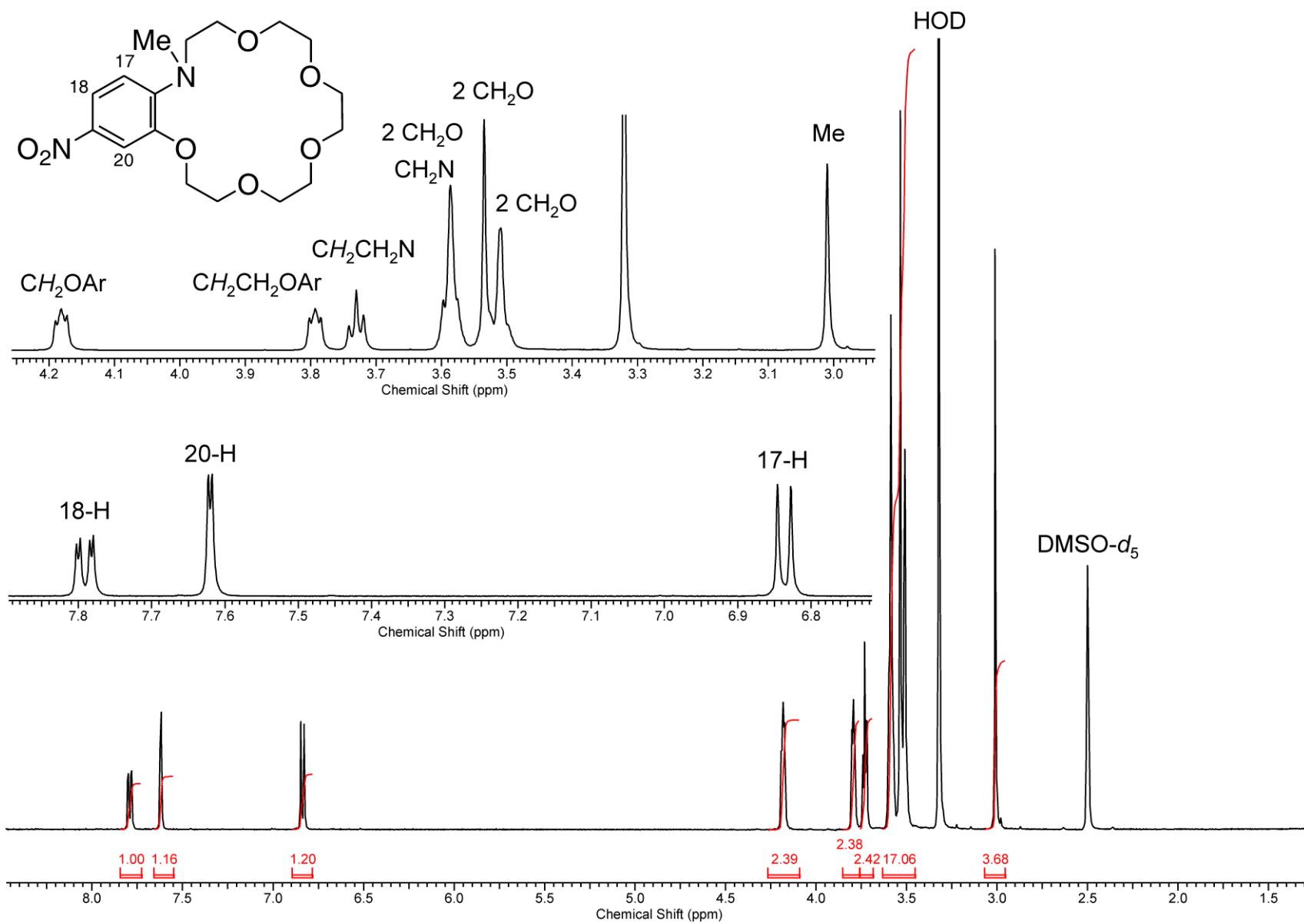


Figure S6. ¹H NMR spectrum of compound **2c** (500.13 MHz, DMSO-*d*₆, 25 °C).

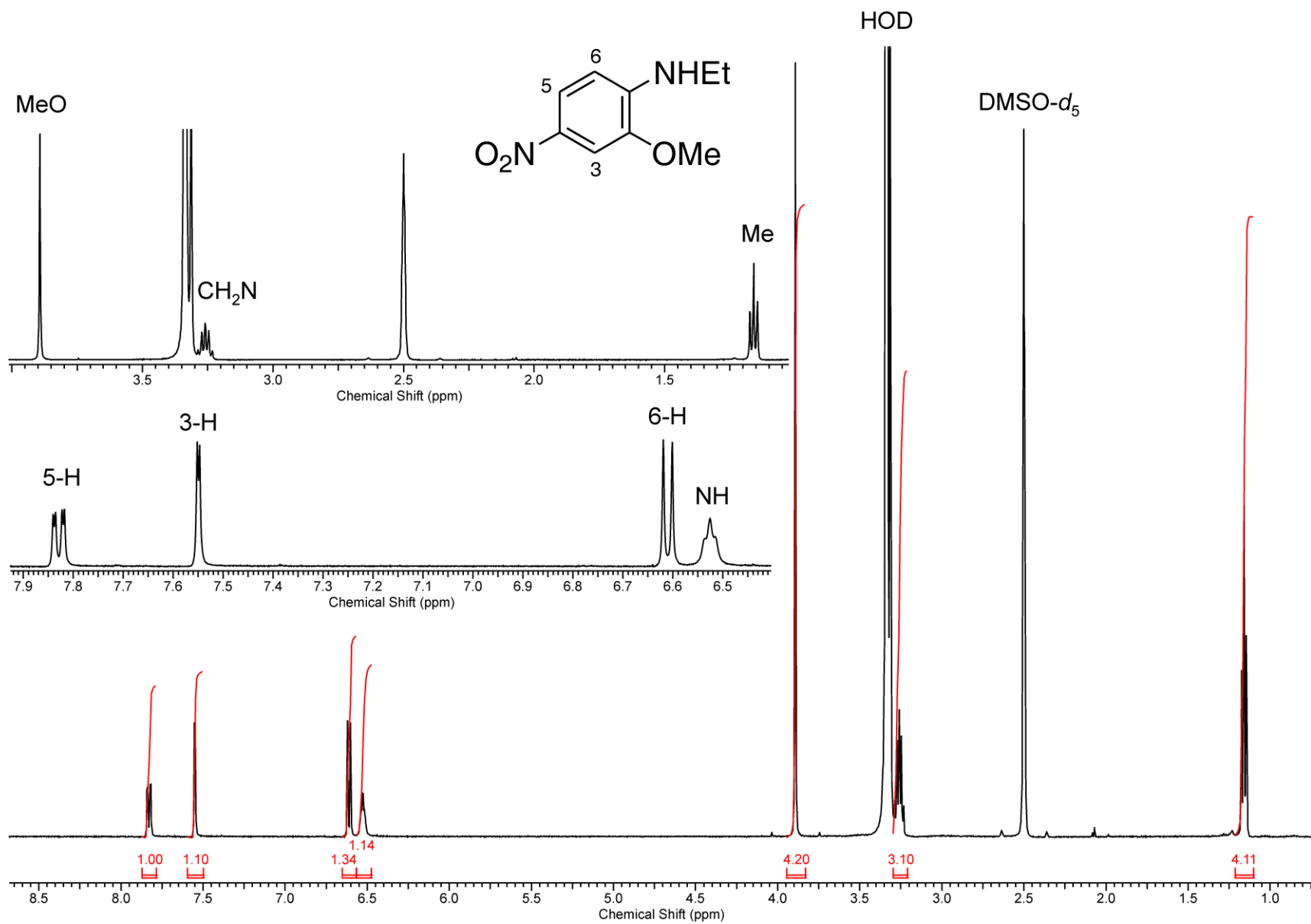


Figure S7. ^1H NMR spectrum of compound **5** (500.13 MHz, $\text{DMSO-}d_6$, $25\text{ }^\circ\text{C}$).

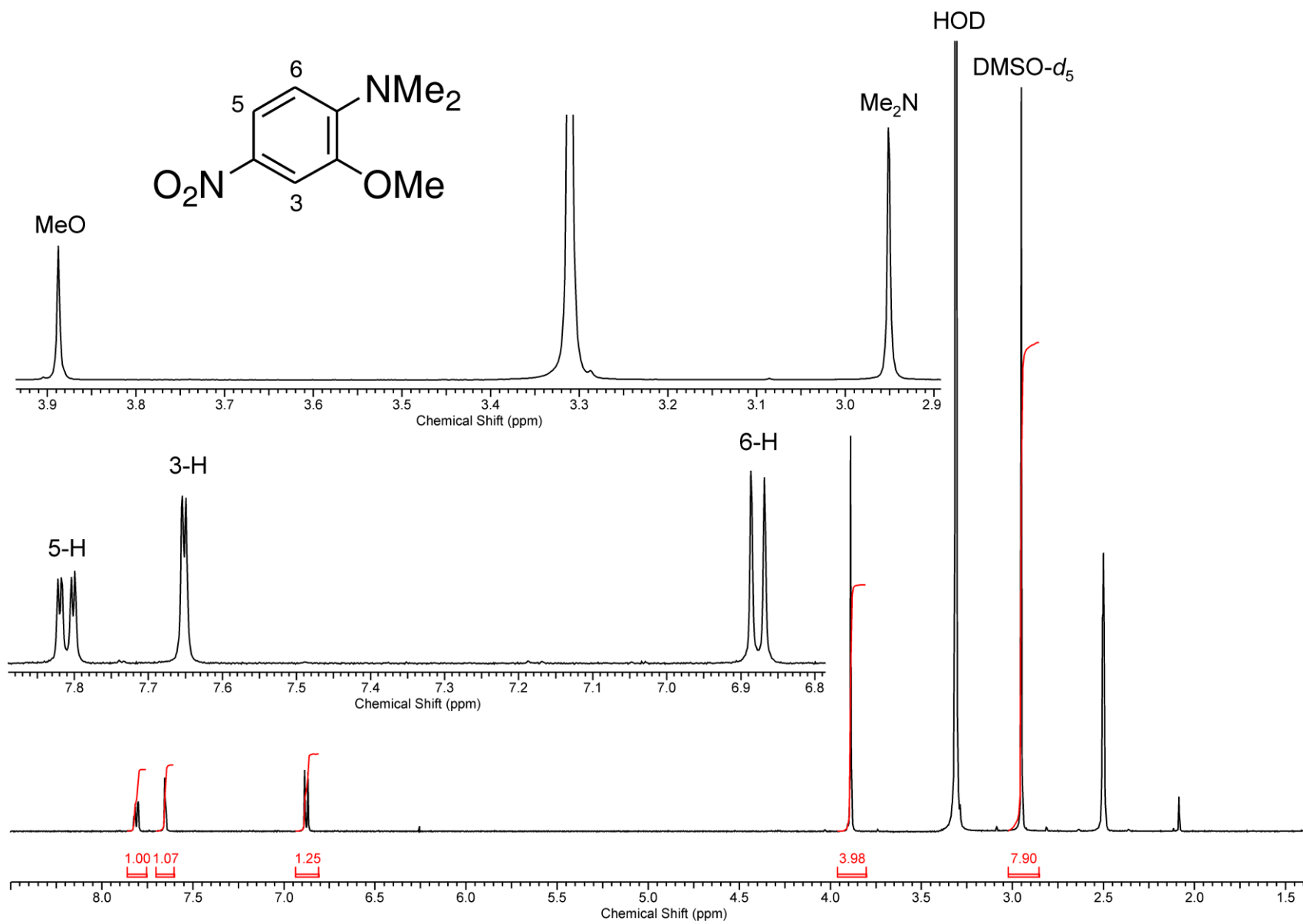


Figure S8. ^1H NMR spectrum of compound **7** (500.13 MHz, $\text{DMSO-}d_6$, 25 $^\circ\text{C}$).

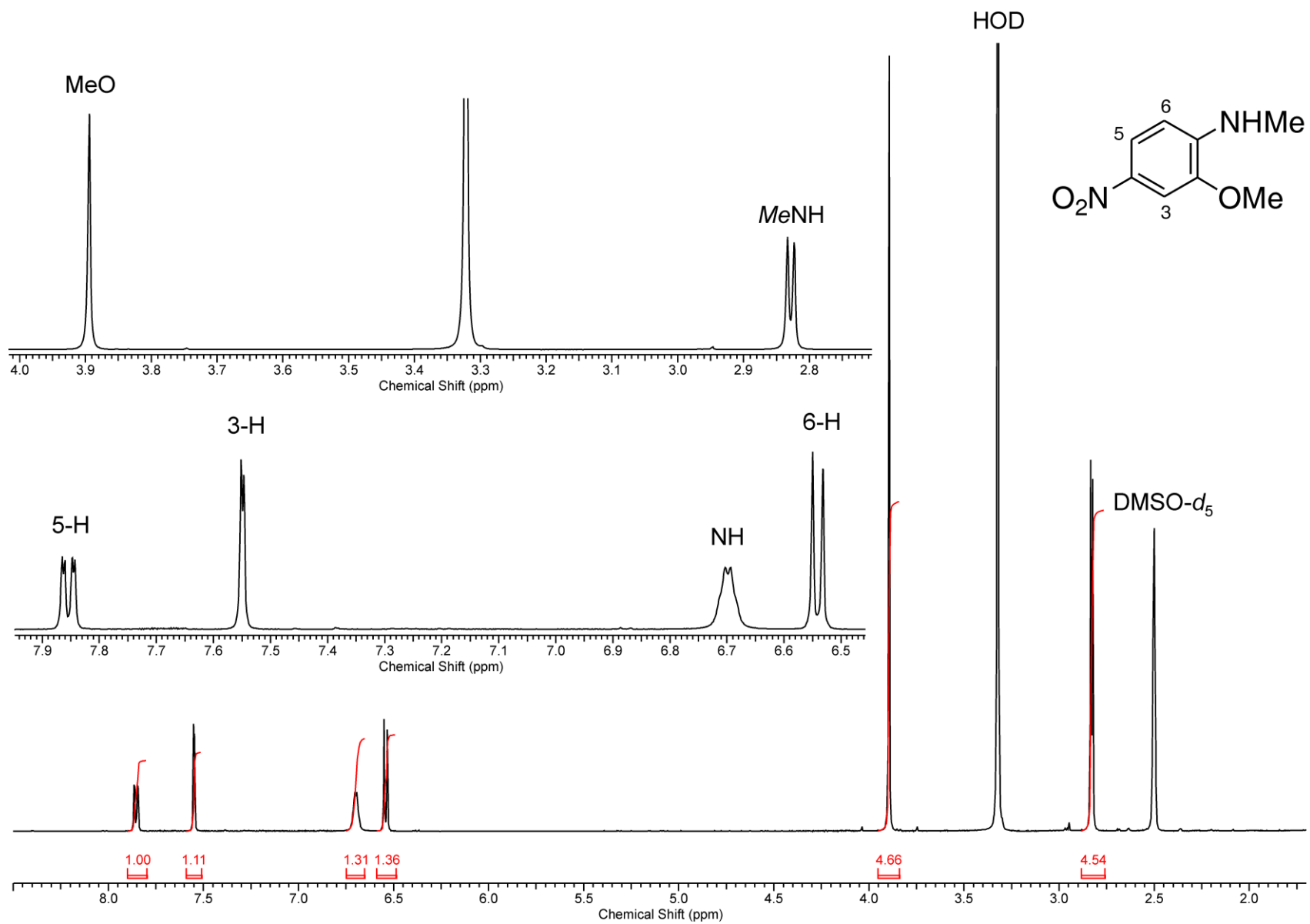


Figure S9. ^1H NMR spectrum of compound **8** (500.13 MHz, $\text{DMSO}-d_6$, 25 $^\circ\text{C}$).

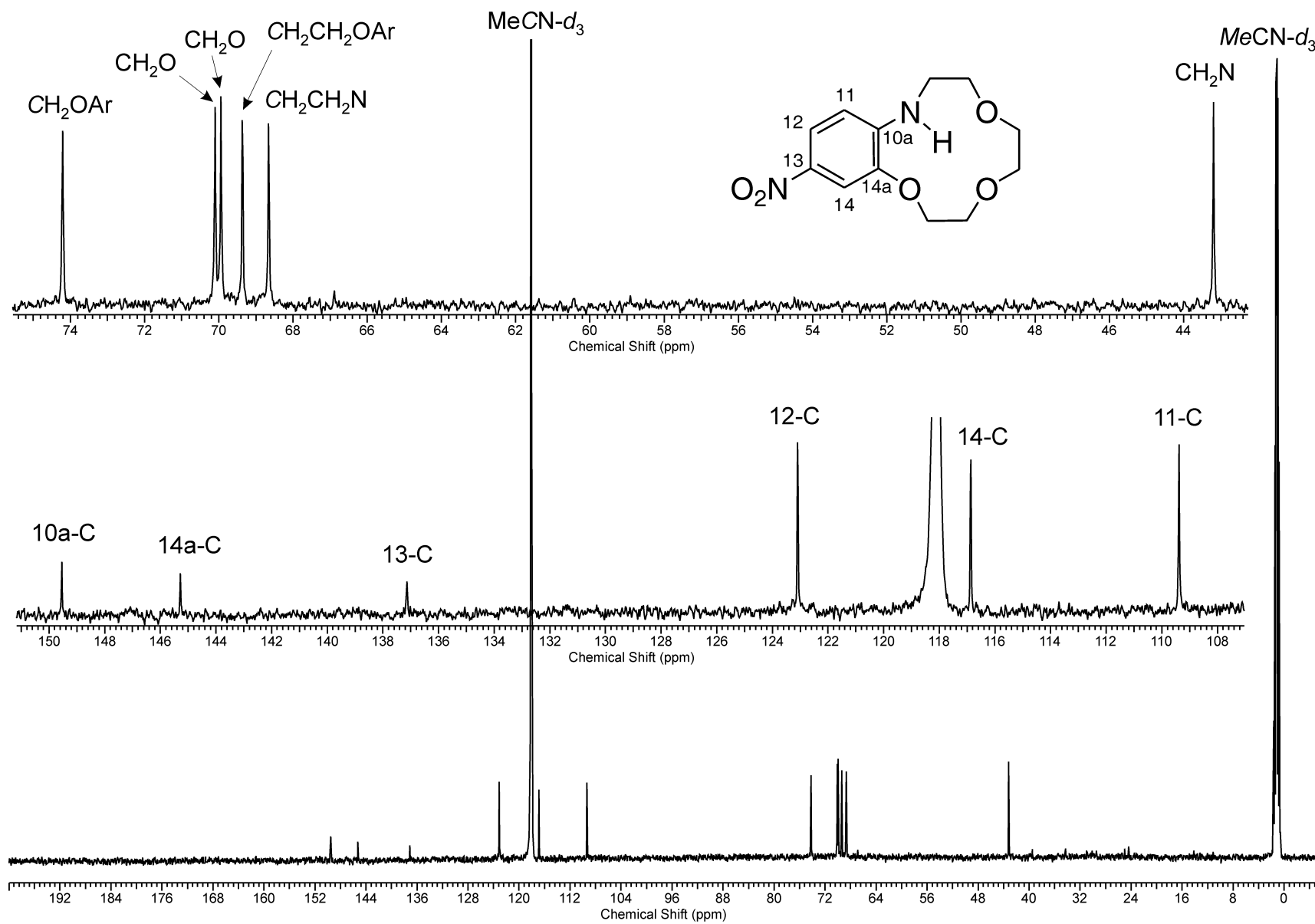


Figure S10. ^{13}C NMR spectrum of compound **1a** (125.76 MHz, $\text{MeCN-}d_3$, 25 $^\circ\text{C}$).

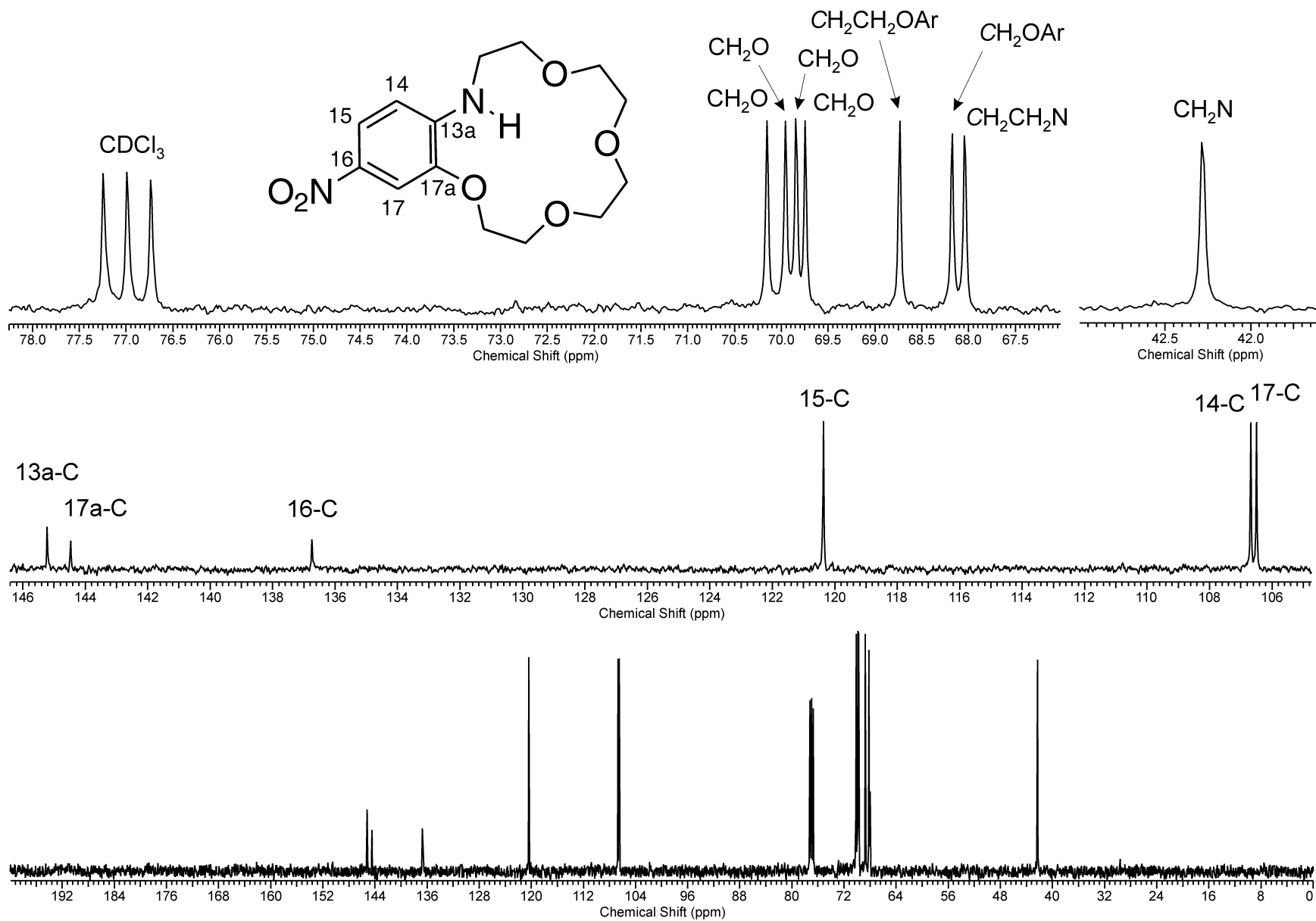


Figure S11. ^{13}C NMR spectrum of compound **1b** (125.76 MHz, CDCl_3 , 25 °C).

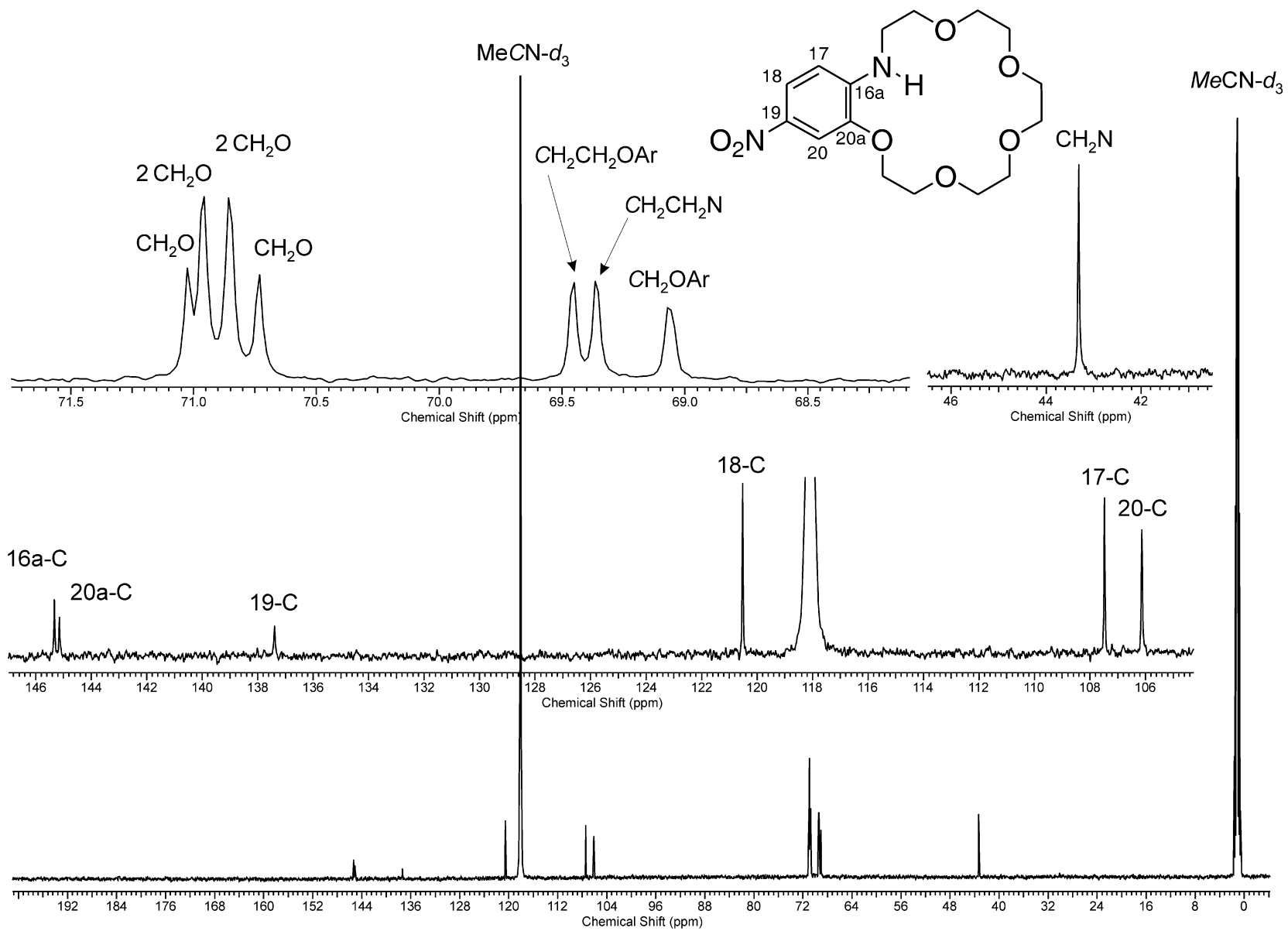


Figure S12. ^{13}C NMR spectrum of compound **1c** (125.76 MHz, $\text{MeCN-}d_3$, 25 °C).

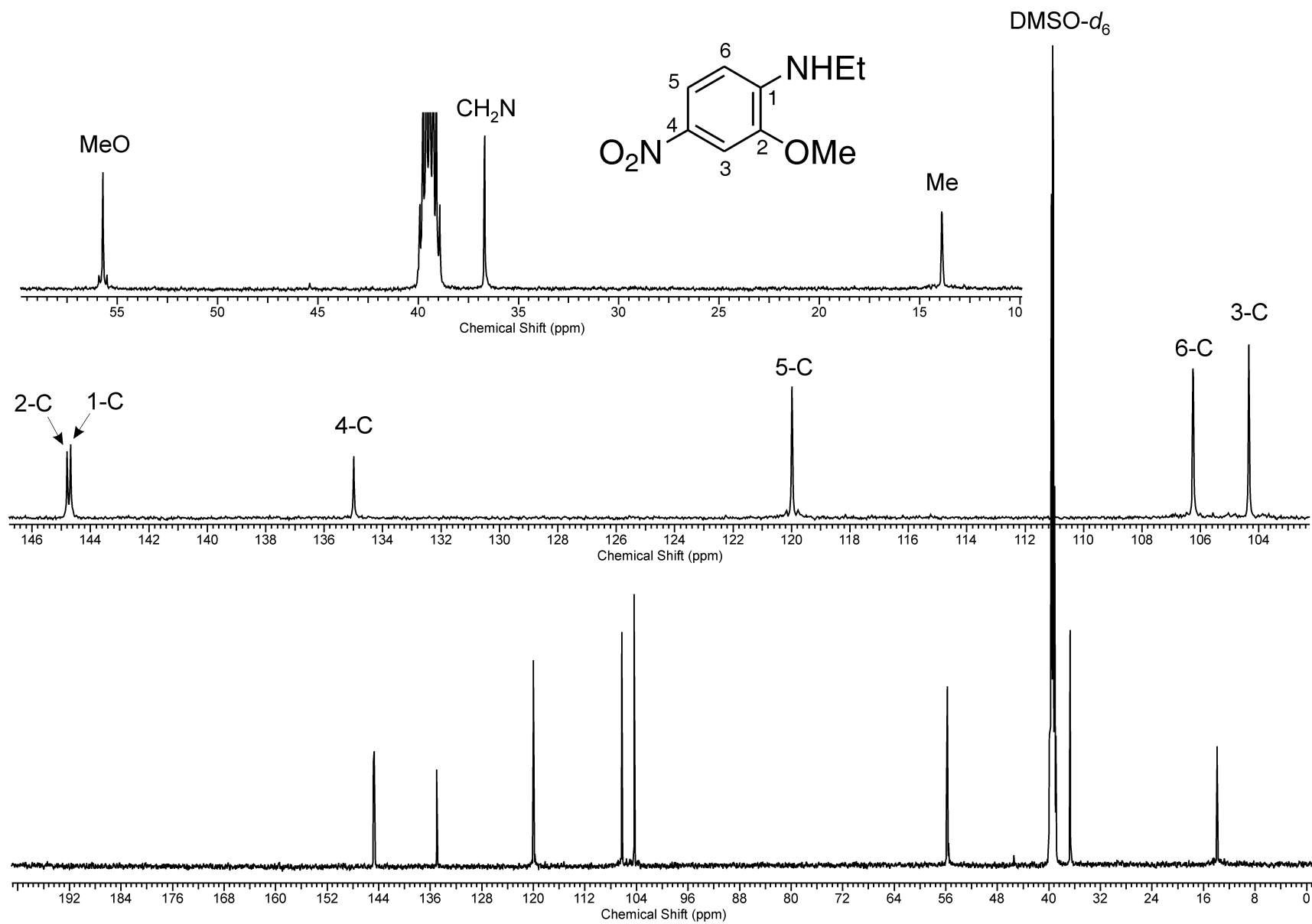


Figure S13. ^{13}C NMR spectrum of compound **5** (125.76 MHz, $\text{DMSO-}d_6$, 25 $^\circ\text{C}$).

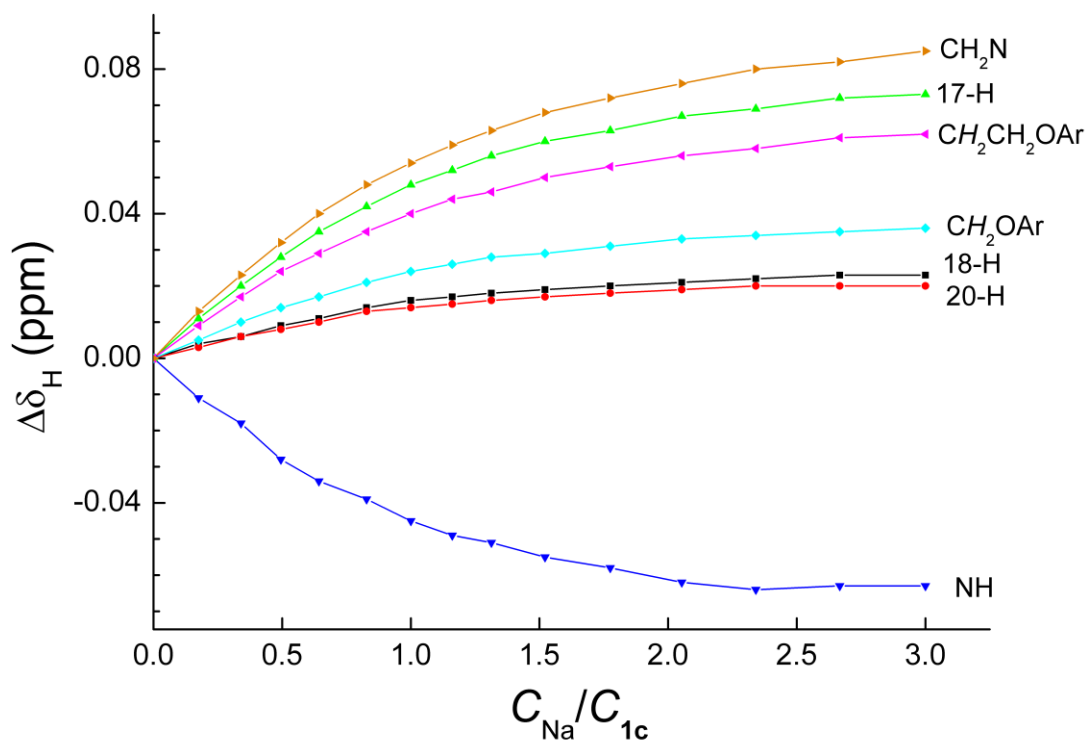


Figure S14. Values of $\Delta\delta_{\text{H}} = \delta_{\text{H}}(\mathbf{1c}/\text{NaClO}_4 \text{ mixture}) - \delta_{\text{H}}(\text{free } \mathbf{1c})$ for some protons of compound **1c** as a function of the $\text{NaClO}_4/\mathbf{1c}$ concentration ratio, $\text{MeCN-}d_3$, 25 °C.

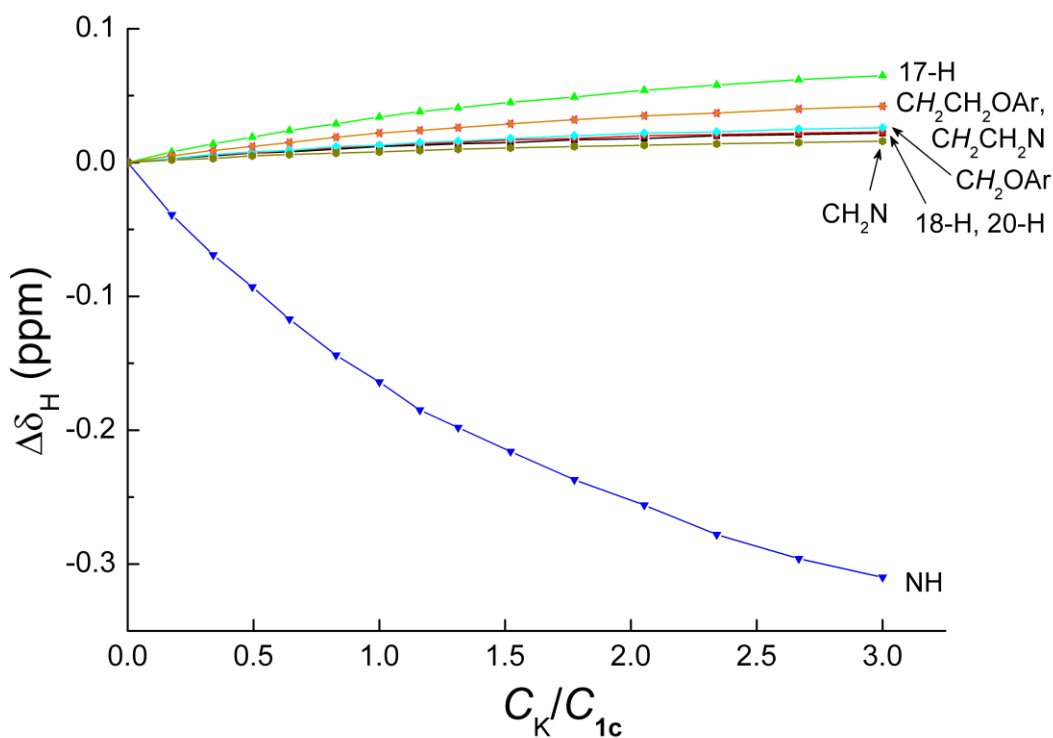


Figure S15. Values of $\Delta\delta_{\text{H}} = \delta_{\text{H}}(\mathbf{1c}/\text{KClO}_4 \text{ mixture}) - \delta_{\text{H}}(\text{free } \mathbf{1c})$ for some protons of compound **1c** as a function of the $\text{KClO}_4/\mathbf{1c}$ concentration ratio, $\text{MeCN-}d_3$, 25 °C.

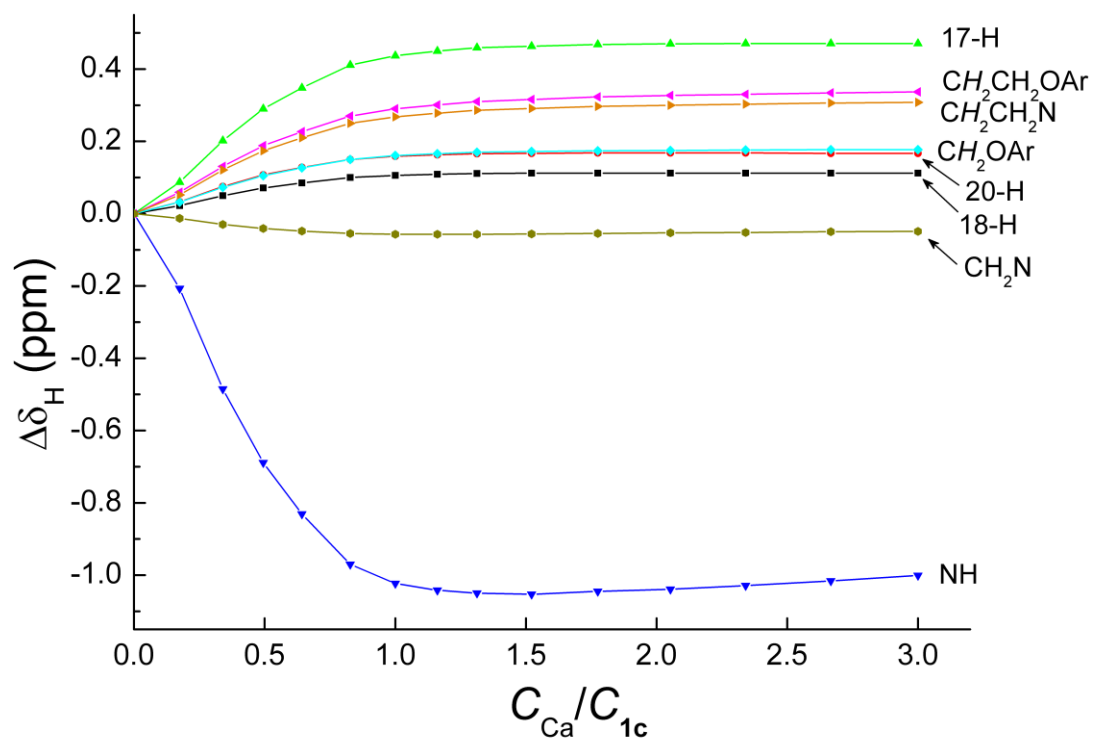


Figure S16. Values of $\Delta\delta_H = \delta_H(\mathbf{1c}/Ca(ClO_4)_2 \text{ mixture}) - \delta_H(\text{free } \mathbf{1c})$ for some protons of compound **1c** as a function of the $Ca(ClO_4)_2/\mathbf{1c}$ concentration ratio, $MeCN-d_3$, 25 °C.

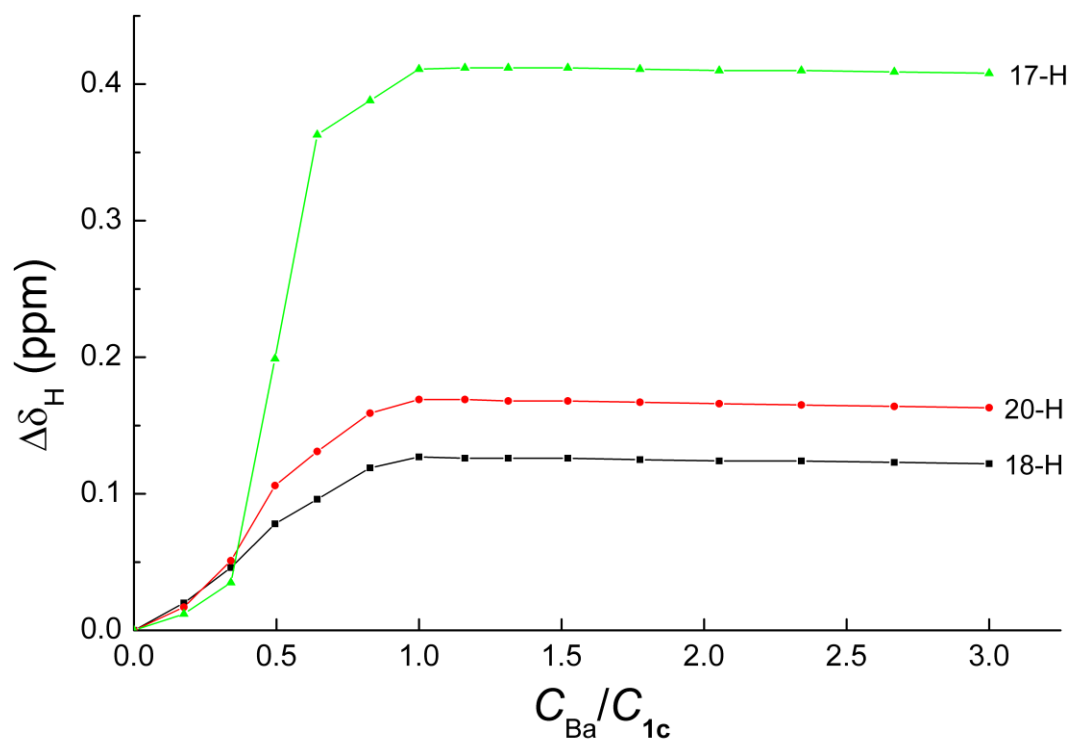


Figure S17. Values of $\Delta\delta_H = \delta_H(\mathbf{1c}/Ba(ClO_4)_2 \text{ mixture}) - \delta_H(\text{free } \mathbf{1c})$ for some protons of compound **1c** as a function of the $Ba(ClO_4)_2/\mathbf{1c}$ concentration ratio, $MeCN-d_3$, 25 °C.