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Supplementary Information

to the article

Title: Self-assembly of cucurbiturils and cyclodextrins to supramolecular millstones with naphthalene derivatives capable of translocations in the host cavities

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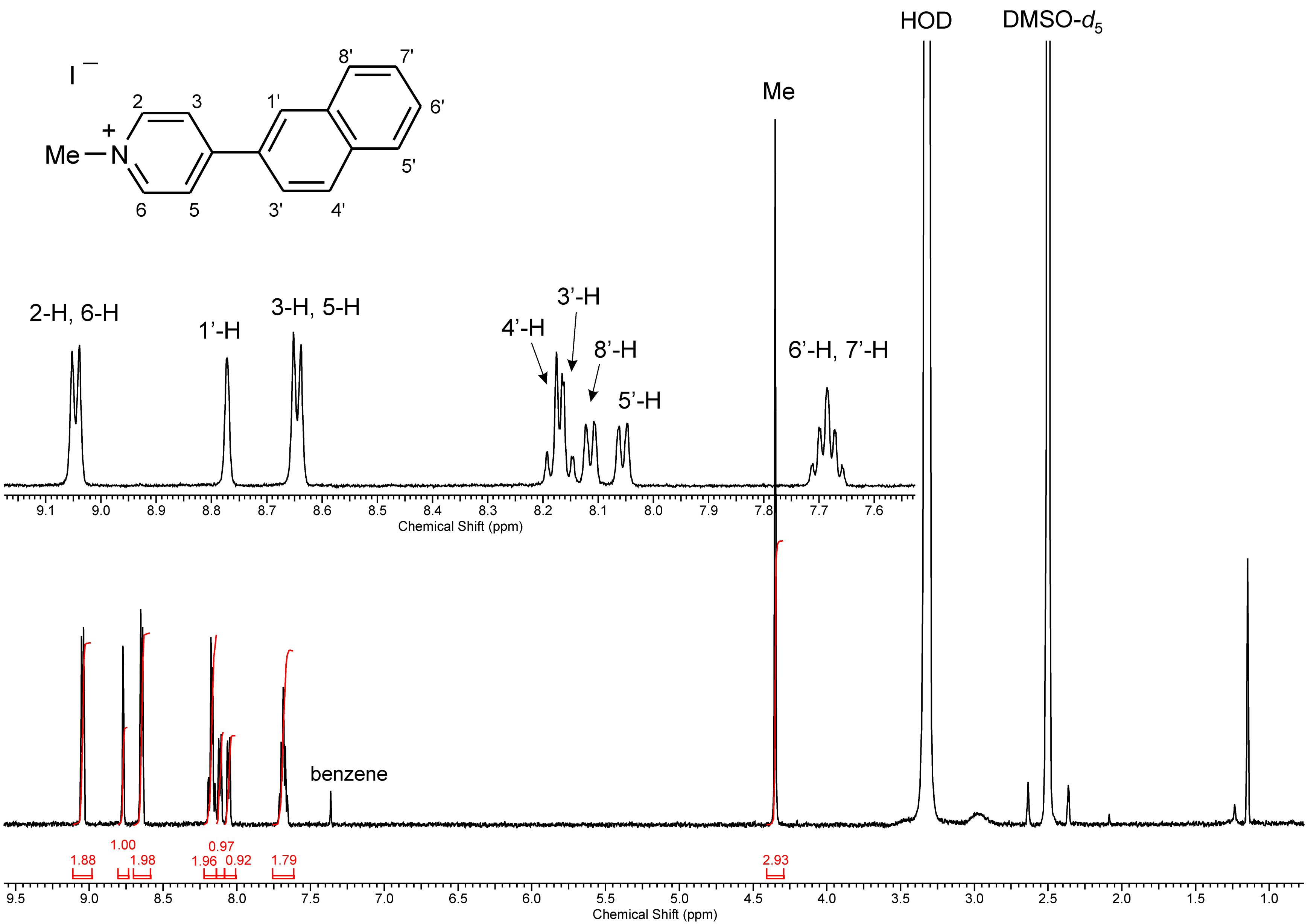


Fig. S1 ^{1}H NMR spectrum of compound **1** (500.13 MHz, DMSO-d_6, 25 °C).

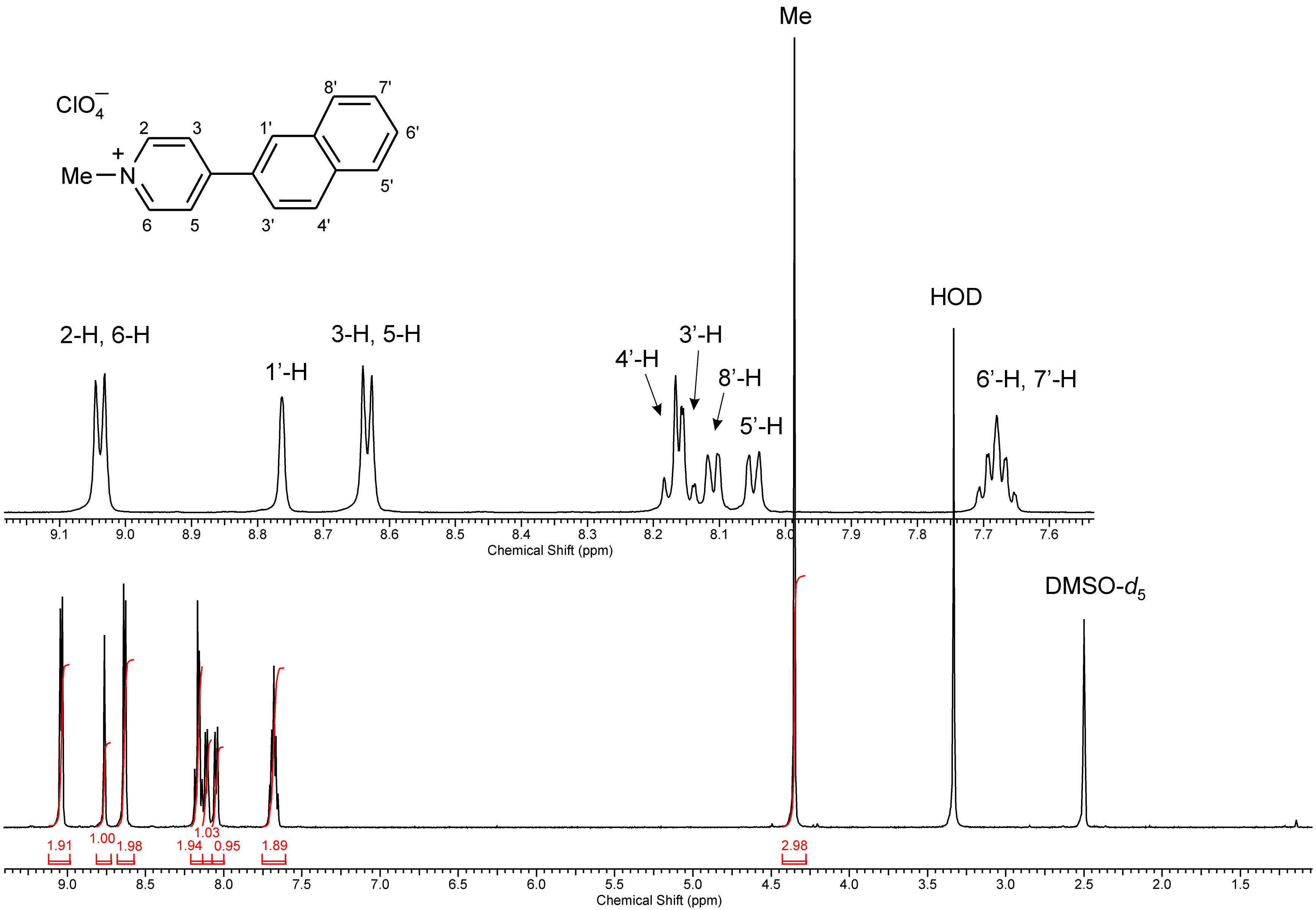


Fig. S2 ^{1}H NMR spectrum of compound **2** (500.13 MHz, DMSO-d_6, 26 °C).

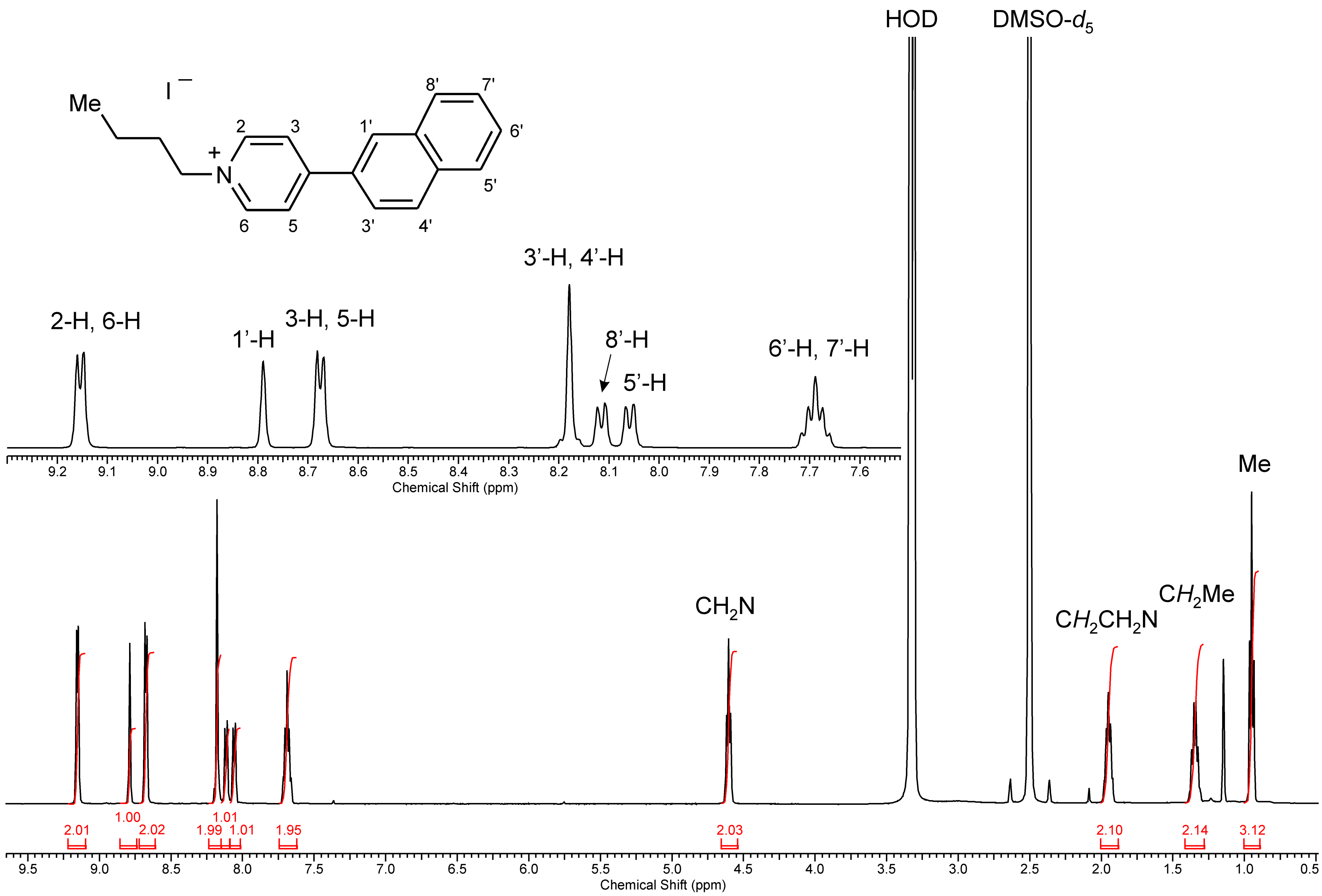


Fig. S3 ^{1}H NMR spectrum of compound **3** (500.13 MHz, DMSO-d_6, 26 °C).

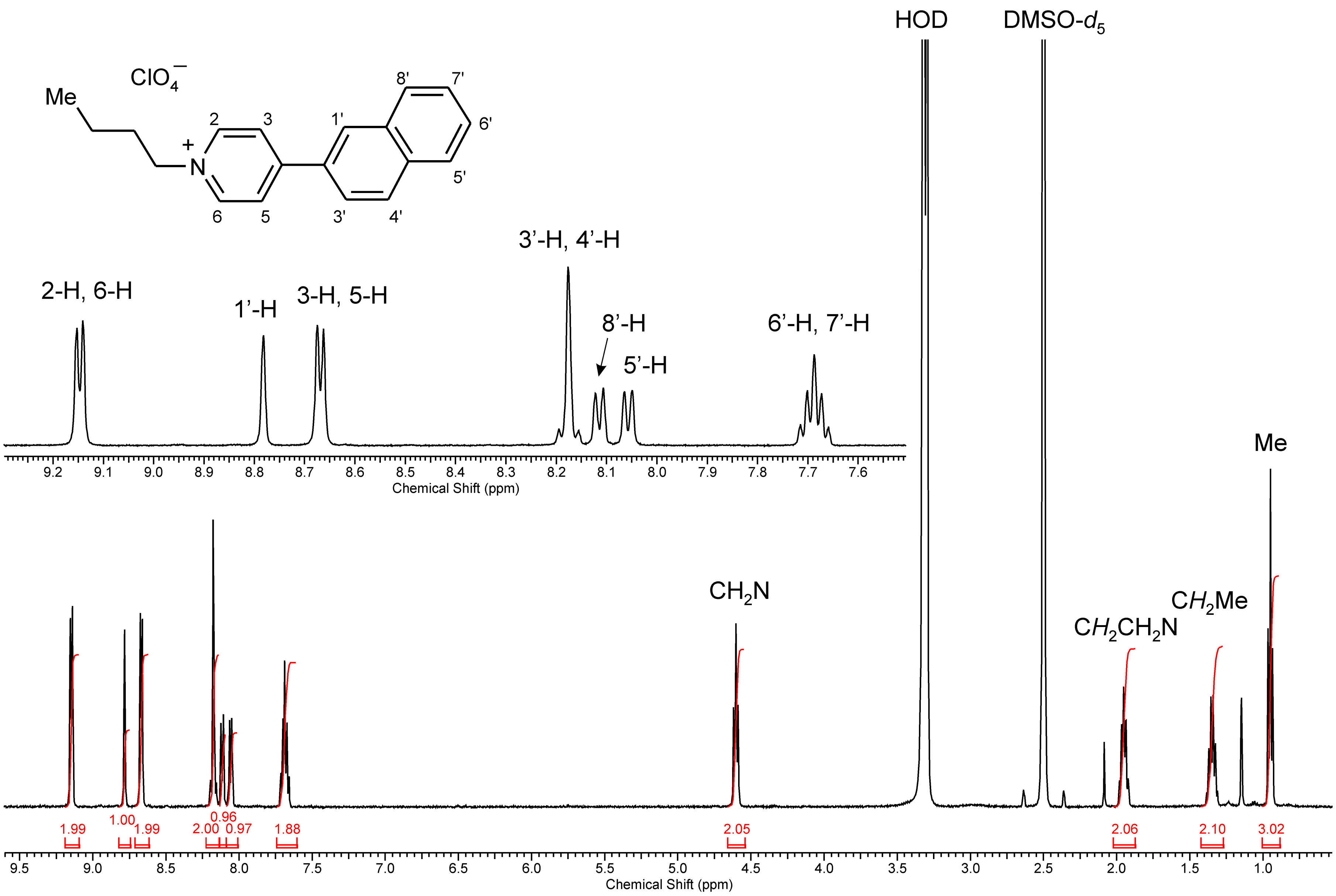


Fig. S4 ^{1}H NMR spectrum of compound **4** (500.13 MHz, DMSO-d_6, 26 °C).

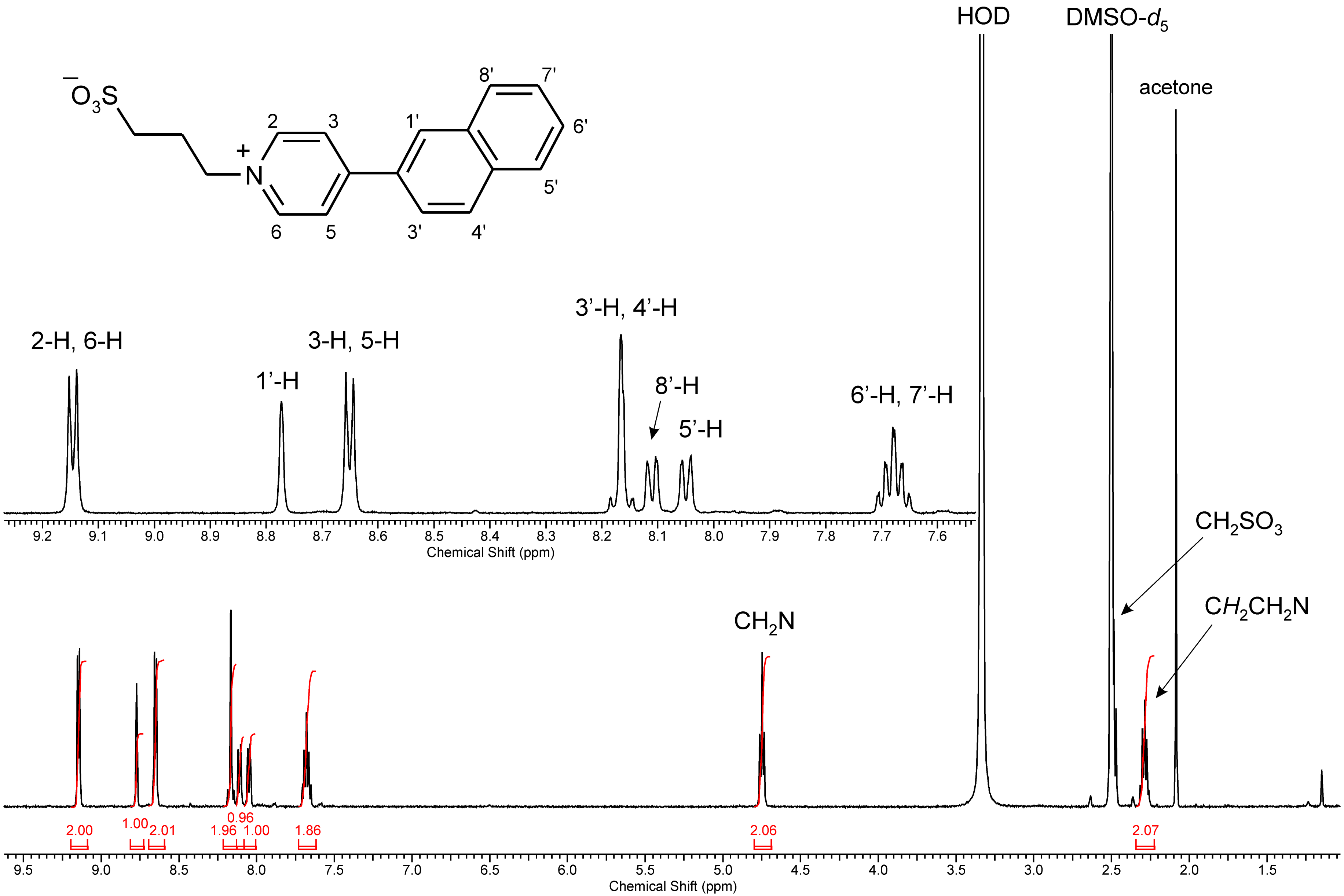


Fig. S5 ^{1}H NMR spectrum of compound **5** (500.13 MHz, DMSO-d_6, 28 °C).

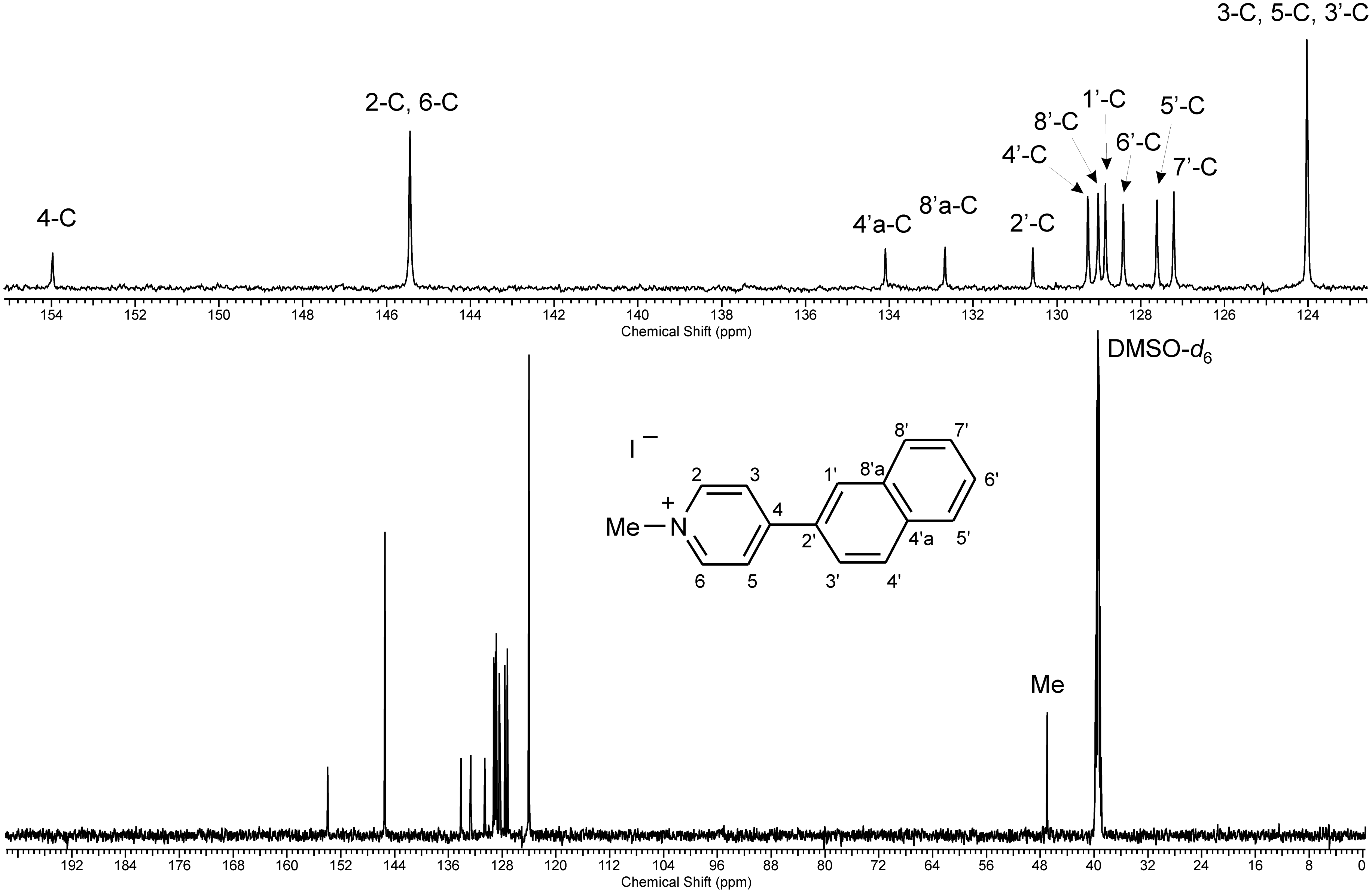


Fig. S6 ^{13}C NMR spectrum of compound **1** (125.76 MHz, DMSO-d_6, 25 °C).

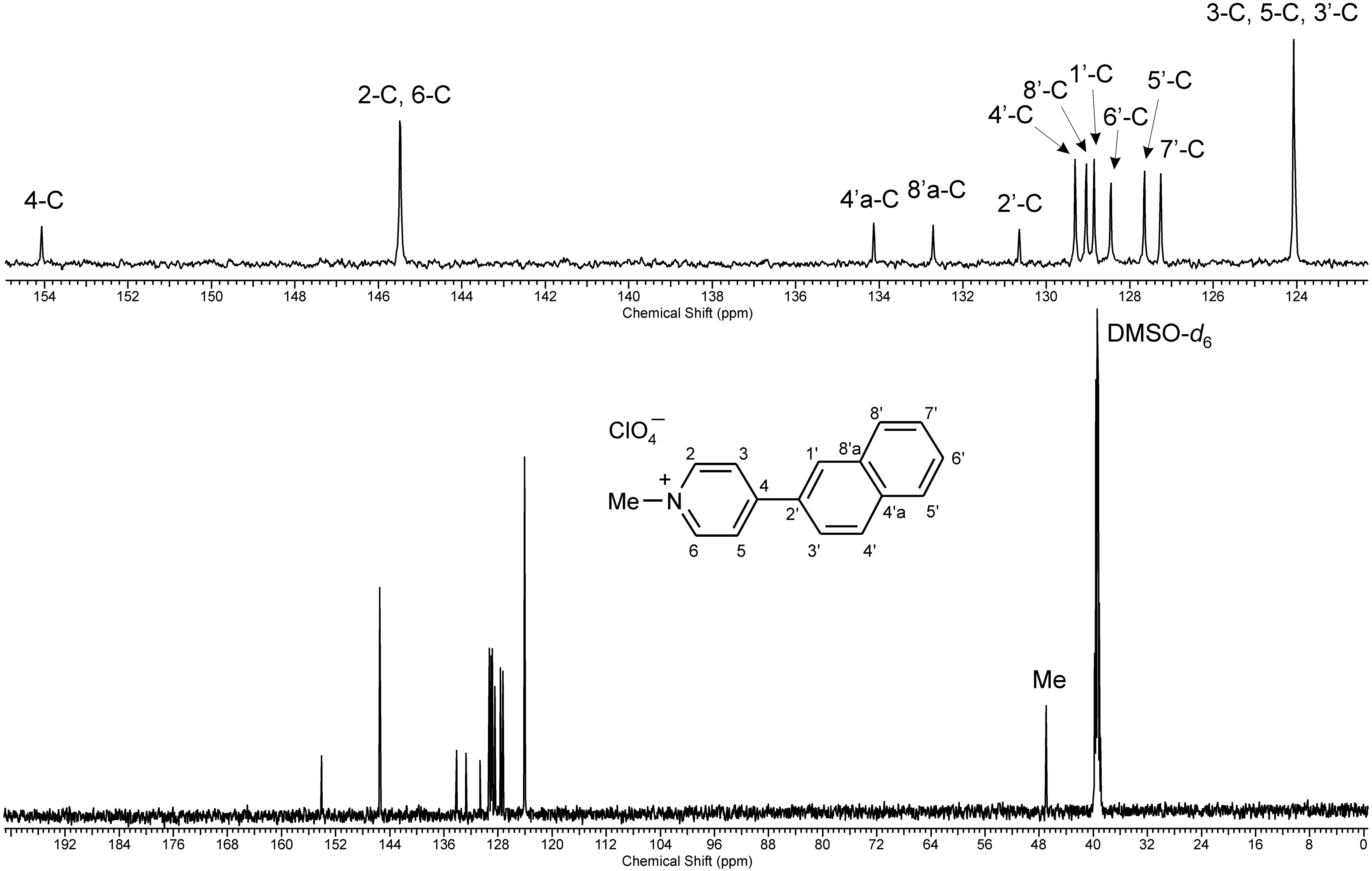


Fig. S7 ^{13}C NMR spectrum of compound **2** (125.76 MHz, DMSO-d_6, 26 °C).

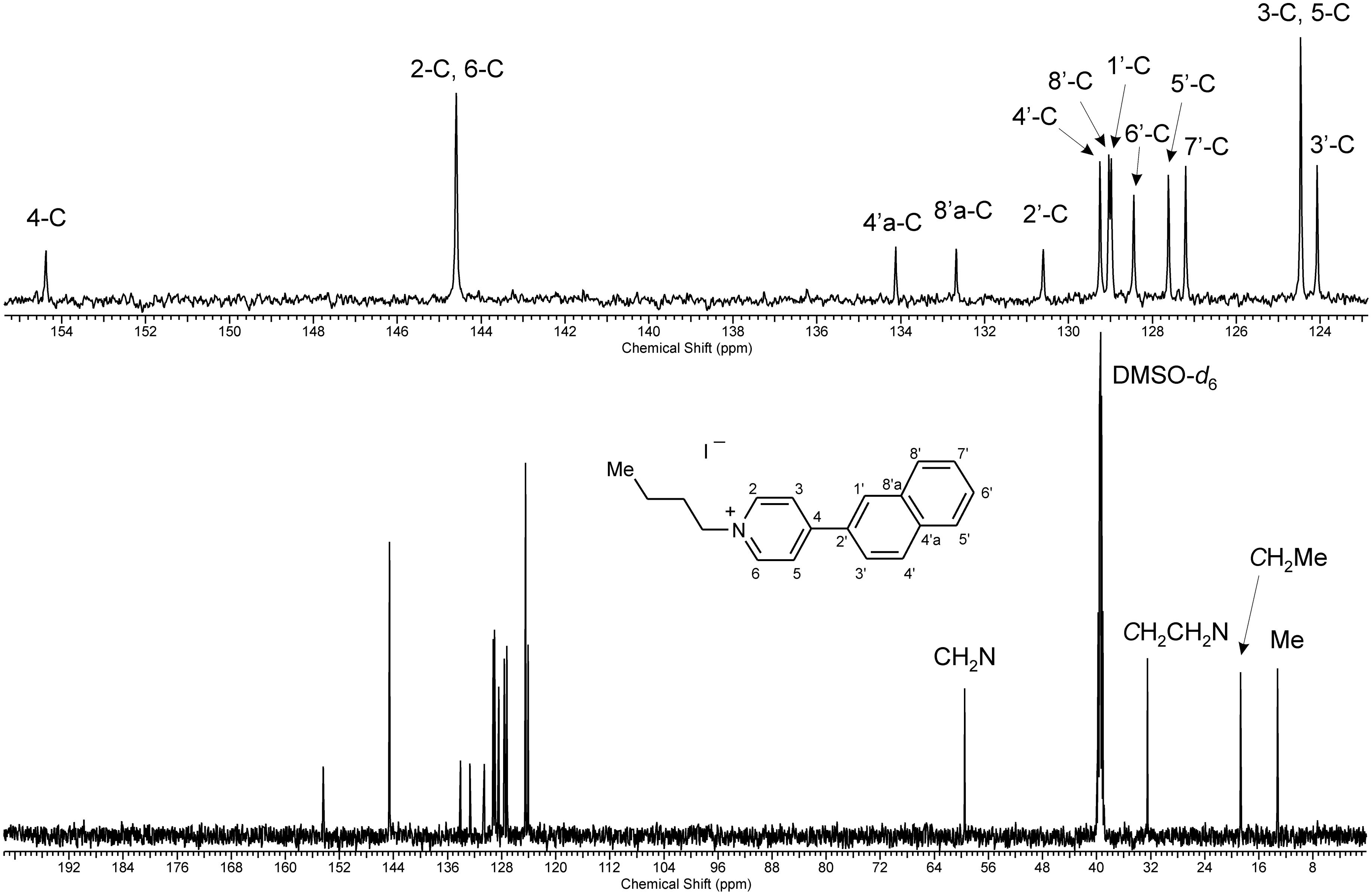


Fig. S8 ^{13}C NMR spectrum of compound **3** (125.76 MHz, DMSO-d_6, 25 °C).

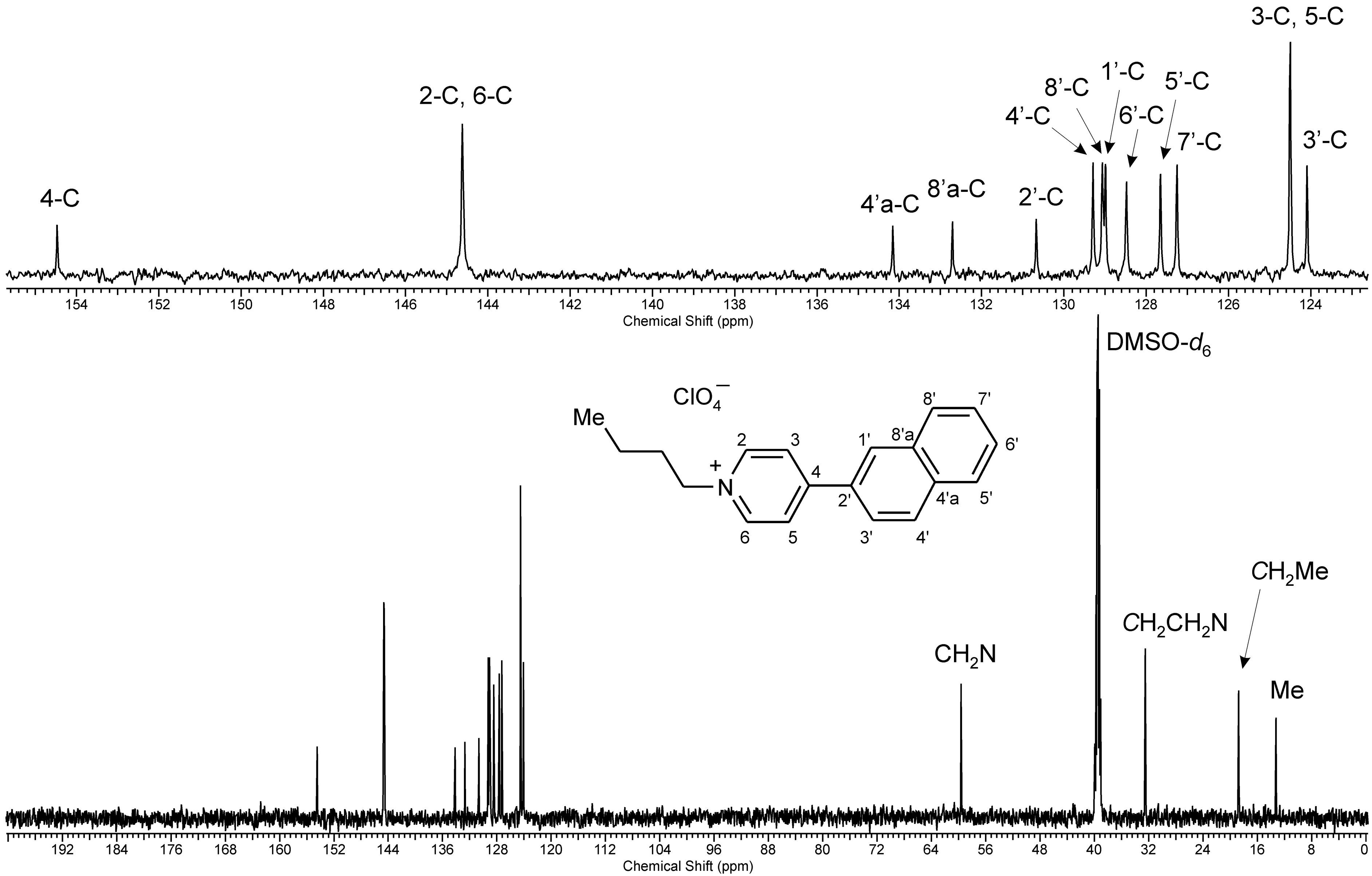


Fig. S9 ^{13}C NMR spectrum of compound **4** (125.76 MHz, DMSO-d_6, 25 °C).

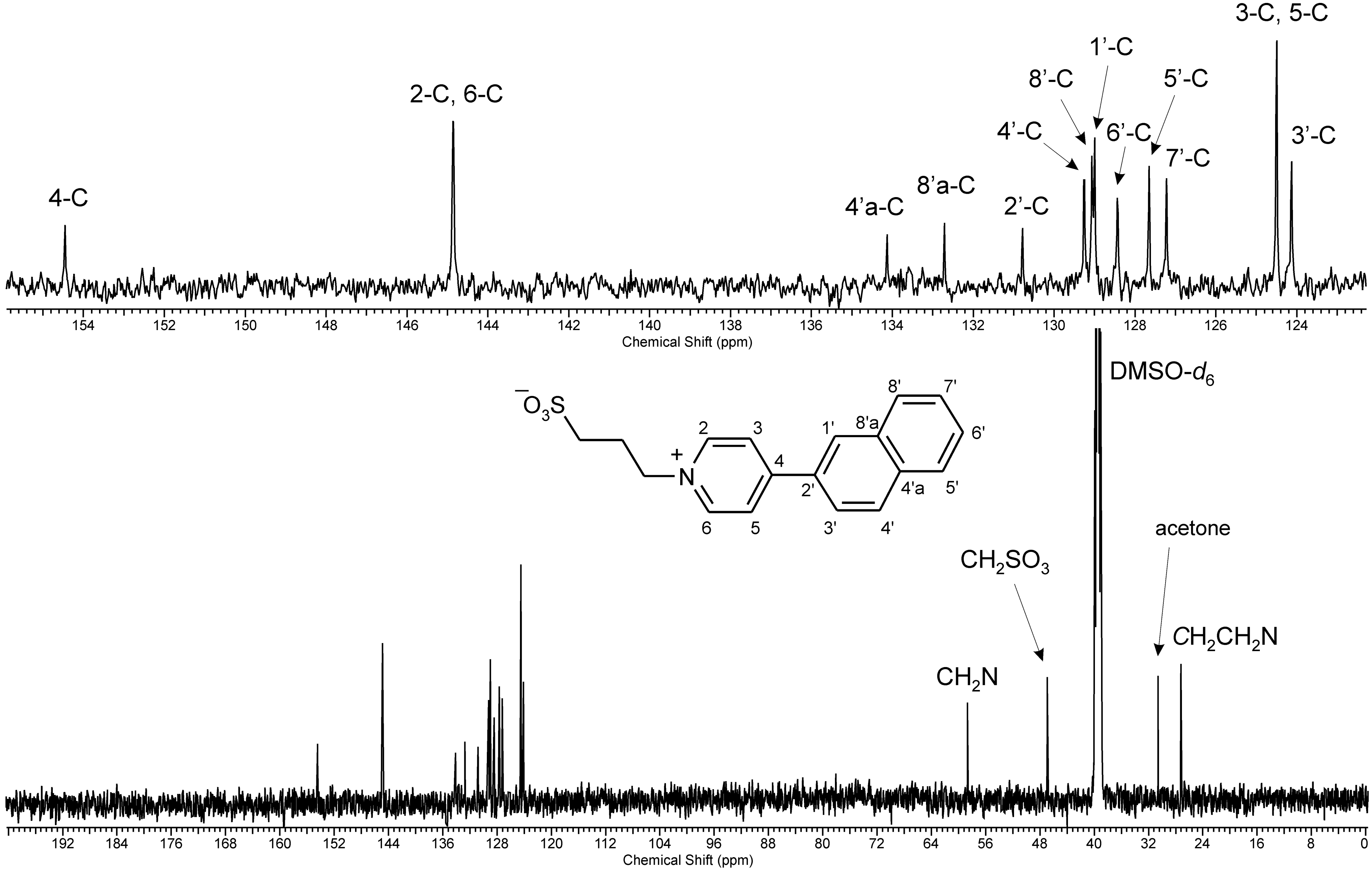


Fig. S10 ^{13}C NMR spectrum of compound **5** (125.76 MHz, DMSO-d_6, 26 °C).

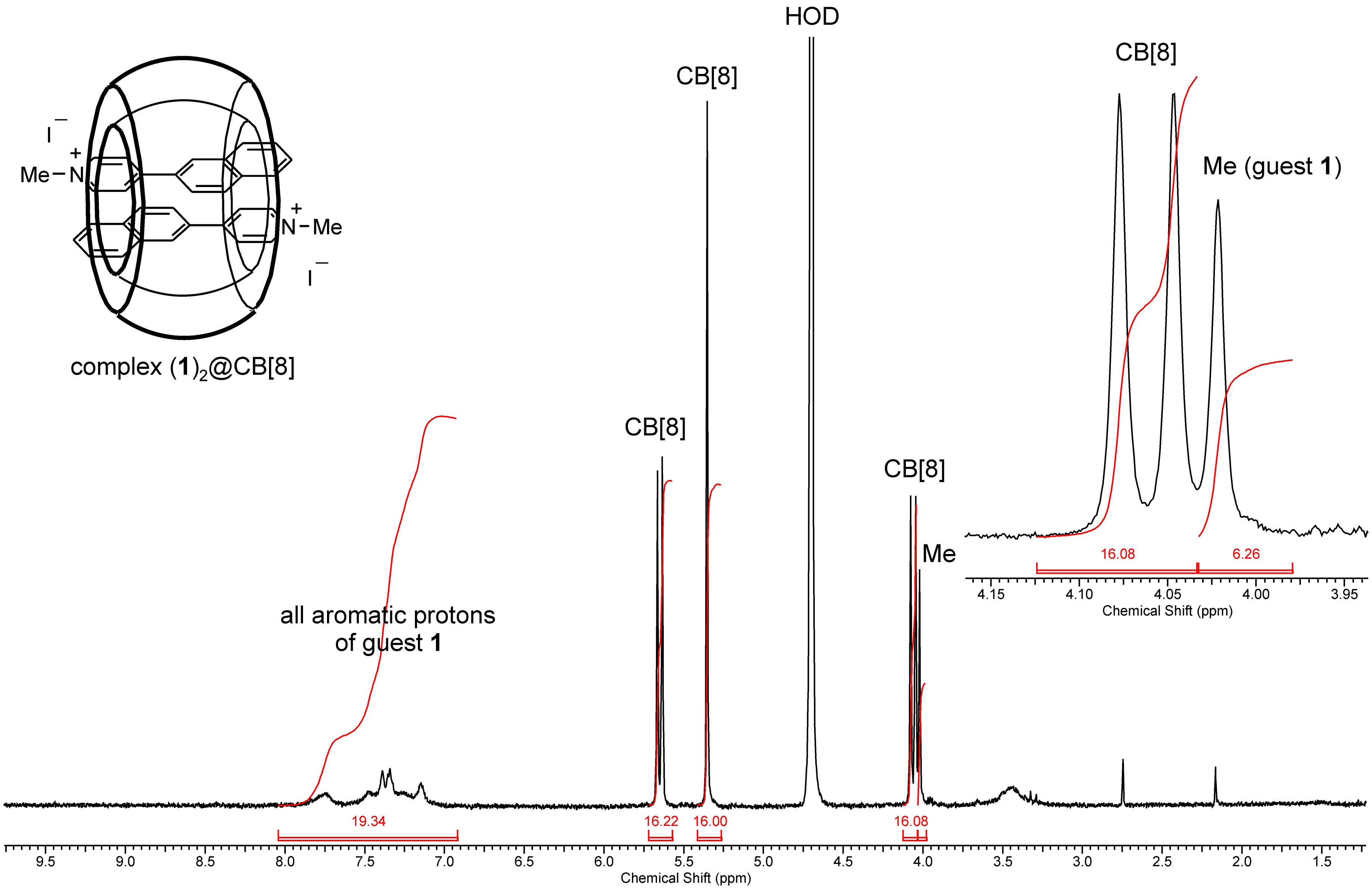


Fig. S11 ^{1}H NMR spectrum of complex (**1**)$_2$@CB[8]·6.5H$_2$O, which was obtained by crystallization ($C_{complex}$ = 3×10^{-4} M), D$_2$O, 25 °C.

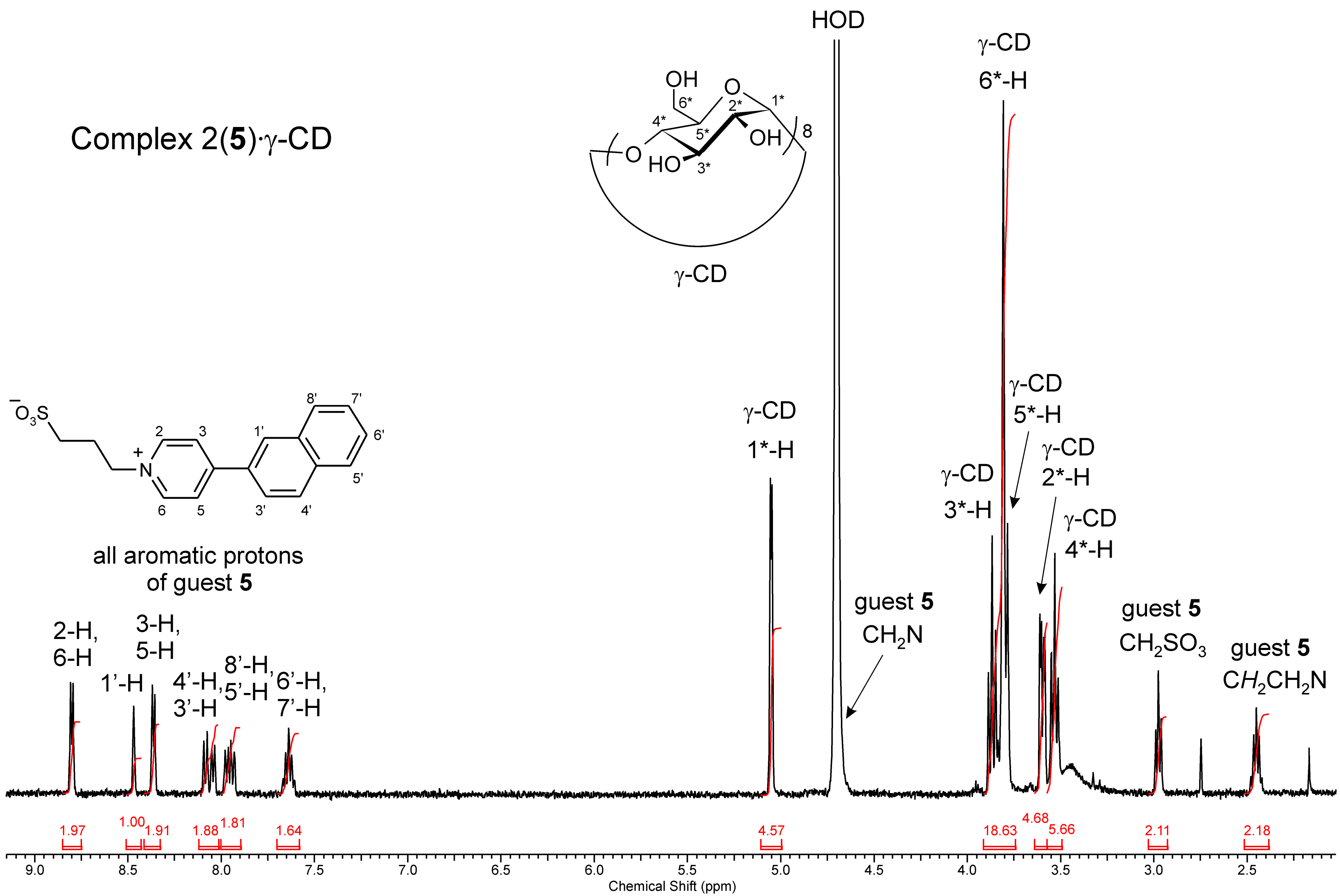


Fig. S12 ^{1}H NMR spectrum of complex 2(**5**)@γ-CD·6H_2O, which was obtained by crystallization ($C_{complex}$ = 3×10^{-4} M), D_2O, 25 °C.

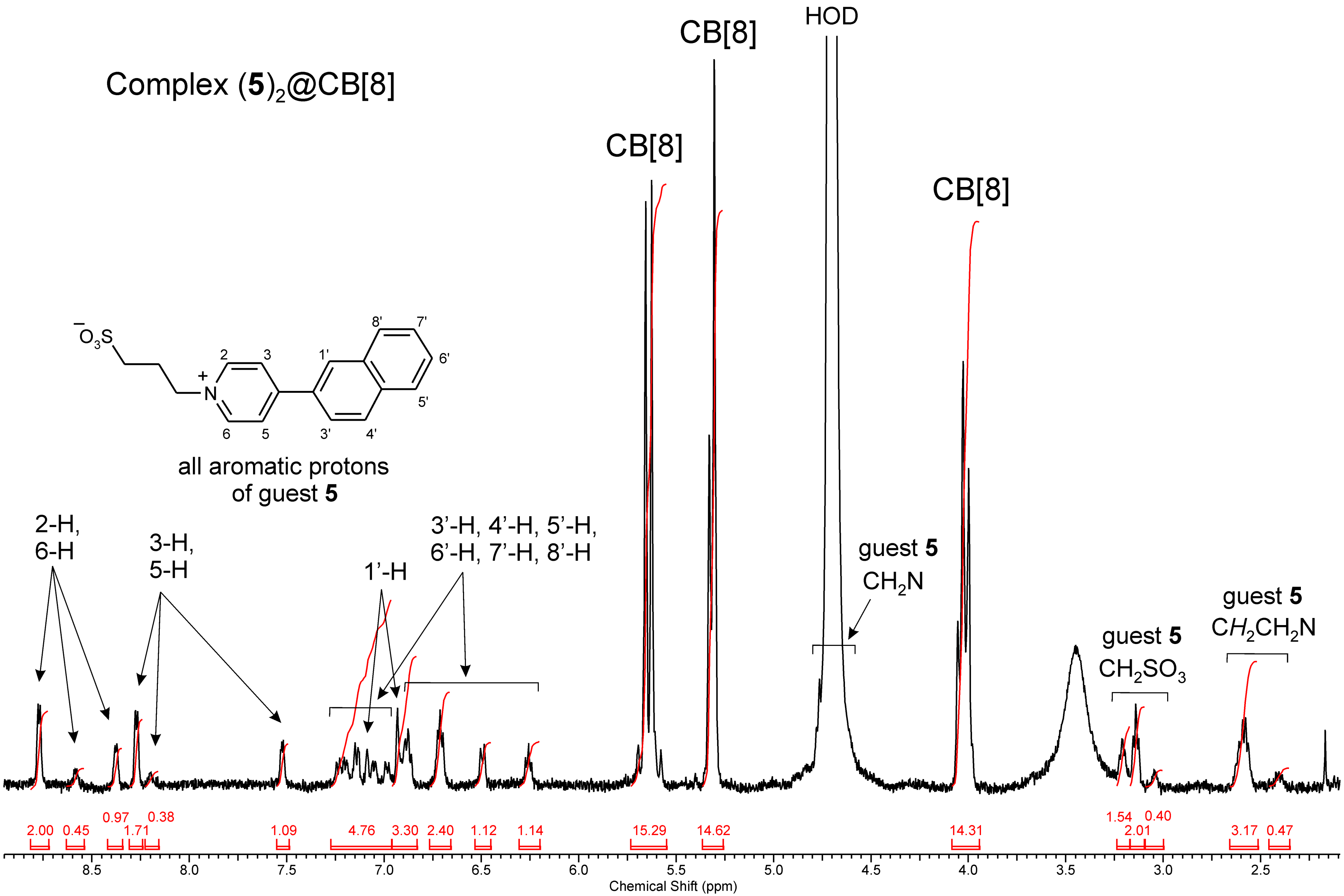


Fig. S13 [1]H NMR spectrum of complex (**5**)$_2$@CB[8]·5H_2O, which was obtained by crystallization (sat., $C_{\text{complex}} < 1\times10^{-4}$ M), D_2O, 25 °C.

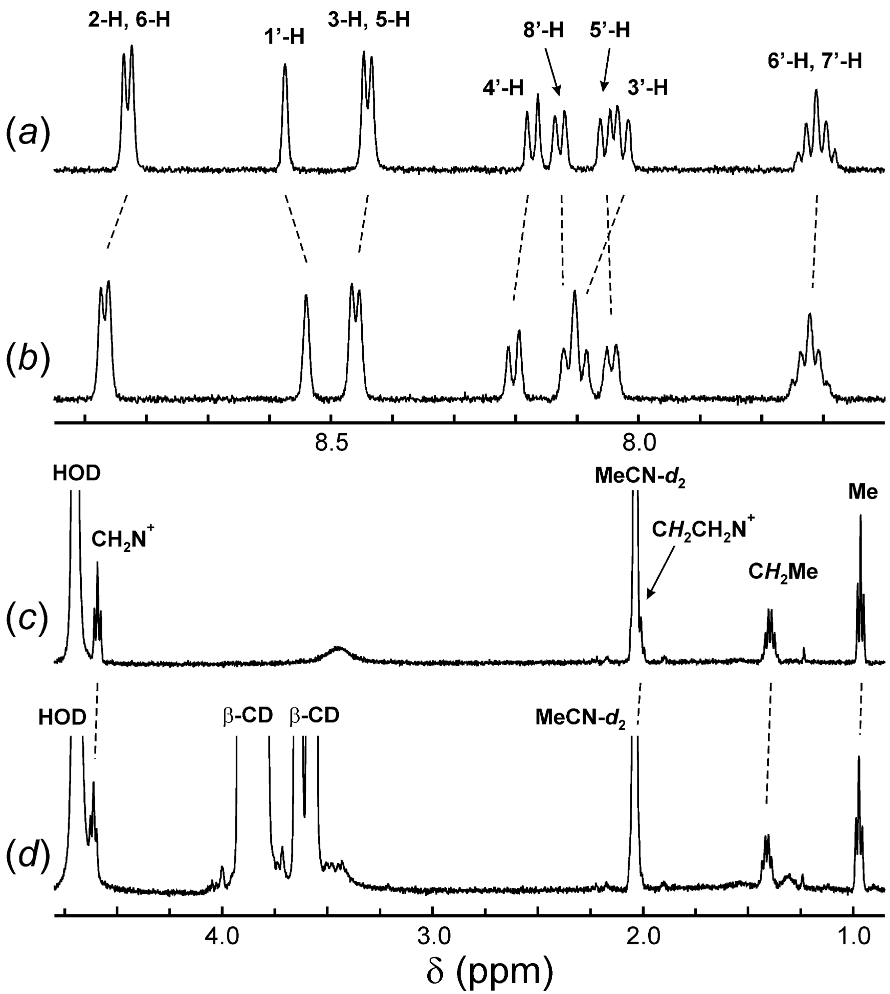


Fig. S14 ^{1}H NMR spectra ((*a*, *b*) aromatic and (*c*, *d*) aliphatic proton regions) of (*a*, *c*) compound **4** and (*b*, *d*) a 1:6.0 mixture of compound **4** and β-CD (C_4 = 5.0×10^{-4} M), D_2O–MeCN-d_3 (10:1, v/v), 25 °C.

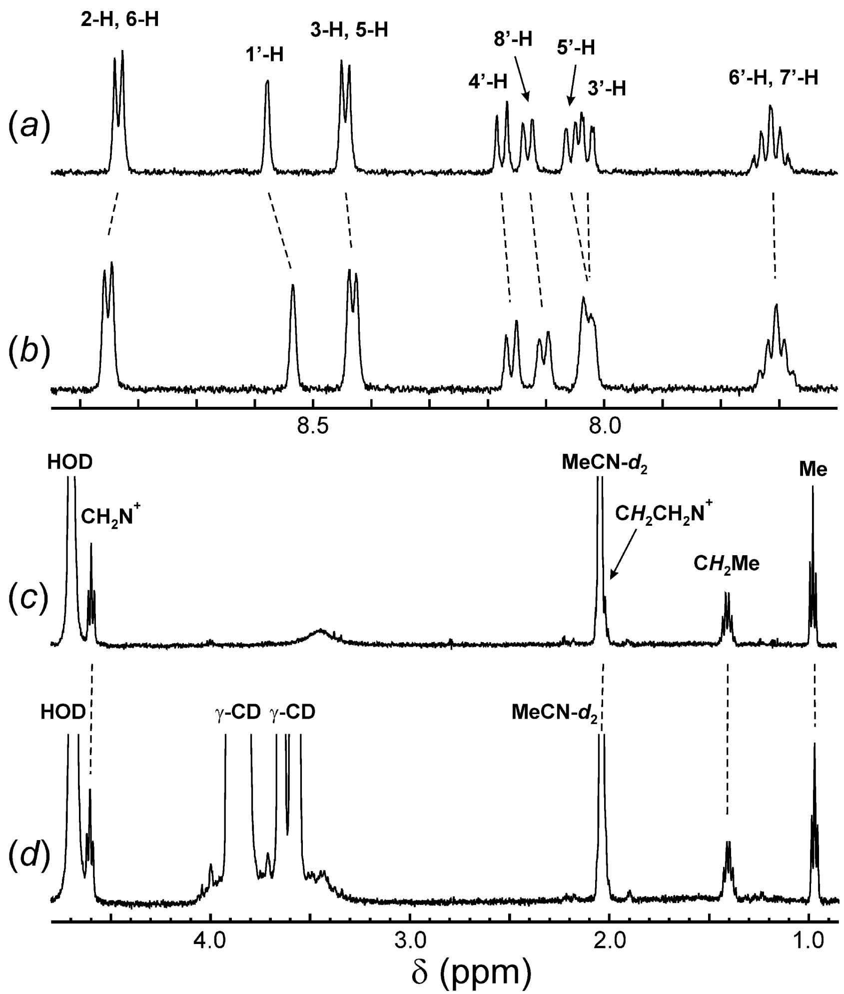


Fig. S15 ^{1}H NMR spectra ((*a*, *b*) aromatic and (*c*, *d*) aliphatic proton regions) of (*a*, *c*) compound **4** and (*b*, *d*) a 1:7.4 mixture of compound **4** and γ-CD (C_4 = 4.3×10^{-4} M), D_2O–MeCN-d_3 (10:1, v/v), 25 °C.

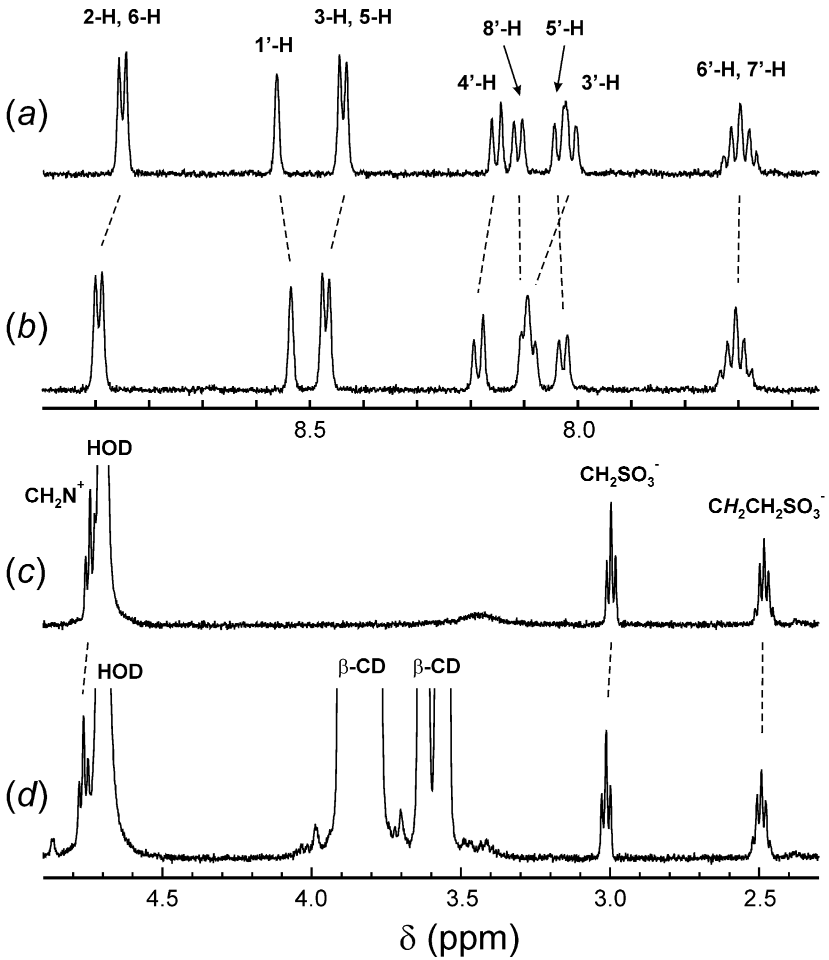


Fig. S16 ^{1}H NMR spectra ((*a*, *b*) aromatic and (*c*, *d*) aliphatic proton regions) of (*a*, *c*) compound **5** and (*b*, *d*) a 1:5.8 mixture of compound **5** and β-CD ($C_5 = 5.2\times10^{-4}$ M), D_2O–MeCN-d_3 (10:1, v/v), 25 °C.

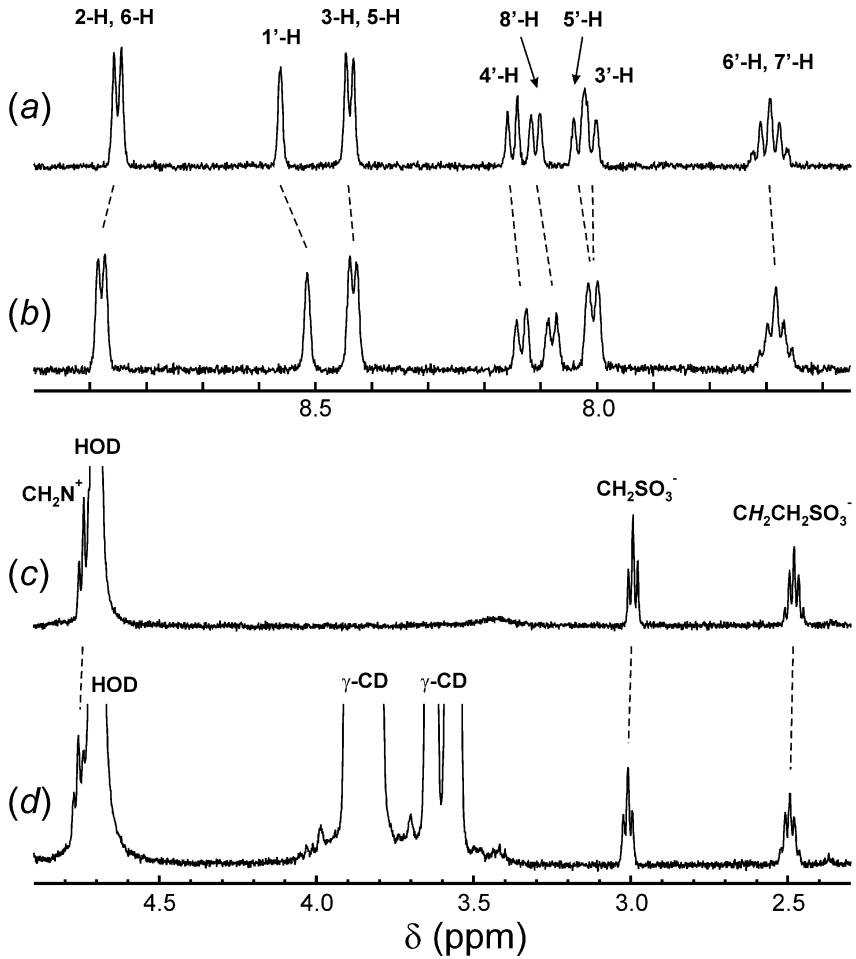


Fig. S17 ^{1}H NMR spectra ((*a*, *b*) aromatic and (*c*, *d*) aliphatic proton regions) of (*a*, *c*) compound **5** and (*b*, *d*) a 1:6.1 mixture of compound **5** and γ-CD ($C_5 = 5.2\times10^{-4}$ M), D_2O–MeCN-d_3 (10:1, v/v), 25 °C.

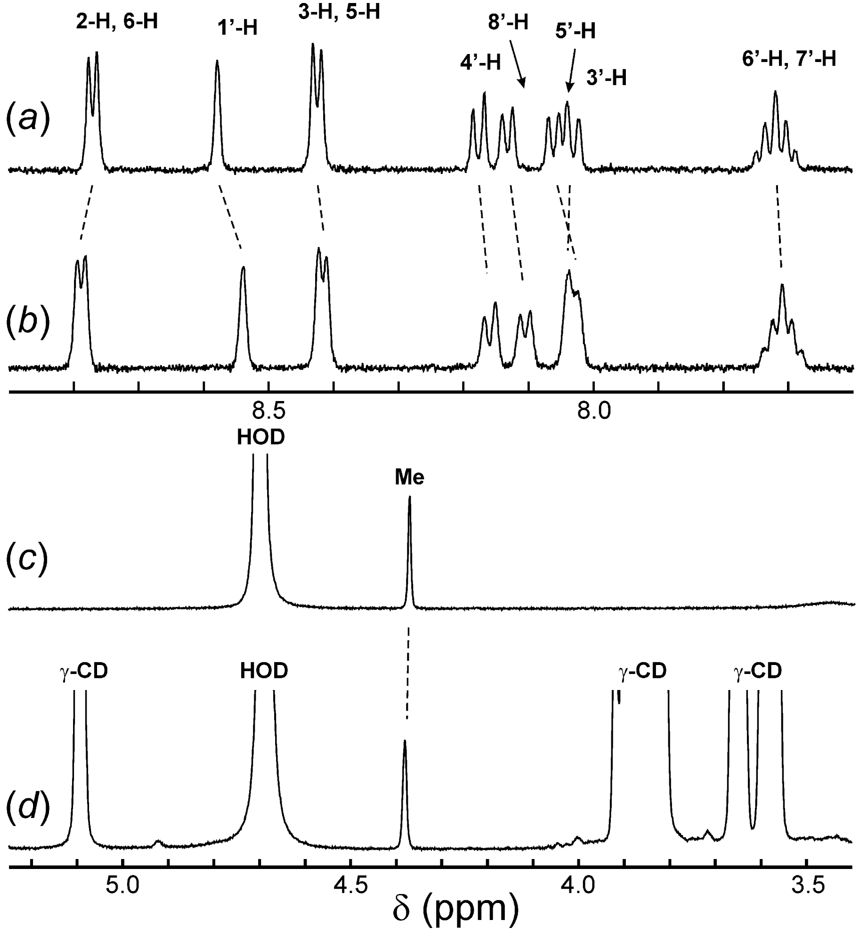


Fig. S18 [1]H NMR spectra ((*a*, *b*) aromatic and (*c*, *d*) aliphatic proton regions) of (*a*, *c*) compound **2** and (*b*, *d*) a 1:6.5 mixture of compound **2** and γ-CD ($C_2 = 4.7\times10^{-4}$ M), D_2O–MeCN-d_3 (10:1, v/v), 25 °C.

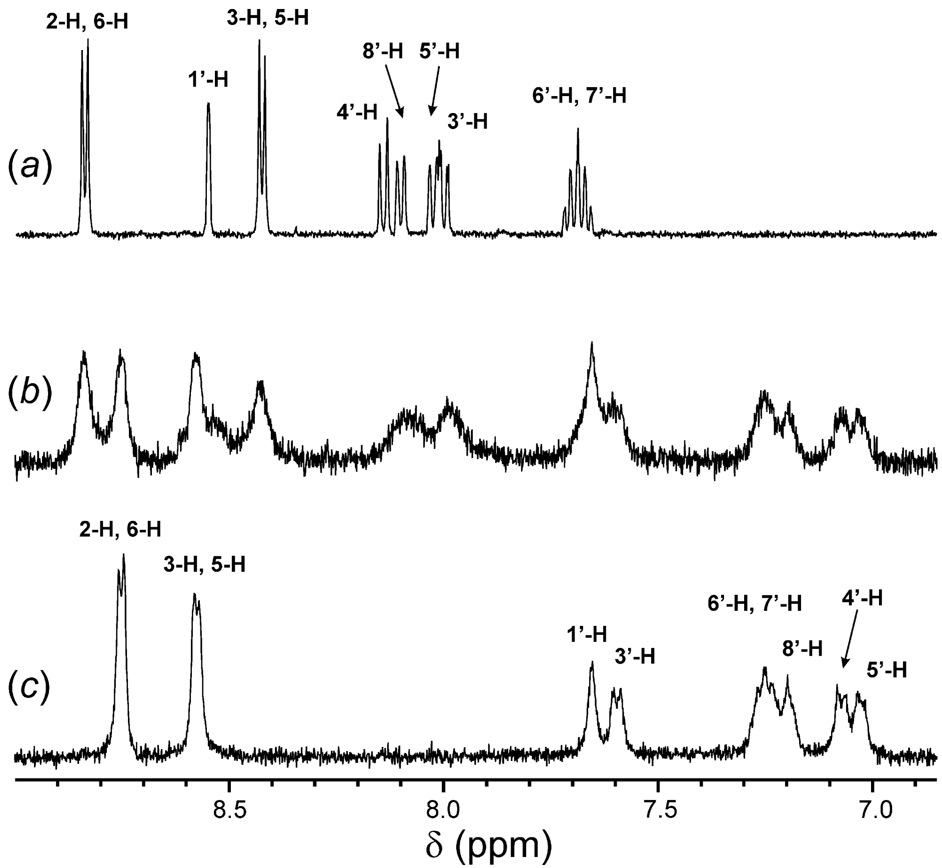


Fig. S19 [1]H NMR spectra (aromatic proton region) of (*a*) compound **5** and (*b*) 1:0.7 and (*c*) 1:1.9 mixtures of compound **5** and CB[7] (C_5 = 6.4×10^{-4} M), D_2O–MeCN-d_3 (10:1, v/v), 25 °C.

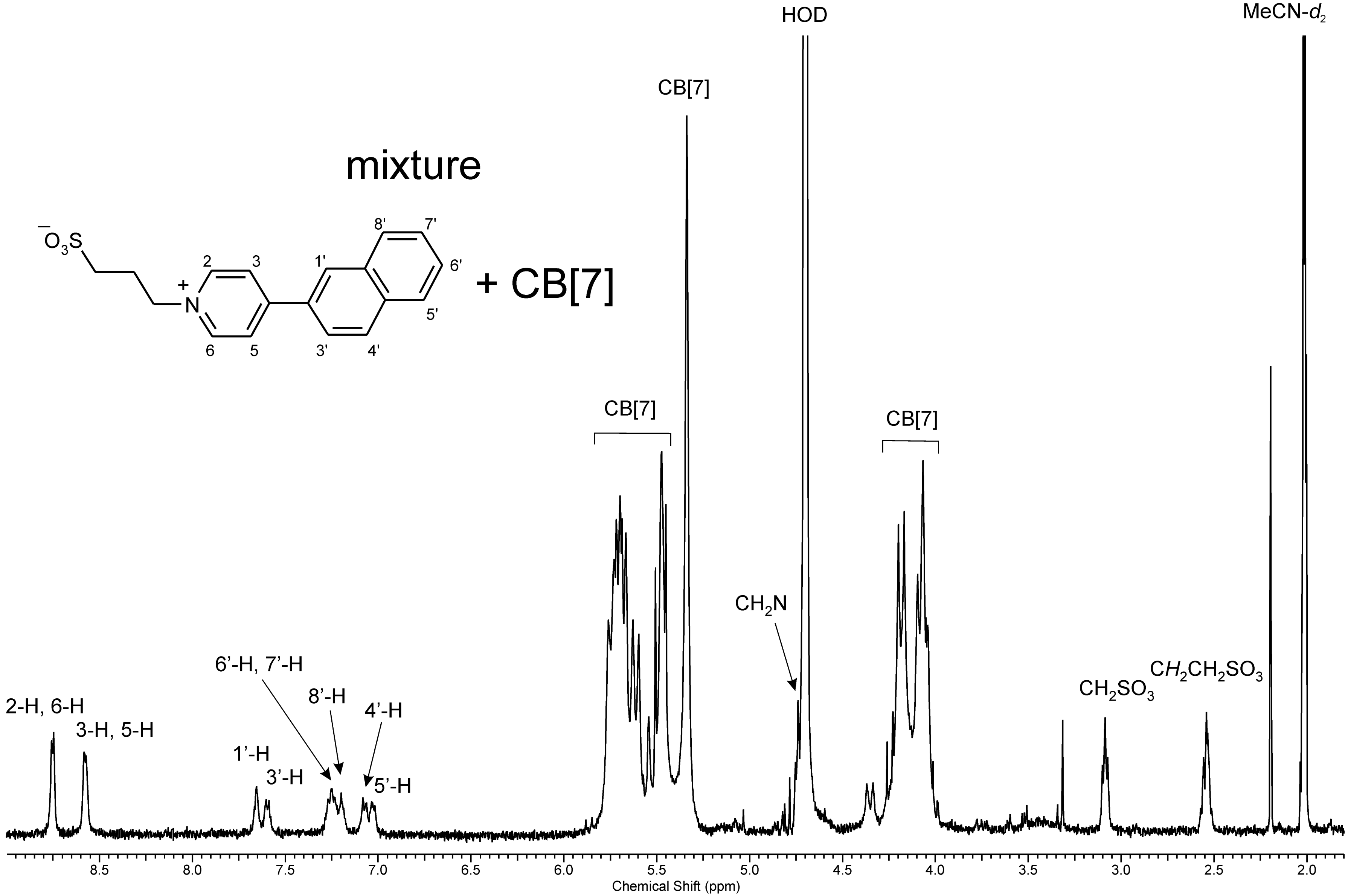


Fig. S20 ^{1}H NMR spectrum of a 1:1.9 mixture of compound **5** and CB[7] (C_5 = 6.4×10^{-4} M), D_2O–MeCN-d_3 (10:1, v/v), 25 °C.

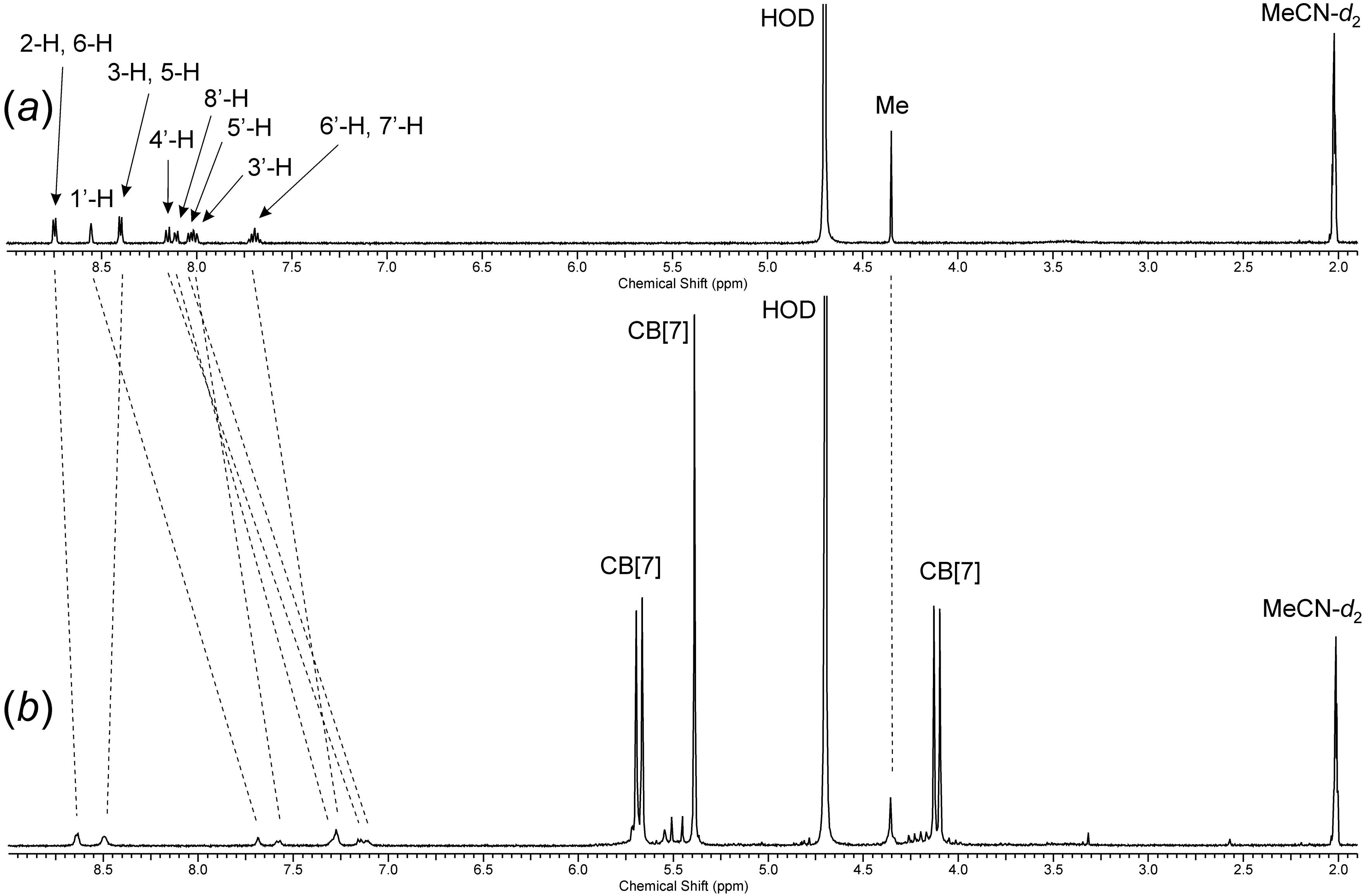


Fig. S21 ^{1}H NMR spectra of (*a*) compound **2** and (*b*) a 1:1.9 mixture of compound **2** and CB[7] (C_2 = 5.7×10^{-4} M), D_2O–MeCN-d_3 (10:1, v/v), 25 °C.

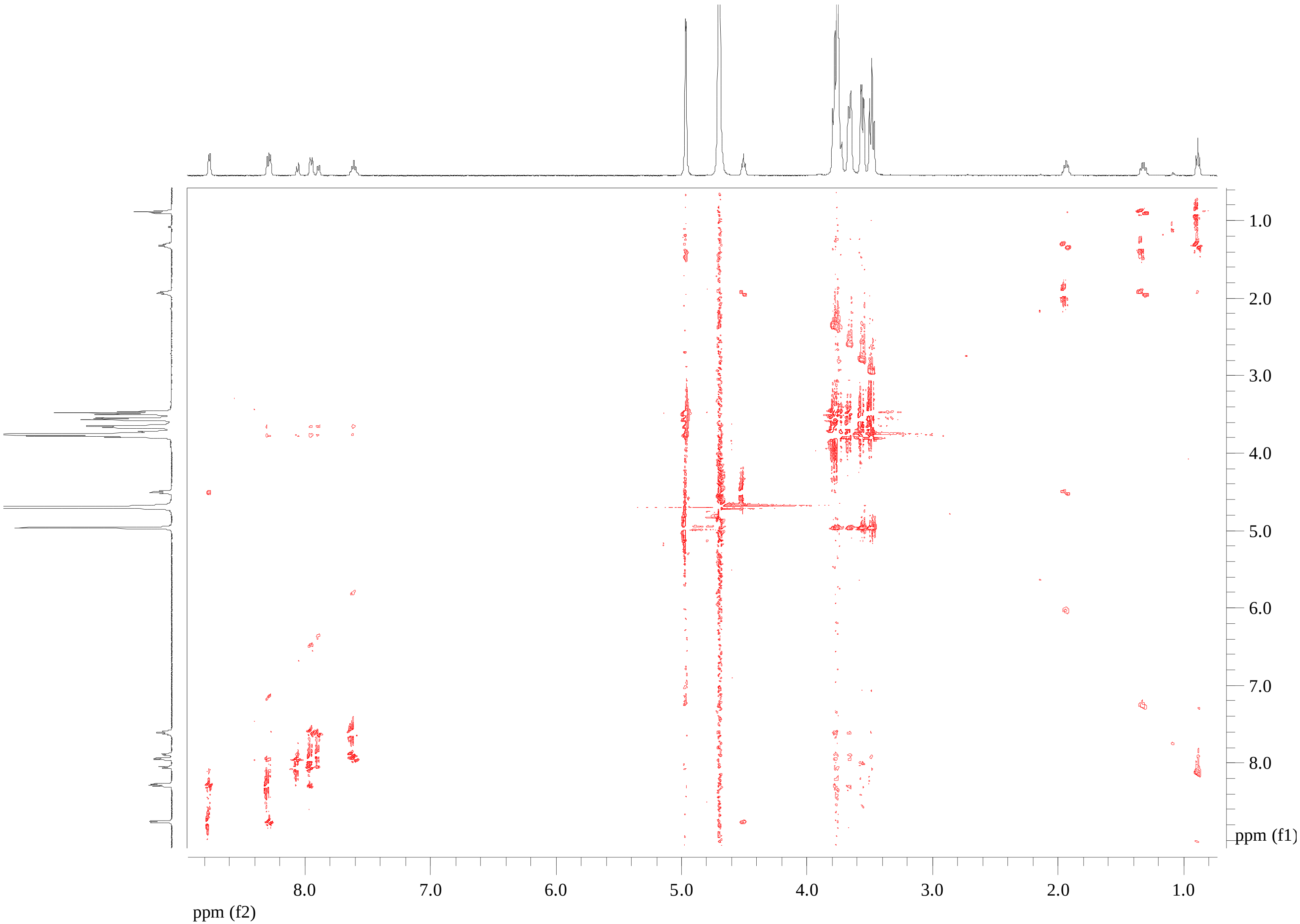
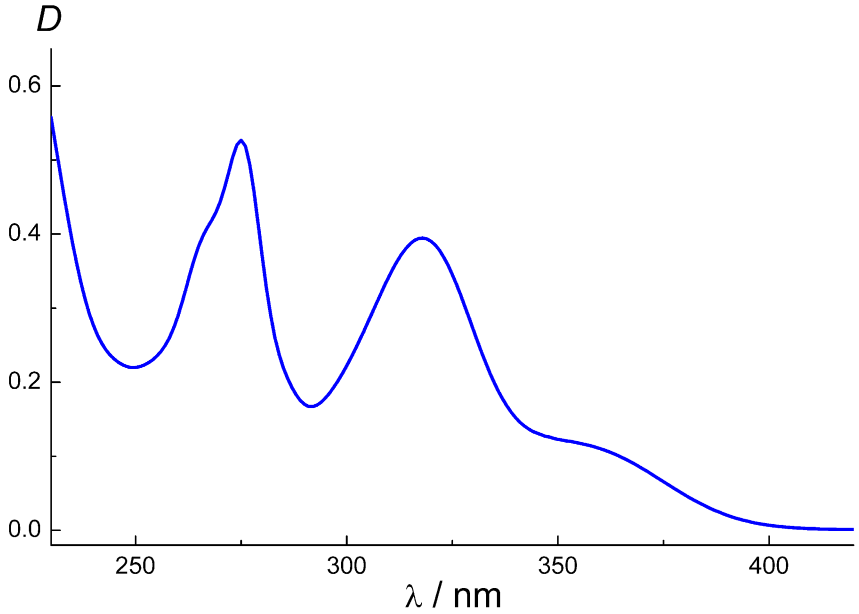


Fig. S22 NOESY spectrum of an equimolar mixture of compound **3** and β-CD ($C_3 = C_{CD} = 6\times10^{-3}$ M), D_2O, 25 °C.



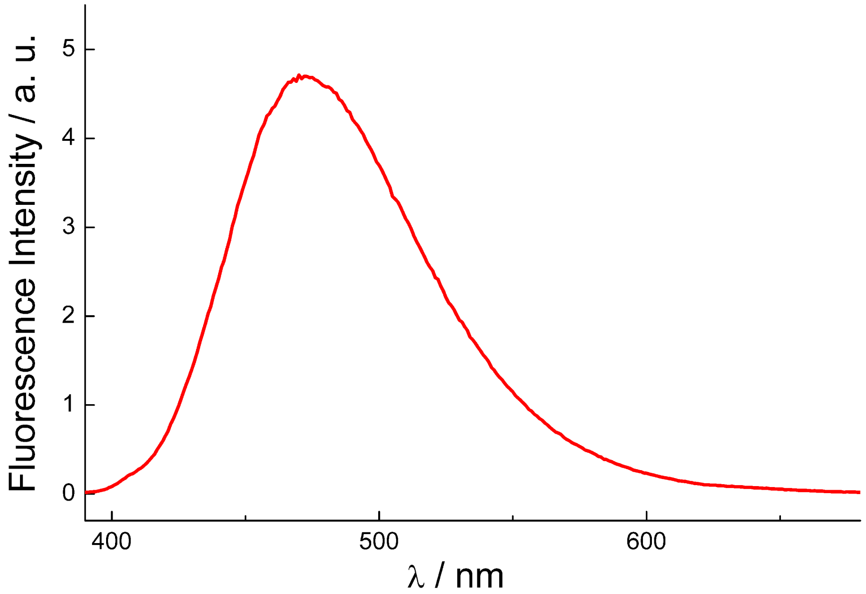
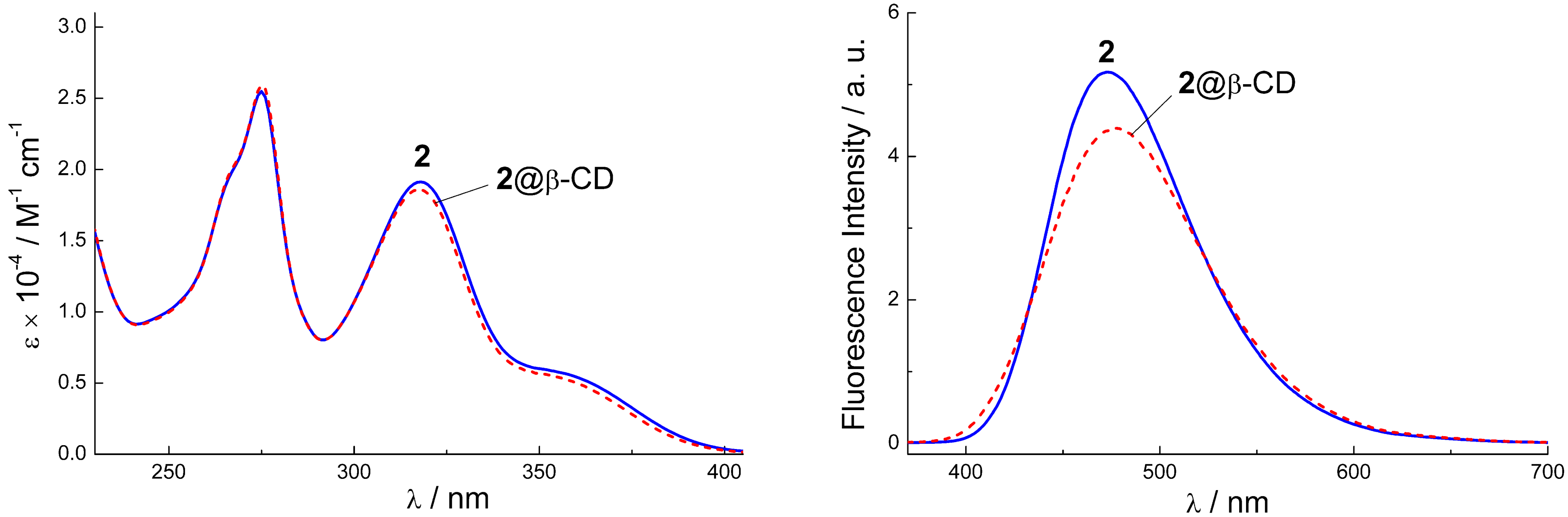


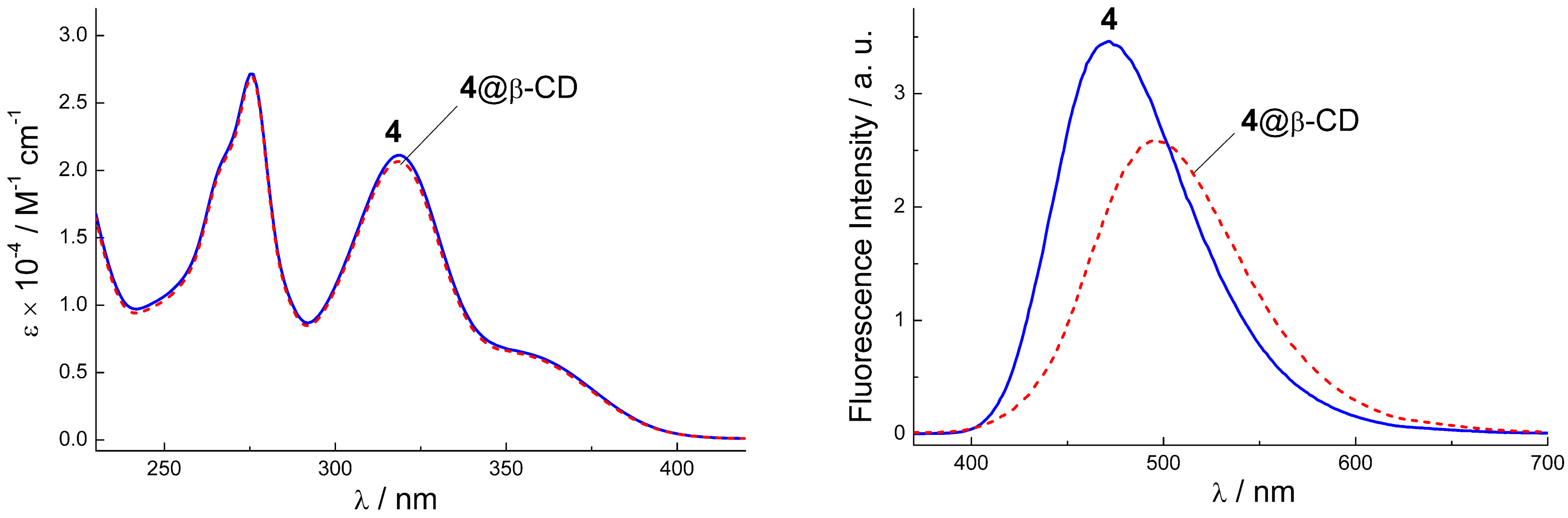
Fig. S23 Absorption spectrum of compound **1** (C = 2×10^{-5} M), water, ambient temperature, 1-cm quartz cell.

Fig. S24 Fluorescence spectrum of compound **1** (C = 1×10^{-6} M), water, ambient temperature. The fluorescence was excited by light at 356 nm.



(*a*) (*b*)

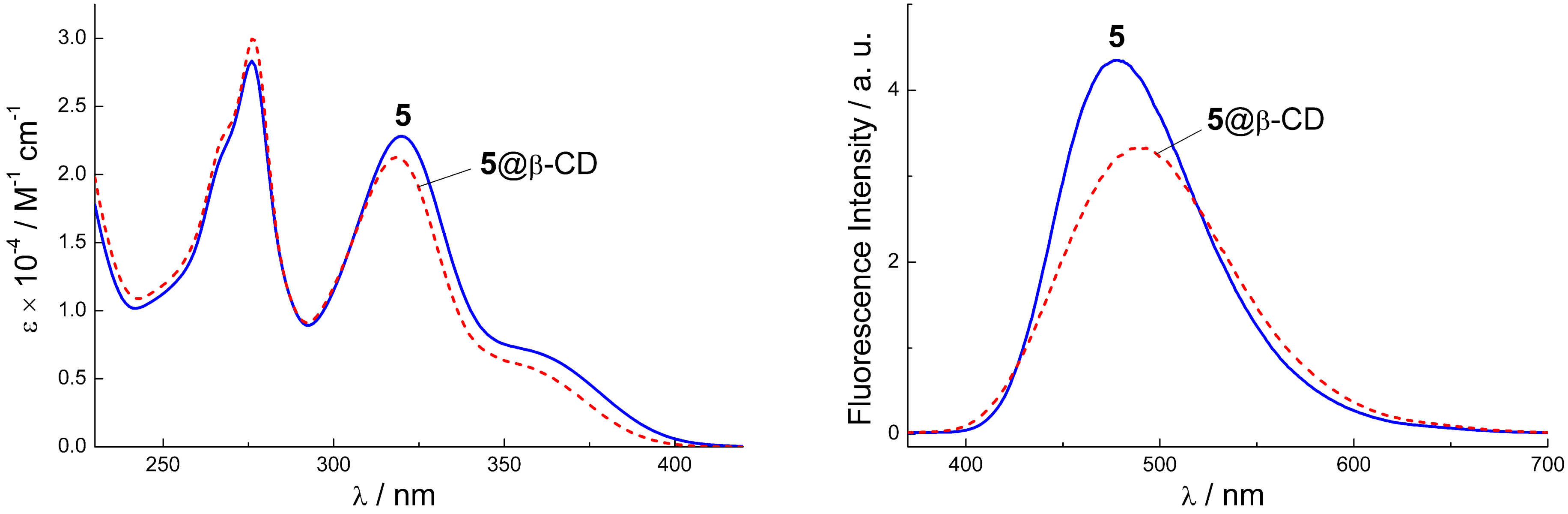
Fig. S25 (*a*) Absorption and (*b*) fluorescence spectra of compound **2** ($C_2 = 2\times10^{-5}$ M for absorption and $C_2 = 1\times10^{-5}$ M for fluorescence) and respective evaluated spectra of complex **2**@β-CD, water, ambient temperature. The fluorescence was excited by light at 313 nm.



(*a*) (*b*)

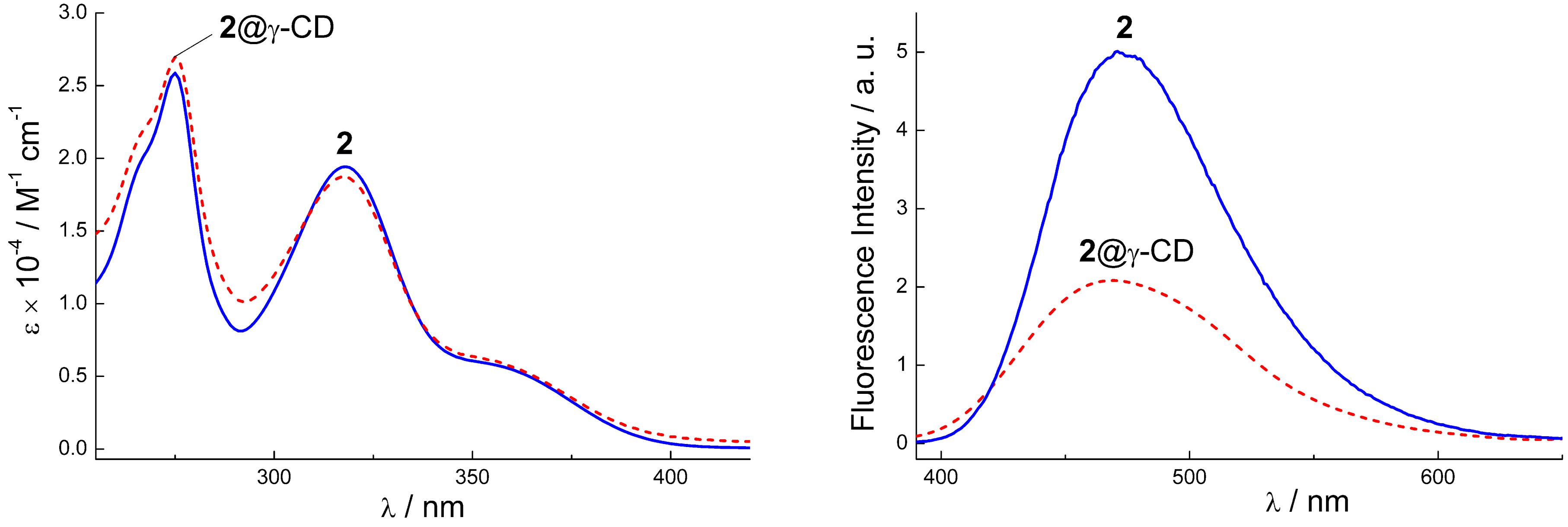
(*l*

Fig. S26 (*a*) Absorption and (*b*) fluorescence spectra of compound **4** ($C_{\mathbf{4}}$ = 2×10^{-5} M for absorption and $C_{\mathbf{4}}$ = 1×10^{-5} M for fluorescence) and respective evaluated spectra of complex **4**@β-CD, water, ambient temperature. The fluorescence was excited by light at 319 nm.



(*a*) (*b*)

Fig. S27 (*a*) Absorption and (*b*) fluorescence spectra of compound **5** ($C_5 = 2\times10^{-5}$ M for absorption and $C_5 = 1\times10^{-5}$ M for fluorescence) and respective evaluated spectra of complex **5**@β-CD, water, ambient temperature. The fluorescence was excited by light at 311 nm.



(*a*) (*b*)

Fig. S28 (*a*) Absorption and (*b*) fluorescence spectra of compound **2** ($C_2 = 2\times10^{-5}$ M for absorption and $C_2 = 1\times10^{-5}$ M for fluorescence) and respective evaluated spectra of complex **2**@γ-CD, water, ambient temperature. The fluorescence was excited by light at 332 nm.

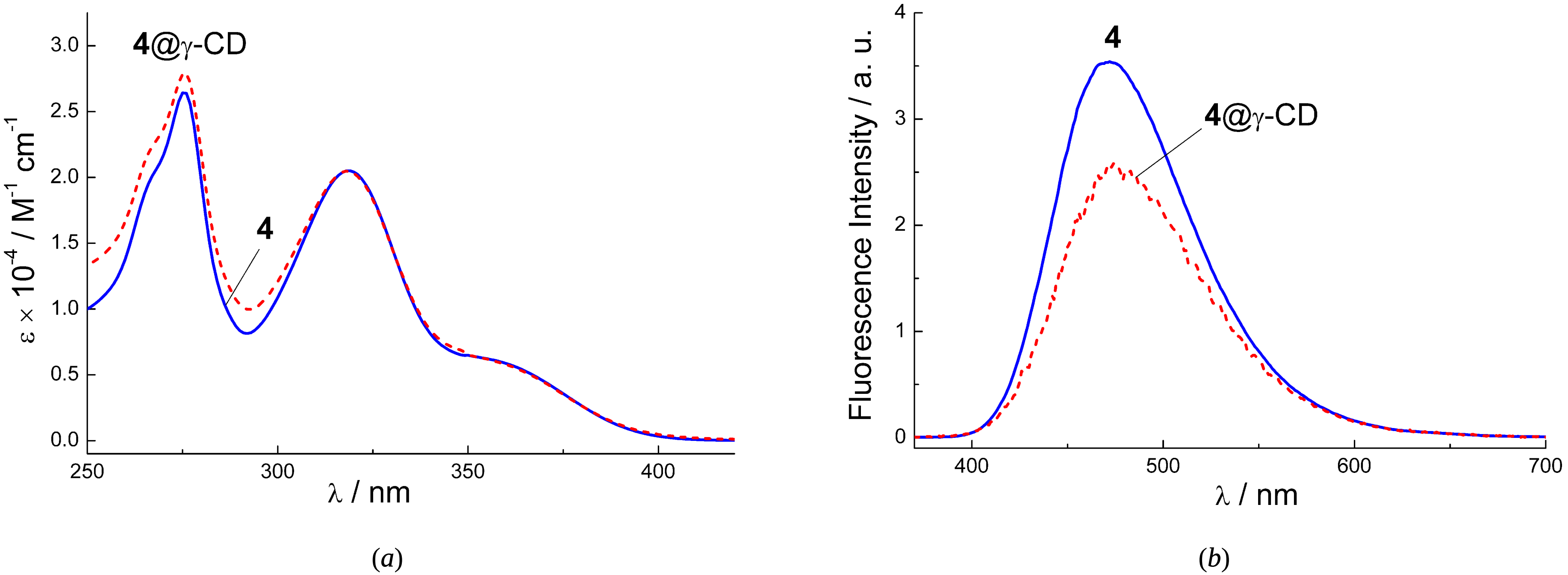
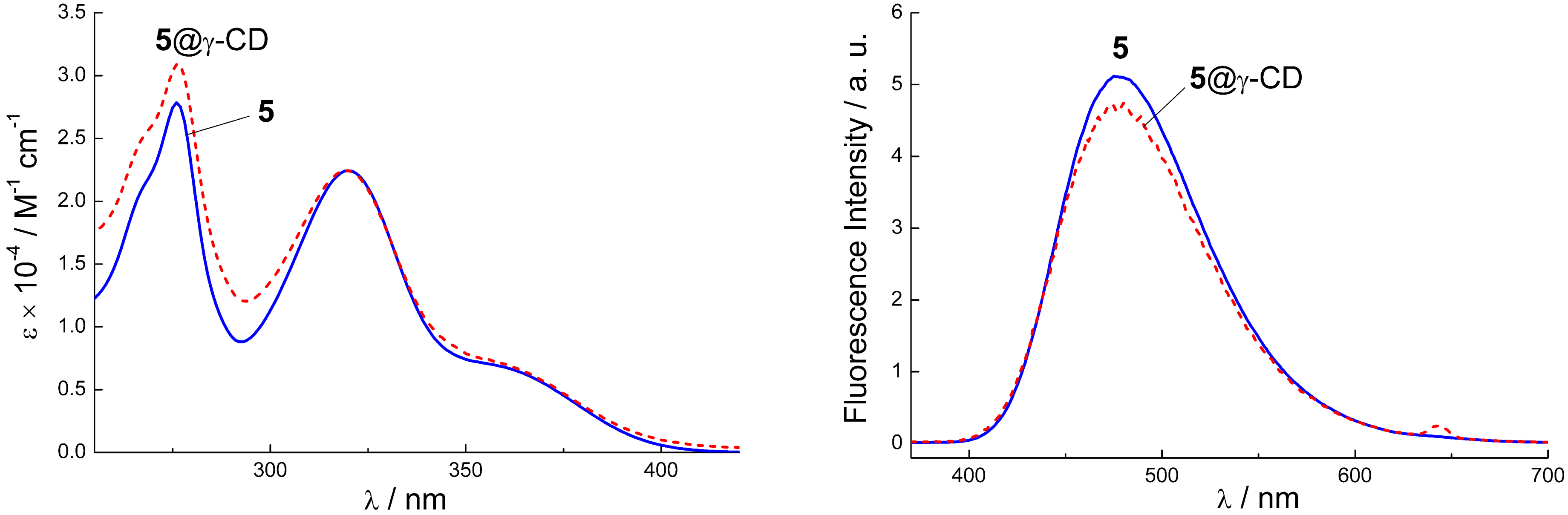
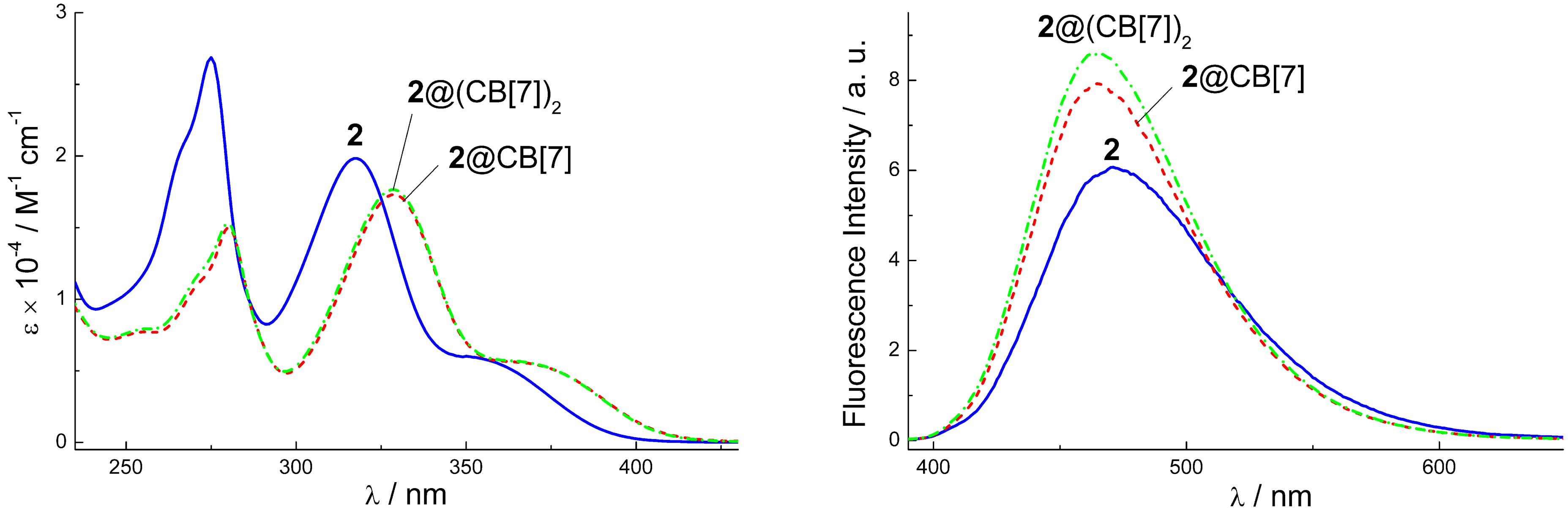


Fig. S29 (*a*) Absorption and (*b*) fluorescence spectra of compound **4** (C_4 = 2×10^{-5} M for absorption and C_4 = 1×10^{-5} M for fluorescence) and respective evaluated spectra of complex **4**@γ-CD, water, ambient temperature. The fluorescence was excited by light at 319 nm.



(*a*) (*b*)

Fig. S30 (*a*) Absorption and (*b*) fluorescence spectra of compound **5** ($C_5 = 2\times10^{-5}$ M for absorption and $C_5 = 1\times10^{-5}$ M for fluorescence) and respective evaluated spectra of complex **5**@γ-CD, water, ambient temperature. The fluorescence was excited by light at 321 nm.



(*a*) (*b*)

Fig. S31 (*a*) Absorption and (*b*) fluorescence spectra of compound **2** (C_2 = 2×10^{-5} M for absorption and C_2 = 1×10^{-6} M for fluorescence) and respective evaluated spectra of complexes **2**@CB[7] and **2**@(CB[7])$_2$, water, ambient temperature. The fluorescence was excited by light at 356 nm.

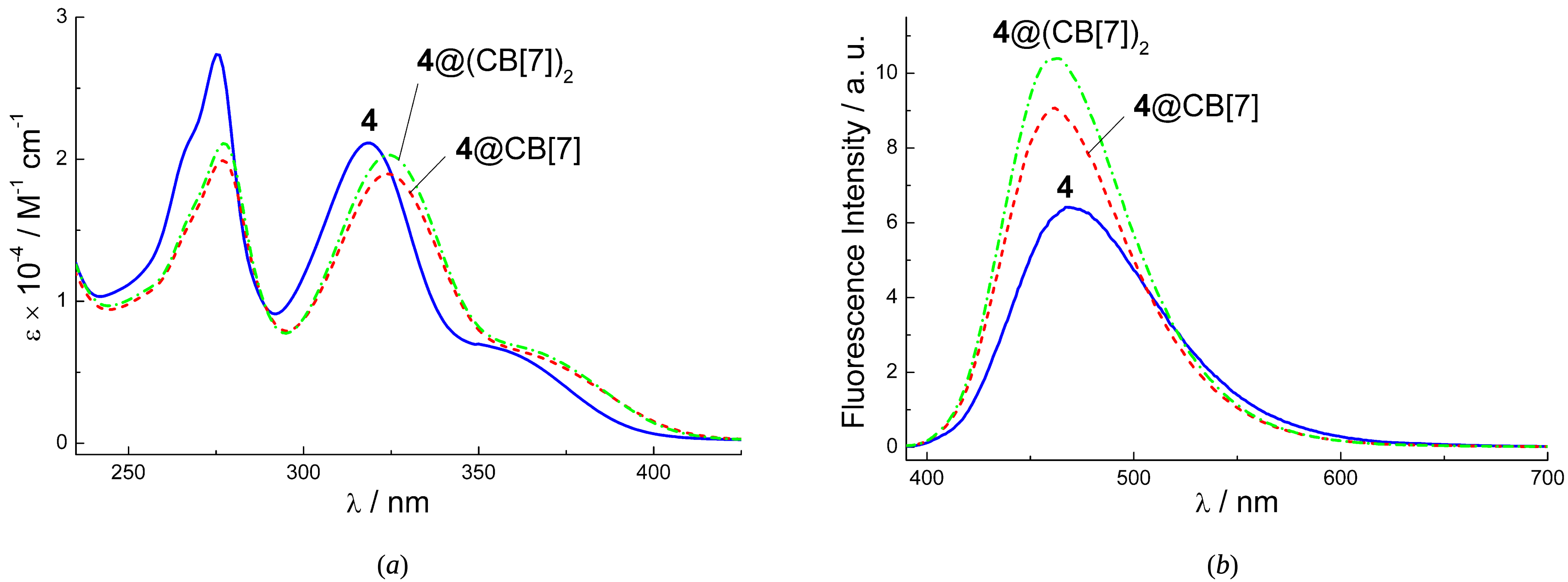
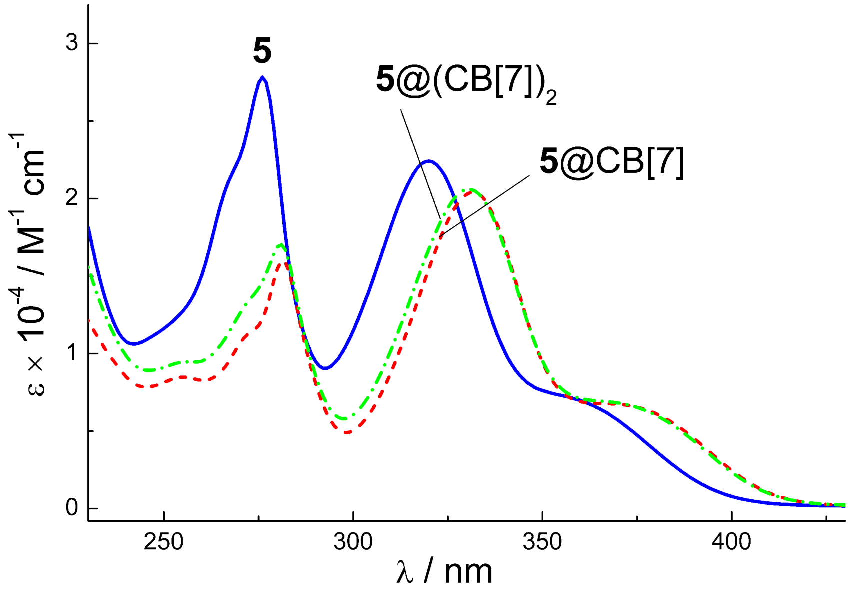
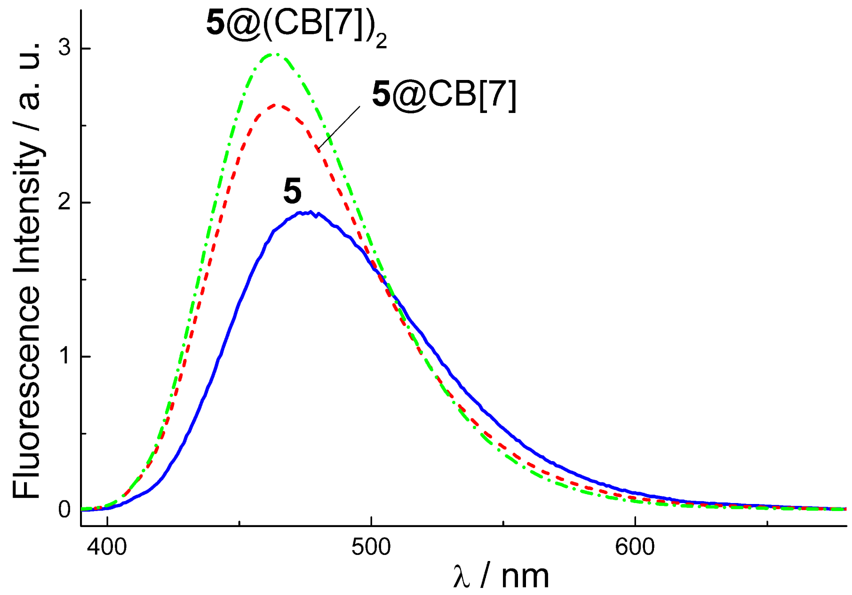


Fig. S32 (*a*) Absorption and (*b*) fluorescence spectra of compound **4** (C_4 = 2×10^{-5} M for absorption and C_4 = 1×10^{-6} M for fluorescence) and respective evaluated spectra of complexes **4**@CB[7] and **4**@(CB[7])$_2$, water, ambient temperature. The fluorescence was excited by light at 356 nm.



(*a*)



(*b*)

Fig. S33 (*a*) Absorption and (*b*) fluorescence spectra of compound **5** (C_5 = 2×10^{-5} M for absorption and C_5 = 1×10^{-6} M for fluorescence) and respective evaluated spectra of complexes **5**@CB[7] and **5**@(CB[7])$_2$, water, ambient temperature. The fluorescence was excited by light at 359 nm.

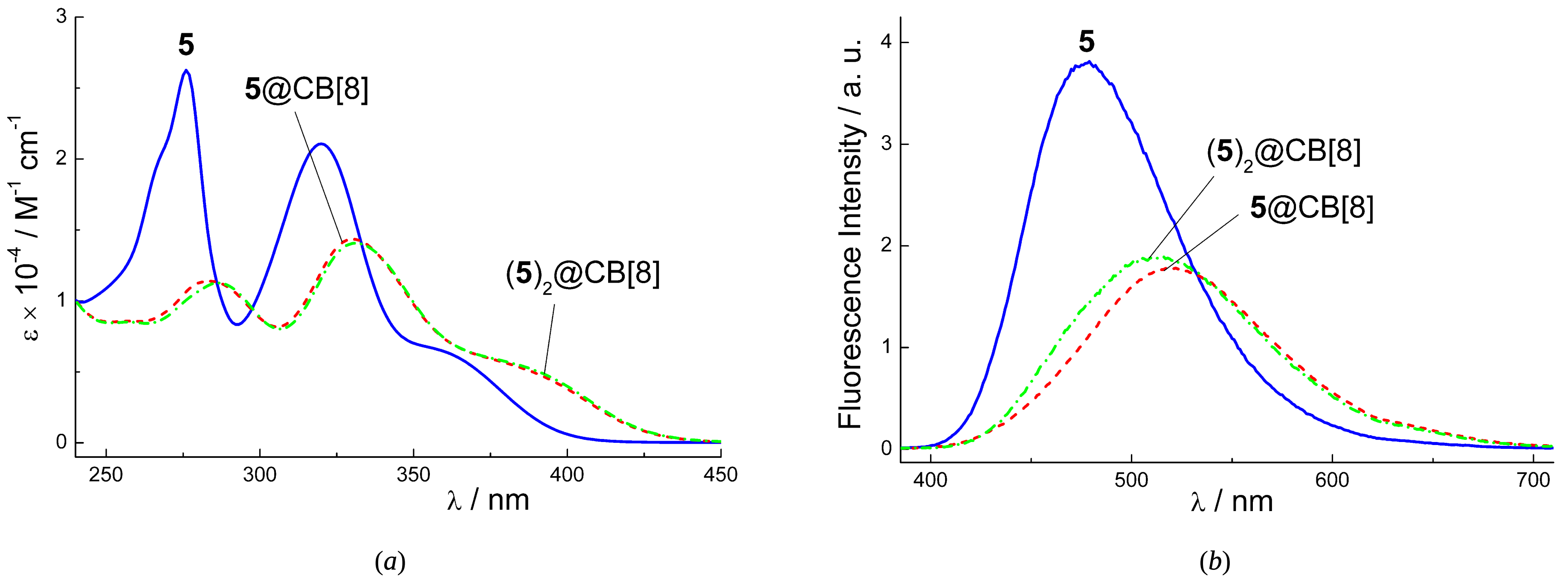


Fig. S34 (*a*) Absorption and (*b*) fluorescence spectra of compound **5** (C_5 = 2×10^{-5} M for absorption and C_5 = 1×10^{-6} M for fluorescence) and respective evaluated spectra of complexes **5**@CB[8] and (**5**)$_2$@CB[8] (per molecule of naphthylpyridine derivative), water, ambient temperature. The fluorescence was excited by light at 333 nm.