Support Information

for

Template-Assisted Stereoselective Photocyclodimerization of 2-Anthracenecarboxylic Acid by Bispyridinio-Appended γ-Cyclodextrin

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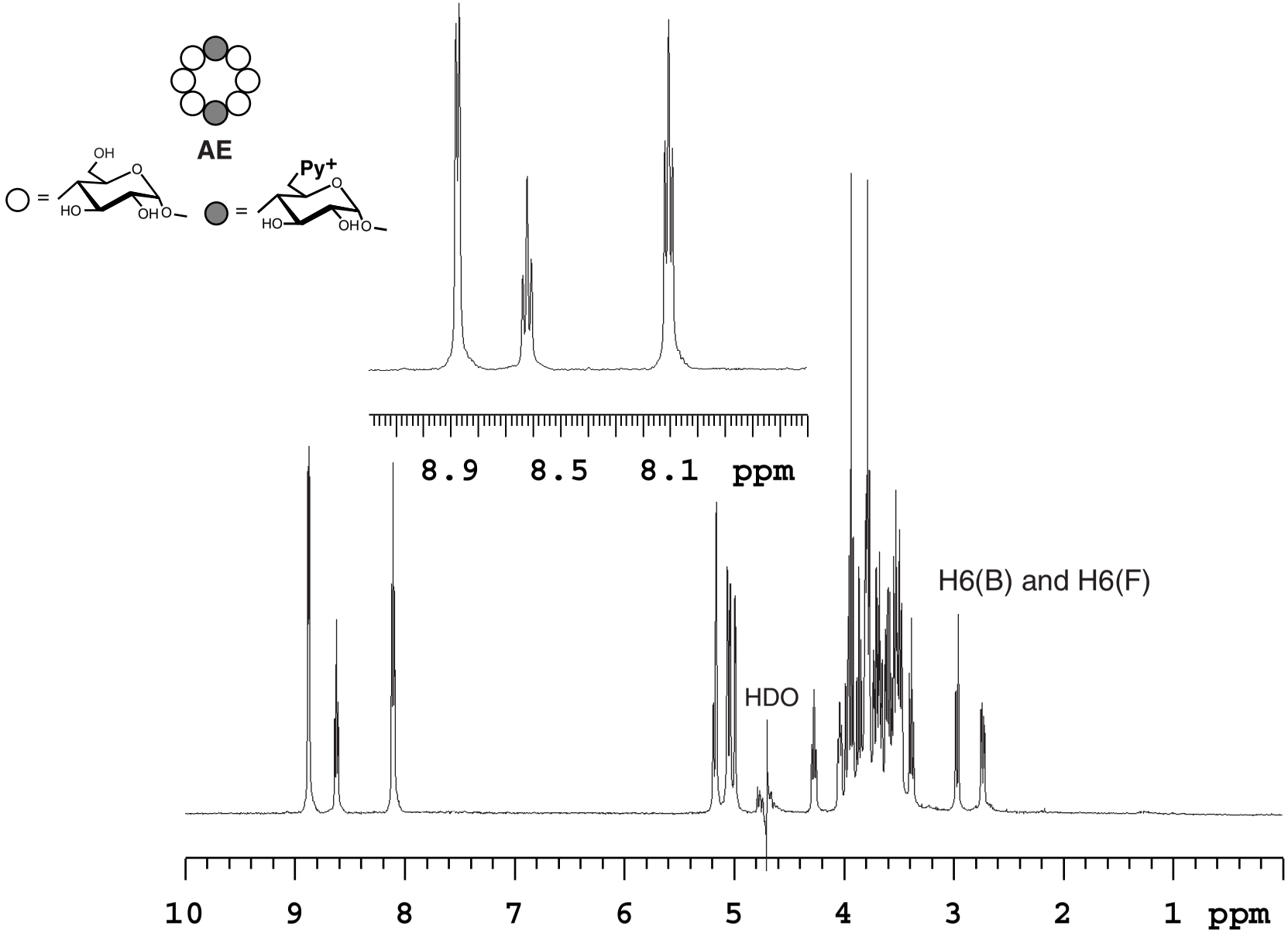

Figure S1 ^{1}H NMR Spectrum of **Py2(AE)-γ-CD** in D_2O at 25 °C.

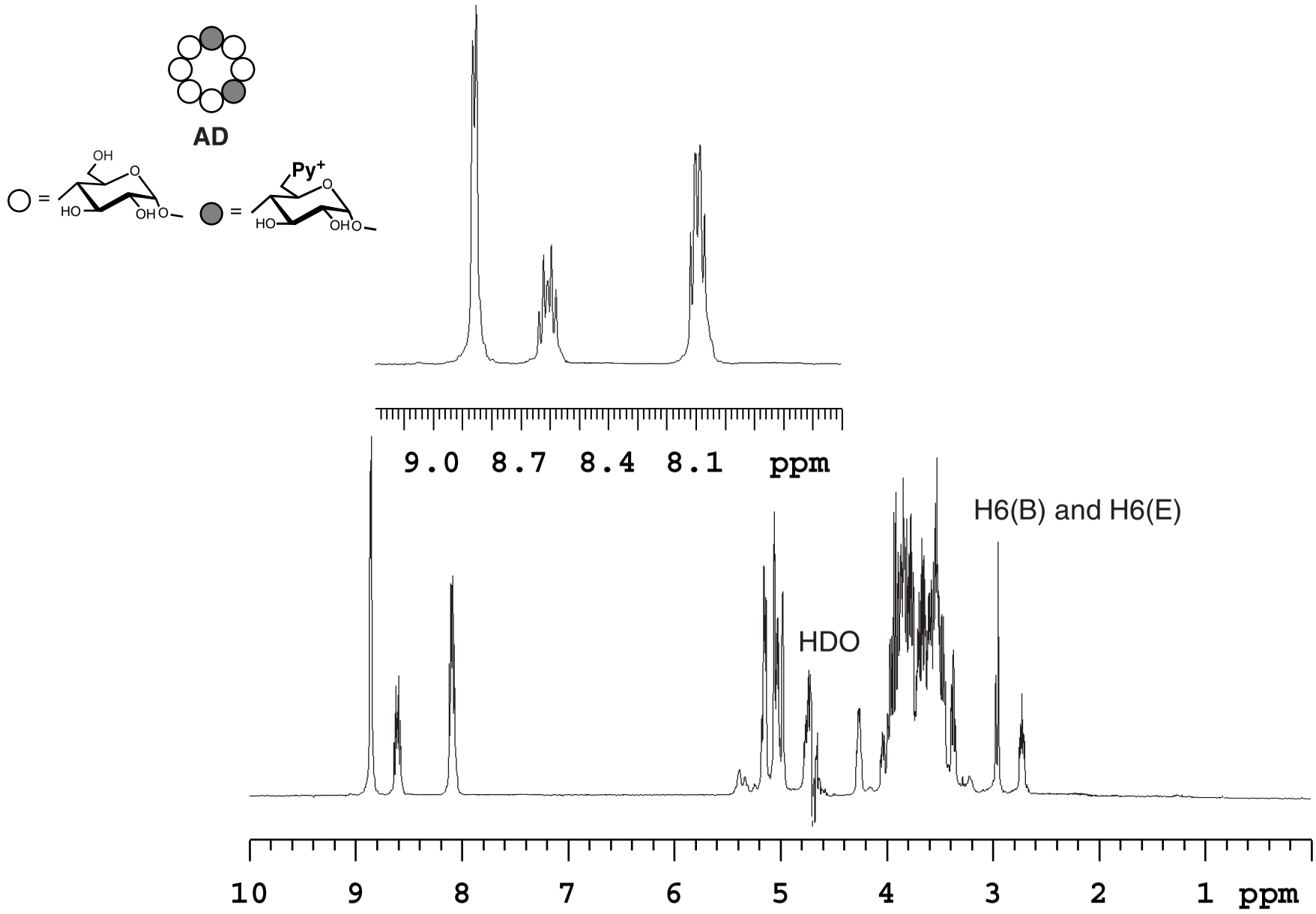

Figure S2 ^{1}H NMR Spectrum of **Py2(AD)-γ-CD** in D_2O at 25 °C.

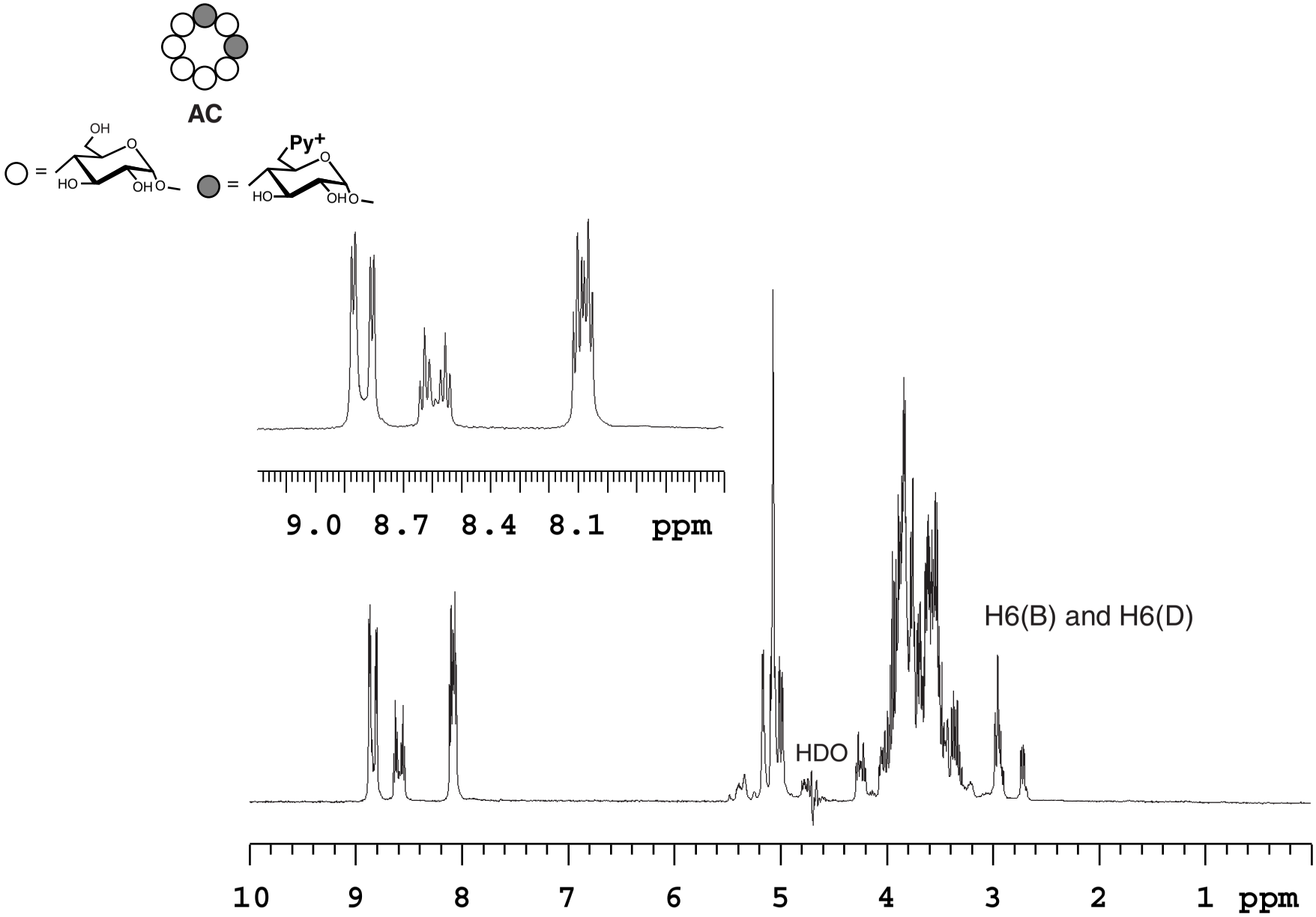

Figure S3 ^{1}H NMR Spectrum of **Py2(AC)-γ-CD** in D_2O at 25 °C

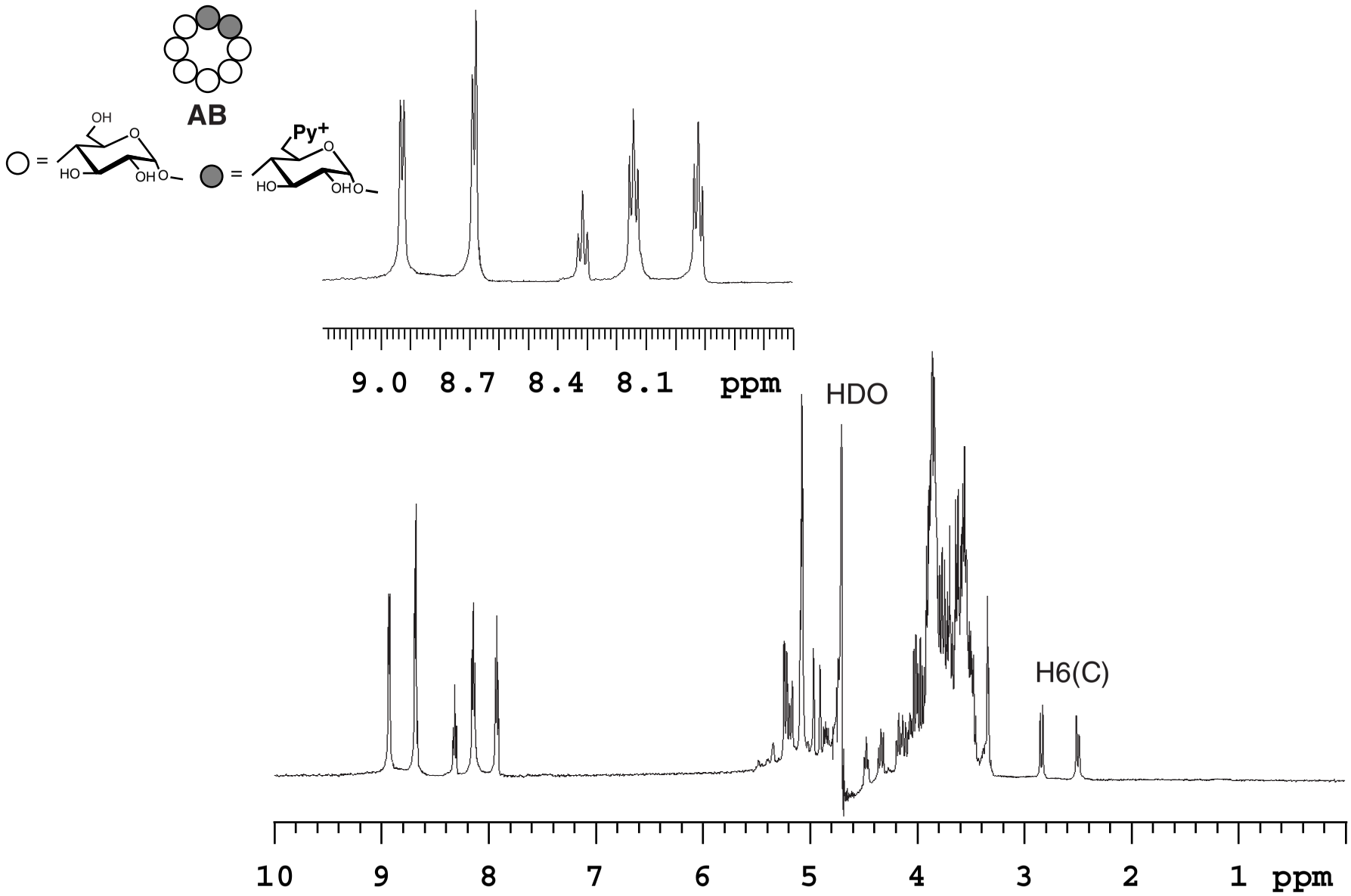

Figure S4 ^{1}H NMR Spectrum of **Py2(AB)-γ-CD** in D_2O at 25 °C.

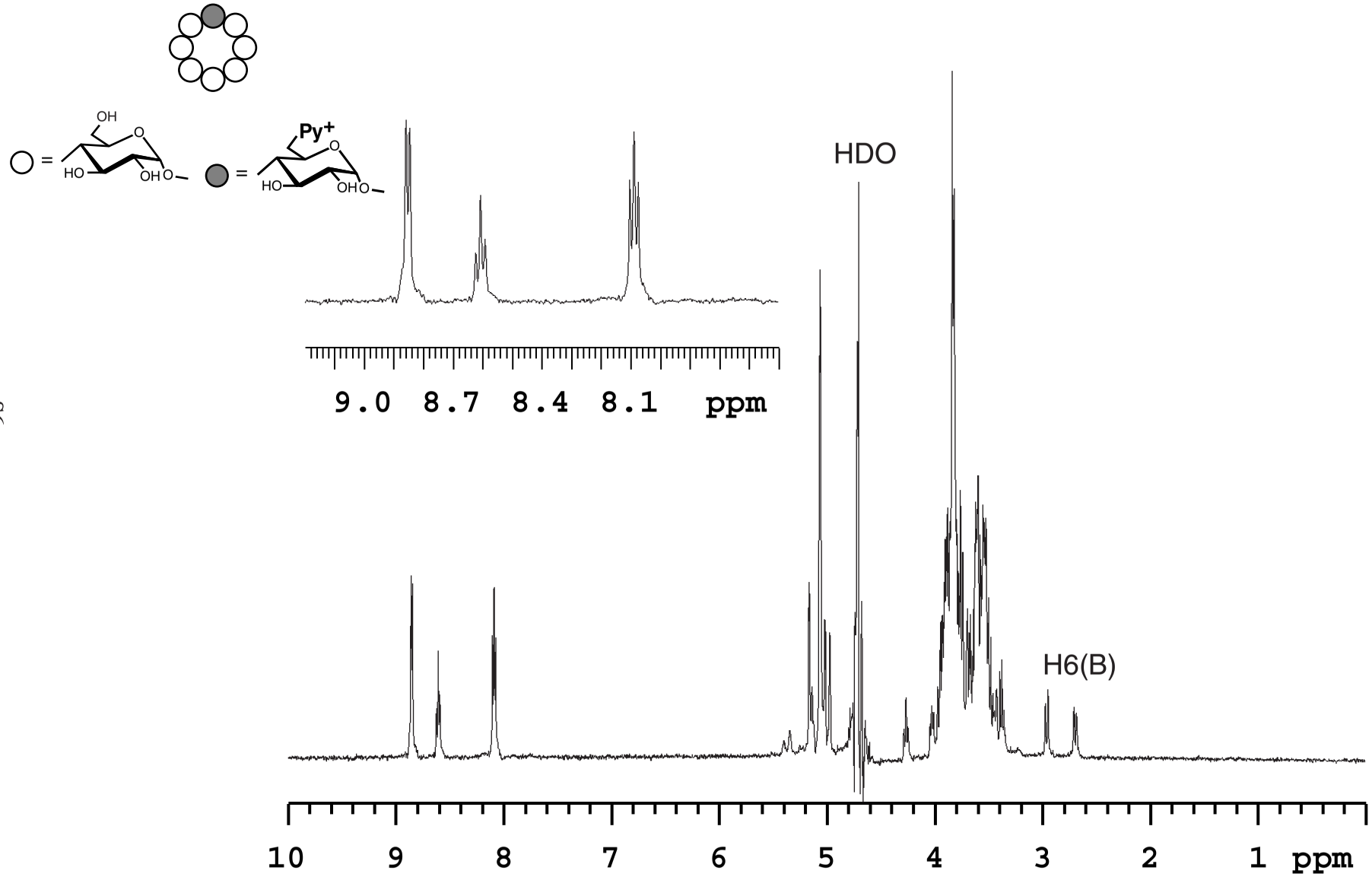

Figure S5 ^{1}H NMR Spectrum of **Py-γ-CD** in D_2O at 25 °C.

Assinments of ^{1}H NMR spectra of pyridinio-modified CDs

Py2(AE)-γ-CD

^{1}H NMR (500 MHz, D_2O): δ =2.73 (dd, *J* = 4.5, 12.3 Hz, 2H, H-6b, H-6b), 2.97 (dd, *J* = 2.2, 12.3 Hz, 2H, H-6a, H-6a), 4.99 (d, *J* = 3.9 Hz, 2H, H-1), 5.03 (d, *J* = 3.9 Hz, 2H, H-1), 5.06 (d, *J* = 4.2 Hz, 2H, H-1), 5.16 (d, *J* = 3.9 Hz, 2H, H-1), 8.10 (dd, *J* = 7.8, 6.8 Hz, 4H, Py-3), 8.62 (tt, *J* = 7.8, 1.2 Hz, 2H, Py-4), 8.87 (dd, *J* = 6.8, 1.2 Hz, 4H, Py-2).

Py2(AD)-γ-CD

^{1}H NMR (500 MHz, D_2O): δ = 2.73 (dd, *J* = 4.4, 12.3 Hz, 1H, H-6b), 2.74 (dd, *J* = 4.8, 12.3 Hz, 1H, H-6b), 2.97 (bd, *J* = 12.3 Hz, 2H, H-6a), 4.99 (bd, *J* = 3.9 Hz, 2H, H-1), 5.03 (d, *J* = 3.9 Hz, 1H, H-1), 5.04 (d, *J* = 3.7 Hz, 1H, H-1), 5.06 (d, *J* = 3.9 Hz, 1H, H-1), 5.07 (d, *J* = 3.9 Hz, 1H, H-1), 5.15 (d, *J* = 3.9 Hz, 1H, H-1), 5.16 (d, *J* = 3.9 Hz, 1H, H-1), 8.09 (t, *J* = 7.2 Hz, 2H, Py-3), 8.11 (t, *J* = 7.2 Hz, 2H, Py-3), 8.60 (t, *J* = 7.2 Hz, 1H, Py-4), 8.63 (t, *J* = 7.2 Hz, 1H, Py-4), 8.87 (d, *J* = 7.2 Hz, 4H, Py-2).

Py2(AC)-γ-CD

^{1}H NMR (500 MHz, D_2O): δ = 2.72 (dd, *J* = 4.3, 12.3 Hz, 1H, H-6b), 2.92 (dd, *J* = 6.4, 12.3 Hz, 1H, H-6b), 2.97 (dd, *J* = 2.2, 12.3 Hz, 1H, H-6a), 2.97 (dd, *J* = 2.2, 12.3 Hz, 1H, H-6a), 4.98 (d, *J* = 3.9 Hz, 1H, H-1), 5.01 (d, *J* = 3.9 Hz, 1H, H-1), 5.07 (d, *J* = 3.9 Hz, 3H, H-1), 5.08 (d, *J* = 3.9 Hz, 1H, H-1), 5.09 (d, *J* = 3.9 Hz, 1H, H-1), 5.17 (d, *J* = 3.9 Hz, 1H, H-1), 8.07 (dd, *J* = 7.8, 6.8 Hz, 2H, Py-3), 8.10 (dd, *J* = 7.8, 6.8 Hz, 2H, Py-3), 8.55 (tt, *J* = 7.8, 1.2 Hz, 1H, Py-4), 8.63 (tt, *J* = 7.8, 1.2 Hz, 1H, Py-4), 8.81 (dd, *J* = 6.8, 1.2 Hz, 2H, Py-2), 8.87 (dd, *J* = 6.8, 1.2 Hz, 2H, Py-2).

Py2(AB)-γ-CD

^{1}H NMR (500 MHz, D_2O): δ = 2.50 (dd, *J* = 4.0, 12.3 Hz, 1H, H-6b), 2.84 (bd, *J* = 12.3 Hz, 1H, H-6a), 4.90 (d, *J* = 3.4 Hz, 1H, H-1), 4.97 (d, *J* = 3.9 Hz, 1H, H-1), 5.07 (d, *J* = 3.9 Hz, 2H, H-1), 5.09 (d, *J* = 3.9 Hz, 2H, H-1), 5.22 (d, *J* = 3.9 Hz, 1H, H-1), 5.24 (d, *J* = 3.9 Hz, 1H, H-1), 7.92 (dd, *J* = 7.8, 6.8 Hz, 2H, Py-3), 8.14 (dd, *J* = 7.8, 6.8 Hz, 2H, Py-3), 8.31 (tt, *J* = 7.8, 1.2 Hz, 1H, Py-4), 8.68 (tt, *J* = 7.8, 1.2 Hz, 1H, Py-4), 8.68 (dd, *J* = 6.8, 1.2 Hz, 2H, Py-2), 8.93 (dd, *J* = 6.8, 1.2 Hz, 2H, Py-2).

Py-γ-CD

^{1}H NMR (500 MHz, D_2O): δ = 2.69 (dd, *J* = 4.2, 12.6 Hz, 1H, H-6b), 2.96 (dd, *J* = 2.0, 12.6 Hz, 1H, H-6a), 4.97 (d, *J* = 3.9 Hz, 1H, H-1), 5.02 (d, *J* = 3.7 Hz, 1H, H-1), 5.06 (bd, *J* = 3.9 Hz, 5H, H-1), 5.16 (d, *J* = 4.1 Hz, 1H, H-1), 8.09 (t, *J* = 7.6 Hz, 2H, Py-3), 8.61 (t, *J* = 7.6 Hz, 1H, Py-4), 8.85 (d, *J* = 7.6 Hz, 2H, Py-2).