Supplementary Information

Fluorescent Arylethynyl Hamilton Receptors for Barbiturate Sensing

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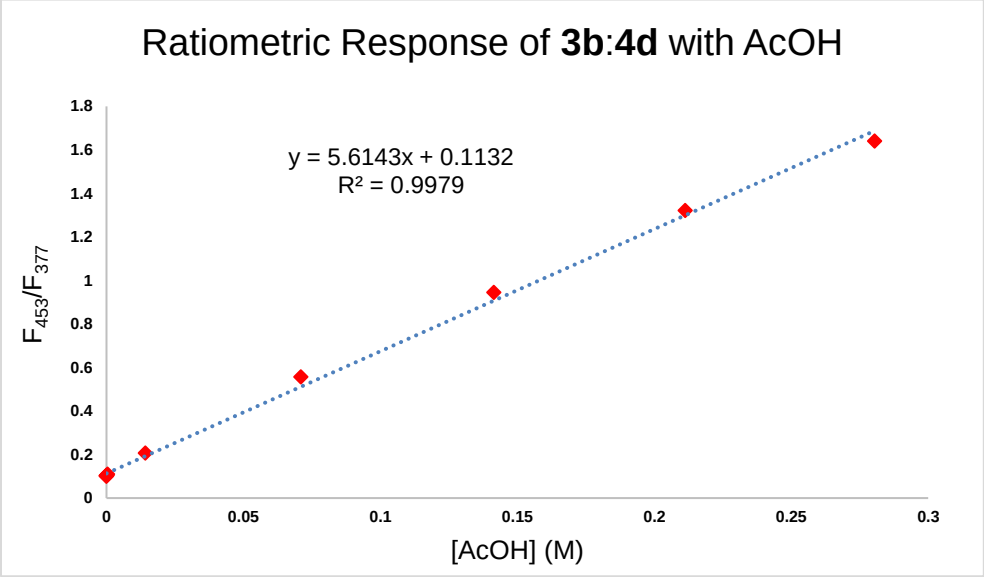

Figure S1. Ratiometric response of **3b:4d** to the addition of AcOH in $CHCl_3$.

Additional Fluorescence and Absorption Spectra

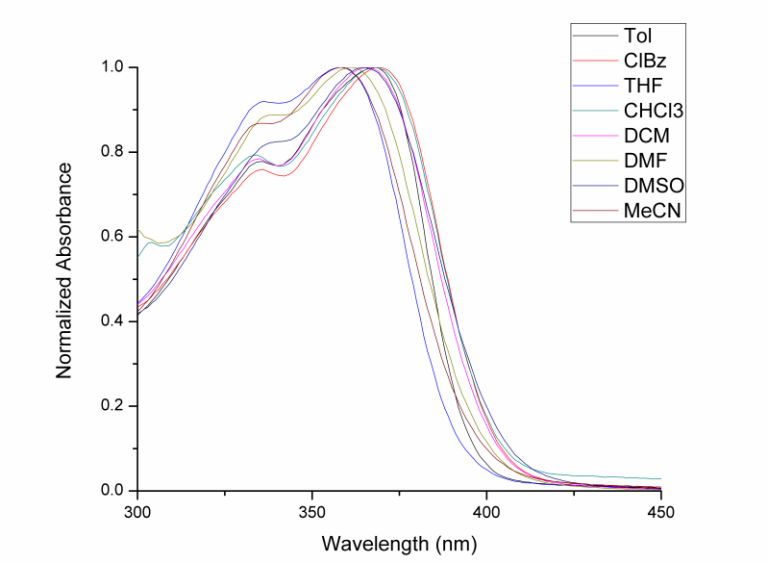

Figure S2. Normalized absorbance spectra of **3e** showing solvatomchromic behavior. [**3e**] = 5.0 µM**.**

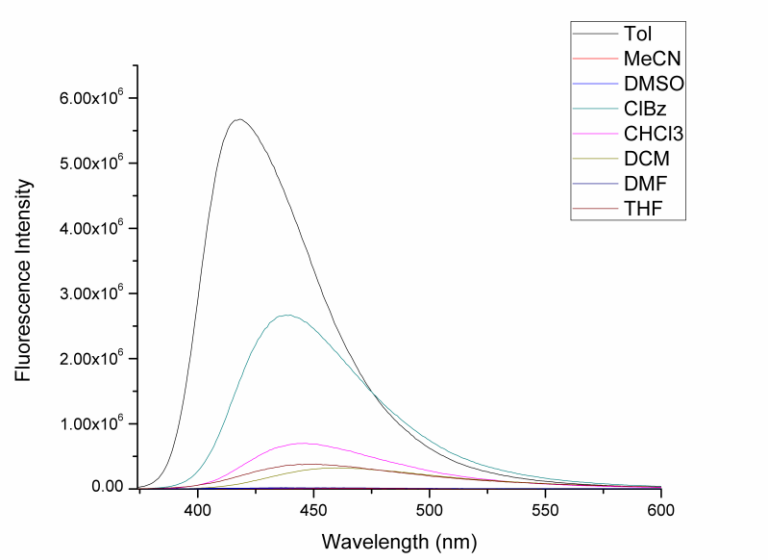

Figure S3. Raw absorbance spectra of **3e** showing decreasing emission intensity as a function of solvent polarity. [**3e**] = 5.0 µM**.**

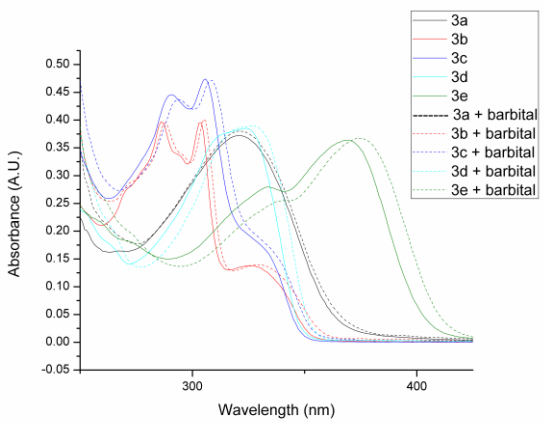

Figure S4. Absorption spectra of **3a-e** in the absence and presence of barbital (100 equiv.) in H_2O sat. $CHCl_3$. [H] = 5 μM.

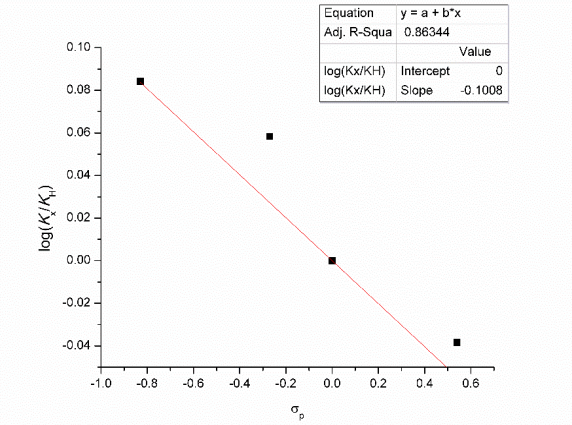

Figure S5. Hammett Plot of binding affinities of **3b-e** with barbital in H_2O sat. $CHCl_3$ at 25 °C.

Table S1. Solvent dependent absorption and emission properties of 3e ([H] = 5 μM).

solvent	absorption λ_{max} (nm)	emission λ_{max} (nm)
toluene	368	418
chloroform	368	447
chlorobenzene	369	440
tetrahydrofuran	359	451
dichloromethane	366	459
acetonitrile	358	479
dimethylformamide	361	438
dimethylsulfoxide	365	464

Representative Binding Isotherms and Raw Fluorescence Data

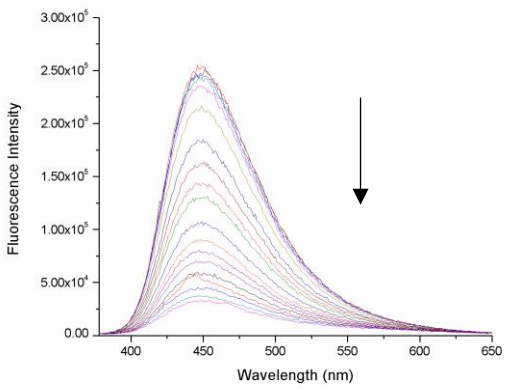

Figure S6. Raw fluorescence data from **3e** with barbital titration.

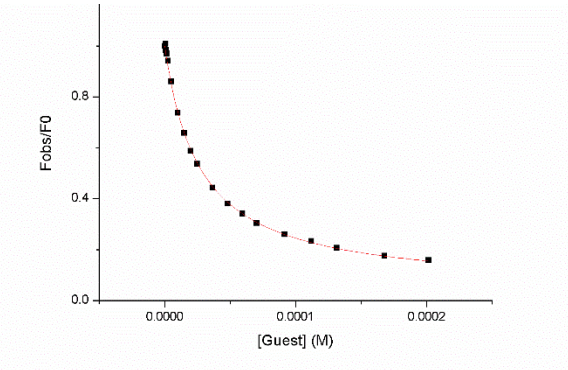

Figure S7. Representative binding isotherm of **3e** with barbital.

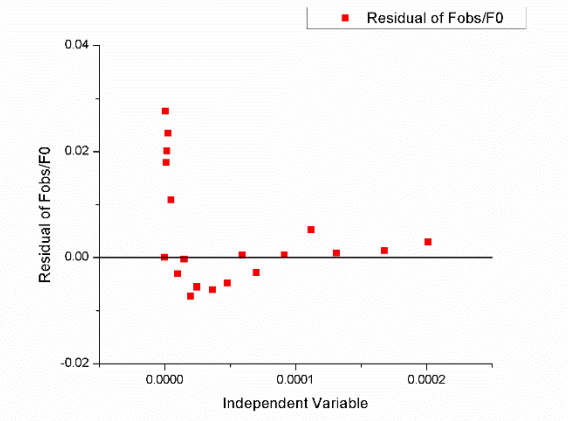

Figure S8. Residuals plot from 1:1 binding model of **3e** with barbital titration.

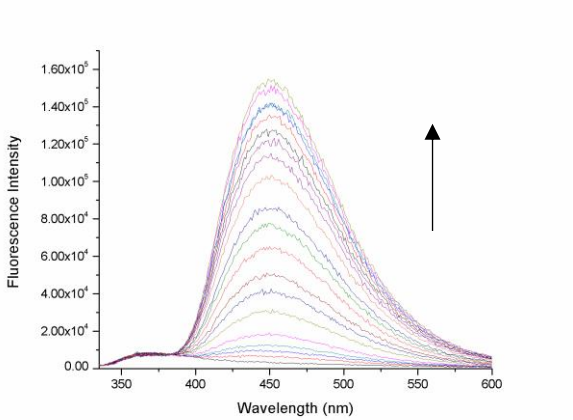

Figure S9. Raw fluorescence data from **3d** with barbital titration.

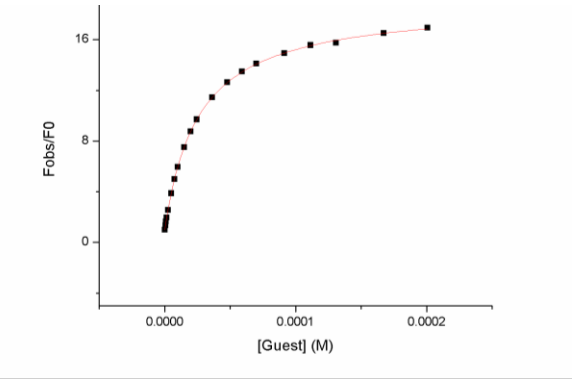

Figure S10. Representative binding isotherm of **3d** with barbital.

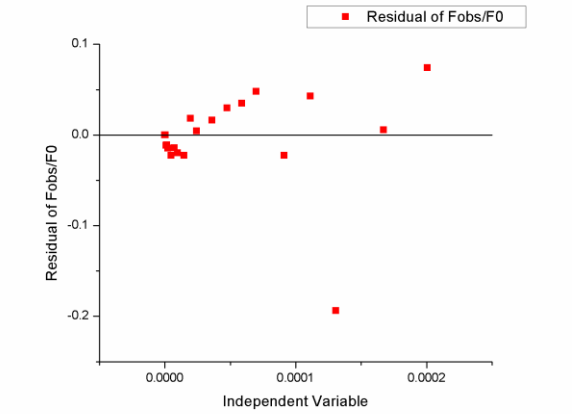

Figure S11. Residuals plot from 1:1 binding model of **3d** with barbital titration.

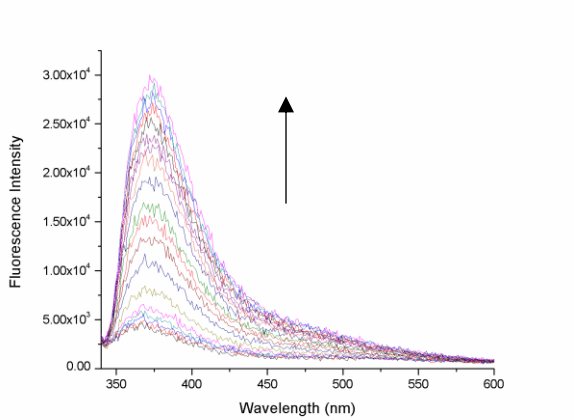

Figure S12 Raw fluorescence data from **3c** with barbital titration.

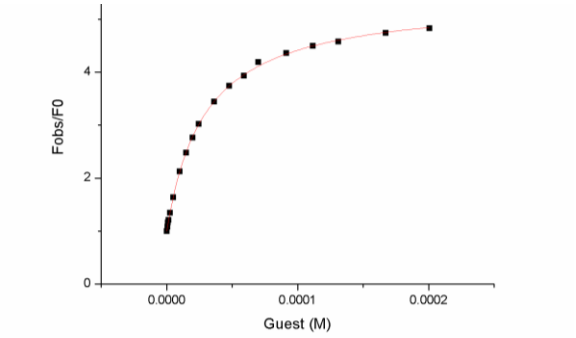

Figure S13. Representative binding isotherm of **3c** with barbital.

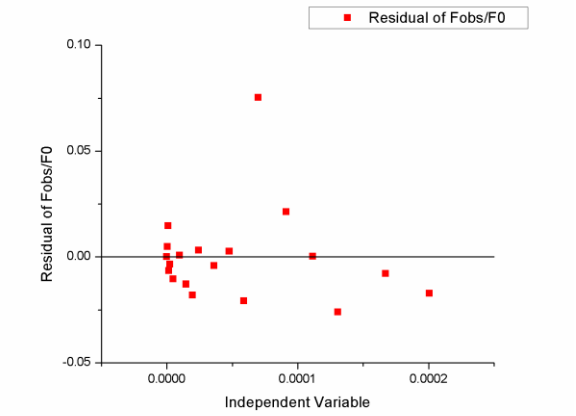

Figure S14. Residuals plot from 1:1 binding model of **3c** with barbital titration.

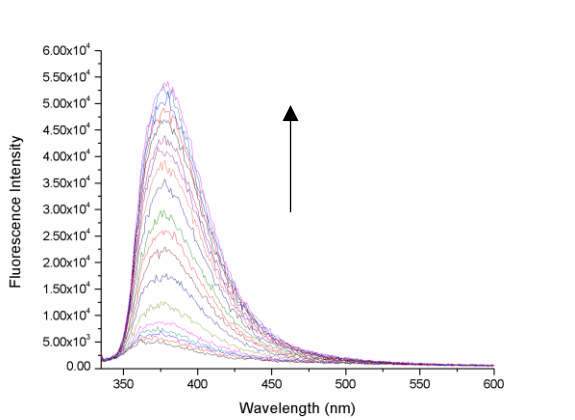

Figure S15. Raw fluorescence data from **3b** with barbital titration

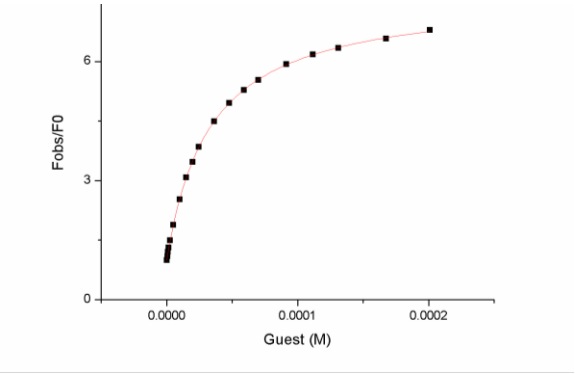

Figure S16. Representative binding isotherm of **3b** with barbital.

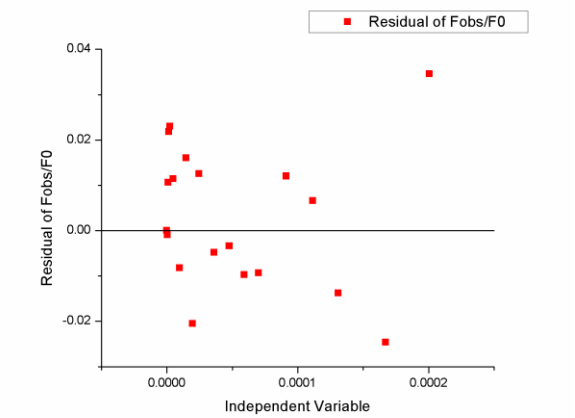

Figure S17. Residuals plot from 1:1 binding model of **3c** with barbital titration.

NMR Spectra.

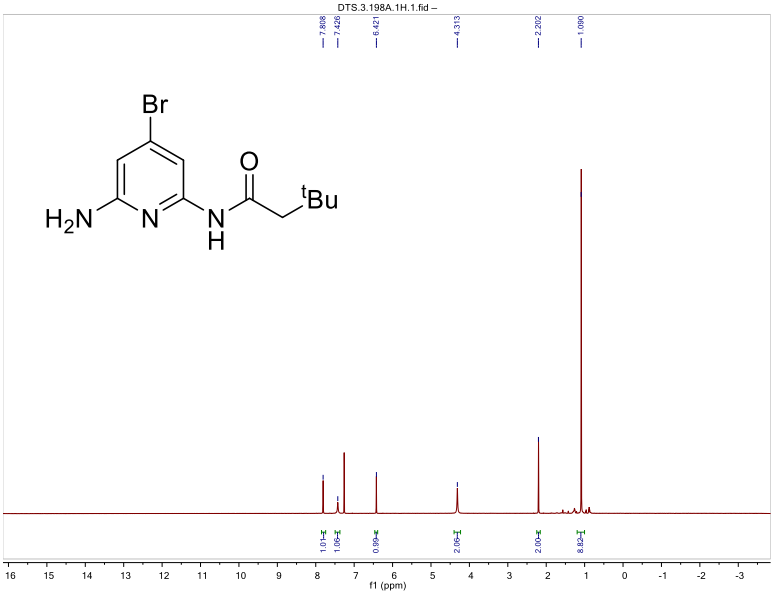

Figure S18. ^{1}H (500 MHz, $CDCl_3$), NMR spectrum of **1**.

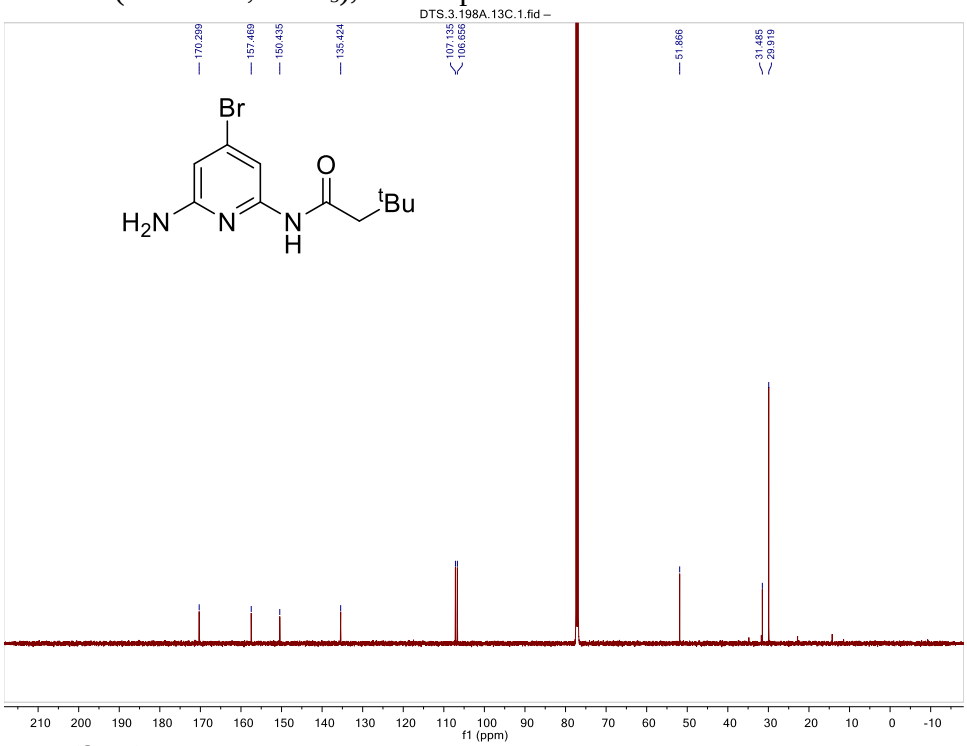

Figure S19. $^{13}C\{^{1}H\}$ (126 MHz, $CDCl_3$) NMR spectrum of **1**.

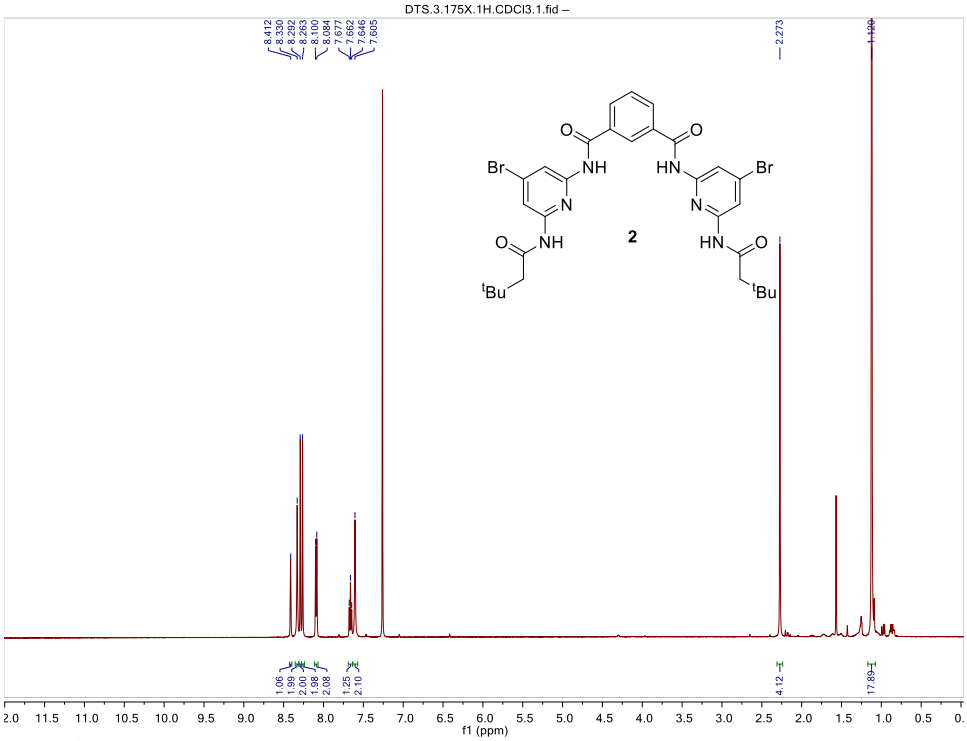

Figure S20. ^{1}H (500 MHz , $CDCl_3$), NMR spectrum of **2**.

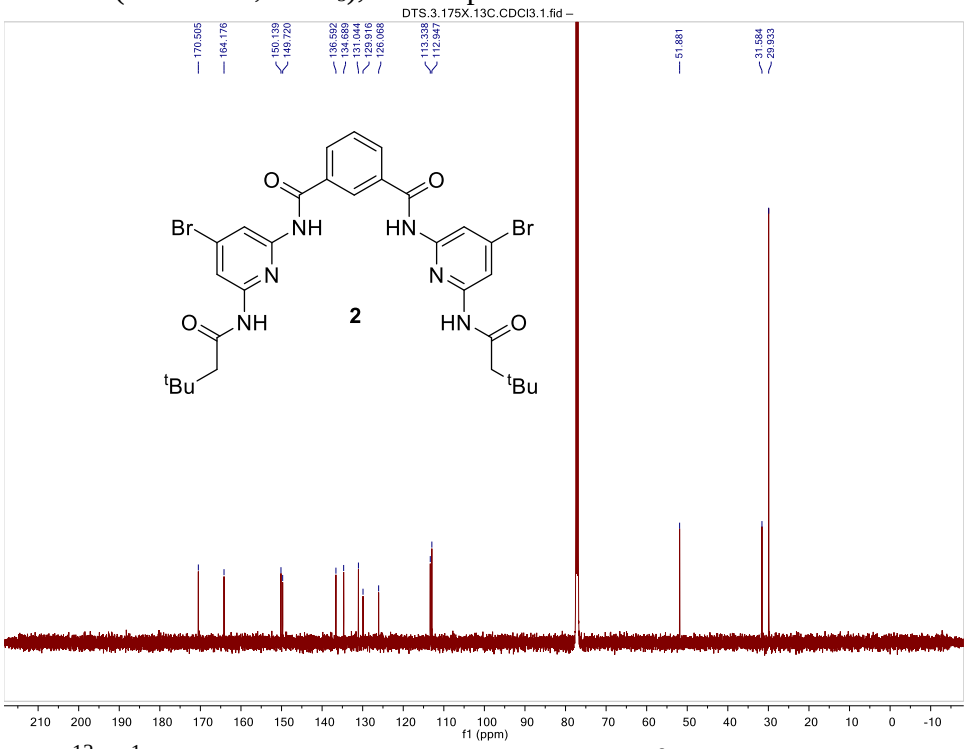

Figure S21. $^{13}C\{^{1}H\}$ (126 MHz, $CDCl_3$) NMR spectrum of **2**.

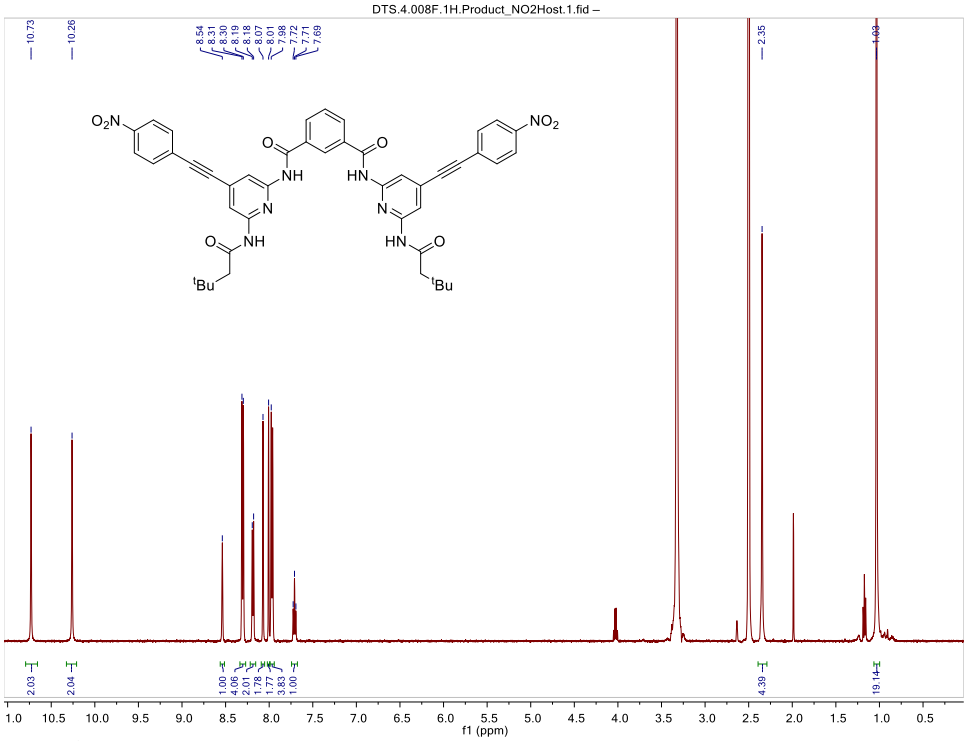

Figure S22. ^{1}H (500 MHz, DMSO-d_6) NMR spectrum of **3a**.

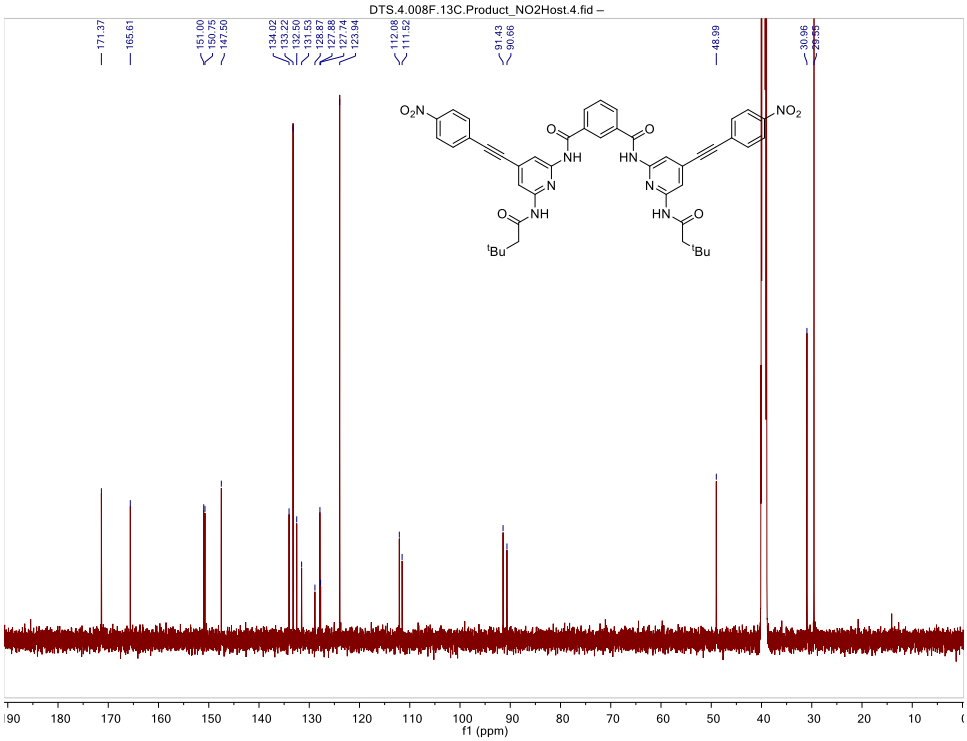

Figure S23. ^{13}C{^{1}H} (126 MHz, DMSO-d_6) NMR spectrum of **3a**.

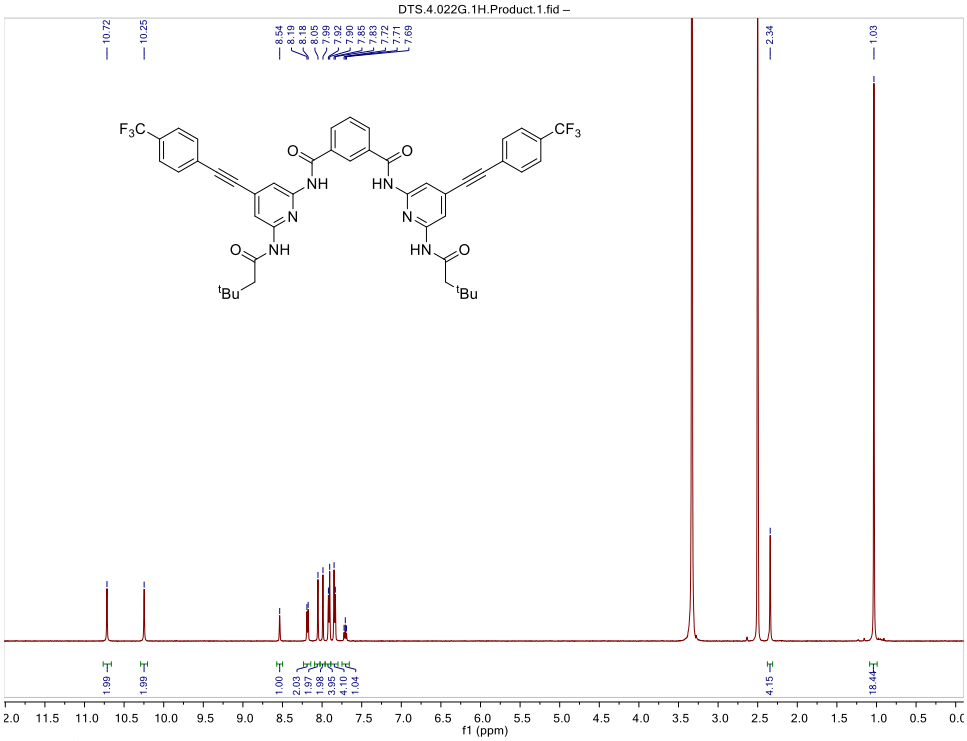

Figure S24. ^{1}H (500 MHz, DMSO-d_6) NMR spectrum of **3b**.

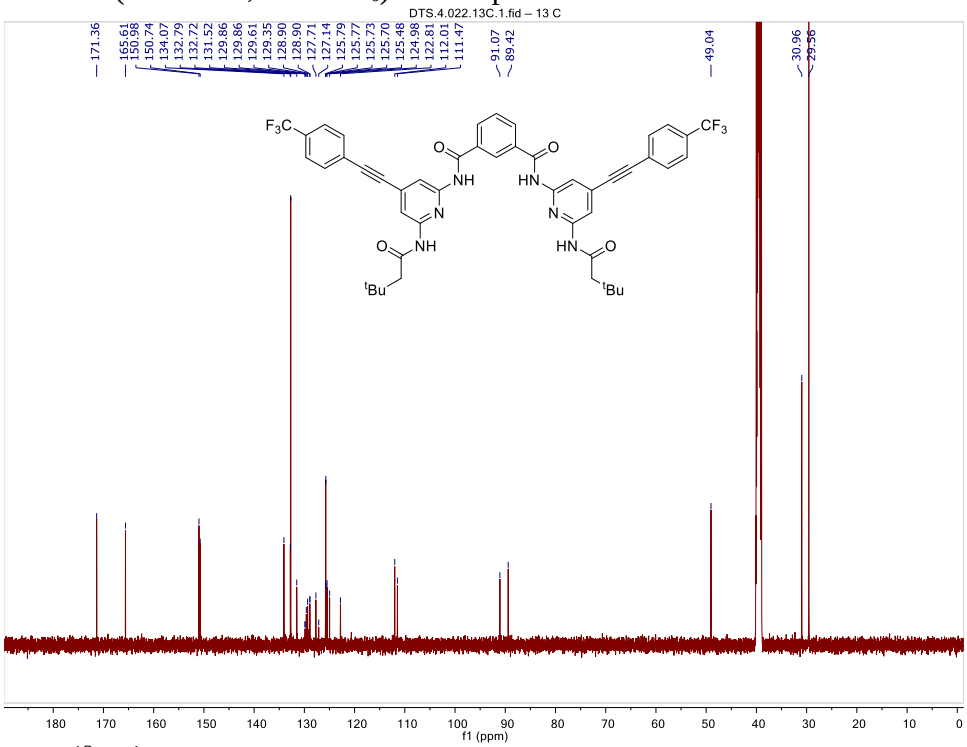

Figure S25. ^{13}C{^{1}H} (126 MHz, DMSO-d_6) NMR spectrum of **3b**.

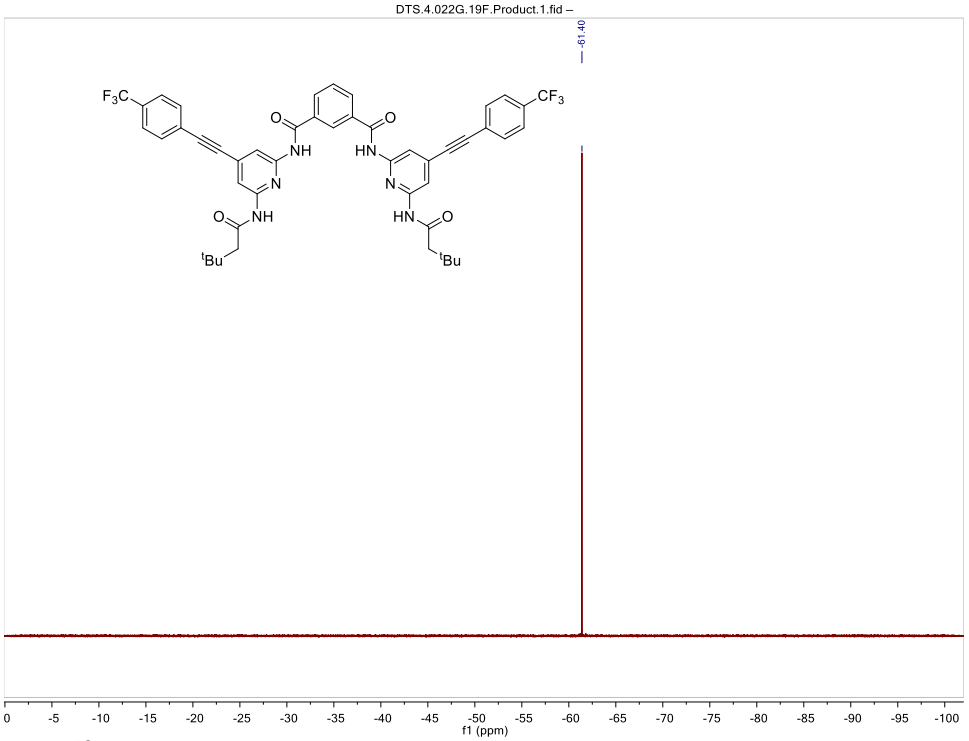

Figure S26. ^{19}F (471 MHz, DMSO-d_6) NMR spectrum of **3b**.

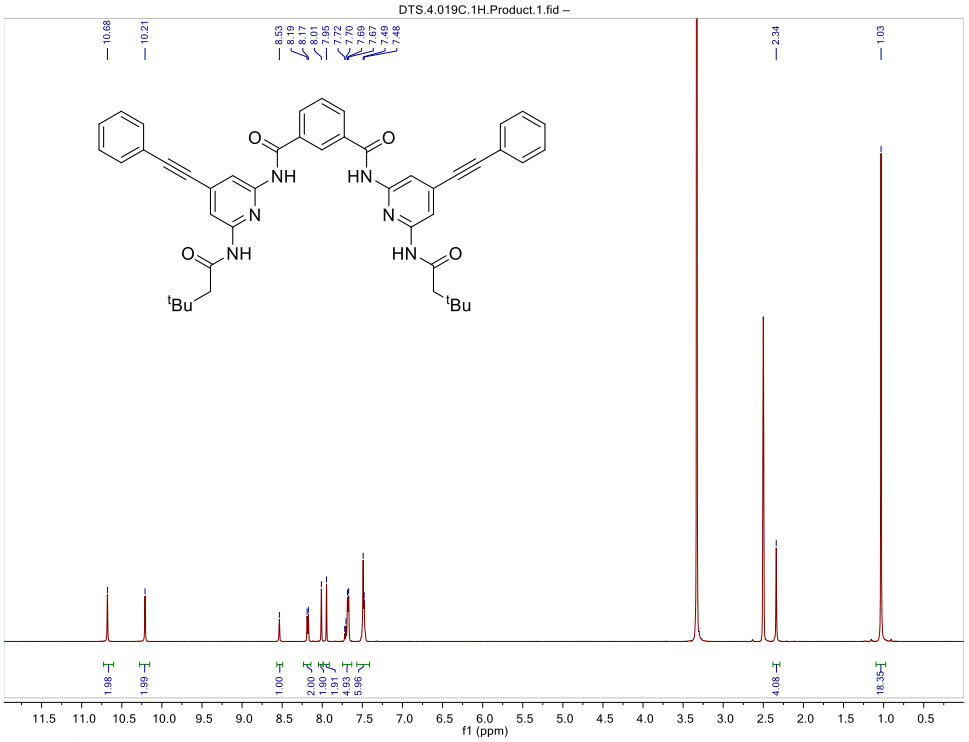

Figure S27. ^{1}H (500 MHz, DMSO-d_6) NMR spectrum of **3c**.

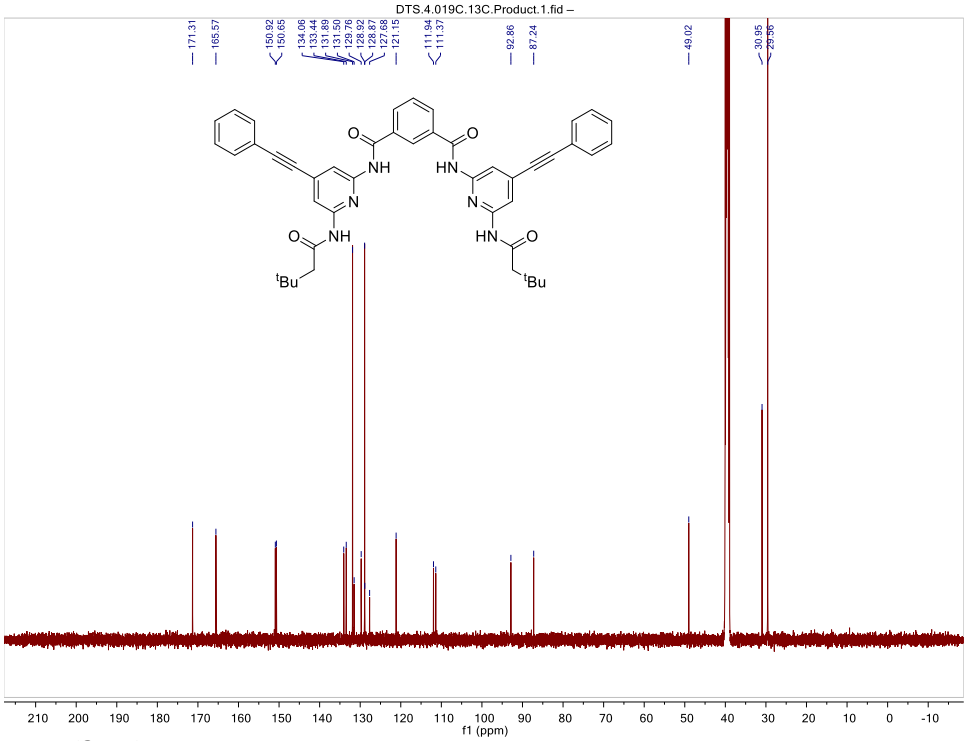

Figure S28. $^{13}C\{^{1}H\}$ (126 MHz, DMSO-d_6) NMR spectrum of **3c**.

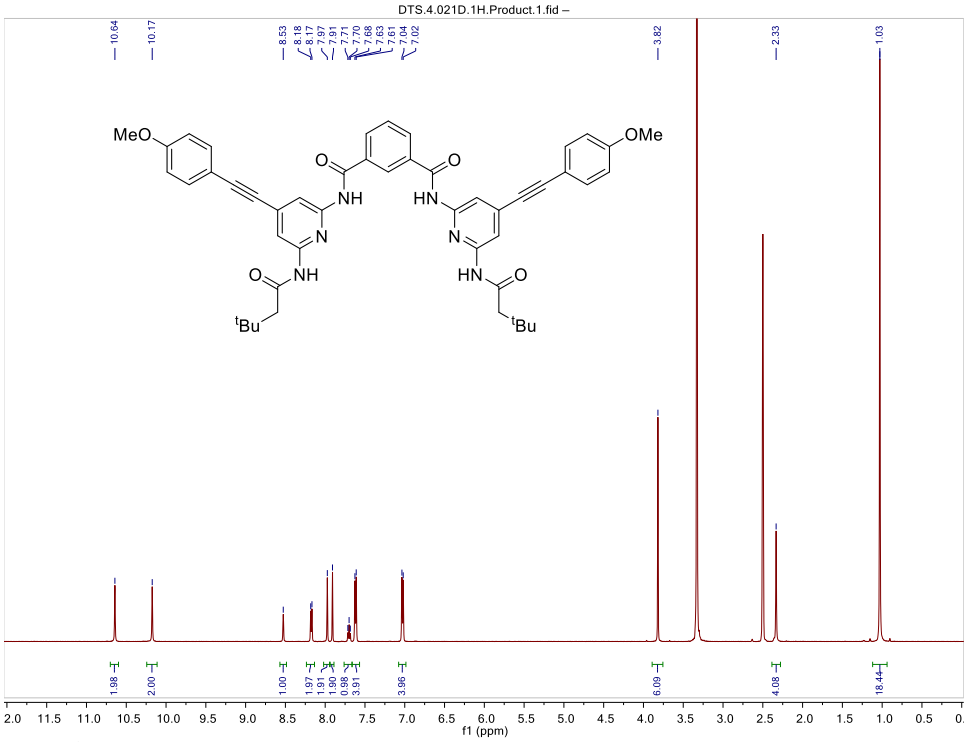

Figure S29. ^{1}H (500 MHz) NMR spectrum of **3d**.

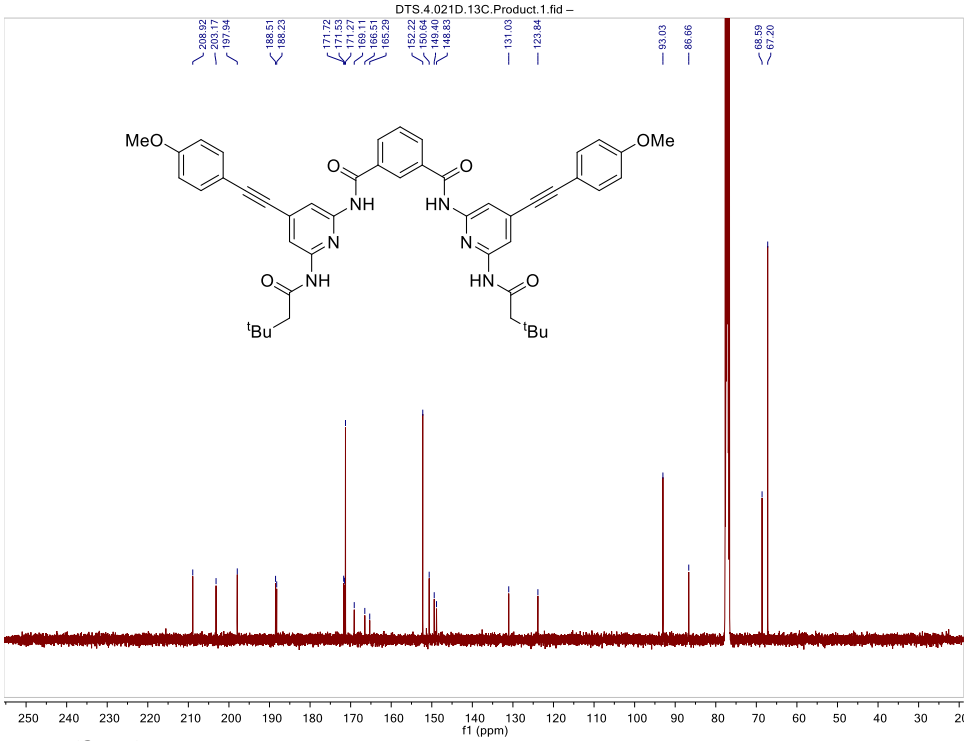

Figure S30. $^{13}C\{^{1}H\}$ (126 MHz, DMSO-d_6) NMR spectrum of **3d**.

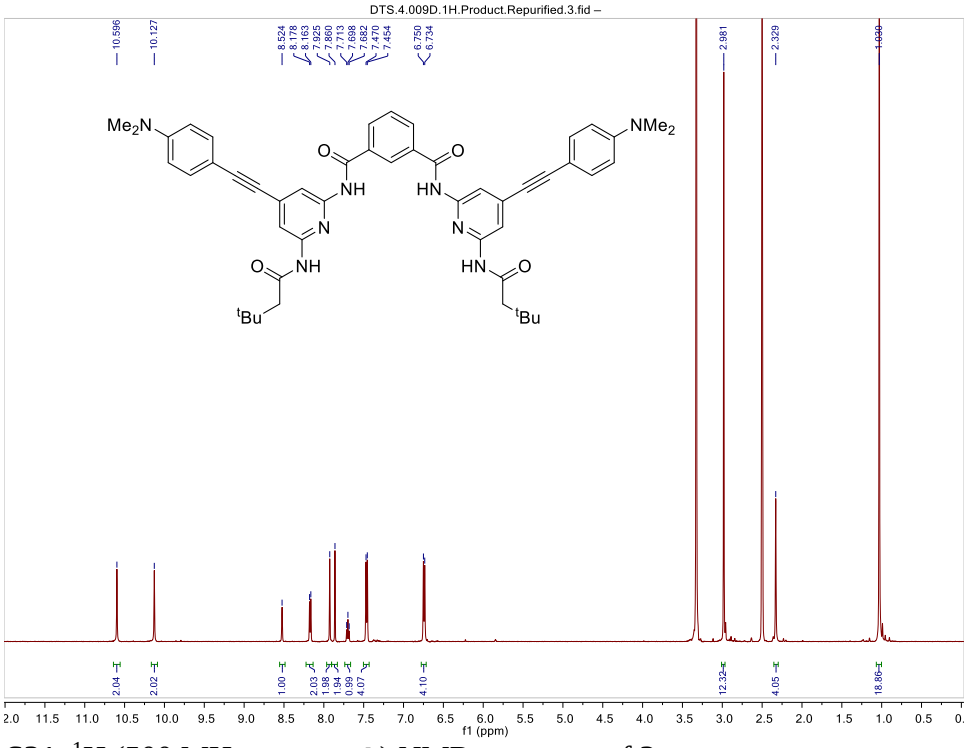

Figure S31. ^{1}H (500 MHz, DMSO-d_6) NMR spectrum of **3e**.

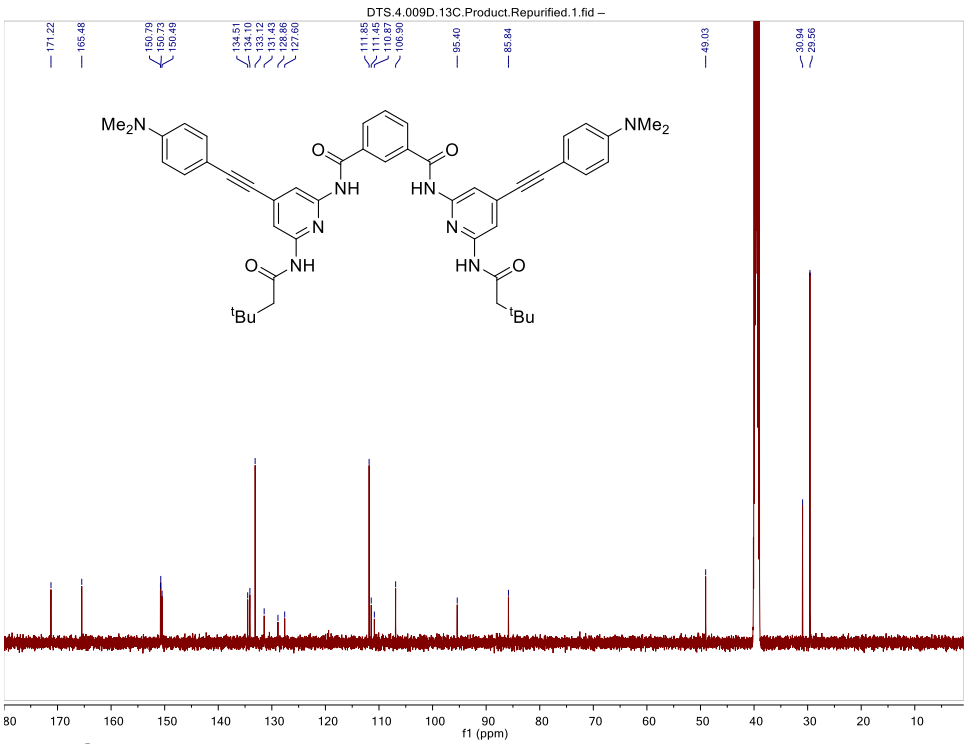

Figure S32. $^{13}C\{^{1}H\}$ (126 MHz, DMSO-d_6) NMR spectrum of **3e**.