SUPPORTING INFORMATION

Synthesis and Optical Properties of Excited-State Intramolecular Proton Transfer (ESIPT) Emitters with Sulfobetaine Fragments

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S1. Materials and methods

All chemicals were received from commercial sources (Sigma Aldrich, Fluorochem) and used without further purification. Tetrahydrofuran (THF) was distilled over metallic sodium (Na). Dichloromethane (DCM) was distilled over P_2O_5 under an argon atmosphere. Triethylamine (Et_3N) was distilled under argon over KOH. Thin layer chromatography (TLC) was performed on silica gel coated with fluorescent indicator. Chromatographic purifications were conducted using 40-63 µm silica gel.

^{1}H NMR (500 MHz) and ^{13}C NMR (126 MHz) spectra were recorded on a Bruker Advance 400 or 500 MHz spectrometers with perdeuterated solvents with residual protonated solvent signals as internal references. Absorption spectra were recorded using a dual-beam grating Schimadzu UV-3000 absorption spectrometer with a quartz cell of 1 cm of optical path length. The steady-state fluorescence emission and excitation spectra were recorded by using a Horiba S2 Jobin Yvon Fluoromax 4. All fluorescence and excitation spectra were corrected. Solvents for spectroscopy were spectroscopic grade and were used as received.

The fluorescence quantum yields (Φ_{exp}) were measured in diluted solution with an absorption value below 0.1 at the excitation wavelength using the following equation:

$$\Phi_{exp} = \Phi_{ref} \frac{I}{I_{ref}} \frac{OD_{ref}}{OD} \frac{\eta^2}{\eta^2_{ref}} \quad (\text{eq } 1)$$

I is the integral of the corrected emission spectrum, OD is the optical density at the excitation wavelength, and η is the refractive index of the medium. The reference system used was Rhodamine 6G, Φ = 88% in ethanol (λ_{exc} = 488 nm).

Luminescence lifetimes were measured on a Horiba Scientific TCSPC system equipped with a nanoLED 370. Lifetimes were deconvoluted with FS-900 software using a light-scattering solution (LUDOX) for instrument response. The excitation source was a laser diode (λ_{exc} = 320 nm).

S2. ^{1}H and ^{13}C NMR spectra

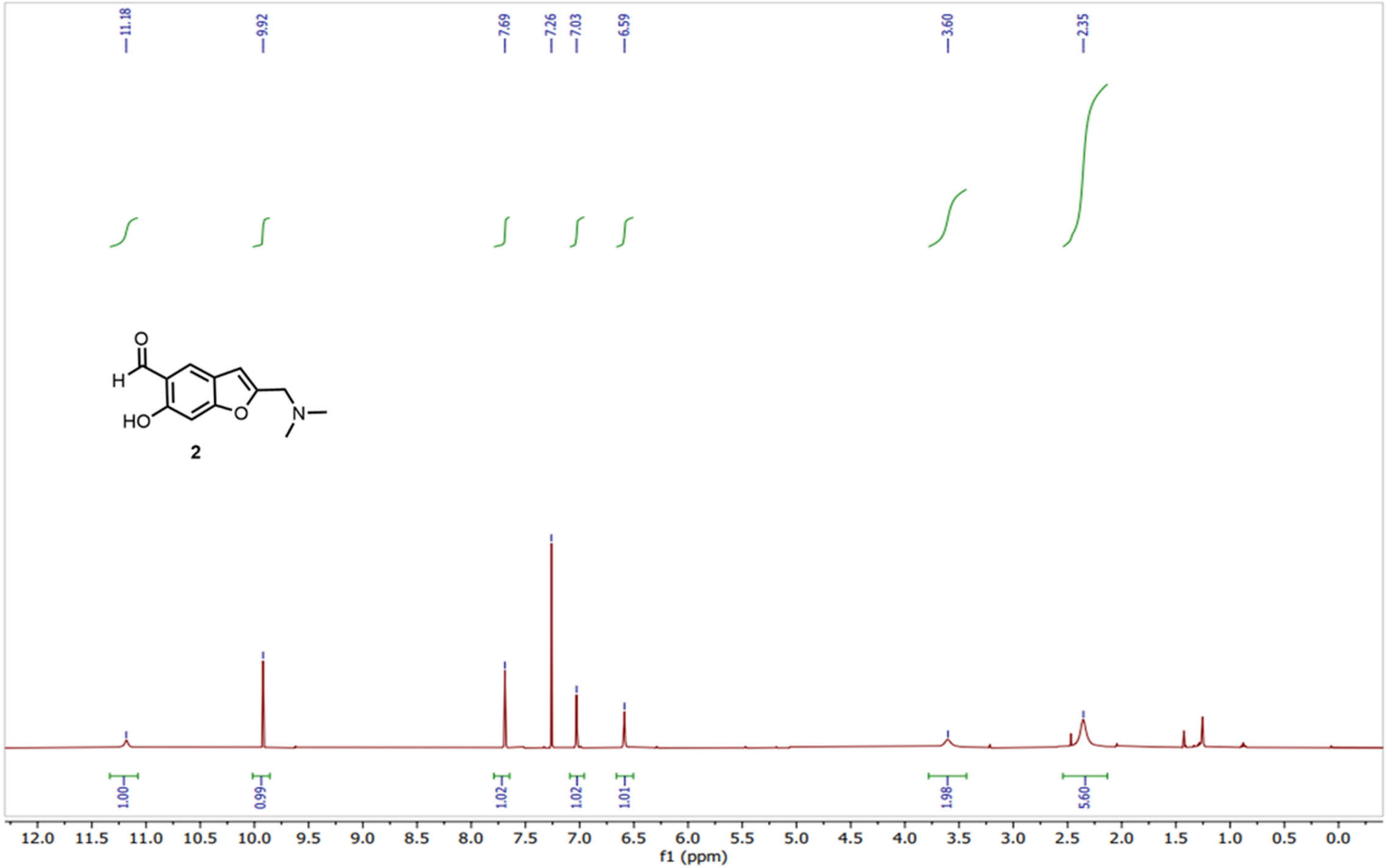

Figure S2.1. ^{1}H NMR spectrum of **2**

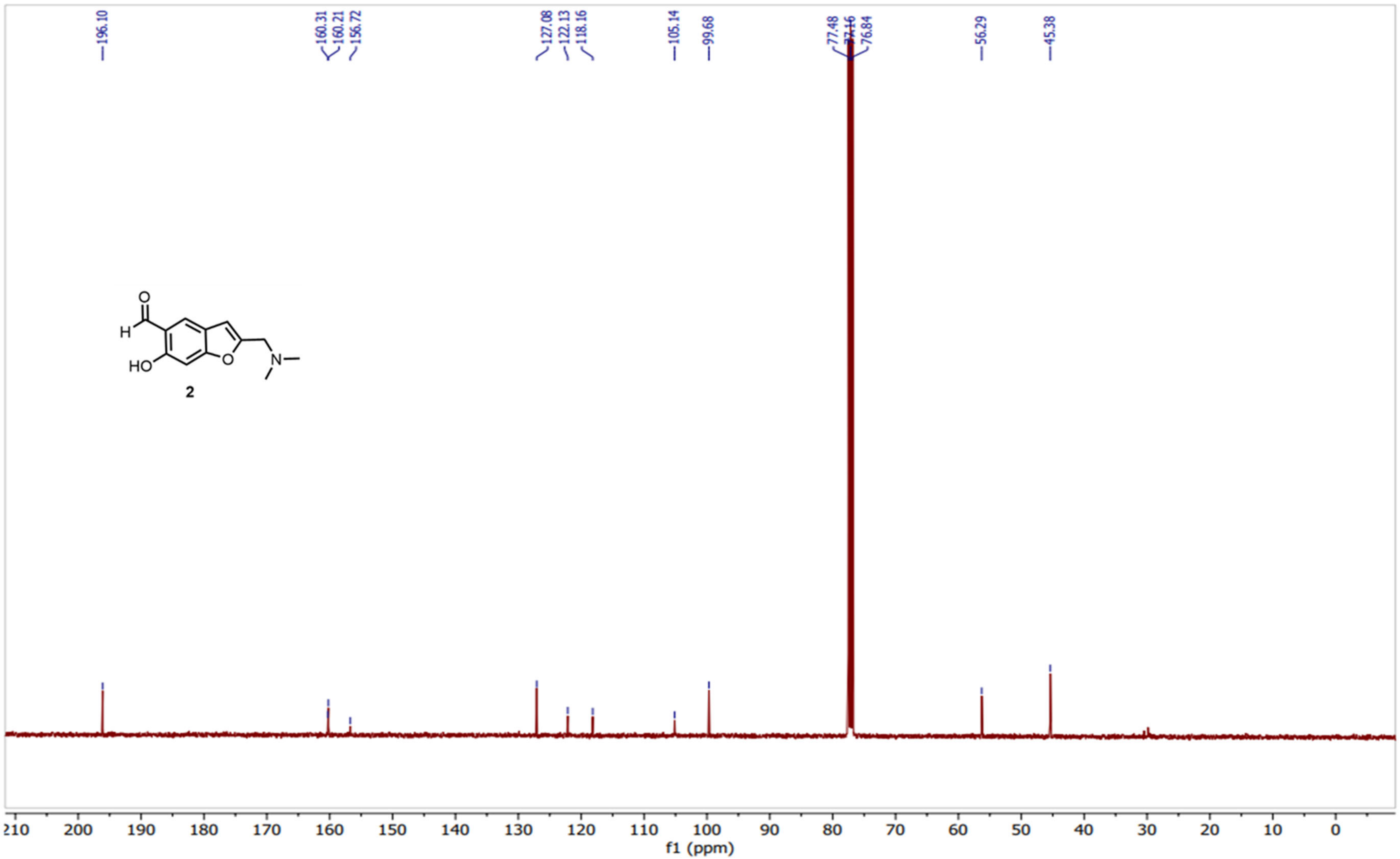

Figure S2.2. ^{13}C NMR spectrum of **2**

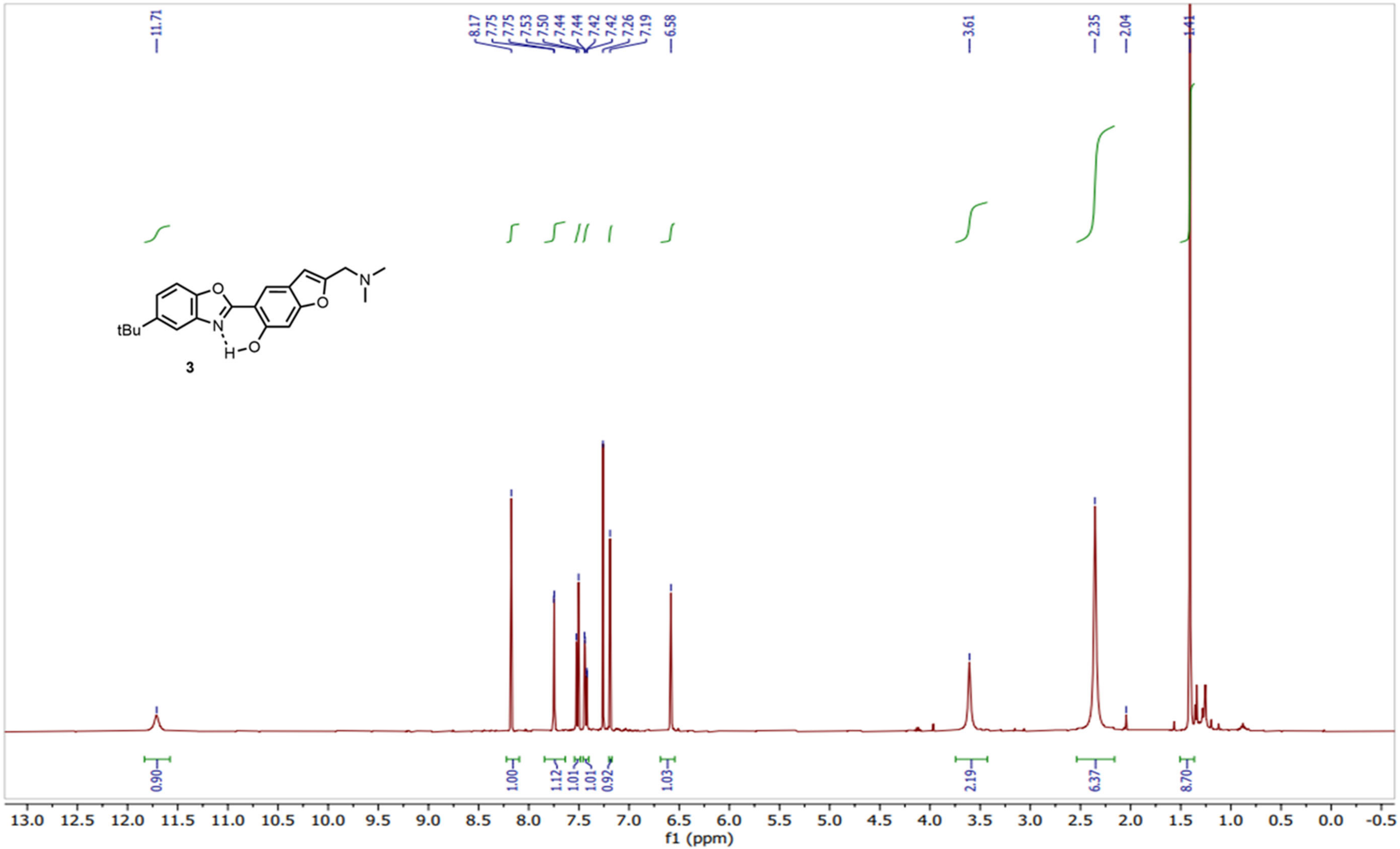

Figure S2.3. ^{1}H NMR spectrum of **3**

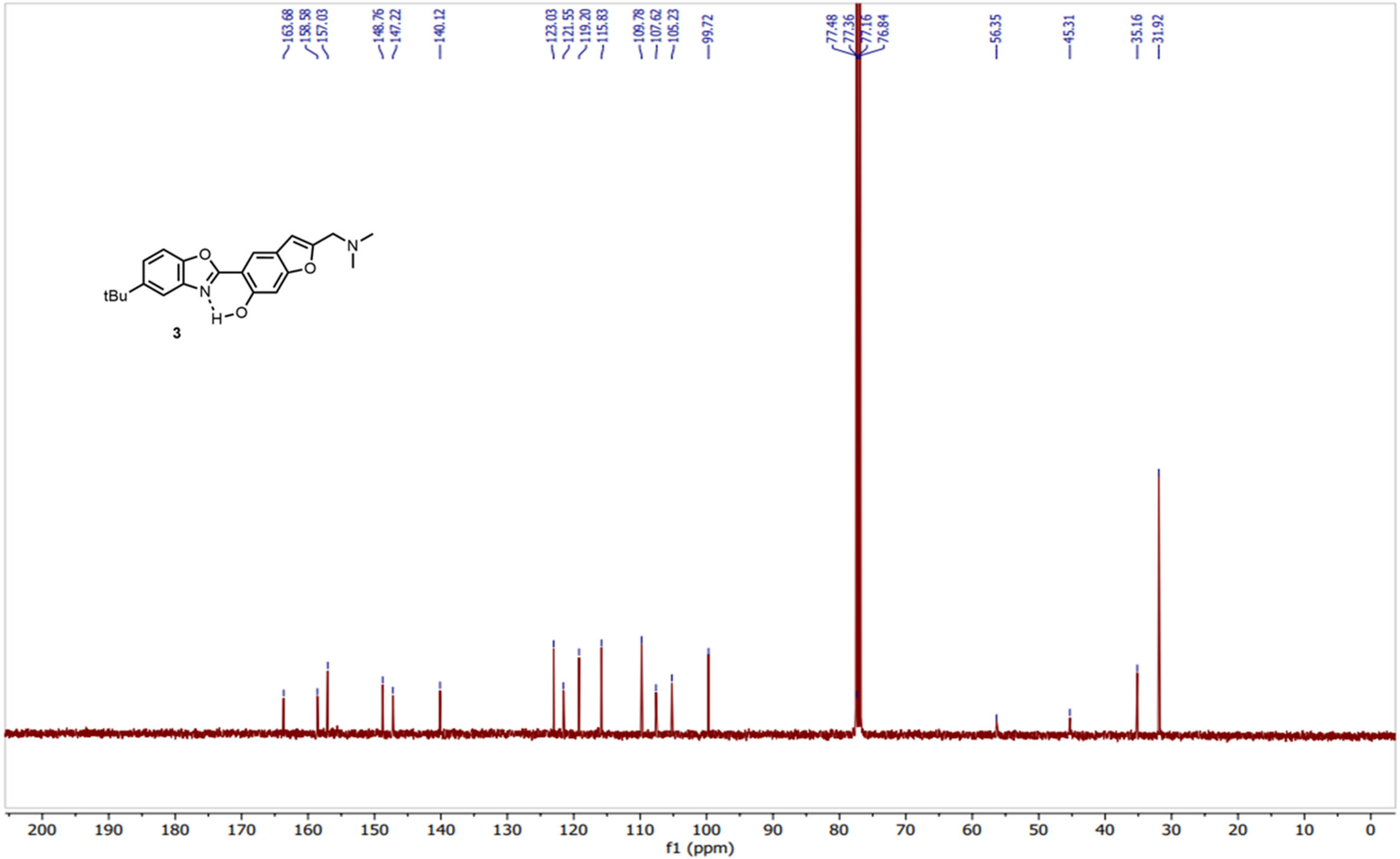

Figure S2.4. ^{13}C NMR spectrum of **3**

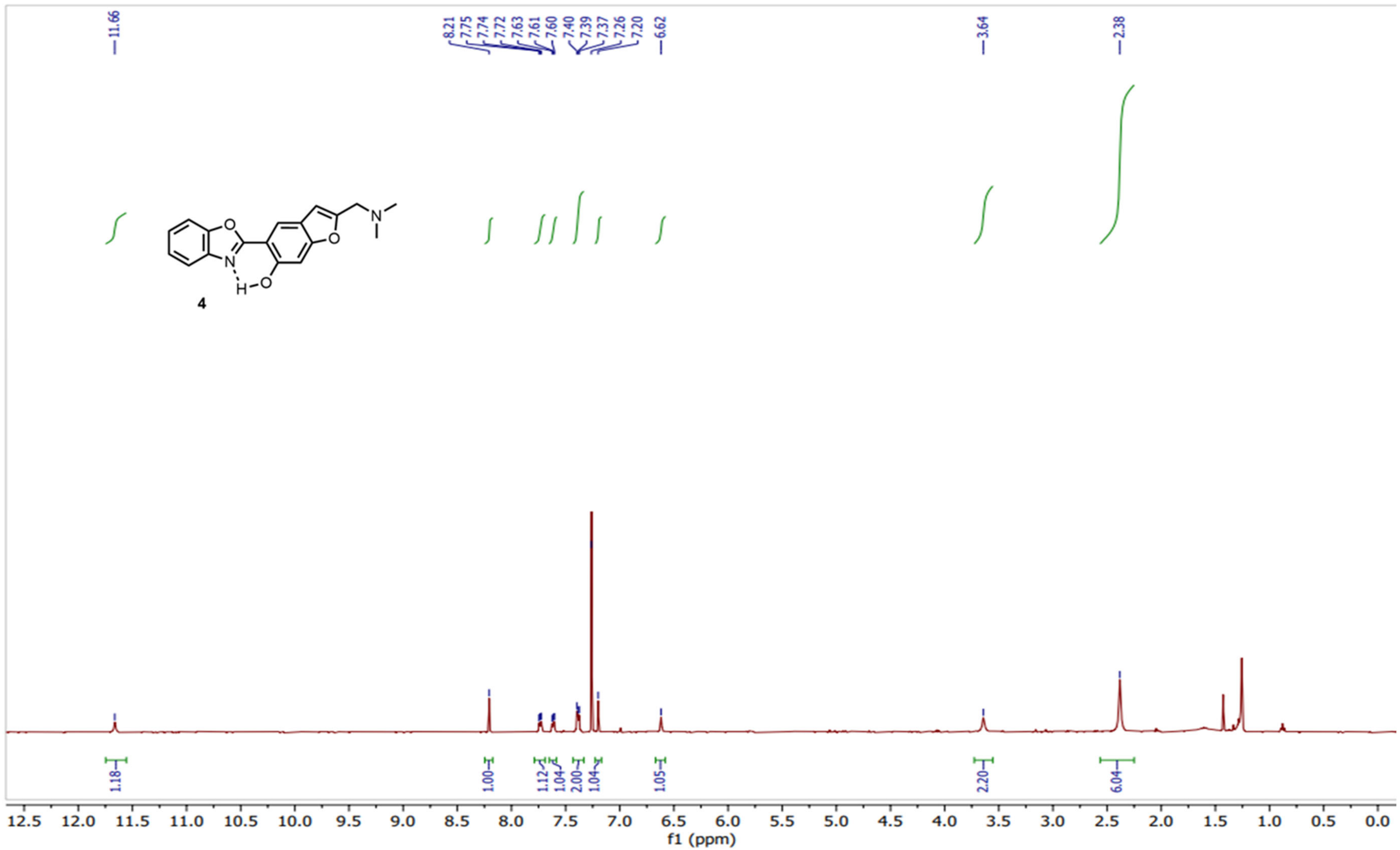

Figure S2.4. [1]H NMR spectrum of **4**

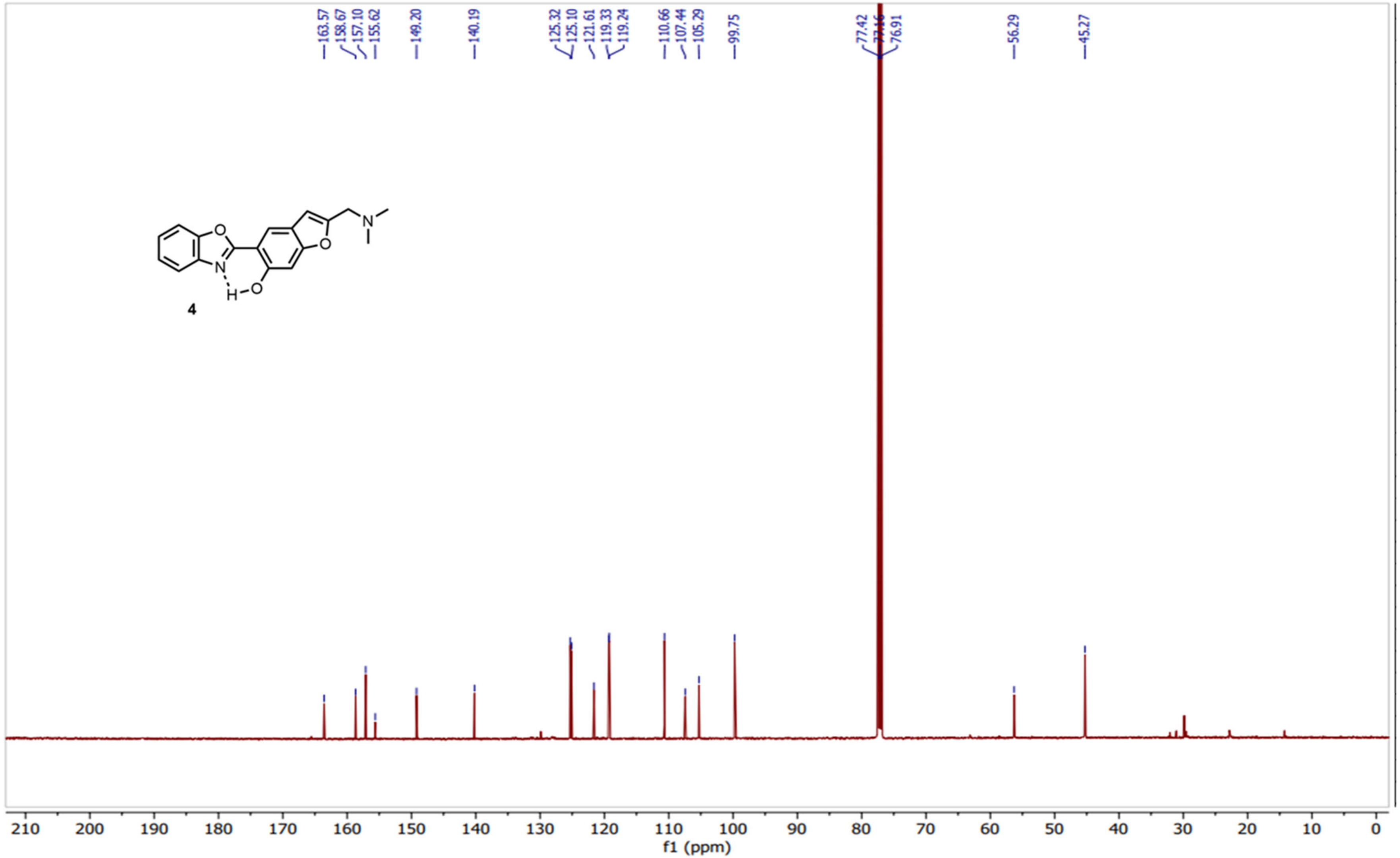

Figure S2.5. ^{13}C NMR spectrum of **4**

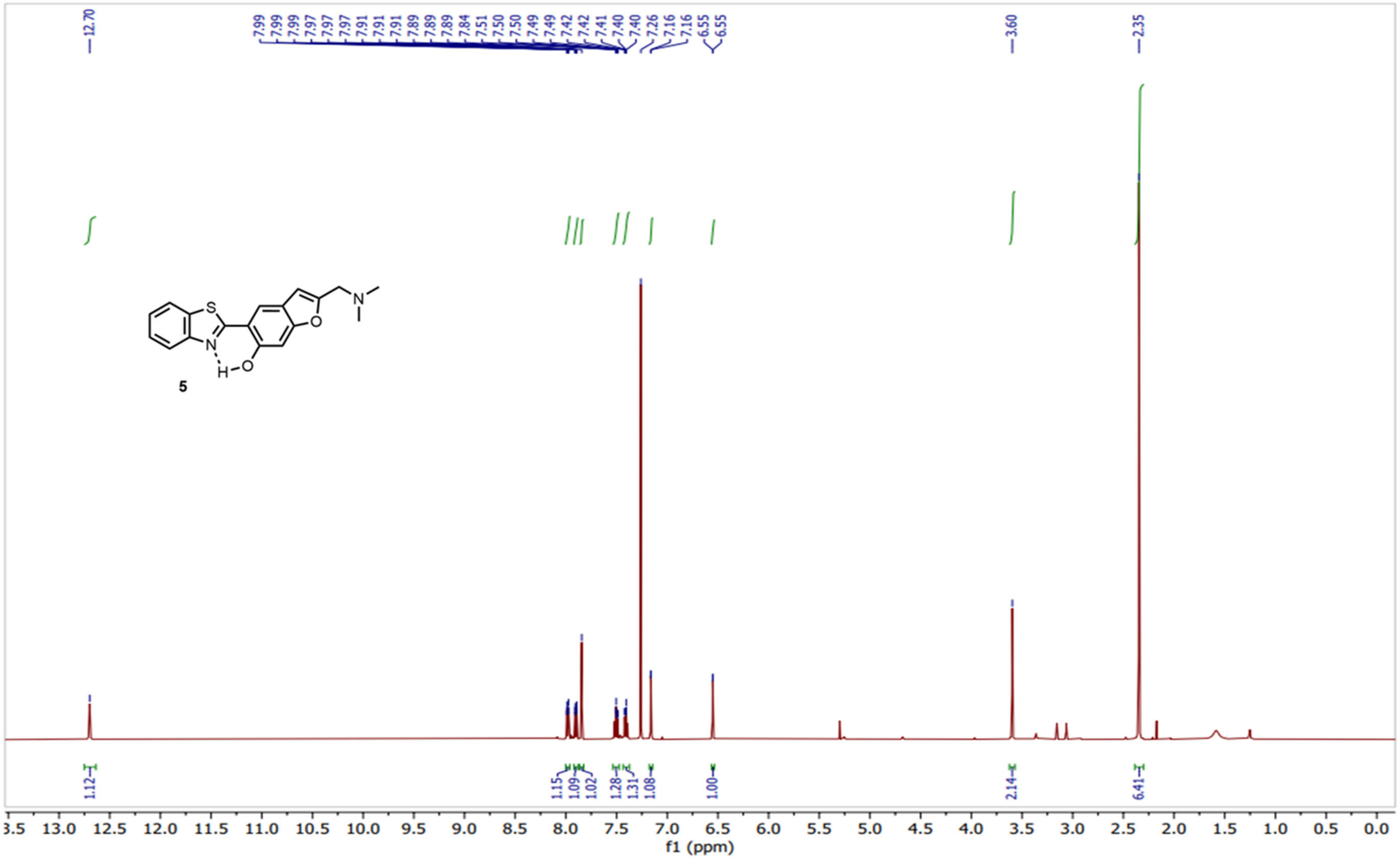

Figure S2.6. ^{1}H NMR spectrum of **5**

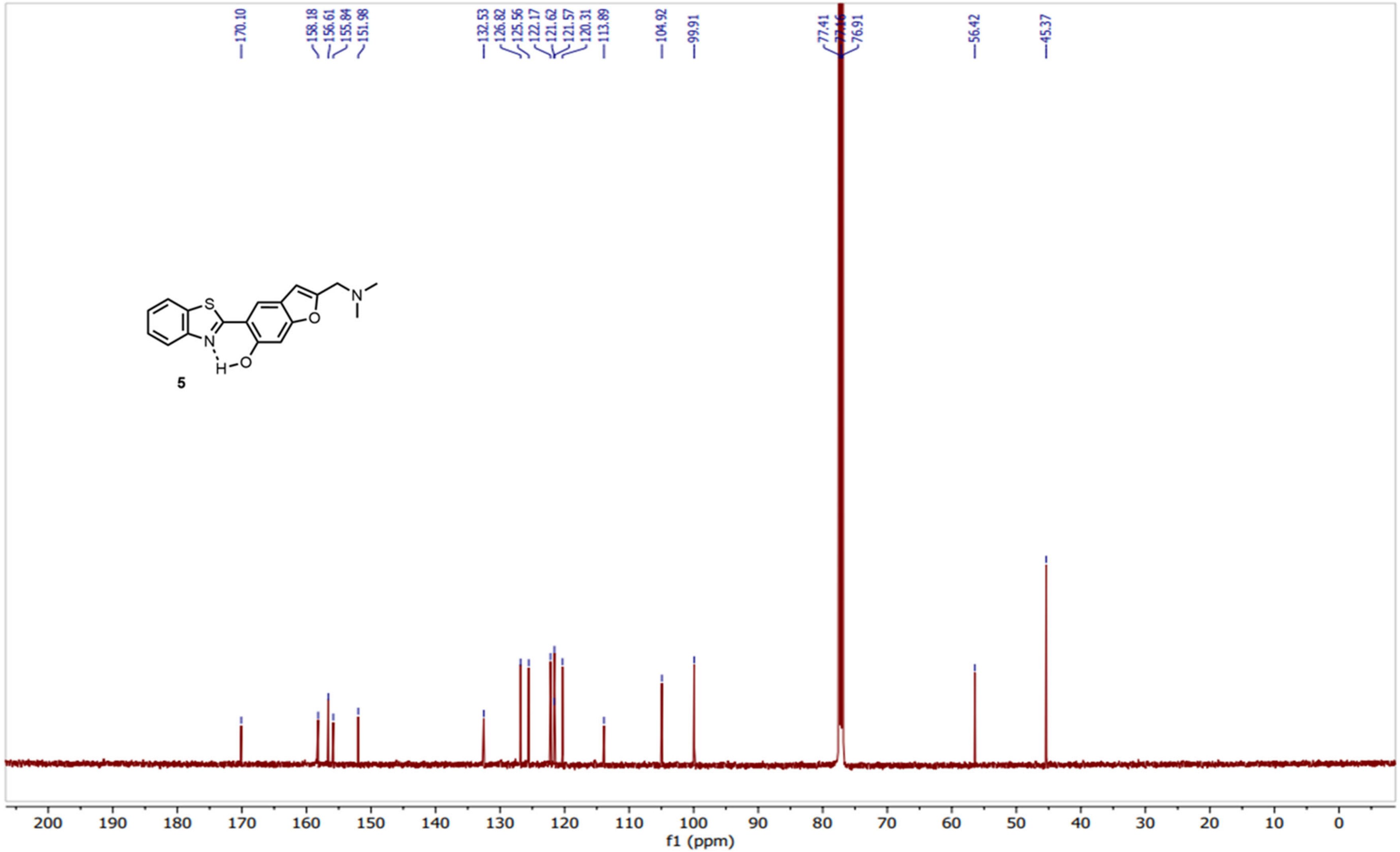

Figure S2.7. ^{13}C NMR spectrum of **5**

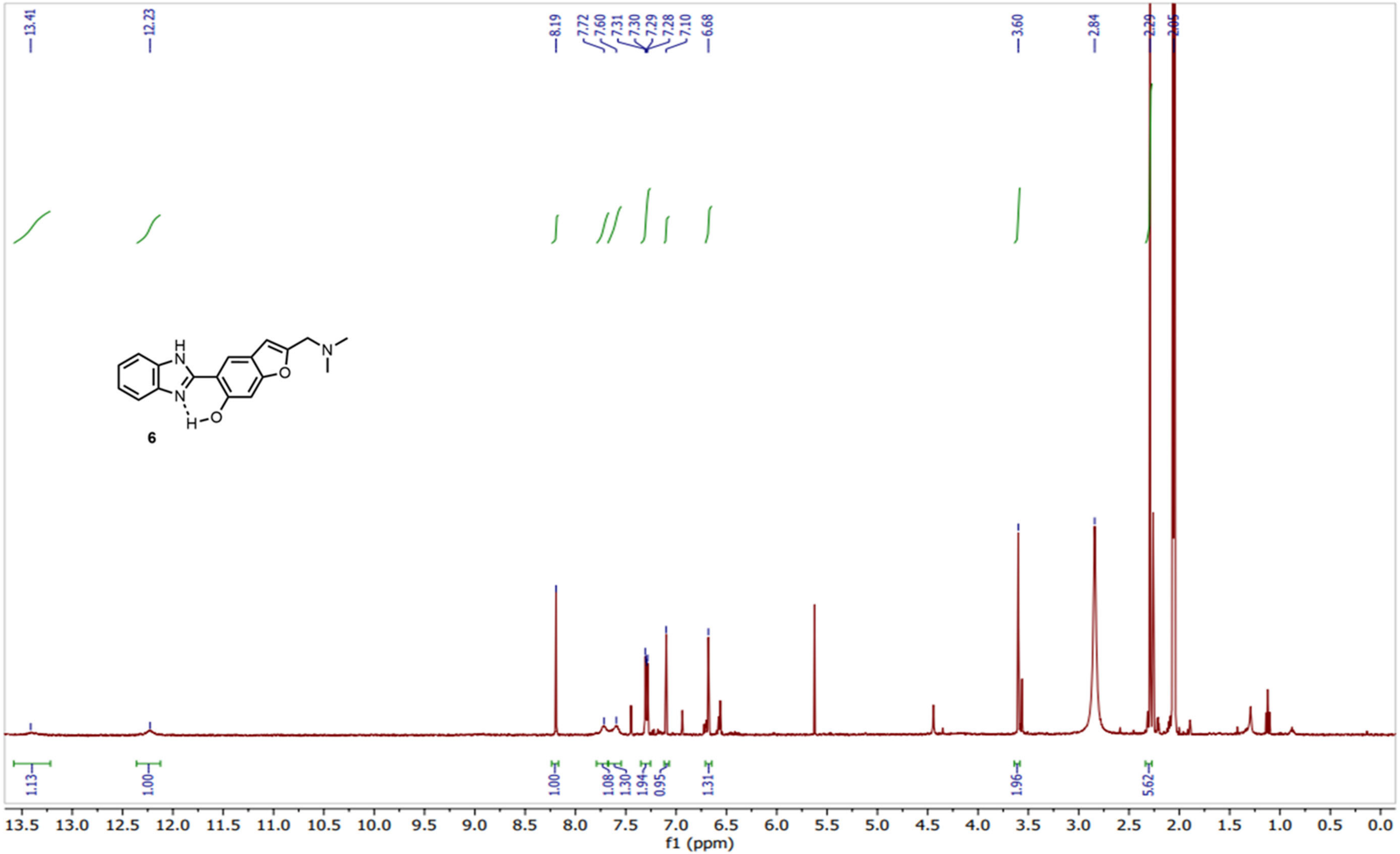

Figure S2.8. ^{1}H NMR spectrum of **6**

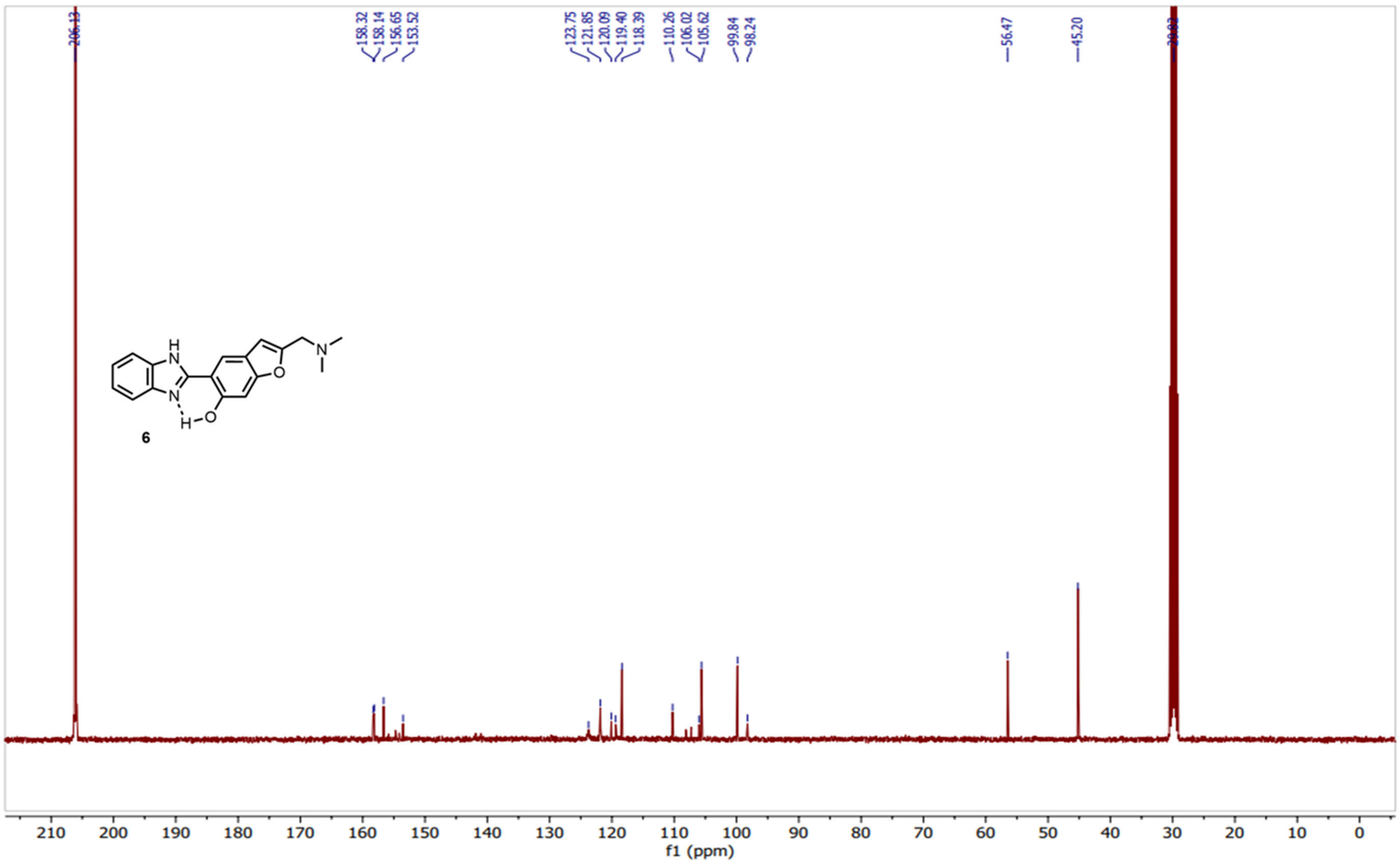

Figure S2.9. ^{13}C NMR spectrum of **6**

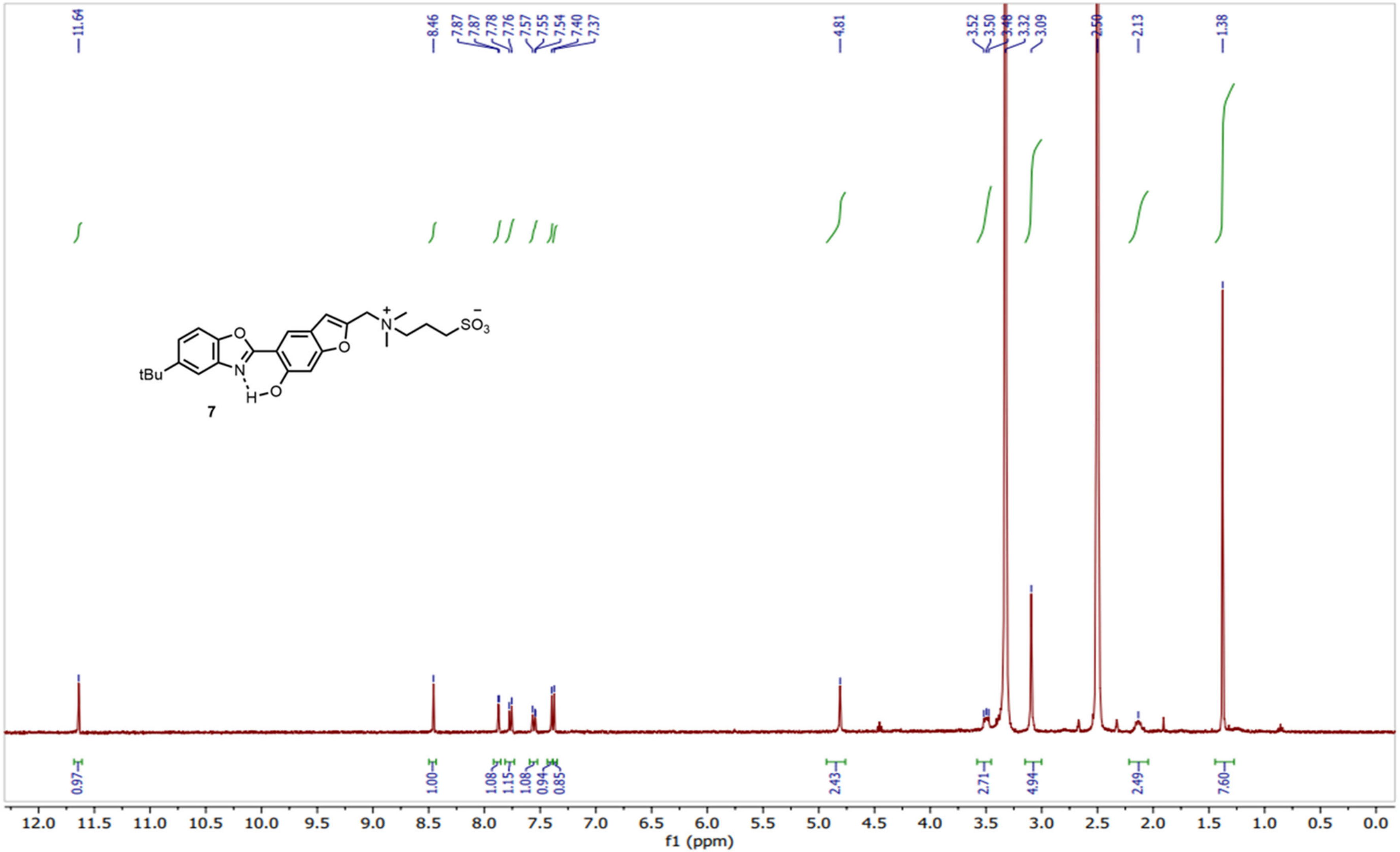

Figure S2.10. [1]H NMR spectrum of **7**

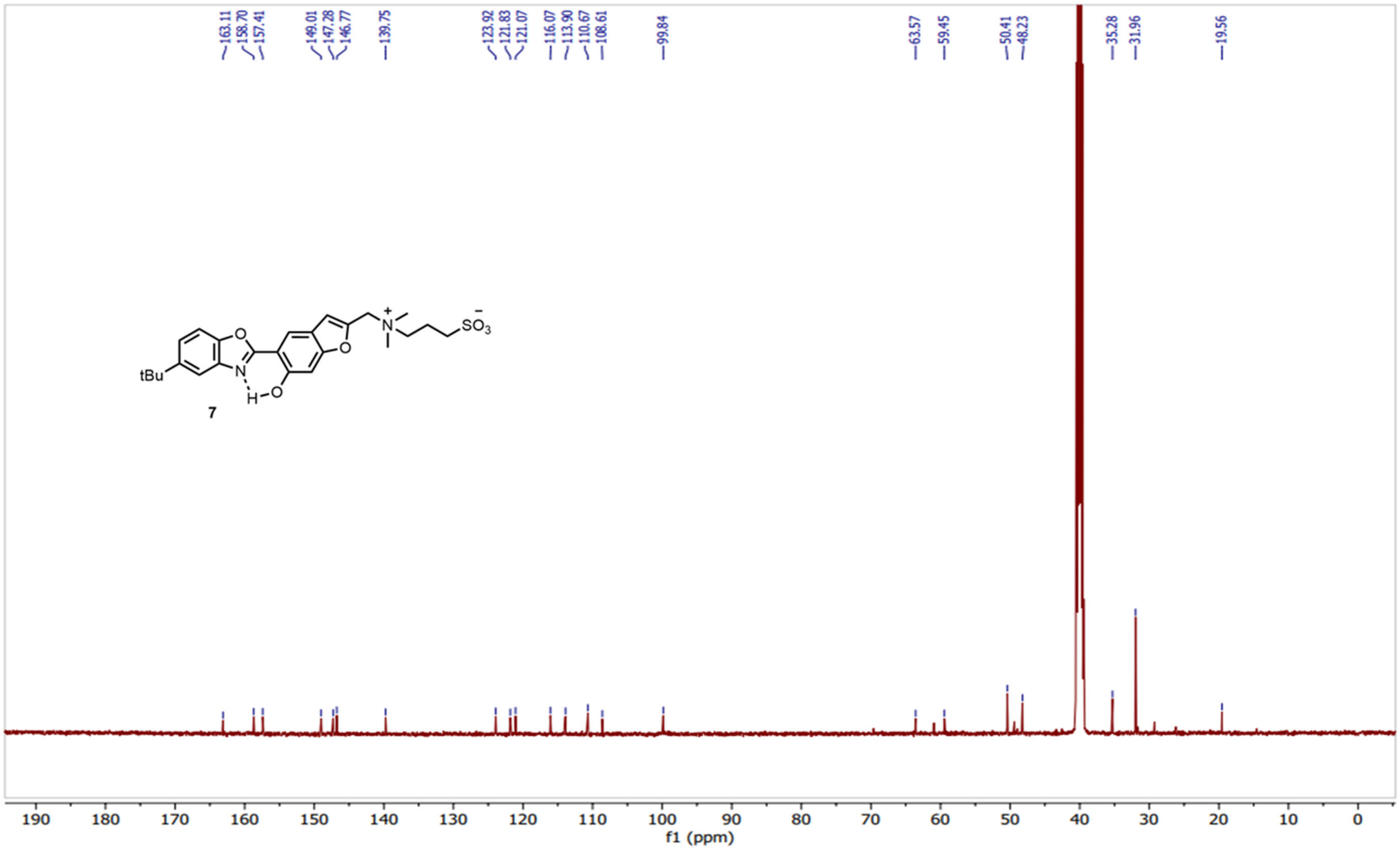

Figure S2.11. ^{13}C NMR spectrum of **7**

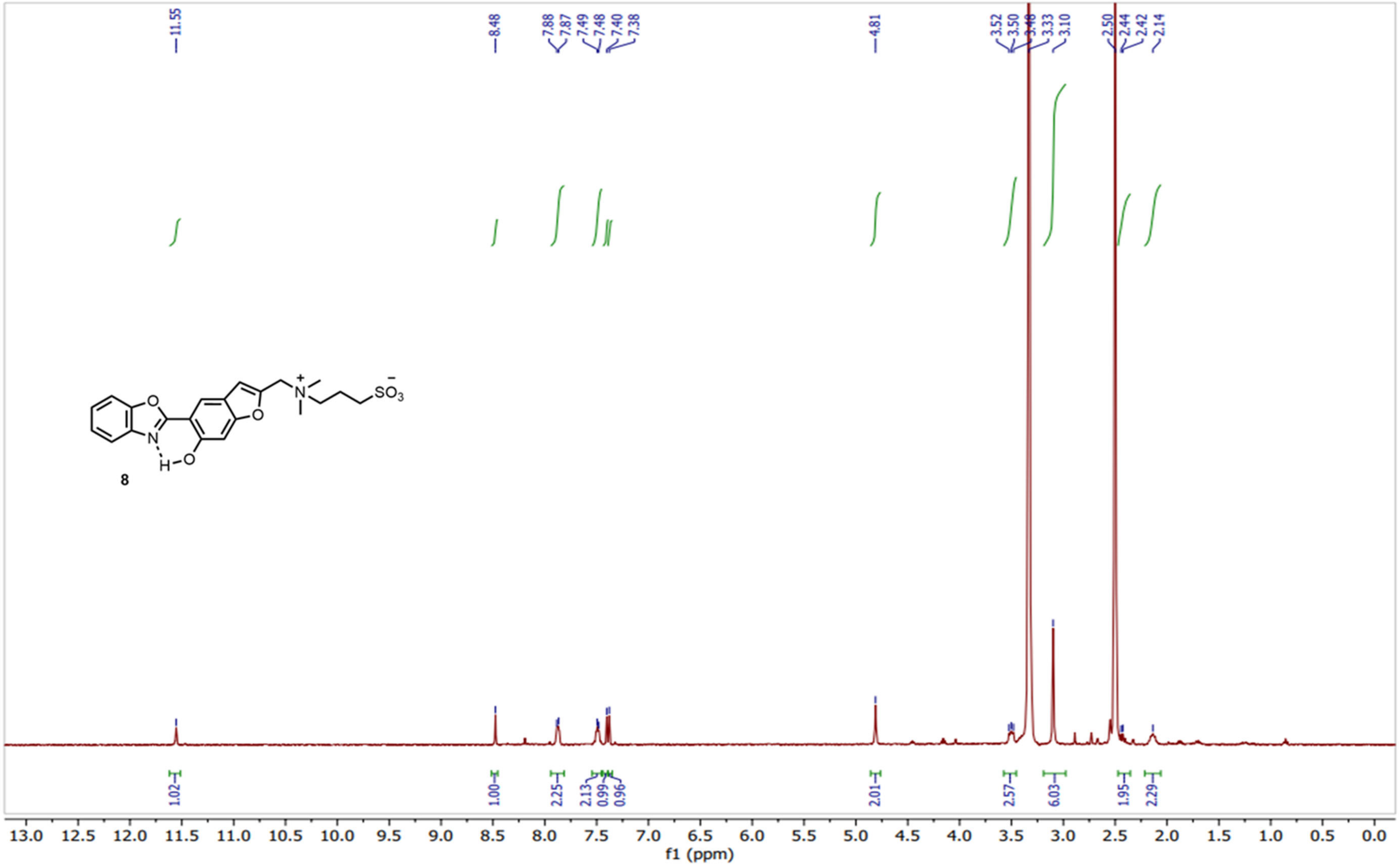

Figure S2.12. [1]H NMR spectrum of **8**

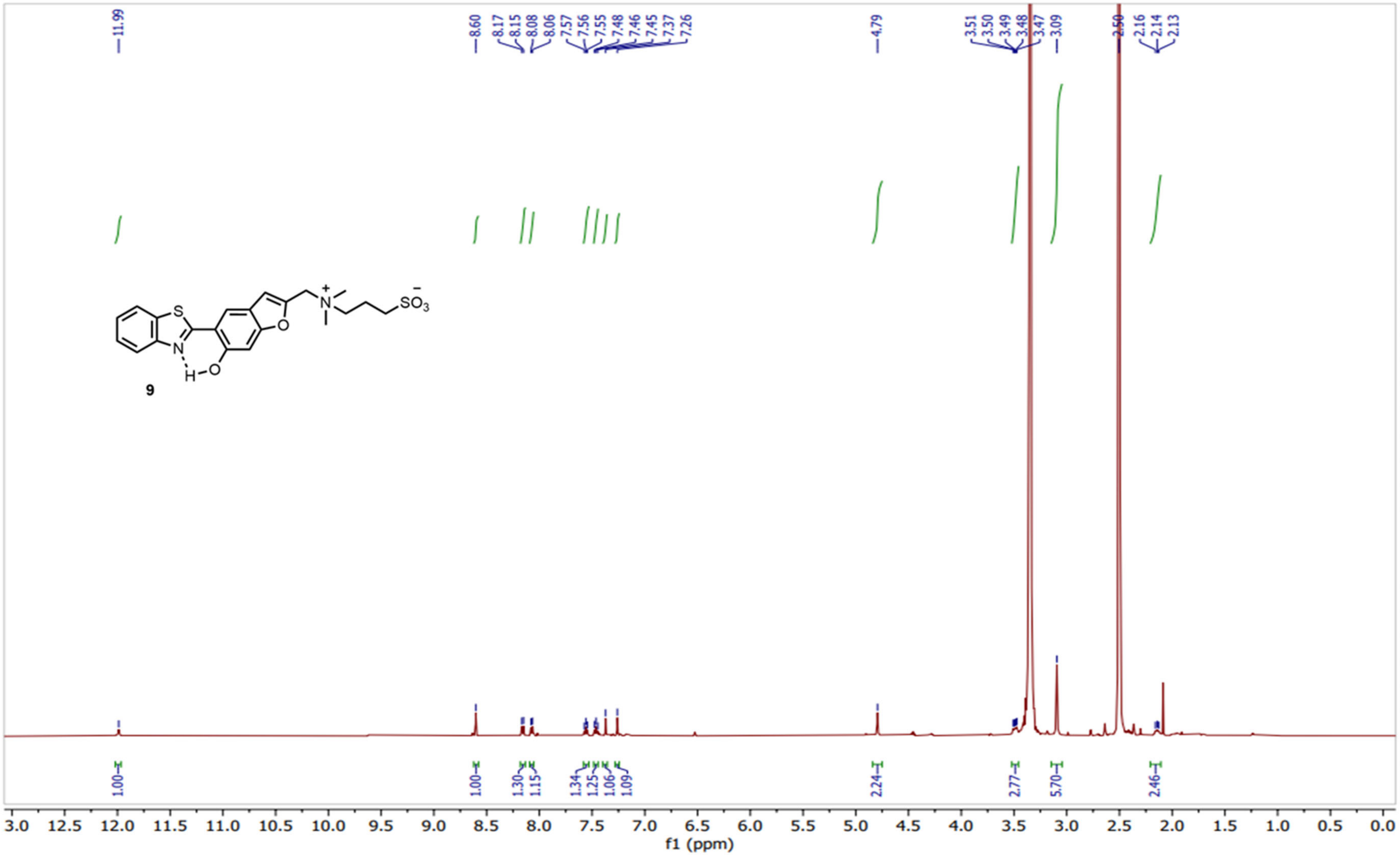

Figure S2.13. [1]H NMR spectrum of **9**

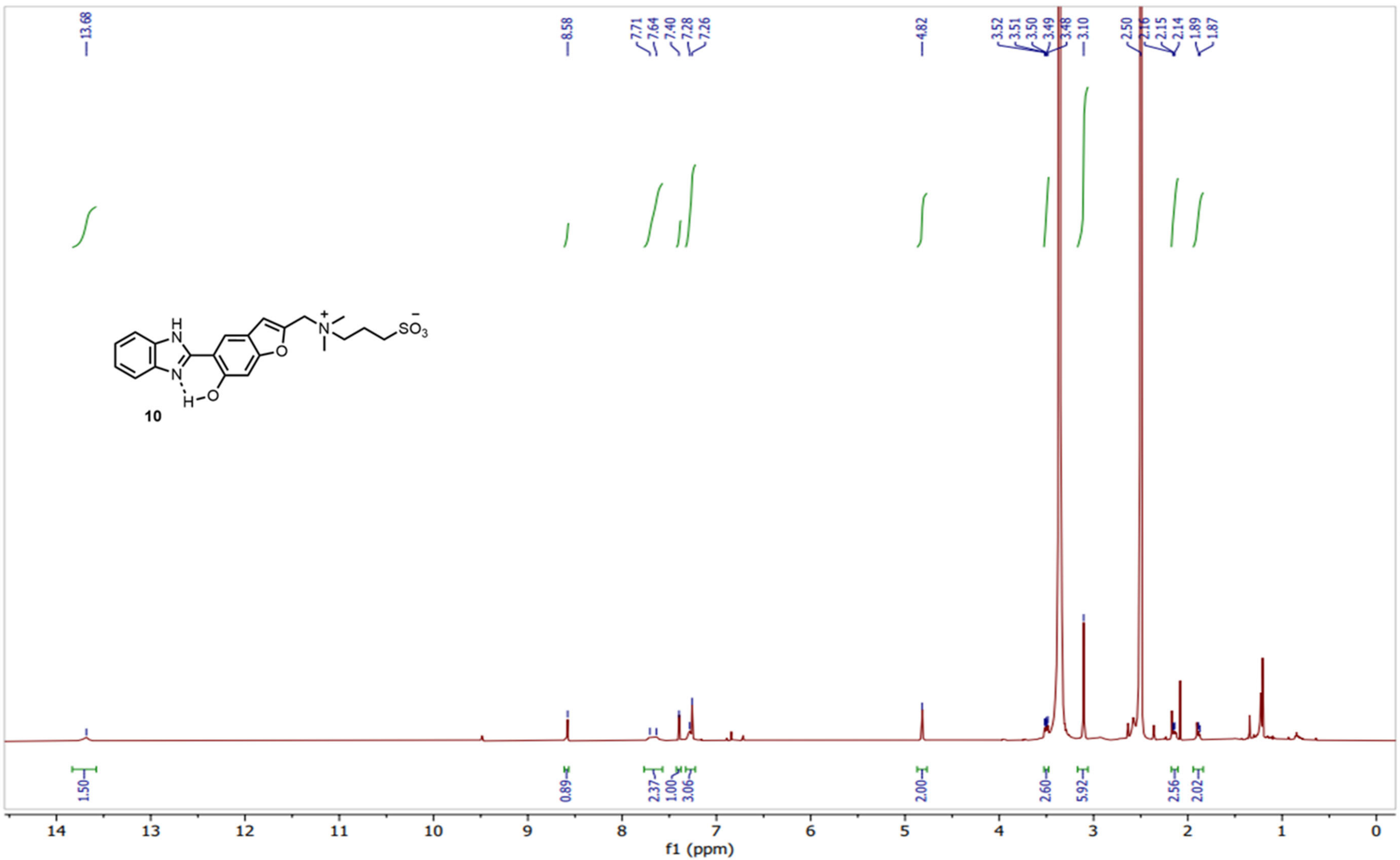

Figure S2.14. ^{1}H NMR spectrum of **10**

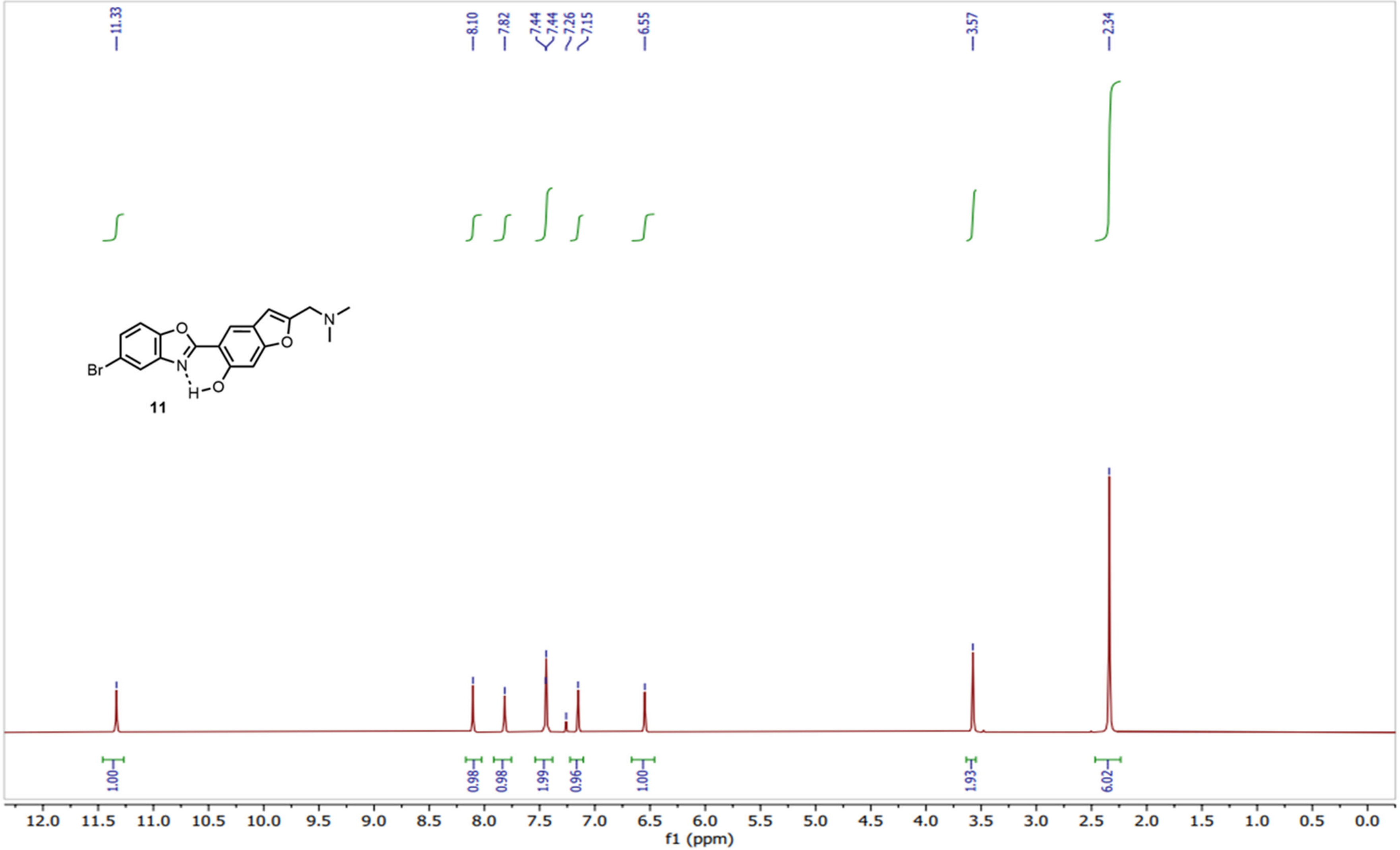

Figure S2.15. ^{1}H NMR spectrum of **11**

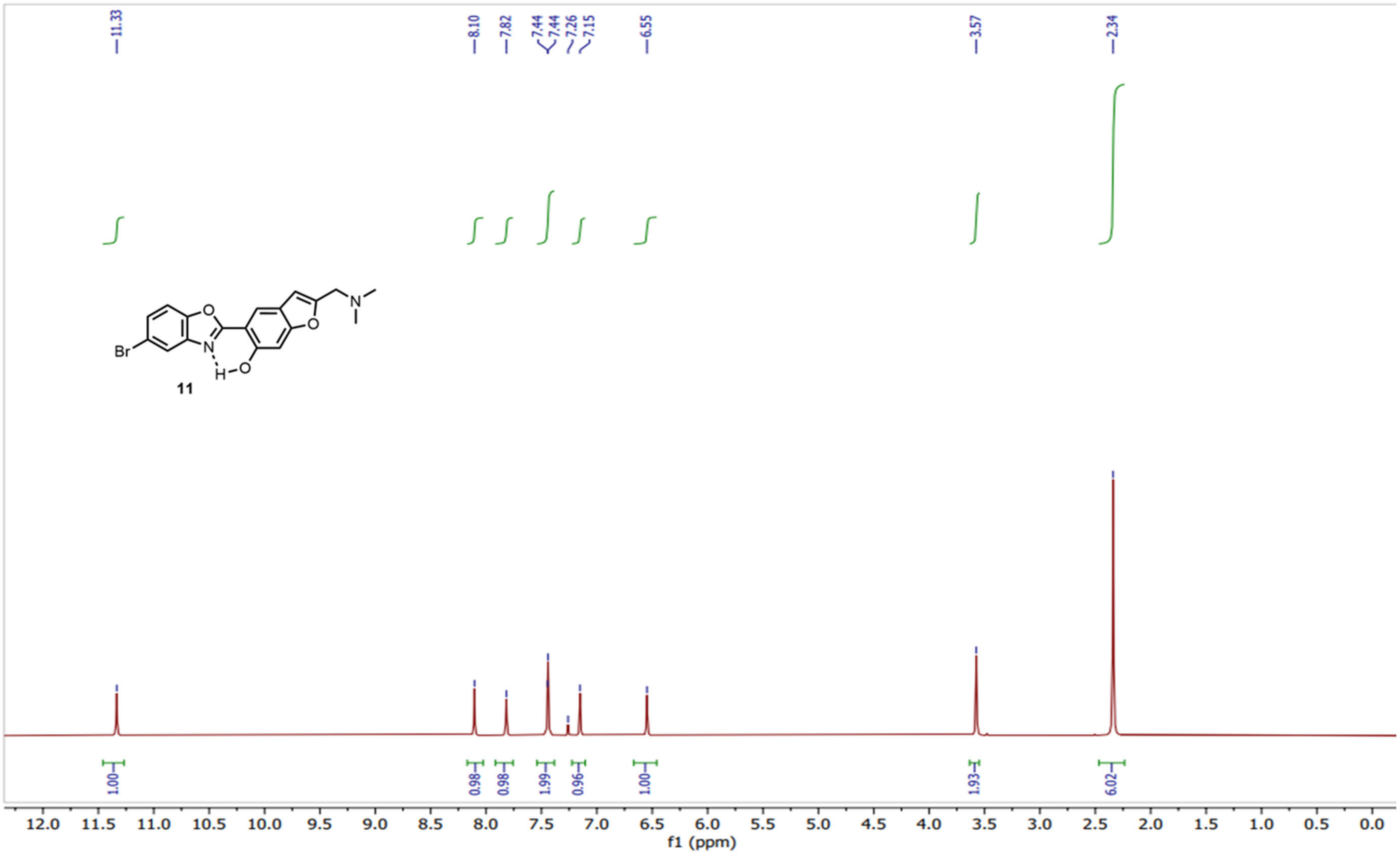

Figure S2.16. ^{13}C NMR spectrum of **11**

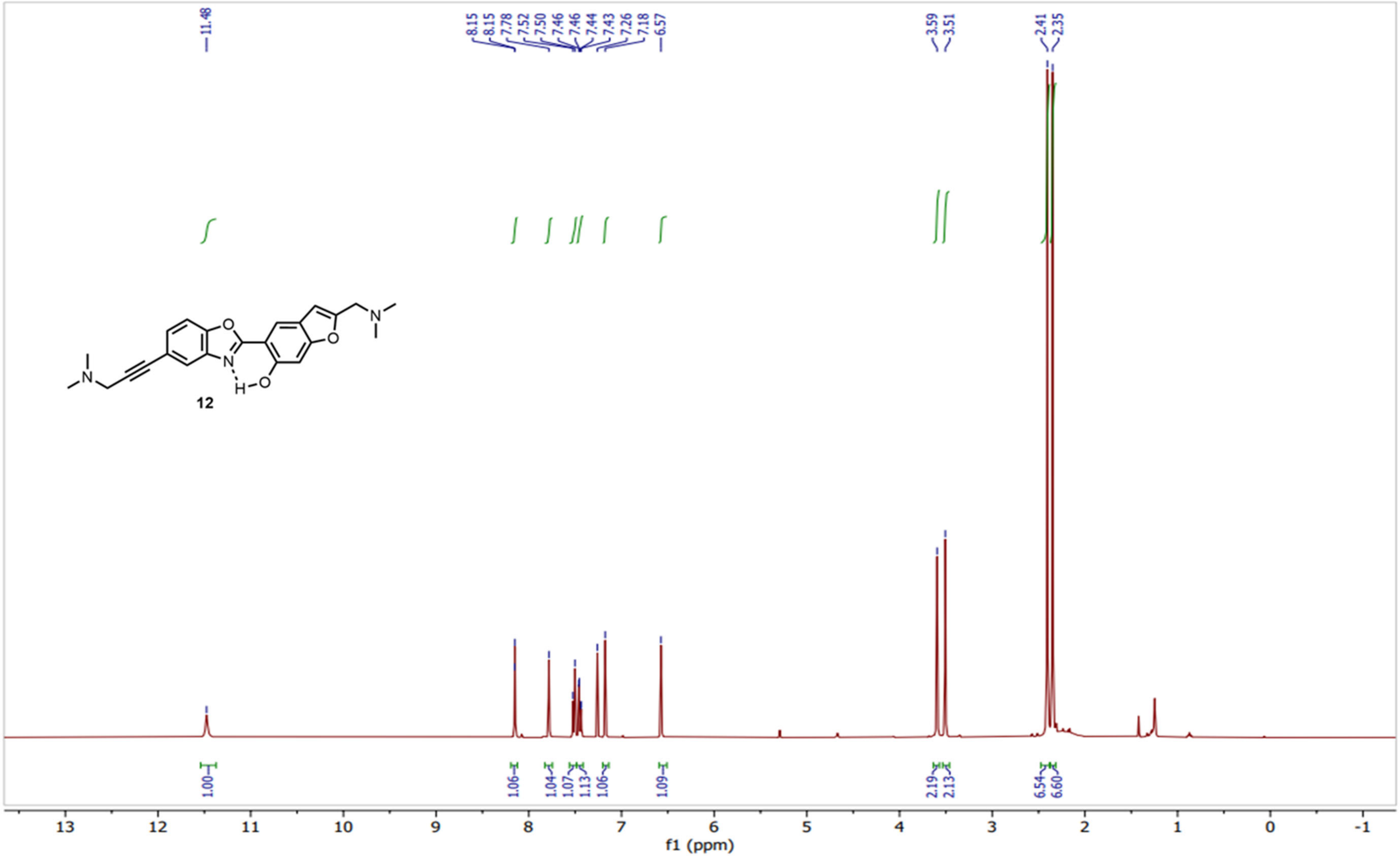

Figure S2.17. ^{1}H NMR spectrum of **12**

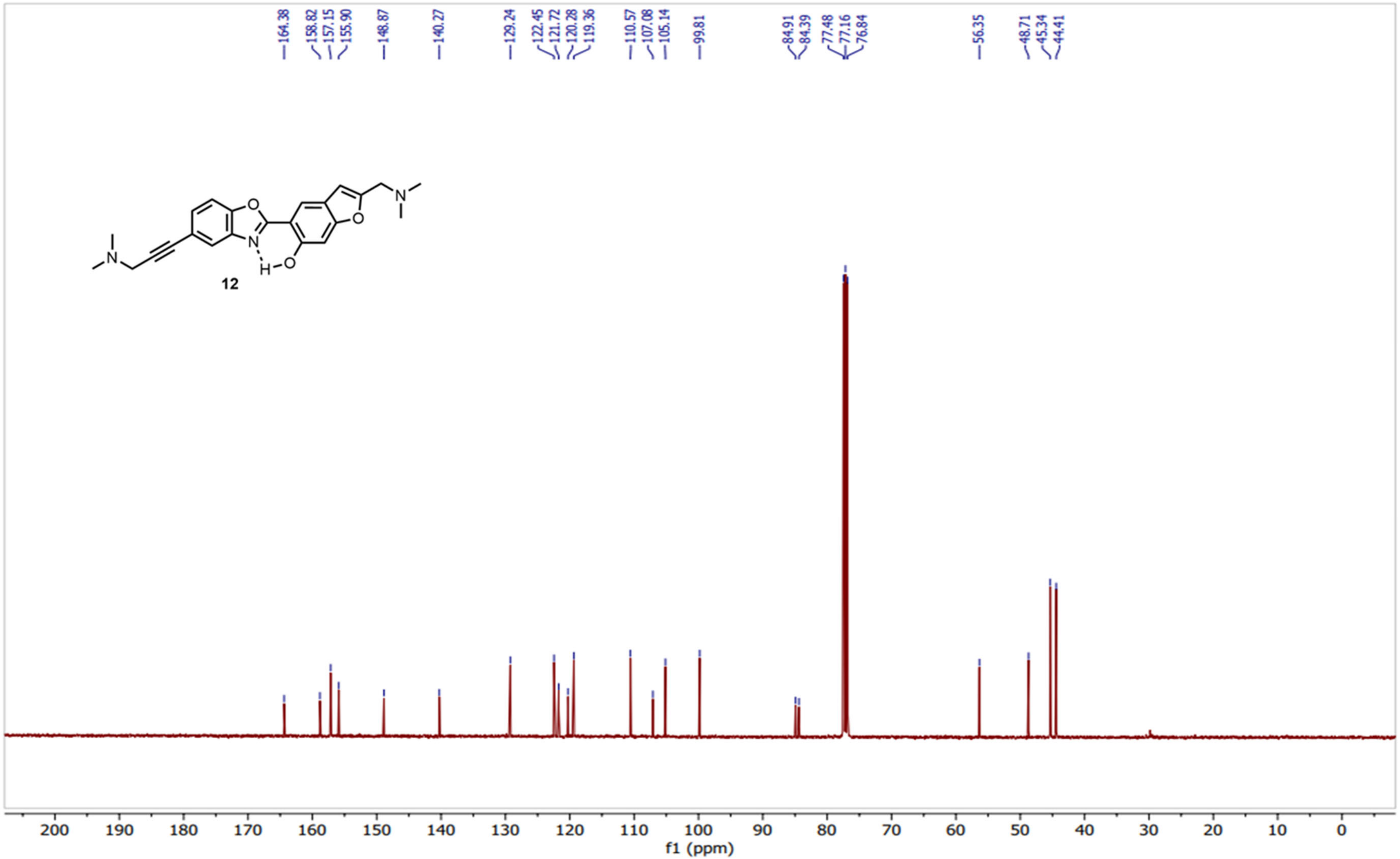

Figure S2.18. ^{13}C NMR spectrum of **12**

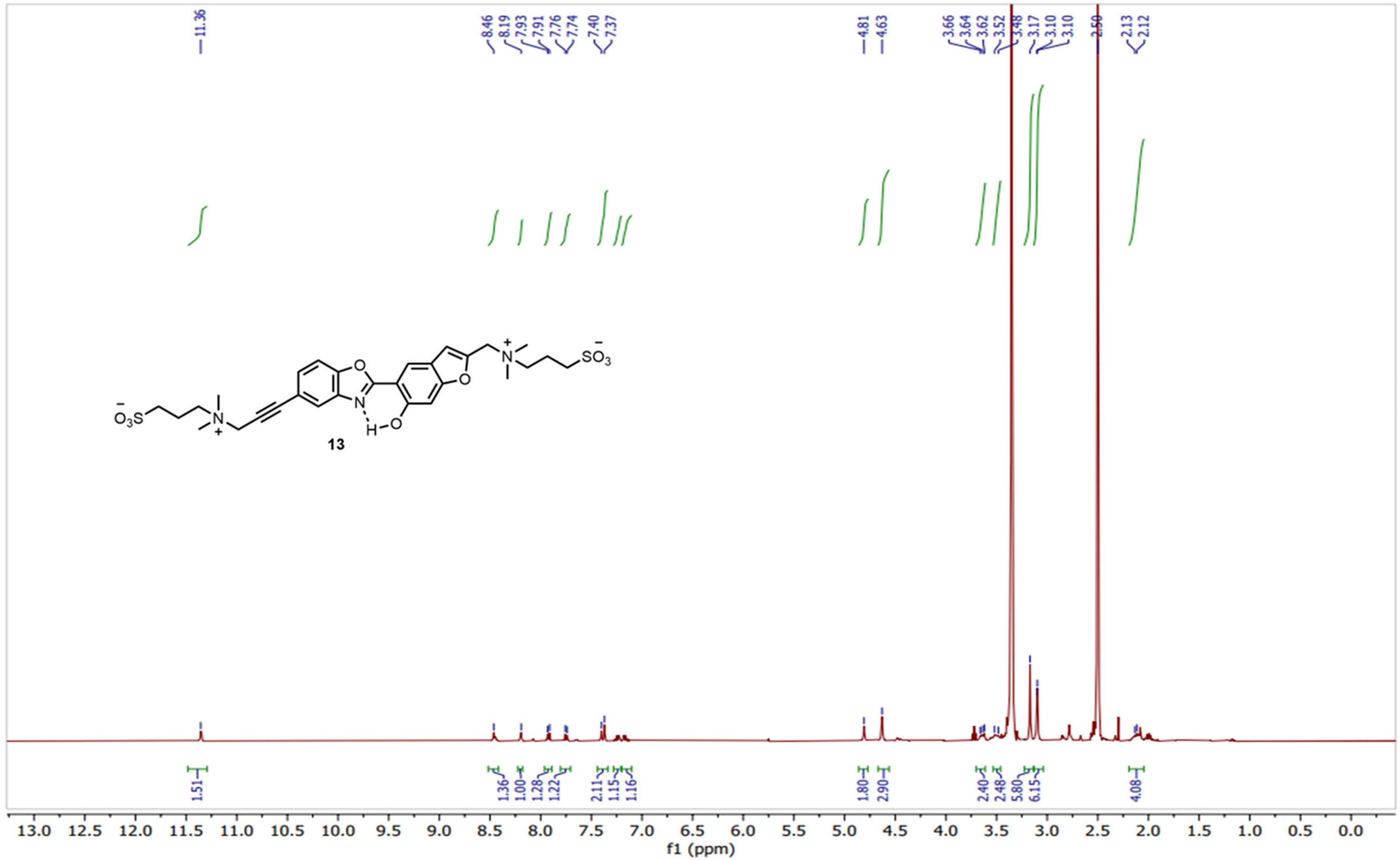

Figure S2.19. ^{1}H NMR spectrum of **13**

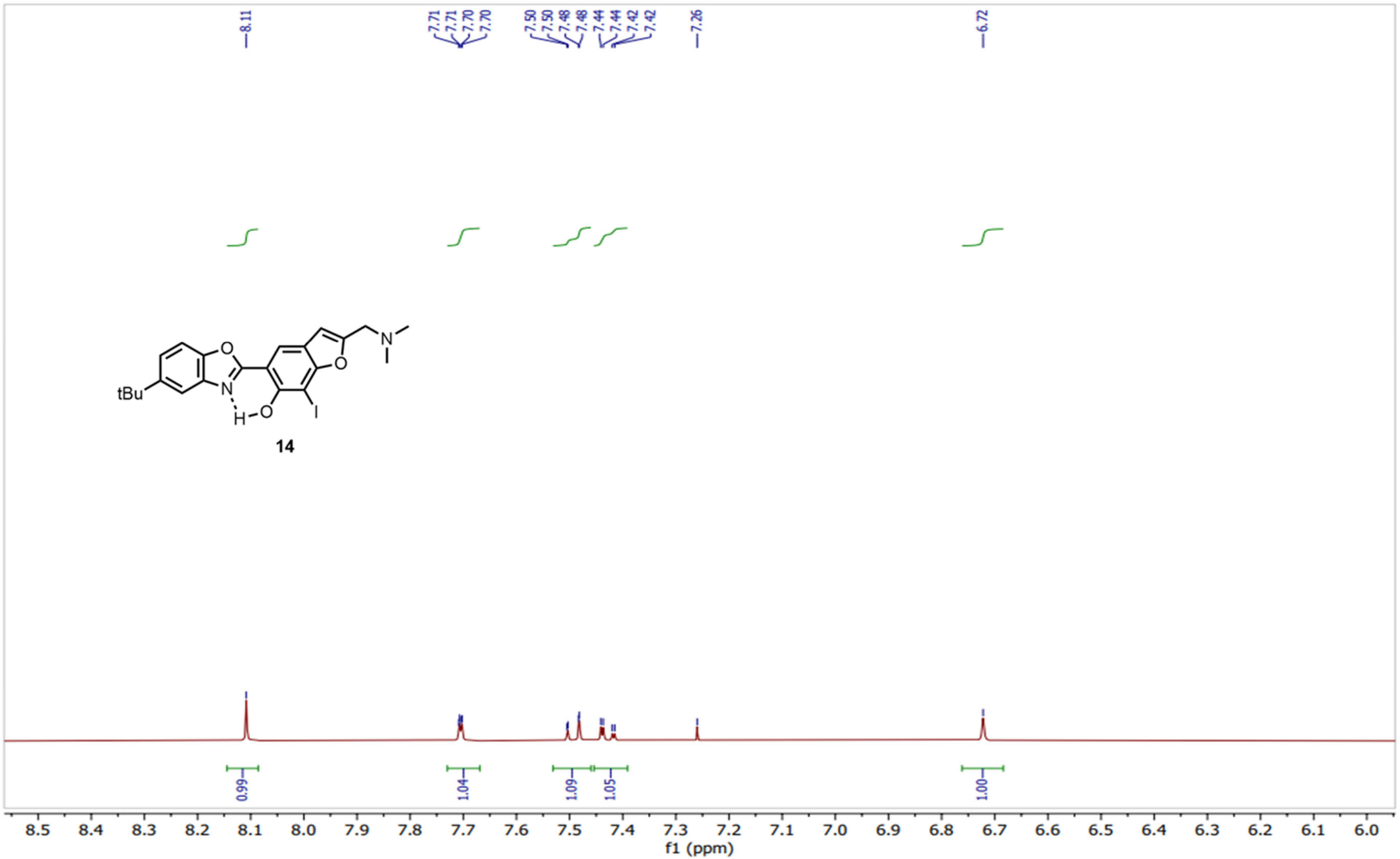

Figure S2.20. ^{1}H NMR spectrum of **14**

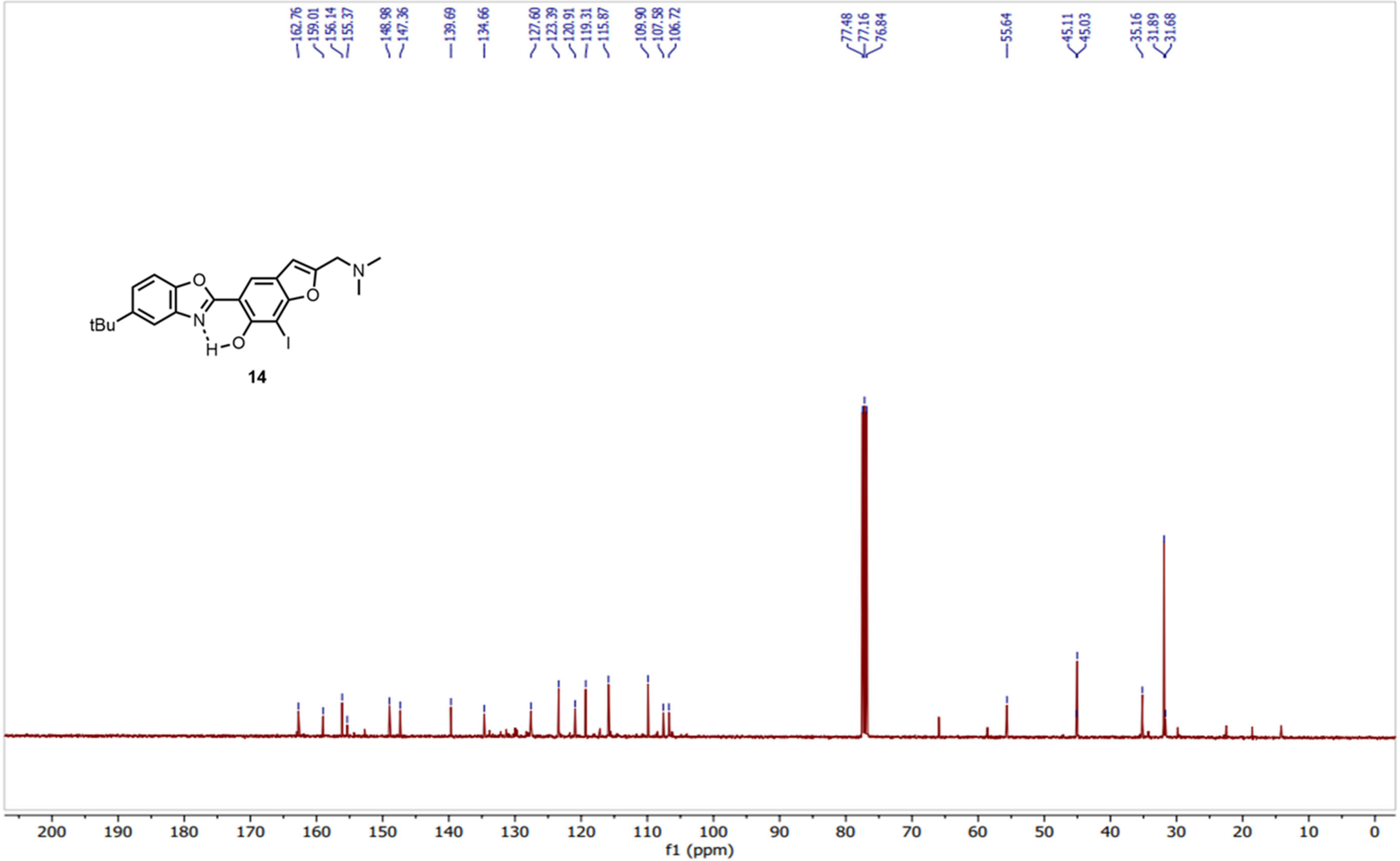

Figure S2.21. ^{13}C NMR spectrum of **14**

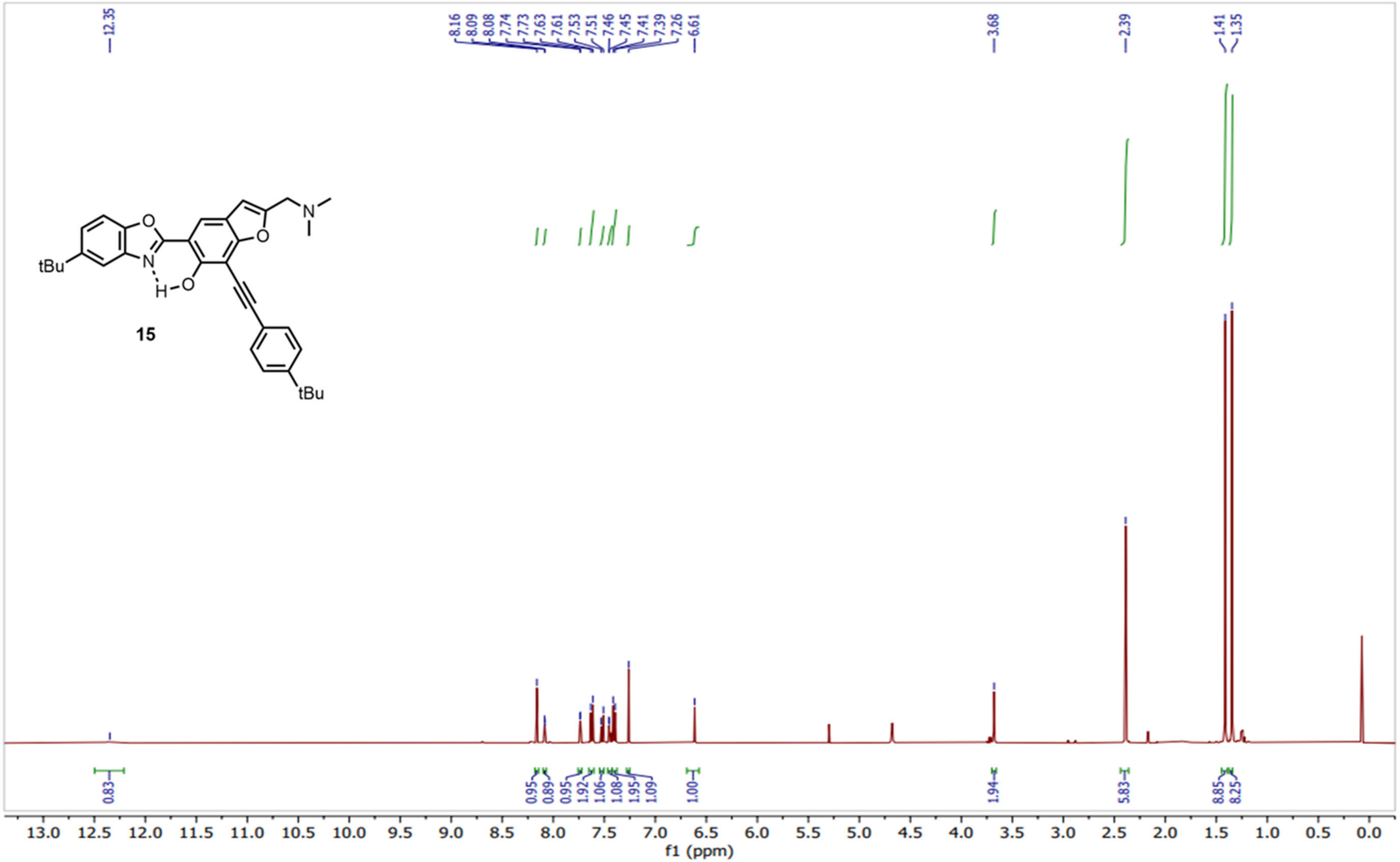

Figure S2.22. ^{1}H NMR spectrum of **15**

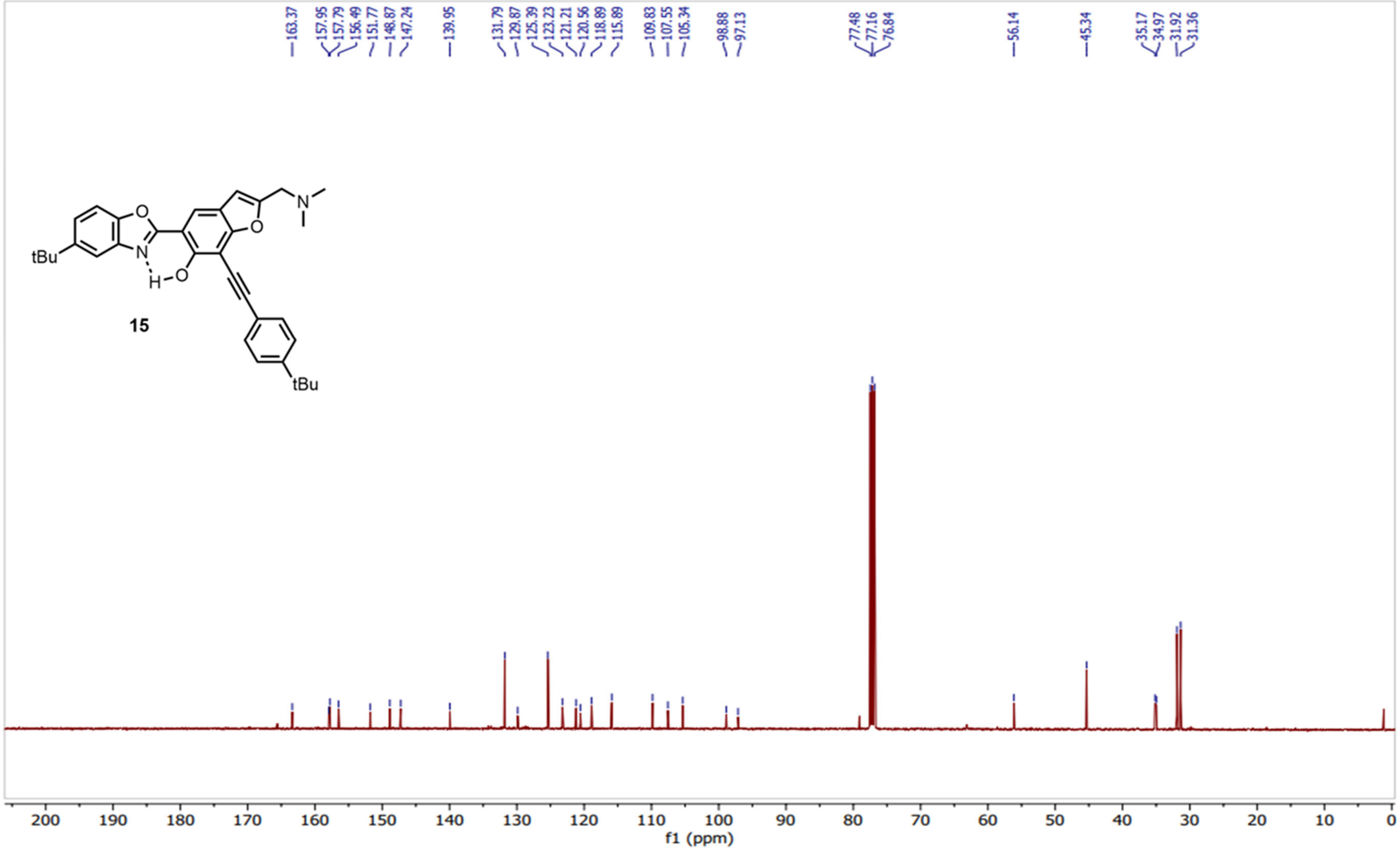

Figure S2.23. ^{13}C NMR spectrum of **15**

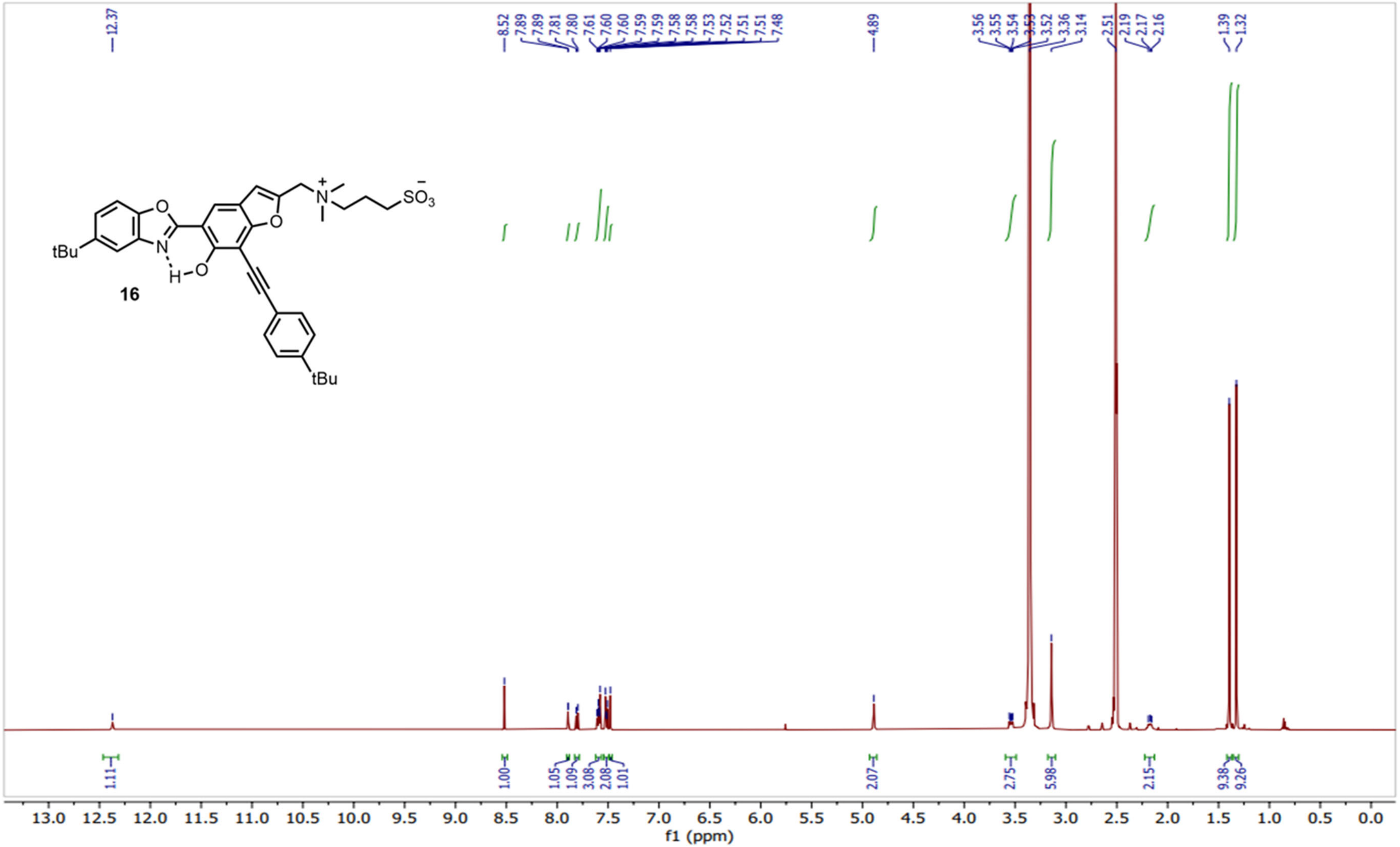

Figure S2.24. ^{1}H NMR spectrum of **16**

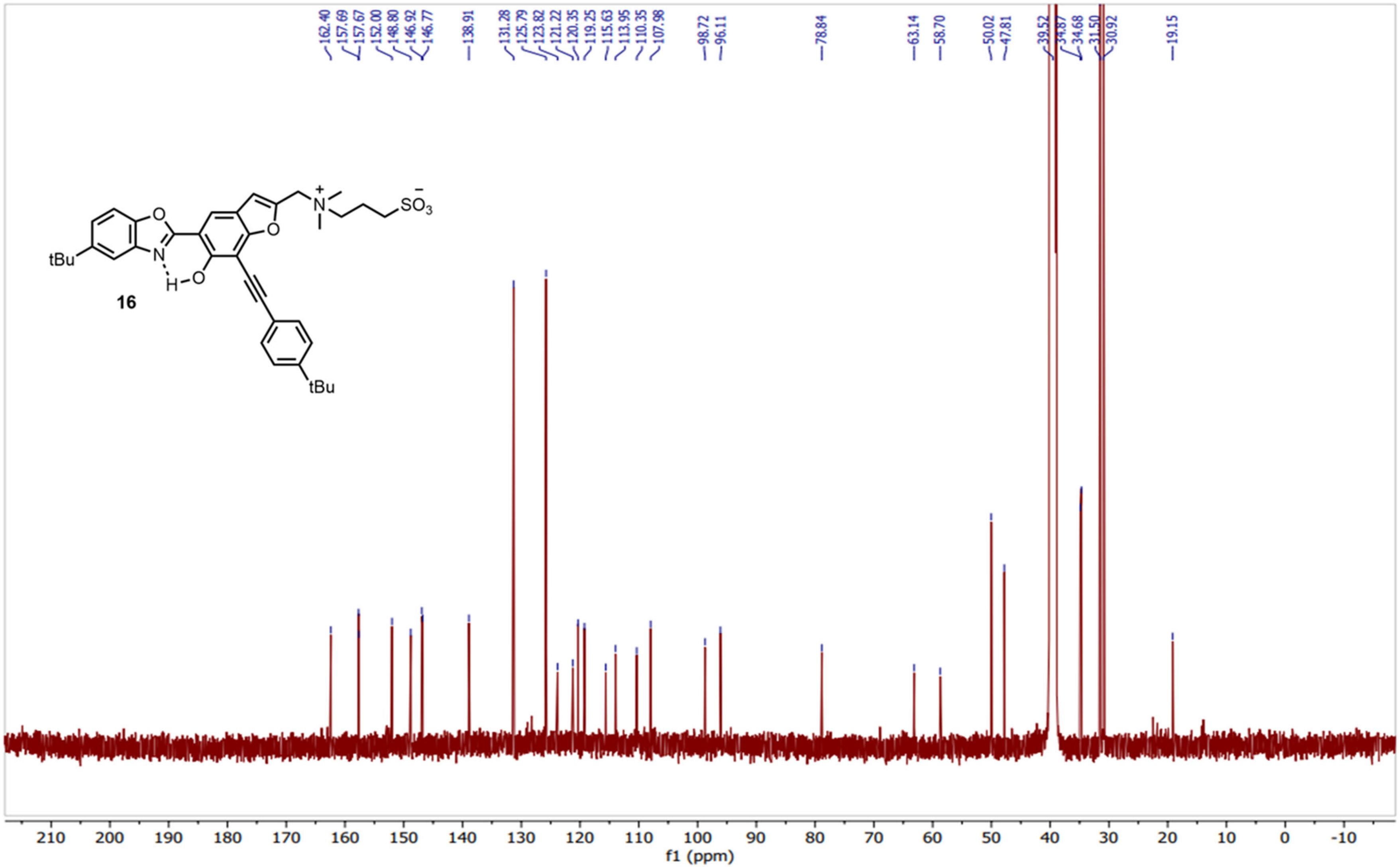

Figure S2.25. ^{13}C NMR spectrum of **16**

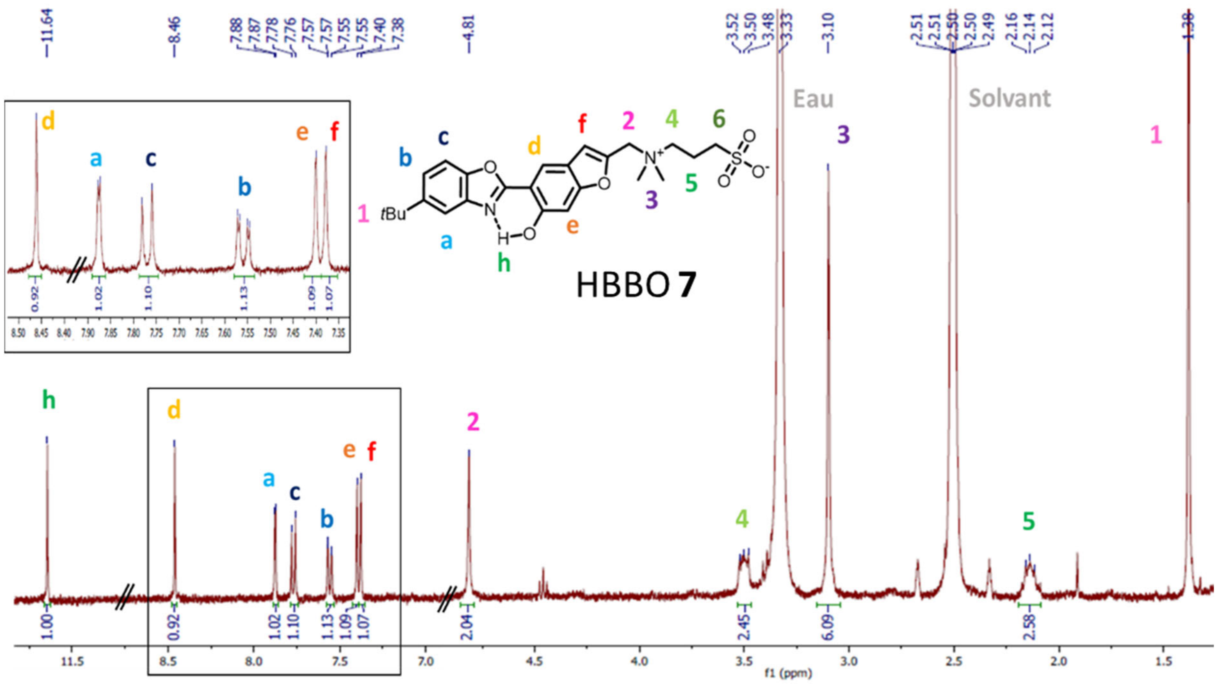

Figure S2.26. ^{1}H NMR spectrum of HBBO **7** in DMSO d^6.

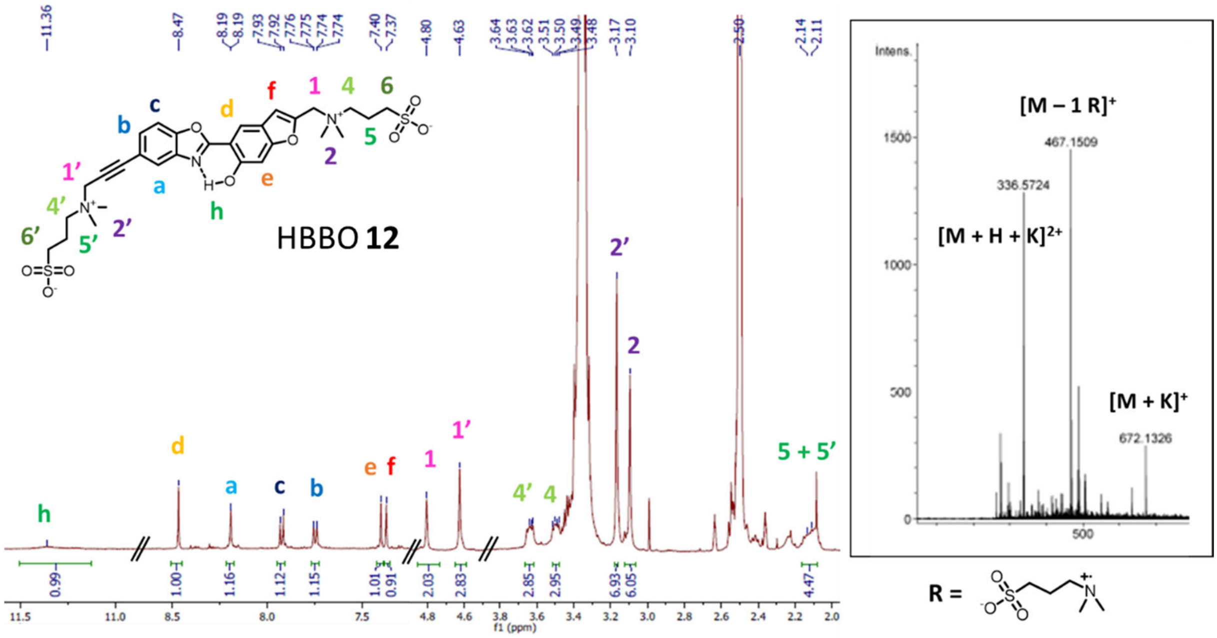

Figure S2.27. (a) ^{1}H NMR spectrum of HBBO **12** in DMSO d^6 and (b) HR-MS spectrum of HBBO **12**.

S3. Spectroscopic data

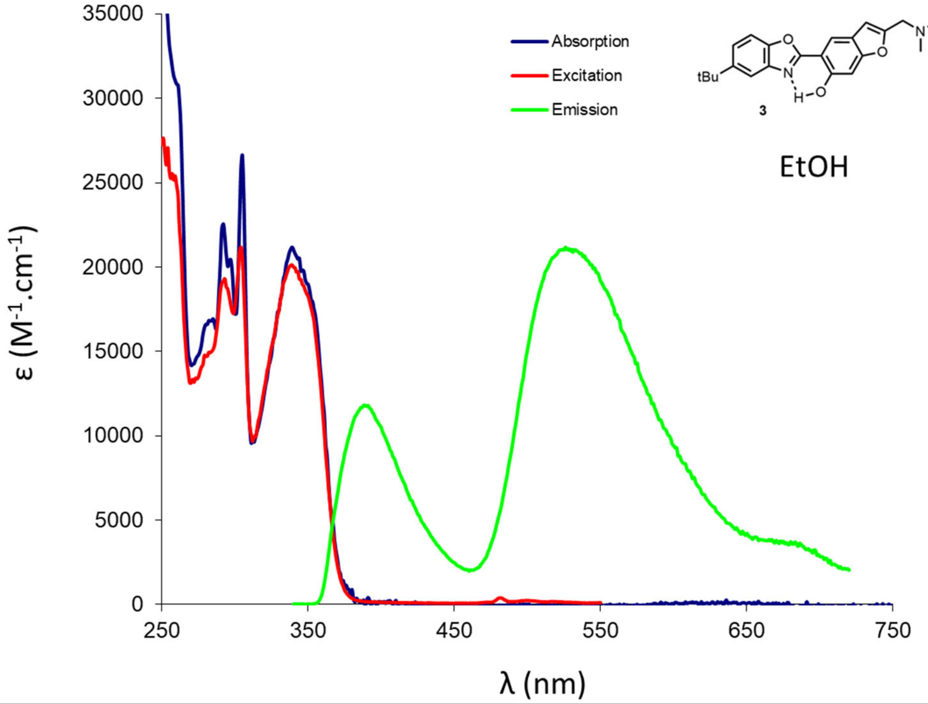

Figure S3.1. Absorption (blue), Emission (green) and Excitation (red) spectra of **HBBO 3** in ethanol.

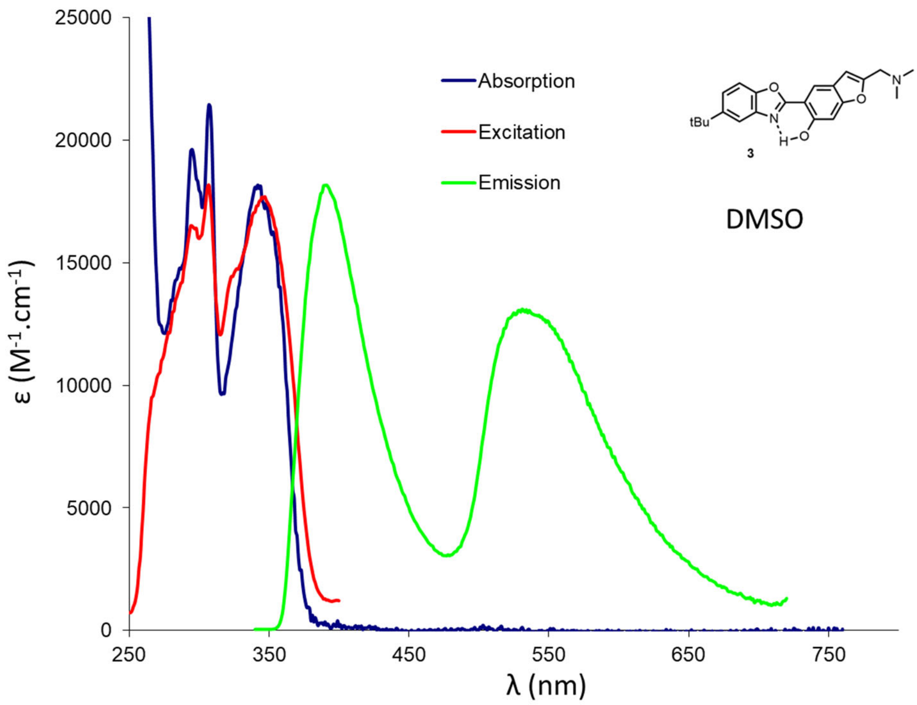

Figure S3.2. Absorption (blue), Emission (green) and Excitation (red) spectra of **HBBO 3** in DMSO.

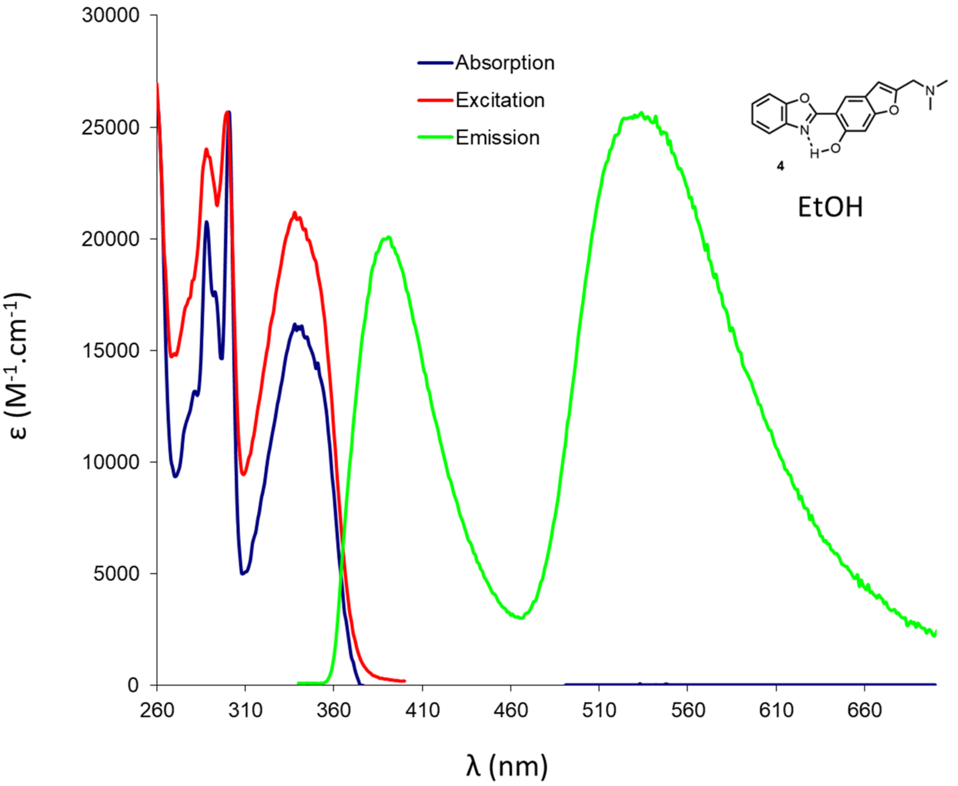

Figure S3.3. Absorption (blue), Emission (green) and Excitation (red) spectra of **HBBO 4** in ethanol.

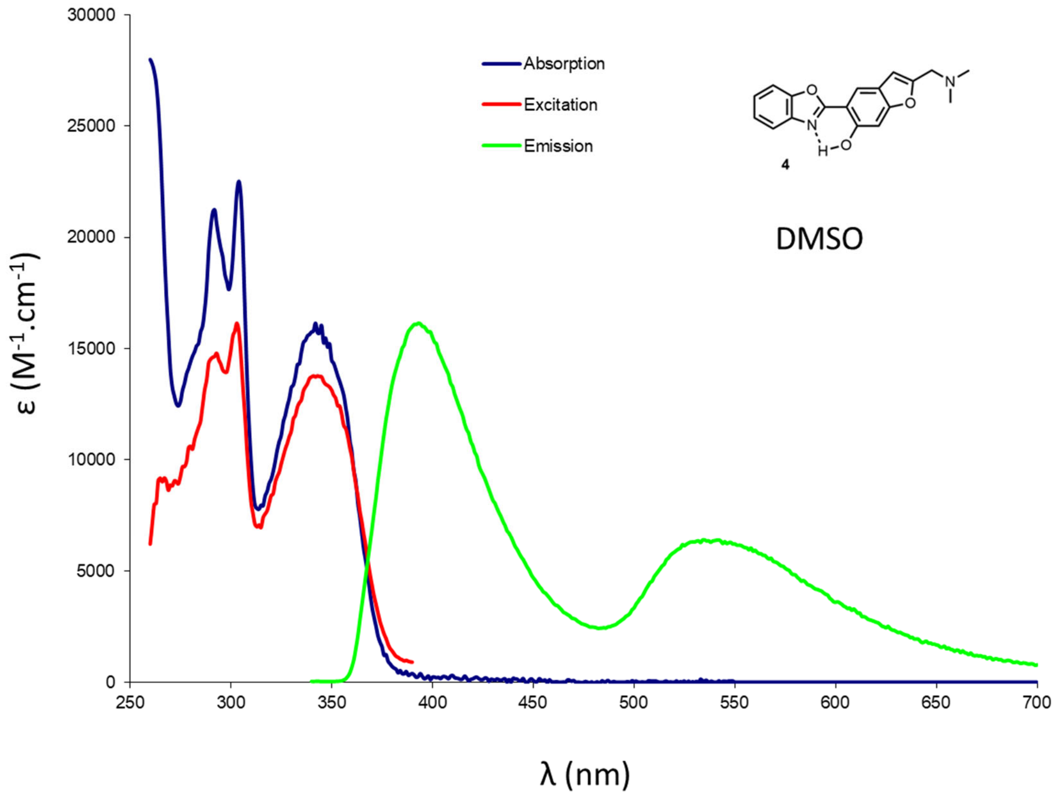

Figure S3.4. Absorption (blue), Emission (green) and Excitation (red) spectra of **HBBO 4** in DMSO.

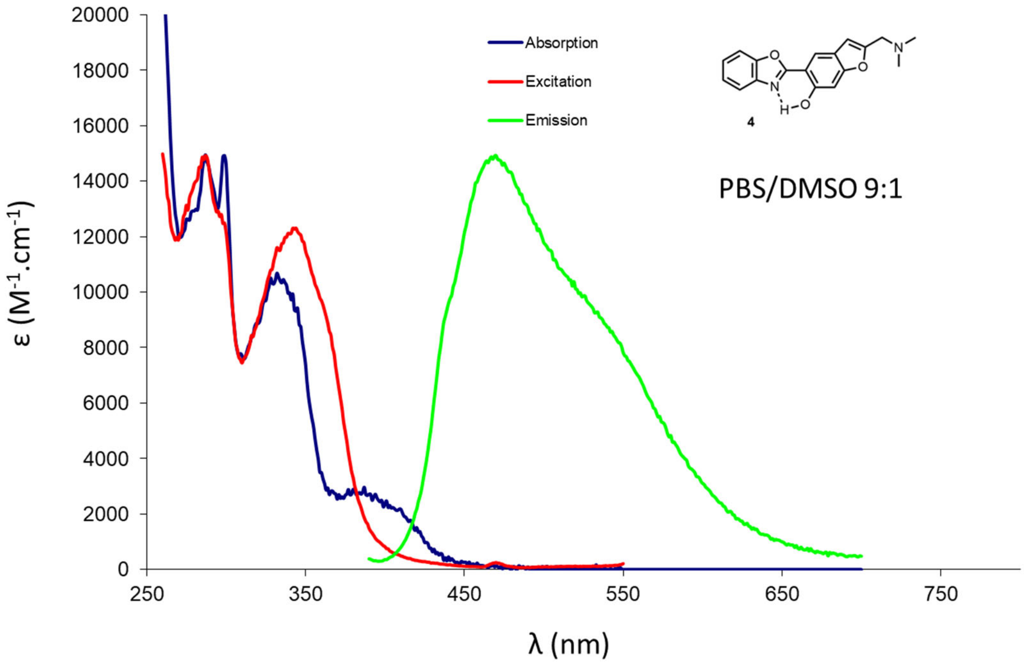

Figure S3.5. Absorption (blue), Emission (green) and Excitation (red) spectra of **HBBO 4** in PBS/DMSO 9:1.

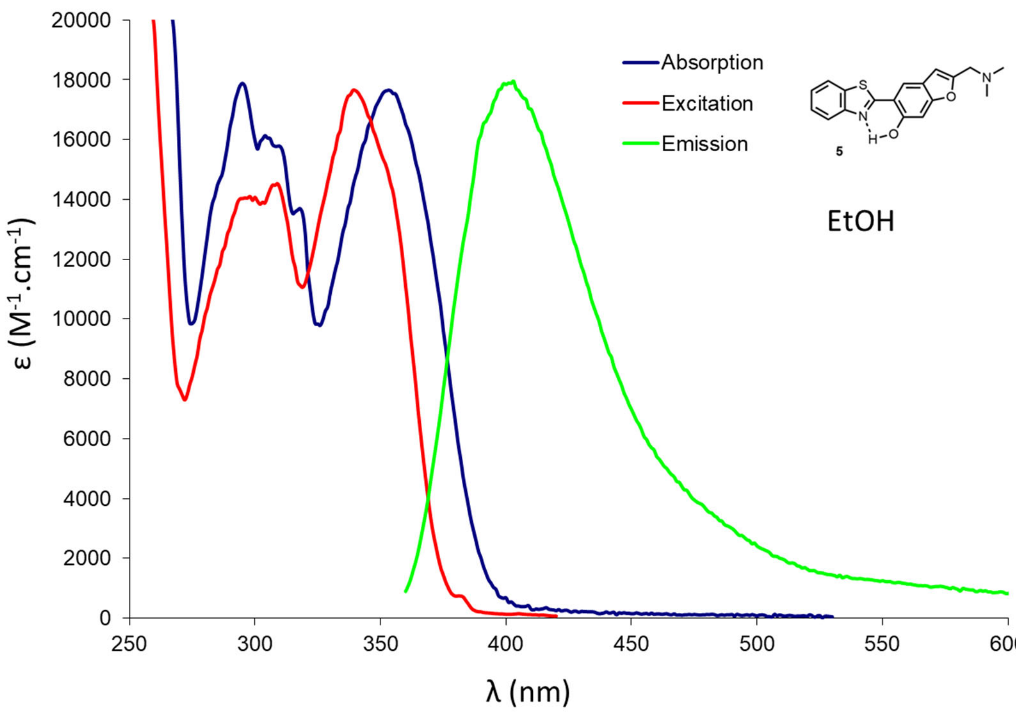

Figure S3.6. Absorption (blue), Emission (green) and Excitation (red) spectra of **HBBT 5** in ethanol.

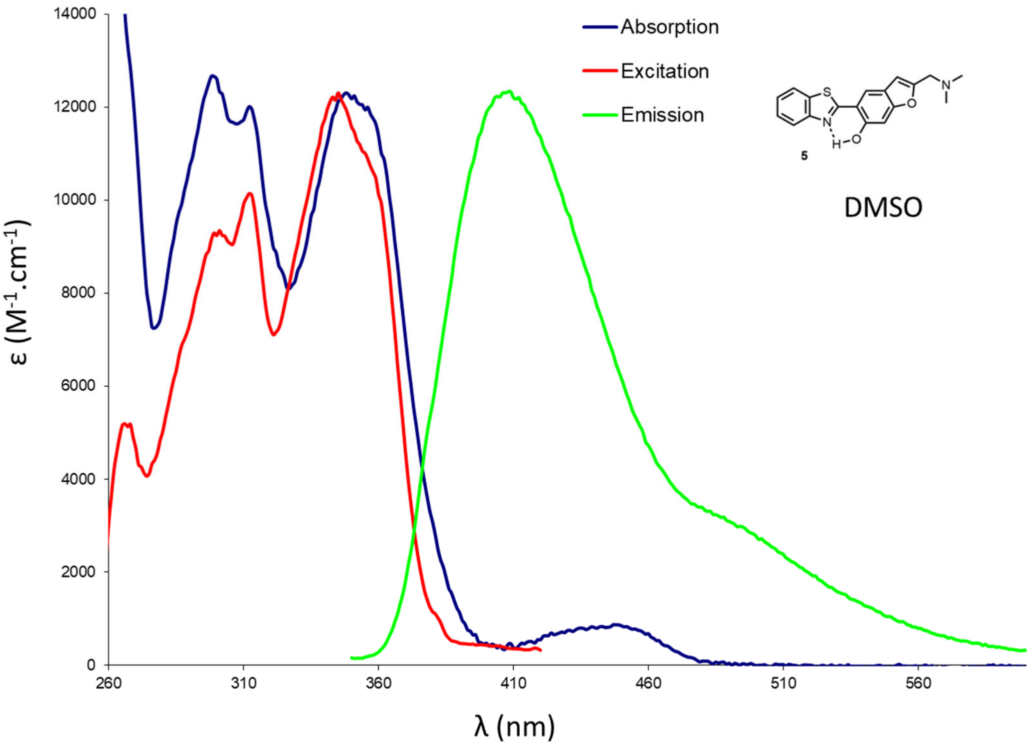

Figure S3.7. Absorption (blue), Emission (green) and Excitation (red) spectra of **HBBT 5** in DMSO.

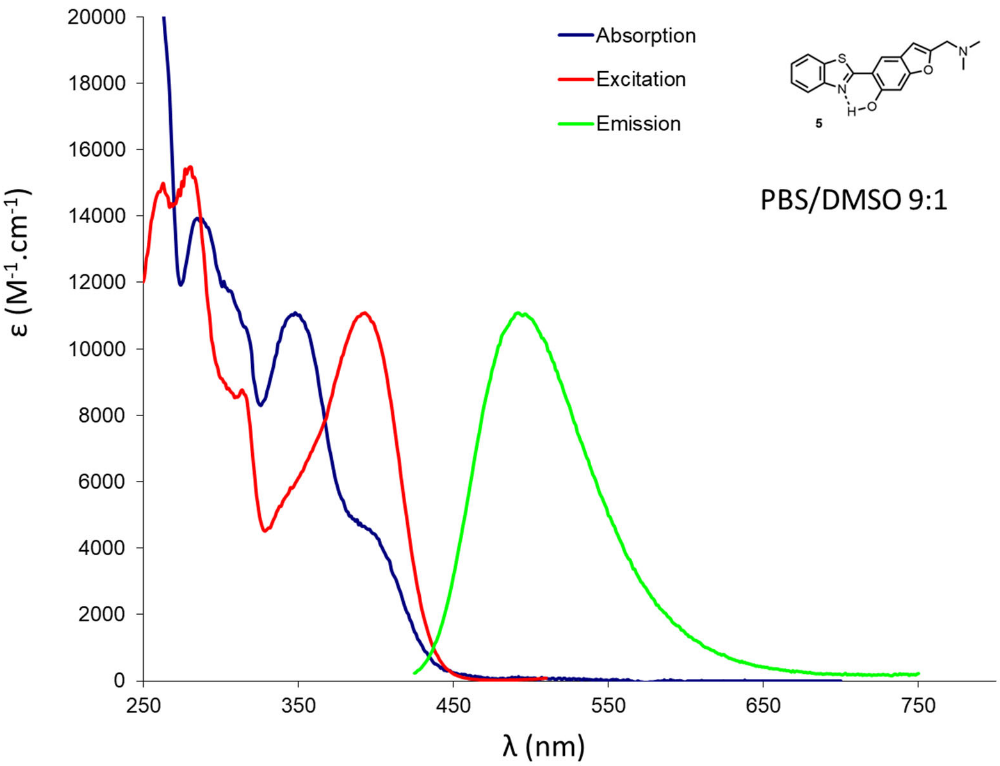

Figure S3.8. Absorption (blue), Emission (green) and Excitation (red) spectra of **HBBT 5** in PBS/DMSO 9:1.

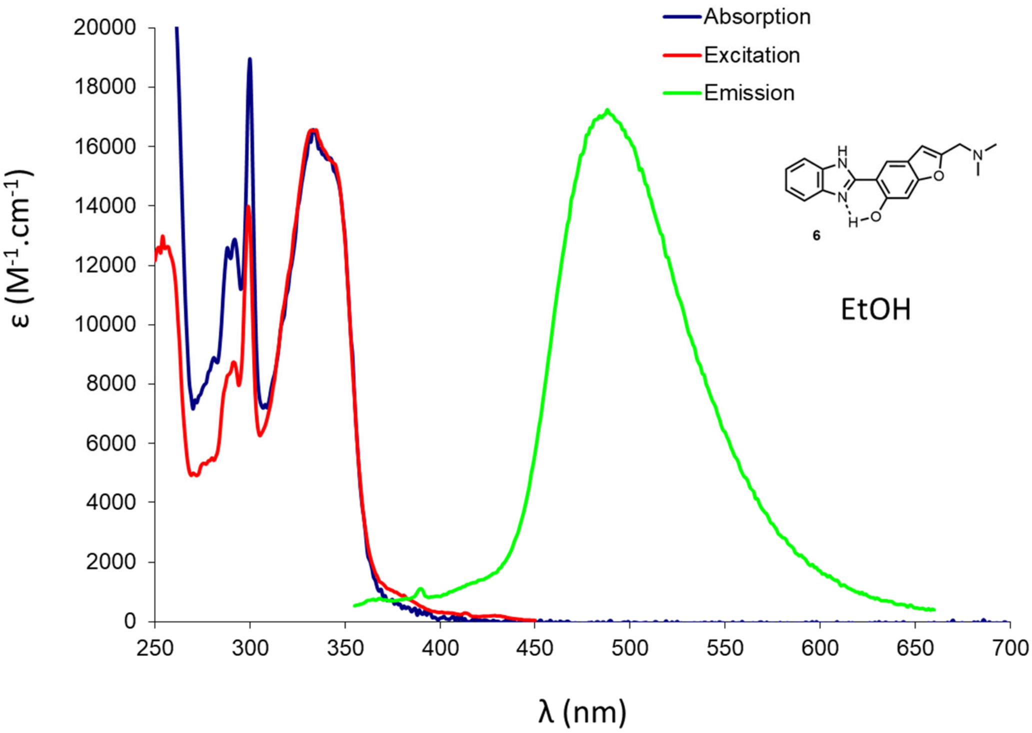

Figure S3.9. Absorption (blue), Emission (green) and Excitation (red) spectra of **HBBI 6** in EtOH.

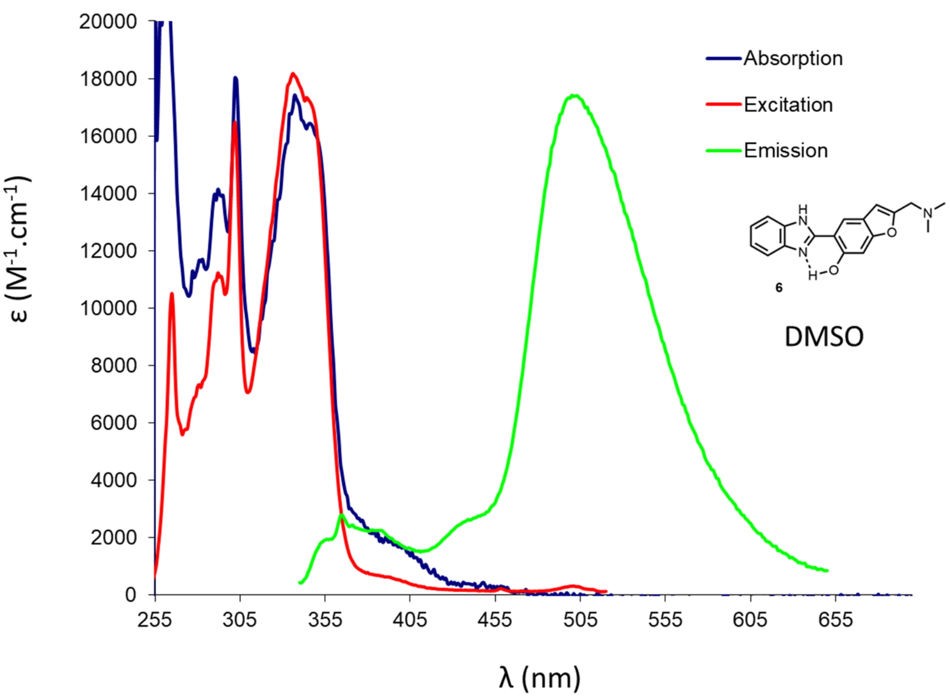

Figure S3.10. Absorption (blue), Emission (green) and Excitation (red) spectra of **HBBI 6** in DMSO.

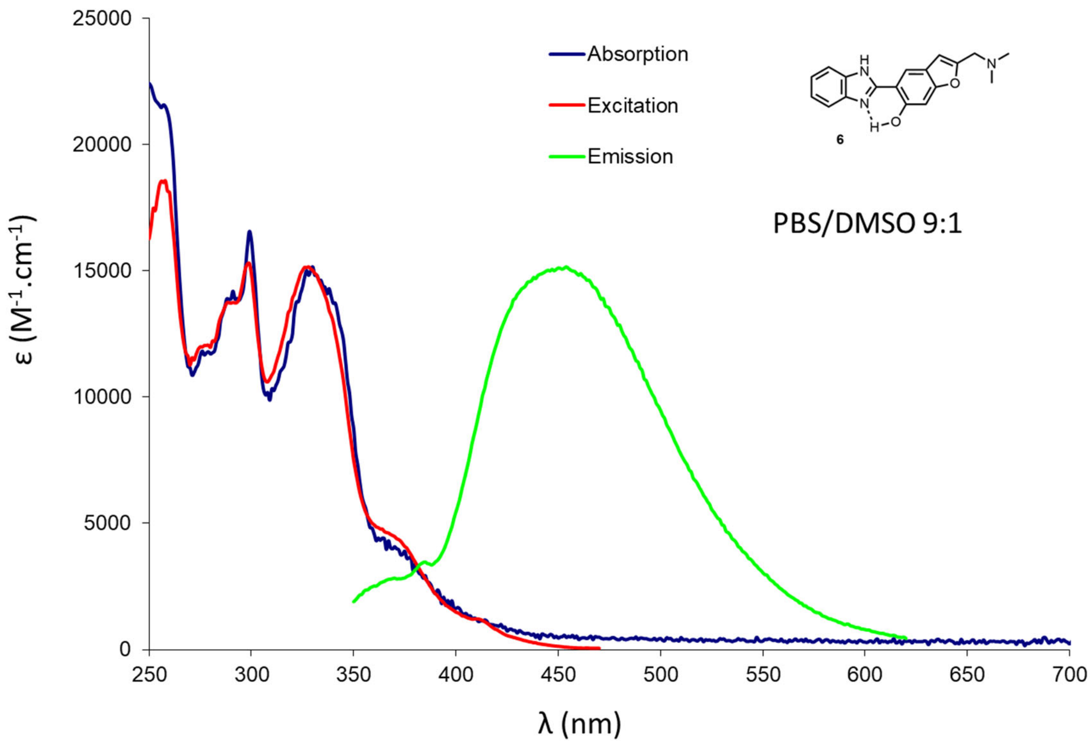

Figure S3.11. Absorption (blue), Emission (green) and Excitation (red) spectra of **HBBI 6** in PBS/DMSO 9:1.

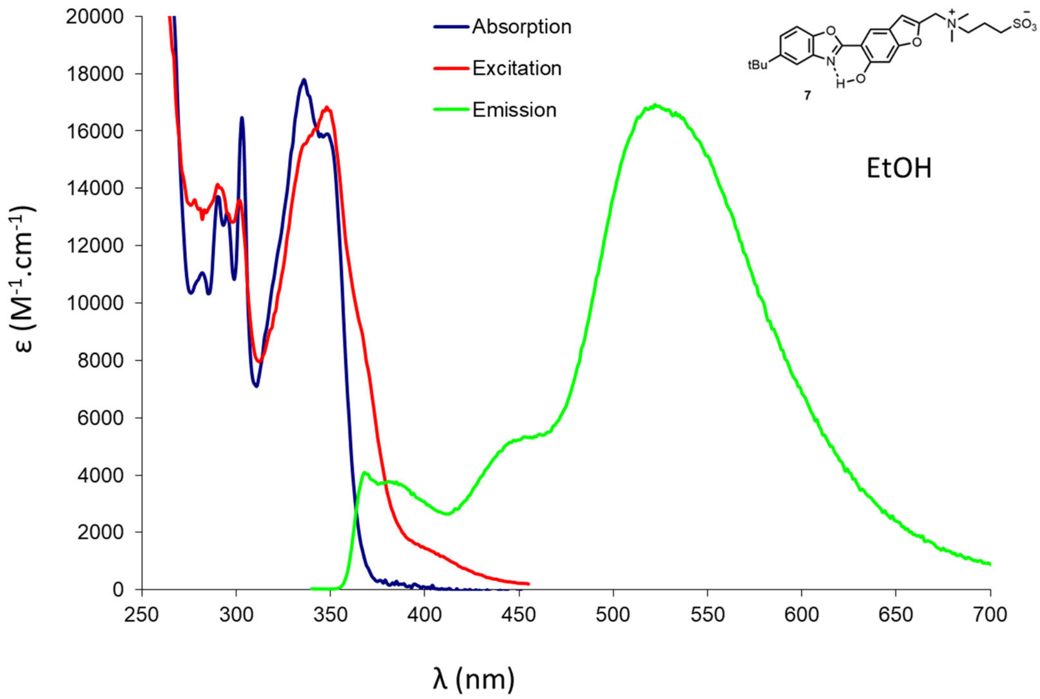

Figure S3.12. Absorption (blue), Emission (green) and Excitation (red) spectra of **HBBO 7** in ethanol.

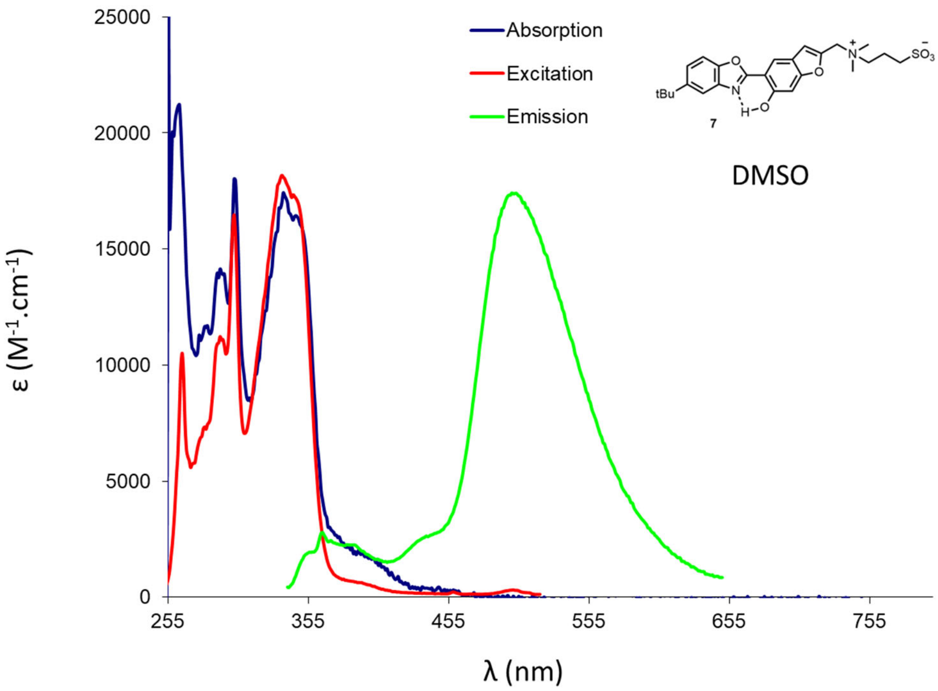

Figure S3.13. Absorption (blue), Emission (green) and Excitation (red) spectra of **HBBO 7** in DMSO.

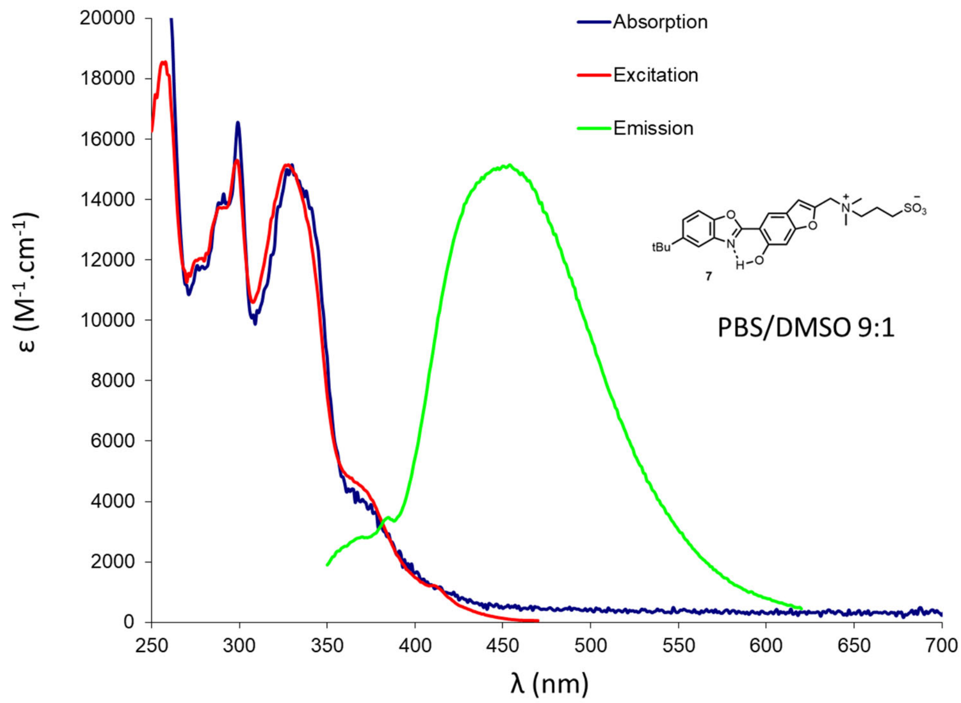

Figure S3.14. Absorption (blue), Emission (green) and Excitation (red) spectra of **HBBO 7** in PBS/DMSO 9:1.

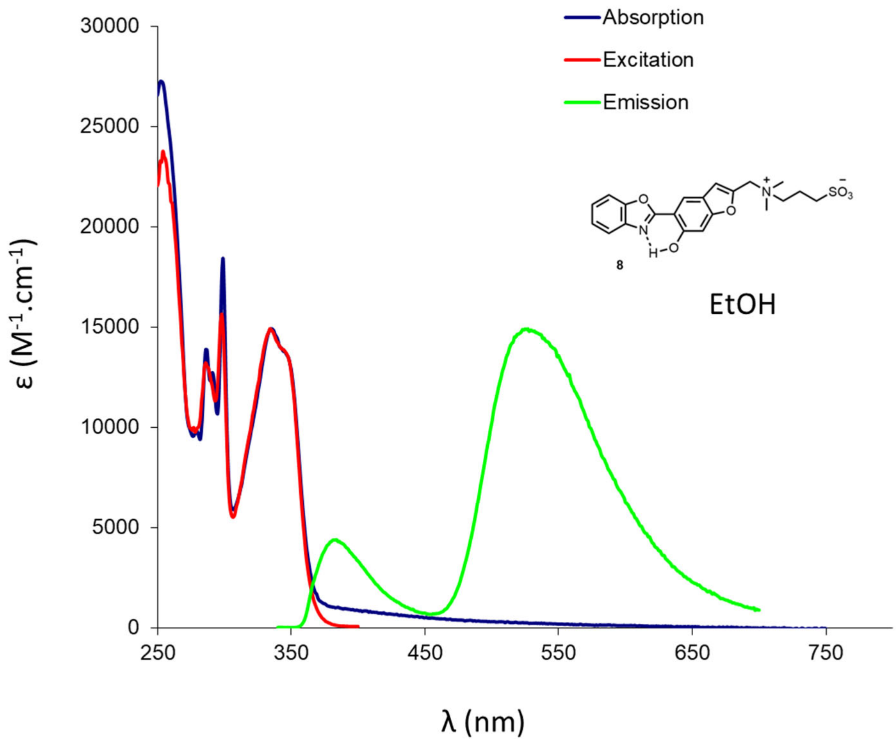

Figure S3.15. Absorption (blue), Emission (green) and Excitation (red) spectra of **HBBO 8** in ethanol.

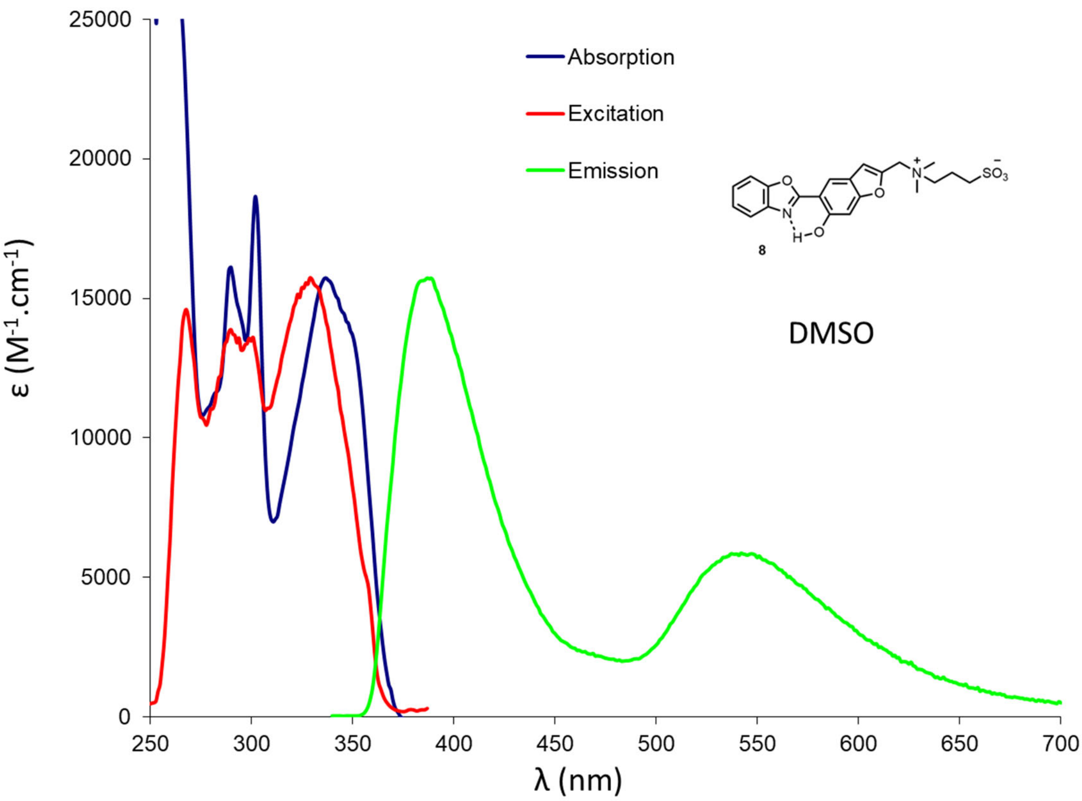

Figure S3.16. Absorption (blue), Emission (green) and Excitation (red) spectra of **HBBO 8** in DMSO.

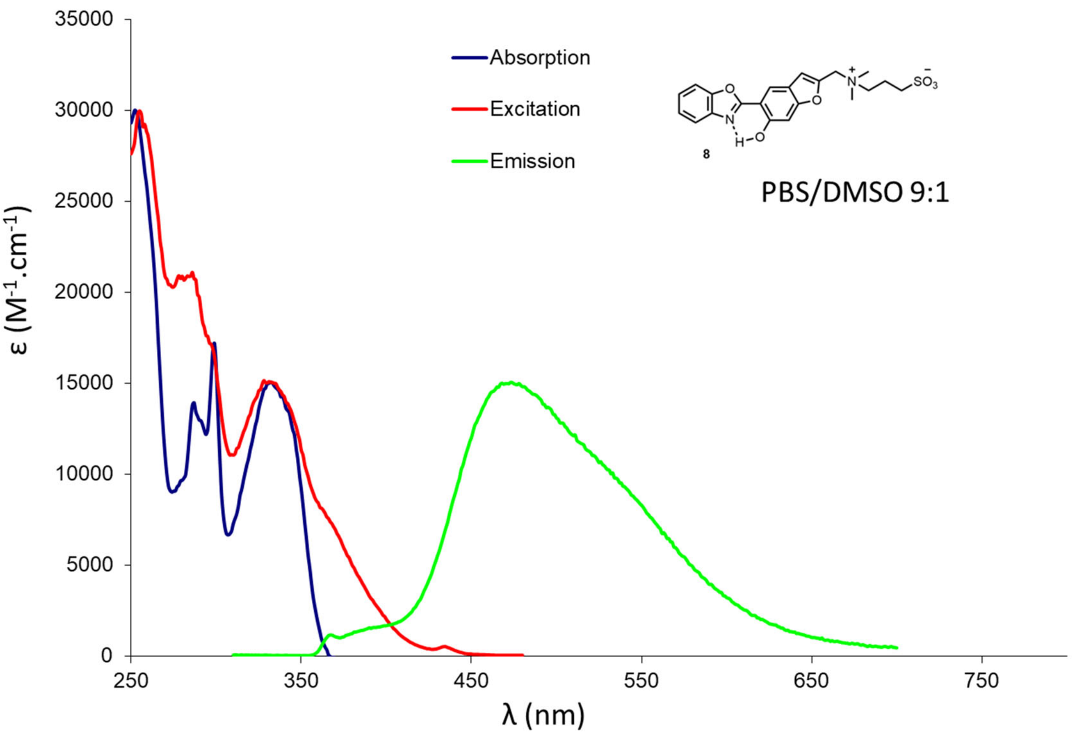

Figure S3.17. Absorption (blue), Emission (green) and Excitation (red) spectra of **HBBO 8** in PBS/DMSO 9:1.

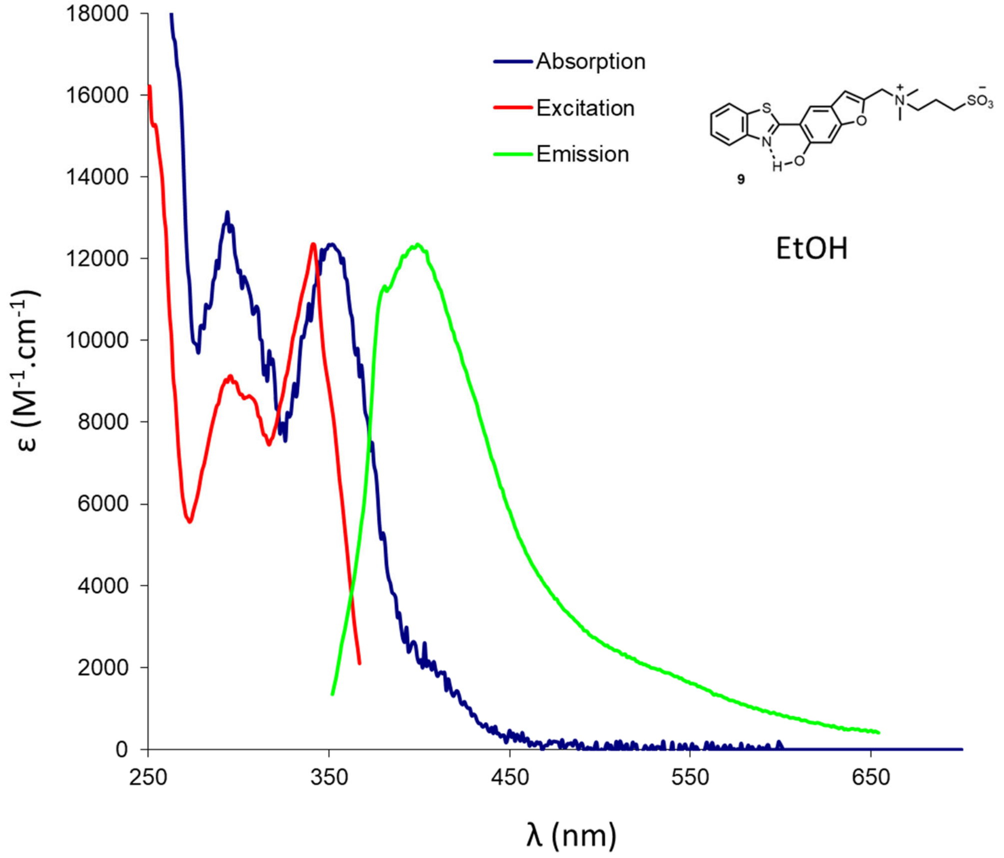

Figure S3.18. Absorption (blue), Emission (green) and Excitation (red) spectra of **HBBT 9** in ethanol.

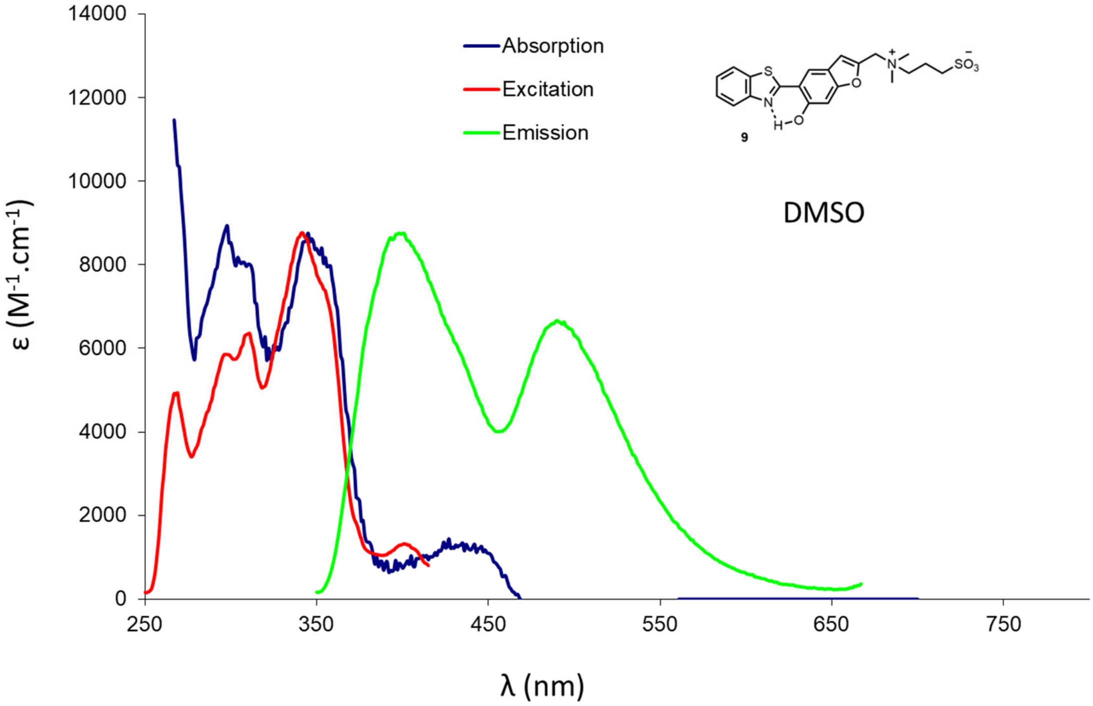

Figure S3.19. Absorption (blue), Emission (green) and Excitation (red) spectra of **HBBT 9** in ethanol.

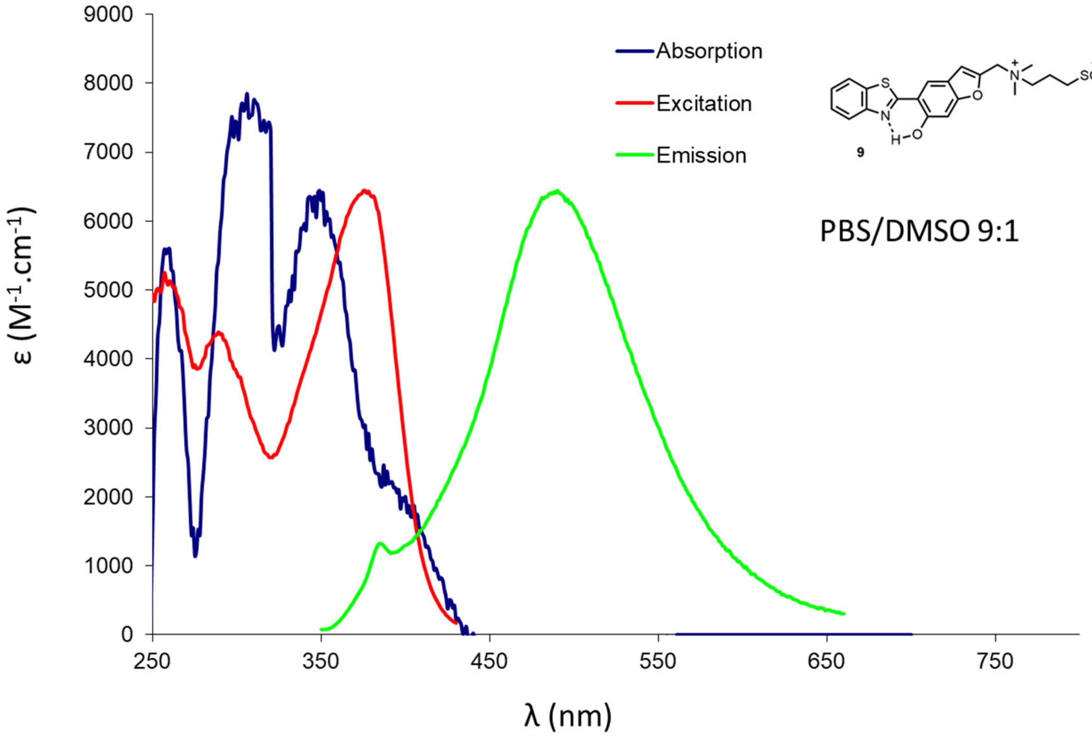

Figure S3.20. Absorption (blue), Emission (green) and Excitation (red) spectra of **HBBT 9** in PBS/DMSO 9:1.

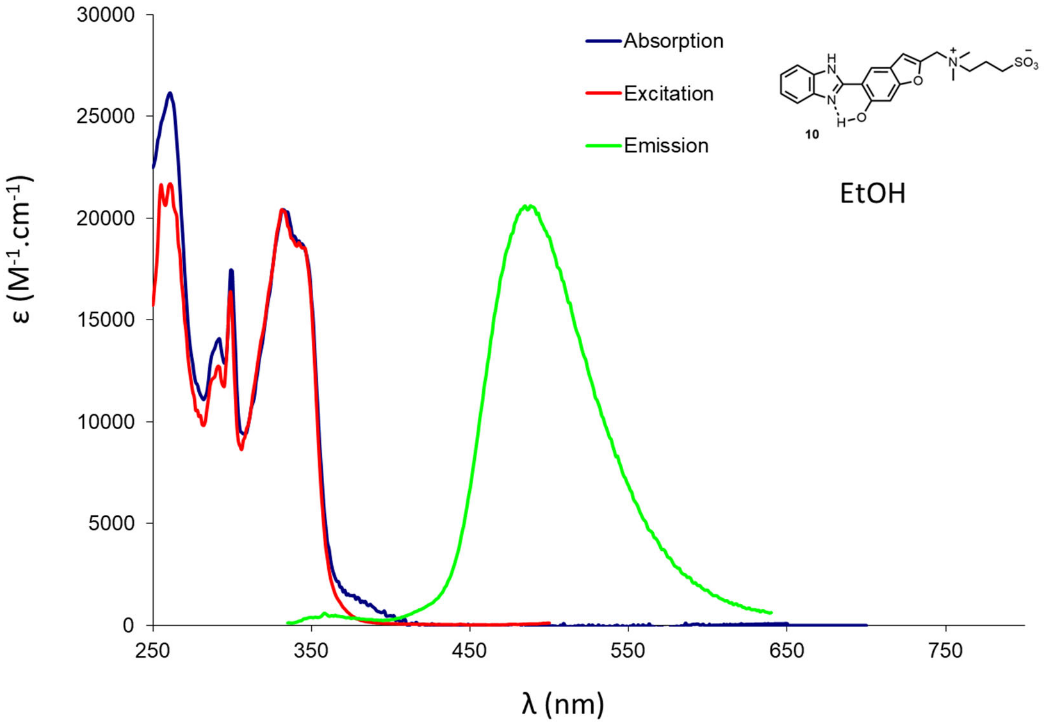

Figure S3.21. Absorption (blue), Emission (green) and Excitation (red) spectra of **HBBI 10** in ethanol.

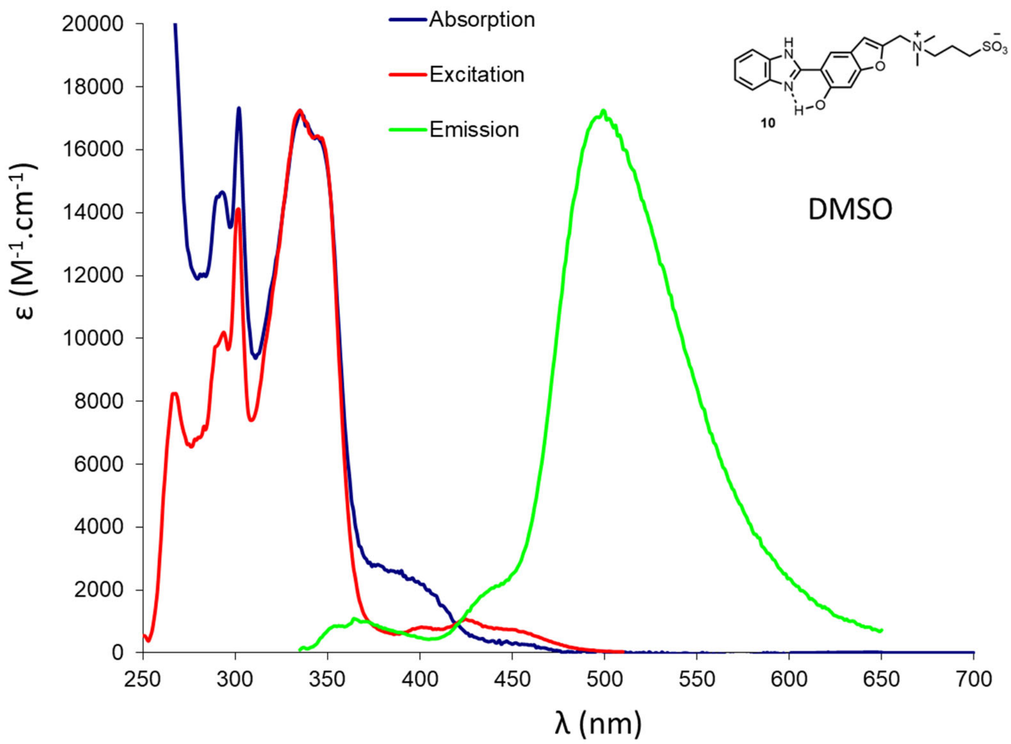

Figure S3.22. Absorption (blue), Emission (green) and Excitation (red) spectra of **HBBI 10** in DMSO.

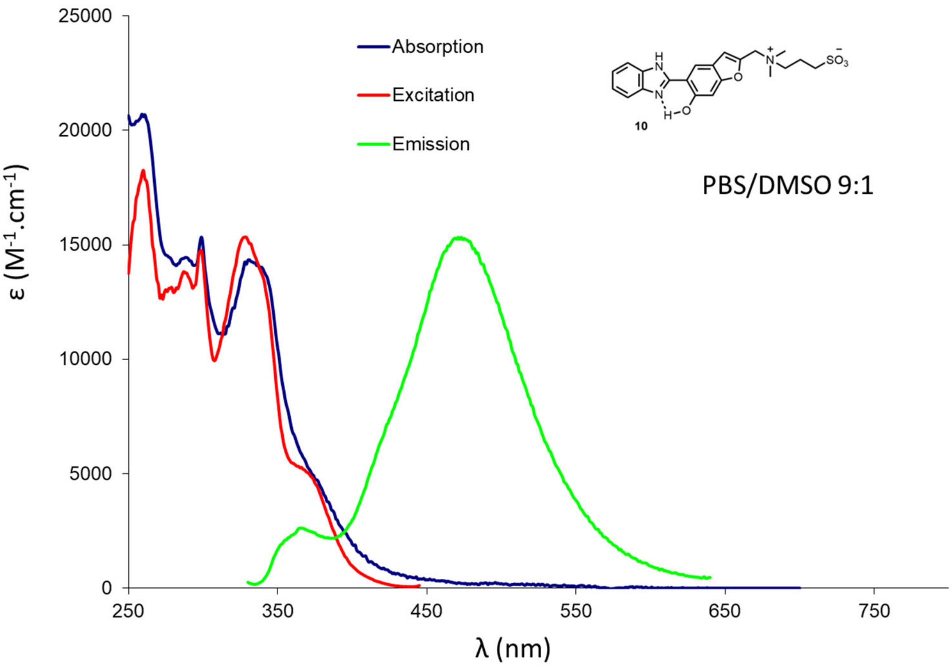

Figure S3.23. Absorption (blue), Emission (green) and Excitation (red) spectra of **HBBI 10** in PBS/DMSO 9:1.

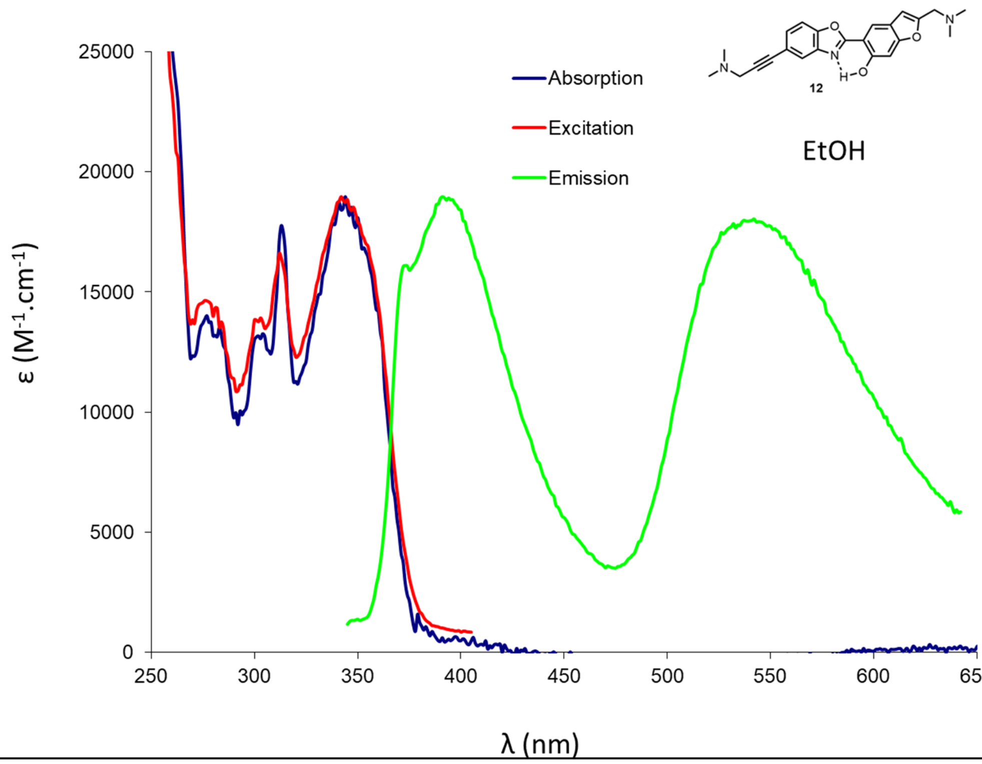

Figure S3.24. Absorption (blue), Emission (green) and Excitation (red) spectra of **HBBO 12** in ethanol.

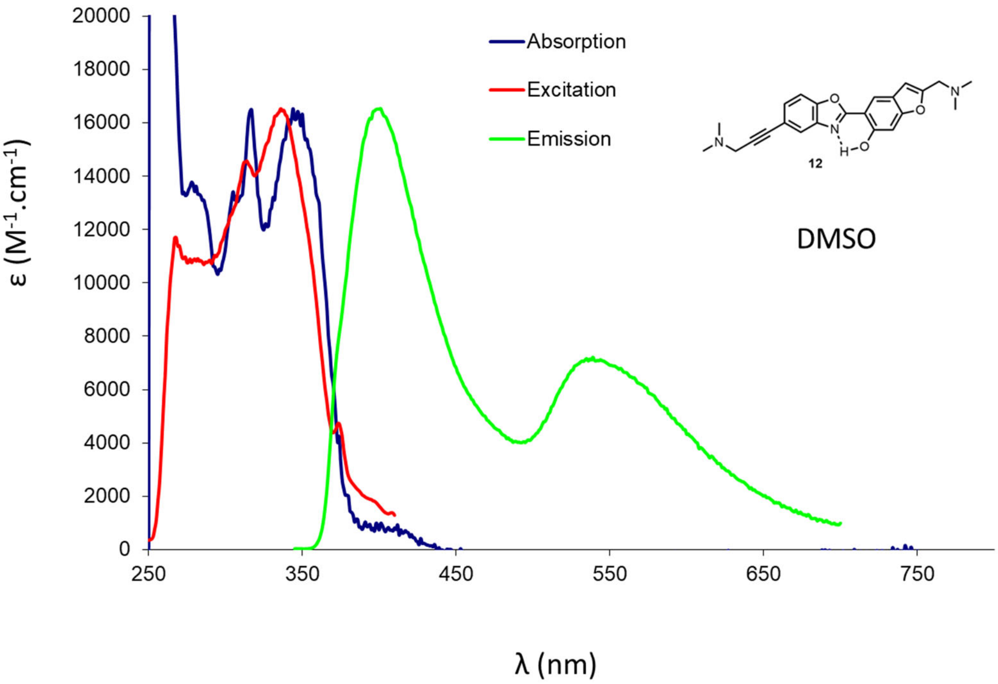

Figure S3.25. Absorption (blue), Emission (green) and Excitation (red) spectra of **HBBO 12** in DMSO.

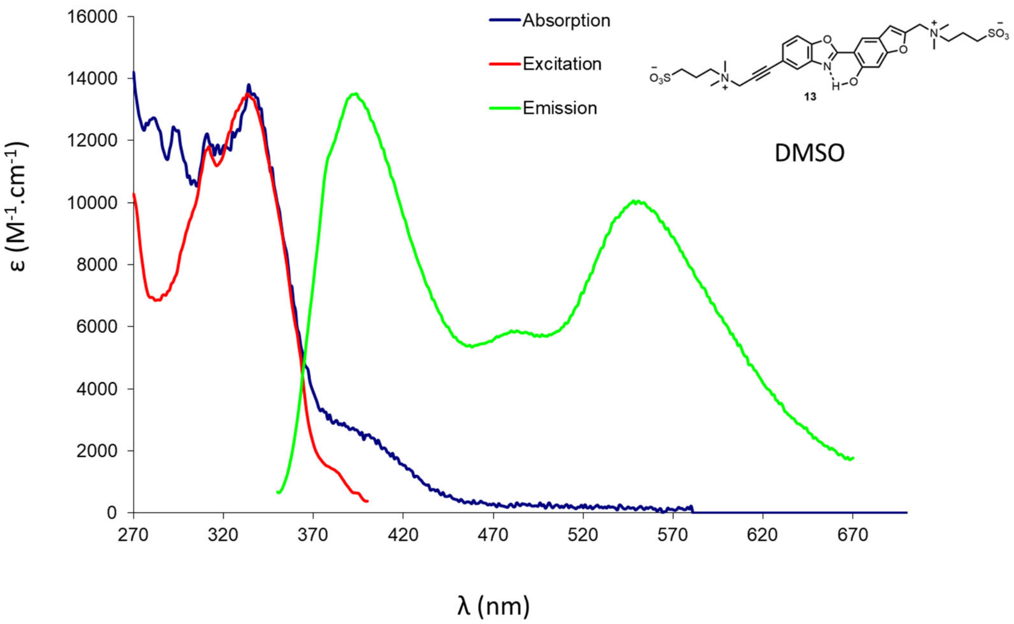

Figure S3.26. Absorption (blue), Emission (green) and Excitation (red) spectra of **HBBO 13** in DMSO.

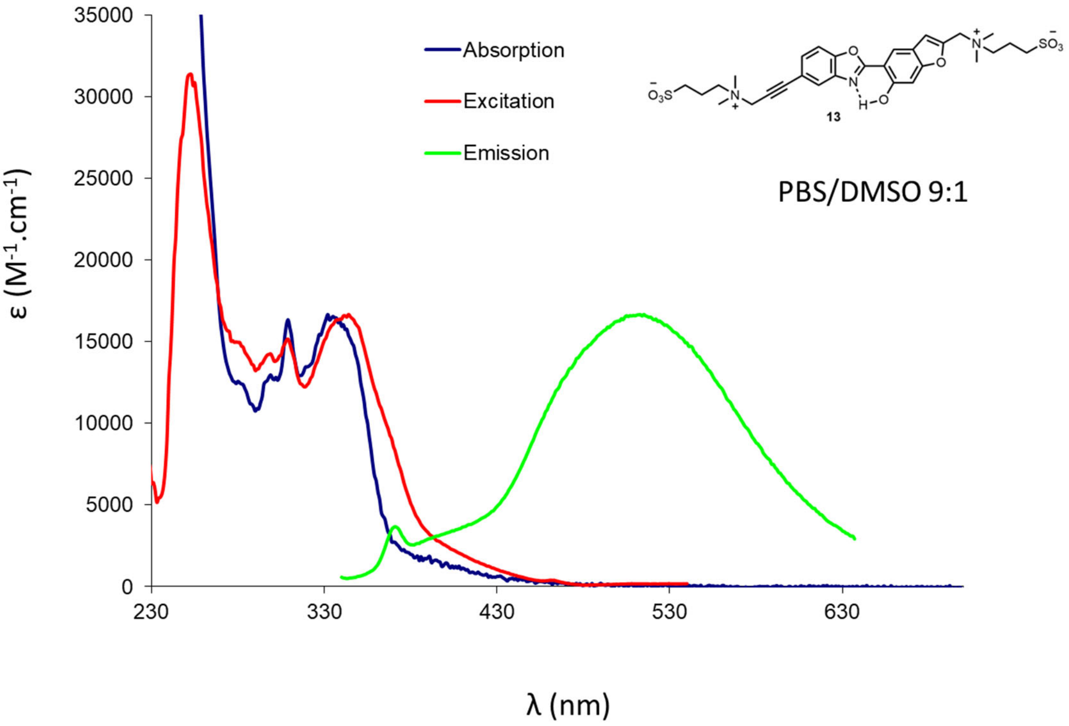

Figure S3.27. Absorption (blue), Emission (green) and Excitation (red) spectra of **HBBO 13** in PBS/DMSO 9:1.

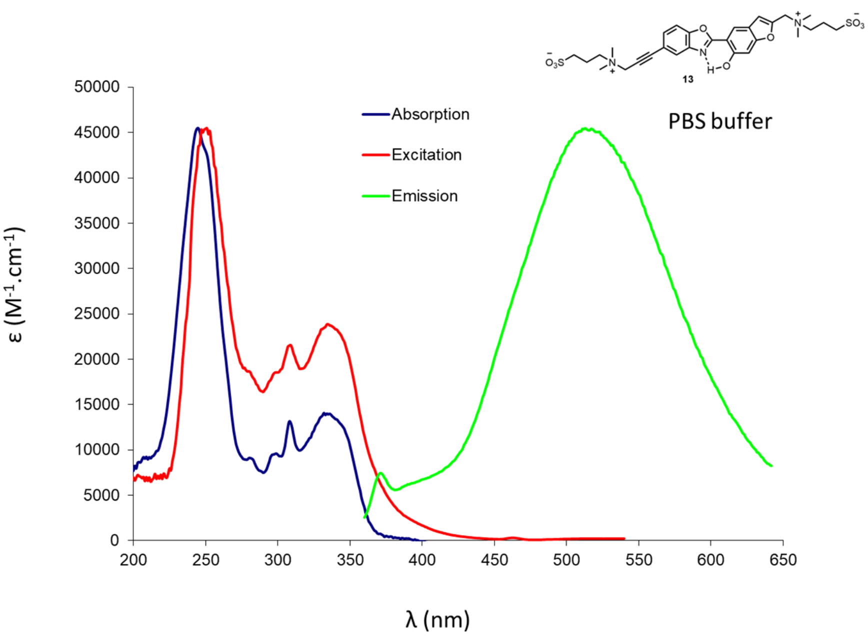

Figure S3.28. Absorption (blue), Emission (green) and Excitation (red) spectra of **HBBO 13** in PBS buffer.

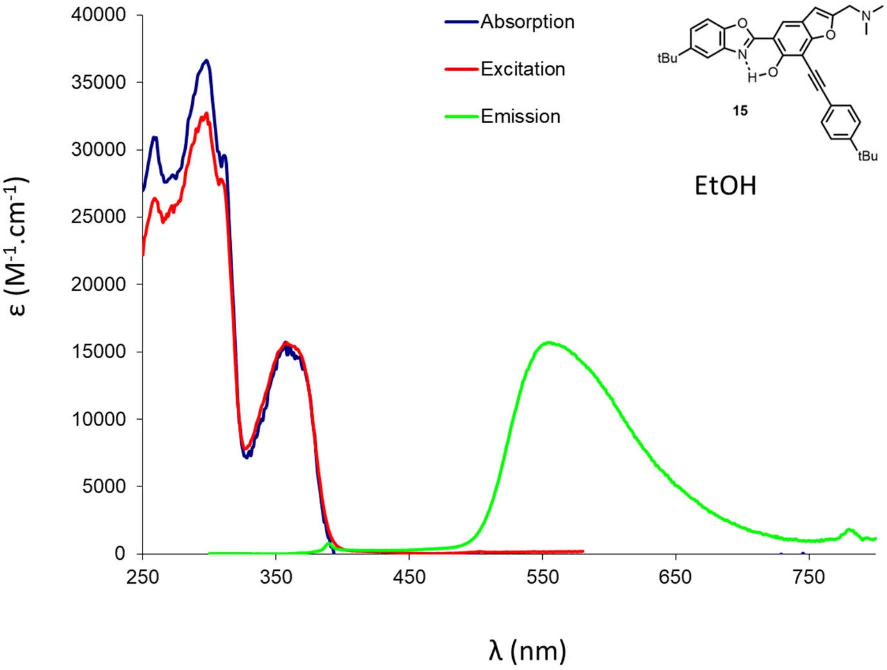

Figure S3.29. Absorption (blue), Emission (green) and Excitation (red) spectra of **HBBO 15** in ethanol.

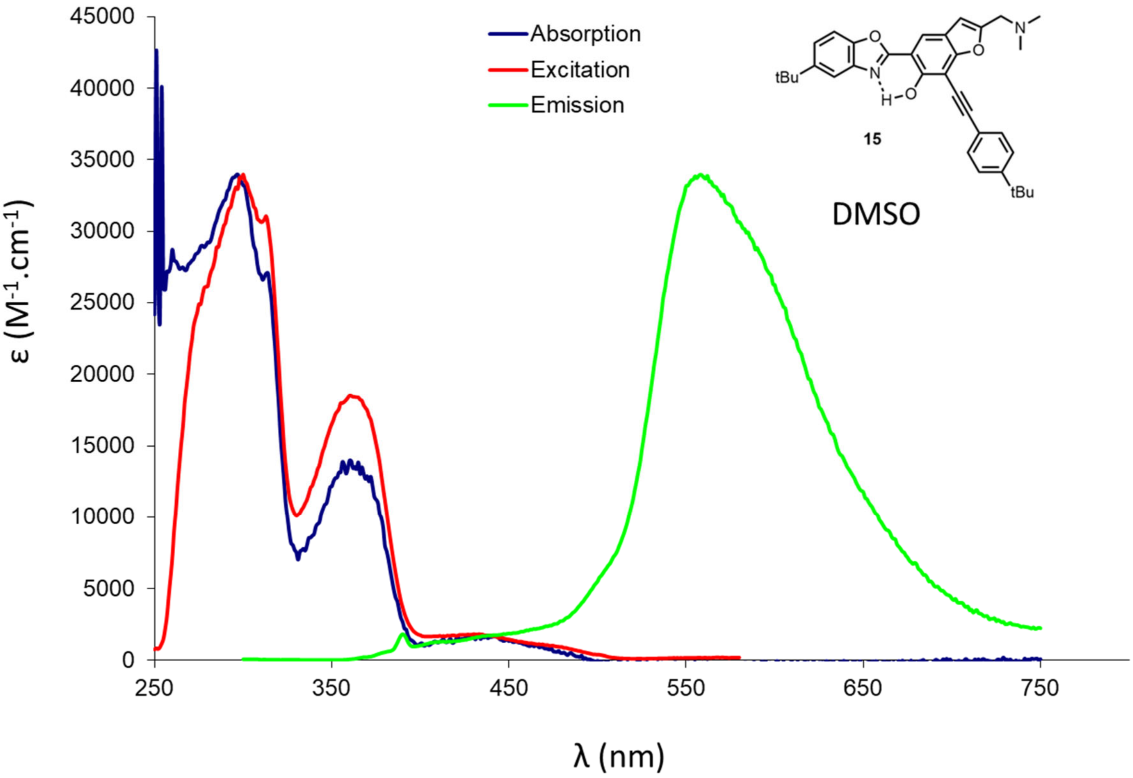

Figure S3.30. Absorption (blue), Emission (green) and Excitation (red) spectra of **HBBO 15** in DMSO.

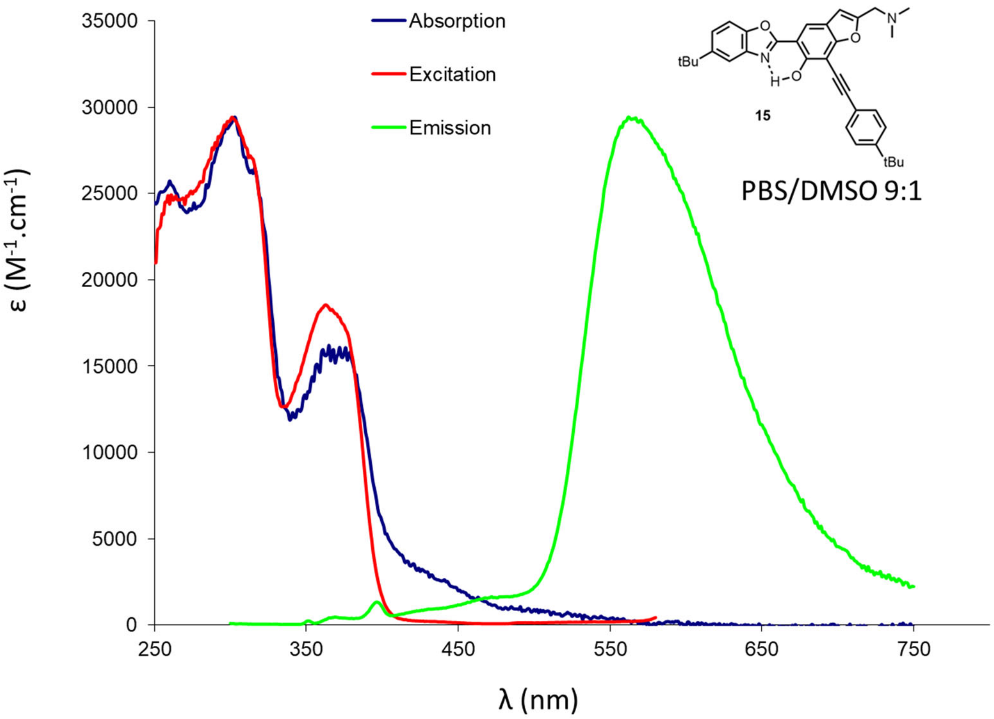

Figure S3.31. Absorption (blue), Emission (green) and Excitation (red) spectra of **HBBO 15** in PBS/DMSO 9:1.

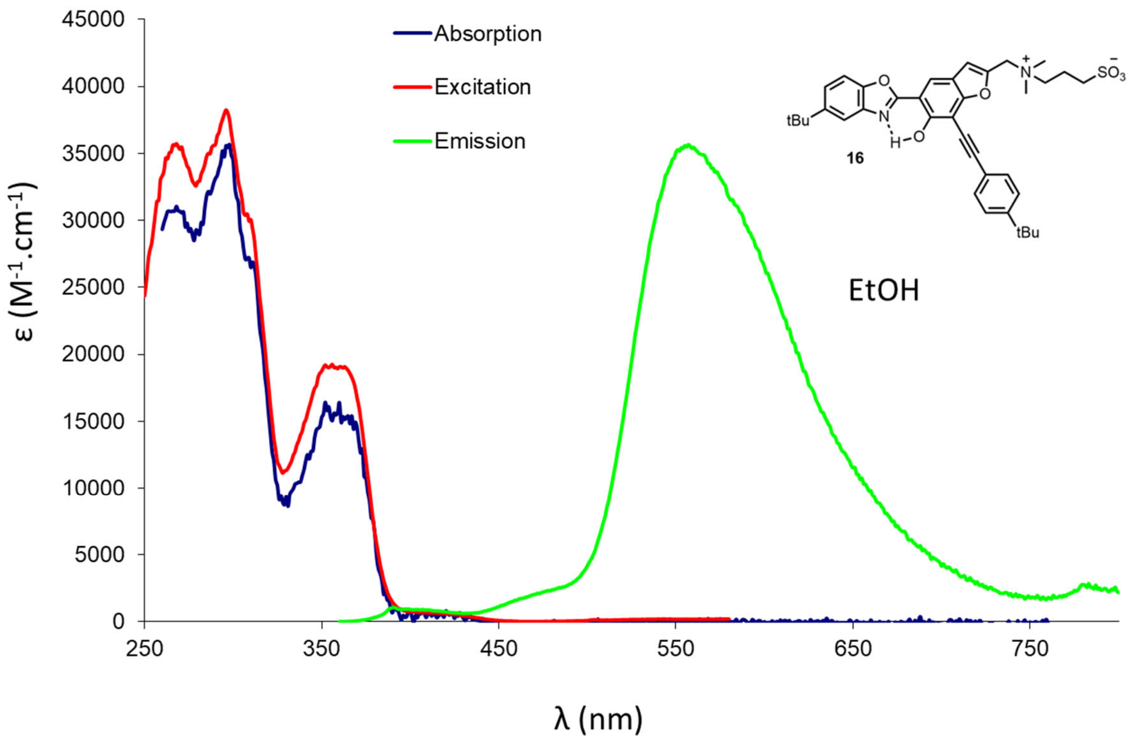

Figure S3.32. Absorption (blue), Emission (green) and Excitation (red) spectra of **HBBO 16** in ethanol.

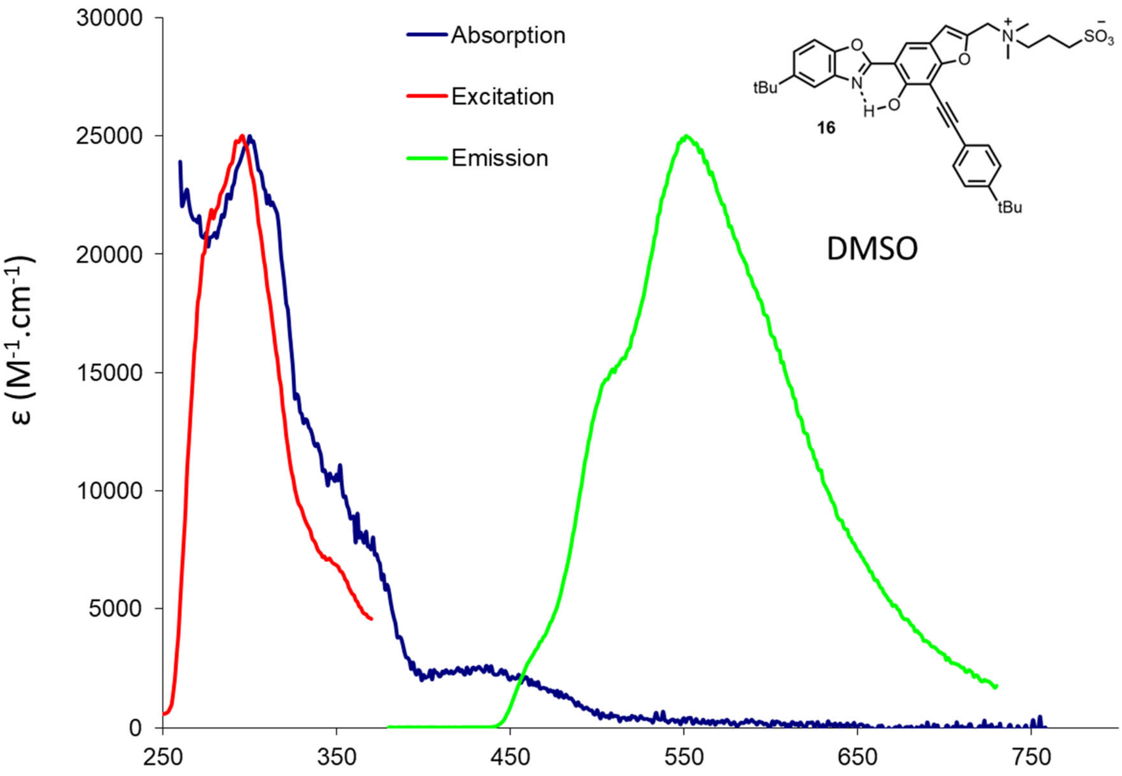

Figure S3.32. Absorption (blue), Emission (green) and Excitation (red) spectra of **HBBO 16** in DMSO .

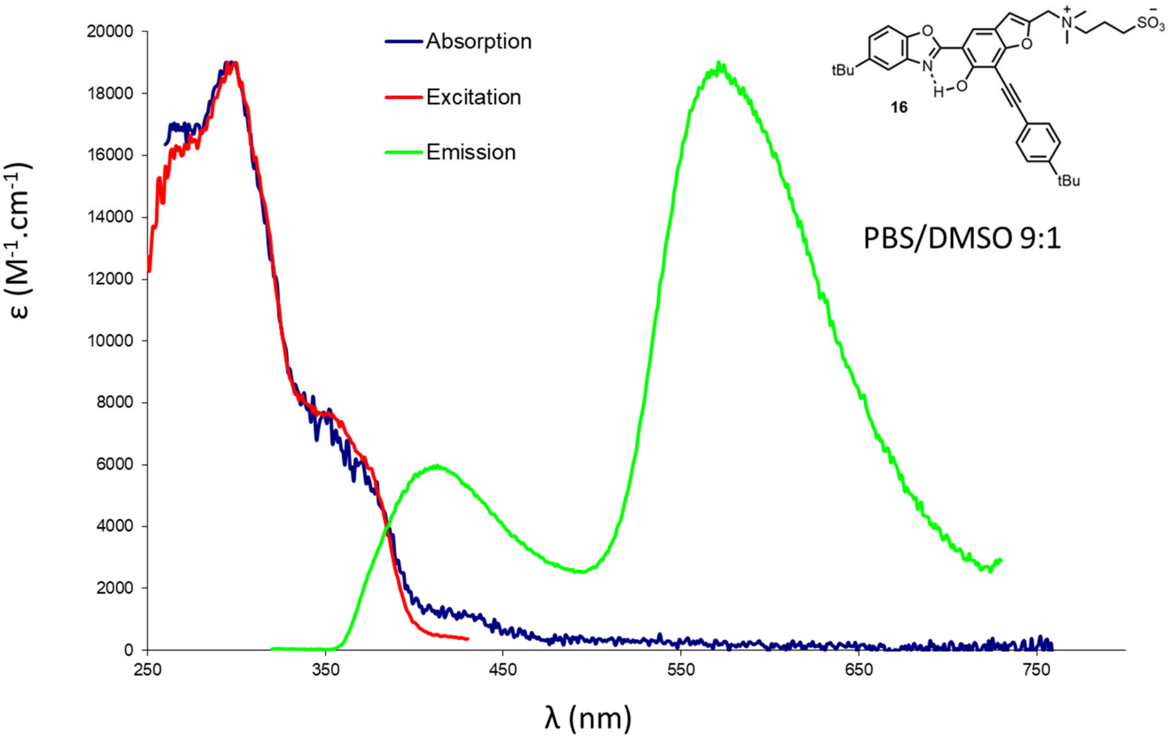

Figure S3.33. Absorption (blue), Emission (green) and Excitation (red) spectra of **HBBO 16** in PBS/DMSO 9:1.