Naphthalimide/ benzimide-based excited-state intramolecualr proton transfer (ESIPT)-active luminogens: aggregation-induced enhanced emission and potential for chemical modification

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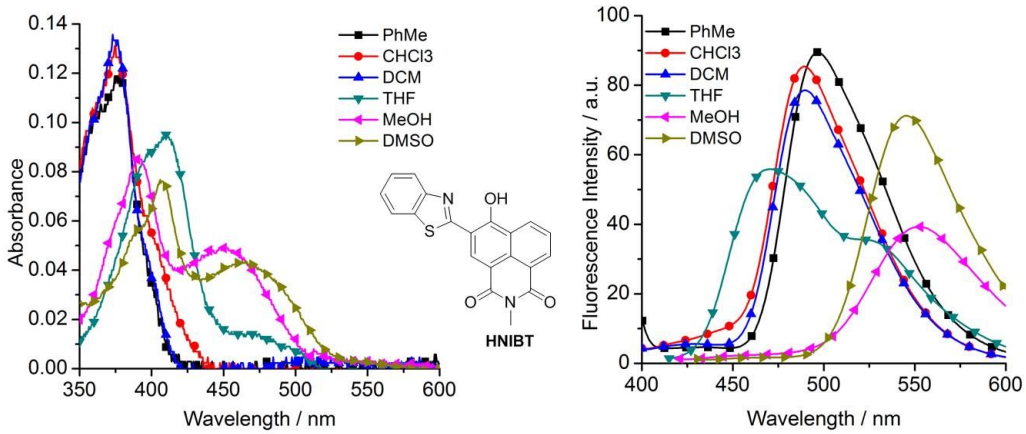


Figure S1. Absorption spectra and fluorescence spectra of HNIBT in various solvents.

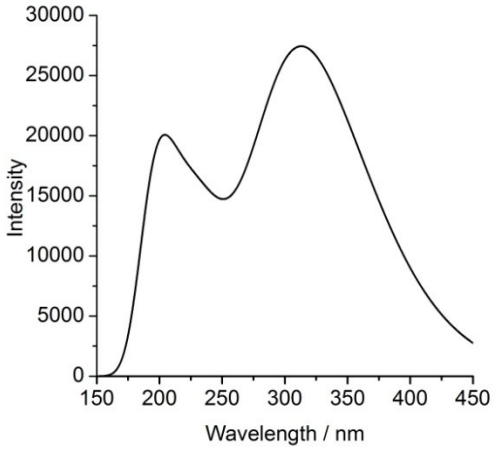


Figure S2. Theoretically calculated absorption spectra of HNIBT.

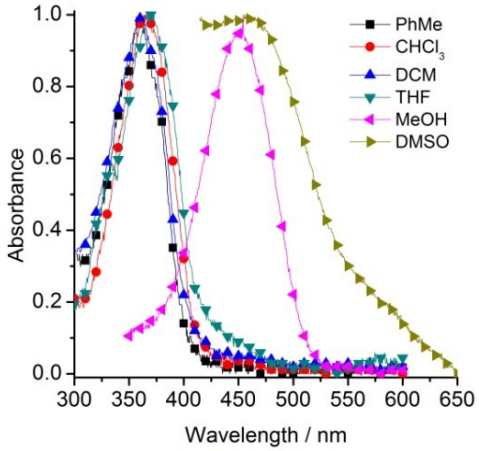
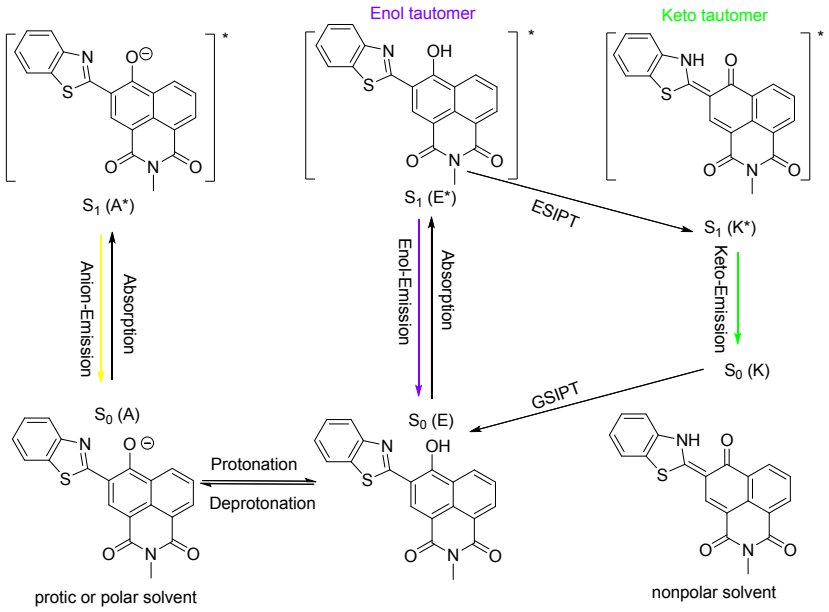


Figure S3. Absorption spectra of HNI in various solvents.



Scheme S1. Schematic representation of the photophysical process of HNIPT.

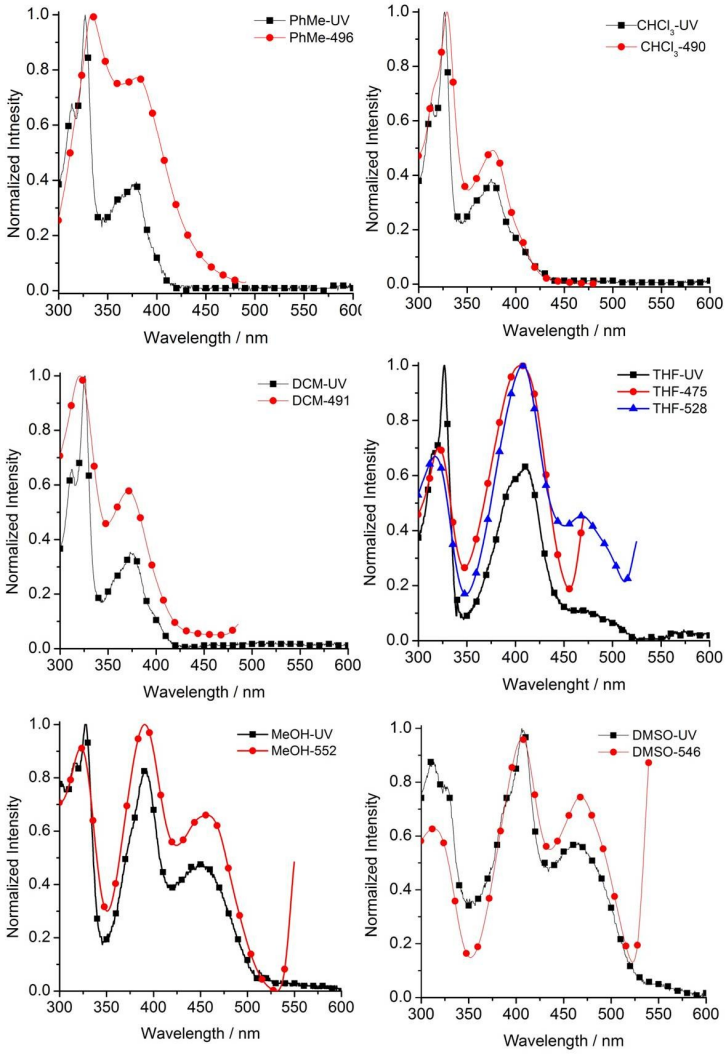
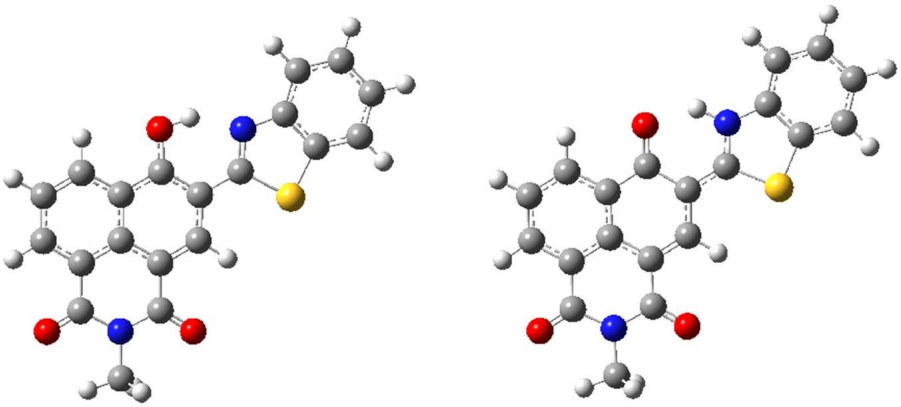


Figure S4. Comparison of the excitation spectra monitored at the fluorescence maximum wavelength and the absorption spectra of HNIBT in various solutions.



-1502.81017920 A.U. -1502.80415945 A.U.

Figure S5. Comparison of energies of enol-tautomer (left) and keto-tautomer (right) of HNIBT at the ground state.

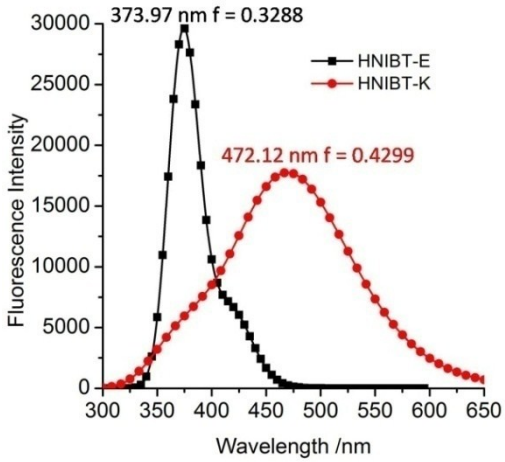


Figure S6. Theoretically calculated emission spectra of enol-tautomer and keto-tautomer of HNIBT.

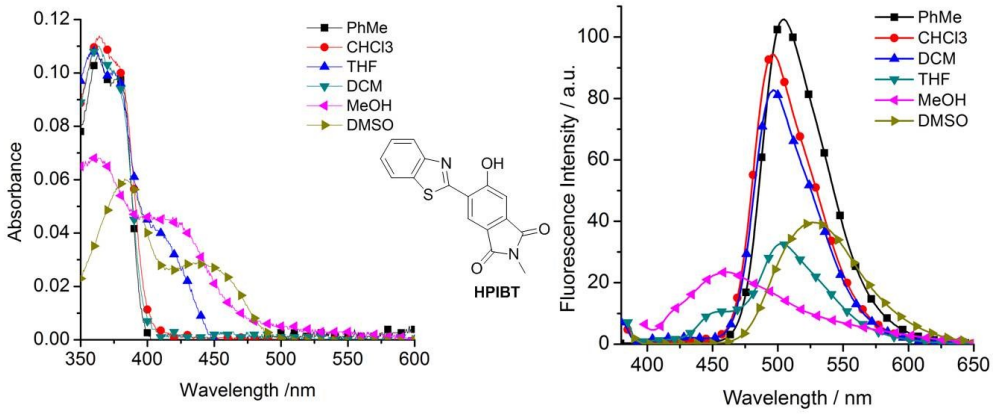


Figure S7. Absorption spectra and fluorescence spectra of HPIBT in various solvents.

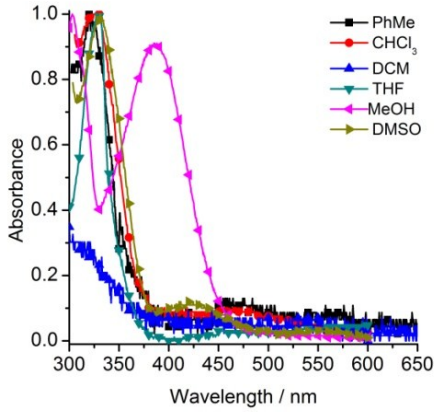


Figure S8. Absorption spectra of HPI in various solvents.

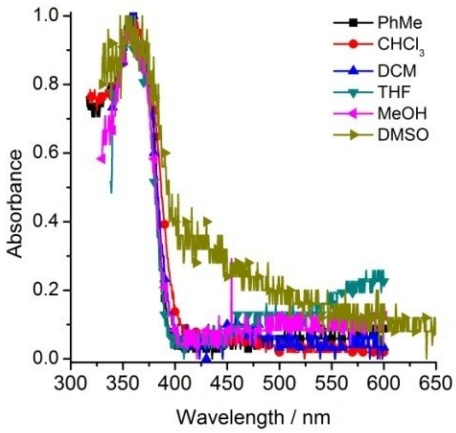


Figure S9. Absorption spectra of MPIBT in various solvents.

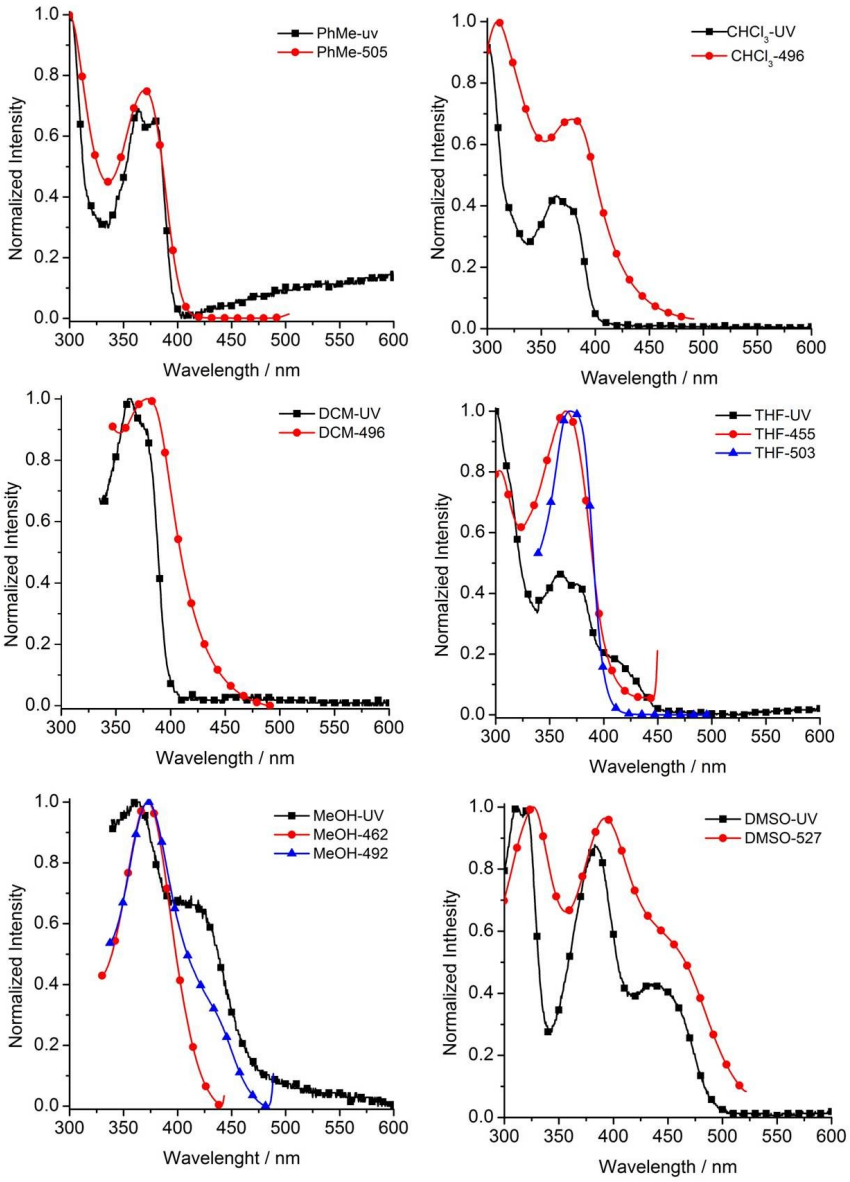
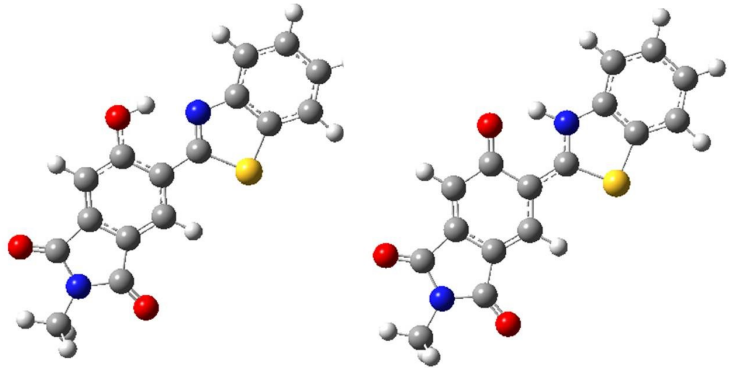


Figure S10. Comparison of the excitation spectra monitored at the fluorescence maximum wavelength and the absorption spectra of HPIBT in various solutions.



-1349.15272018 A.U -1349.14022084 A.U.

Figure S11. Comparison of energies of enol-tautomer (left) and keto-tautomer (right) of HPIBT at the ground state.

Table S1. Comparison of the relevant H-bonding parameters of HNIBT and HPIBT in S_0 and S_1.

		H-O	H---N	O---N
HNIBT	S_0	1.00296	1.70079	2.60220
	S_1	1.00464	1.69702	2.60337
	$\Delta(S_0 \rightarrow S$	**0.00168**	**-0.00377**	**0.00117**
HPIBT	S_0	0.99742	1.72621	2.61867
	S_1	1.00795	1.69143	2.60492
	$\Delta(S_0 \rightarrow S$	**0.01053**	**-0.03478**	**-0.01375**

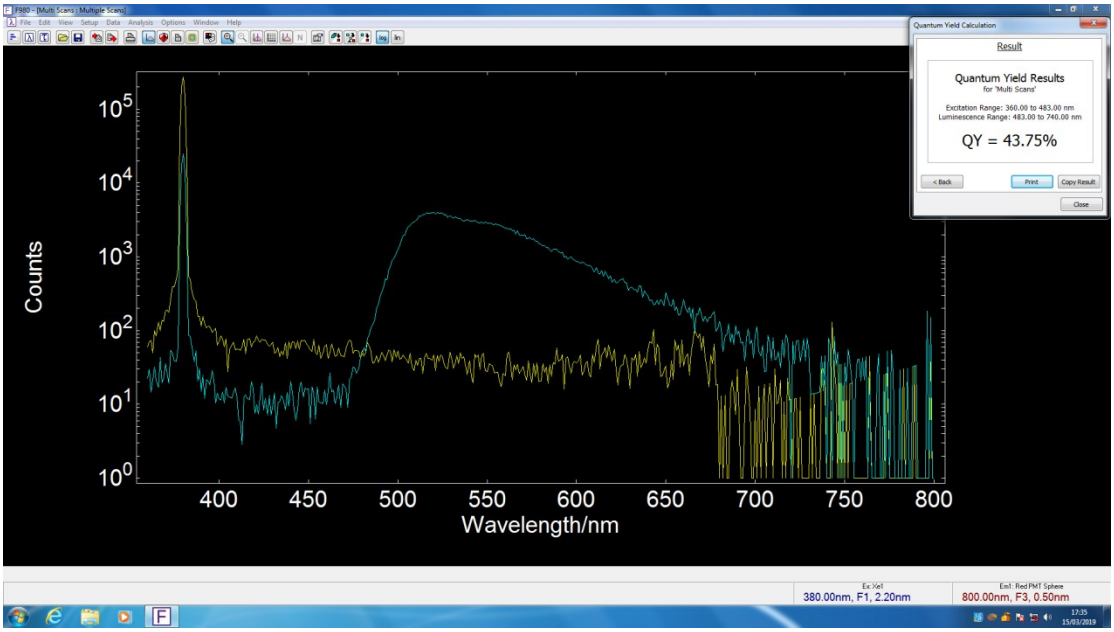


Figure S12. The Φ_f of HNIBT powder measured by integrating sphere.

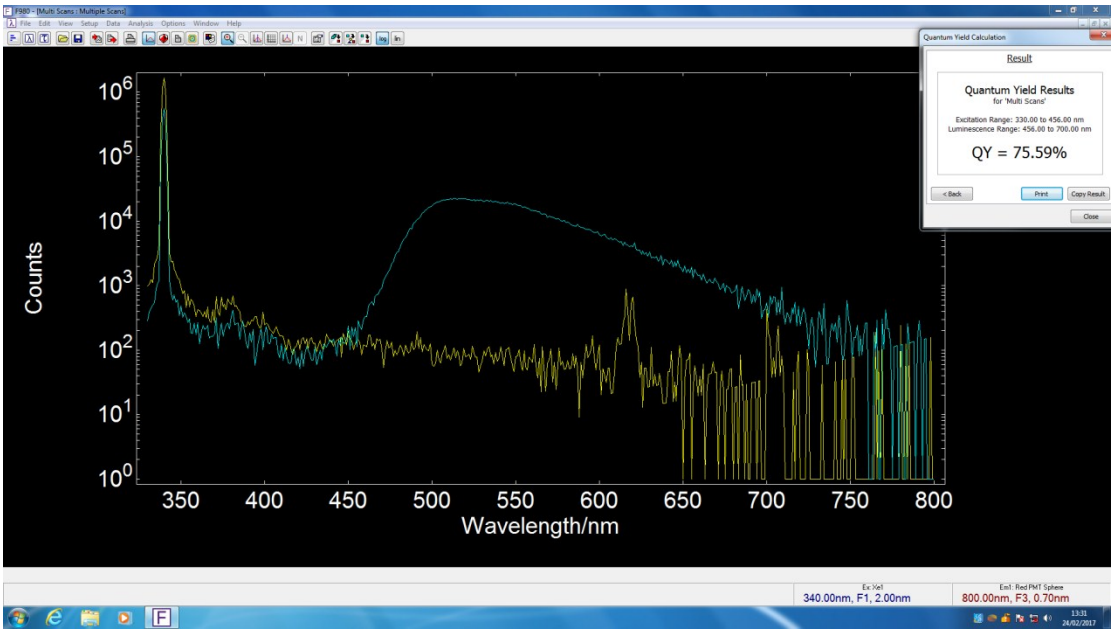


Figure S13. The Φ_f of HPIBT powder measured by integrating sphere.

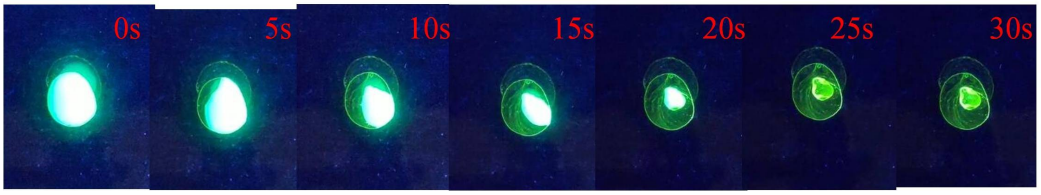


Figure S14. Digital photographs showing changes in fluorescence of HPIBT-Pe upon DCM evaporation and irradiation with 365 nm UV light.

Crystal data and structure refinement

Table S2. Crystal data and structure refinement for HPIBT (CCDC number: 1906721).

Identification code	190113a
Empirical formula	C16 H10 N2 O3 S
Formula weight	310.32
Temperature	298(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 5.6795(5) A alpha = 90 deg. b = 28.701(3) A beta = 90.117(2) deg. c = 7.8681(7) A gamma = 90 deg.
Volume	1282.6(2) A^3
Z, Calculated density	4, 1.607 Mg/m^3
Absorption coefficient	0.268 mm^-1
F(000)	640
Crystal size	0.30 x 0.06 x 0.03 mm
Theta range for data collection	2.68 to 25.02 deg.
Limiting indices	-5<=h<=6, -34<=k<=24, -9<=l<=9
Reflections collected / unique	6289 / 2242 [R(int) = 0.0573]
Completeness to theta = 25.02	98.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9920 and 0.9240
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2242 / 0 / 200
Goodness-of-fit on F^2	1.025
Final R indices [I>2sigma(I)]	R1 = 0.0623, wR2 = 0.1607
R indices (all data)	R1 = 0.0913, wR2 = 0.1735
Largest diff. peak and hole	0.257 and -0.276 e.A^-3

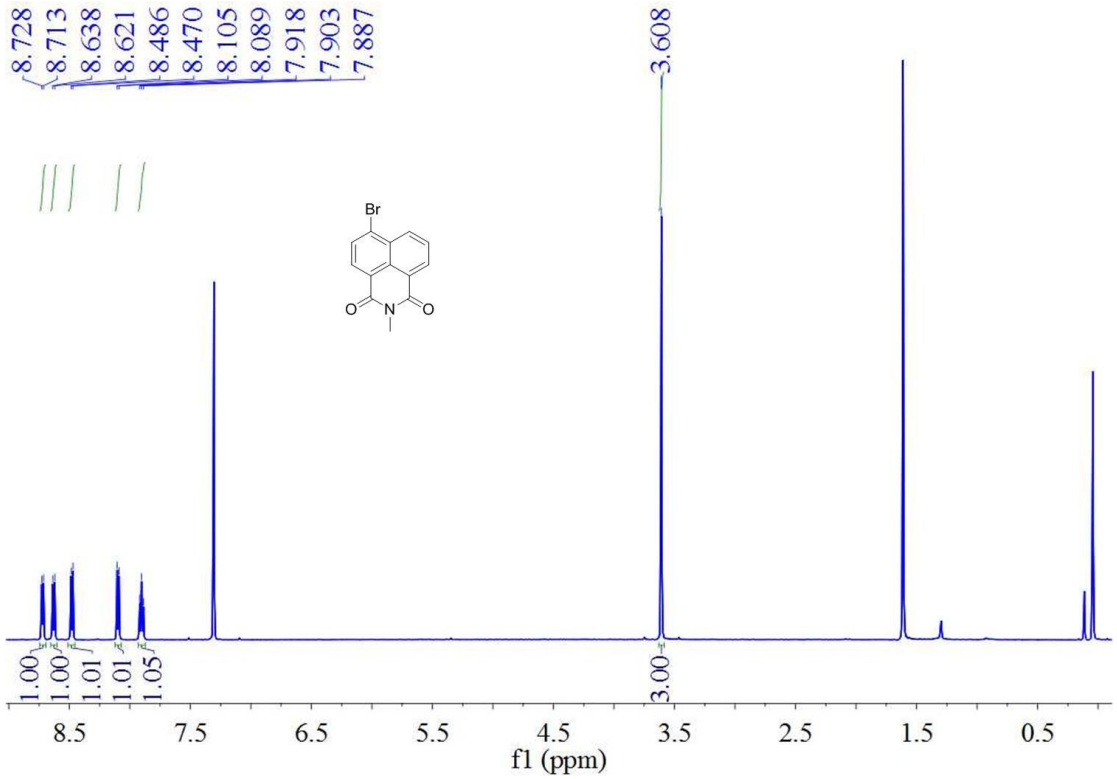


Figure S15. ^{1}H NMR spectrum of compound **1** in $CDCl_3$.

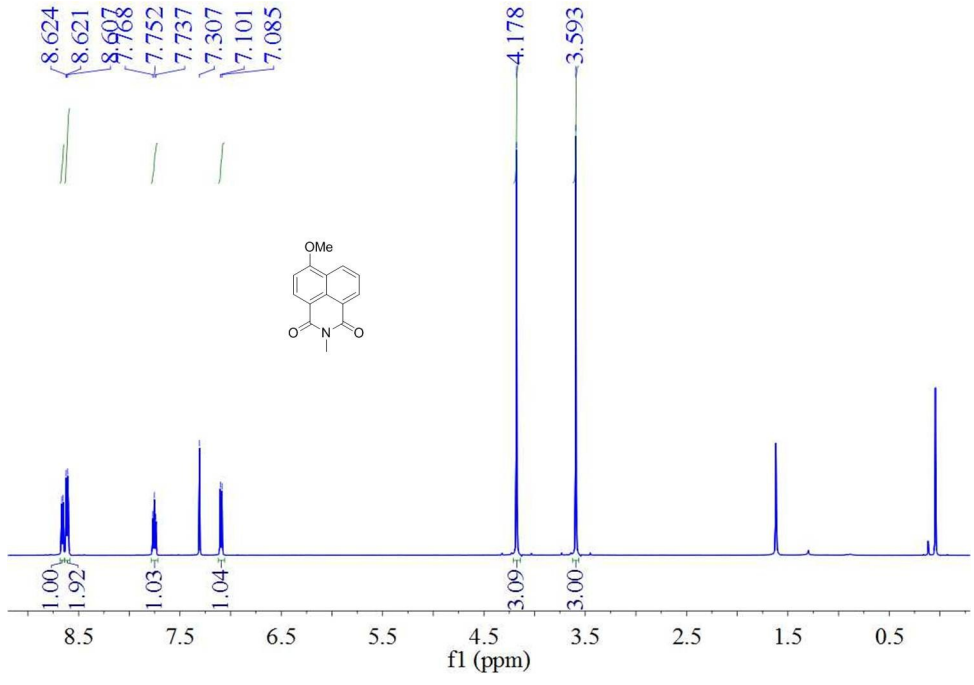


Figure S16. ^{1}H NMR spectrum of compound **2**in $CDCl_3$.

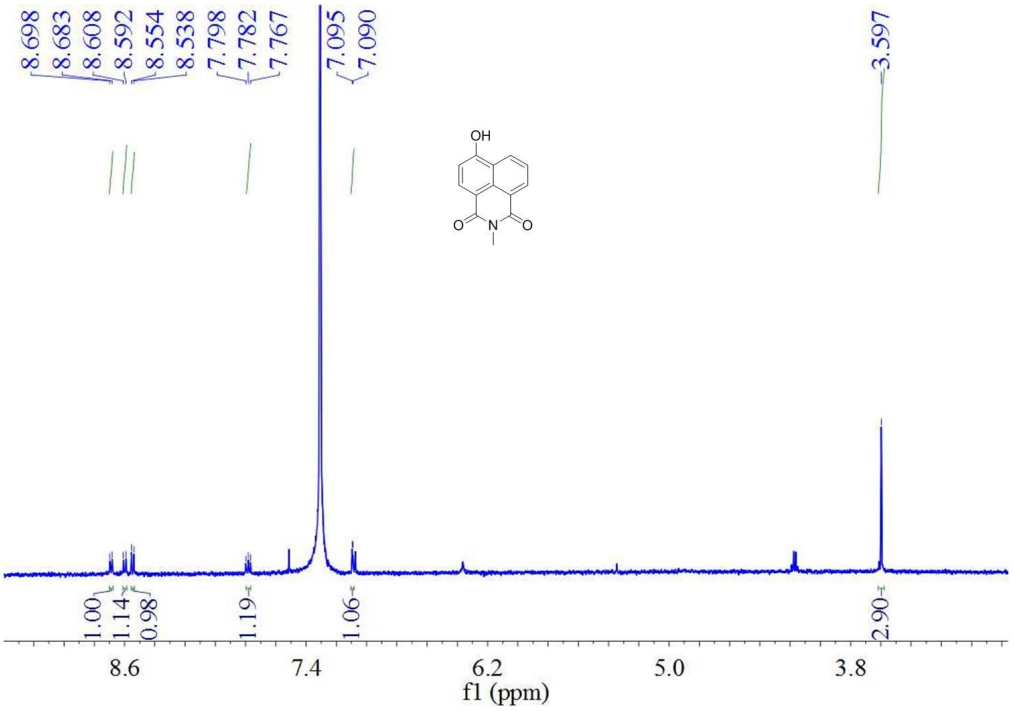


Figure S17. ^{1}H NMR spectrum of **HNI** in $CDCl_3$.

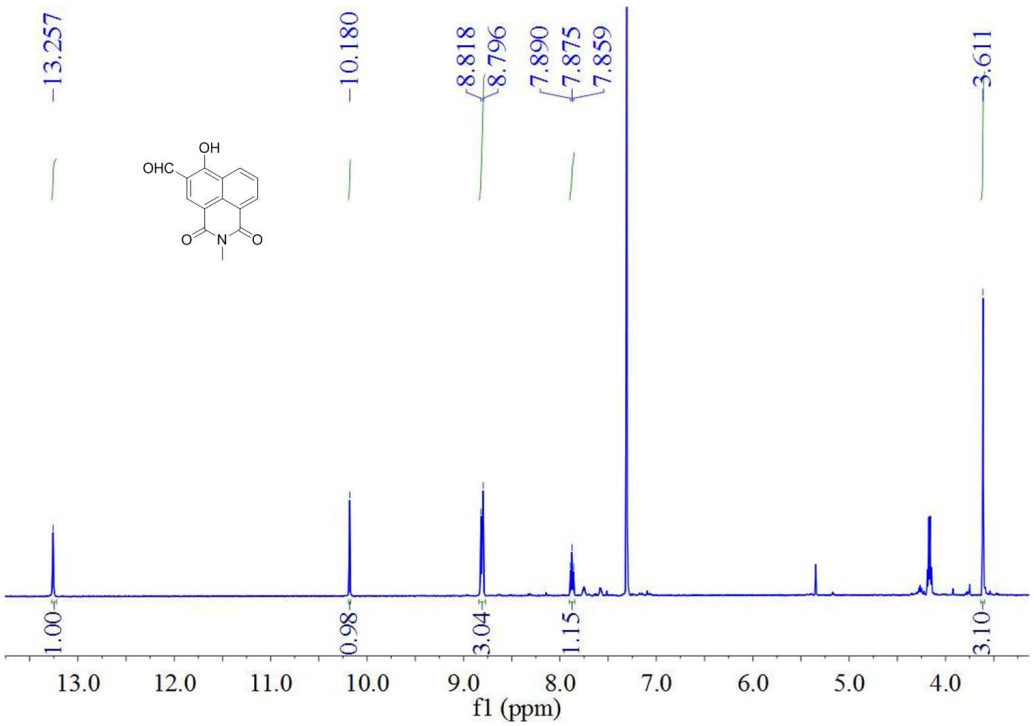


Figure S18. ^{1}H NMR spectrum of compound **3** in $CDCl_3$.

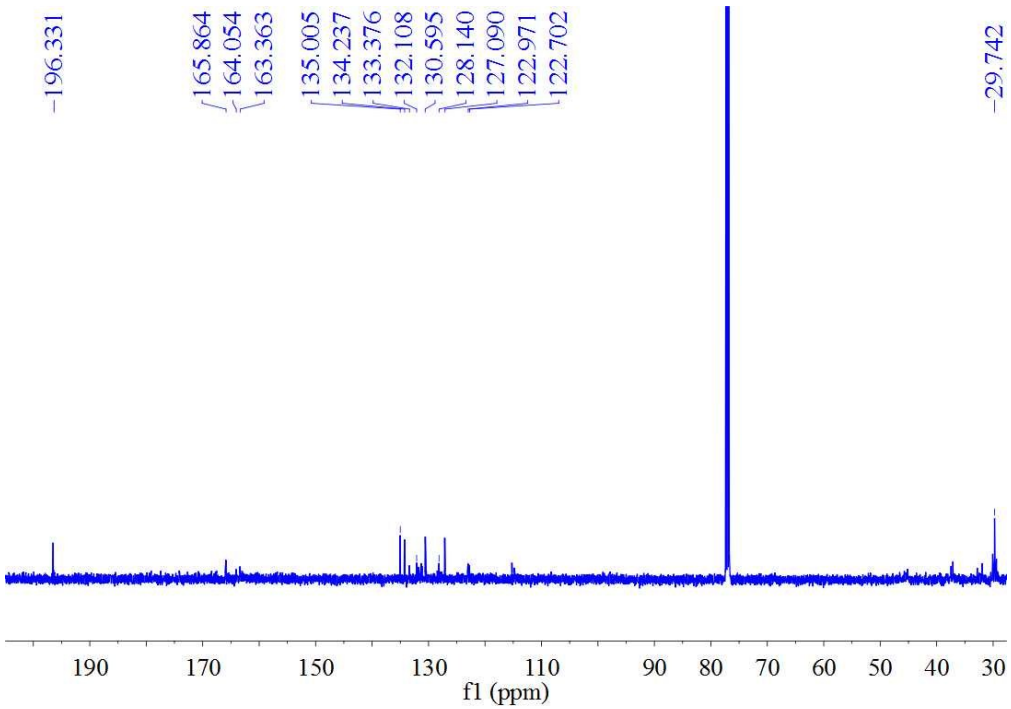


Figure S19. ^{13}C NMR spectrum of compound **3** in $CDCl_3$.

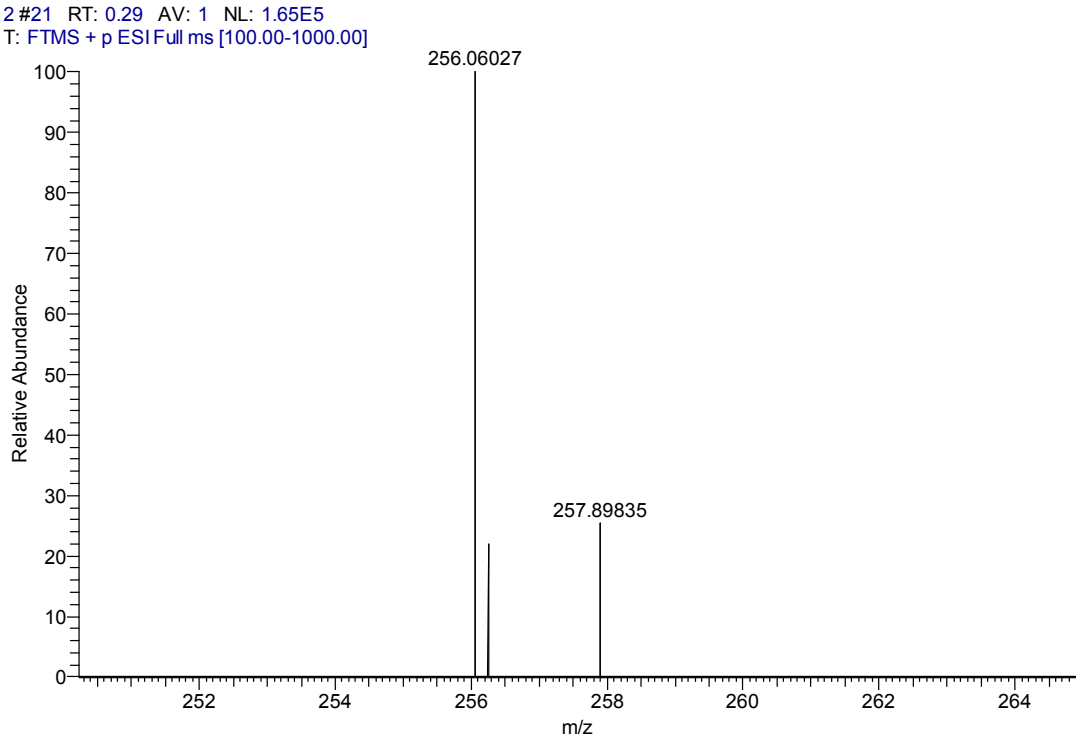


Figure S20. HRMS spectrum of compound **3**.

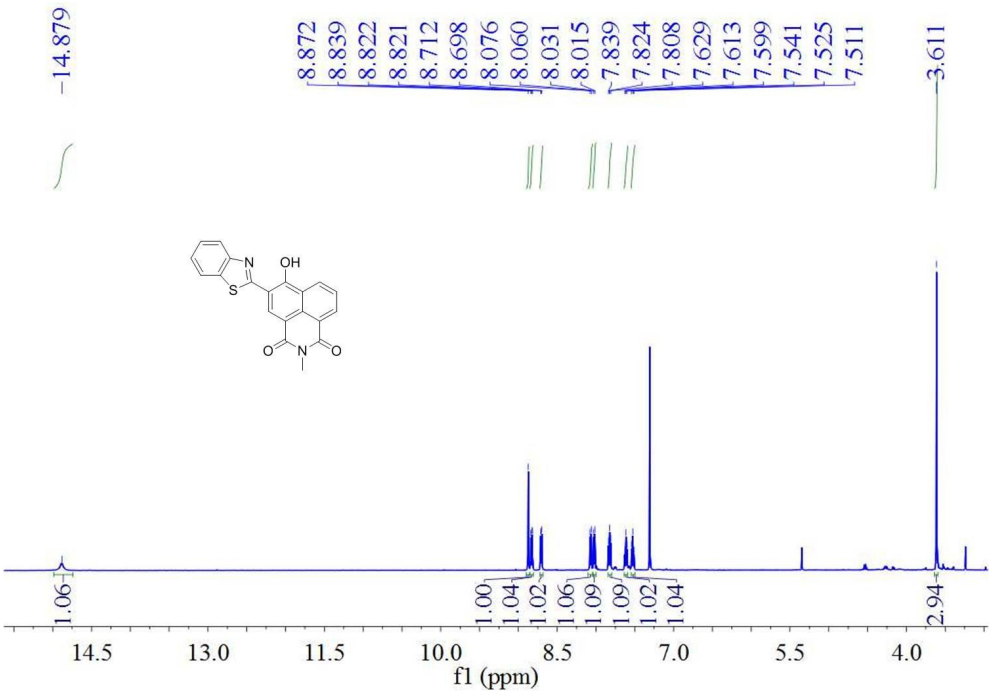


Figure S21. ^{1}H NMR spectrum of **HNIBT** in $CDCl_3$.

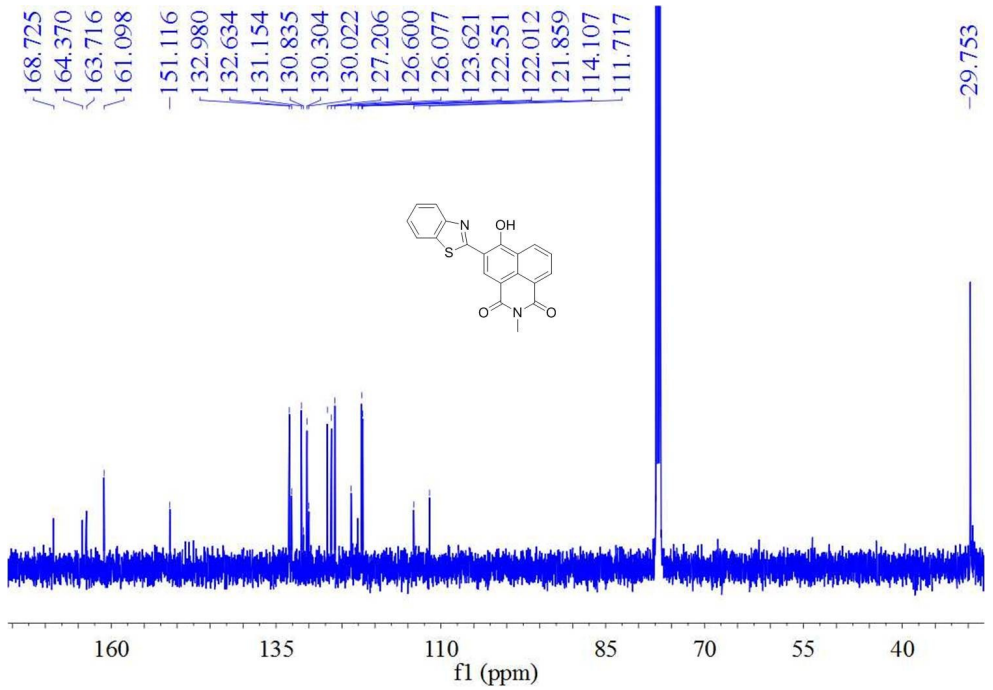


Figure S22. ^{13}C NMR spectrum of **HNIBT** in $CDCl_3$.

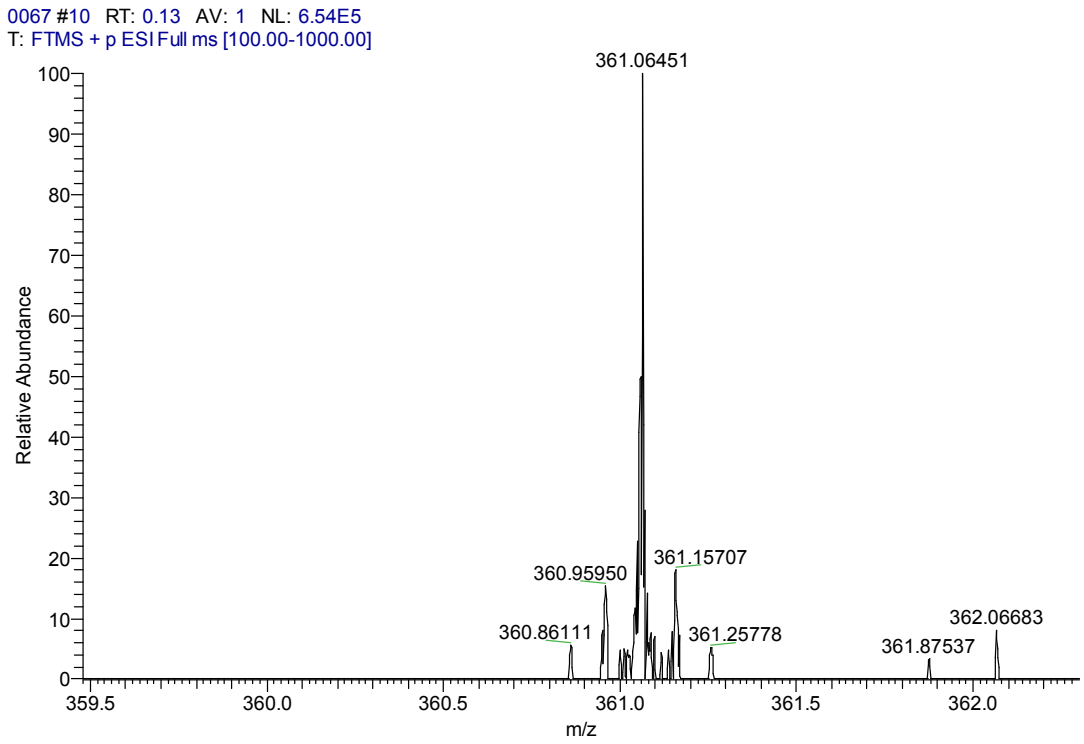


Figure S23. HRMS spectrum of **HNIBT**.

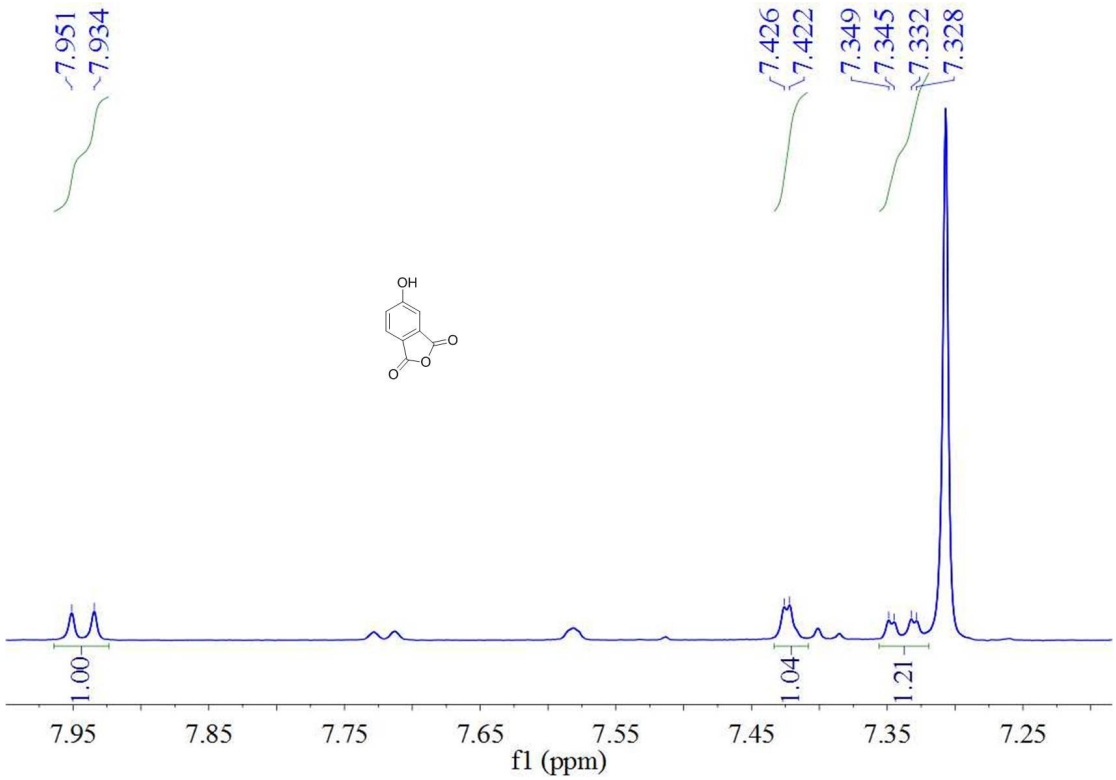


Figure S24. ^{1}H NMR spectrum of compound **4** in $CDCl_3$.

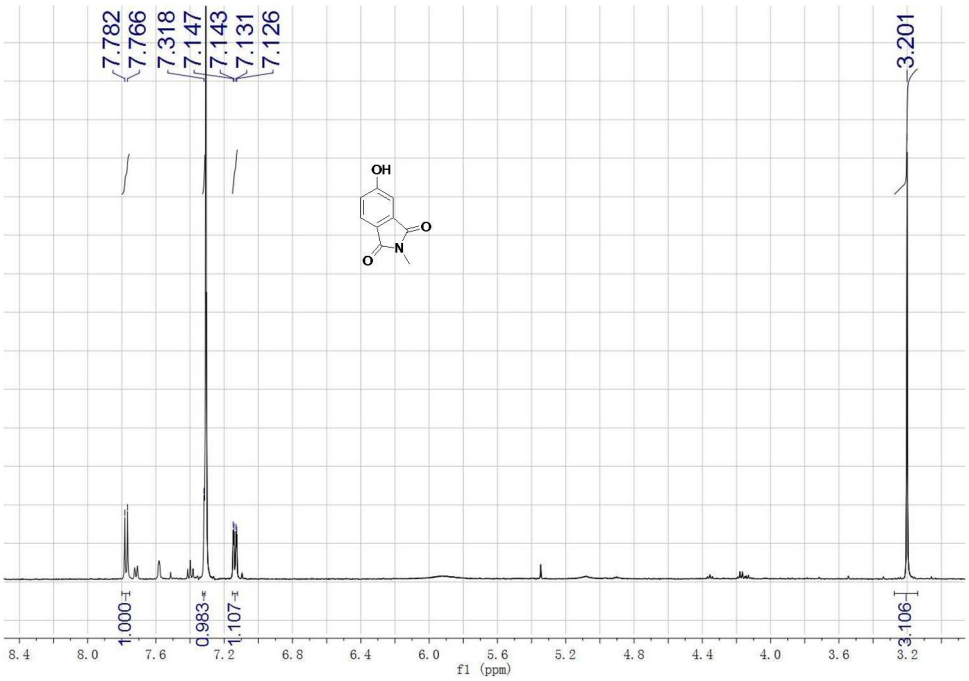


Figure S25. ^{1}H NMR spectrum of HPI in $CDCl_3$.

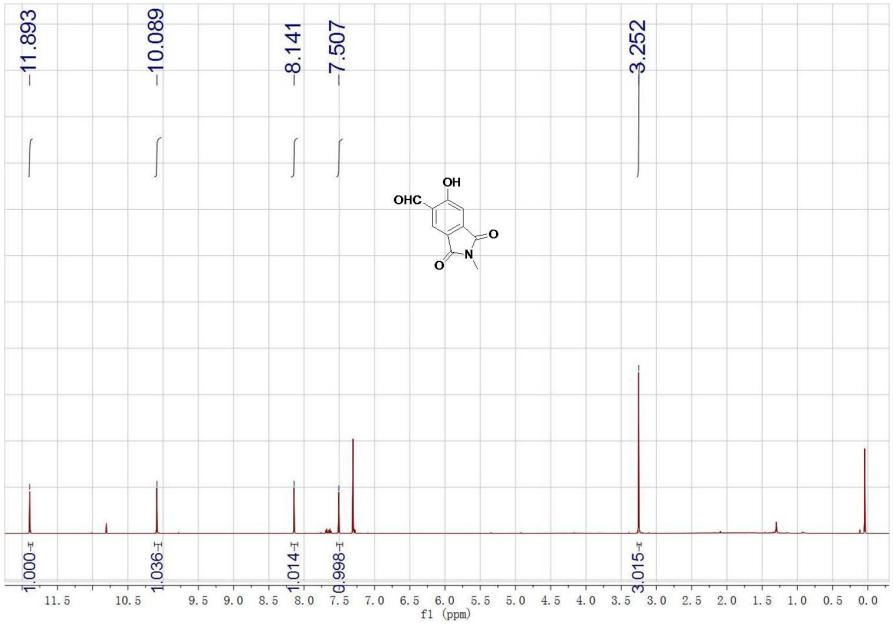


Figure S26. ^{1}H NMR spectrum of compound 5 in $CDCl_3$.

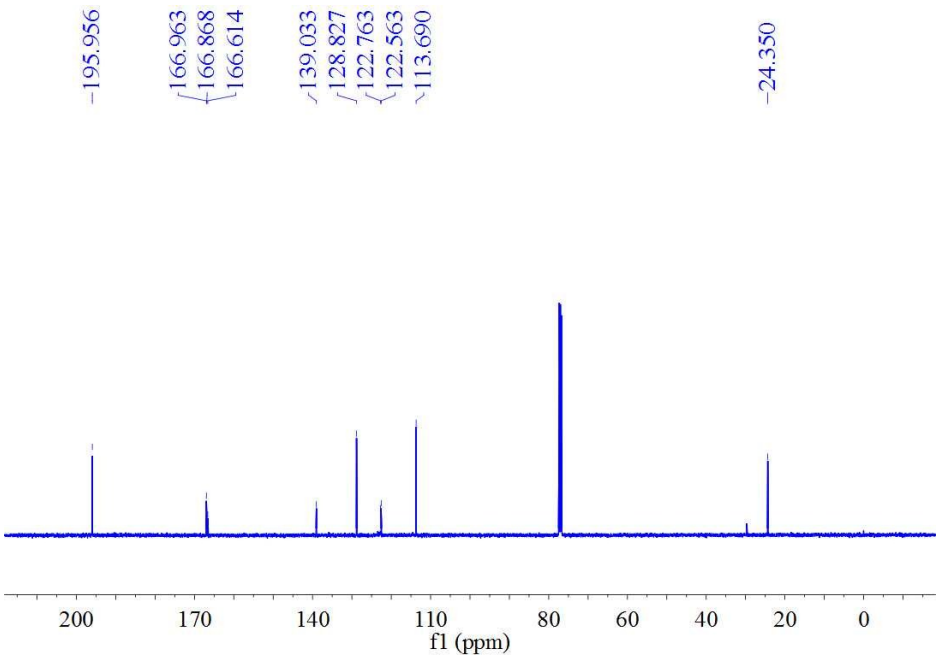


Figure S27. ^{13}C NMR spectrum of compound **5** in $CDCl_3$.

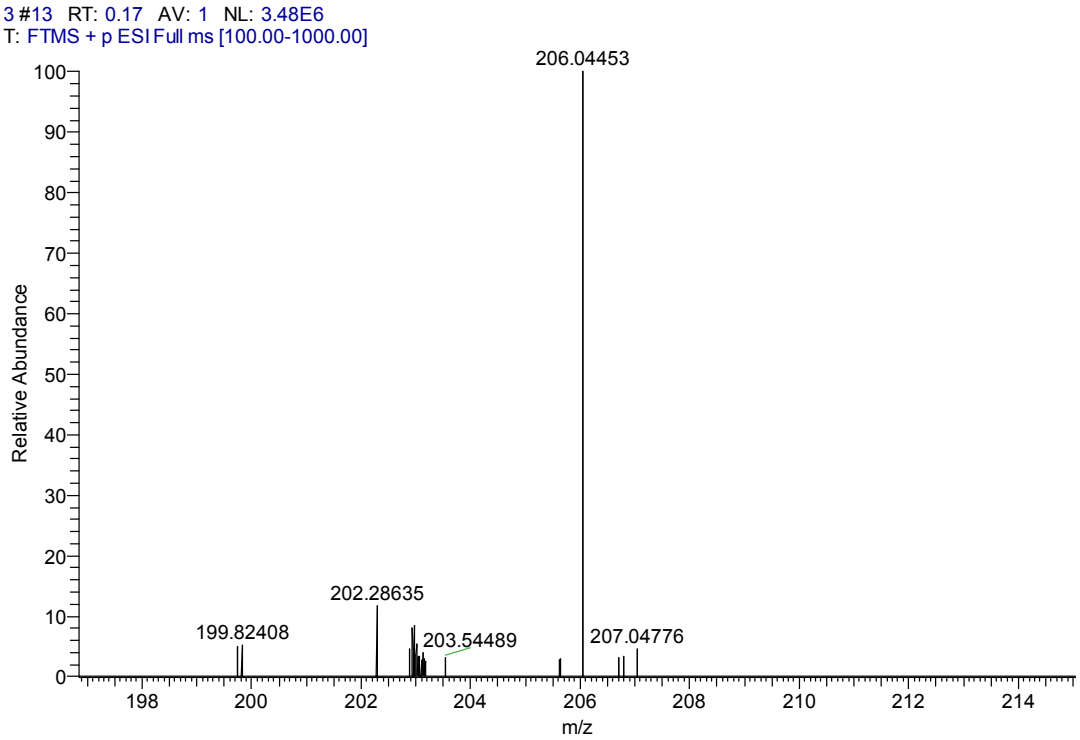


Figure S28. HRMS spectrum of compound **5**.

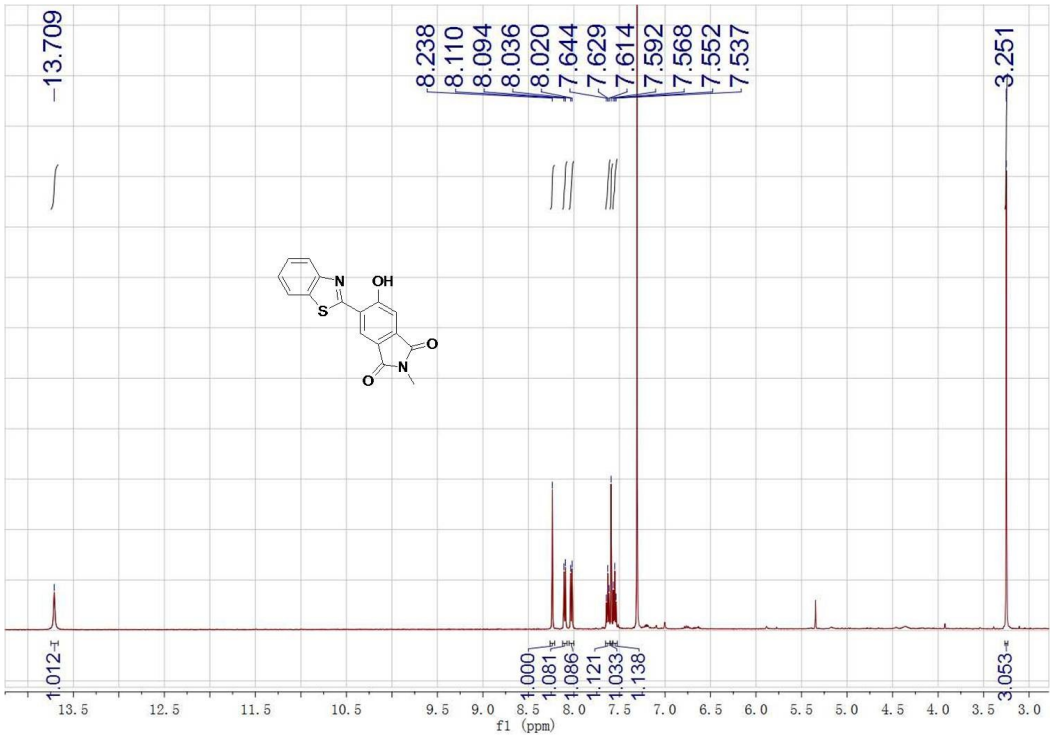


Figure S29. ^{1}H NMR spectrum of HPIBT in $CDCl_3$.

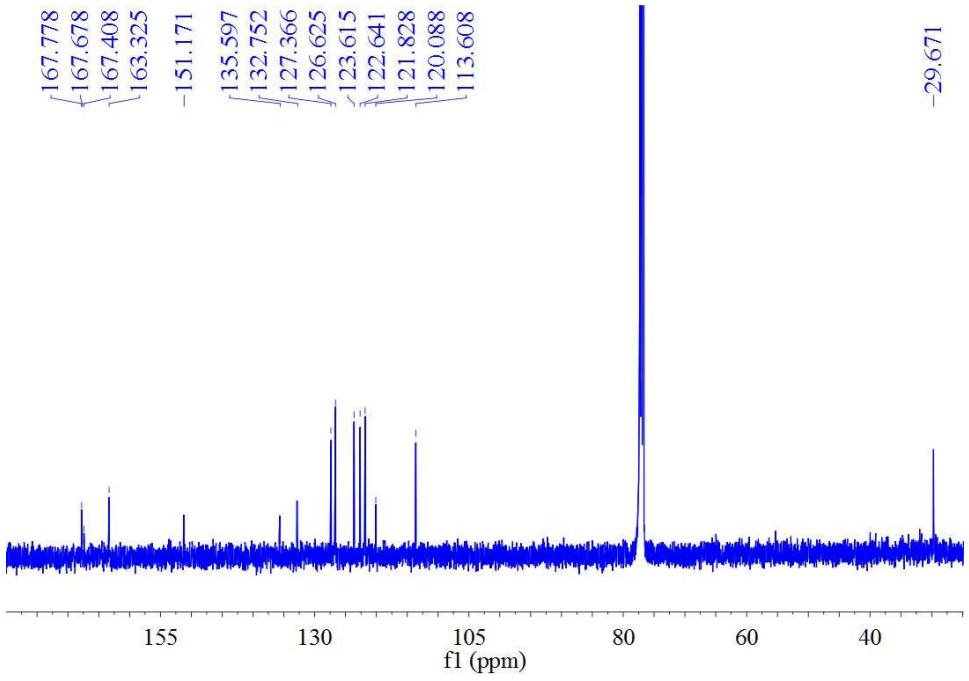


Figure S30. ^{13}C NMR spectrum of HPIBT in $CDCl_3$.

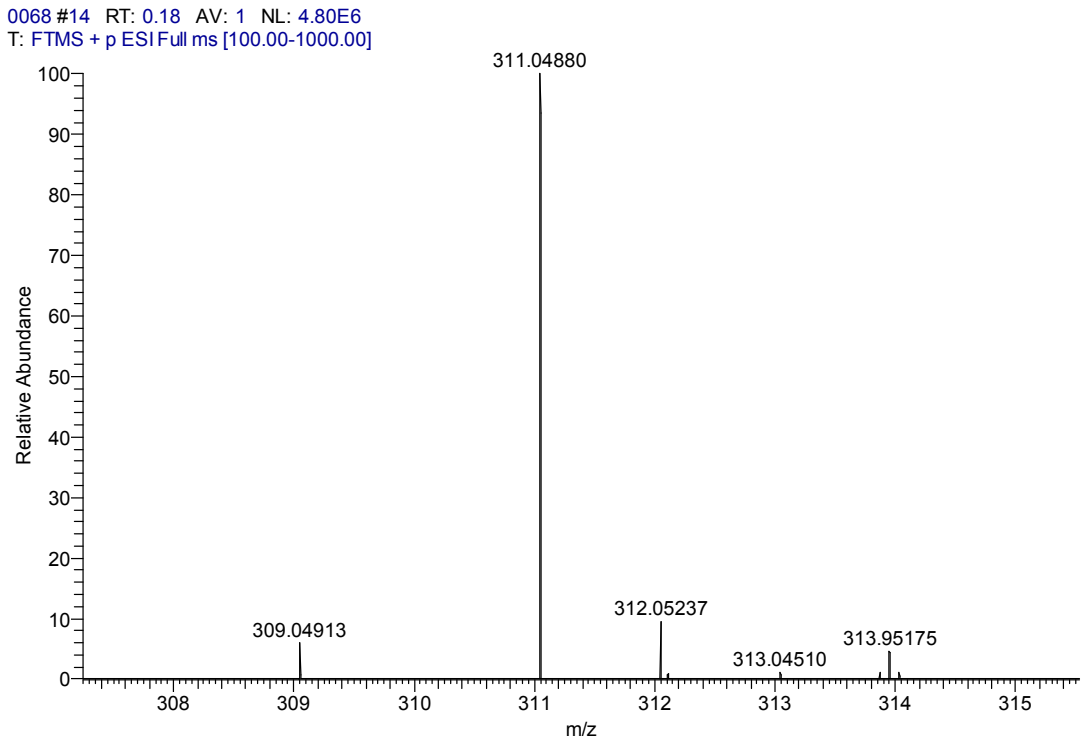


Figure S31. HRMS spectrum of HPIBT.

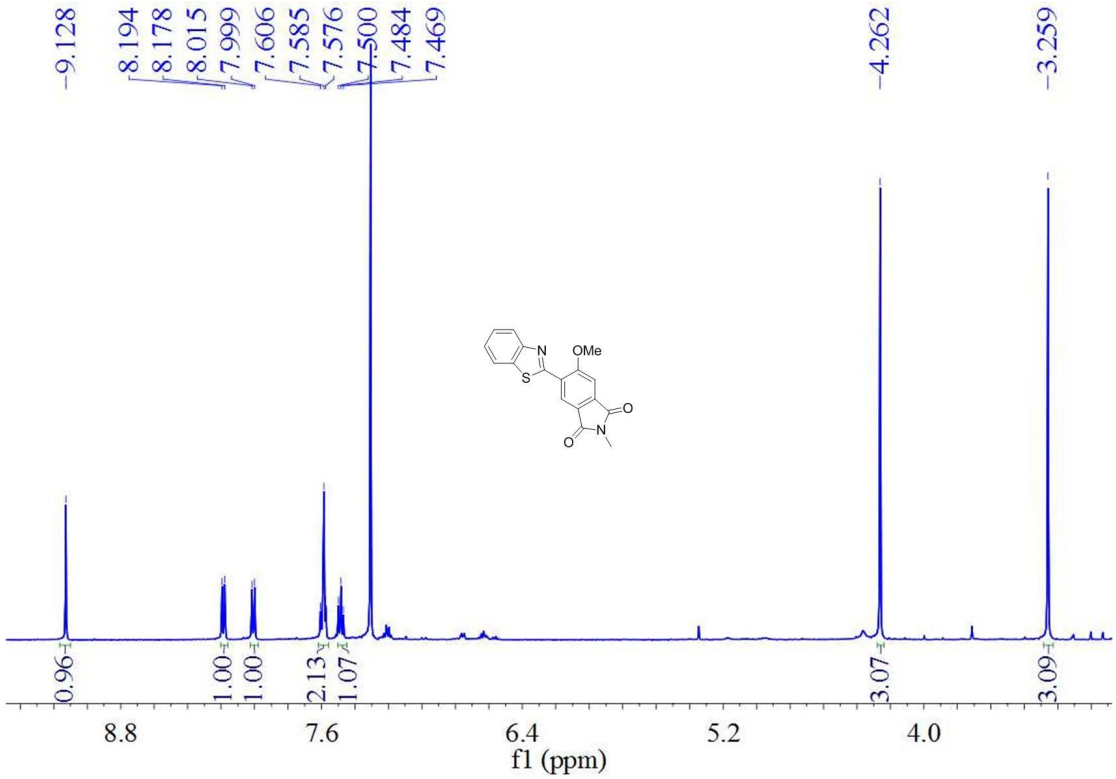


Figure S32. ^{1}H NMR spectrum of MPIBT in $CDCl_3$.

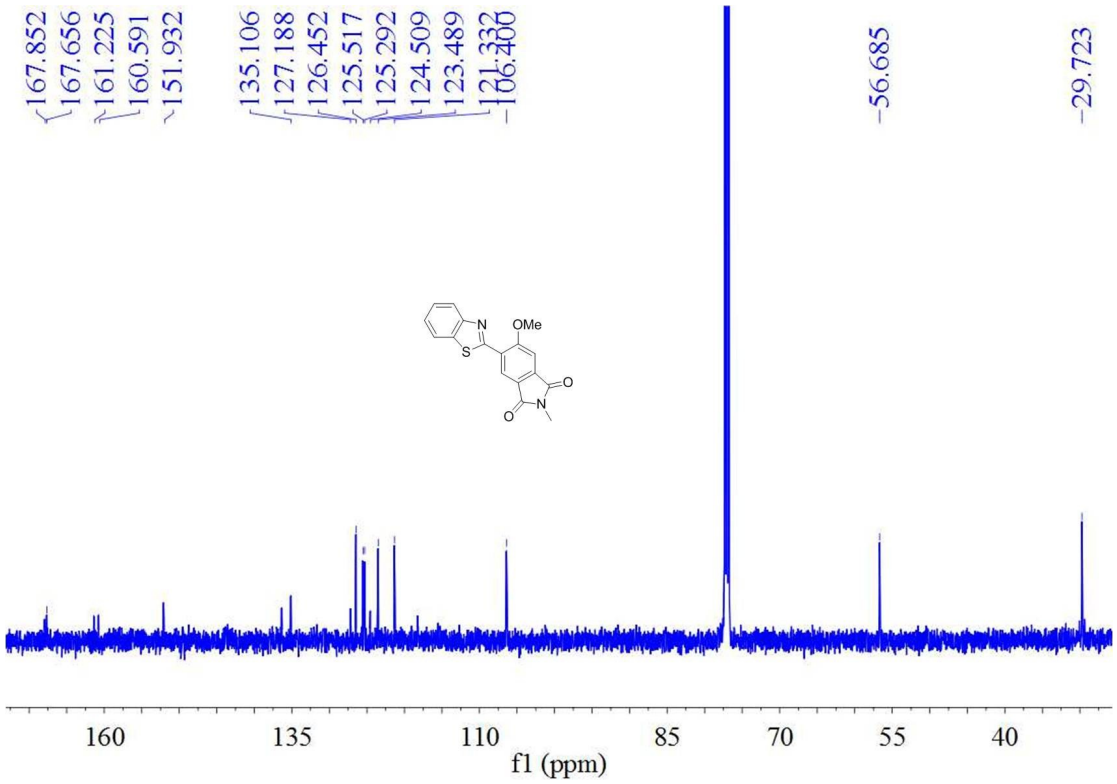


Figure S33. ^{13}C NMR spectrum of MPIBT in $CDCl_3$.

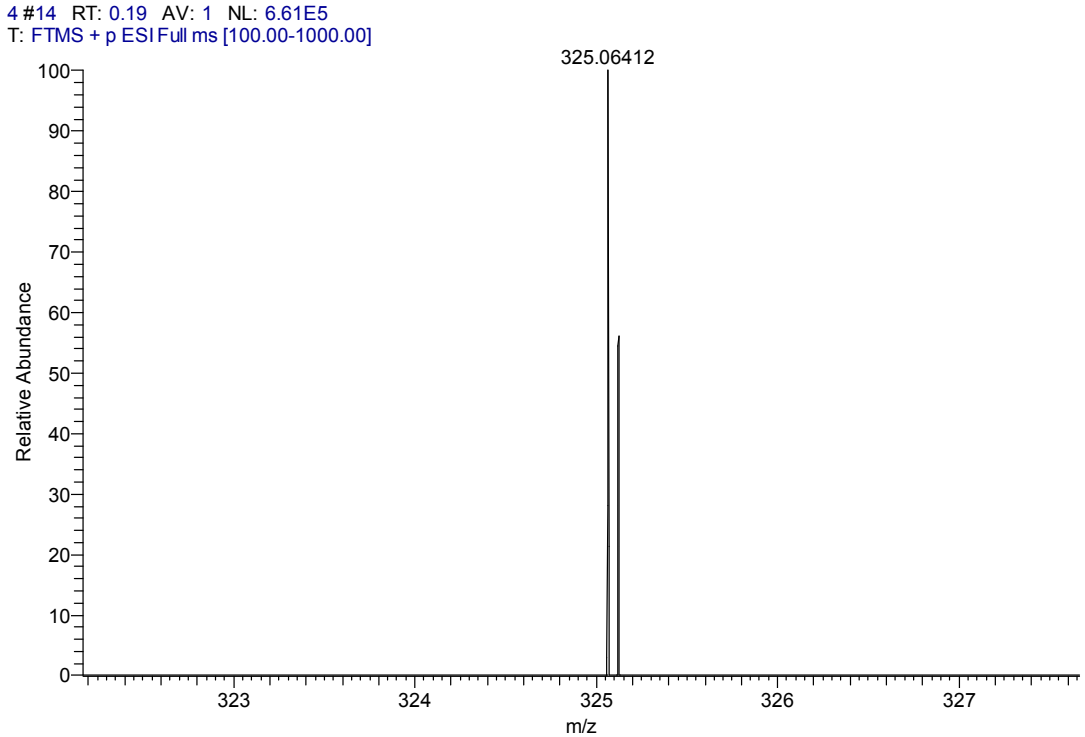


Figure S34. HRMS spectrum of **MPIBT**.

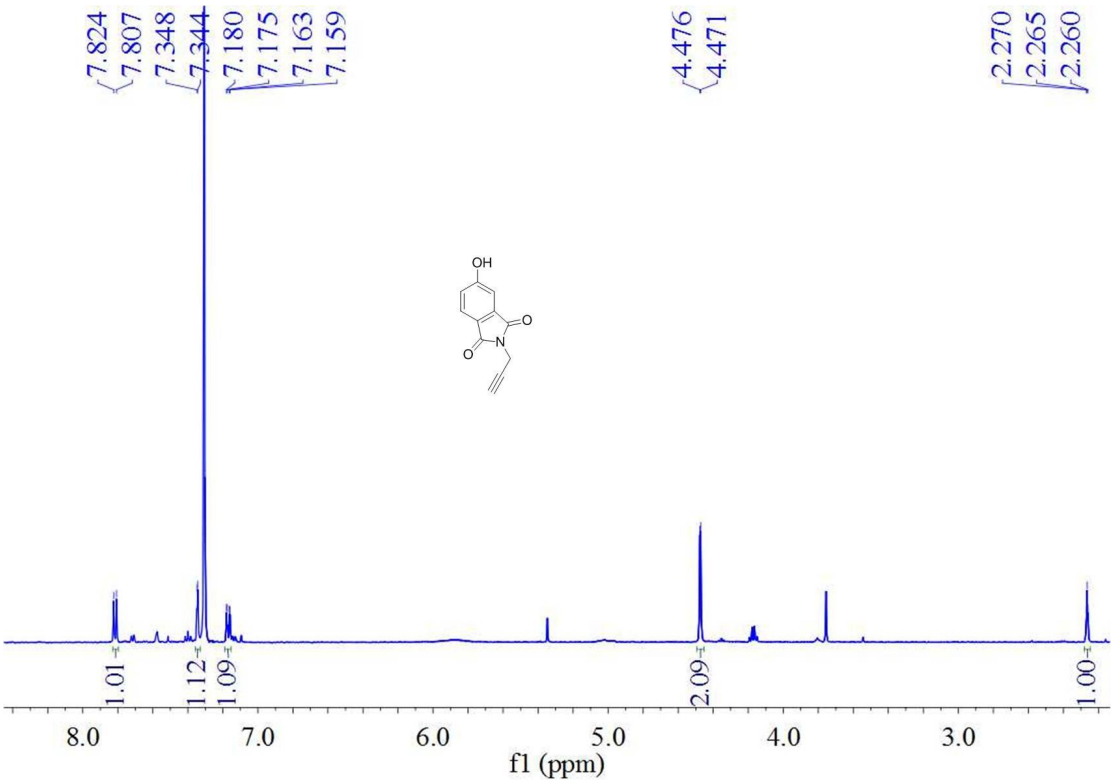


Figure S35. ^{1}H NMR spectrum of compound 6 in $CDCl_3$.

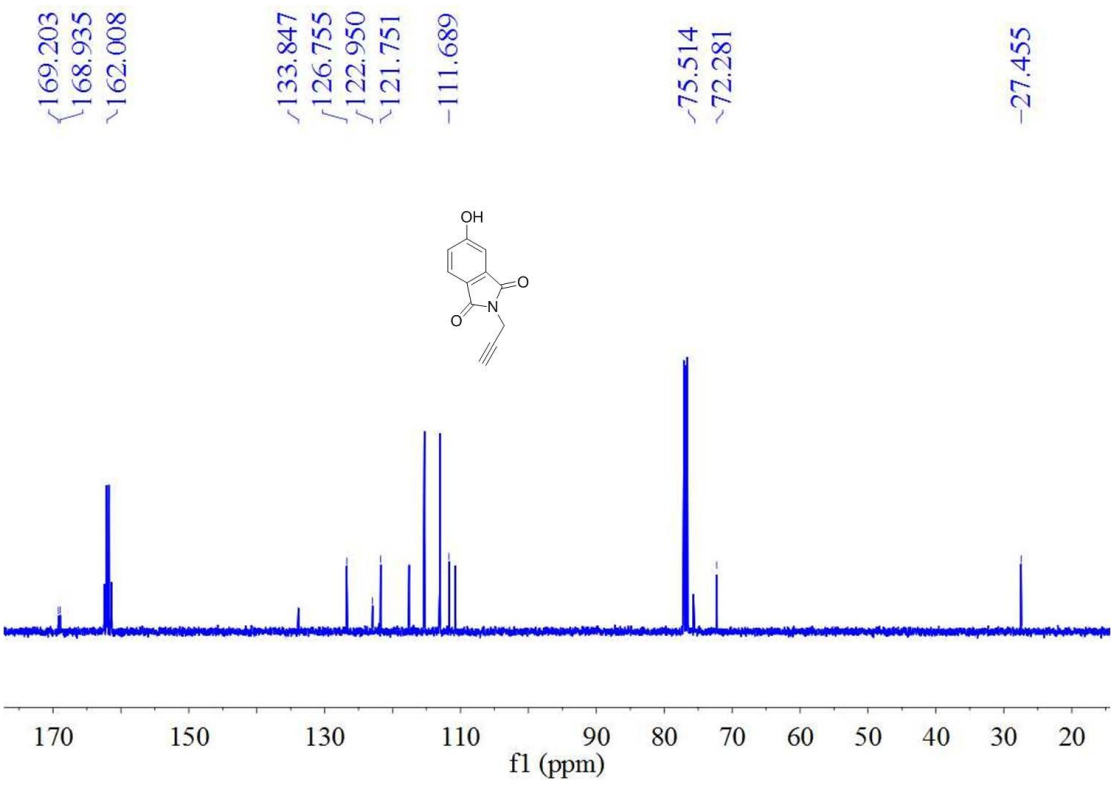


Figure S36. ^{13}C NMR spectrum of compound 6 in $CDCl_3$ + CF_3COOH.

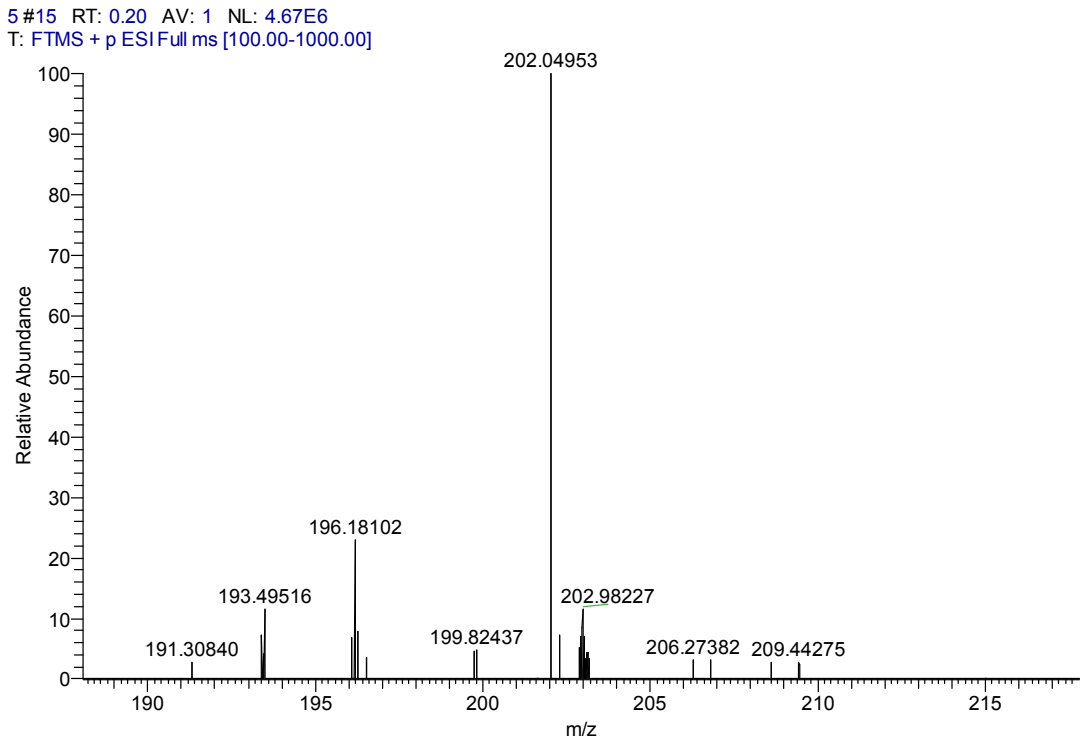


Figure S37. HRMS spectrum of compound 7.

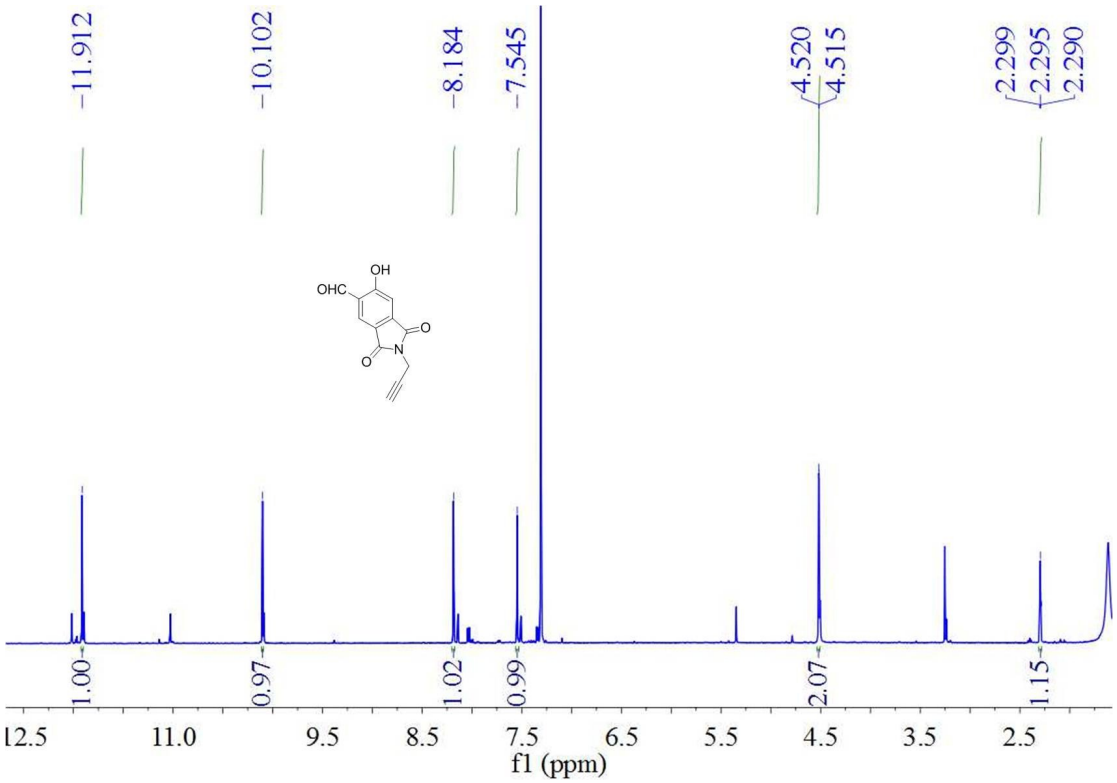


Figure S38. ^{1}H NMR spectrum of compound 7 in $CDCl_3$.

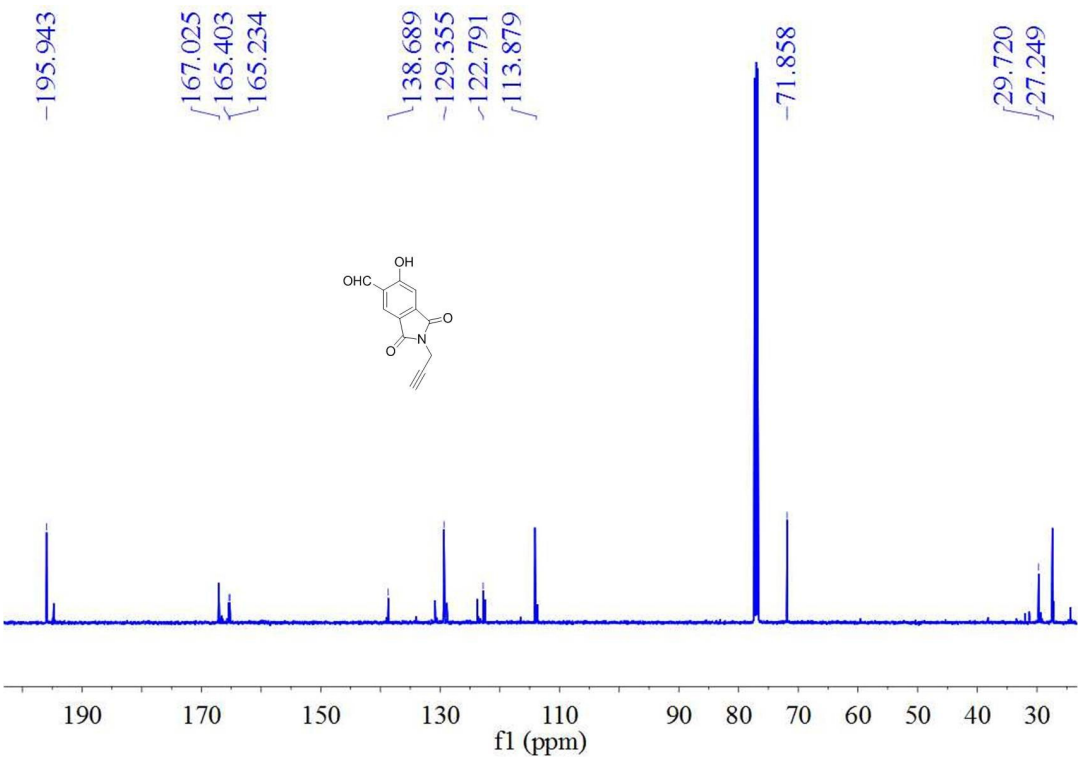


Figure S39. ^{13}C NMR spectrum of compound 7 in $CDCl_3$.

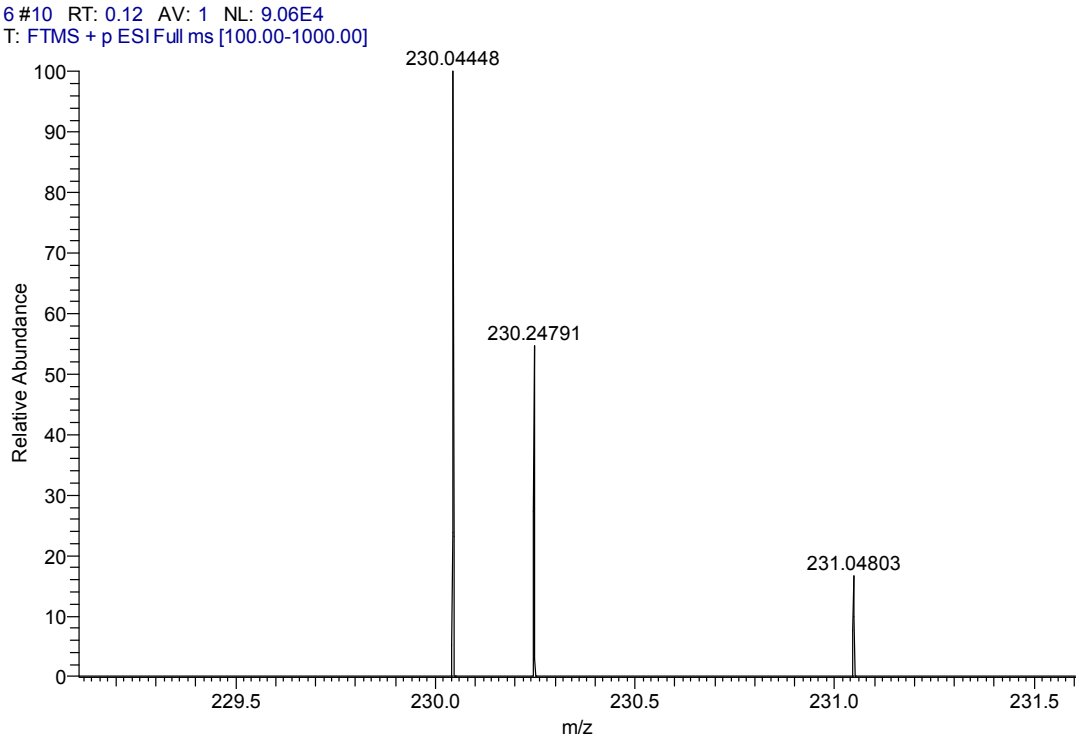


Figure S40. HRMS spectrum of compound 7.

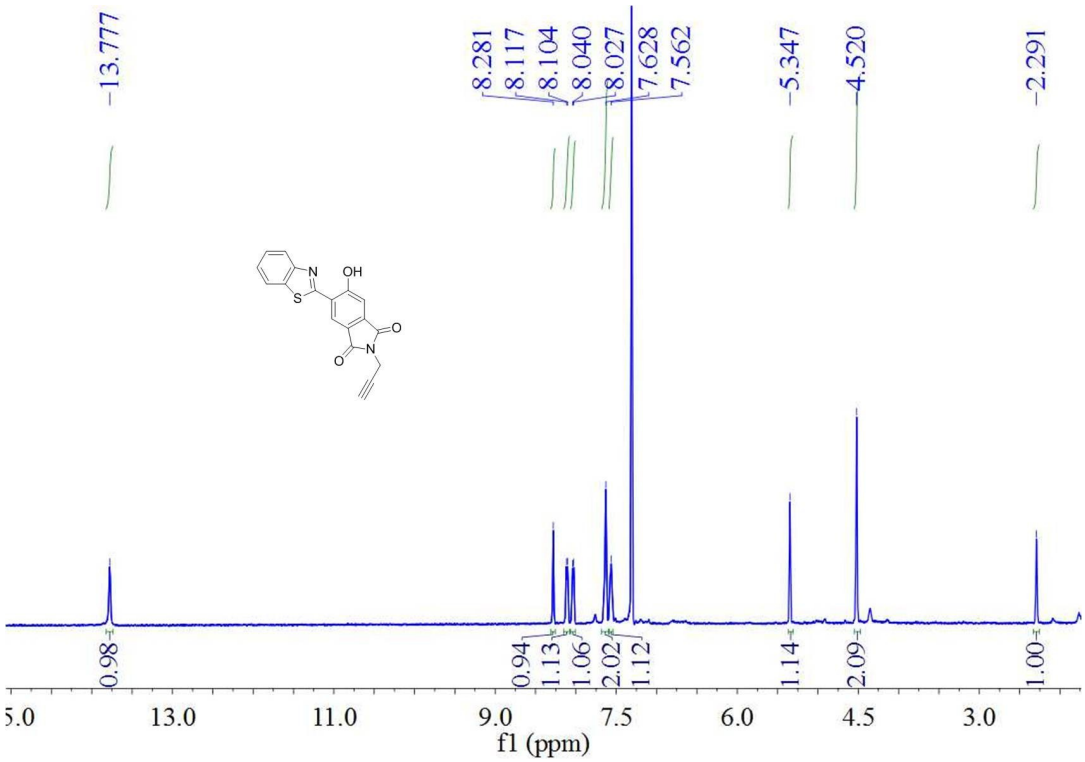


Figure S41. ^{1}H NMR spectrum of HPIBT-yl in $CDCl_3$.

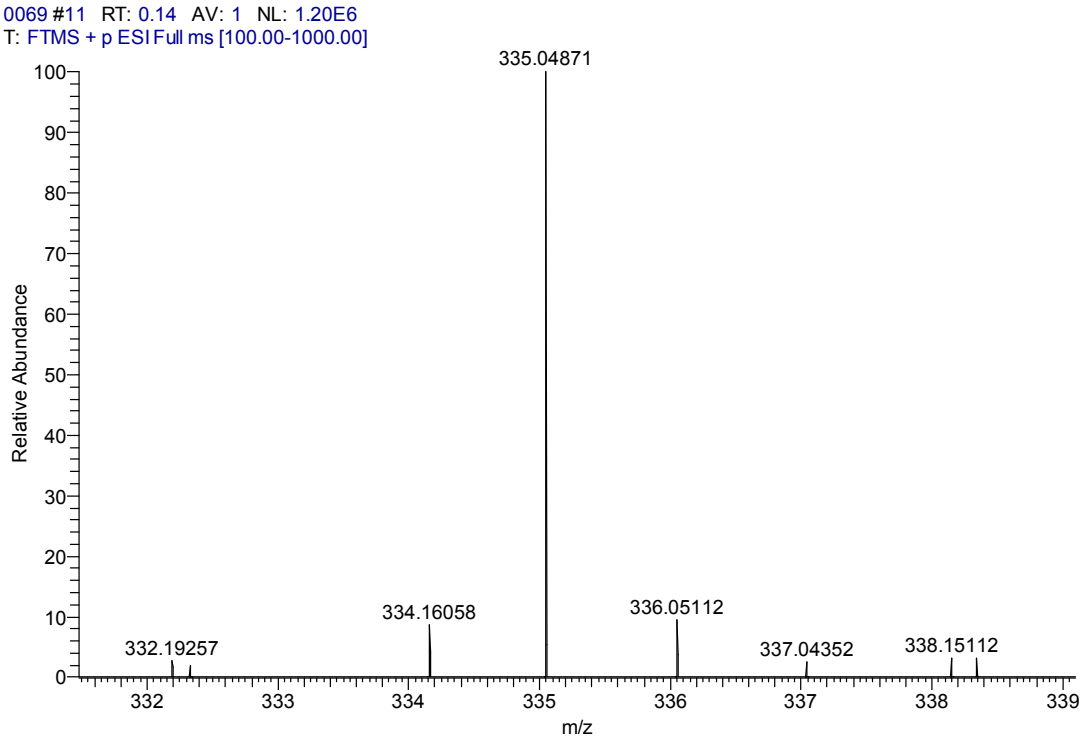


Figure S42. HRMS spectrum of HPIBT-yl**.**

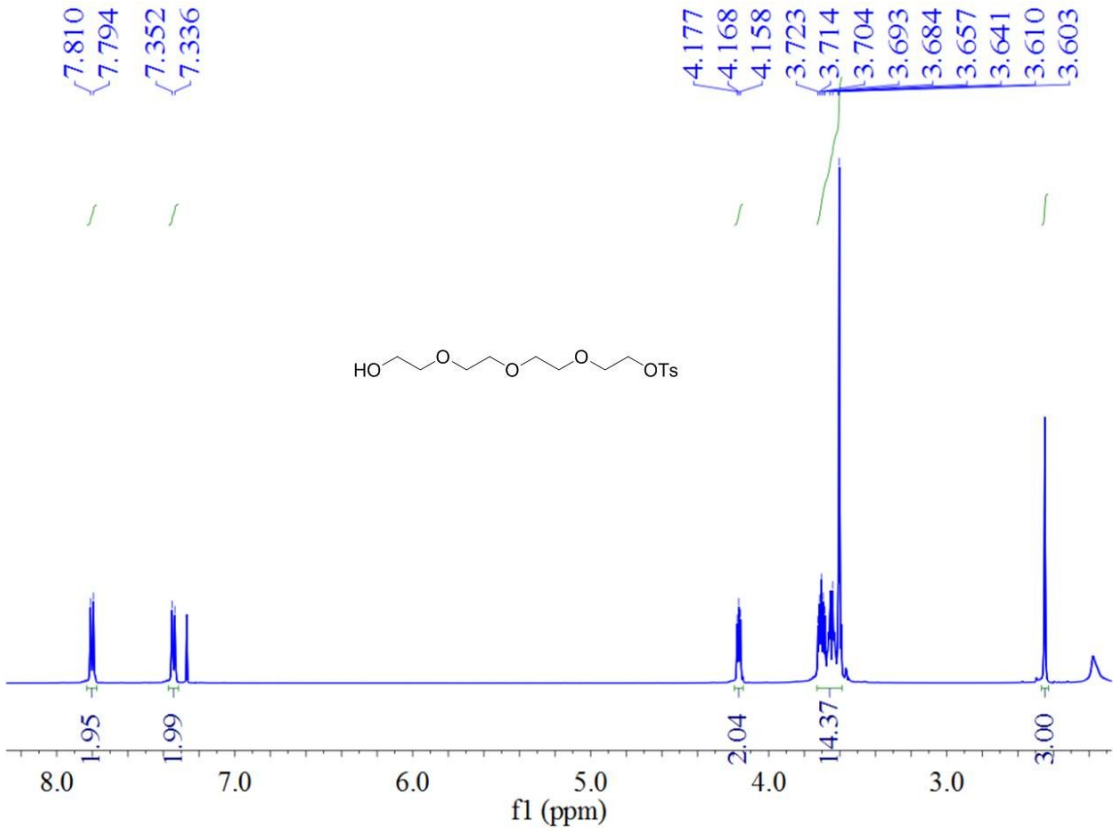


Figure S43. ^{1}H NMR spectrum of compound 8 in $CDCl_3$

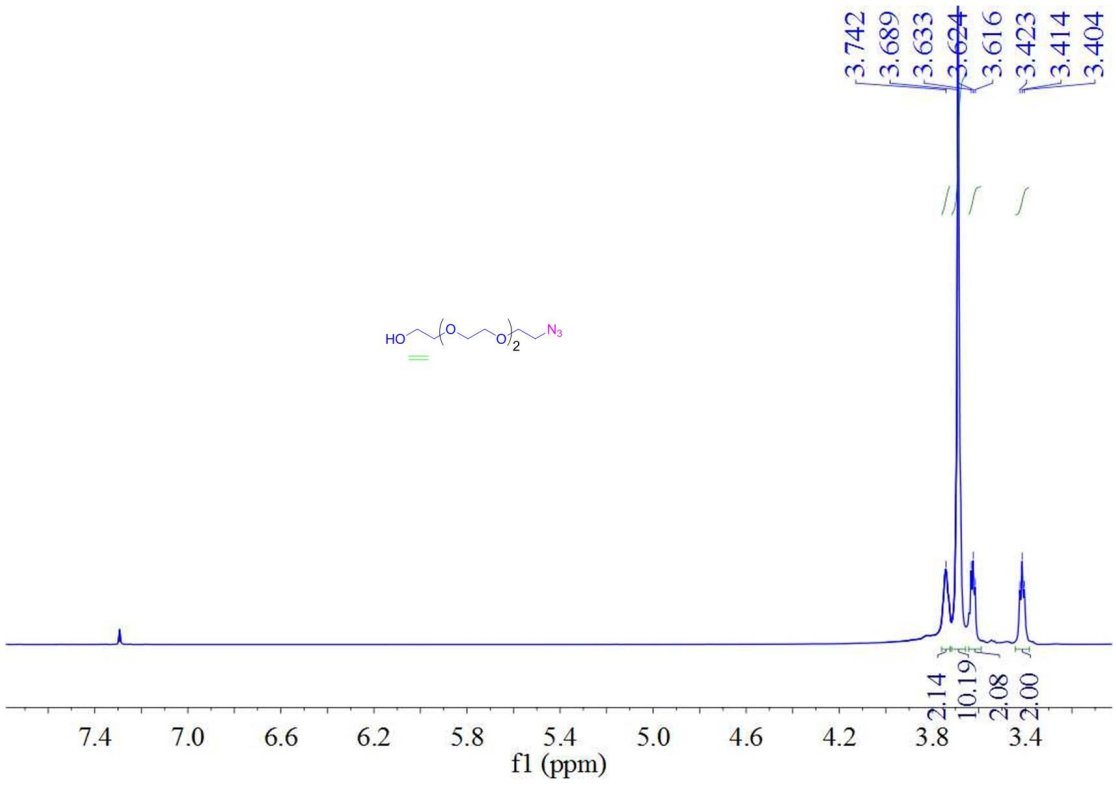


Figure S44. ^{1}H NMR spectrum of compound 9 in $CDCl_3$

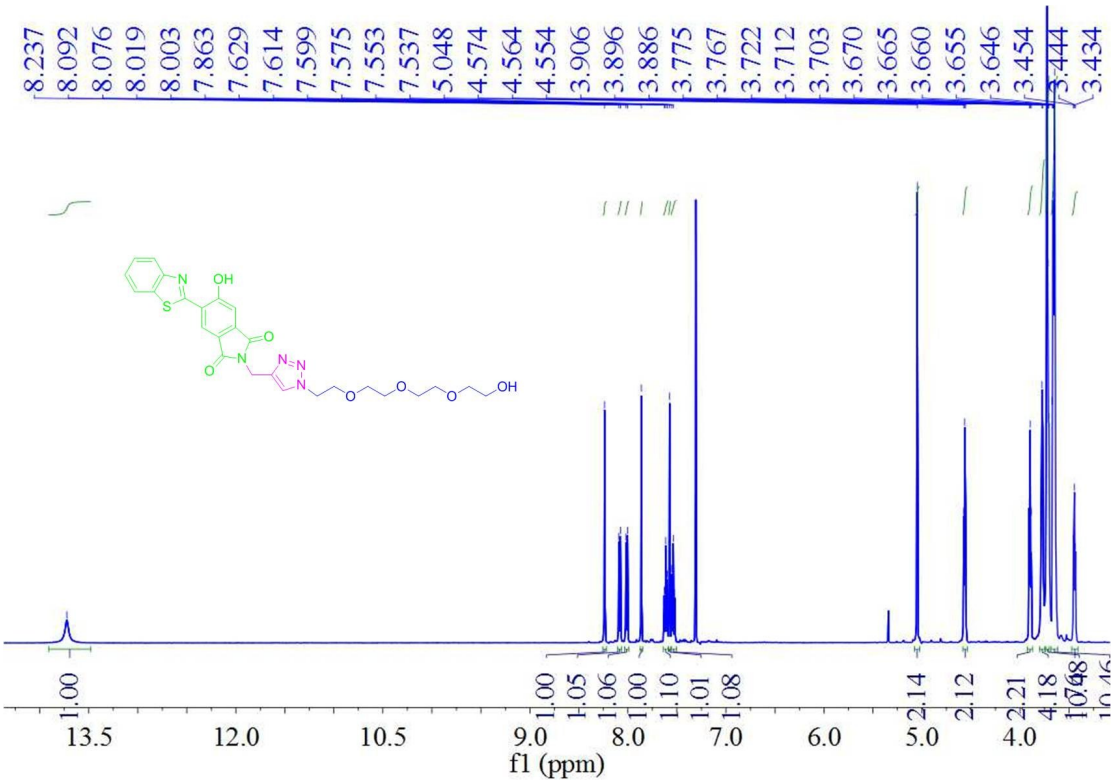


Figure S45. ^{1}H NMR spectrum of HPIBT-Pe in $CDCl_3$.

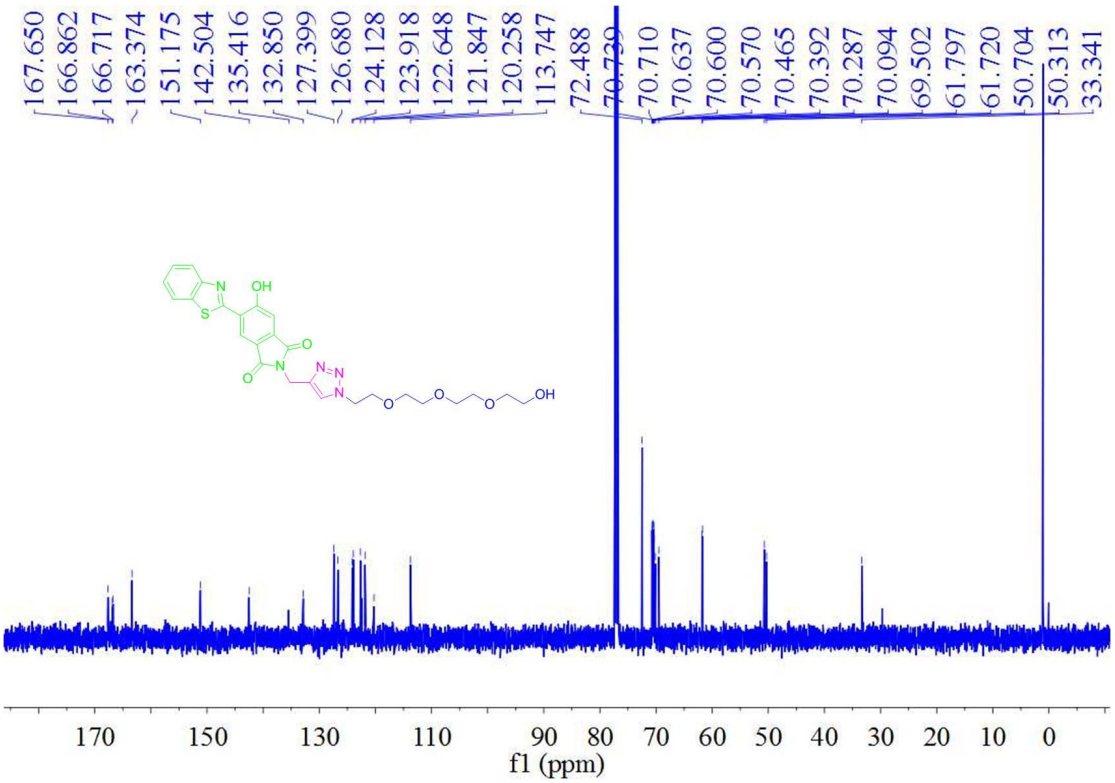


Figure S46. ^{13}C NMR spectrum of HPIBT-Pe in $CDCl_3$.

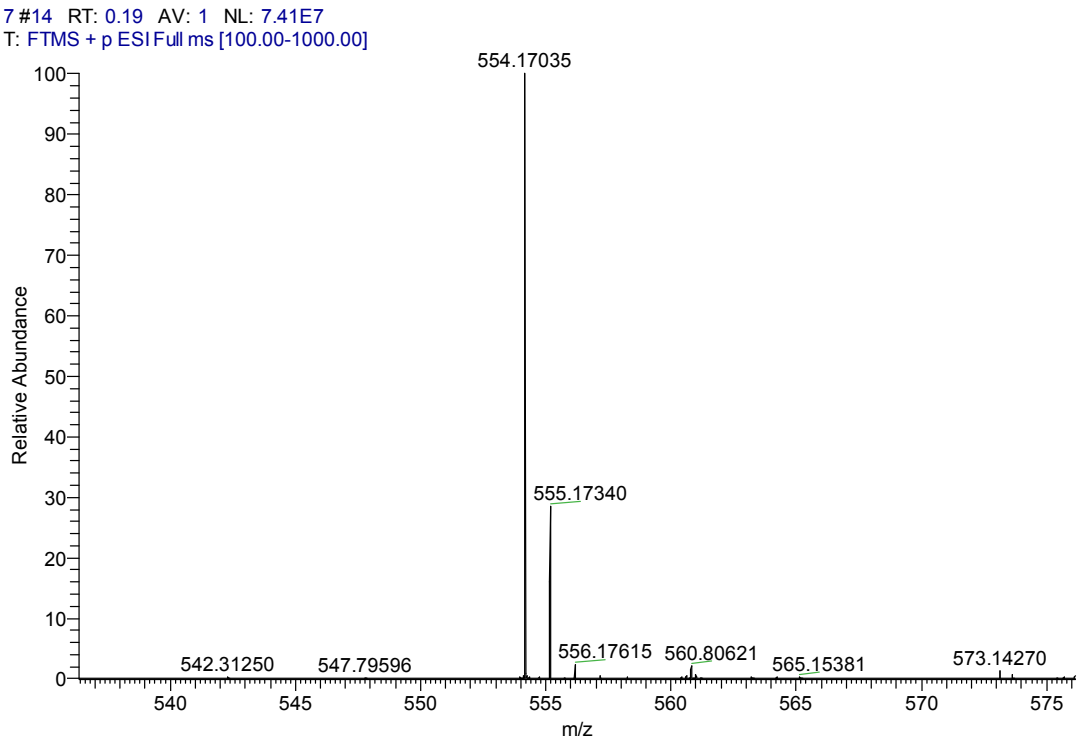


Figure S47. HRMS spectrum of HPIBT-Pe**.**