Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Experimental and DFT studies of disubstituted 2-(2-hydroxyphenyl)benzothiazole-based fluorophores synthesized by Suzuki coupling

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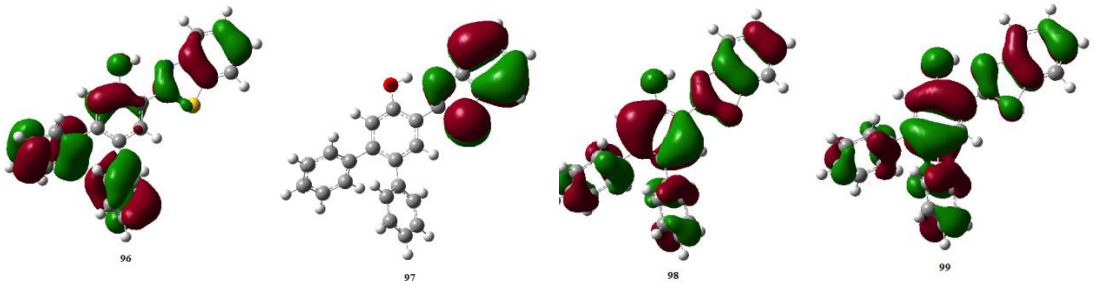
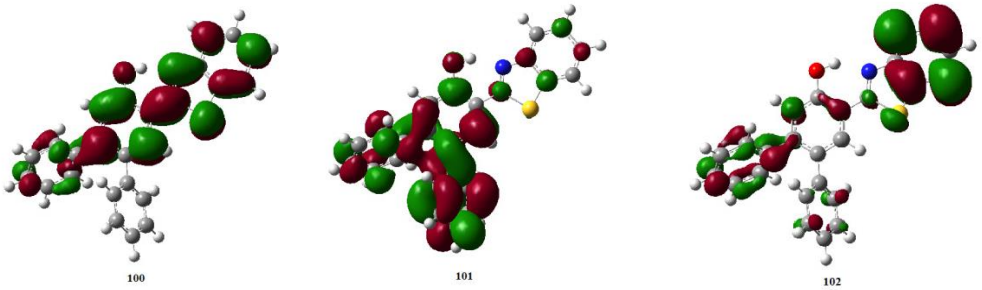
Table S1. TDDFT vertical excitation wavelengths and oscillator strengths (*f*) of HBT-H-H.

TDDFT－PCM			
λ(nm)	*f*	assign	%
369.01	0.6470	HOMO >LUMO	97.6
317.12	0.4621	HOMO-1 > LUMO	92.9
299.10	0.0468	HOMO-2> LUMO	75.3
		HOMO-3> LUMO	14.6
294.55	0.1183	HOMO > LUMO	2.8
		HOMO-3> LUMO	78.9
		HOMO-2> LUMO	13.6
		HOMO > LUMO+1	3.2



HOMO-3 HOMO-2 HOMO-1 HOMO



LUMO LUMO+1 LUMO+2

Figure S1. Molecular orbital amplitude plots of HBT-H-H calculated by using B3LYP/6-31+G(d) basis set with G09 program.

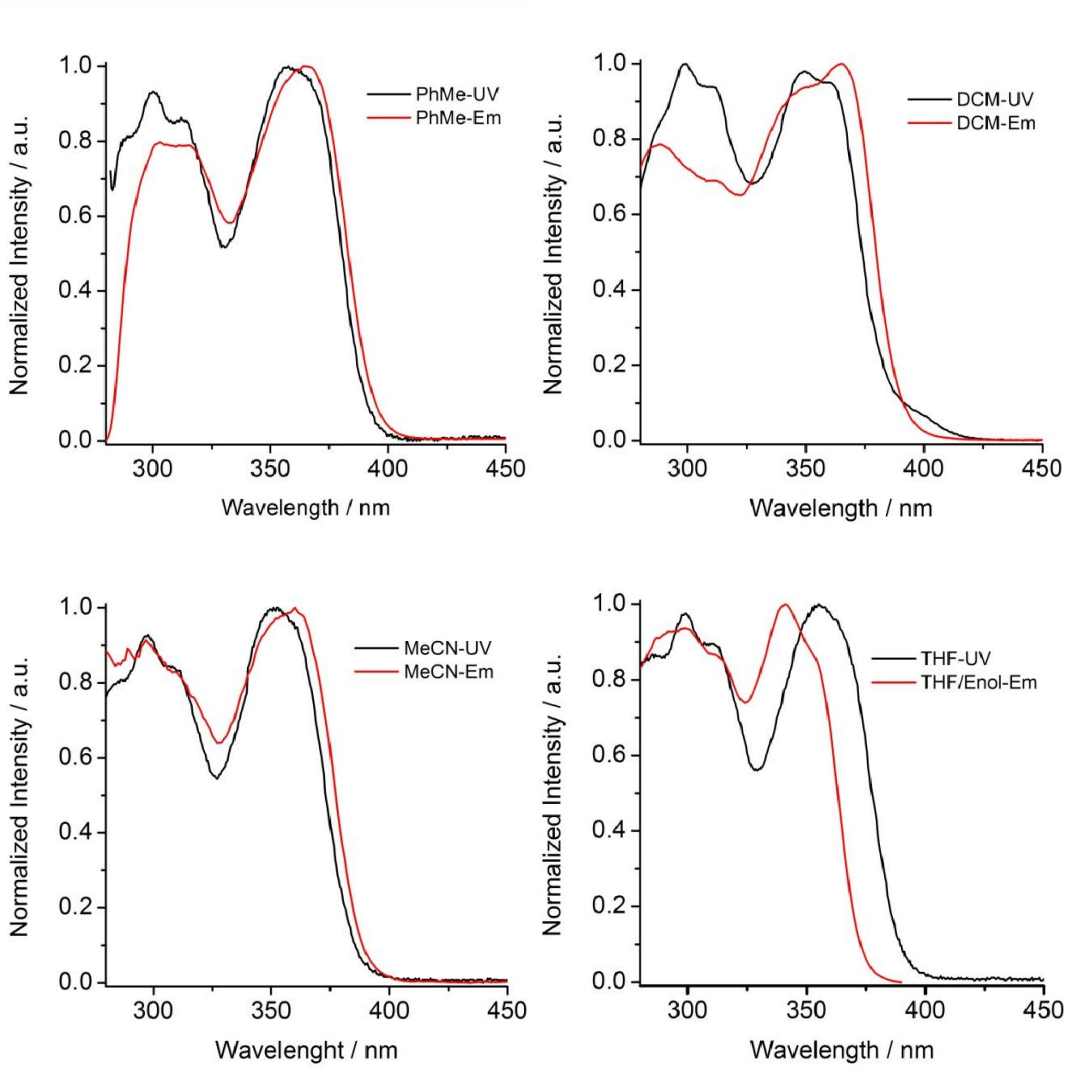


Figure S2. Comparison of the excitation spectra monitored at the fluorescence maximum wavelength and the absorption spectra of HBT-H-H in various solution.

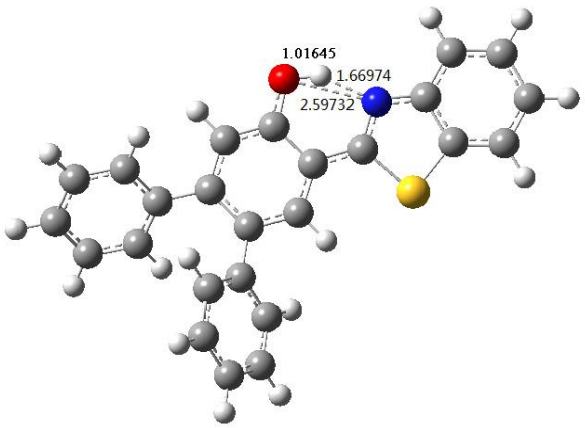


Figure S3 The energy-optimized geometric structures of enol-tautomer of HBT- -H in excited state and the relevant H-bond parameters.

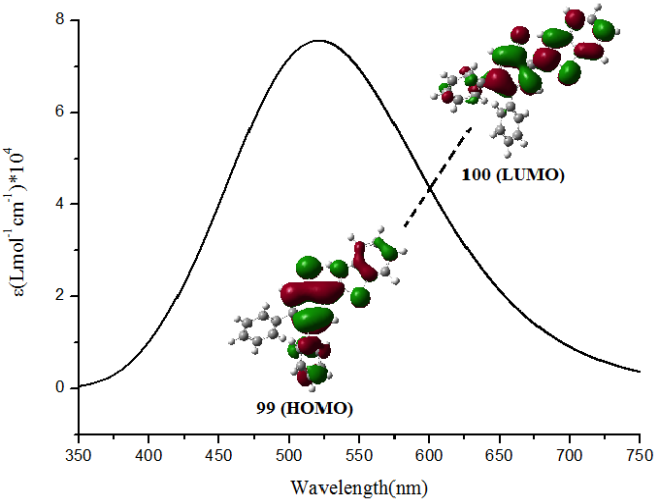


Figure S4. The theoretically calculated fluorescence spectrum of HBT-H-H in toluene. (λ_{em} = 532.23 nm)

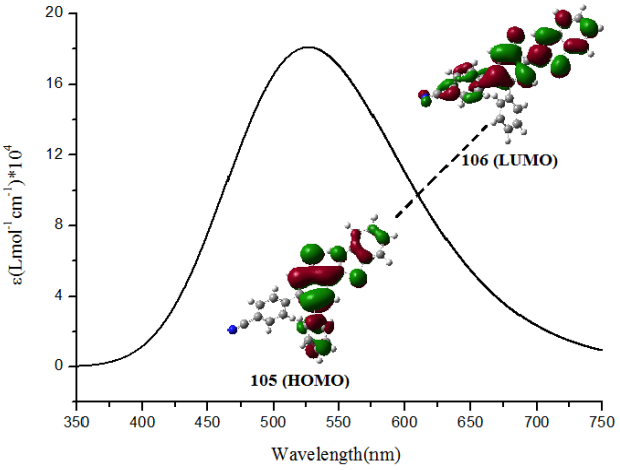


Figure S5. The theoretically calculated fluorescence spectrum of HBT-CN-H in toluene. (λ_{em} = 536.72 nm)

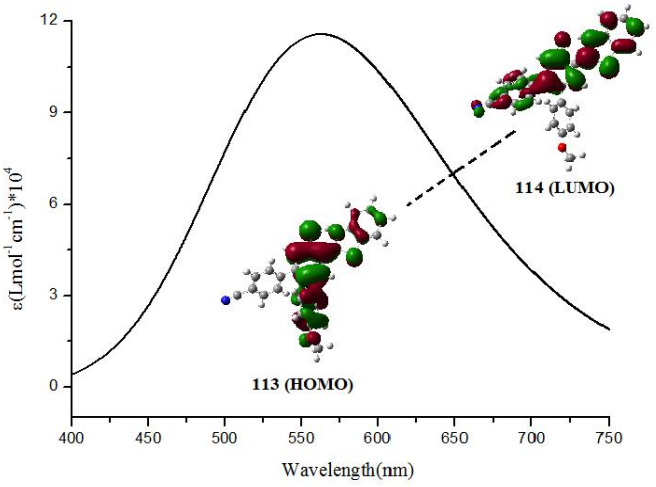


Figure S6. The theoretically calculated fluorescence spectrum of HBT-CN-OMe in toluene. (λ_{em} = 570.62 nm)

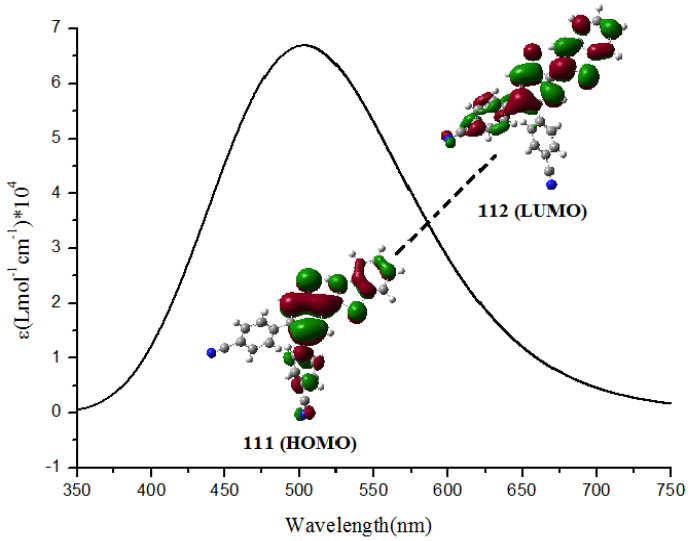


Figure S7. The theoretically calculated fluorescence spectrum of HBT-CN-CN in toluene. (λ_{em} = 516.23 nm)

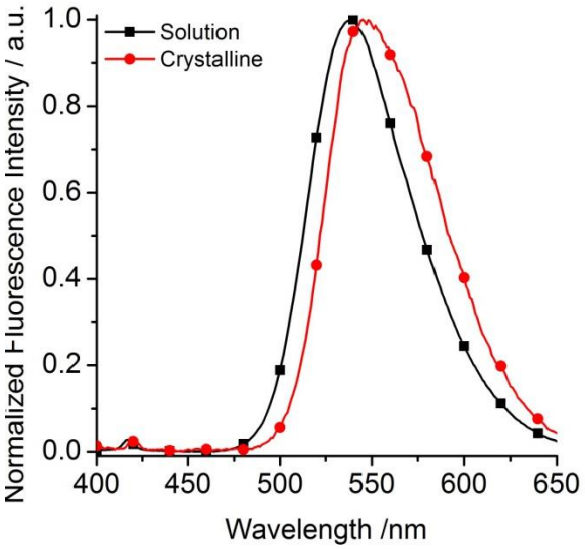


Figure S8. Comparison of the fluorescence spectra of HBT-H-H in toluene and in crystalline.

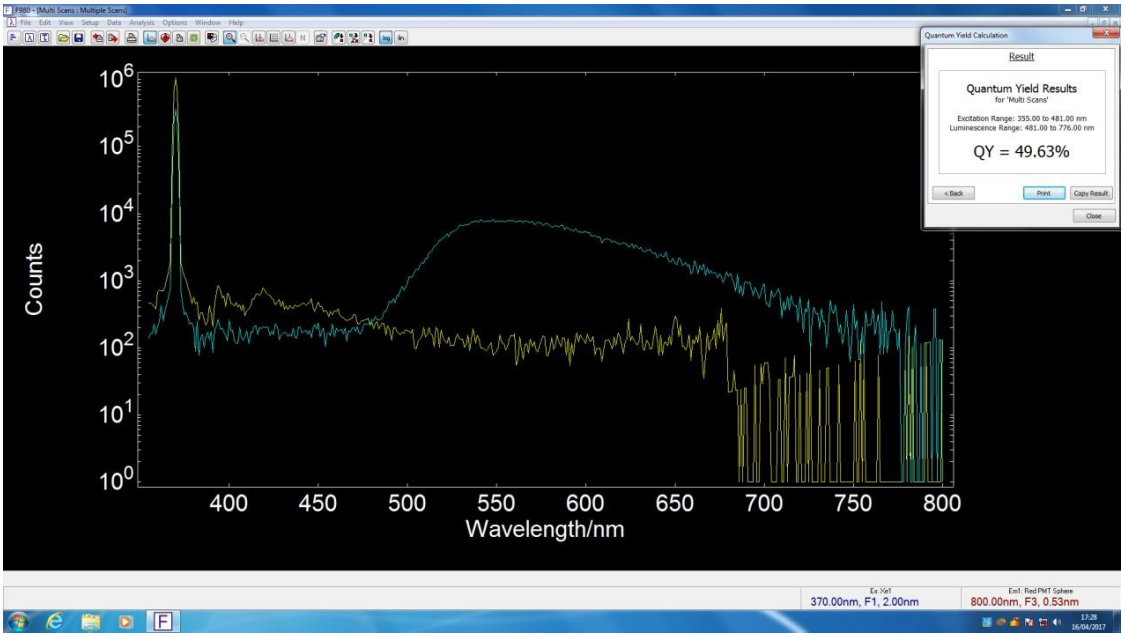


Figure S9. Fluorescence quantum yield of HBT-H-H crystal (Φ_f =49.63%).

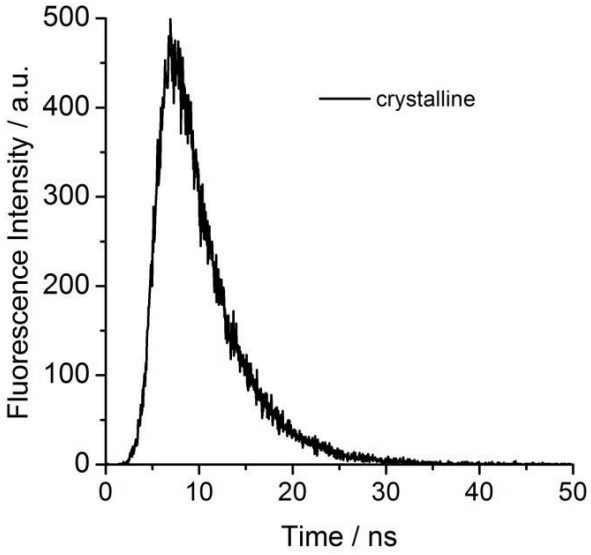


Figure S10. Fluorescence lifetime profiles of HBT-H-H crystal.

Table S2. Crystallographic data for HBT-H-H (CCDC 1546814)

Empirical formula	$C_{25}H_{17}NOS$
Å Formula weight	379.46
Crystal system	Triclinic
space group	P-1
Crystal size/mm	0.40 x 0.30 x 0.20
a/ Å , α/deg.	9.9130(8)/ 78.3830(10)
b/ Å, β/deg.	10.2709(9)/ 71.218(2)
c/ Å, γ/deg.	10.8021(9)/ 67.6380(10)
V/ Å^3	959.04(14)
GOF	1.047

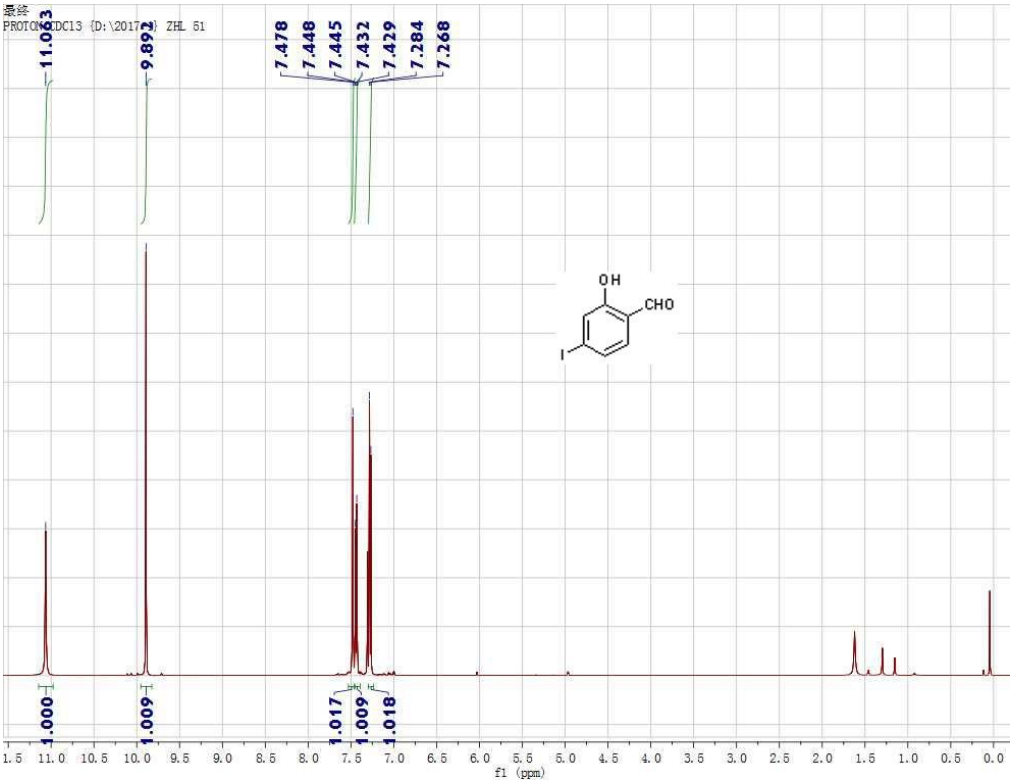


Figure S11. ^{1}H NMR spectrum of 2-hydroxy-4-iodobenzaldehyde (Compound **1**) in $CDCl_3$.

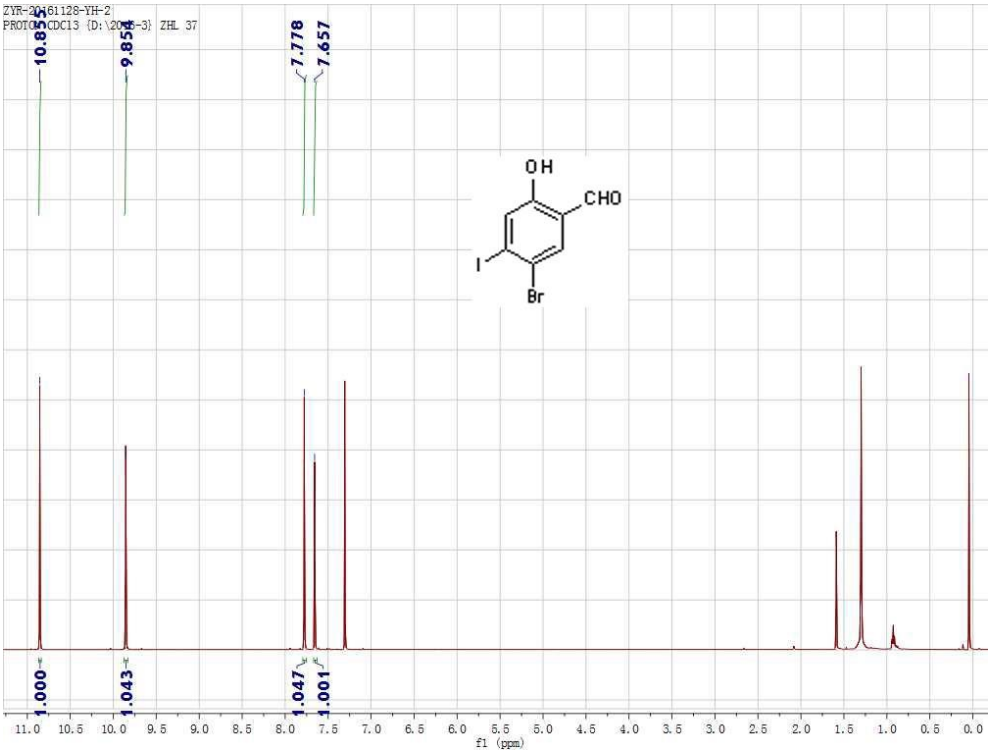


Figure S12. ^{1}H NMR spectrum of 5-bromo-2-hydroxy-4-iodobenzaldehyde (Compound **2**) in $CDCl_3$.

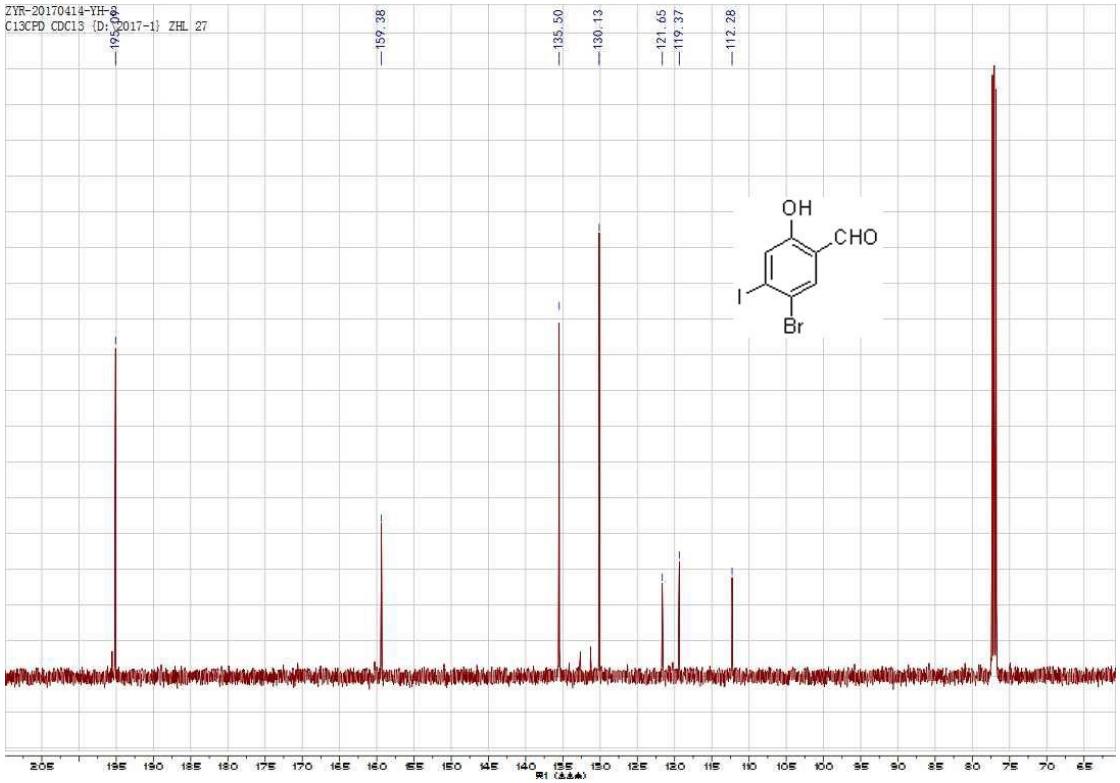


Figure S13. ^{13}C NMR spectrum of 5-bromo-2-hydroxy-4-iodobenzaldehyde (Compound **2**) in $CDCl_3$.

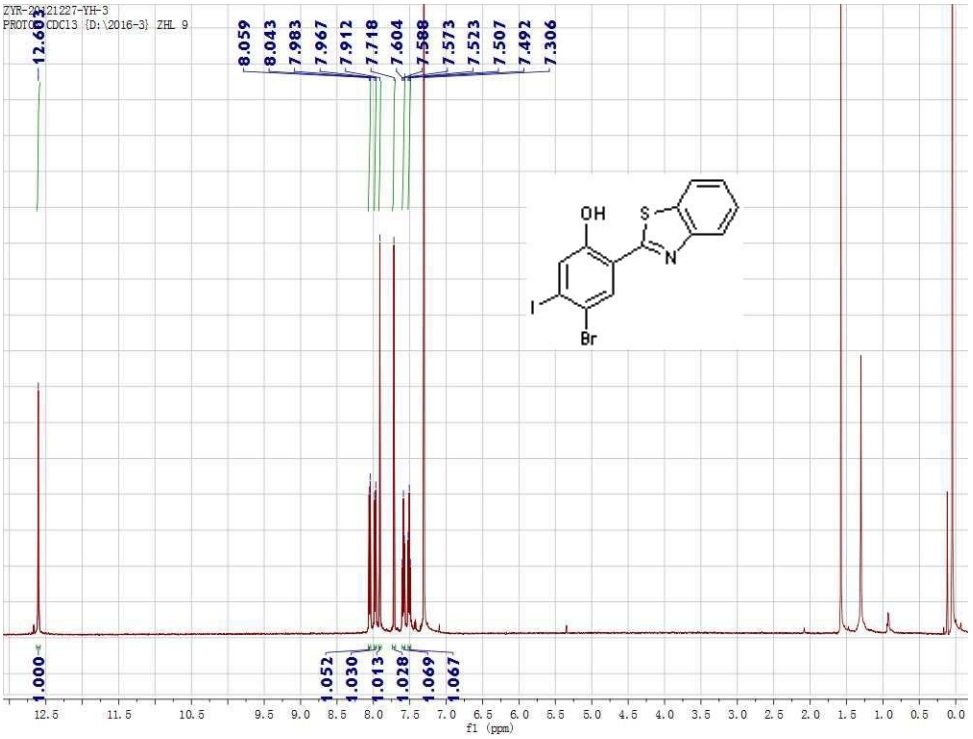


Figure S14. ^{1}H NMR spectrum of 2-(benzo[*d*]thiazol-2-yl)-4-bromo-5-iodophenol (Compound **3**) in $CDCl_3$

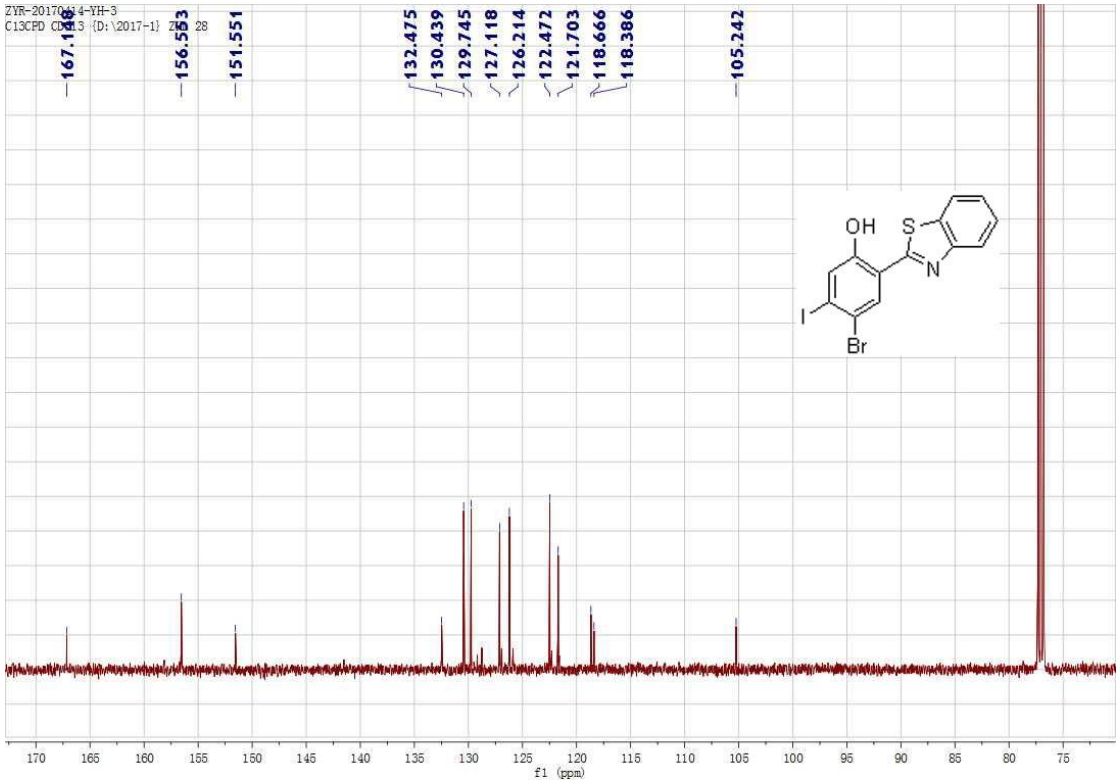


Figure S15. ^{13}C NMR spectrum of 2-(benzo[*d*]thiazol-2-yl)-4-bromo-5-iodophenol (Compound 3) in $CDCl_3$

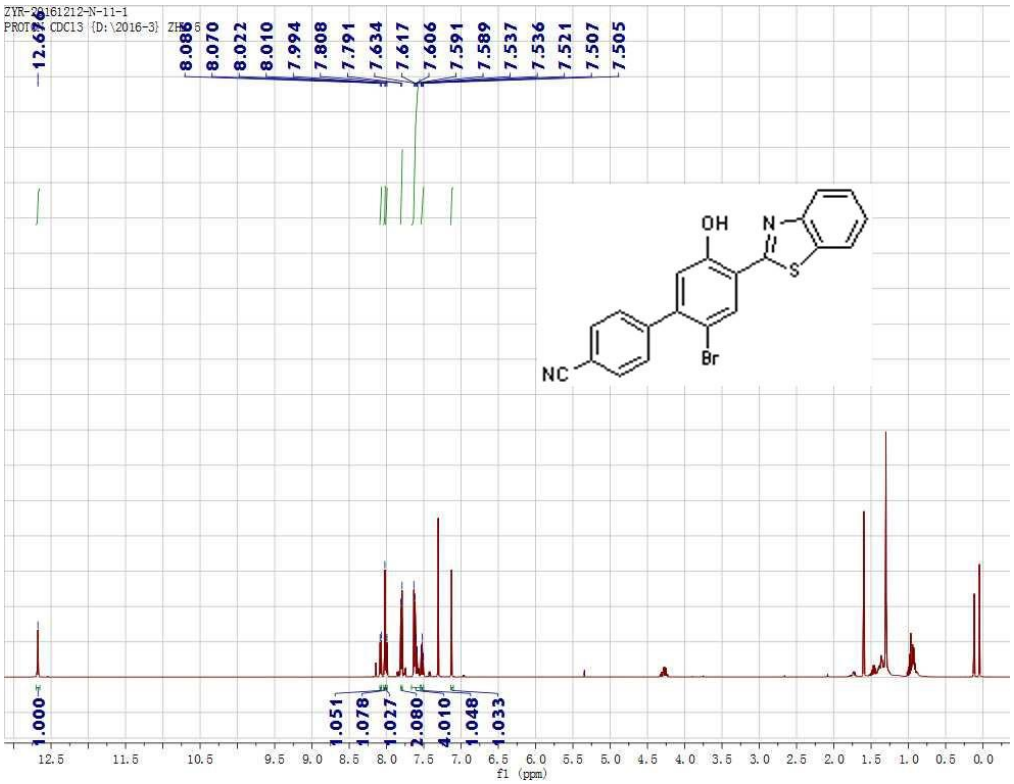


Figure S16. ^{1}H NMR spectrum of Compound **4** in $CDCl_3$.

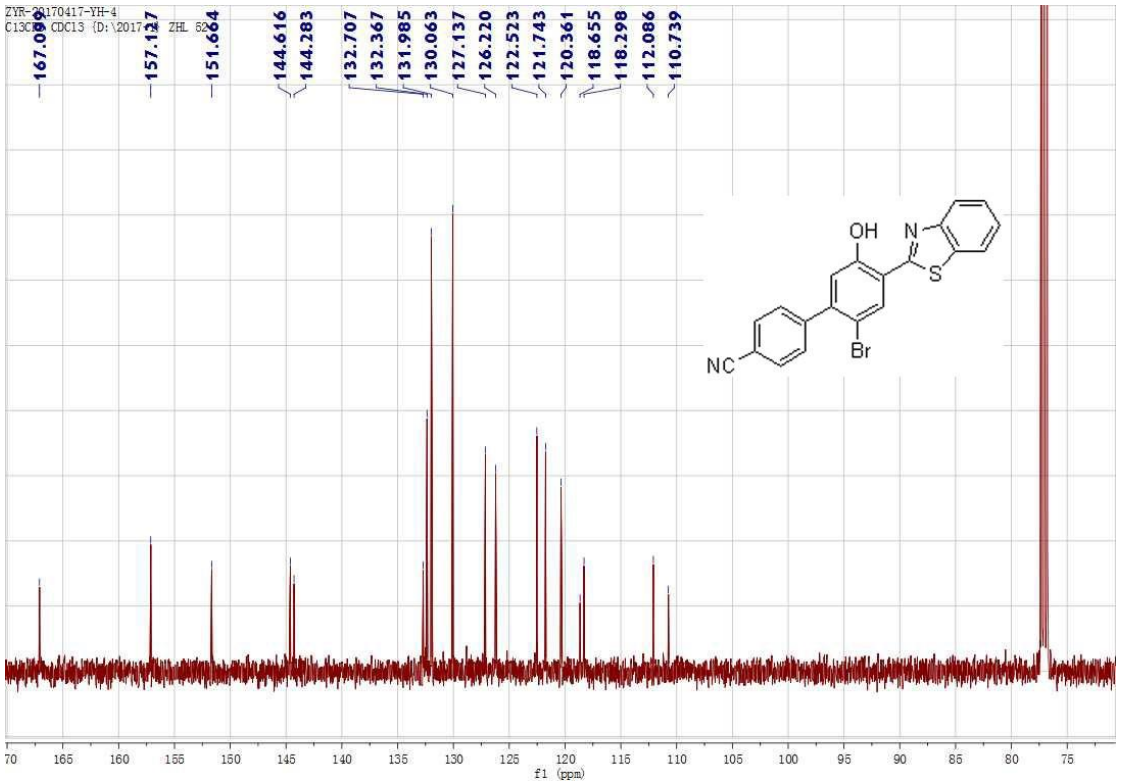


Figure S17. ^{13}C NMR spectrum of Compound **4** in $CDCl_3$

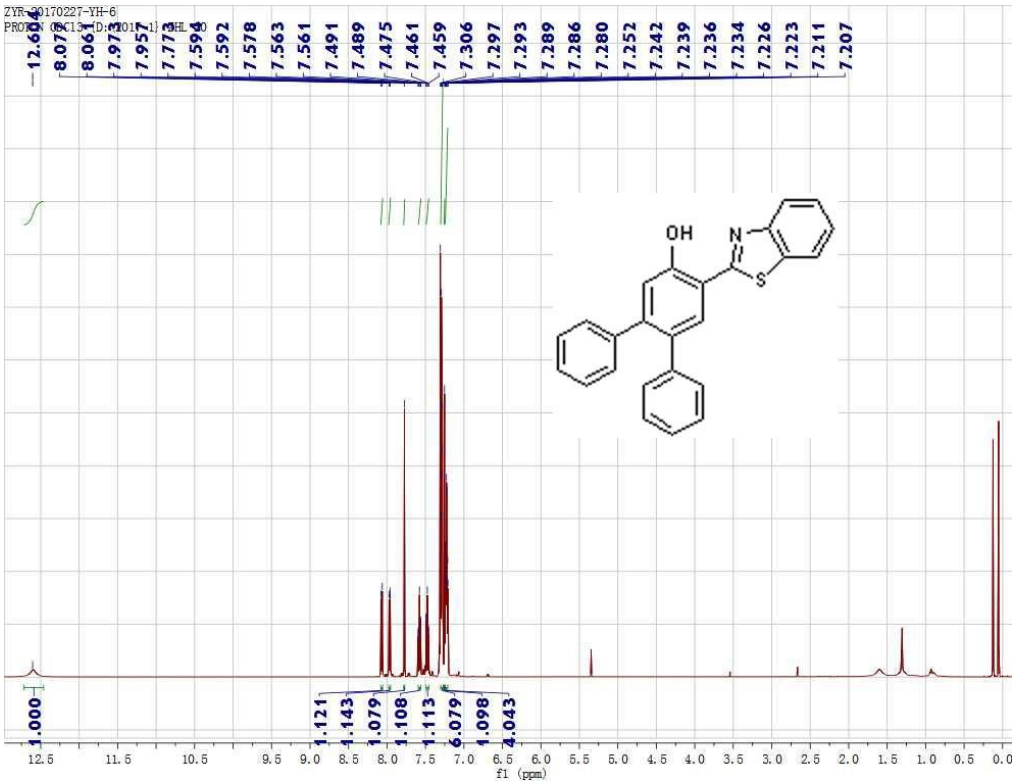


Figure S18. ^{1}H NMR spectrum of HBT-H-H in $CDCl_3$.

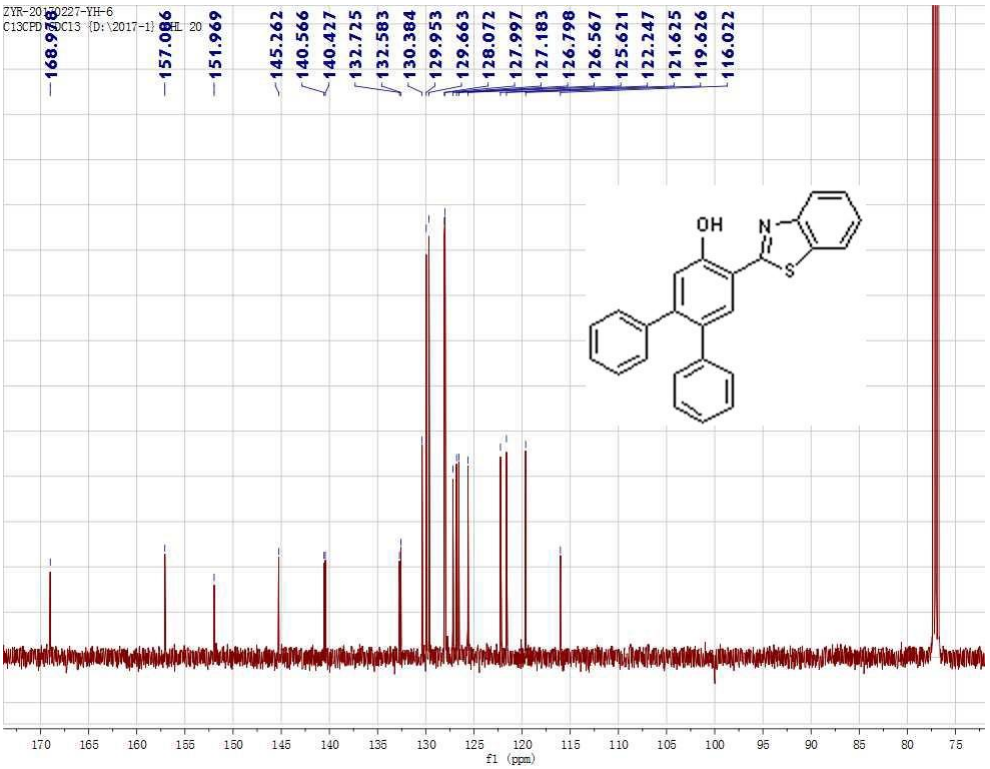


Figure S19. ^{13}C NMR spectrum of HBT-H-H in $CDCl_3$

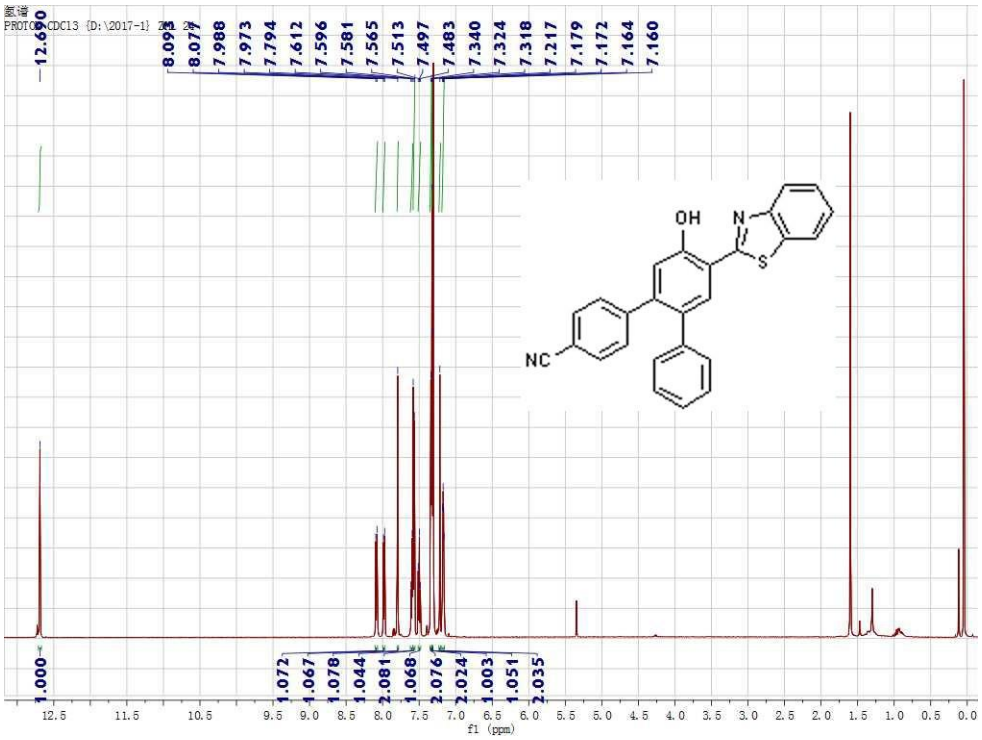


Figure S20. ^{1}H NMR spectrum of HBT-CN-H in $CDCl_3$

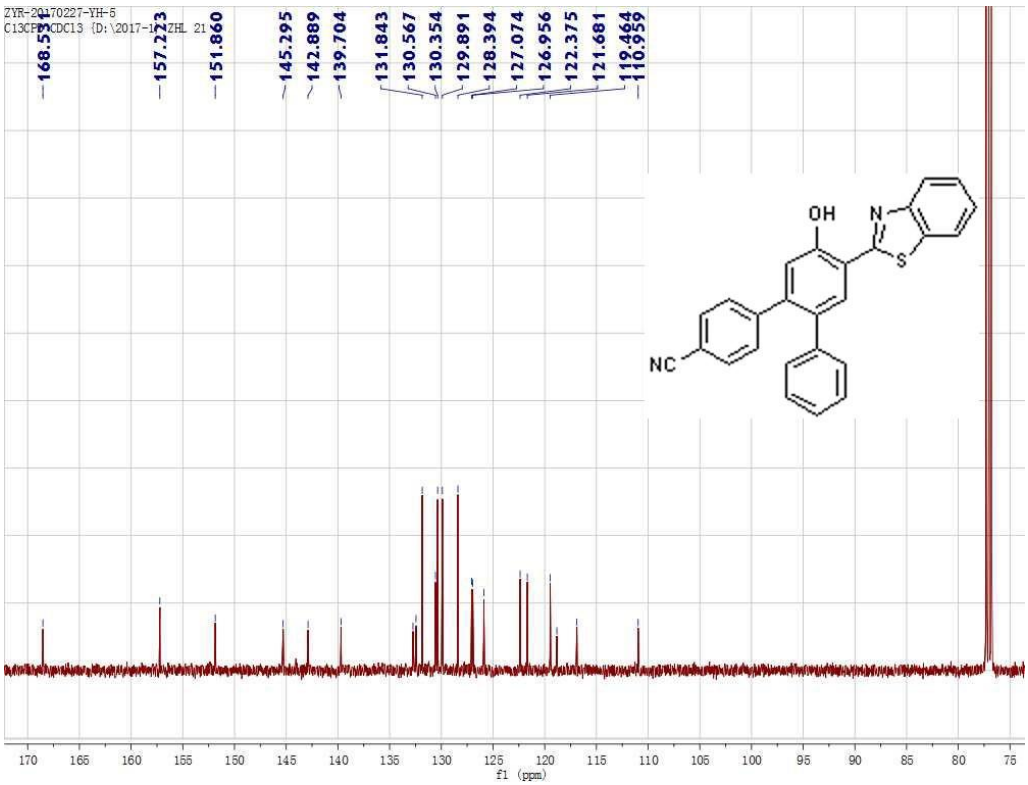


Figure S21. ^{13}C NMR spectrum of HBT-CN-H in $CDCl_3$

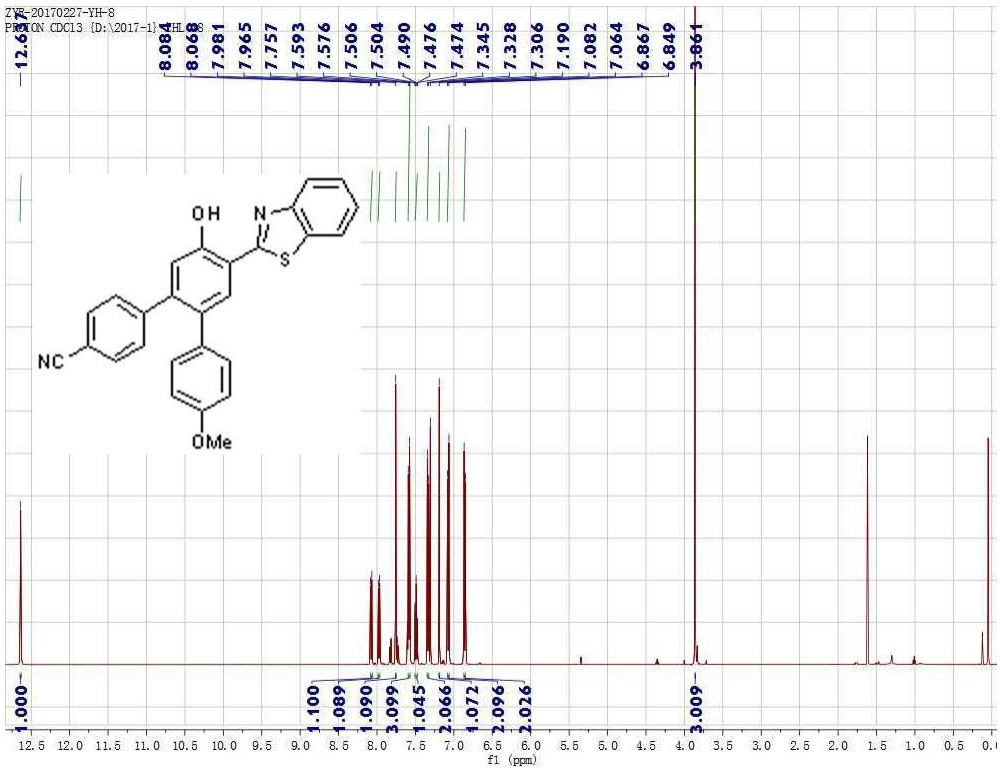


Figure S22. ^{1}H NMR spectrum of HBT-CN-MeO in $CDCl_3$

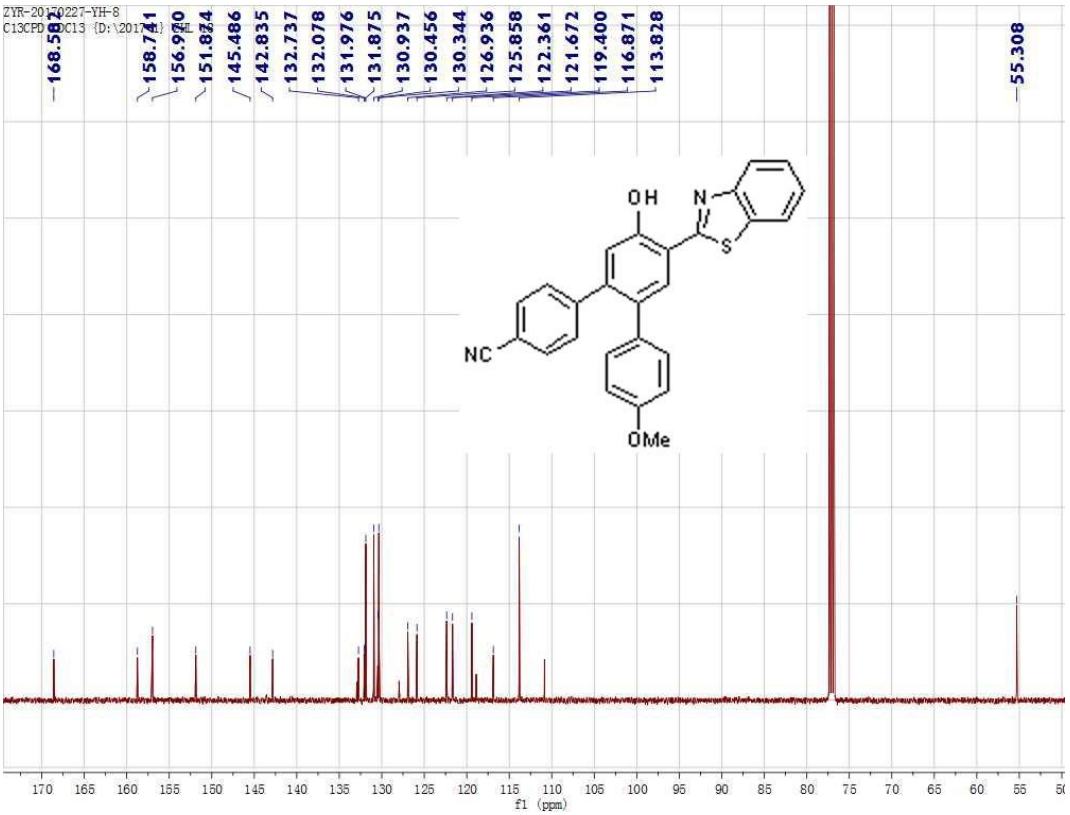


Figure S23. ^{13}C NMR spectrum of HBT- CN-MeO in $CDCl_3$

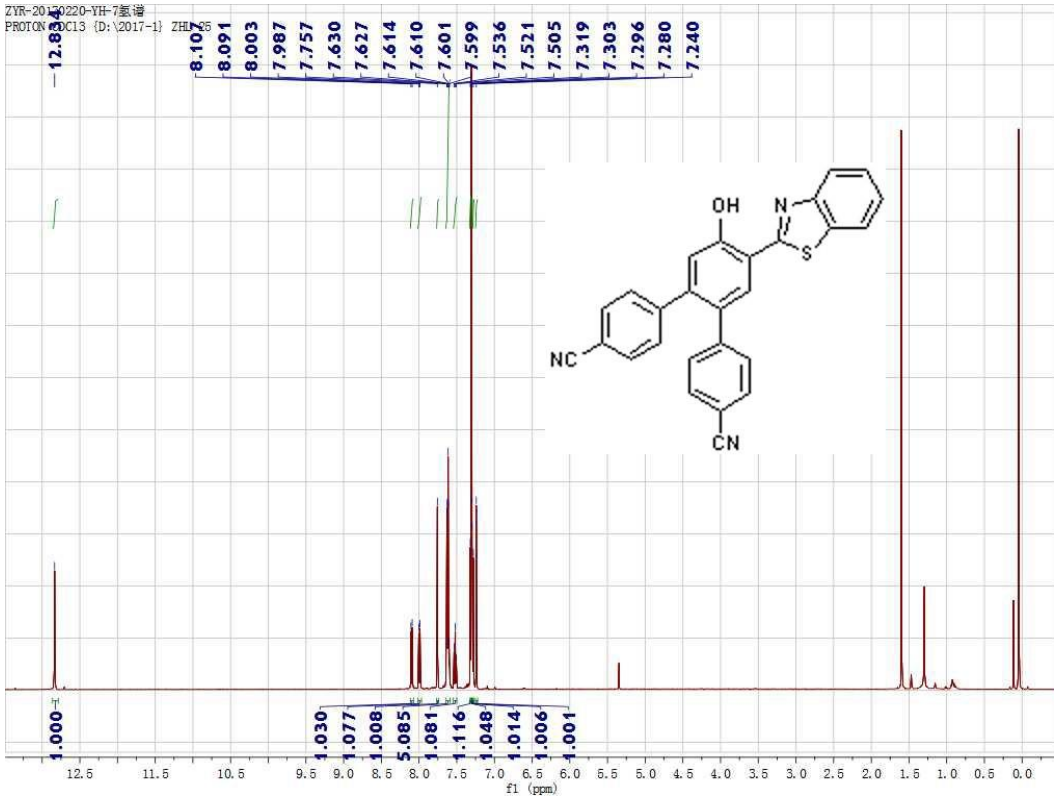


Figure S24. ^{1}H NMR spectrum of HBT-CN-CN in $CDCl_3$

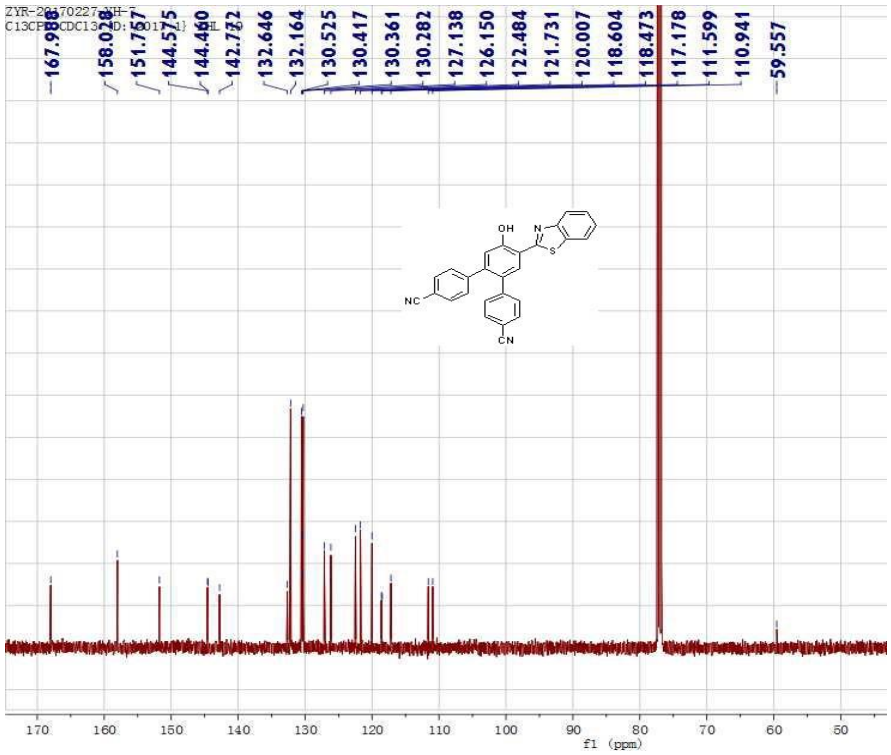


Figure S25. ^{13}C NMR spectrum of HBT- CN-CN in $CDCl_3$

YH-6: HRMS (ESI) m/z calcd for $C_{25}H_{18}NOS^+$ $(M+H)^+$ 380.11036, found 380.11078.

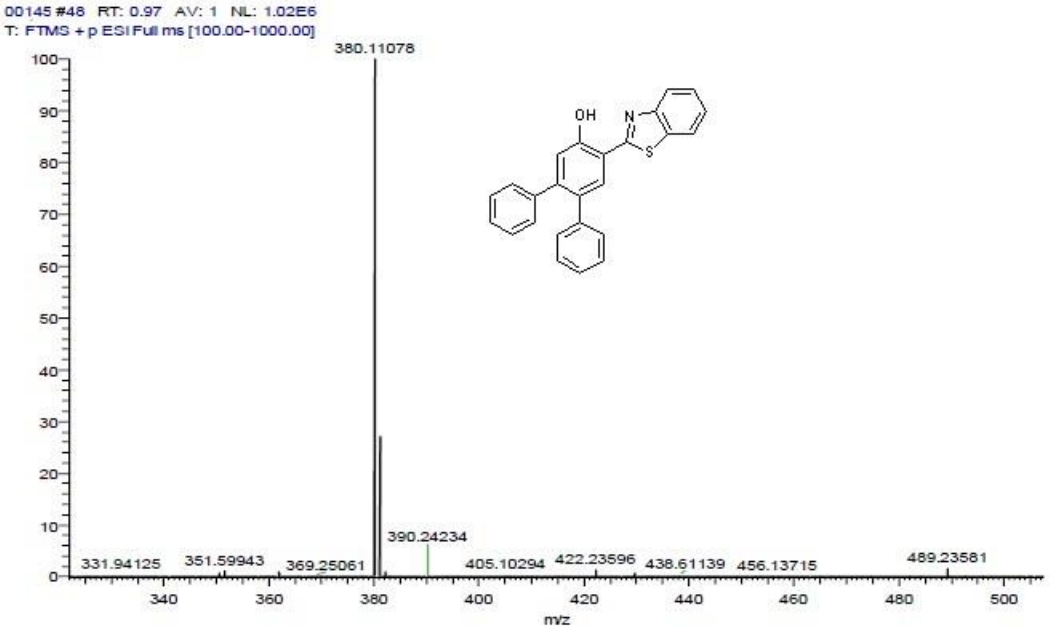


Figure S26. HRMS spectrum of HBT-H-H.

YH-7: HRMS (ESI) m/z calcd for $C_{27}H_{16}N_3OS^+$ $(M+H)^+$ 430.10086, found 430.10101.

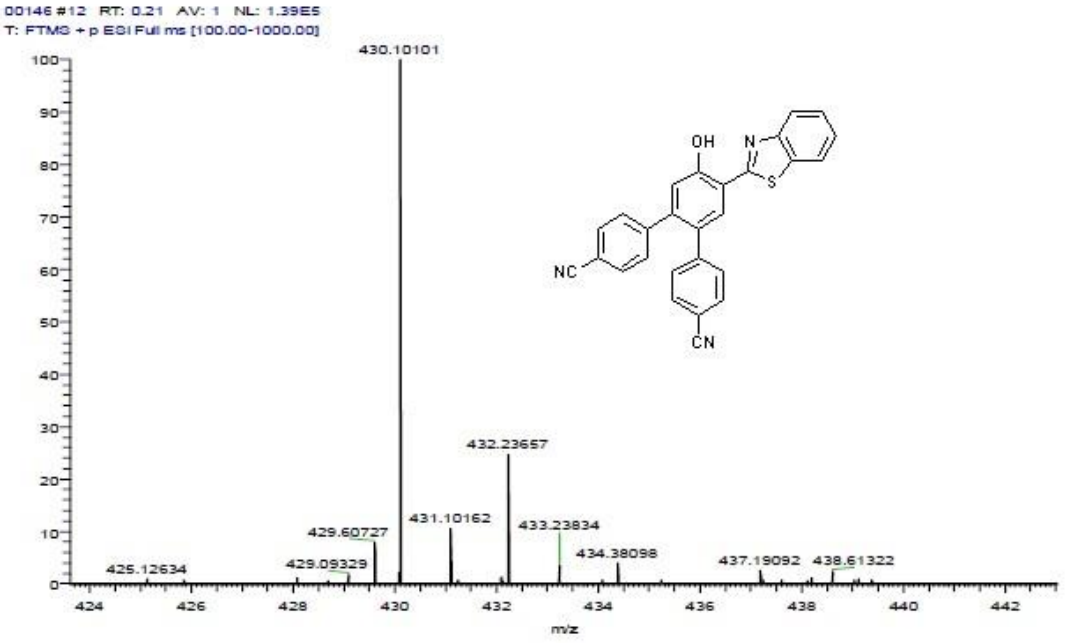


Figure S27. HRMS spectrum of HBT-CN-CN.

YH-11: HRMS (ESI) m/z calcd for $C_{20}H_{12}BrN_2OS^+$ $(M+H)^+$ 406.98482, found 406.98447.

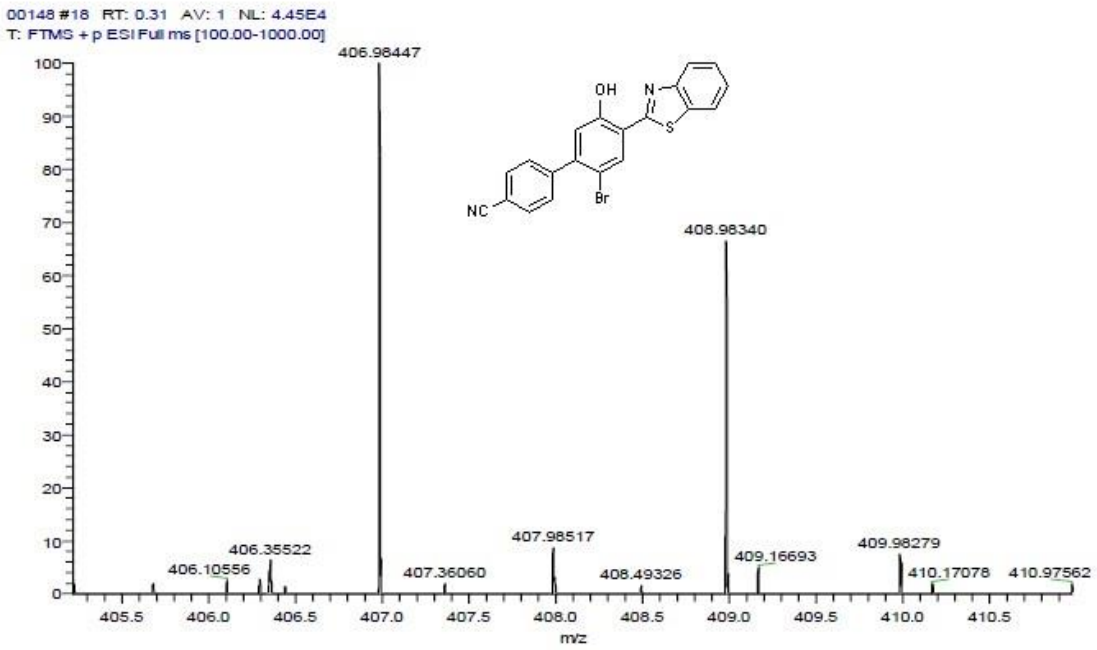


Figure S28. HRMS spectrum of Compound **4**.

YH-5: HRMS (ESI) m/z calcd for $C_{26}H_{17}N_2OS^+$ $(M+H)^+$ 405.10561, found 405.10568.

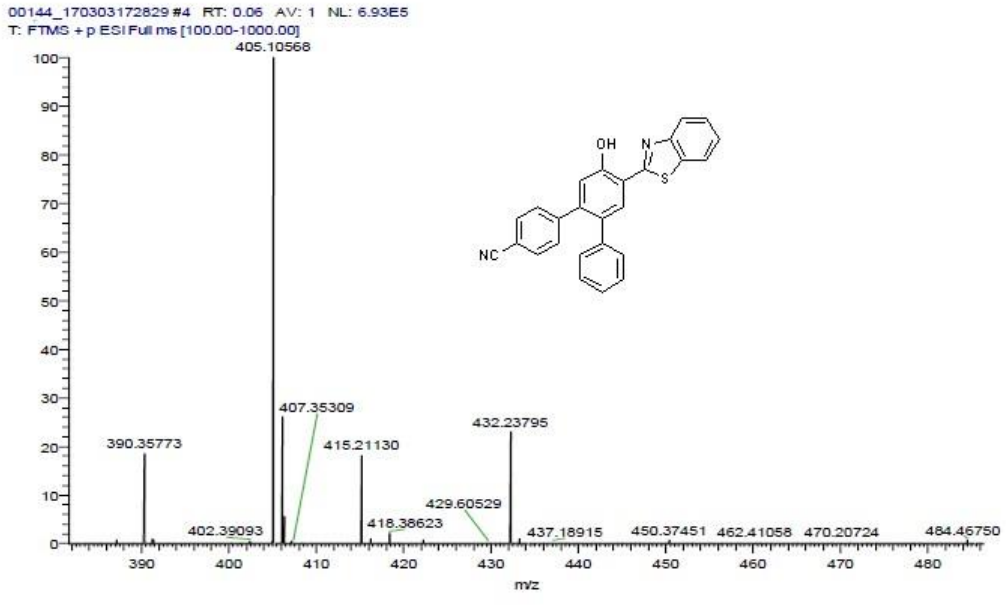


Figure S29. HRMS spectrum of HBT-CN-H.

YH-8: HRMS (ESI) m/z calcd for $C_{27}H_{19}N_2O_2S^+$ $(M+H)^+$ 435.11617, found 435.11618.

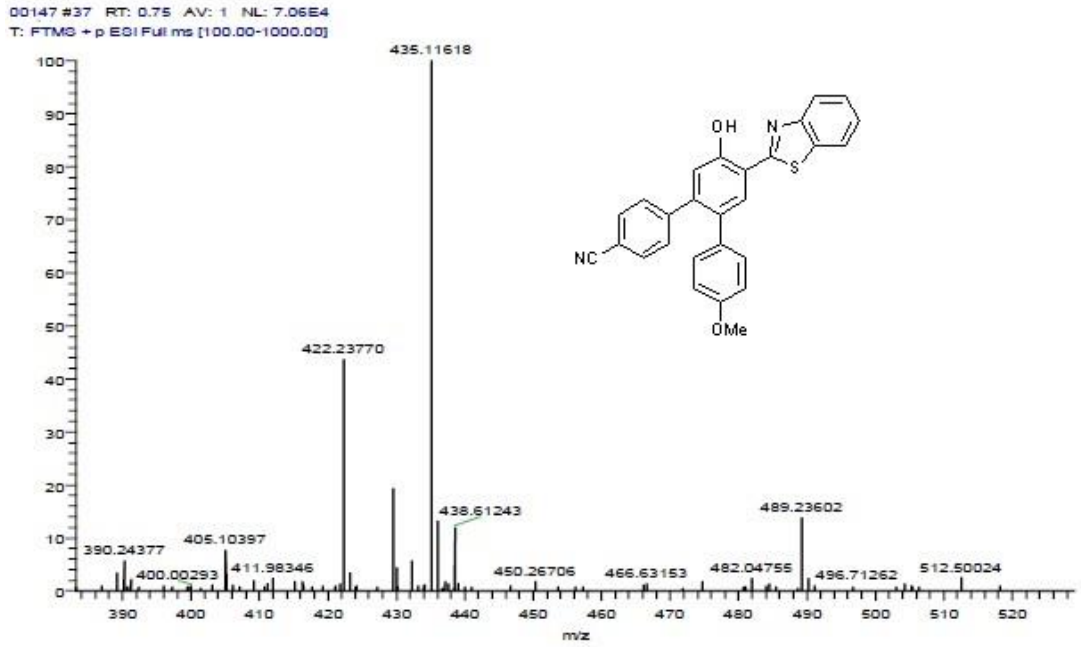


Figure S30. HRMS spectrum of HBT-CN-OMe.