

Electronic Supporting Information for

BODIPY Based Hyperbranched Conjugated Polymers for Detecting Organic Vapors

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1. ^1H and ^{13}C NMR and mass spectra of monomers

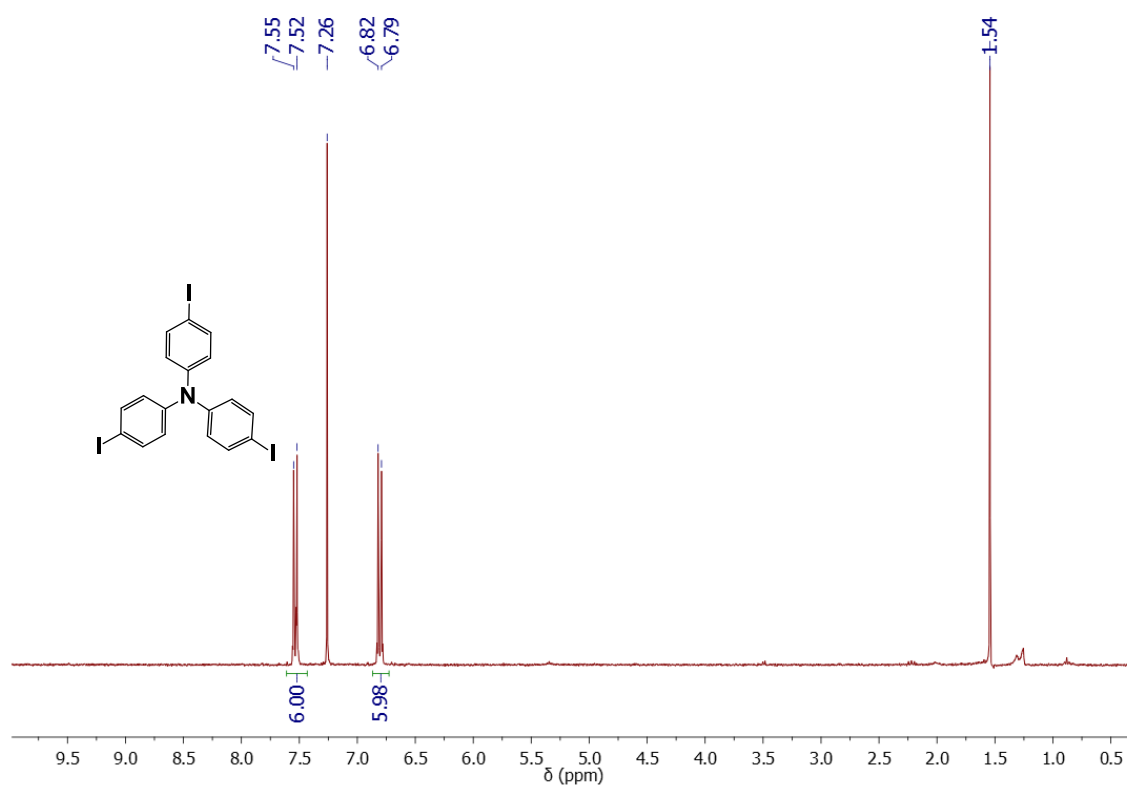


Figure S1. ^1H NMR spectrum of tris(4-iodophenyl)amine in CDCl₃.

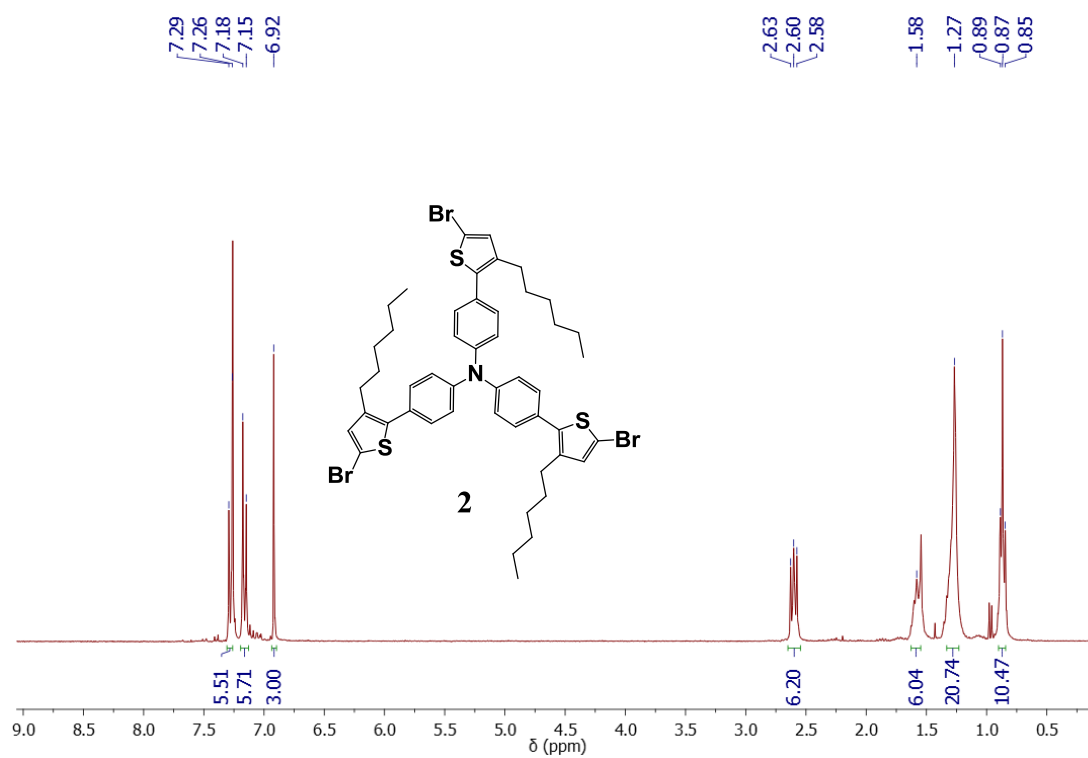


Figure S2. ^1H NMR spectrum of compound **2** in CDCl₃.

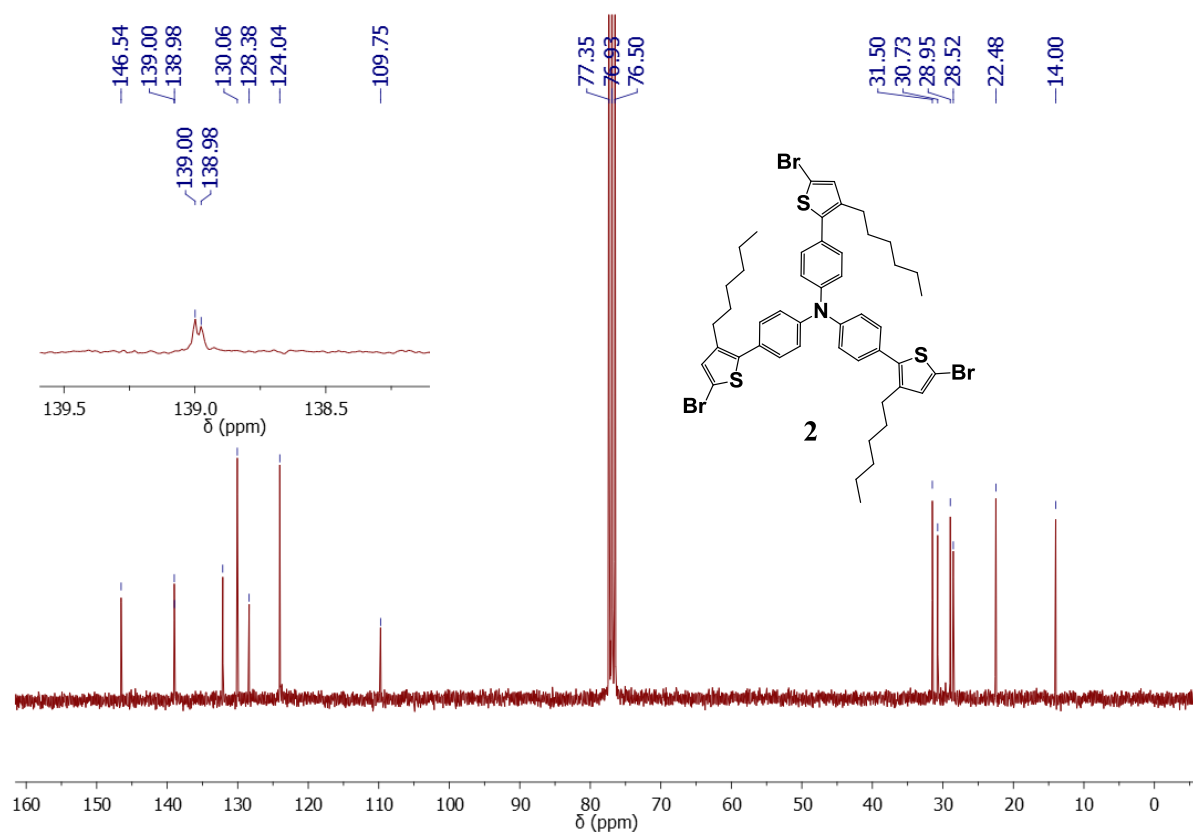


Figure S3. ¹³C NMR spectrum of compound **2** in CDCl₃.

Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	2500 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Waste

Meas. m/z	#	Formula	m/z	err [ppm]	rdB	e ⁻ Conf	N-Rule
978.1045	1	C 48 H 55 Br 3 N S 3	978.1041	-0.3	20.5	even	ok

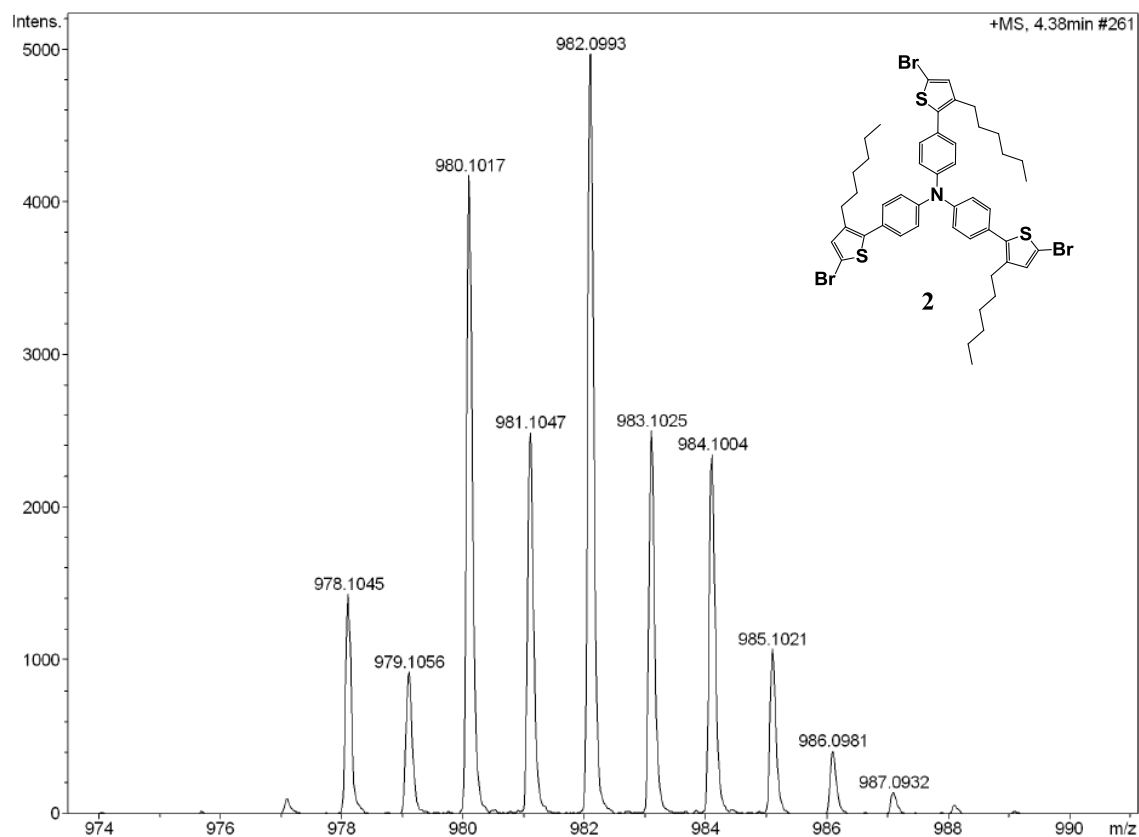


Figure S4. High resolution atmospheric-pressure chemical ionization mass spectrum of compound **2**.

2. ^1H NMR spectra of HP1-HP3

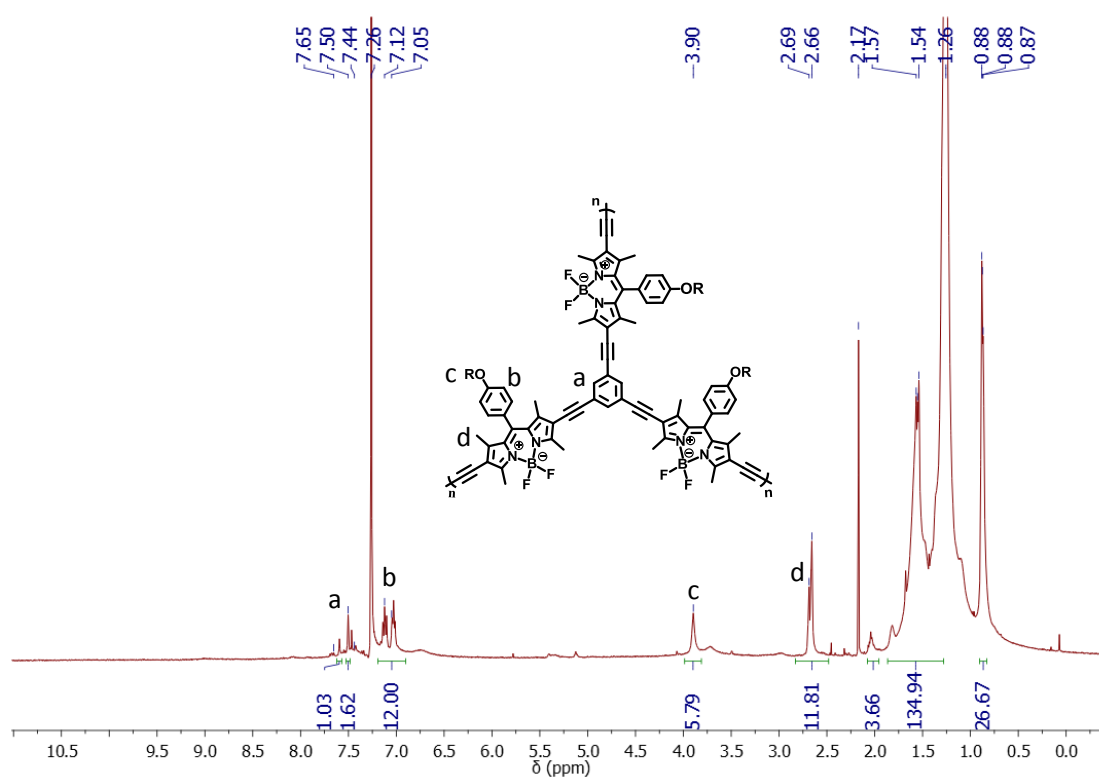


Figure S5. ^1H NMR spectrum of **HP1** in CDCl_3 .

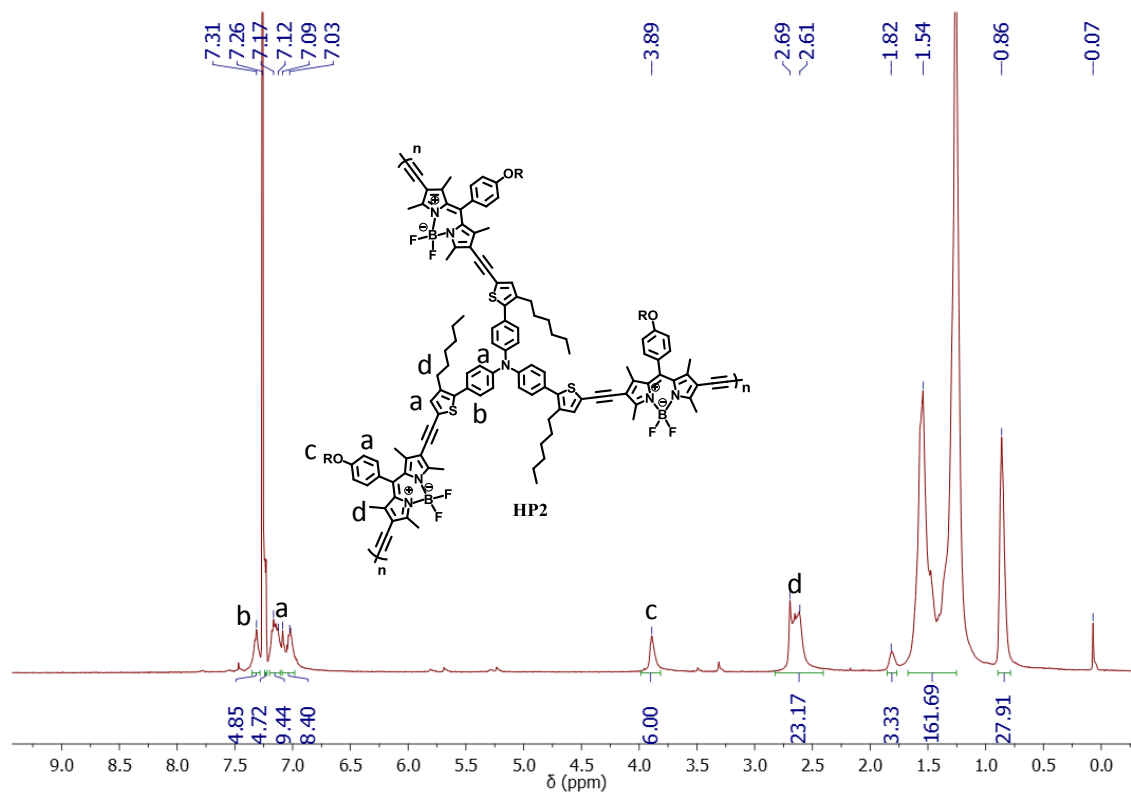


Figure S6. ¹H NMR spectrum of **HP2** in CDCl₃.

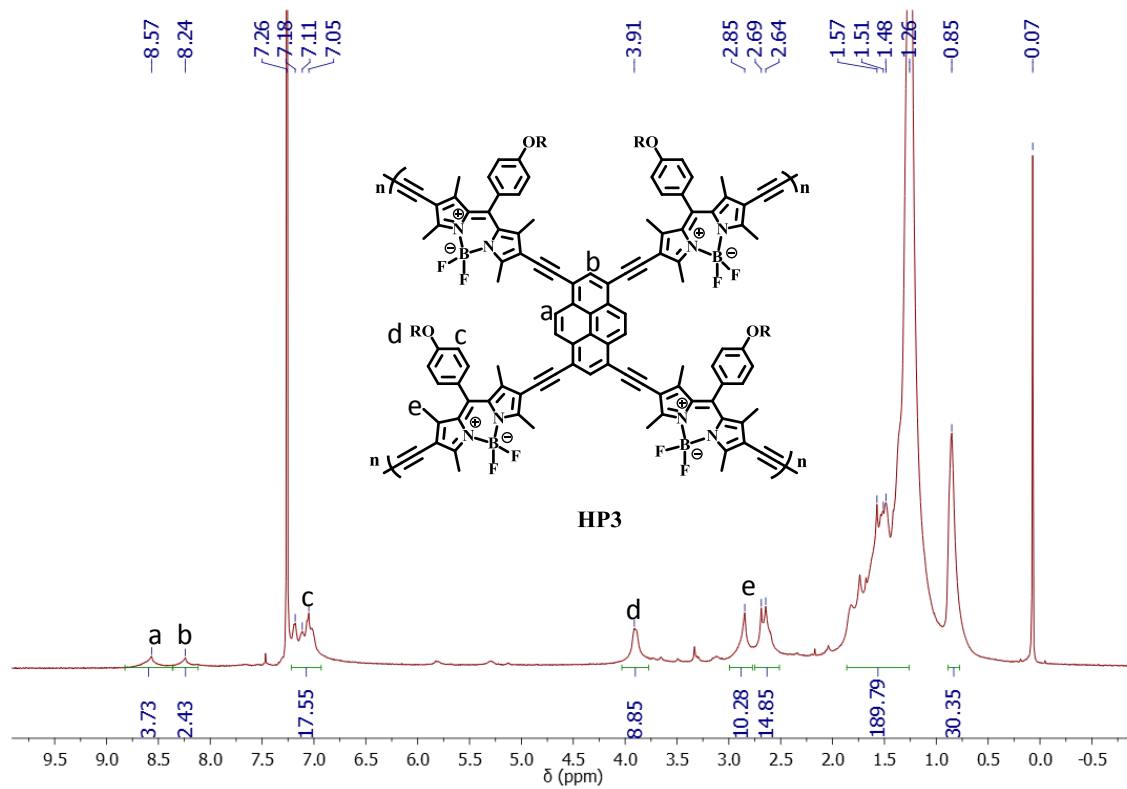
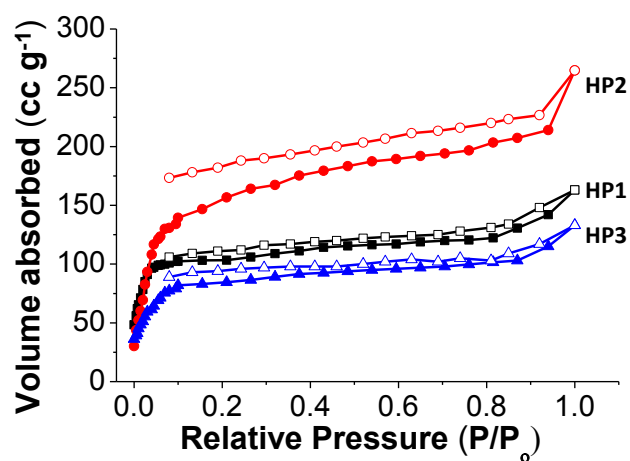


Figure S7. ¹H NMR spectrum of **HP3** in CDCl₃.

3. BET analysis of HP1-3



	Surface Area (m ² /g)	Pore Size (nm)
HP1	362.21	11.03
HP2	513.67	16.54
HP3	259.03	12.41

Figure S8. Nitrogen sorption isotherms of **HP1-3** with adsorption (solid symbols) and desorption (open symbols) traces at 77 K.

4. Absorption and emission spectra

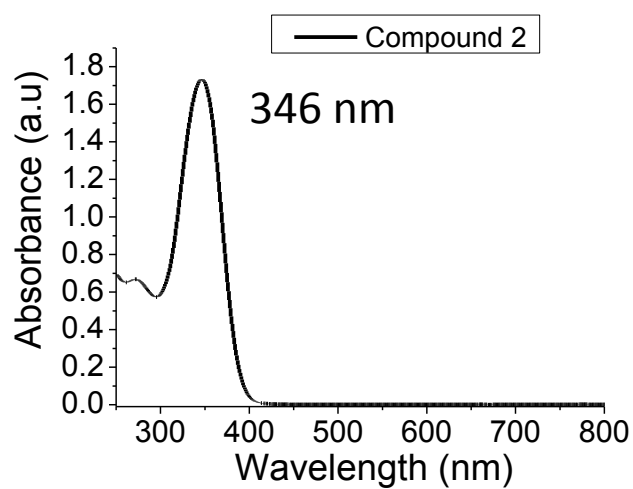


Figure S9. Absorption spectrum of compound 2 in THF.

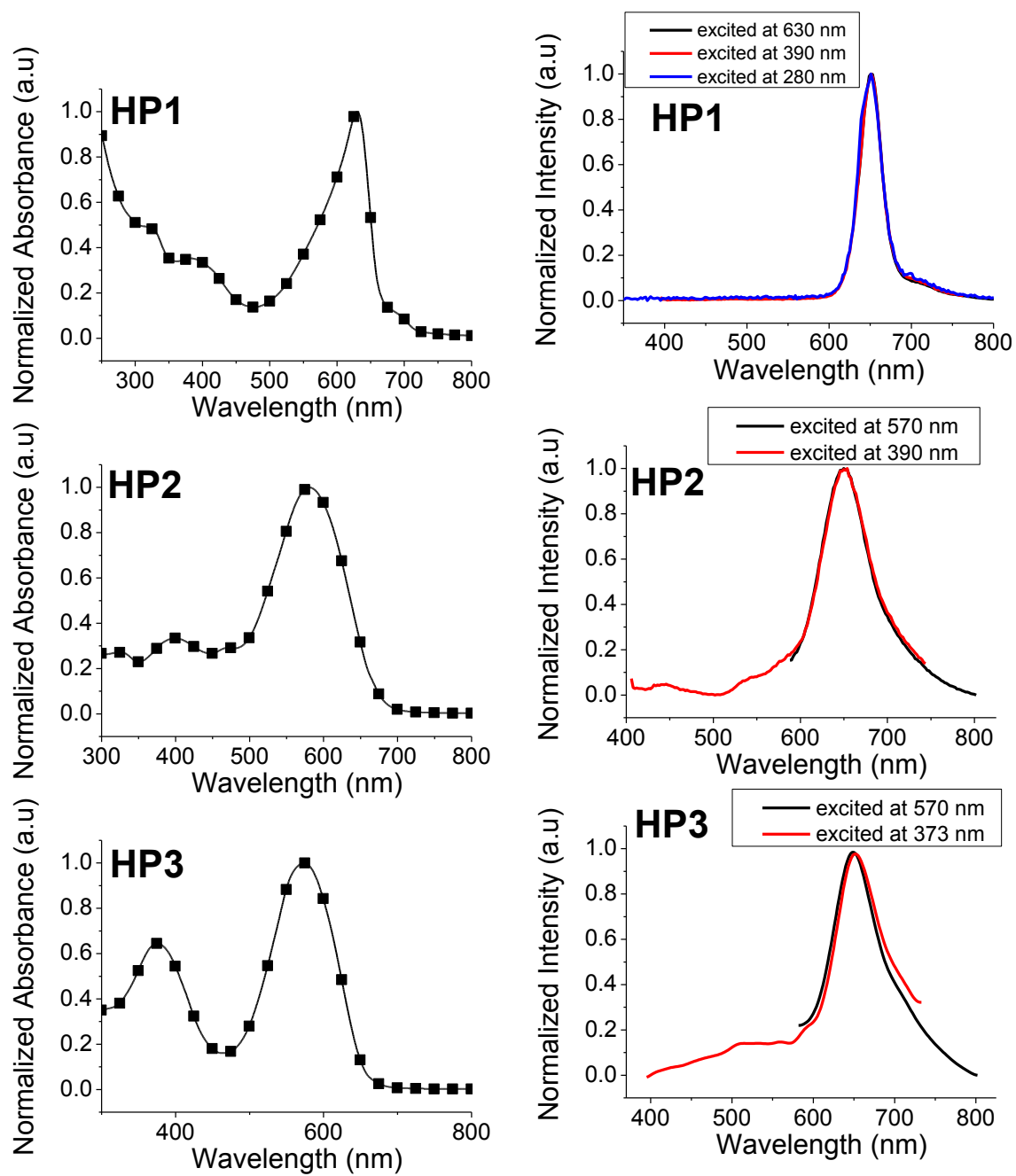


Figure S10. Absorption (left) and emission spectra (right) of **HP1-HP3** in chloroform.

5. Optimized molecular geometry of HP2 by DFT

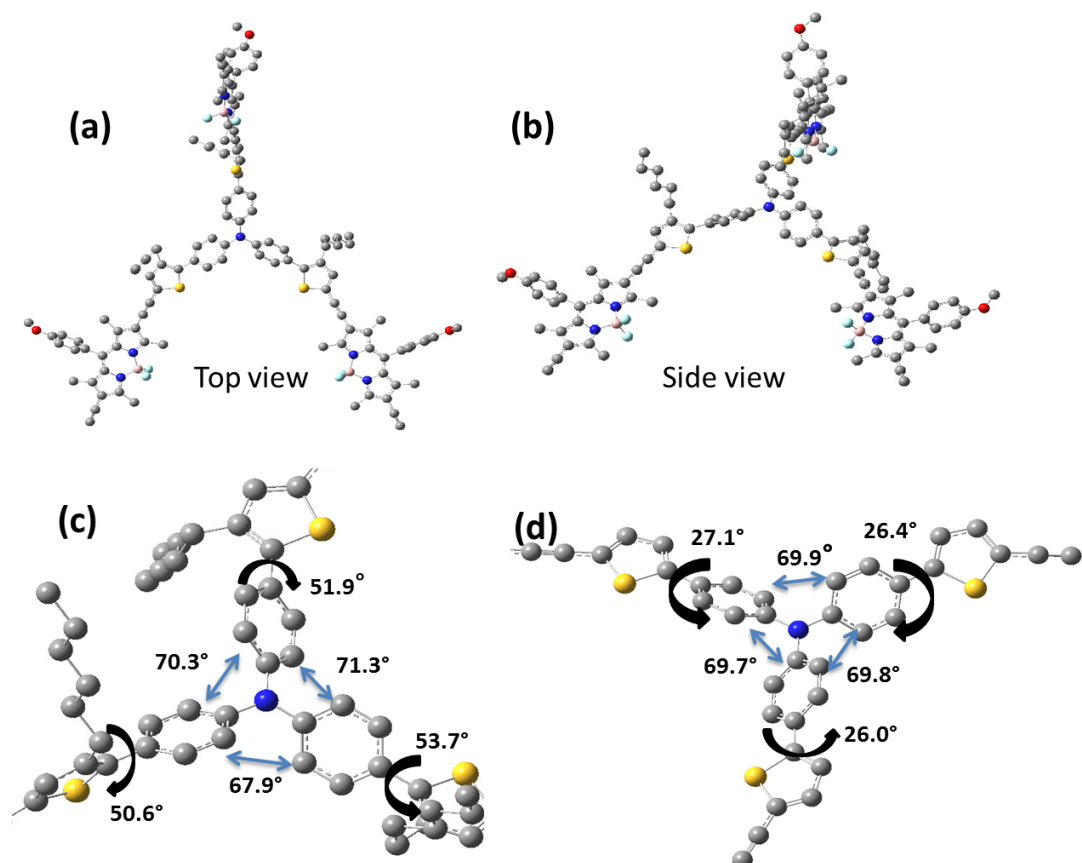


Figure S11. The optimized molecular geometry of **HP2** by using DFT at B3LYP/6-311g (d, p) level. Top view (a) and side view (b) of **HP2** model molecule, dihedral angles of the tris(4-(5-bromo-3-hexylthiophen-2-yl)phenyl)amine (c), and dihedral angles of the tris(4-(5-bromothiophen-2-yl)phenyl)amine (d).

6. SEM images of HP1-HP3

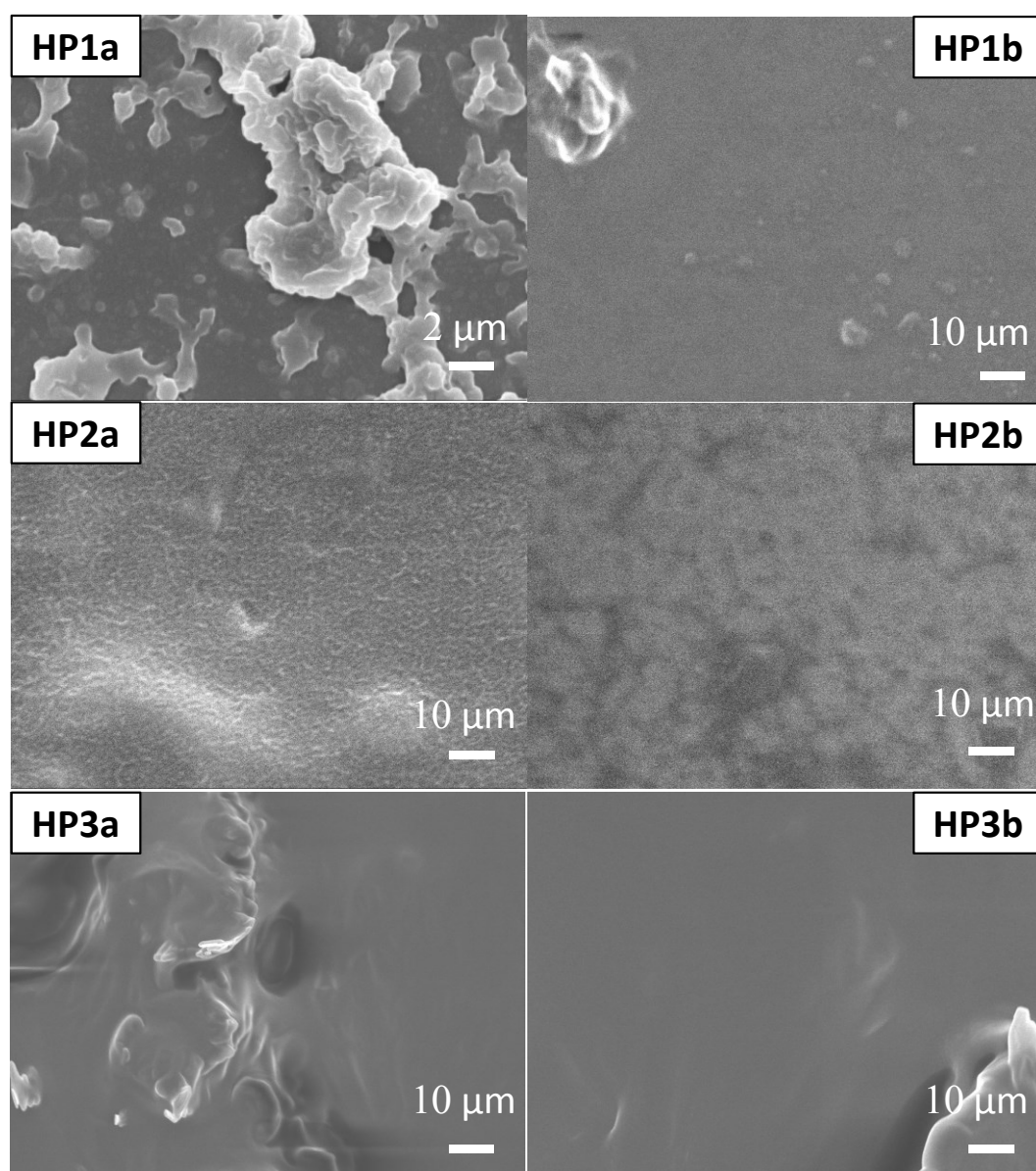


Figure S12. SEM micrographs of **HP1-3** thin film prepared by drop-casting polymer solution in (a) THF, and (b) toluene on a glass substrate. The solvent was evaporated slowly at room temperature.

7. QCM measurement of HP2 to different aromatic vapors.

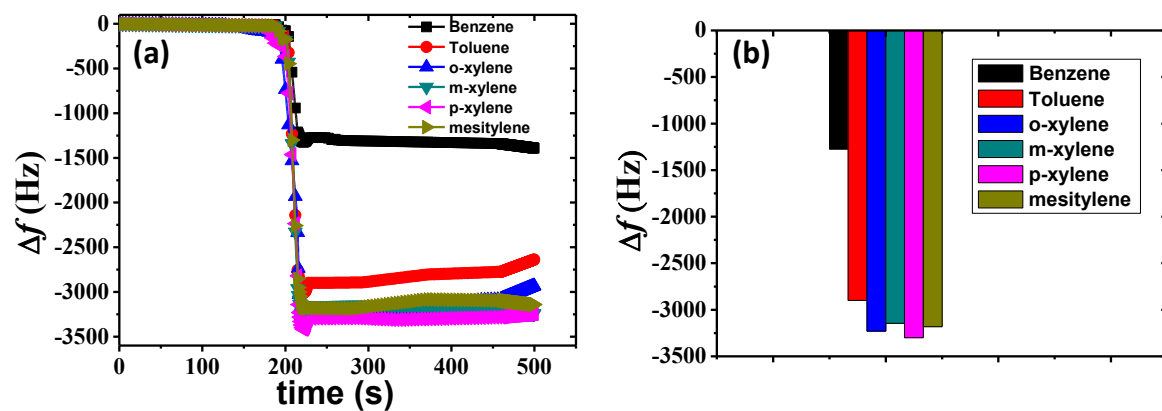


Figure S13. (a) QCM frequency shifts of **HP2** electrode upon exposure to different solvent vapors (benzene, toluene, o-xylene, m-xylene, p-xylene, and mesitylene), (b) summary of vapor sensing performance of **HP2**.