

## Supporting information

### Efficient solution-processable non-doped hybridized local and charge-transfer (HLCT) emitter for a simplified organic light-emitting diode

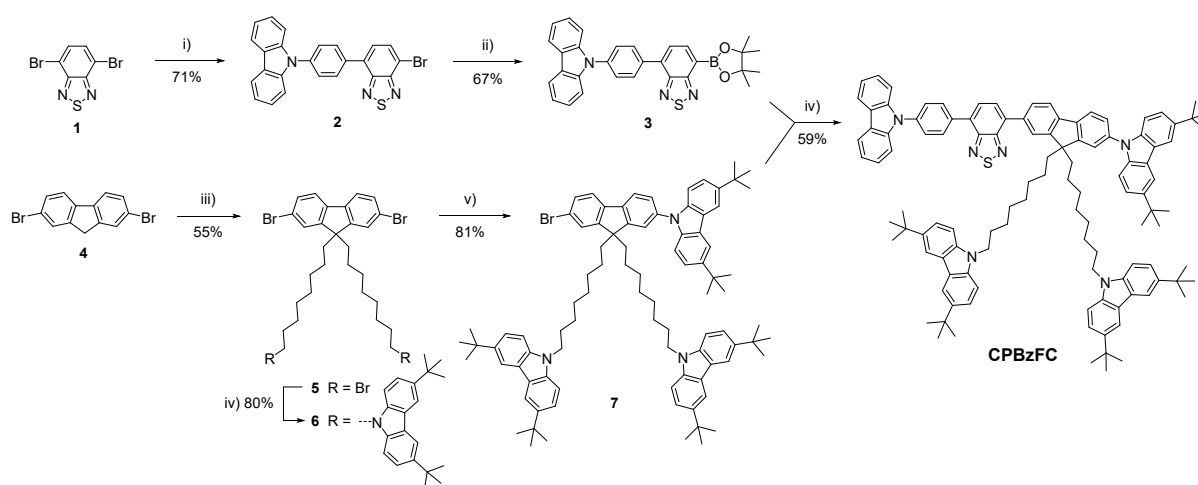
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#### Synthesis and characterization



**Scheme 1** Synthesis of **CPBzFC**. *Reagents and conditions:* i) (4-(carbazol-9-yl)phenyl)boronic acid, Pd(PPh<sub>3</sub>)<sub>4</sub>, 10% K<sub>2</sub>CO<sub>3</sub> (aq), THF, reflux; ii) bispinacolatodiboron, KOAc, Pd(dppf)<sub>2</sub>Cl<sub>2</sub>, toluene, reflux; iii) 1,8-dibromooctane, *tert*-BuNH<sub>4</sub>Br, KOH, DMF, H<sub>2</sub>O; iv) 3,6-di-*tert*-butylcarbazole, KOH, DMF; v) 3,6-di-*tert*-butylcarbazole, CuI, K<sub>3</sub>PO<sub>4</sub>, (±)-*trans*-1,2-diaminocyclohexane, toluene, reflux; vi) Pd(PPh<sub>3</sub>)<sub>4</sub>, 10% K<sub>2</sub>CO<sub>3</sub> (aq), THF, reflux.

#### 4-(4-(Carbazol-9-yl)phenyl)-7-bromobenzothiadiazole (2)

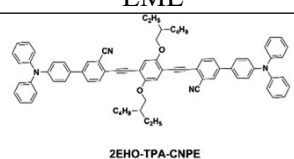
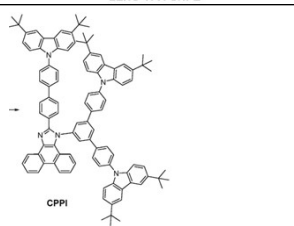
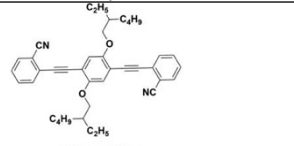
4,7-Dibromobenzothiadiazole (**3**) (2.0 g, 7.0 mmol) and (4-(carbazol-9-yl)phenyl)boronic acid (**4**) (1.0 g, 3.5 mmol) were dissolved in dried THF (75 mL) under nitrogen atmosphere. 10% K<sub>2</sub>CO<sub>3</sub> (aq) (10 ml) was added, the mixture was stirred at ambient temperature. Tetrakis(triphenylphosphene)palladium(0) Pd(PPh<sub>3</sub>)<sub>4</sub> (0.2 g, 0.17 mmol) was then added to reaction flask and degassed for 10 minutes. The reaction mixture was heated to reflux for 16 hours. After completion, allowed to room temperature, water was added to reaction mixture and extracted by dichloromethane (3 x 50 mL). The organic layer was washed with brine (3 x 20 mL), dried (Na<sub>2</sub>SO<sub>4</sub>)

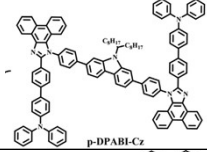
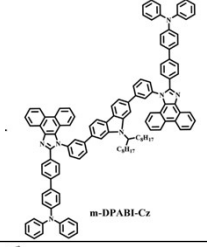
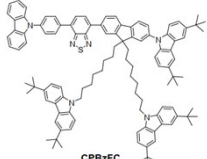
and concentrated *in vacuo*. The product was purified by column chromatography on silica gel eluting with dichloromethane:hexane (1:2) to give yellow solids (1.1 g, 71%). <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) δ 8.20 – 8.15 (4H, m, Ar-*H*), 8.00 (1H, d, *J* = 7.5 Hz, Ar-*H*), 7.76 (2H, d, *J* = 8.4 Hz, Ar-*H*), 7.71 (1H, d, *J* = 7.5 Hz, Ar-*H*), 7.55 (2H, d, *J* = 8.2 Hz, Ar-*H*), 7.44 (2H, t, *J* = 7.4 Hz, Ar-*H*), 7.31 (2H, t, *J* = 7.4 Hz, Ar-*H*); <sup>13</sup>C NMR (151 MHz, CDCl<sub>3</sub>) δ 154.0, 153.1, 140.7, 138.2, 135.5, 133.0, 132.3, 130.6, 128.4, 127.2, 126.1, 123.6, 120.4, 120.2, 113.7, 109.9. HRMS MALDI-TOF (*m/z*) calcd (M<sup>+</sup>) for C<sub>24</sub>H<sub>14</sub>BrN<sub>3</sub>S: 456.3610; found: 457.2473 (M+H<sup>+</sup>).

**9,9'-((2,7-Bibromo-9H-fluorene-9,9-diyl)bis(octane-8,1-diyl))bis(3,6-di-*tert*-butyl-9H-carbazole) (6)**  
 2,7-Dibromofluorene (**4**) (2.00 g, 6.17 mmol) and *t*-butyl ammonium bromide (0.198 g, 0.617 mmol) were weighted into round bottom flask, and then solution of KOH (3.461, 61.17 mmol) in water (3.5 mL) was added, the mixtures were stirred at room temperature for 30 min, after that 1,8-dibromooctane (3.4 mL, 18.51 mmol) was added and stirred at 70 °C for 4 h. After cooling down the reaction to the room temperature, the mixtures were poured in water, extracted with dichloromethane (DCM, 3 x 20 mL) and brine solution (50 mL), dried over Na<sub>2</sub>SO<sub>4</sub> and concentrated on a rotary evaporator. Finally, the residue was purified by column chromatography eluting with hexane to give pale-yellow solids (compound **5**). <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>): δ = 7.43 (s, 2H), 7.52 (d, 2H, *J* = 7.92 Hz), 7.46 (d, 2H, *J* = 8.04 Hz), 3.34 (t, 4H, *J* = 6.72, 6.72 Hz), 1.91 (t, 4H, *J* = 7.74, 8.10 Hz), 1.79-1.75 (m, 4H), 1.33-1.28 (m, 4H), 1.12-1.06 (m, 12H), 0.58 (brs, 4H). HRMS APCI (*m/z*) calcd (M<sup>+</sup>) for C<sub>29</sub>H<sub>38</sub>Br<sub>4</sub>: 705.9666; found 706.9927.

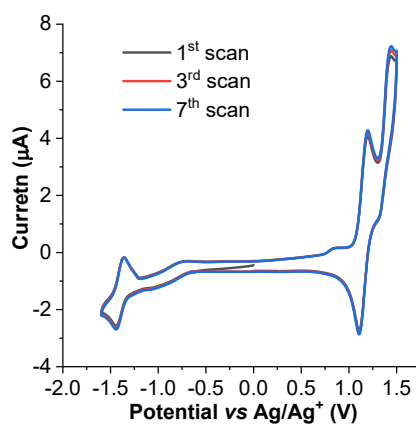
3,6-Di-*tert*-butylcarbazole (8.90 g, 31.897 mmol) and KOH (5.72 g, 0.10 mol) were dissolved in DMF (80 mL) and then compound **5** (8.00 g, 12.759 mmol) was added and stirred at room temperature for 4.5 h. The mixtures were poured in water, extracted with dichloromethane (DCM, 3 x 10 mL) and brine solution (20 mL), dried over Na<sub>2</sub>SO<sub>4</sub> and evaporated by a rotary evaporator. Finally, the residue was purified by column chromatography eluting with DCM/hexane (1:5) (v/v) to give white solids (9.92 g, 80%). <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>): δ = 8.08 (s, 4H), 7.48-7.45 (m, 6H), 7.41 (d, 4H, *J* = 7.5 Hz), 7.24 (s, 4H), 4.16 (t, 4H, *J* = 6.96, 6.90 Hz), 1.89-1.86 (m, 4H), 1.76-1.74 (m, 4H), 1.45 (s, 36H), 1.29-1.25 (m, 5H), 1.12 (m, 4H), 1.01 (s, 8H), 0.55 (brs, 4H). HRMS APCI (*m/z*) calcd (M<sup>+</sup>) for C<sub>69</sub>H<sub>86</sub>Br<sub>2</sub>N<sub>2</sub>: 1102.5564; found 1103.5642.

**Table S1.** Electroluminescent data of the previously reported solution-processed non-doped HLCT OLEDs.

EML	V <sub>on</sub> (V)	L <sub>max</sub> (cd m <sup>-2</sup> )	EQE <sub>max</sub> (%)	CE <sub>max</sub> (cd A <sup>-1</sup> )	Ref
 2EHO-TPA-CNPE	3.5	~2000	4.5%	12.0	1
 CPPH	3.2	4050	3.3	2.61	2
 2EHO-CNPE	4.0	~500	2.36	2.23	3

	5.1	5521	2.88	3.71	4
	5.7	4403	2.28	2.74	4
	<b>3.2</b>	<b>30300</b>	<b>6.74</b>	<b>14.38</b>	<b>This work</b>

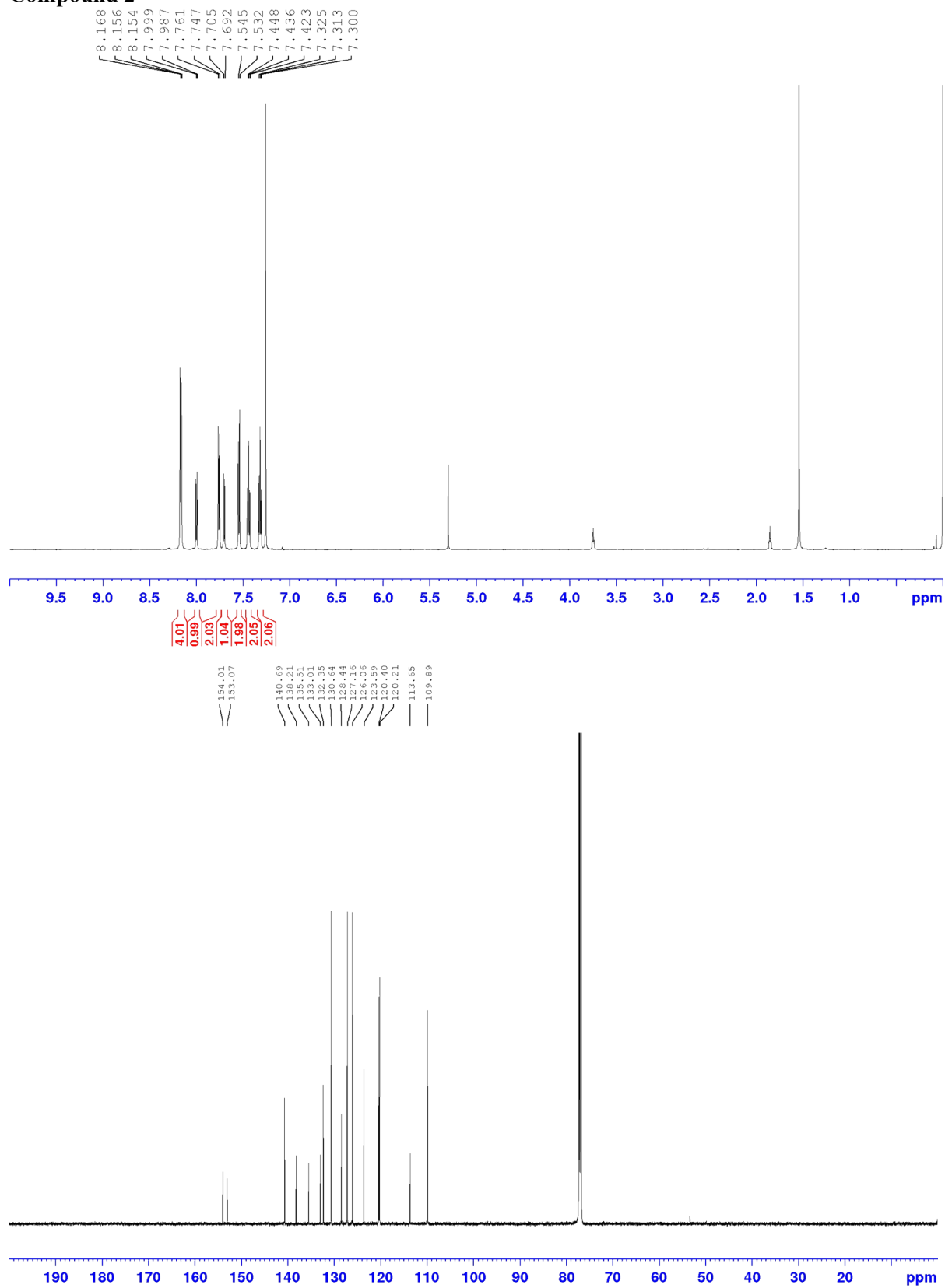
1. H. Usta, D. Alimli, R. Ozdemir, E. Tekin, F. Alkan, R. Kacar, A. G. Altas, S. Dabak, A. G. Gürek, E. Mutlugun, A. F. Yazici and A. Can, *J. Mater. Chem. C*, 2020, 8, 8047–8060.
2. T. Sudyoardsuk, S. Petdee, P. Chasing, P. Therdkatanyuphong, C. Kaiyasuan, W. Waengdongbung, S. Namuangruk and V. Promarak, *Dye. Pigment.*, 2021, 195, 109712.
3. H. Usta, D. Alimli, R. Ozdemir, S. Dabak, Y. Zorlu, F. Alkan, E. Tekin and A. Can, *ACS Appl. Mater. Interfaces*, 2019, 11, 44474–44486.
4. Y. Bai, L. Hong, T. Lei, L. Zhang, X. Ouyang, Z. Liu, Y. Chen, W. Li and Z. Ge, *Dye. Pigment.*, 2016, 132, 94–102



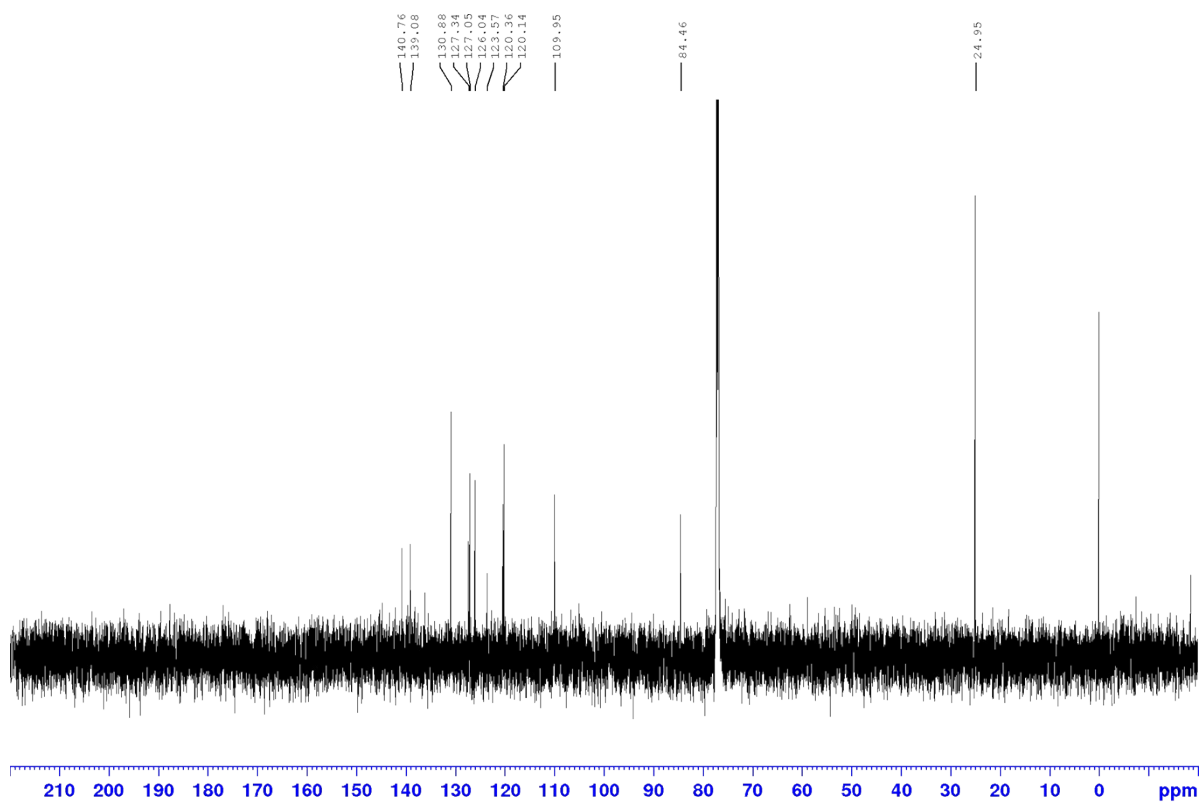
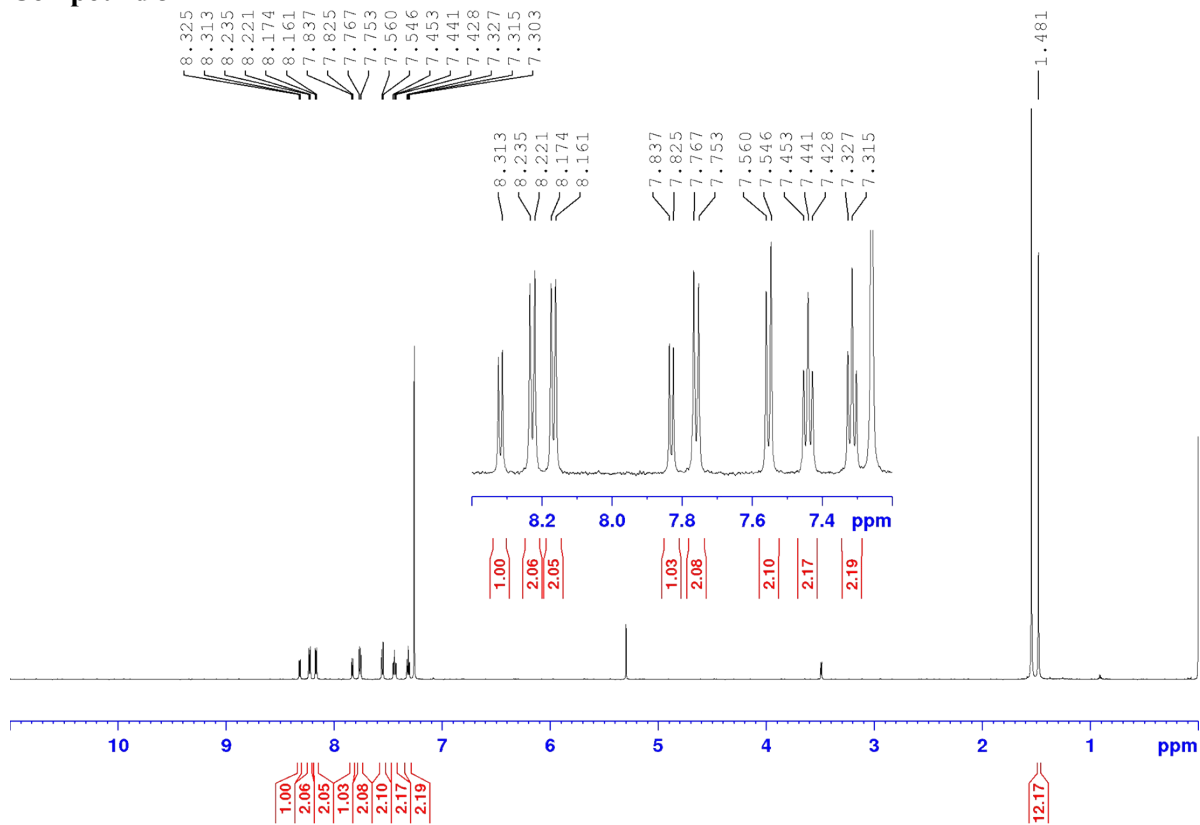
**Fig. S1** Repeated CV scan.

**Fig. S2** Copies of  $^1\text{H}$ -NMR (600 MHz,  $\text{CDCl}_3$ ) and  $^{13}\text{C}$ -NMR (151 MHz,  $\text{CDCl}_3$ ) and HRMS mass spectra

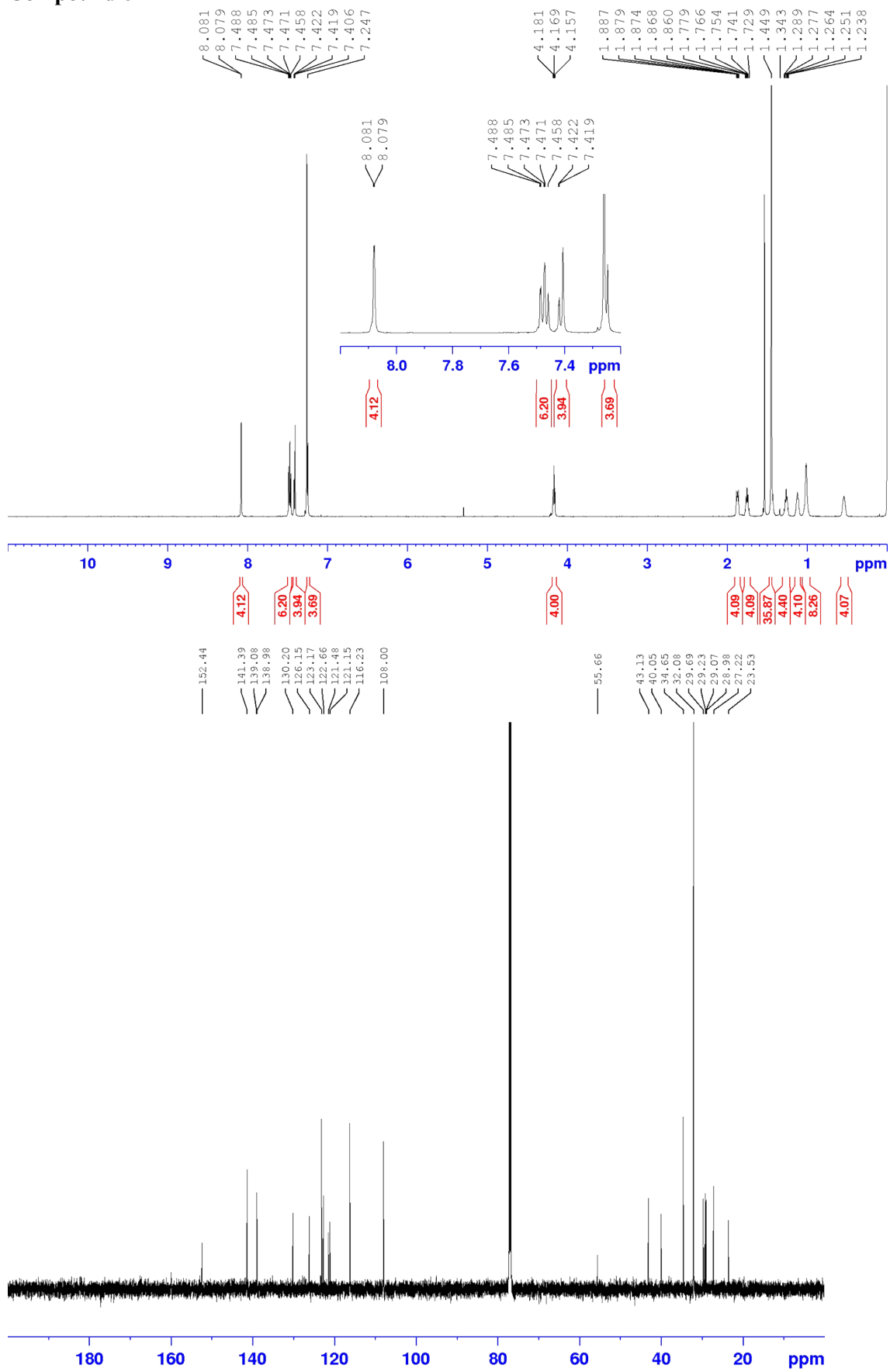
**Compound 2**



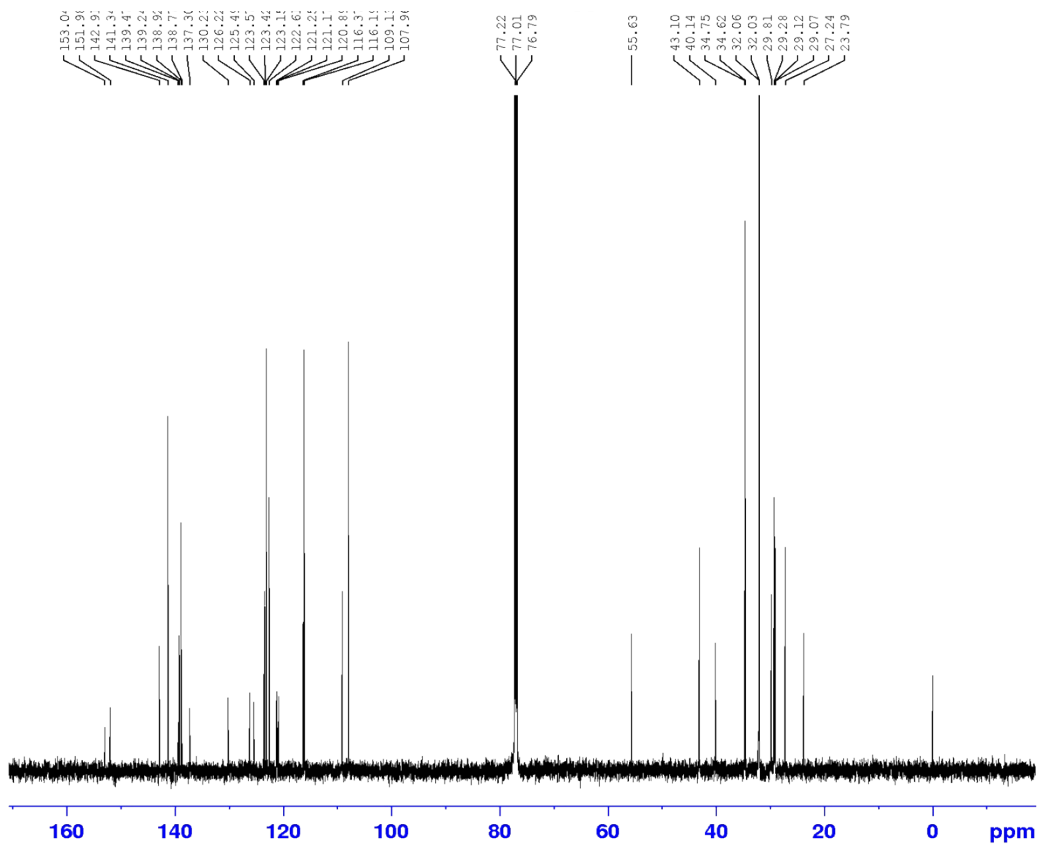
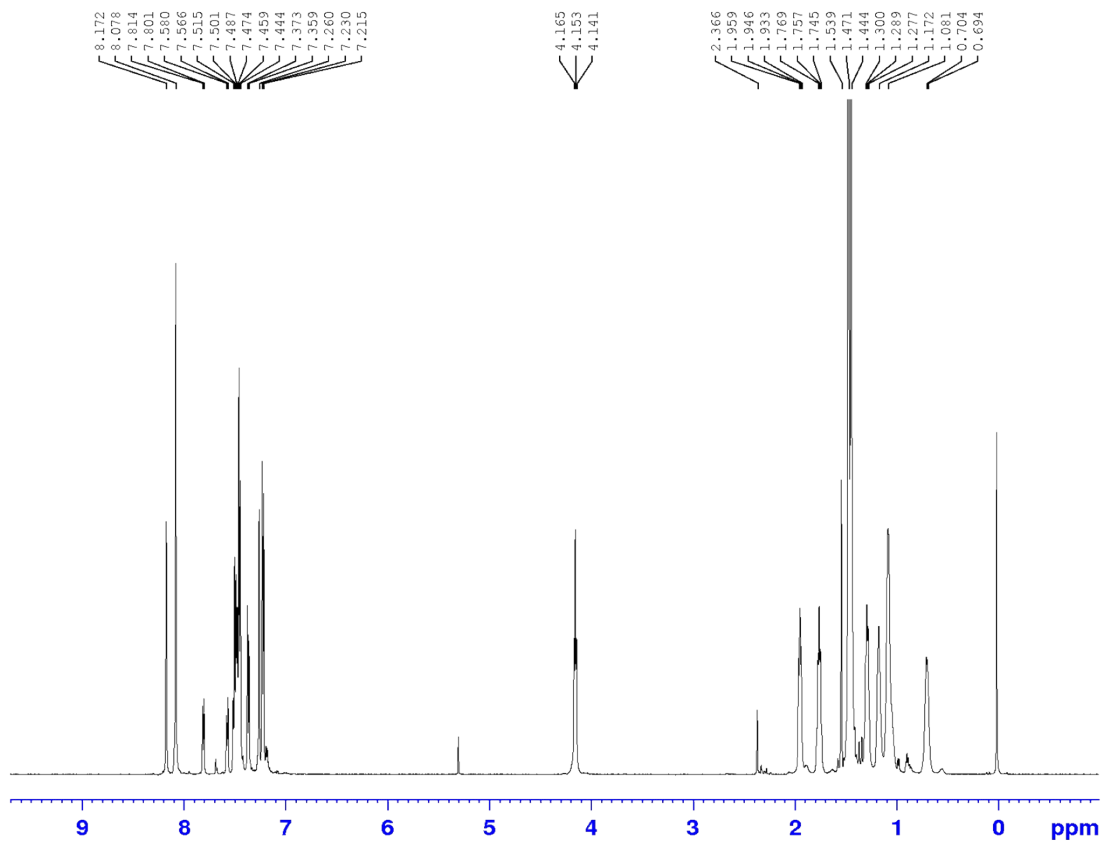
# Compound 3



# Compound 6



# Compound 7



# Compound CPBzFC

