Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting Information

Solution-processable hole-transporting material containing fluorenyl core and triple-carbazolyl terminals: Synthesis and application to enhancement of electroluminescence

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The ^{1}H NMR of **FC** is shown in Figure S1. The chemical shifts at 0.70~2.30 ppm was attributed to the characteristic protons on the alkyl chain of **FC**. The chemical shifts at 4.42~4.51 ppm were assigned to the proton (a) beside the nitrogen atom of carbazole moieties. In addition, the chemical shifts at 7.20~8.60 ppm was attributed to the protons of aromatic and vinylene moieties. The ratio of peak area among the chemical shifts at 0.70~2.30 ppm, 4.42~4.51 ppm and 7.20~8.60 ppm was about 63 : 6 : 33 which is acceptable compared to theoretical ratio (59 : 6 : 32). However, assignments of all protons were not successful by only ^{1}H NMR spectrum, two dimensional COSY, and NOESY spectra further were employed to clearly assign other protons.

As shown in Figure S2(a), there was an off-diagonal peak between 4.42~4.51 ppm (a) and 1.87~1.95 ppm assigned clearly the peak at 1.87~1.95 ppm to be b proton. The peak at 1.28~1.44 ppm can be assigned as proton c, as judging from the off-diagonal peak between b proton and 1.28~1.44 ppm. The chemical shift at 1.28~1.44 ppm was further assigned as proton d by the off-diagonal peak between proton c and 1.28~1.44 ppm. The peak at 0.84~0.88 ppm can be assigned as proton f due to the interaction between proton d and 0.84~0.88 ppm. The chemical shift at 1.28~1.44 ppm can also assigned as proton e because of the off-diagonal peak between proton f and 1.28~1.44 ppm.

The chemical shift at 2.20~2.24 ppm can be assigned as proton g due to the closest to the C-9 position of fluorene moiety (Figure S1). As shown in Figure S2(b), the peak at 0.74~0.77 pm was assigned as proton h from the interaction between proton g and 0.74~0.77 pm. Moreover, the proton at end of alkyl chain also assigned clearly the chemical shift at 0.74~0.77 pm to be proton l. The chemical shift at 1.09~1.15 ppm can further be assigned as proton i by the off-diagonal peak between proton h and 1.09~1.15 ppm. There was also an off-diagonal peak between proton l and 1.09~1.15 ppm assigned the chemical shift at 1.09~1.15 ppm to be k proton. The peak at 1.09~1.15 ppm further can be assigned as proton j, as judging from the interaction between proton k and 1.09~1.15 ppm.

As shown in Figure S2(c) (NOESY spectrum of **FC**), the existence of an off-diagonal peak between the proton g and 7.81 ppm as well as that between the proton g and 7.72 ppm assigned the peaks at 7.81 ppm and 7.72 ppm as protons m and n, respectively. The chemical shift at 7.90 ppm was assigned as proton o by the off-diagonal peak between proton m and 7.90 ppm [Figure S2(d)]. As shown in Figure S2(e), There was an off-diagonal peak between proton m and 7.63, 7.67 ppm assigned clearly the chemical shift at 7.63, 7.67 ppm to be proton B. The chemical shift at 7.52, 7.57 ppm assigned as proton C because of the interaction between proton o and 7.52, 7.57 ppm. The existence of an off-diagonal peak between proton n and 7.54, 7.59 ppm assigned the peak at 7.54, 7.59 ppm to be proton A.

There were three off-diagonal peaks between the proton A and the peaks at 7.37, 7.41 ppm, the proton B and the peaks at 7.43, 7.47 ppm, and the proton C and the peaks at 8.05~8.09 ppm, respectively [Figure S2(f); COSY spectrum of **FC**]. Thus the peaks at 7.37, 7.41 ppm, 7.43, 7.47 ppm and 8.05~8.09 ppm also can be assigned as proton A, B and C, respectively. As shown in Figure S2(e) (NOESY spectrum of **FC**), the existence of three off-diagonal peaks between proton A and the peak at 8.41 ppm, proton B and the peak at 8.45

ppm, and proton C and the peaks at 8.59, 7.94~7.96 ppm, respectively, assigned the chemical shifts at 8.41 ppm, 8.45 ppm, and 8.59, 7.94~7.96 ppm as protons t, s, p and q.

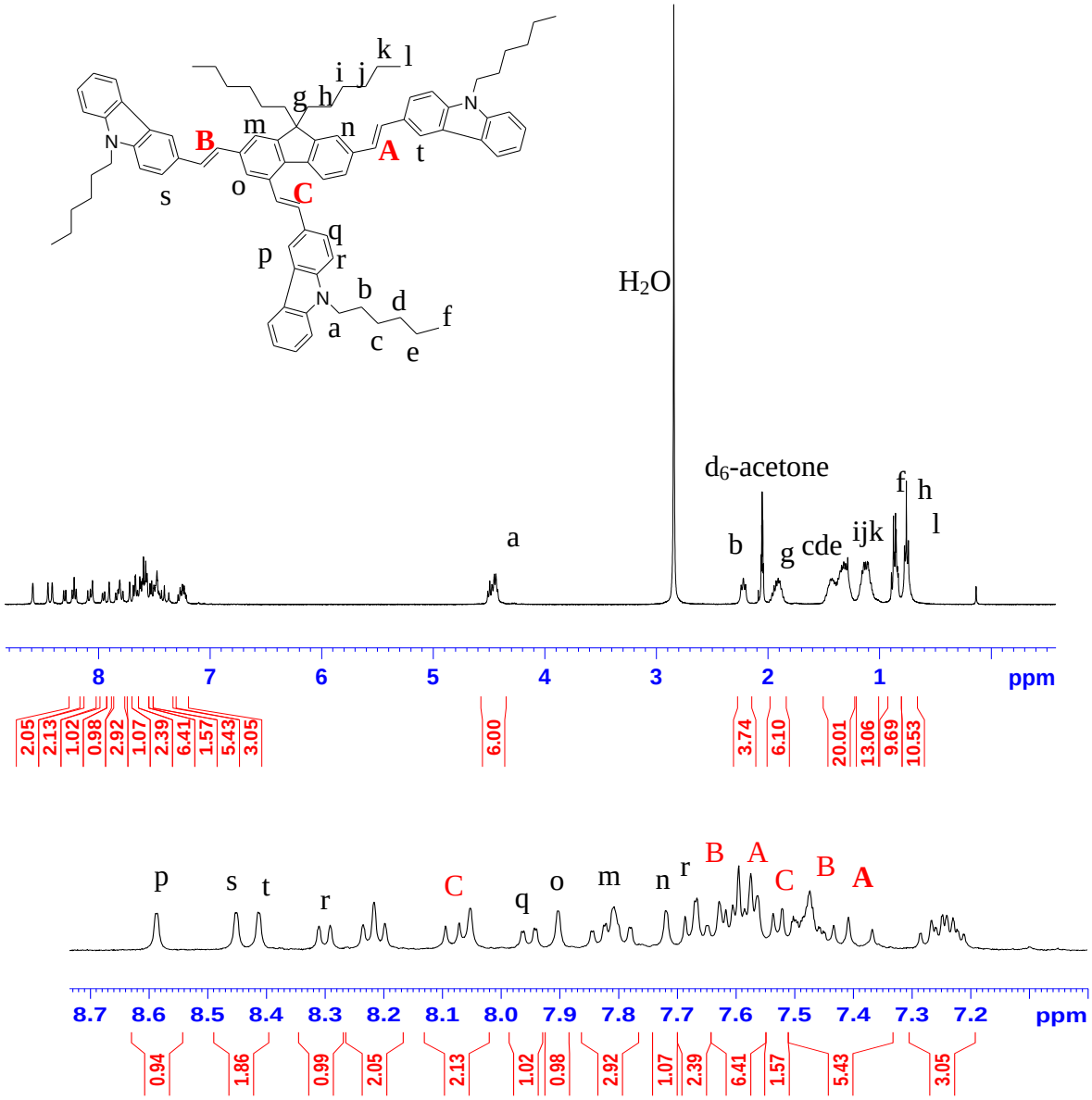
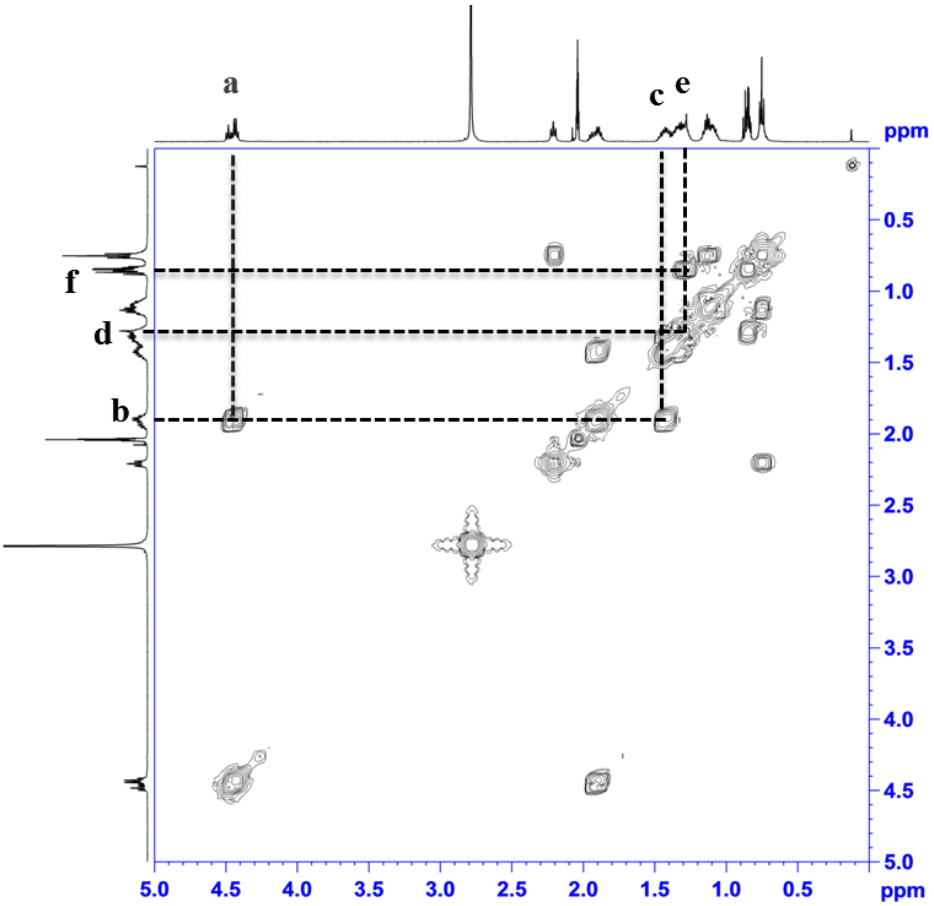
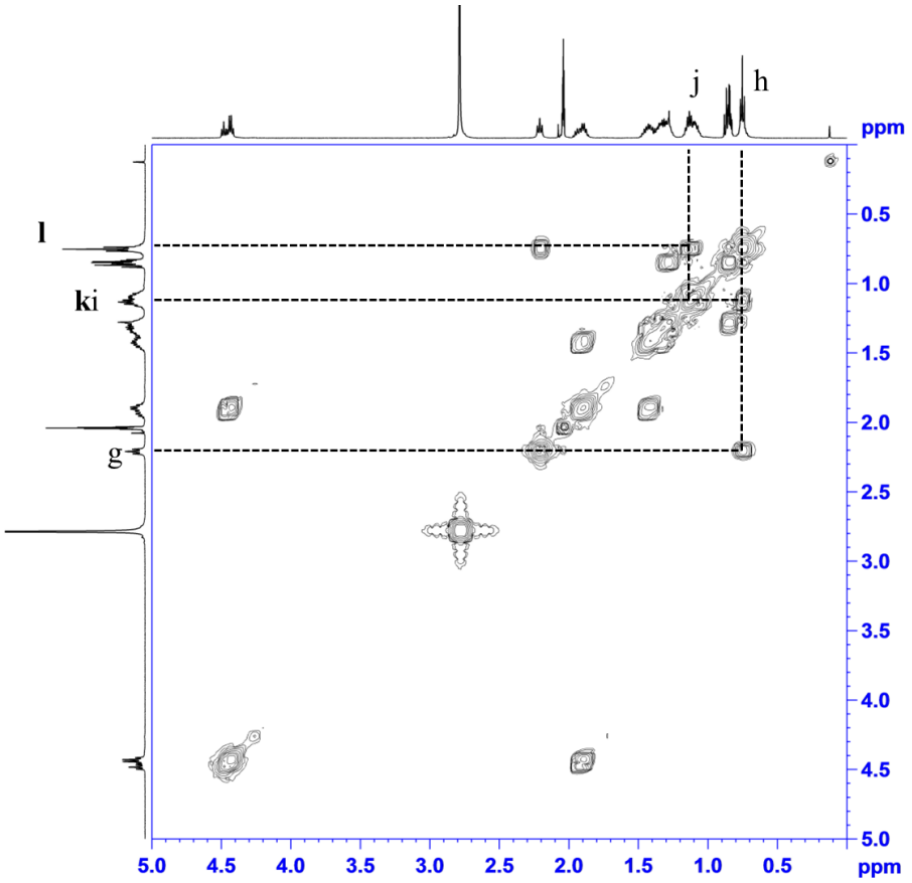


Figure S1 ^{1}H NMR spectrum of compound **FC** in d_6-acetone.

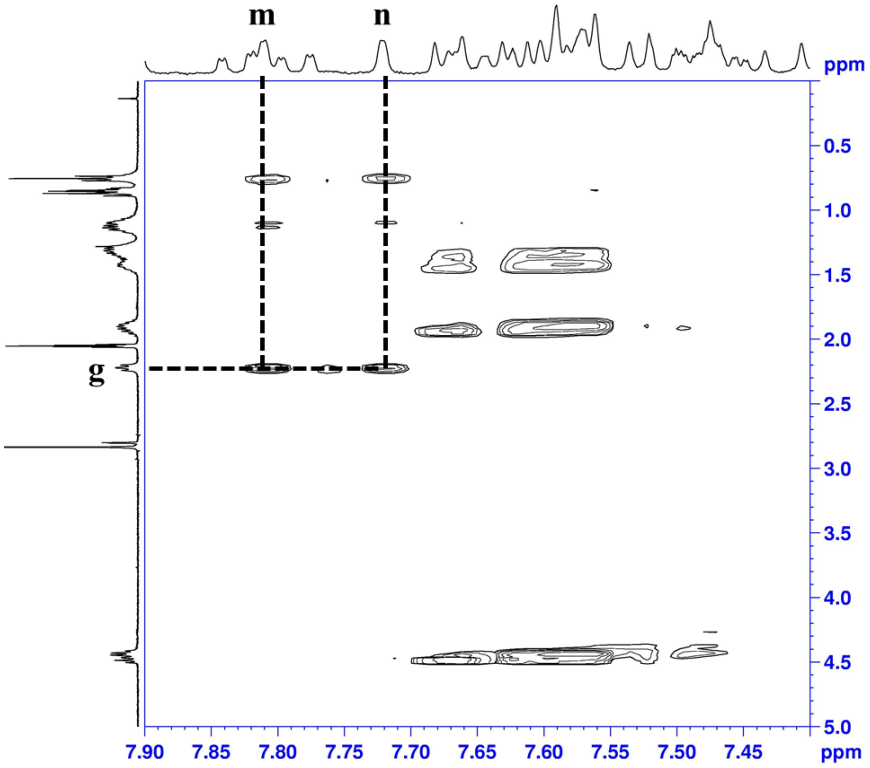
(a)



(b)



(c)


m
n
g
ppm
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1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
5.0
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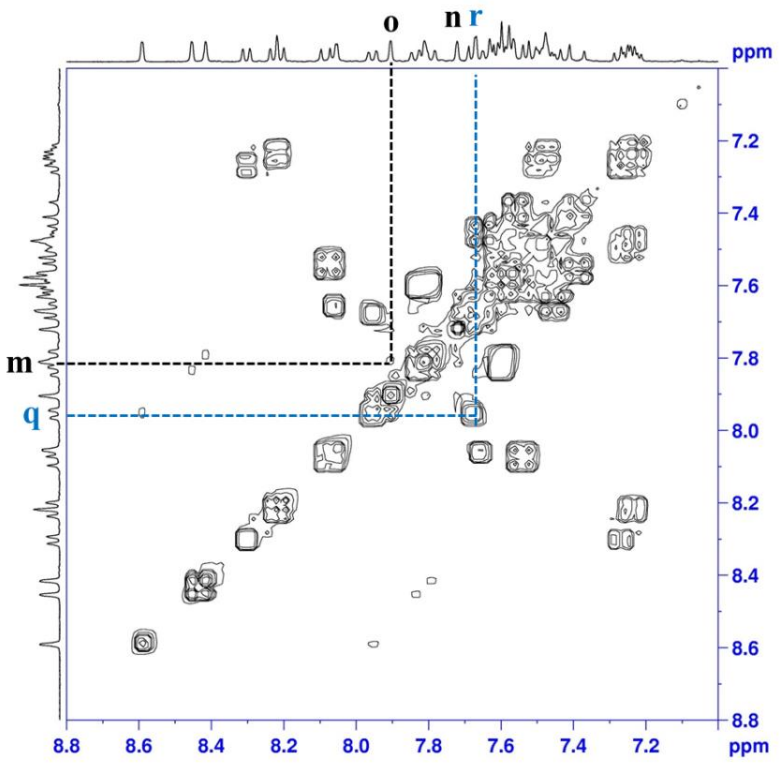
7.85
7.80
7.75
7.70
7.65
7.60
7.55
7.50
7.45
ppm

(d)


o
n
r
ppm
m
q
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7.4
7.6
7.8
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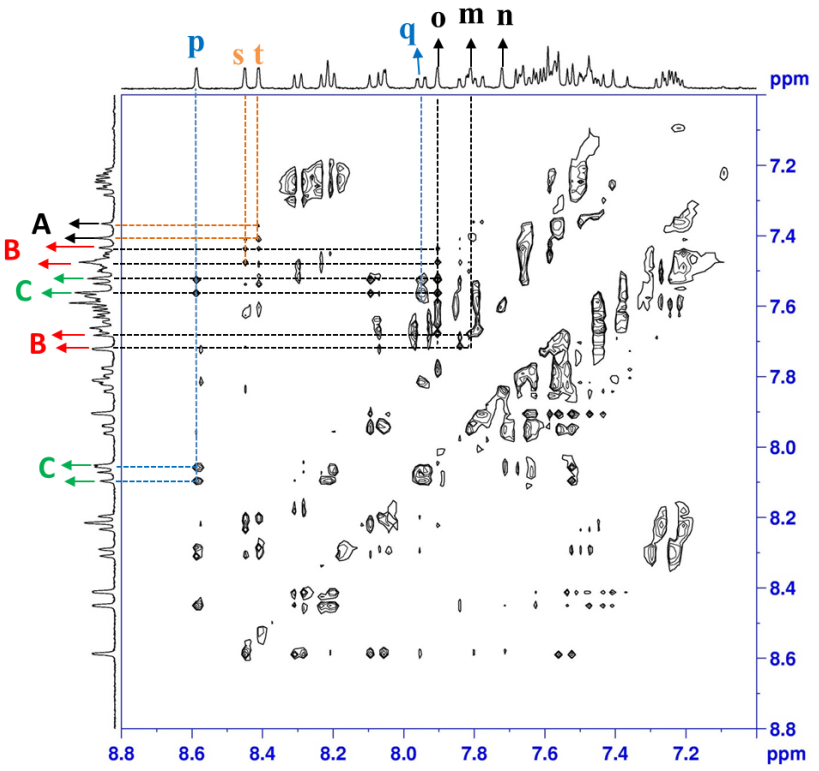
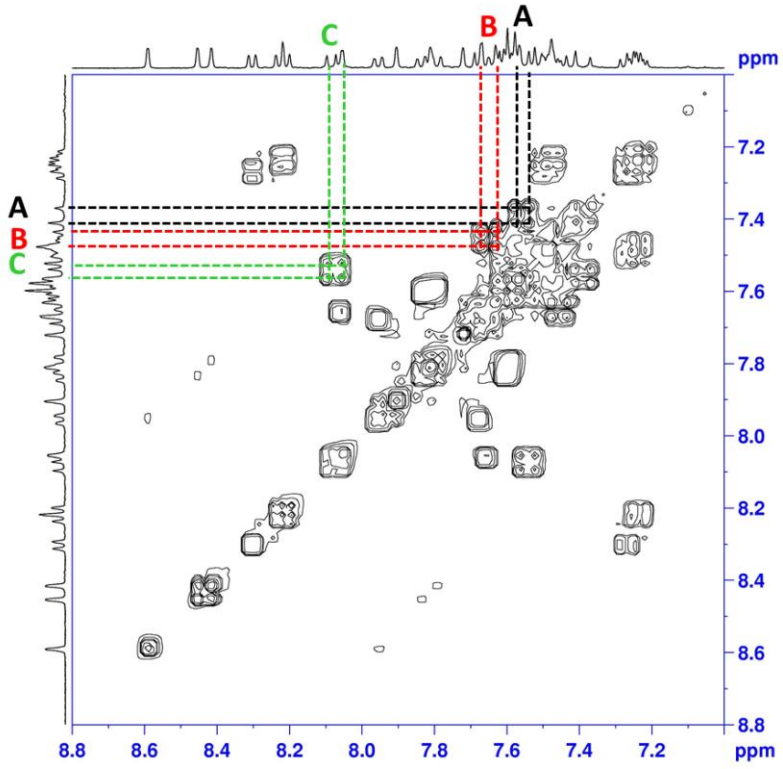
8.2
8.4
8.6
8.8
8.8
8.6
8.4
8.2
8.0
7.8
7.6
7.4
7.2
ppm

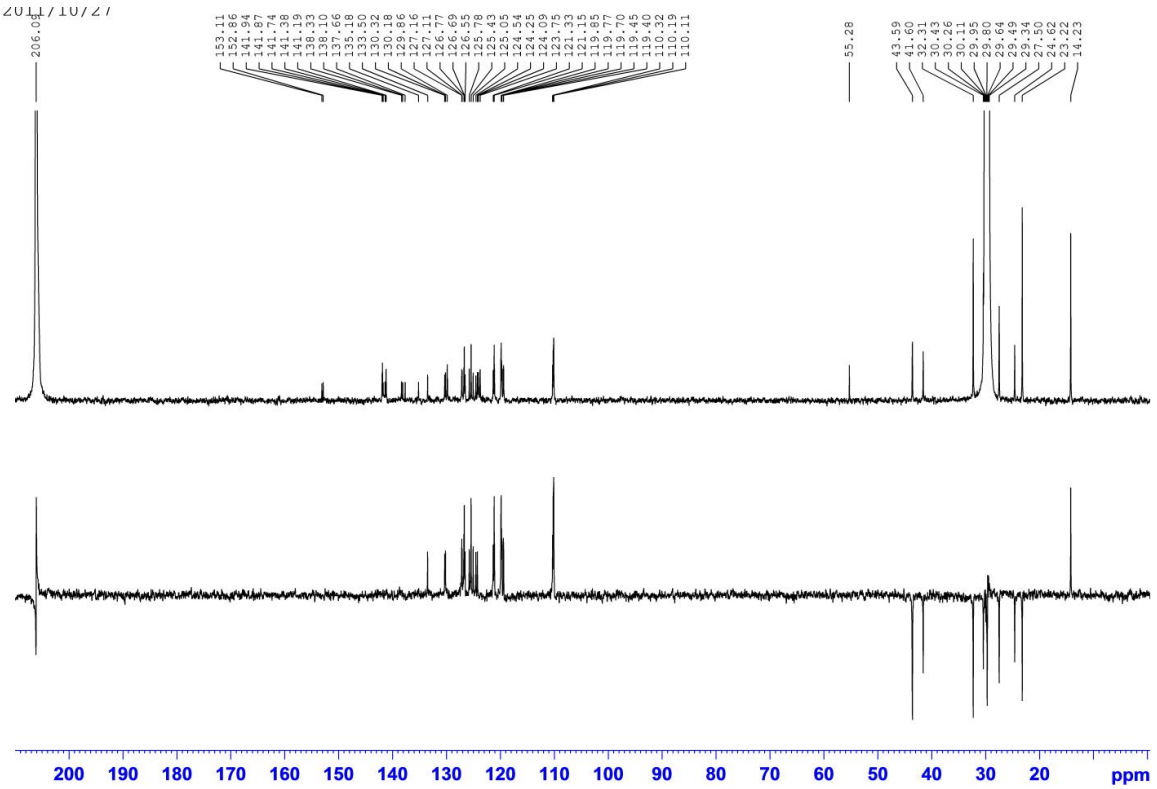
(e)



(f)



(g)



(h)

Figure S2 (a) (b) (d) (f) H-H COSY, (c) (e) H-H NOESY, (g) ^{13}C NMR and (h) DEPT135 spectra of **FC** in d_6-acetone.

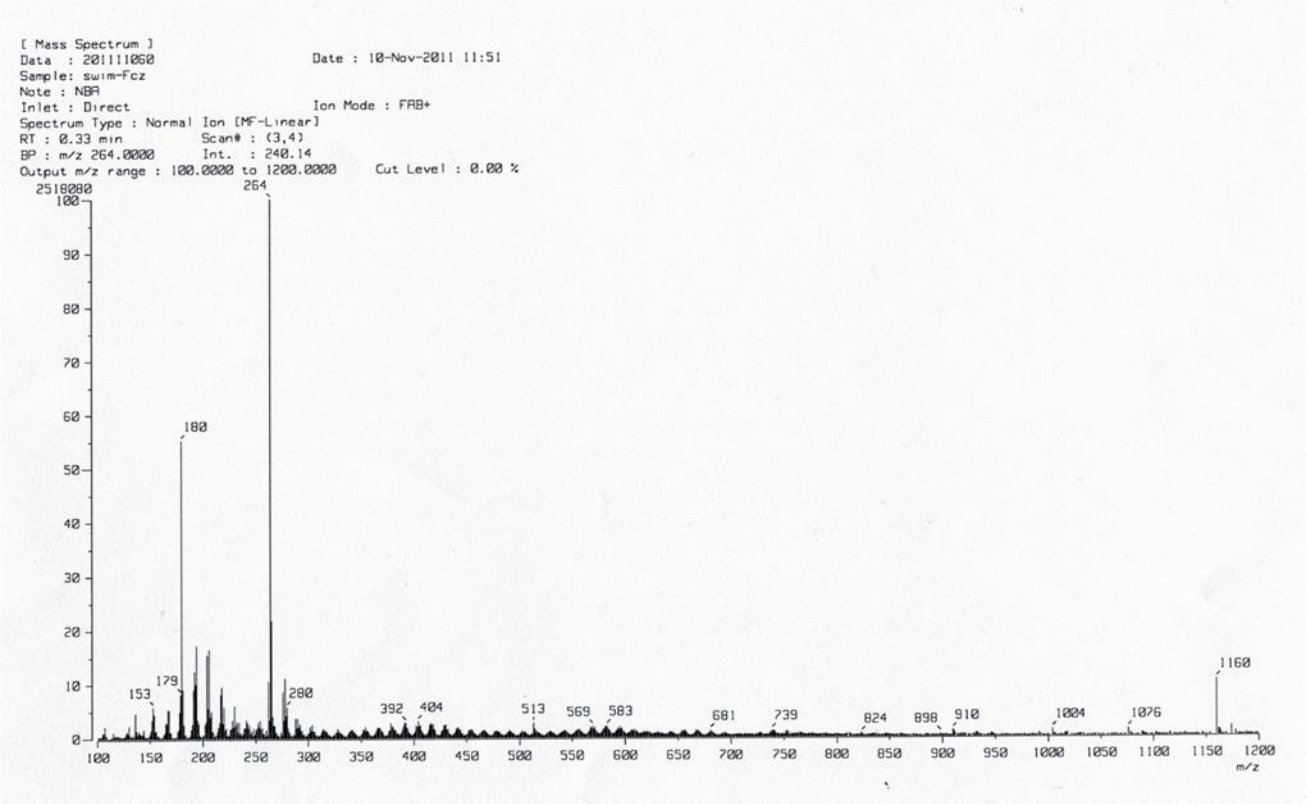


Figure S3 Mass spectrum of **FC**.

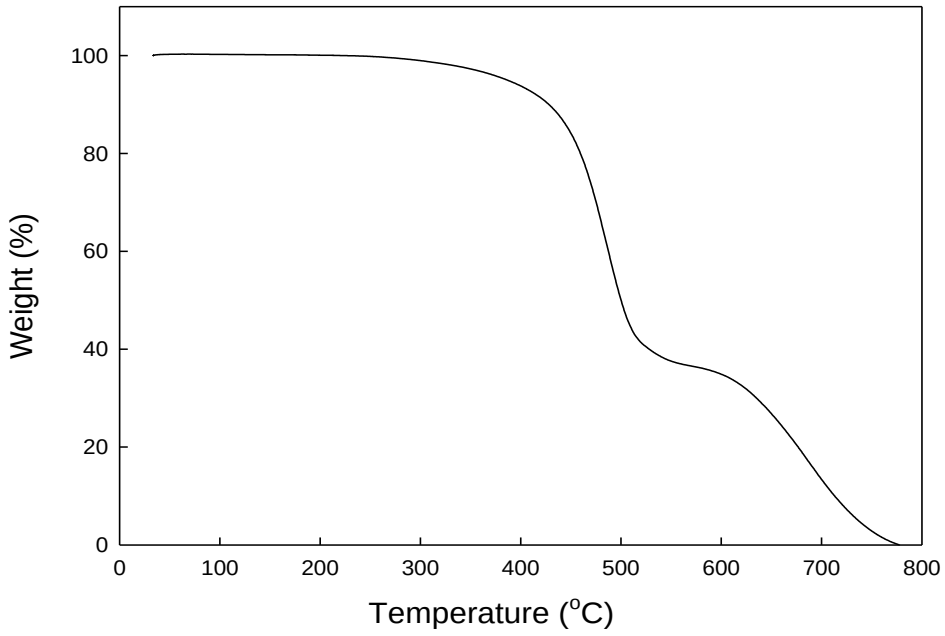


Figure S4 Thermogravimetric curves of **FC** with heating rate of 10 °C/min under nitrogen.