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Novel liquid crystalline organogelators based on terephthalic acid and terephthalaldehyde derivatives: Properties and promotion through the formation of halogen bonding

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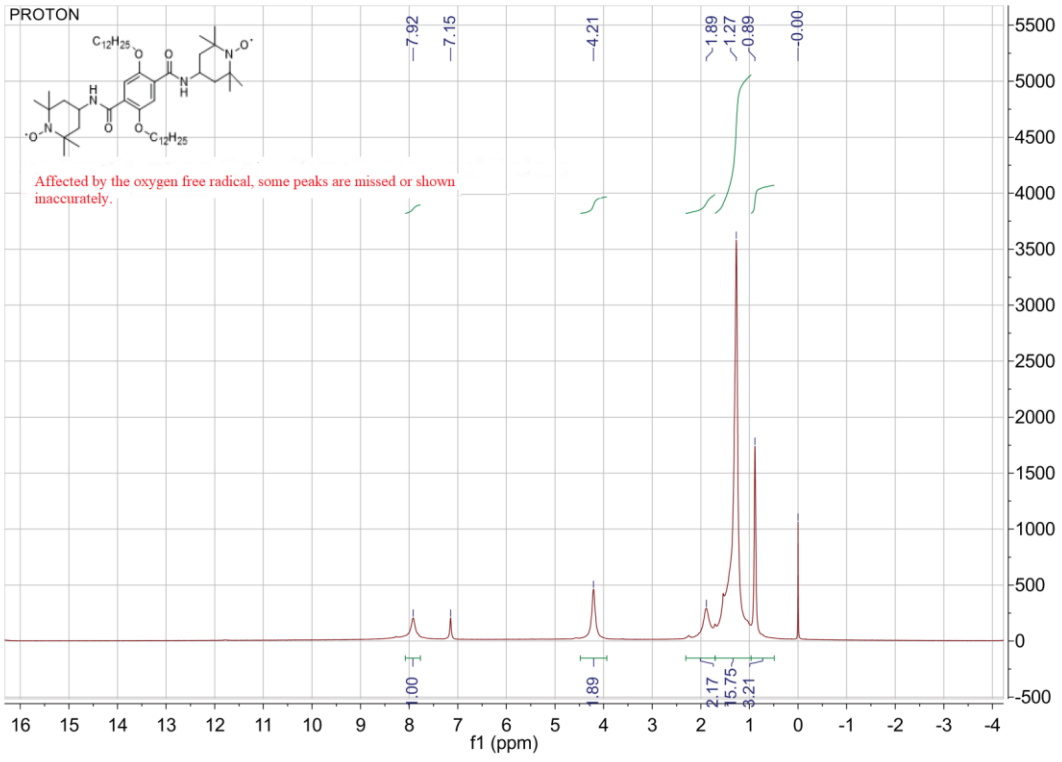

Fig. S1 ^{1}H NMR of **A1**

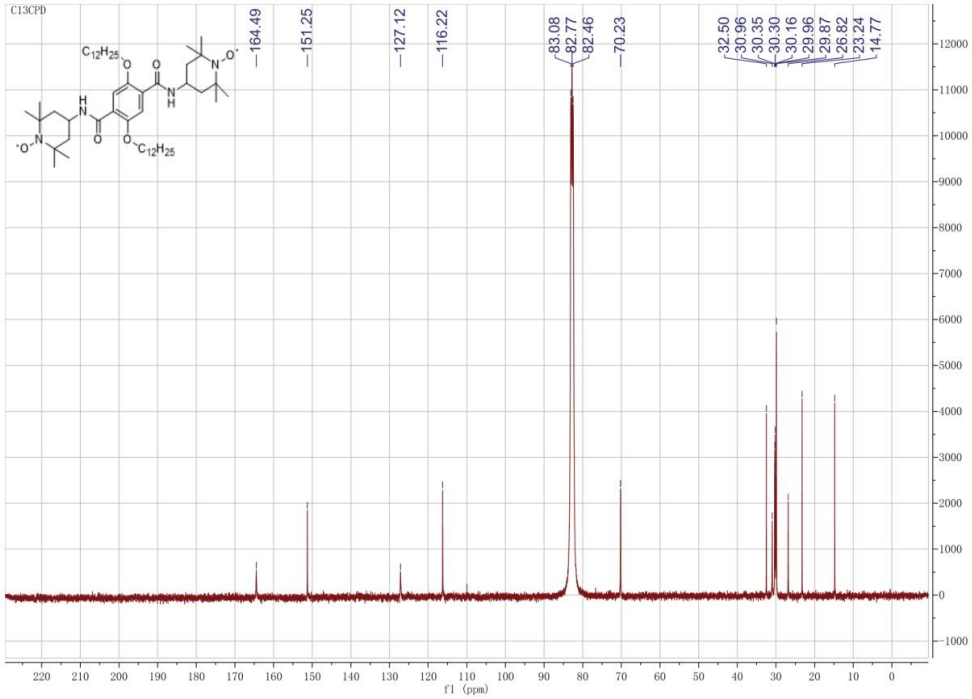

Fig. S2 ^{13}C NMR of **A1**

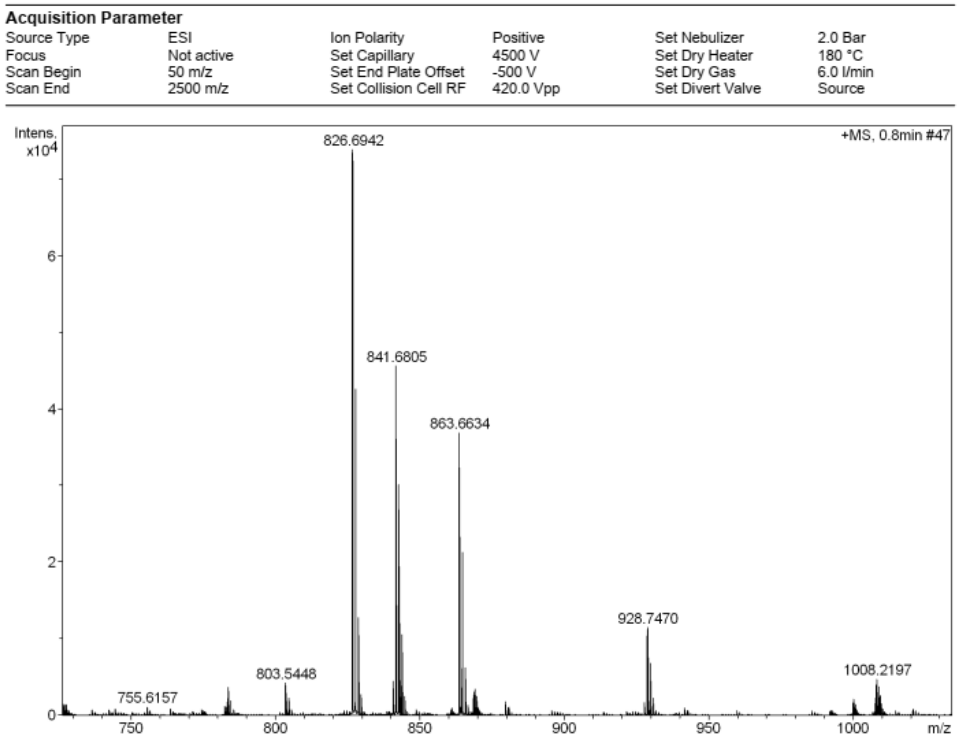

Fig. S3 HRMS of **A1**

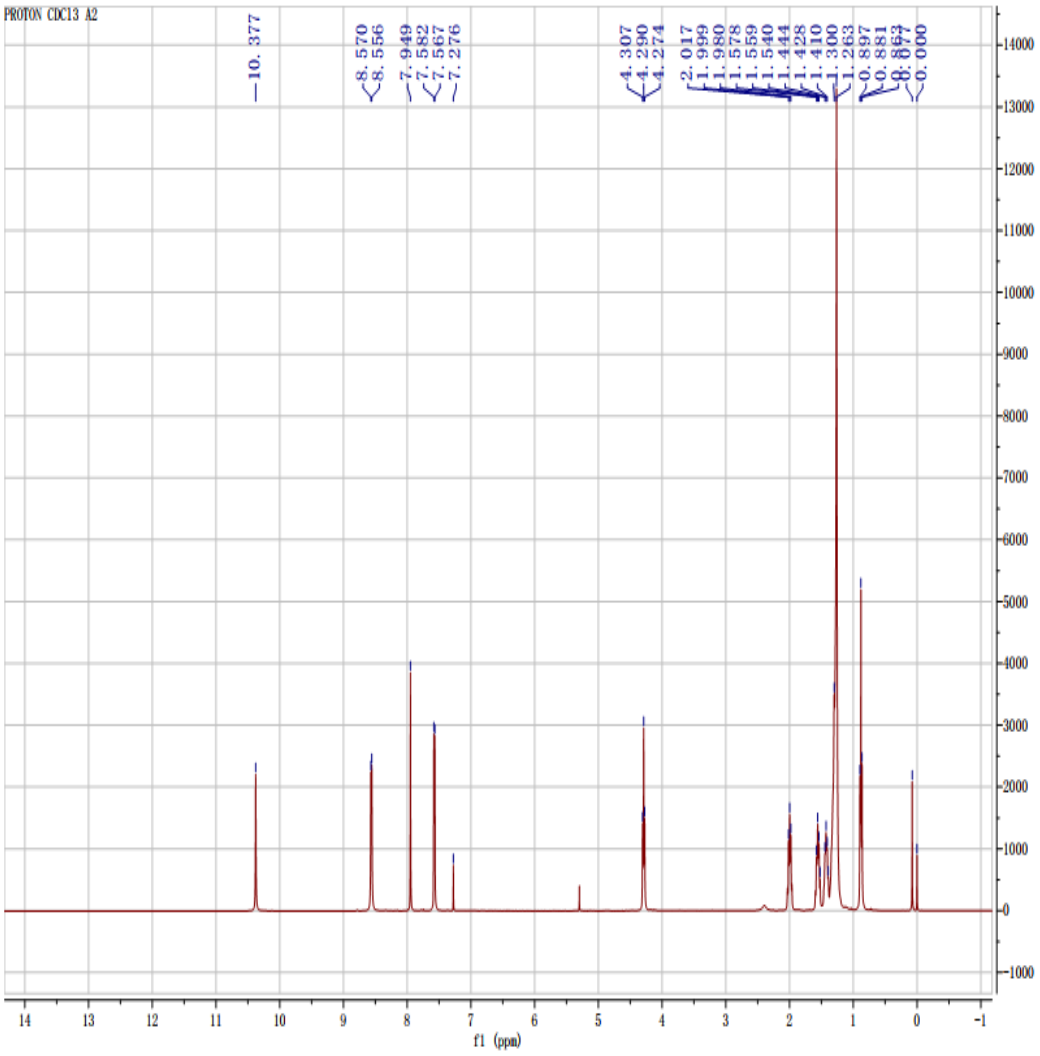

Fig. S4 ^{1}H NMR of **A2**

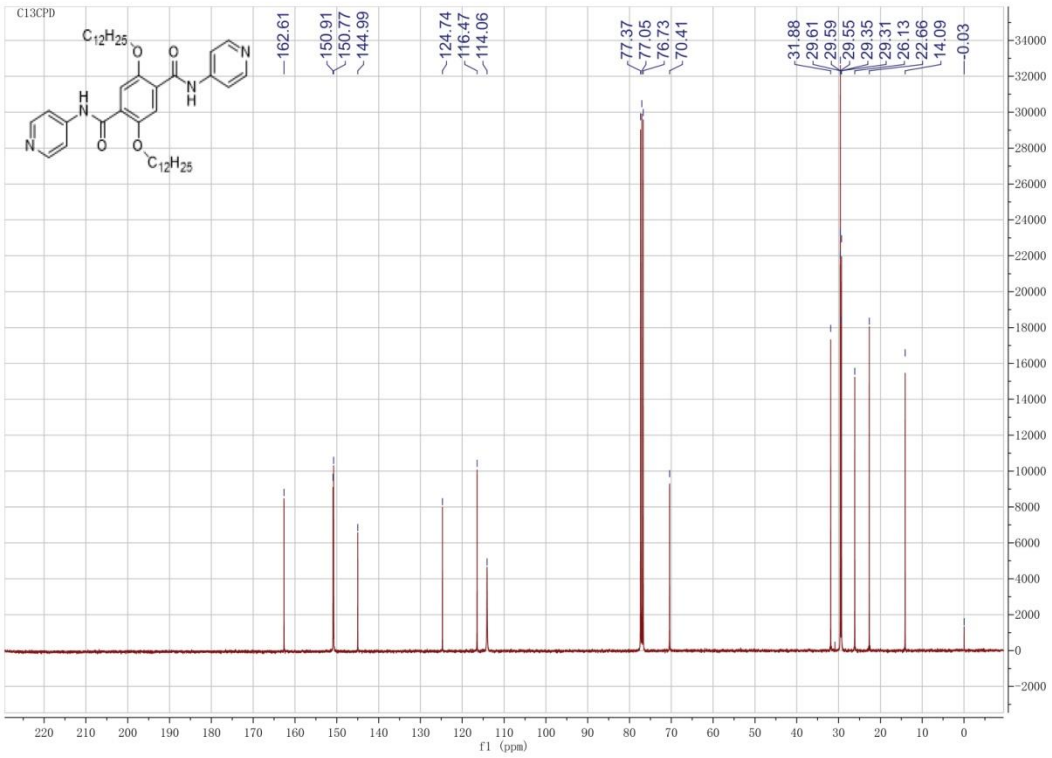

Fig. S5 ^{13}C NMR of **A2**

Acquisition Parameter					
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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	420.0 Vpp	Set Divert Valve	Source

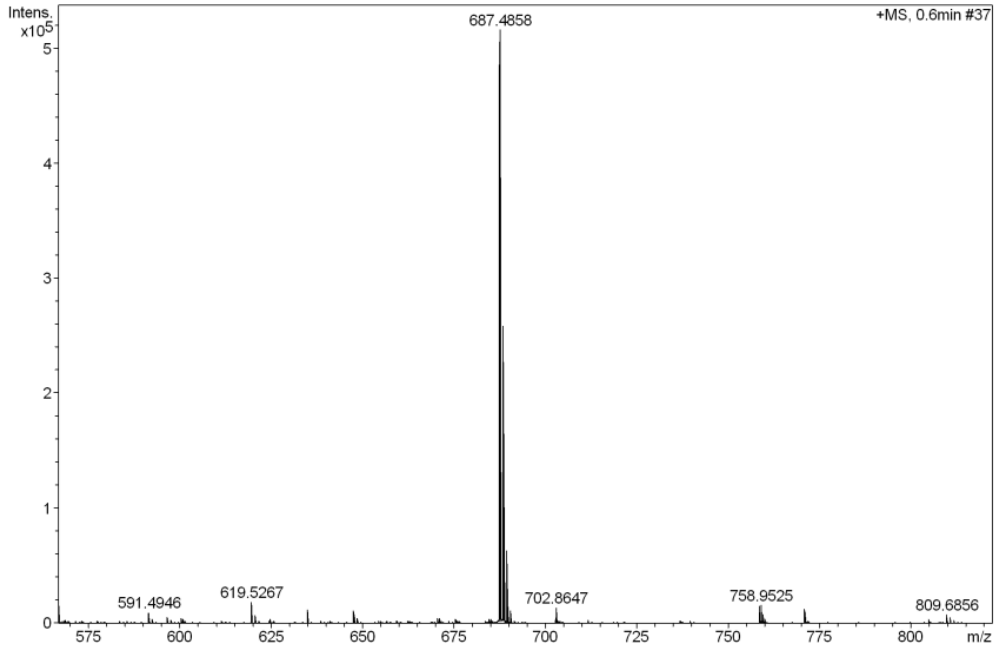

Fig. S6 HRMS of **A2**

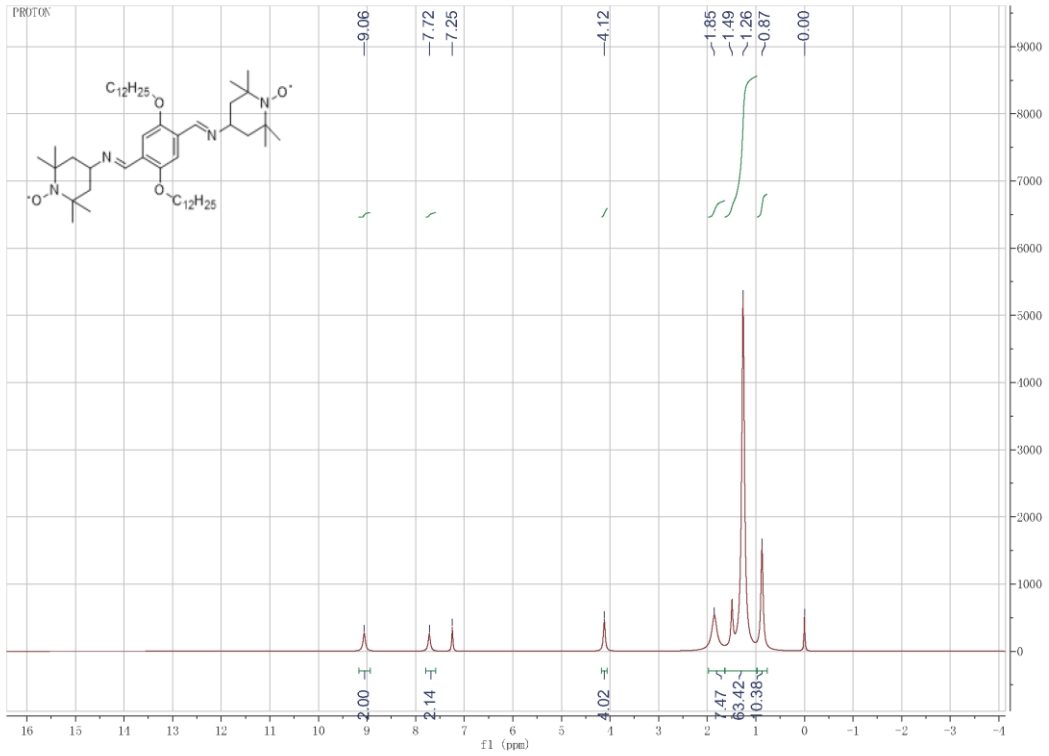

Fig. S7 ^{1}H NMR of **SB**

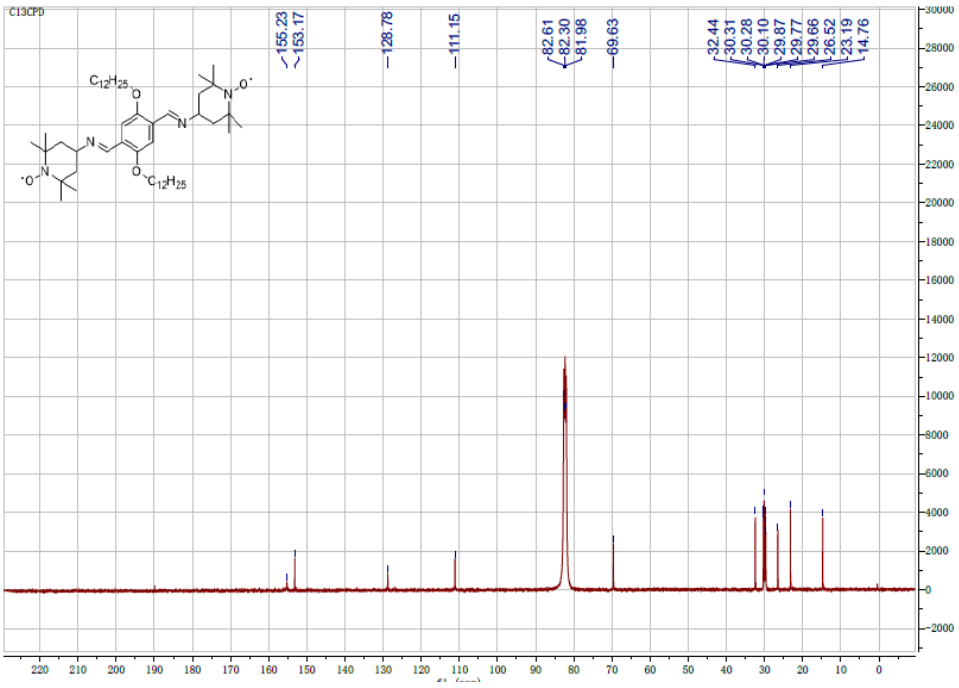

Fig. S8 ^{13}C NMR of **SB**

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
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Scan End	2500 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Source

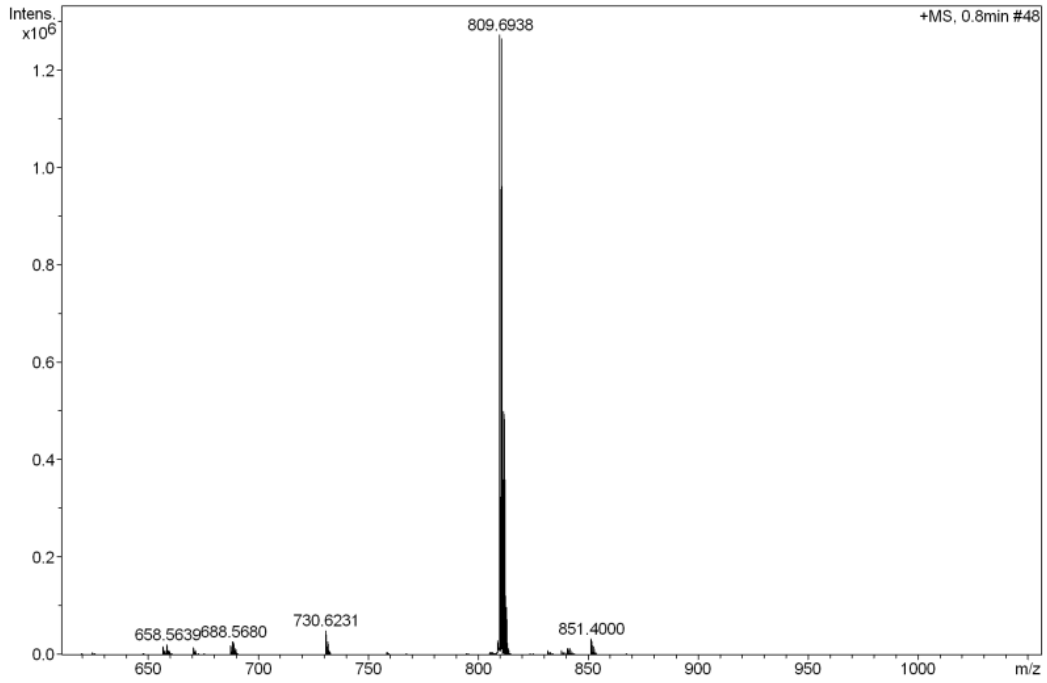

Fig. S9 HRMS of **SB**

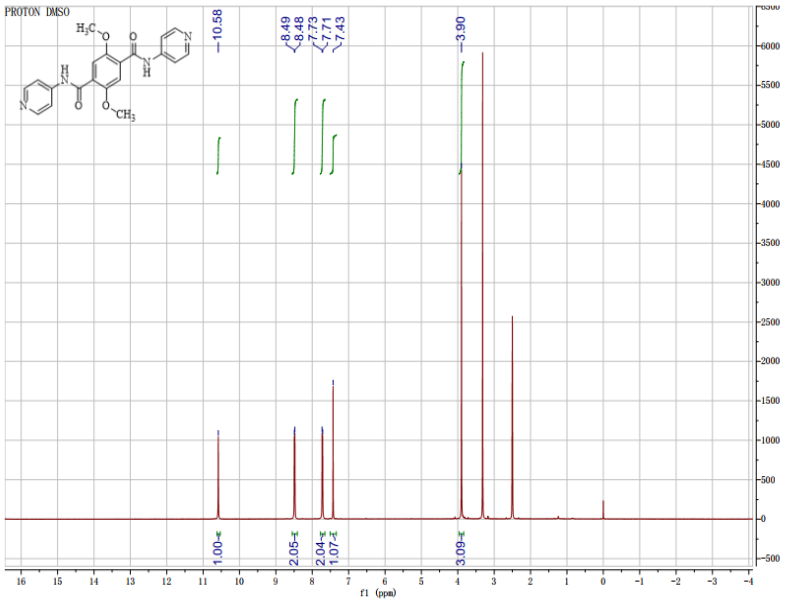

Fig. S10 ^{1}H NMR of **A2-OMe**

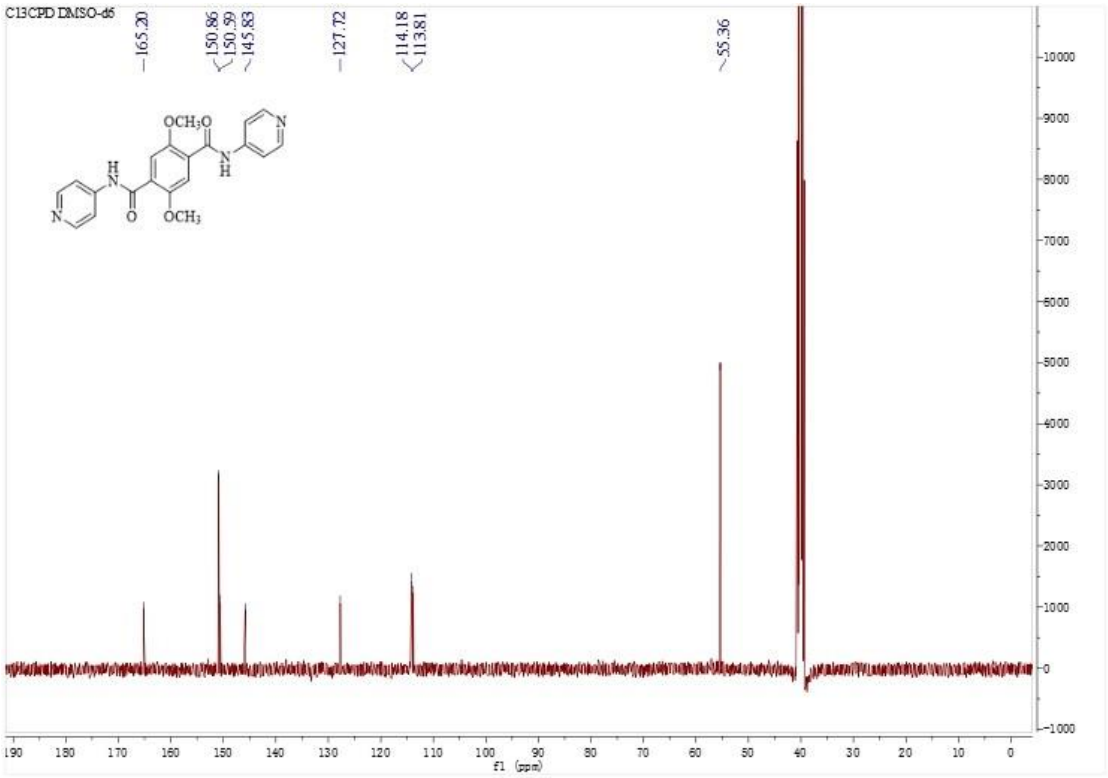

Fig. S11 ^{13}C NMR of **A2-OMe**

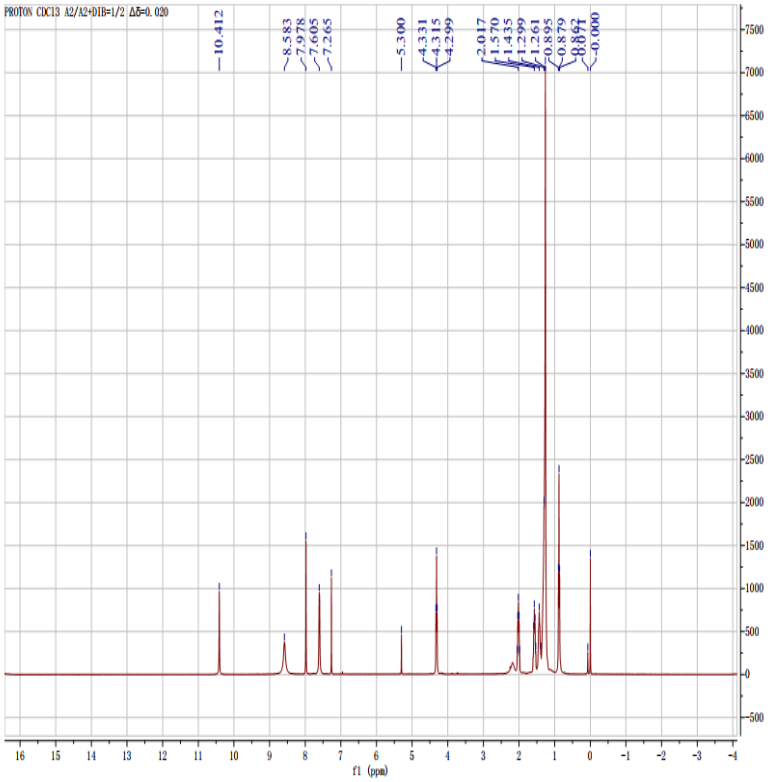

Fig. S12 ^{1}H NMR of **A2/(A2+DIB)=1/2 Δδ=0.020**

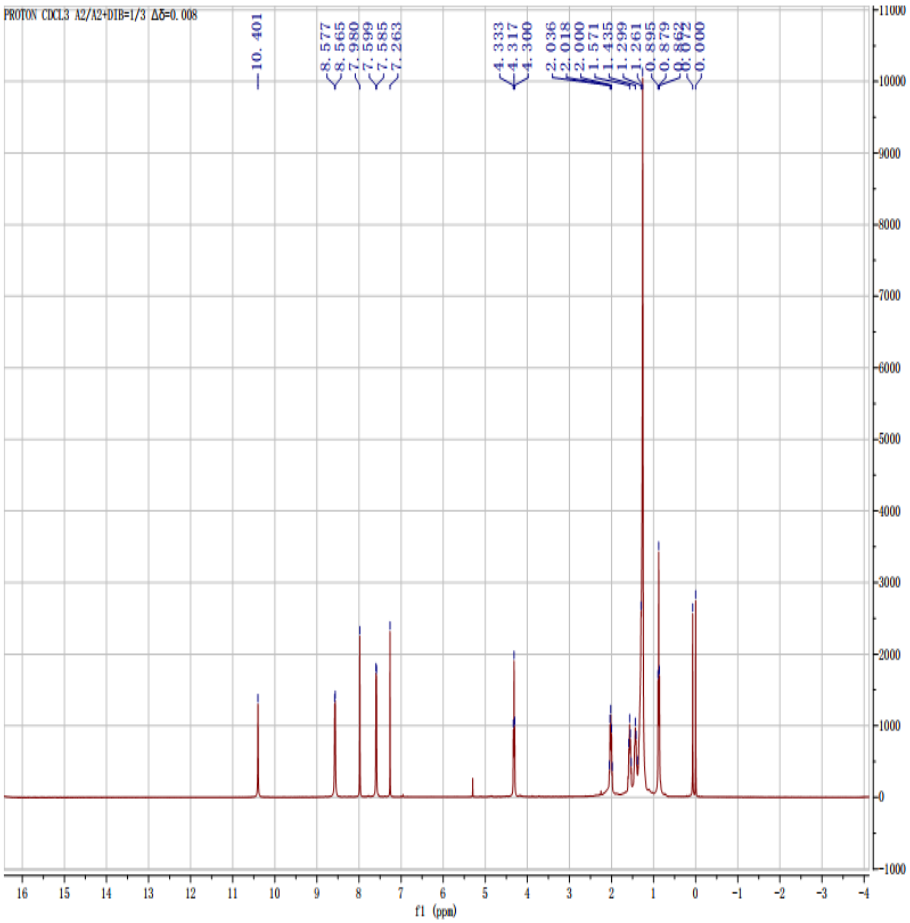

Fig. S13 ^{1}H NMR of **A2/(A2+DIB)=1/3 Δδ=0.008**

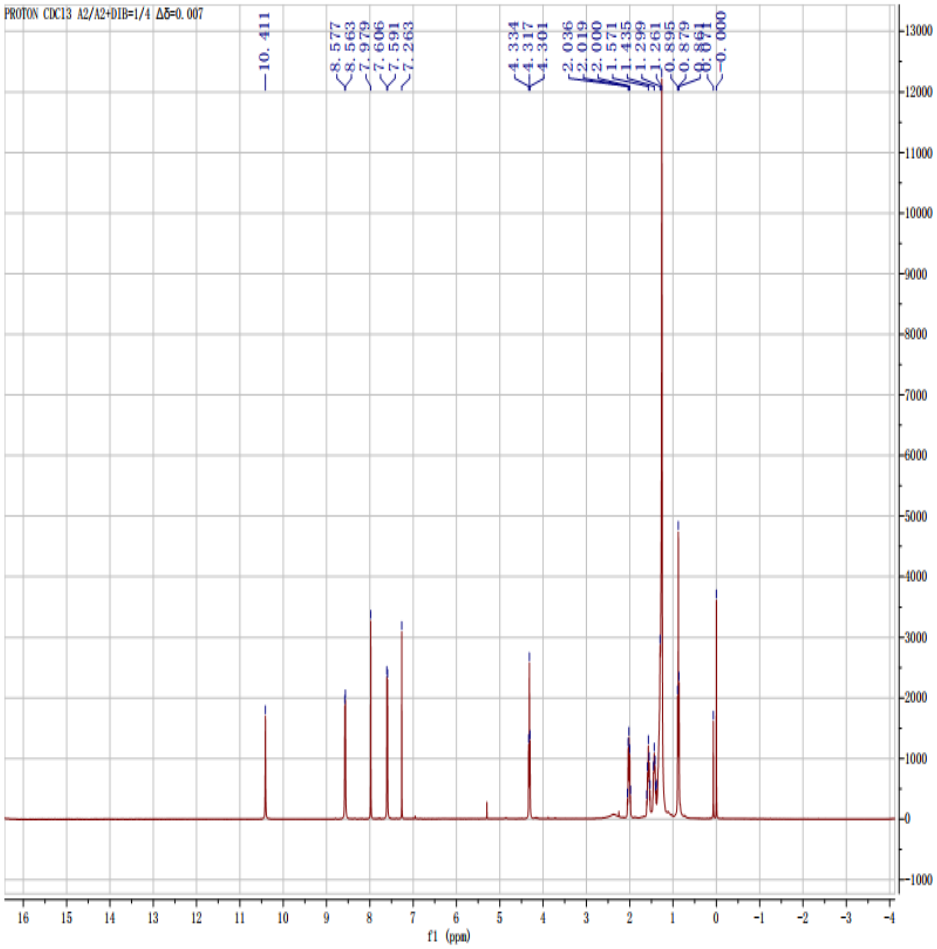

Fig. S14 ^{1}H NMR of **A2/(A2+DIB)=1/4 Δδ=0.007**

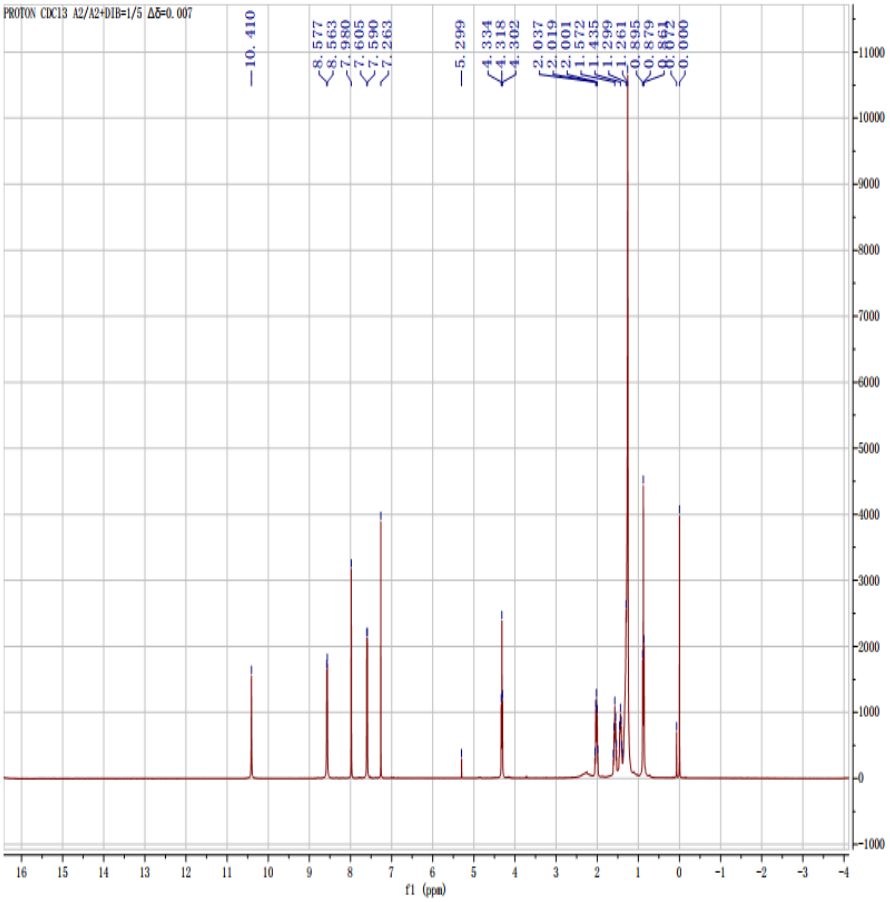

Fig. S15 ^{1}H NMR of **A2/(A2+DIB)=1/5 Δδ=0.007**

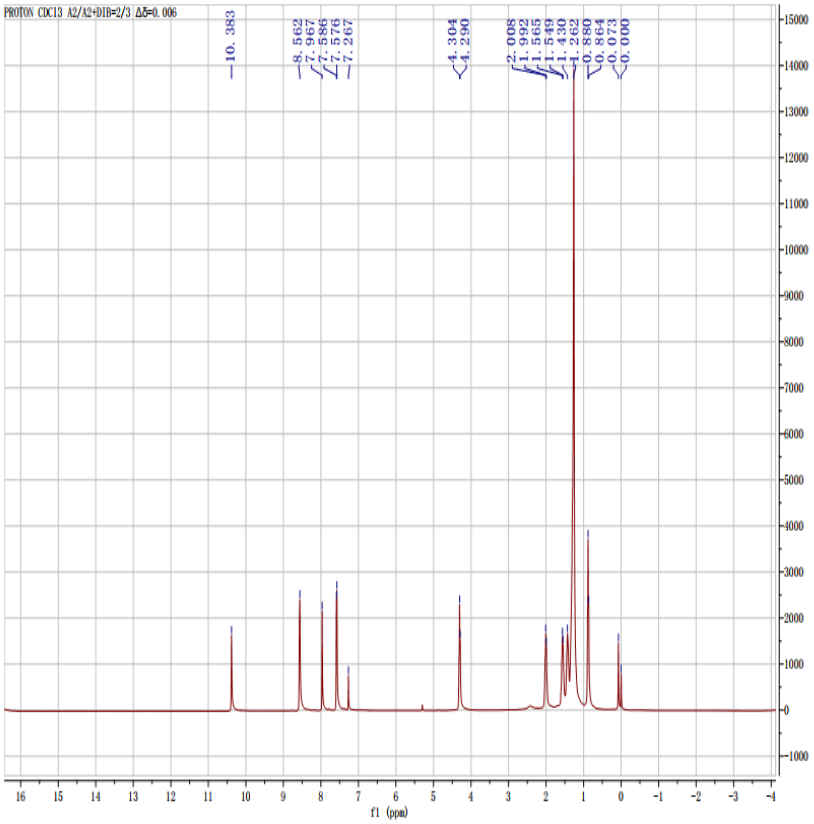

Fig. S16 ^{1}H NMR of **A2/(A2+DIB)=2/3 Δδ=0.006**

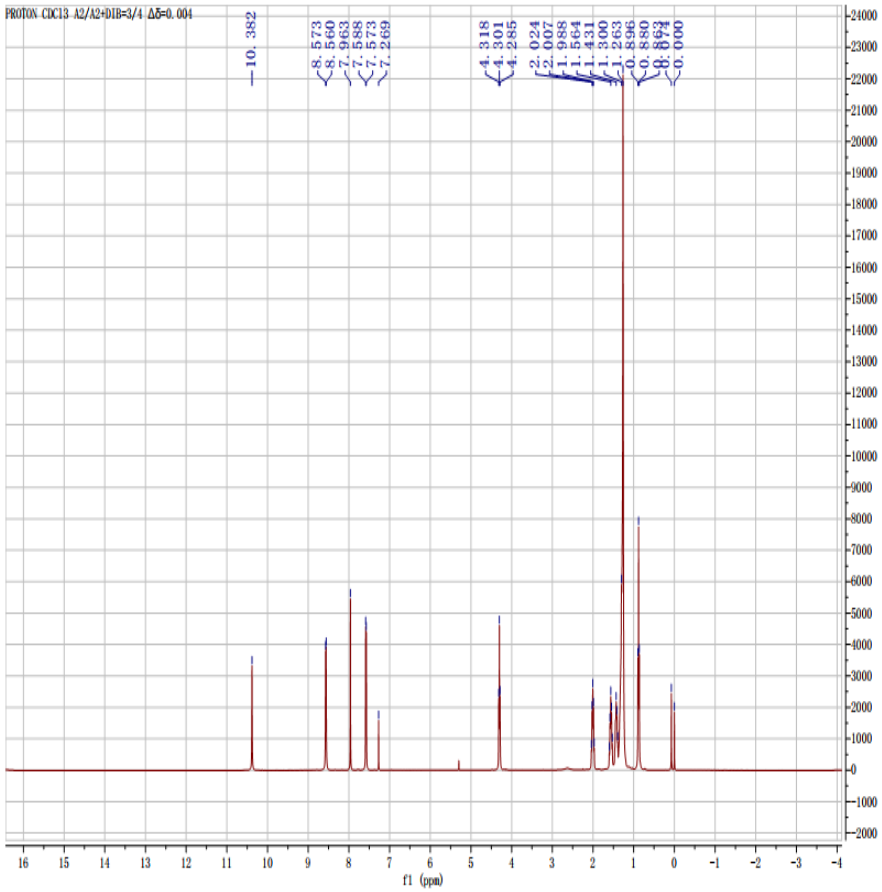

Fig. S17 ^{1}H NMR of **A2/(A2+DIB)=3/4 Δδ=0.004**

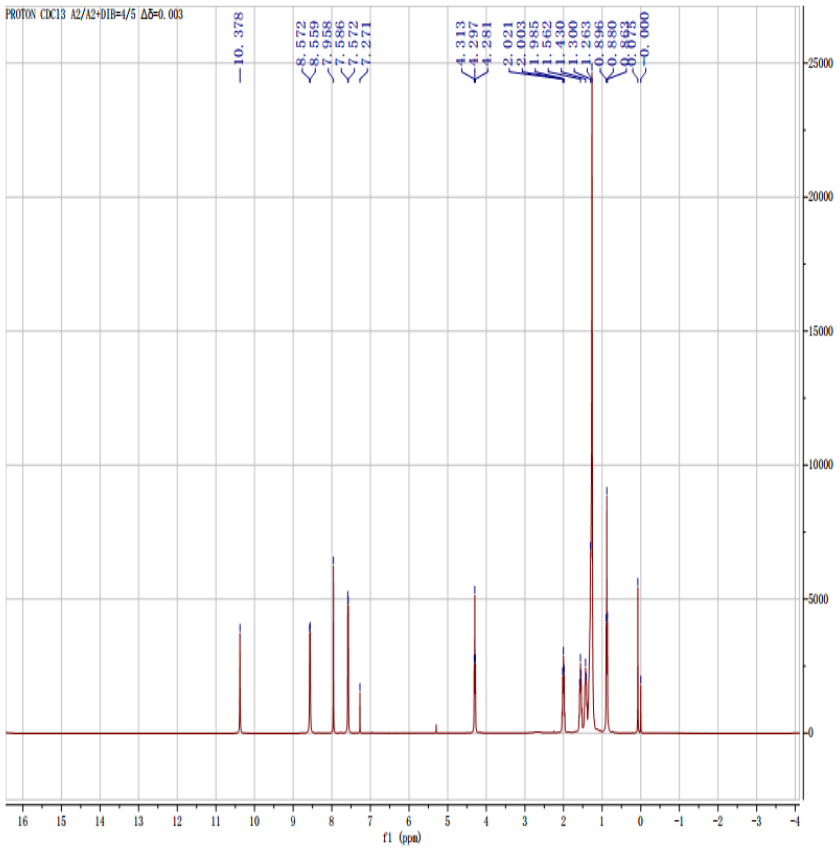

Fig. S18 ^{1}H NMR of **A2/(A2+DIB)=1/5 Δδ=0.003**

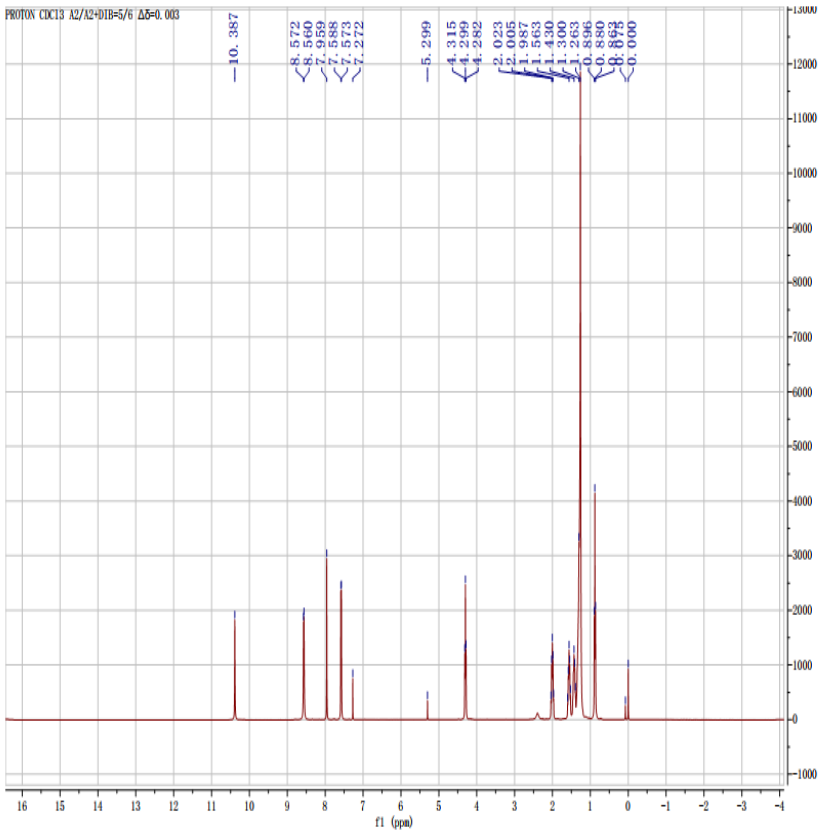

Fig. S19 ^{1}H NMR of **A2/(A2+DIB)=5/6 Δδ=0.003**

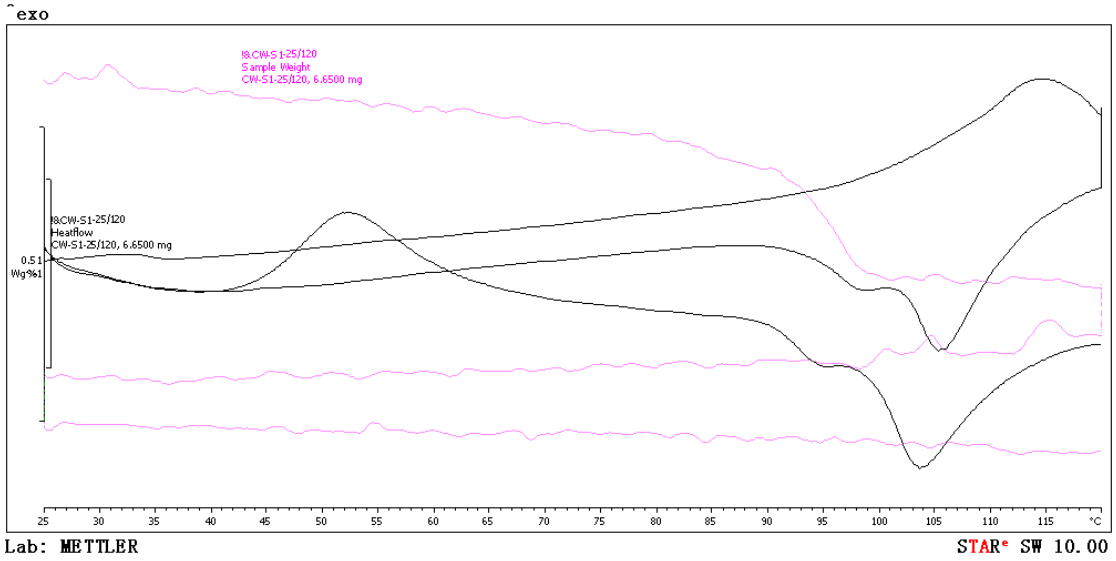

Fig. S20 TG and DSC curves of **SB**.

Table S1 Crystal data for complex **A2-OMe**-DIB

Identification code	A2-OMe-DIB
Empirical formula	$C_{26}H_{18}F_4I_2N_4O_4$
Formula weight	780.24
Temperature/K	160.00(10)

Crystal system	triclinic
Space group	P-1
a/Å	8.3364(3)
b/Å	8.9922(2)
c/Å	9.09840(10)
α/°	82.895(2)
β/°	73.539(2)
γ/°	84.883(2)
Volume/Å^3	648.01(3)
Z	1
ρ_{calc}g/cm^3	1.999
μ/mm^{-1}	19.699
F(000)	376.0
Crystal size/mm^3	0.12 ×0.11 ×0.08
Radiation	CuKα (λ = 1.54184)
2θ range for data collection/ °	9.928 to 154.17
Index ranges	-10 ≤ h ≤ 10, -11 ≤ k ≤ 11, -11 ≤ l ≤ 11
Reflections collected	10921
Independent reflections	2624 [R_{int} = 0.0373, R_{sigma} = 0.0232]
Data/restraints/parameters	2624/0/182
Goodness-of-fit on F^2	1.064
Final R indexes [I> = 2σ (I)]	R_1 = 0.0248, wR_2 = 0.0629
Final R indexes [all data]	R_1 = 0.0281, wR_2 = 0.0637
Largest diff. peak/hole/e Å^{-3}	0.77/-1.01

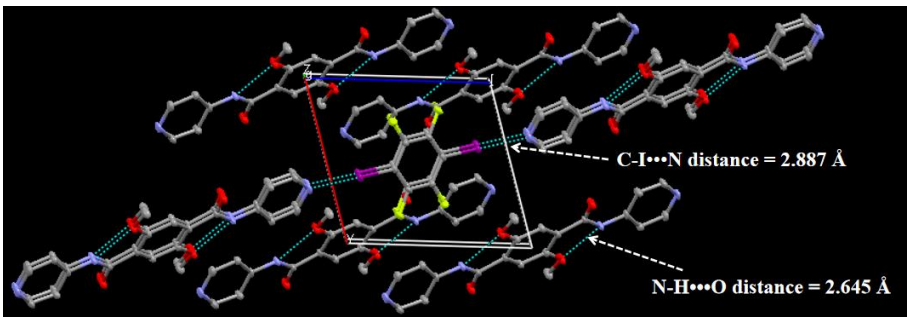

Fig. S21 Crystal-packing modes of **A2-OMe**-DIB exhibiting a C−I···N XB interaction with a distance of 2.887 Å and a N−H ··O HB interaction with a distance of 2.645 Å