Supporting information

Aggregation tuned dual emission of silole's derivatives: Synthesis, Crystal Structure and Photophysical Properties

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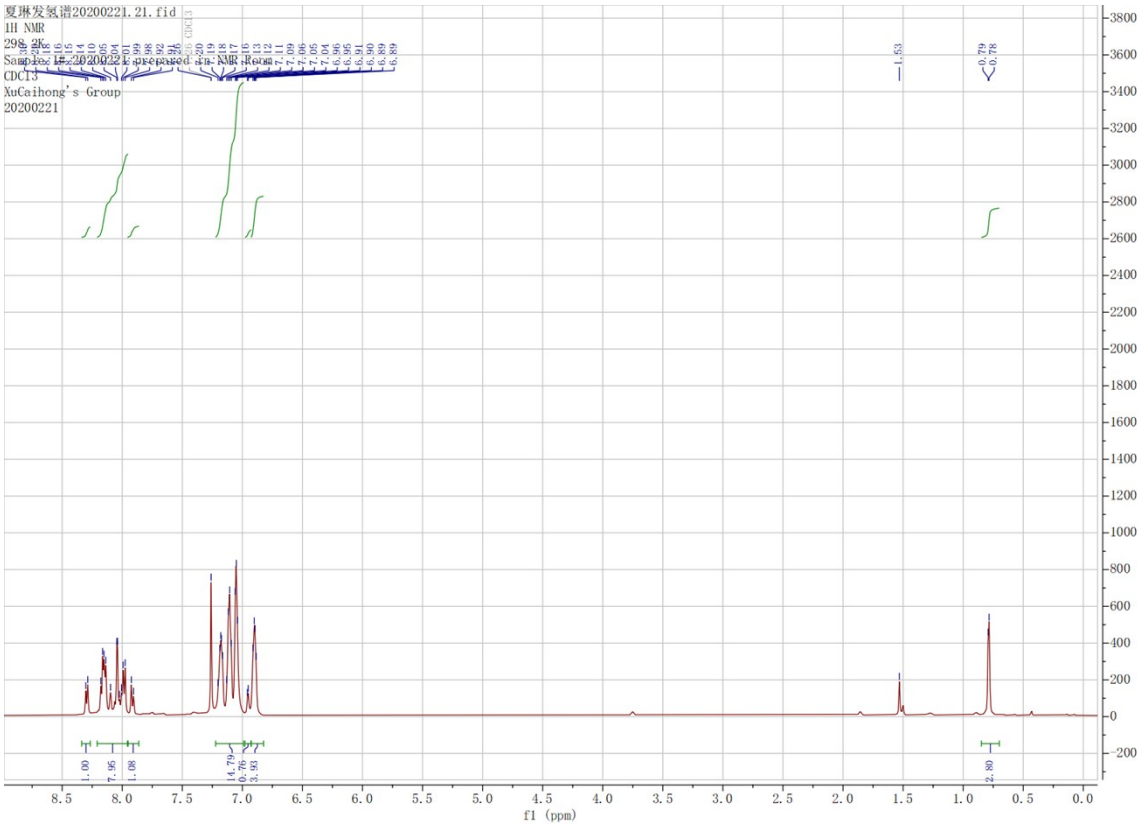


Figure 1S ^{1}H NMR spectrum of compound **1**

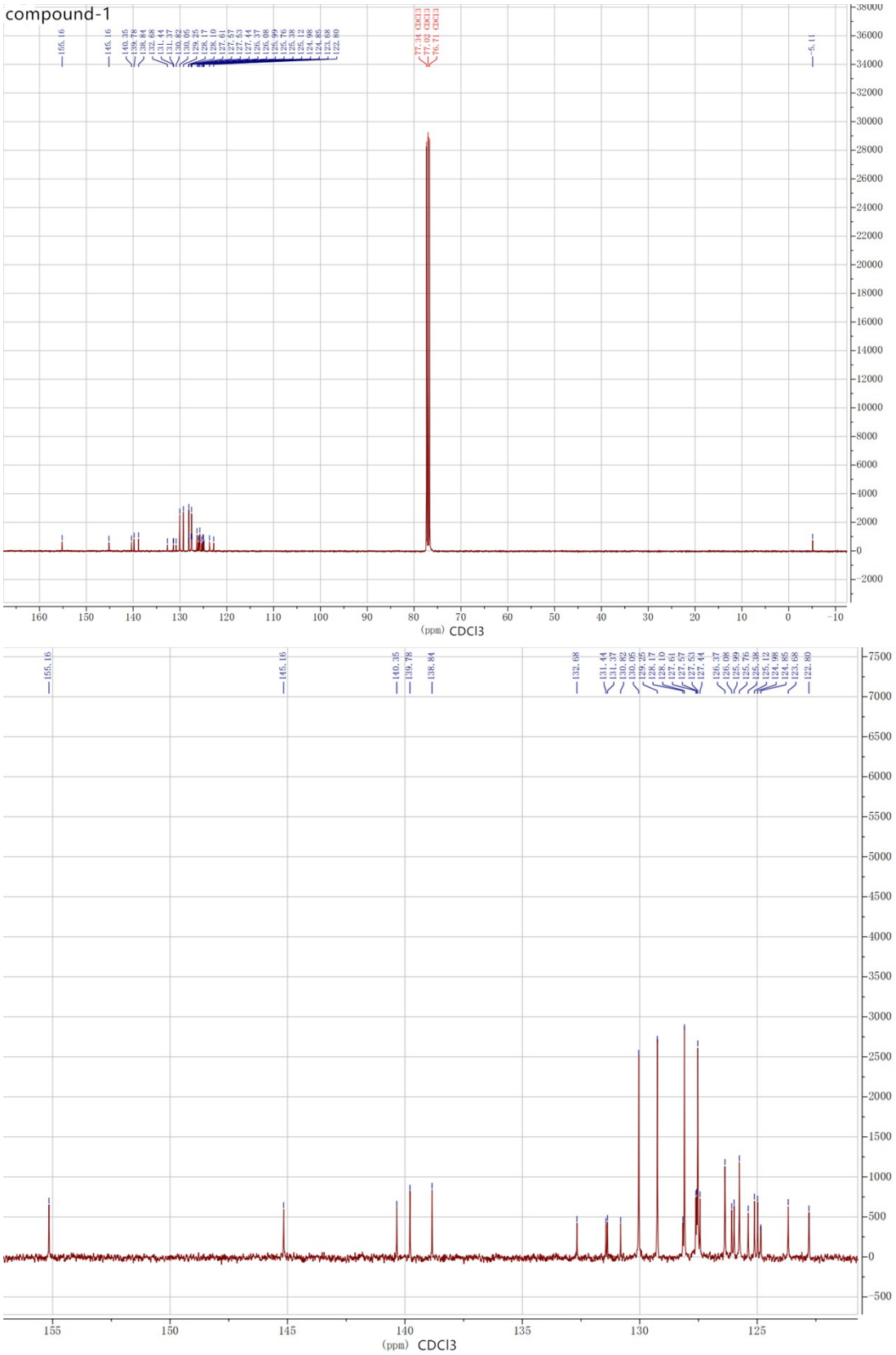


Figure 2S ^{13}C NMR spectrum of compound 1

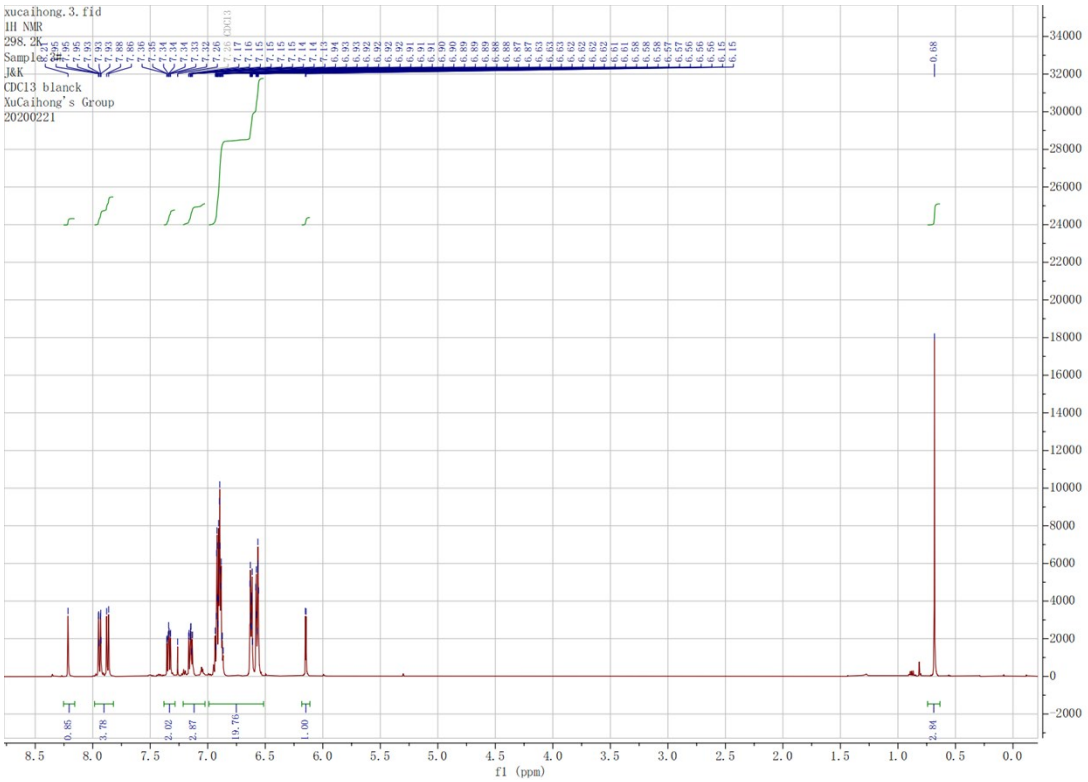
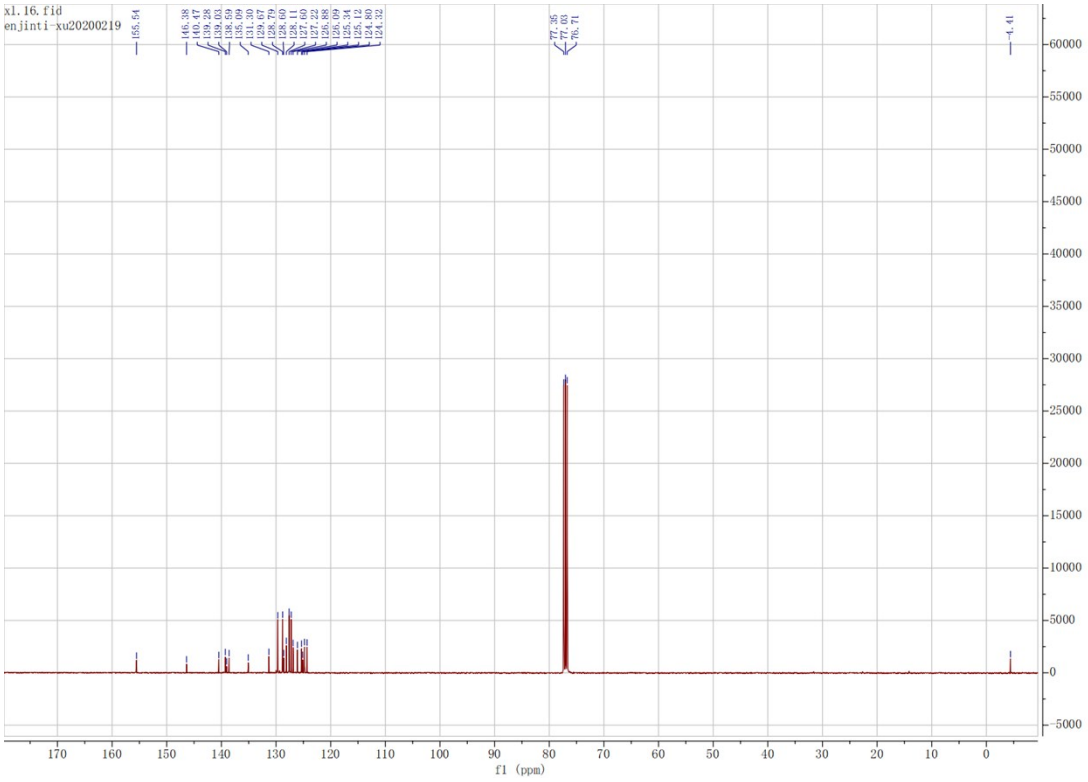


Figure 3S ^{1}H NMR spectrum of compound **2**



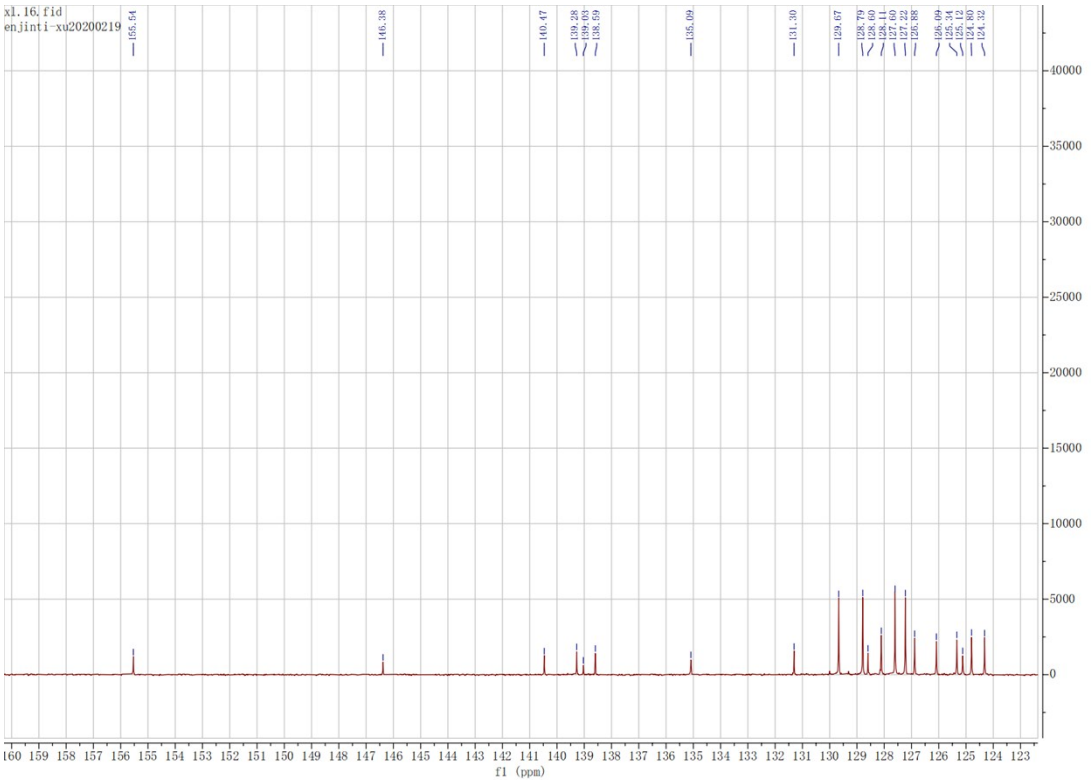


Figure 4S ^{13}C NMR spectrum of compound **2**

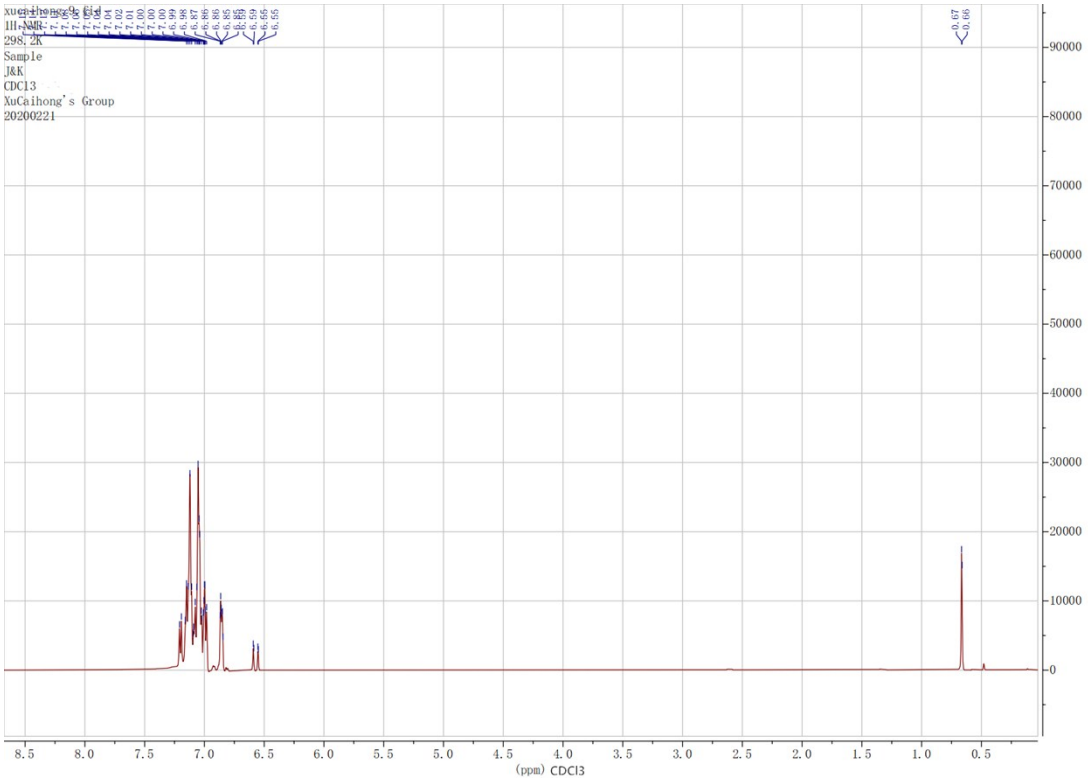


Figure 5S ^{1}H NMR spectrum of compound **3**

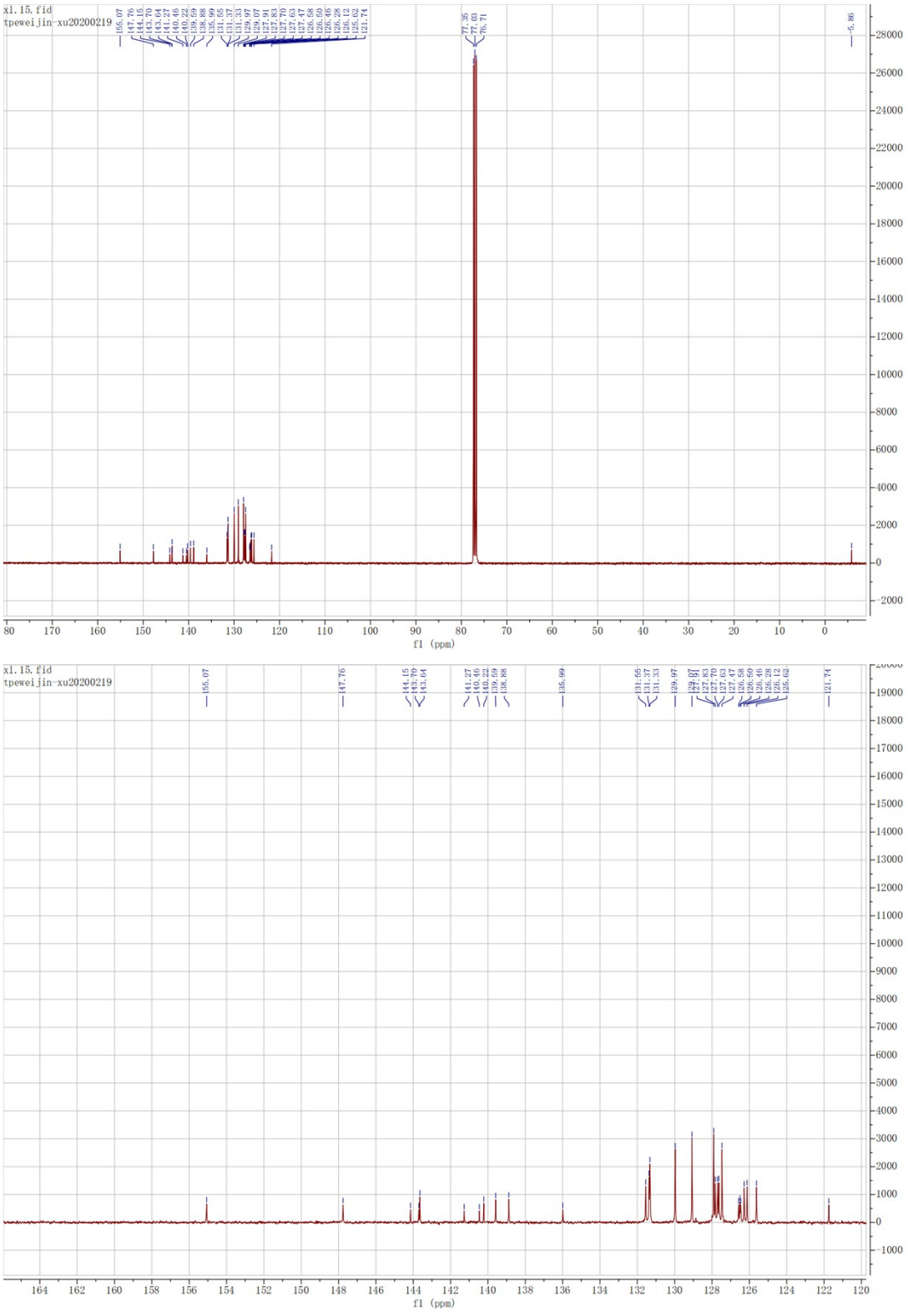


Figure 6S ^{13}C NMR spectrum of compound **3**

Table S1. Crystal data and structure refinements for compounds **1**，**2** and **3**

Compound	**1**	**2**	**3**
Empirical Formula	$C_{47}H_{34}Si$	$C_{45}H_{34}Si$	$C_{57}H_{44}Si$
Formula Weight	626.83	602.81	757.01
Temperature	173.1500 K	173.1500 K	293(2) K
Crystal System	Triclinic	Triclinic	Triclinic
Space Group	P -1	P -1	P -1
Unit Cell	a = 10.390(3) Å b = 11.261(3) Å c = 16.275(4) Å α= 97.171(2)° β= 103.230(3)°. γ = 111.096(3)°.	a = 10.685(3) Å b = 13.039(3) Å c = 13.504(3) Å α= 104.0750(10)° β= 103.729(3)°. γ = 108.671(3)°	a = 11.170(2) Å b = 12.894(3) Å c = 17.928(4) Å α= 73.46(3)°. β= 73.56(3)° γ = 76.03(3)°.
Volume	1683.8(7) $Å^3$	1623.9(7) $Å^3$	2337.3(10) $Å^3$
Z	2	2	2
Density (Calculated)	1.236 Mg/m^3	1.233 Mg/m^3	1.076 Mg/m^3
F(000)	660	636	800
Crystal Size	0.41 x 0.3 x 0.28 mm^3	0.4 x 0.38 x 0.14 mm^3	0.4 x 0.3 x 0.20 mm^3
Index Ranges	-13<=h<=13 -14<=k<=14 -21<=l<=21	-13<=h<=13 -16<=k<=16 -17<=l<=17	-14<=h<=14 -16<=k<=16 -23<=l<=22
Reflection Collected	22311	20820	32715
Independent Reflections	7700 [R(int) = 0.0306]	7397 [R(int) = 0.0352]	10680 [R(int) = 0.0609]
Completeness	99.6 %	99.5 %	99.8 %
Data / restraints / parameters	7700 / 0 / 434	7397 / 0 / 416	10680 / 0 / 524
Goodness-of-fit on F^2	1.134	1.300	1.142
R_1 [$I > 2\sigma(I)$][a]	R1 = 0.0572 wR2 = 0.1156	R1 = 0.0582 wR2 = 0.1751	R1 = 0.0765 wR2 = 0.1470

wR_2 (all data)[b]	R1 = 0.0665 wR2 = 0.1200	R1 = 0.0649 wR2 = 0.1803	R1 = 0.0891 wR2 = 0.1536

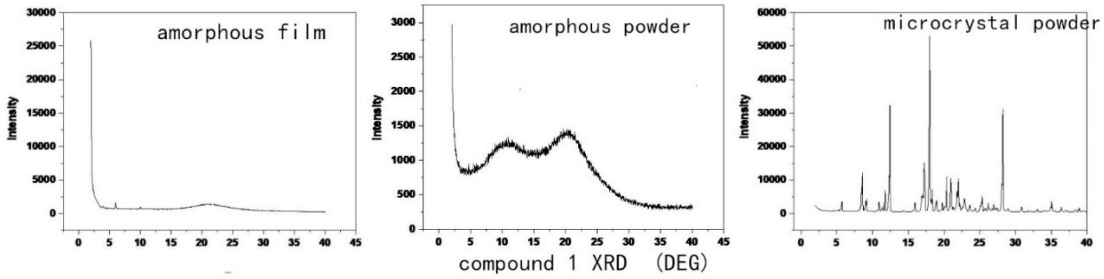


Figure 7S XRD patterns of compound **1** in different morphologic state, amorphous film was obtained by drop-casting of **1** dichloromethane solution, amorphous powder was obtained by grinding the sample which was separated through column separation. Microcrystal powder was obtained by grinding the crystal of **1** which crystallizing in the mixing solvent.

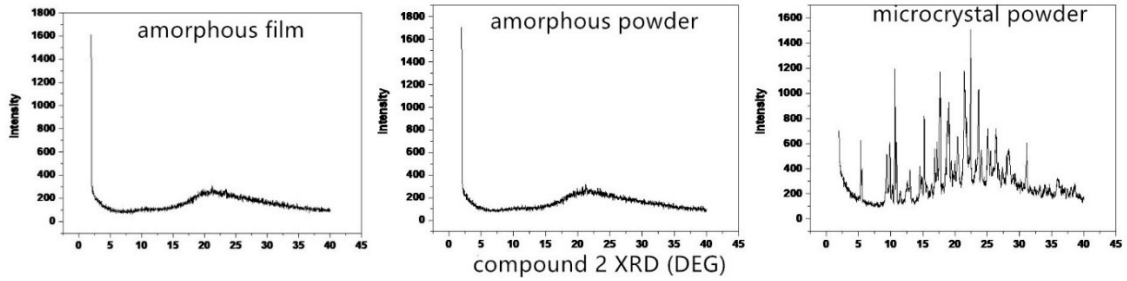


Figure 8S XRD patterns of compound **2** in different morphologic state, amorphous film was obtained by drop-casting of **2** dichloromethane solution, amorphous powder was obtained by grinding the sample which was separated through column separation. Microcrystal powder was obtained by grinding the crystal of **2** which crystallizing in the mixing solvent.

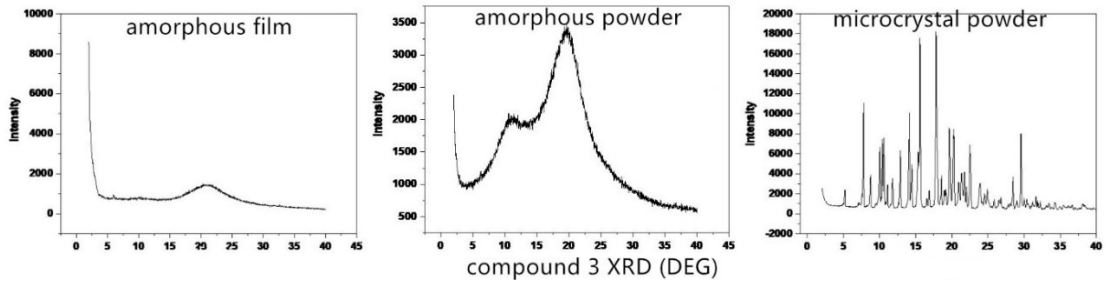


Figure 9S XRD patterns of compound **3** in different morphologic state, amorphous film was obtained by drop-casting of **3** dichloromethane solution, amorphous powder was obtained by grinding the sample which was separated through column separation. Microcrystal powder was obtained by grinding the crystal of **3** which crystallizing in the mixing solvent.

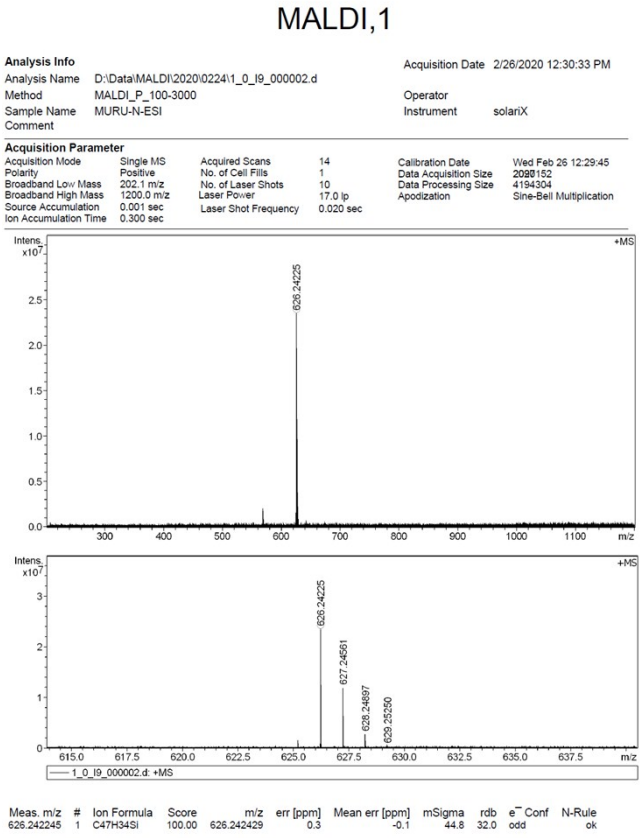


Figure 10S HRMS spectrum of compound **1**

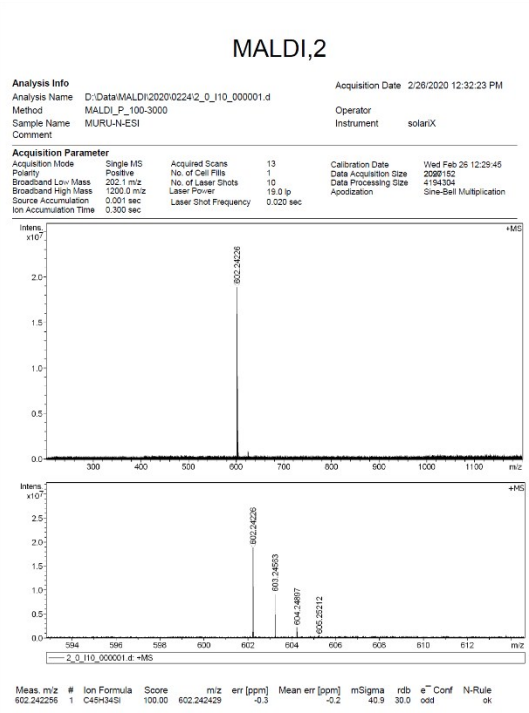


Figure 11S HRMS spectrum of compound **2**

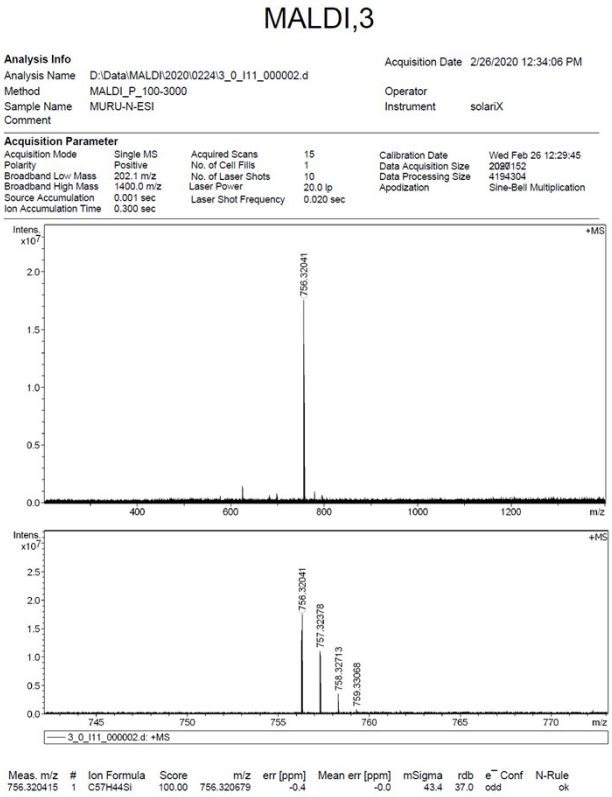


Figure 12S HRMS spectrum of compound **3**