

Supporting information

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

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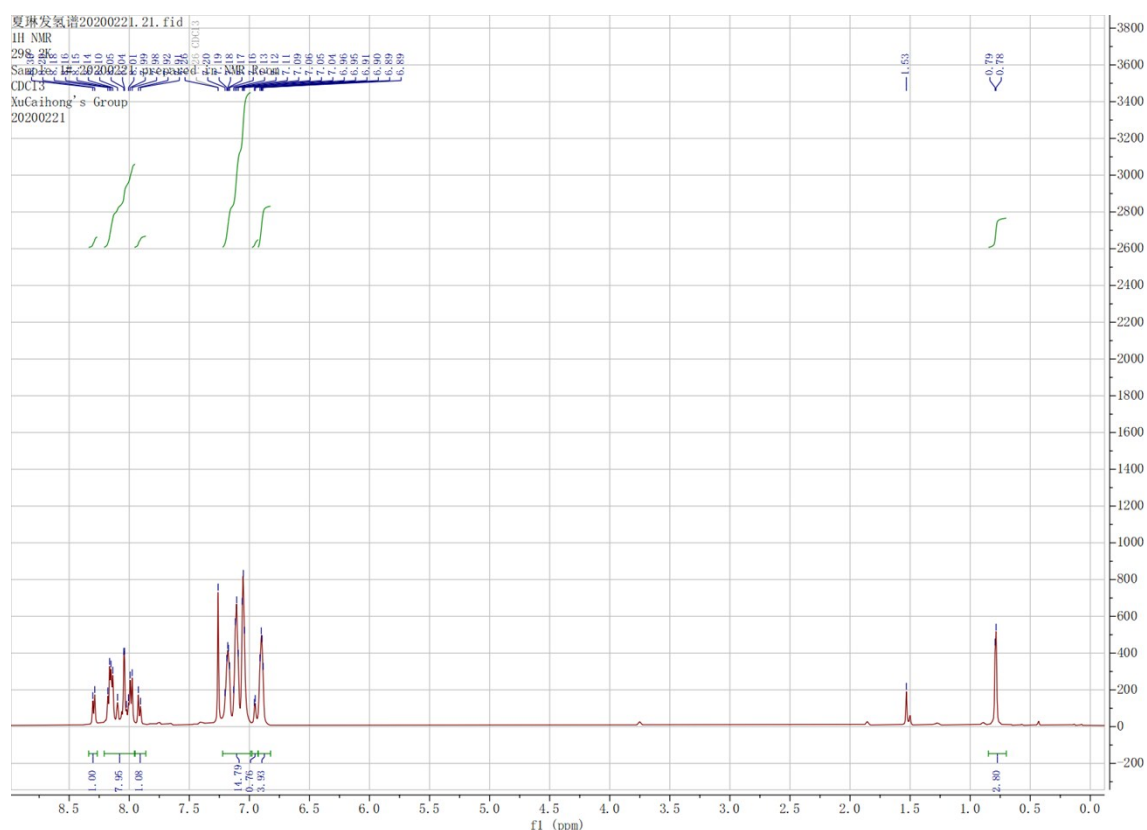


Figure 1S ¹H NMR spectrum of compound 1

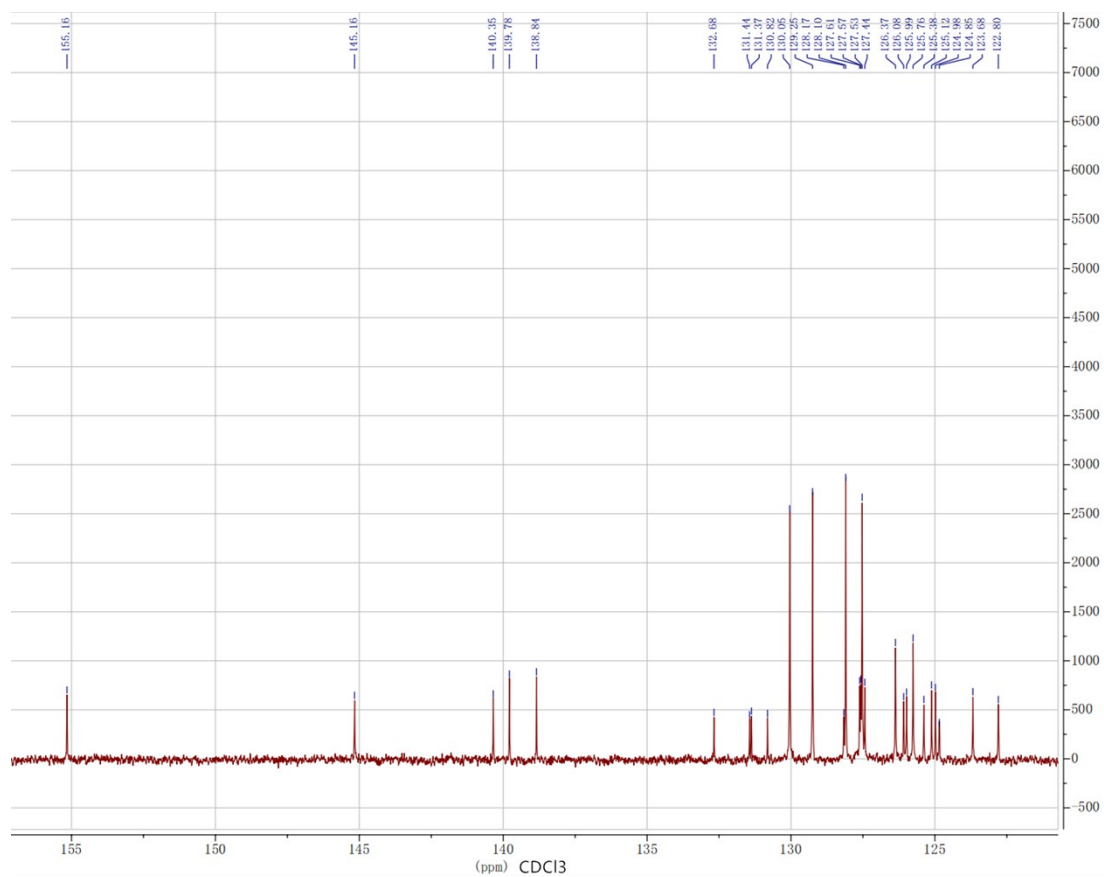
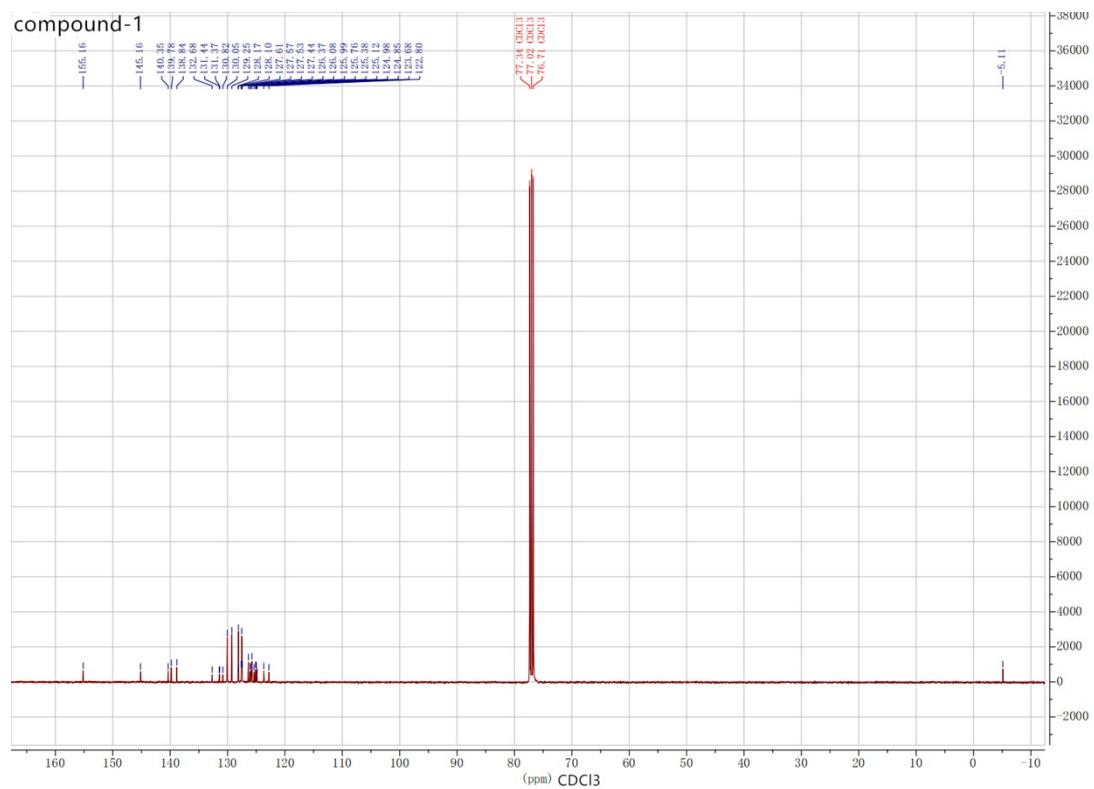


Figure 2S ^{13}C NMR spectrum of compound 1

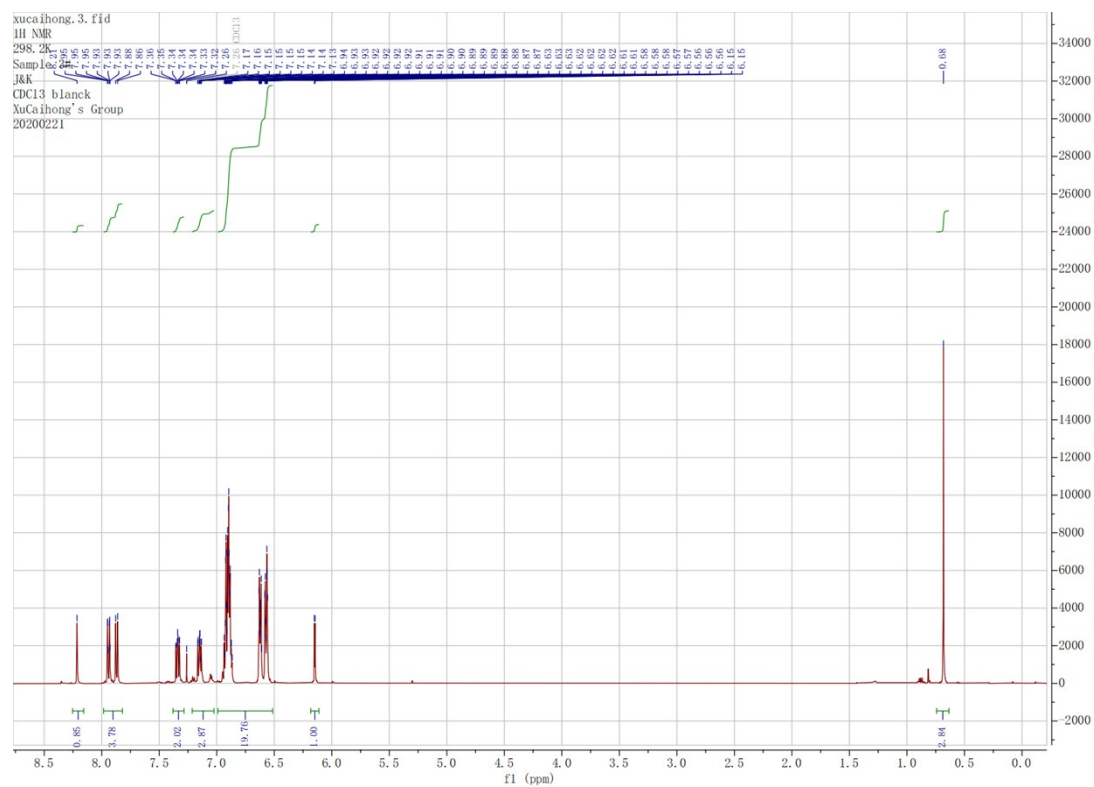
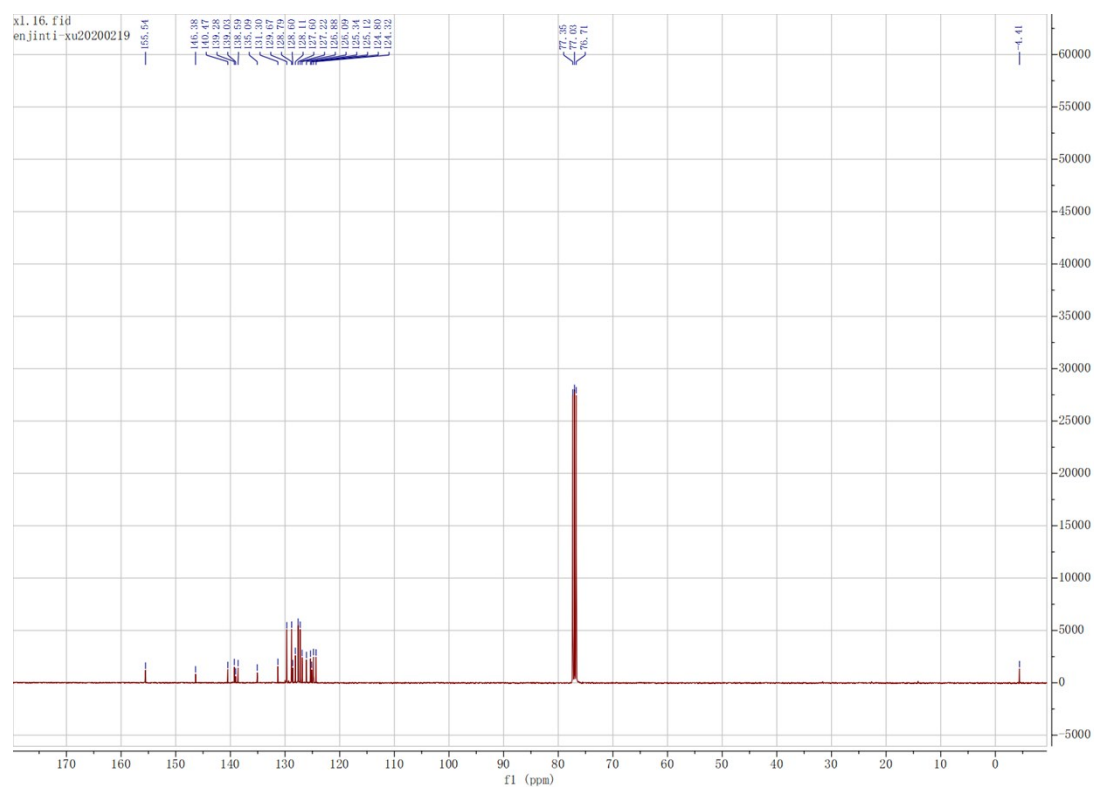


Figure 3S ^1H NMR spectrum of compound **2**



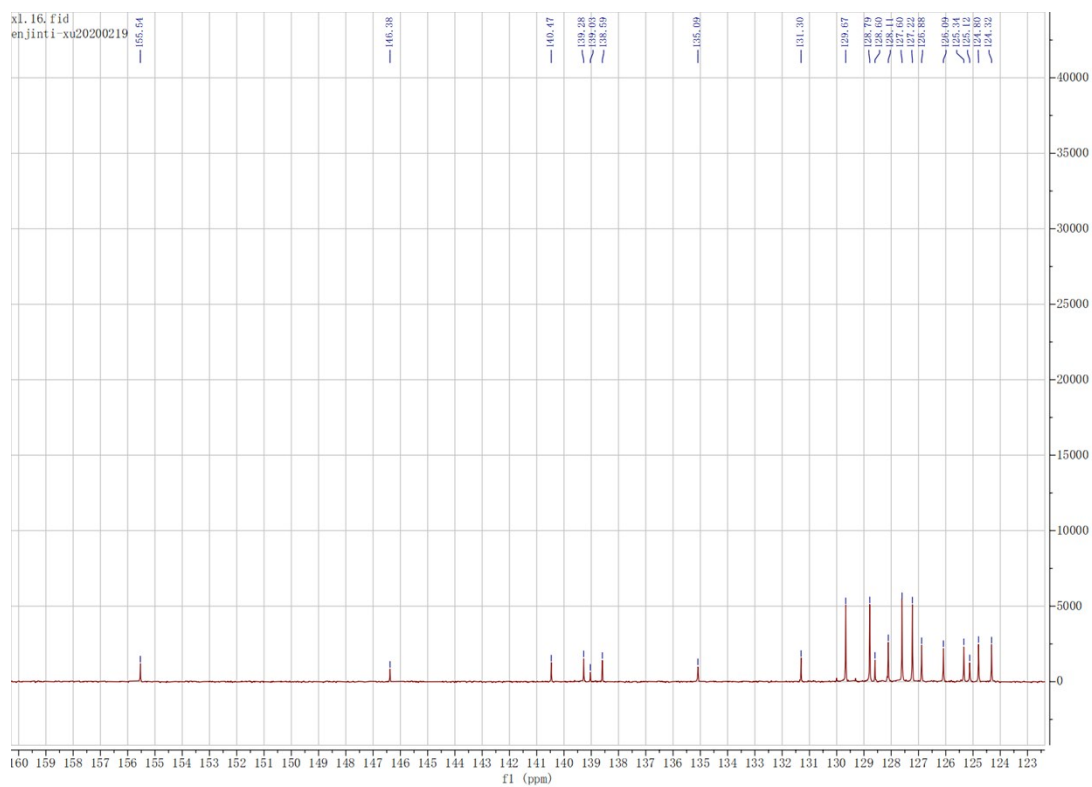


Figure 4S ^{13}C NMR spectrum of compound **2**

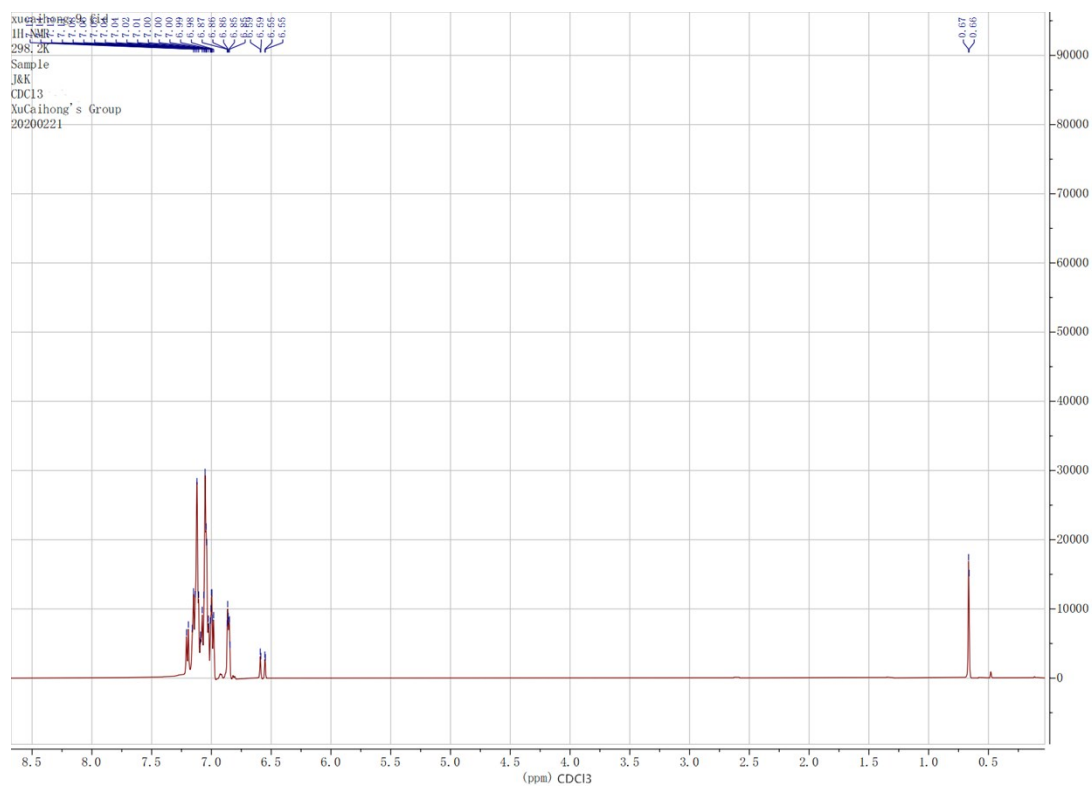


Figure 5S ^1H NMR spectrum of compound **3**

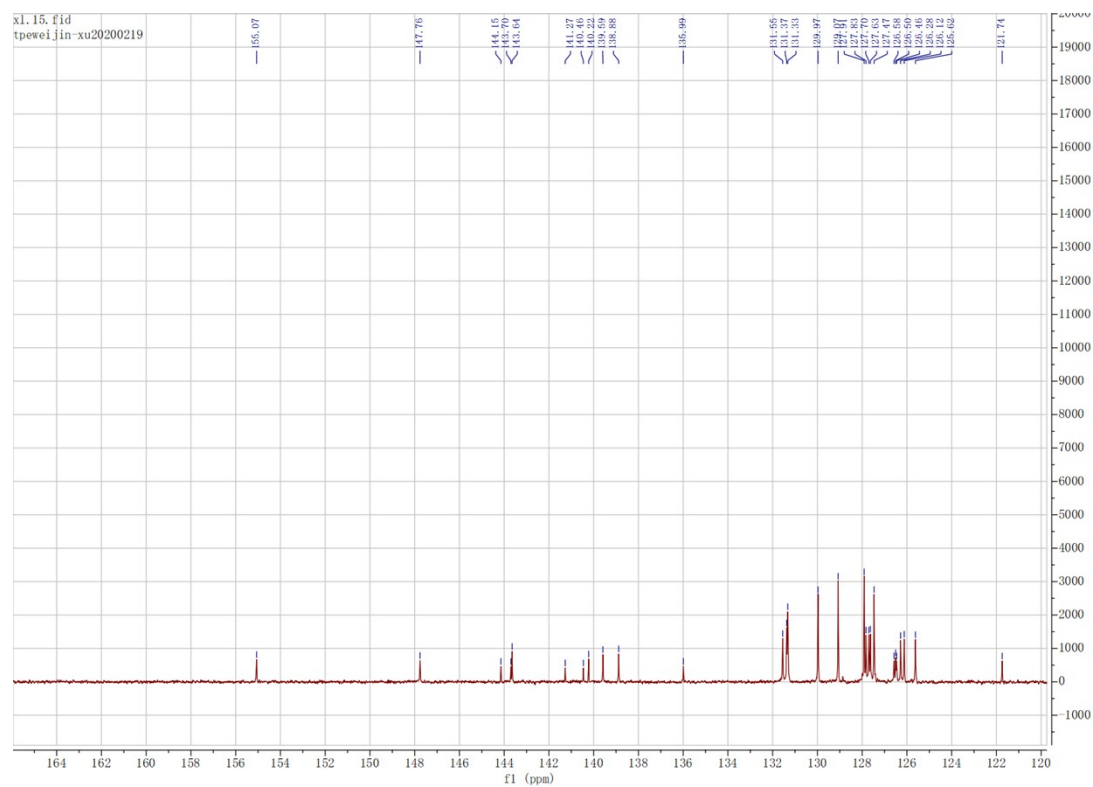
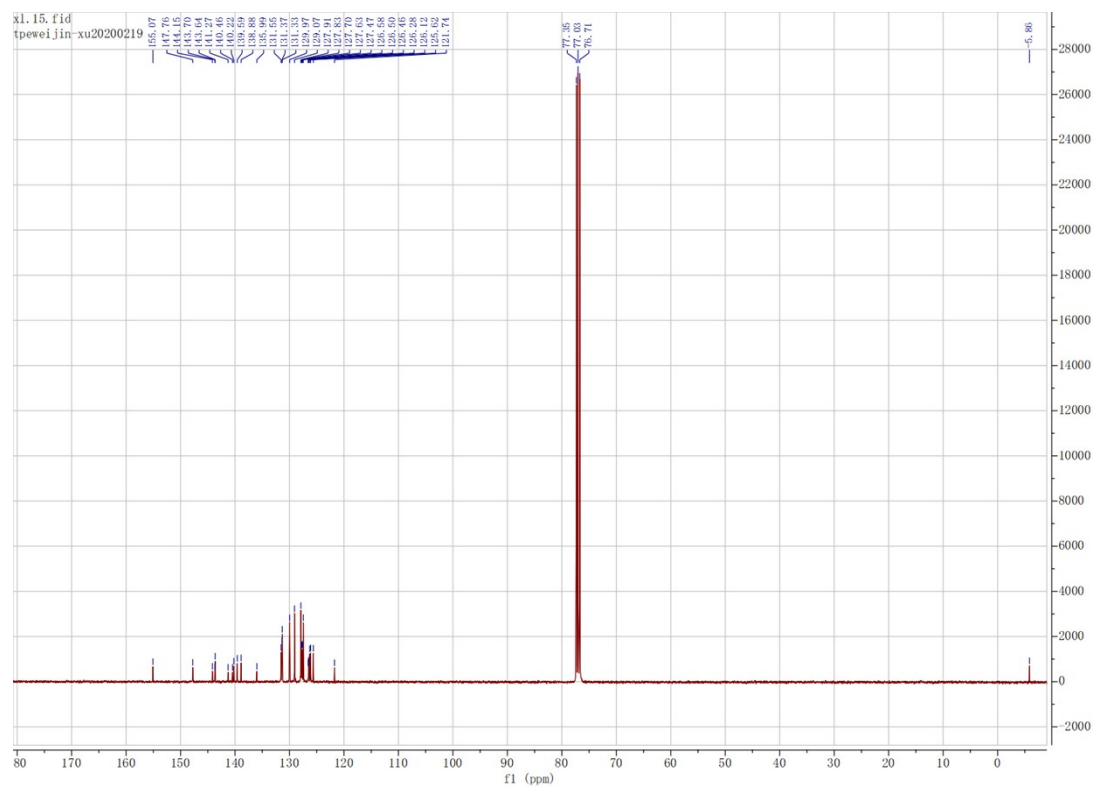


Figure 6S ¹³C NMR spectrum of compound **3**

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	a = 10.685(3) Å	a = 11.170(2) Å
	b = 11.261(3) Å	b = 13.039(3) Å	b = 12.894(3) Å
	c = 16.275(4) Å	c = 13.504(3) Å	c = 17.928(4) Å
	α = 97.171(2)°	α = 104.0750(10)°	α = 73.46(3)°
	β = 103.230(3)°	β = 103.729(3)°	β = 73.56(3)°
	γ = 111.096(3)°	γ = 108.671(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	-13 ≤ h ≤ 13	-14 ≤ h ≤ 14
	-14 ≤ k ≤ 14	-16 ≤ k ≤ 16	-16 ≤ k ≤ 16
	-21 ≤ l ≤ 21	-17 ≤ l ≤ 17	-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 <i>F</i> ²	1.134	1.300	1.142
R ₁ [<i>I</i> > 2σ(<i>I</i>)] ^a	R1 = 0.0572	R1 = 0.0582	R1 = 0.0765
	wR2 = 0.1156	wR2 = 0.1751	wR2 = 0.1470

 wR_2 (all data)^b

R1 = 0.0665

R1 = 0.0649

R1 = 0.0891

 wR_2 = 0.1200 wR_2 = 0.1803 wR_2 = 0.1536

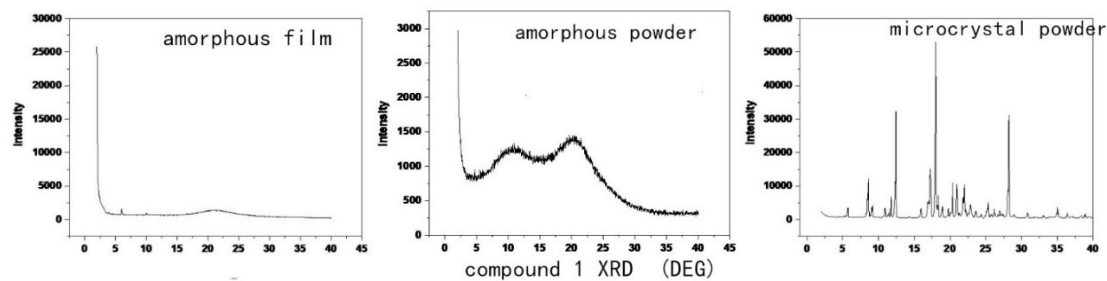


Figure 7S XRD patterns of compound **1** in different morphologic state, amorphous film was obtained by drop-casting of **1** dichloromethane solution, amorphous powder was obtained by grinding the sample which was separated through column separation. Microcrystal powder was obtained by grinding the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

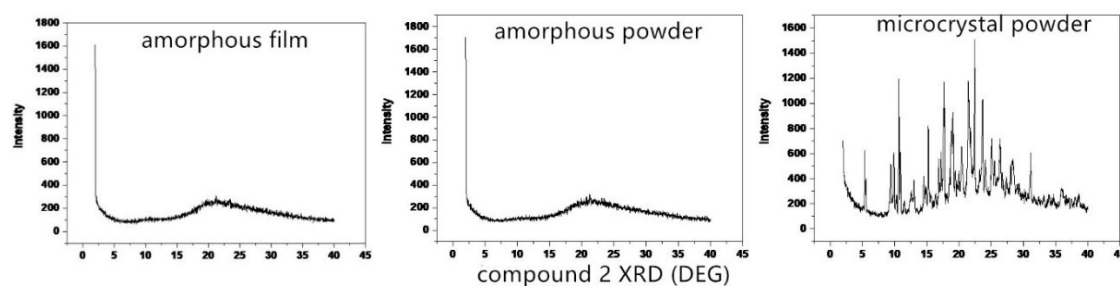


Figure 8S XRD patterns of compound **2** in different morphologic state, amorphous film was obtained by drop-casting of **2** dichloromethane solution, amorphous powder was obtained by grinding the sample which was separated through column separation. Microcrystal powder was obtained by grinding the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

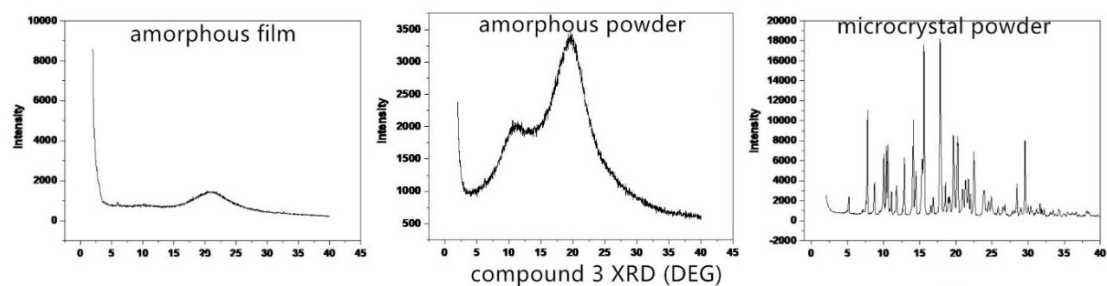


Figure 9S XRD patterns of compound **3** in different morphologic state, amorphous film was obtained by drop-casting of **3** dichloromethane solution, amorphous powder was obtained by grinding the sample which was separated through column separation. Microcrystal powder was obtained by grinding the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

MALDI,1

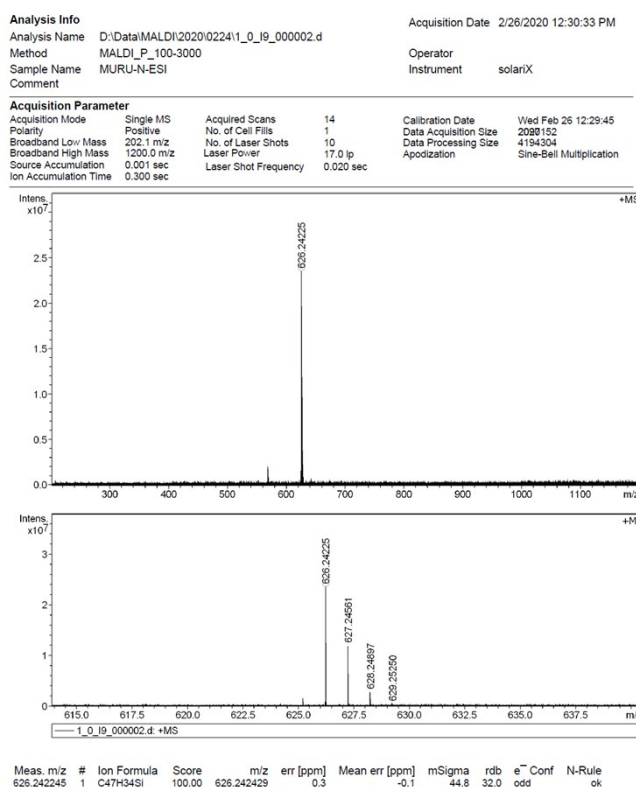
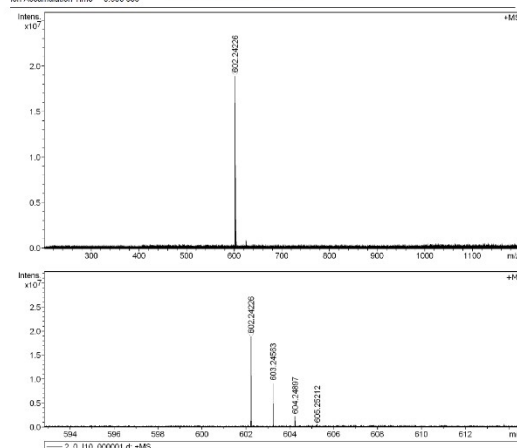


Figure 10S HRMS spectrum of compound **1**

MALDI,2

Analysis Info
 Analysis Name: D:\Data\MALDI\2020\0224\2_0_110_000001.d
 Method: MALDI_P_100-3000
 Sample Name: MURU-N-ESI
 Comment:
 Acquisition Date: 2/26/2020 12:32:23 PM
 Operator: solarix
 Instrument: solarix

Acquisition Parameter
 Acquisition Mode: Single MS
 Polarity: Positive
 Broadband Low Mass: 202.1 m/z
 Broadband High Mass: 1200.0 m/z
 Source Accumulation: 0.001 sec
 Ion Accumulation Time: 0.300 sec
 Acquired Scans: 13
 No. of Cell Fills: 1
 No. of Laser Shots: 10
 Laser Power: 19.0 Ip
 Laser Shot Frequency: 0.020 sec
 Calibration Date: Wed Feb 26 12:29:45
 Data Acquisition Size: 2098152
 Data Processing Size: 4194304
 Apodization: Sine-Bell Multiplication



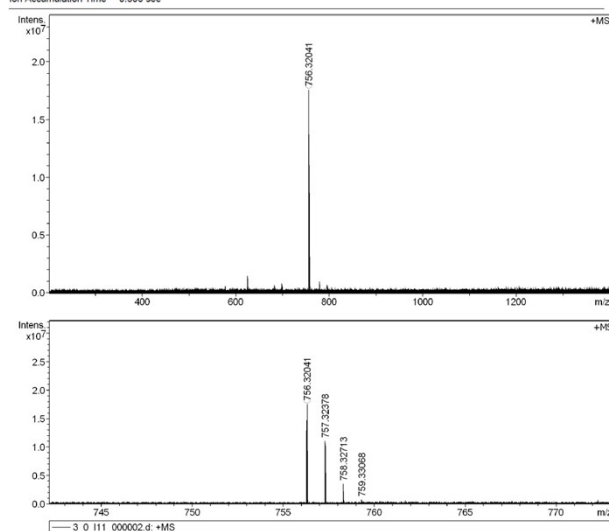
Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdB	e ⁻ Conf	N-Rule
602.242256	1	C ₄₅ H ₃₄ Si	100.00	602.242429	-0.3	-0.2	40.9	30.0	odd	ok

Figure 11S HRMS spectrum of compound 2

MALDI,3

Analysis Info
 Analysis Name: D:\Data\MALDI\2020\0224\3_0_111_000002.d
 Method: MALDI_P_100-3000
 Sample Name: MURU-N-ESI
 Comment:
 Acquisition Date: 2/26/2020 12:34:06 PM
 Operator: solarix
 Instrument: solarix

Acquisition Parameter
 Acquisition Mode: Single MS
 Polarity: Positive
 Broadband Low Mass: 202.1 m/z
 Broadband High Mass: 1400.0 m/z
 Source Accumulation: 0.001 sec
 Ion Accumulation Time: 0.300 sec
 Acquired Scans: 15
 No. of Cell Fills: 1
 No. of Laser Shots: 10
 Laser Power: 20.0 Ip
 Laser Shot Frequency: 0.020 sec
 Calibration Date: Wed Feb 26 12:29:45
 Data Acquisition Size: 2098152
 Data Processing Size: 4194304
 Apodization: Sine-Bell Multiplication



Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdB	e ⁻ Conf	N-Rule
756.320415	1	C ₅₇ H ₄₄ Si	100.00	756.320679	-0.4	-0.0	43.4	37.0	odd	ok

Figure 12S HRMS spectrum of compound 3