

Supporting Information for

Copper Catalyzed Preparation of Benzo[3,4]indolo[1,2-*b*]isoquinoline-8-ones and Photoluminescence Exploration

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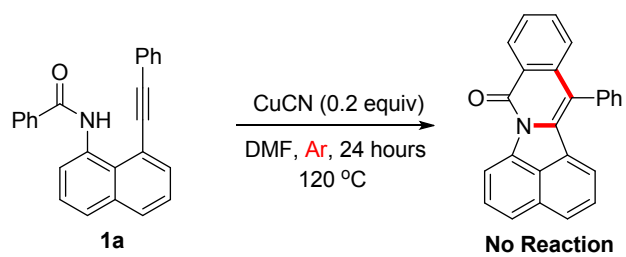
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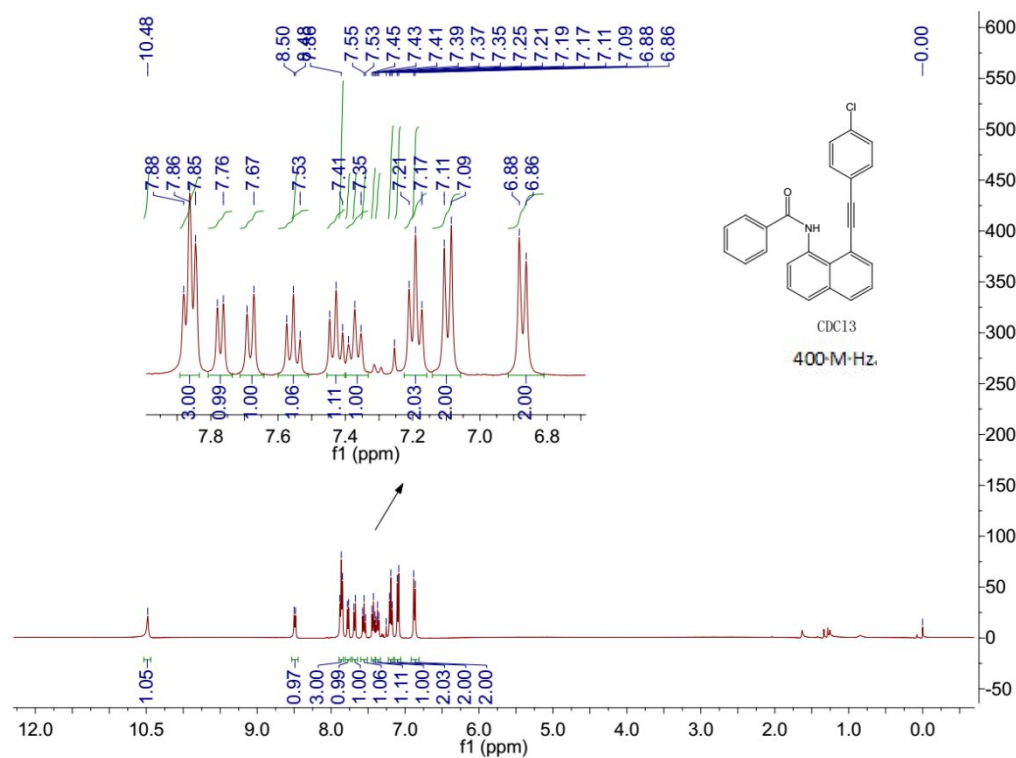
1. Control experiment (Scheme S1)
2. The deuterium labeling studies
3. The photophysical properties of products
4. Copies of the Products ^1H NMR, ^{13}C NMR

1. Control experiment (Scheme S1)

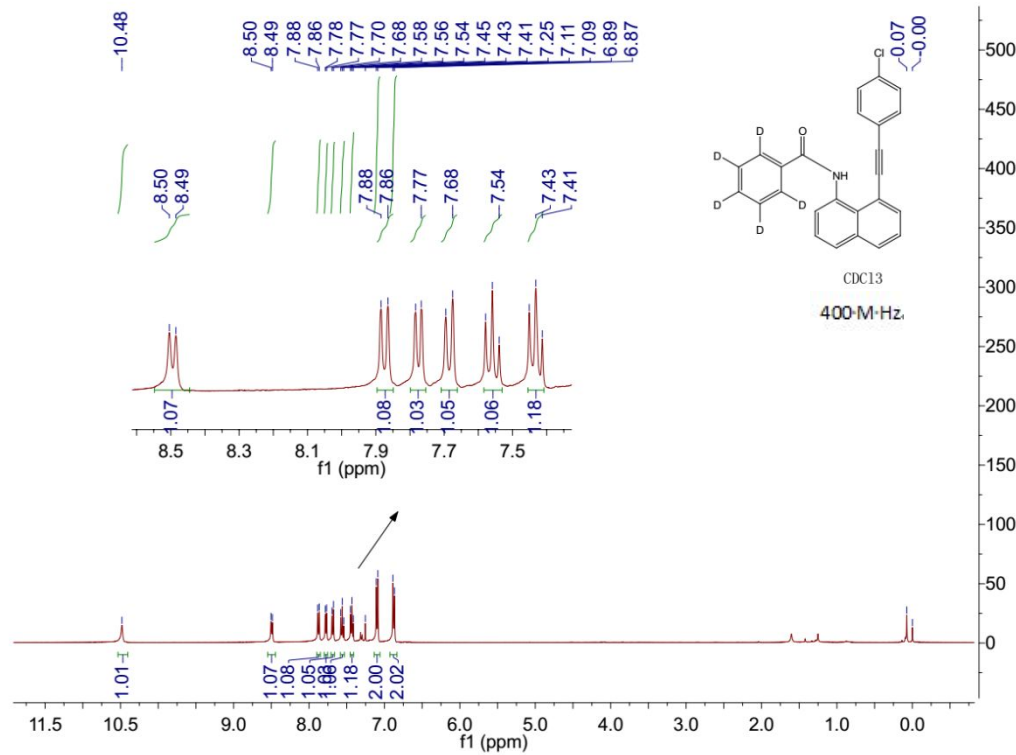


2. The deuterium labeling studies

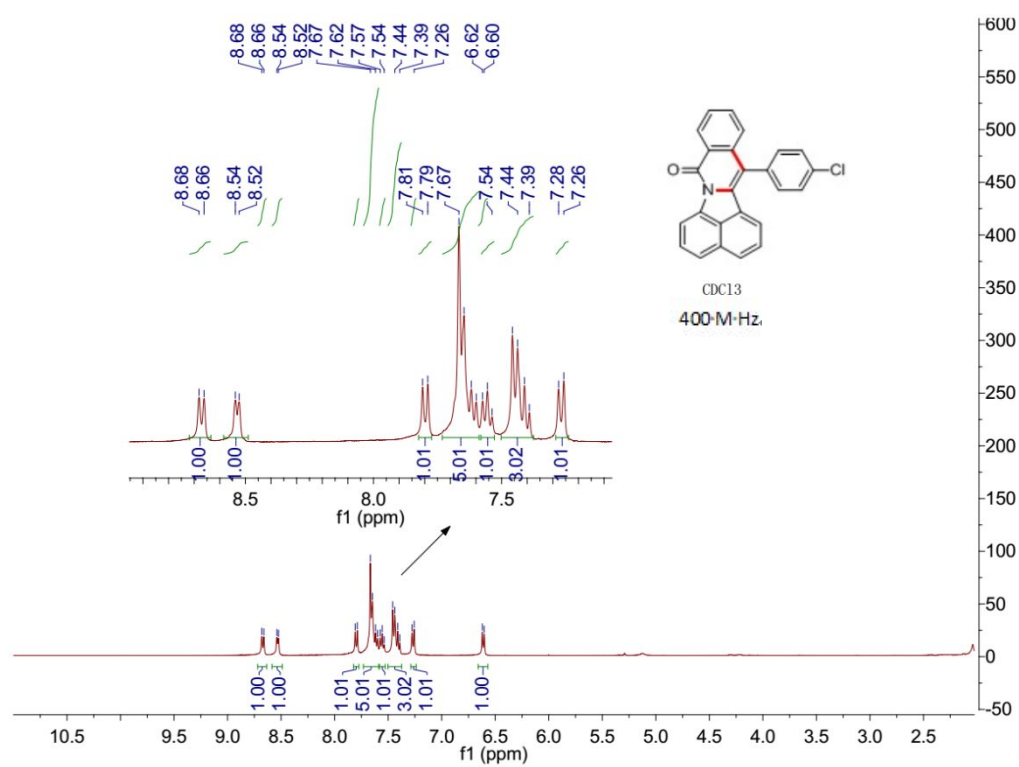
^1H NMR of **1a-H₅**



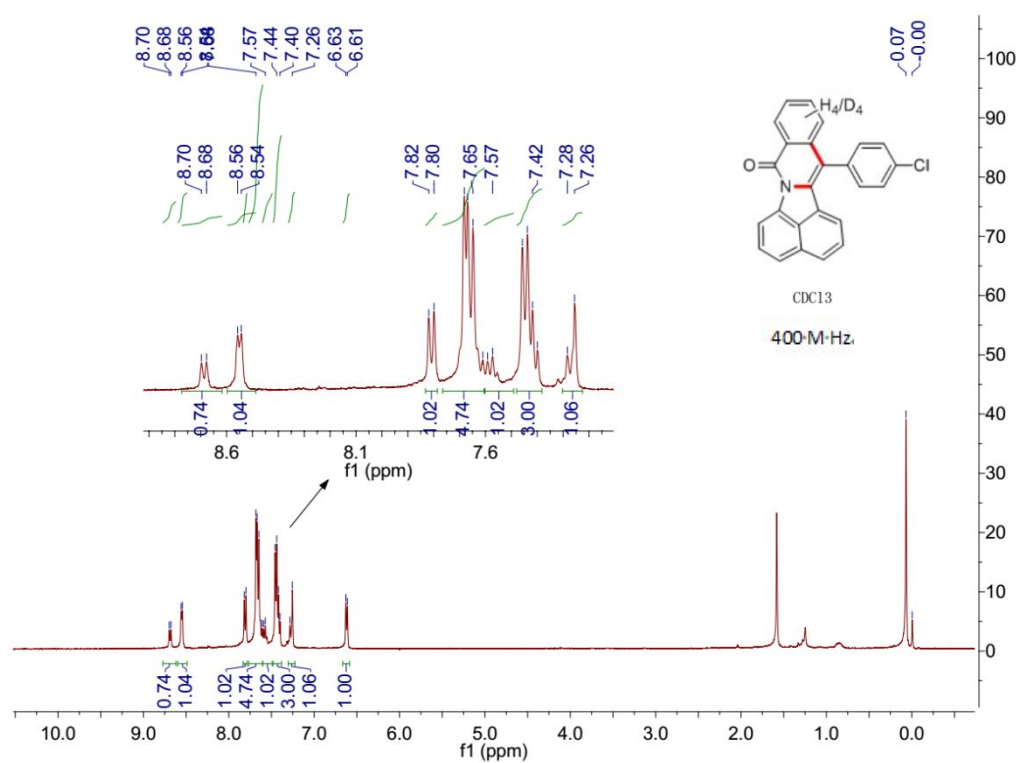
^1H NMR of **1a-D₅**



^1H NMR of **2a-H₅**

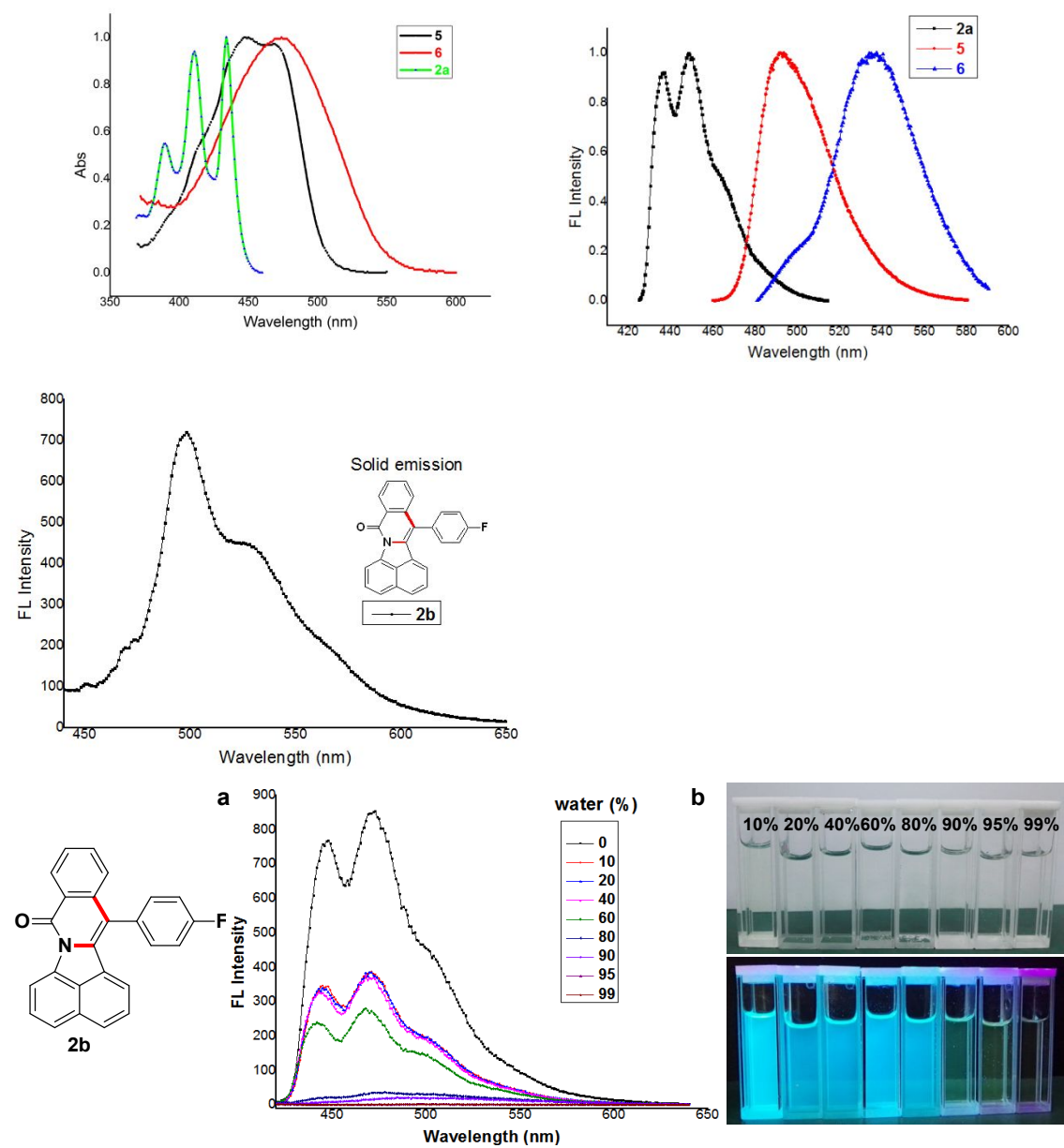


^1H NMR of **2a-D₅**



3. The photophysical properties of products

Absorption and emission spectra of these compounds in solutions were measured in Tetrahydrofuran (THF) with a concentration of 10^{-5} M.



4. Copies of the Products ^1H NMR, ^{13}C NMR

Figure S1 ^1H -NMR spectrum of **2a**

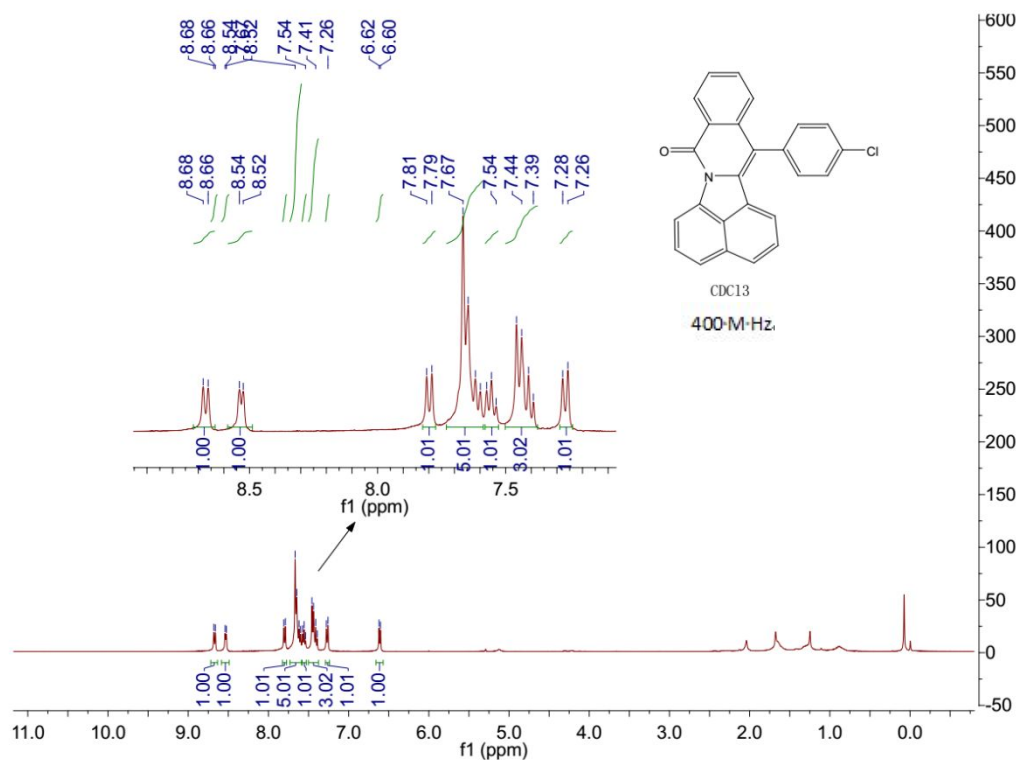


Figure S2 ^{13}C -NMR spectrum of **2a**

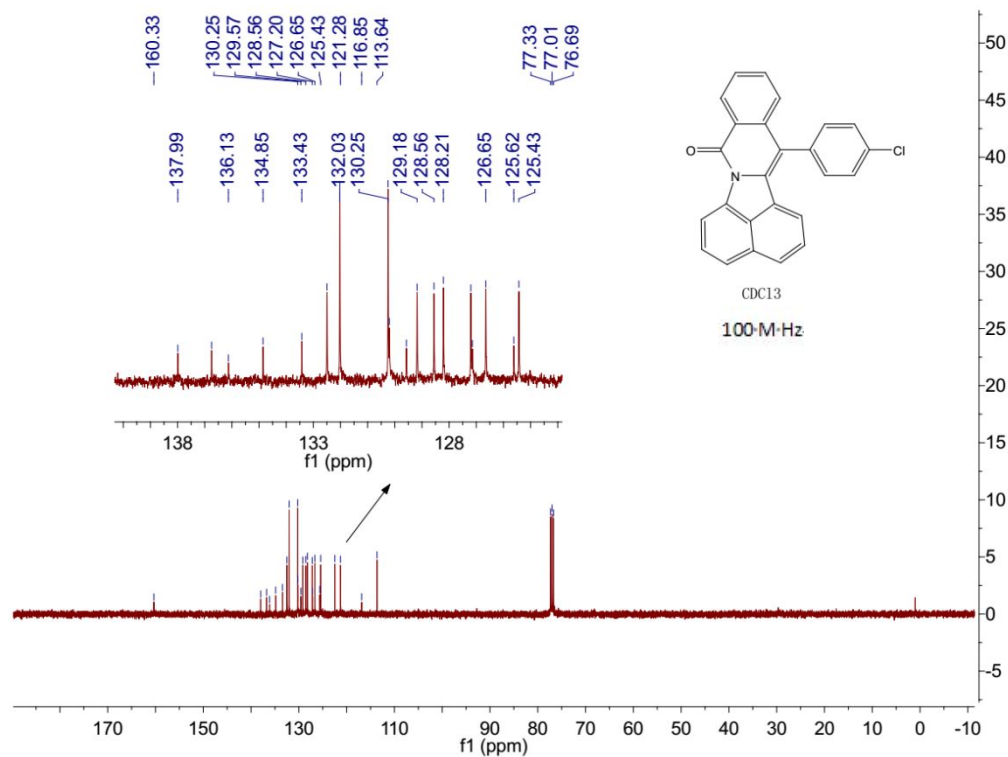


Figure S3 ^1H -NMR spectrum of **2b**

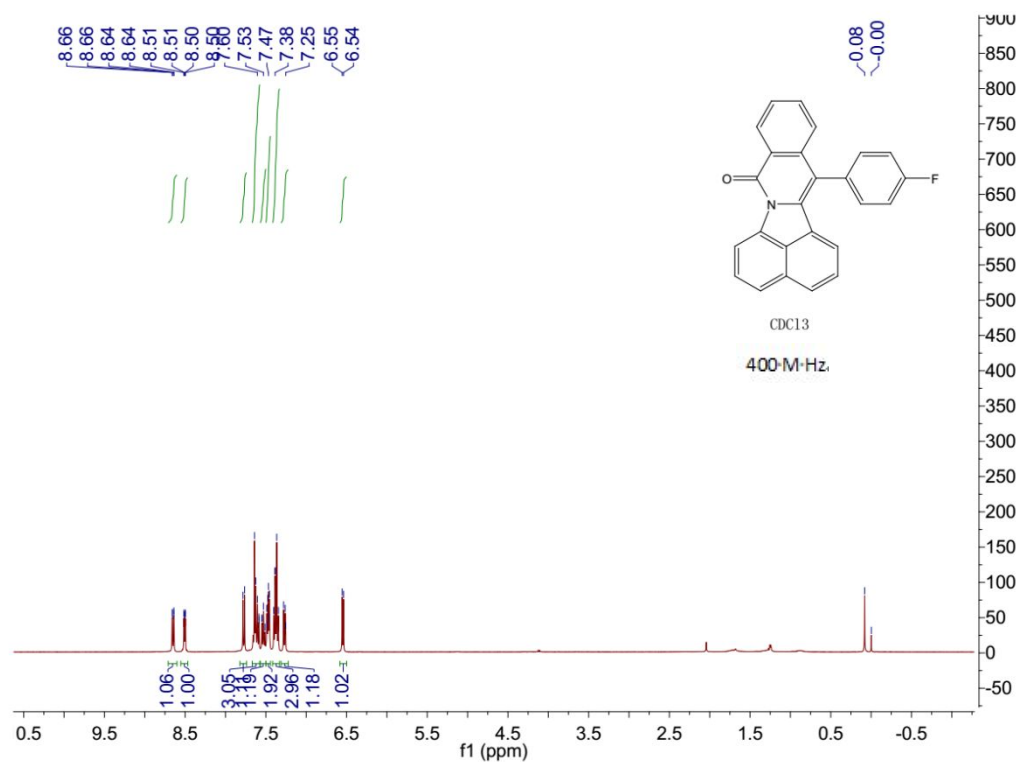


Figure S4 ^{13}C -NMR spectrum of **2b**

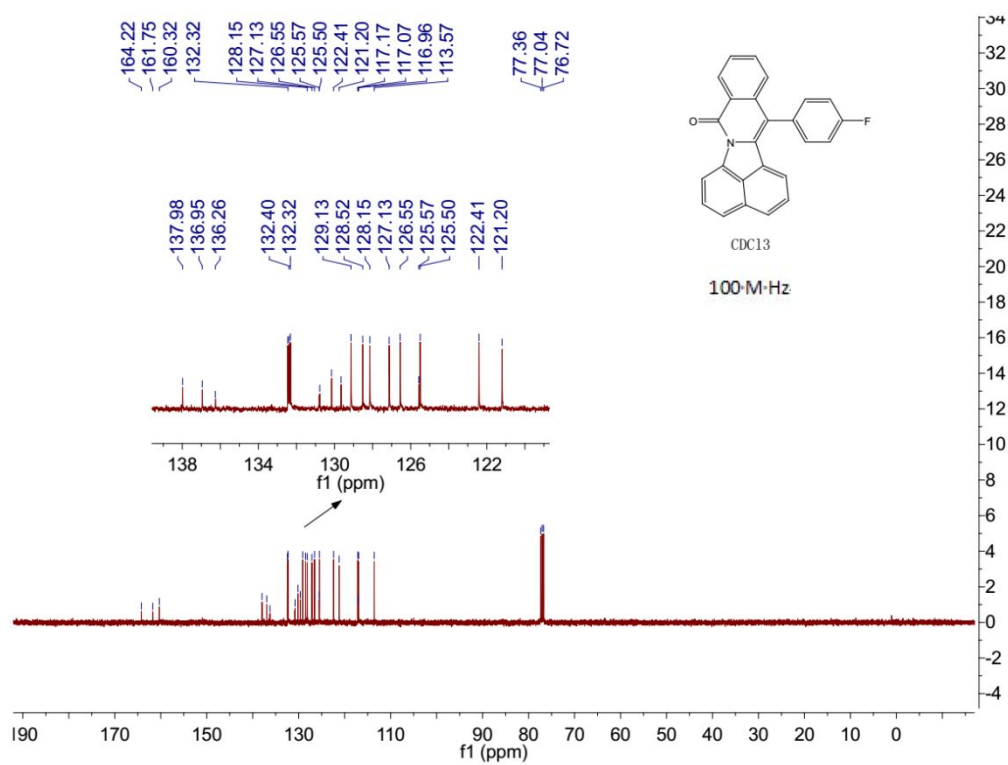


Figure S5 ^1H -NMR spectrum of **2c**

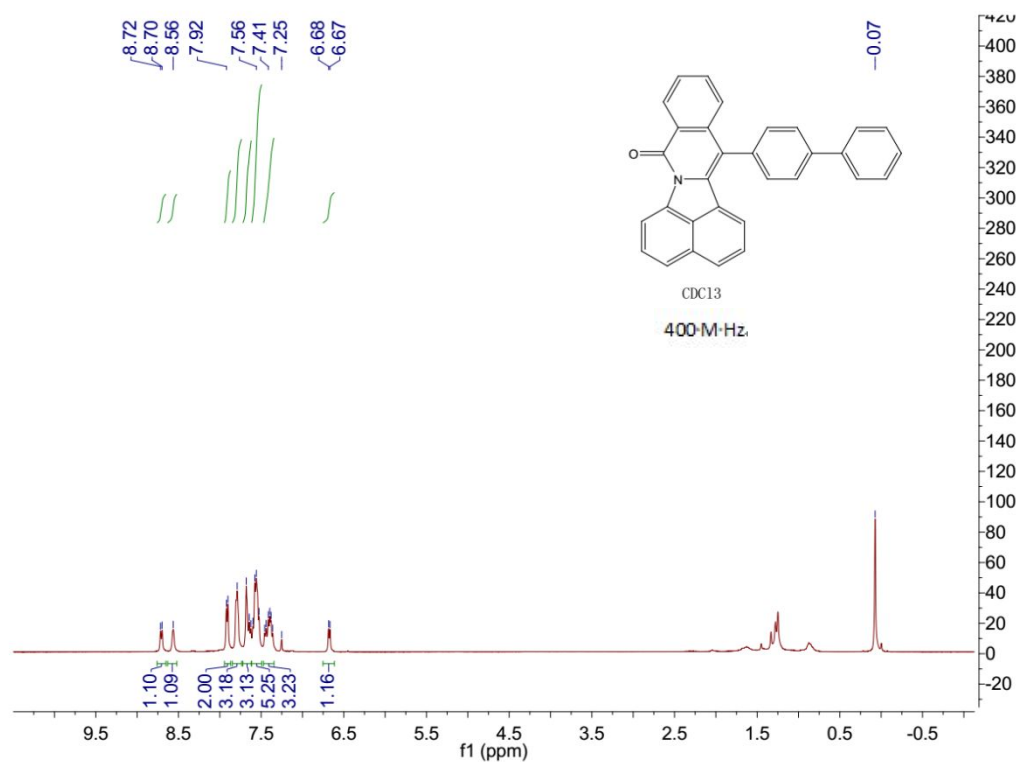


Figure S6 ^{13}C -NMR spectrum of **2c**

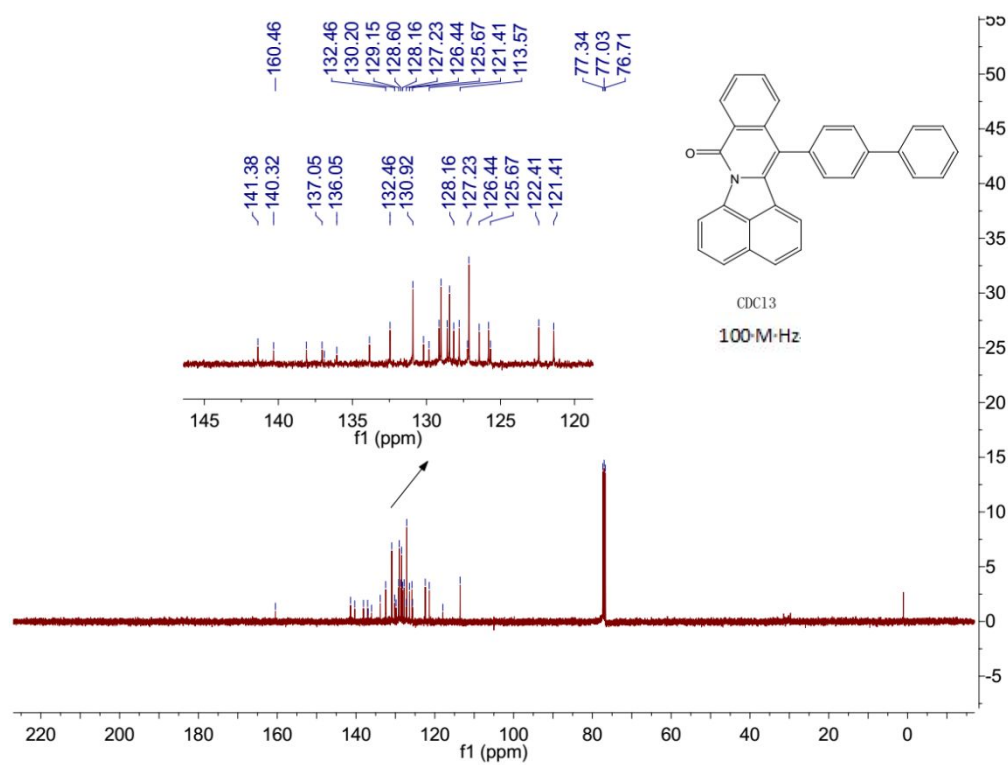


Figure S7 ^1H -NMR spectrum of **2d**

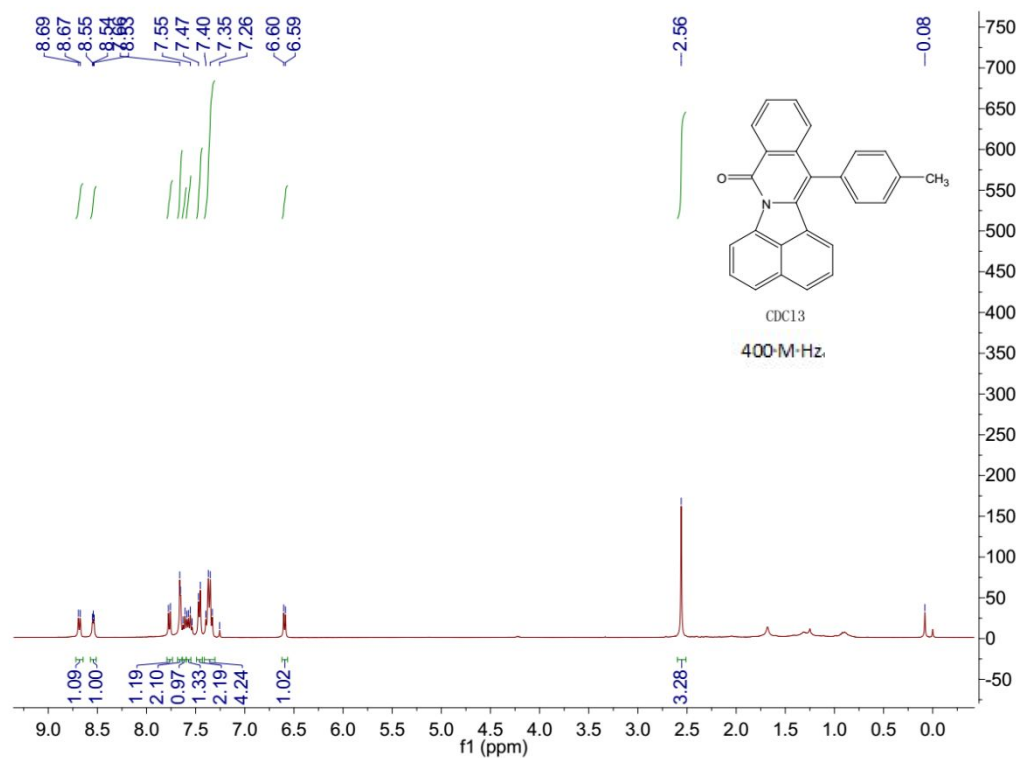


Figure S8 ^{13}C -NMR spectrum of **2d**

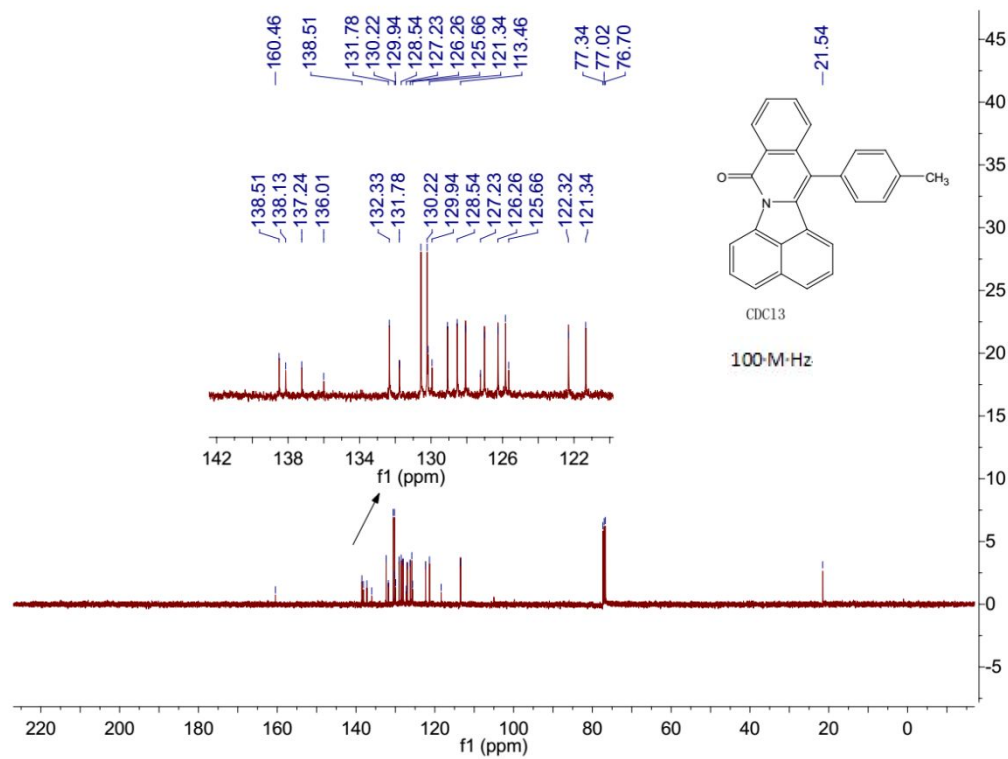


Figure S9 ^1H -NMR spectrum of **2e**

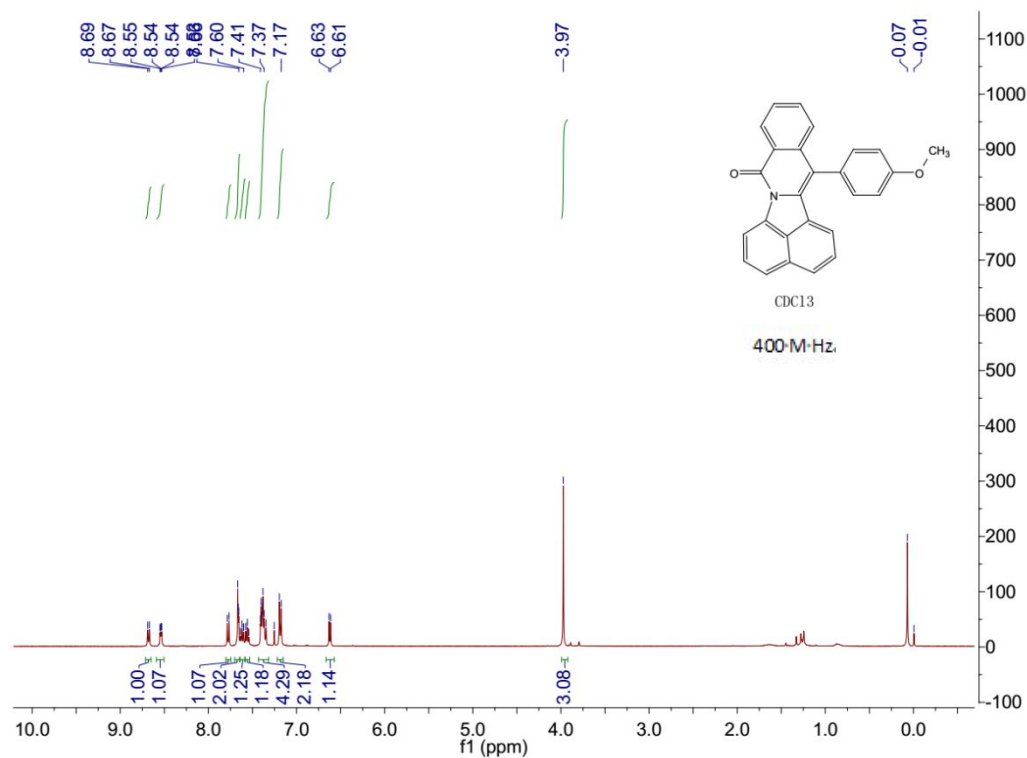


Figure S10 ^{13}C -NMR spectrum of **2e**

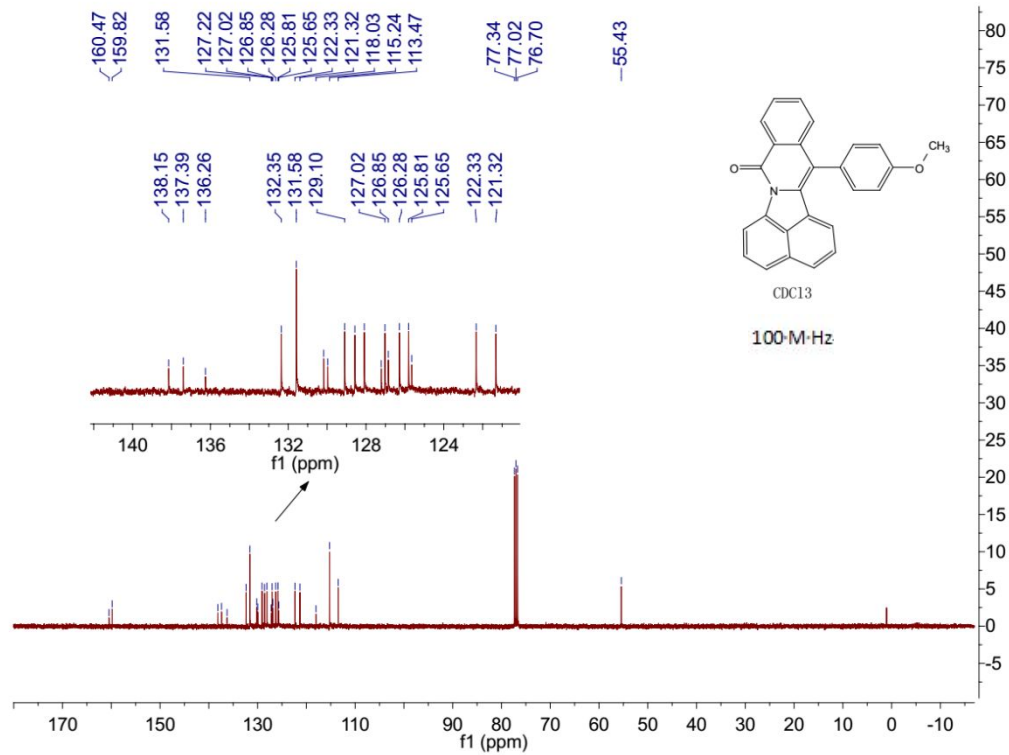


Figure S11 ^1H -NMR spectrum of **2f**

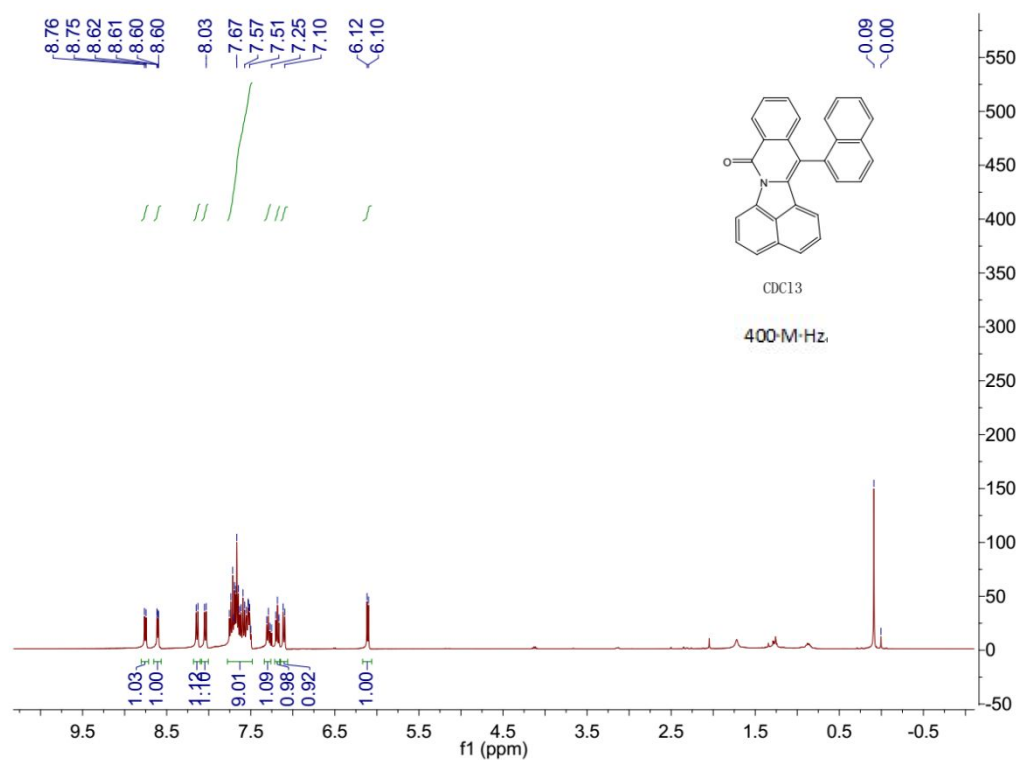


Figure S12 ^{13}C -NMR spectrum of **2f**

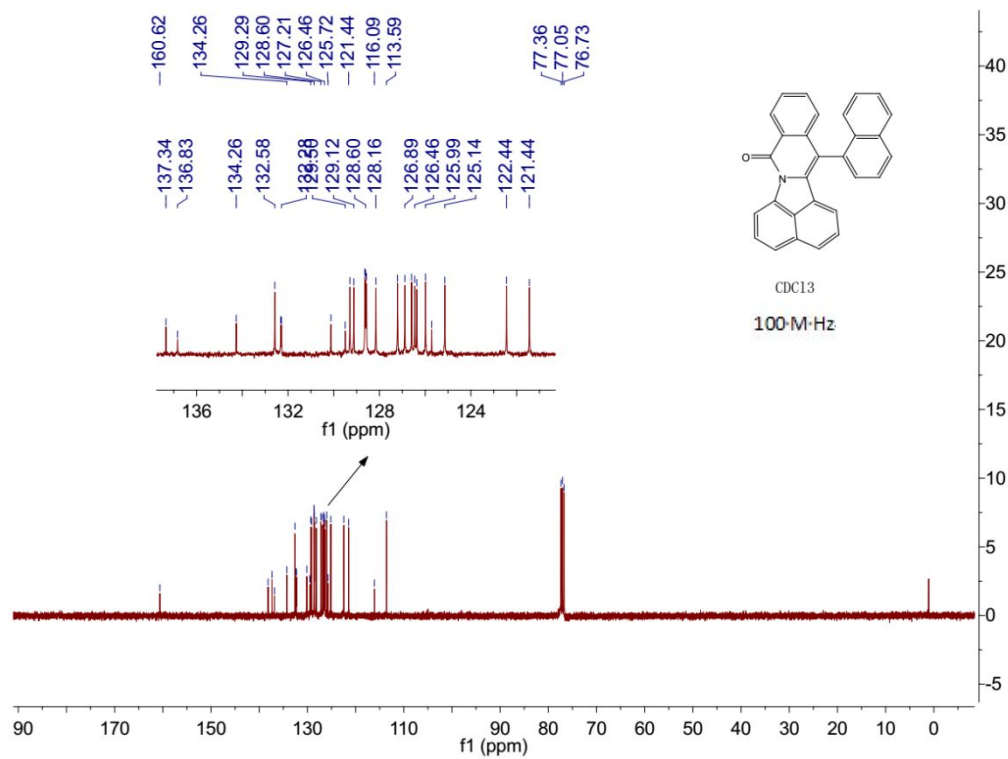


Figure S13 ^1H -NMR spectrum of **2g**

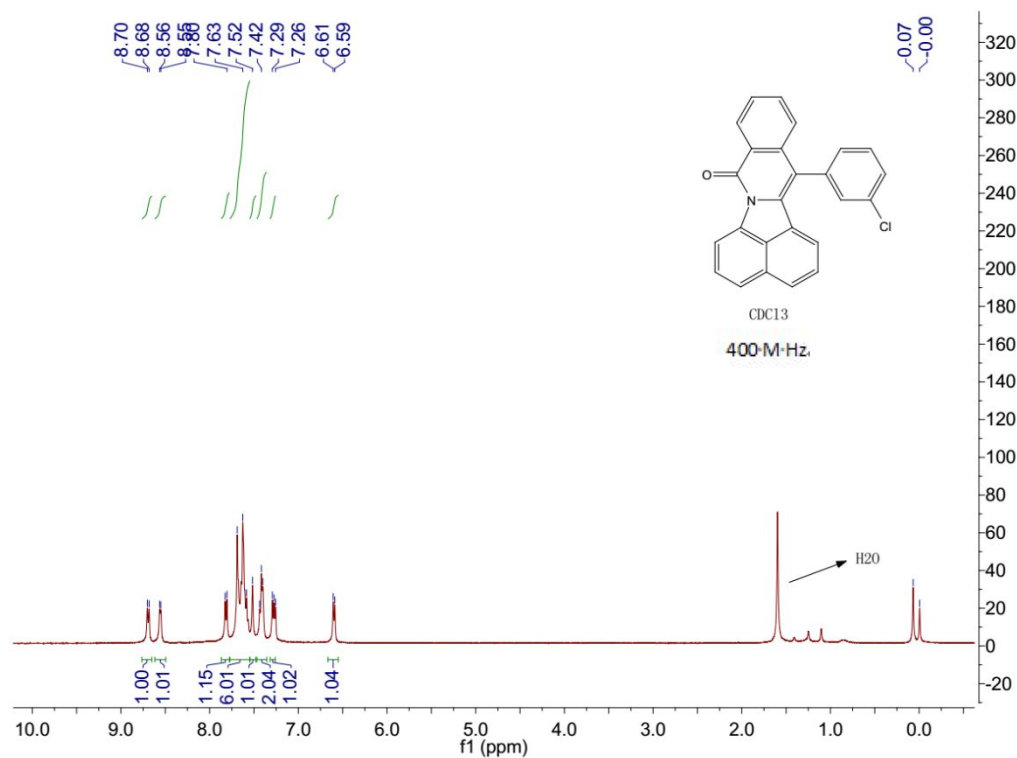


Figure S14 ^{13}C -NMR spectrum of **2g**

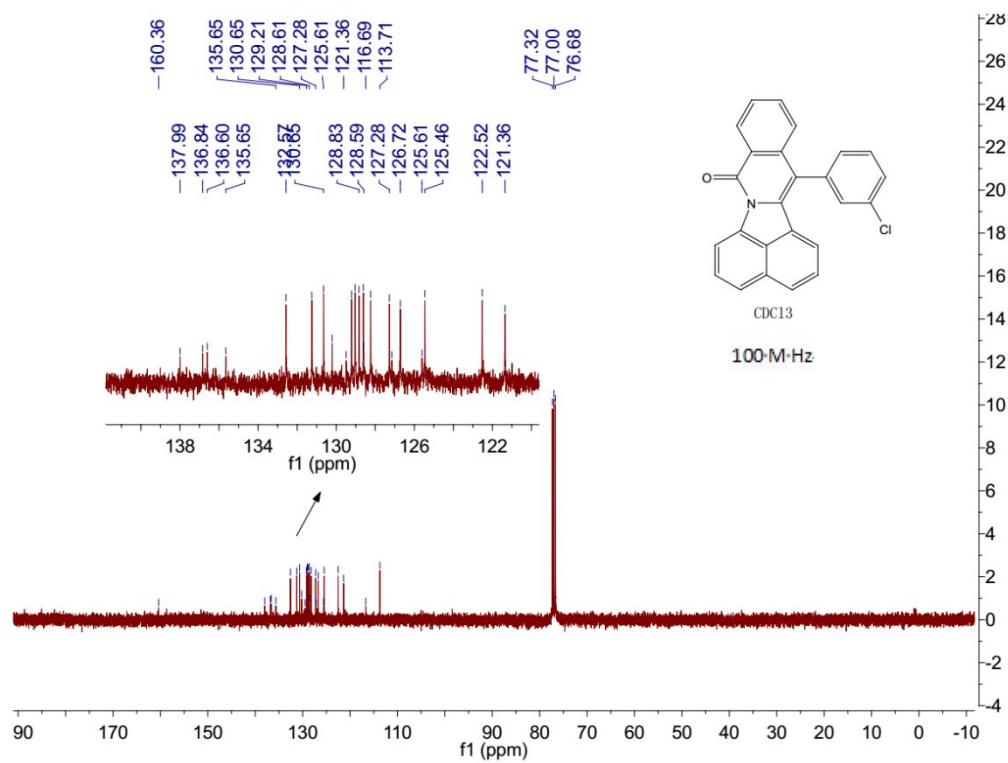


Figure S15 ^1H -NMR spectrum of **2h**

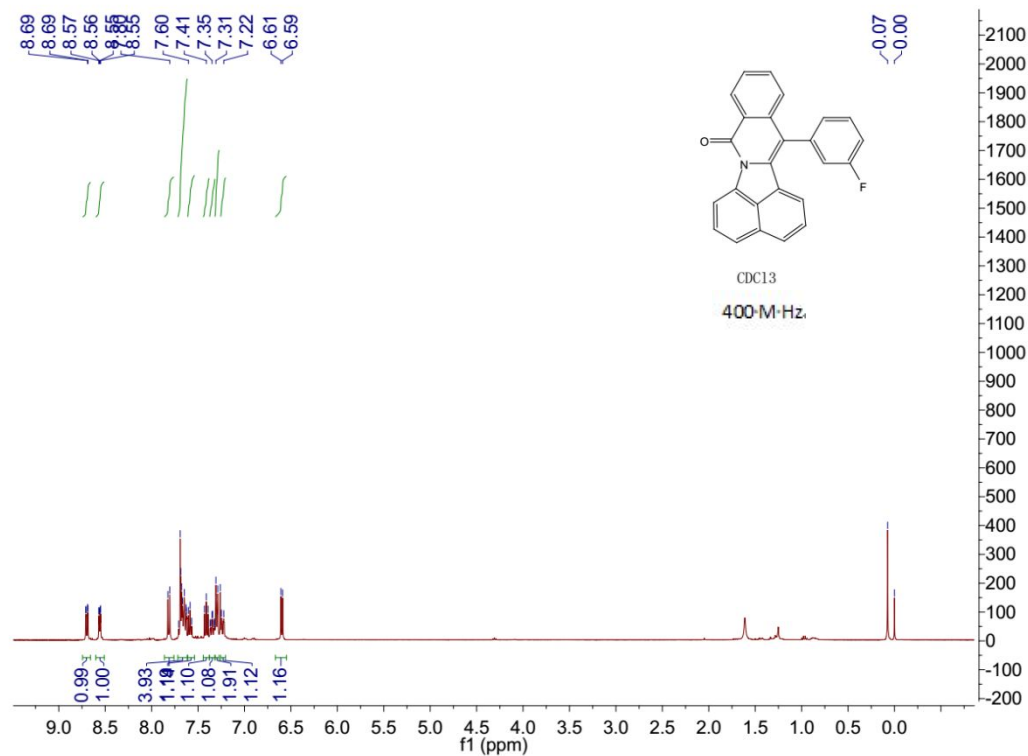


Figure S16 ^{13}C -NMR spectrum of **2h**

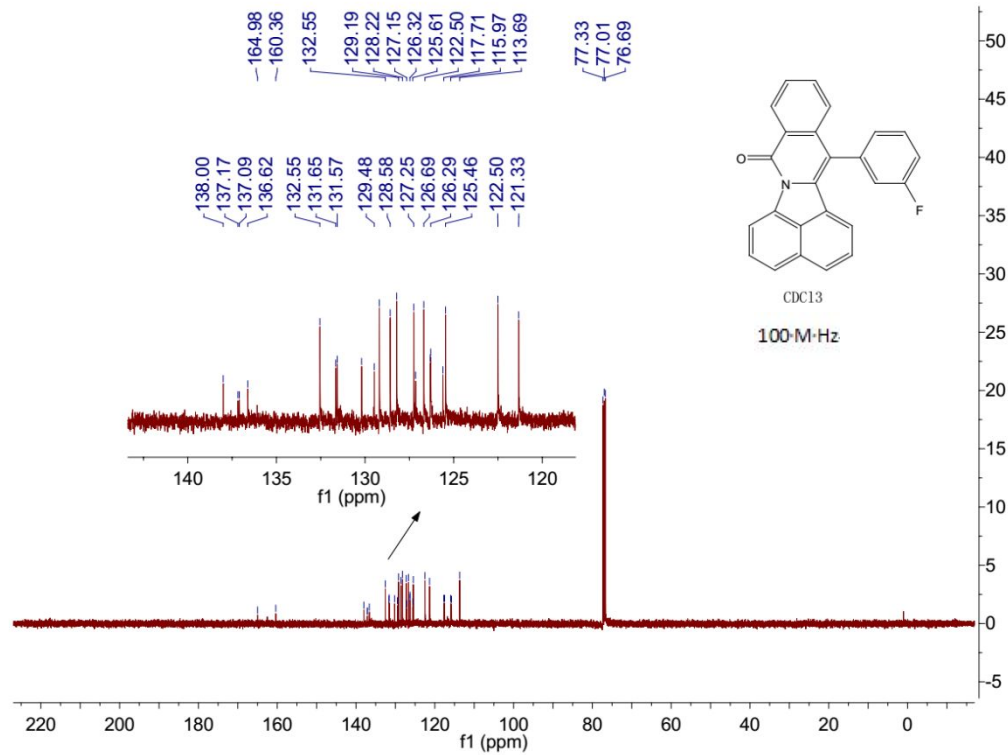


Figure S17 ^1H -NMR spectrum of **2i**

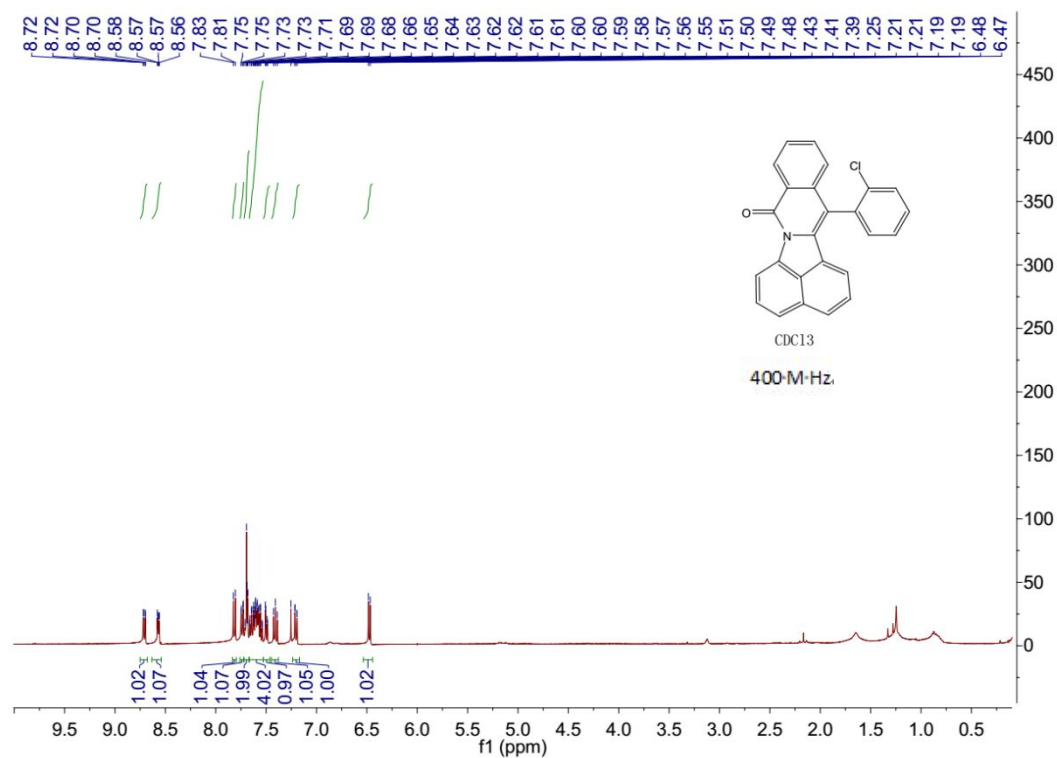


Figure S18 ^{13}C -NMR spectrum of **2i**

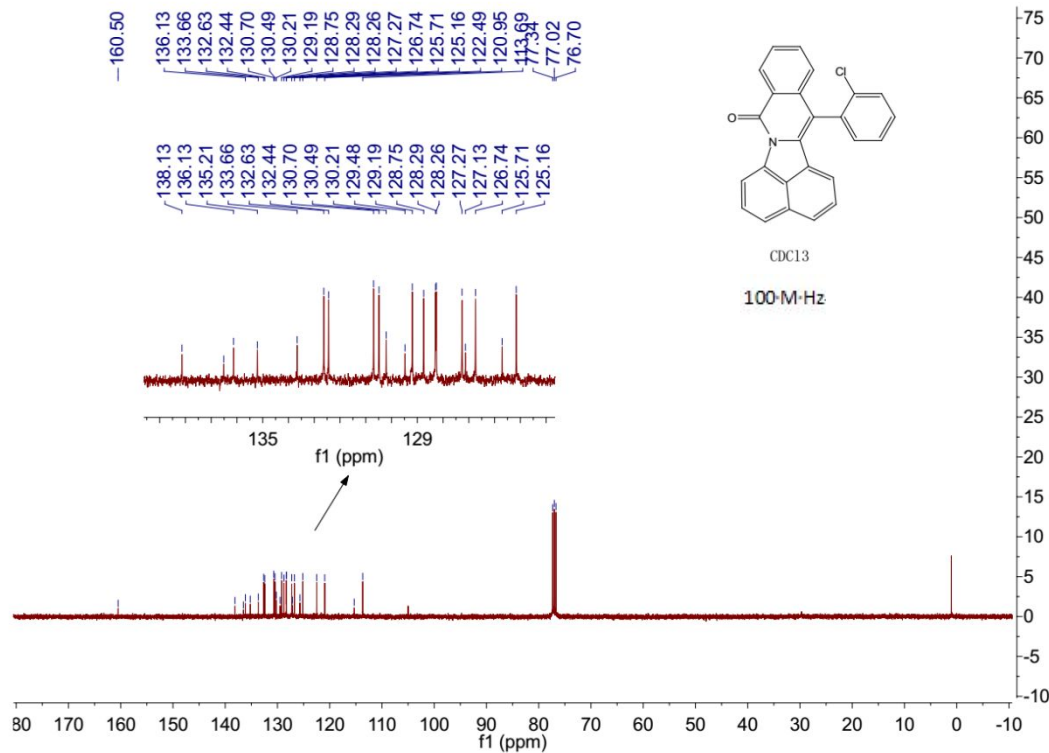


Figure S19 ^1H -NMR spectrum of **2j**

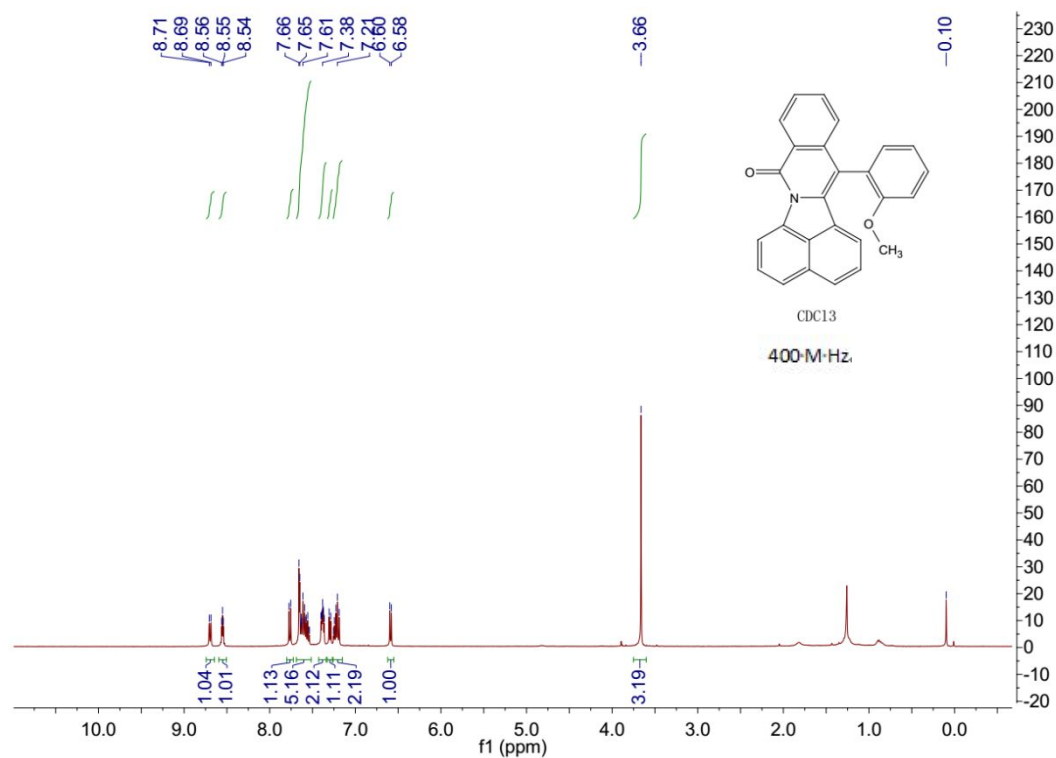


Figure S20 ^{13}C -NMR spectrum of **2j**

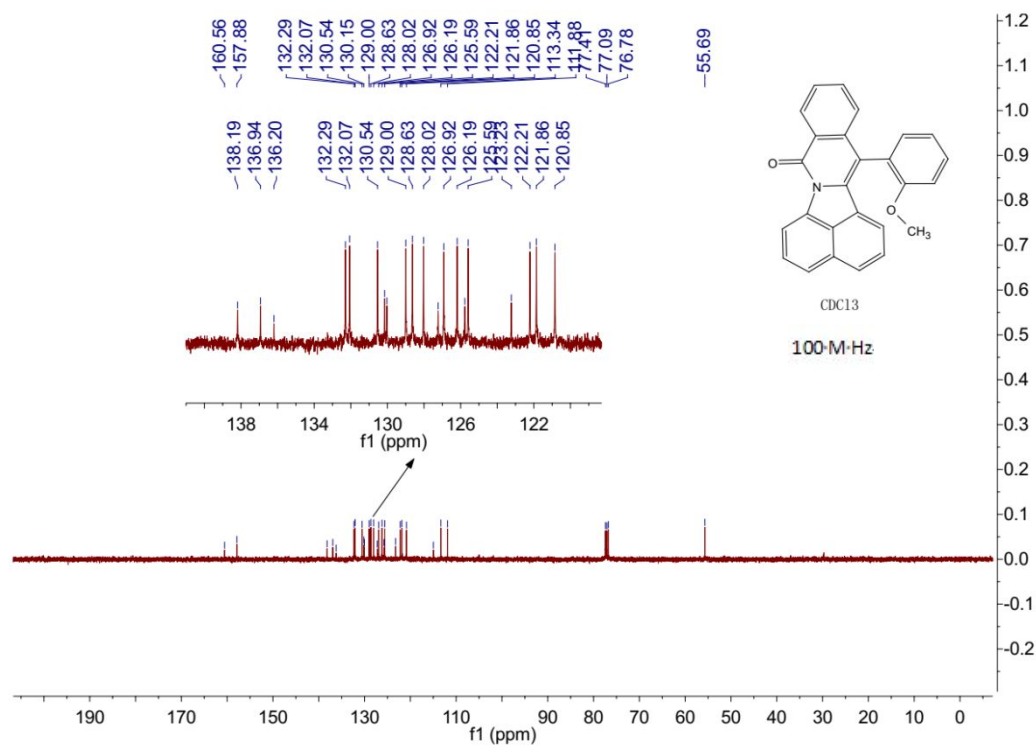


Figure S21 ^1H -NMR spectrum of **2k**

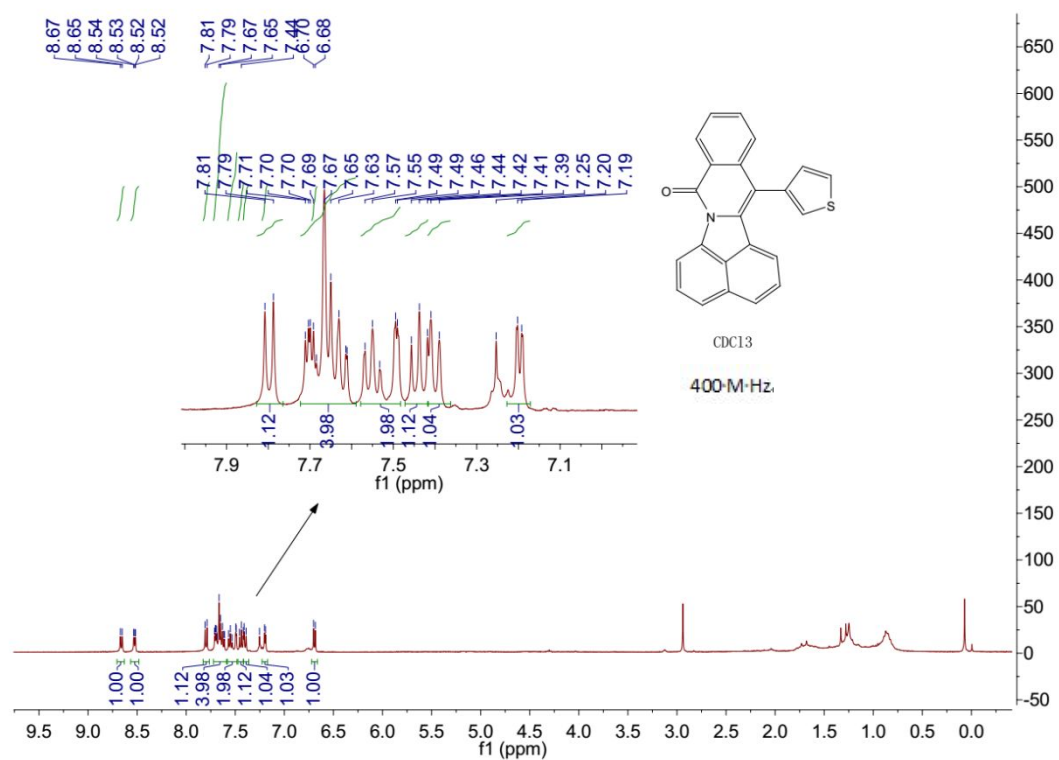


Figure S22 ^{13}C -NMR spectrum of **2k**

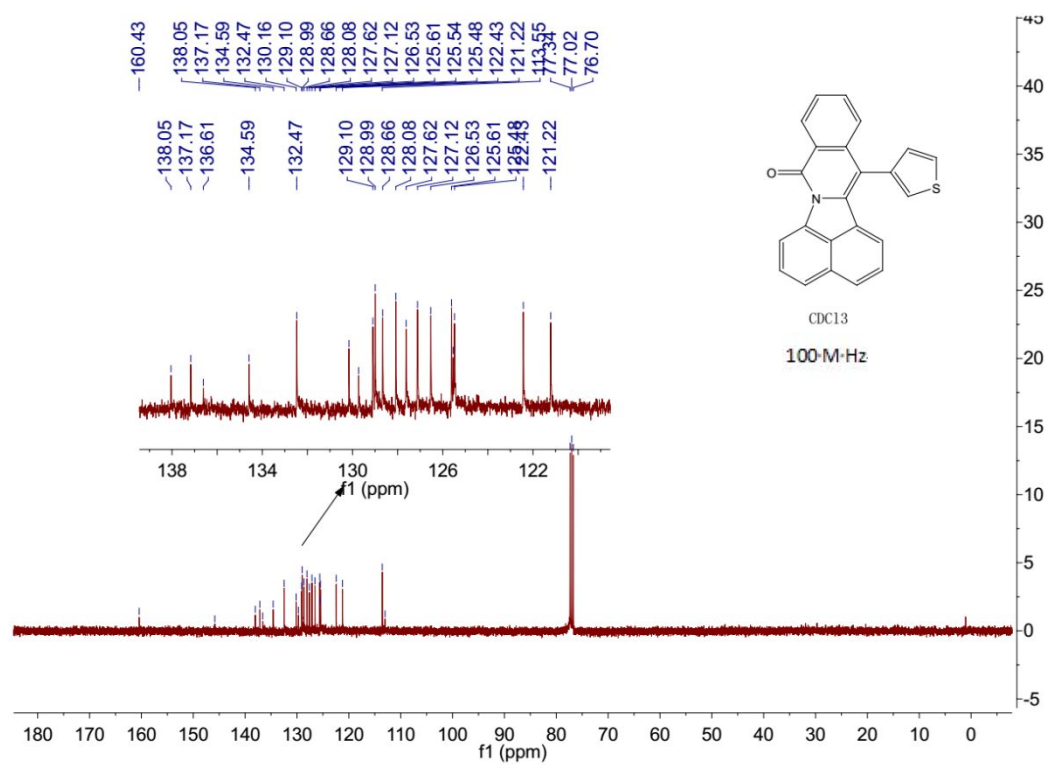


Figure S23 ^1H -NMR spectrum of **2l**

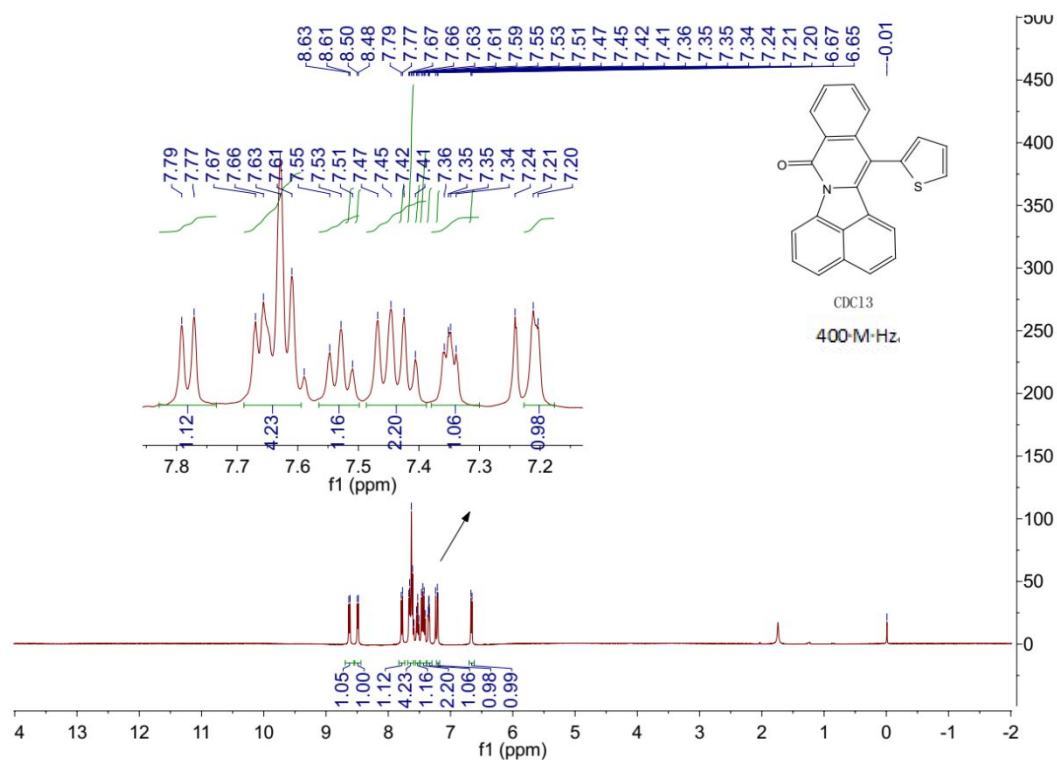


Figure S24 ^{13}C -NMR spectrum of **2l**

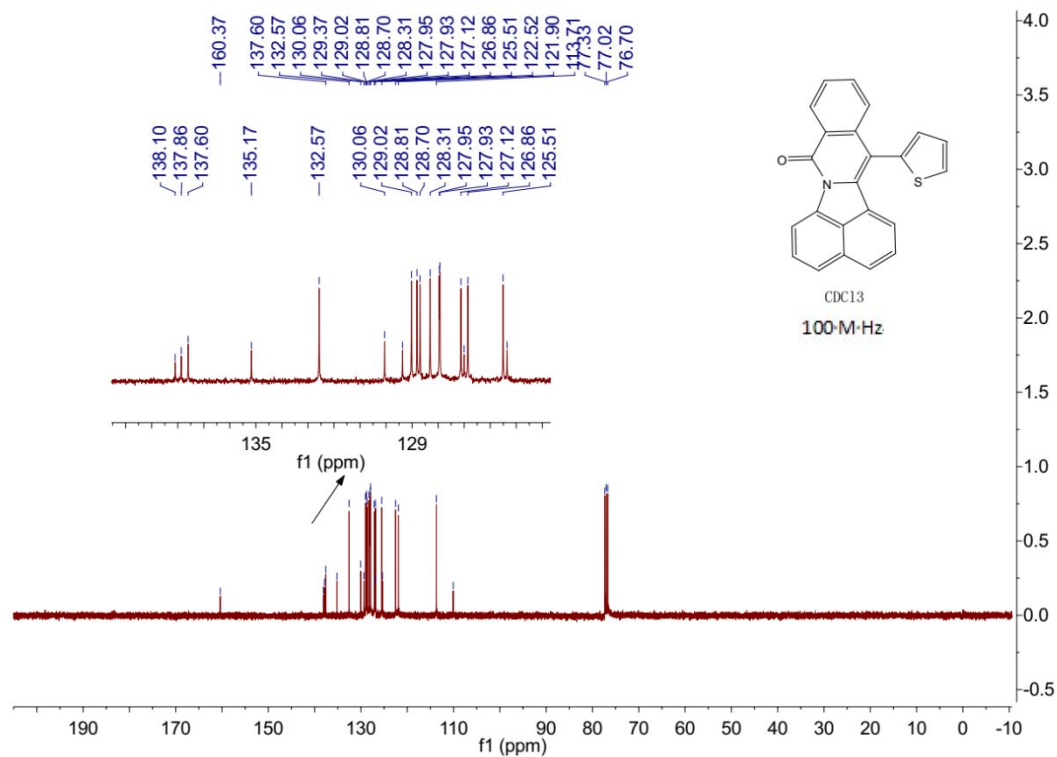


Figure S25 ^1H -NMR spectrum of **2m**

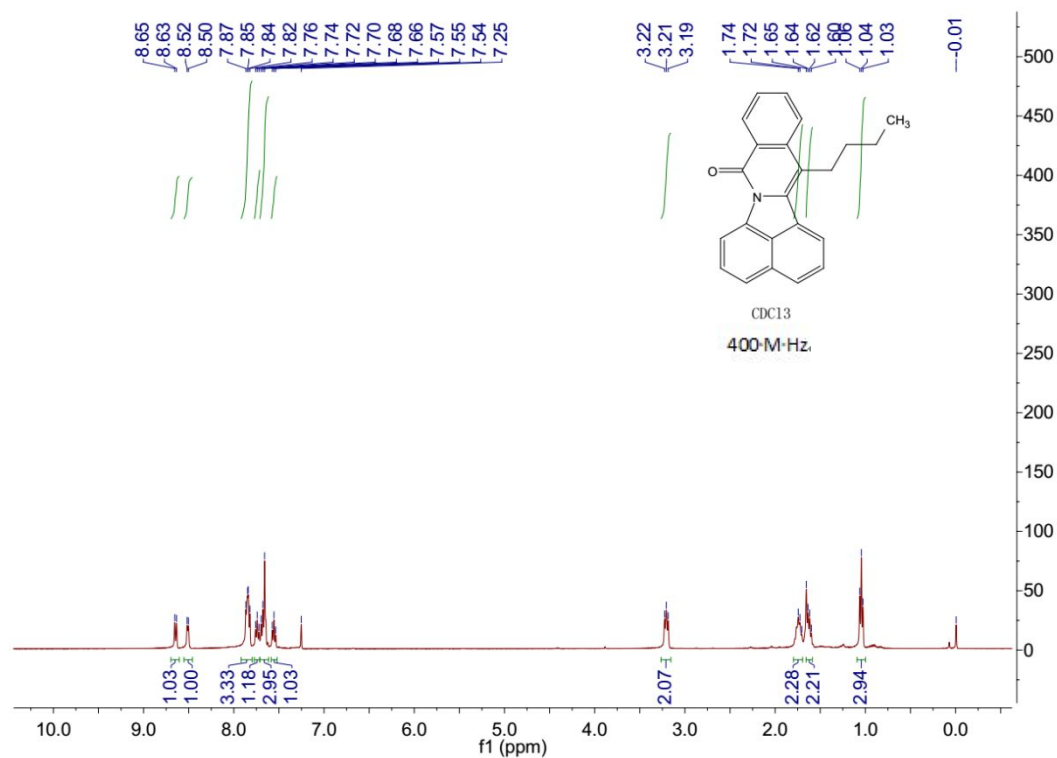


Figure S26 ^{13}C -NMR spectrum of **2m**

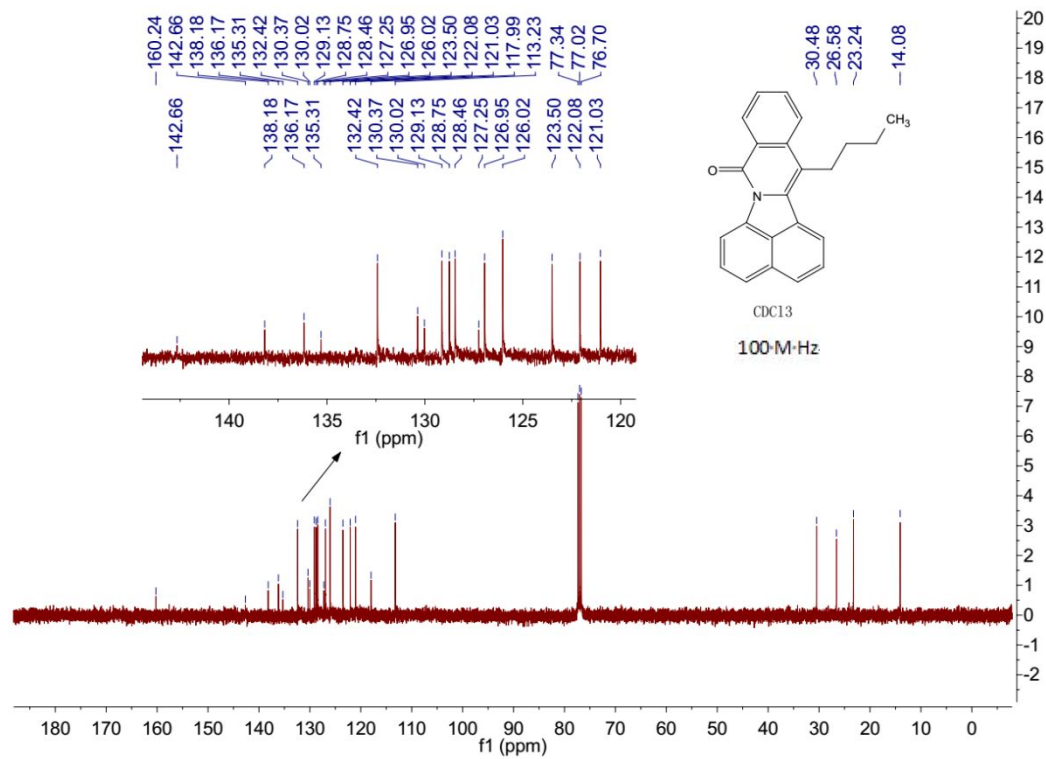


Figure S27 ^1H -NMR spectrum of **4a**

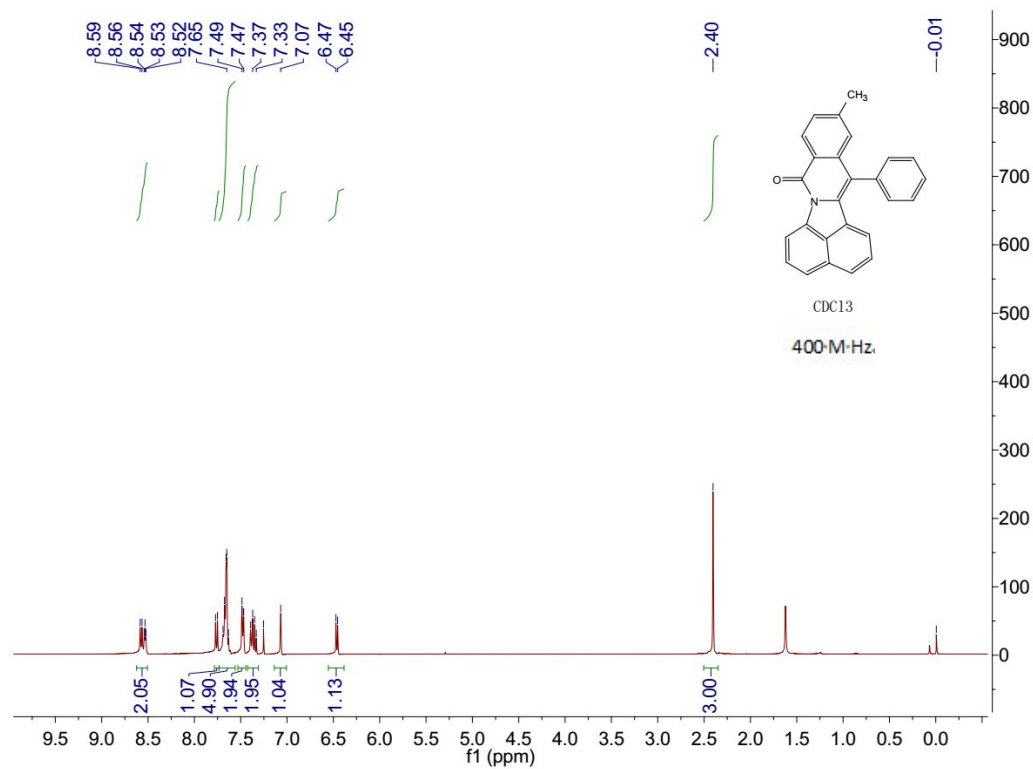


Figure S28 ^{13}C -NMR spectrum of **4a**

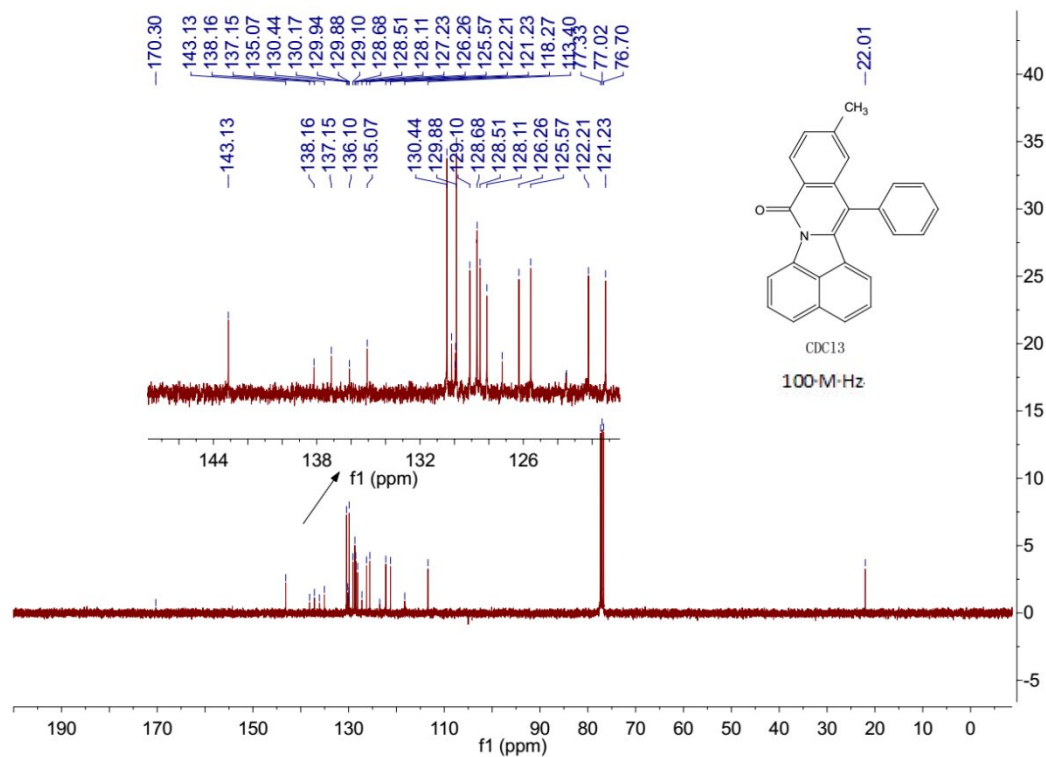


Figure S29 ^1H -NMR spectrum of **4b**

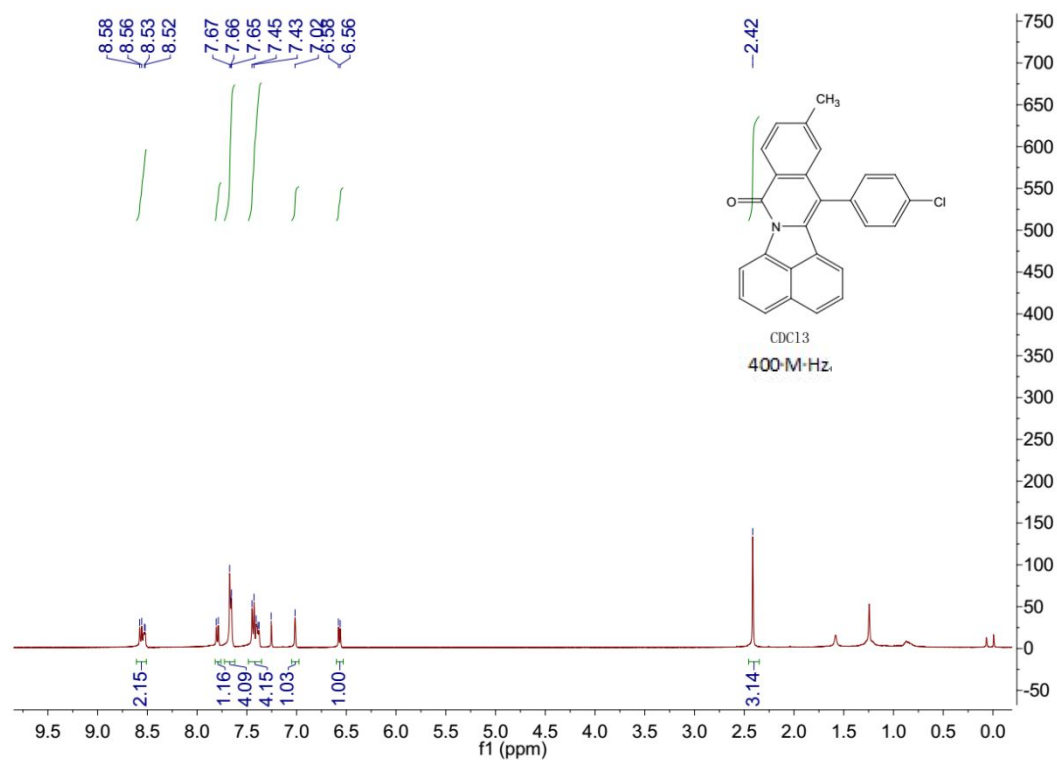
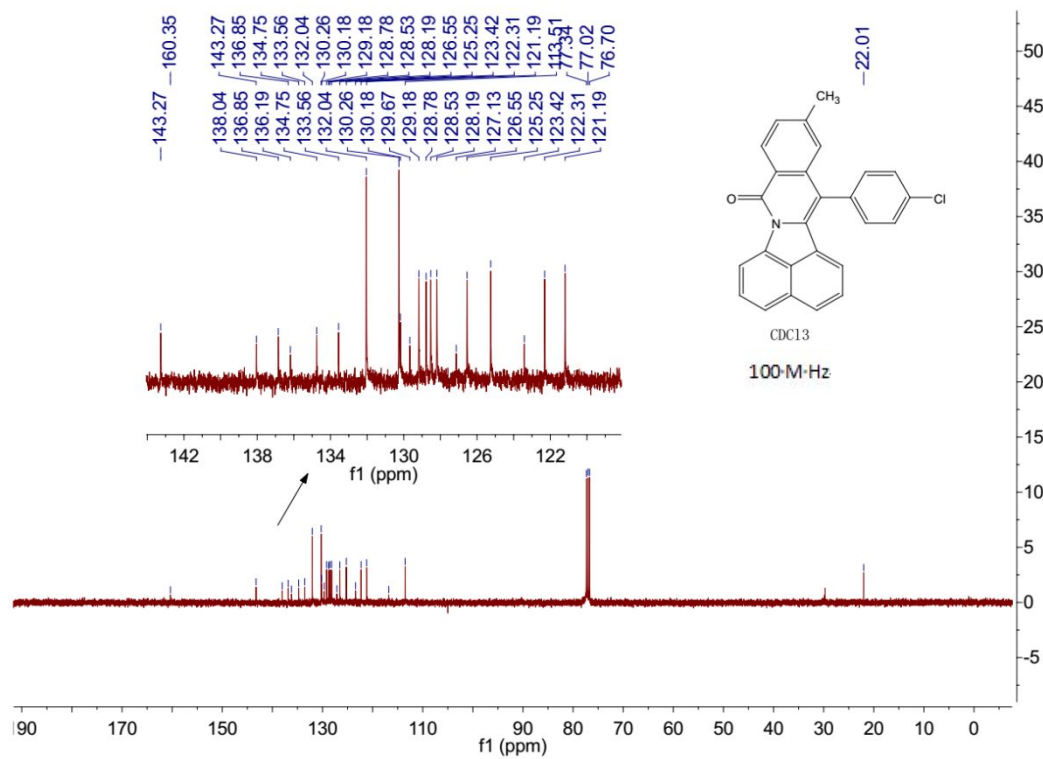


Figure S30 ^{13}C -NMR spectrum of **4b**



Chemical structure of 2-(2,6-dichlorophenyl)-1-phenylisoquinolin-3(1H)-one is shown. The ^1H NMR spectrum (400 MHz, CDCl_3) displays peaks corresponding to the structure. The x-axis represents the chemical shift in ppm (δ), ranging from 10.5 to -0.5. The y-axis represents the intensity. The spectrum shows aromatic signals between 6.5 and 8.7 ppm, a solvent triplet at 7.26 ppm, and aliphatic signals at 1.50 and 1.55 ppm. Integration values are provided below the peaks.

Chemical Shift (δ , ppm)	Integration
8.68, 8.67, 8.53, 8.51	1.05, 1.04
7.78, 7.69, 7.64, 7.59, 7.47, 7.46	1.12, 3.24, 2.91, 1.98, 1.24
7.26 (solvent)	1.00
6.05	1.00
1.55	1.00
1.50	1.00

Chemical structure of 100-M-Hz (100-M-Hz) is shown as an inset. The structure is a tricyclic system consisting of a benzene ring fused to a pyridine ring, which is further fused to a benzene ring. The pyridine ring has a carbonyl group (C=O) at position 2 and a chlorine atom (Cl) at position 4. The benzene ring at position 3 has a phenyl group (C6H5) attached. The solvent is CDCl3 and the concentration is 100-M-Hz.

The ¹³C NMR spectrum (f1 (ppm)) shows peaks at the following chemical shifts (ppm): 137.15, 136.87, 135.75, 132.70, 132.58, 131.79, 131.07, 130.54, 129.97, 129.86, 129.52, 129.21, 129.07, 128.94, 128.78, 128.72, 128.64, 128.64, 128.41, 127.08, 127.01, 127.01, 123.11, 123.04, 116.61, 114.10, 77.32, 77.00, 76.68.

Chemical structure of compound 10: O=C1c2cc(Cl)c(Cl)cc2C3=C(N1C4=CC=CC=C4)C5=CC=CC=C5C6=CC=C(C=C6)Cl

¹H NMR spectrum (CDCl₃) of compound 10. The x-axis represents the chemical shift in ppm (f1), ranging from 0.0 to 9.0. The y-axis represents the intensity in arbitrary units, ranging from -50 to 750. The spectrum shows several peaks in the aromatic region (6.2-8.7 ppm) and a reference peak at 0.0 ppm. Integration values are provided below the peaks.

Chemical Shift (ppm)	Integration
8.68, 8.54, 8.52	1.00, 1.12
7.72, 7.68, 7.60, 7.43, 7.39, 7.25	1.15, 3.20, 2.07, 3.23
6.22, 6.20	1.17
0.06, 0.01	-

13

Chemical structure of **13** is shown, a fluorene derivative with two 4-chlorophenyl groups and a carbonyl group.

¹³C NMR spectrum (CDCl₃) of **13**. The spectrum shows peaks corresponding to the structure, with the solvent triplet (CDCl₃) visible at 77.00 ppm.

Chemical shift values (ppm) labeled on the spectrum:

- 158.32
- 135.82
- 132.12
- 129.88
- 129.05
- 128.83
- 127.49
- 127.40
- 123.24
- 122.98
- 114.24
- 138.18
- 135.82
- 135.49
- 135.38
- 134.80
- 132.89
- 132.33
- 132.12
- 130.02
- 129.88
- 129.61
- 129.05
- 128.83
- 128.69
- 127.49
- 127.40
- 77.32
- 77.00
- 76.69

Figure S35 ^1H -NMR spectrum of **4e**

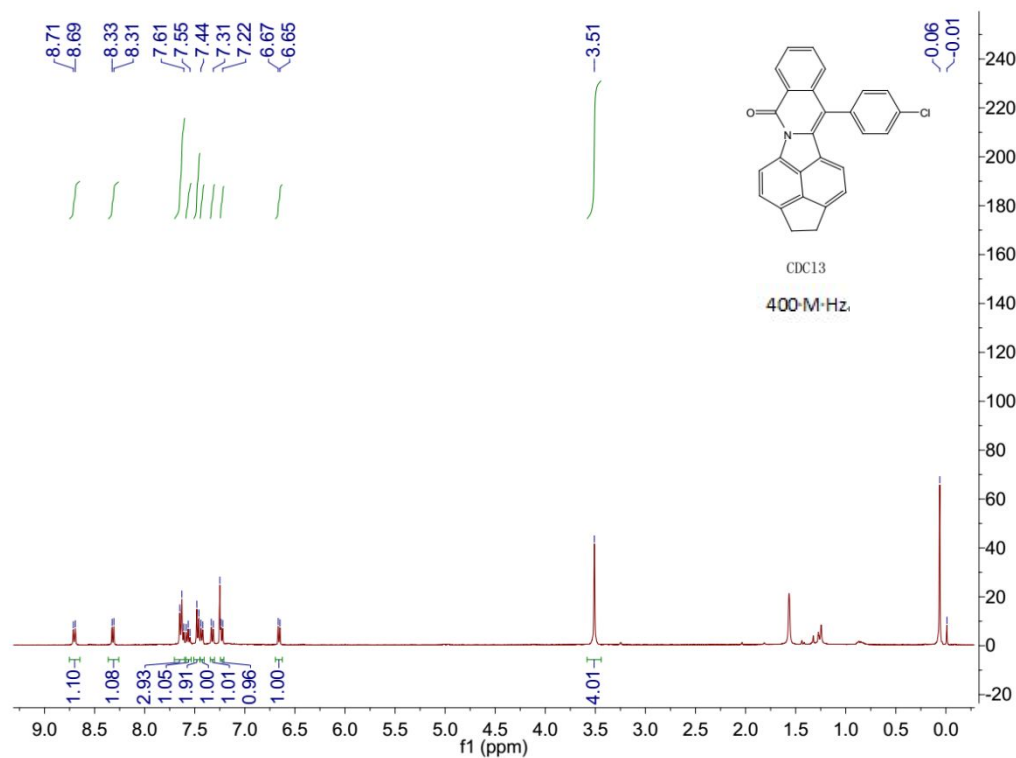


Figure S36 ^{13}C -NMR spectrum of **4e**

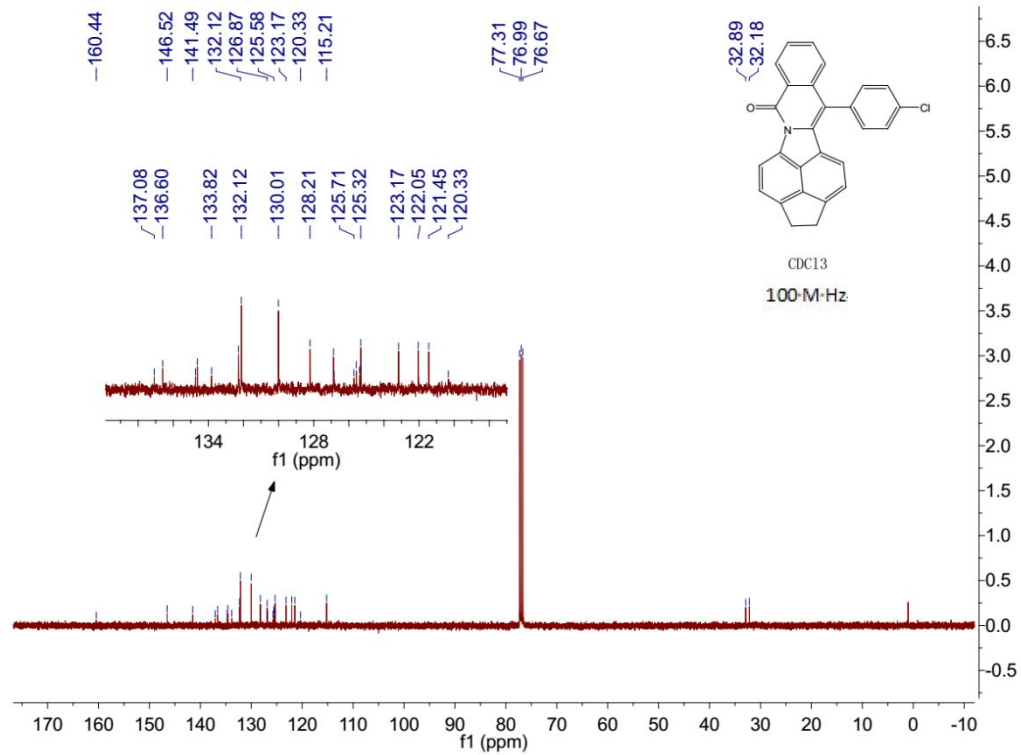


Figure S37 ^1H -NMR spectrum of **4f**

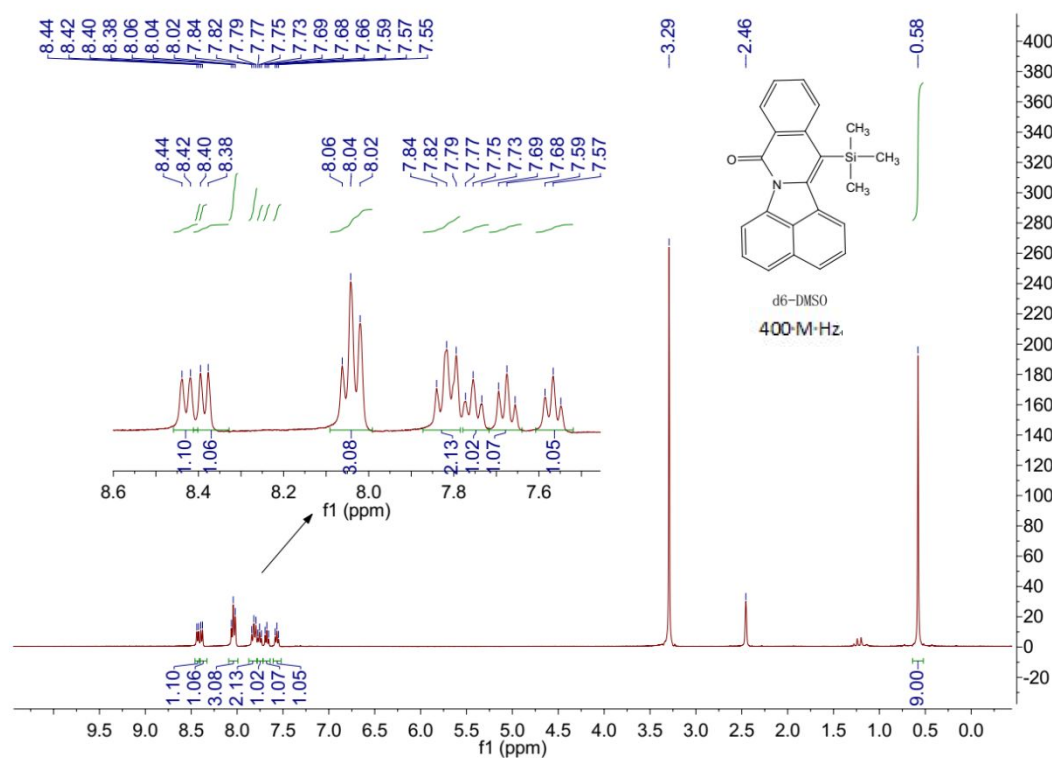


Figure S38 ^{13}C -NMR spectrum of **4f**

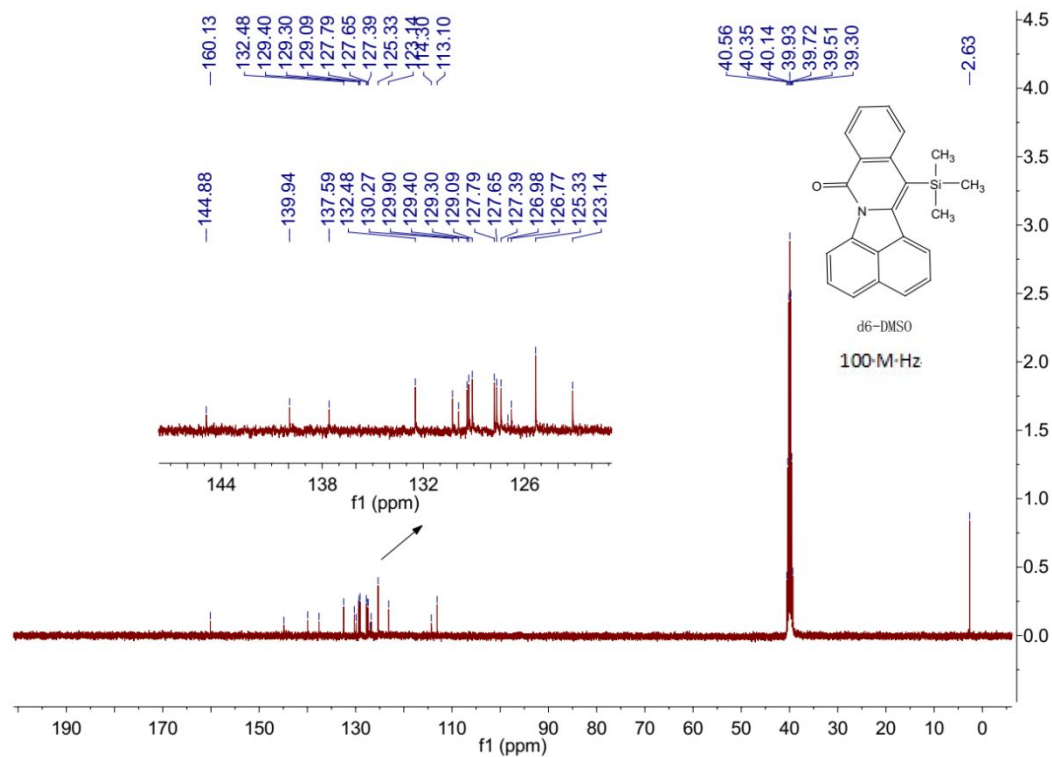


Figure S39 ^1H -NMR spectrum of **5**

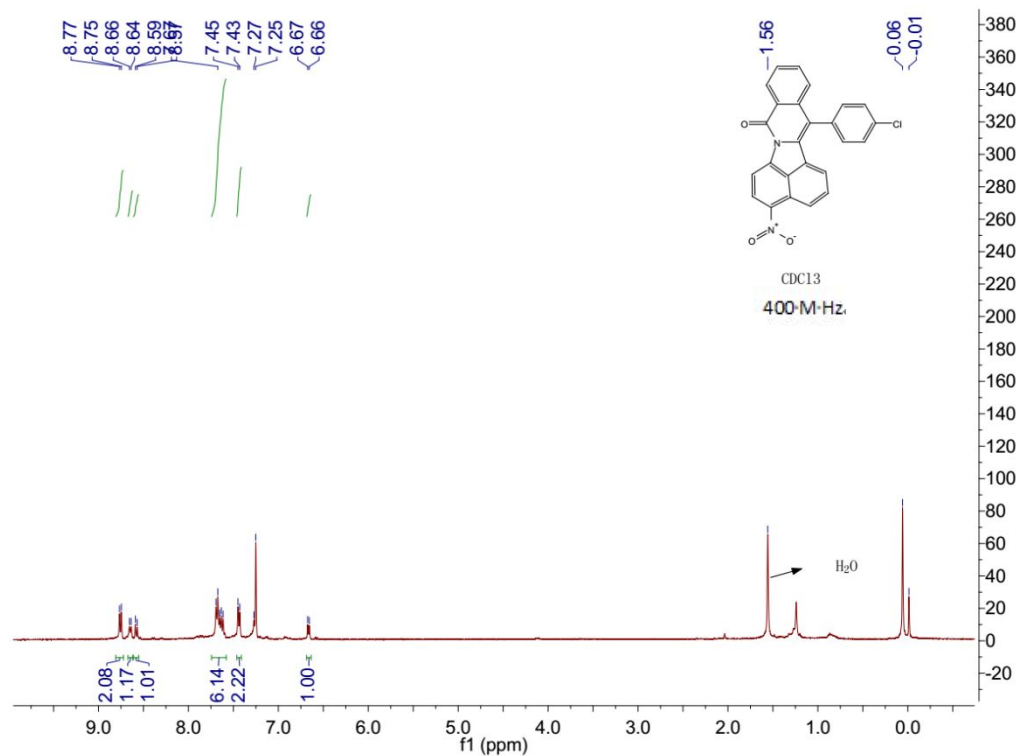


Figure S40 ^{13}C -NMR spectrum of **5**

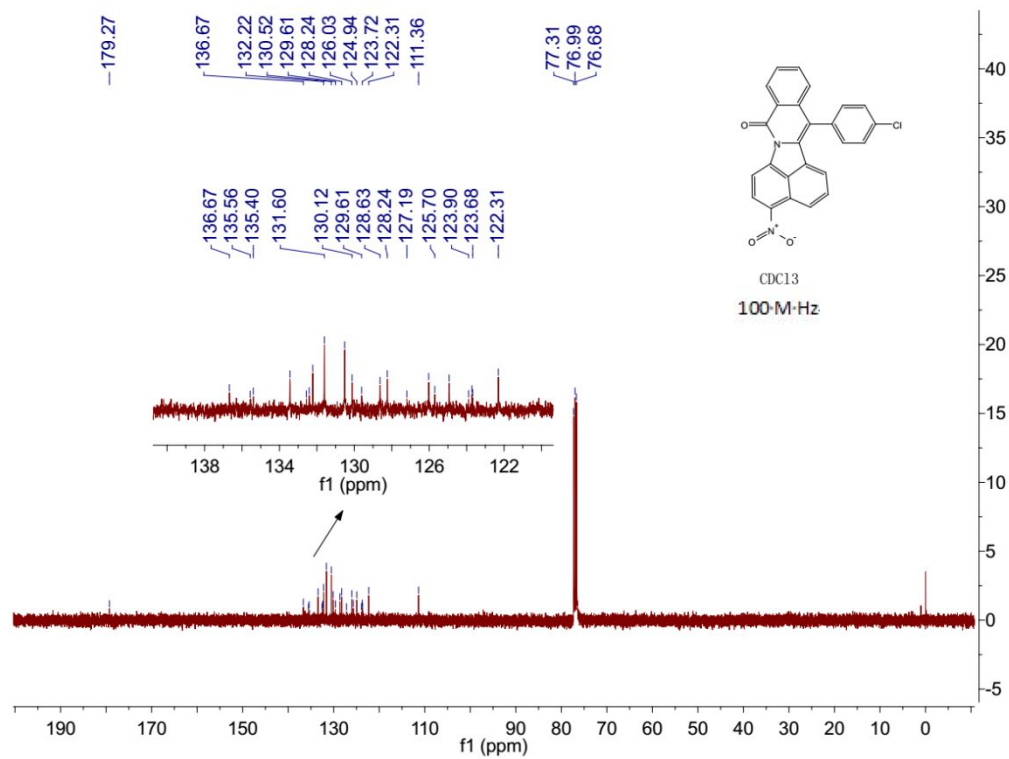


Figure S41 ^1H -NMR spectrum of **6**

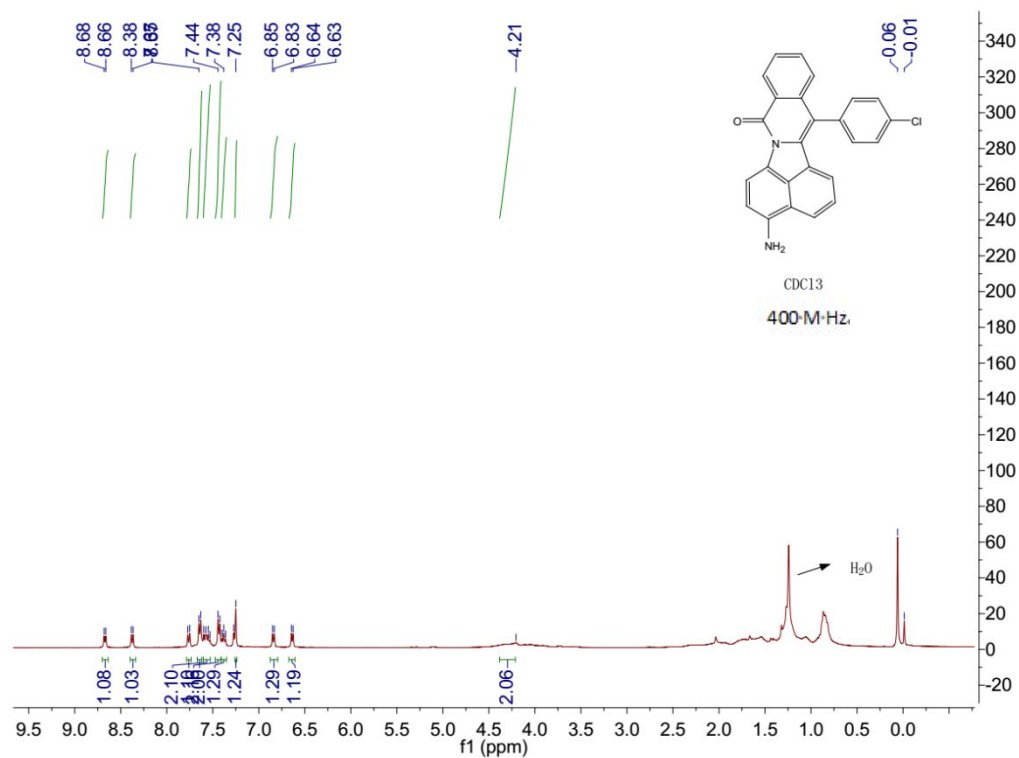


Figure S42 ^{13}C -NMR spectrum of **6**

