

Supporting Information for

**Chemodivergent Tandem Cyclizations of 2-Indolylmethanols
with Tryptophols: C–N versus C–C Bond Formation**

Jing-Yi Wang, Ping Wu, Jia-Le Wu, Guang-Jian Mei* and Feng Shi*

School of Chemistry and Materials Science, Jiangsu Normal University, Xuzhou, 221116, China

E-mail: fshi@jsnu.edu.cn; guangjianM@jsnu.edu.cn

Contents:

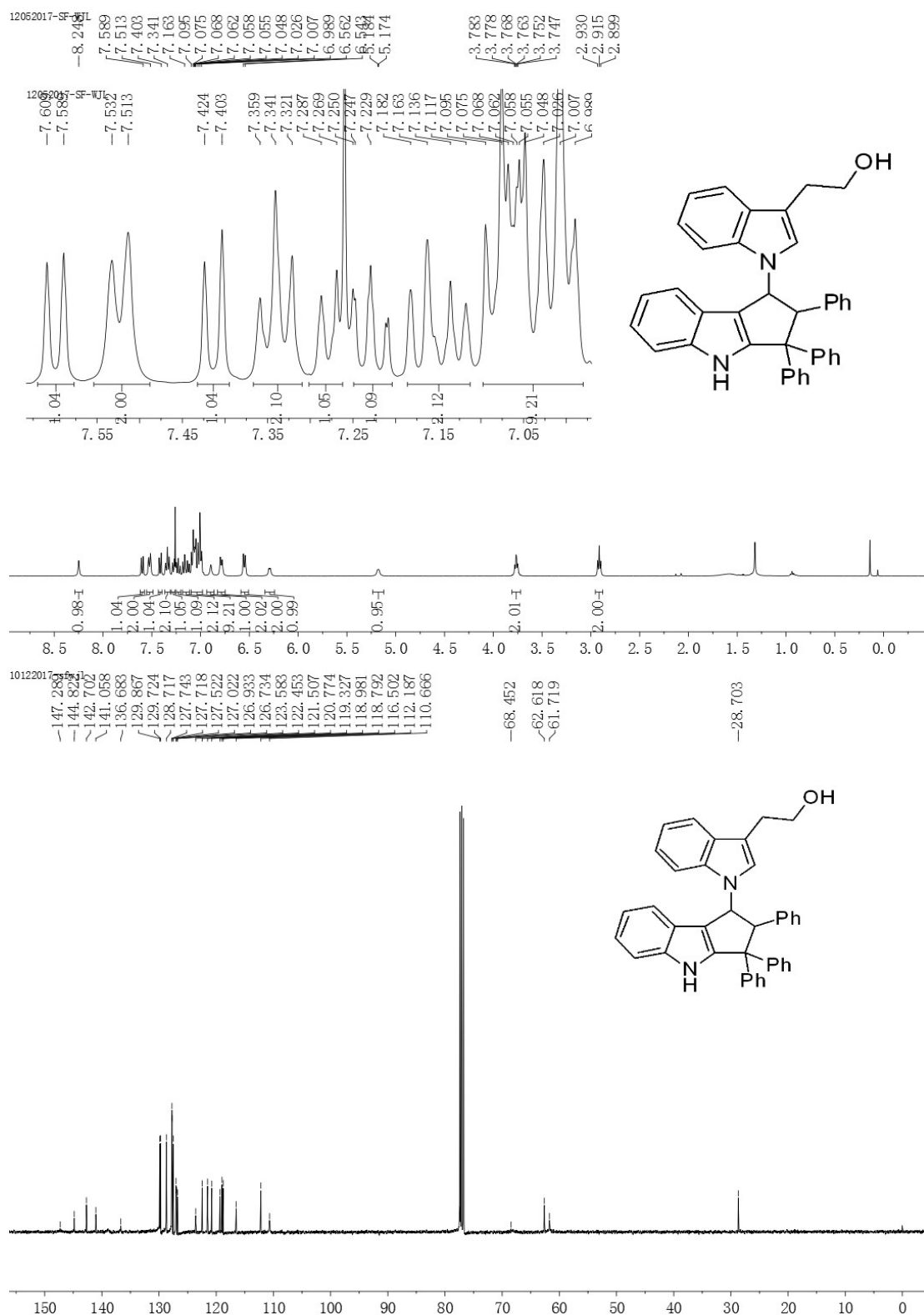
- 1. NMR spectra of products 3-4 and 6-8 (S2-S46)**

- 2. HPLC copies of product 3aa (S47)**

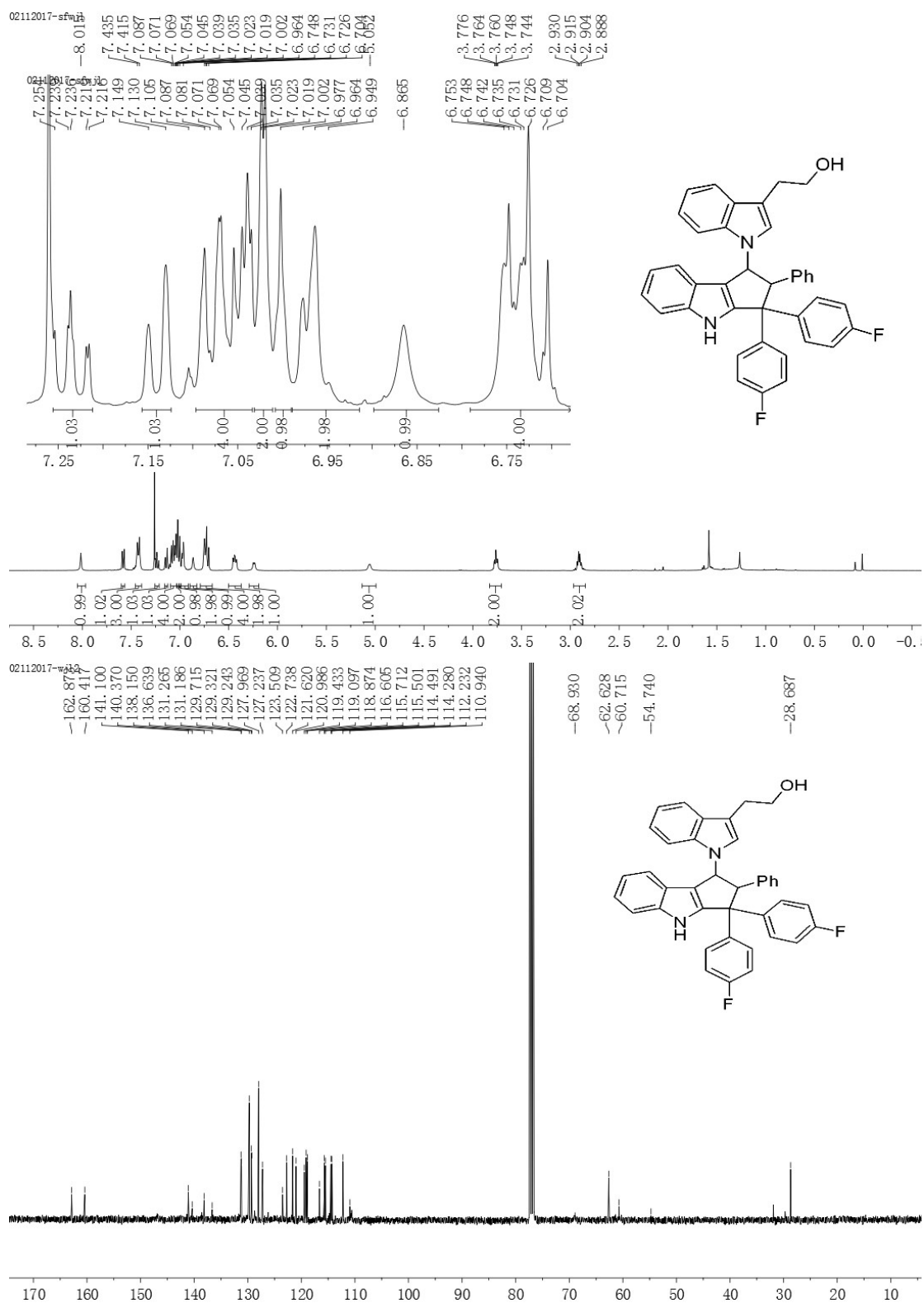
- 3. X-ray single crystal data for products 3aa and 4aa (S48-S51)**

1. NMR spectra of products 3 and 4

3aa



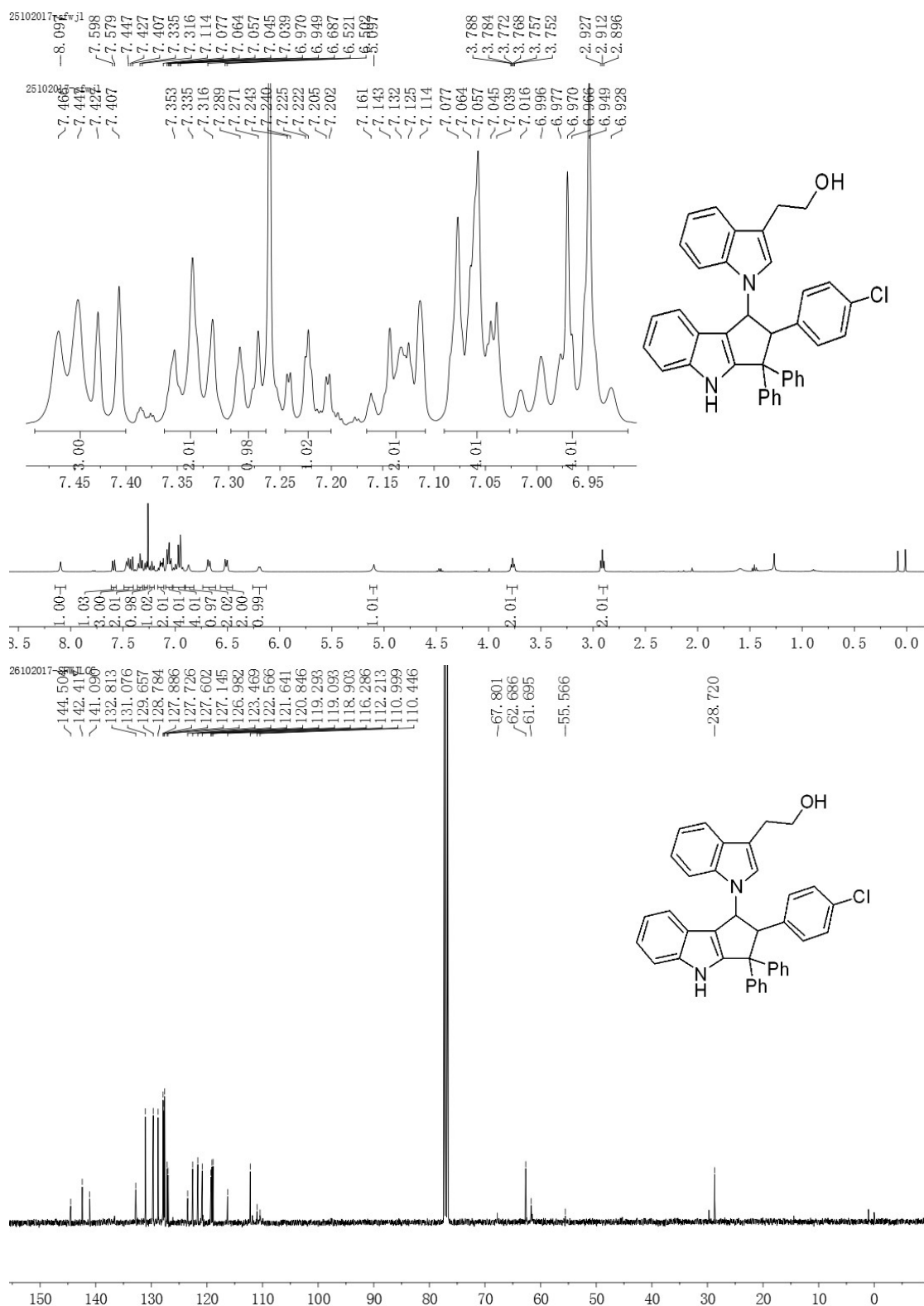
3ba



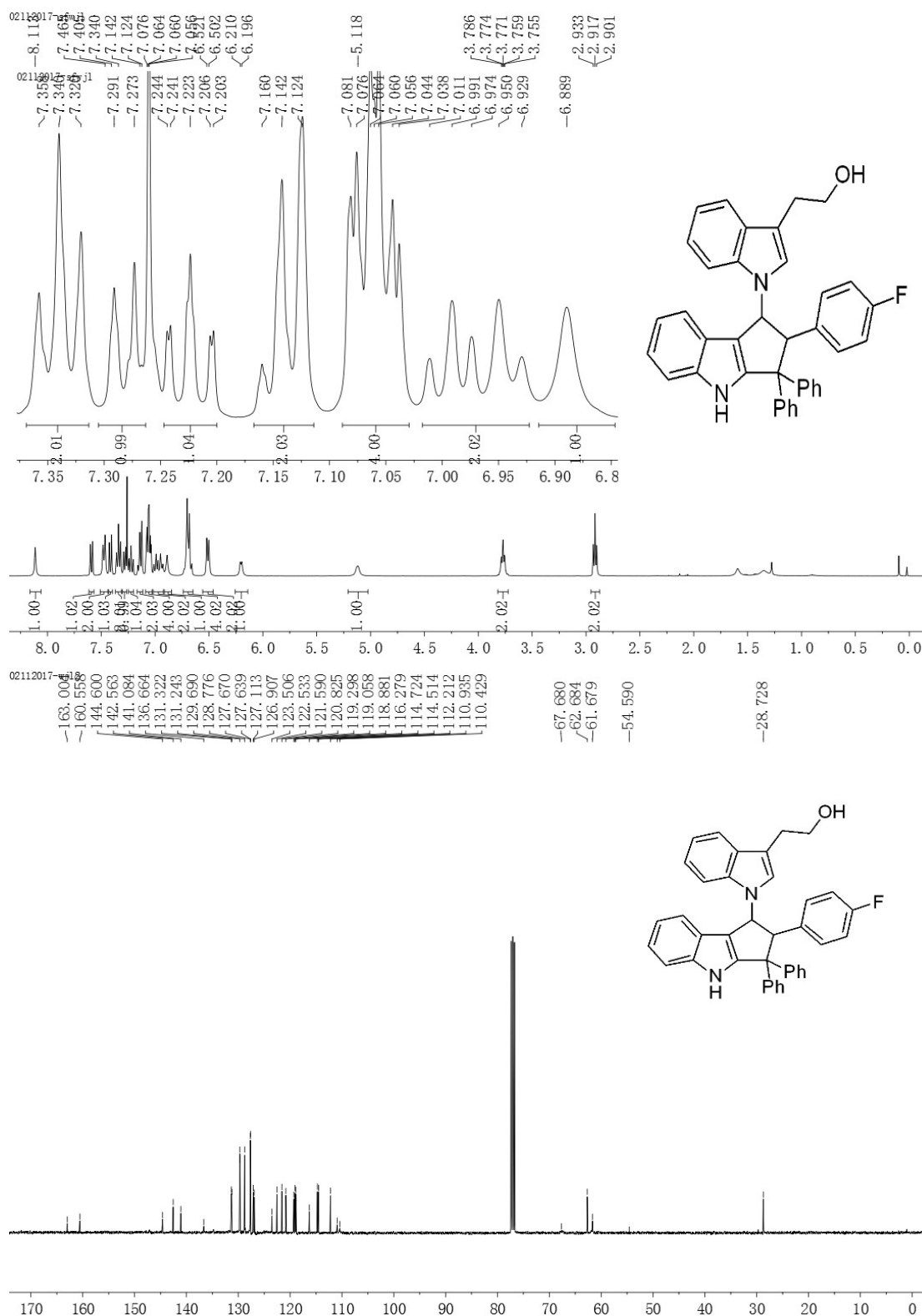
08092017-sfwjl2



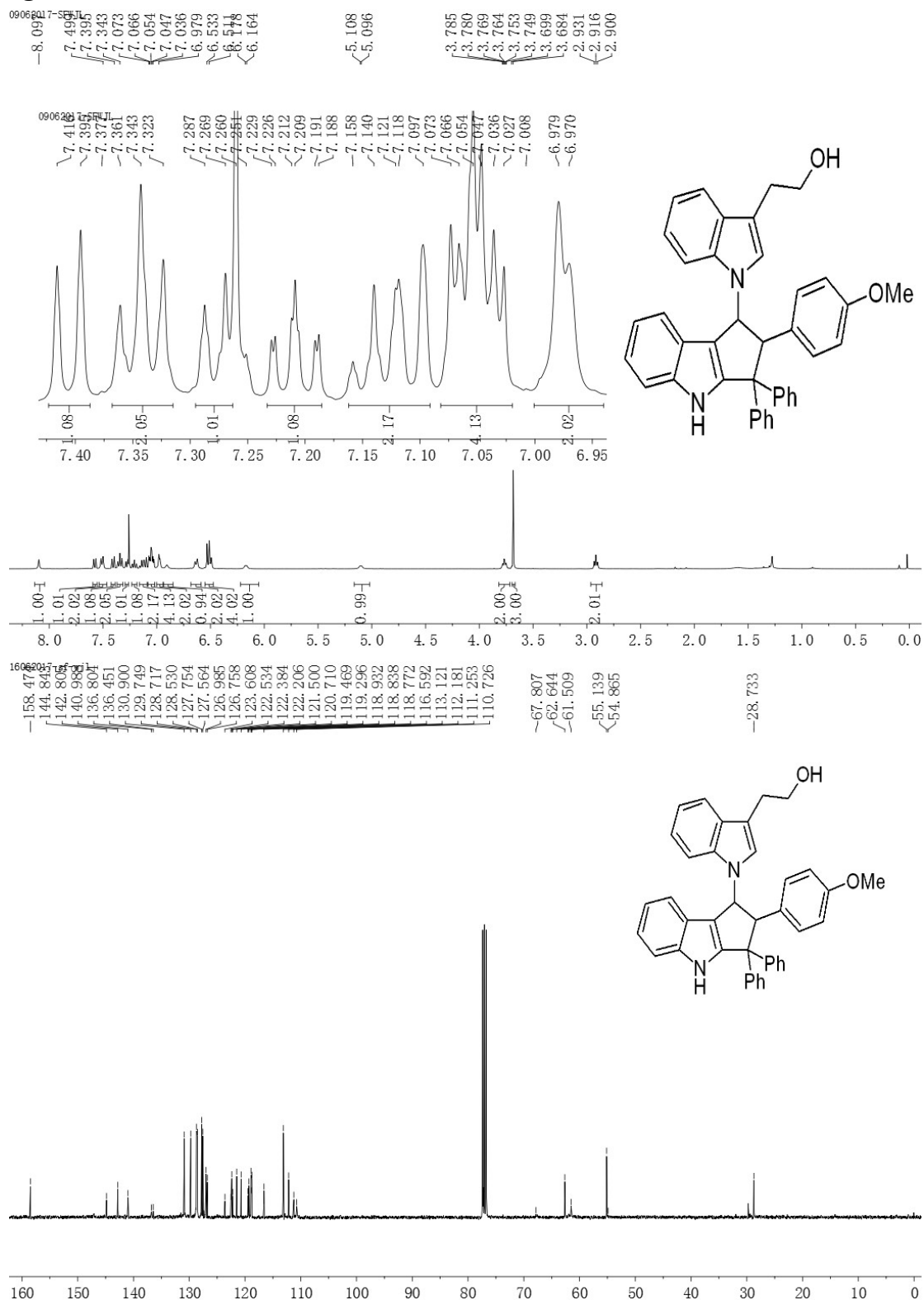
3ea

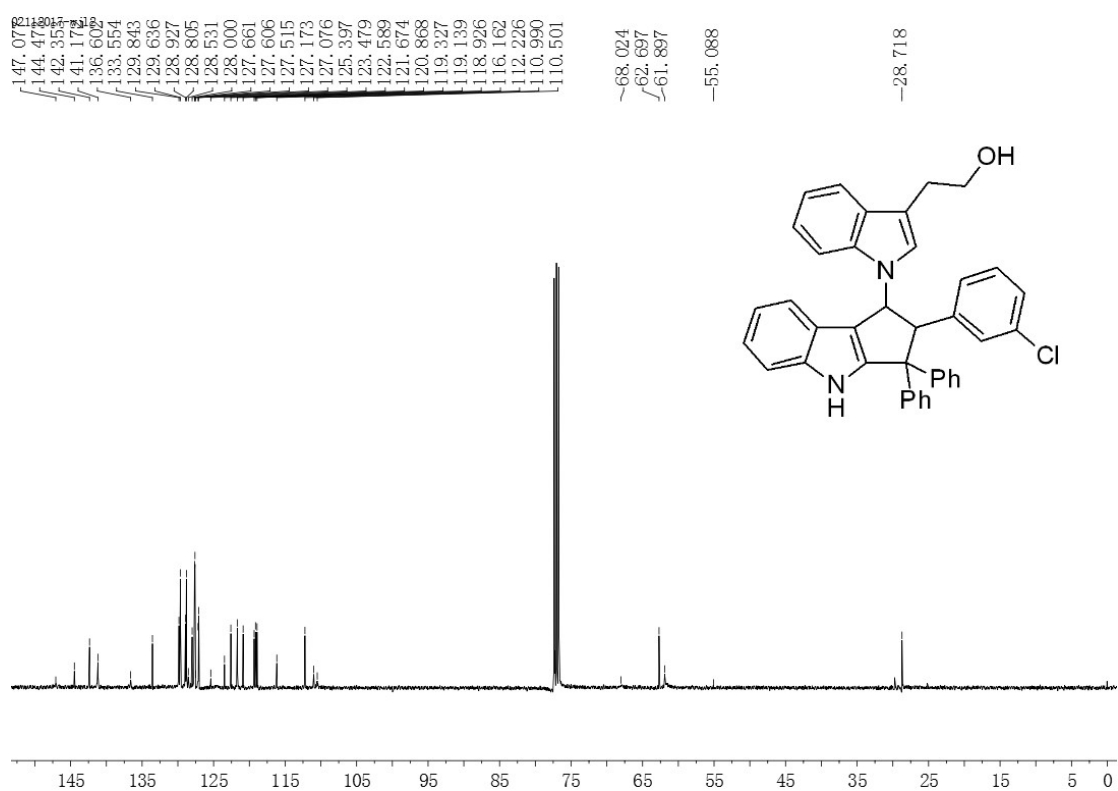
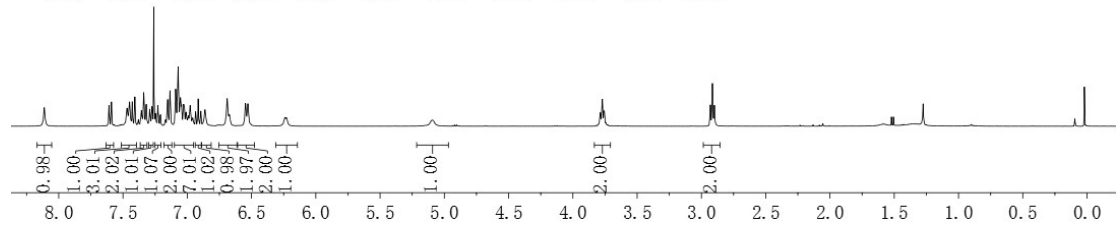


3fa

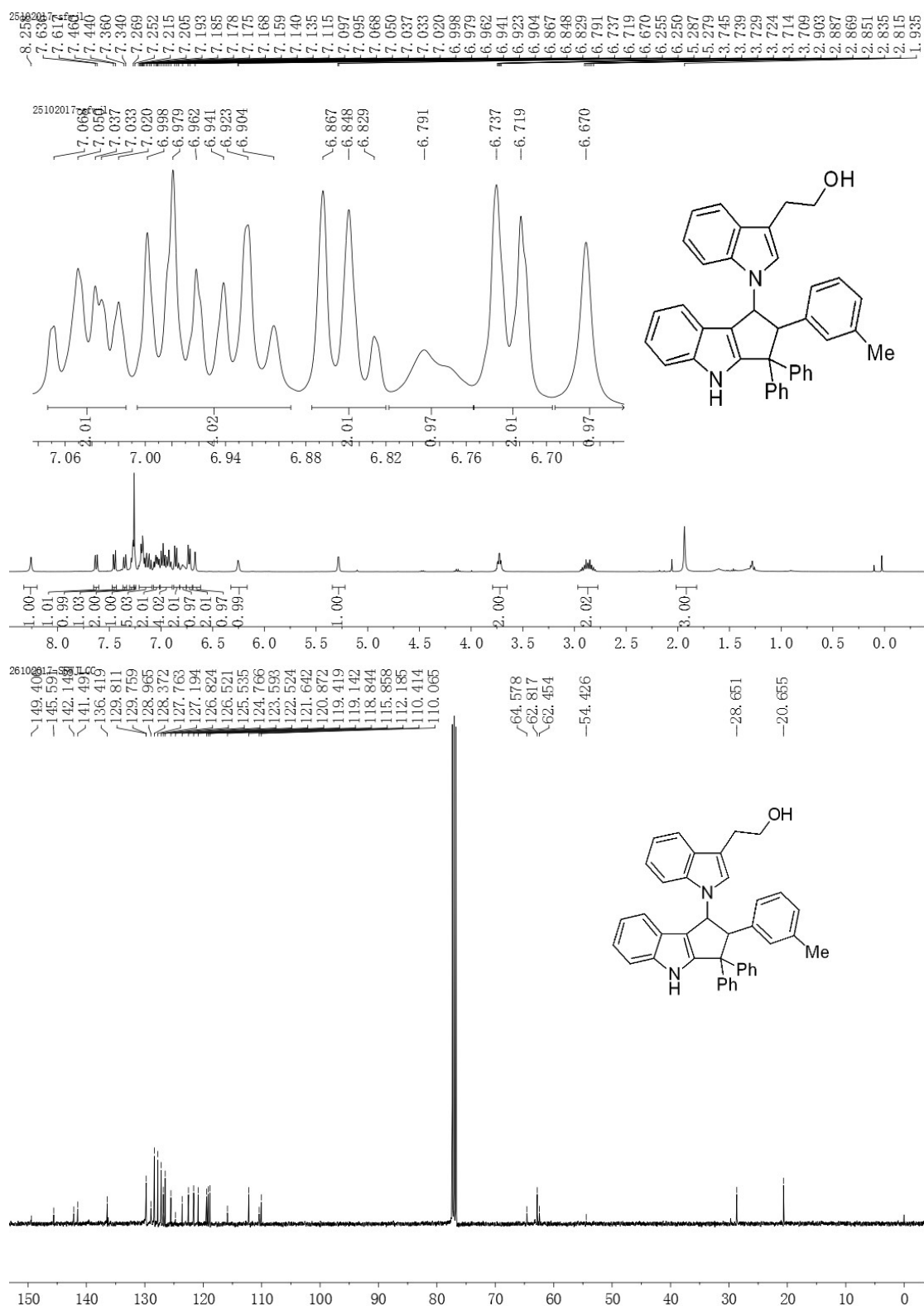


3ga

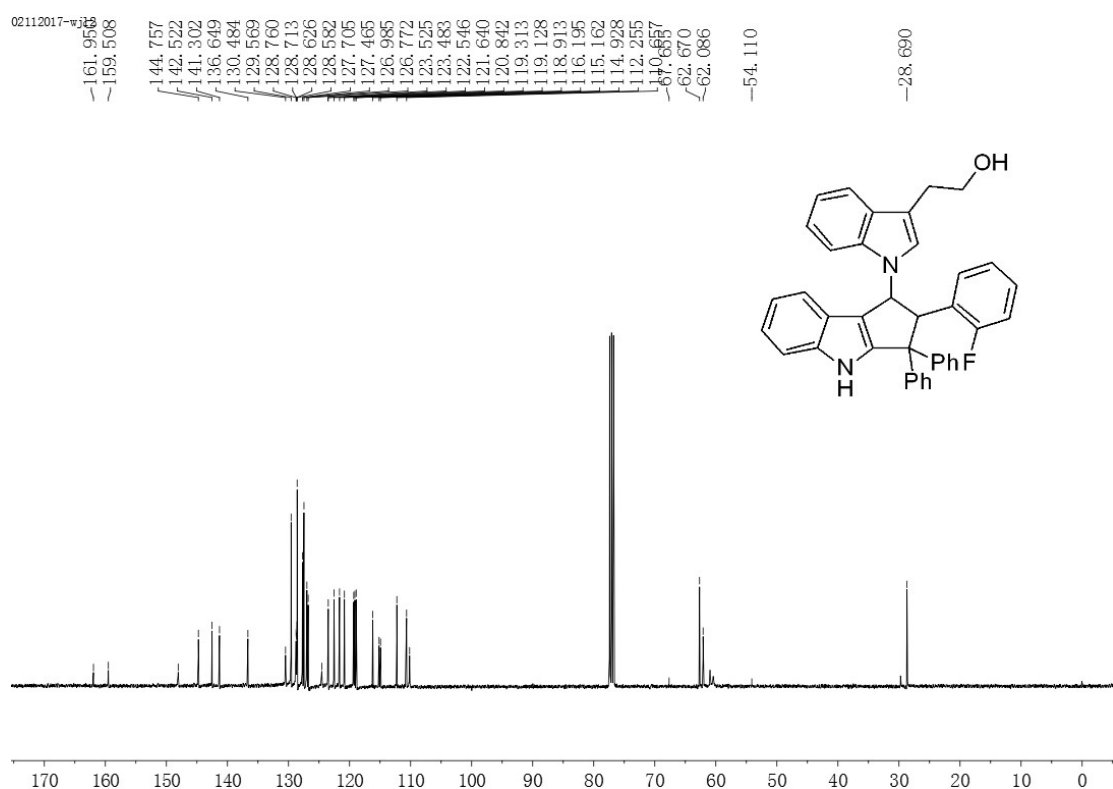
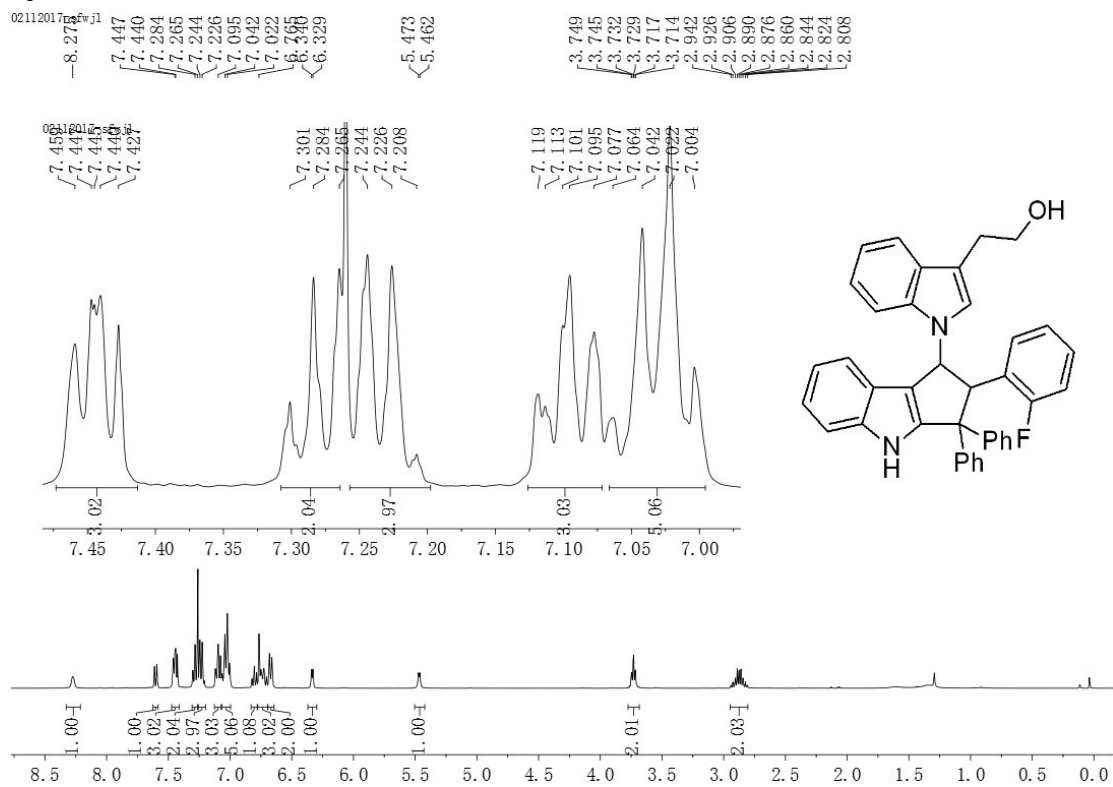




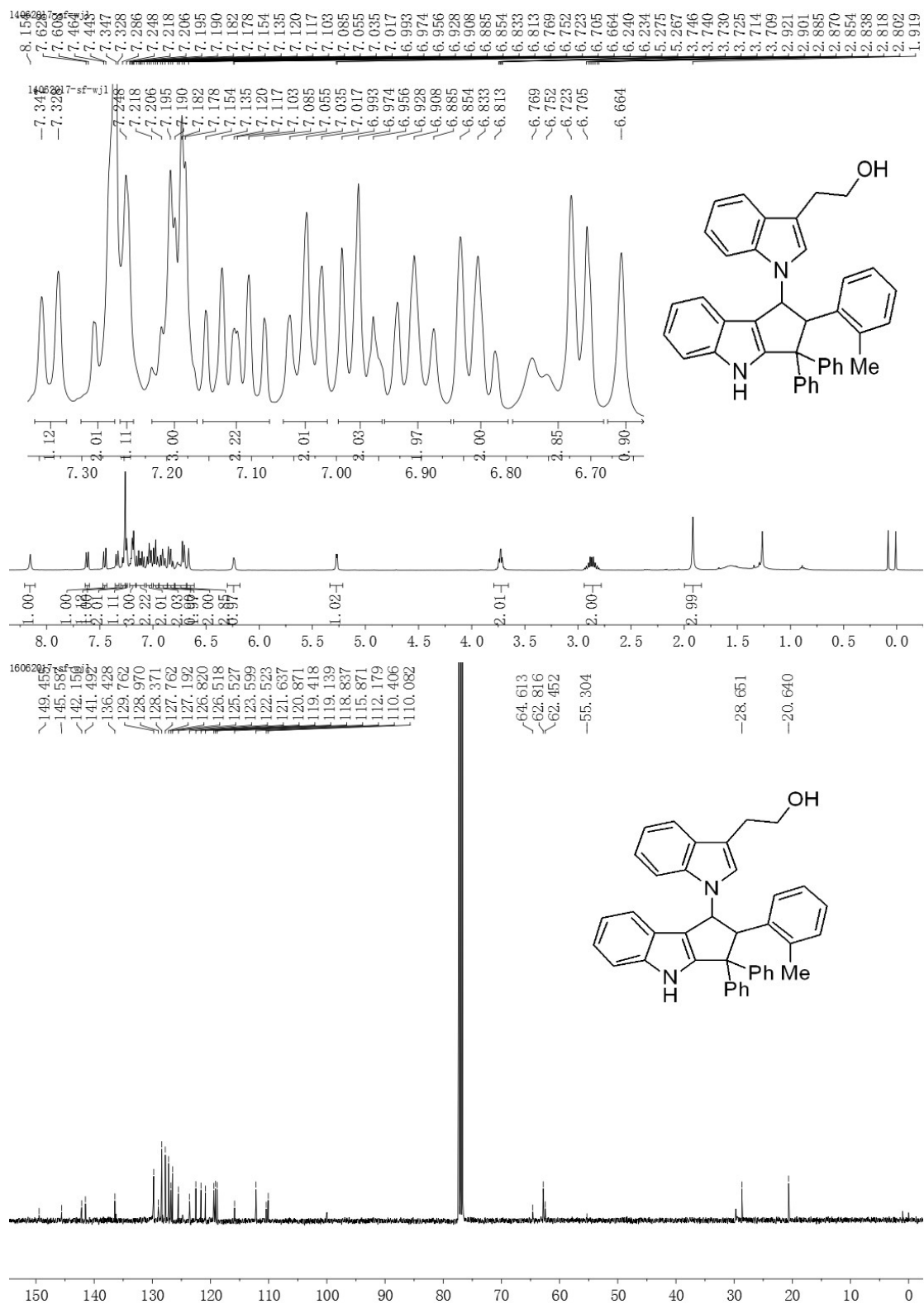
3ia



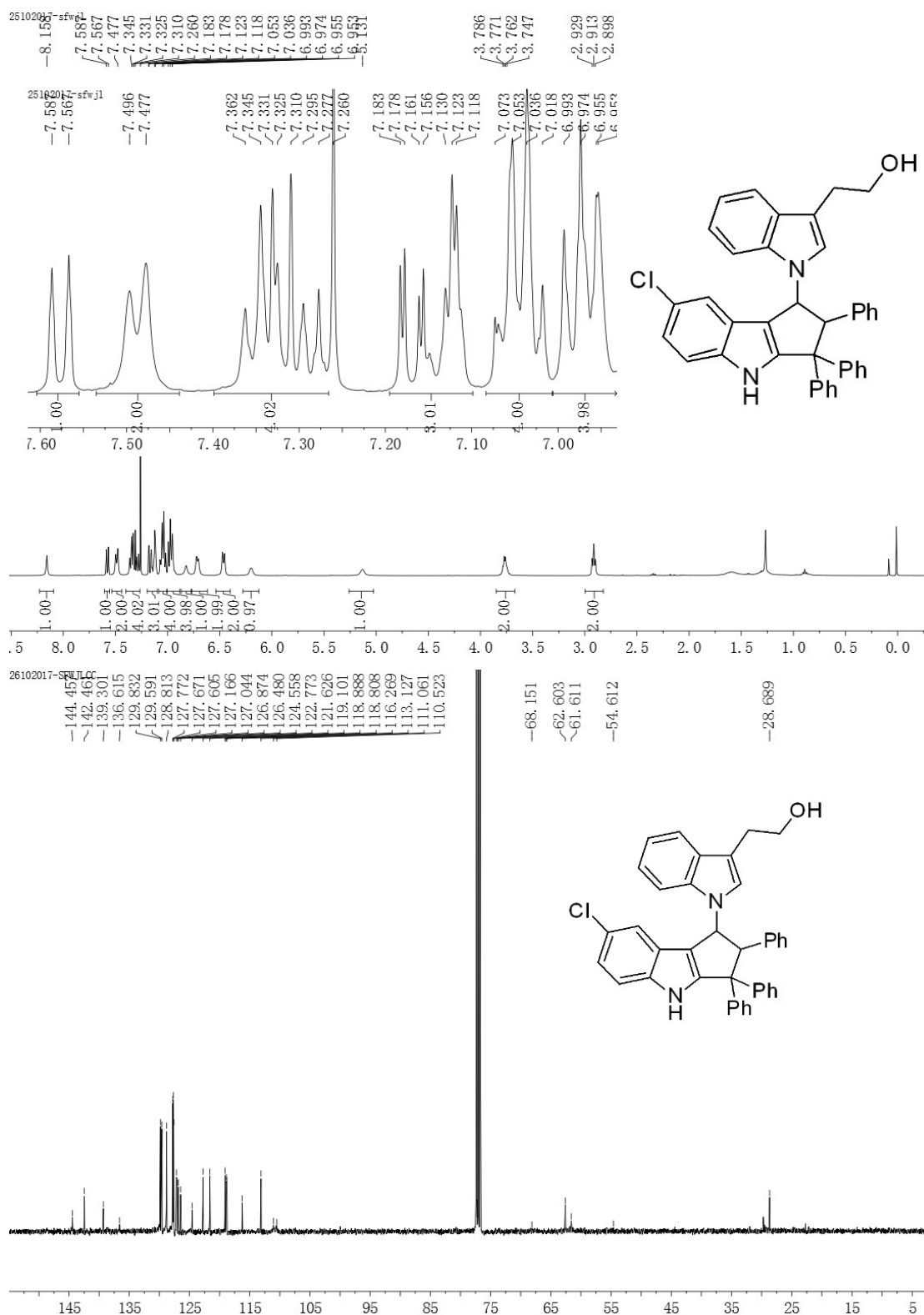
3ja



3ka

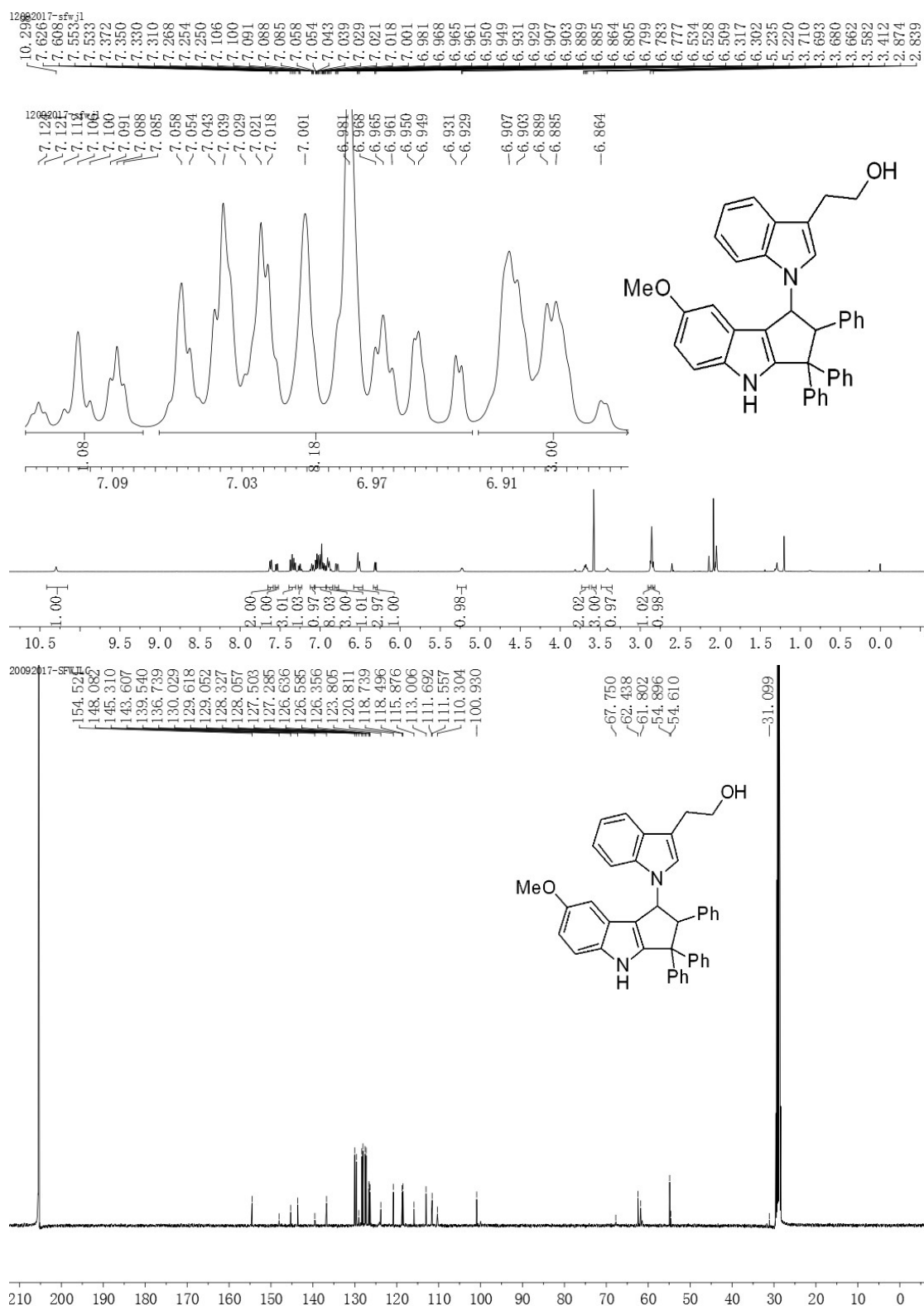


3la

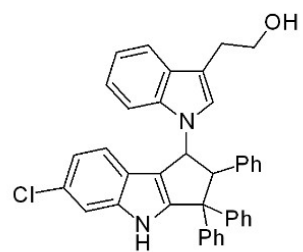


[illegible]

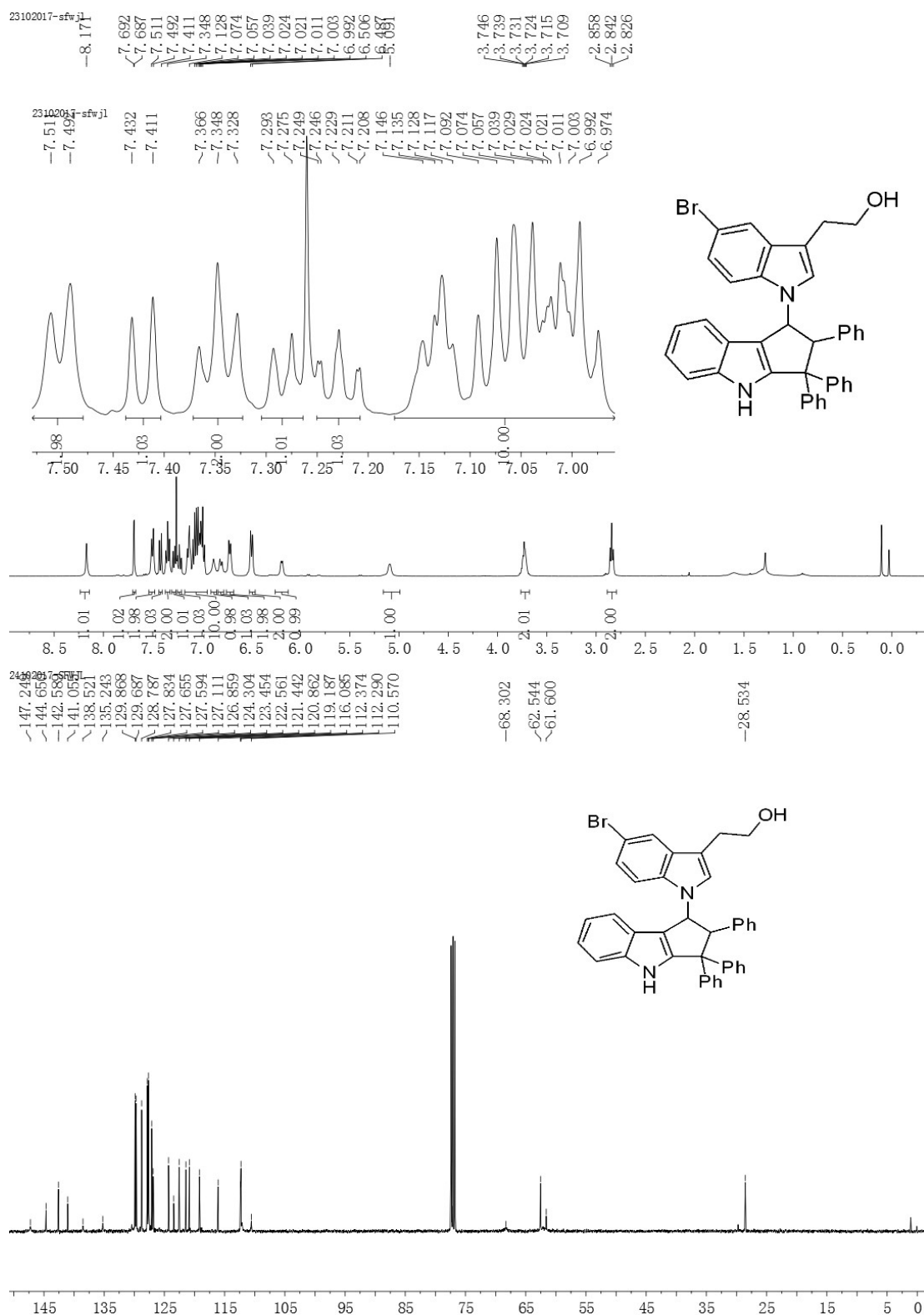
3na



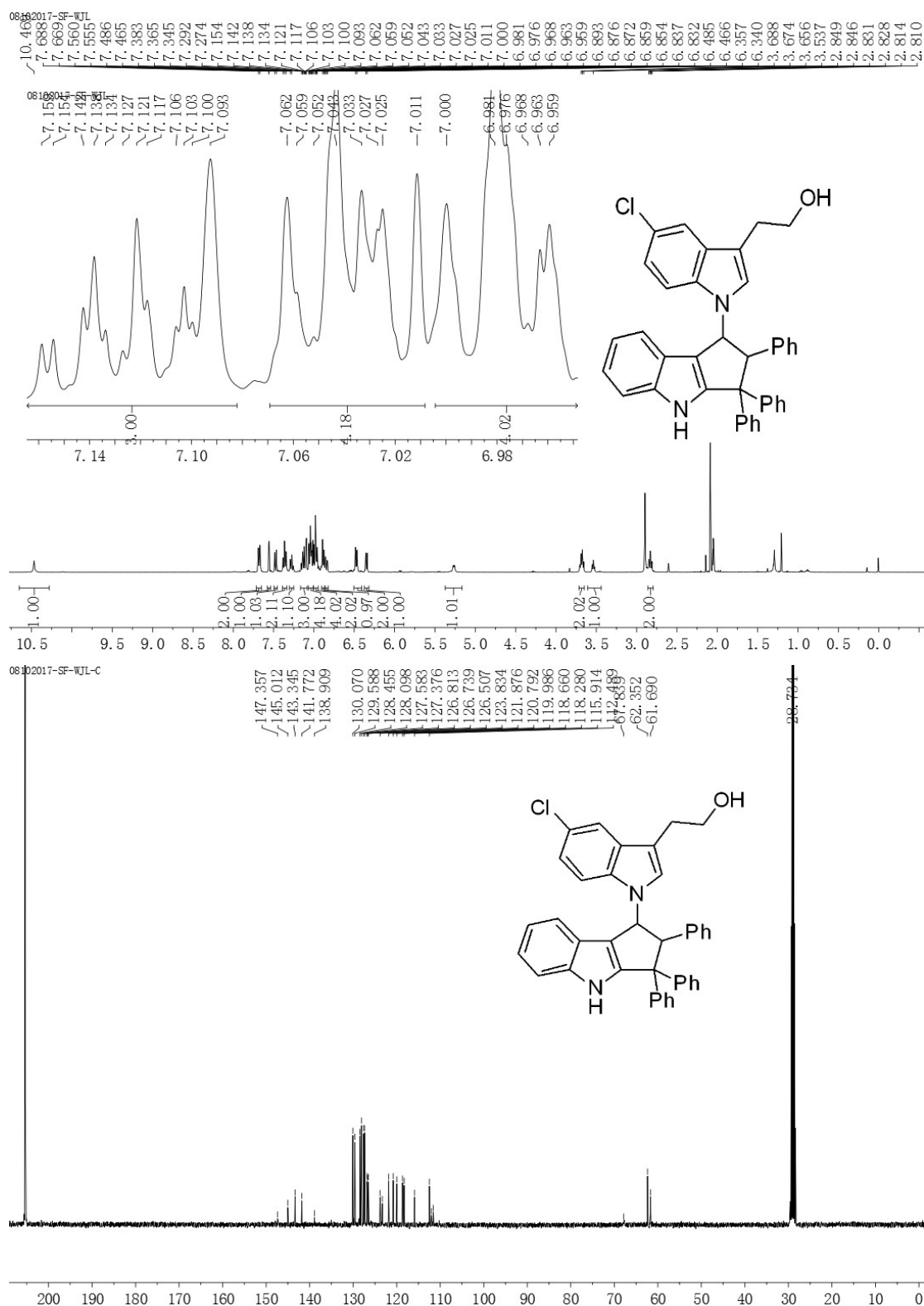
25102017sfwjlc



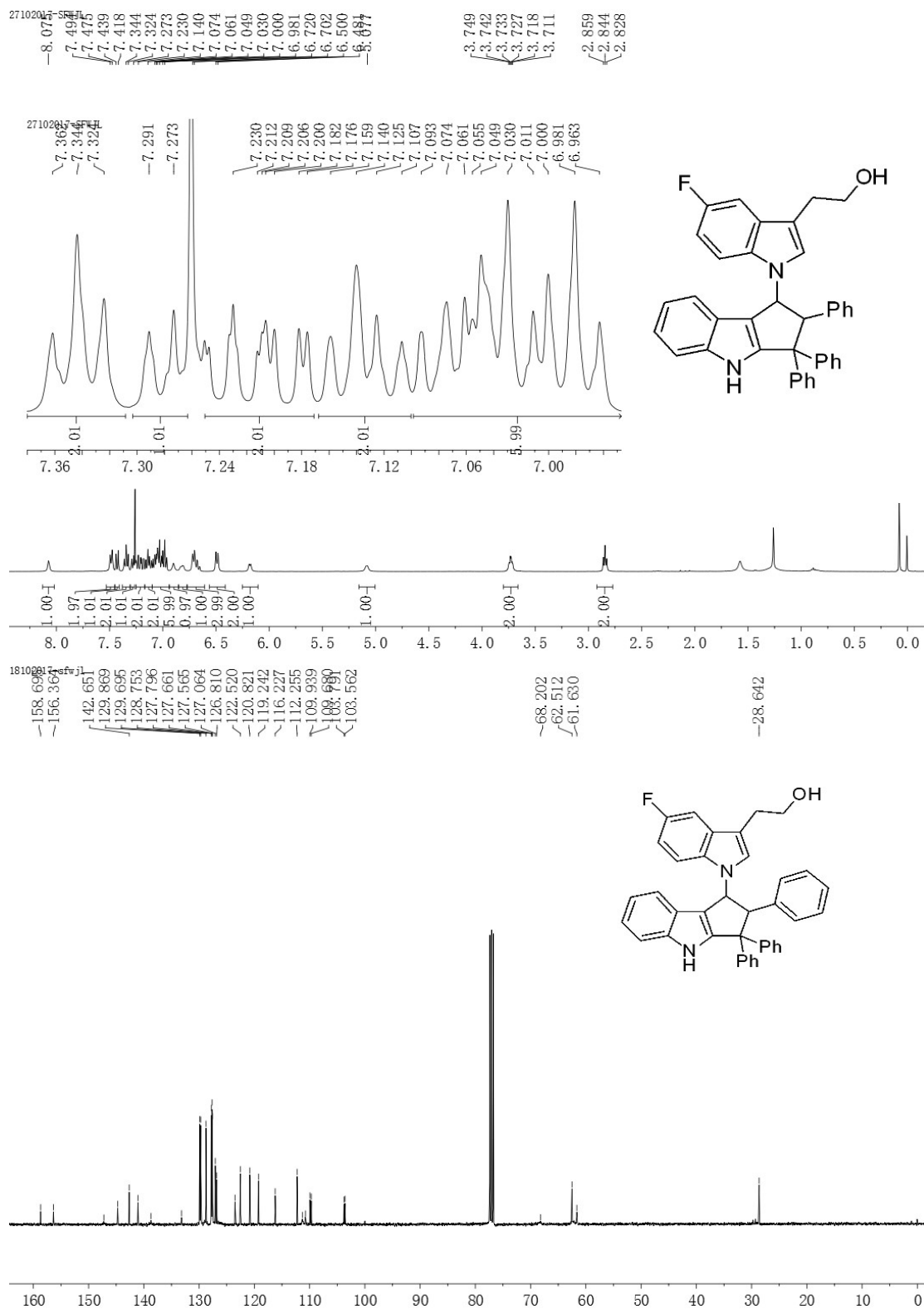
3ab



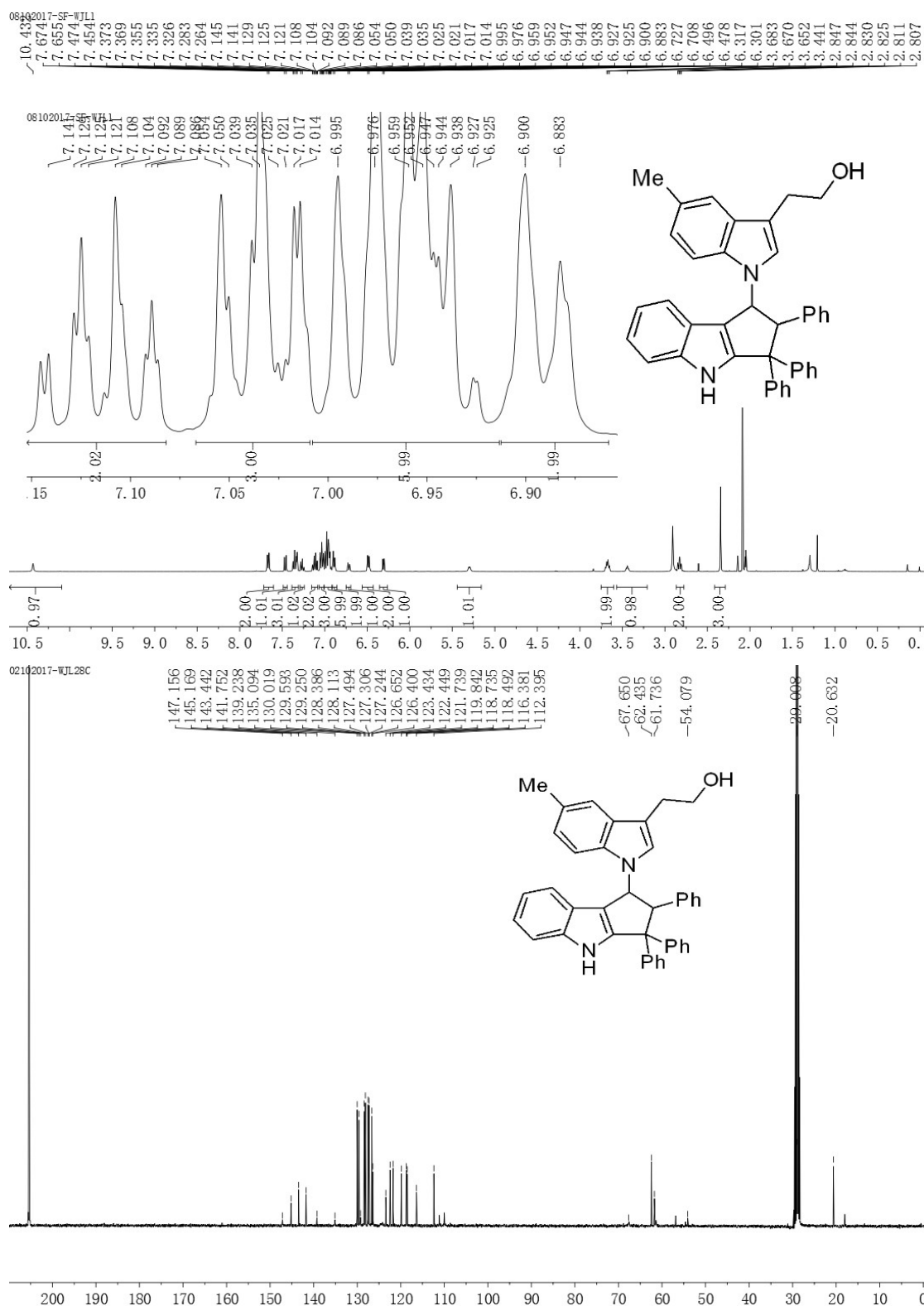
3ac



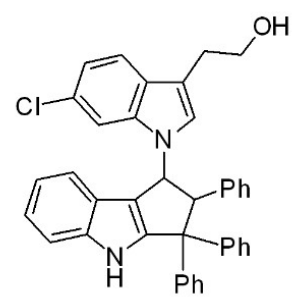
3ad



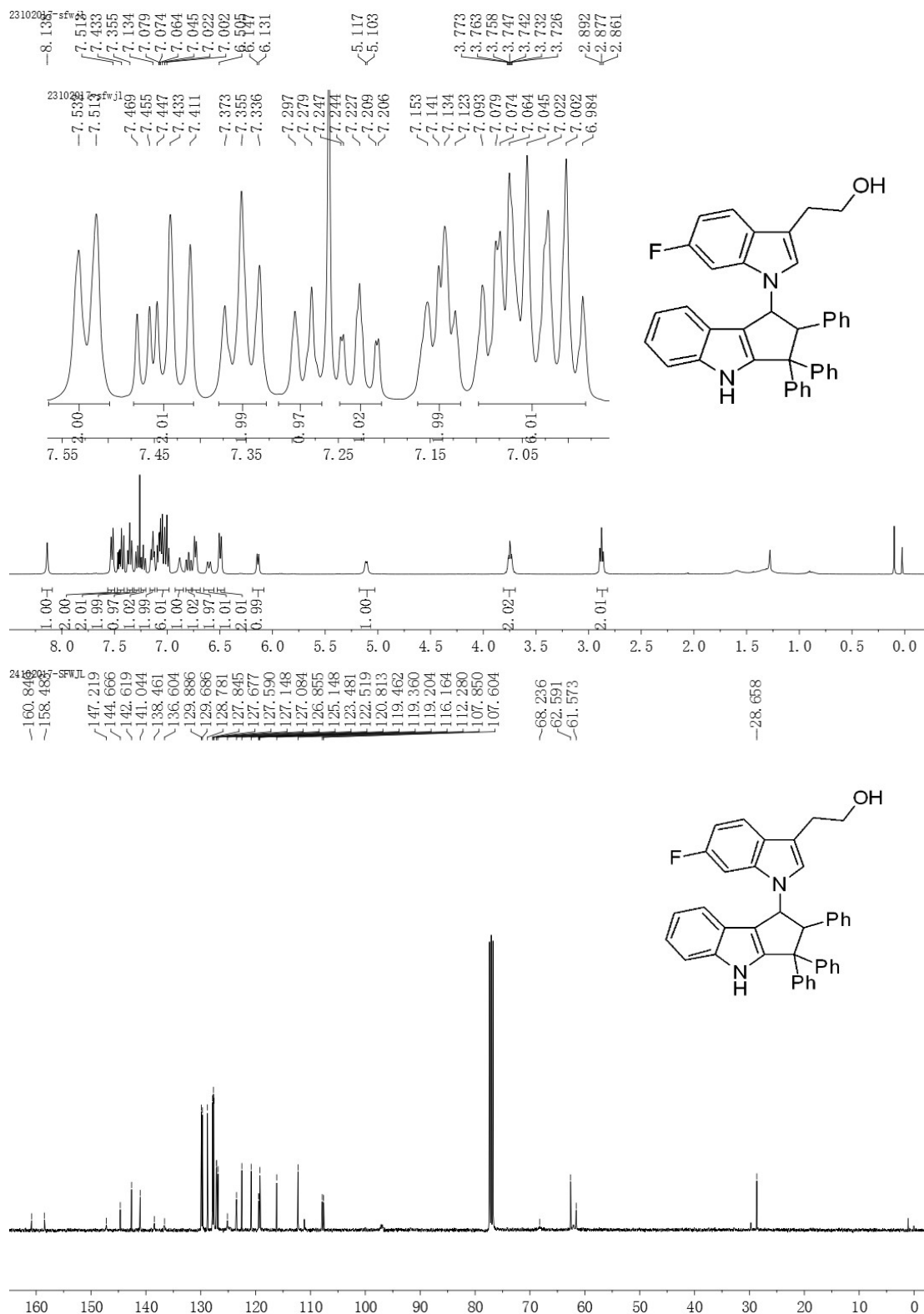
3ae



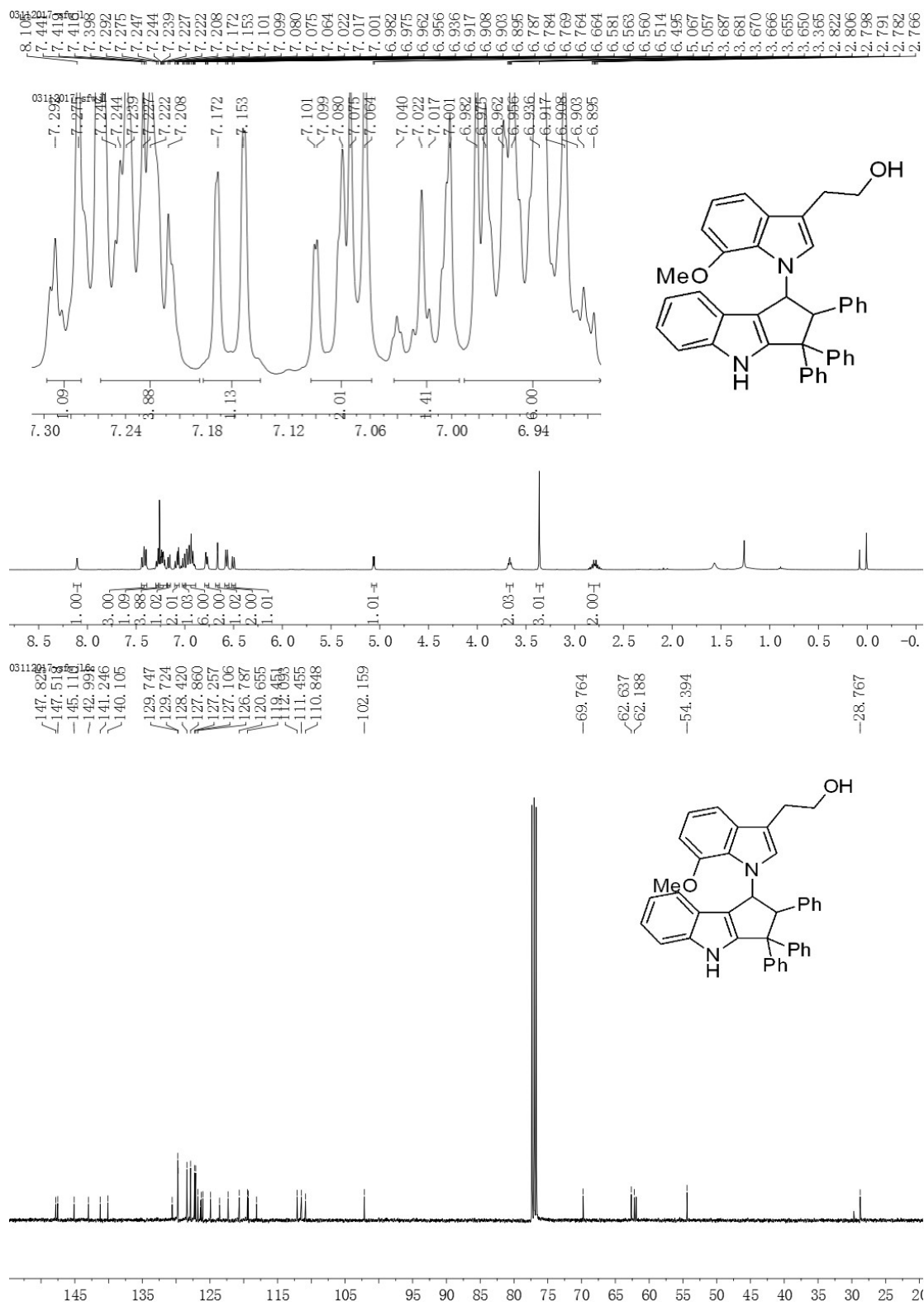
02112017
8.08



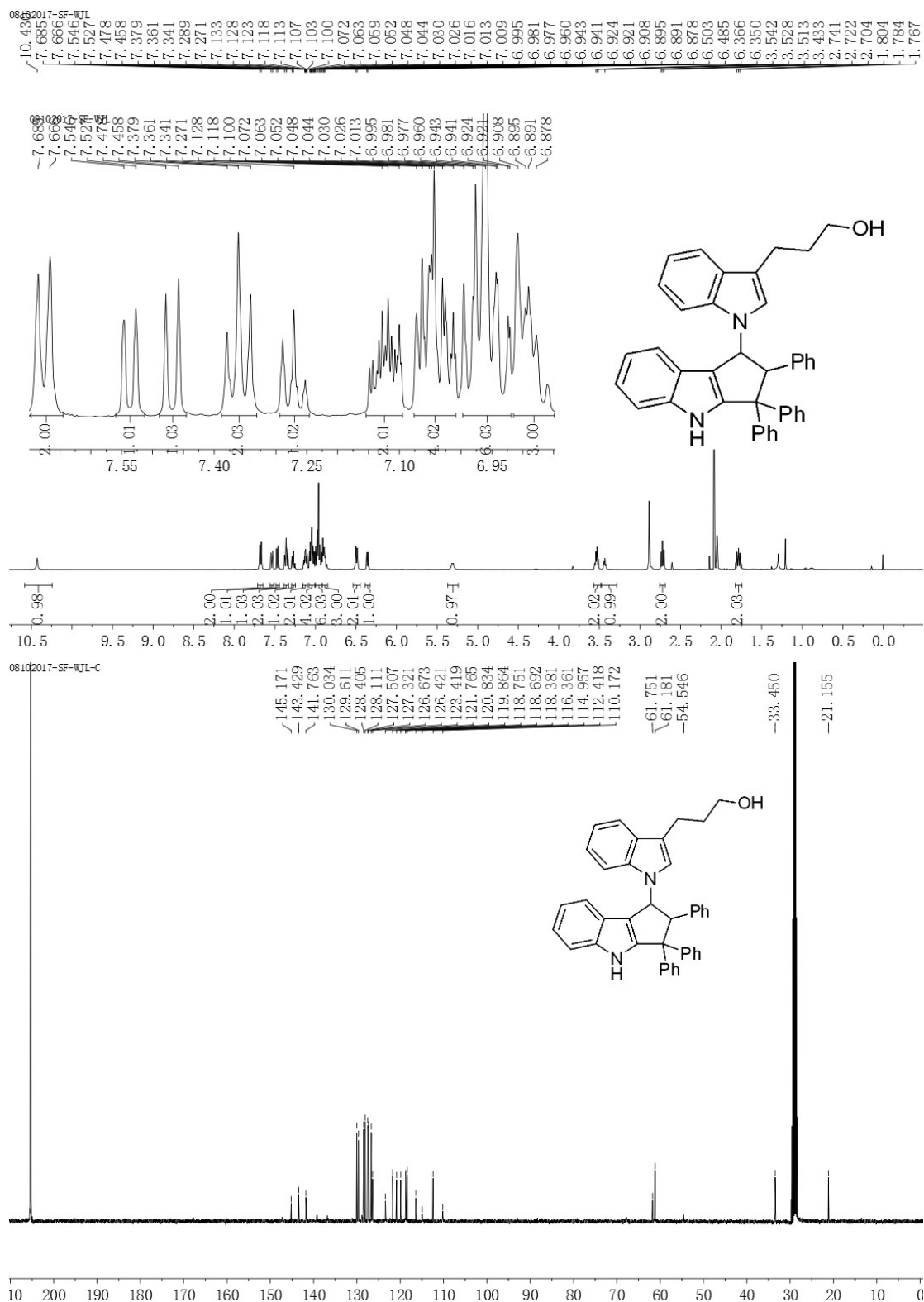
3ah



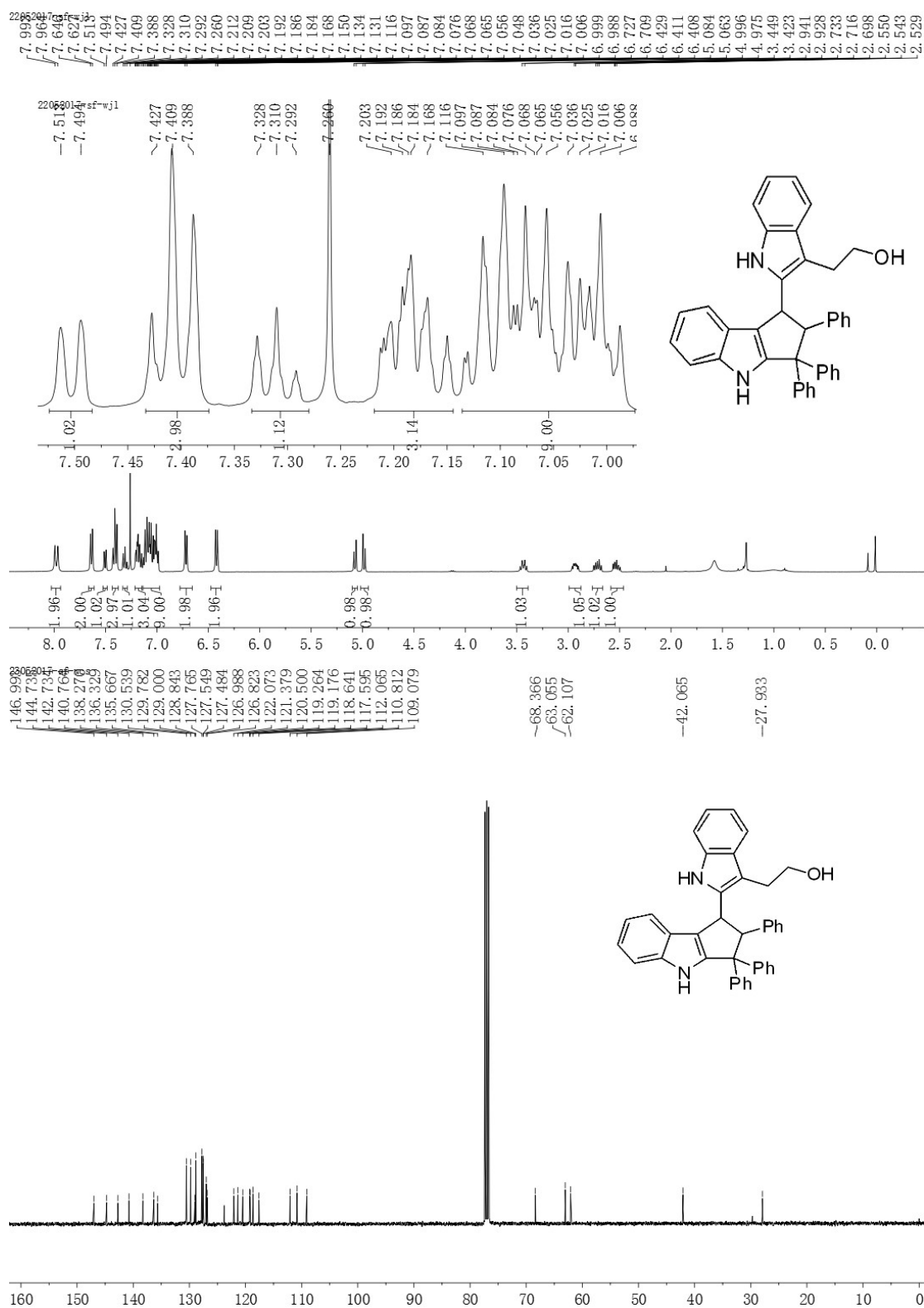
3ak



3al



4aa

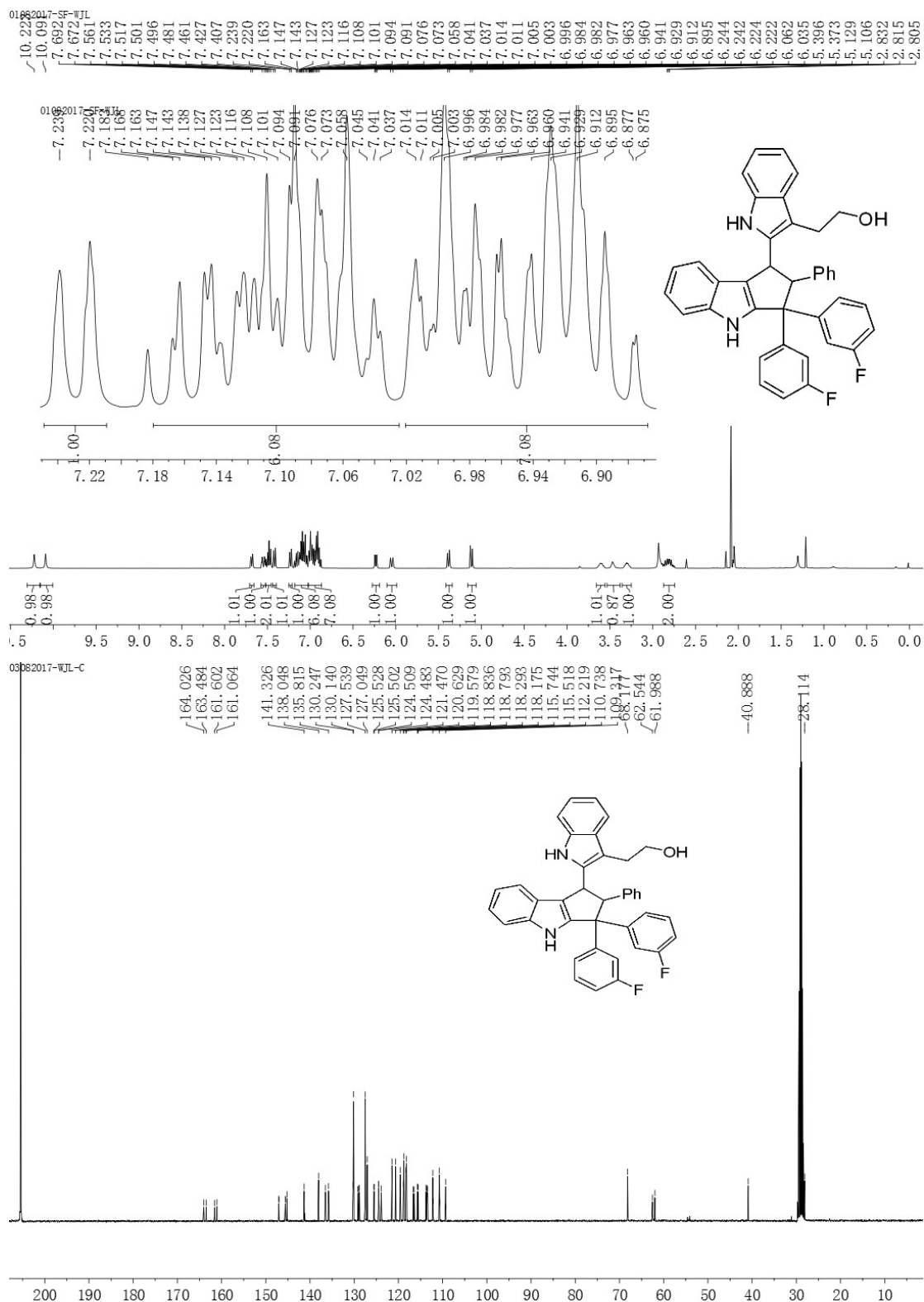


S27

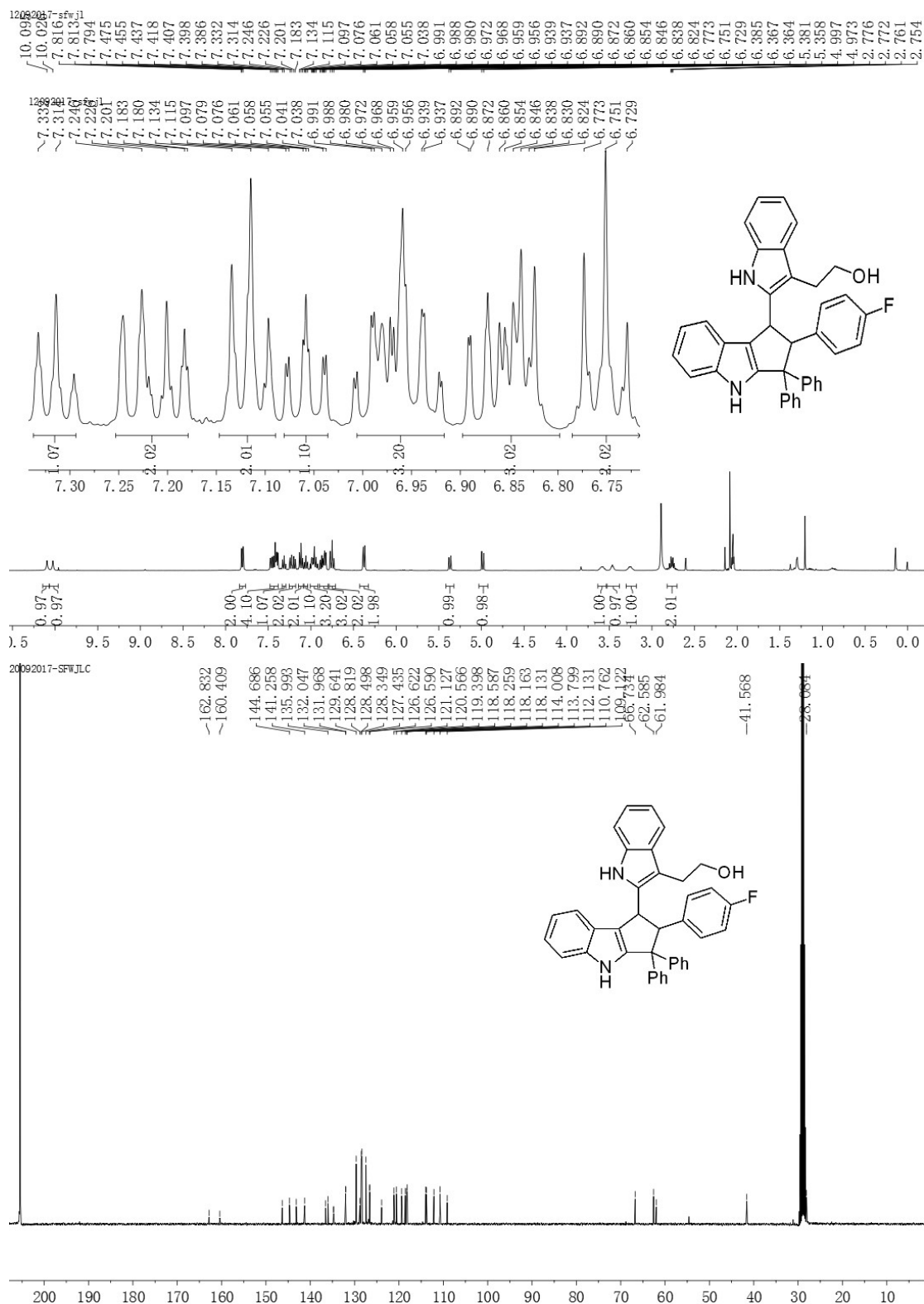
12692017-sfw.jl



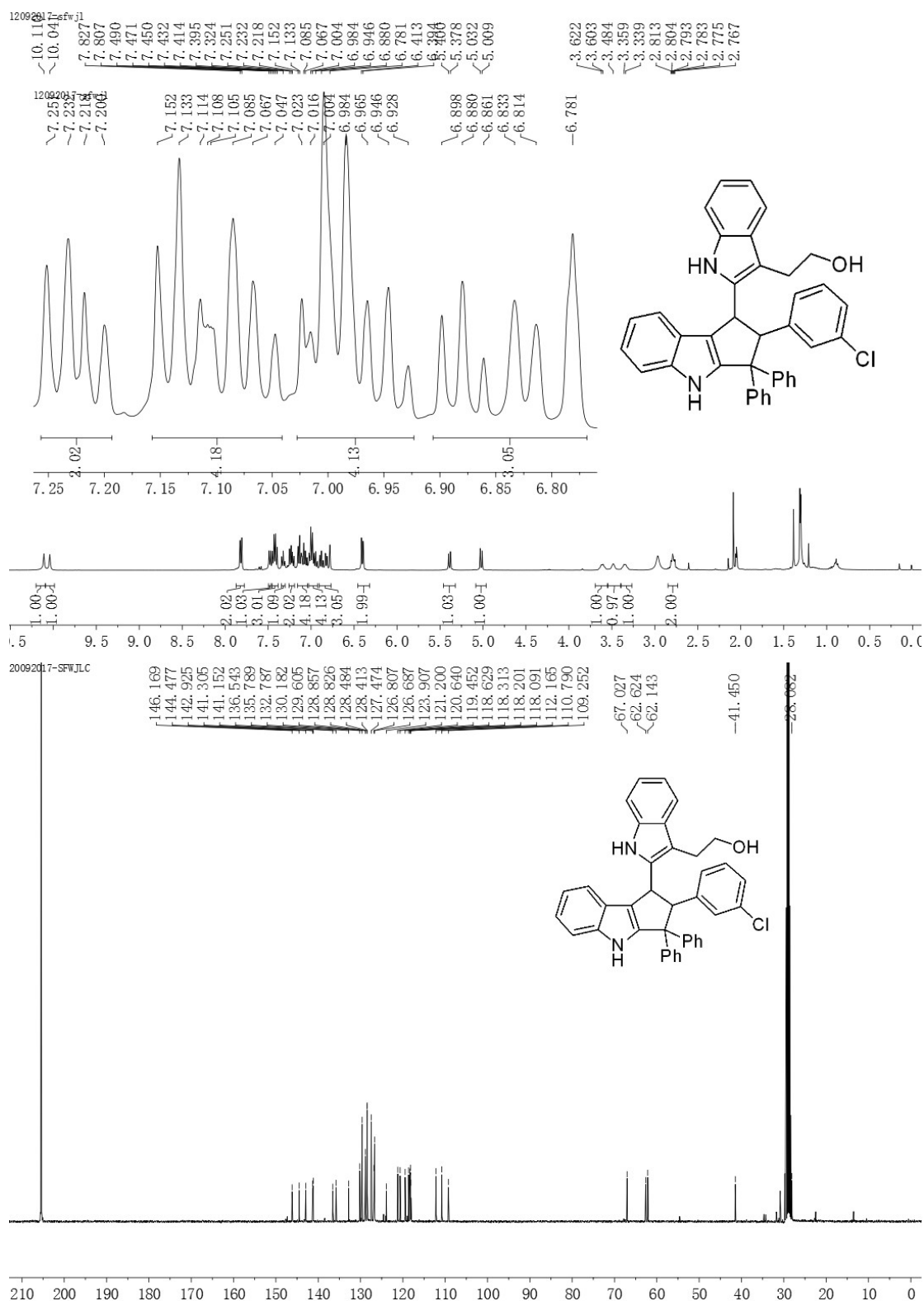
4da



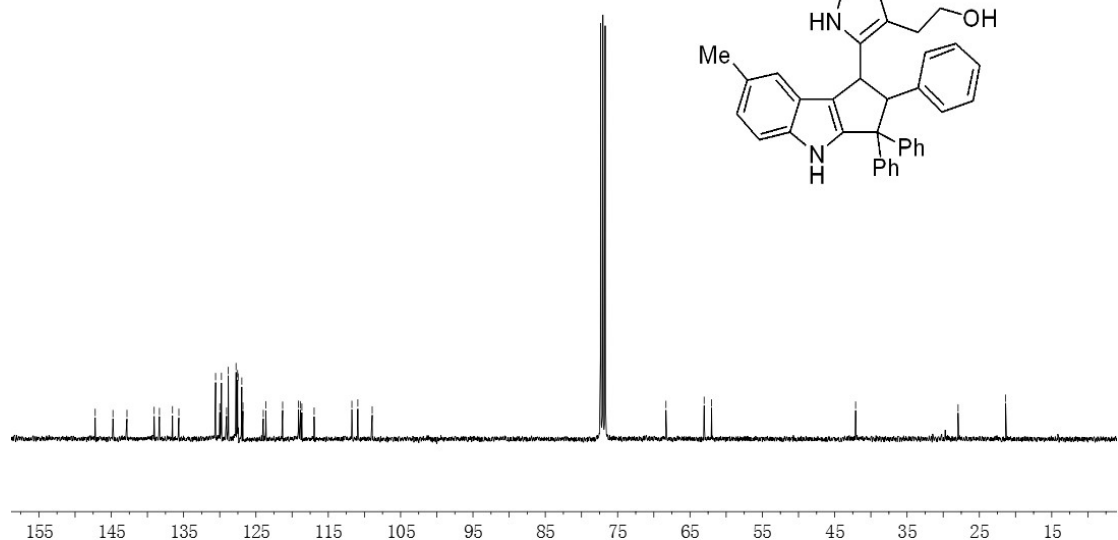
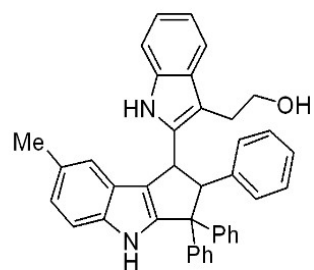
4fa



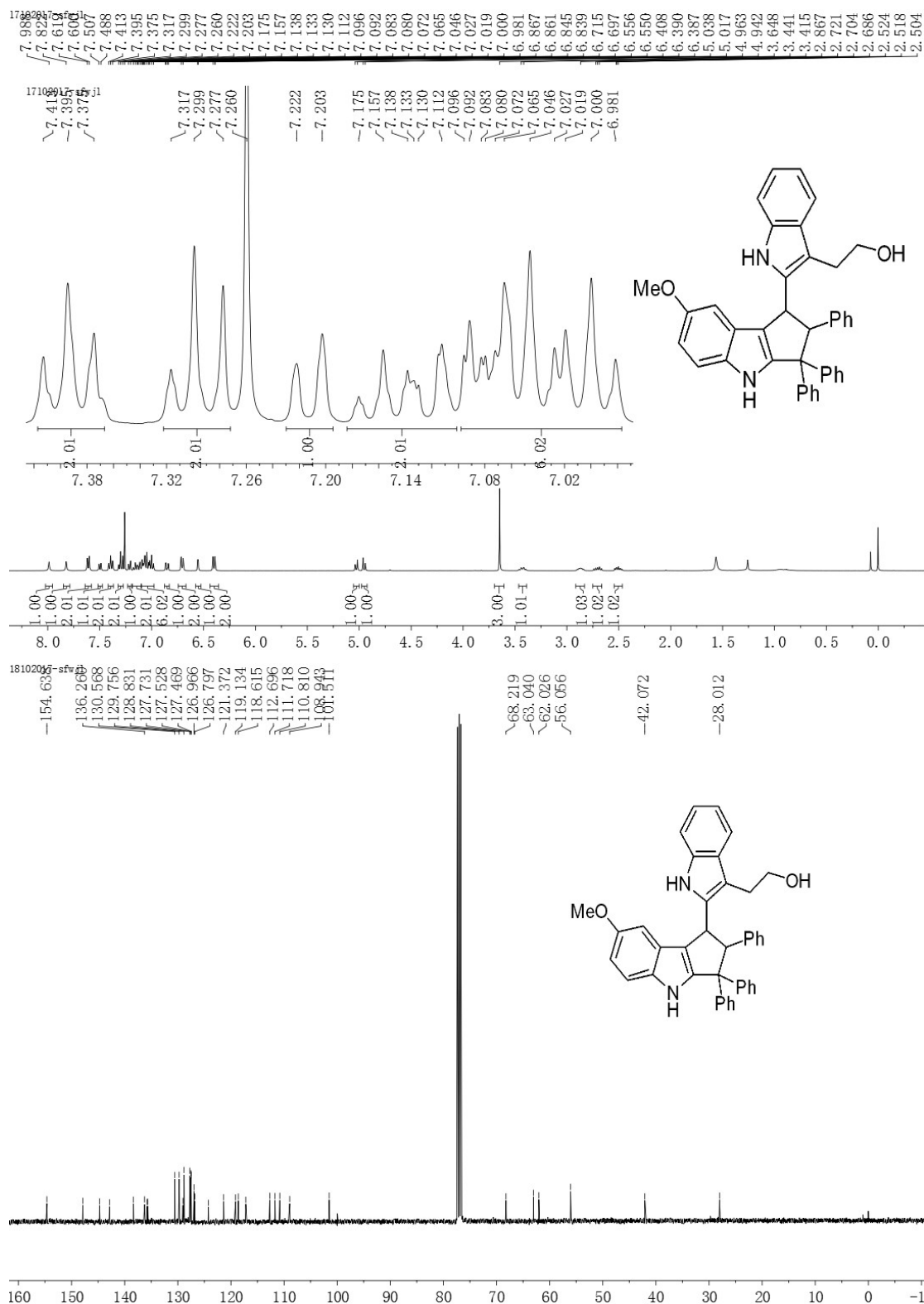
4ha

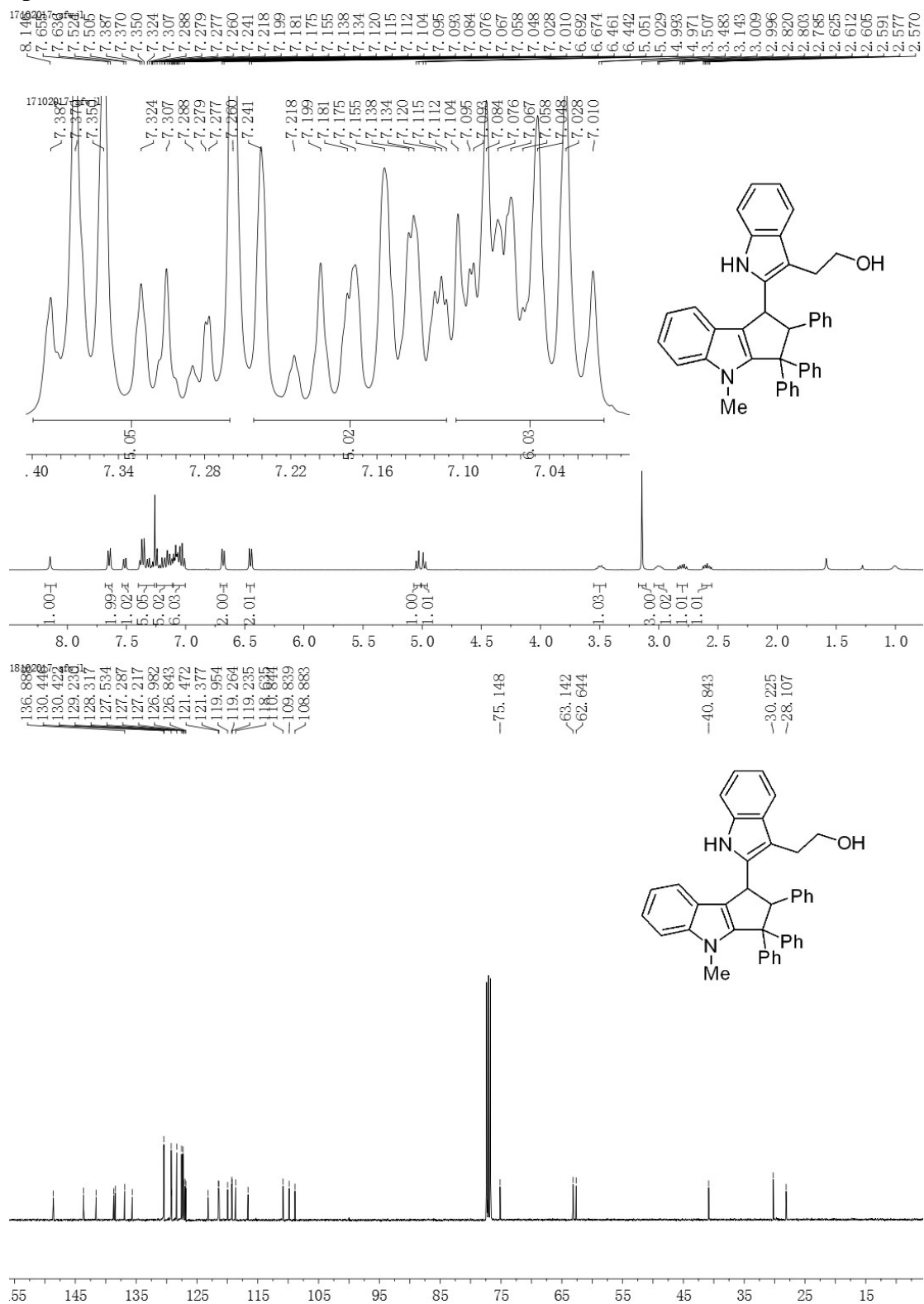


20160205

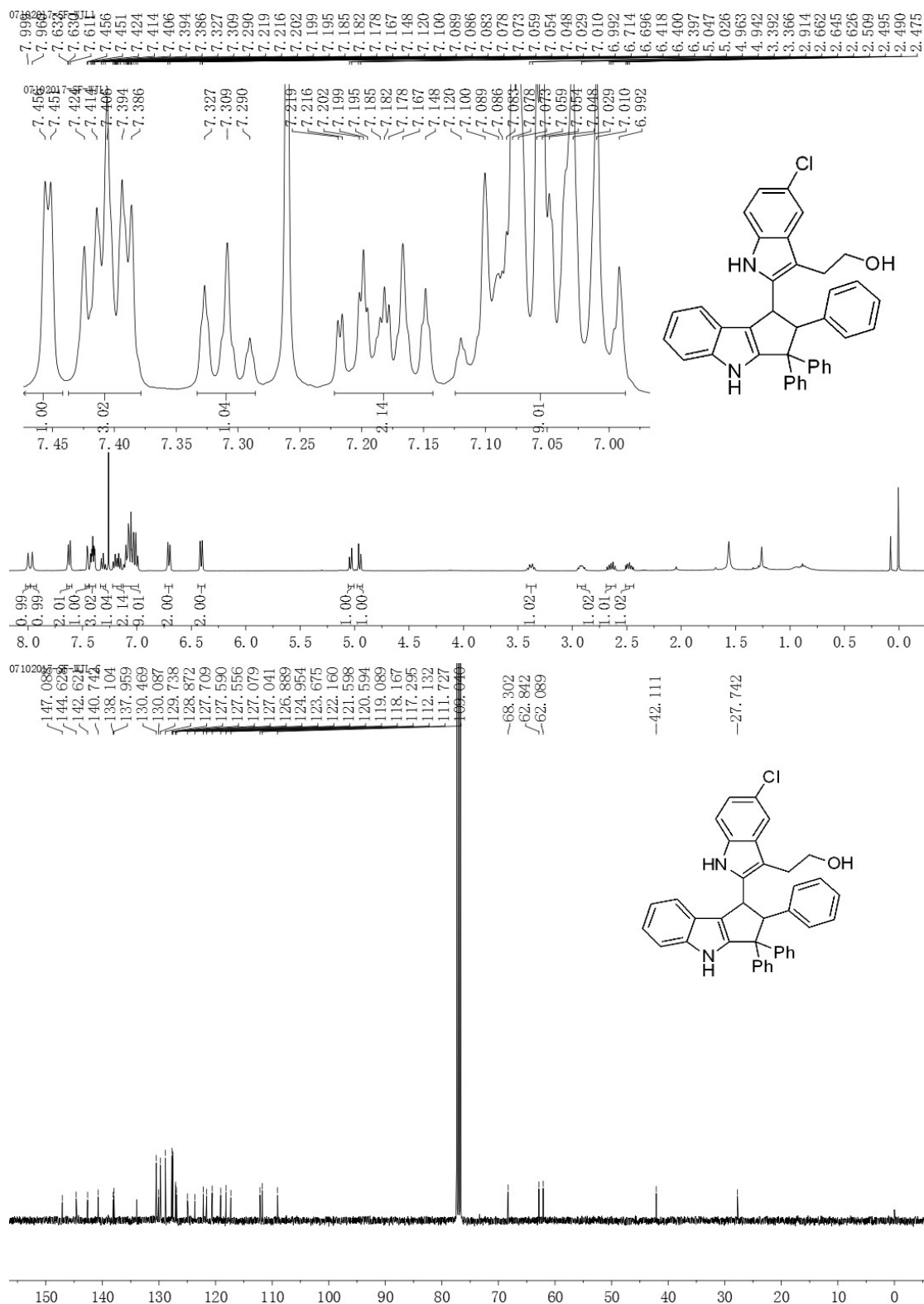


4na

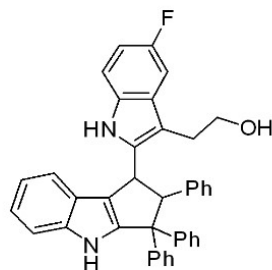
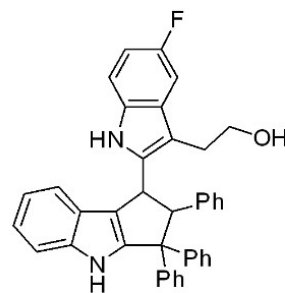




4ac



1504245-stj



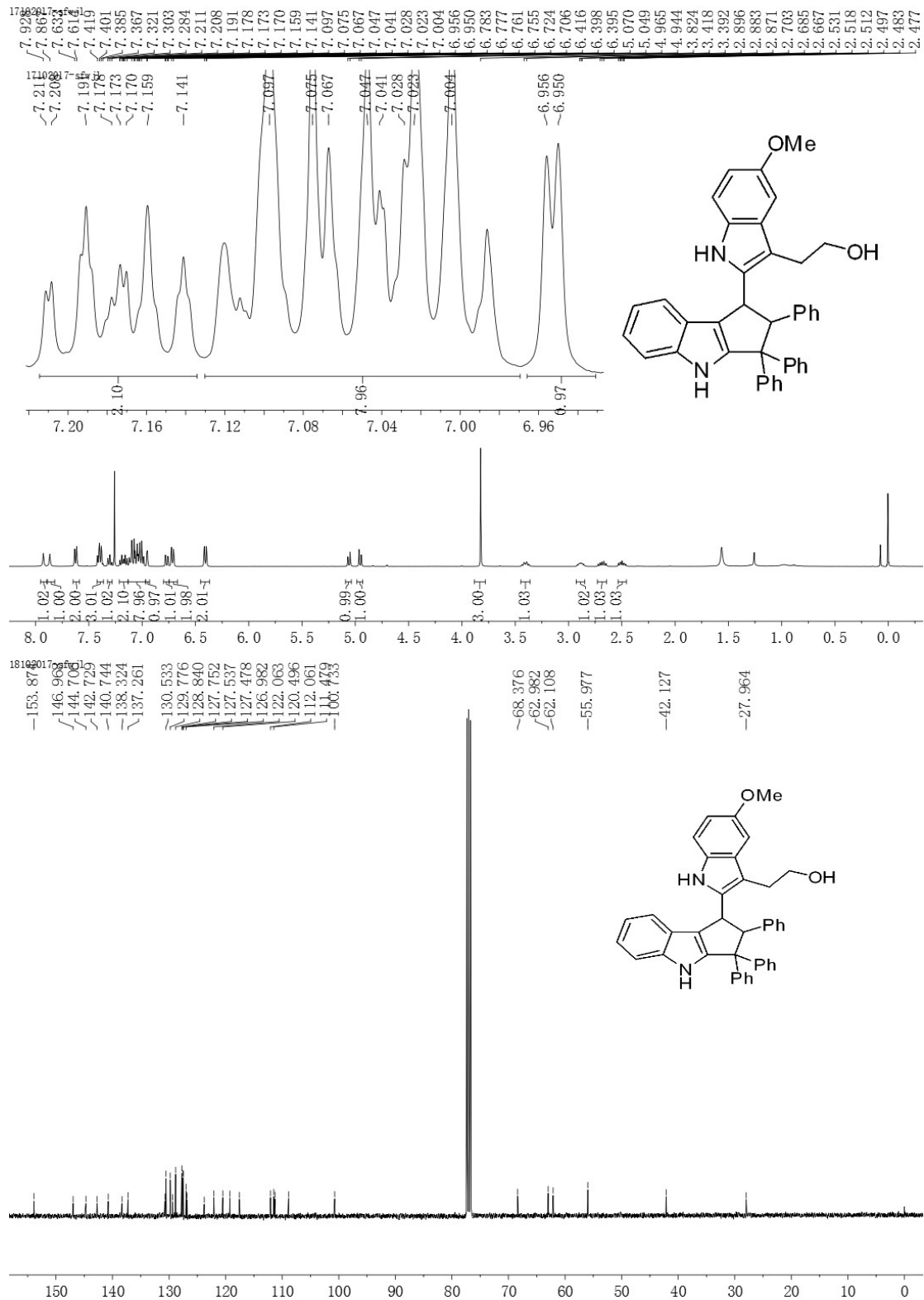
The figure displays the ^1H and ^{13}C NMR spectra of compound 10, along with its chemical structure.

Chemical Structure: The structure of compound 10 is shown, featuring a central indole ring system substituted with a 2-methyl-3-(2-hydroxyethyl)indol-5-yl group, a 2-phenyl-3-phenyl-4-phenyl-1H-indol-5-yl group, and a 2-phenyl-3-phenyl-4-phenyl-1H-indol-5-yl group.

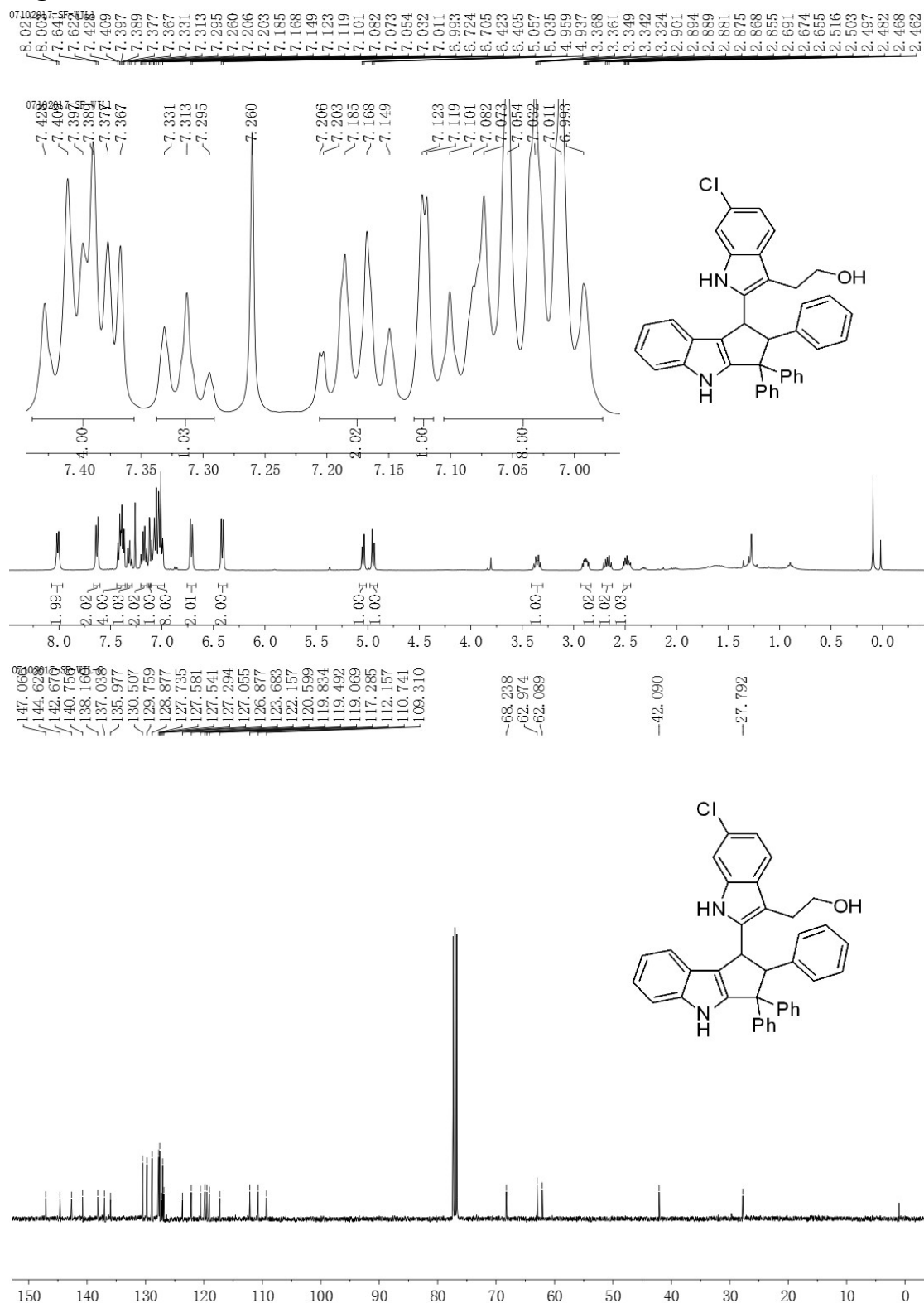
^1H NMR Spectrum: The ^1H NMR spectrum (top) shows peaks in the aromatic region (6.94–7.18 ppm) and the aliphatic region (2.42–2.99 ppm). Integration values are provided below the peaks.

^{13}C NMR Spectrum: The ^{13}C NMR spectrum (bottom) shows peaks in the aromatic region (108.60–140.74 ppm) and the aliphatic region (21.50–42.10 ppm).

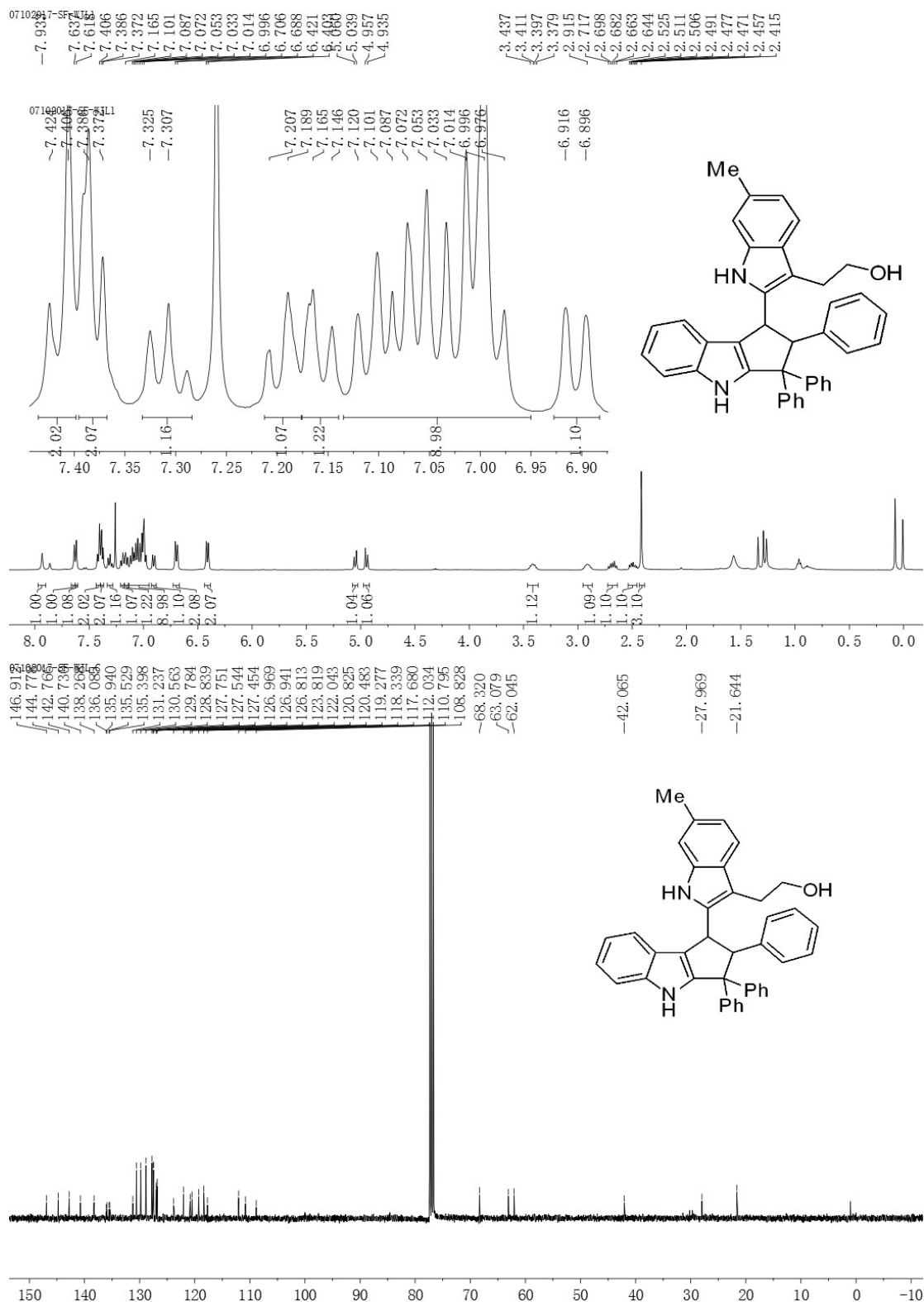
4af



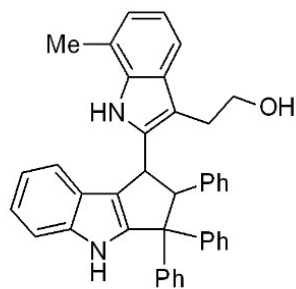
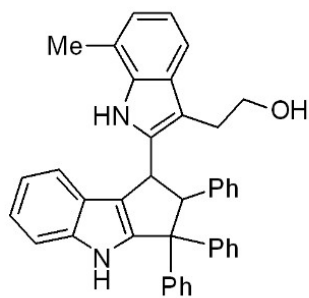
4ag



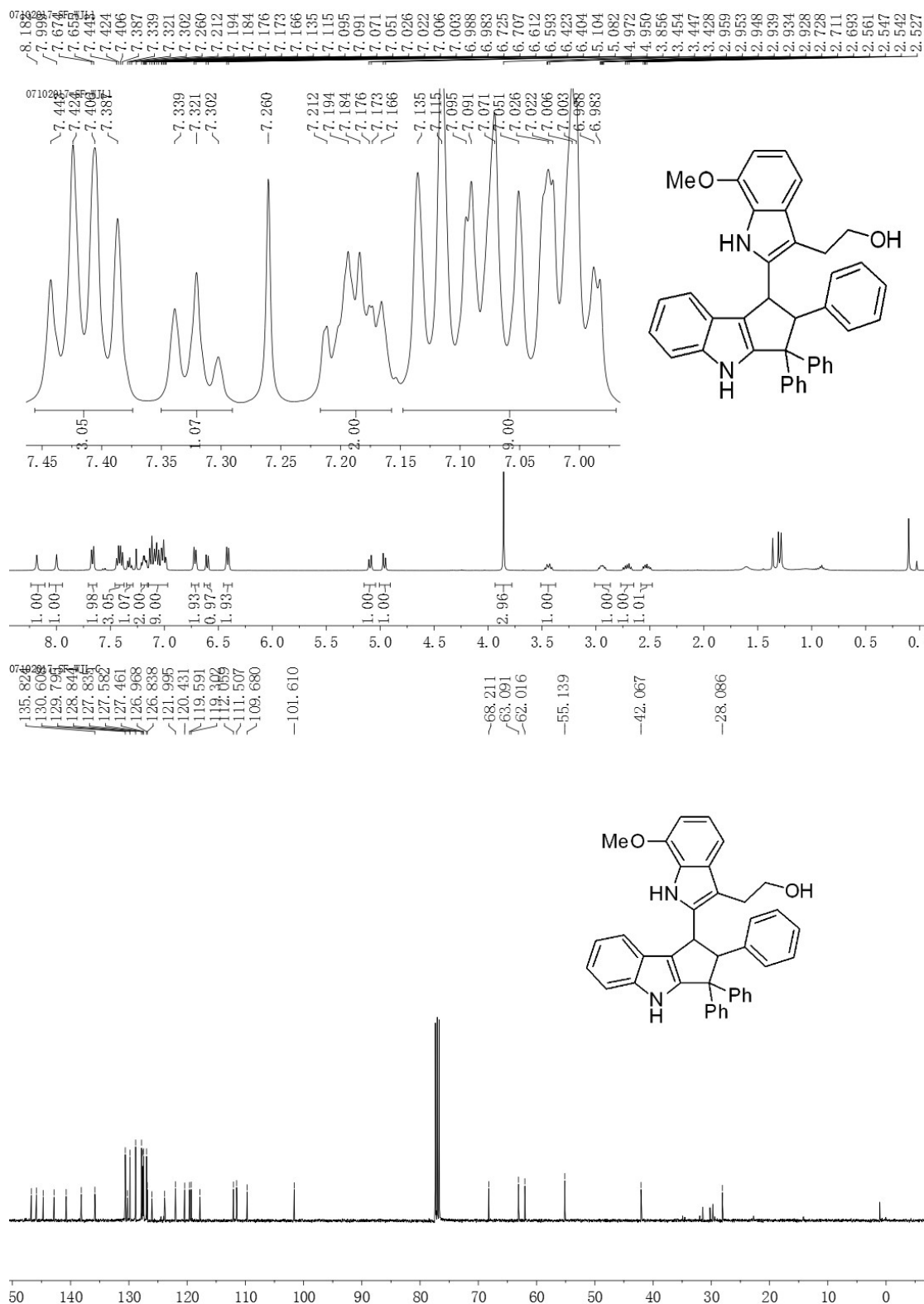
4ai



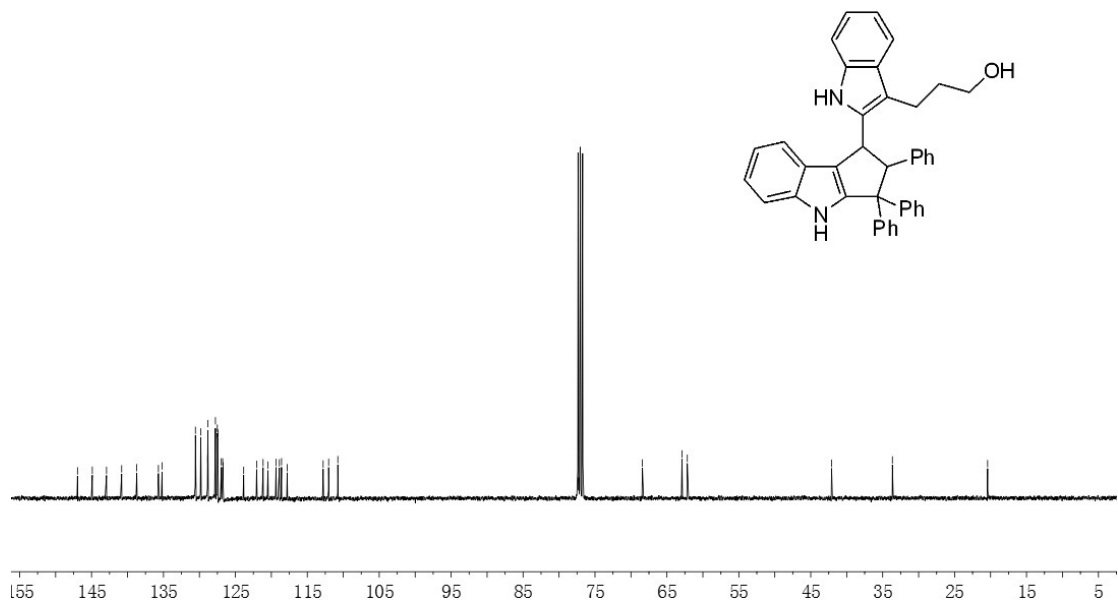
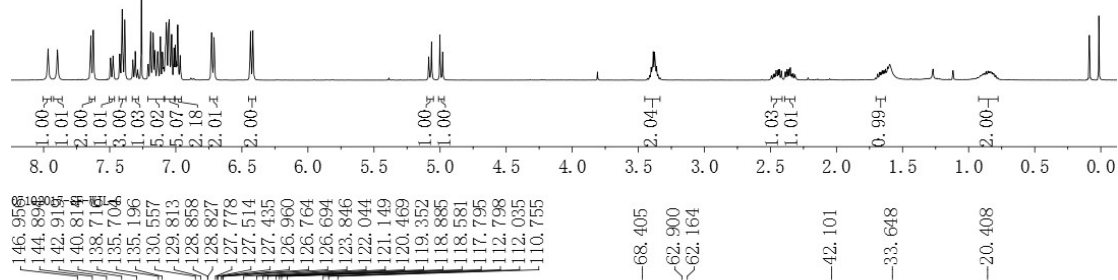
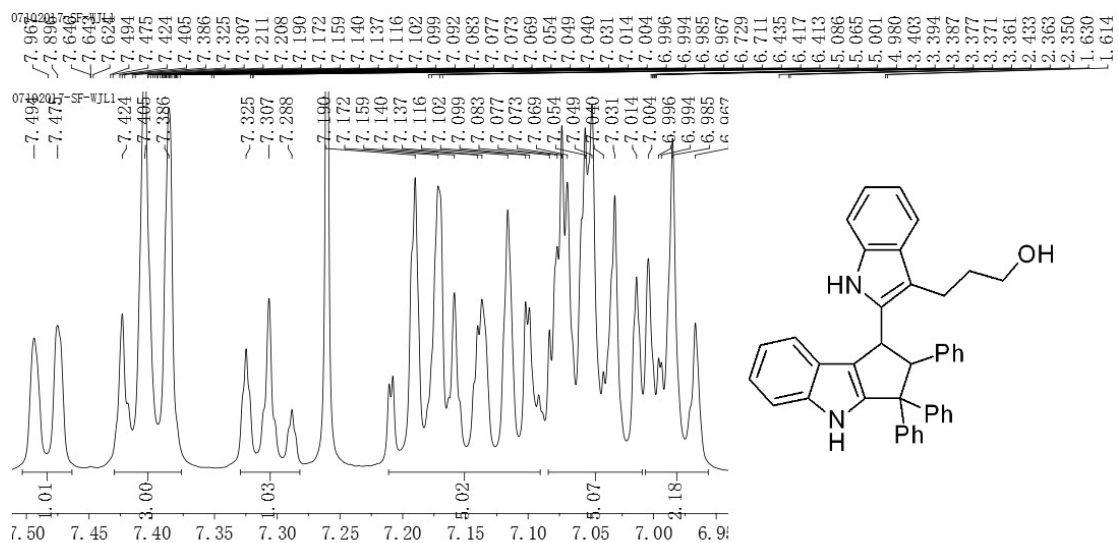
26520



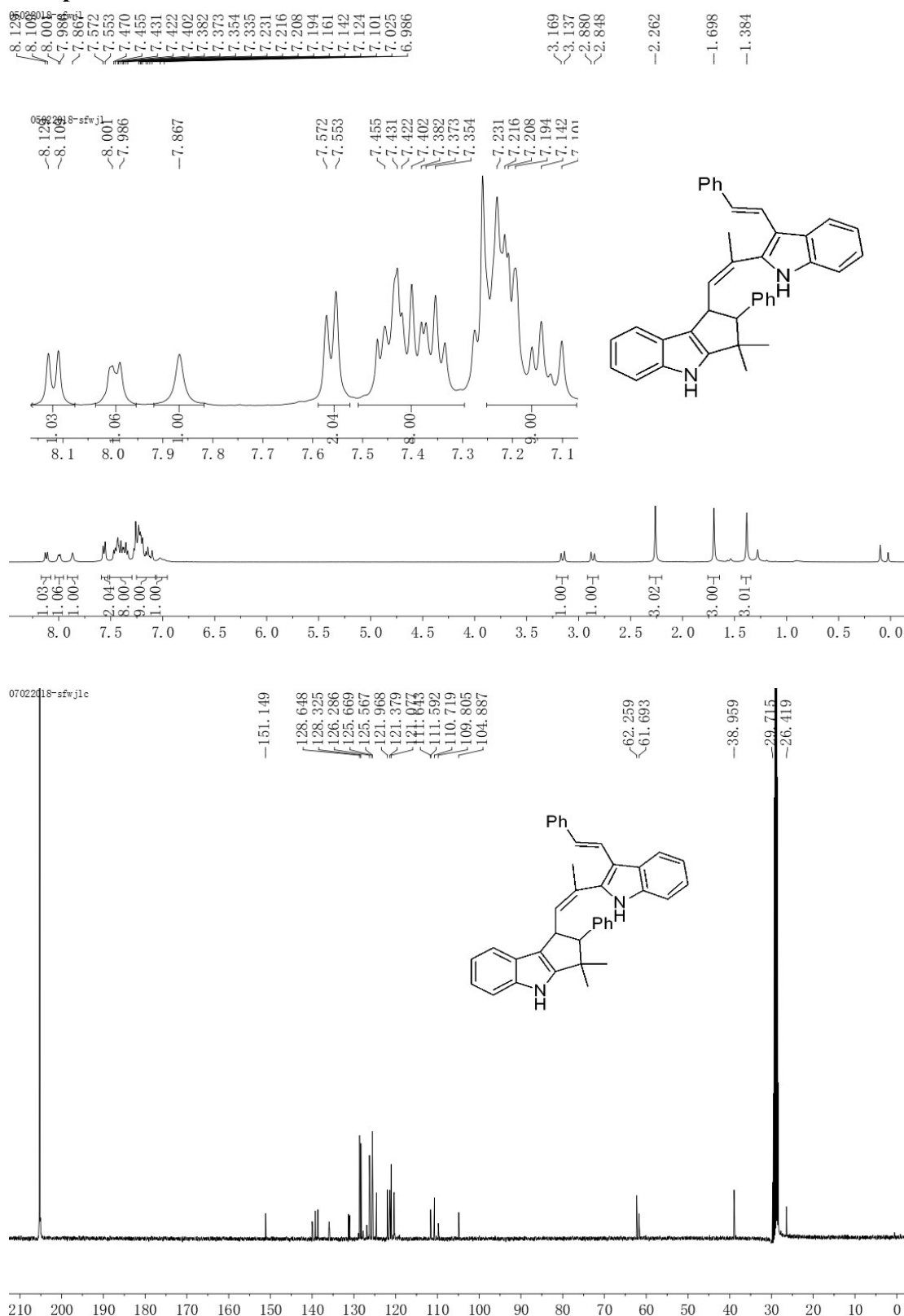
4ak



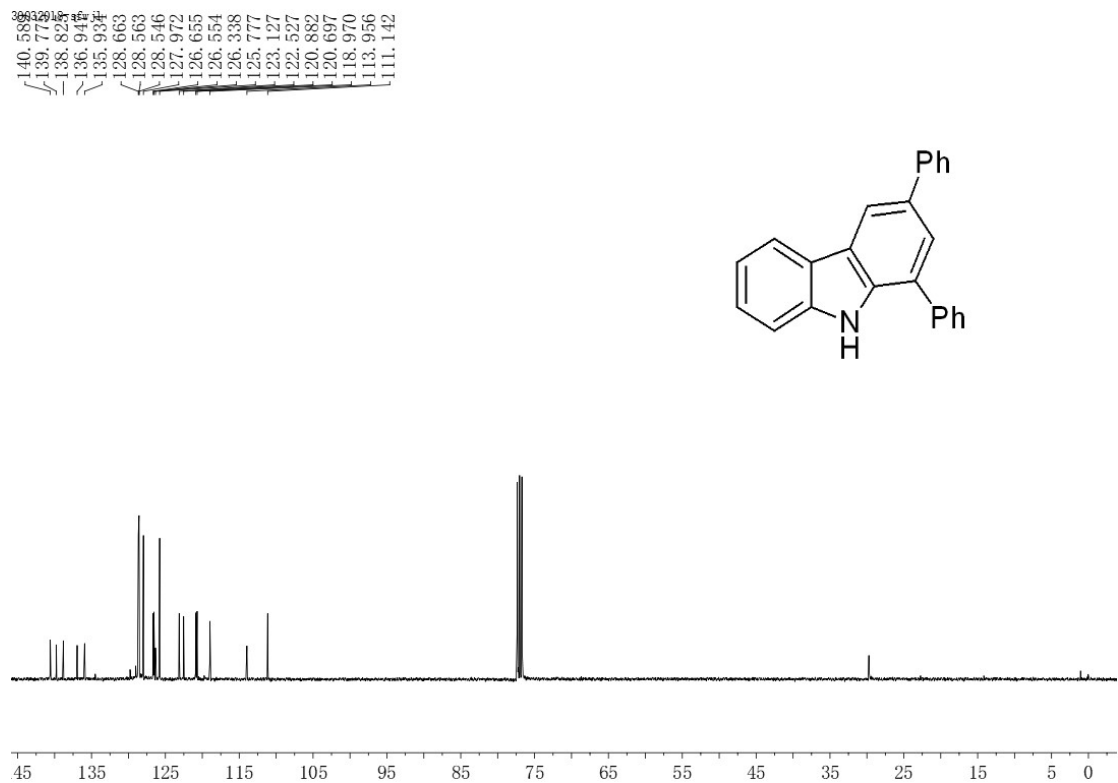
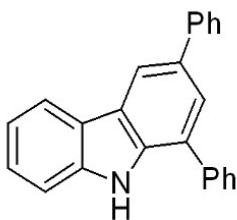
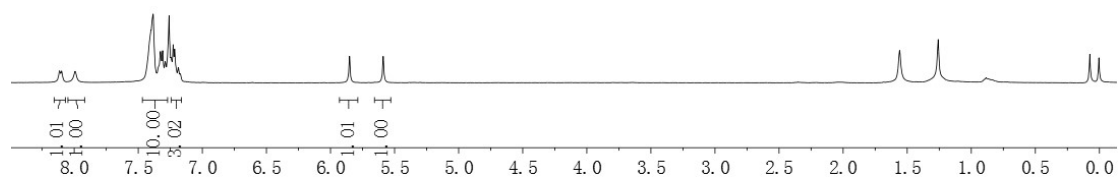
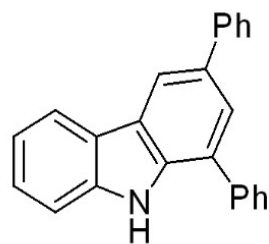
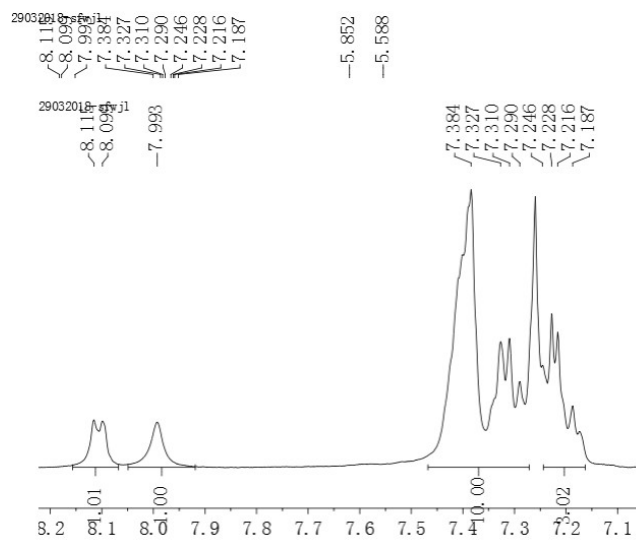
4al



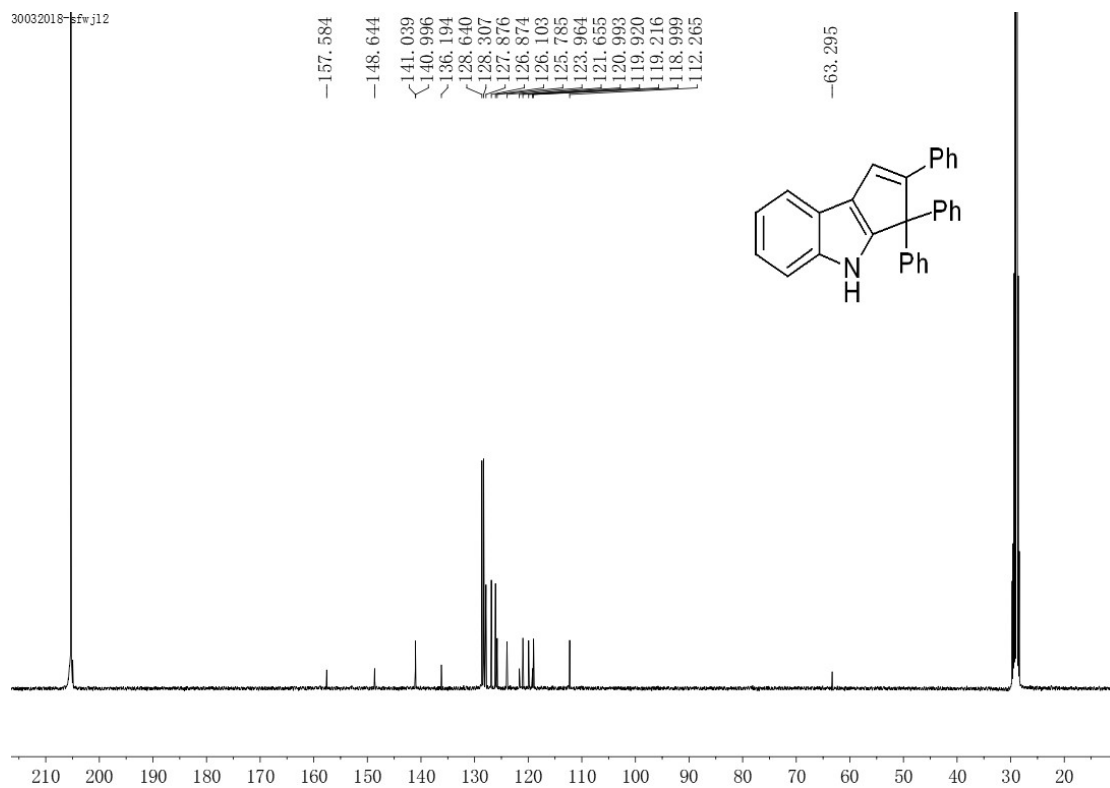
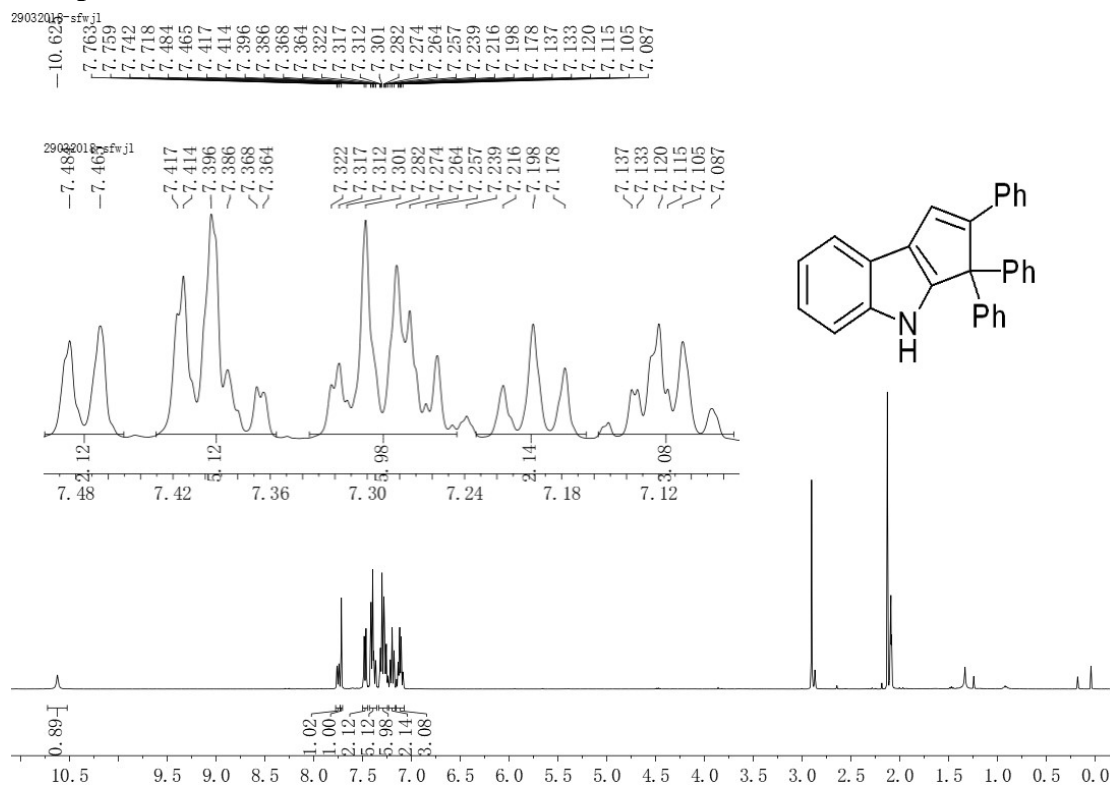
Compound 6



Compound 7

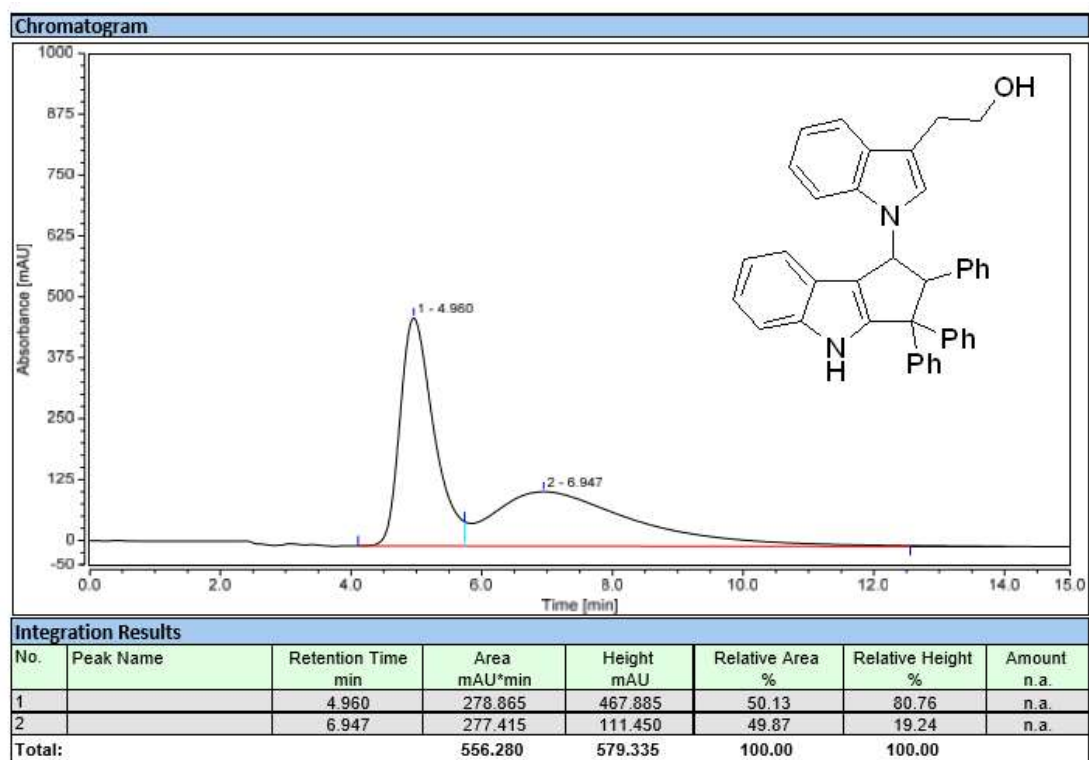


Compound 8

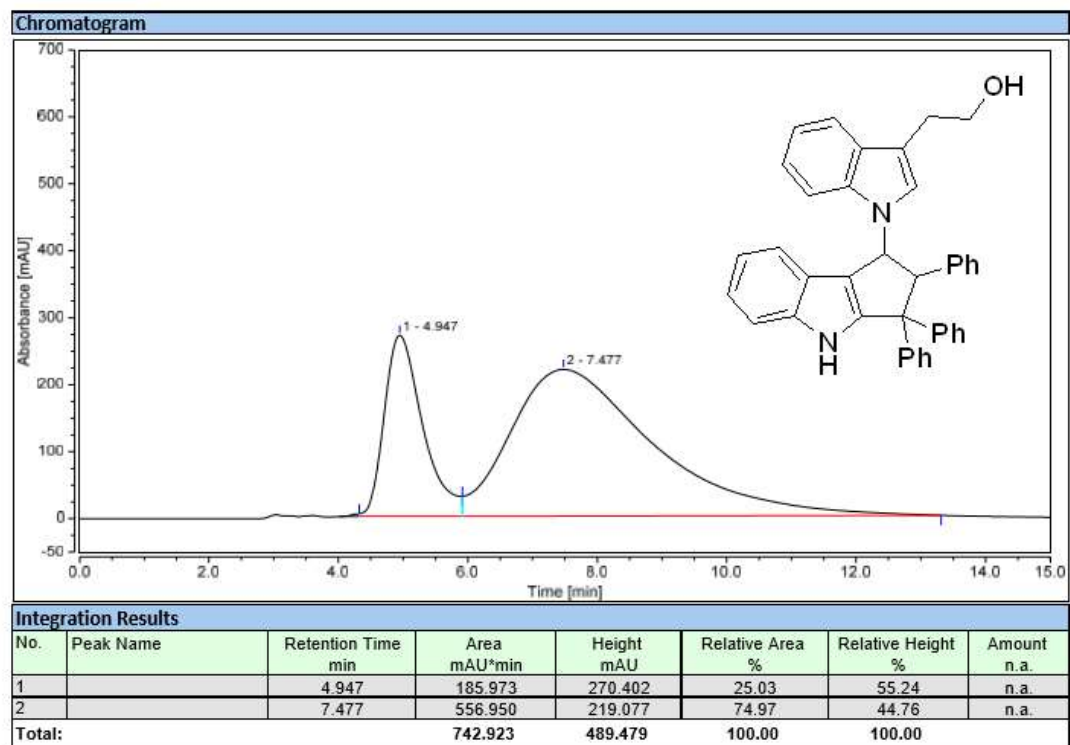


2. HPLC copies of product 3aa

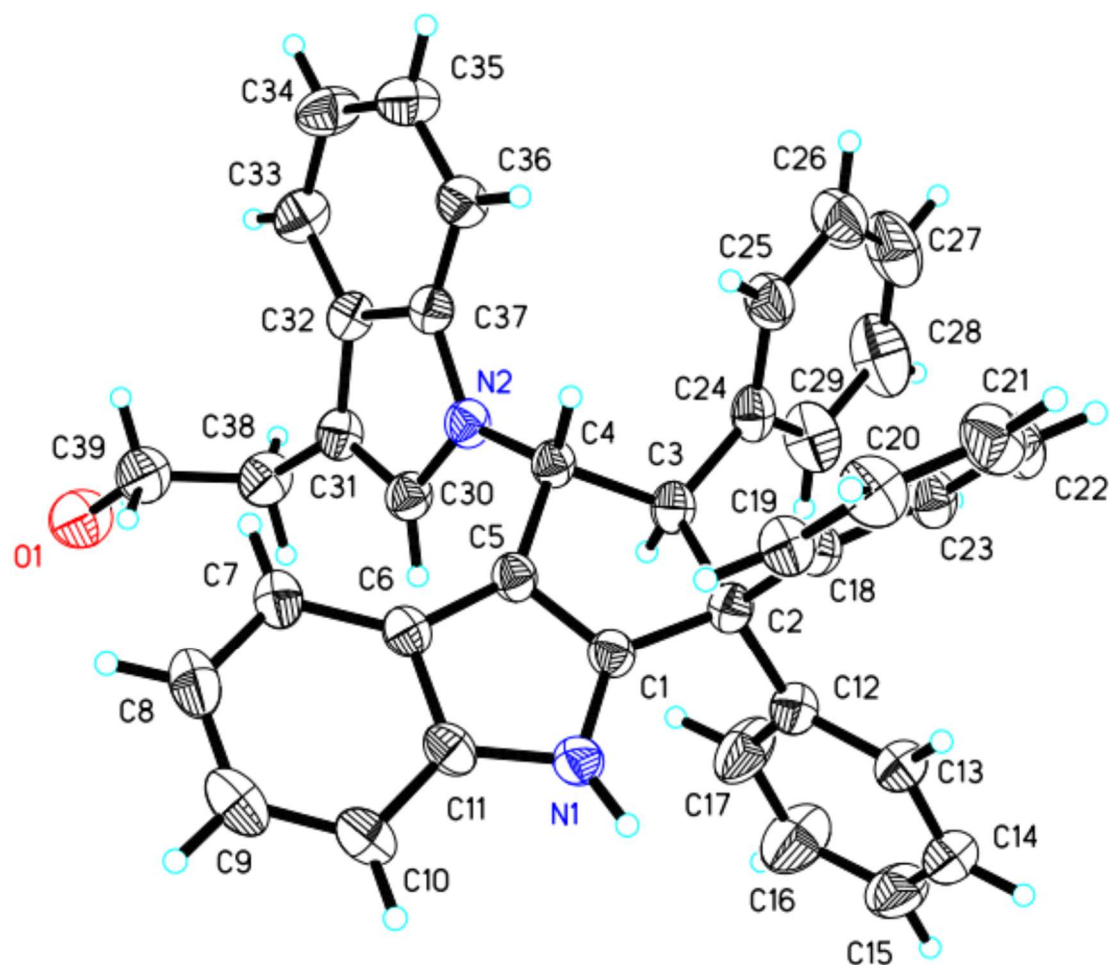
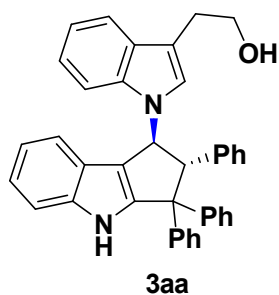
Racemic:



Enantioselective:



3. X-ray analysis of product 3aa and 4aa

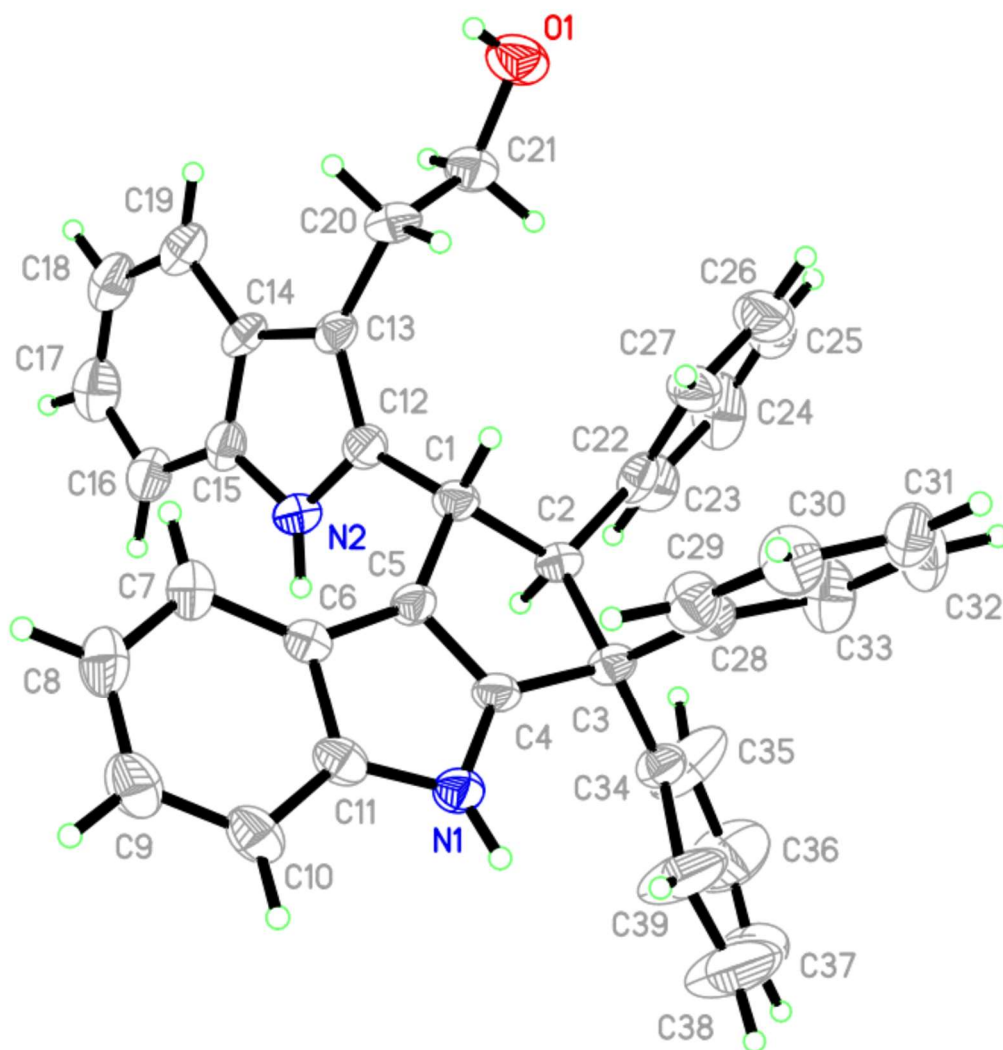
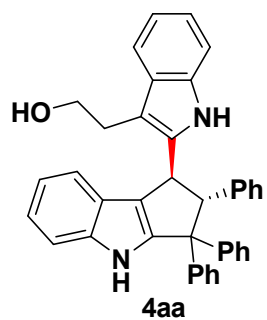


The thermal ellipsoid was drawn at the 30% probability level.

Figure S1. Single crystal structure of **3aa**

Temperature	296.15 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C 1 2/c 1	
Unit cell dimensions	a = 23.869(3) Å	$\alpha = 90^\circ$.
	b = 13.815(2) Å	$\beta = 103.665(2)^\circ$.
	c = 19.332(3) Å	$\gamma = 90^\circ$.

Volume	6194.3(15) Å ³
Z	8
Density (calculated)	1.259 Mg/m ³
Absorption coefficient	0.158 mm ⁻¹
F(000)	2472
Crystal size	0.3 x 0.3 x 0.1 mm ³
Theta range for data collection	2.447 to 27.484°.
Index ranges	-30<= <i>h</i> <=21, -16<= <i>k</i> <=17, -24<= <i>l</i> <=25
Reflections collected	18186
Independent reflections	6952 [R(int) = 0.0339]
Completeness to theta = 25.242°	99.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7456 and 0.6720
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	6952 / 0 / 394
Goodness-of-fit on F ²	1.034
Final R indices [I>2sigma(I)]	R1 = 0.0648, wR2 = 0.1705
R indices (all data)	R1 = 0.1219, wR2 = 0.2013
Extinction coefficient	n/a
Largest diff. peak and hole	0.387 and -0.483 e.Å ⁻³



The thermal ellipsoid was drawn at the 30% probability level.

Figure S2. Single crystal structure of **4aa**

Empirical formula	C ₃₉ H ₃₂ N ₂ O
Formula weight	544.66
Temperature	296.15 K
Wavelength	0.71073 Å
Crystal system	Orthorhombic

Space group	P2 ₁ 2 ₁ 2 ₁	
Unit cell dimensions	a = 11.228(6) Å	α = 90°.
	b = 16.224(8) Å	β = 90°.
	c = 18.542(9) Å	γ = 90°.
Volume	3378(3) Å ³	
Z	4	
Density (calculated)	1.071 Mg/m ³	
Absorption coefficient	0.064 mm ⁻¹	
F(000)	1152	
Crystal size	0.25 x 0.22 x 0.2 mm ³	
Theta range for data collection	2.530 to 26.749°.	
Index ranges	-10 ≤ h ≤ 14, -20 ≤ k ≤ 20, -23 ≤ l ≤ 23	
Reflections collected	19183	
Independent reflections	6988 [R(int) = 0.0381]	
Completeness to theta = 25.242°	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7455 and 0.6449	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	6988 / 0 / 380	
Goodness-of-fit on F ²	0.934	
Final R indices [I > 2σ(I)]	R1 = 0.0762, wR2 = 0.2088	
R indices (all data)	R1 = 0.1074, wR2 = 0.2341	
Absolute structure parameter	0.0(9)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.469 and -0.319 e.Å ⁻³	