Supporting Information

Vinylogous elimination/Heck coupling/allylation domino reactions: access to 2-substituted 2,3-dihydrobenzofurans and indolines

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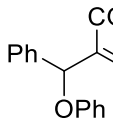
The copies of ^{1}H or ^{13}C NMR and NOESY spectra for compounds **2-4** and **6** S2

X-Ray Crystallographic Data for compounds **3a**, **6t**, and **6w** S65



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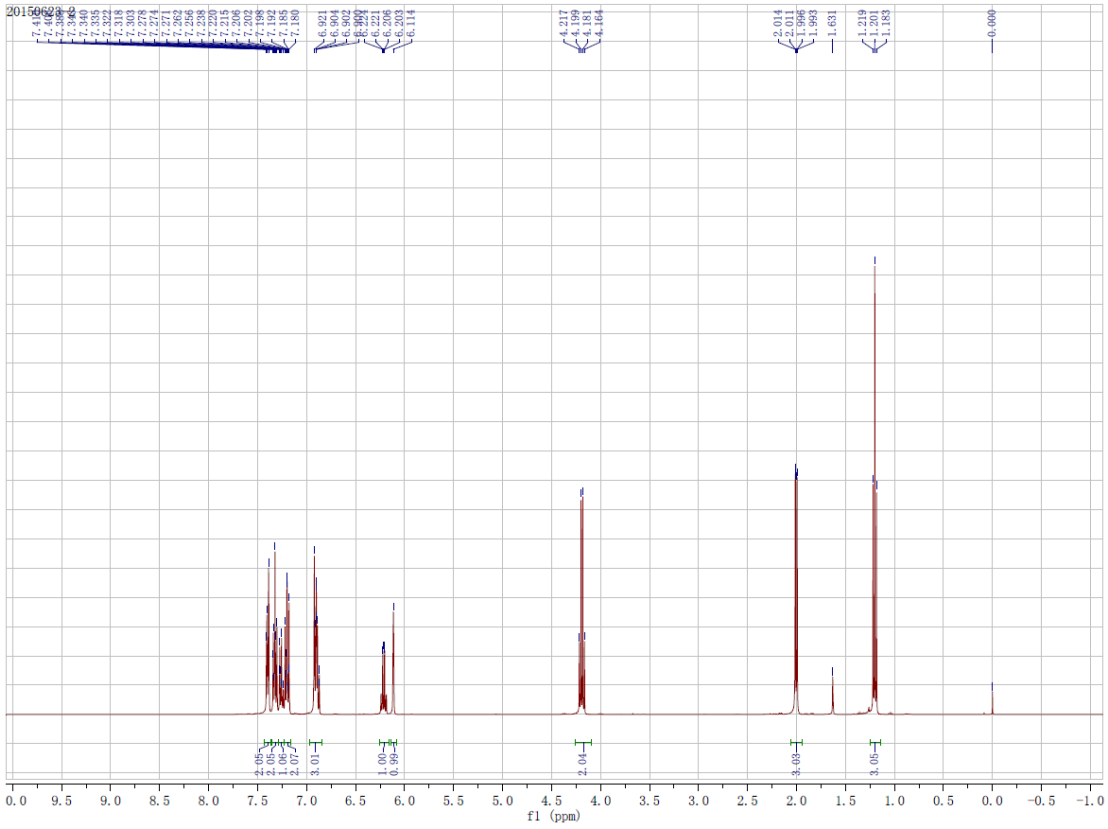

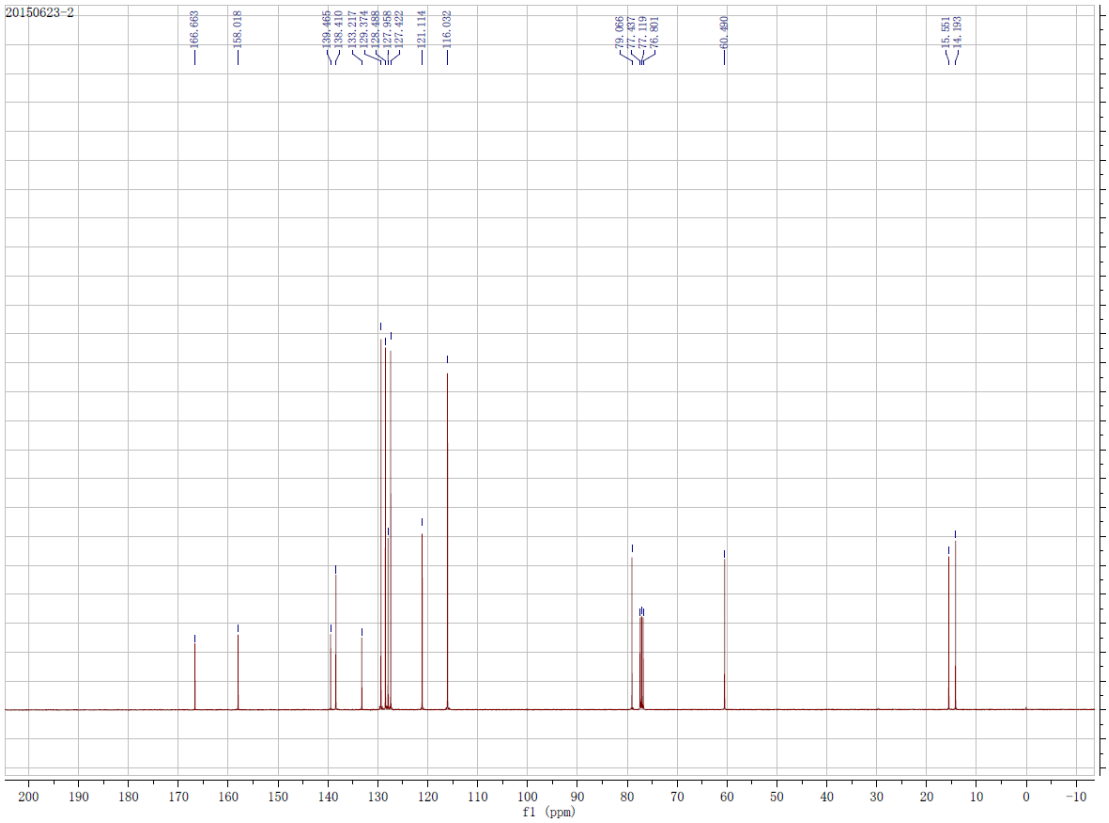

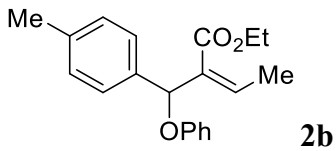

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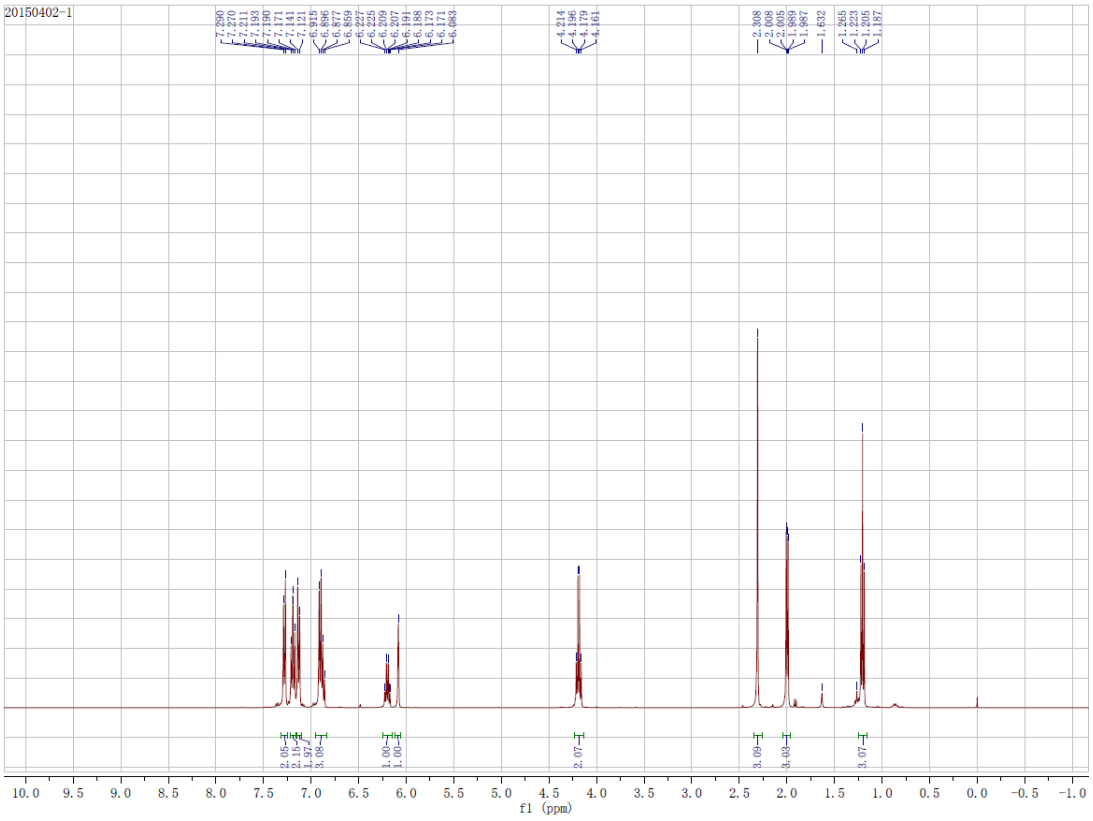

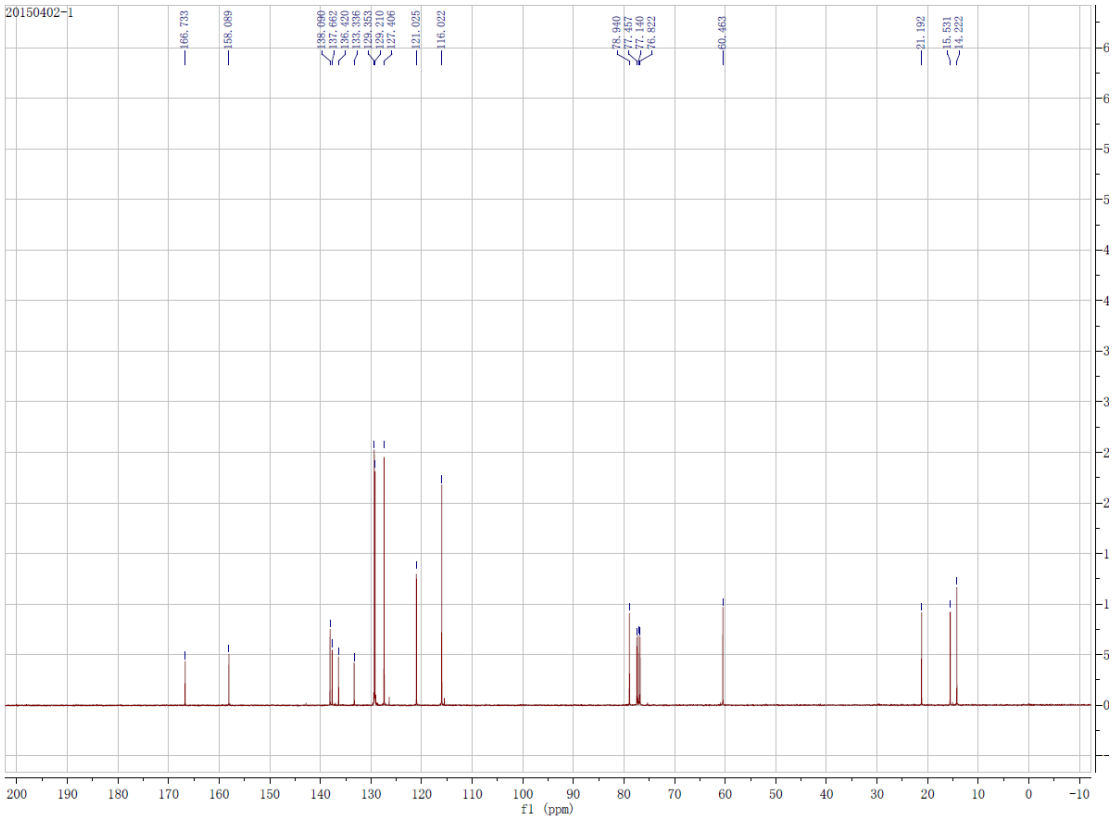

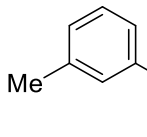

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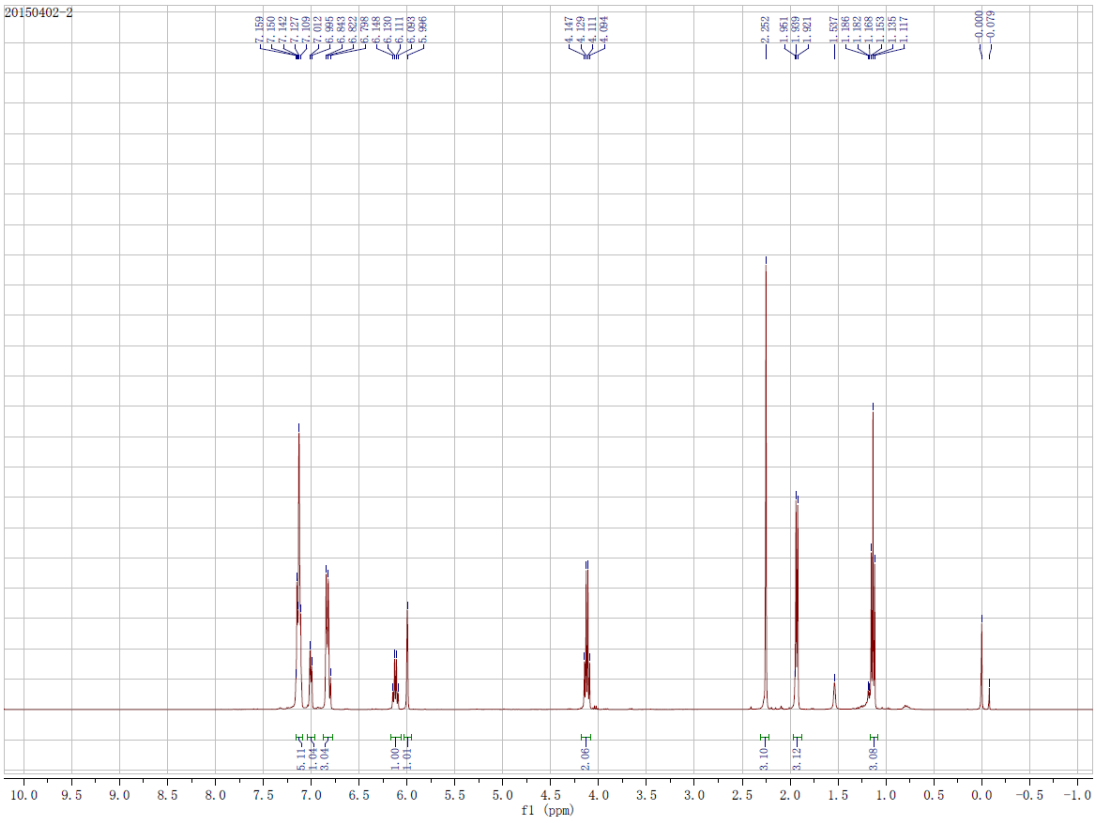

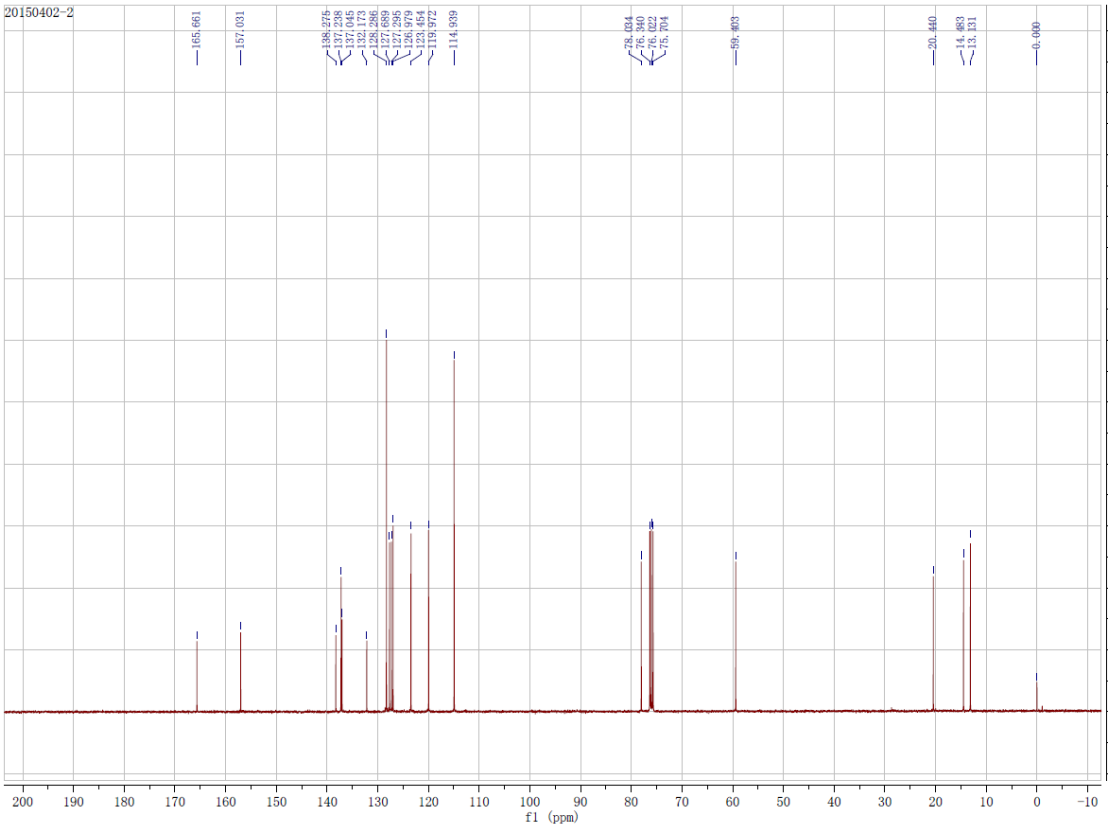

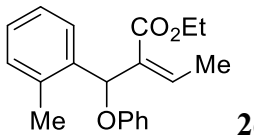

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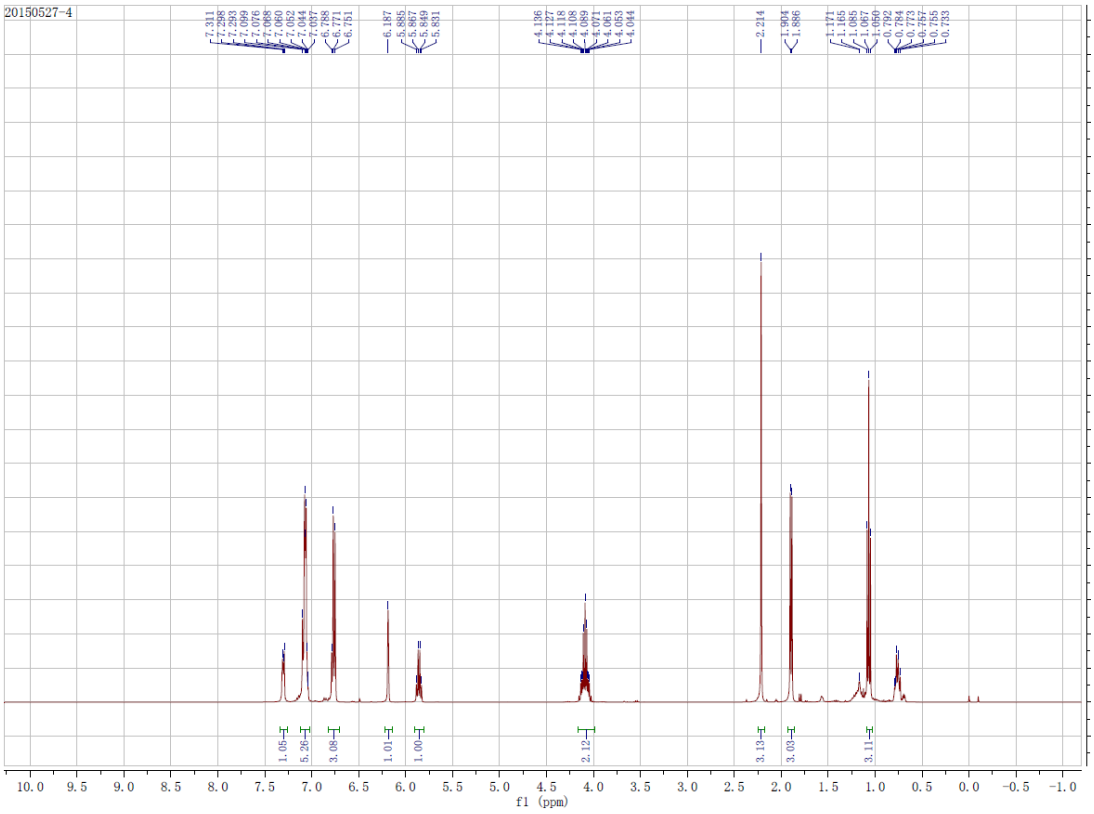

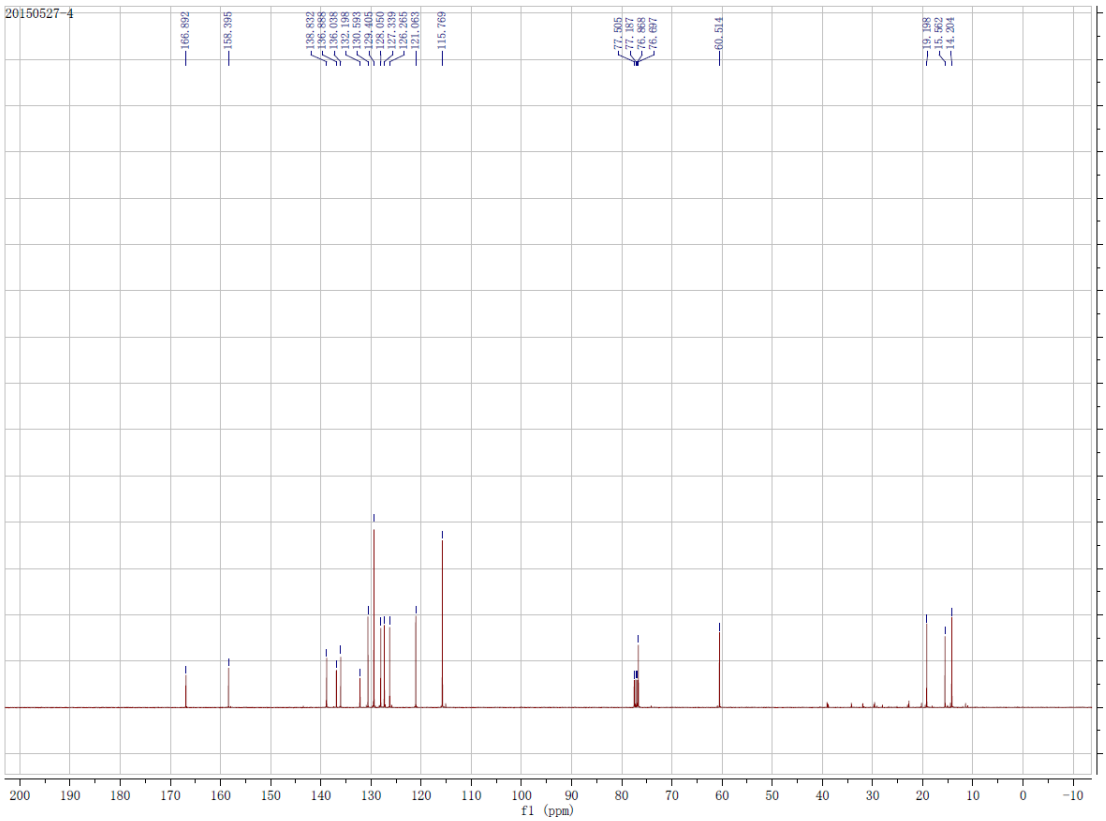

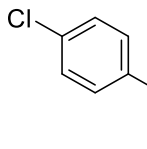

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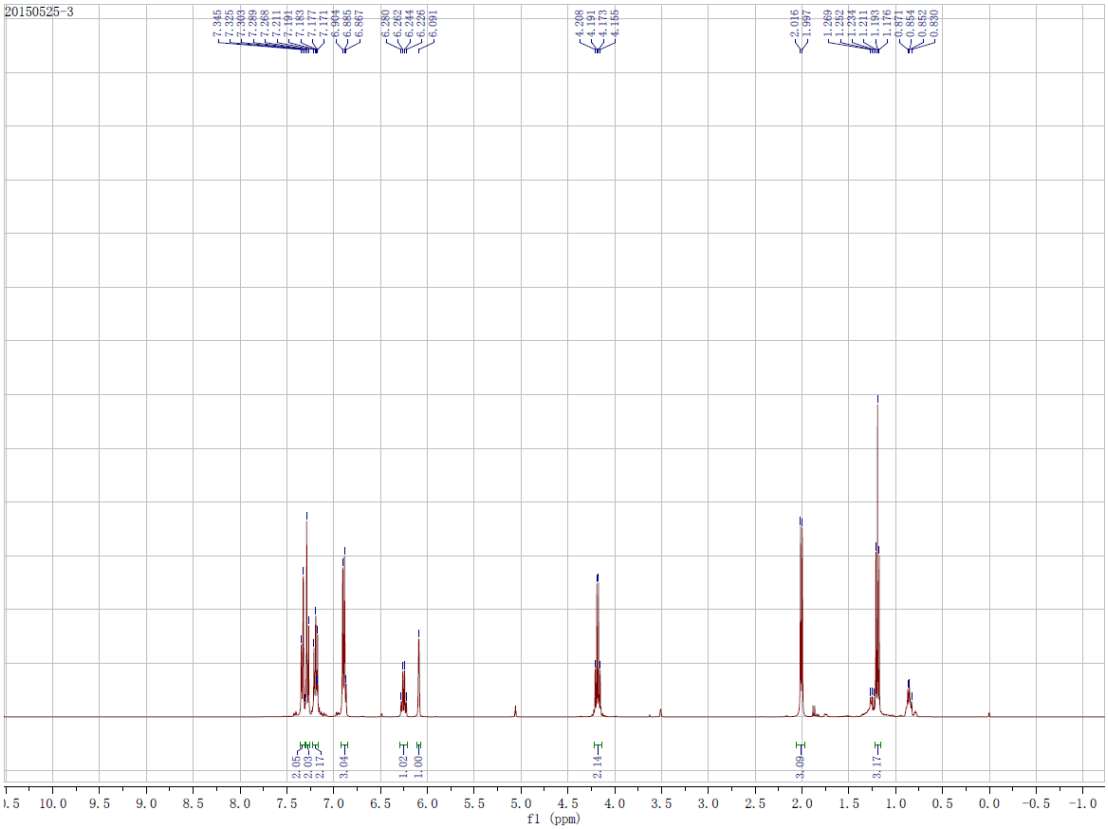

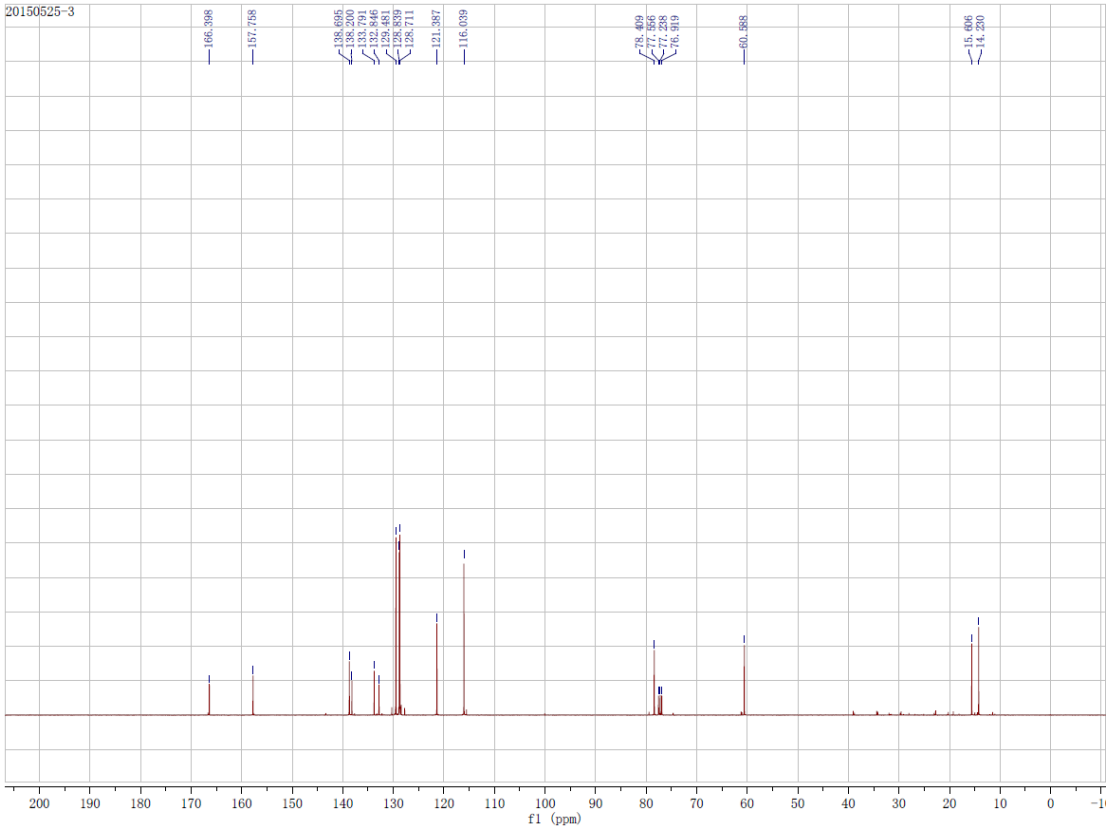

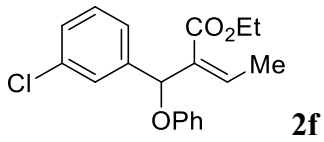

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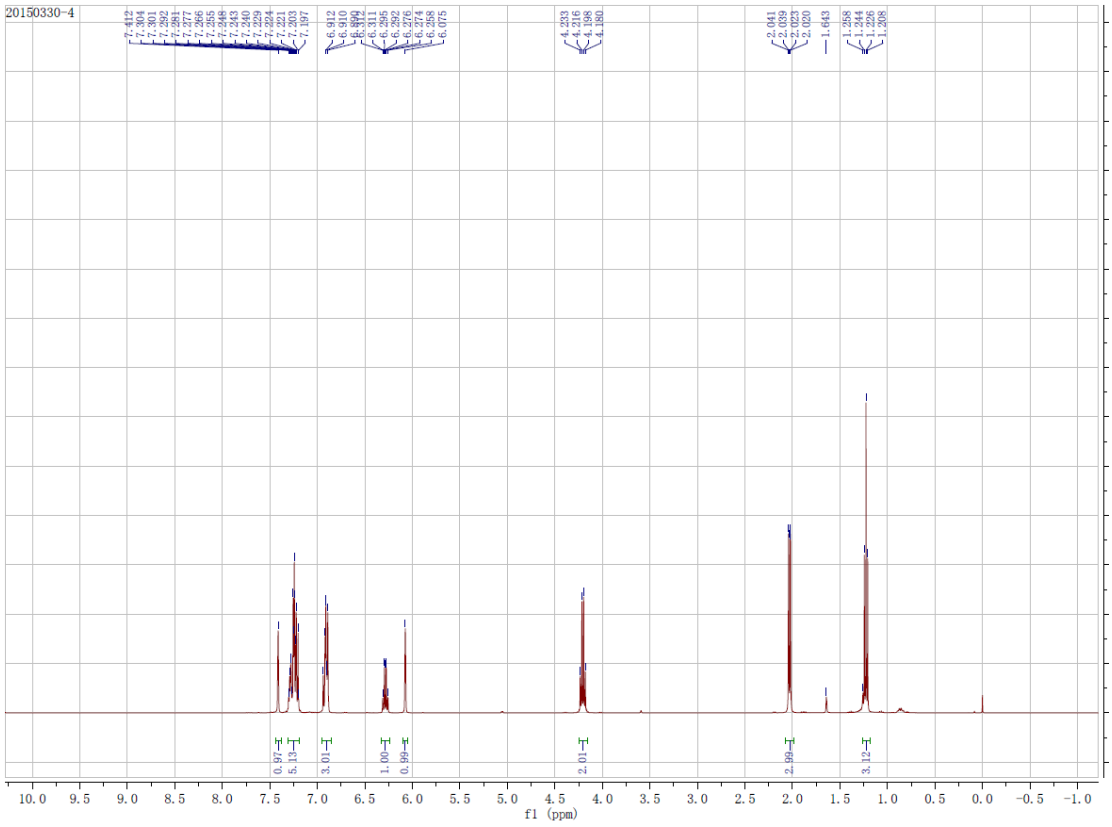

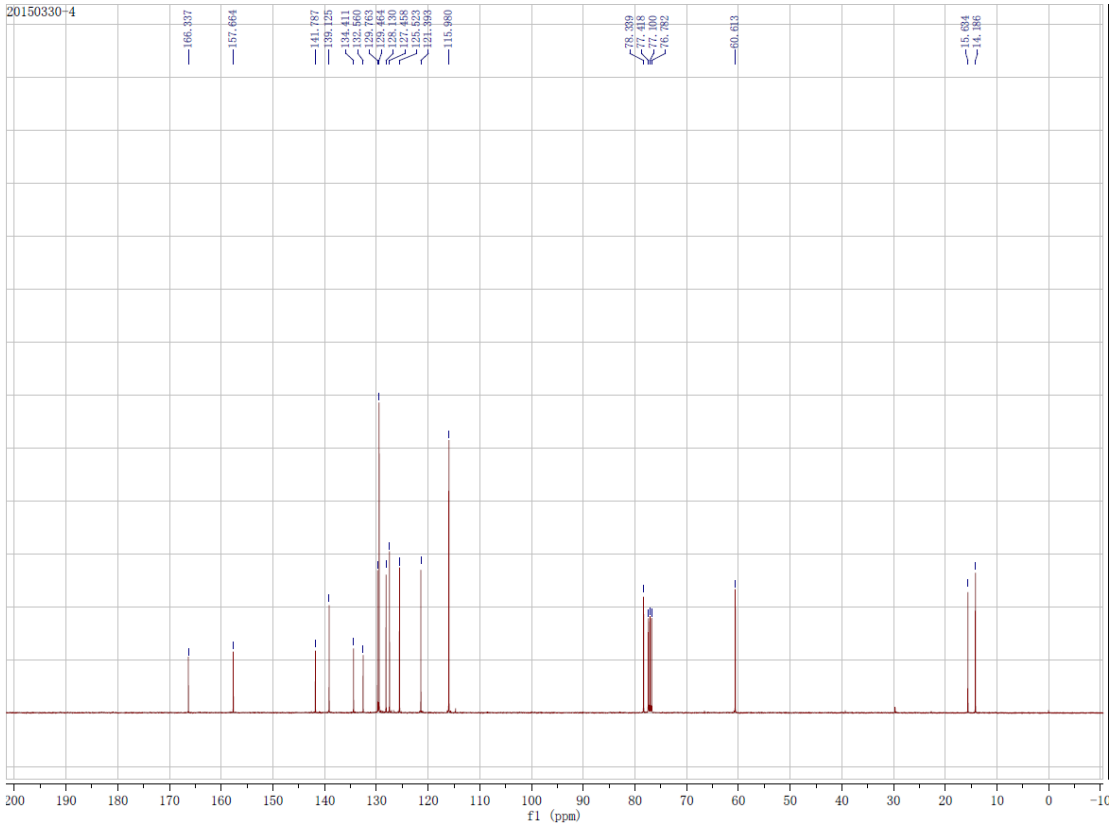

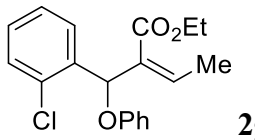

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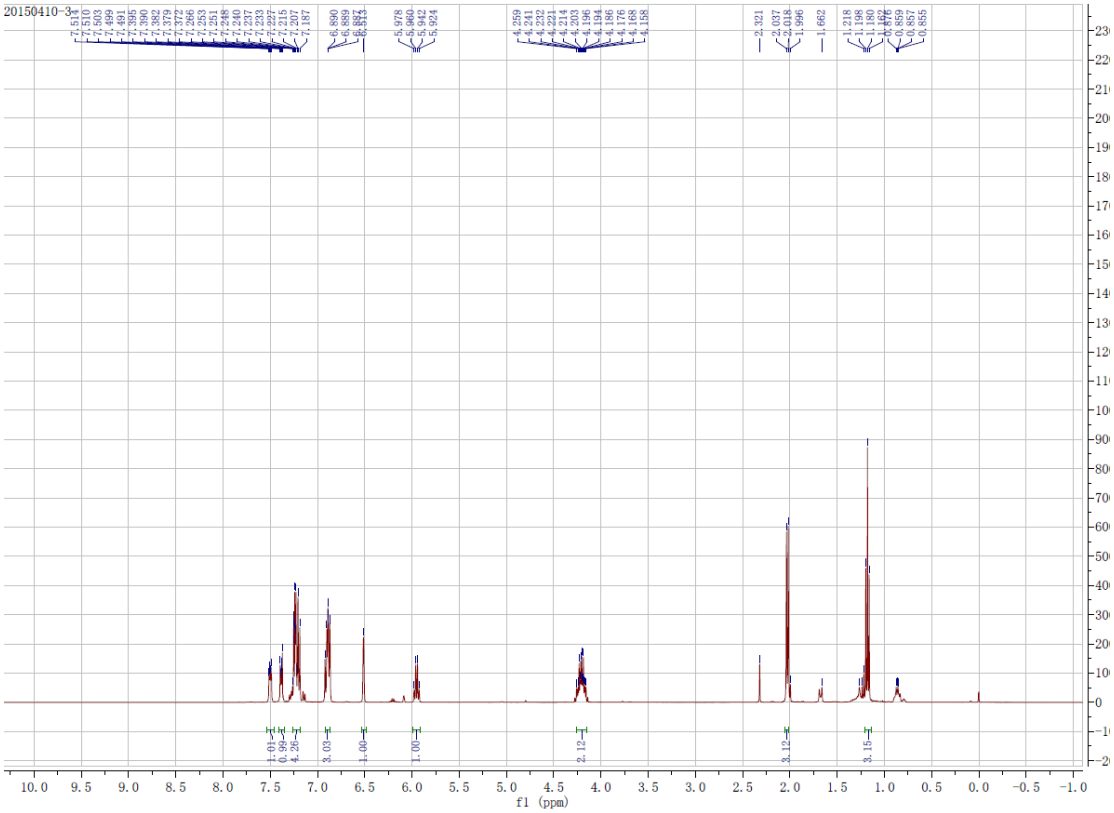

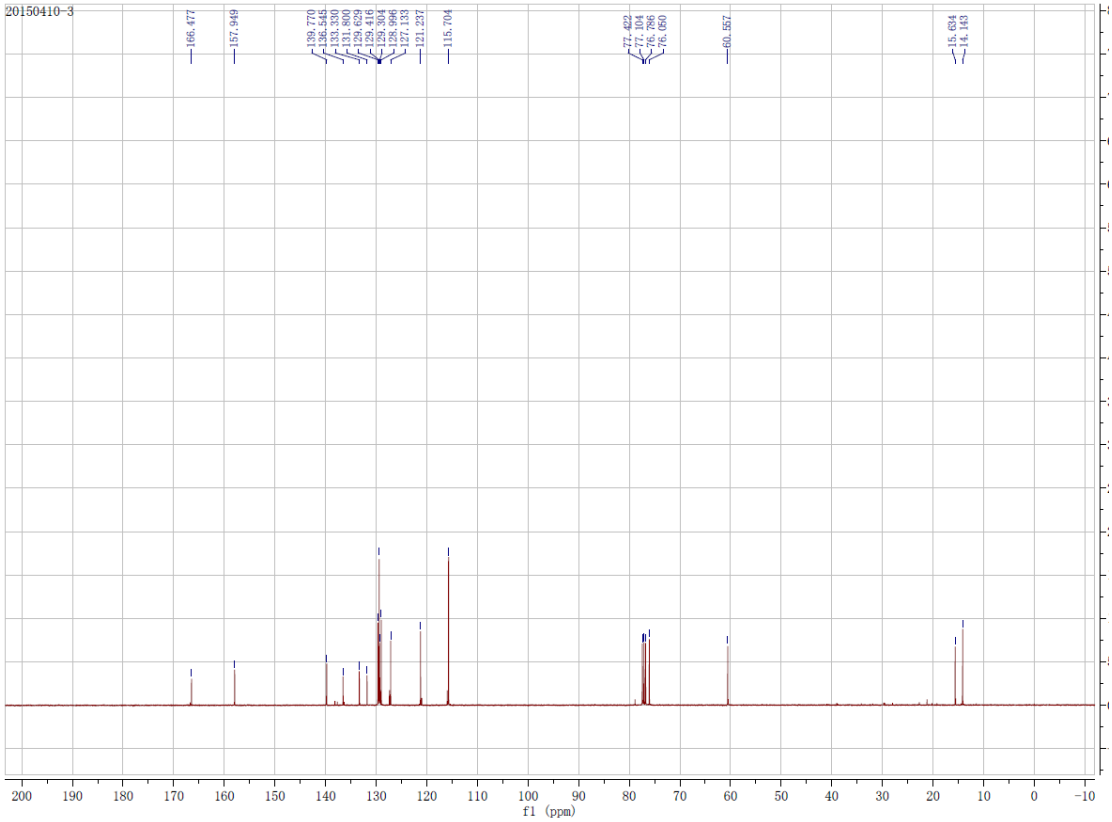

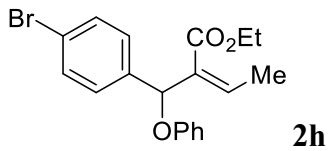

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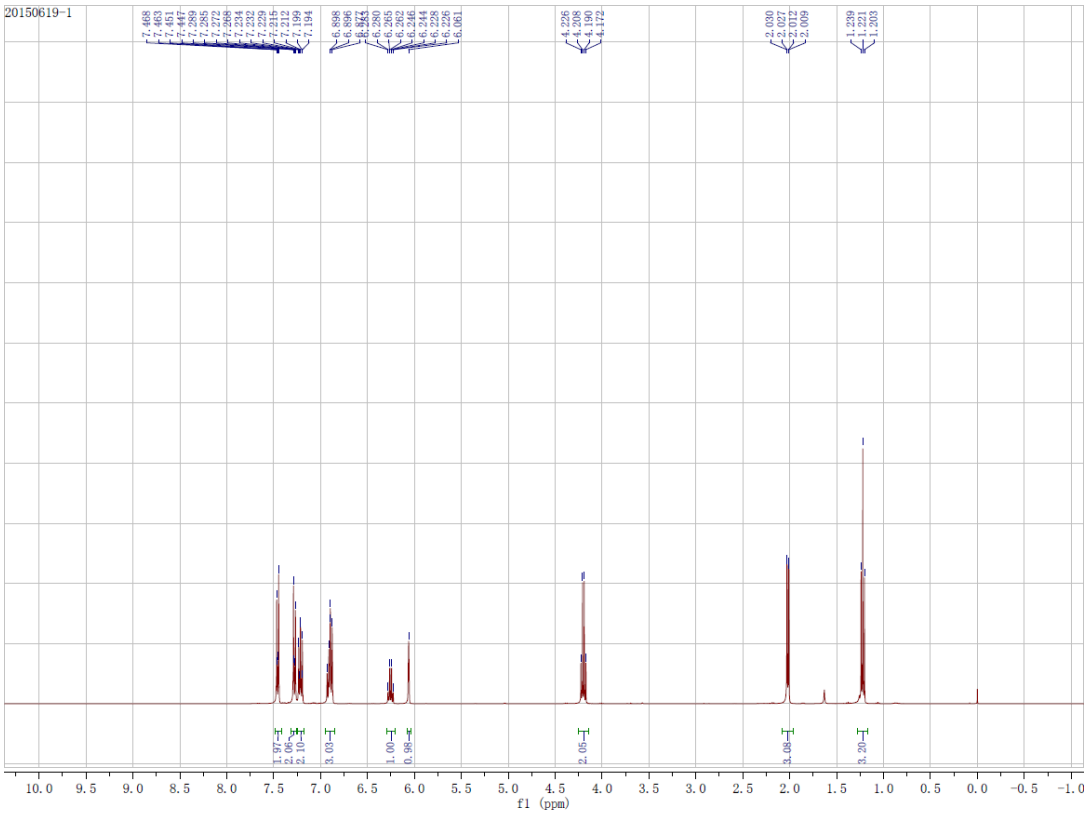

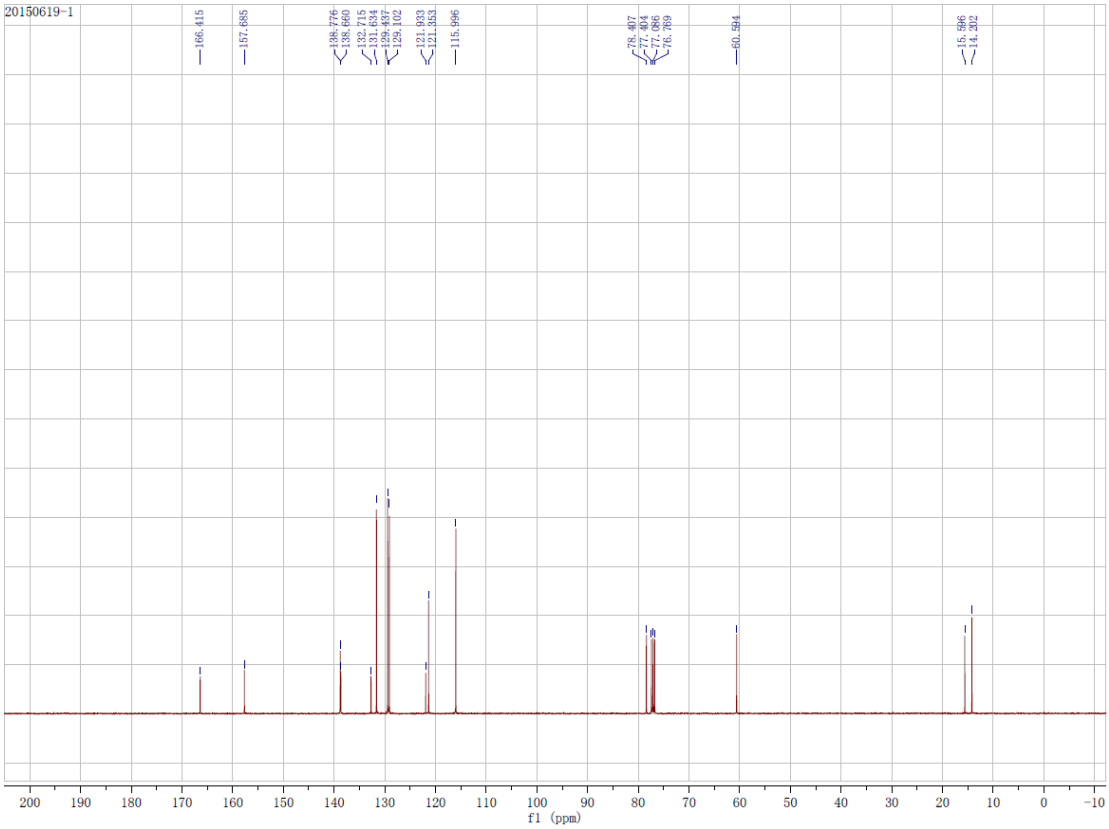

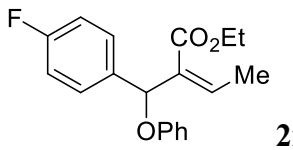

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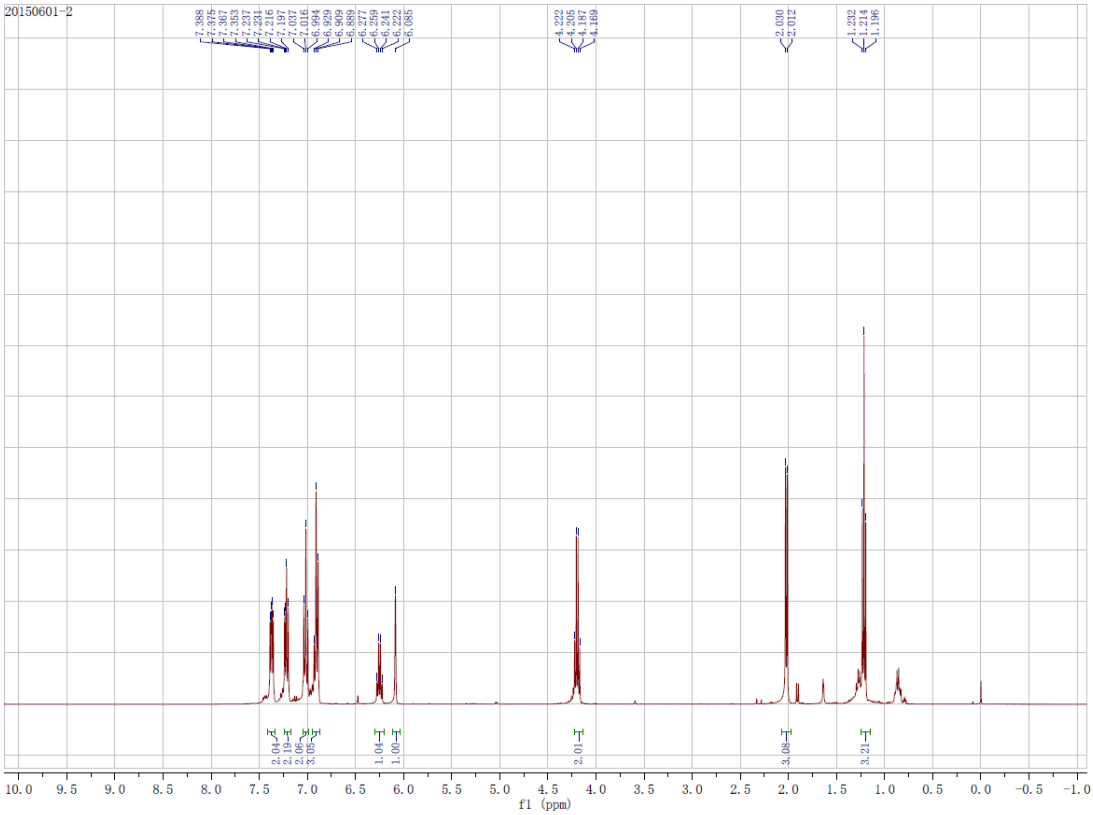

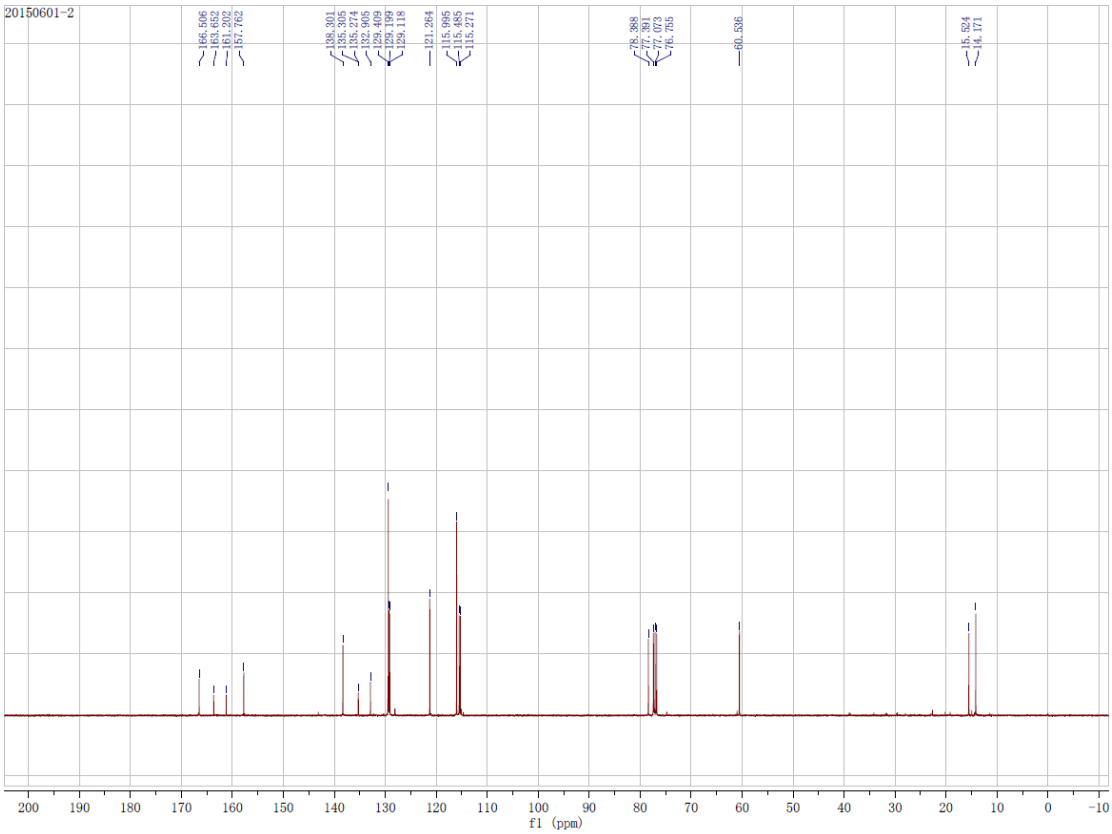

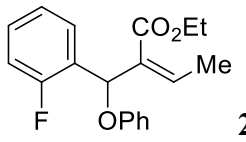

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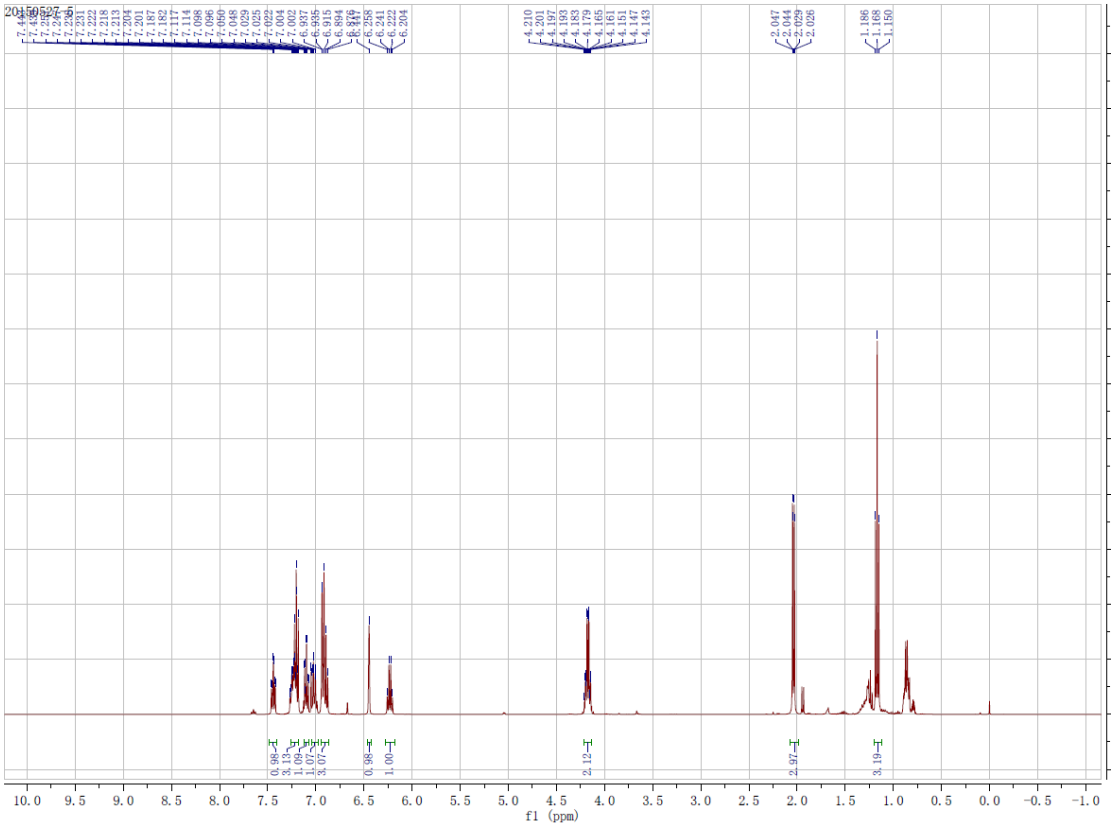

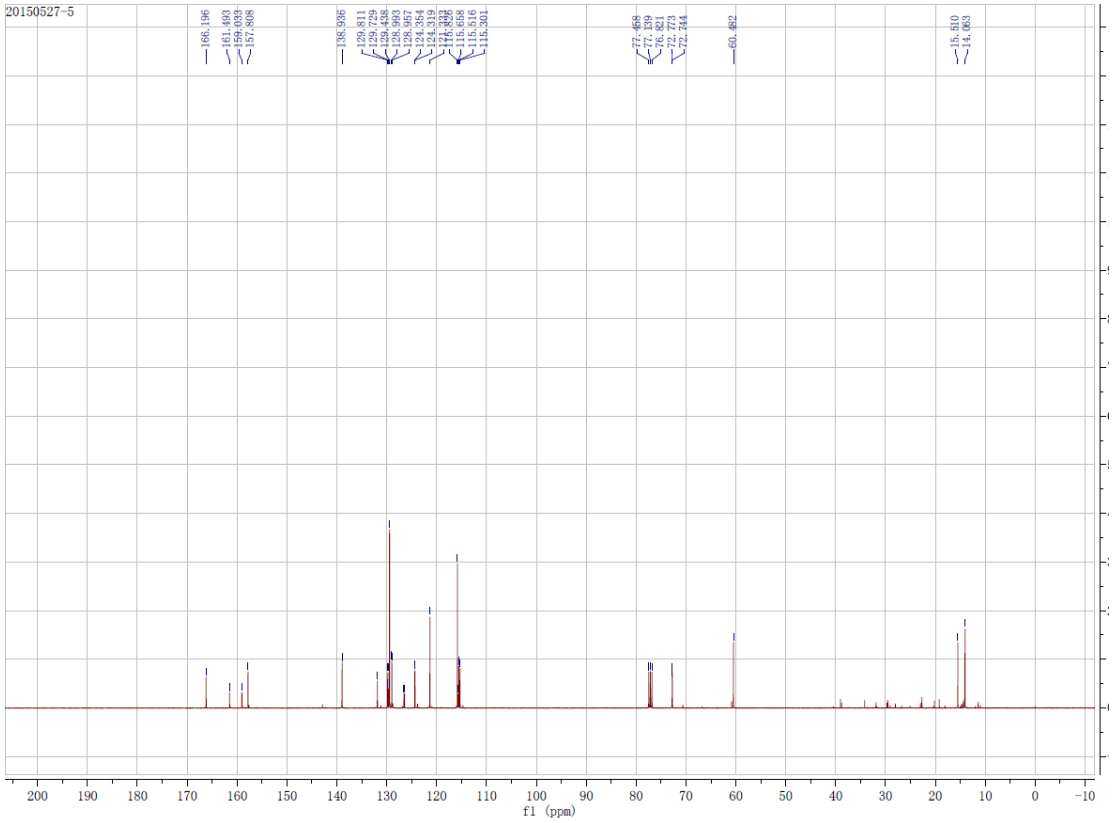

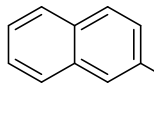

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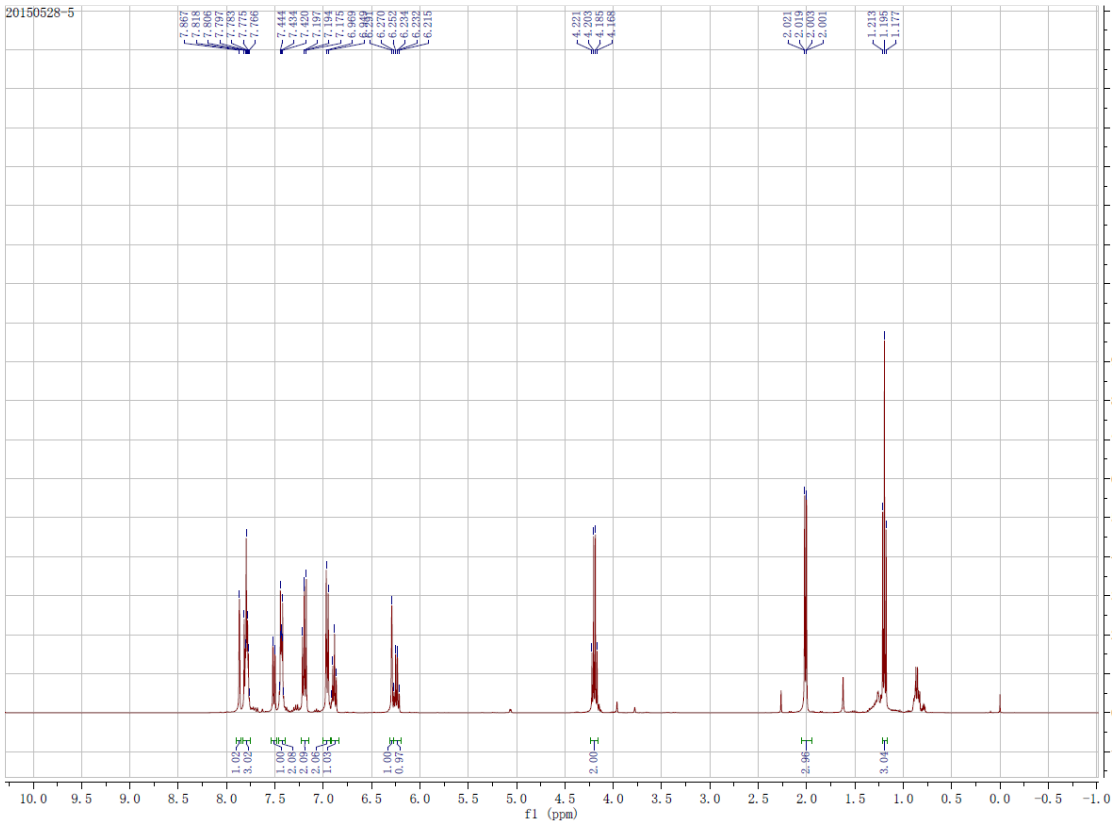

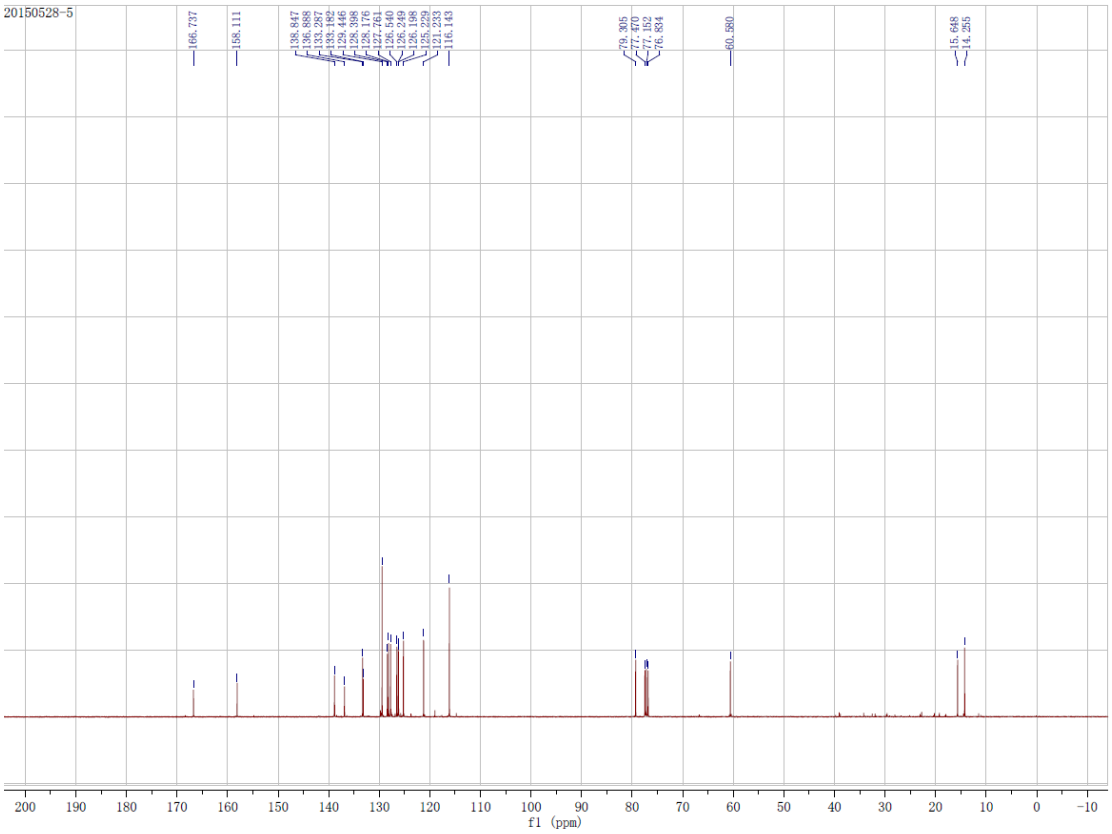

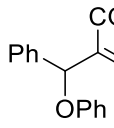
CO2Me
Ph
Me
OPh

2l


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7.336
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7.291
7.273
7.249
7.233
7.214
7.193
6.921
6.904
6.889
6.287
6.286
6.269
6.267
6.251
6.249
6.233
6.231
6.112
3.736
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2.019
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2.02
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1.00
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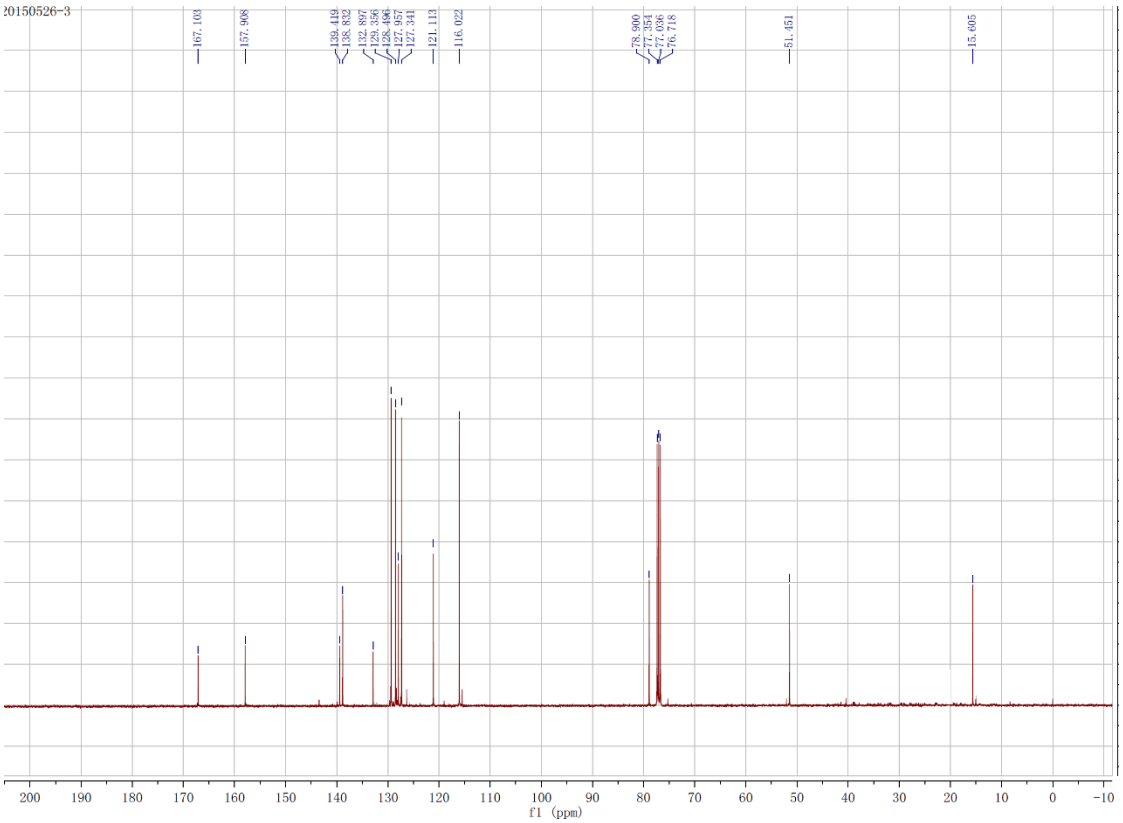
3.13
f1 (ppm)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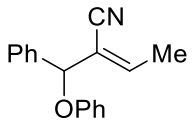
f1 (ppm)



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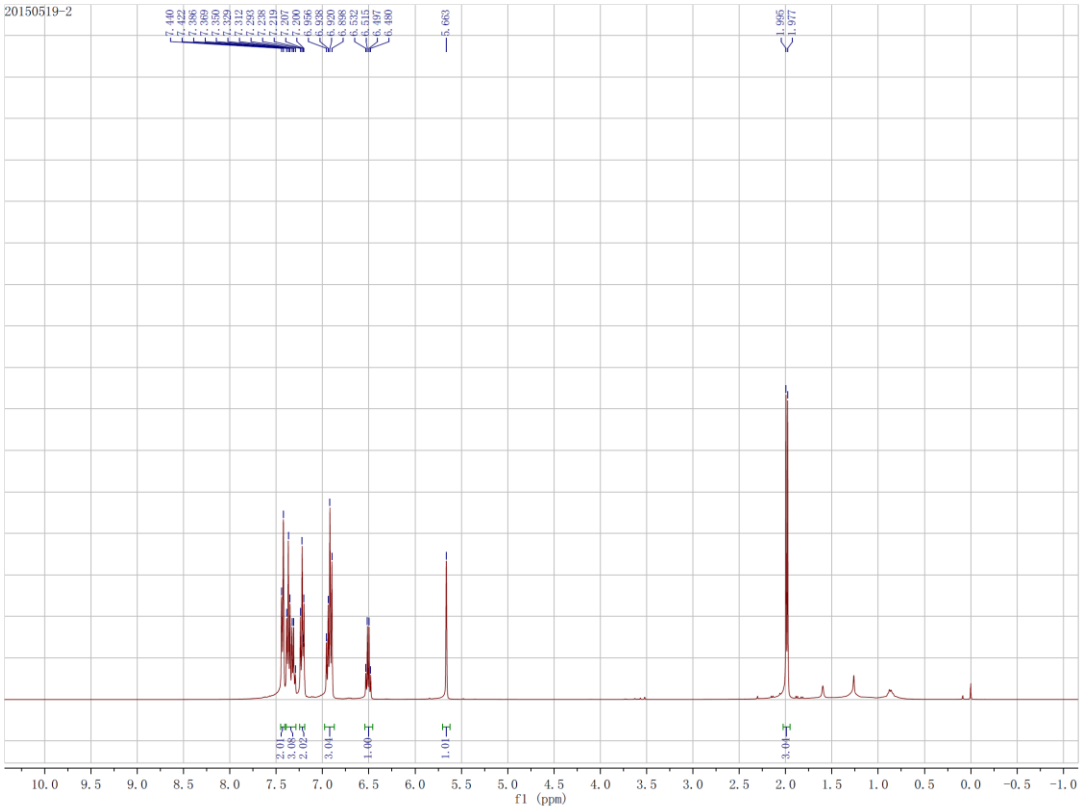

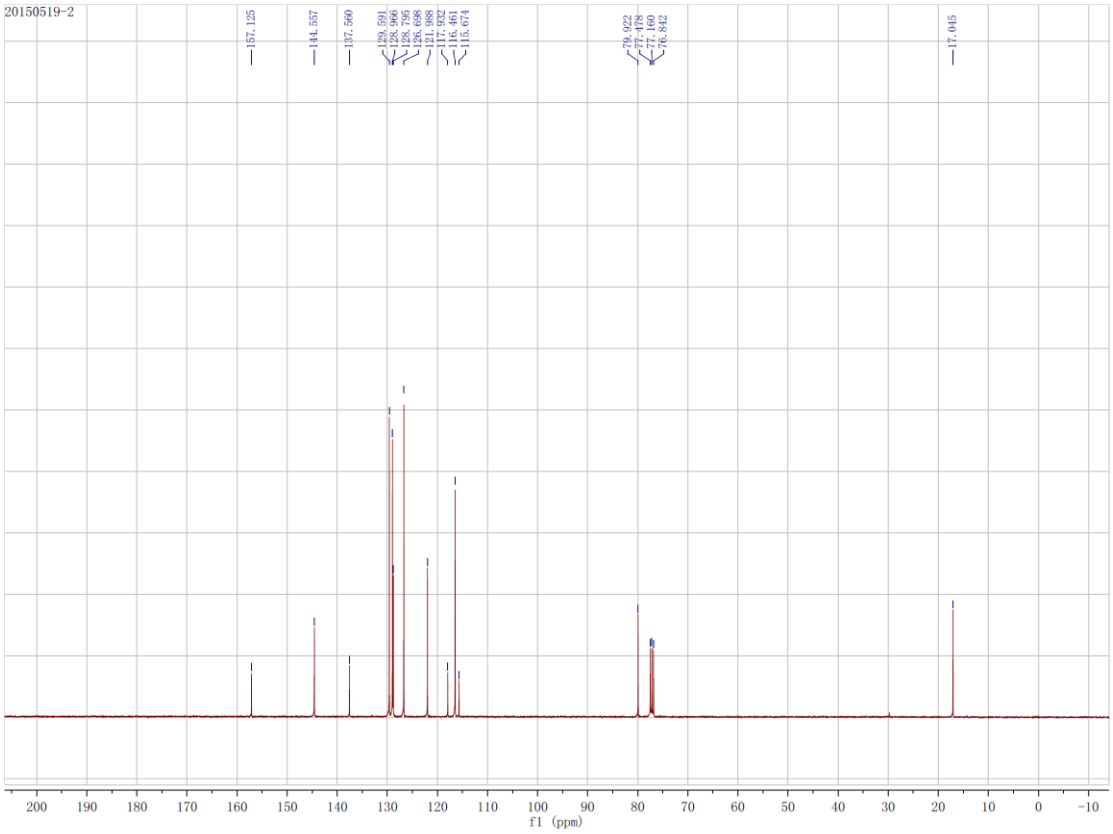

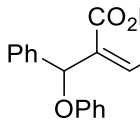

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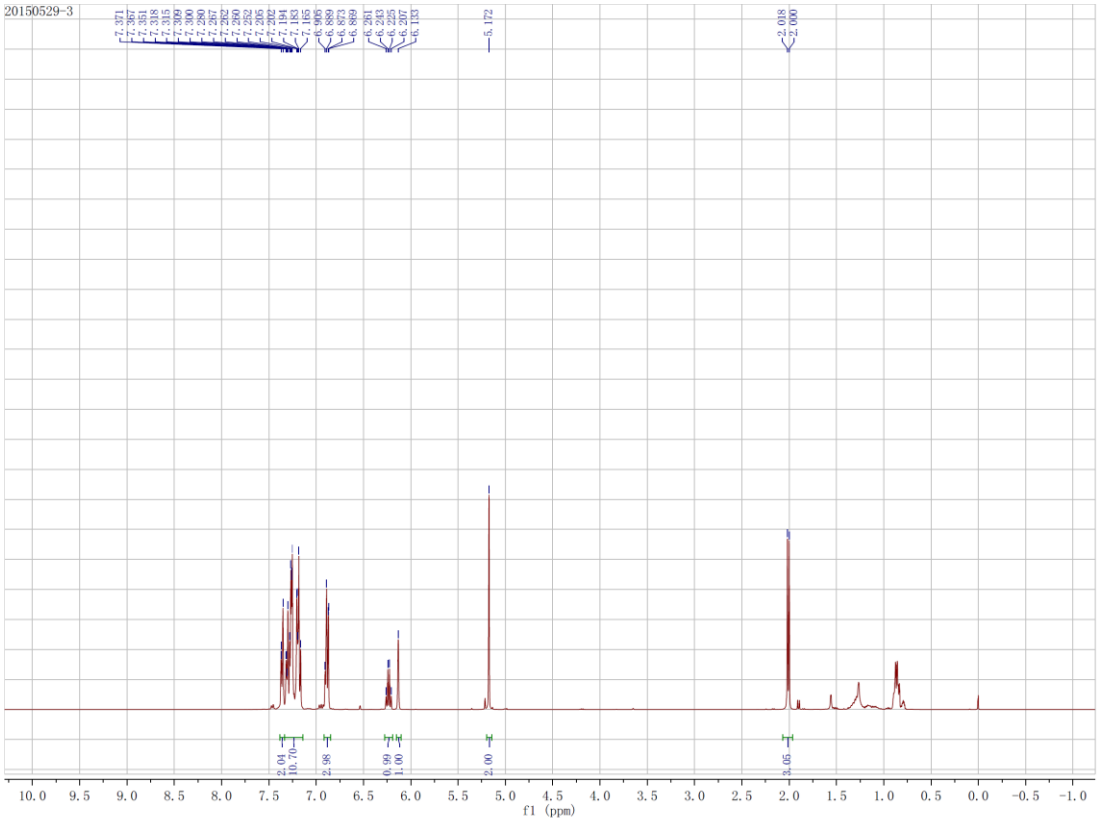

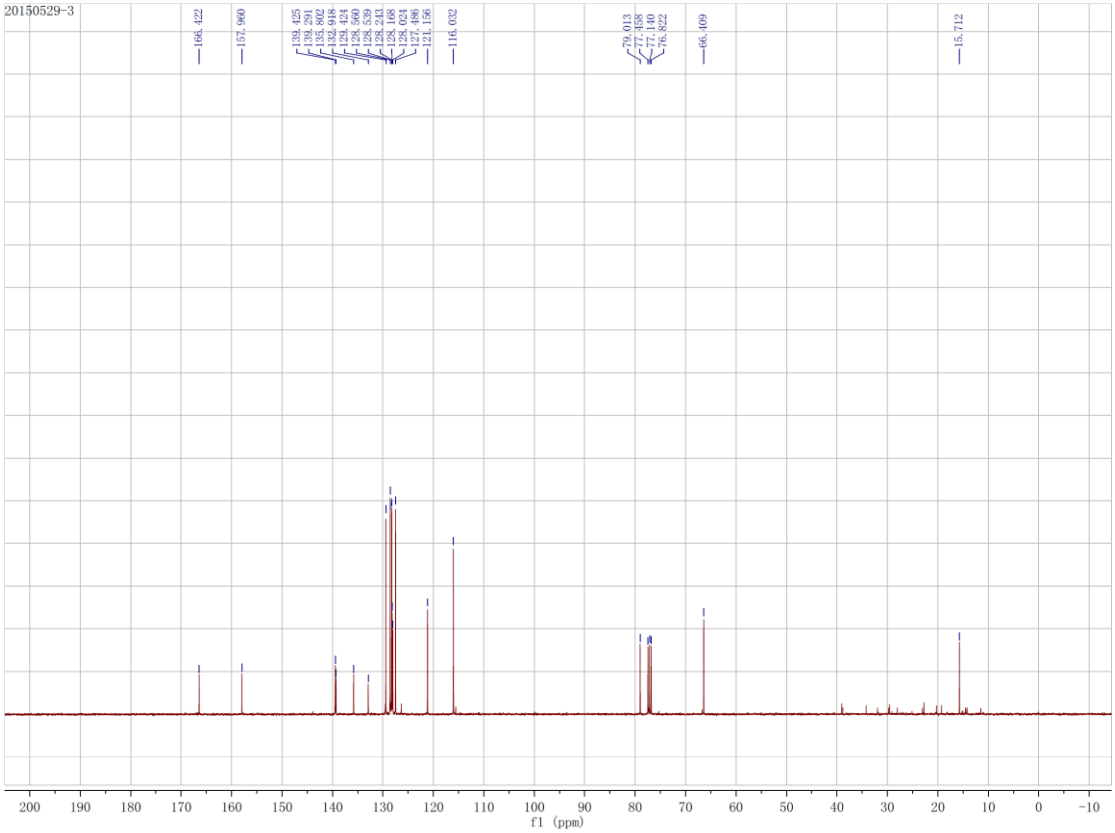

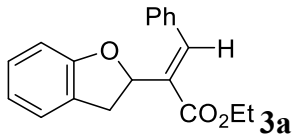

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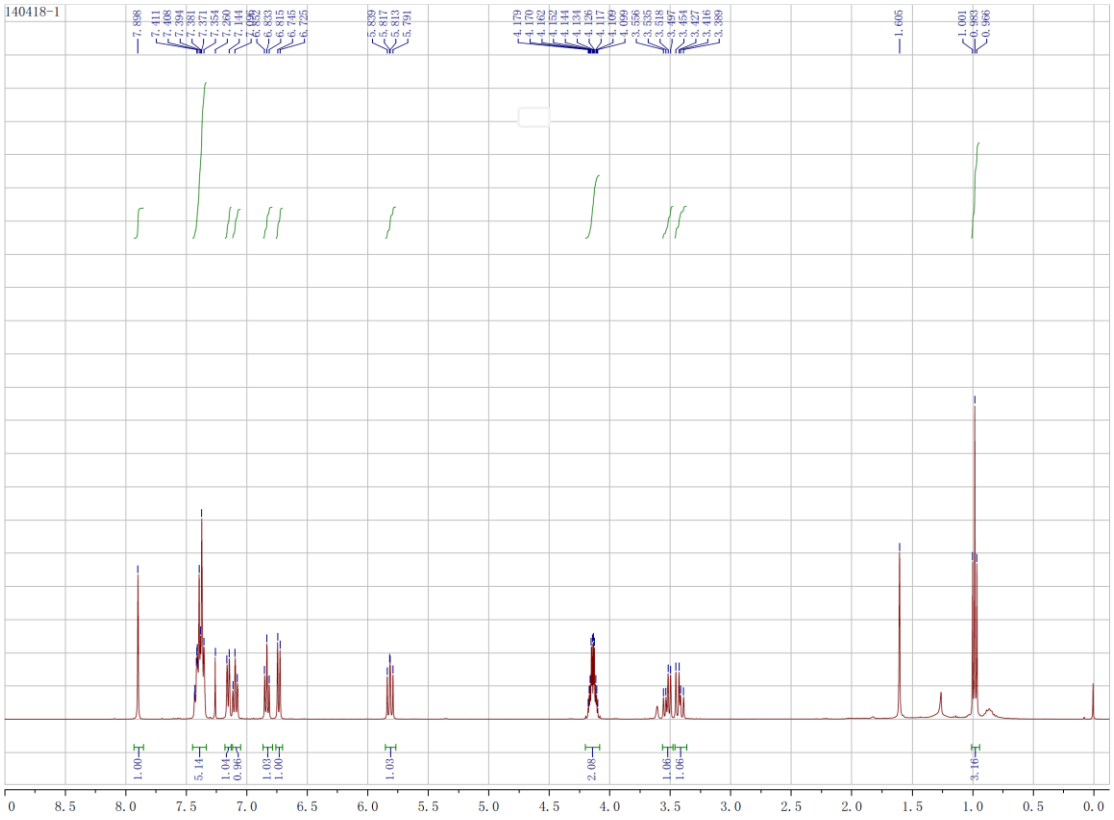

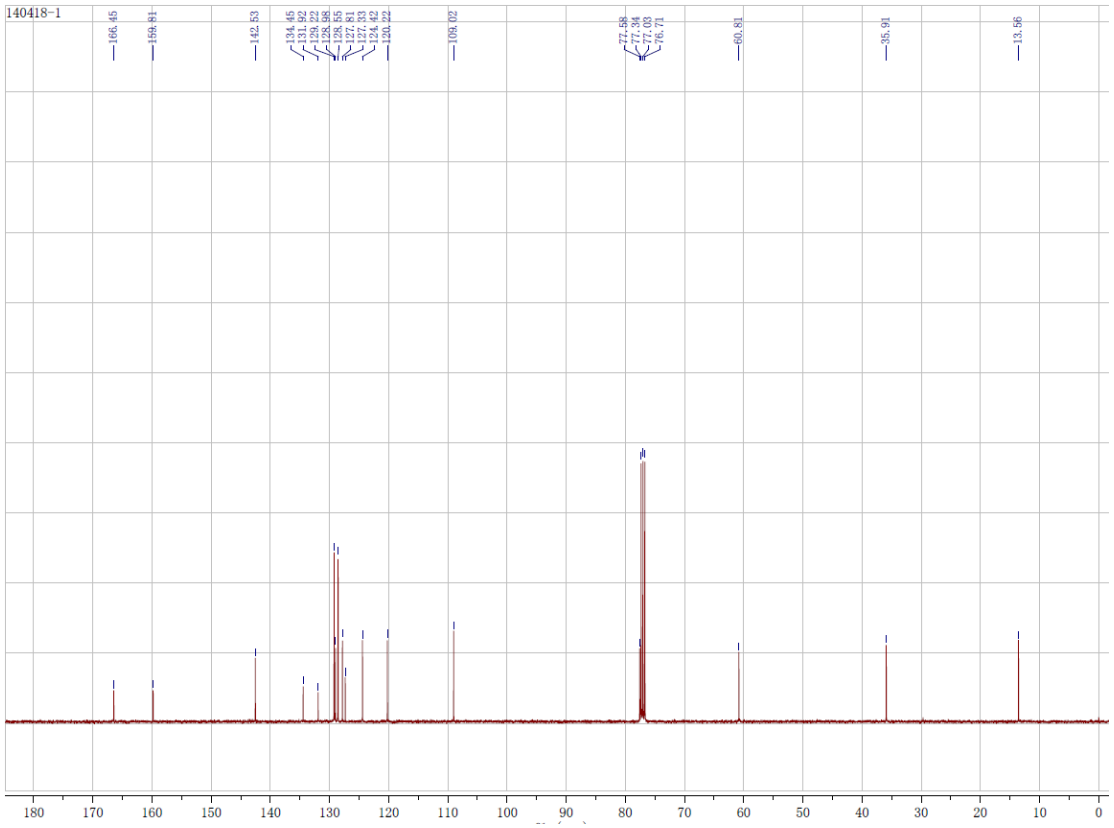

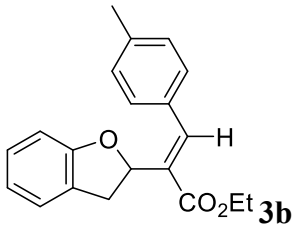

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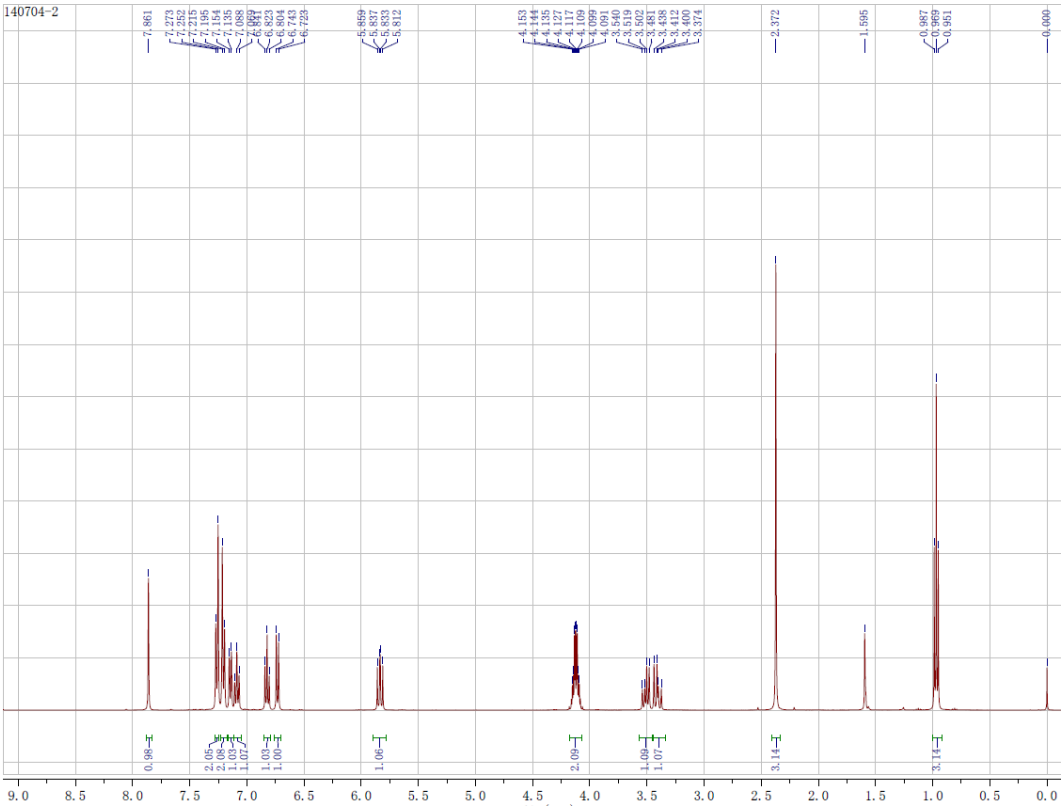
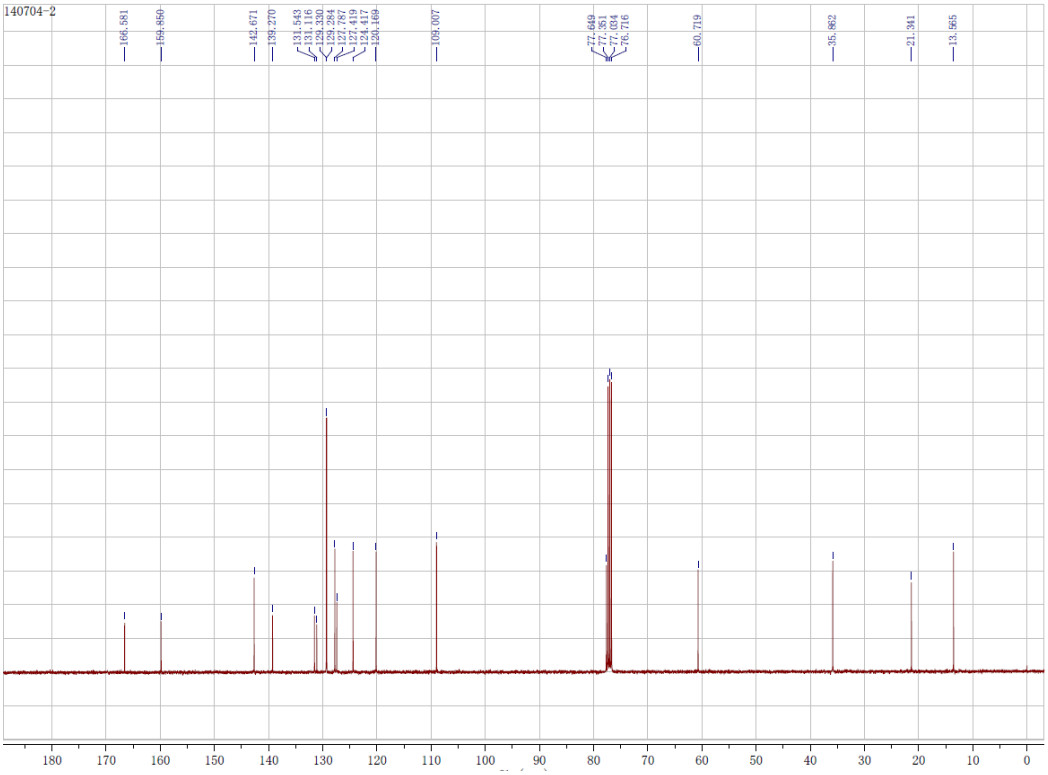
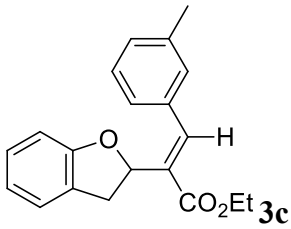
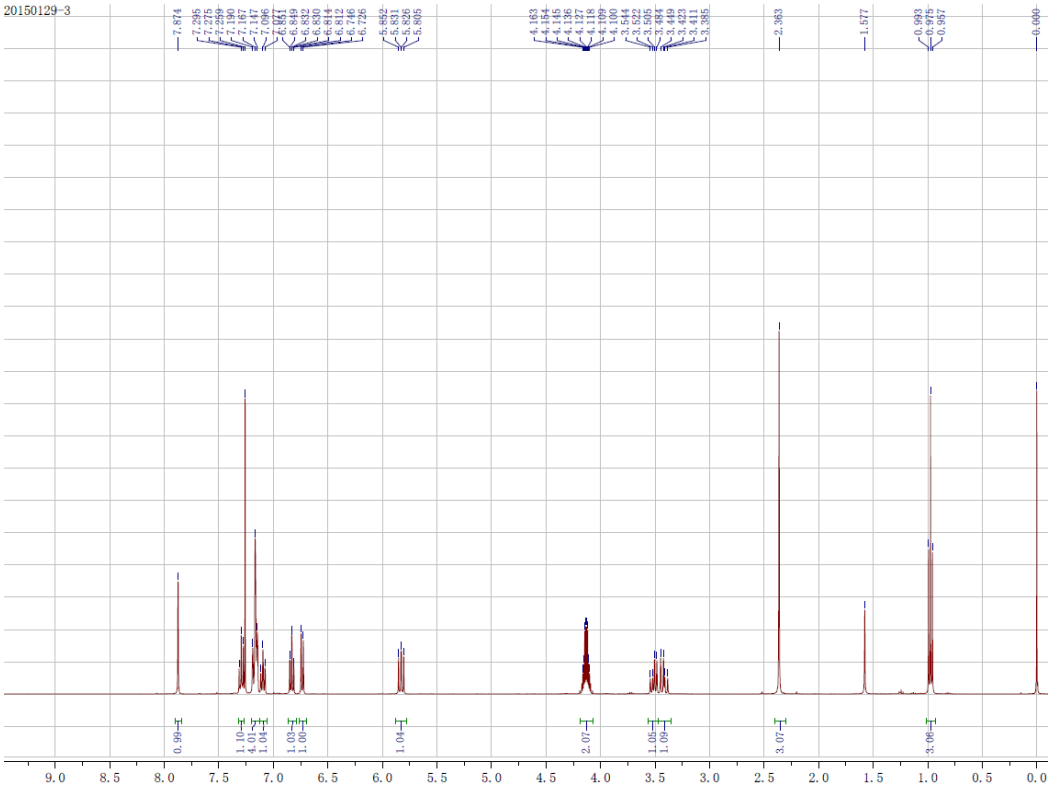





O
H
CO2Et

3c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6.812
6.746
6.726
5.852
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4.154
4.145
4.136
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4.109
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3.522
3.505
3.484
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0.000
0.99
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4.01
1.04
1.03
1.06
1.04
2.07
1.05
1.09
3.07
3.06
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8.5
8.0
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7.0
6.5
6.0
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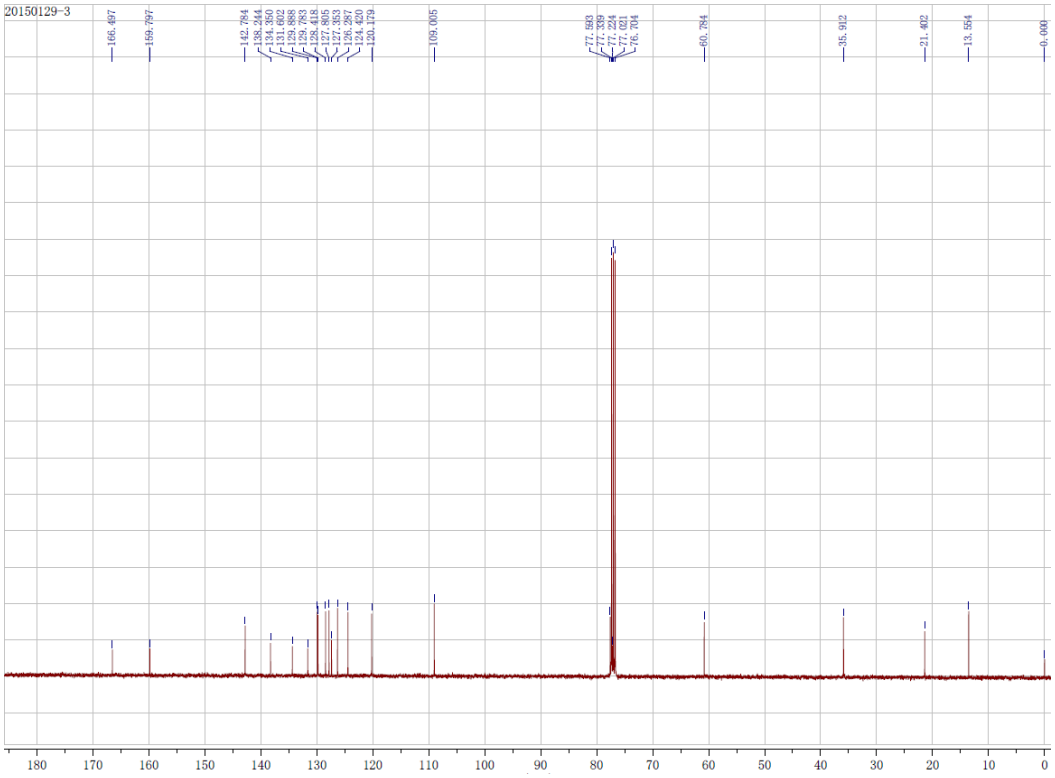
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120.179
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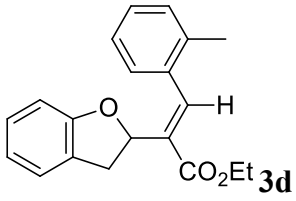

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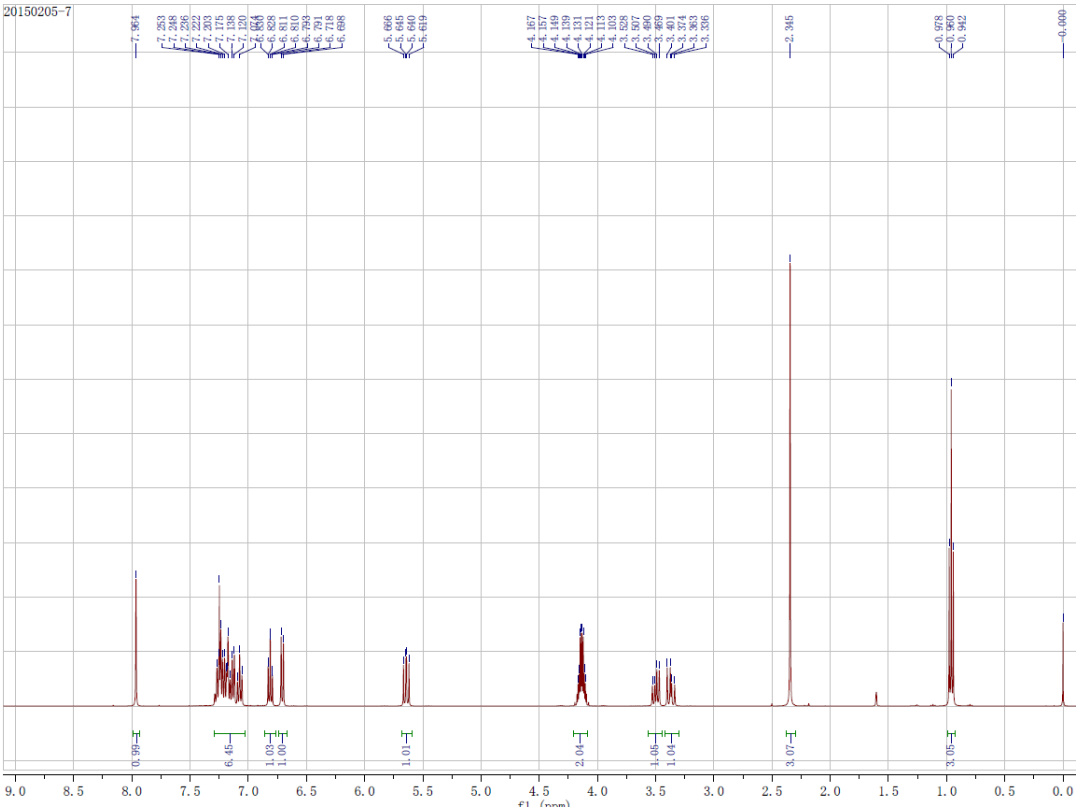

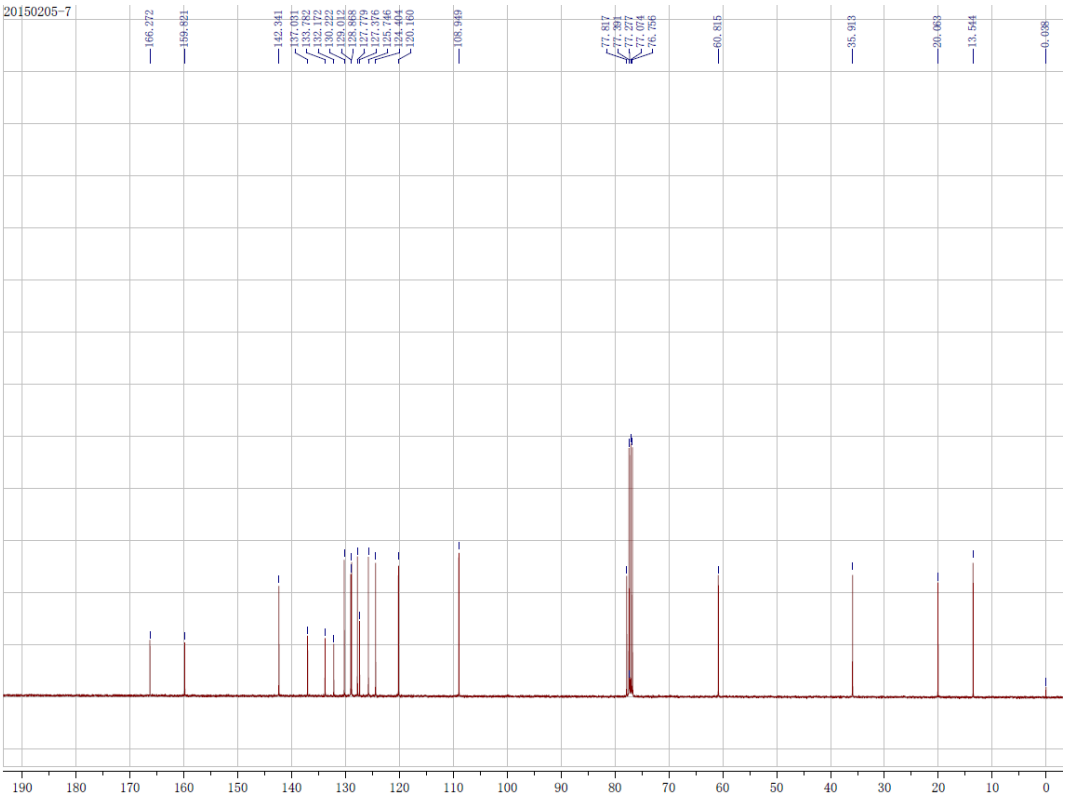

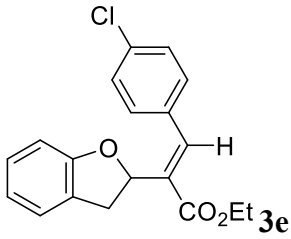
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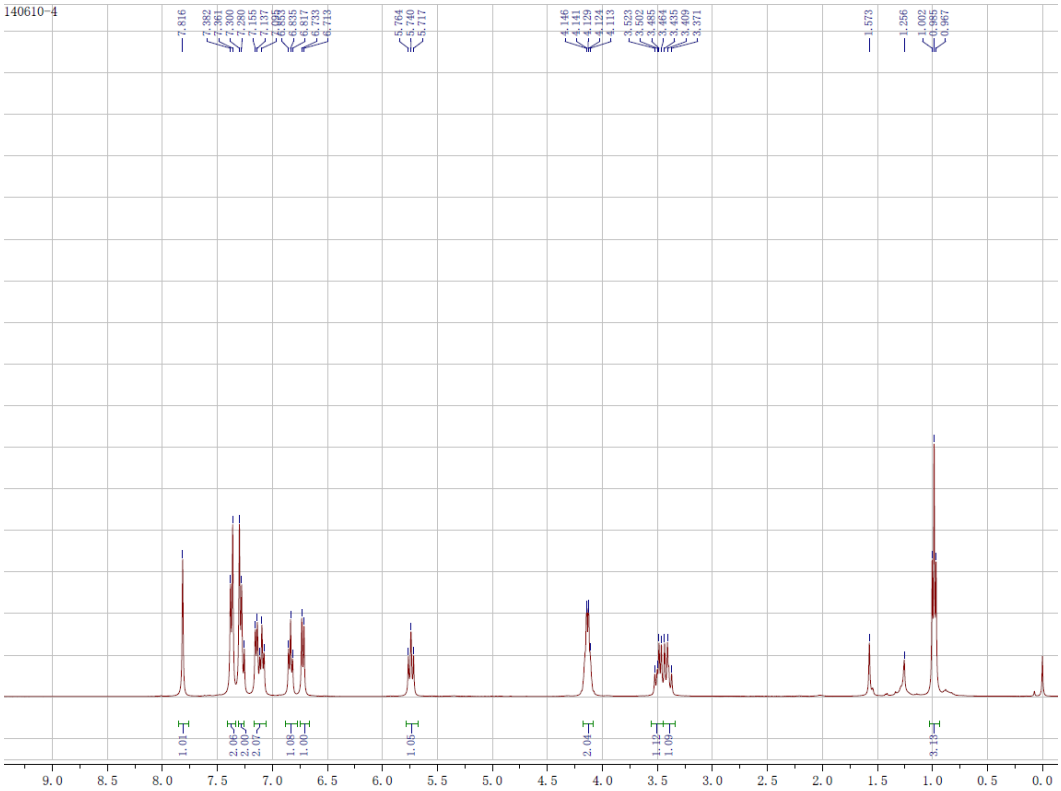
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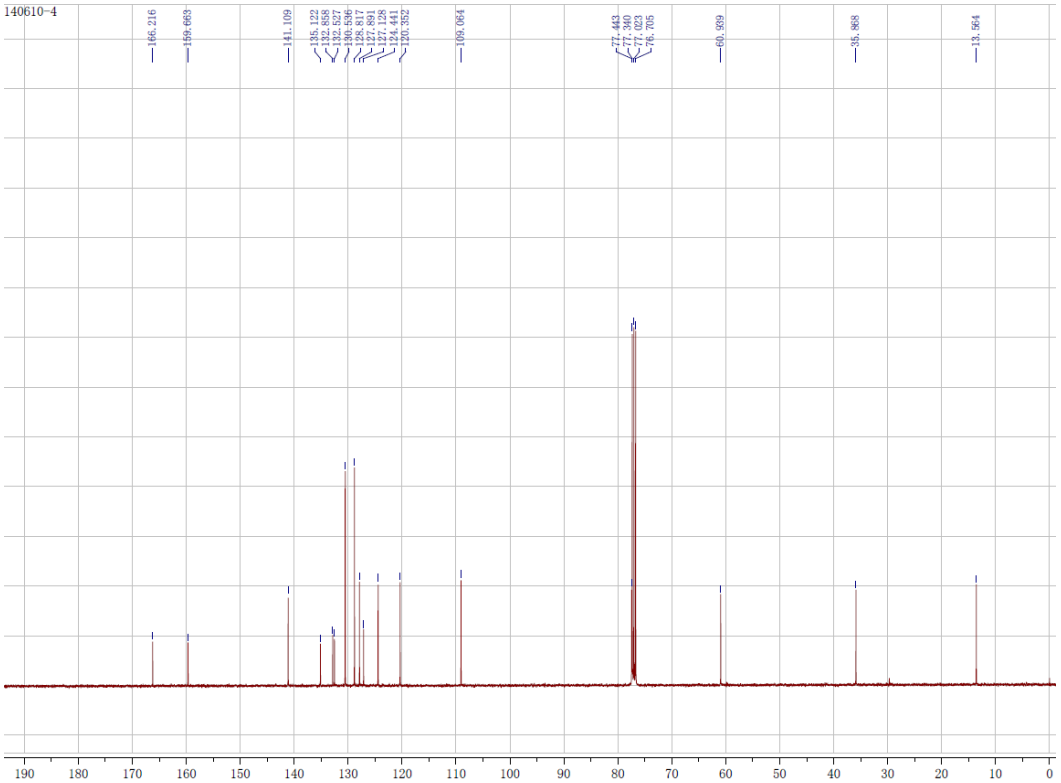
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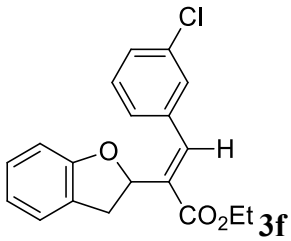

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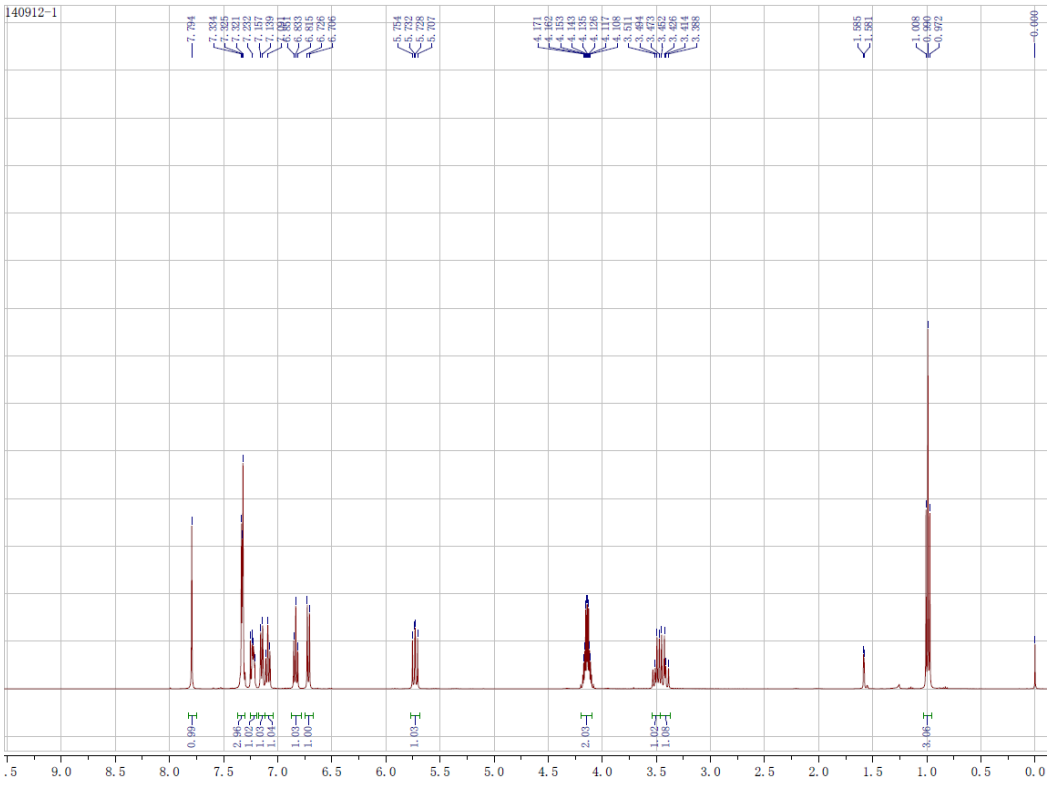

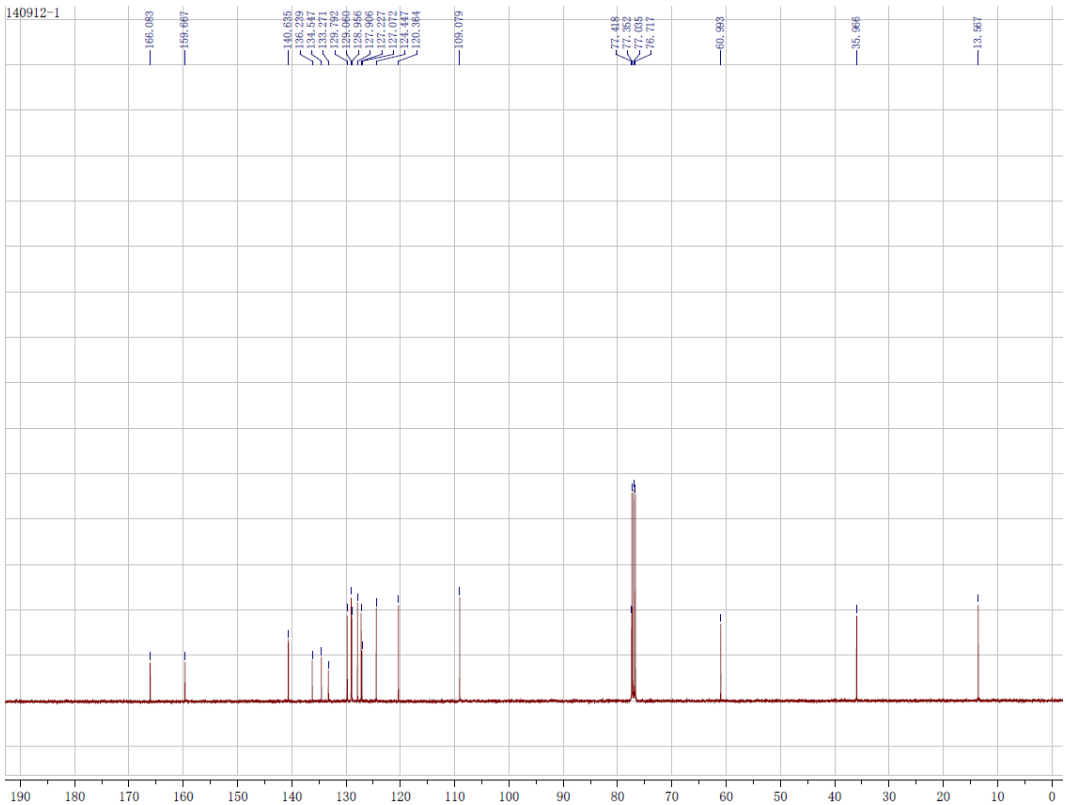

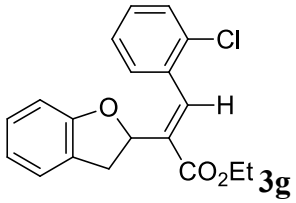

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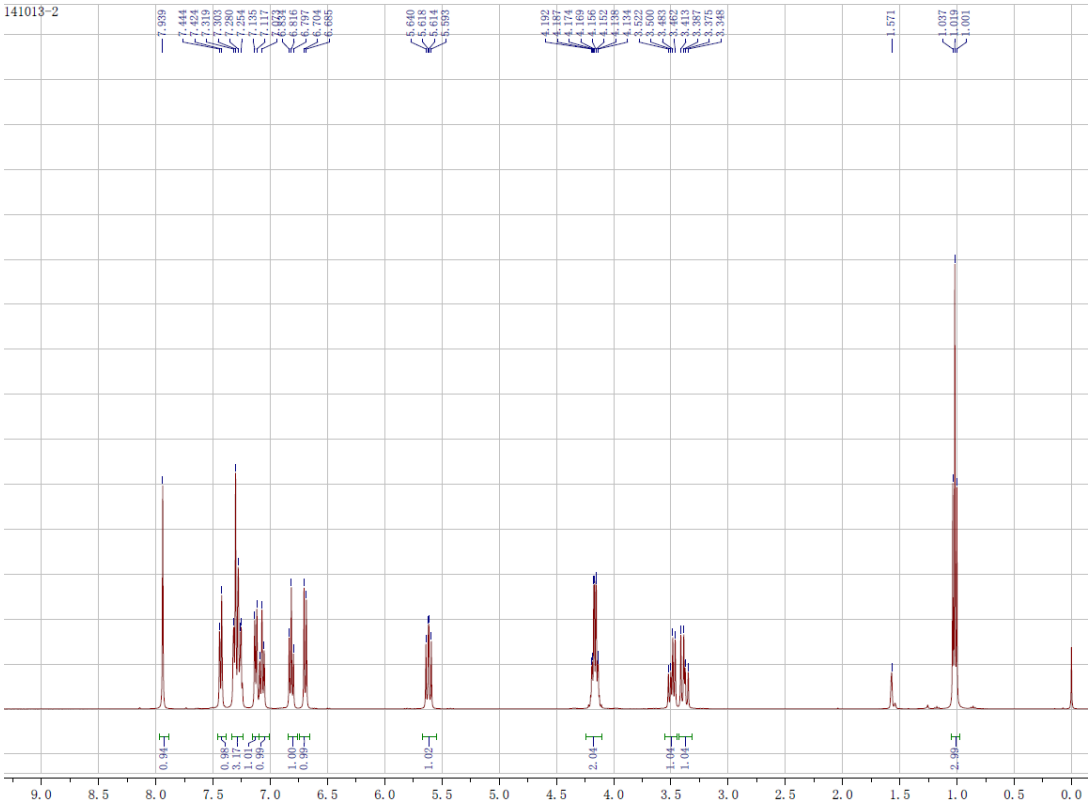

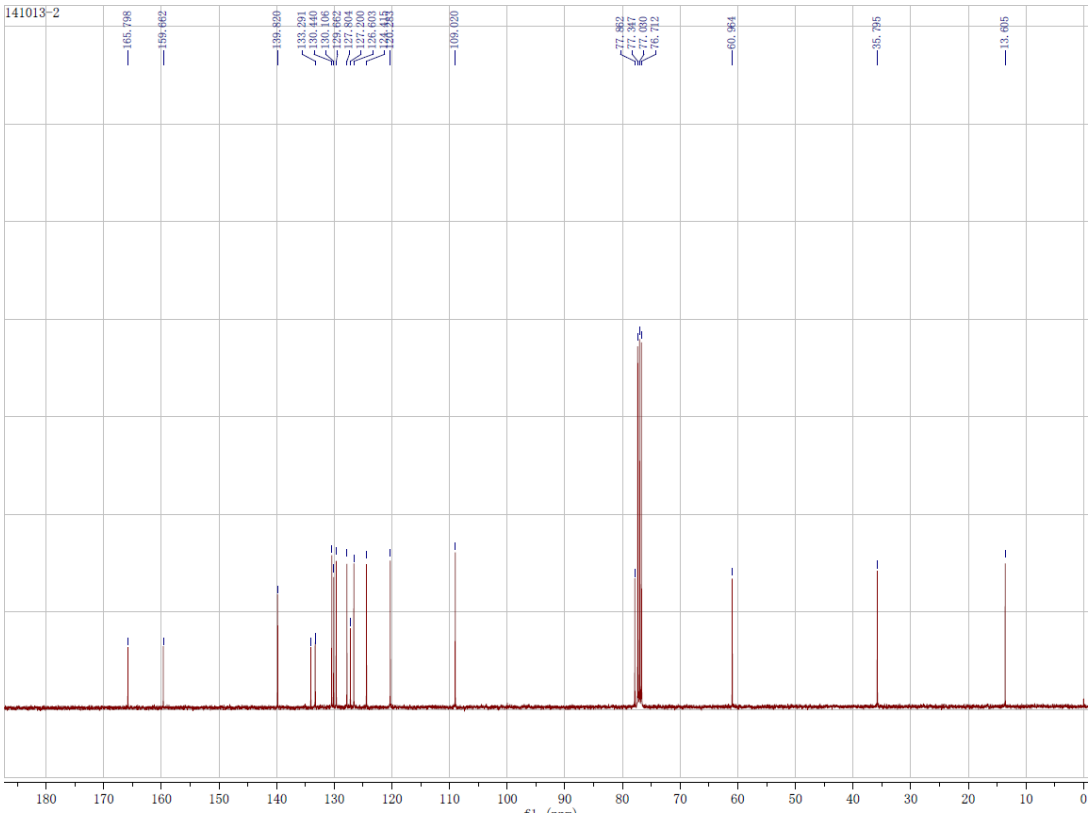

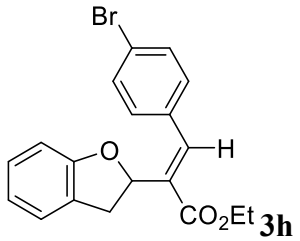

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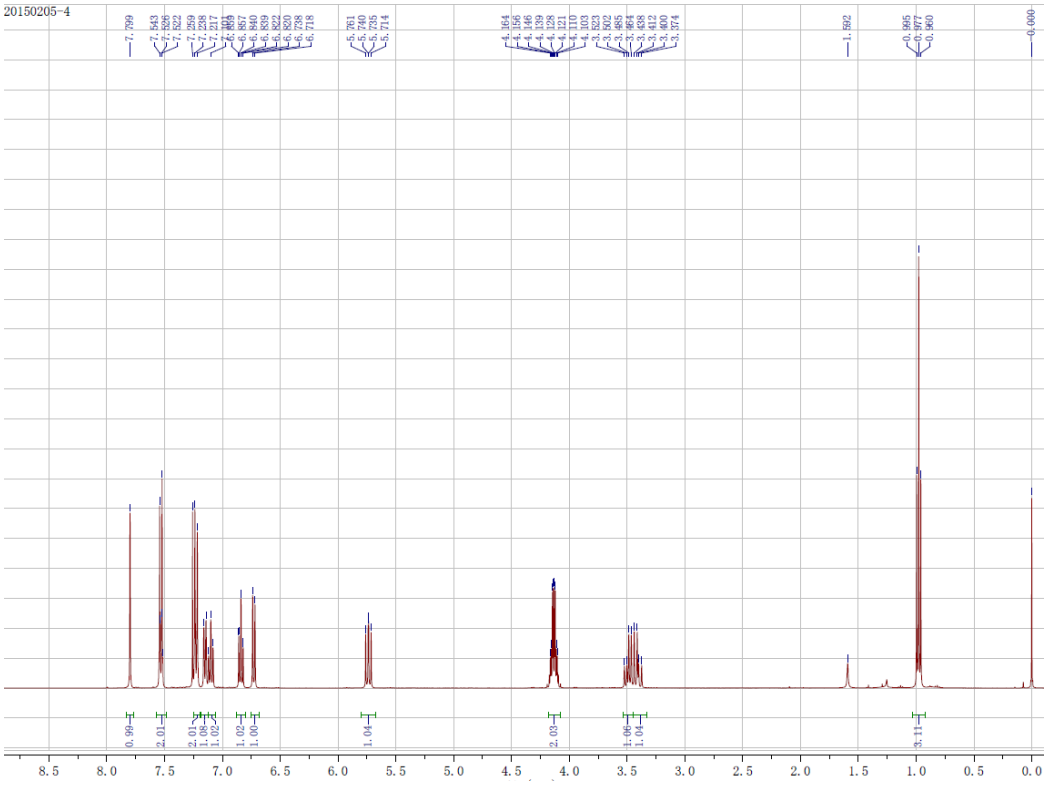

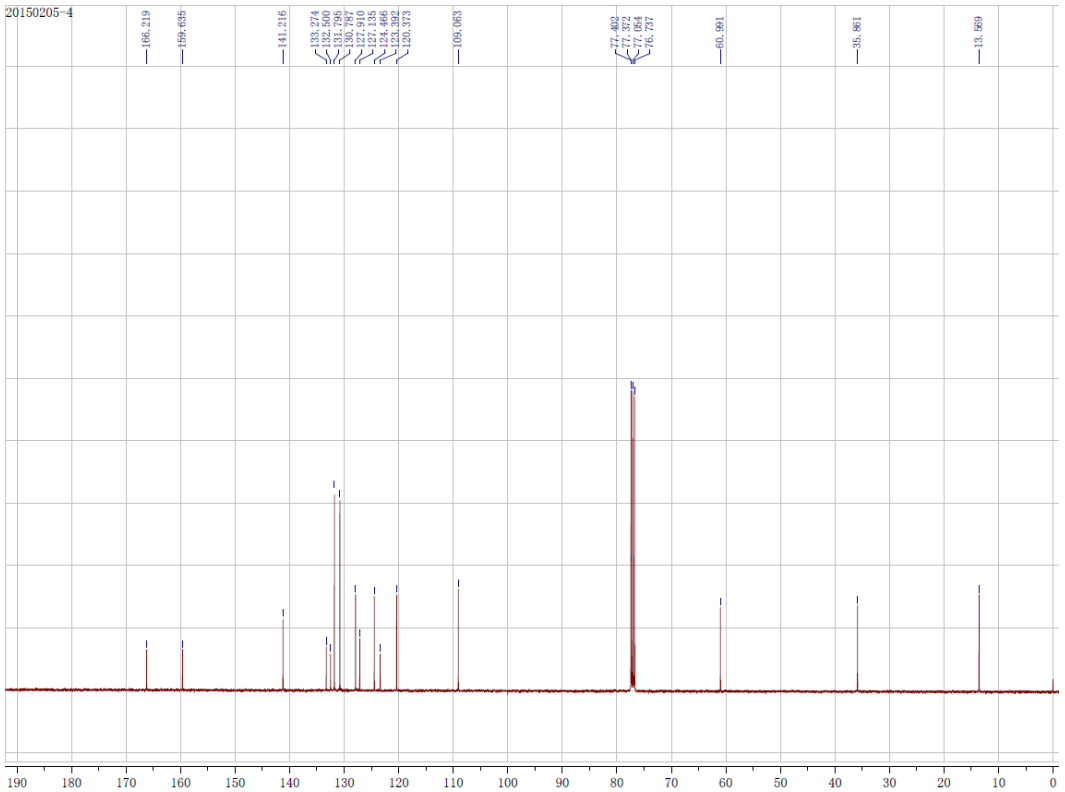

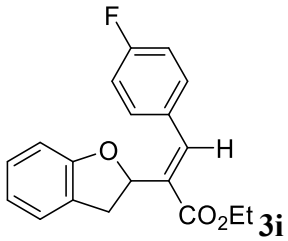

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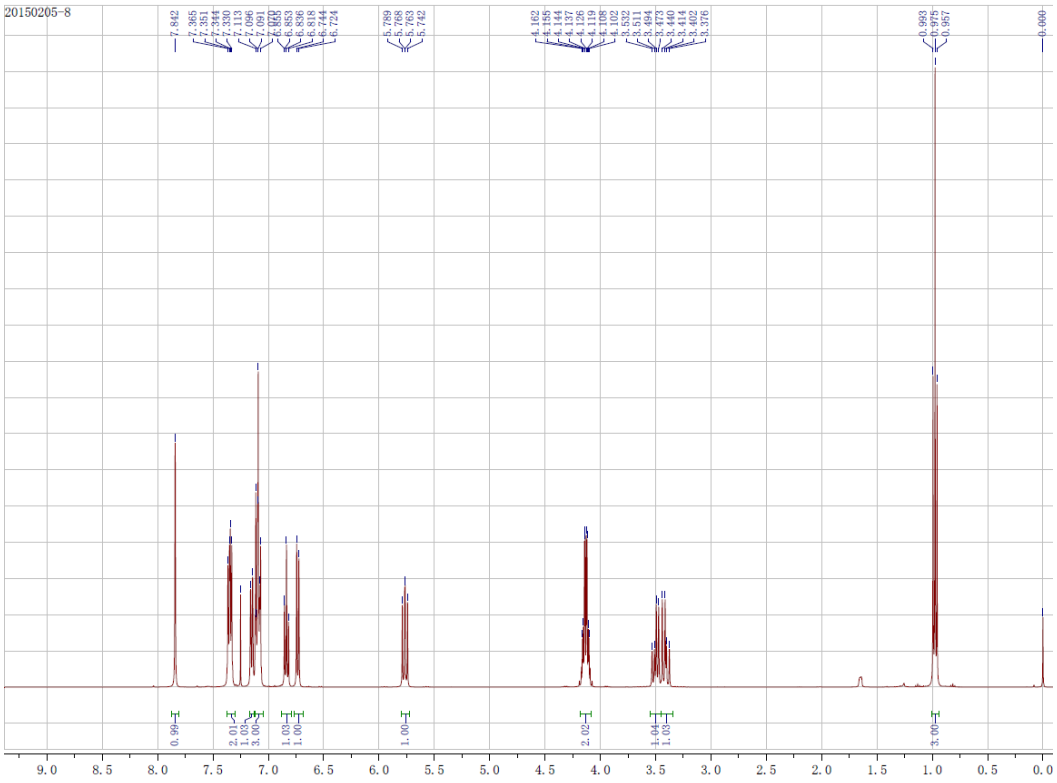

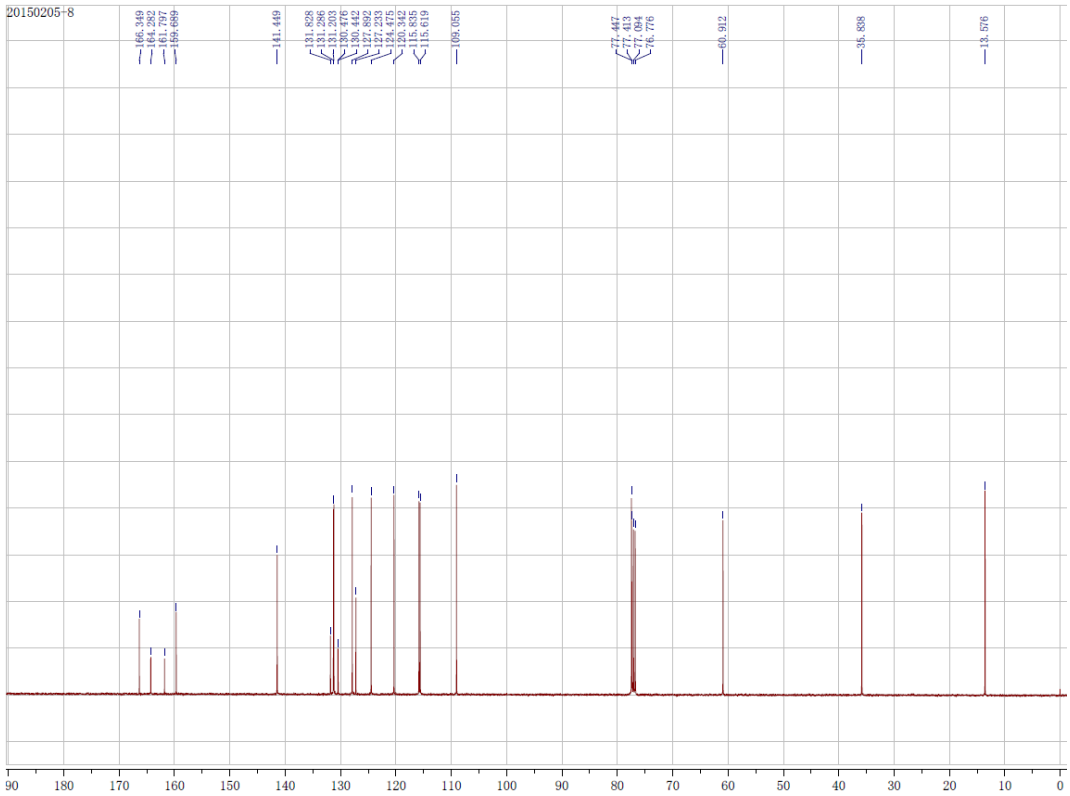

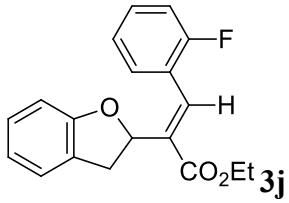

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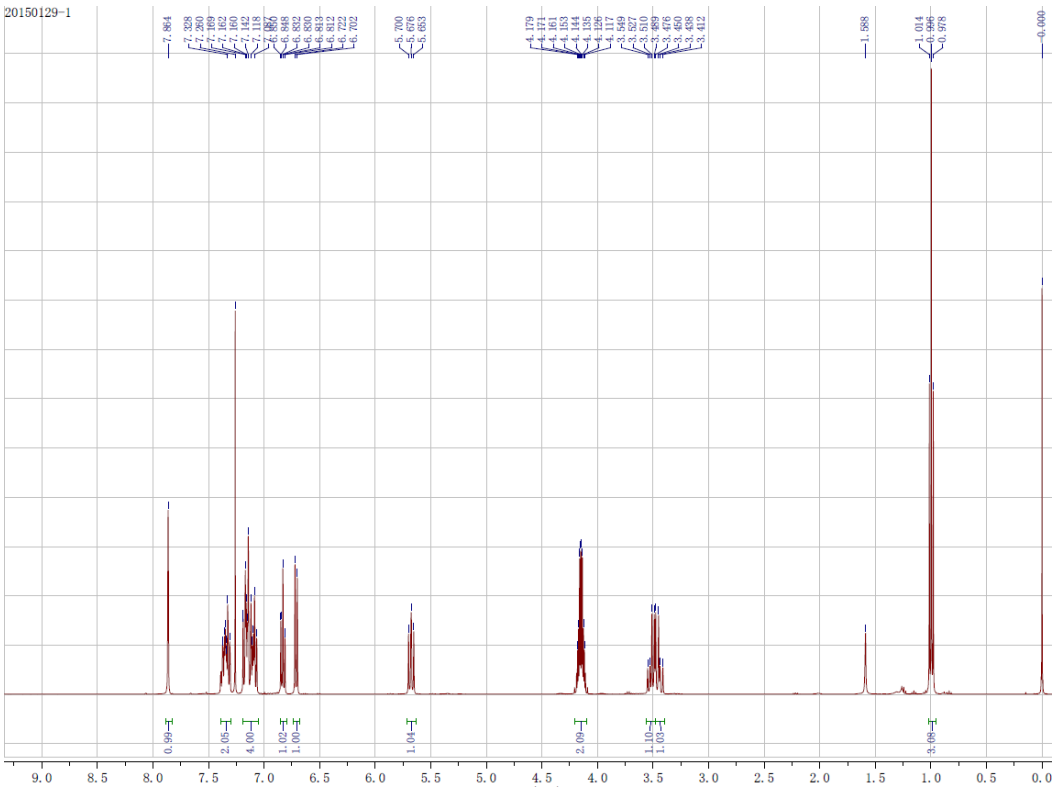

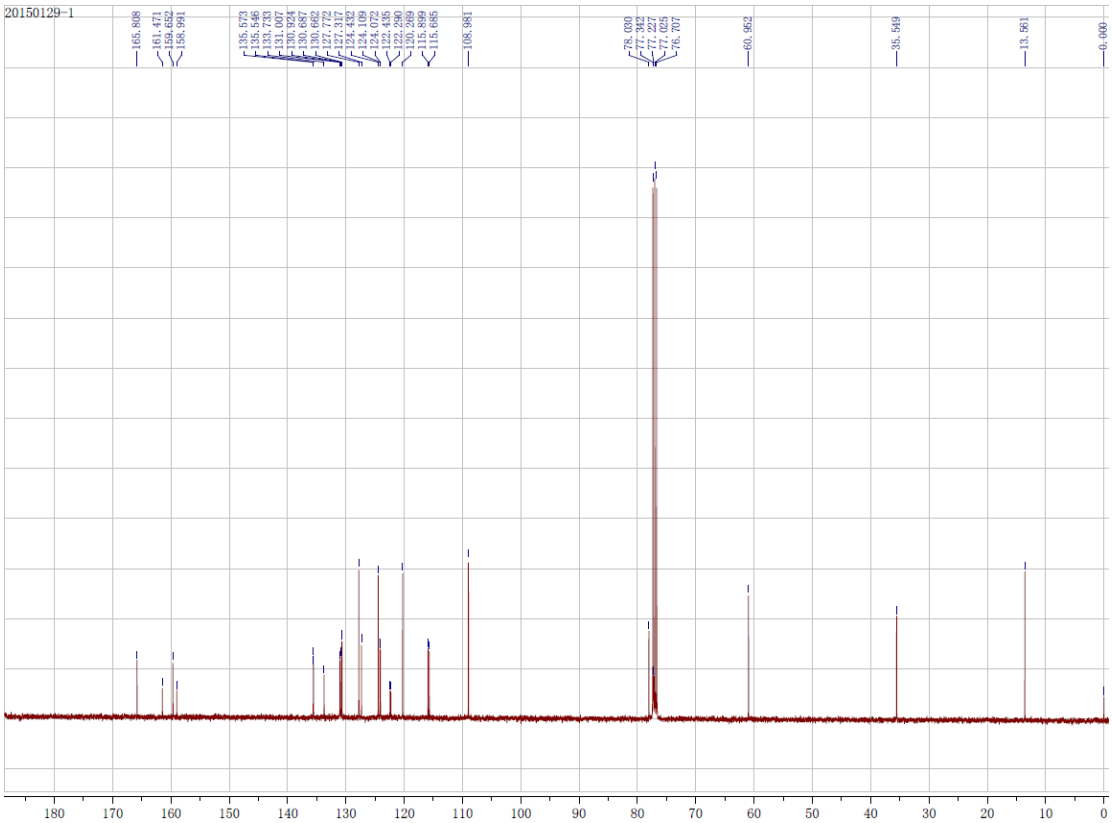

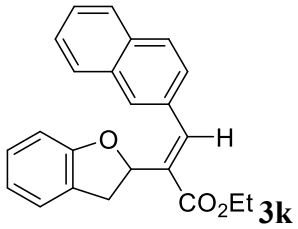

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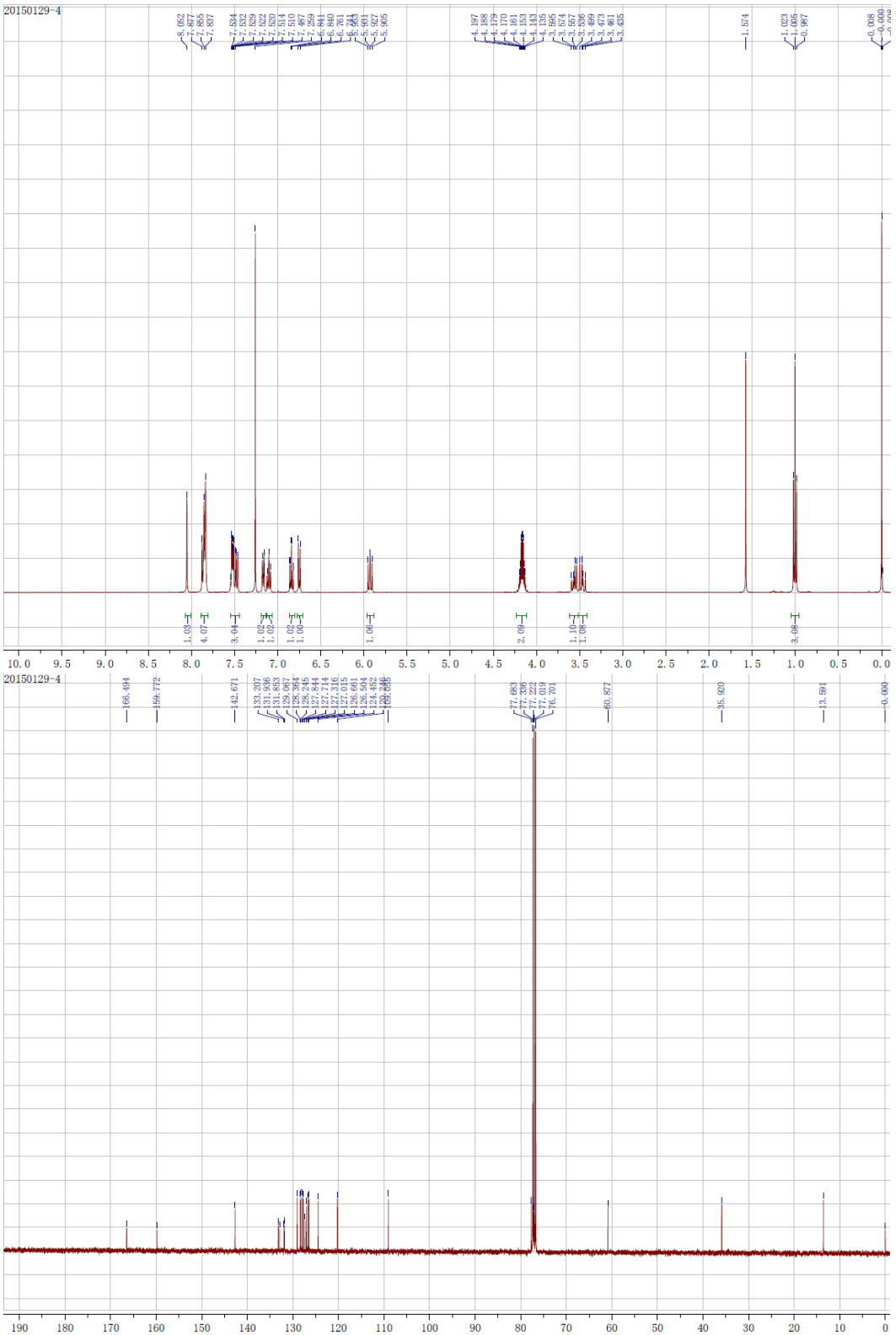

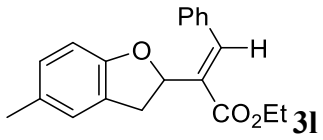
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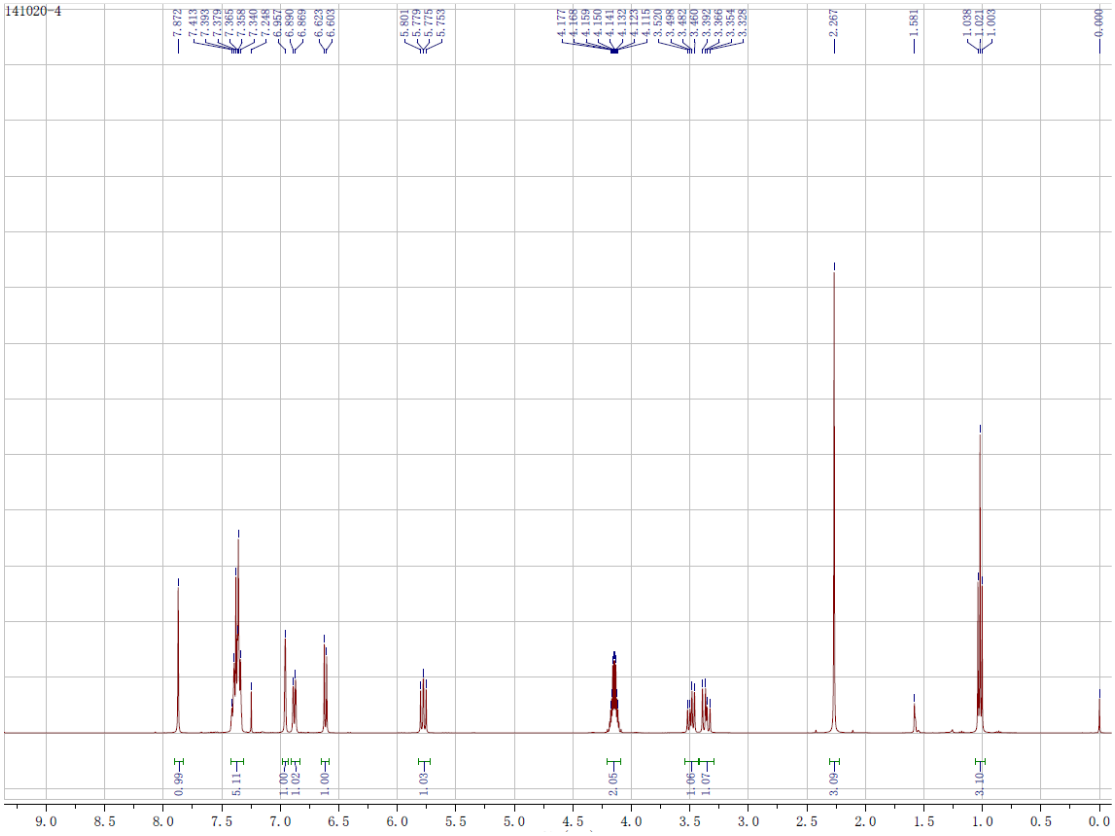
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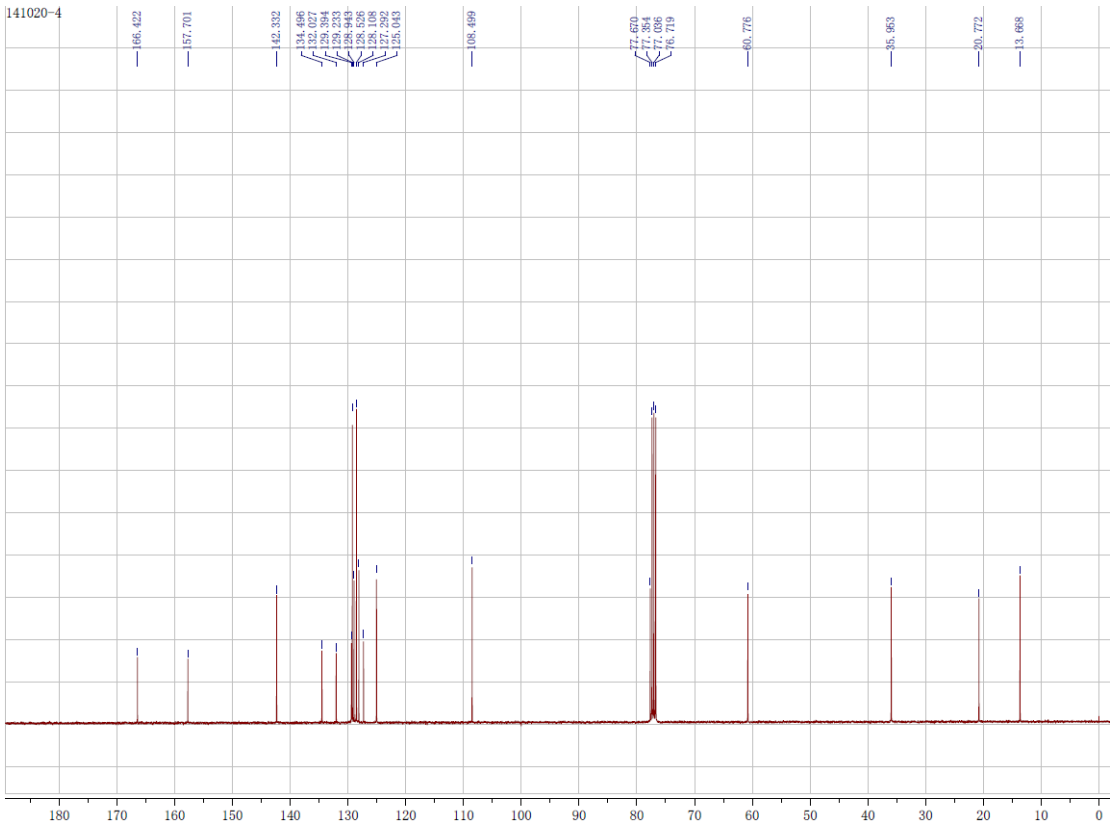
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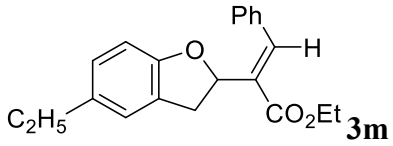

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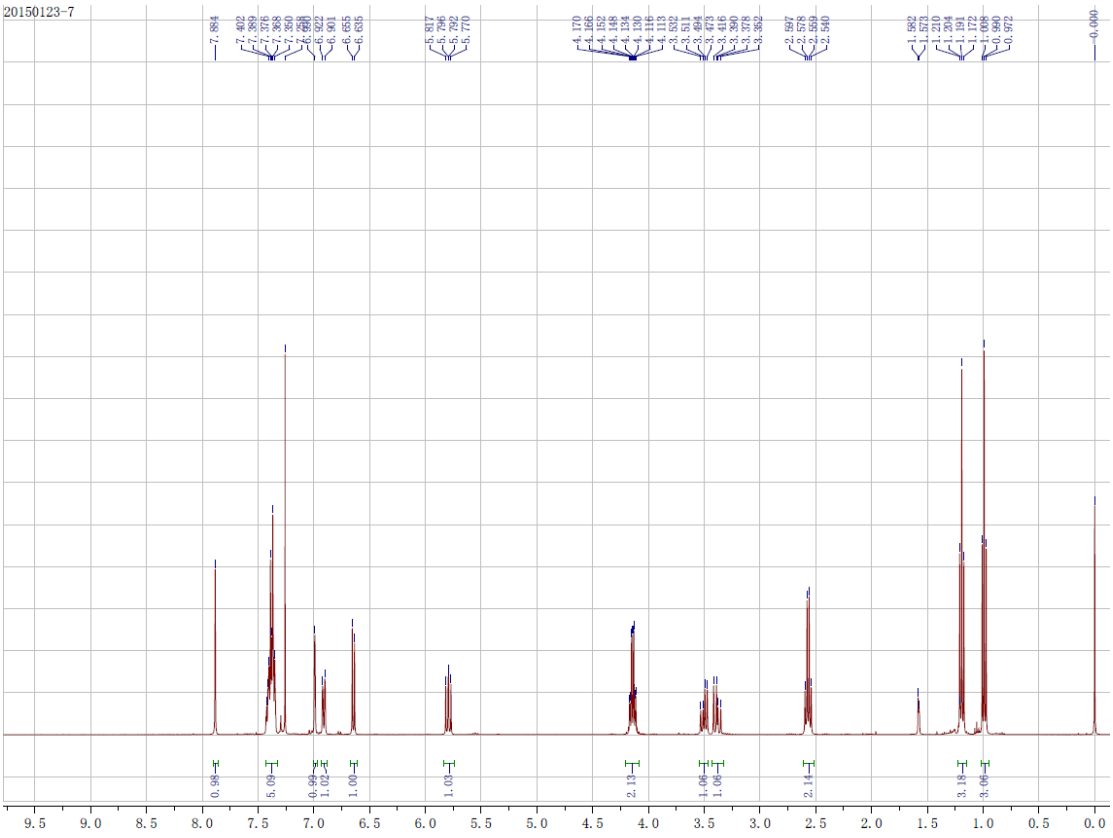

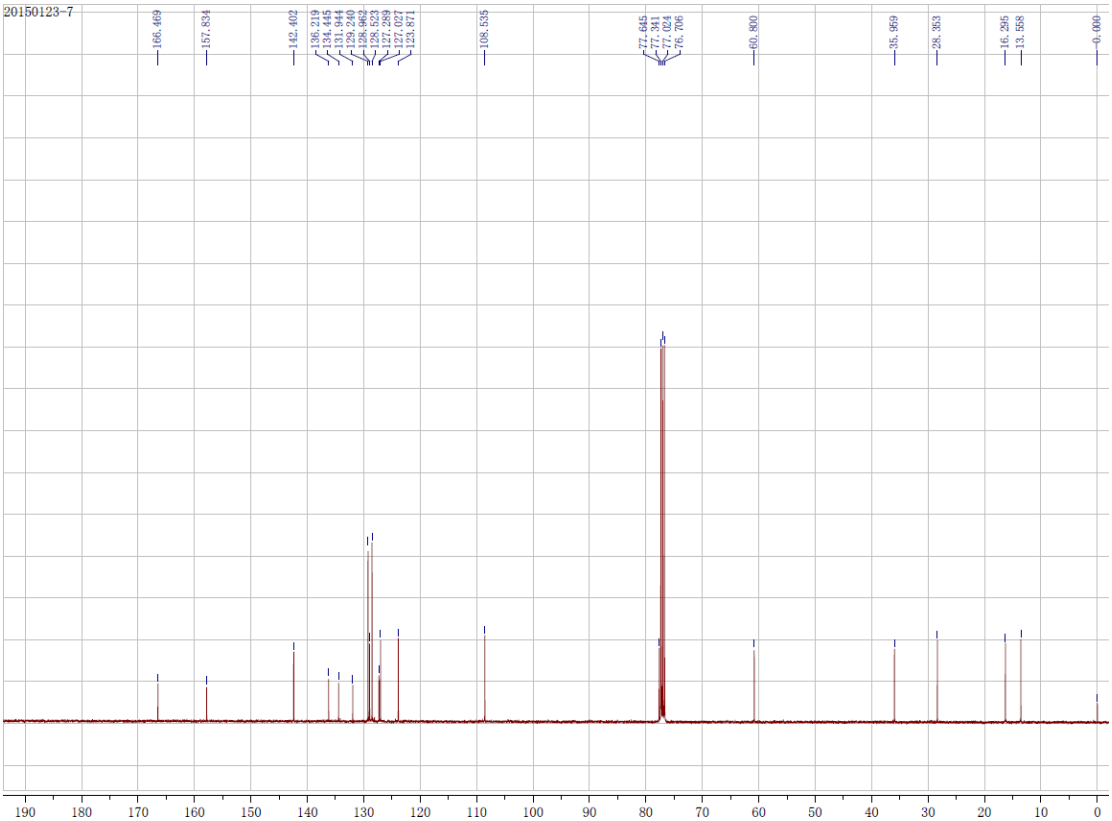

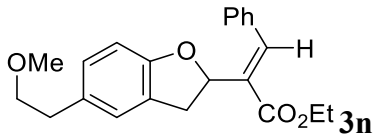

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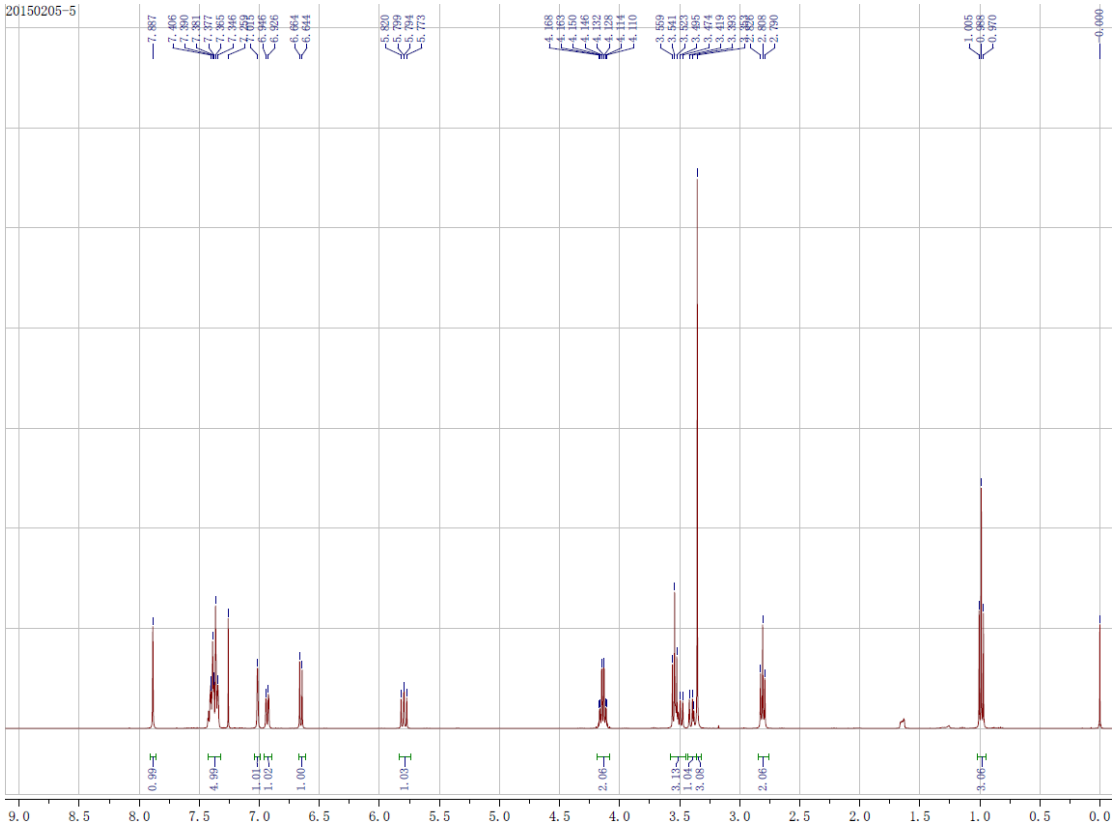

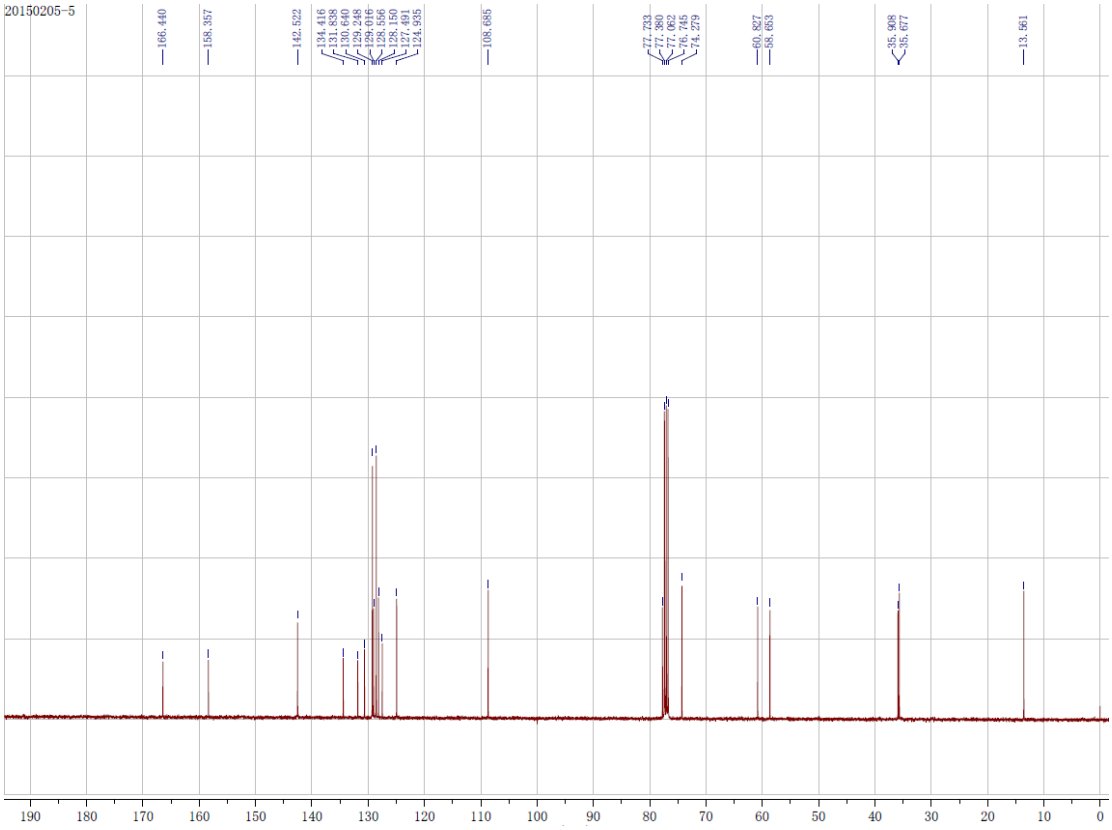

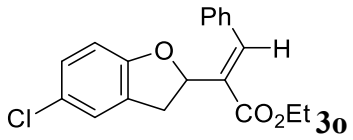

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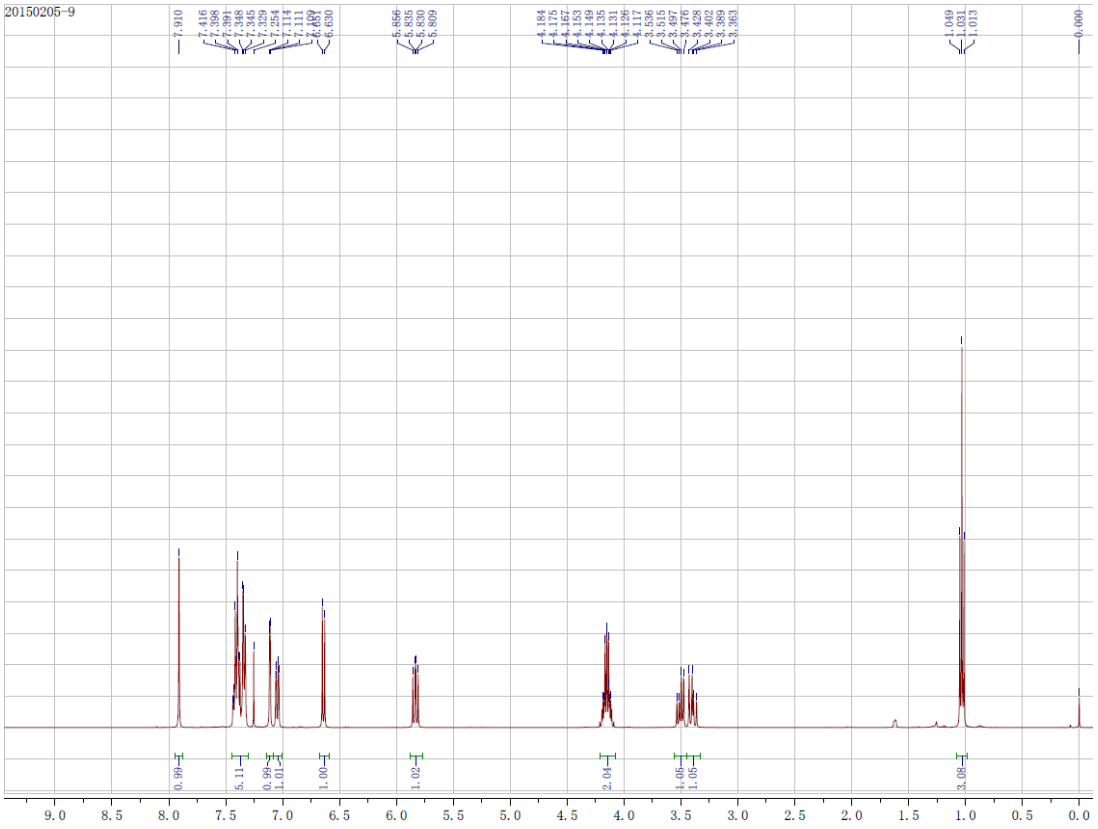

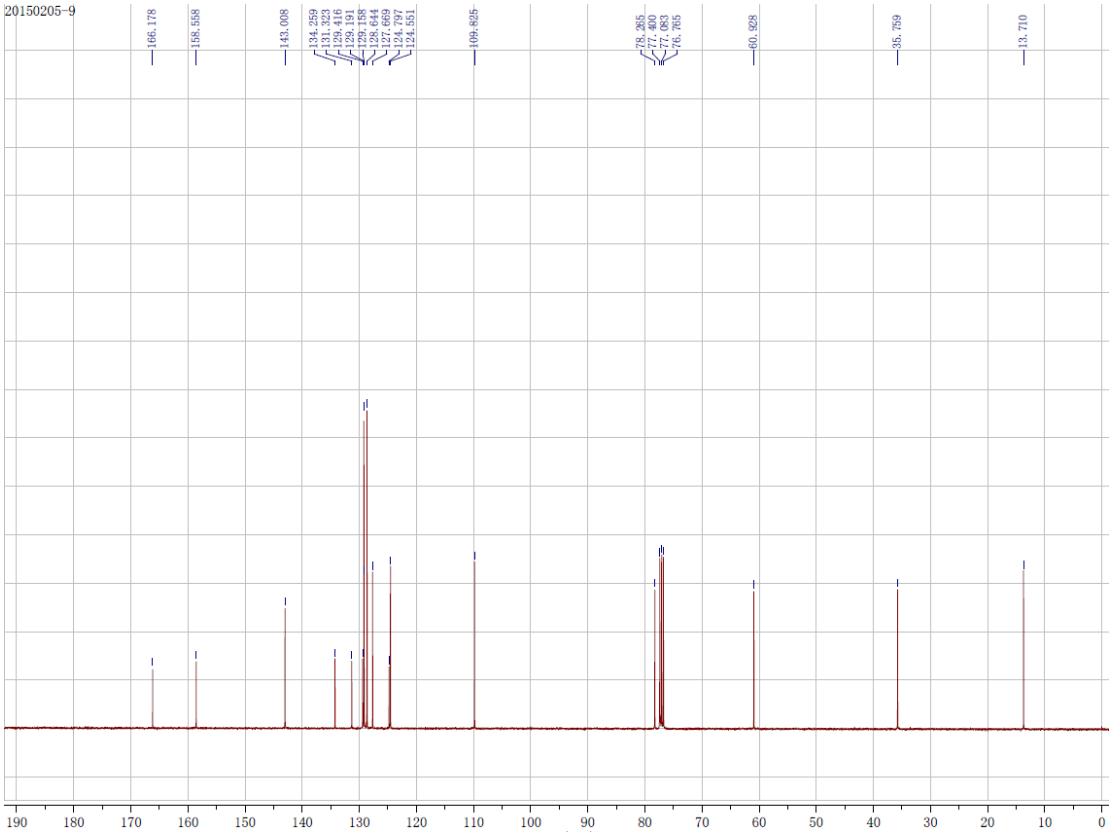

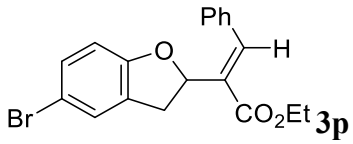

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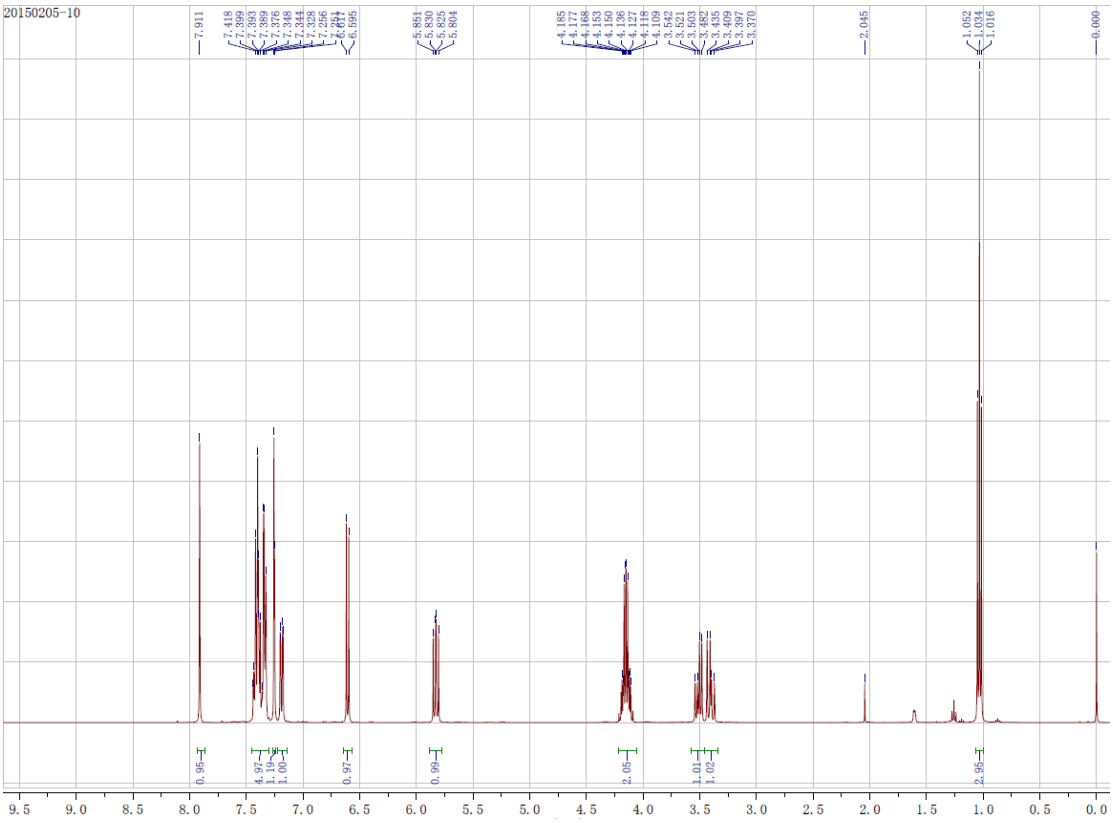

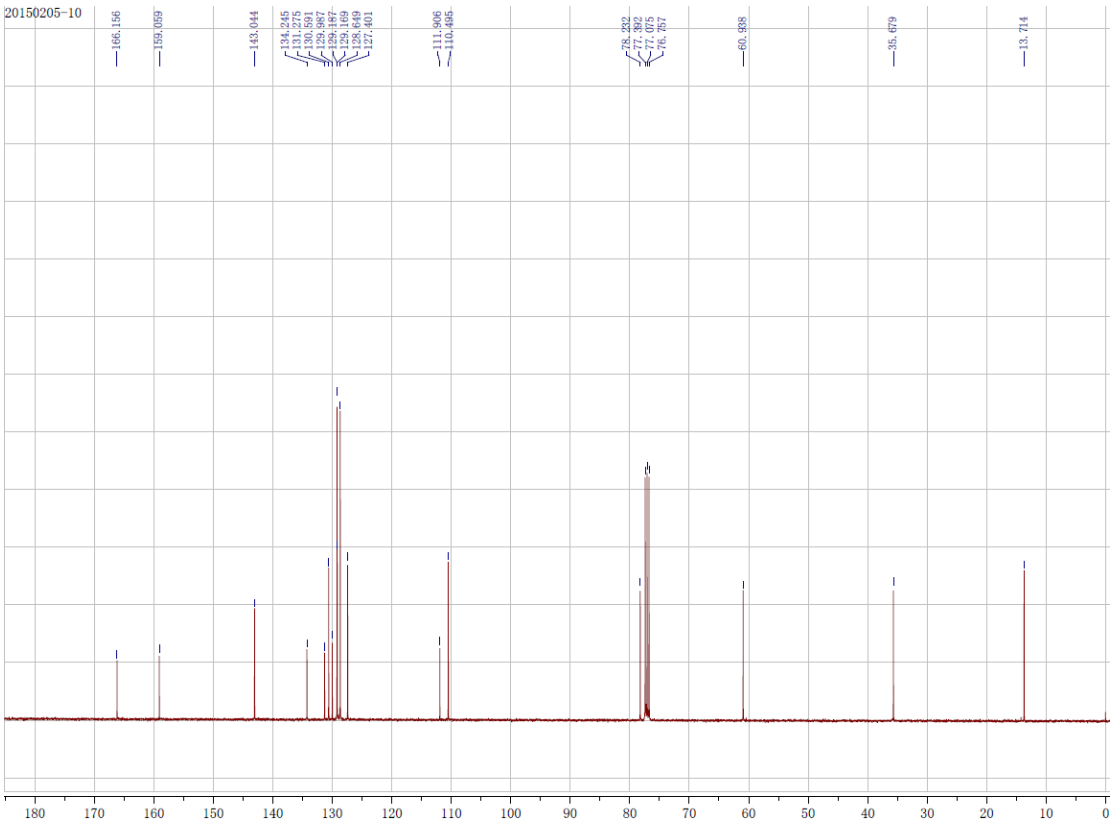

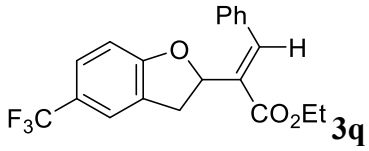

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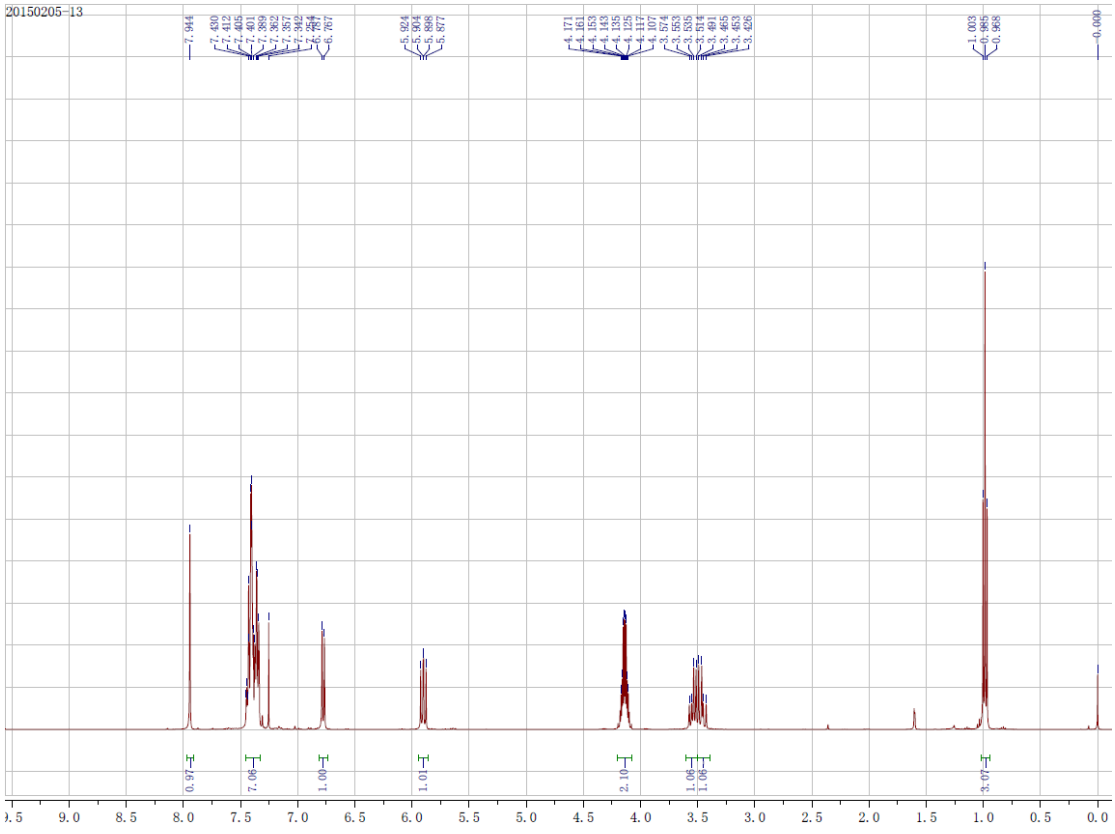

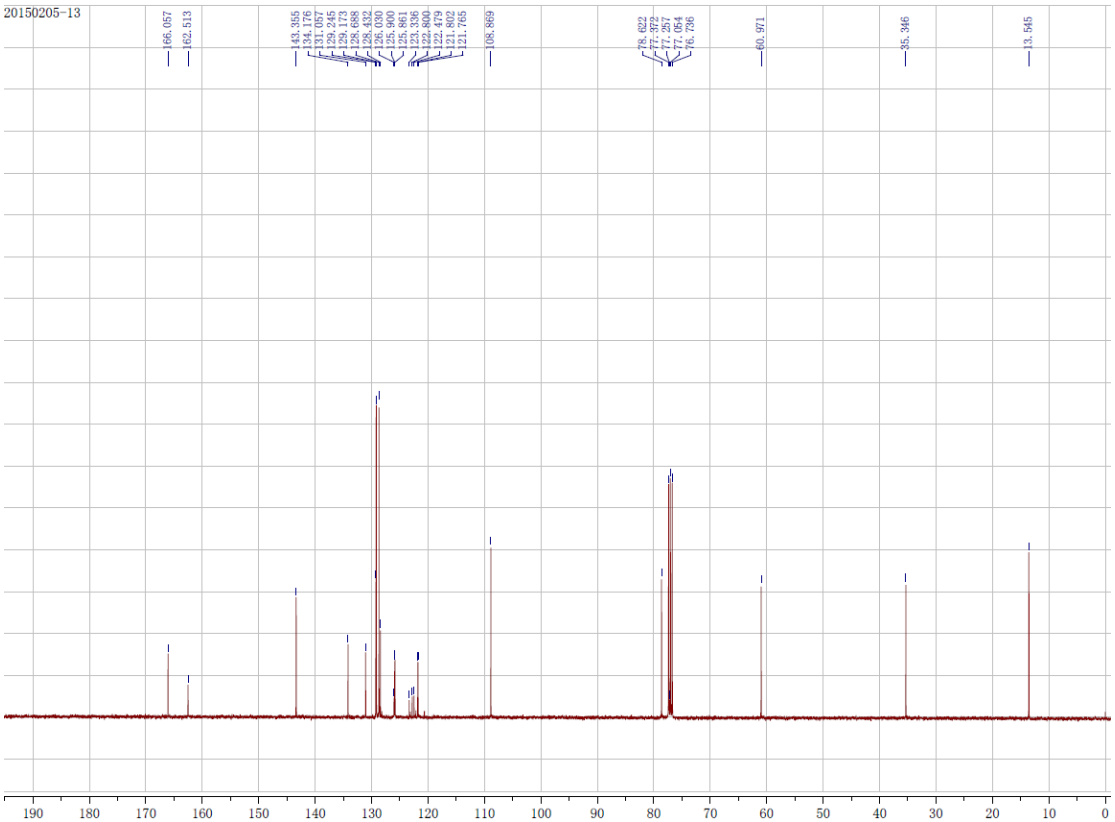

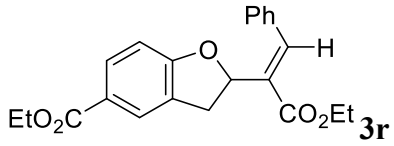

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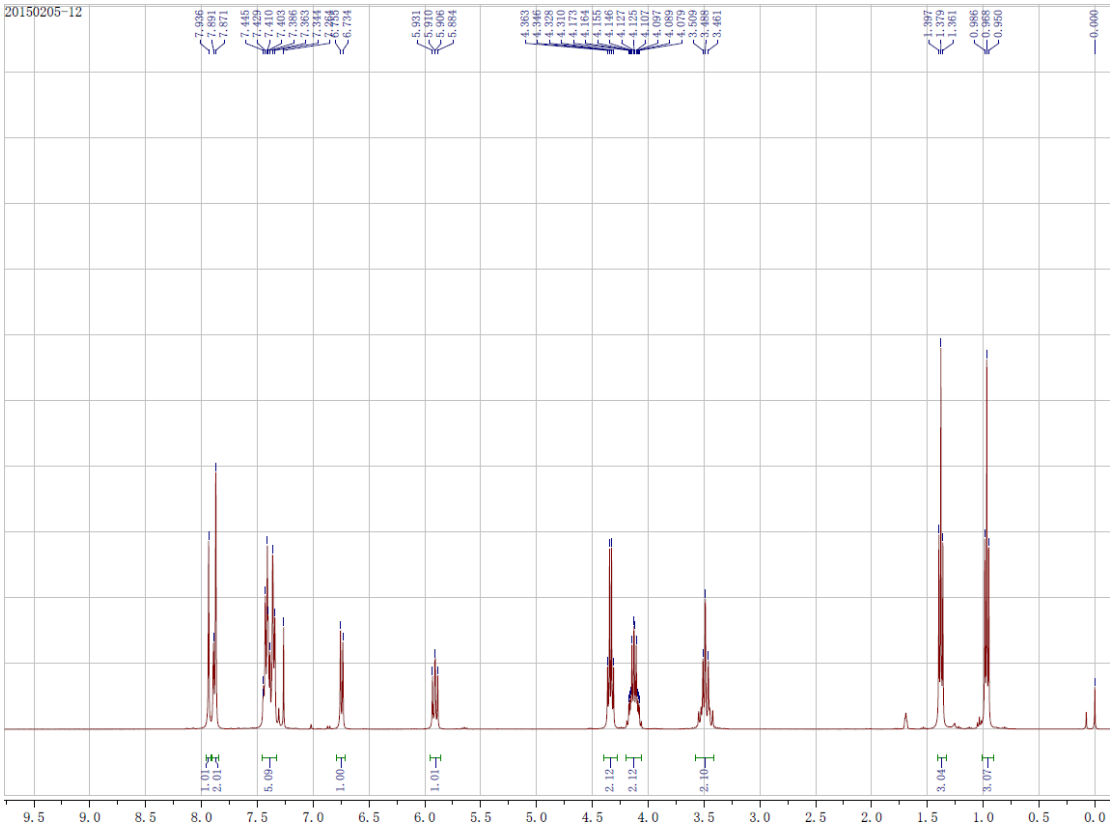

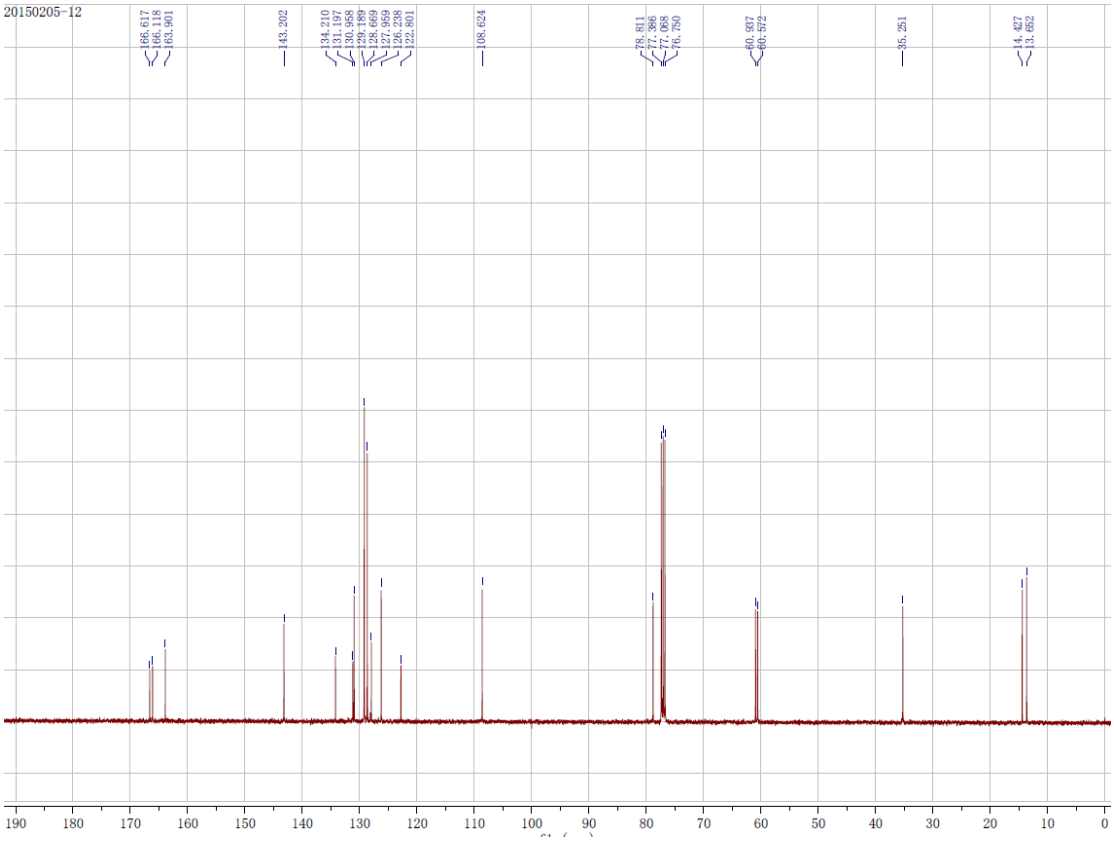

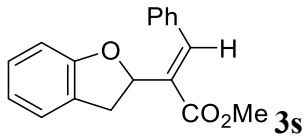
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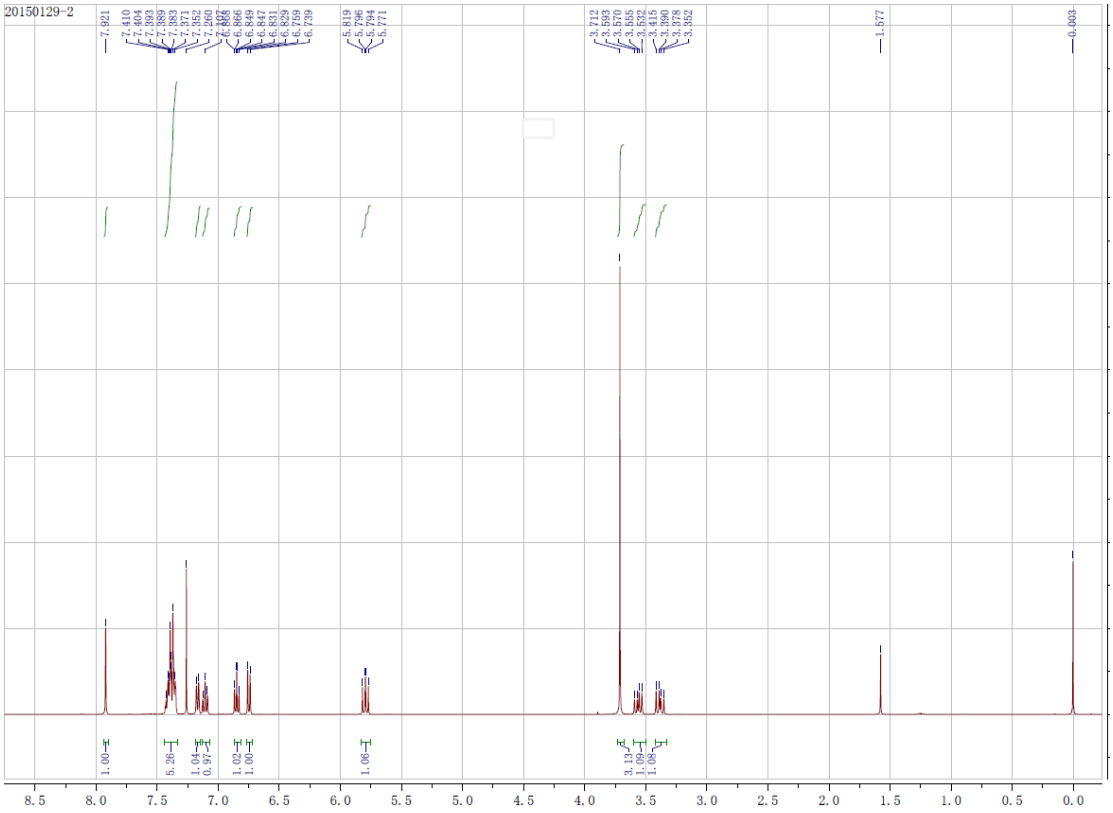
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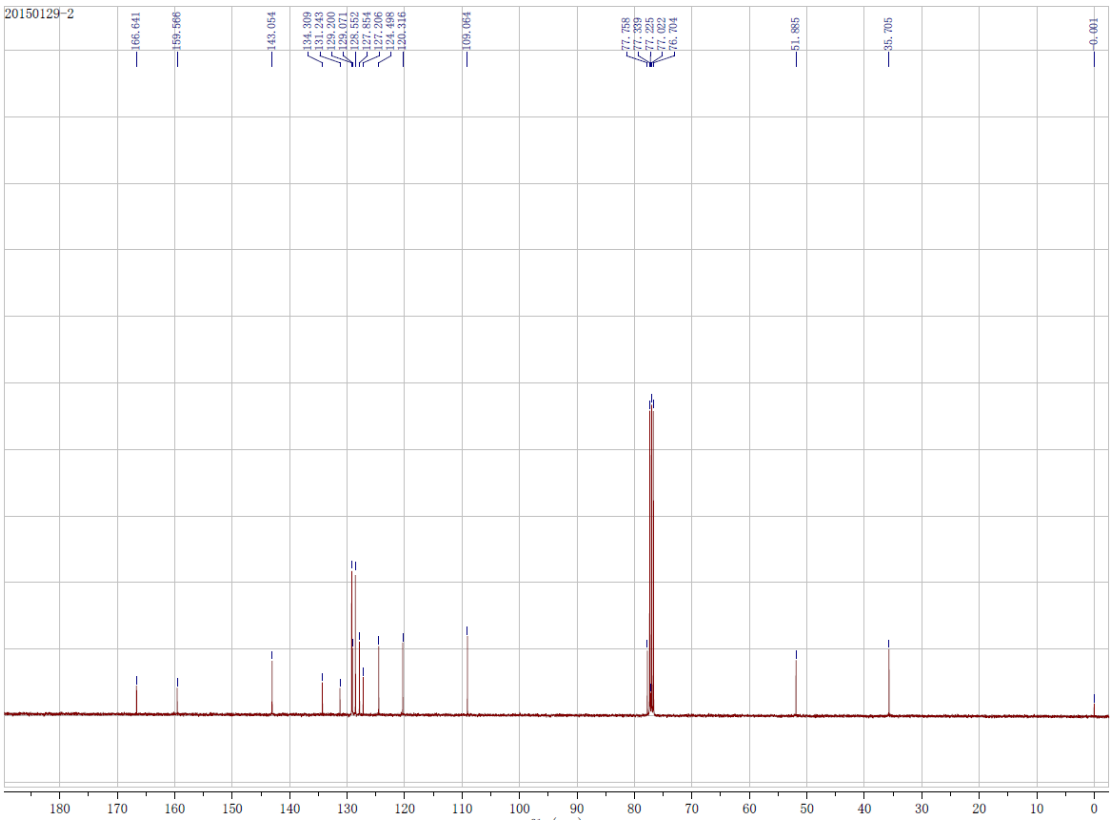
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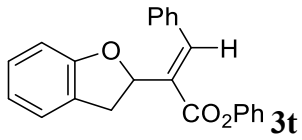

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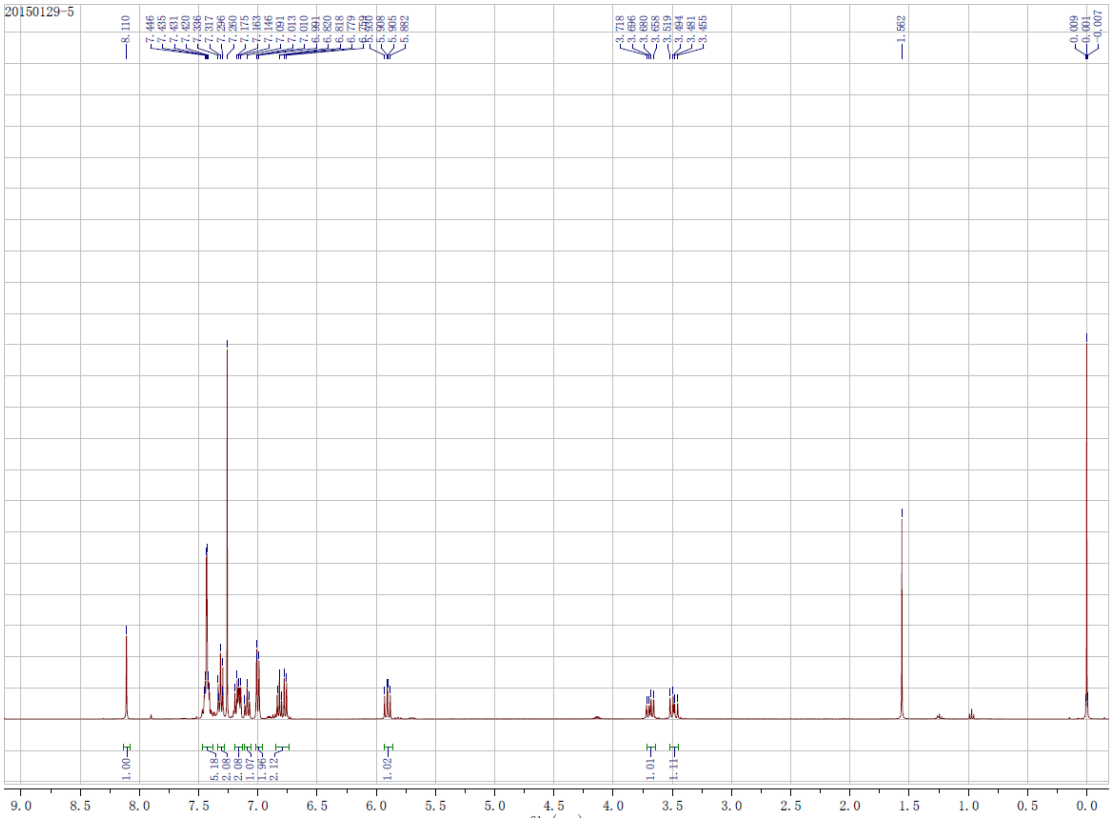

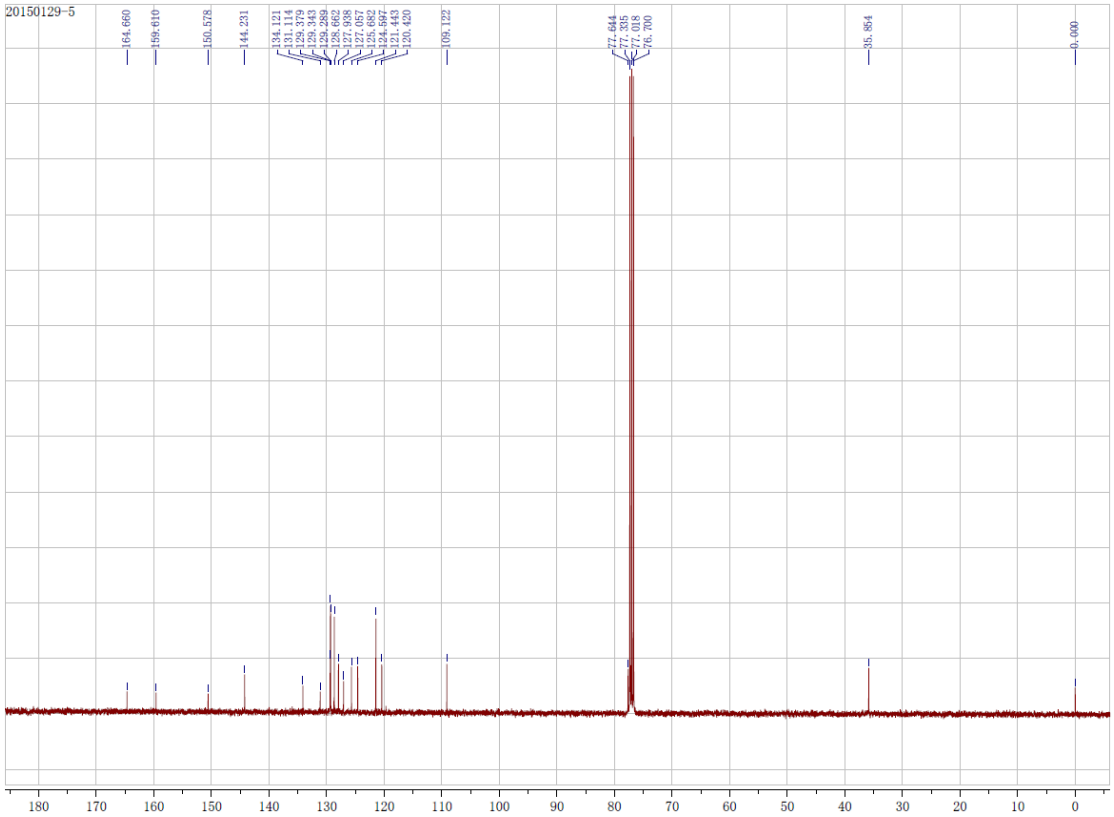

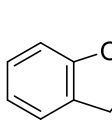
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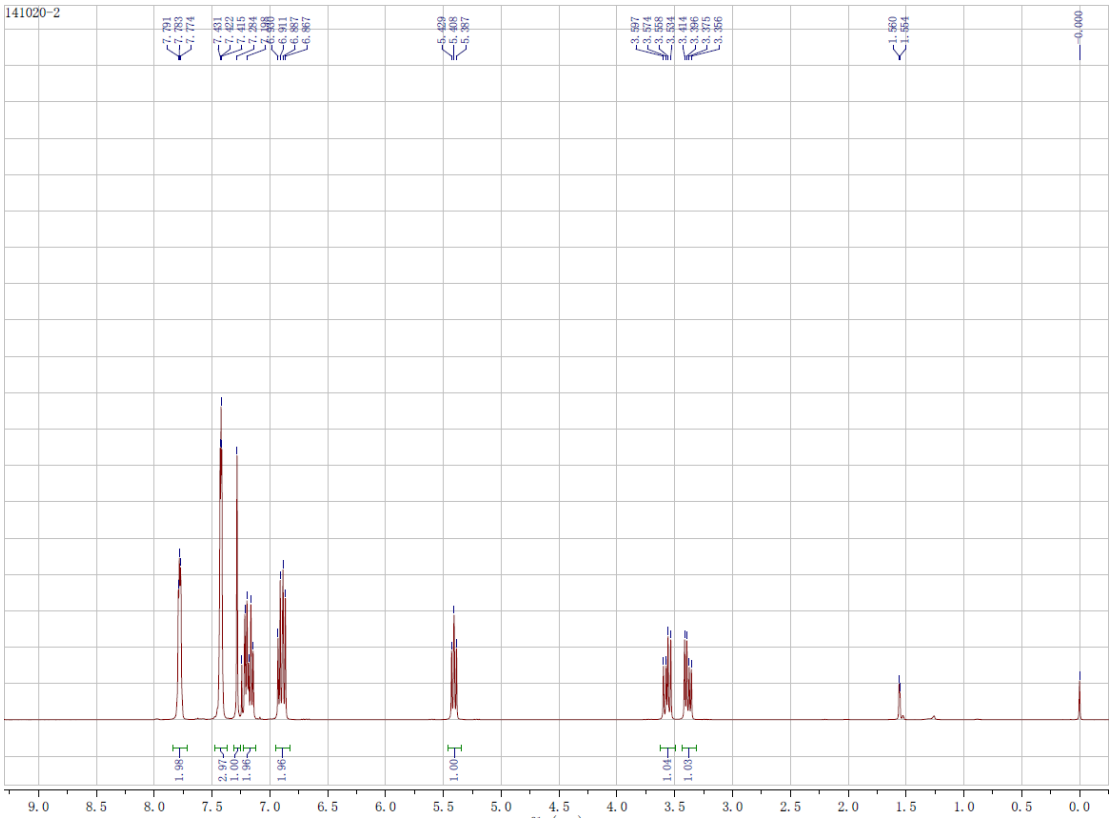
CN

3u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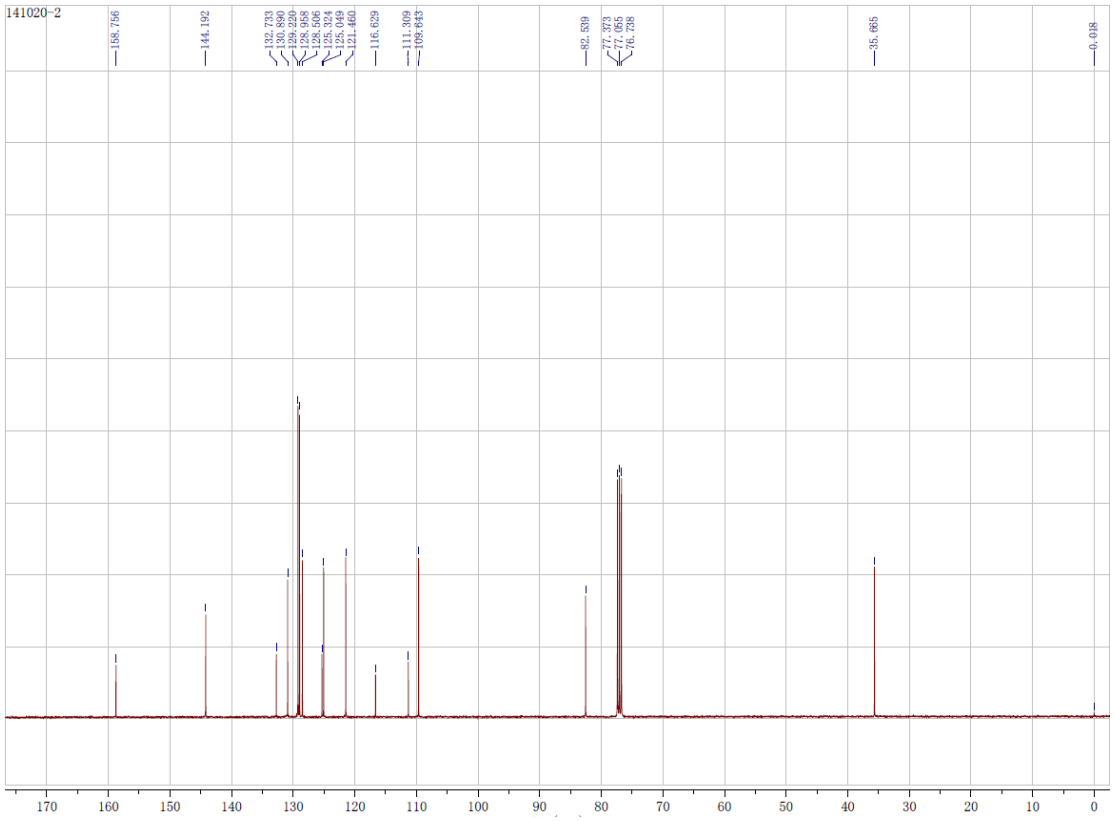
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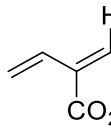
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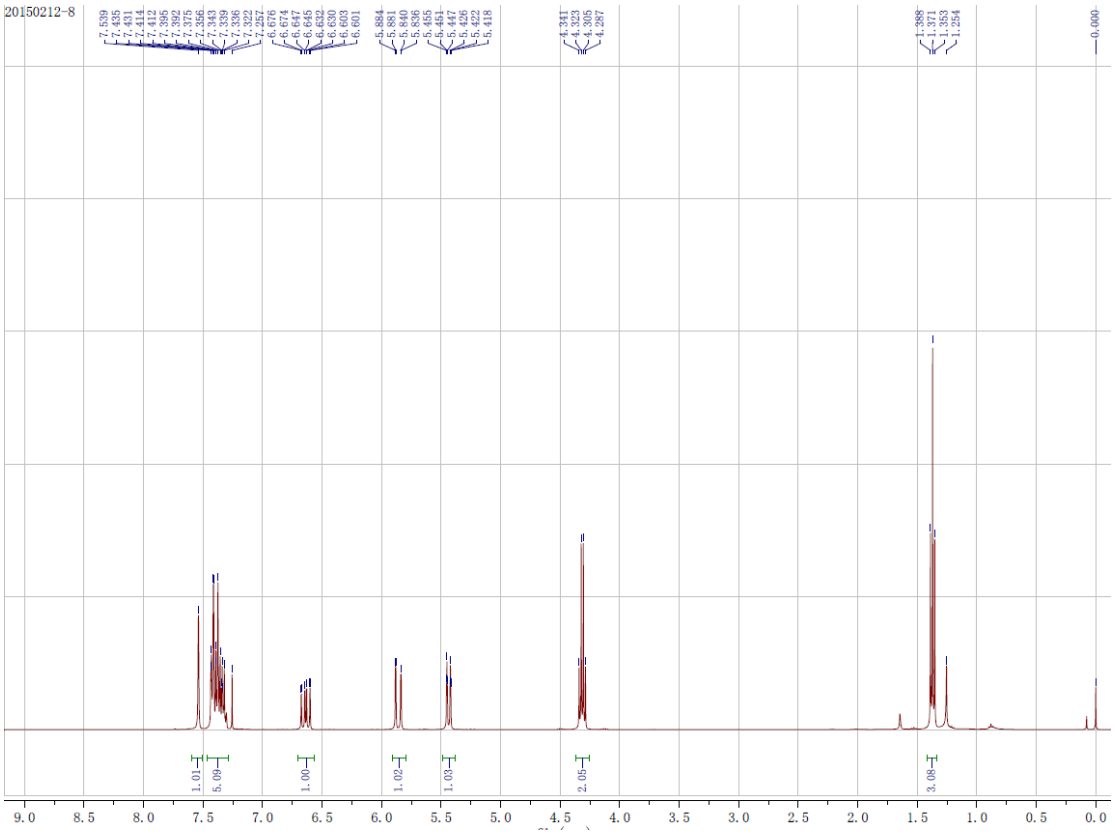
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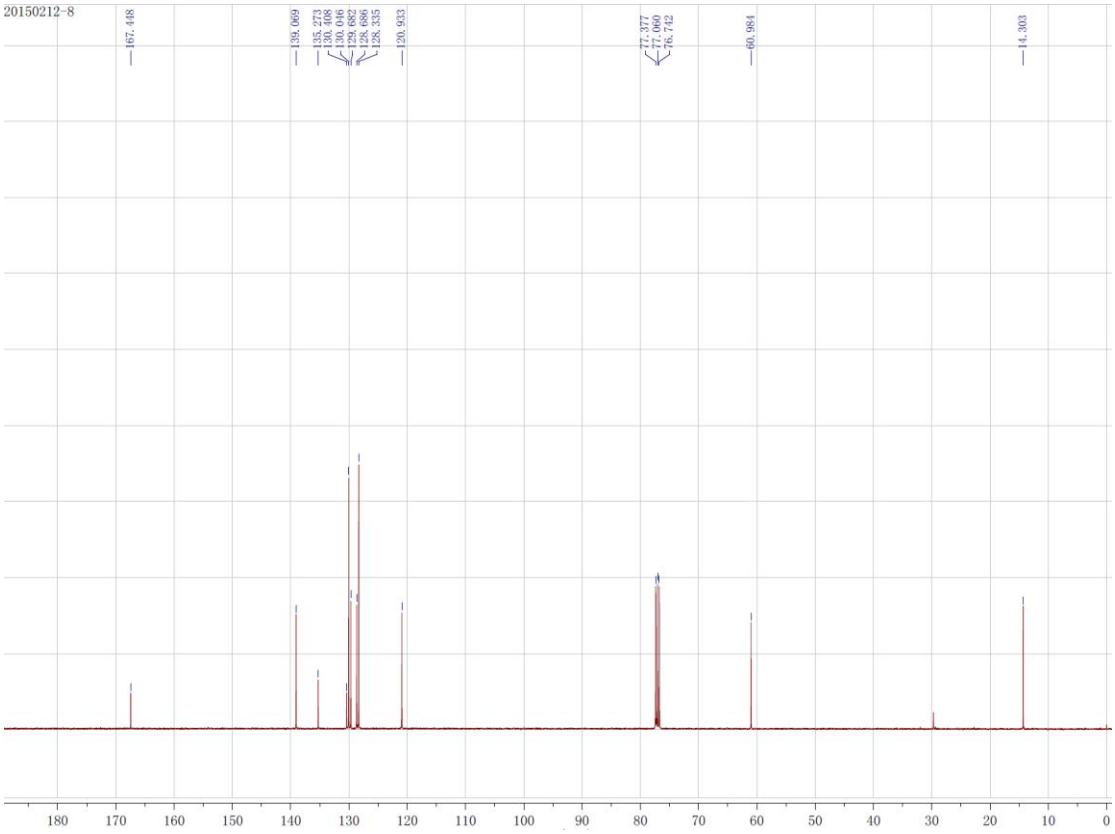
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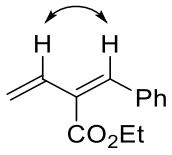
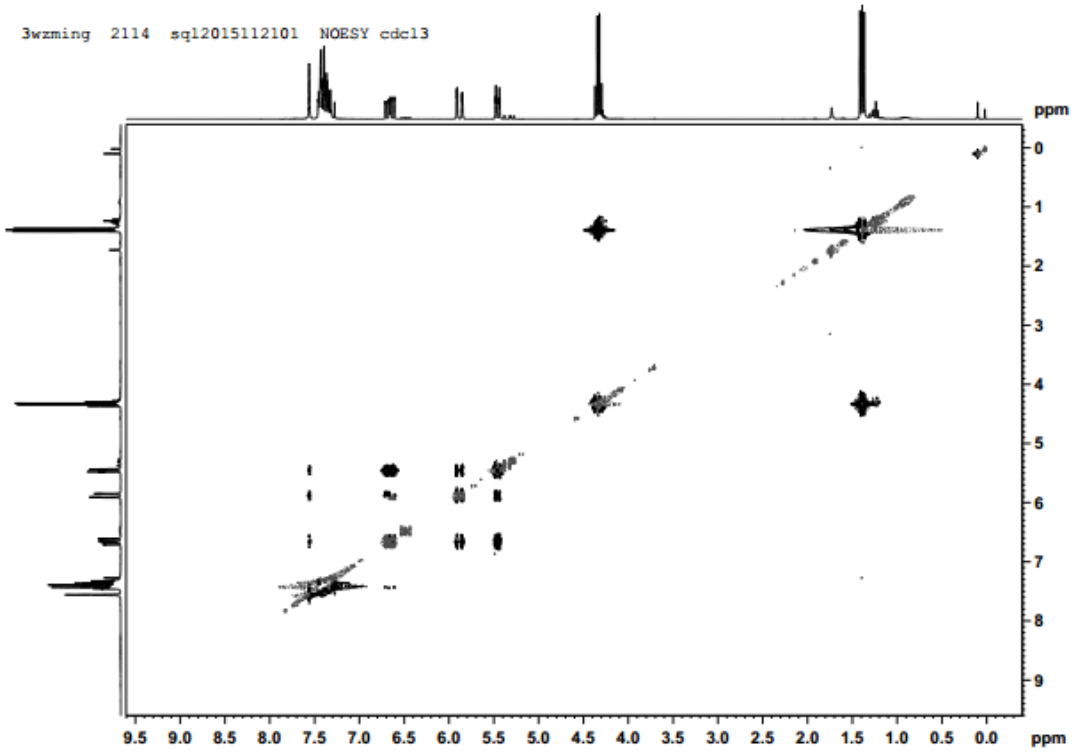
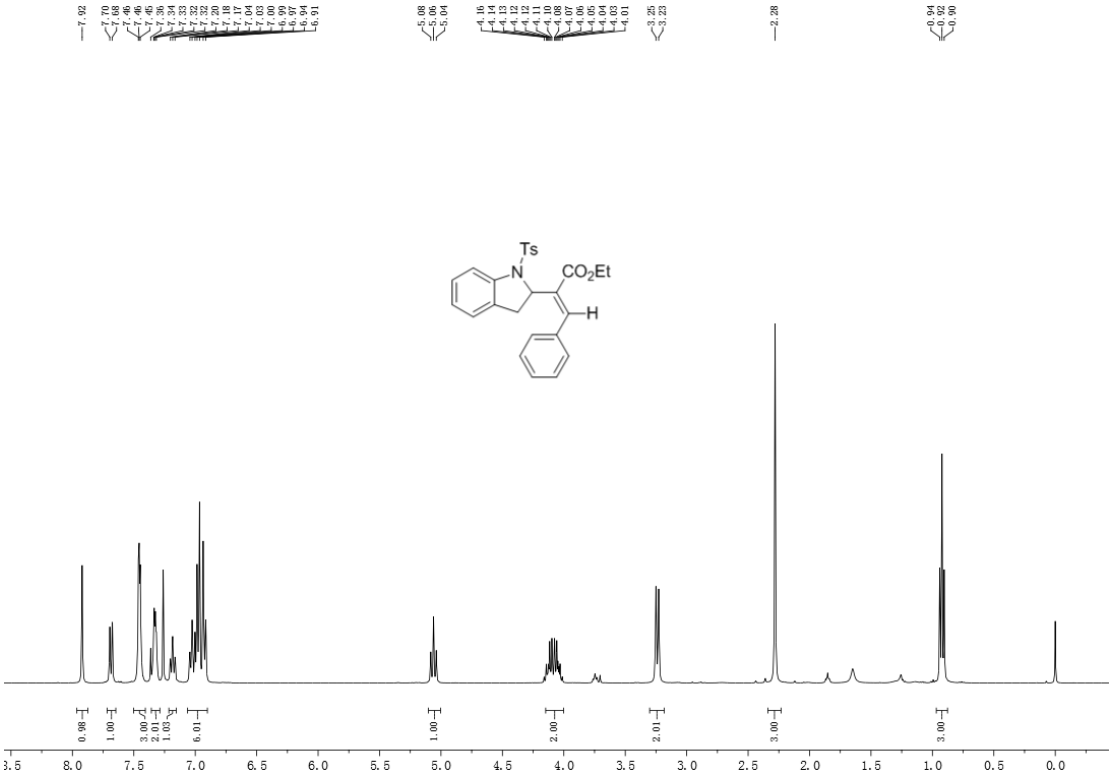
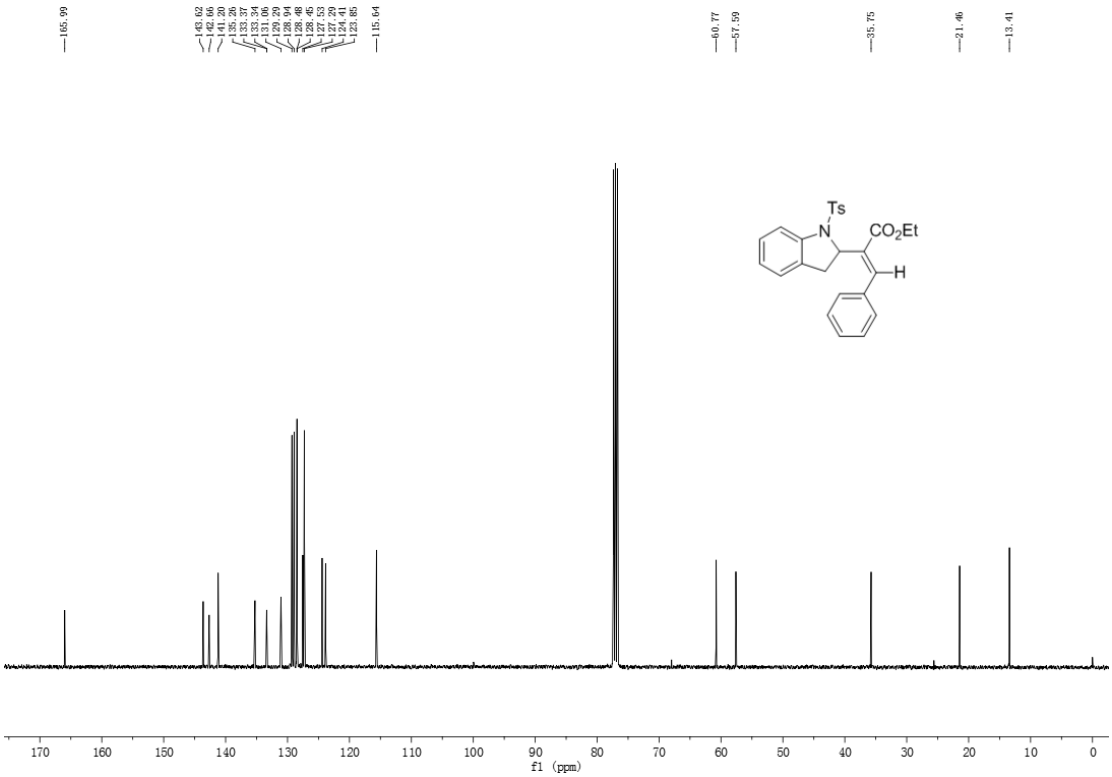


NOESY (δ 7.54 and 6.64)

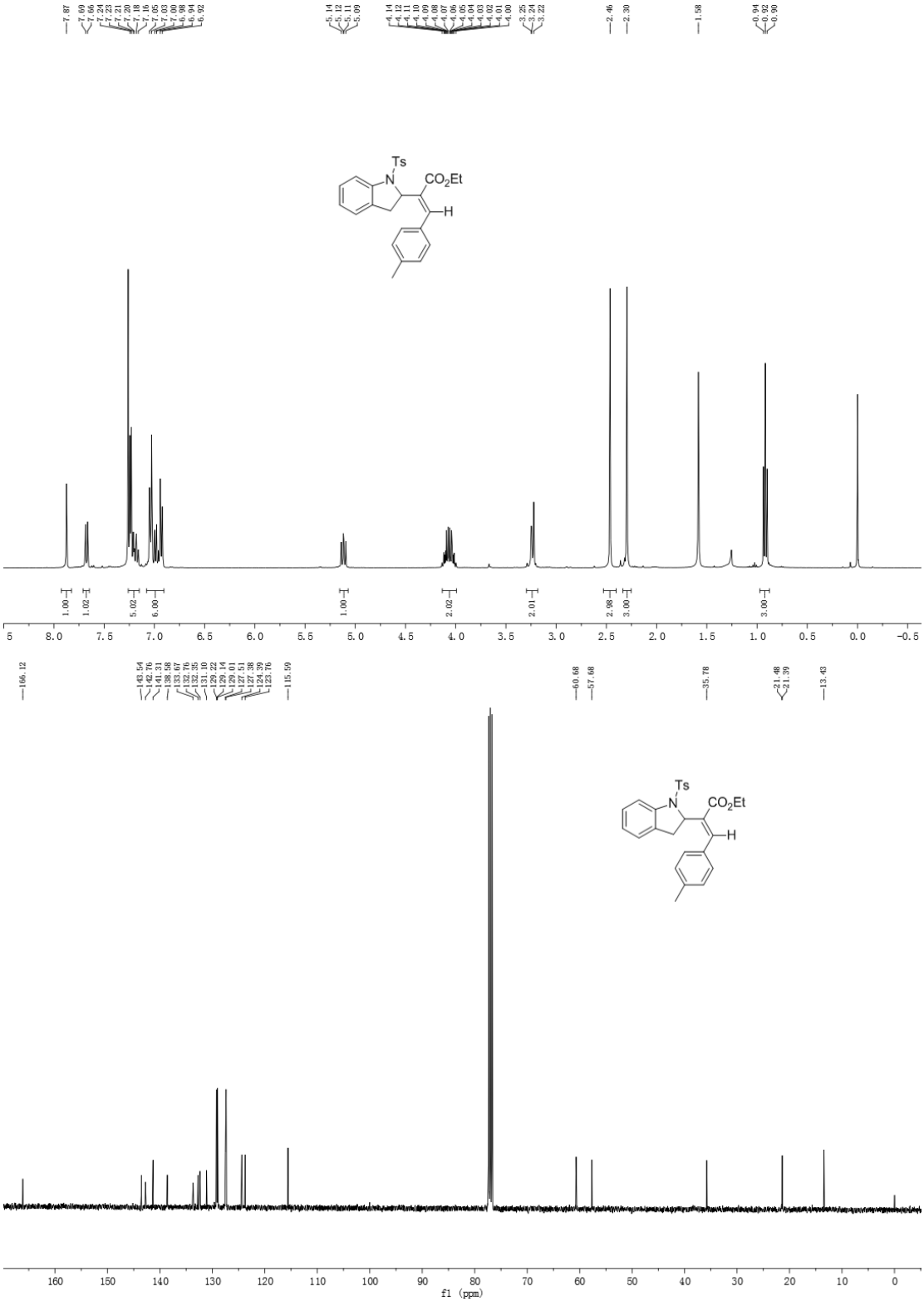


6a HNMR 400 MHz, CNMR 100 MHz

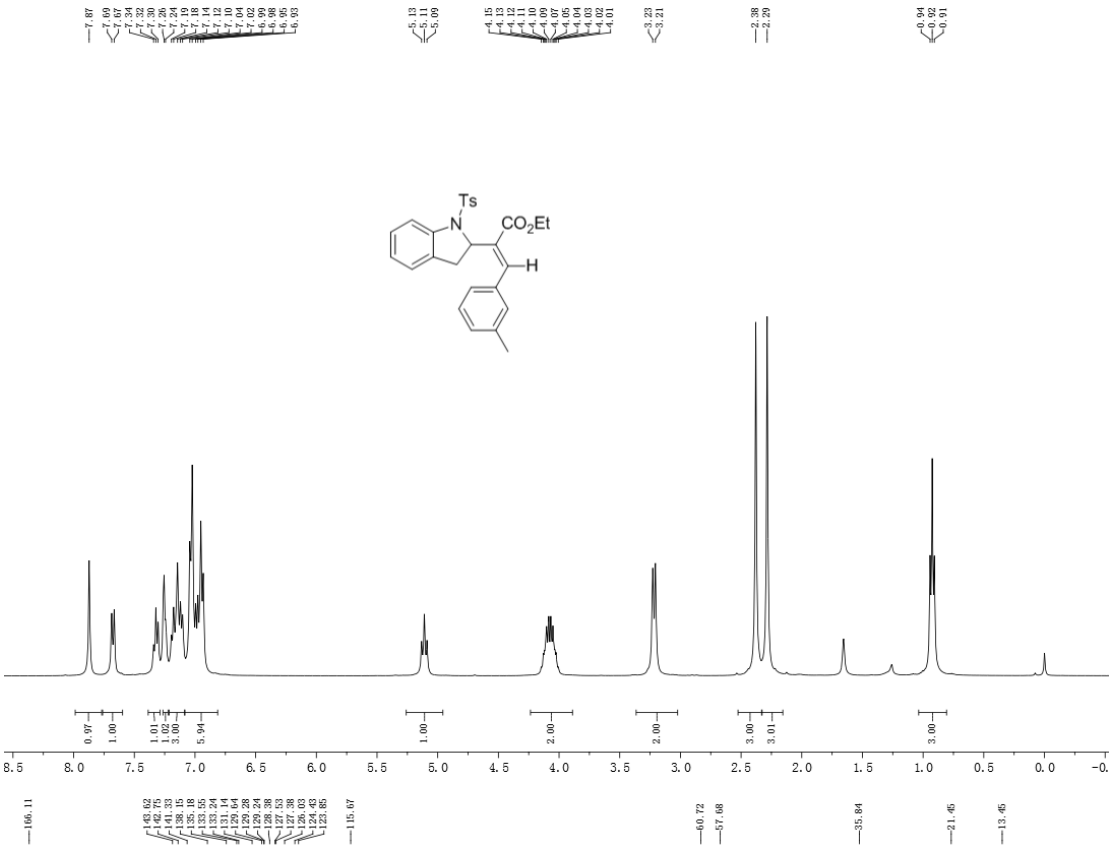


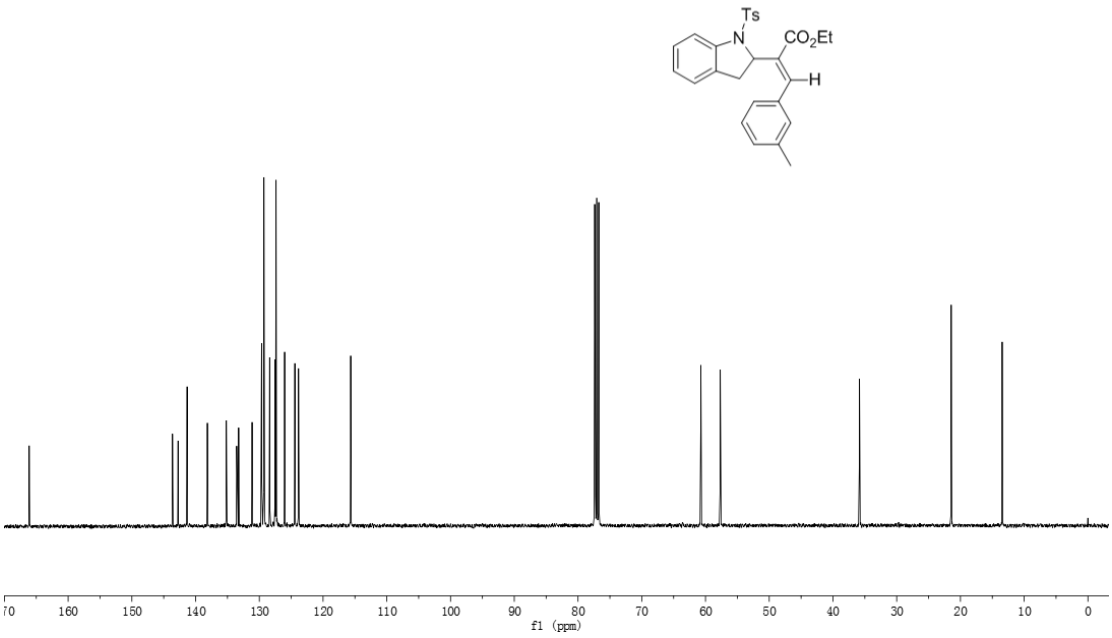


6b HNMR 400 MHz, CNMR 100 MHz

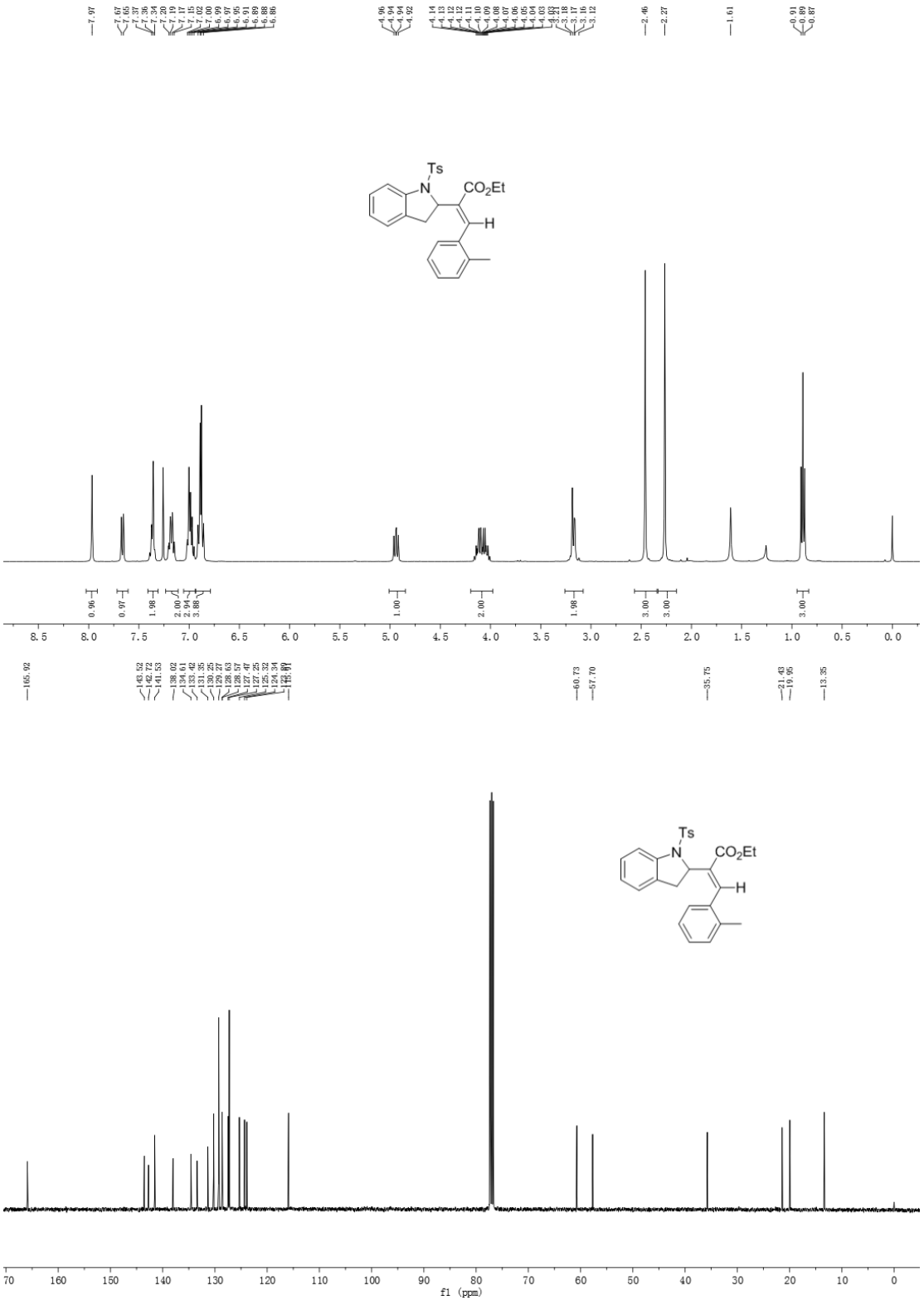


6c HNMR 400 MHz, CNMR 100 MHz

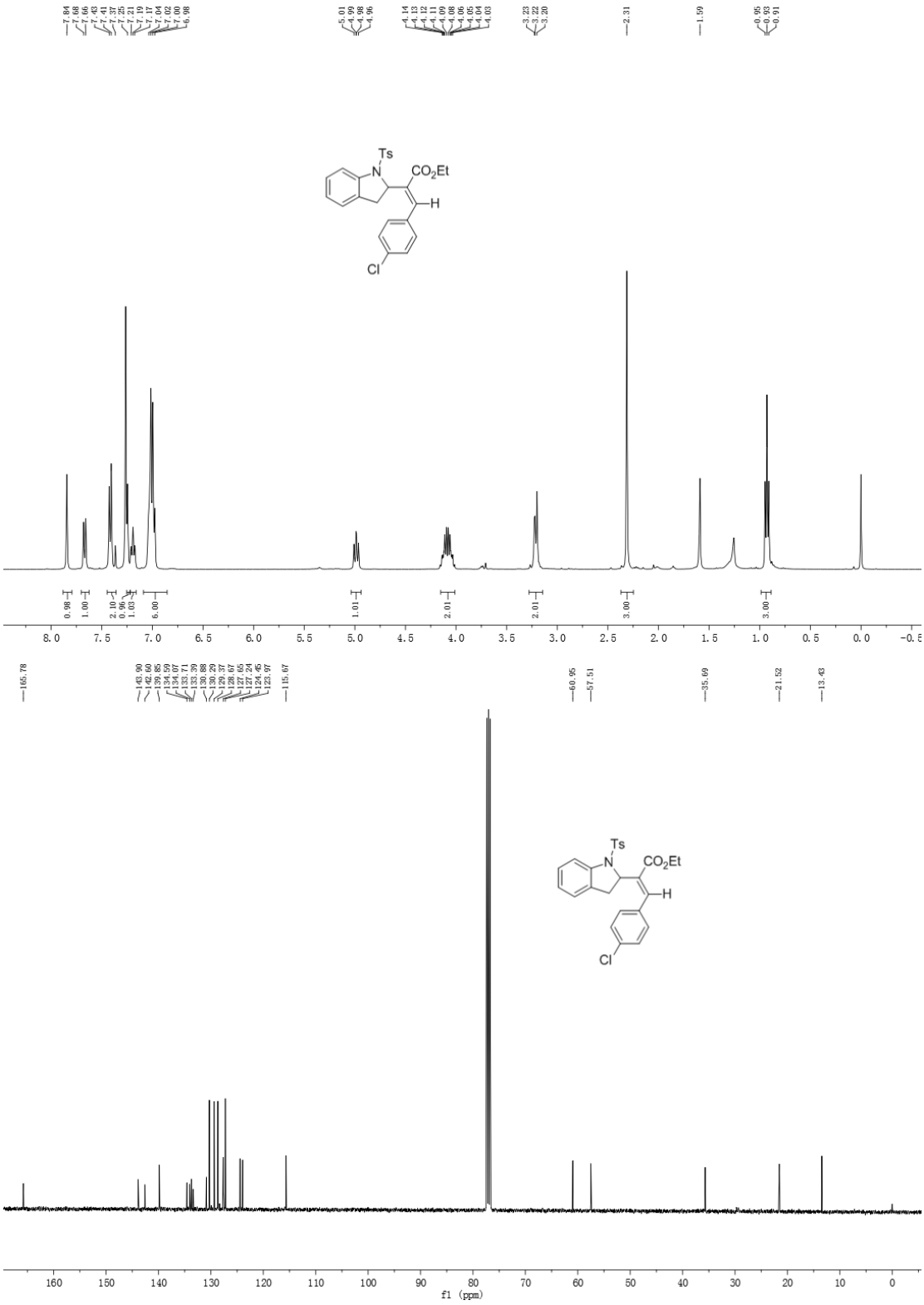




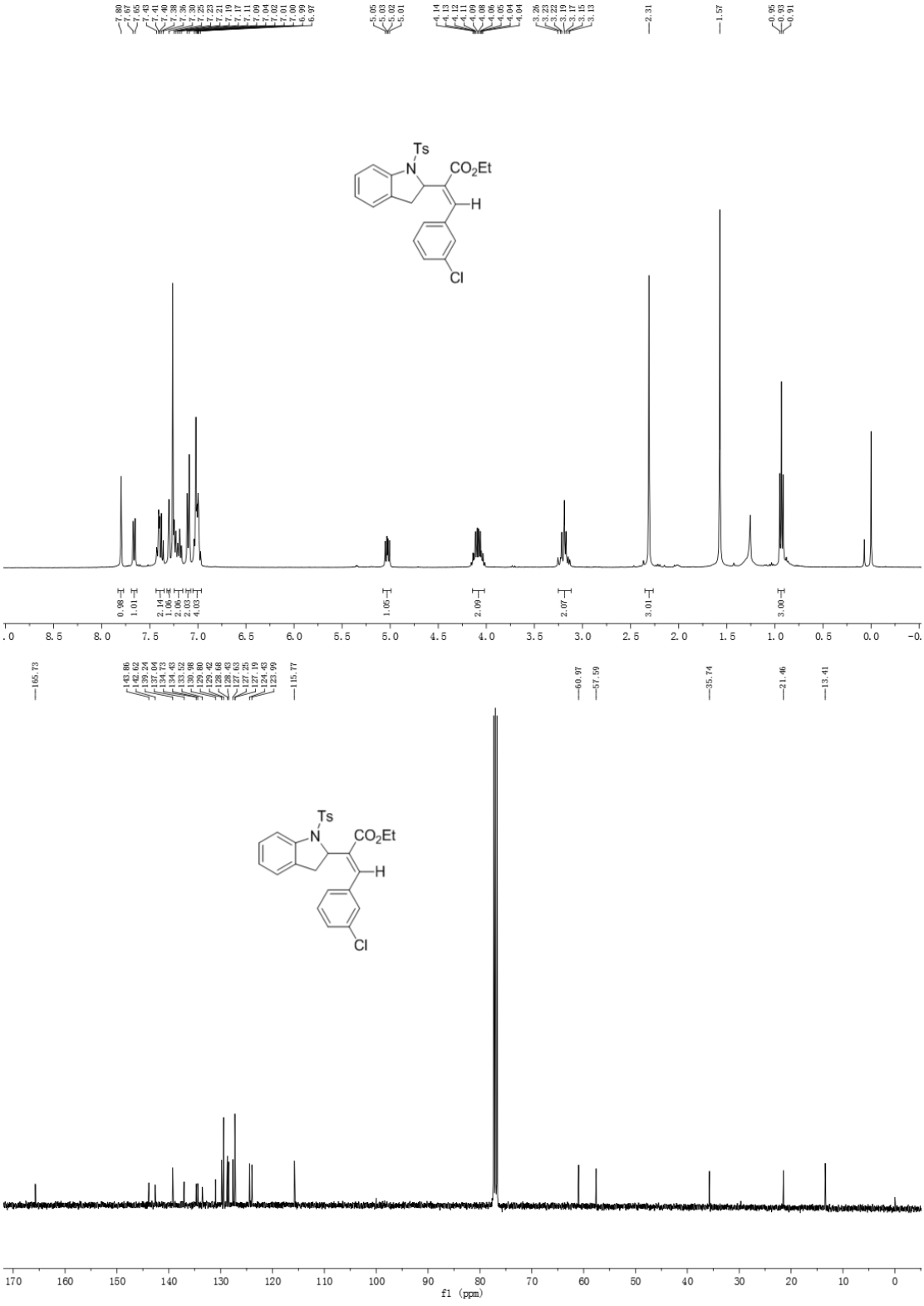
6d HNMR 400 MHz, CNMR 100 MHz



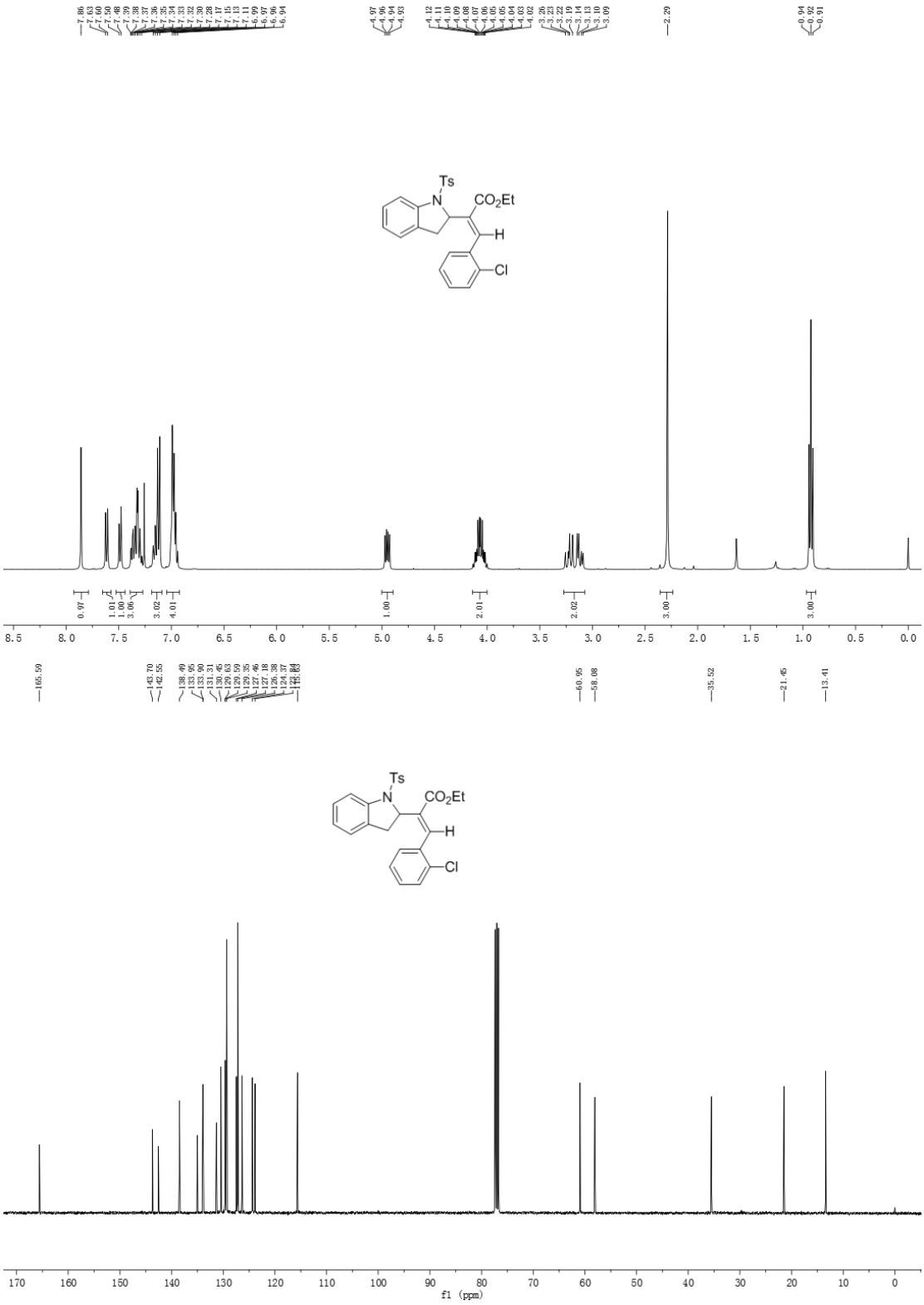
6e HNMR 400 MHz, CNMR 100 MHz



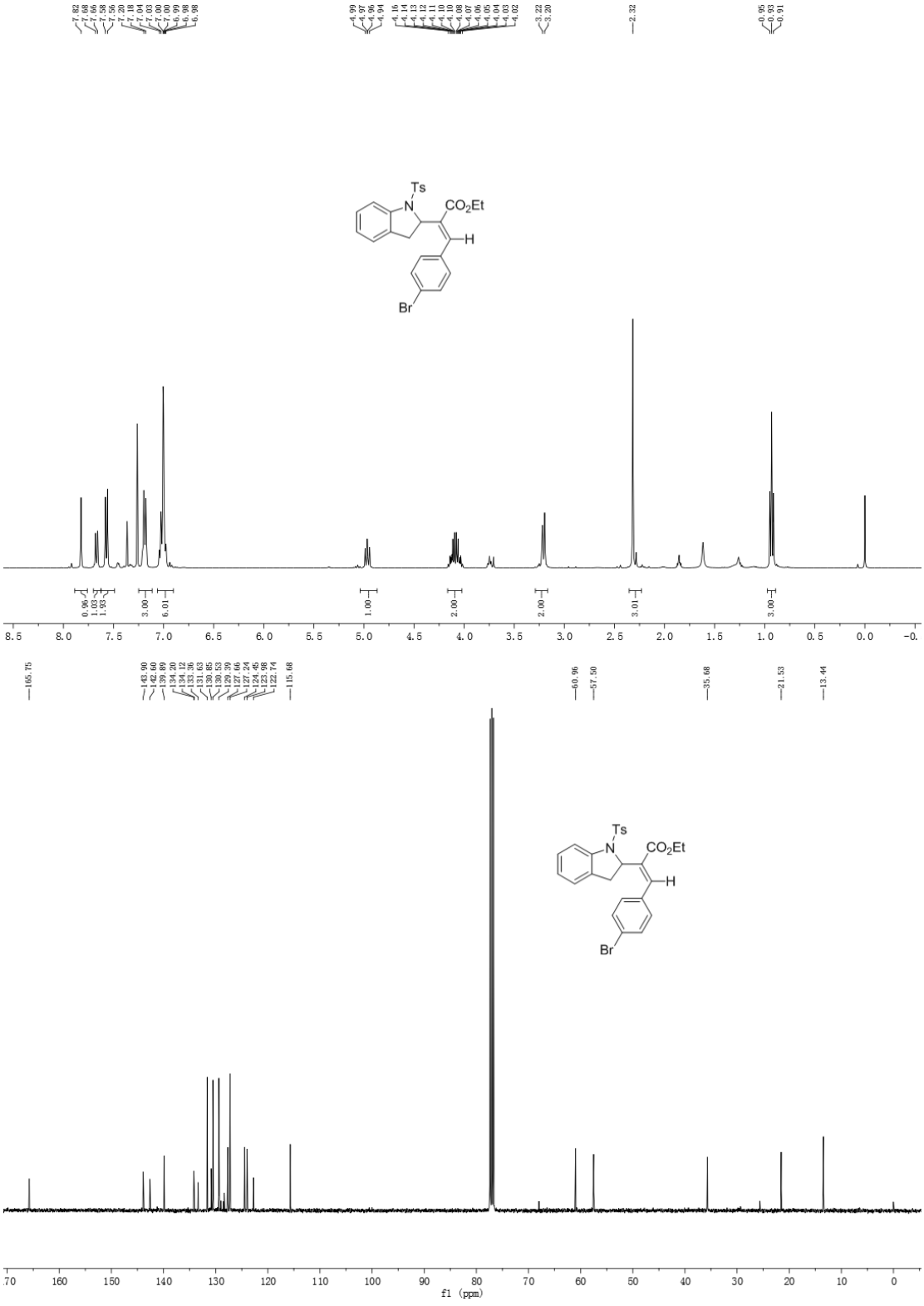
6f HNMR 400 MHz, CNMR 100 MHz



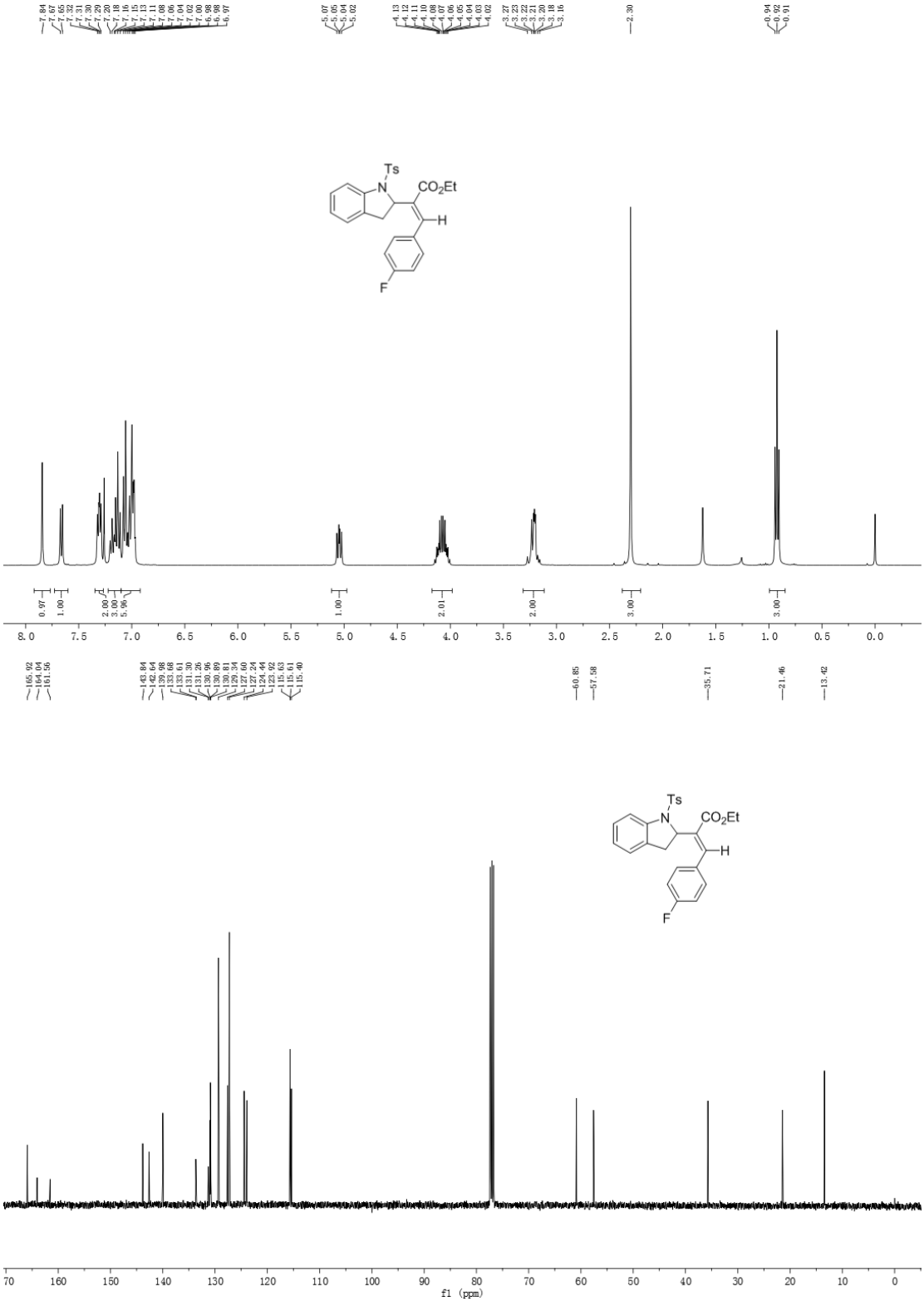
6g HNMR 400 MHz, CNMR 100 MHz



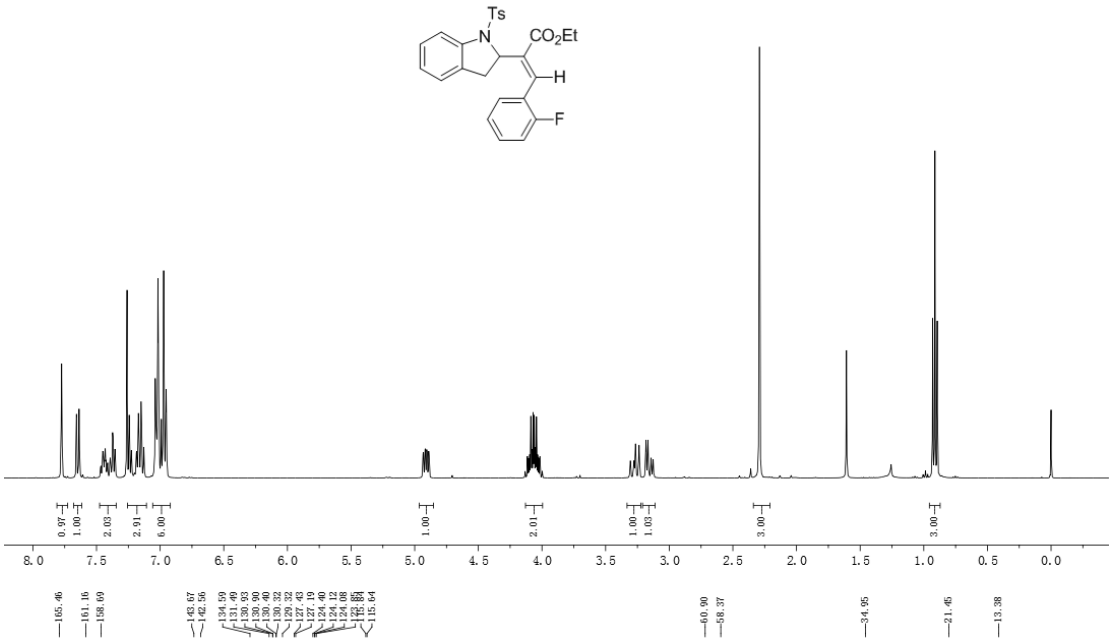
6h HNMR 400 MHz, CNMR 100 MHz

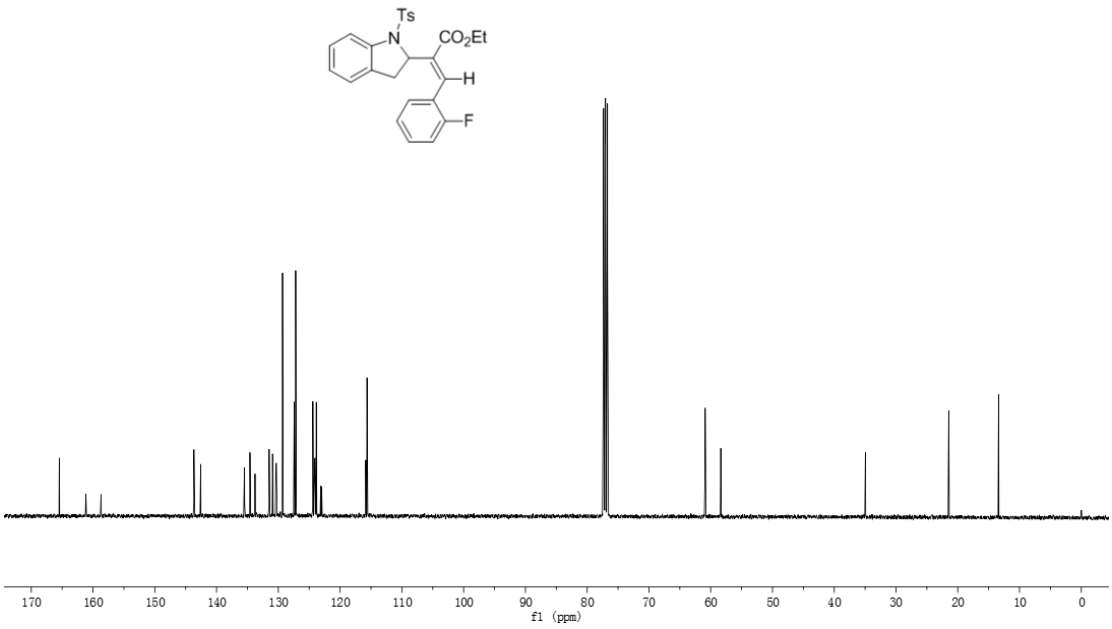


6i HNMR 400 MHz, CNMR 100 MHz

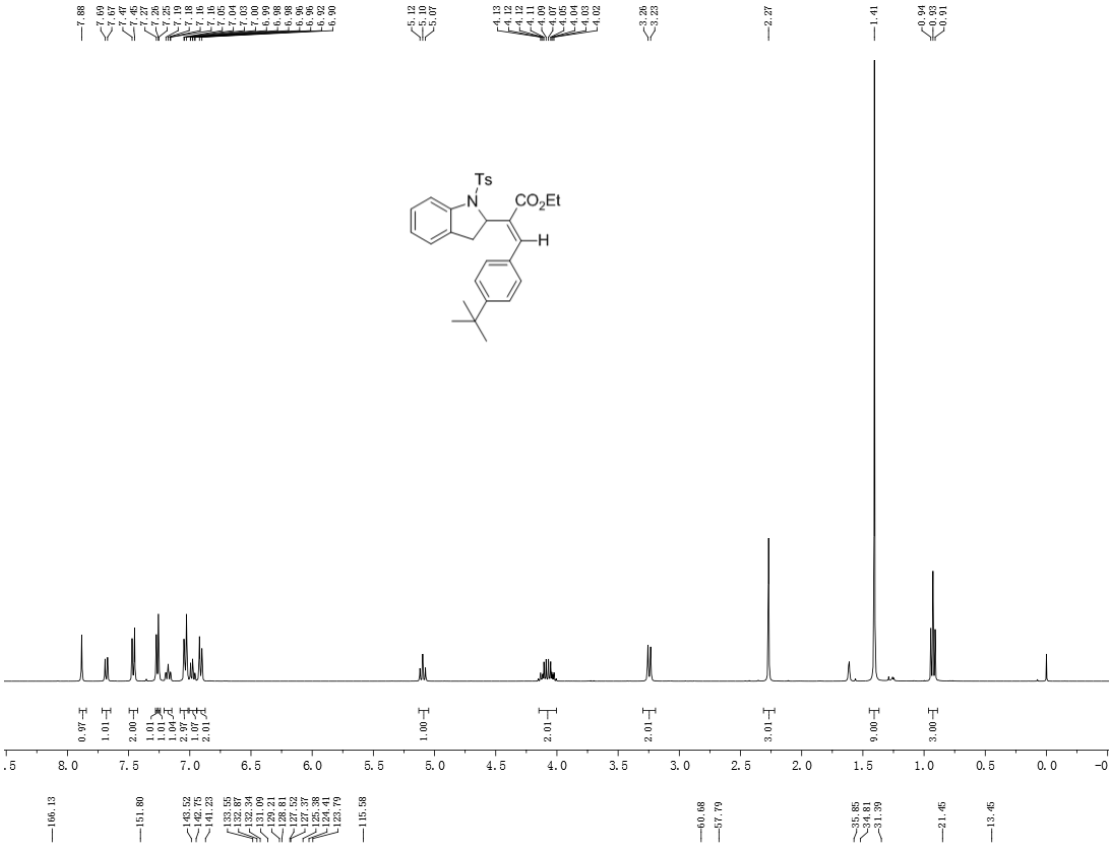


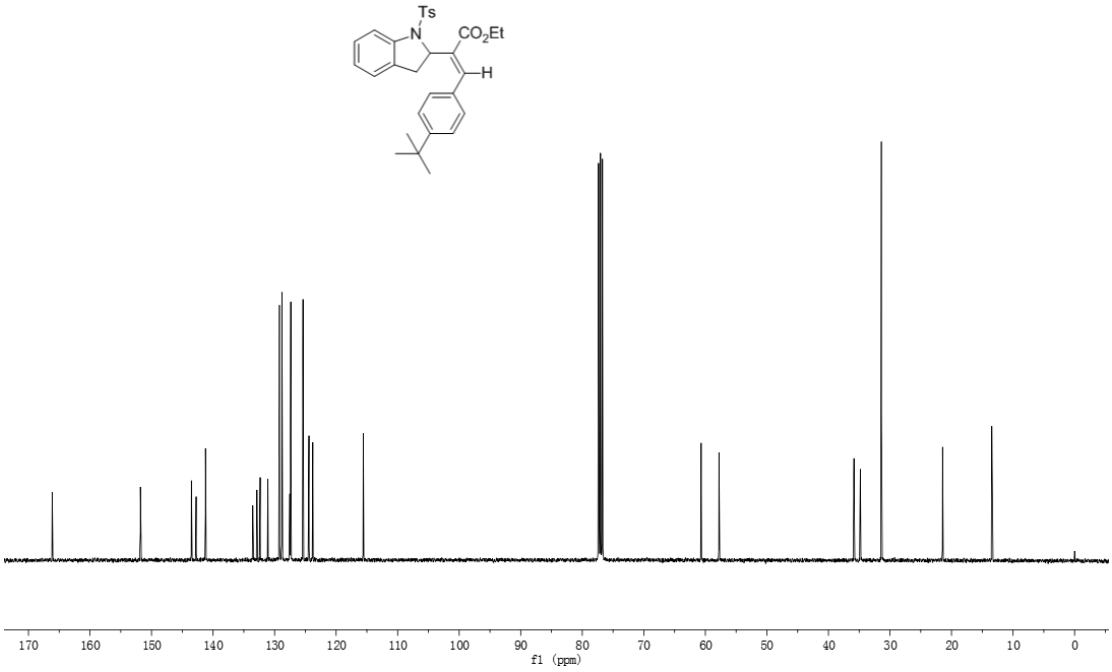
6j HNMR 400 MHz, CNMR 100 MHz



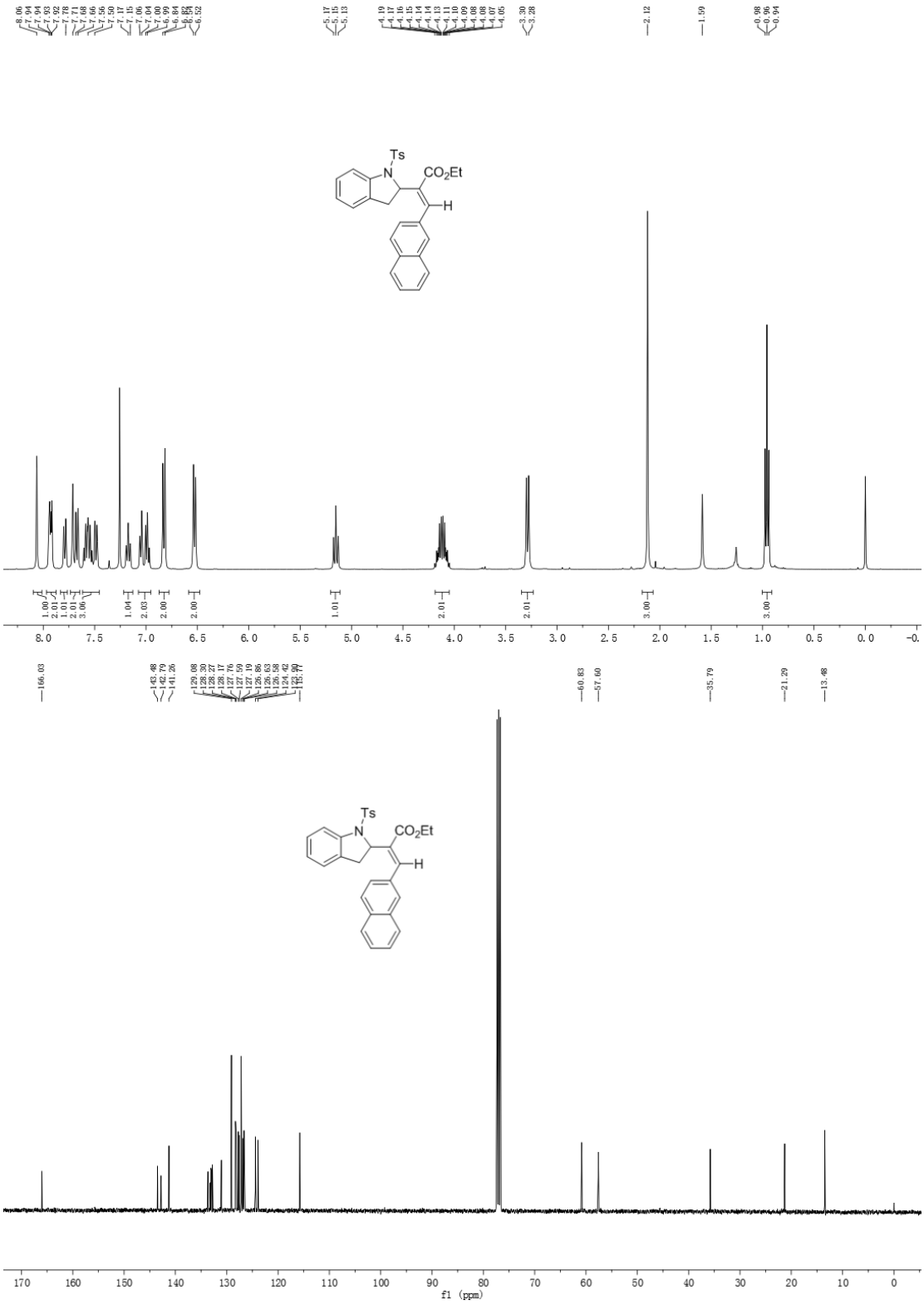


6k HNMR 400 MHz, CNMR 100 MHz

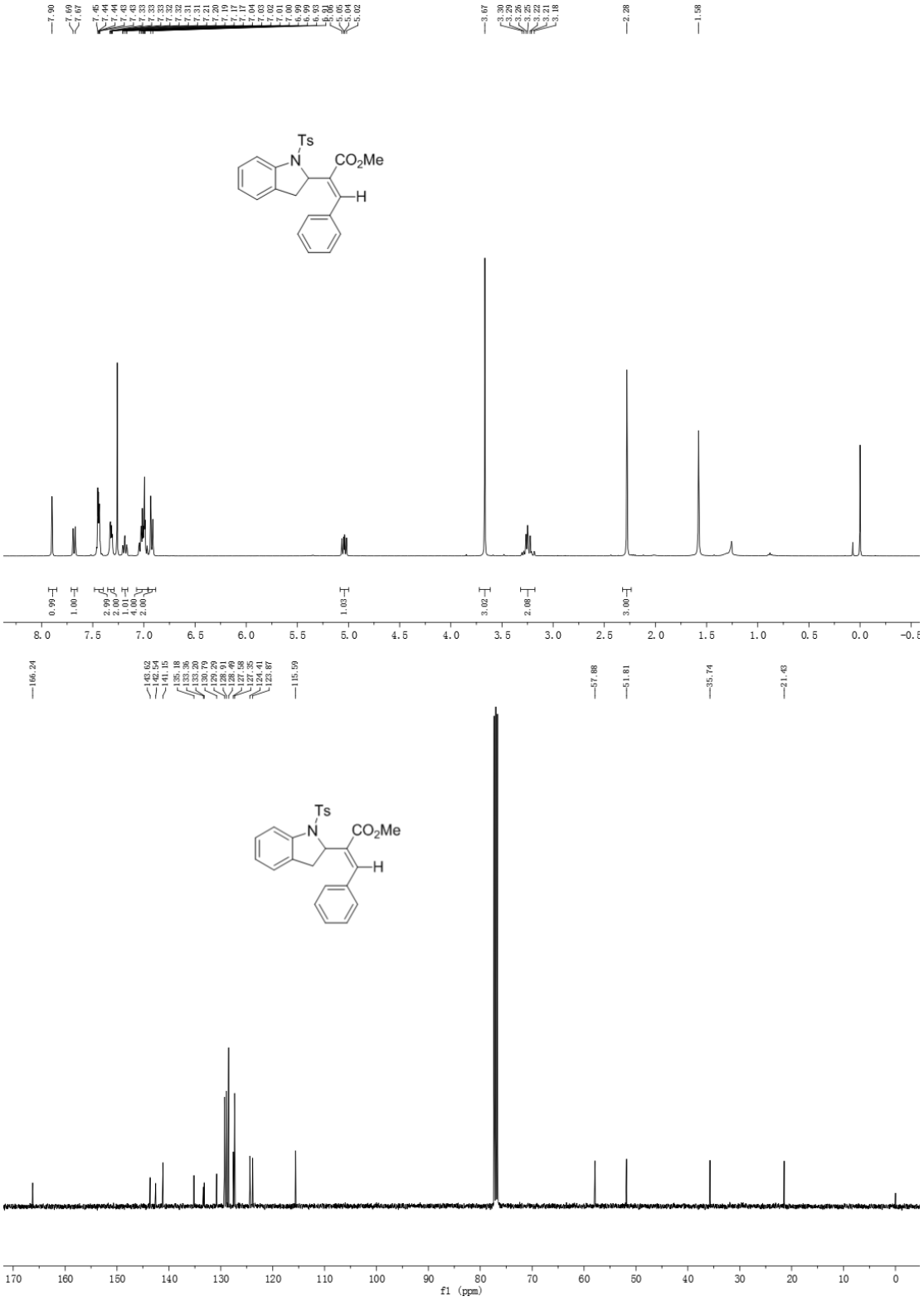




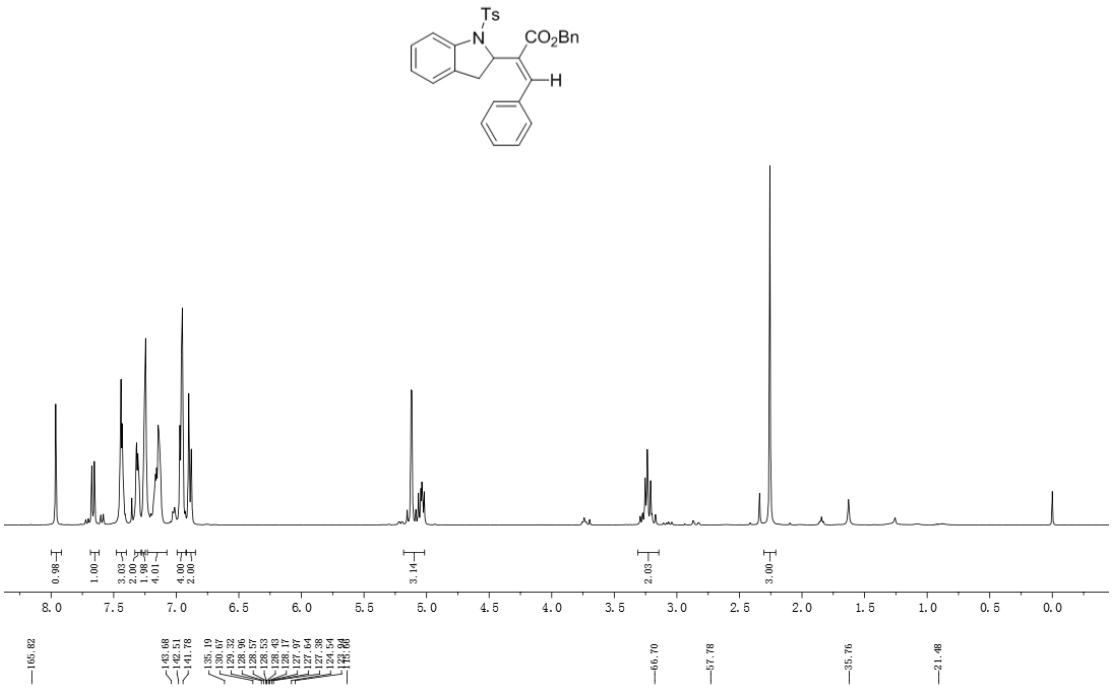
6l HNMR 400 MHz, CNMR 100 MHz

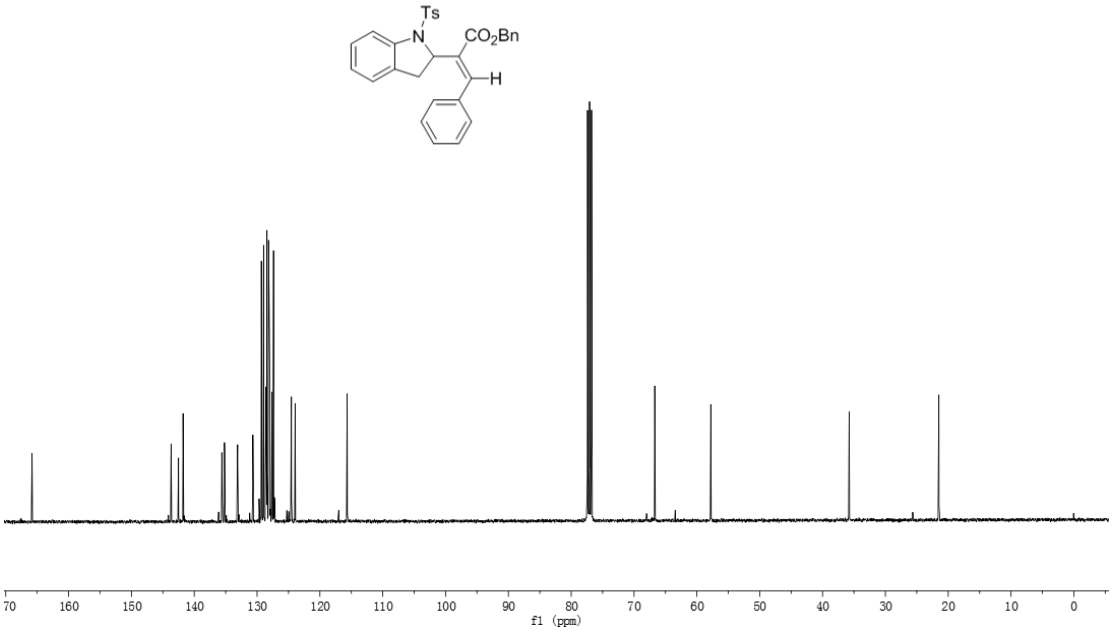


6m HNMR 400 MHz, CNMR 100 MHz

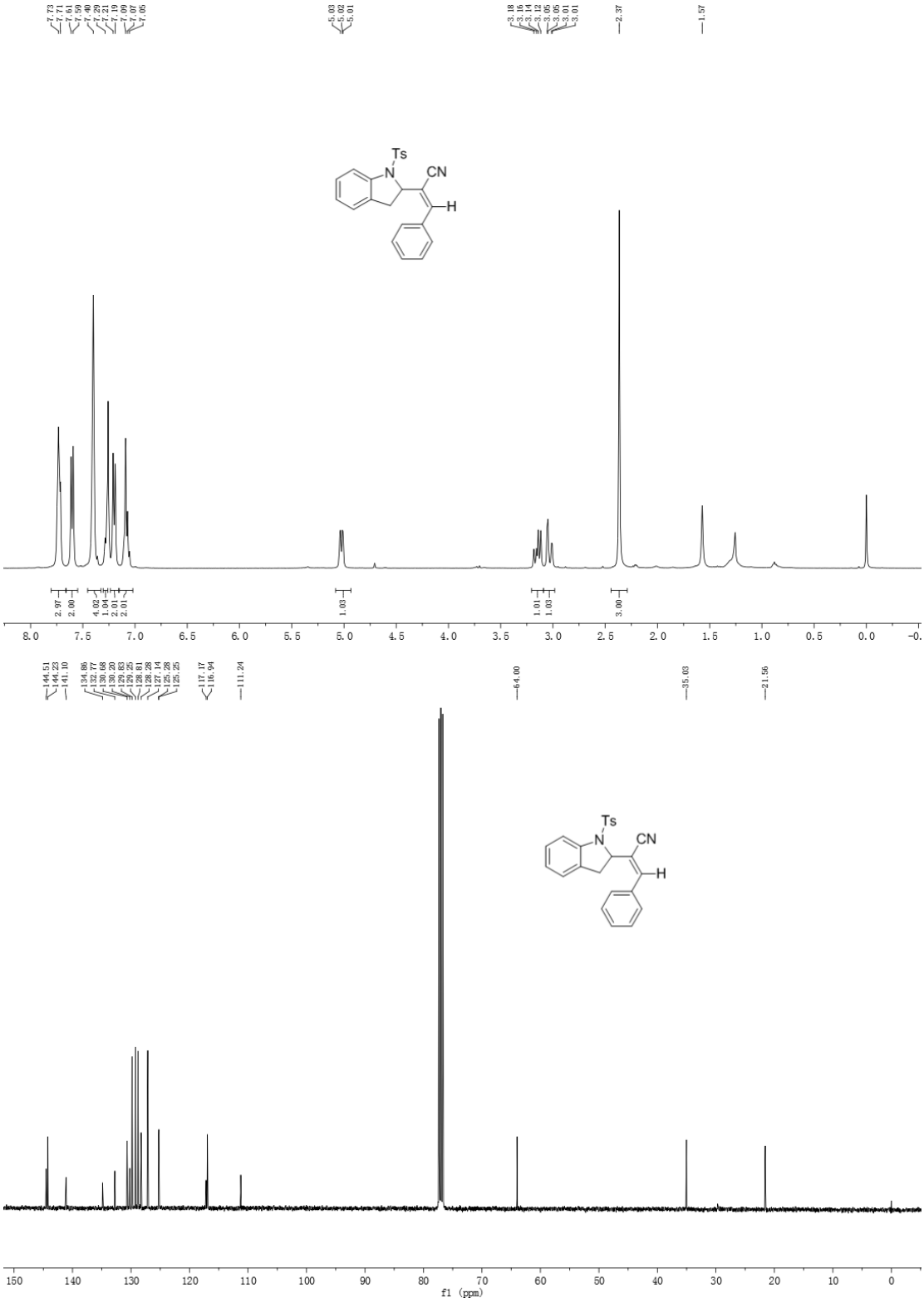


6n HNMR 400 MHz, CNMR 100 MHz





6o HNMR 400 MHz, CNMR 100 MHz



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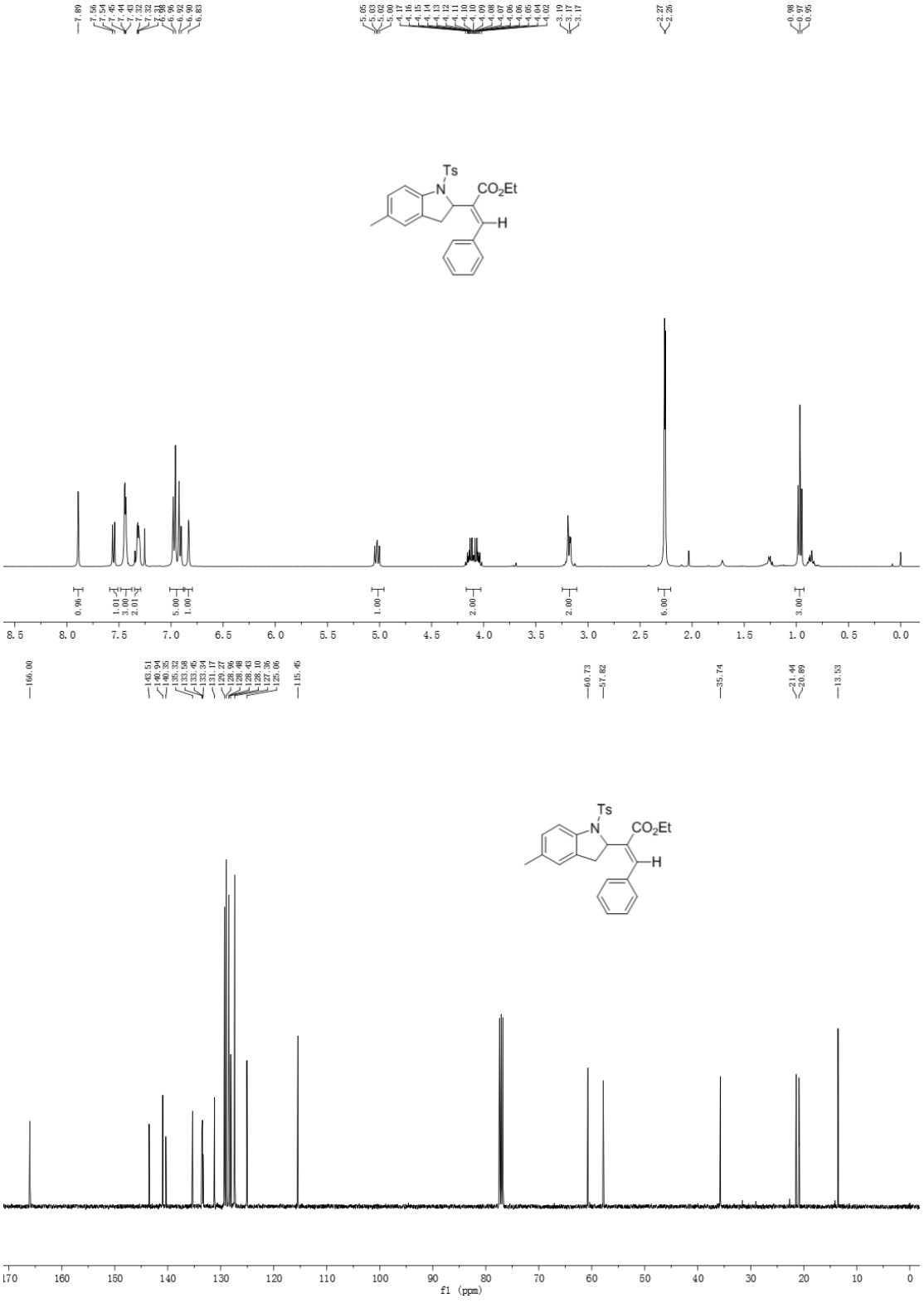
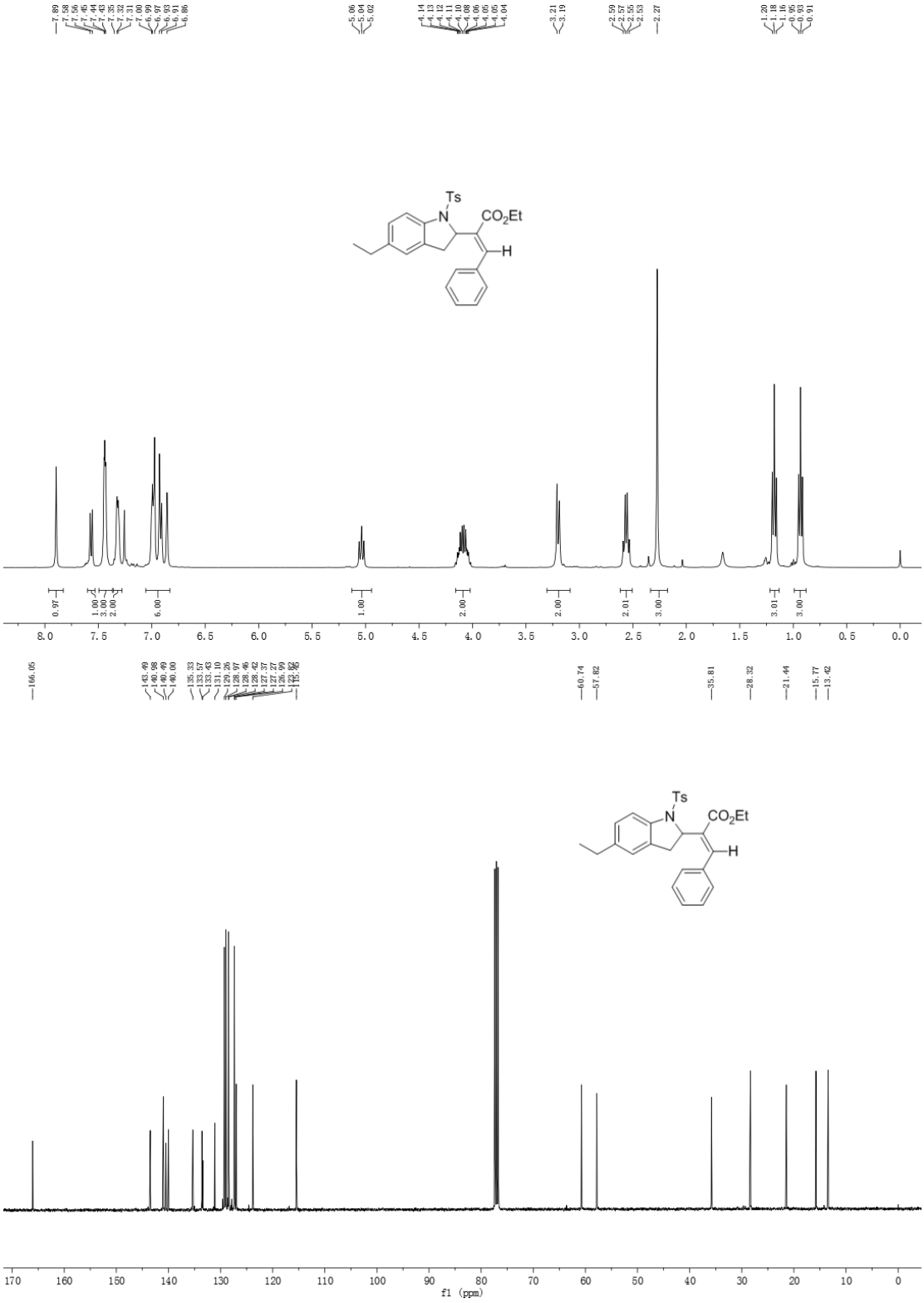
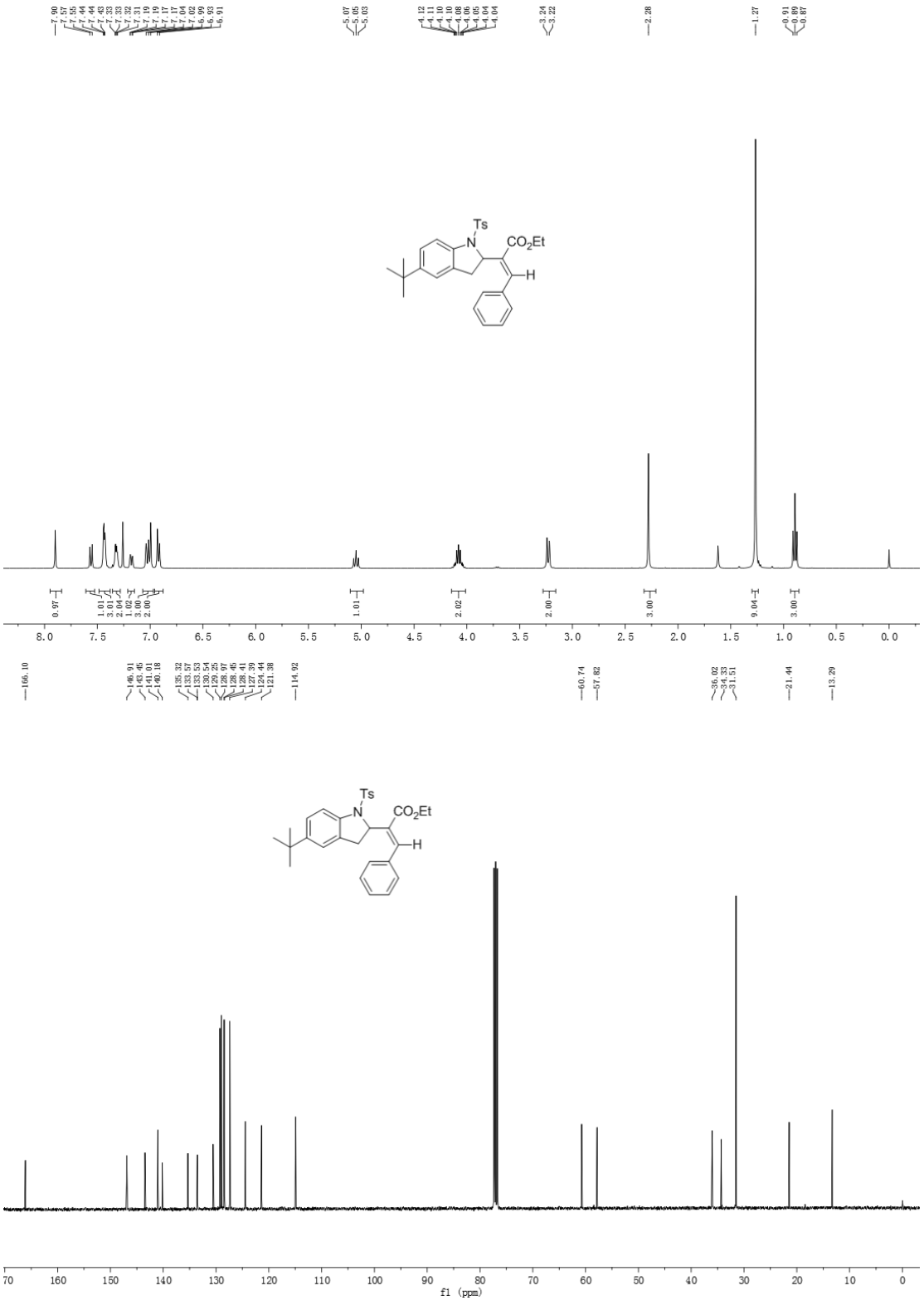


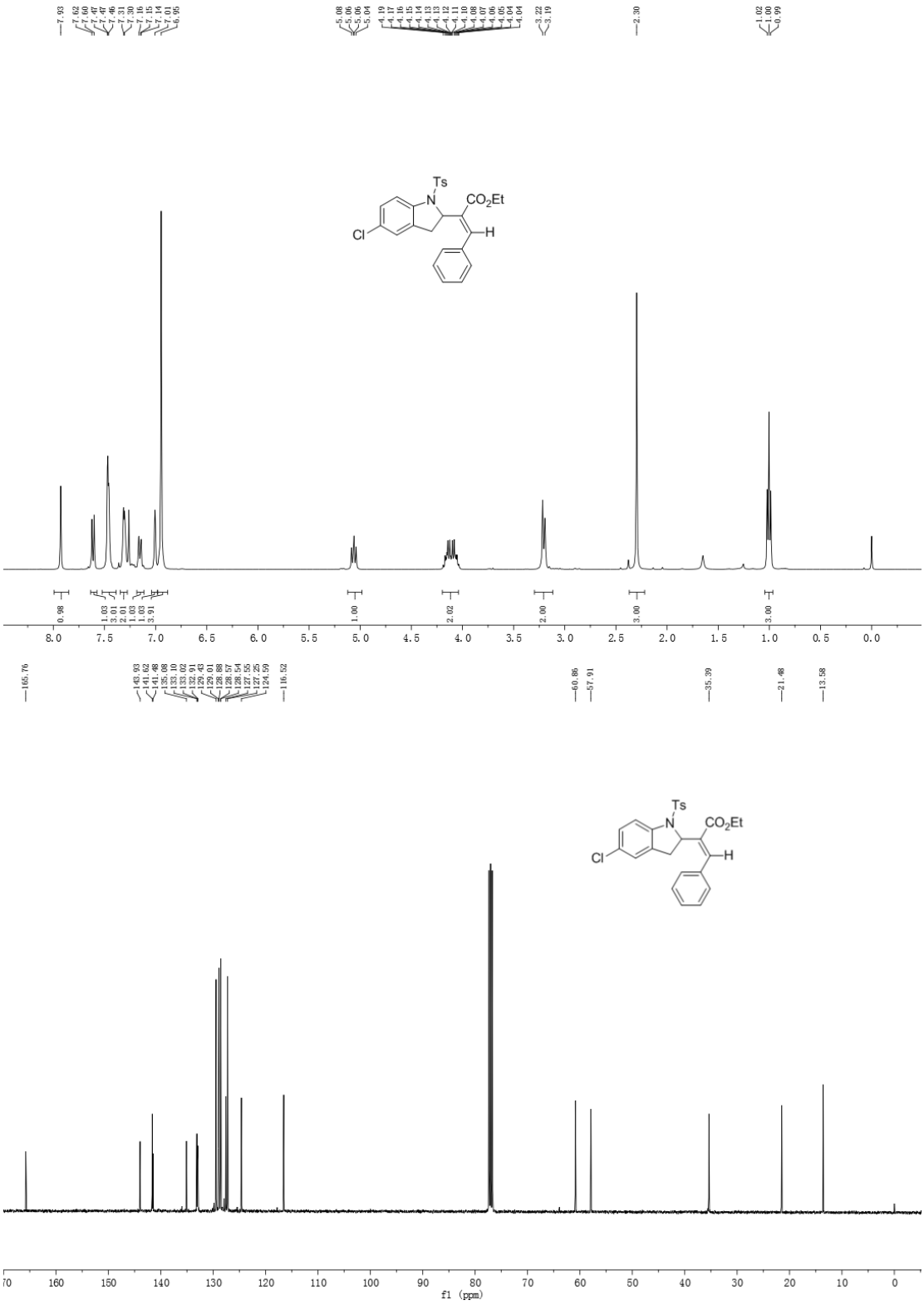
6q HNMR 400 MHz, CNMR 100 MHz



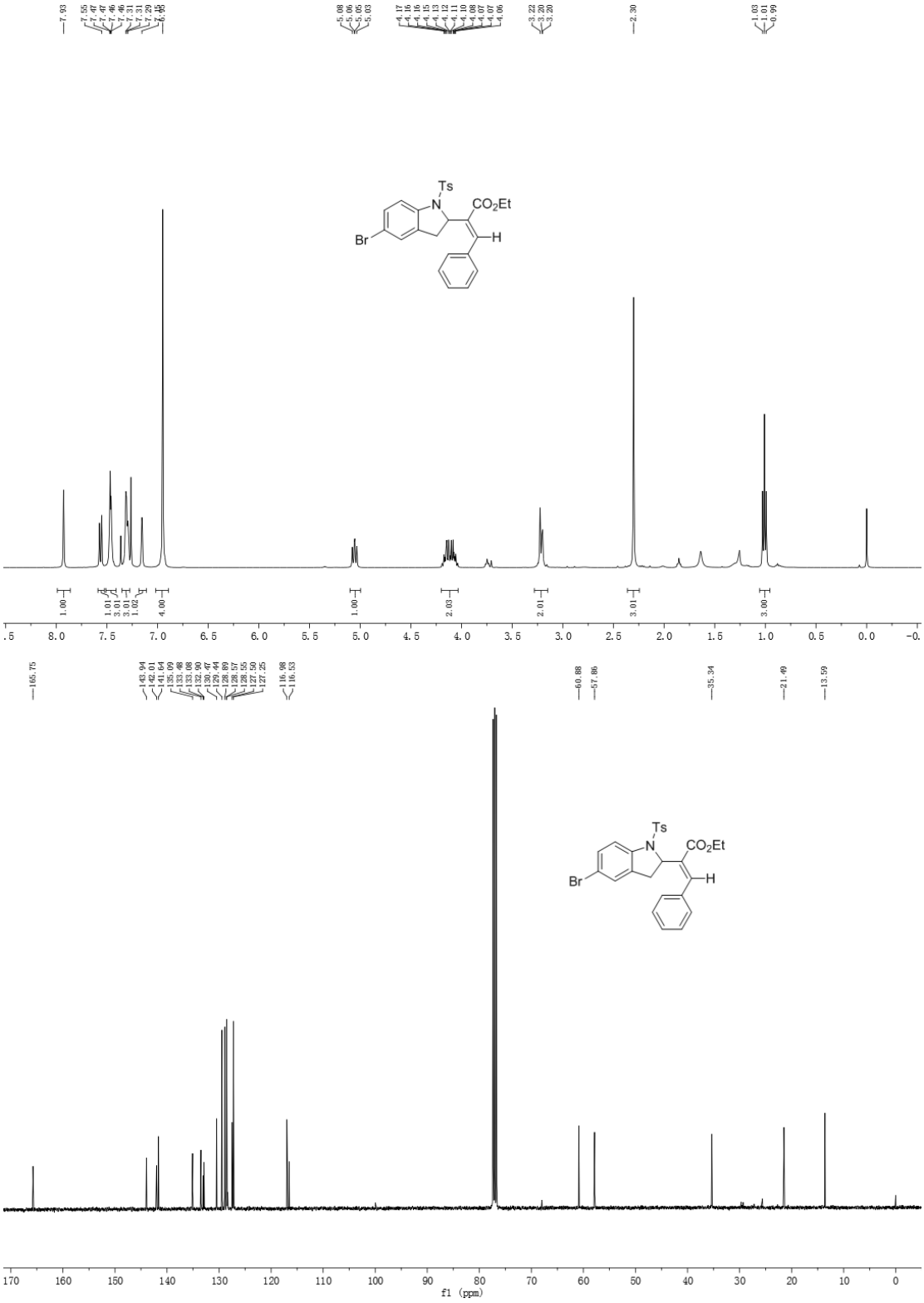
6r HNMR 400 MHz, CNMR 100 MHz



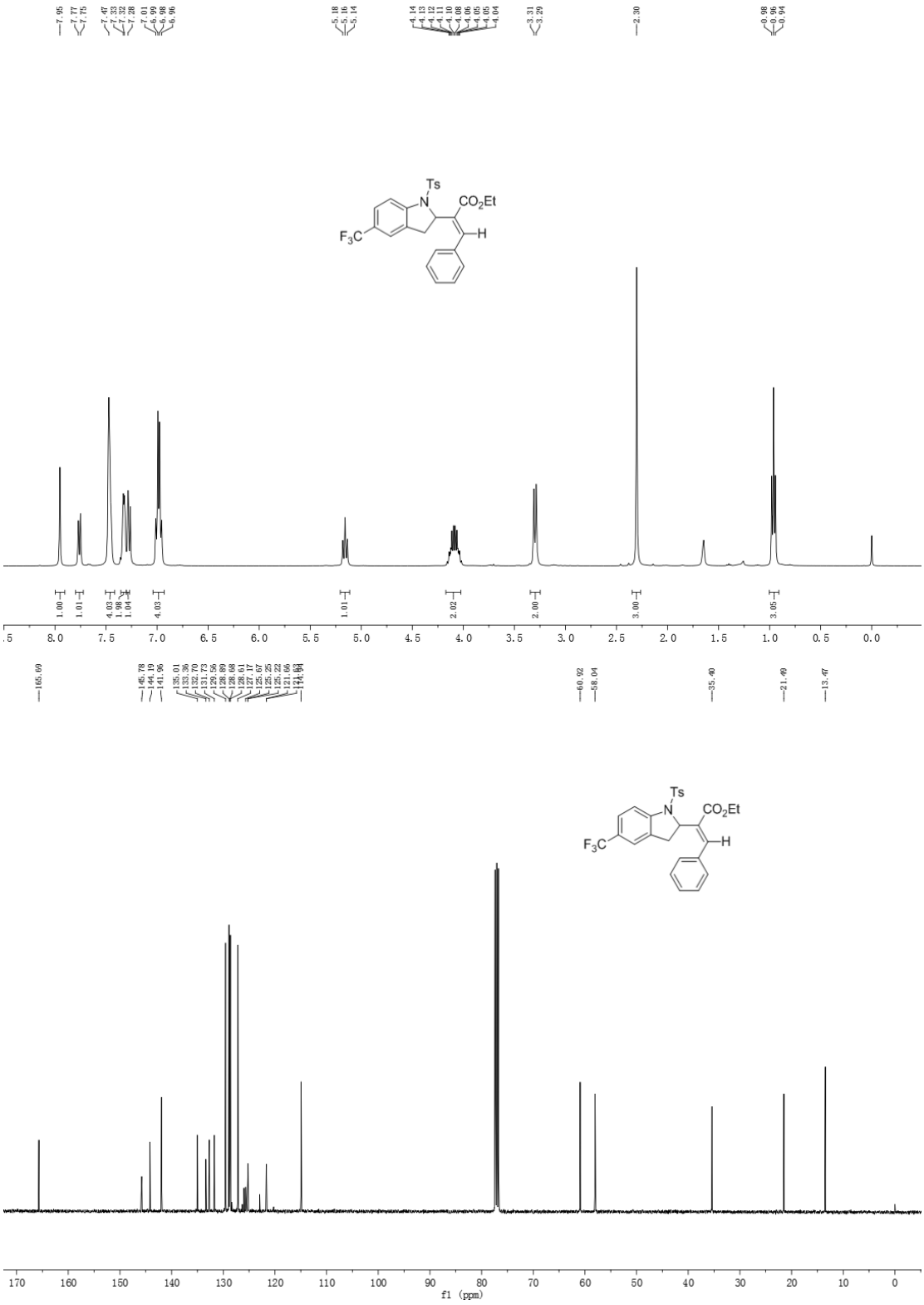
6s HNMR 400 MHz, CNMR 100 MHz



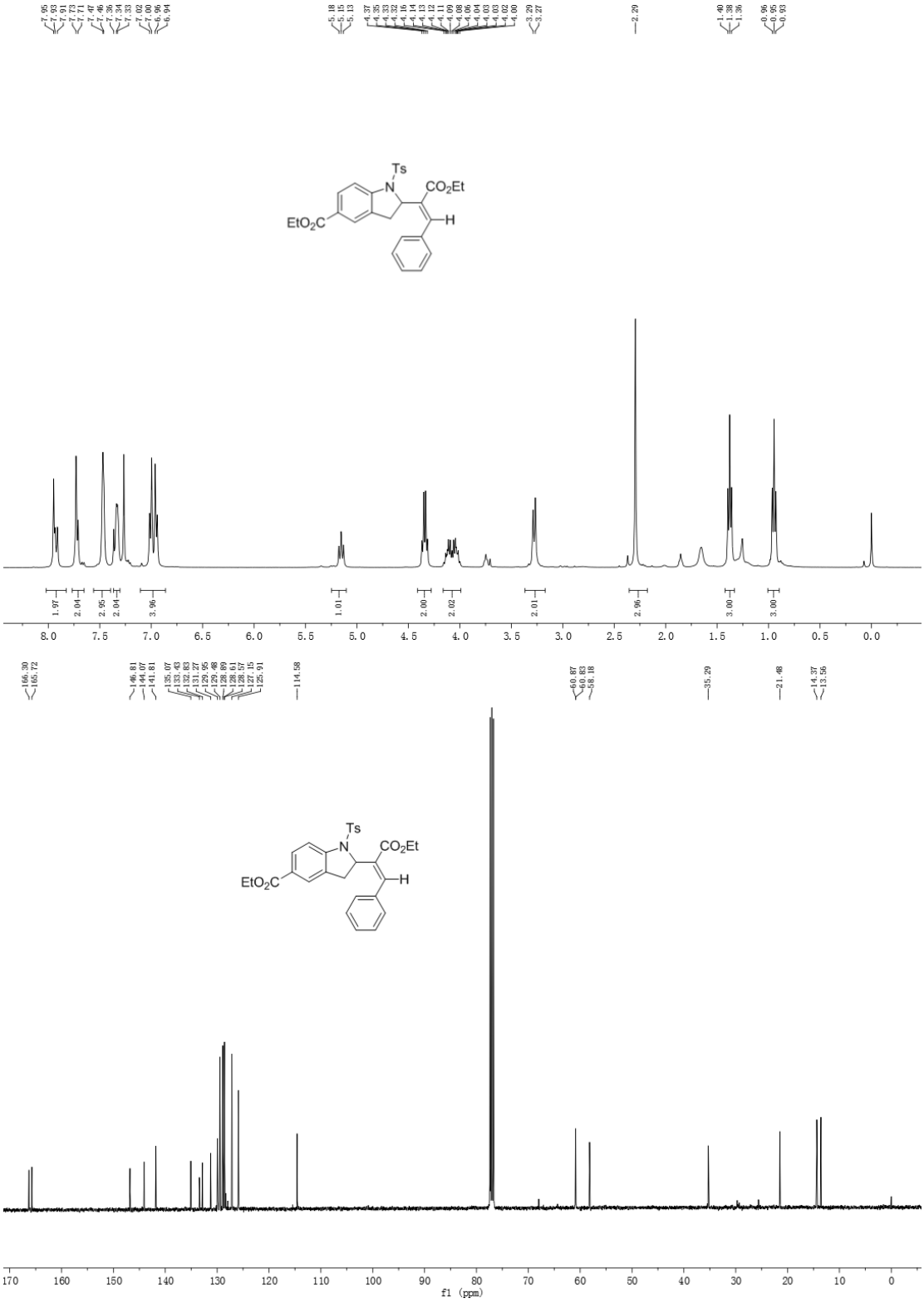
6t HNMR 400 MHz, CNMR 100 MHz



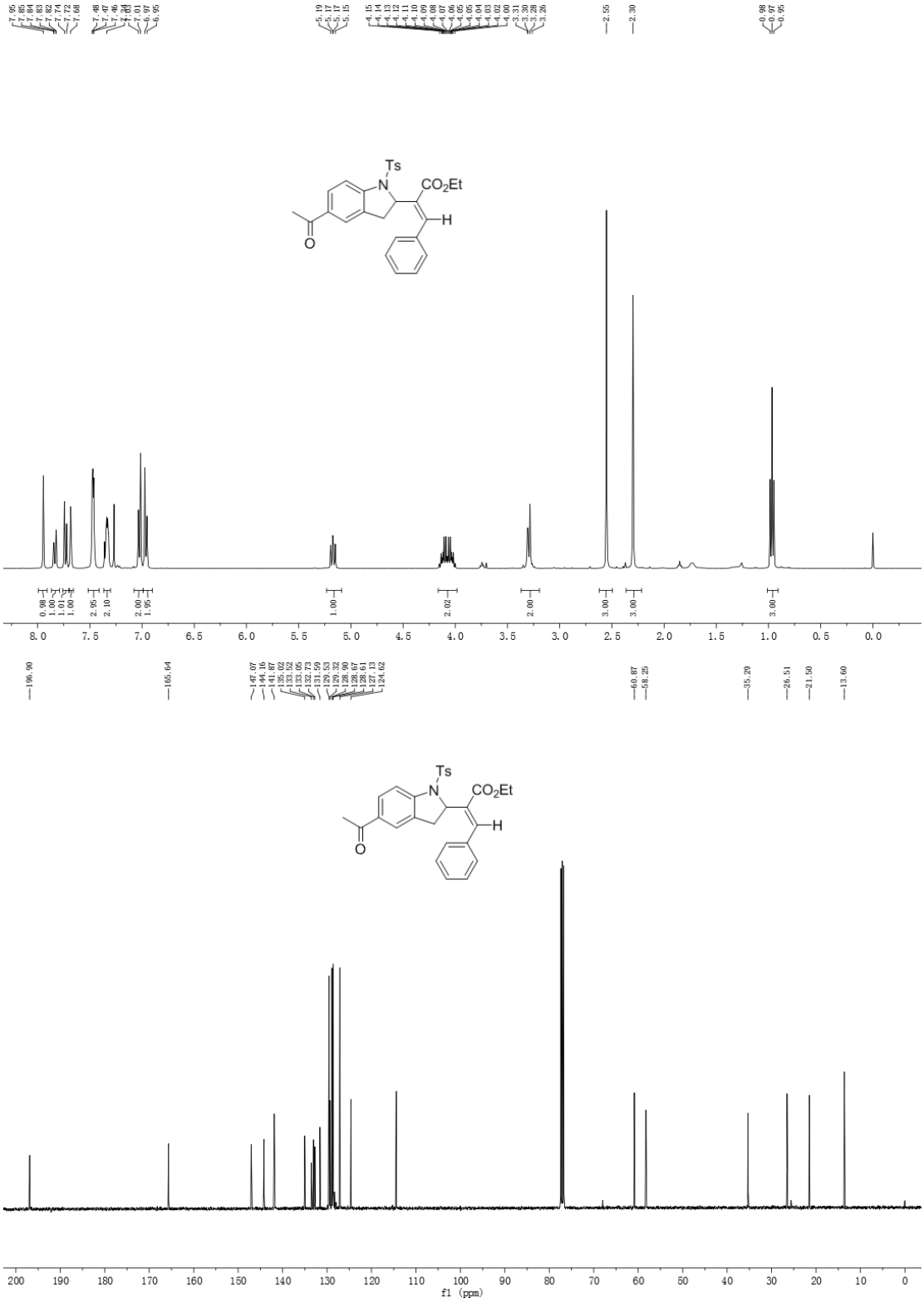
6u HNMR 400 MHz, CNMR 100 MHz



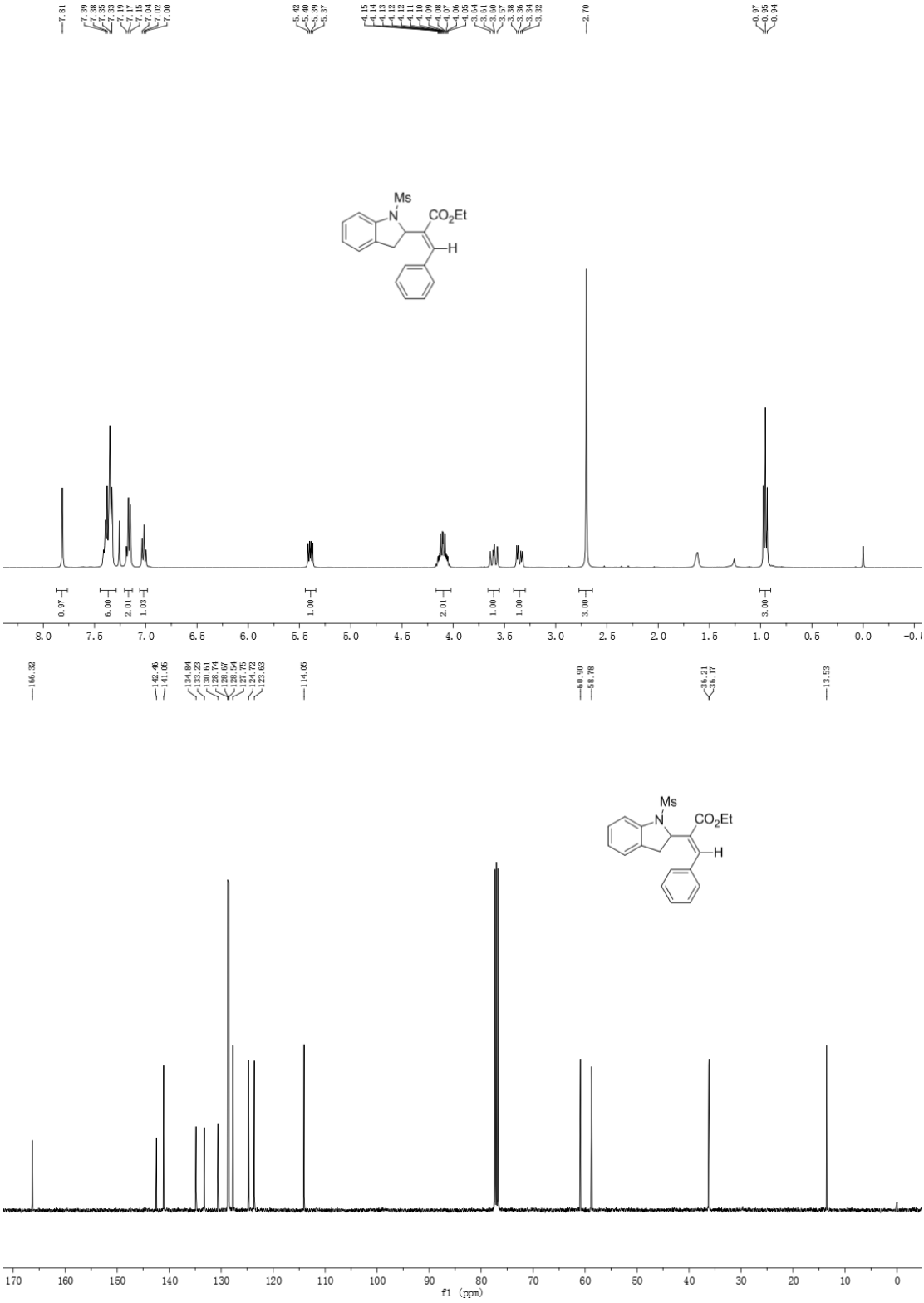
6v HNMR 400 MHz, CNMR 100 MHz



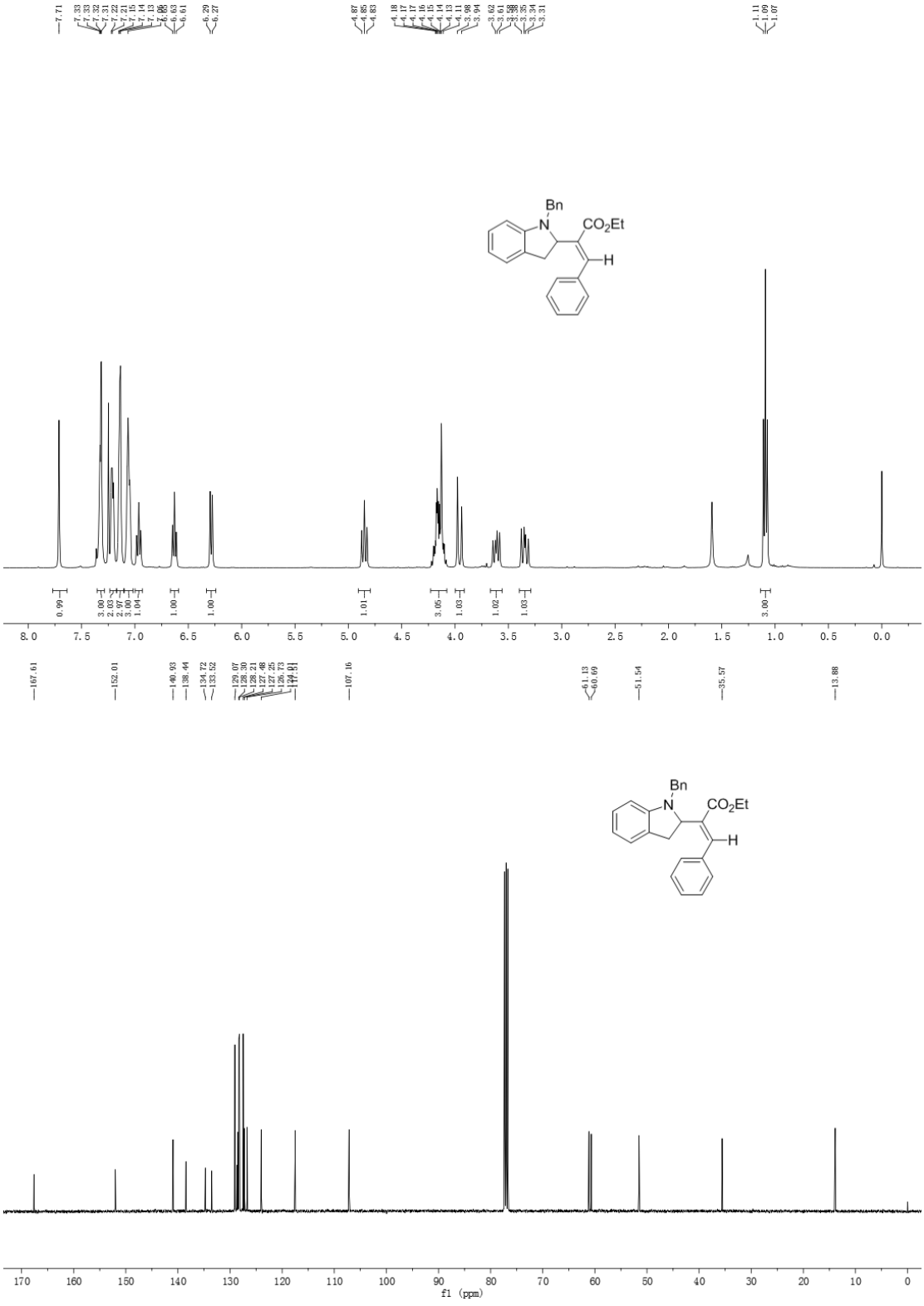
6w HNMR 400 MHz, CNMR 100 MHz



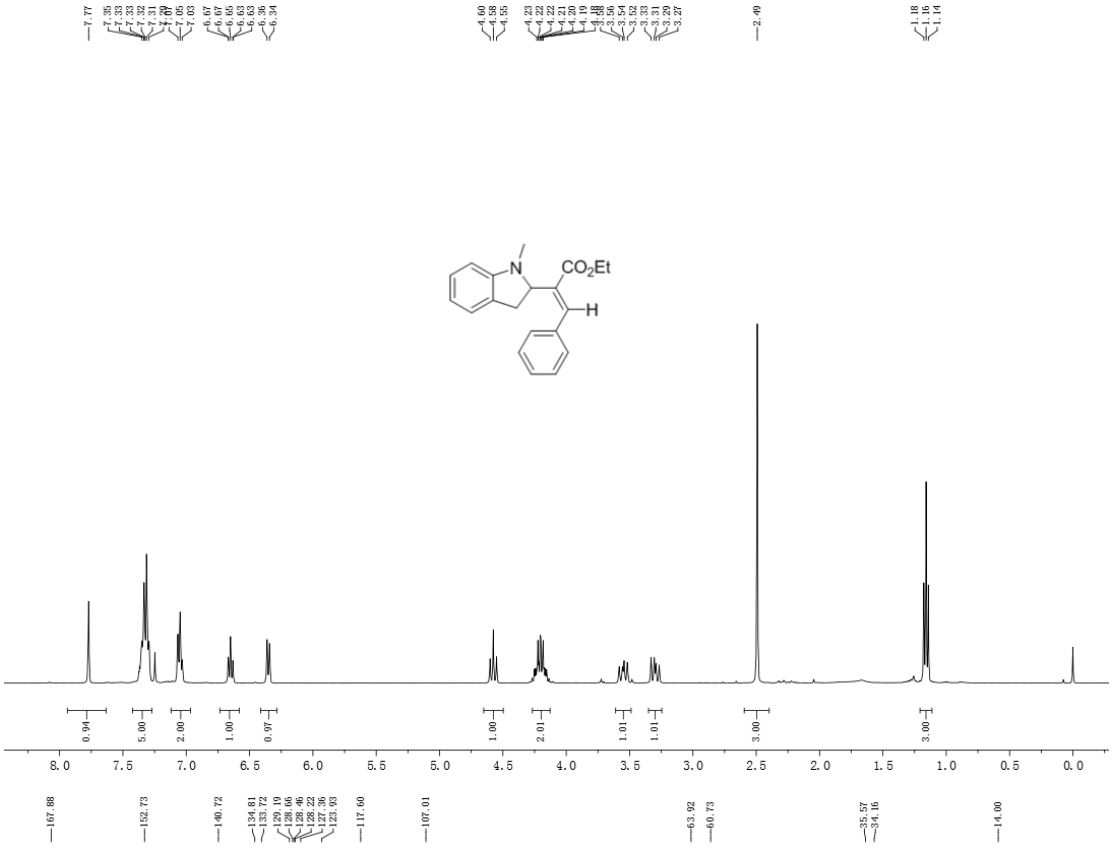
6x HNMR 400 MHz, CNMR 100 MHz

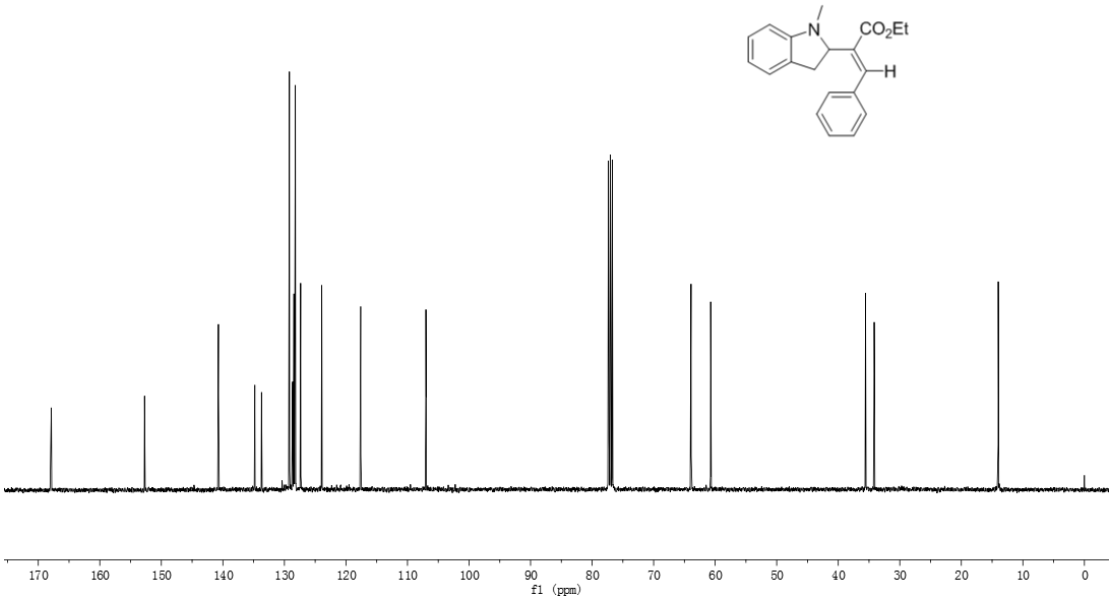


6y HNMR 400 MHz, CNMR 100 MHz



6z HNMR 400 MHz, CNMR 100 MHz





X-Ray Crystallographic Data

Experimental single crystals of **3a**, **6t** and **6w** were recrystallized from mounted in inert oil and transferred to the cold gas stream of the diffractometer. Crystallographic data for **3a**, **6t** and **6w** have been deposited with the Cambridge Crystallographic Data Centre as 15759999, 1576284 and 1576283. These data can be obtained free of charge via www.ccdc.cam. ac.uk/data_request/cif, or by emailing data_request@ccdc.cam.ac.uk, or by contacting The Cambridge Crystallographic Data Centre, 12, Union Road, Cambridge CB2 1EZ, UK; fax: +44 1223 336033.

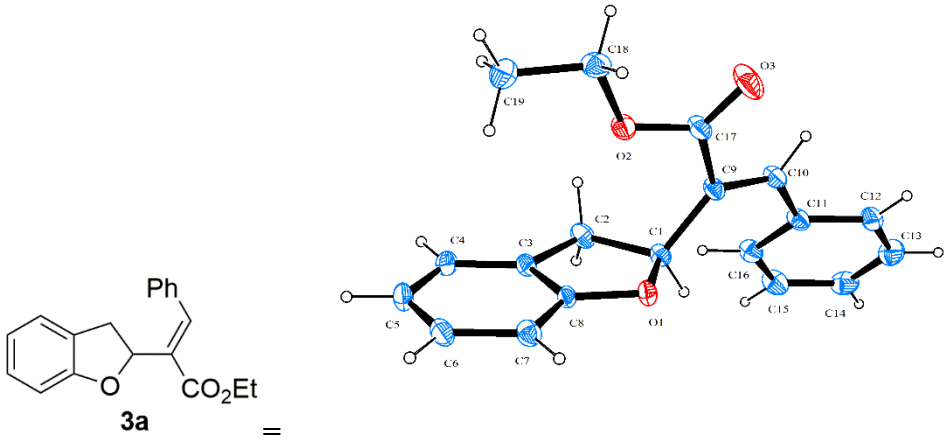


Figure S1. ORTEP representation of 3a draw with 50% probability thermal ellipsoids

Table S1. Crystal data and structure refinement for 3a

Identification code	**3a**	
Empirical formula	$C_{19}H_{18}O_3$	
Formula weight	294.33	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 6.776(2) Å	a= 90.537(11)°.
	b = 10.643(3) Å	b=

106.826(9)°.	
	c = 11.371(4) Å g = 94.317(8)°.
Volume	782.2(5) $Å^3$
Z	2
Density (calculated)	1.250 Mg/m^3
Absorption coefficient	0.084 mm^{-1}
F(000)	312
Crystal size	0.210 x 0.200 x 0.190 mm^3
Theta range for data collection	1.872 to 27.540°.
Index ranges	-8<=h<=7, -11<=k<=13, -9<=l<=14
Reflections collected	5206
Independent reflections	3410 [R(int) = 0.0478]
Completeness to theta = 25.242°	98.9 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3410 / 1 / 200
Goodness-of-fit on F^2	0.875
Final R indices [I>2sigma(I)]	R1 = 0.0586, wR2 = 0.1347
R indices (all data)	R1 = 0.1633, wR2 = 0.2079
Extinction coefficient	n/a
Largest diff. peak and hole	0.227 and -0.218 $e.Å^{-3}$

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 3a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor

	x	y	z	U(eq)

C(1)	897(4)	5207(3)	3126(3)	44(1)
C(2)	3058(5)	5208(3)	2964(3)	56(1)
C(3)	3877(5)	4057(3)	3630(3)	45(1)
C(4)	5706(5)	3526(4)	3796(3)	60(1)
C(5)	6014(6)	2425(4)	4448(4)	68(1)
C(6)	4517(5)	1873(3)	4904(4)	61(1)
C(7)	2640(5)	2391(3)	4724(3)	53(1)
C(8)	2373(4)	3475(3)	4068(3)	39(1)
C(9)	-860(5)	5179(3)	1961(3)	47(1)
C(10)	-2044(5)	6125(3)	1554(3)	53(1)
C(11)	-1829(5)	7432(3)	2065(3)	53(1)
C(12)	-3630(6)	8058(3)	1854(4)	60(1)
C(13)	-3479(7)	9300(4)	2270(4)	78(1)
C(14)	-1636(7)	9917(4)	2868(4)	73(1)
C(15)	163(7)	9316(3)	3050(4)	71(1)
C(16)	61(6)	8076(3)	2646(3)	58(1)
C(17)	-1401(5)	4001(3)	1178(3)	54(1)
C(18)	-99(6)	2139(3)	665(4)	66(1)
C(19)	1937(6)	1576(4)	1015(4)	76(1)
O(1)	605(3)	4083(2)	3817(2)	46(1)
O(2)	183(3)	3302(2)	1379(2)	58(1)
O(3)	-3024(4)	3718(3)	436(3)	100(1)

Table S3. Bond lengths [Å] and angles [°] for 3a

C(1)-O(1)	1.469(4)
C(1)-C(9)	1.502(4)
C(1)-C(2)	1.527(4)
C(1)-H(1)	0.9800
C(2)-C(3)	1.503(4)
C(2)-H(2A)	0.9700
C(2)-H(2B)	0.9700
C(3)-C(4)	1.364(4)
C(3)-C(8)	1.370(4)
C(4)-C(5)	1.389(5)
C(4)-H(4)	0.9300
C(5)-C(6)	1.365(6)
C(5)-H(5)	0.9300
C(6)-C(7)	1.386(5)
C(6)-H(6)	0.9300
C(7)-C(8)	1.373(4)
C(7)-H(7)	0.9300
C(8)-O(1)	1.363(3)
C(9)-C(10)	1.336(4)
C(9)-C(17)	1.490(5)
C(10)-C(11)	1.483(5)
C(10)-H(10)	0.9300
C(11)-C(16)	1.384(5)
C(11)-C(12)	1.395(5)
C(12)-C(13)	1.385(5)
C(12)-H(12)	0.9300
C(13)-C(14)	1.353(6)
C(13)-H(13)	0.9300

C(14)-C(15)	1.383(5)
C(14)-H(14)	0.9300
C(15)-C(16)	1.383(5)
C(15)-H(15)	0.9300
C(16)-H(16)	0.9300
C(17)-O(3)	1.192(4)
C(17)-O(2)	1.319(4)
C(18)-O(2)	1.443(4)
C(18)-C(19)	1.494(5)
C(18)-H(18A)	0.9700
C(18)-H(18B)	0.9700
C(19)-H(19A)	0.9600
C(19)-H(19B)	0.9600
C(19)-H(19C)	0.9600

O(1)-C(1)-C(9)	108.4(2)
O(1)-C(1)-C(2)	106.8(2)
C(9)-C(1)-C(2)	115.8(3)
O(1)-C(1)-H(1)	108.5
C(9)-C(1)-H(1)	108.5
C(2)-C(1)-H(1)	108.5
C(3)-C(2)-C(1)	102.9(3)
C(3)-C(2)-H(2A)	111.2
C(1)-C(2)-H(2A)	111.2
C(3)-C(2)-H(2B)	111.2
C(1)-C(2)-H(2B)	111.2
H(2A)-C(2)-H(2B)	109.1
C(4)-C(3)-C(8)	119.6(3)
C(4)-C(3)-C(2)	131.7(3)
C(8)-C(3)-C(2)	108.6(3)

C(3)-C(4)-C(5)	118.6(4)
C(3)-C(4)-H(4)	120.7
C(5)-C(4)-H(4)	120.7
C(6)-C(5)-C(4)	121.0(3)
C(6)-C(5)-H(5)	119.5
C(4)-C(5)-H(5)	119.5
C(5)-C(6)-C(7)	120.9(3)
C(5)-C(6)-H(6)	119.6
C(7)-C(6)-H(6)	119.6
C(8)-C(7)-C(6)	116.8(3)
C(8)-C(7)-H(7)	121.6
C(6)-C(7)-H(7)	121.6
O(1)-C(8)-C(3)	113.8(3)
O(1)-C(8)-C(7)	123.2(3)
C(3)-C(8)-C(7)	123.0(3)
C(10)-C(9)-C(17)	115.5(3)
C(10)-C(9)-C(1)	125.7(3)
C(17)-C(9)-C(1)	118.8(3)
C(9)-C(10)-C(11)	128.8(3)
C(9)-C(10)-H(10)	115.6
C(11)-C(10)-H(10)	115.6
C(16)-C(11)-C(12)	119.3(3)
C(16)-C(11)-C(10)	123.3(3)
C(12)-C(11)-C(10)	117.2(3)
C(13)-C(12)-C(11)	118.9(4)
C(13)-C(12)-H(12)	120.6
C(11)-C(12)-H(12)	120.6
C(14)-C(13)-C(12)	121.7(4)
C(14)-C(13)-H(13)	119.1
C(12)-C(13)-H(13)	119.1

C(13)-C(14)-C(15)	119.8(4)
C(13)-C(14)-H(14)	120.1
C(15)-C(14)-H(14)	120.1
C(14)-C(15)-C(16)	119.7(4)
C(14)-C(15)-H(15)	120.1
C(16)-C(15)-H(15)	120.1
C(15)-C(16)-C(11)	120.5(4)
C(15)-C(16)-H(16)	119.8
C(11)-C(16)-H(16)	119.8
O(3)-C(17)-O(2)	123.0(3)
O(3)-C(17)-C(9)	125.6(3)
O(2)-C(17)-C(9)	111.3(3)
O(2)-C(18)-C(19)	106.7(3)
O(2)-C(18)-H(18A)	110.4
C(19)-C(18)-H(18A)	110.4
O(2)-C(18)-H(18B)	110.4
C(19)-C(18)-H(18B)	110.4
H(18A)-C(18)-H(18B)	108.6
C(18)-C(19)-H(19A)	109.5
C(18)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(18)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(8)-O(1)-C(1)	107.8(2)
C(17)-O(2)-C(18)	117.6(3)

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 3a. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	42(2)	41(2)	45(2)	-1(2)	4(2)	4(1)
C(2)	45(2)	56(2)	58(2)	1(2)	1(2)	-6(2)
C(3)	33(2)	52(2)	44(2)	-4(2)	5(2)	3(1)
C(4)	31(2)	94(3)	55(2)	-8(2)	11(2)	6(2)
C(5)	49(2)	85(3)	66(3)	-9(2)	4(2)	31(2)
C(6)	57(2)	57(2)	56(2)	-8(2)	-6(2)	18(2)
C(7)	51(2)	48(2)	55(2)	-1(2)	8(2)	5(2)
C(8)	29(2)	44(2)	42(2)	-7(2)	4(1)	6(1)
C(9)	38(2)	47(2)	48(2)	-5(2)	1(2)	2(1)
C(10)	53(2)	50(2)	47(2)	0(2)	-2(2)	10(2)
C(11)	57(2)	48(2)	47(2)	3(2)	1(2)	11(2)
C(12)	58(2)	64(2)	56(2)	7(2)	9(2)	18(2)
C(13)	97(3)	65(3)	78(3)	5(2)	27(3)	39(2)
C(14)	103(4)	51(2)	65(3)	-3(2)	23(3)	13(2)
C(15)	77(3)	52(2)	70(3)	-3(2)	2(2)	2(2)
C(16)	64(2)	46(2)	57(2)	2(2)	7(2)	8(2)
C(17)	47(2)	53(2)	51(2)	-3(2)	-4(2)	5(2)
C(18)	82(3)	52(2)	55(3)	-12(2)	5(2)	9(2)
C(19)	85(3)	69(3)	75(3)	-5(2)	22(2)	26(2)
O(1)	32(1)	52(1)	54(2)	6(1)	9(1)	8(1)

O(2)	55(1)	51(1)	59(2)	-15(1)	1(1)	11(1)
O(3)	72(2)	77(2)	111(3)	-36(2)	-35(2)	18(1)

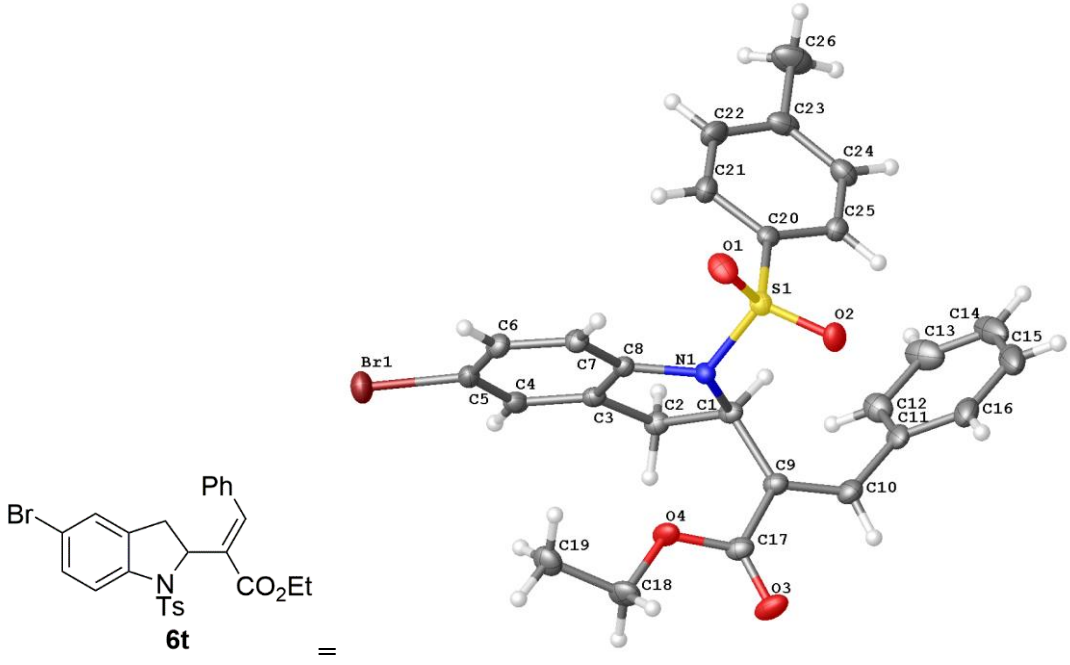


Figure S2. ORTEP representation of 6t draw with 50% probability thermal ellipsoids

Table S5. Crystal data and structure refinement for 6t

Identification code	**6t**	
Empirical formula	C_{26} H_{24} Br N O_4 S	
Formula weight	526.43	
Temperature	130 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 1 21/c 1	
Unit cell dimensions	a = 14.0516(10) Å	a= 90°.
	b = 12.5217(9) Å	b= 117.4870(10)°.
	c = 15.0866(11) Å	g = 90°.
Volume	2354.8(3) $Å^3$	

Z	4
Density (calculated)	1.485 Mg/m^3
Absorption coefficient	1.868 mm^{-1}
F(000)	1080
Crystal size	0.33 x 0.3 x 0.25 mm^3
Theta range for data collection	2.227 to 30.789°.
Index ranges	-20<=h<=15, -17<=k<=18, -21<=l<=21
Reflections collected	23536
Independent reflections	7290 [R(int) = 0.0363]
Completeness to theta = 25.242°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7461 and 0.4664
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7290 / 0 / 300
Goodness-of-fit on F^2	1.005
Final R indices [I>2sigma(I)]	R1 = 0.0330, wR2 = 0.0748
R indices (all data)	R1 = 0.0520, wR2 = 0.0815
Extinction coefficient	n/a
Largest diff. peak and hole	0.569 and -0.475 $e.Å^{-3}$

Table S6. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 6t. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor

	x	y	z	U(eq)

Br(1)	1064(1)	3104(1)	5158(1)	31(1)
S(1)	4102(1)	7422(1)	4498(1)	18(1)
O(1)	4886(1)	6618(1)	5026(1)	28(1)
O(2)	4212(1)	8071(1)	3769(1)	25(1)
O(3)	1173(1)	6762(1)	709(1)	31(1)
O(4)	1360(1)	5822(1)	2048(1)	25(1)
N(1)	2938(1)	6800(1)	3892(1)	16(1)
C(1)	1974(1)	7520(1)	3369(1)	17(1)
C(2)	1094(1)	7015(1)	3589(1)	19(1)
C(3)	1582(1)	5988(1)	4121(1)	17(1)
C(4)	1105(1)	5162(1)	4384(1)	20(1)
C(5)	1722(1)	4266(1)	4839(1)	21(1)
C(6)	2785(1)	4183(1)	5036(1)	22(1)
C(7)	3262(1)	5010(1)	4761(1)	19(1)
C(8)	2649(1)	5908(1)	4311(1)	16(1)
C(9)	1704(1)	7663(1)	2279(1)	19(1)
C(10)	1771(1)	8611(1)	1896(1)	23(1)
C(11)	2061(1)	9645(1)	2422(1)	23(1)
C(12)	1528(1)	10059(1)	2933(1)	29(1)
C(13)	1837(2)	11034(2)	3431(2)	40(1)
C(14)	2684(2)	11597(2)	3427(2)	45(1)
C(15)	3205(2)	11202(2)	2912(2)	42(1)
C(16)	2896(2)	10243(2)	2410(1)	32(1)
C(17)	1389(1)	6726(1)	1585(1)	22(1)
C(18)	1057(2)	4853(1)	1445(1)	29(1)
C(19)	1229(2)	3935(1)	2146(1)	29(1)
C(20)	4000(1)	8286(1)	5372(1)	18(1)
C(21)	3993(1)	7860(2)	6226(1)	26(1)
C(22)	3984(2)	8550(2)	6938(1)	31(1)
C(23)	3983(1)	9653(2)	6818(1)	28(1)

C(24)	3959(1)	10058(1)	5946(1)	26(1)
C(25)	3965(1)	9381(1)	5218(1)	21(1)
C(26)	4038(2)	10387(2)	7635(2)	44(1)

Table S7. Bond lengths [Å] and angles [°] for 6t

Br(1)-C(5)	1.9005(16)
S(1)-O(1)	1.4330(12)
S(1)-O(2)	1.4327(12)
S(1)-N(1)	1.6549(13)
S(1)-C(20)	1.7617(16)
O(3)-C(17)	1.213(2)
O(4)-C(17)	1.342(2)
O(4)-C(18)	1.4576(19)
N(1)-C(1)	1.5102(18)
N(1)-C(8)	1.4307(19)
C(1)-H(1)	1.0000
C(1)-C(2)	1.555(2)
C(1)-C(9)	1.517(2)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(2)-C(3)	1.503(2)
C(3)-C(4)	1.387(2)
C(3)-C(8)	1.393(2)
C(4)-H(4)	0.9500
C(4)-C(5)	1.390(2)
C(5)-C(6)	1.385(2)
C(6)-H(6)	0.9500
C(6)-C(7)	1.397(2)
C(7)-H(7)	0.9500

C(7)-C(8)	1.388(2)
C(9)-C(10)	1.343(2)
C(9)-C(17)	1.497(2)
C(10)-H(10)	0.9500
C(10)-C(11)	1.474(2)
C(11)-C(12)	1.398(3)
C(11)-C(16)	1.399(2)
C(12)-H(12)	0.9500
C(12)-C(13)	1.394(3)
C(13)-H(13)	0.9500
C(13)-C(14)	1.387(3)
C(14)-H(14)	0.9500
C(14)-C(15)	1.381(3)
C(15)-H(15)	0.9500
C(15)-C(16)	1.378(3)
C(16)-H(16)	0.9500
C(18)-H(18A)	0.9900
C(18)-H(18B)	0.9900
C(18)-C(19)	1.504(3)
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-C(21)	1.398(2)
C(20)-C(25)	1.388(2)
C(21)-H(21)	0.9500
C(21)-C(22)	1.383(3)
C(22)-H(22)	0.9500
C(22)-C(23)	1.393(3)
C(23)-C(24)	1.395(2)
C(23)-C(26)	1.511(3)

C(24)-H(24)	0.9500
C(24)-C(25)	1.391(2)
C(25)-H(25)	0.9500
C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800
C(26)-H(26C)	0.9800
O(1)-S(1)-N(1)	106.69(7)
O(1)-S(1)-C(20)	108.84(8)
O(2)-S(1)-O(1)	119.83(7)
O(2)-S(1)-N(1)	105.82(7)
O(2)-S(1)-C(20)	107.55(7)
N(1)-S(1)-C(20)	107.52(7)
C(17)-O(4)-C(18)	116.58(12)
C(1)-N(1)-S(1)	115.30(10)
C(8)-N(1)-S(1)	122.23(10)
C(8)-N(1)-C(1)	109.17(11)
N(1)-C(1)-H(1)	108.0
N(1)-C(1)-C(2)	104.78(12)
N(1)-C(1)-C(9)	110.67(12)
C(2)-C(1)-H(1)	108.0
C(9)-C(1)-H(1)	108.0
C(9)-C(1)-C(2)	116.92(12)
C(1)-C(2)-H(2A)	110.9
C(1)-C(2)-H(2B)	110.9
H(2A)-C(2)-H(2B)	108.9
C(3)-C(2)-C(1)	104.44(12)
C(3)-C(2)-H(2A)	110.9
C(3)-C(2)-H(2B)	110.9
C(4)-C(3)-C(2)	128.96(14)
C(4)-C(3)-C(8)	120.25(14)

C(8)-C(3)-C(2)	110.74(13)
C(3)-C(4)-H(4)	121.0
C(3)-C(4)-C(5)	118.00(14)
C(5)-C(4)-H(4)	121.0
C(4)-C(5)-Br(1)	118.49(12)
C(6)-C(5)-Br(1)	119.37(12)
C(6)-C(5)-C(4)	122.11(15)
C(5)-C(6)-H(6)	120.1
C(5)-C(6)-C(7)	119.87(15)
C(7)-C(6)-H(6)	120.1
C(6)-C(7)-H(7)	120.9
C(8)-C(7)-C(6)	118.15(14)
C(8)-C(7)-H(7)	120.9
C(3)-C(8)-N(1)	110.48(13)
C(7)-C(8)-N(1)	127.62(13)
C(7)-C(8)-C(3)	121.62(14)
C(10)-C(9)-C(1)	122.58(14)
C(10)-C(9)-C(17)	116.62(14)
C(17)-C(9)-C(1)	120.75(13)
C(9)-C(10)-H(10)	116.5
C(9)-C(10)-C(11)	126.97(15)
C(11)-C(10)-H(10)	116.5
C(12)-C(11)-C(10)	122.51(16)
C(12)-C(11)-C(16)	118.30(17)
C(16)-C(11)-C(10)	119.19(16)
C(11)-C(12)-H(12)	119.7
C(13)-C(12)-C(11)	120.64(18)
C(13)-C(12)-H(12)	119.7
C(12)-C(13)-H(13)	120.1
C(14)-C(13)-C(12)	119.8(2)

C(14)-C(13)-H(13)	120.1
C(13)-C(14)-H(14)	120.0
C(15)-C(14)-C(13)	119.97(19)
C(15)-C(14)-H(14)	120.0
C(14)-C(15)-H(15)	119.8
C(16)-C(15)-C(14)	120.4(2)
C(16)-C(15)-H(15)	119.8
C(11)-C(16)-H(16)	119.6
C(15)-C(16)-C(11)	120.8(2)
C(15)-C(16)-H(16)	119.6
O(3)-C(17)-O(4)	123.12(15)
O(3)-C(17)-C(9)	125.39(15)
O(4)-C(17)-C(9)	111.49(13)
O(4)-C(18)-H(18A)	110.3
O(4)-C(18)-H(18B)	110.3
O(4)-C(18)-C(19)	106.98(13)
H(18A)-C(18)-H(18B)	108.6
C(19)-C(18)-H(18A)	110.3
C(19)-C(18)-H(18B)	110.3
C(18)-C(19)-H(19A)	109.5
C(18)-C(19)-H(19B)	109.5
C(18)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(21)-C(20)-S(1)	119.55(13)
C(25)-C(20)-S(1)	119.34(12)
C(25)-C(20)-C(21)	121.08(15)
C(20)-C(21)-H(21)	120.5
C(22)-C(21)-C(20)	118.95(16)

C(22)-C(21)-H(21)	120.5
C(21)-C(22)-H(22)	119.4
C(21)-C(22)-C(23)	121.22(16)
C(23)-C(22)-H(22)	119.4
C(22)-C(23)-C(24)	118.75(16)
C(22)-C(23)-C(26)	120.04(18)
C(24)-C(23)-C(26)	121.18(18)
C(23)-C(24)-H(24)	119.5
C(25)-C(24)-C(23)	121.09(16)
C(25)-C(24)-H(24)	119.5
C(20)-C(25)-C(24)	118.85(15)
C(20)-C(25)-H(25)	120.6
C(24)-C(25)-H(25)	120.6
C(23)-C(26)-H(26A)	109.5
C(23)-C(26)-H(26B)	109.5
C(23)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S8. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 6t. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}

Br(1)	37(1)	25(1)	34(1)	2(1)	18(1)	-9(1)
S(1)	16(1)	17(1)	21(1)	0(1)	8(1)	0(1)
O(1)	17(1)	23(1)	37(1)	2(1)	8(1)	4(1)
O(2)	30(1)	24(1)	27(1)	-1(1)	19(1)	-5(1)
O(3)	45(1)	28(1)	16(1)	1(1)	12(1)	9(1)
O(4)	38(1)	16(1)	17(1)	-3(1)	10(1)	0(1)
N(1)	16(1)	14(1)	16(1)	2(1)	5(1)	1(1)
C(1)	18(1)	14(1)	16(1)	1(1)	5(1)	4(1)
C(2)	19(1)	18(1)	19(1)	1(1)	8(1)	4(1)
C(3)	18(1)	17(1)	14(1)	-2(1)	6(1)	1(1)
C(4)	20(1)	24(1)	16(1)	-4(1)	8(1)	-3(1)
C(5)	27(1)	19(1)	17(1)	-1(1)	10(1)	-6(1)
C(6)	25(1)	17(1)	19(1)	3(1)	8(1)	2(1)
C(7)	18(1)	18(1)	19(1)	1(1)	7(1)	2(1)
C(8)	19(1)	14(1)	14(1)	0(1)	7(1)	0(1)
C(9)	20(1)	18(1)	17(1)	0(1)	6(1)	3(1)
C(10)	24(1)	23(1)	19(1)	4(1)	7(1)	3(1)
C(11)	24(1)	18(1)	20(1)	7(1)	4(1)	2(1)
C(12)	27(1)	21(1)	32(1)	2(1)	8(1)	4(1)
C(13)	41(1)	24(1)	37(1)	-4(1)	5(1)	11(1)
C(14)	48(1)	17(1)	38(1)	3(1)	-8(1)	0(1)
C(15)	37(1)	30(1)	37(1)	14(1)	-1(1)	-8(1)
C(16)	29(1)	31(1)	28(1)	12(1)	7(1)	-2(1)
C(17)	22(1)	21(1)	18(1)	1(1)	6(1)	6(1)
C(18)	38(1)	21(1)	24(1)	-9(1)	11(1)	0(1)
C(19)	35(1)	19(1)	33(1)	-7(1)	15(1)	-3(1)
C(20)	15(1)	20(1)	16(1)	0(1)	6(1)	-2(1)
C(21)	28(1)	26(1)	22(1)	4(1)	10(1)	-5(1)
C(22)	34(1)	41(1)	19(1)	0(1)	15(1)	-8(1)

C(23)	22(1)	39(1)	23(1)	-11(1)	11(1)	-8(1)
C(24)	26(1)	22(1)	29(1)	-6(1)	12(1)	-5(1)
C(25)	21(1)	22(1)	19(1)	1(1)	9(1)	-2(1)
C(26)	44(1)	56(1)	35(1)	-22(1)	23(1)	-12(1)

Table S9. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 6t

	x	y	z	U(eq)
H(1)	2160	8236	3698	21
H(2A)	919	7491	4017	23
H(2B)	432	6875	2960	23
H(4)	378	5208	4258	24
H(6)	3188	3564	5357	26
H(7)	3985	4960	4880	23
H(10)	1616	8616	1213	28
H(12)	950	9671	2940	35
H(13)	1467	11312	3773	47
H(14)	2906	12255	3777	54
H(15)	3781	11593	2905	50
H(16)	3254	9986	2051	38
H(18A)	1506	4764	1102	35
H(18B)	296	4889	934	35
H(19A)	1047	3264	1769	44
H(19B)	769	4025	2470	44

H(19C)	1982	3917	2655	44
H(21)	3994	7109	6315	31
H(22)	3978	8266	7519	37
H(24)	3939	10809	5849	31
H(25)	3945	9663	4625	25
H(26A)	4778	10422	8169	65
H(26B)	3571	10112	7905	65
H(26C)	3799	11103	7360	65

Table S10. Torsion angles [°] for 6t

Br(1)-C(5)-C(6)-C(7)	176.92(12)
S(1)-N(1)-C(1)-C(2)	-137.62(10)
S(1)-N(1)-C(1)-C(9)	95.51(13)
S(1)-N(1)-C(8)-C(3)	137.96(11)
S(1)-N(1)-C(8)-C(7)	-48.2(2)
S(1)-C(20)-C(21)-C(22)	175.80(13)
S(1)-C(20)-C(25)-C(24)	-175.62(12)
O(1)-S(1)-N(1)-C(1)	173.89(10)
O(1)-S(1)-N(1)-C(8)	37.23(14)
O(1)-S(1)-C(20)-C(21)	-42.39(15)
O(1)-S(1)-C(20)-C(25)	135.47(13)
O(2)-S(1)-N(1)-C(1)	-57.45(12)
O(2)-S(1)-N(1)-C(8)	165.88(11)
O(2)-S(1)-C(20)-C(21)	-173.62(12)
O(2)-S(1)-C(20)-C(25)	4.23(15)
N(1)-S(1)-C(20)-C(21)	72.82(14)
N(1)-S(1)-C(20)-C(25)	-109.32(13)
N(1)-C(1)-C(2)-C(3)	-5.99(15)
N(1)-C(1)-C(9)-C(10)	-115.38(16)

N(1)-C(1)-C(9)-C(17)	61.97(18)
C(1)-N(1)-C(8)-C(3)	-0.97(16)
C(1)-N(1)-C(8)-C(7)	172.89(14)
C(1)-C(2)-C(3)-C(4)	-171.60(15)
C(1)-C(2)-C(3)-C(8)	5.78(16)
C(1)-C(9)-C(10)-C(11)	-2.7(3)
C(1)-C(9)-C(17)-O(3)	-179.03(16)
C(1)-C(9)-C(17)-O(4)	1.7(2)
C(2)-C(1)-C(9)-C(10)	124.80(16)
C(2)-C(1)-C(9)-C(17)	-57.85(19)
C(2)-C(3)-C(4)-C(5)	177.24(14)
C(2)-C(3)-C(8)-N(1)	-3.17(17)
C(2)-C(3)-C(8)-C(7)	-177.46(13)
C(3)-C(4)-C(5)-Br(1)	-177.58(11)
C(3)-C(4)-C(5)-C(6)	0.3(2)
C(4)-C(3)-C(8)-N(1)	174.47(13)
C(4)-C(3)-C(8)-C(7)	0.2(2)
C(4)-C(5)-C(6)-C(7)	-1.0(2)
C(5)-C(6)-C(7)-C(8)	1.2(2)
C(6)-C(7)-C(8)-N(1)	-174.05(14)
C(6)-C(7)-C(8)-C(3)	-0.8(2)
C(8)-N(1)-C(1)-C(2)	4.45(15)
C(8)-N(1)-C(1)-C(9)	-122.42(13)
C(8)-C(3)-C(4)-C(5)	0.1(2)
C(9)-C(1)-C(2)-C(3)	116.92(14)
C(9)-C(10)-C(11)-C(12)	-54.1(2)
C(9)-C(10)-C(11)-C(16)	126.23(19)
C(10)-C(9)-C(17)-O(3)	-1.5(2)
C(10)-C(9)-C(17)-O(4)	179.21(14)
C(10)-C(11)-C(12)-C(13)	179.21(16)

C(10)-C(11)-C(16)-C(15)	-178.52(16)
C(11)-C(12)-C(13)-C(14)	-0.4(3)
C(12)-C(11)-C(16)-C(15)	1.8(3)
C(12)-C(13)-C(14)-C(15)	1.3(3)
C(13)-C(14)-C(15)-C(16)	-0.6(3)
C(14)-C(15)-C(16)-C(11)	-0.9(3)
C(16)-C(11)-C(12)-C(13)	-1.1(3)
C(17)-O(4)-C(18)-C(19)	172.27(14)
C(17)-C(9)-C(10)-C(11)	179.85(15)
C(18)-O(4)-C(17)-O(3)	0.4(2)
C(18)-O(4)-C(17)-C(9)	179.68(13)
C(20)-S(1)-N(1)-C(1)	57.27(12)
C(20)-S(1)-N(1)-C(8)	-79.40(13)
C(20)-C(21)-C(22)-C(23)	-0.1(3)
C(21)-C(20)-C(25)-C(24)	2.2(2)
C(21)-C(22)-C(23)-C(24)	1.9(3)
C(21)-C(22)-C(23)-C(26)	-176.46(17)
C(22)-C(23)-C(24)-C(25)	-1.7(3)
C(23)-C(24)-C(25)-C(20)	-0.3(2)
C(25)-C(20)-C(21)-C(22)	-2.0(2)
C(26)-C(23)-C(24)-C(25)	176.64(16)

Symmetry transformations used to generate equivalent atoms:

Table S11. Hydrogen bonds for 6t [Å and °]

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)

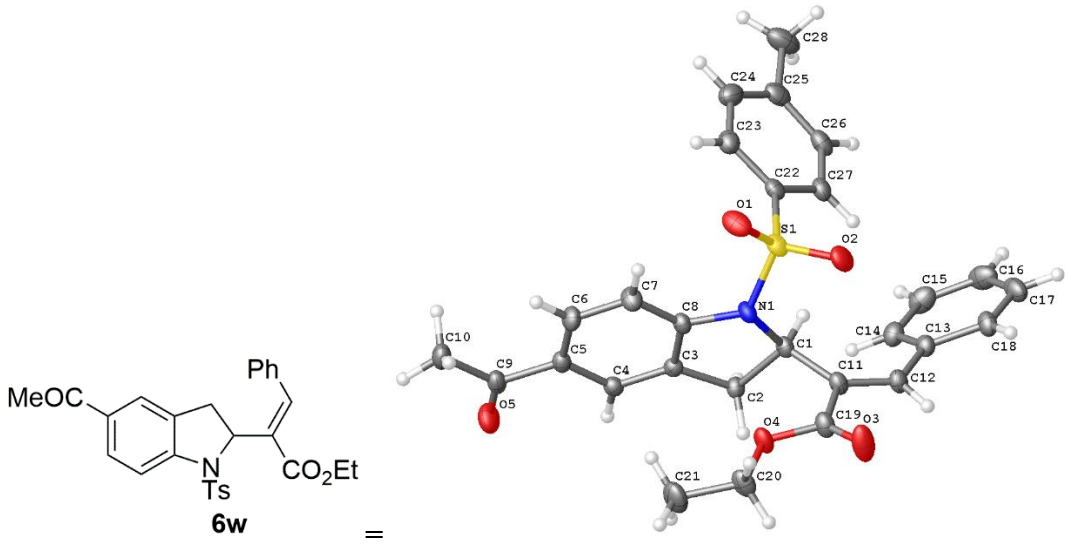


Figure S3. ORTEP representation of 6w draw with 50% probability thermal ellipsoids

Table S12 Crystal data and structure refinement for 6w

Identification code	**6w**
Empirical formula	$C_{28}H_{27}NO_5S$
Formula weight	489.56
Temperature/K	130
Crystal system	orthorhombic
Space group	Pbca
a/Å	15.4536(15)
b/Å	12.9941(12)
c/Å	24.233(2)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	4866.1(8)
Z	8
ρ_{calc}g/cm^3	1.336
μ/mm^{-1}	0.173

F(000)	2064.0
Crystal size/mm^3	0.18 × 0.15 × 0.03
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.362 to 61.234
Index ranges	$-19 \leq h \leq 22$, $-18 \leq k \leq 18$, $-34 \leq l \leq 34$
Reflections collected	47045
Independent reflections	7479 [R_{int} = 0.0660, R_{sigma} = 0.0446]
Data/restraints/parameters	7479/0/319
Goodness-of-fit on F^2	1.009
Final R indexes [I>=2σ (I)]	R_1 = 0.0486, wR_2 = 0.1030
Final R indexes [all data]	R_1 = 0.0817, wR_2 = 0.1182
Largest diff. peak/hole / e $Å^{-3}$	0.33/-0.39

Table S13 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 6w. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor

Atom	*x*	*y*	*z*	U(eq)
S1	5258.2(3)	3591.2(3)	7138.5(2)	23.23(10)
O1	5405.2(9)	2817.0(9)	7547.6(5)	33.0(3)
O2	5930.3(8)	4304.8(10)	6999.0(5)	31.6(3)
O3	7214.1(8)	3297.8(10)	5668.1(7)	43.6(4)
O4	6076.3(7)	2222.2(8)	5678.2(5)	25.6(3)
O5	2419.6(9)	-377.6(10)	5658.1(5)	36.4(3)
N1	5026.0(9)	2997.3(10)	6552.5(5)	21.0(3)
C1	4915.9(10)	3660.0(11)	6045.6(6)	19.6(3)
C2	4329.3(10)	3013.2(11)	5655.1(6)	19.3(3)
C3	4078.1(9)	2089.7(11)	5996.6(6)	17.8(3)
C4	3535.5(10)	1284.6(11)	5861.4(6)	19.4(3)

C5	3401.8(10)	488.7(12)	6243.5(7)	20.9(3)
C6	3822.1(11)	522.6(12)	6753.2(7)	24.7(3)
C7	4371.1(11)	1329.1(12)	6893.4(7)	25.9(3)
C8	4484.2(10)	2113.8(11)	6512.2(6)	19.2(3)
C9	2805.4(10)	-376.3(12)	6099.3(7)	24.5(3)
C10	2686.9(12)	-1242.4(13)	6507.8(8)	30.1(4)
C11	5780(1)	3970.4(12)	5808.6(7)	21.4(3)
C12	5999.4(10)	4936.1(12)	5670.8(7)	22.9(3)
C13	5476.3(10)	5885.9(12)	5708.2(6)	21.8(3)
C14	4582.5(11)	5923.4(13)	5621.3(7)	25.4(3)
C15	4138.4(12)	6850.8(14)	5667.8(7)	33.0(4)
C16	4576.0(14)	7749.6(14)	5793.9(8)	37.0(4)
C17	5464.5(13)	7728.6(13)	5868.9(7)	32.8(4)
C18	5909.7(12)	6811.5(12)	5821.4(7)	26.0(3)
C19	6446.0(11)	3152.6(12)	5714.6(7)	25.4(3)
C20	6635.2(11)	1353.3(12)	5559.9(8)	29.9(4)
C21	6064.2(14)	427.4(14)	5492.5(10)	42.5(5)
C22	4352.4(10)	4318.6(12)	7344.0(6)	21.8(3)
C23	3822.9(11)	3959.9(13)	7769.3(7)	27.6(4)
C24	3154.0(12)	4580.8(15)	7959.5(7)	33.2(4)
C25	3000.9(11)	5545.9(14)	7730.5(7)	30.6(4)
C26	3517.1(11)	5873.5(13)	7292.7(7)	28.4(4)
C27	4200.2(11)	5279.4(12)	7104.5(7)	24.5(3)
C28	2315.9(13)	6257.2(17)	7959.0(9)	44.7(5)

Table S14. Anisotropic Displacement Parameters ($Å^2×10^3$) for 6w. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
S1	24.10(19)	20.84(18)	24.74(18)	-3.62(15)	-7.04(15)	0.15(15)
O1	43.1(7)	28.4(6)	27.4(6)	-0.9(5)	-13.9(5)	9.2(6)
O2	24.0(6)	32.9(7)	37.7(7)	-10.6(5)	-4.6(5)	-7.7(5)
O3	20.9(6)	25.8(7)	84.0(11)	-3.2(7)	2.0(6)	0.5(5)
O4	21.7(6)	14.8(5)	40.2(7)	-4.5(5)	-0.5(5)	1.2(4)
O5	36.0(7)	33.6(7)	39.5(7)	0.0(6)	-7.3(6)	-13.3(6)
N1	26.6(7)	14.6(6)	21.9(6)	-1.1(5)	-4.5(5)	-1.7(5)
C1	21.6(7)	13.7(6)	23.5(7)	0.3(6)	-1.7(6)	0.2(6)
C2	18.8(7)	17.5(7)	21.7(7)	1.6(6)	-2.2(5)	-0.9(6)
C3	17.9(7)	15.6(7)	20.0(7)	0.6(5)	1.1(5)	3.4(5)
C4	18.9(7)	18.2(7)	21.3(7)	-1.6(6)	0.2(6)	1.6(6)
C5	19.4(7)	16.6(7)	26.7(8)	-0.9(6)	2.3(6)	0.6(6)
C6	28.2(8)	17.7(7)	28.1(8)	5.5(6)	-0.7(6)	-1.4(6)
C7	32.1(9)	21.6(8)	24.0(8)	3.5(6)	-6.5(6)	-1.1(7)
C8	20.0(7)	14.5(7)	23.1(7)	-0.4(6)	-1.3(6)	1.0(6)
C9	20.9(8)	18.6(8)	33.9(9)	-3.0(6)	4.4(6)	-1.8(6)
C10	29.6(9)	21.1(8)	39.7(10)	-0.1(7)	7.5(7)	-5.3(7)
C11	19.8(7)	16.4(7)	27.9(8)	-2.0(6)	-1.9(6)	-0.3(6)
C12	20.5(7)	18.6(7)	29.4(8)	-0.7(6)	-0.9(6)	-2.8(6)
C13	25.3(8)	17.3(7)	22.8(7)	2.3(6)	-0.4(6)	-0.6(6)
C14	25.6(8)	23.8(8)	26.9(8)	5.4(6)	-0.5(6)	-1.5(6)
C15	29.3(9)	33.2(9)	36.6(9)	9.4(8)	5.1(7)	8.9(8)
C16	50.3(12)	24.9(9)	35.8(10)	3.6(7)	10.4(9)	13.9(8)
C17	51.3(11)	17.8(8)	29.4(9)	-0.9(7)	0.0(8)	-0.7(8)
C18	31.7(9)	18.4(7)	27.9(8)	3.0(6)	-4.0(7)	-3.5(7)
C19	23.4(8)	17.2(7)	35.5(9)	-0.2(6)	-2.3(7)	0.5(6)

C20	27.1(8)	18.4(8)	44.1(10)	-5.1(7)	-2.3(7)	7.0(7)
C21	46.6(12)	19.4(8)	61.4(13)	-6.8(9)	4.8(10)	1.0(8)
C22	24.3(8)	19.0(7)	22.1(7)	-4.3(6)	-4.6(6)	-2.2(6)
C23	32.4(9)	25.4(8)	25.0(8)	0.3(6)	-3.1(7)	-4.5(7)
C24	31.9(9)	39.8(10)	27.9(9)	-4.8(8)	3.5(7)	-6.7(8)
C25	25.2(8)	32.5(9)	34.2(9)	-12.8(7)	-4.9(7)	-2.2(7)
C26	30.5(9)	19.2(8)	35.4(9)	-5.7(7)	-8.0(7)	-1.0(7)
C27	29.0(8)	17.8(7)	26.7(8)	-1.7(6)	-3.1(6)	-4.0(6)
C28	36.4(11)	46.8(12)	51.0(12)	-24.2(10)	-1.6(9)	5.4(9)

Table S15. Bond Lengths for 6w

Atom	Atom	Length/Å	Atom	Atom	Length/Å
S1	O1	1.4305(12)	C7	C8	1.387(2)
S1	O2	1.4328(13)	C9	C10	1.510(2)
S1	N1	1.6554(13)	C11	C12	1.342(2)
S1	C22	1.7609(16)	C11	C19	1.497(2)
O3	C19	1.207(2)	C12	C13	1.478(2)
O4	C19	1.3401(19)	C13	C14	1.398(2)
O4	C20	1.4502(19)	C13	C18	1.404(2)
O5	C9	1.224(2)	C14	C15	1.391(2)
N1	C1	1.5099(19)	C15	C16	1.384(3)
N1	C8	1.4243(19)	C16	C17	1.385(3)
C1	C2	1.557(2)	C17	C18	1.381(2)
C1	C11	1.509(2)	C20	C21	1.501(3)
C2	C3	1.509(2)	C22	C23	1.396(2)
C3	C4	1.380(2)	C22	C27	1.397(2)
C3	C8	1.398(2)	C23	C24	1.390(3)
C4	C5	1.403(2)	C24	C25	1.392(3)

C5	C6	1.396(2)	C25	C26	1.394(3)
C5	C9	1.495(2)	C25	C28	1.510(3)
C6	C7	1.390(2)	C26	C27	1.385(2)

Table S16. Bond Angles for dm17012

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
O1	S1	O2	120.23(8)	C5	C9	C10	118.82(14)
O1	S1	N1	107.52(7)	C12	C11	C1	124.63(14)
O1	S1	C22	107.92(8)	C12	C11	C19	116.89(14)
O2	S1	N1	104.86(7)	C19	C11	C1	118.48(13)
O2	S1	C22	107.19(7)	C11	C12	C13	128.85(15)
N1	S1	C22	108.70(7)	C14	C13	C12	124.07(14)
C19	O4	C20	117.48(13)	C14	C13	C18	118.09(15)
C1	N1	S1	117.16(10)	C18	C13	C12	117.80(15)
C8	N1	S1	124.20(10)	C15	C14	C13	120.36(16)
C8	N1	C1	109.73(11)	C16	C15	C14	120.52(17)
N1	C1	C2	104.61(11)	C15	C16	C17	119.78(17)
C11	C1	N1	111.26(12)	C18	C17	C16	119.99(17)
C11	C1	C2	115.36(13)	C17	C18	C13	121.20(17)
C3	C2	C1	104.23(12)	O3	C19	O4	123.65(15)
C4	C3	C2	128.98(13)	O3	C19	C11	125.41(15)
C4	C3	C8	120.11(14)	O4	C19	C11	110.93(13)
C8	C3	C2	110.91(13)	O4	C20	C21	107.18(14)
C3	C4	C5	119.43(14)	C23	C22	S1	119.71(13)
C4	C5	C9	119.38(14)	C23	C22	C27	120.43(15)
C6	C5	C4	119.47(14)	C27	C22	S1	119.74(13)
C6	C5	C9	121.15(14)	C24	C23	C22	119.14(16)
C7	C6	C5	121.59(15)	C23	C24	C25	121.14(17)

C8	C7	C6	117.91(15)	C24	C25	C26	118.78(16)
C3	C8	N1	110.07(13)	C24	C25	C28	121.62(18)
C7	C8	N1	128.38(14)	C26	C25	C28	119.56(18)
C7	C8	C3	121.47(14)	C27	C26	C25	121.11(16)
O5	C9	C5	120.36(15)	C26	C27	C22	119.32(16)
O5	C9	C10	120.82(15)				

Table S17. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 6w

Atom	*x*	*y*	*z*	U(eq)
H1	4594.93	4297.56	6152.96	24
H2A	3811.45	3409.74	5542.72	23
H2B	4650.21	2801.01	5320.29	23
H4	3254.97	1269.27	5512.66	23
H6	3730.75	-18.26	7010.46	30
H7	4659.76	1342.19	7239.47	31
H10A	2371.04	-988.59	6830.93	45
H10B	3254.72	-1500.49	6623.05	45
H10C	2358.1	-1800.42	6334.39	45
H12	6568.64	5020.88	5529.9	27
H14	4276.79	5312.43	5530.09	31
H15	3529.93	6867.04	5612.45	40
H16	4268.11	8379.09	5828.82	44
H17	5767.5	8345.04	5953.09	39
H18	6520.41	6806.84	5866.2	31
H20A	7048.41	1244.7	5866.64	36
H20B	6968.04	1479.08	5217.4	36
H21A	5678.21	530.42	5176.46	64

H21B	5718.51	330.52	5827.59	64
H21C	6422.96	-183.31	5429.61	64
H23	3918.6	3300.04	7926.67	33
H24	2795.04	4342.15	8250.95	40
H26	3398.4	6514.99	7120.56	34
H27	4561.49	5522.94	6815.44	29
H28A	2590.91	6788.93	8186	67
H28B	1909.6	5861.42	8185.66	67
H28C	2002.87	6582.88	7653.76	67