Electronic Supplementary Information

Preparation of Cyclic Imides from Alkene-tethered Amides: an Application of Homogeneous Cu(II) Catalytical System

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Abstract: A Cu-based homogeneous catalytic system was put forward for the preparation of imides from alkene-tethered amides. O_2 acted as a cheap and easily available oxygen source and a terminal oxidant. Cleavage of C=C bonds and formation of C-N bond were catalyzed by Cu(II) salts with proper nitrogen-containing ligand under 100 ^oC. The synthetic approach has potential of applying onto pharmaceutical synthesis. Moreover, scaled-up experiment confirmed the practical application ability.

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1. Reaction condition screening of catalytic system

Table S1 Ligand information

Entry	Code	Name
1	A	2,9-dimethyl-1,10-phenanthroline
2	B	2,2'-bipyridine
3	C	2,2'-bipyrimidine
4	D	5*H*-cyclopenta[2,1-*b*:3,4-*b*']dipyridin-5-one
5	E	4-methyl-2-(pyridin-2-yl)-4,5-dihydrooxazole
6	F	(*S*)-4-isopropyl-2-(pyridin-2-yl)-4,5-dihydrooxazole
7	G	2,2'-(propane-2,2-diyl)bis(4,5-dihydrooxazole)
8	H	2,2'-(propane-2,2-diyl)bis(4-isopropyl-4,5-dihydrooxazole)
9	I	N^1,N^1,N^2,N^2-tetramethylethane-1,2-diamine
10	J	N^1,N^1,N^3,N^3-tetramethylpropane-1,3-diamine
11	K	N^1,N^1,N^4,N^4-tetramethylbutane-1,4-diamine
12	L	N^1,N^1,N^5,N^5-tetramethylpentane-1,5-diamine
13	M	triethylamine
14	N	1*H*-imidazole
15	O	(1*E*,2*E*)-N^1,N^2-dicyclohexylethane-1,2-diimine
16	P	7-(tert-butyl)-2,5-dimethyl-3,4-dihydro-2*H*-pyrano[2,3-*b*]quinoline
17	Q	1,2-bis(phenylsulfinyl)ethane
18	R	ethyl(4-methoxyphenyl)sulfane
19	S	triphenylphosphane
20	T	1,2-bis(diphenylphosphanyl)ethane
21	U	2,2'-bis(diphenylphosphanyl)-1,1'-binaphthalene
22	V	(oxybis(2,1-phenylene))bis(diphenylphosphane)

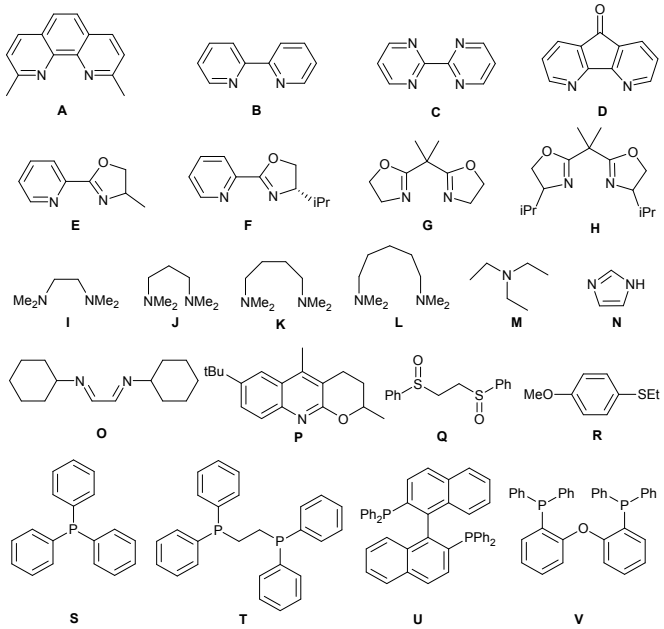
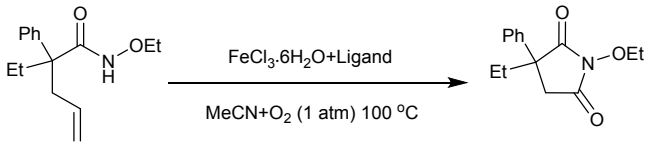


Table S2 Catalytic performance of $FeCl_3·6H_2O$: effect of ligands[a]



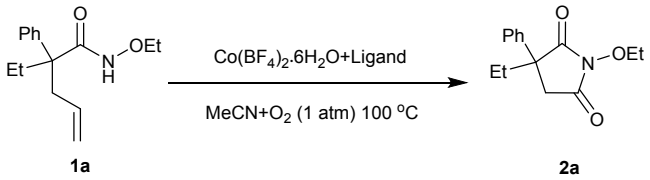
1a 2a

Entry	Ligand Code	Yield/%[b]
1	A	0.5
2	B	Not detected
3	C	Not detected
4	D	0.2
5	E	0.5
6	F	Not detected
7	G	Not detected
8	H	Not detected
9	I	Not detected
10	J	Not detected
11	K	Not detected
12	L	Not detected
13	M	Not detected
14	N	Not detected
15	O	Not detected
16	P	0.8
17	Q	Not detected
18	R	Not detected
19	S	Not detected
20	T	Not detected
21	U	Not detected
22	V	Not detected

[a] Reaction conditions: **1a**, 0.1 mmol; $FeCl_3·6H_2O$, 0.01 mmol (10 mol%); Ligand, 0.015 mmol (15 mol%); MeCN, 1.5 mL; O_2 (1 atm); 100 °C; 24 h.

[b] Determined by ^1H NMR analysis using 1,1,2,2-tetrachloroethane as an internal standard.

Table S3 Catalytic performance of $Co(BF_4)_2{\cdot}6H_2O$: effect of ligands[a]



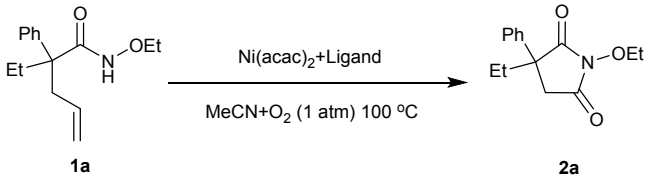
1a **2a**

Entry	Ligand Code	Yield/%[b]
1	A	Not detected
2	B	Not detected
3	C	4.8
4	D	3.2
5	E	Not detected
6	F	Not detected
7	G	Not detected
8	H	Not detected
9	I	0.5
10	J	1
11	K	Not detected
12	L	Not detected
13	M	Not detected
14	N	Not detected
15	O	0.8
16	P	1.2
17	Q	Not detected
18	R	Not detected
19	S	Not detected
20	T	Not detected
21	U	Not detected
22	V	Not detected

[a] Reaction conditions: **1a**, 0.1 mmol; $Co(BF_4)_2{\cdot}6H_2O$, 0.01 mmol (10 mol%); Ligand, 0.015 mmol (15 mol%); MeCN, 1.5 mL; O_2 (1 atm); 100 °C; 24 h.

[b] Determined by ^1H NMR analysis using 1,1,2,2-tetrachloroethane as an internal standard.

Table S4 Catalytic performance of $Ni(acac)_2$: effect of ligands[a]



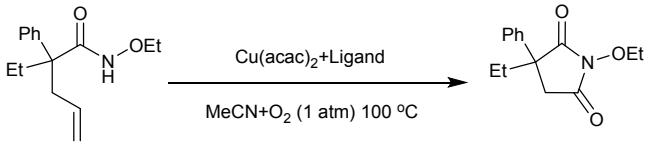
1a **2a**

Entry	Ligand Code	Yield/%[b]
1	A	0.5
2	B	0.4
3	C	0.6
4	D	Not detected
5	E	Not detected
6	F	Not detected
7	G	Not detected
8	H	Not detected
9	I	Not detected
10	J	Not detected
11	K	Not detected
12	L	0.5
13	M	0.8
14	N	0.6
15	O	Not detected
16	P	0.5
17	Q	Not detected
18	R	Not detected
19	S	Not detected
20	T	Not detected
21	U	Not detected
22	V	Not detected

[a] Reaction conditions: **1a**, 0.1 mmol; $Ni(acac)_2$, 0.01 mmol (10 mol%); Ligand, 0.015 mmol (15 mol%); MeCN, 1.5 mL; O_2 (1 atm); 100 °C; 24 h.

[b] Determined by ^1H NMR analysis using 1,1,2,2-tetrachloroethane as an internal standard.

Table S5 Catalytic performance of $Cu(acac)_2$: effect of ligands[a]



1a **2a**

Entry	Ligand Code	Yield/%[b]
1	A	85
2	B	63
3	C	72
4	D	28
5	E	51
6	F	44
7	G	42
8	H	25
9	I	8
10	J	6
11	K	5
12	L	3
13	M	5
14	N	33
15	O	8
16	P	18
17	Q	2
18	R	1
19	S	Not detected
20	T	Not detected
21	U	Not detected
22	V	Not detected

[a] Reaction conditions: **1a**, 0.1 mmol; $Cu(acac)_2$, 0.01 mmol (10 mol%); Ligand, 0.015 mmol (15 mol%); MeCN, 1.5 mL; O_2 (1 atm); 100 °C; 24 h.

[b] Determined by ^1H NMR analysis using 1,1,2,2-tetrachloroethane as an internal standard.

Table S6 Catalytic performance of $ZnCl_2$: effect of ligands[a]

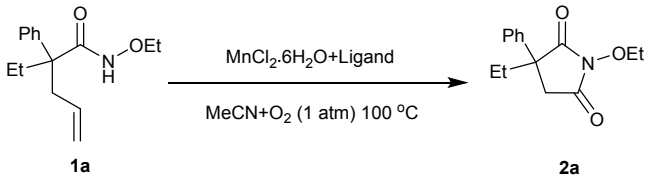
1a **2a**

Entry	Ligand Code	Yield/%[b]
1	A	0.5
2	B	0.5
3	C	0.3
4	D	Not detected
5	E	Not detected
6	F	Not detected
7	G	Not detected
8	H	Not detected
9	I	Not detected
10	J	Not detected
11	K	Not detected
12	L	0.8
13	M	0.4
14	N	0.3
15	O	Not detected
16	P	0.5
17	Q	0.6
18	R	Not detected
19	S	Not detected
20	T	Not detected
21	U	Not detected
22	V	Not detected

[a] Reaction conditions: **1a**, 0.1 mmol; $ZnCl_2$, 0.01 mmol (10 mol%); Ligand, 0.015 mmol (15 mol%); MeCN, 1.5 mL; O_2 (1 atm); 100 °C; 24 h.

[b] Determined by ^1H NMR analysis using 1,1,2,2-tetrachloroethane as an internal standard.

Table S7 Catalytic performance of $MnCl_2·4H_2O$: effect of ligands[a]



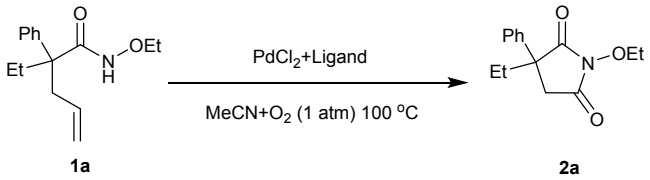
1a **2a**

Entry	Ligand Code	Yield/%[b]
1	A	Not detected
2	B	Not detected
3	C	Not detected
4	D	Not detected
5	E	Not detected
6	F	0.4
7	G	0.5
8	H	0.6
9	I	0.3
10	J	Not detected
11	K	Not detected
12	L	Not detected
13	M	Not detected
14	N	Not detected
15	O	Not detected
16	P	Not detected
17	Q	0.3
18	R	0.5
19	S	Not detected
20	T	Not detected
21	U	Not detected
22	V	Not detected

[a] Reaction conditions: **1a**, 0.1 mmol; $MnCl_2·4H_2O$, 0.01 mmol (10 mol%); Ligand, 0.015 mmol (15 mol%); MeCN, 1.5 mL; O_2 (1 atm); 100 °C; 24 h.

[b] Determined by ^1H NMR analysis using 1,1,2,2-tetrachloroethane as an internal standard.

Table S8 Catalytic performance of $PdCl_2$: effect of ligands[a]



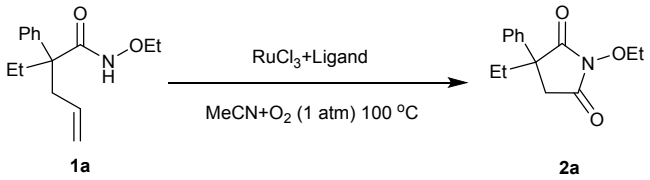
1a **2a**

Entry	Ligand Code	Yield/%[b]
1	A	0.5
2	B	0.6
3	C	5.6
4	D	3.2
5	E	Not detected
6	F	Not detected
7	G	Not detected
8	H	Not detected
9	I	Not detected
10	J	Not detected
11	K	Not detected
12	L	1.2
13	M	Not detected
14	N	1
15	O	Not detected
16	P	0.8
17	Q	0.5
18	R	Not detected
19	S	Not detected
20	T	Not detected
21	U	Not detected
22	V	Not detected

[a] Reaction conditions: **1a**, 0.1 mmol; $PdCl_2$, 0.01 mmol (10 mol%); Ligand, 0.015 mmol (15 mol%); MeCN, 1.5 mL; O_2 (1 atm); 100 °C; 24 h.

[b] Determined by ^1H NMR analysis using 1,1,2,2-tetrachloroethane as an internal standard.

Table S9 Catalytic performance of $RuCl_3$: effect of ligands[a]



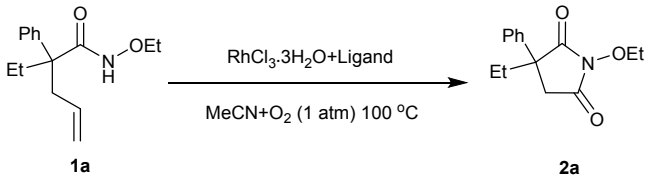
1a **2a**

Entry	Ligand Code	Yield/%[b]
1	A	Not detected
2	B	Not detected
3	C	Not detected
4	D	Not detected
5	E	Not detected
6	F	Not detected
7	G	Not detected
8	H	4.8
9	I	Not detected
10	J	1
11	K	Not detected
12	L	Not detected
13	M	Not detected
14	N	0.5
15	O	1.5
16	P	2
17	Q	0.5
18	R	Not detected
19	S	Not detected
20	T	Not detected
21	U	Not detected
22	V	Not detected

[a] Reaction conditions: **1a**, 0.1 mmol; $RuCl_3$, 0.01 mmol (10 mol%); Ligand, 0.015 mmol (15 mol%); MeCN, 1.5 mL; O_2 (1 atm); 100 °C; 24 h.

[b] Determined by ^1H NMR analysis using 1,1,2,2-tetrachloroethane as an internal standard.

Table S10 Catalytic performance of $RhCl_3 \cdot 3H_2O$: effect of ligands[a]



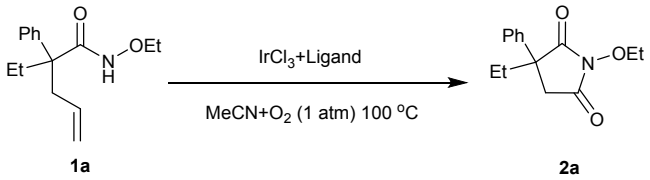
1a **2a**

Entry	Ligand Code	Yield/%[b]
1	A	Not detected
2	B	Not detected
3	C	1
4	D	0.5
5	E	Not detected
6	F	0.6
7	G	5.5
8	H	Not detected
9	I	Not detected
10	J	Not detected
11	K	Not detected
12	L	Not detected
13	M	Not detected
14	N	Not detected
15	O	Not detected
16	P	0.5
17	Q	Not detected
18	R	0.2
19	S	Not detected
20	T	Not detected
21	U	Not detected
22	V	Not detected

[a] Reaction conditions: **1a**, 0.1 mmol; $RhCl_3 \cdot 3H_2O$, 0.01 mmol (10 mol%); Ligand, 0.015 mmol (15 mol%); MeCN, 1.5 mL; O_2 (1 atm); 100 °C; 24 h.

[b] Determined by ^1H NMR analysis using 1,1,2,2-tetrachloroethane as an internal standard.

Table S11 Catalytic performance of $IrCl_3$: effect of ligands[a]



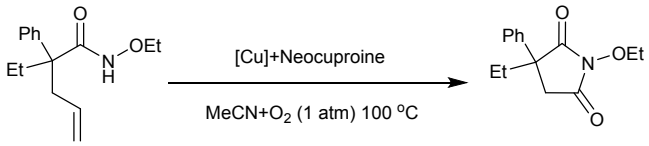
1a **2a**

Entry	Ligand Code	Yield/%[b]
1	A	3.2
2	B	0.5
3	C	0.2
4	D	Not detected
5	E	Not detected
6	F	Not detected
7	G	Not detected
8	H	Not detected
9	I	0.5
10	J	Not detected
11	K	1
12	L	Not detected
13	M	0.5
14	N	Not detected
15	O	Not detected
16	P	Not detected
17	Q	Not detected
18	R	Not detected
19	S	Not detected
20	T	Not detected
21	U	Not detected
22	V	Not detected

[a] Reaction conditions: **1a**, 0.1 mmol; $IrCl_3$, 0.01 mmol (10 mol%); Ligand, 0.015 mmol (15 mol%); MeCN, 1.5 mL; O_2 (1 atm); 100 °C; 24 h.

[b] Determined by ^1H NMR analysis using 1,1,2,2-tetrachloroethane as an internal standard.

Table S12 Screening of Cu salts[a]



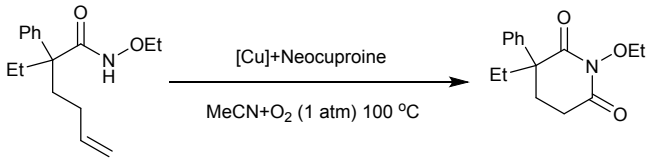
1a **2a**

Entry	Cu Salt	Yield/%[b]
1	$CuSO_4·5H_2O$	75
2	$Cu(NO_3)_2·2.5H_2O$	78
3	$Cu(BF_4)_2·2H_2O$	82
4	CuF_2	81
5	$CuCl_2·2H_2O$	80
6	$CuBr_2$	77
7	$Cu(acac)_2$	85
8	$CuAc_2·H_2O$	78

[a] Reaction conditions: **1a**, 0.1 mmol; Cu salts, 0.01 mmol (10 mol%); Neocuproine, 0.015 mmol (15 mol%); MeCN, 1.5 mL; O_2 (1 atm); 100 °C; 24 h.

[b] Determined by ^1H NMR analysis using 1,1,2,2-tetrachloroethane as an internal standard.

Table S13 Screening of Cu salts[a]



3a **4a**

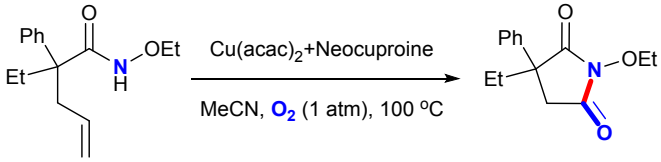
Entry	Cu Salt	Yield/%[b]
1	$CuSO_4·5H_2O$	44
2	$Cu(NO_3)_2·2.5H_2O$	47
3	$Cu(BF_4)_2·2H_2O$	50
4	CuF_2	58
5	$CuCl_2·2H_2O$	49
6	$CuBr_2$	45
7	$Cu(acac)_2$	52
8	$CuAc_2·H_2O$	48

[a] Reaction conditions: **3a**, 0.1 mmol; Cu salts, 0.01 mmol (10 mol%); Neocuproine, 0.015 mmol (15 mol%); MeCN, 1.5 mL; O_2 (1 atm); 100 °C; 24 h.

[b] Determined by ^1H NMR analysis using 1,1,2,2-tetrachloroethane as an internal standard.

2. Studies on the catalytic system

Table S14 Control experiments[a]

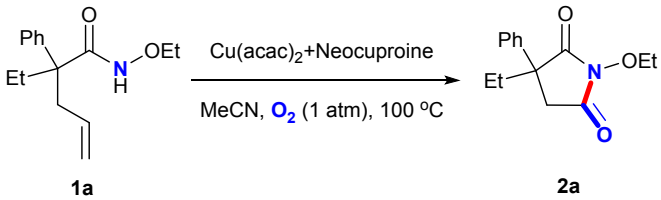


1a **2a**

Entry	Deviation from standard conditions	**2a** yield / %[b]
1	No $Cu(acac)_2$	0
2	No neocuproine	0
3	No O_2	0
4	No neocuproine or O_2	0

[a] Stangard conditions: **1a**, 0.1 mmol; $Cu(acac)_2$, 0.01 mmol (10 mol%); ligand neocuproine, 0.015 mmol (15 mol%); MeCN, 1.5 mL; O_2 (1 atm); 100 °C; 24 h. [b] Determined by ^1H NMR analysis using 1,1,2,2-tetrachloroethane as an internal standard.

Table S15 Quantitative data for the kinetic studies[a,b]

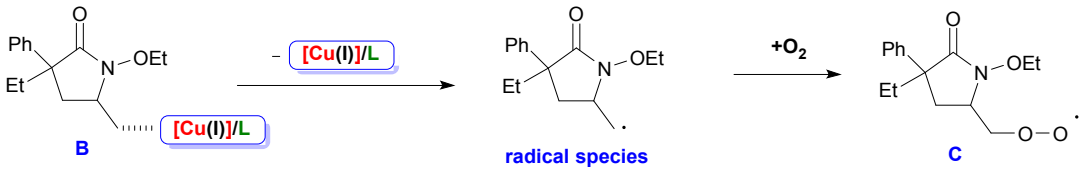


1a **2a**

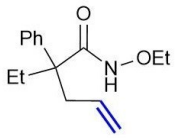
Entry	Time / h	1a / %	E / %	2a / %
1	0	100	0	0
2	0.5	60	30	8
3	1	40	27	18
4	1.5	35	21	25
5	2	25	18	38
6	3	19	16	49
7	6	17	13	58
8	9	16	10	63
9	12	15	8	68
10	15	12	5	72
11	18	10	3	79
12	21	9	2	82
13	24	8	2	85
14	27	8	2	85

[a] Reaction conditions: 1a, 0.1 mmol; $Cu(acac)_2$, 0.01 mmol (10 mol%); ligand neocuproine, 0.015 mmol (15 mol%); MeCN, 1.5 mL; O_2 (1 atm); 100 °C. [b] Yields were determined by ^1H NMR analysis using 1,1,2,2-tetrachloroethane as an internal standard.

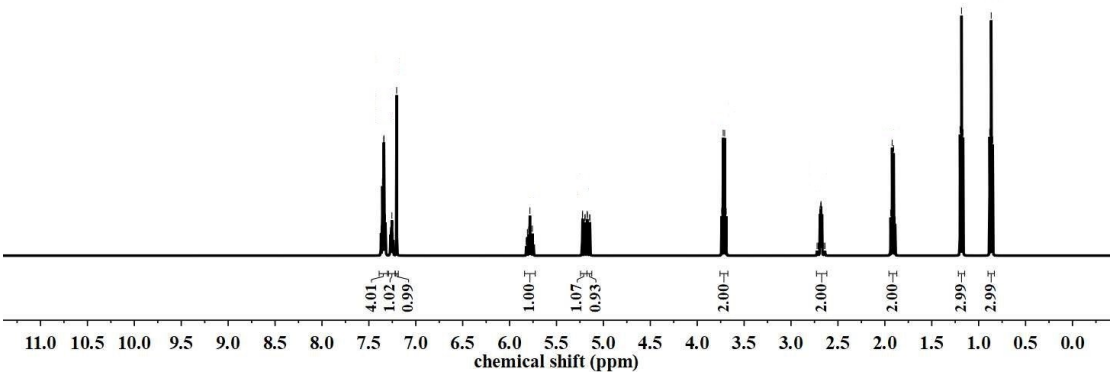
Scheme S1 Process between intermediate B and C

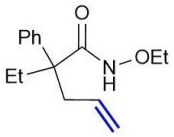


3. NMR spectra of substrates, products and intermediate

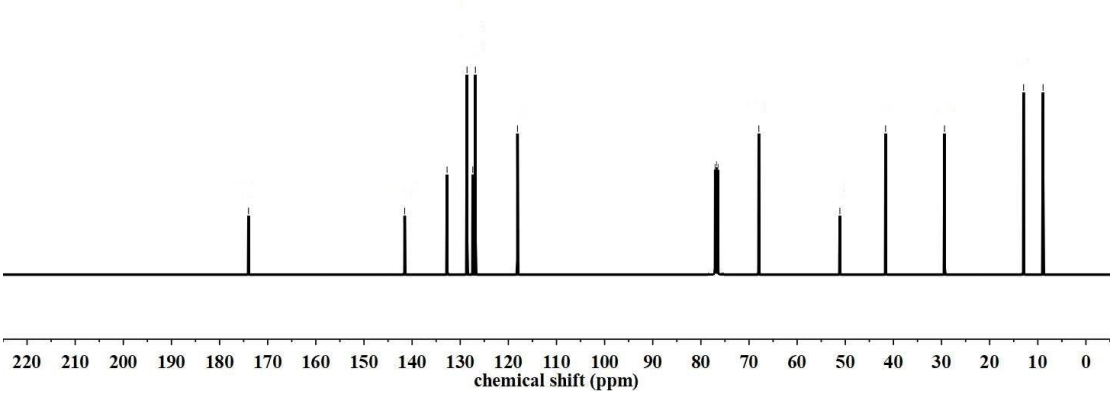


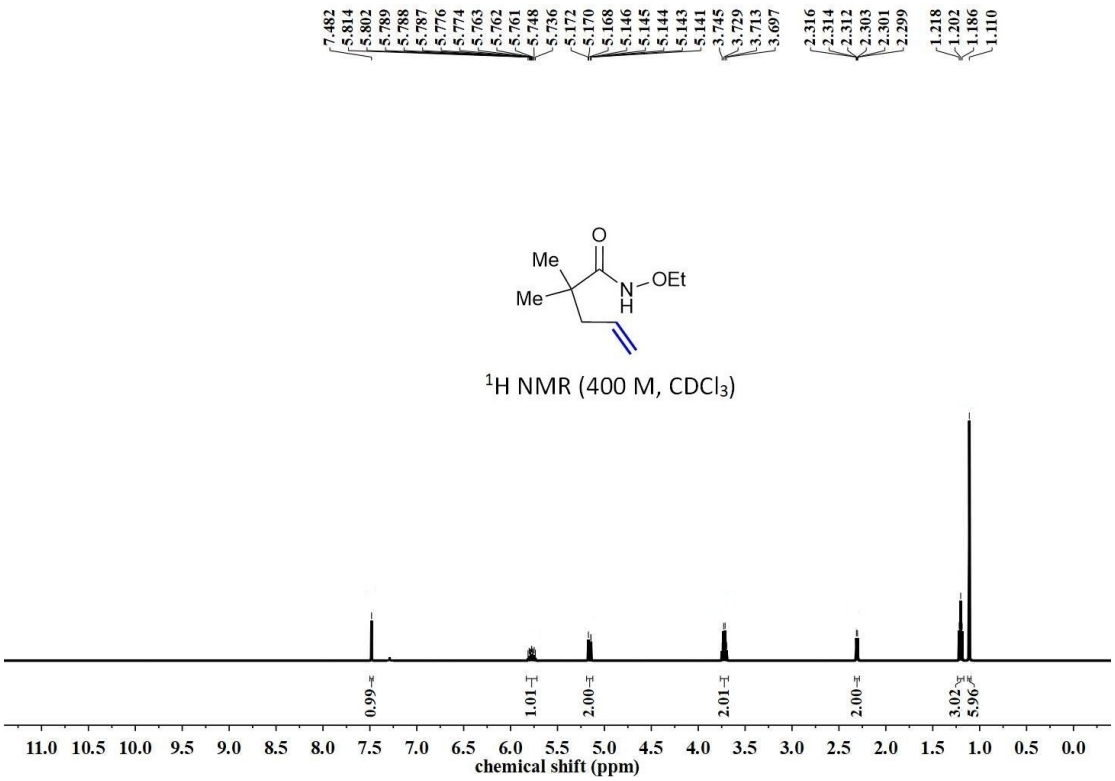
^{1}H NMR (400 M, $CDCl_3$)



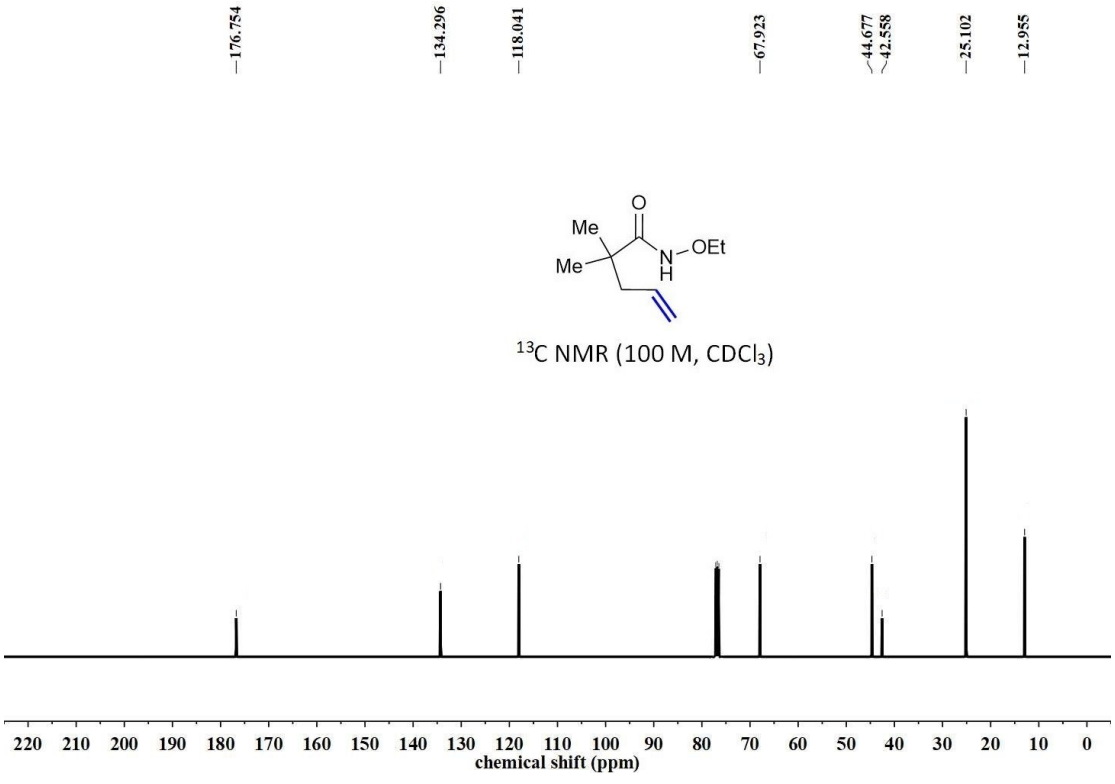


^{13}C NMR (100 M, $CDCl_3$)

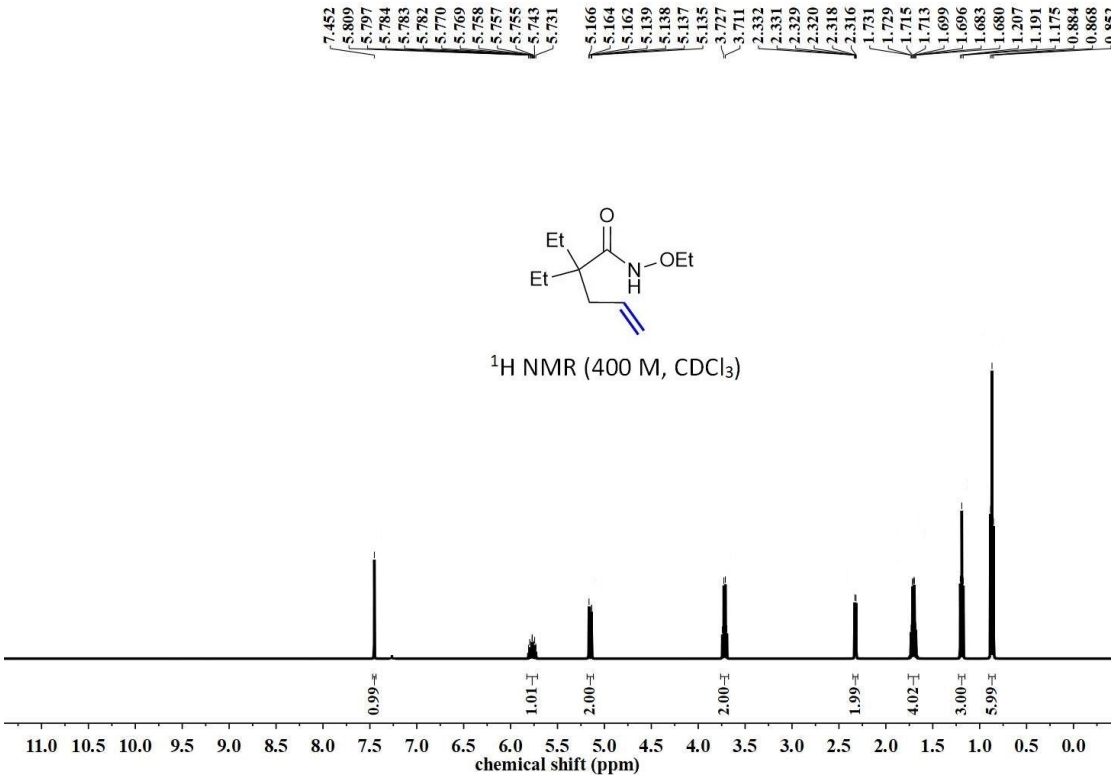


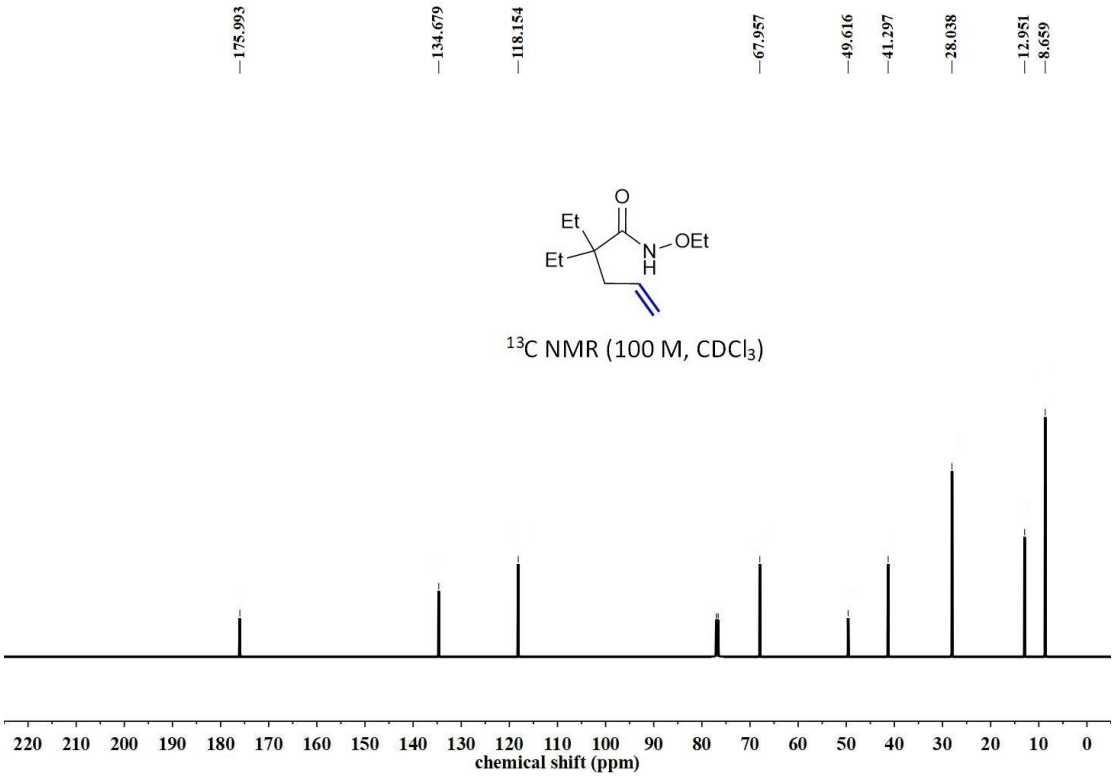


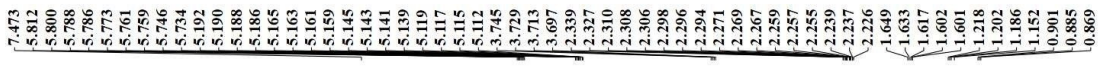
^{1}H NMR (400 M, $CDCl_3$)

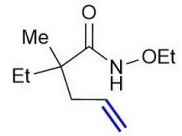


^{13}C NMR (100 M, $CDCl_3$)

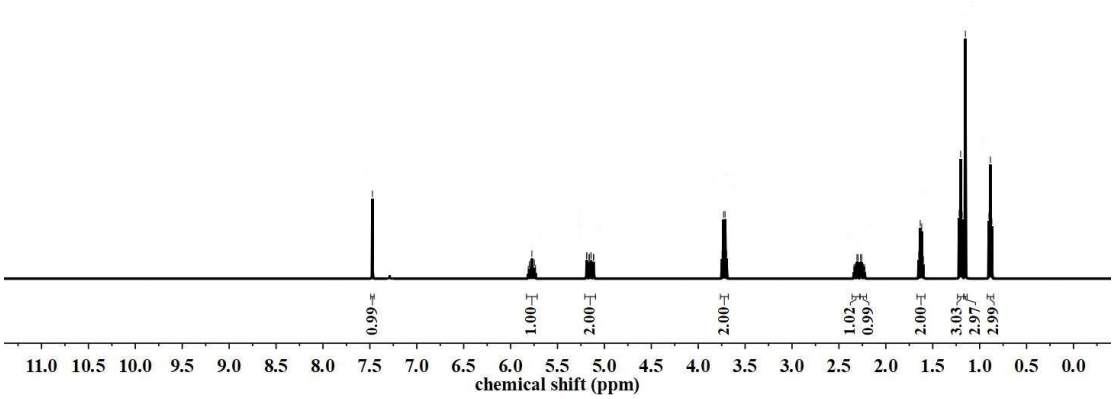

7.452
5.809
5.797
5.784
5.783
5.782
5.770
5.769
5.758
5.757
5.755
5.743
5.731
5.166
5.164
5.162
5.139
5.138
5.137
5.135
3.727
3.711
2.332
2.331
2.329
2.320
2.318
2.316
1.731
1.729
1.715
1.713
1.699
1.696
1.683
1.680
1.207
1.191
1.175
0.884
0.868
O
Et
N
OEt
H
Et
^{1}H NMR (400 M, CDCl$_3$)
0.99
1.01
2.00
2.00
1.99
4.02
3.00
5.99
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
chemical shift (ppm)

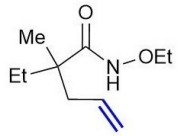

175.993
134.679
118.154
67.957
49.616
41.297
28.038
12.951
8.659
O
Et
N
OEt
H
Et
^{13}C NMR (100 M, CDCl$_3$)
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
chemical shift (ppm)



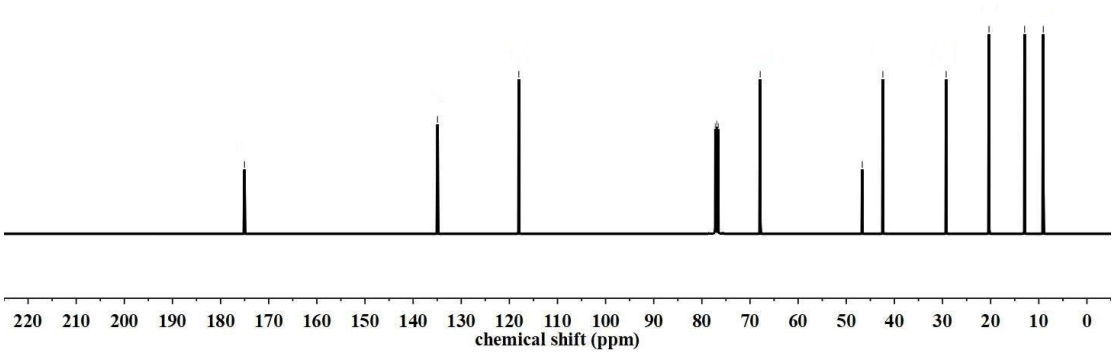


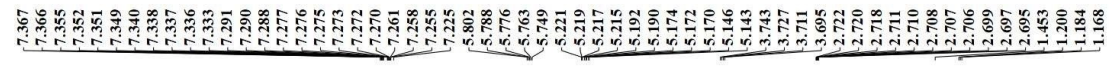
^{1}H NMR (400 M, $CDCl_3$)

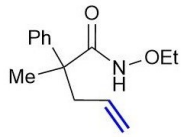




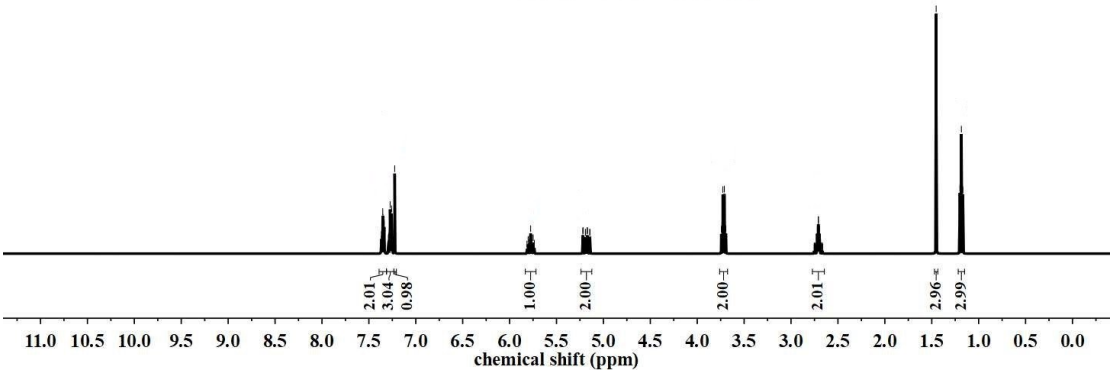
^{13}C NMR (100 M, $CDCl_3$)

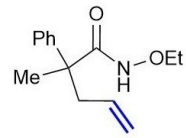




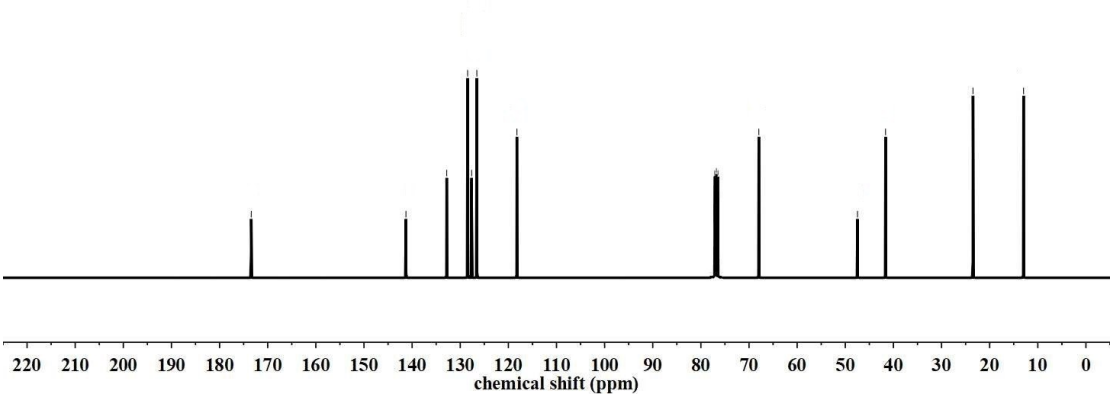


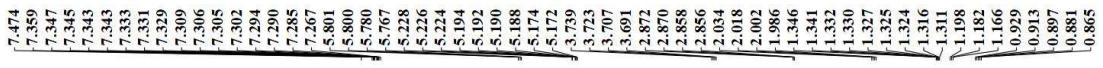
^{1}H NMR (400 M, $CDCl_3$)



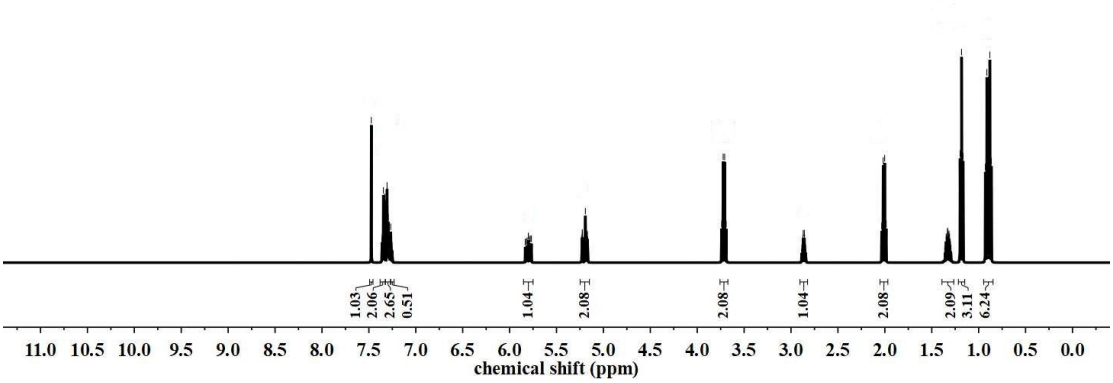


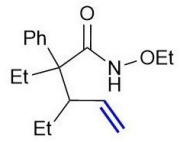
^{13}C NMR (100 M, $CDCl_3$)



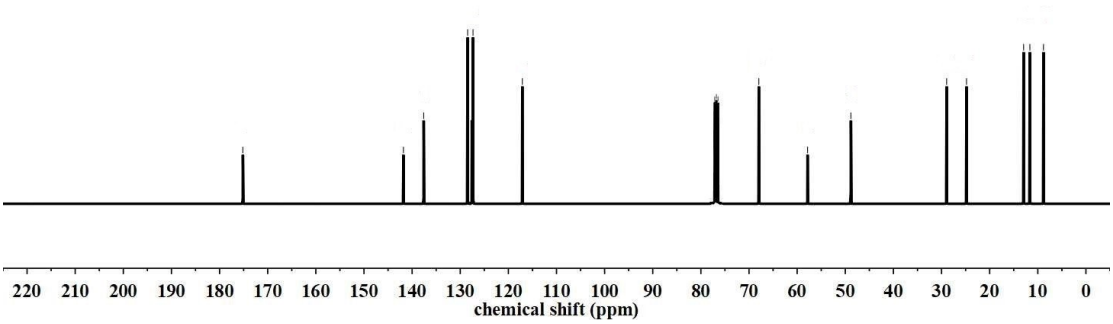


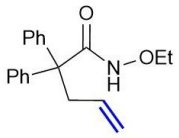
^{1}H NMR (400 M, $CDCl_3$)



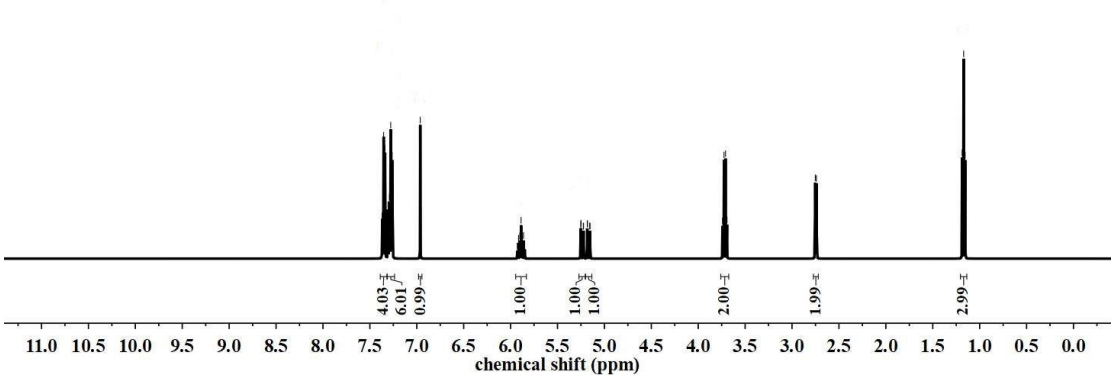


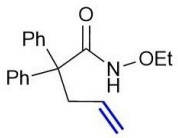
^{13}C NMR (100 M, $CDCl_3$)



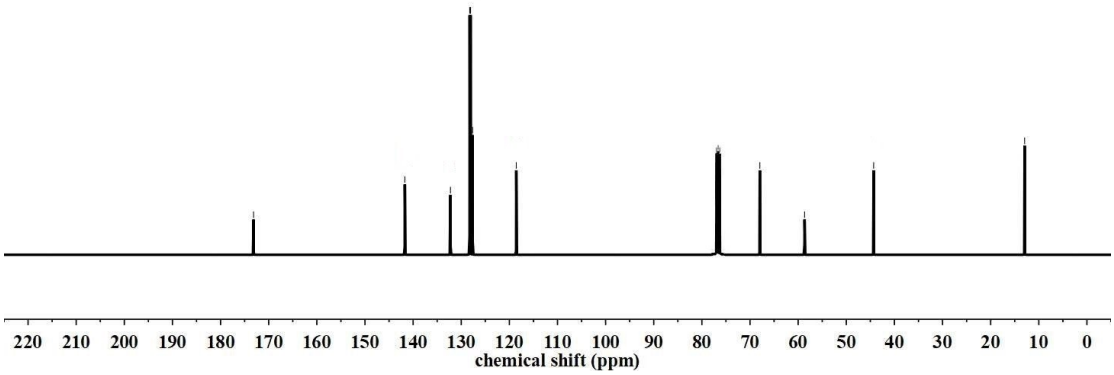


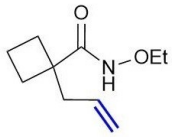
^{1}H NMR (400 M, $CDCl_3$)



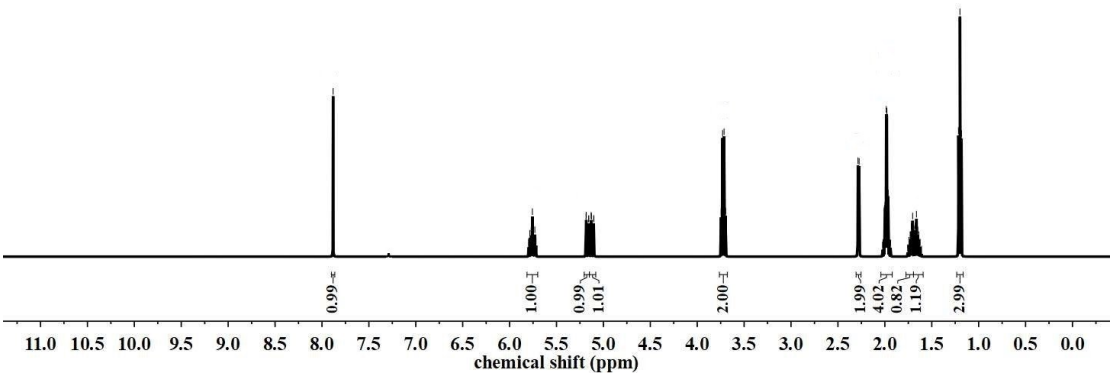


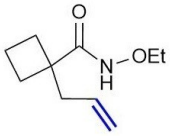
^{13}C NMR (100 M, $CDCl_3$)





^{1}H NMR (400 M, $CDCl_3$)





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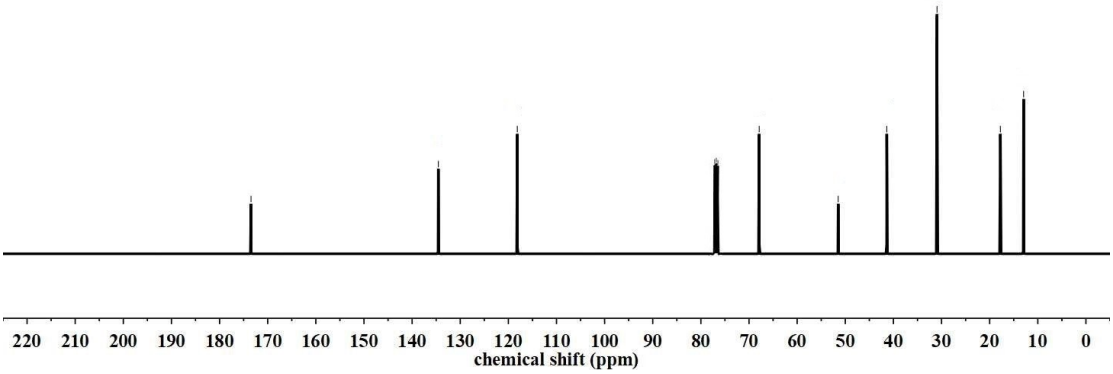

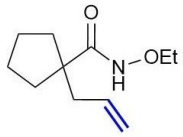

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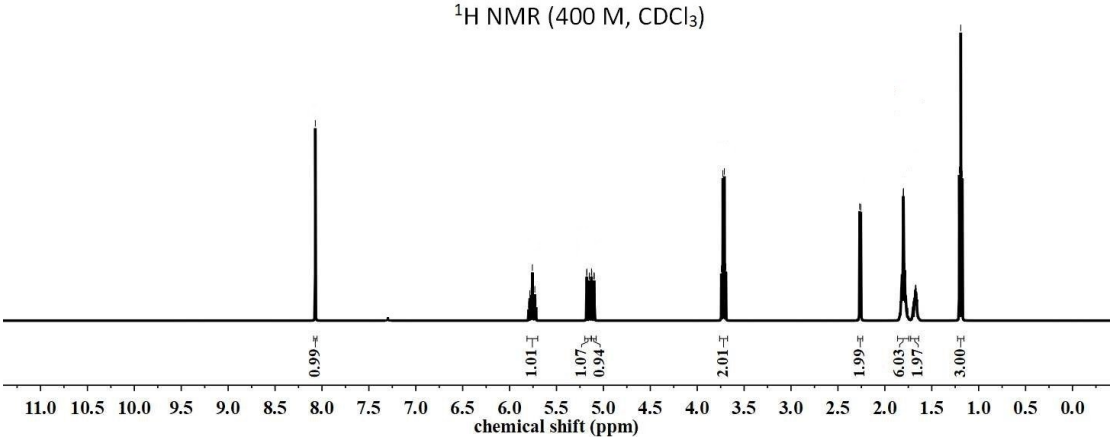
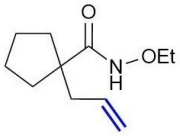
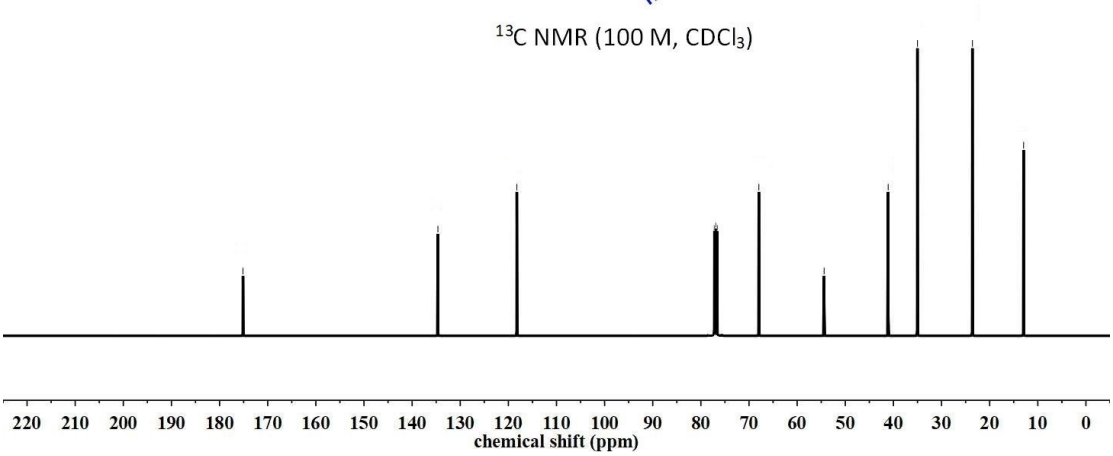
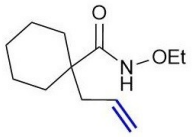


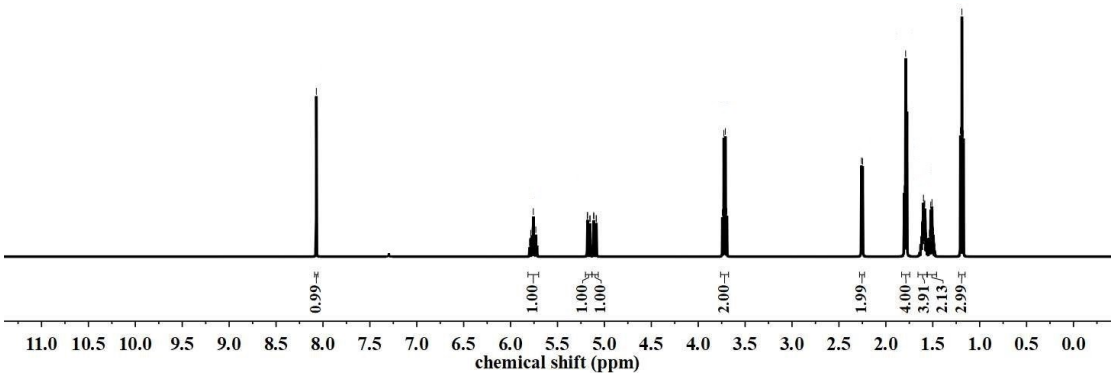


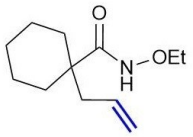
^{13}C NMR (100 M, $CDCl_3$)



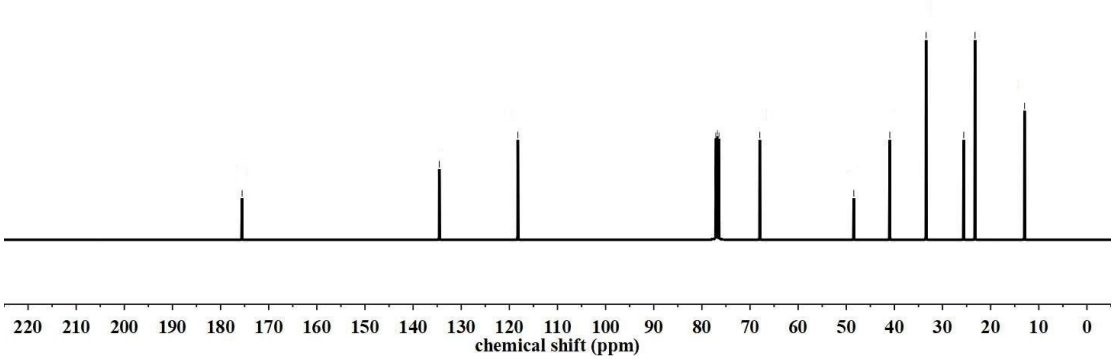


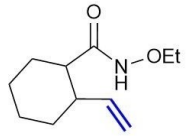
^{1}H NMR (400 M, $CDCl_3$)



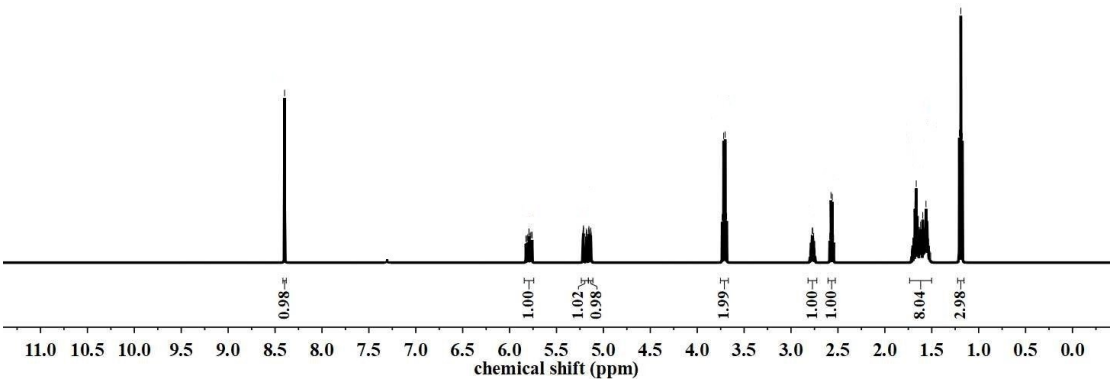


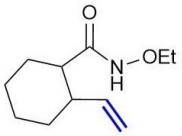
^{13}C NMR (100 M, $CDCl_3$)



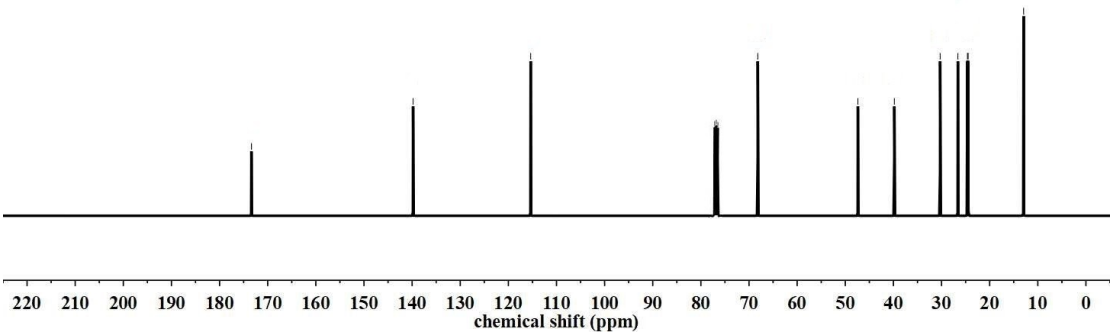


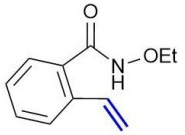
^{1}H NMR (400 M, $CDCl_3$)



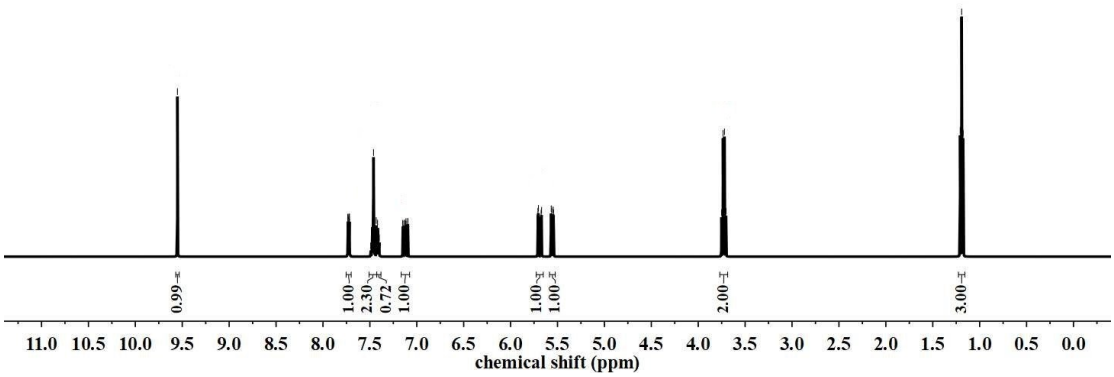


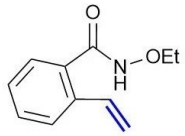
^{13}C NMR (100 M, $CDCl_3$)



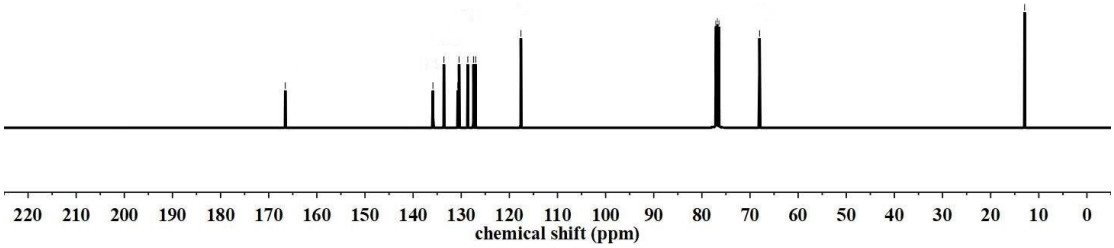


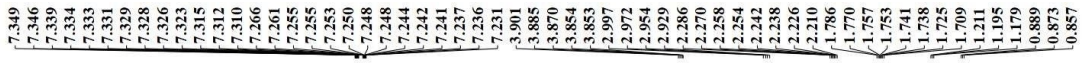
^{1}H NMR (400 M, $CDCl_3$)

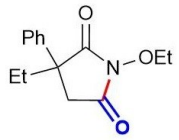




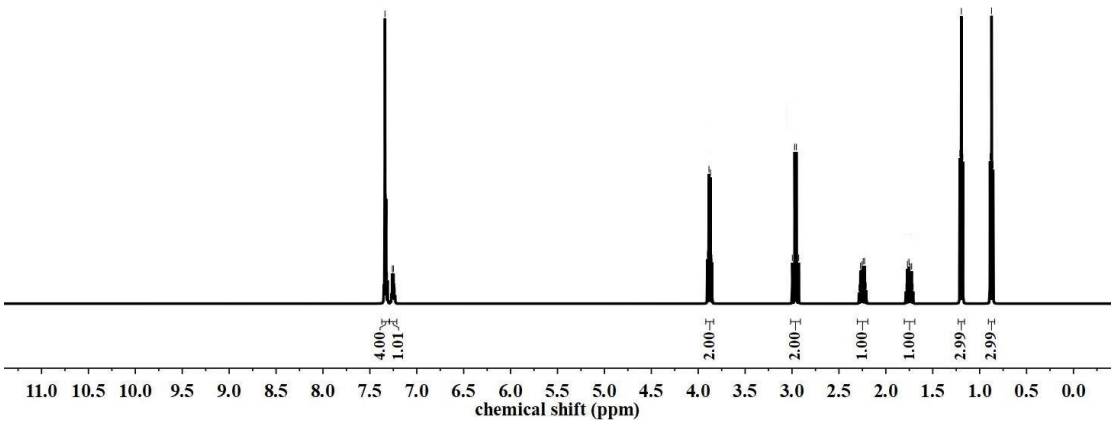
^{13}C NMR (100 M, $CDCl_3$)

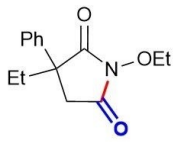




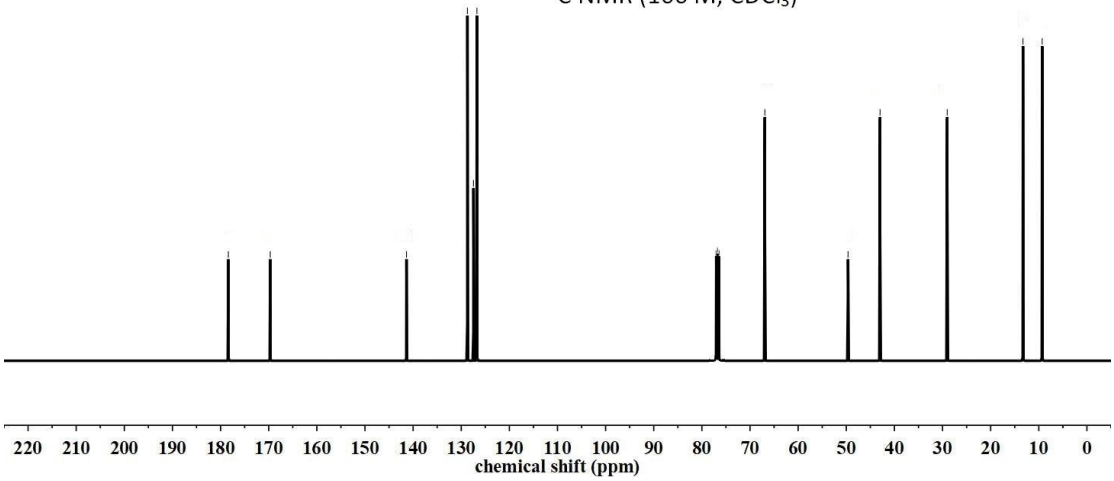


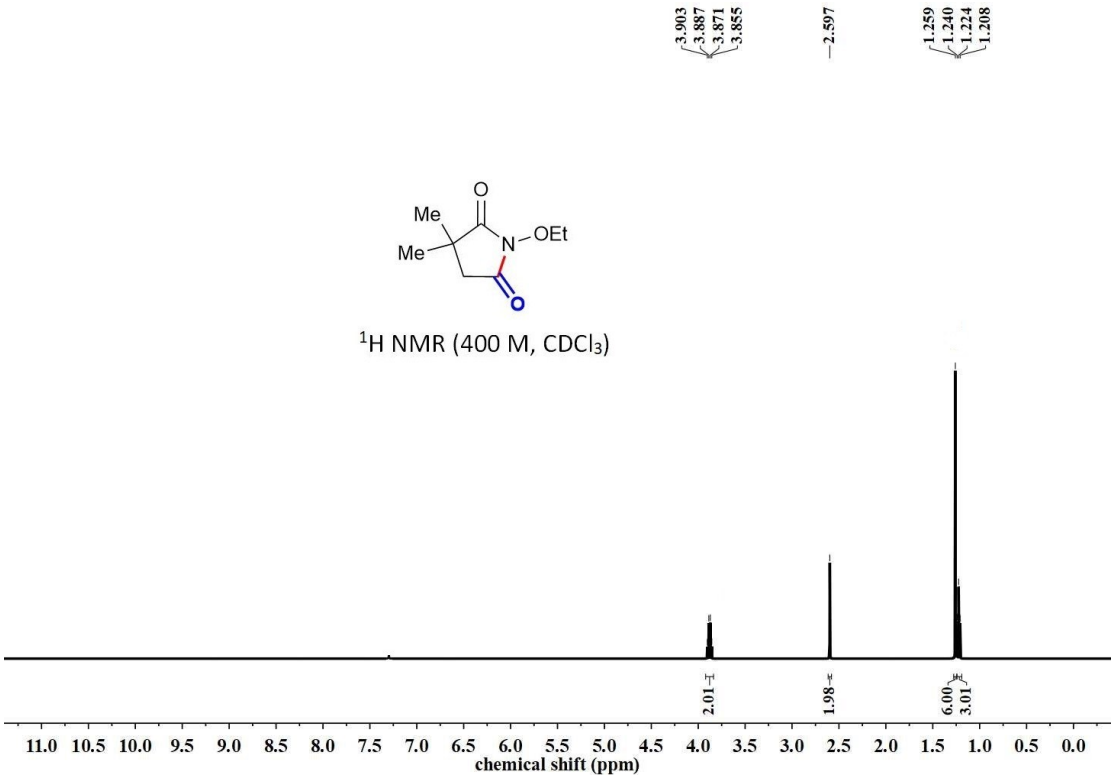
^{1}H NMR (400 M, $CDCl_3$)



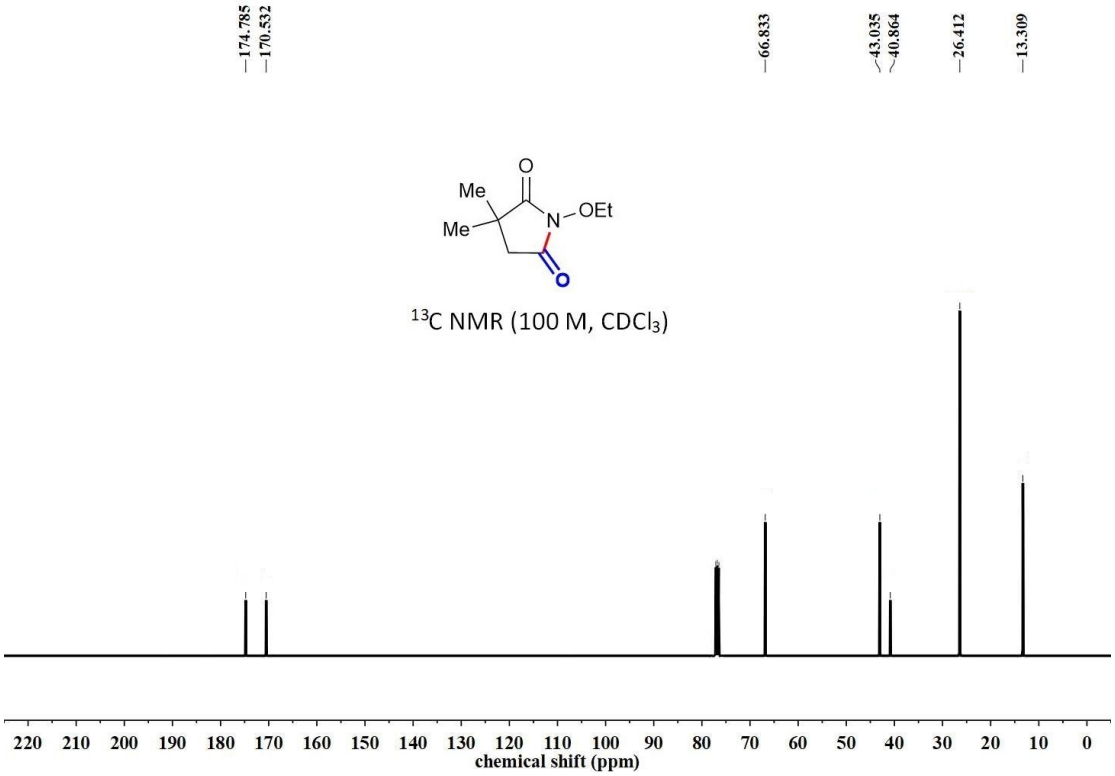


^{13}C NMR (100 M, $CDCl_3$)

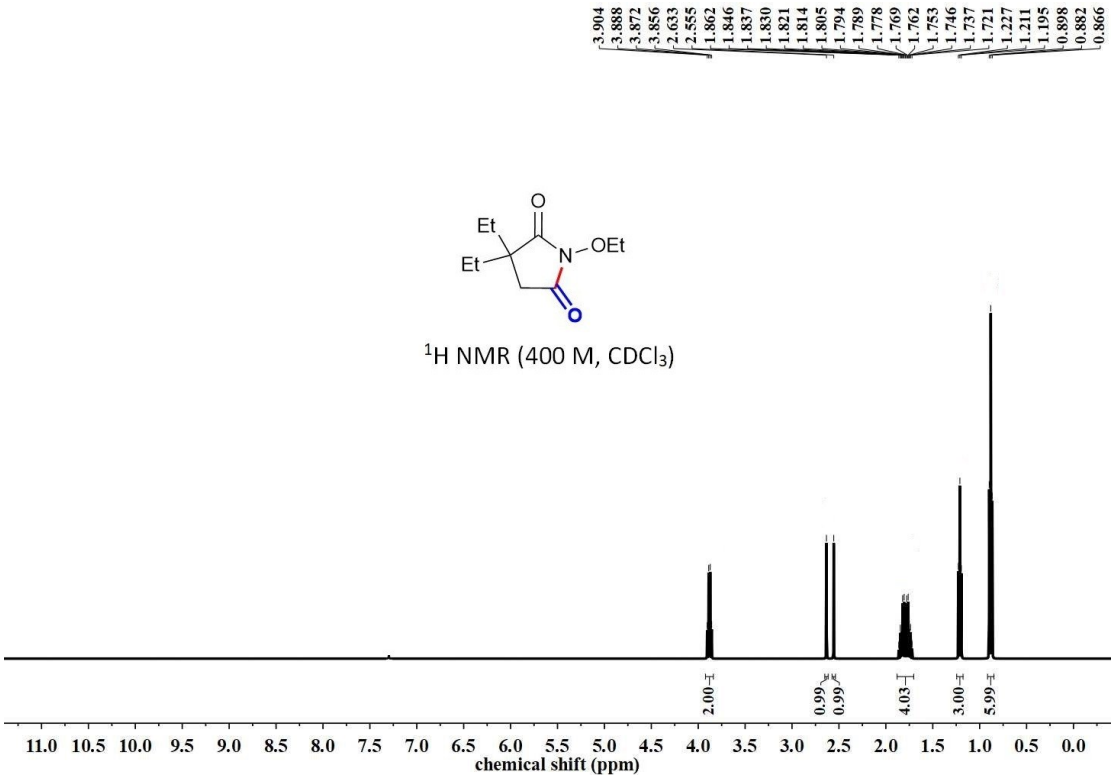




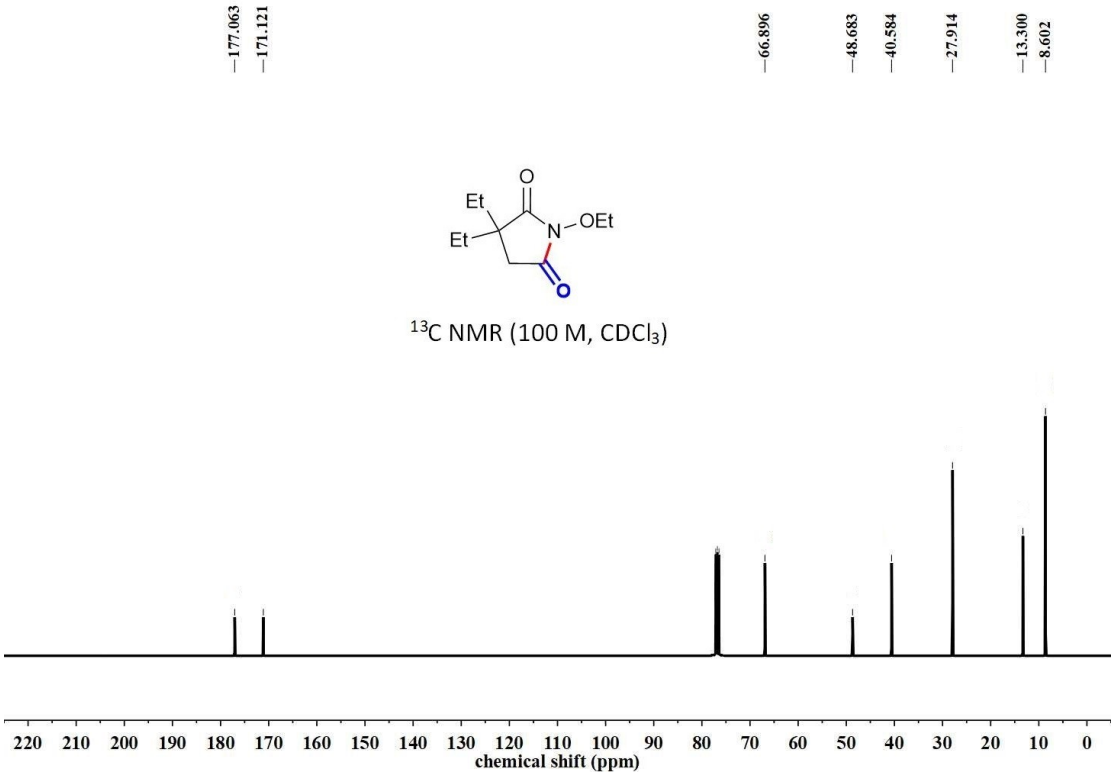
^{1}H NMR (400 M, $CDCl_3$)



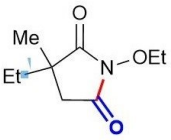
^{13}C NMR (100 M, $CDCl_3$)



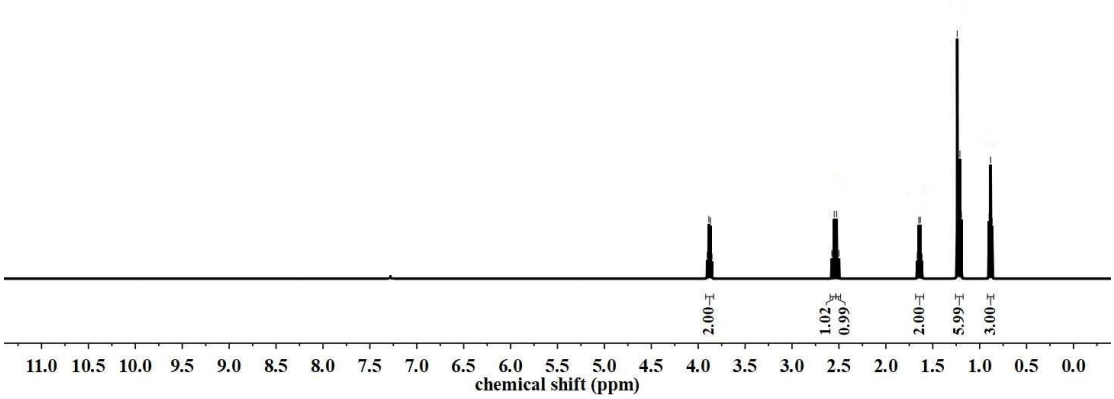
^{1}H NMR (400 M, $CDCl_3$)

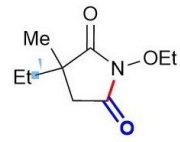


^{13}C NMR (100 M, $CDCl_3$)

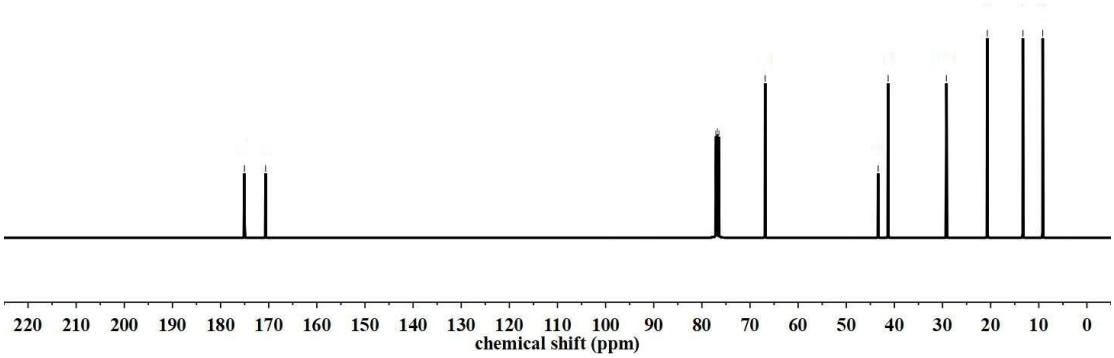


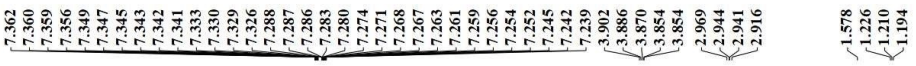
^{1}H NMR (400 M, $CDCl_3$)

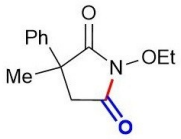




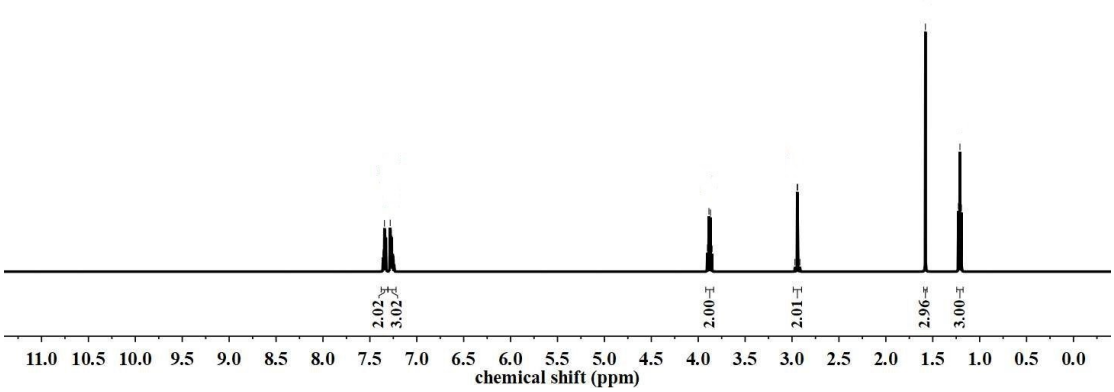
^{13}C NMR (100 M, $CDCl_3$)

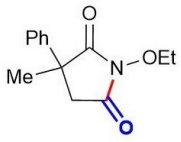




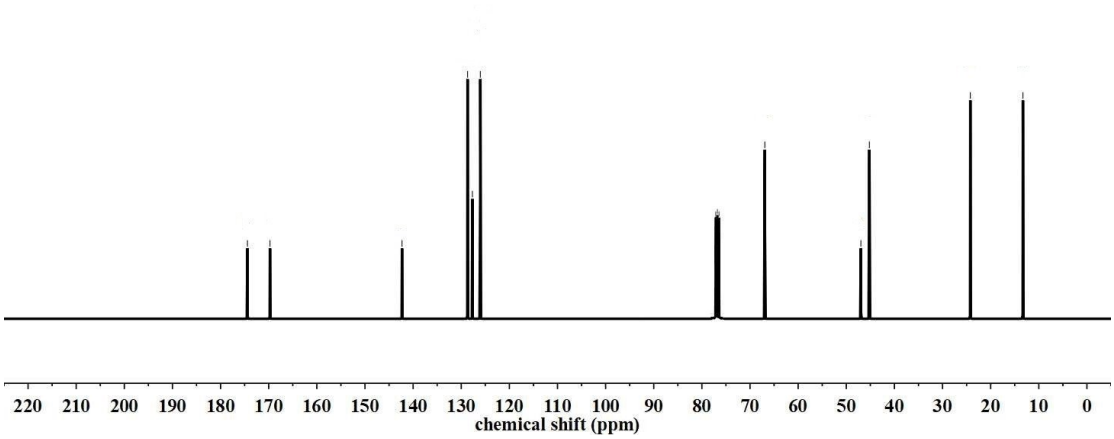


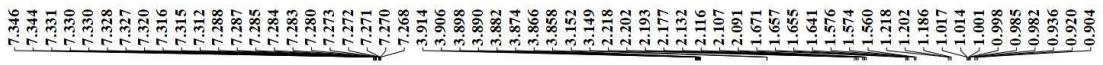
^{1}H NMR (400 M, $CDCl_3$)

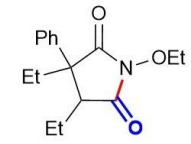




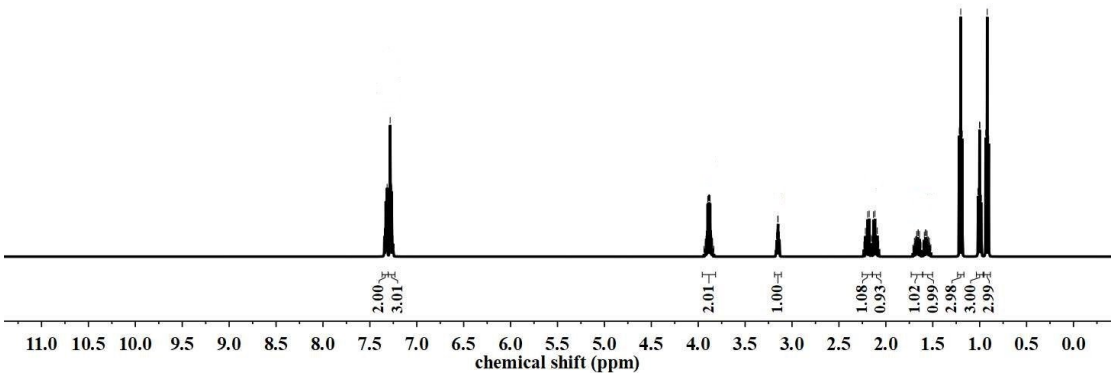
^{13}C NMR (100 M, $CDCl_3$)

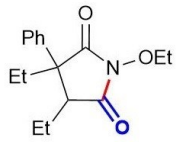




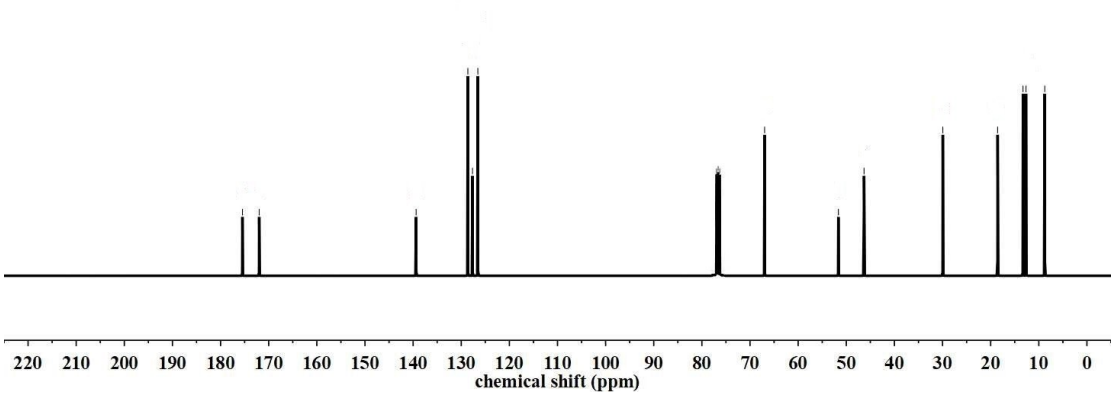


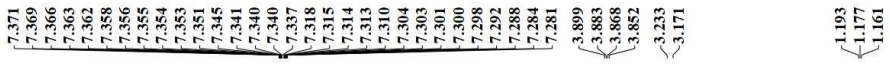
^{1}H NMR (400 M, $CDCl_3$)

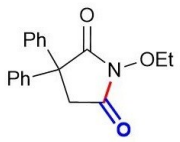




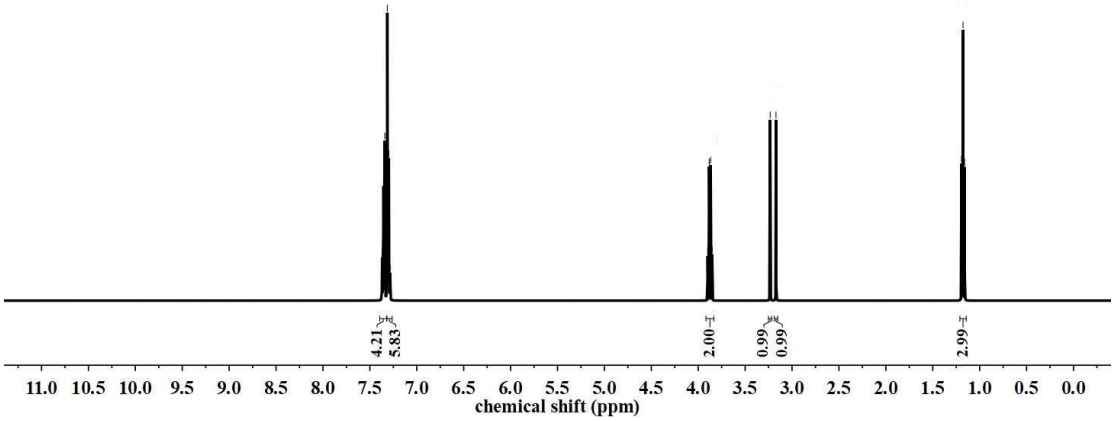
^{13}C NMR (100 M, $CDCl_3$)

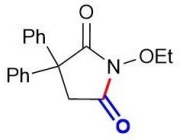




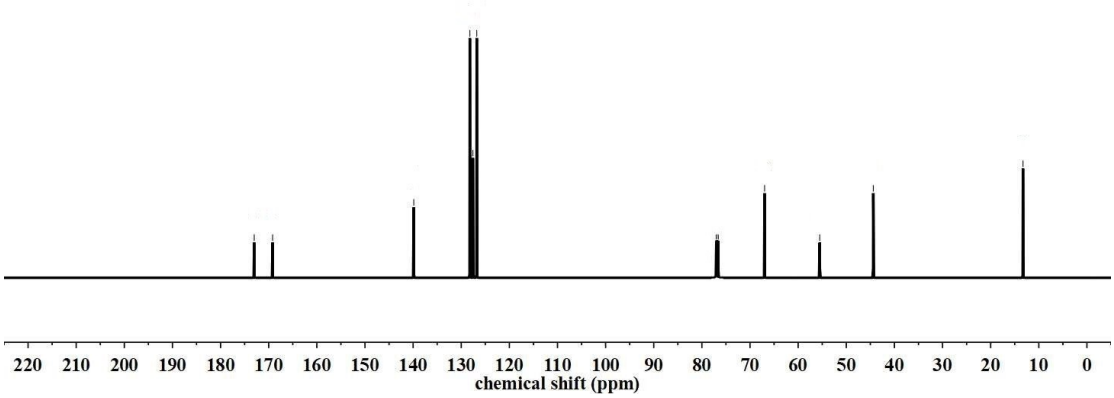


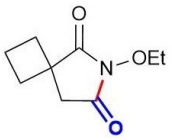
^{1}H NMR (400 M, $CDCl_3$)





^{13}C NMR (100 M, $CDCl_3$)





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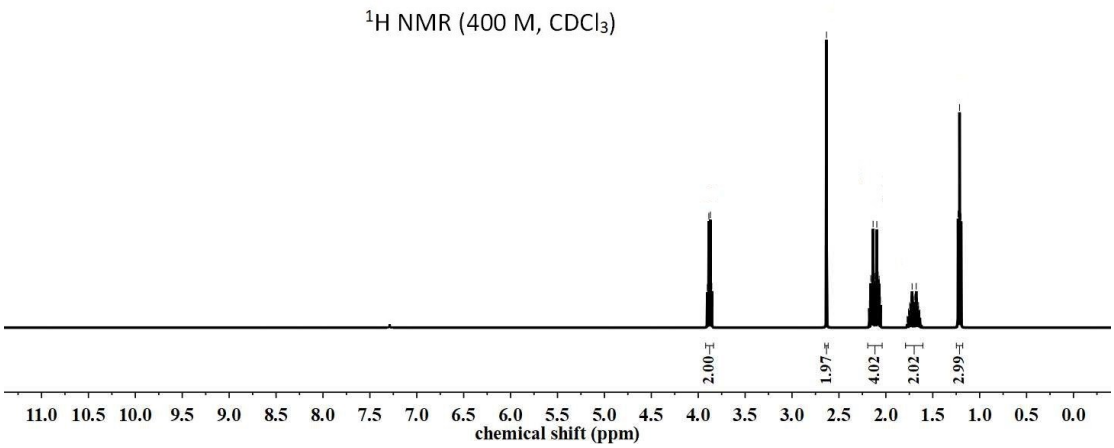
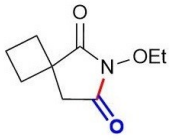
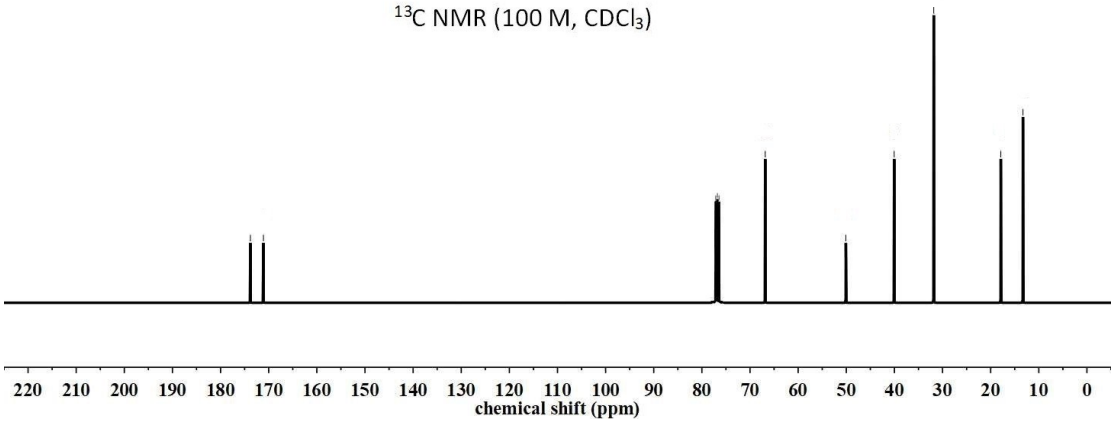
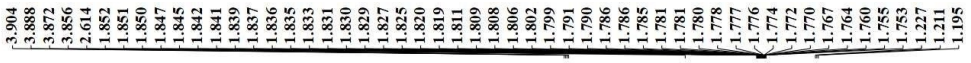
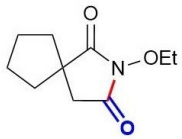




^{13}C NMR (100 M, $CDCl_3$)







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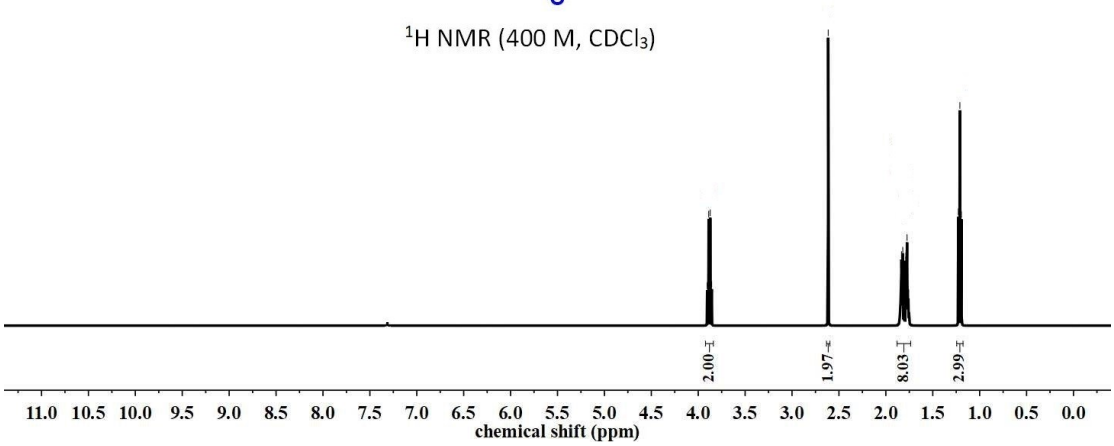
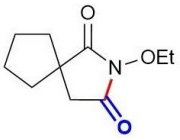
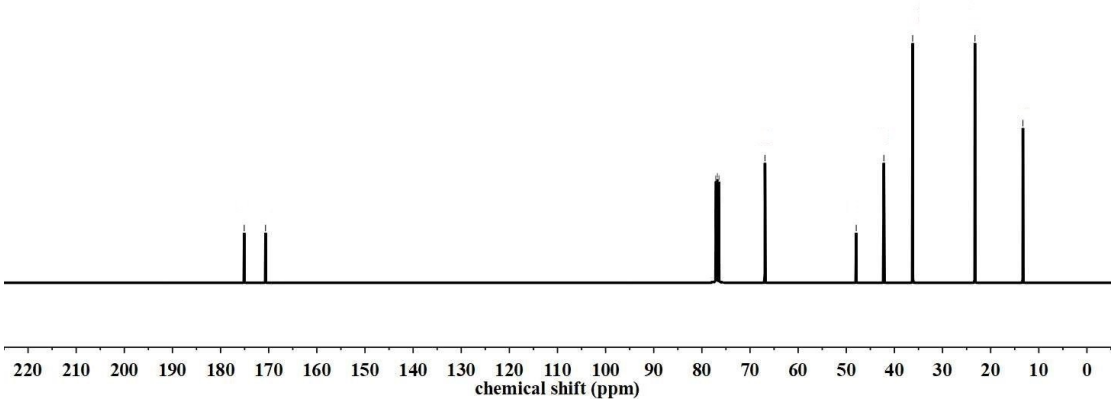
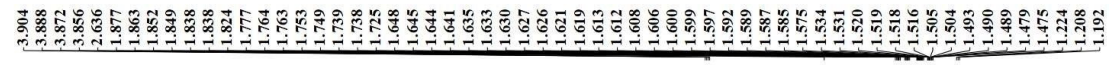
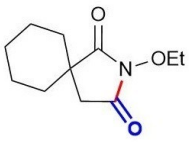




^{13}C NMR (100 M, $CDCl_3$)







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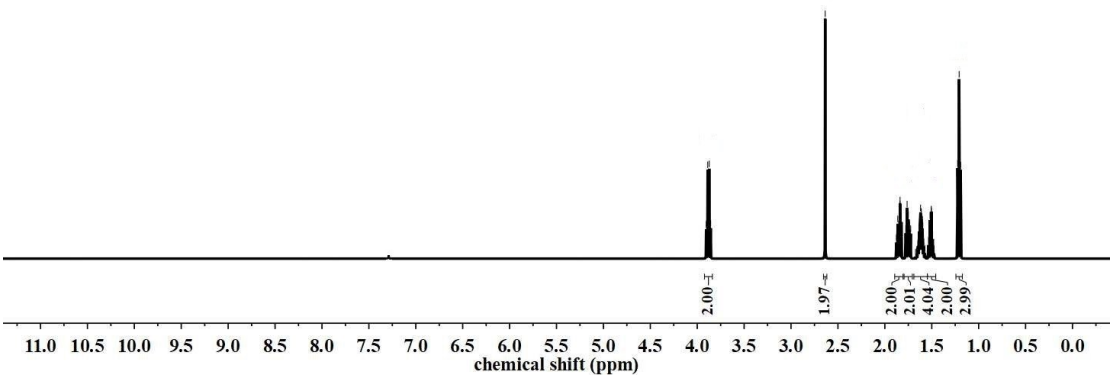
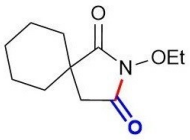
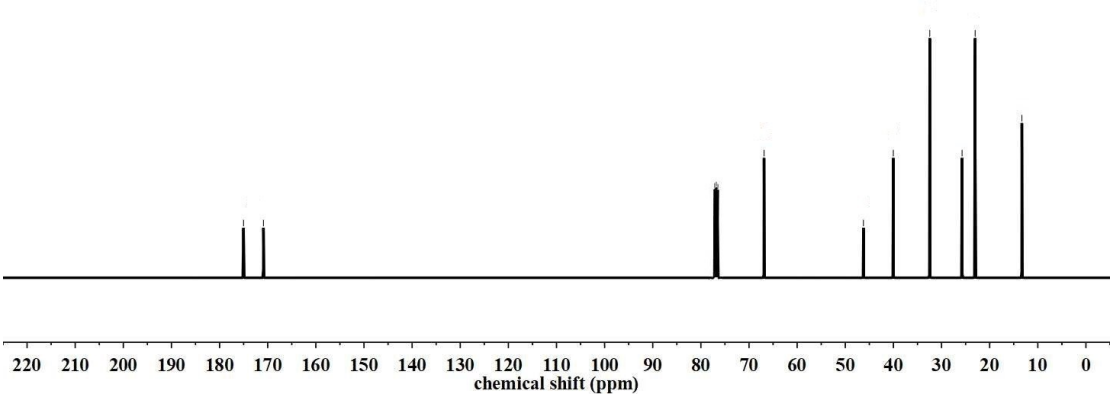
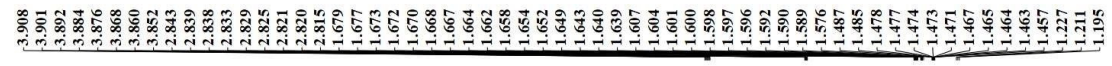




^{13}C NMR (100 M, $CDCl_3$)





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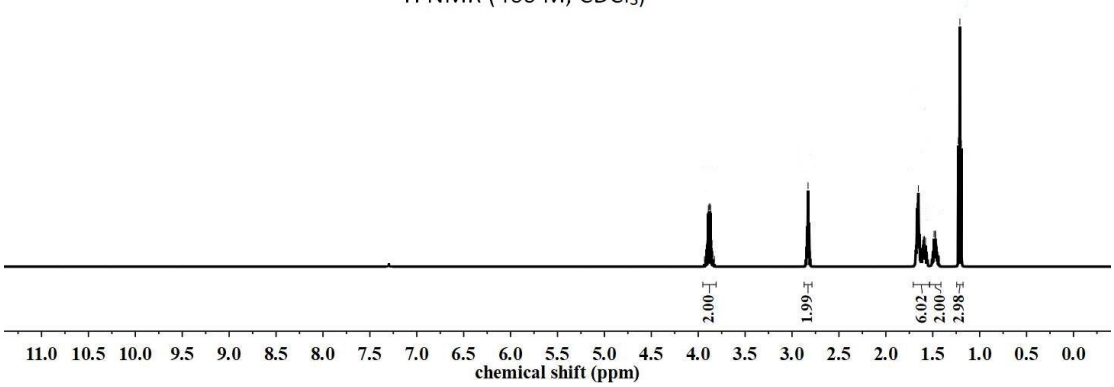

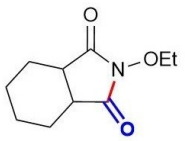

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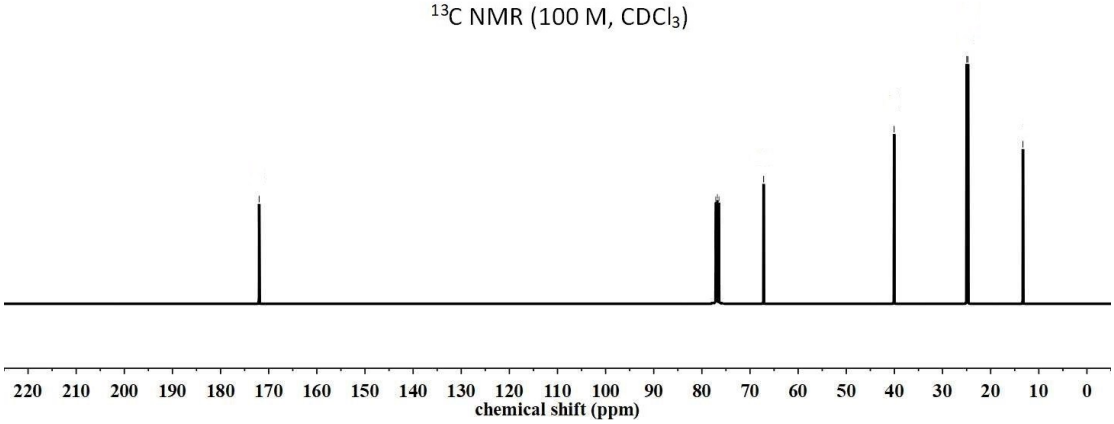

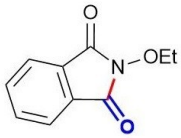

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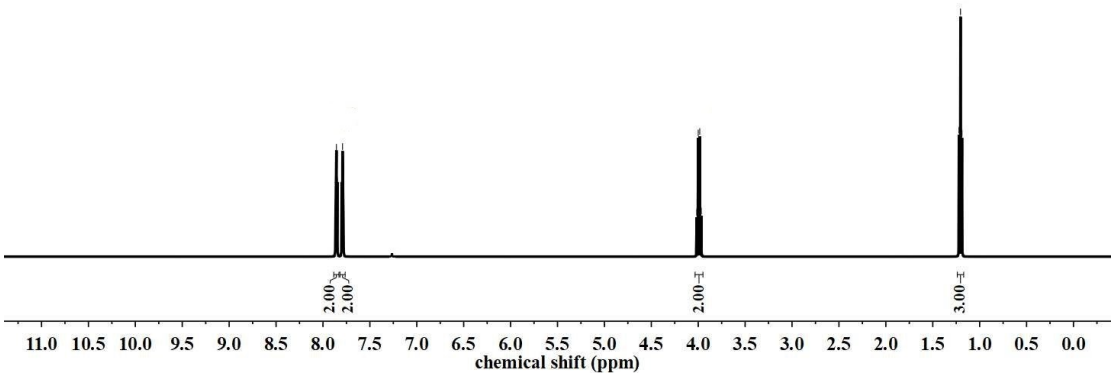

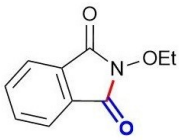

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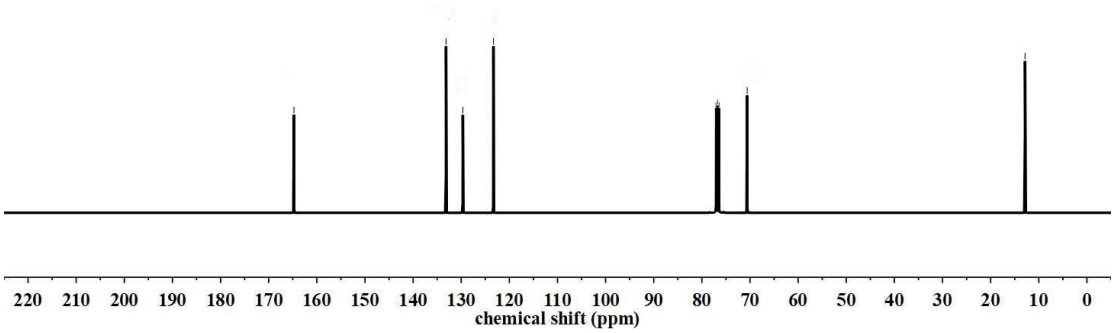

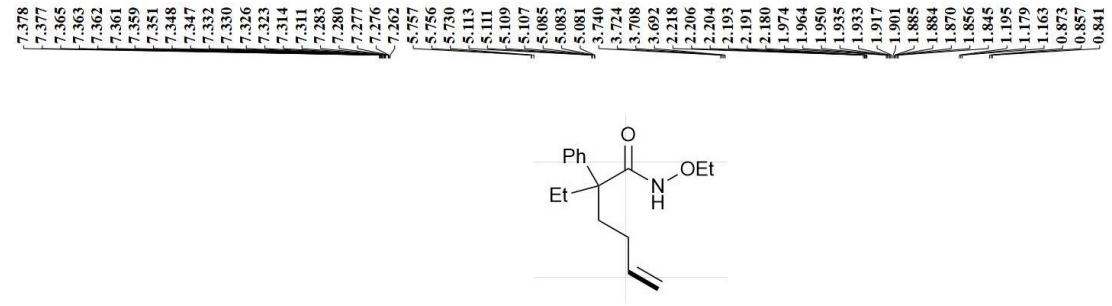

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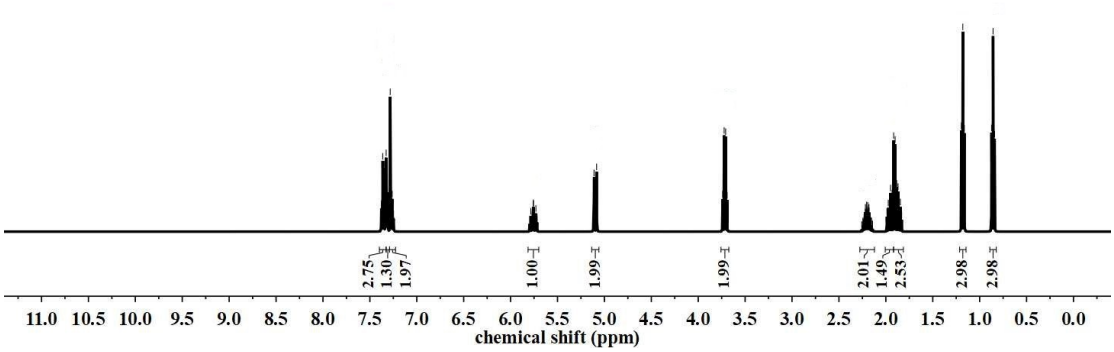
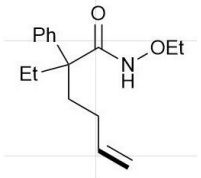
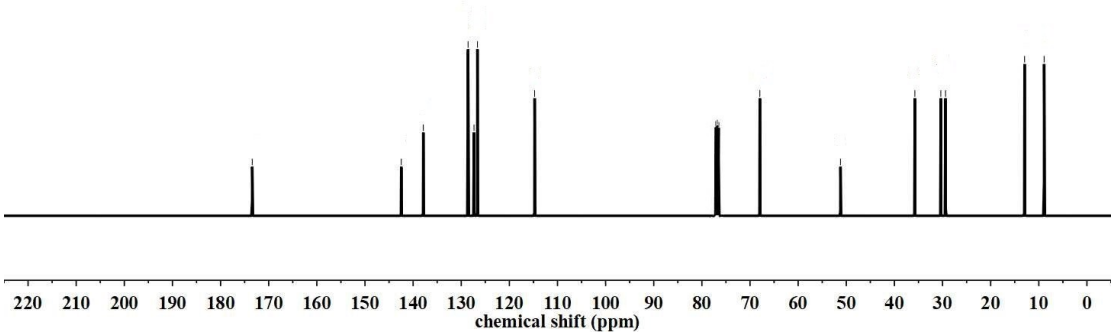
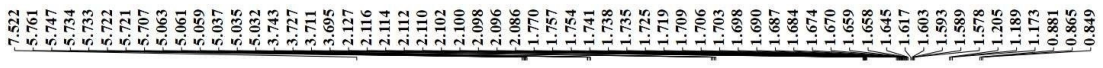
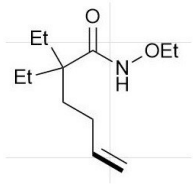




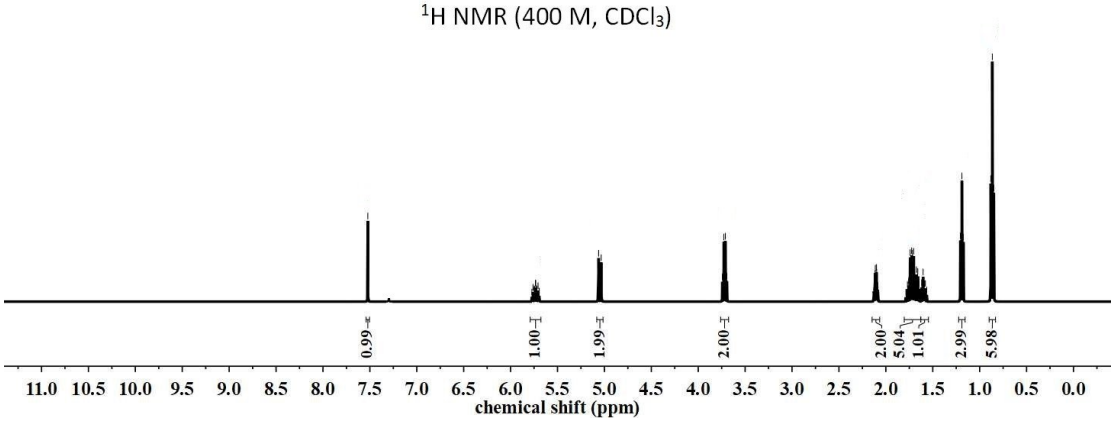
^{13}C NMR (100 M, $CDCl_3$)

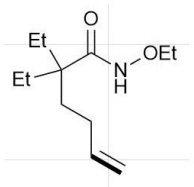




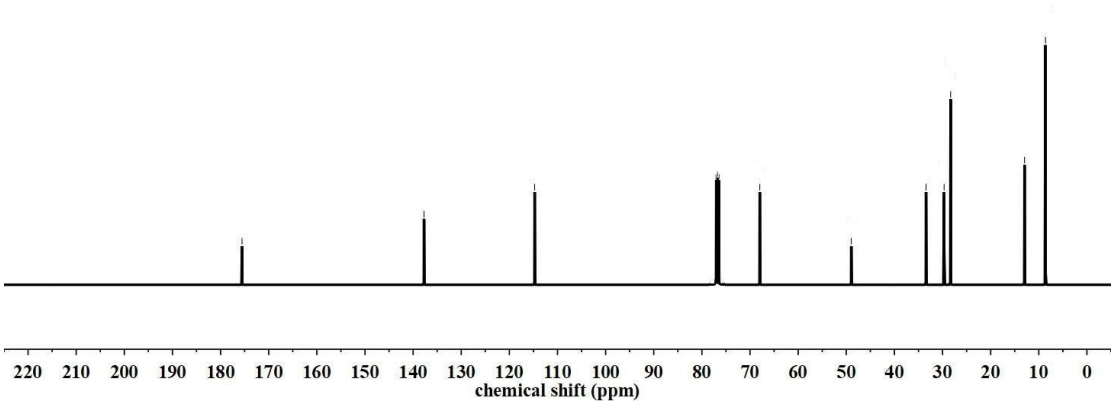


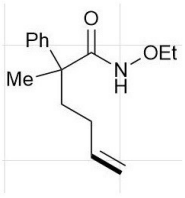
^{1}H NMR (400 M, $CDCl_3$)





^{13}C NMR (100 M, $CDCl_3$)





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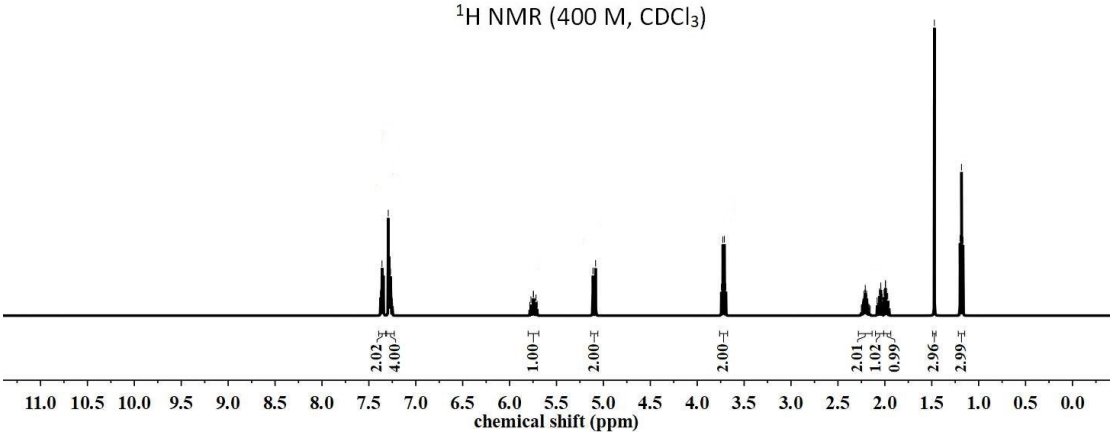
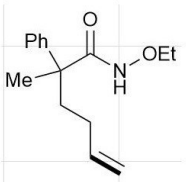
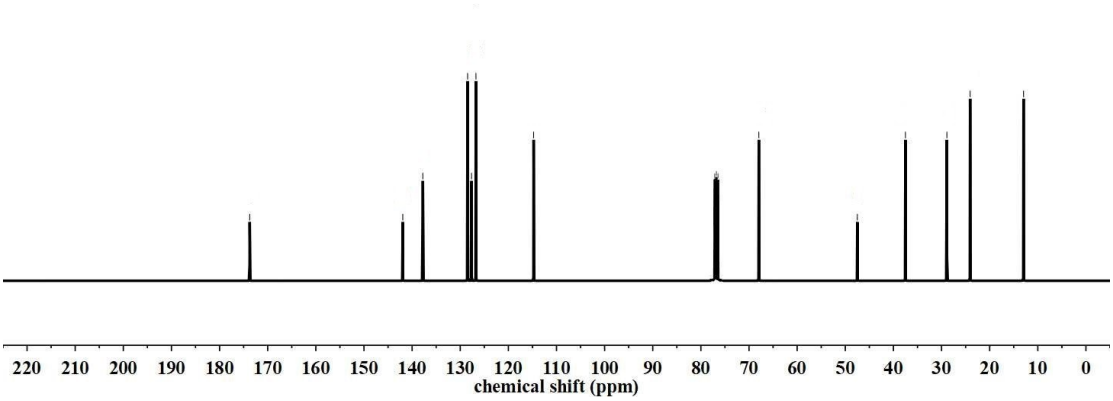
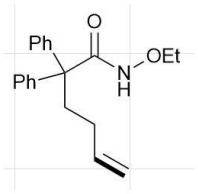


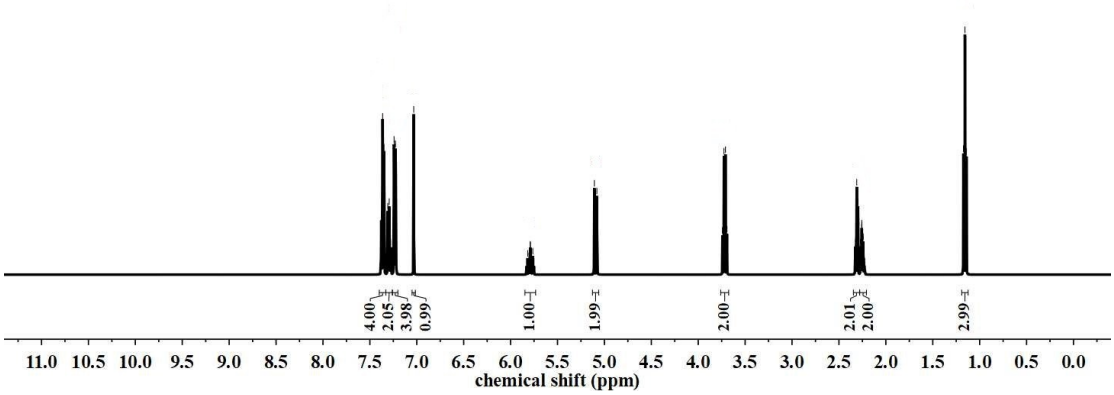


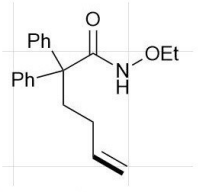
^{13}C NMR (100 M, $CDCl_3$)





^{1}H NMR (400 M, $CDCl_3$)





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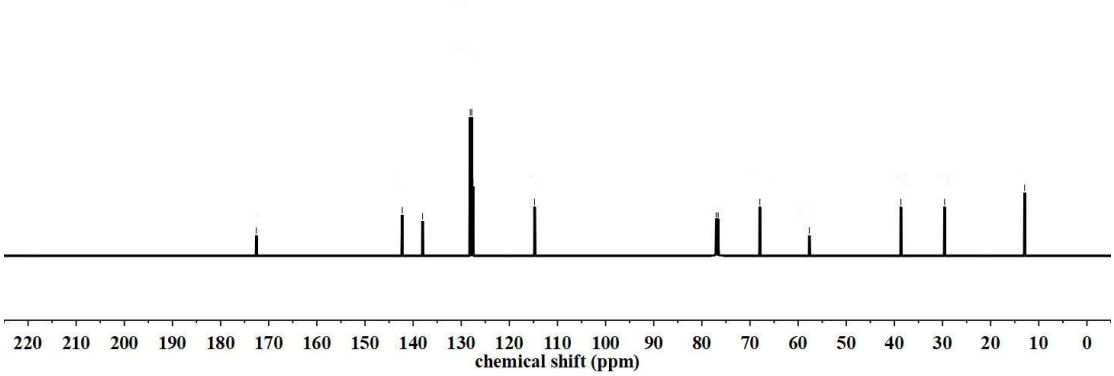

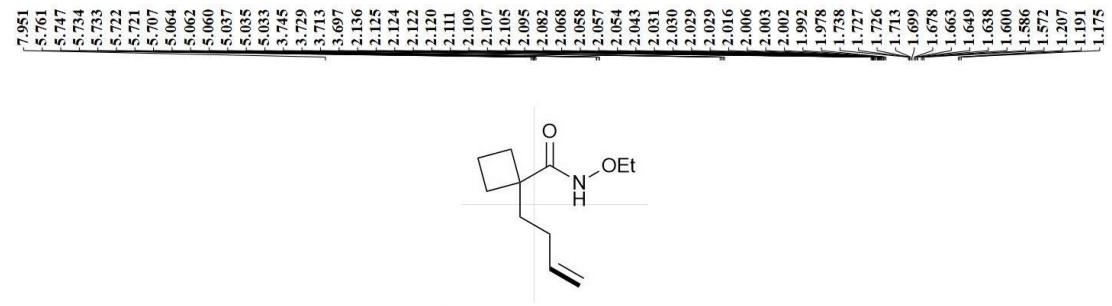

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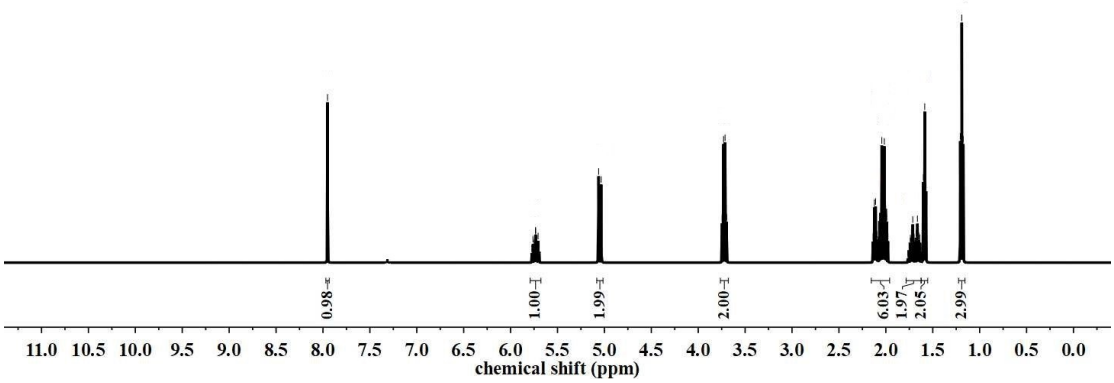
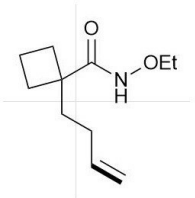
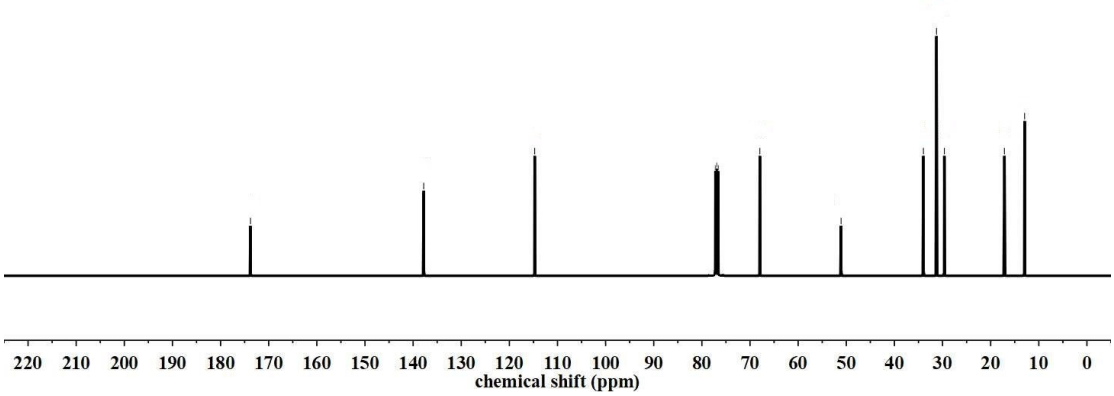
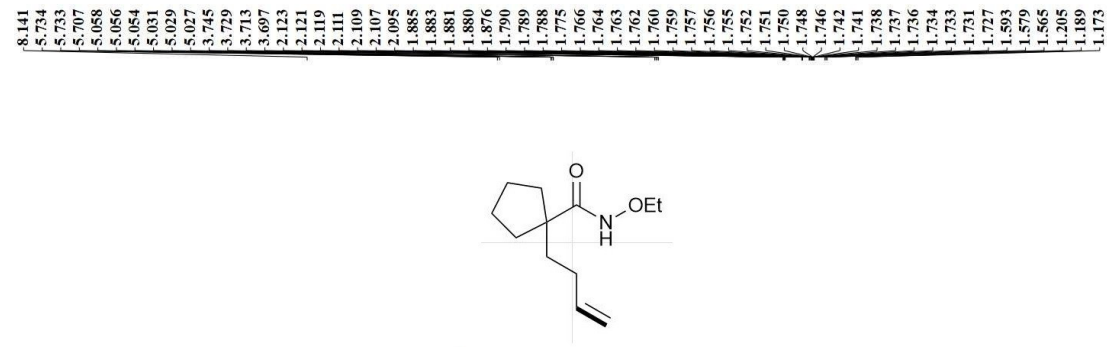


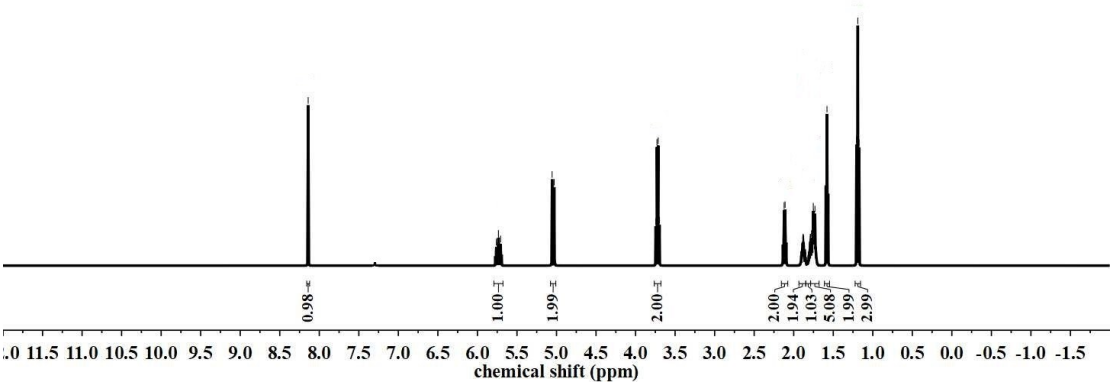


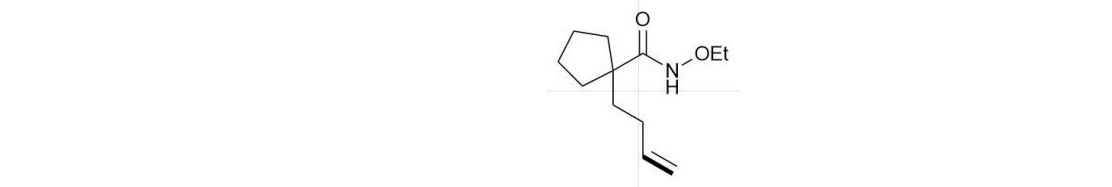
^{13}C NMR (100 M, $CDCl_3$)



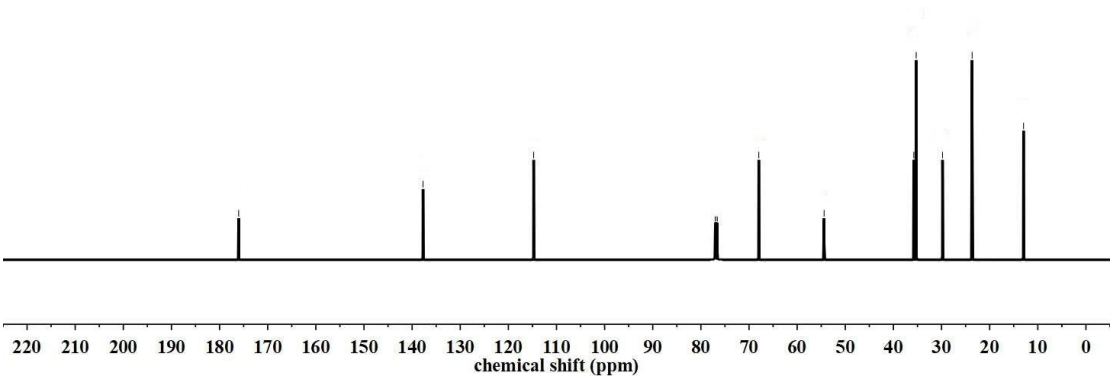


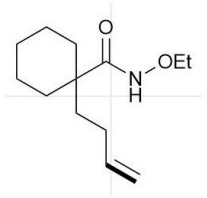
^{1}H NMR (400 M, $CDCl_3$)



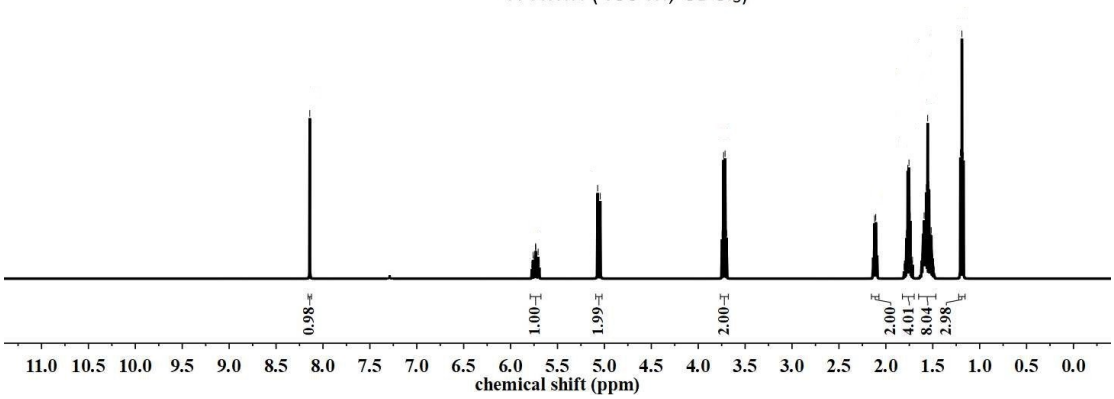


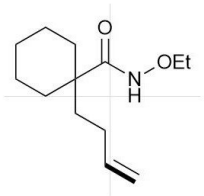
^{13}C NMR (100 M, $CDCl_3$)



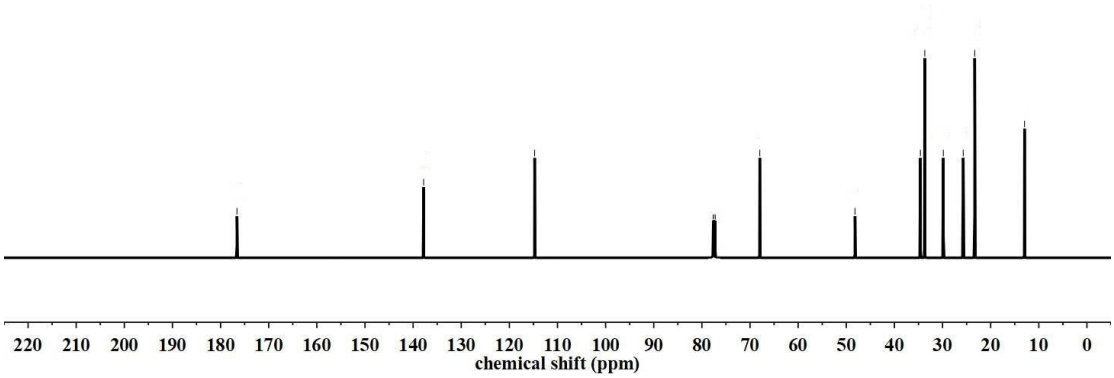


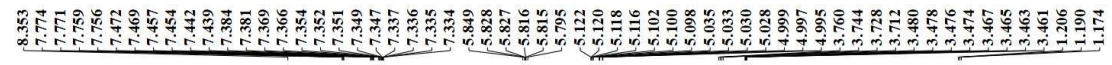
^{1}H NMR (400 M, $CDCl_3$)

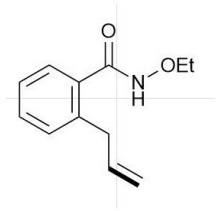




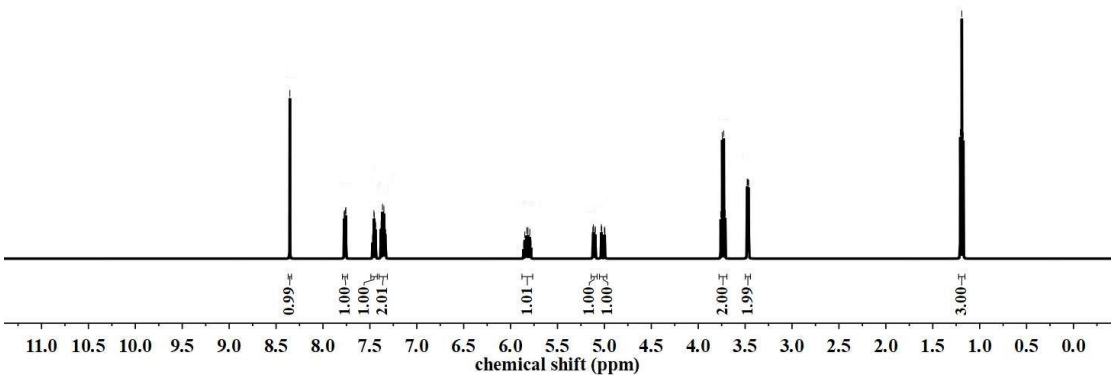
^{13}C NMR (100 M, $CDCl_3$)

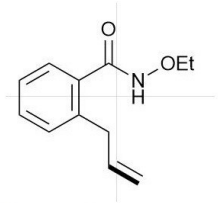




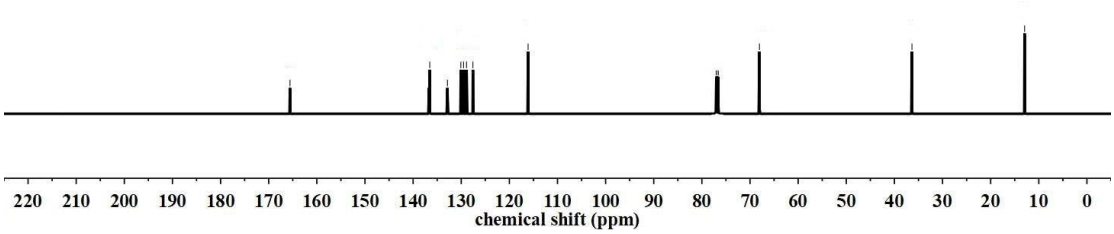


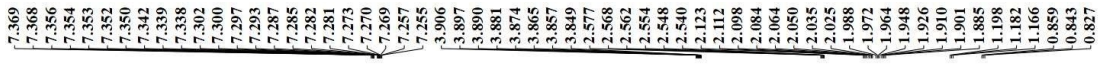
^{1}H NMR (400 M, $CDCl_3$)

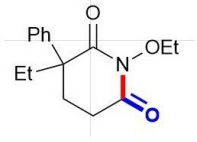




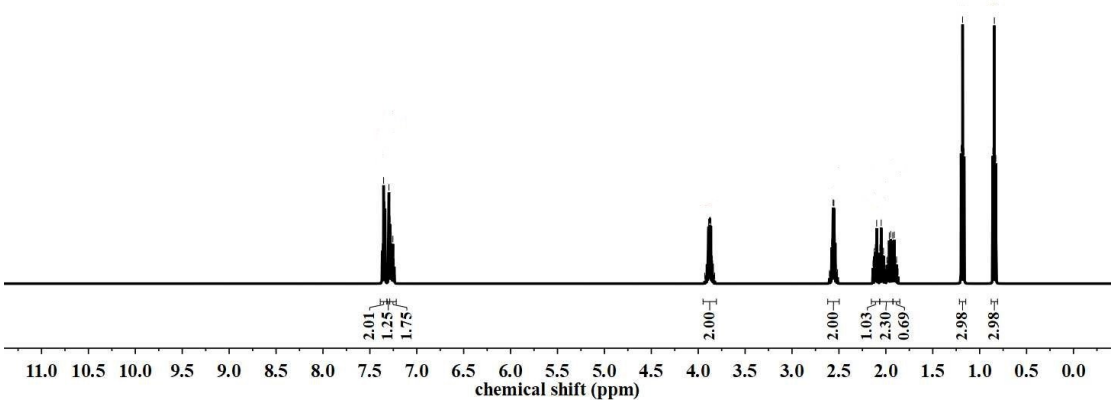
^{13}C NMR (100 M, $CDCl_3$)

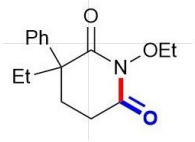




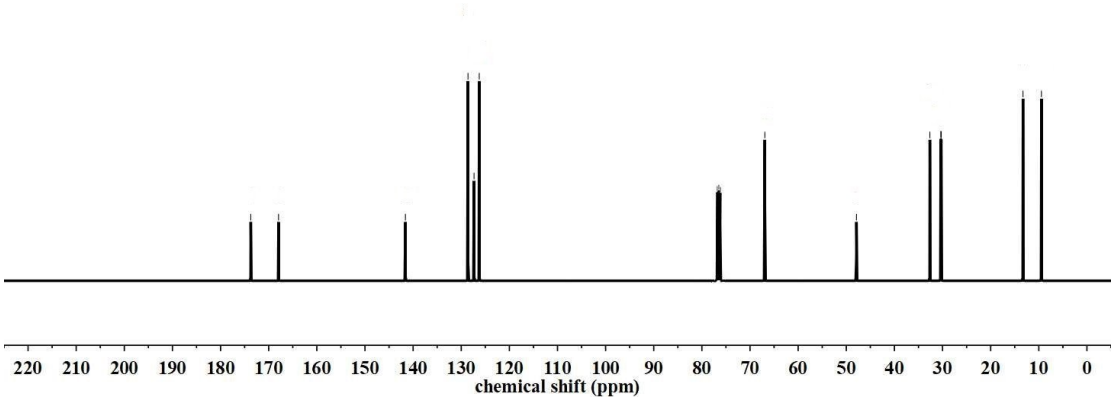


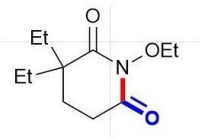
^{1}H NMR (400 M, $CDCl_3$)





^{13}C NMR (100 M, $CDCl_3$)





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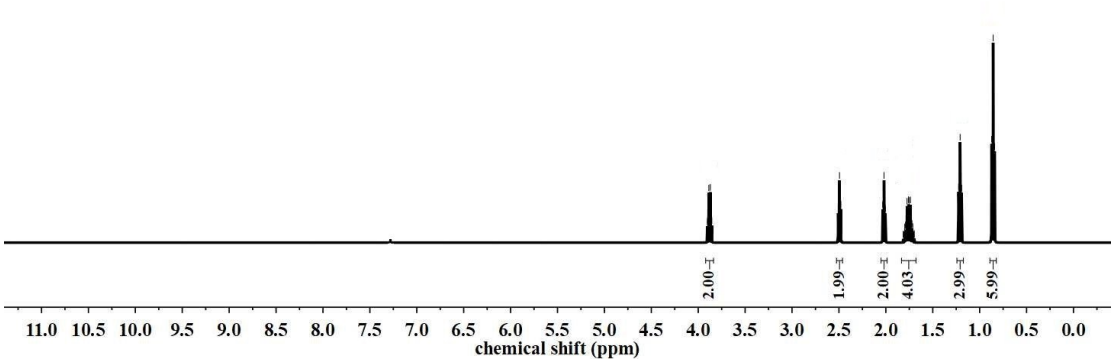
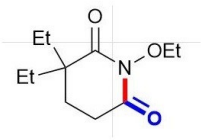
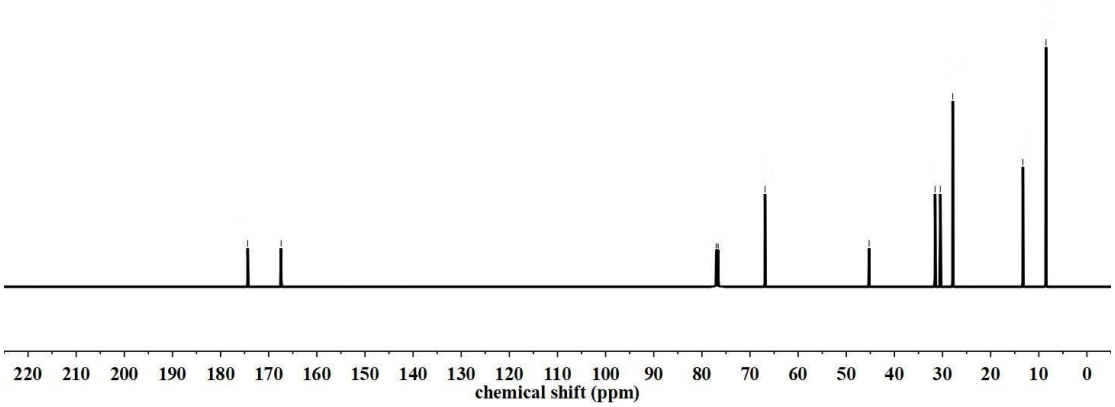
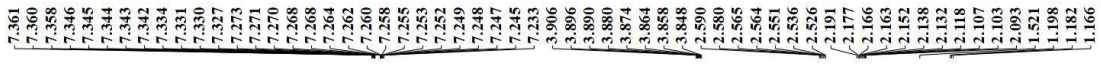
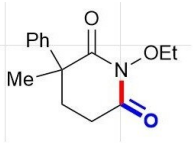




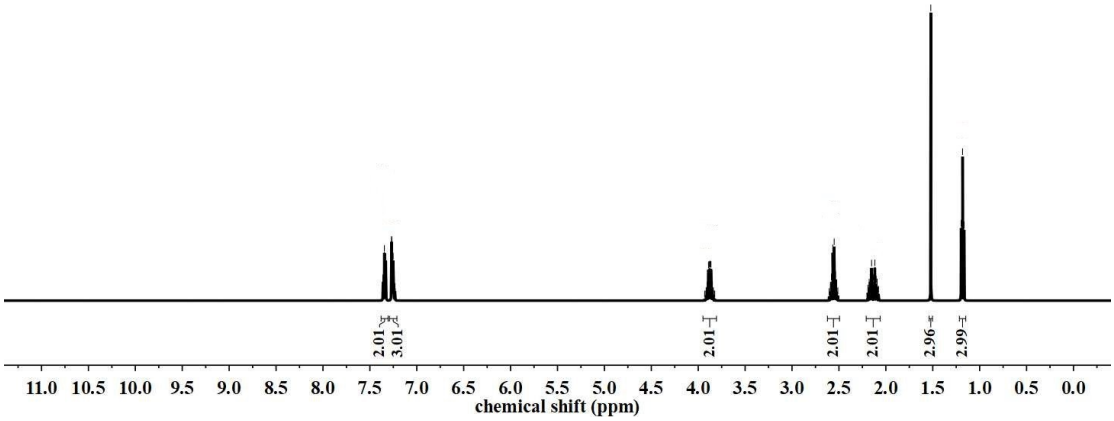
^{13}C NMR (100 M, $CDCl_3$)

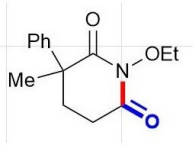




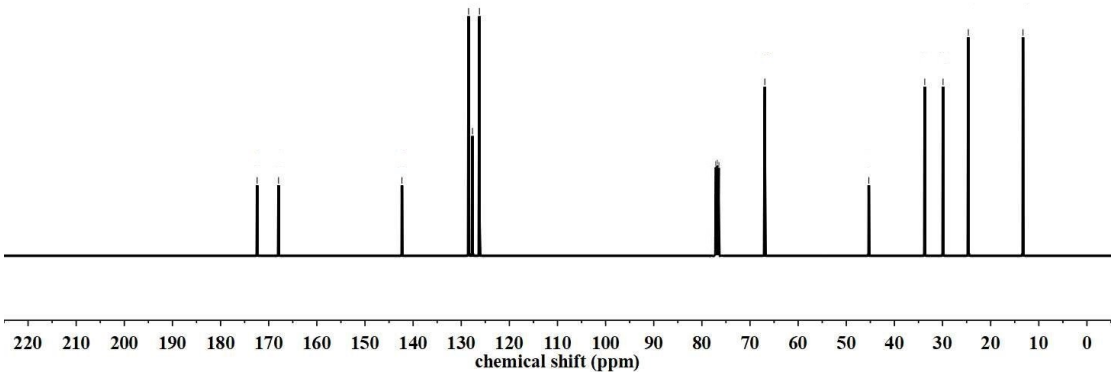


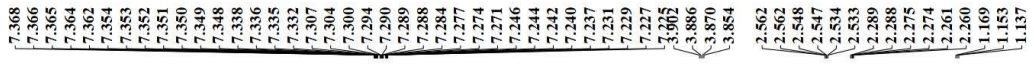
^{1}H NMR (400 M, $CDCl_3$)

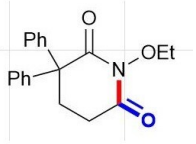




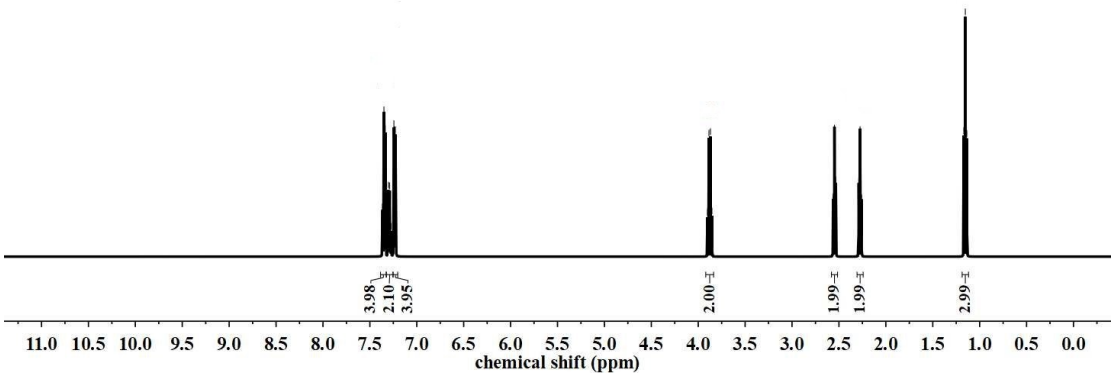
^{13}C NMR (100 M, $CDCl_3$)

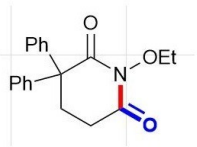




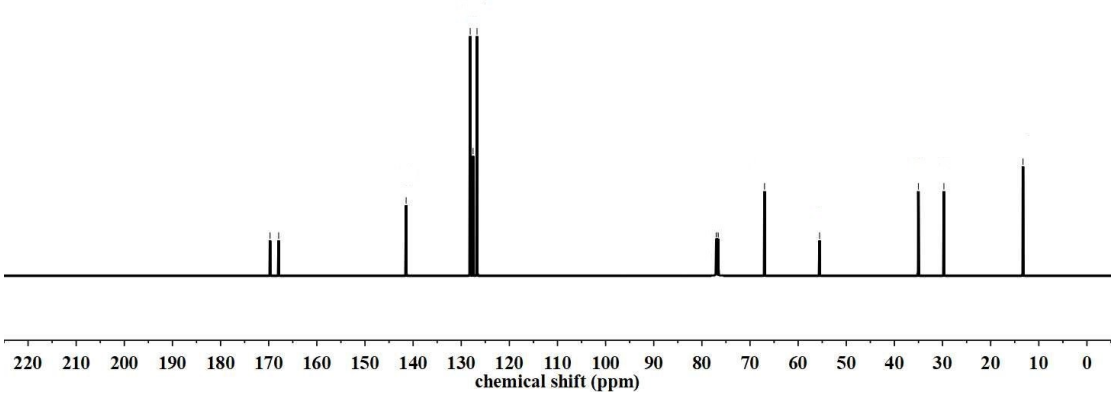


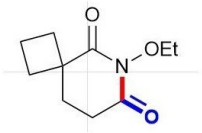
^{1}H NMR (400 M, $CDCl_3$)



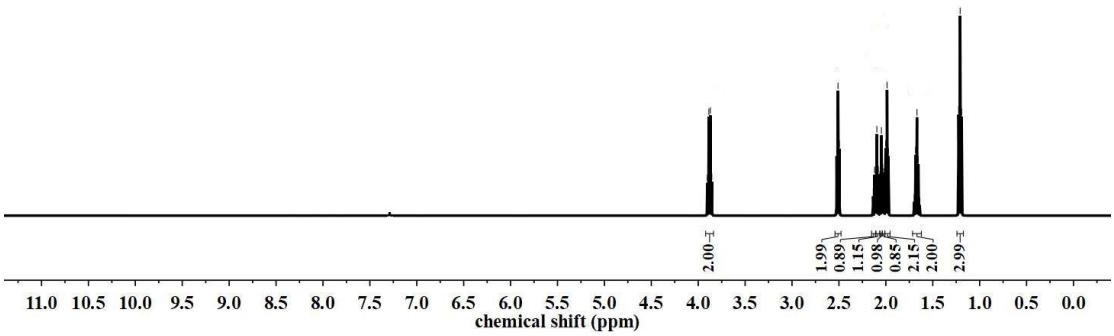


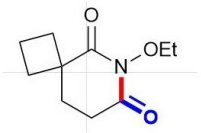
^{13}C NMR (100 M, $CDCl_3$)



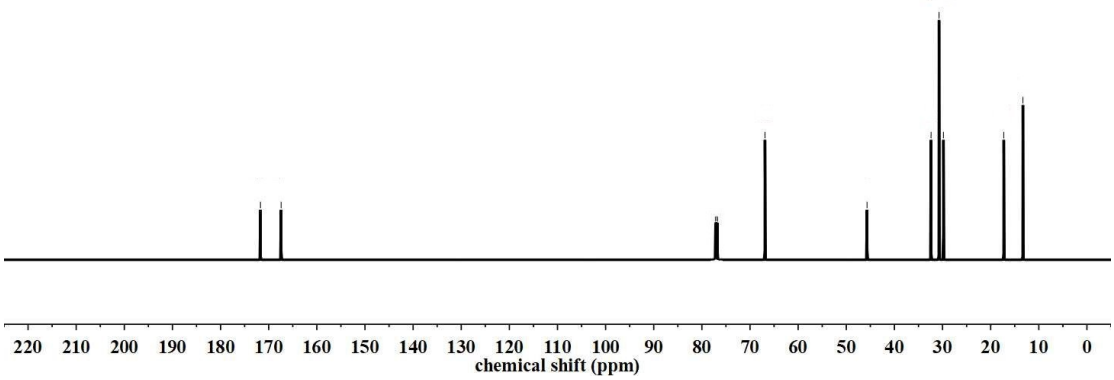


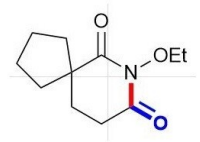
^{1}H NMR (400 M, $CDCl_3$)



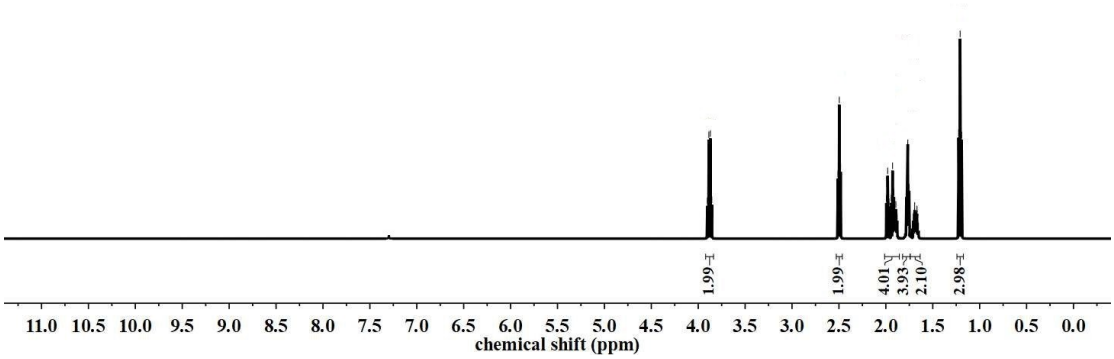


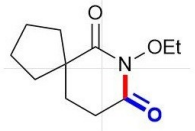
^{13}C NMR (100 M, $CDCl_3$)



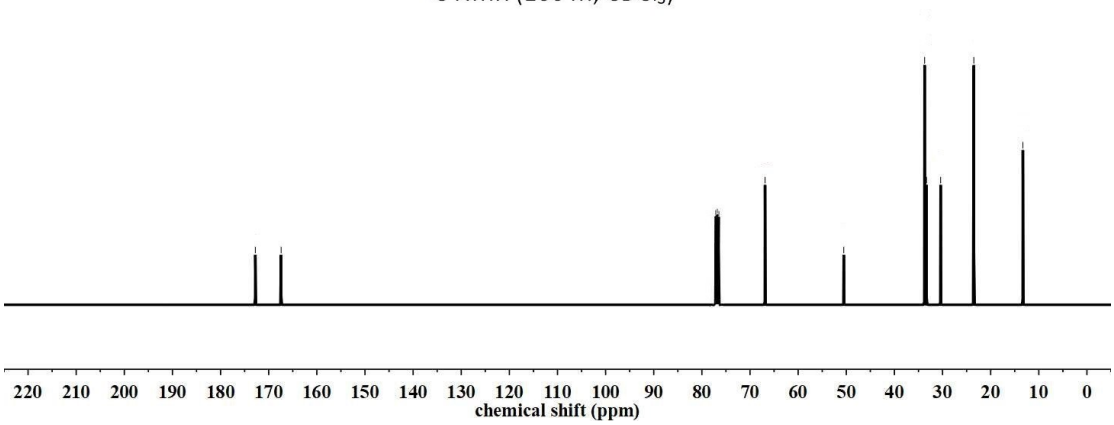


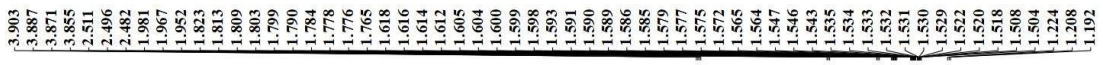
^{1}H NMR (400 M, $CDCl_3$)



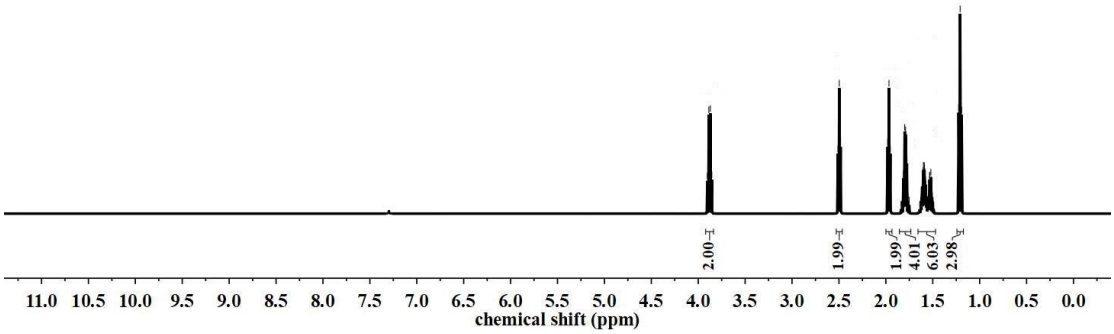


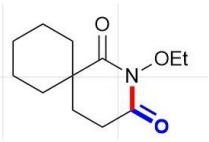
^{13}C NMR (100 M, $CDCl_3$)



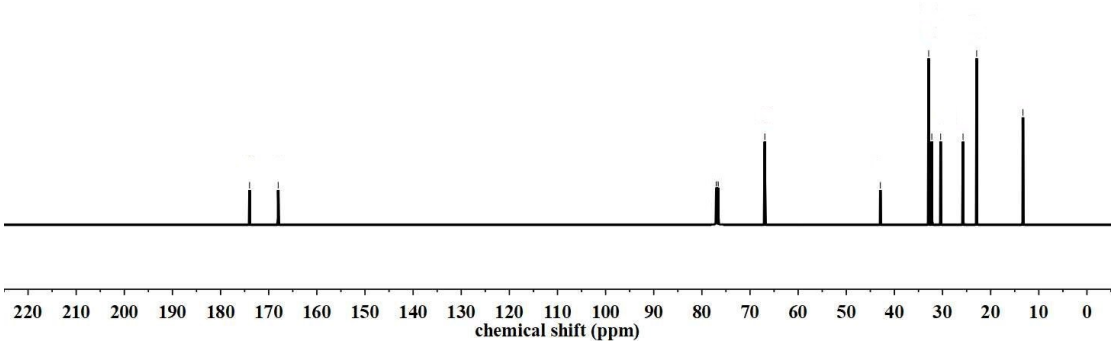


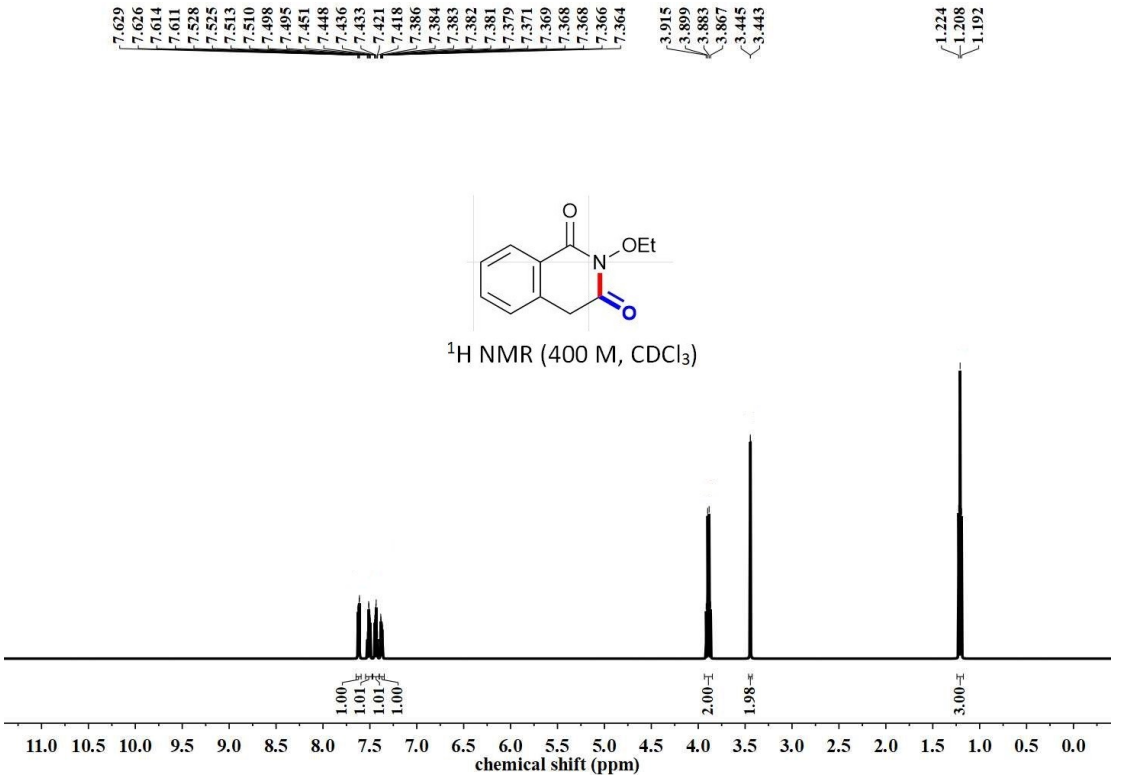
^{1}H NMR (400 M, $CDCl_3$)





^{13}C NMR (100 M, $CDCl_3$)

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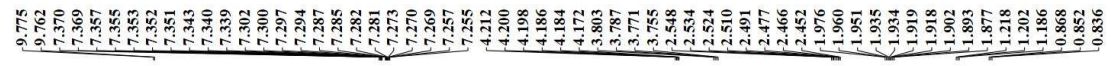
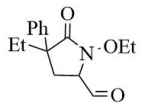
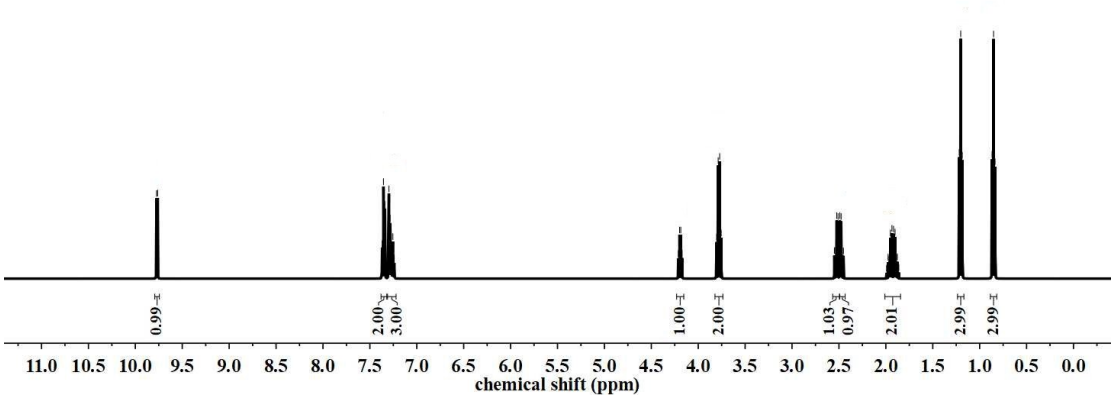
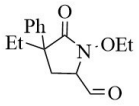
7.626
7.614
7.611
7.528
7.525
7.513
7.510
7.498
7.495
7.451
7.448
7.436
7.433
7.421
7.418
7.386
7.384
7.383
7.382
7.381
7.379
7.371
7.369
7.368
7.368
7.366
7.364
3.915
3.899
3.883
3.867
3.445
3.443
1.224
1.208
1.192
O
N
OEt
O
1H NMR (400 M, CDCl3)
1.00
1.01
1.01
1.00
2.00
1.98
3.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
chemical shift (ppm)
172.527
162.878
135.204
131.032
129.809
127.438
126.494
125.531
67.013
35.820
13.308
O
N
OEt
O
13C NMR (100 M, CDCl3)
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
chemical shift (ppm)



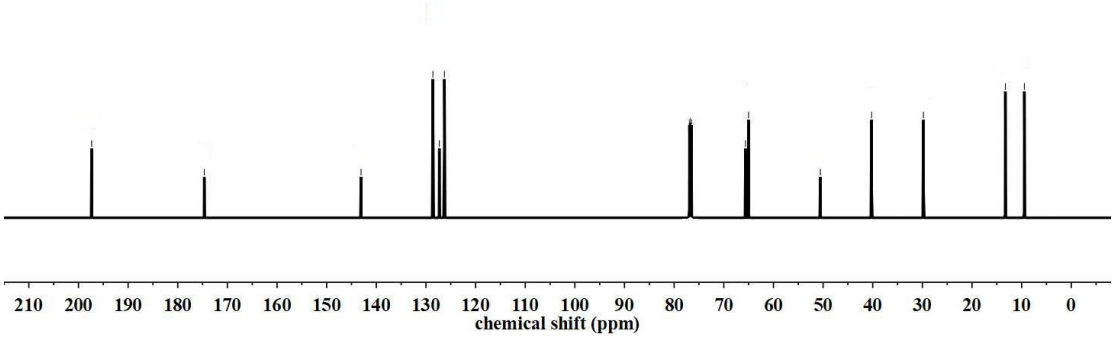


^{1}H NMR ($CDCl_3$, 400 MHz)





^{13}C NMR ($CDCl_3$, 101 MHz)



4. ESI-MS measurement: instrument parameters and results

Acquisition Mass Control	
Detection Mode	Broad band
TD (Acquisition)	1 M
Low Mass	57.75 m/z
High Mass	2000.00 m/z
Estimated R.P.	38000
Transient Length	0.2097 sec
Data transfer mode	standard

API Source		Source Gas Tune		Source Gas Control	
Source Type	ESI	Dry Gas	4.0 L/min	Drying Gas Flow	Yes
Capillary -	2600 V	Dry Temp	100 ^{o}C	Drying Gas Heater	Yes
End Plate Offset	-500 V	Nebulizer	1.0 bar	Nebulizer Gas Flow	Yes
Corona Needle	0.0 nA	Vaporizar Temp	10.0 ^{o}C	Nebulizer Gas Heater	No

Figure S1 ESI-MS spectra of mechanism research