Divergent Synthesis of 2,3-Dihydro-1*H*-pyrroles, 3-Alkyl-1*H*-pyrroles and 3-Alkenyl-1*H*-pyrroles from 2,4-Pentadienenitriles and Isocyanoacetate

Xiaoqing Xin,[a] Xu Liu,[a] Dingyuan Zhang,[a] Rui Zhang,[a] Yongjiu Liang*,[a] Fushe Han,[a] and Dewen Dong*,[a,b]

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[b] *Changzhou Institute of Energy Storage Materials & Devices, Changzhou, 213000, P. R. China*

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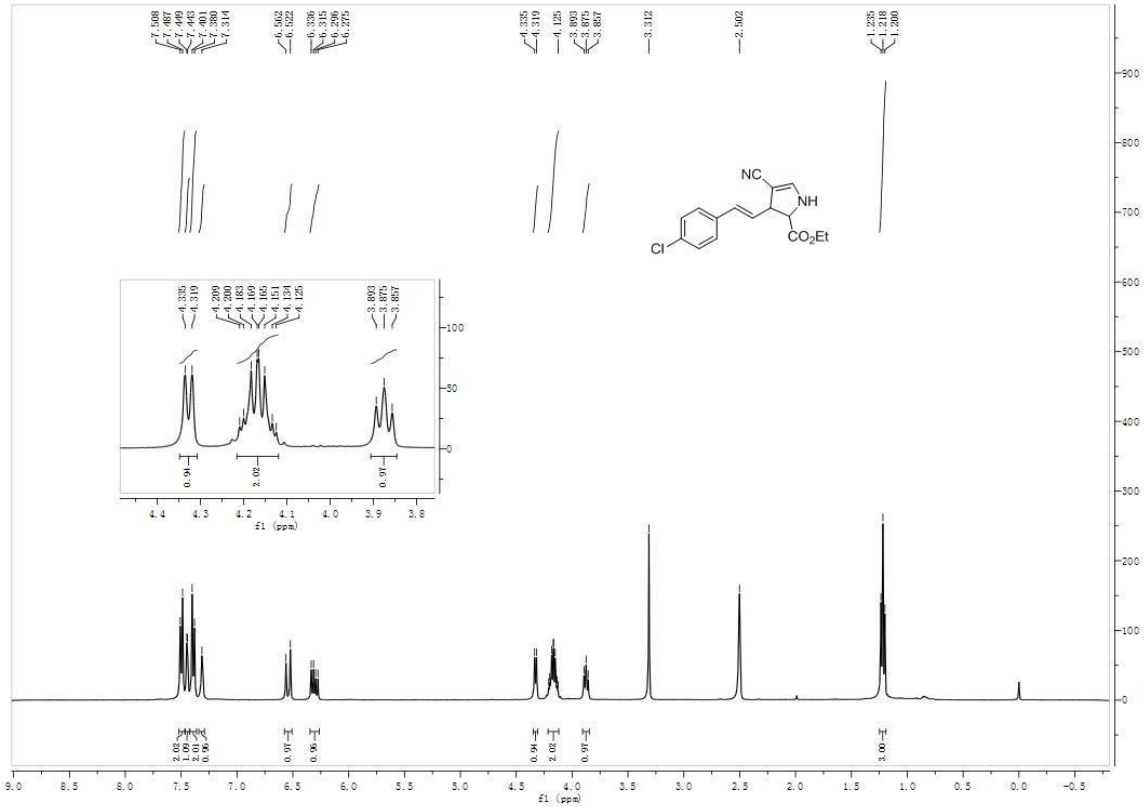
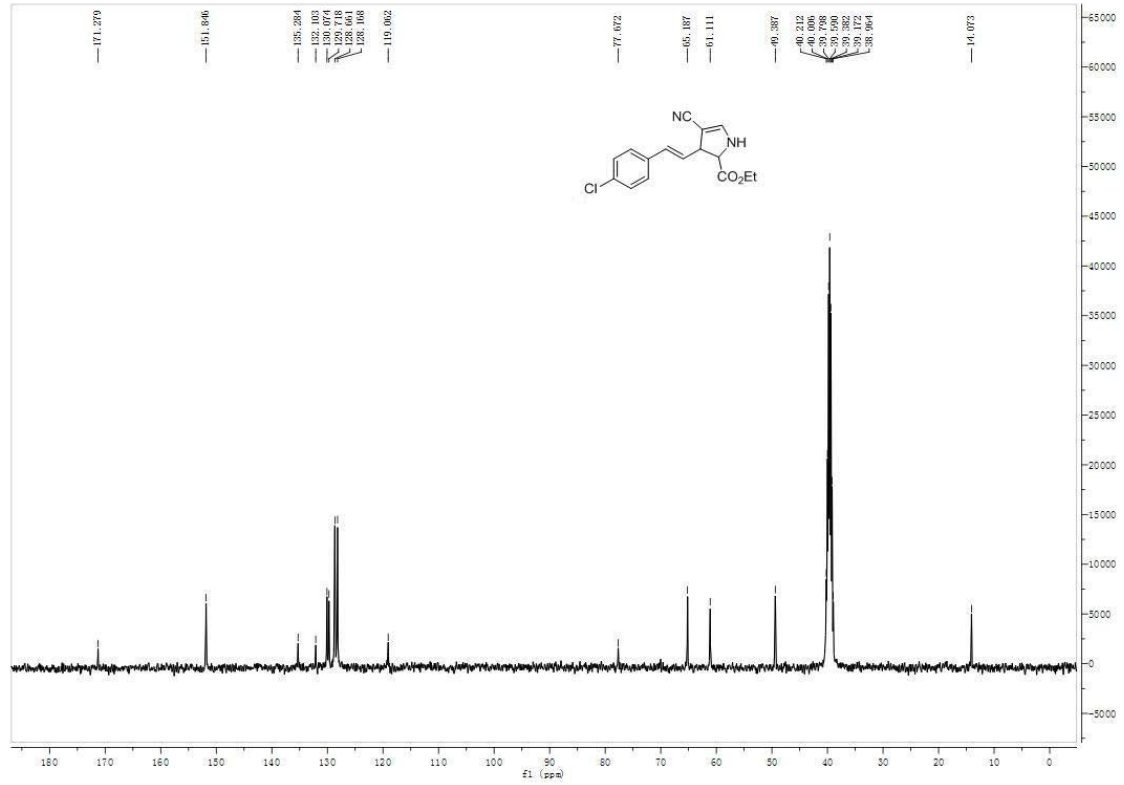
Electronic Supplementary Information

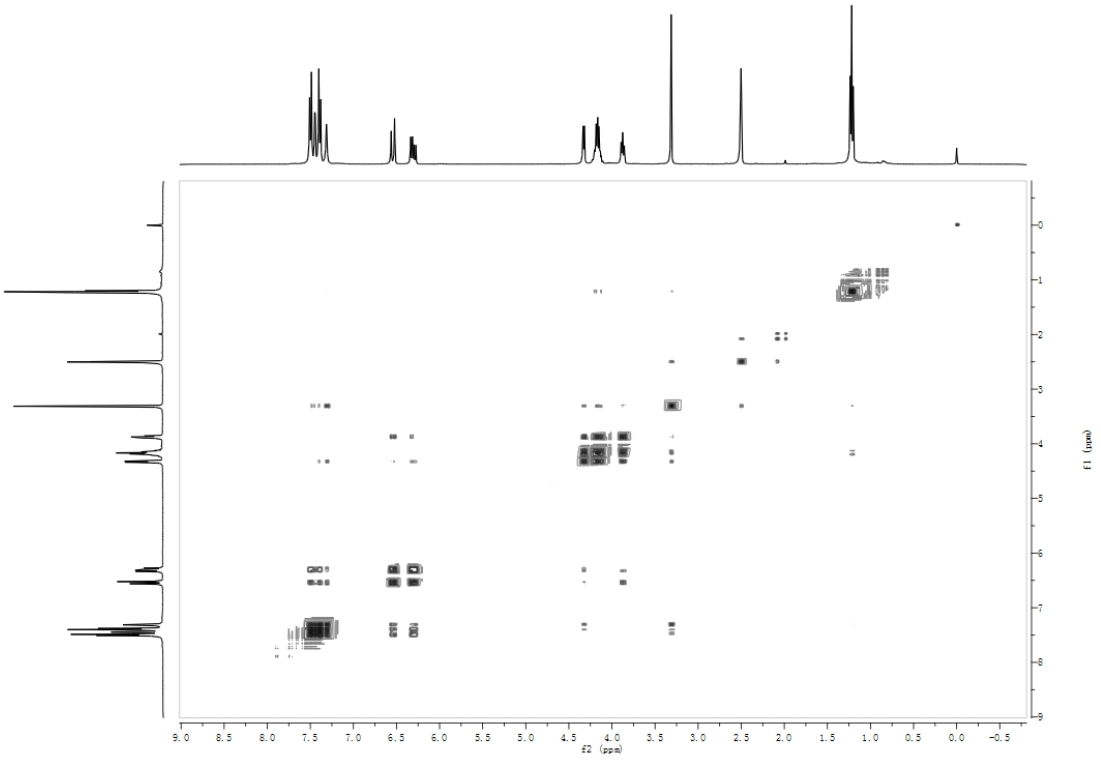
Copies of NMR spectra for compounds **2-4** S2-S23

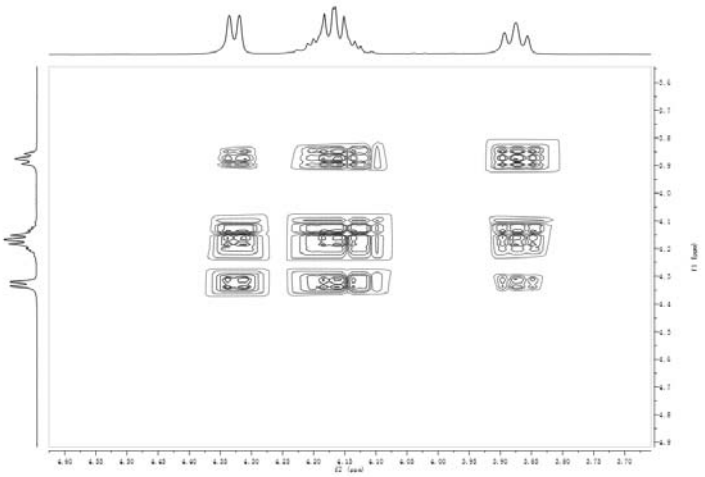
Copies of NMR spectra for compounds 2-4

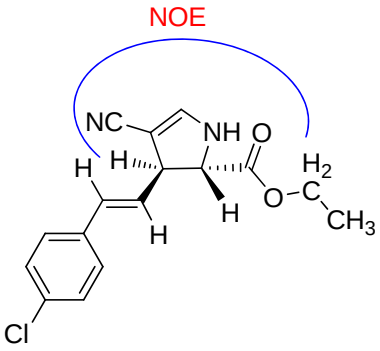
2a







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H
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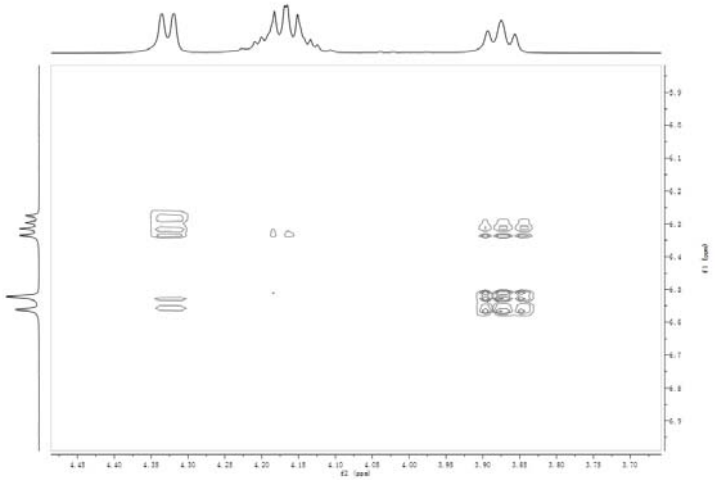

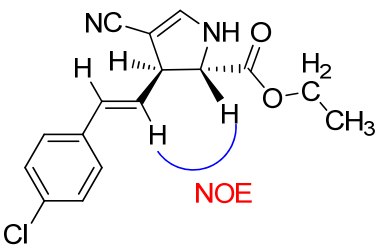
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H
H
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O
C
CH3
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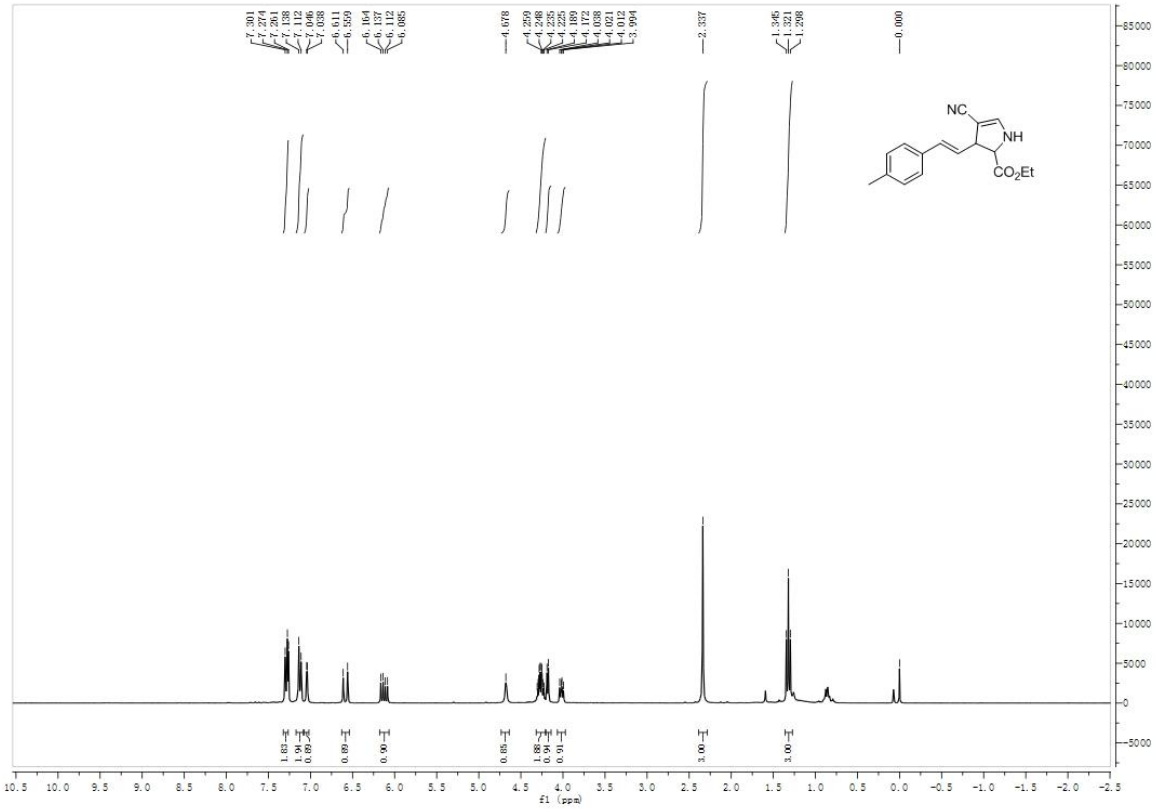
Cl

2b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4.678
4.259
4.248
4.225
4.199
4.172
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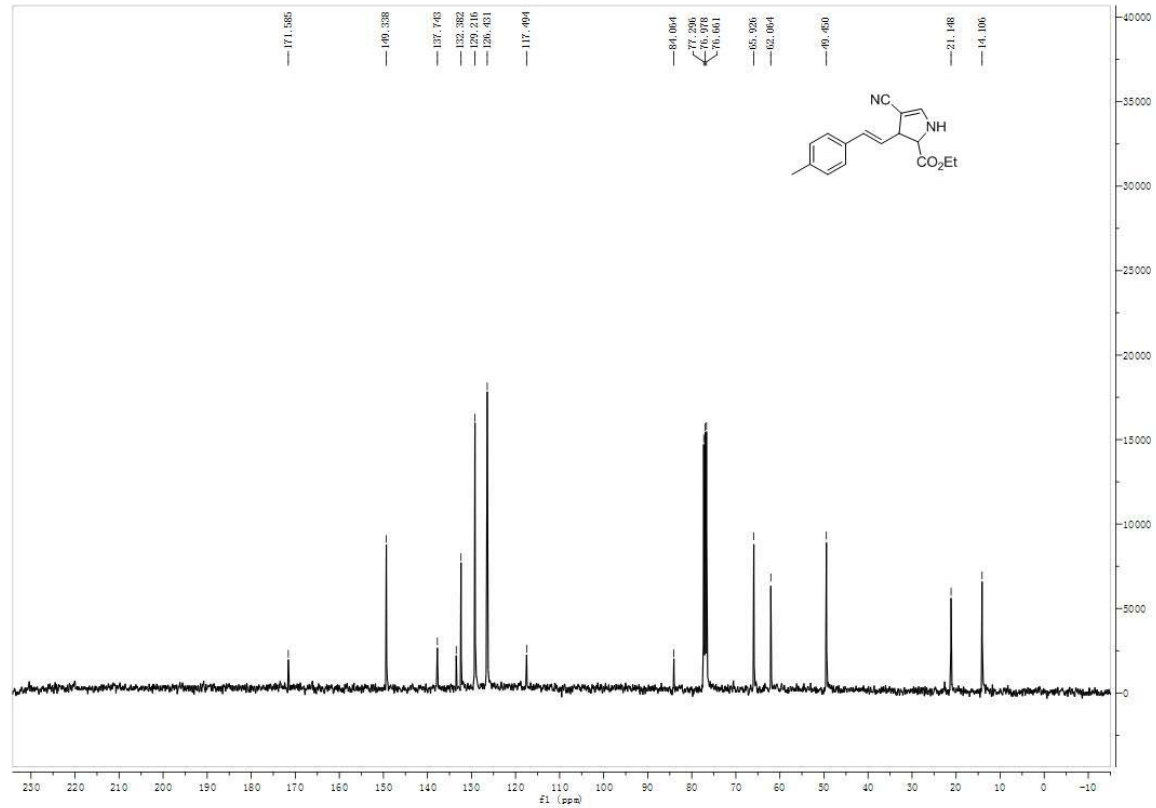
CO2Et
f1 (ppm)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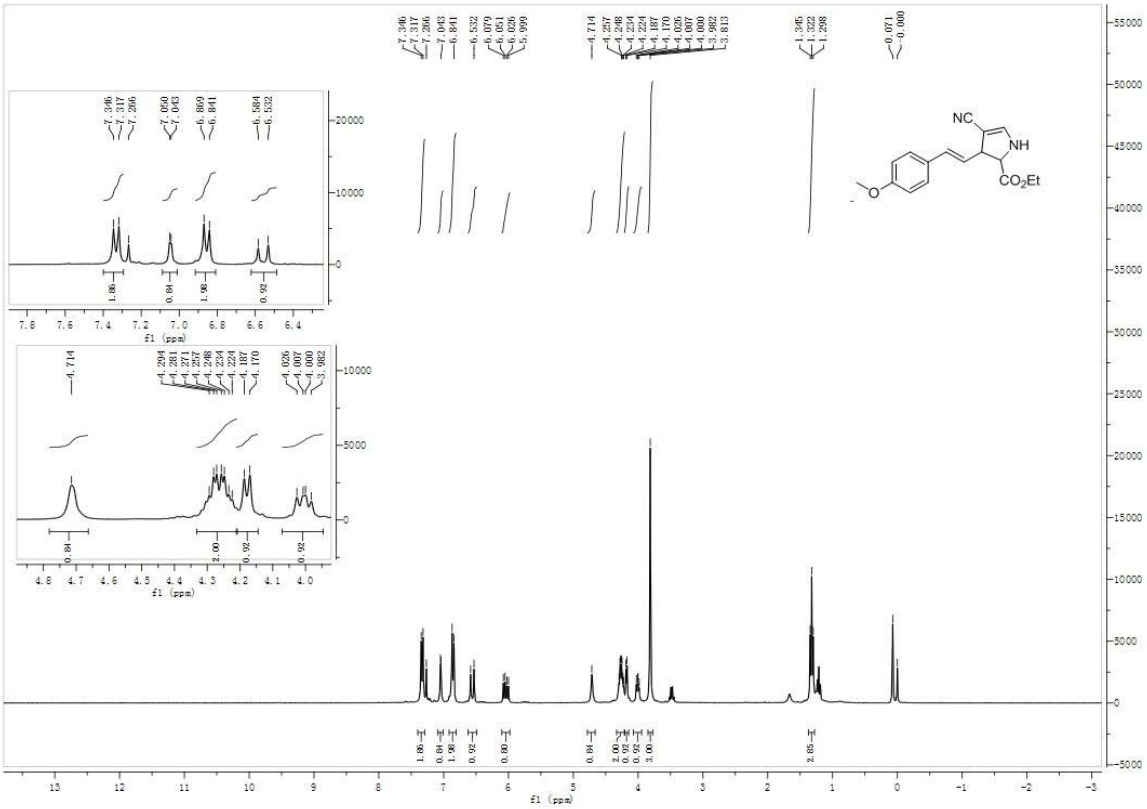
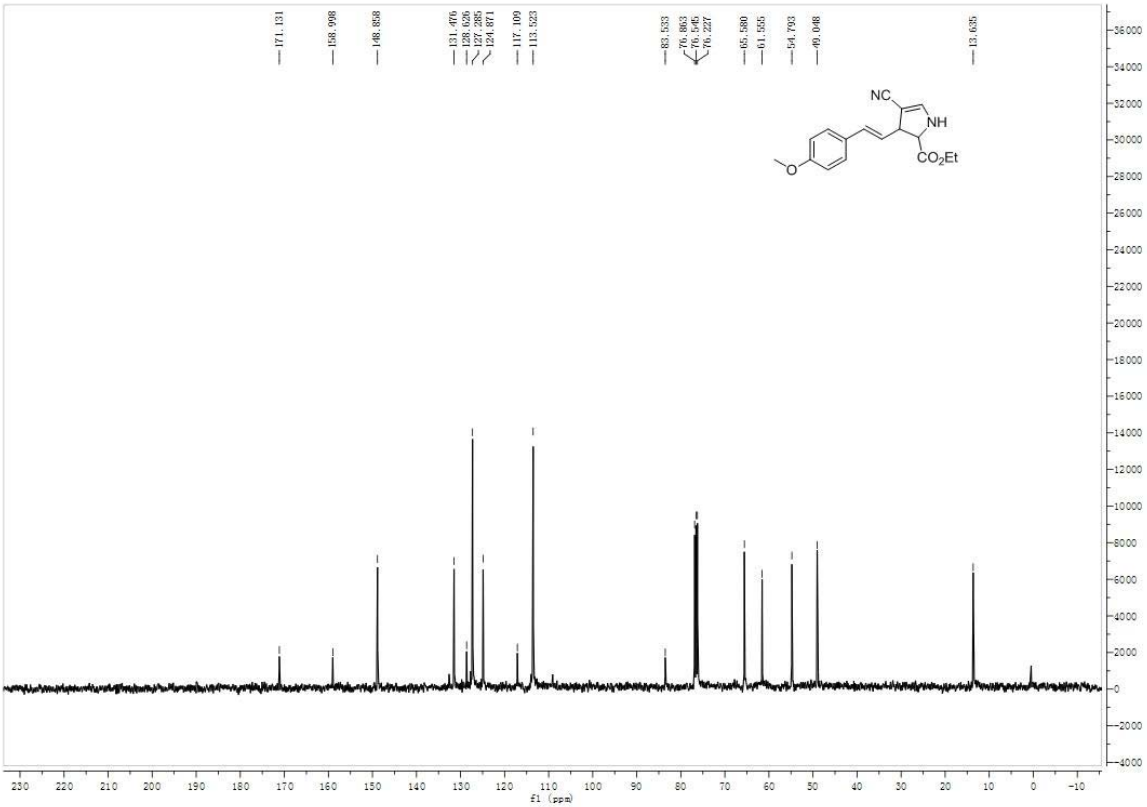
NC
NH
CO2Et
f1 (ppm)

2c





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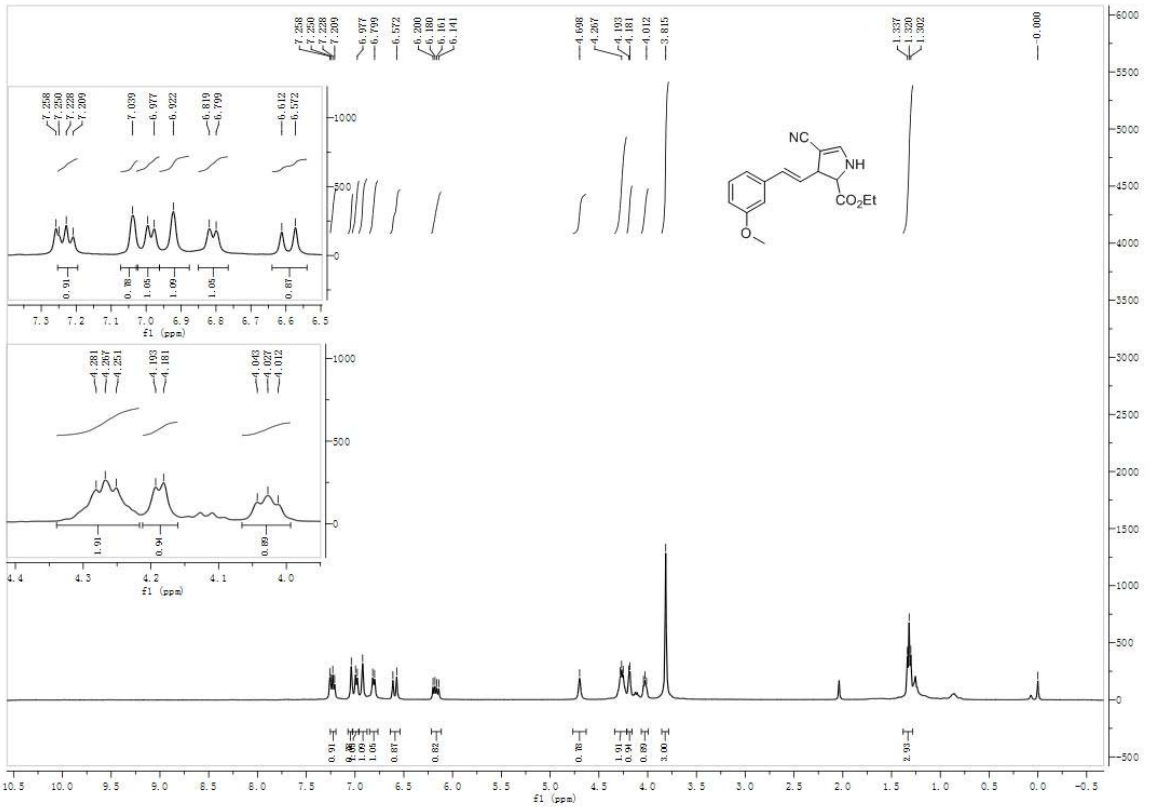

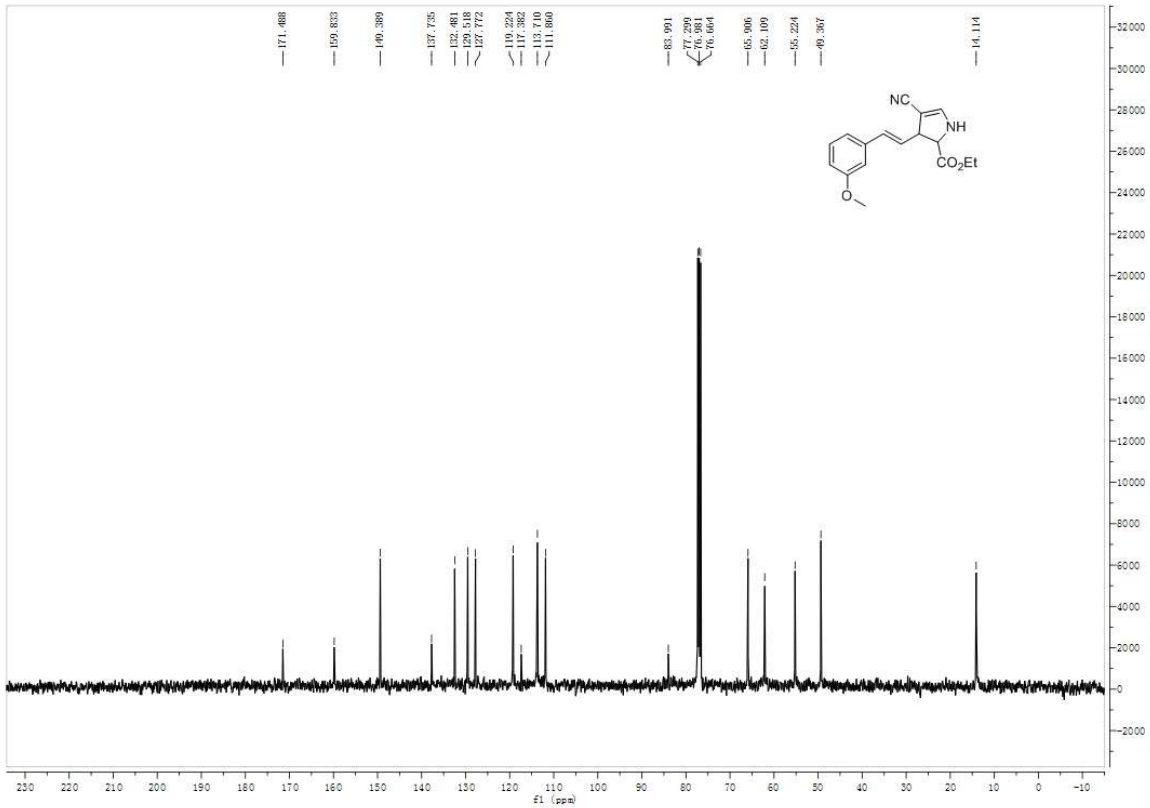

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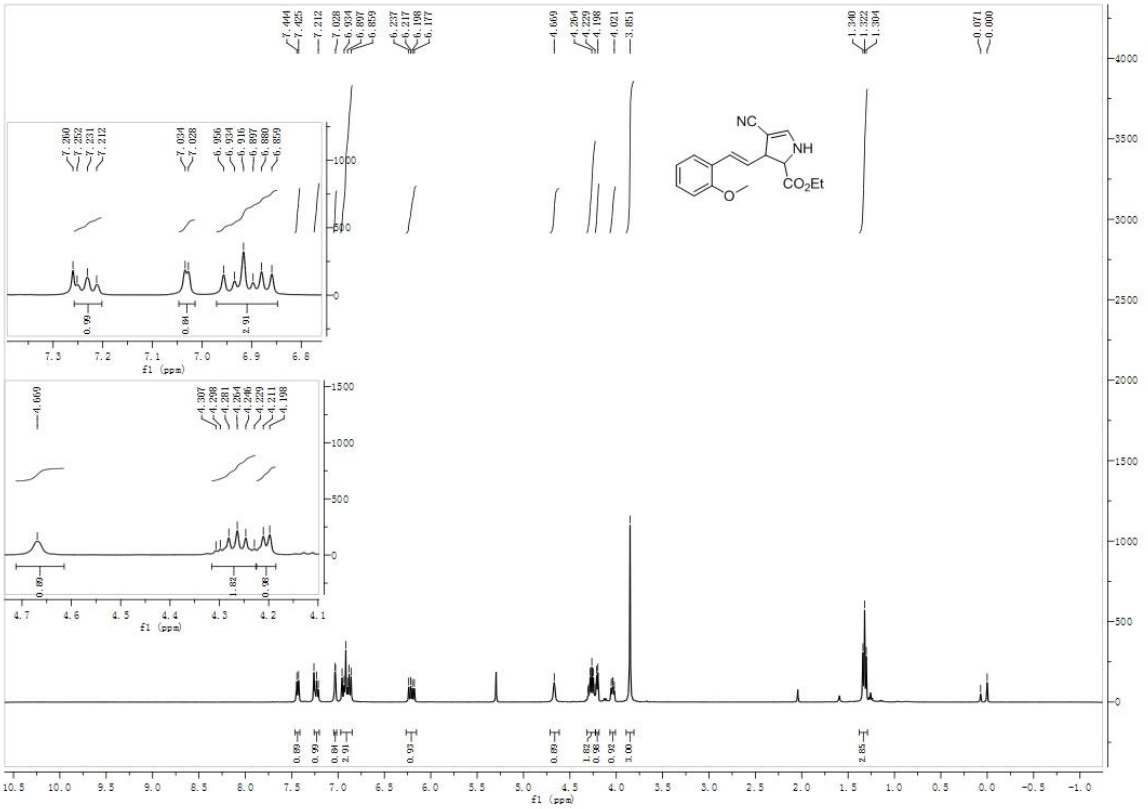

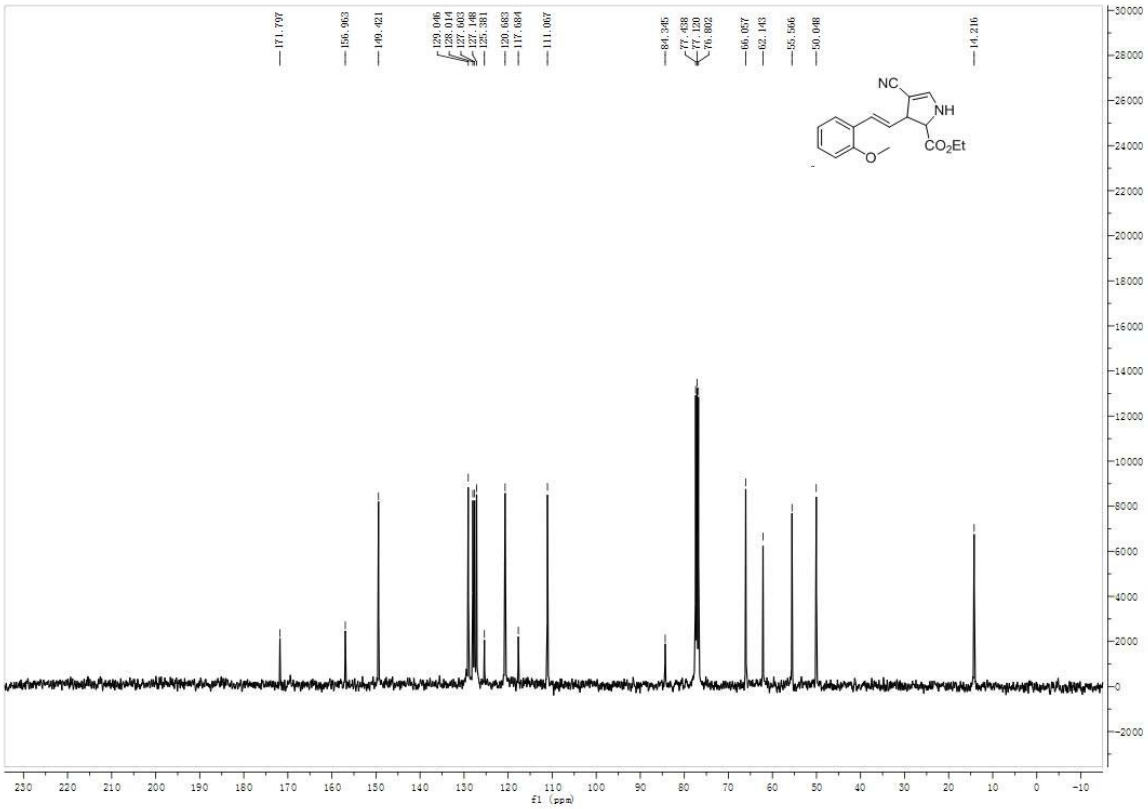

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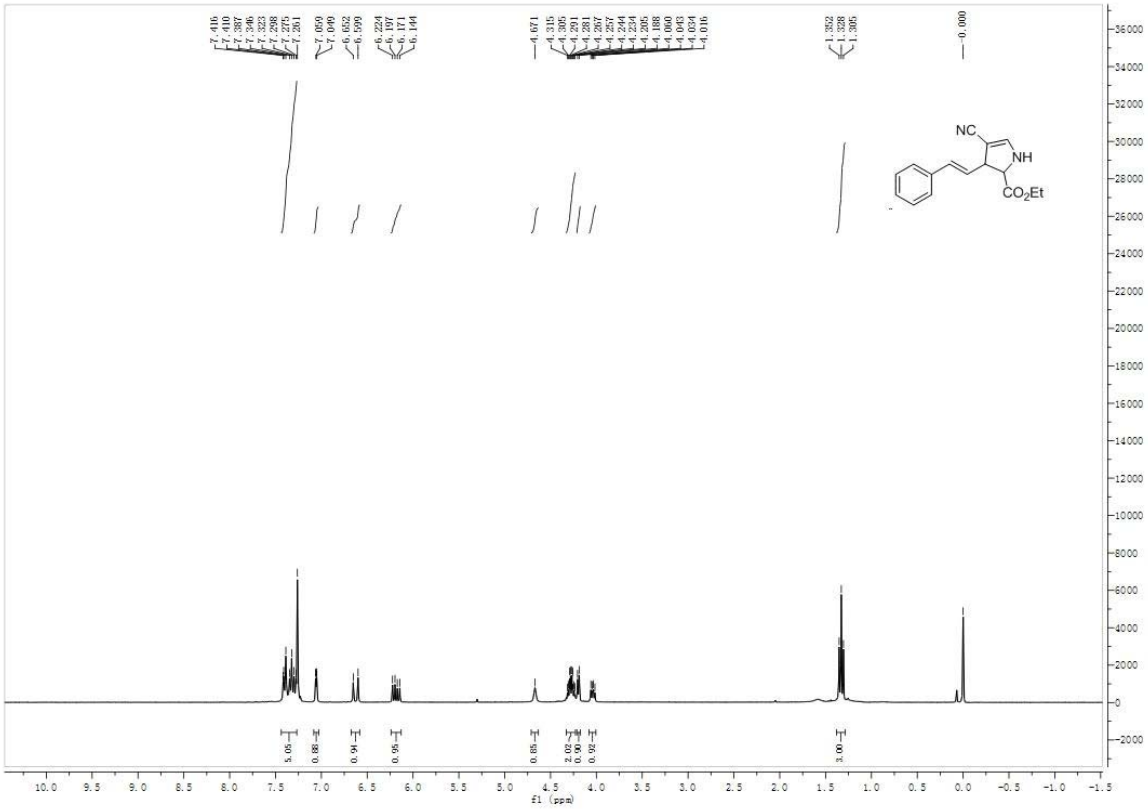
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6.197
6.171
6.144
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4.315
4.305
4.291
4.281
4.267
4.257
4.244
4.234
4.205
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4.060
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4.034
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1.328
1.305
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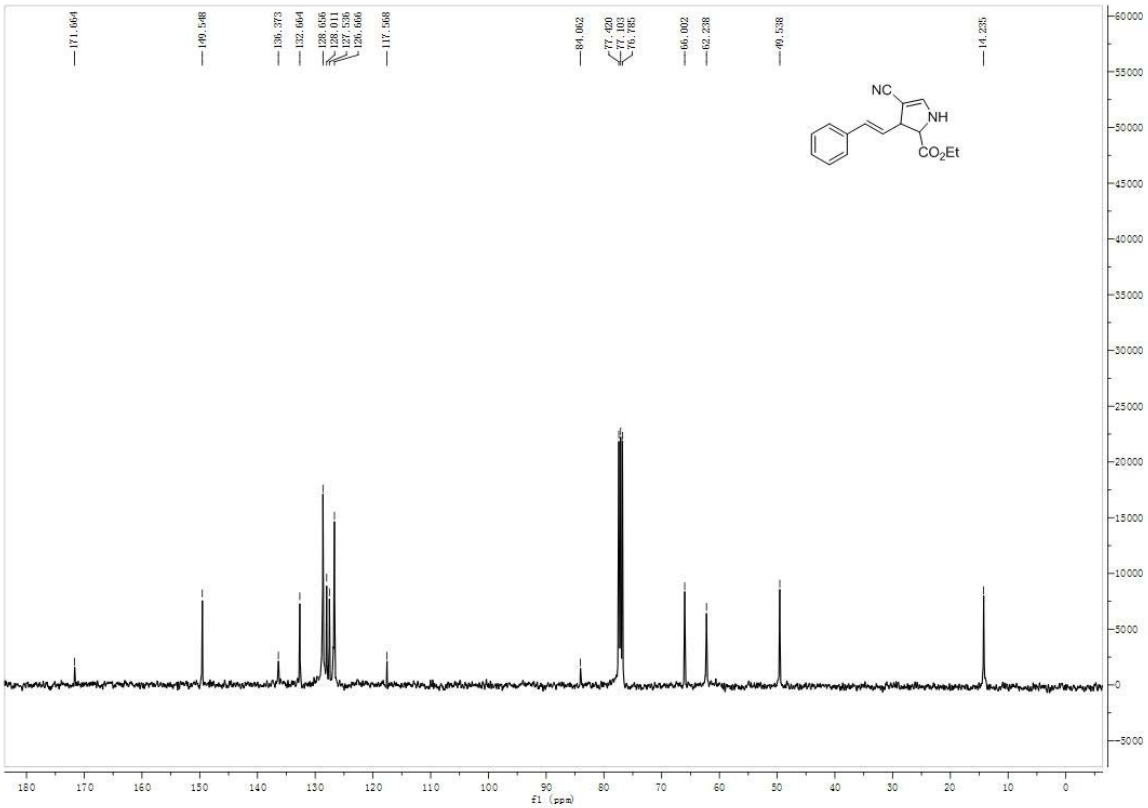
3.00
f1 (ppm)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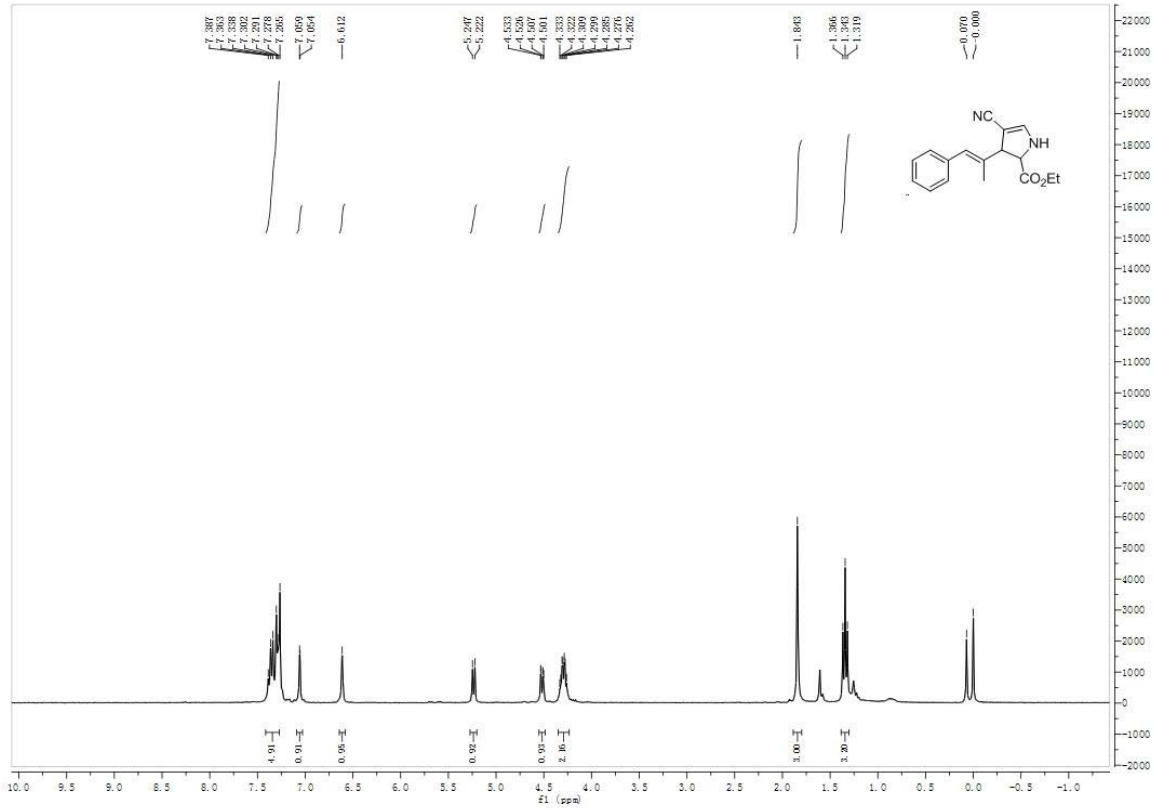
NC
NH
CO2Et
f1 (ppm)

2g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7.265
7.059
7.054
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5.247
5.222
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4.526
4.507
4.501
4.333
4.322
4.309
4.299
4.285
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1.366
1.343
1.319
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3.30
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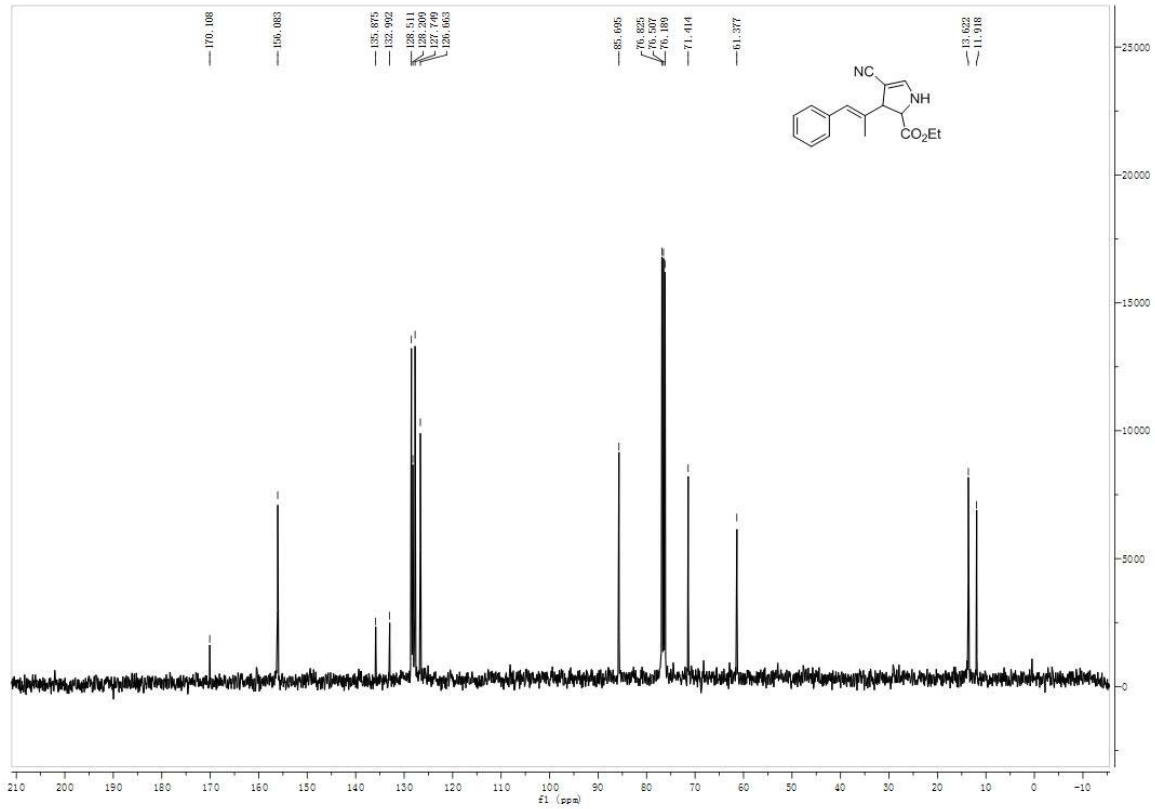
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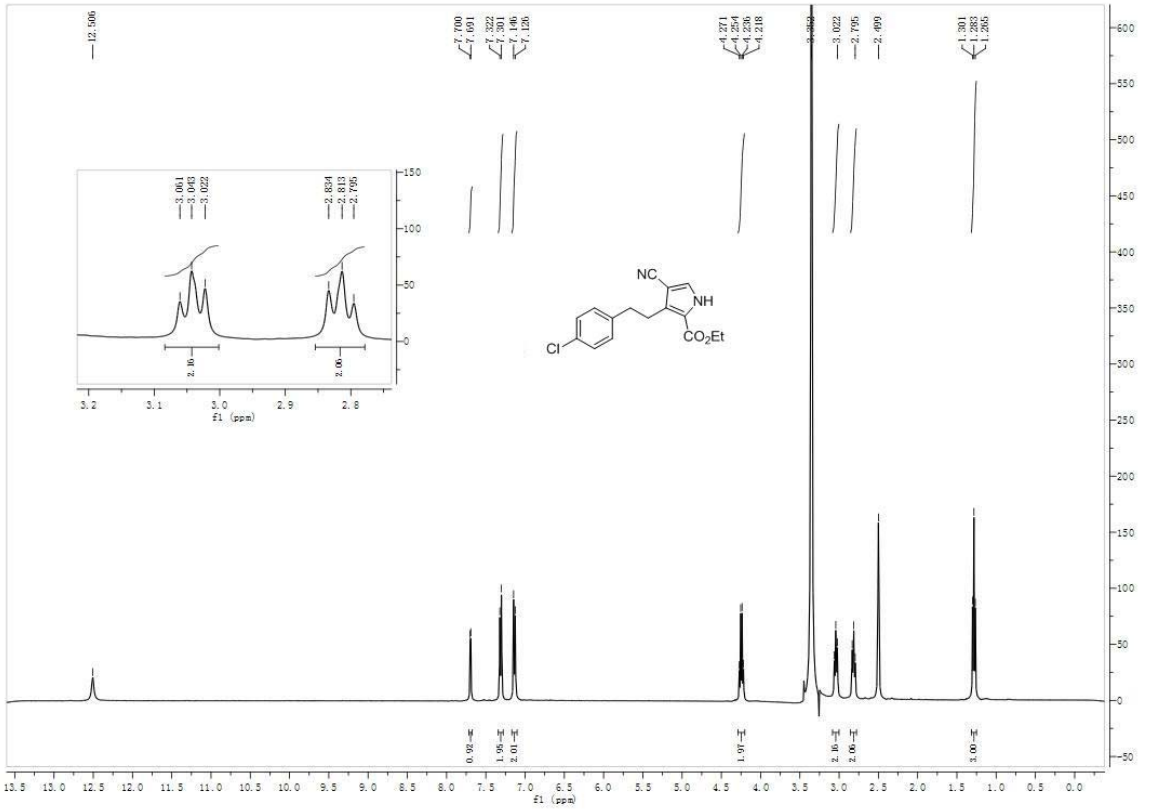
NH
CO2Et
f1 (ppm)

3a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4.218
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2.795
2.499
1.301
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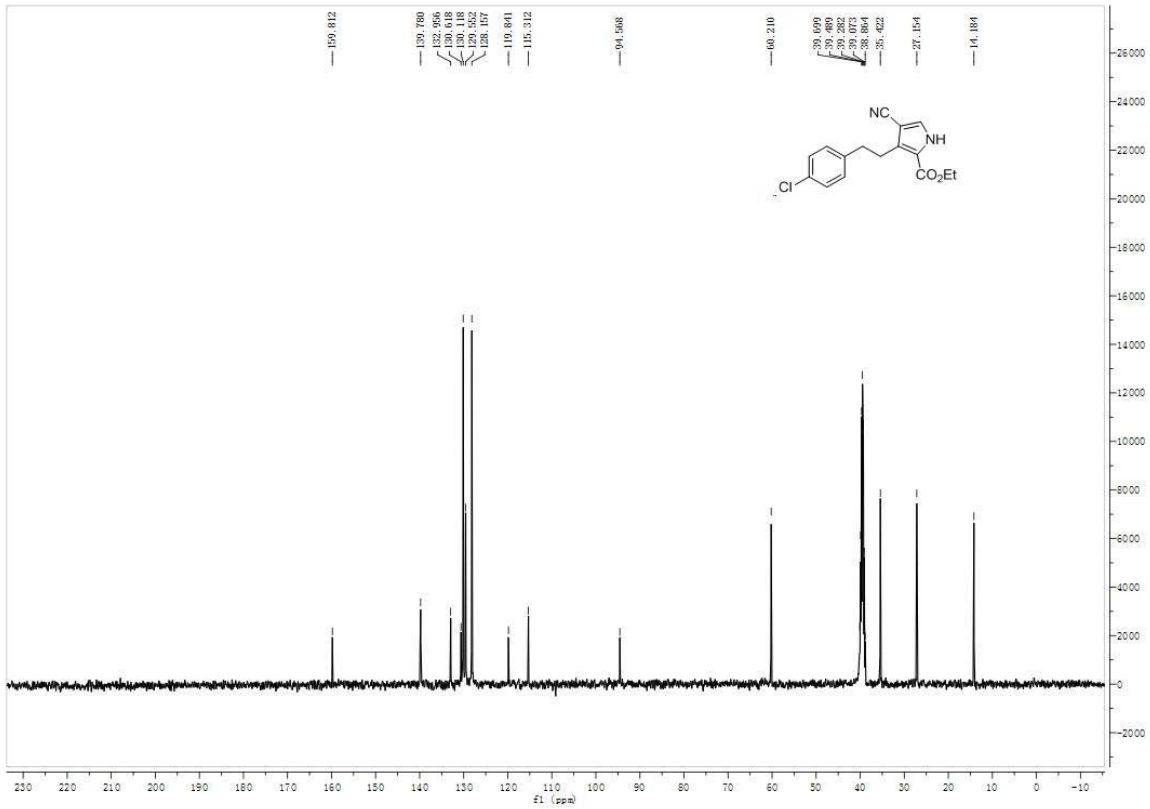
Cl
f1 (ppm)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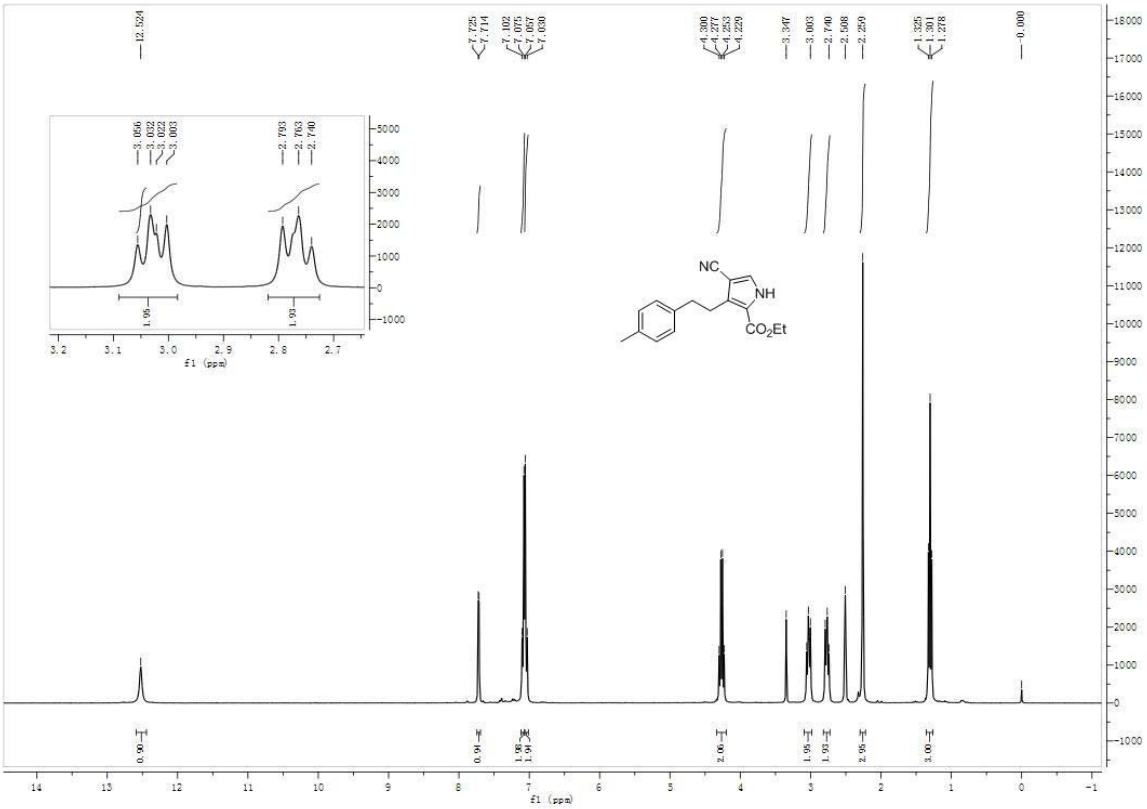
CO2Et
Cl
f1 (ppm)

3b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2.740
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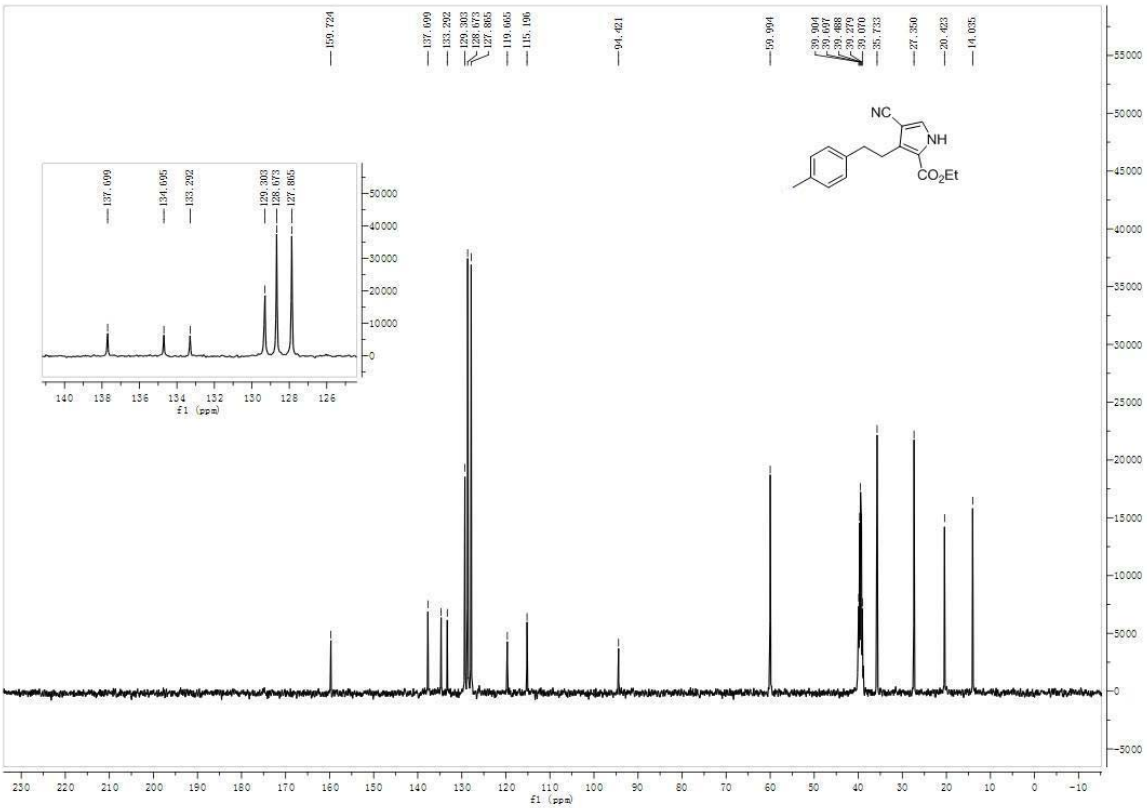
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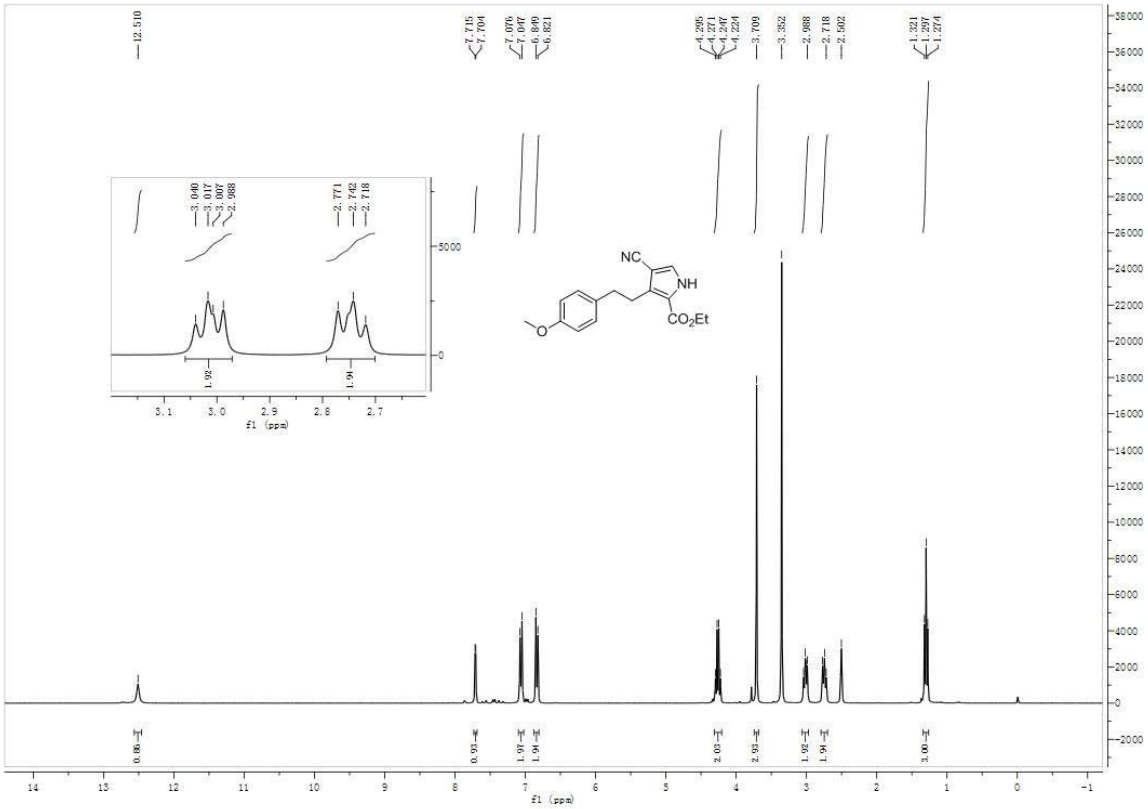
f1 (ppm)

3c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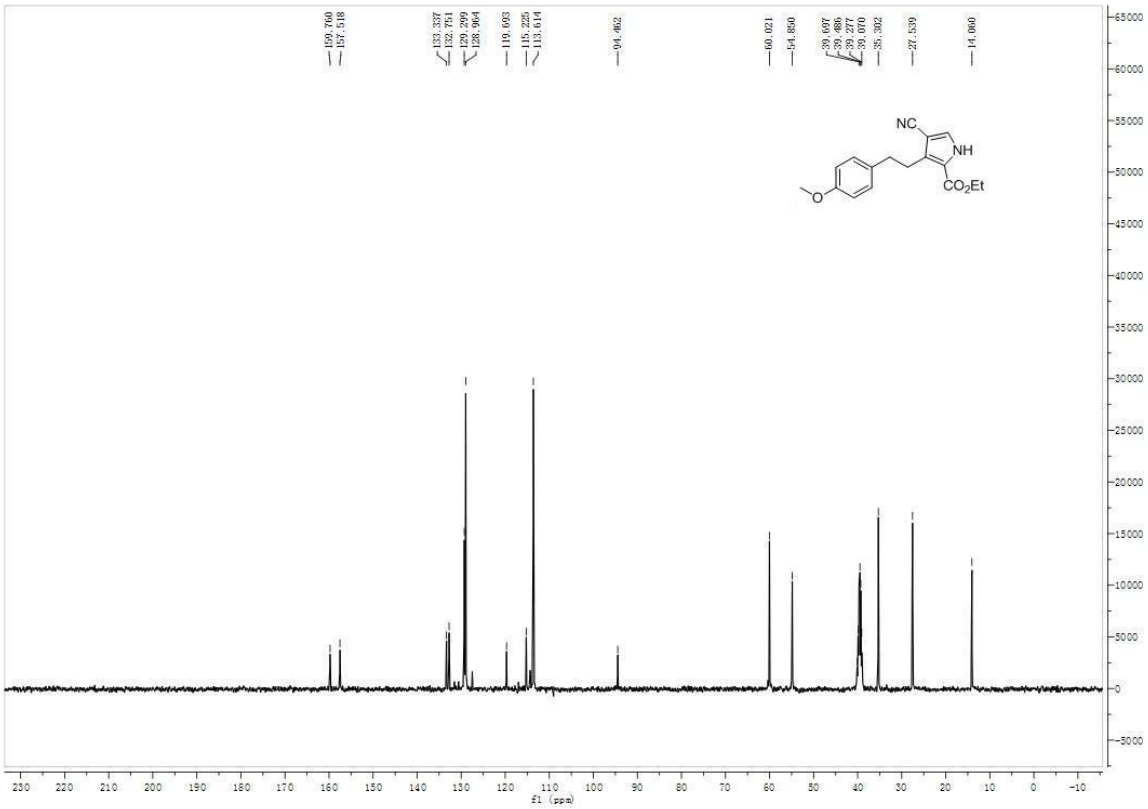
f1 (ppm)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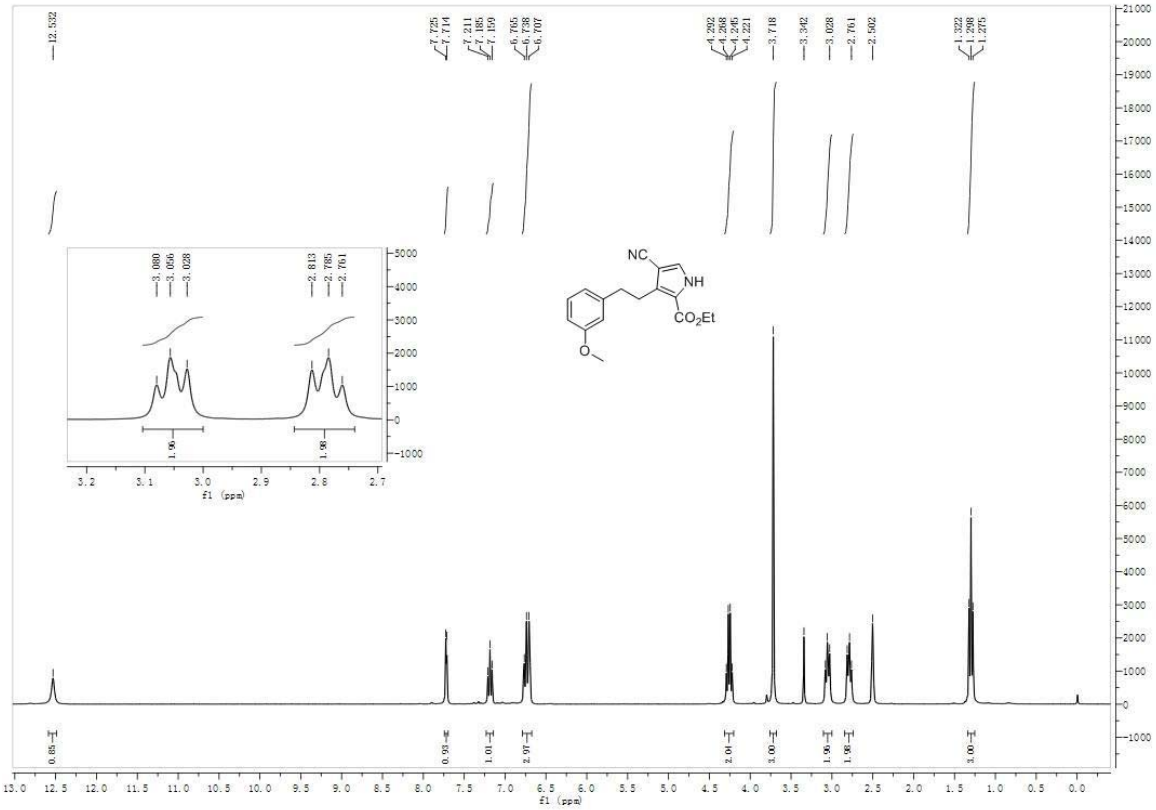
3d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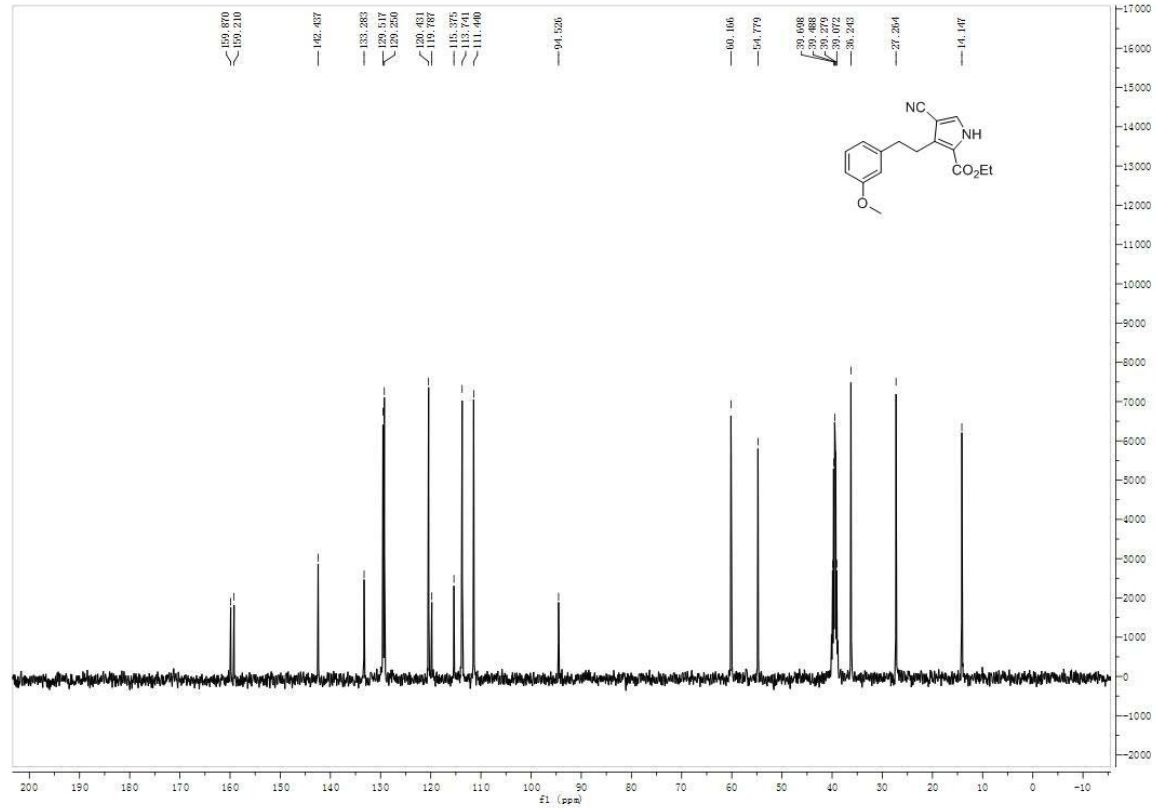
f1 (ppm)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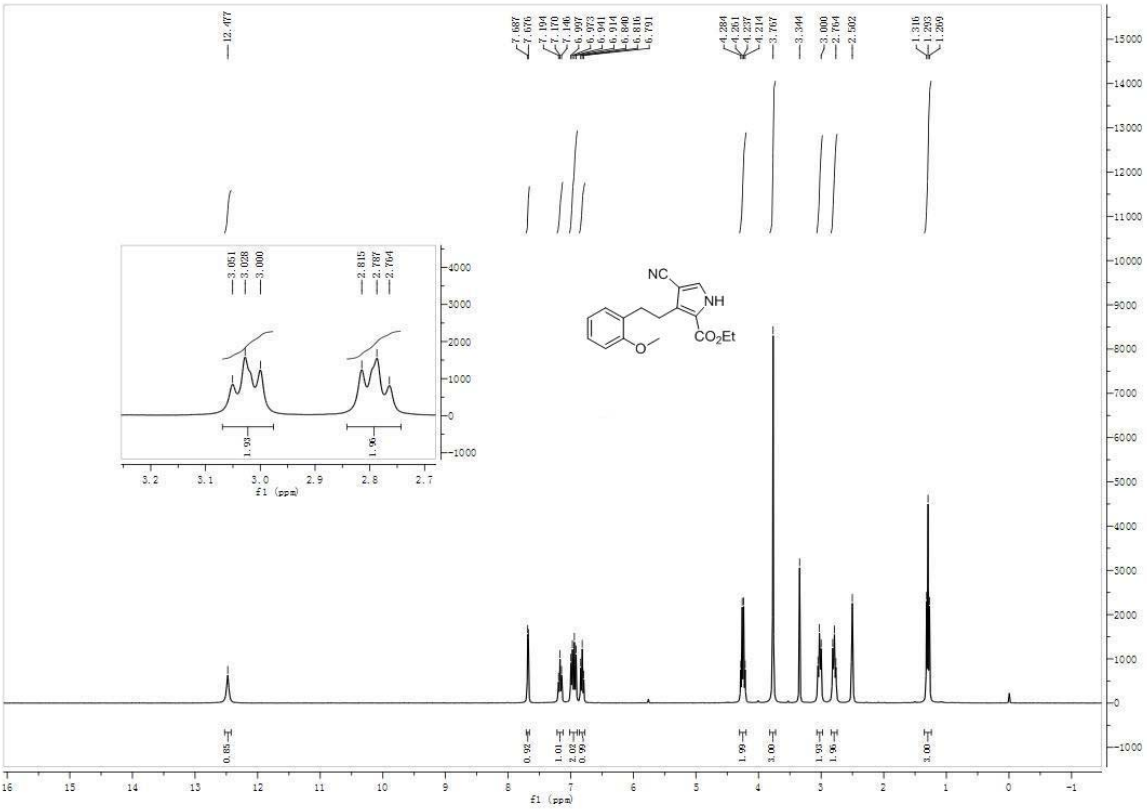
3e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4.214
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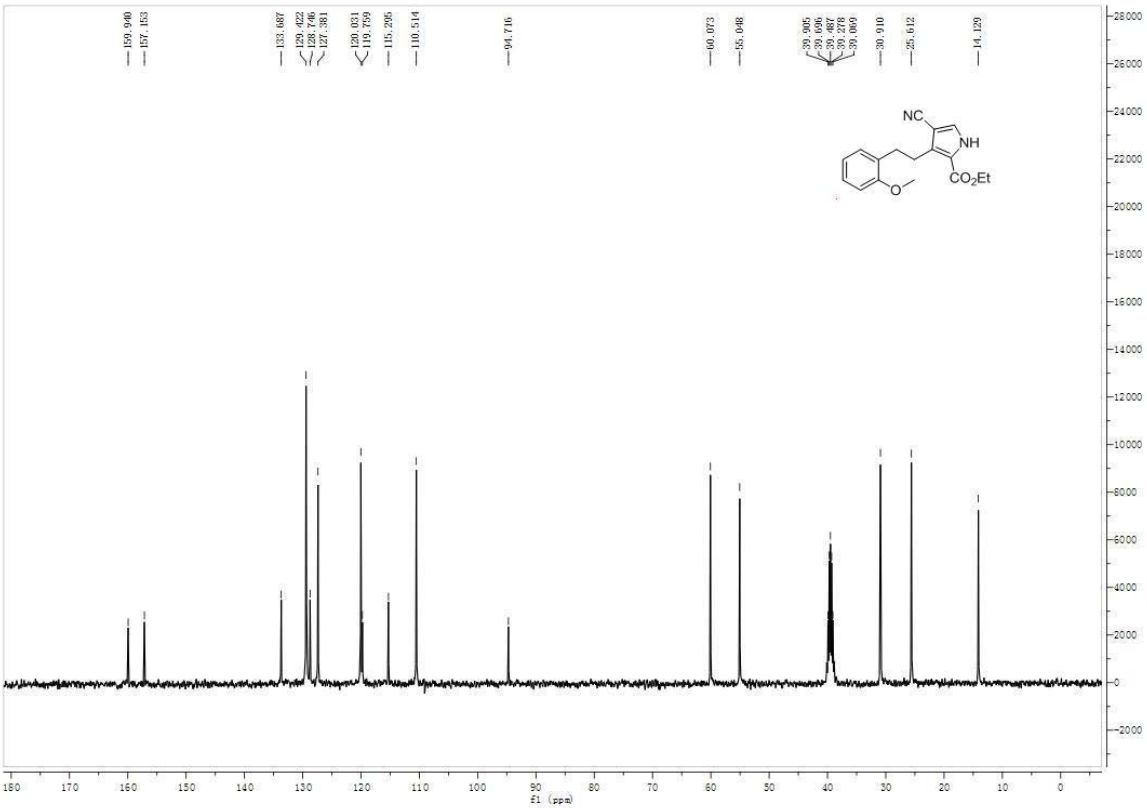
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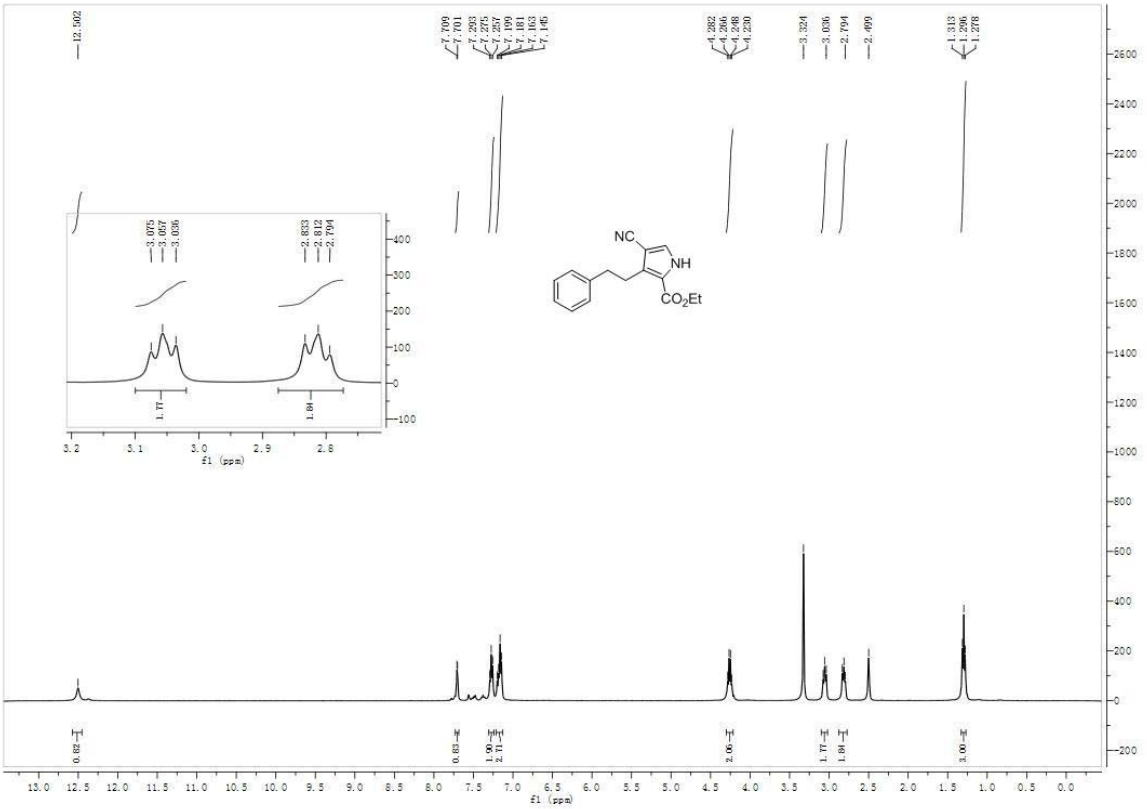
f1 (ppm)

3f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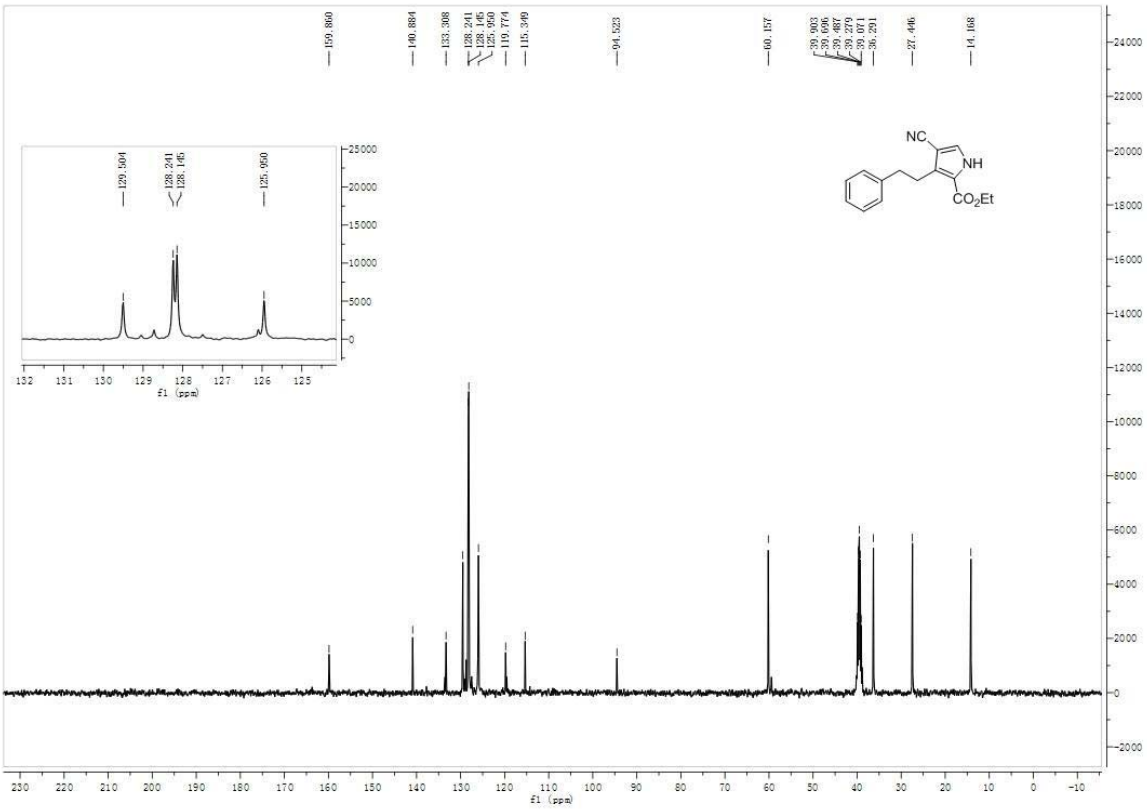
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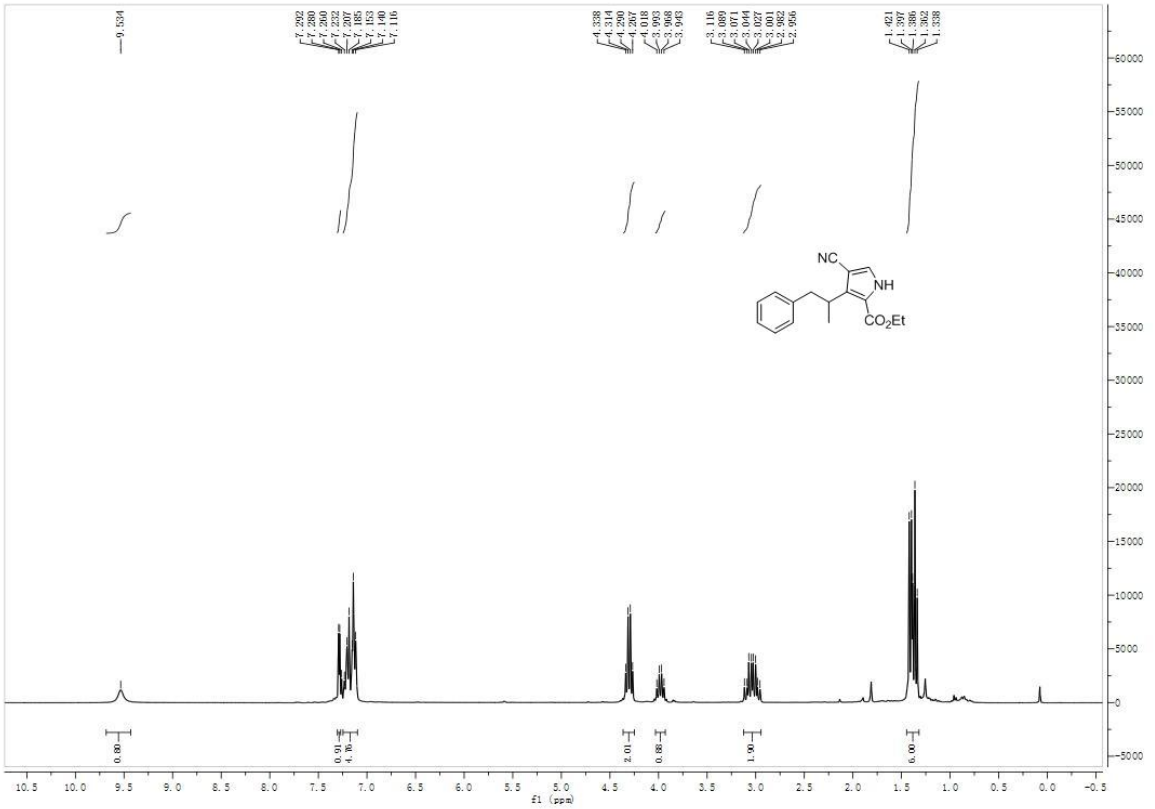
3g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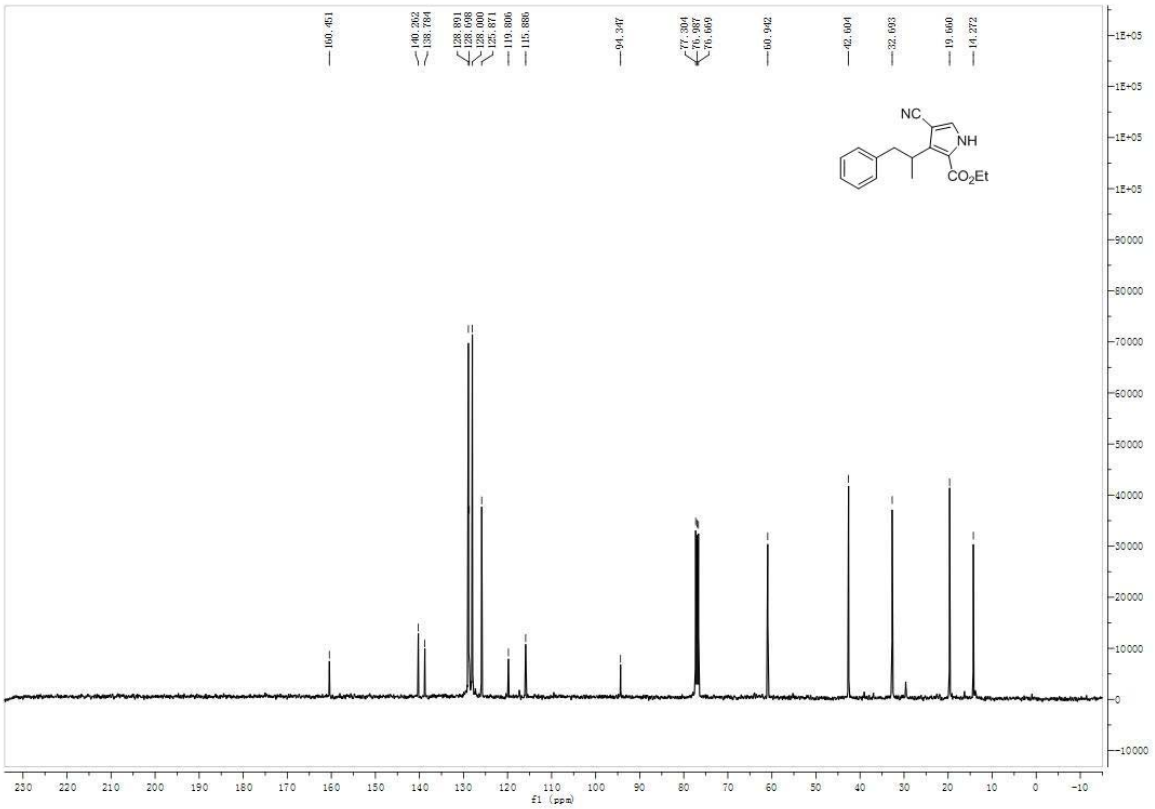
f1 (ppm)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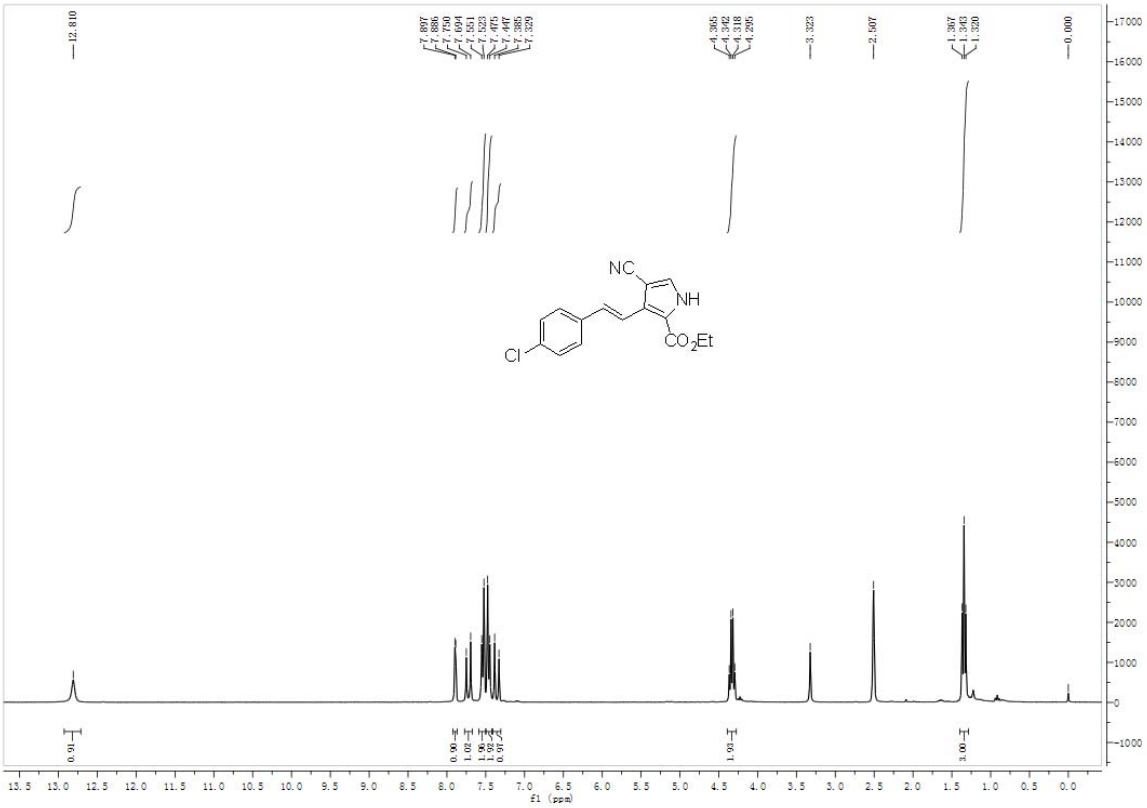
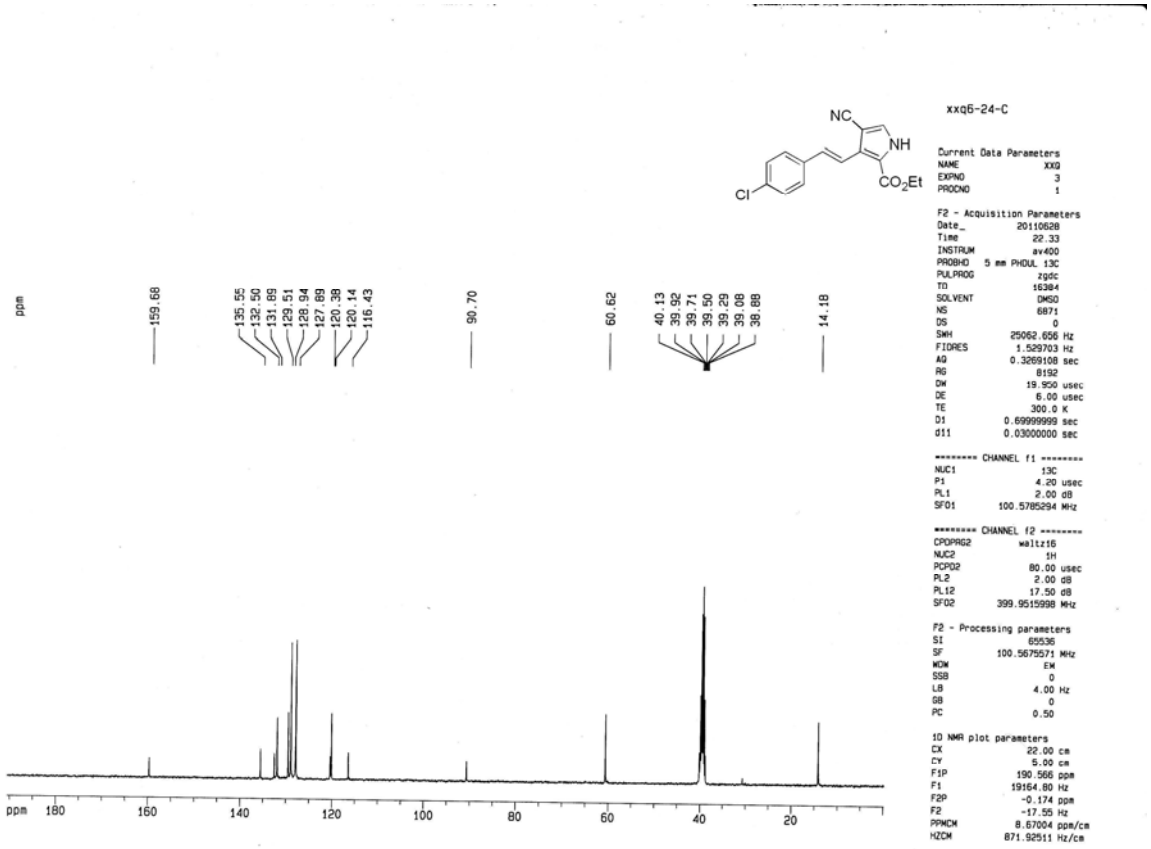
4a



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xxq6-24-C

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EXPNO                   3
PROCNO                  1

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TD                   16384
SOLVENT               DMSO
NS                    6871
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FIDRES             1.529703 Hz
AQ                0.3269108 sec
RG                    8192
DW                  19.950 usec
DE                   6.00 usec
TE                  300.0 K
D1             0.69999999 sec
d11            0.03000000 sec

======== CHANNEL f1 ========
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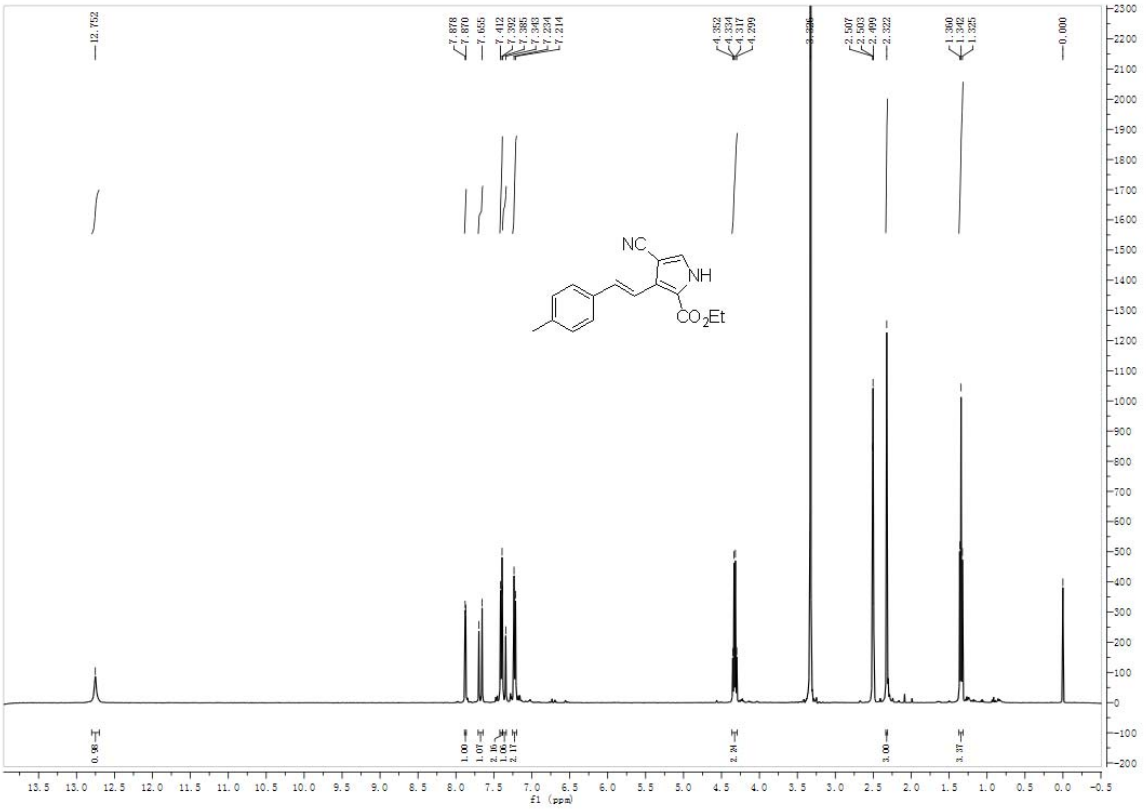
P1                  4.20 usec
PL1                 2.00 dB
SFO1          100.5785294 MHz

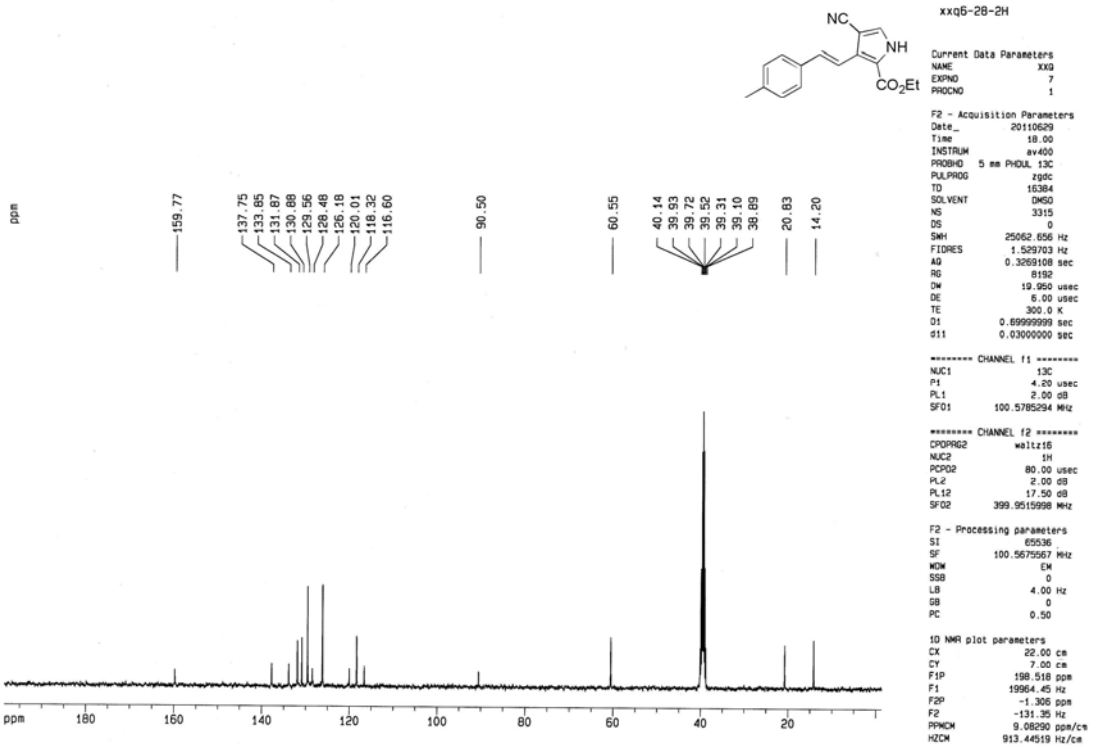
======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2              80.00 usec
PL2                 2.00 dB
PL12               17.50 dB
SFO2          399.9515998 MHz

F2 - Processing parameters
SI                    65536
SF            100.5675571 MHz
WDW                     EM
SSB                      0
LB                  4.00 Hz
GB                       0
PC                    0.50

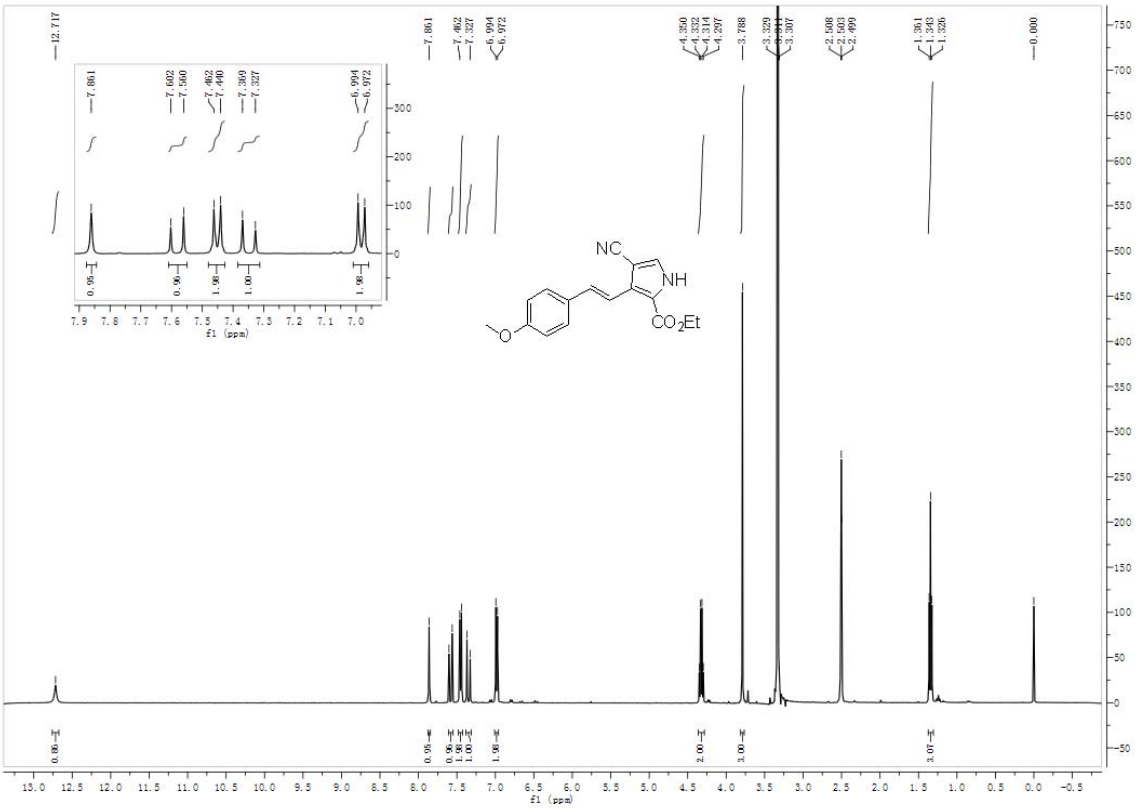
1D NMR plot parameters
CX                  22.00 cm
CY                   5.00 cm
F1P               190.566 ppm
F1                19164.80 Hz
F2P                -0.174 ppm
F2                 -17.55 Hz
PPMCM              8.67004 ppm/cm
HZCM           871.92511 Hz/cm
```

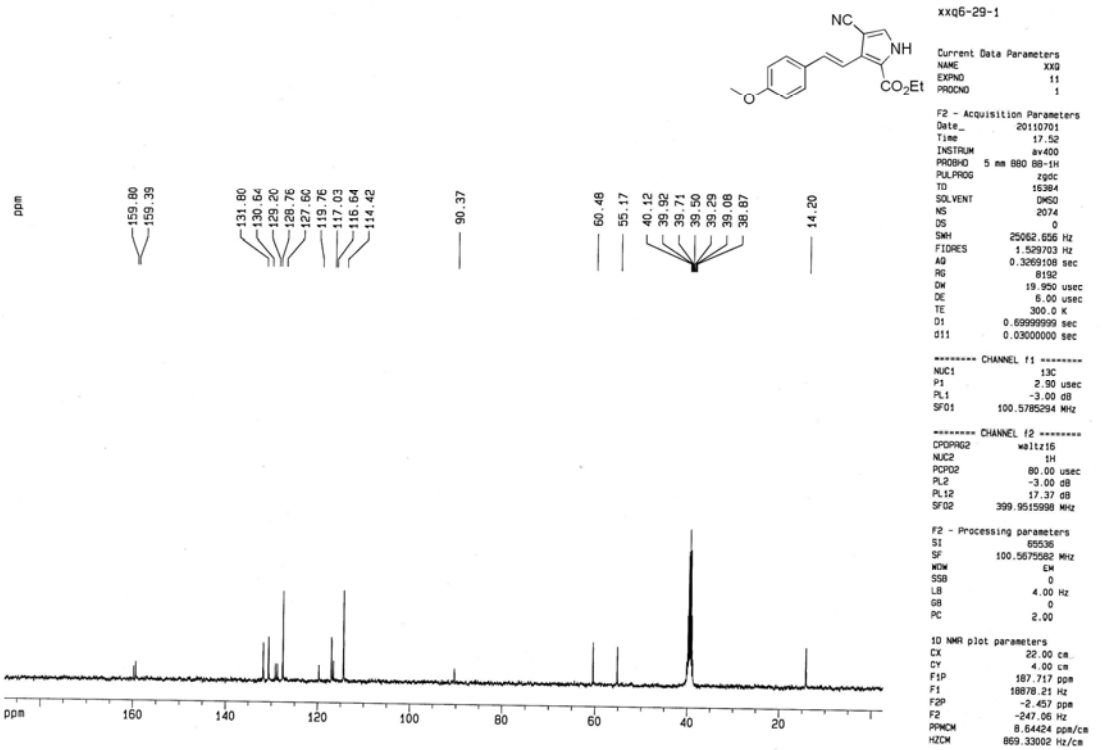
4b


12.752
7.878
7.870
7.655
7.412
7.392
7.385
7.365
7.234
7.214
4.352
4.334
4.317
4.299
3.326
2.507
2.503
2.499
2.322
1.360
1.342
1.325
0.000
NC
NH
CO2Et
f1 (ppm)

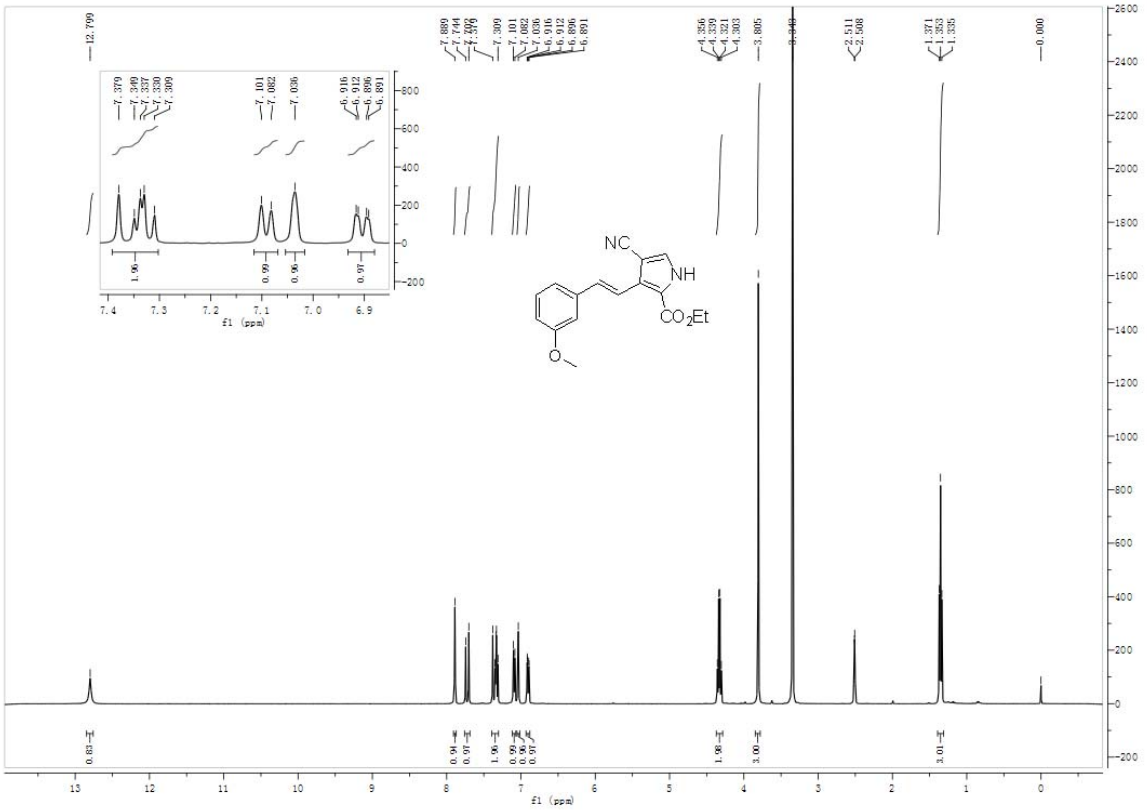

xxq6-28-2H
NC
NH
CO2Et
ppm
159.77
137.75
133.85
131.87
130.88
129.56
128.48
126.18
120.01
118.32
116.60
90.50
60.55
40.14
39.93
39.72
39.52
39.31
39.10
38.89
20.83
14.20
Current Data Parameters
NAME XXQ
EXPNO 7
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110629
Time 18.00
INSTRUM av400
PROBHD 5 mm PHOUL 13C
PULPROG zgdc
TD 16384
SOLVENT DMSO
NS 3315
DS 0
SWH 25062.656 Hz
FIDRES 1.529703 Hz
AQ 0.3269108 sec
RG 8192
DW 19.950 usec
DE 6.00 usec
TE 300.0 K
D1 0.69999999 sec
d11 0.03000000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.20 usec
PL1 2.00 dB
SF01 100.5785294 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.00 dB
PL12 17.50 dB
SF02 399.9515998 MHz
F2 - Processing parameters
SI 65536
SF 100.5675567 MHz
WDW EM
SSB 0
LB 4.00 Hz
GB 0
PC 0.50
1D NMR plot parameters
CX 22.00 cm
CY 7.00 cm
F1P 198.518 ppm
F1 19964.45 Hz
F2P -1.306 ppm
F2 -131.35 Hz
PPMCM 9.08290 ppm/cm
HZCM 913.44519 Hz/cm

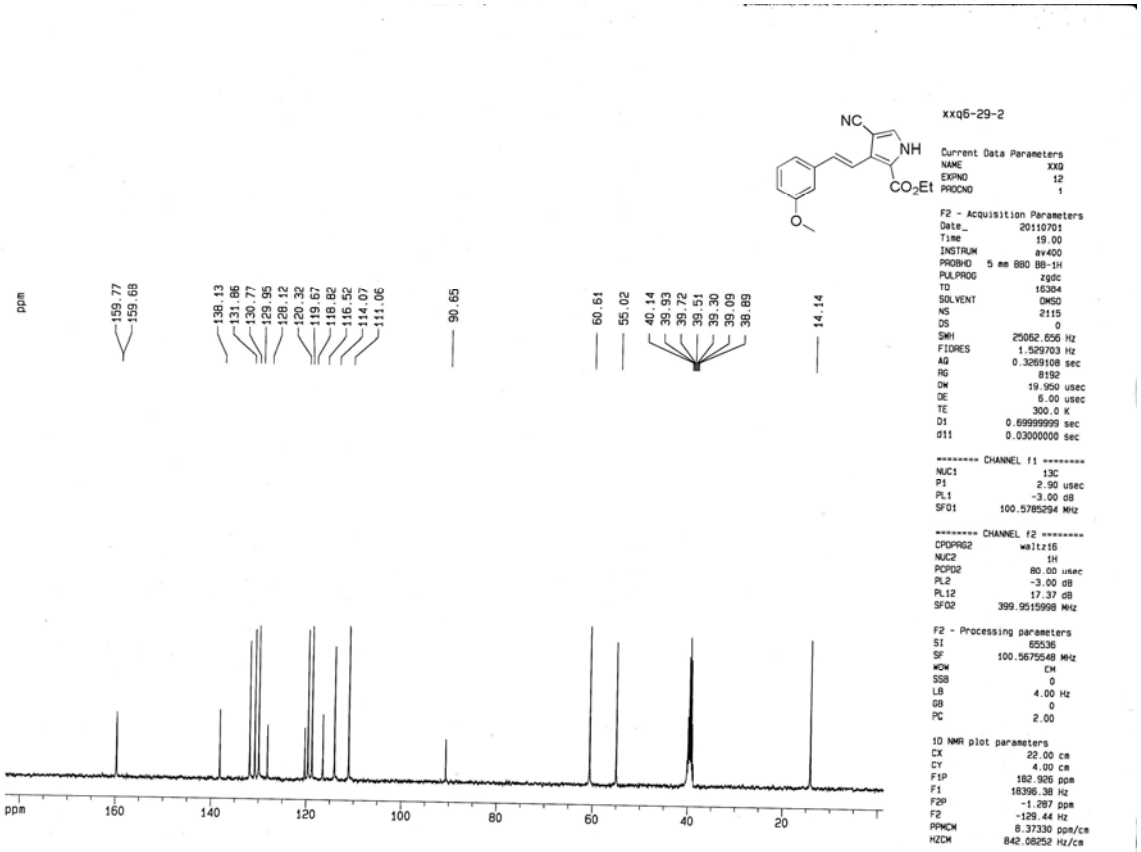
4c


NC
NH
CO2Et
O
f1 (ppm)

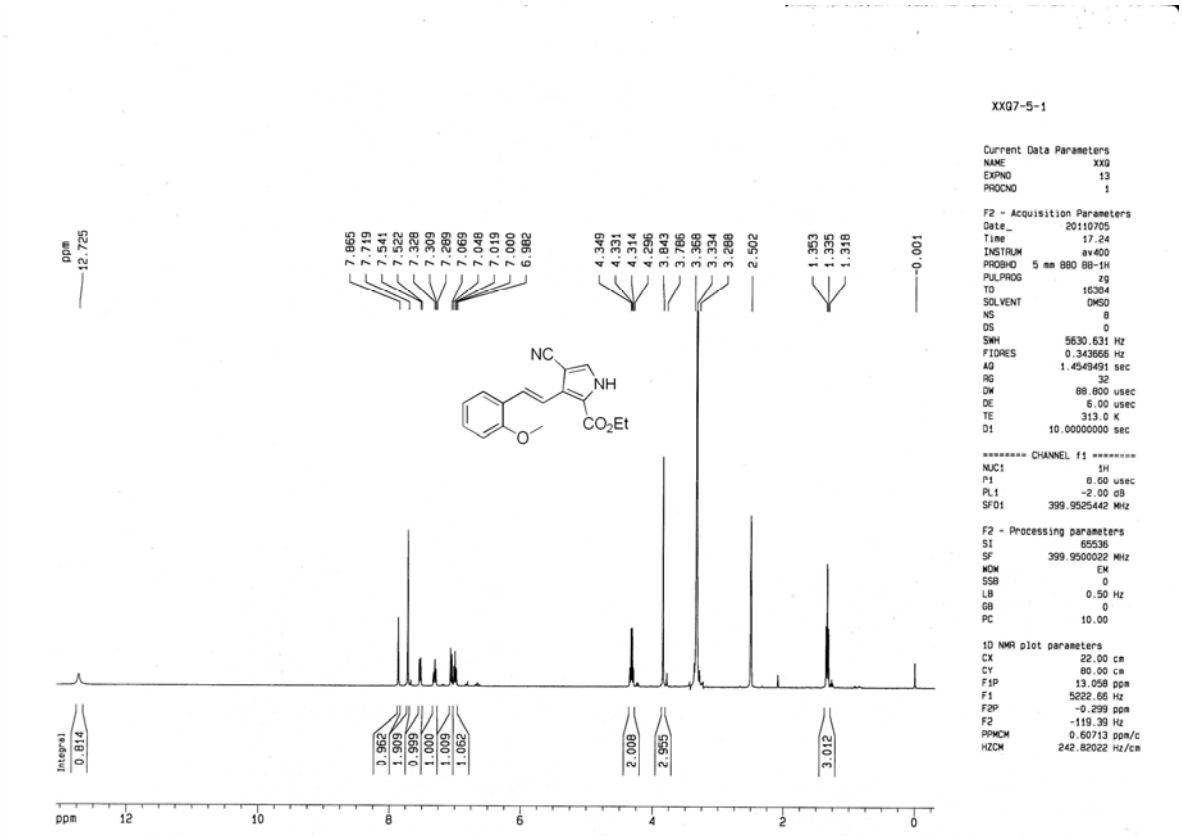

NC
NH
CO2Et
O
ppm
xxq6-29-1
Current Data Parameters
NAME XXQ
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110701
Time 17.52
INSTRUM av400
PROBHD 5 mm BBO BB-1H
PULPROG zgdc
TD 16384
SOLVENT DMSO
NS 2074
DS 0
SWH 25062.656 Hz
FIDRES 1.529703 Hz
AQ 0.3269108 sec
RG 8192
DW 19.950 usec
DE 6.00 usec
TE 300.0 K
D1 0.69999999 sec
d11 0.03000000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 2.90 usec
PL1 -3.00 dB
SFO1 100.5785294 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 17.37 dB
SFO2 399.9515998 MHz
F2 - Processing parameters
SI 65536
SF 100.5675582 MHz
WDW EM
SSB 0
LB 4.00 Hz
GB 0
PC 2.00
1D NMR plot parameters
CX 22.00 cm
CY 4.00 cm
F1P 187.717 ppm
F1 18870.21 Hz
F2P -2.457 ppm
F2 -247.06 Hz
PPMCM 8.64424 ppm/cm
HZCM 869.33002 Hz/cm

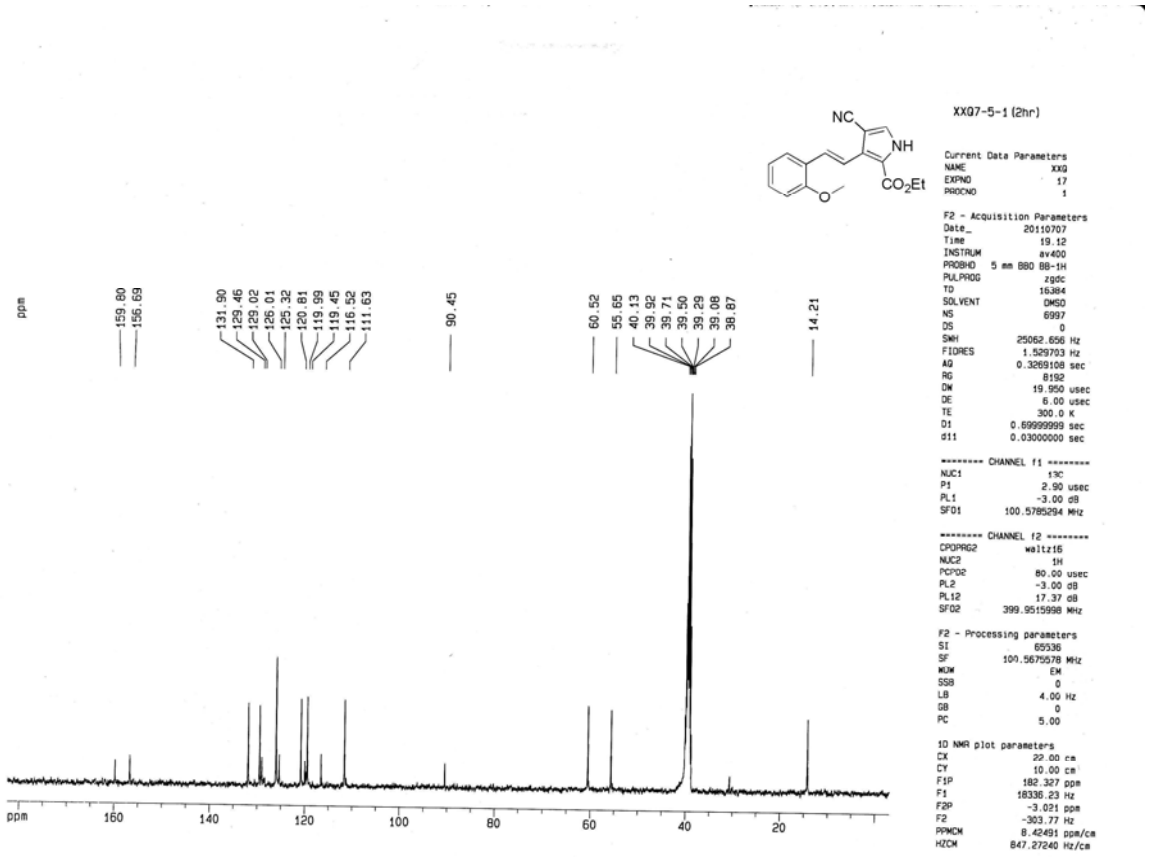
4d


NC
NH
CO2Et
O
f1 (ppm)

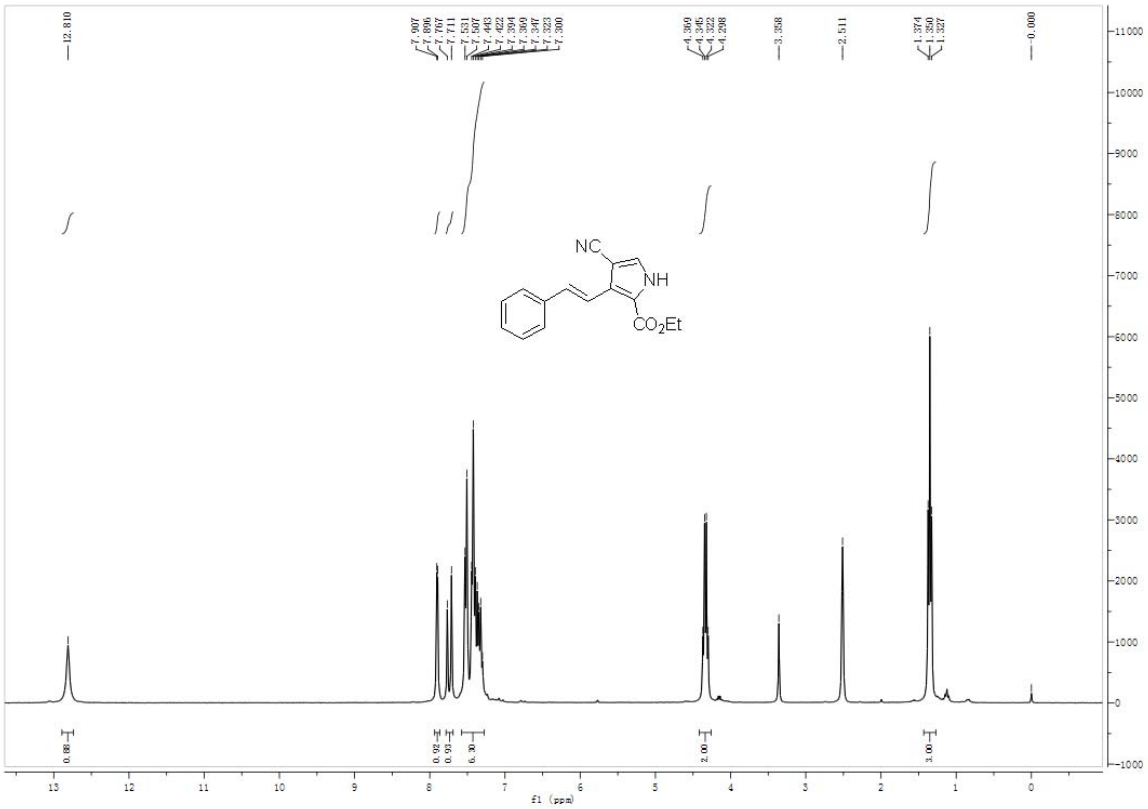

NC
NH
CO2Et
O
ppm
xxq6-29-2
Current Data Parameters
NAME XXQ
EXPNO 12
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110701
Time 19.00
INSTRUM av400
PROBHD 5 mm BB-1H
PULPROG zgdc
TD 16384
SOLVENT DMSO
NS 2115
DS 0
SWH 25062.656 Hz
FIDRES 1.529703 Hz
AQ 0.3269108 sec
RG 8192
DW 19.950 usec
DE 6.00 usec
TE 300.0 K
D1 0.69999999 sec
d11 0.03000000 sec
CHANNEL f1
NUC1 13C
P1 2.90 usec
PL1 -3.00 dB
SFO1 100.5785294 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 17.37 dB
SFO2 399.9515998 MHz
F2 - Processing parameters
SI 65536
SF 100.5675548 MHz
WDW EM
SSB 0
LB 4.00 Hz
GB 0
PC 2.00
1D NMR plot parameters
CX 22.00 cm
CY 4.00 cm
F1P 182.926 ppm
F1 18396.38 Hz
F2P -1.287 ppm
F2 -129.44 Hz
PPMCM 8.37330 ppm/cm
HZCM 842.08252 Hz/cm

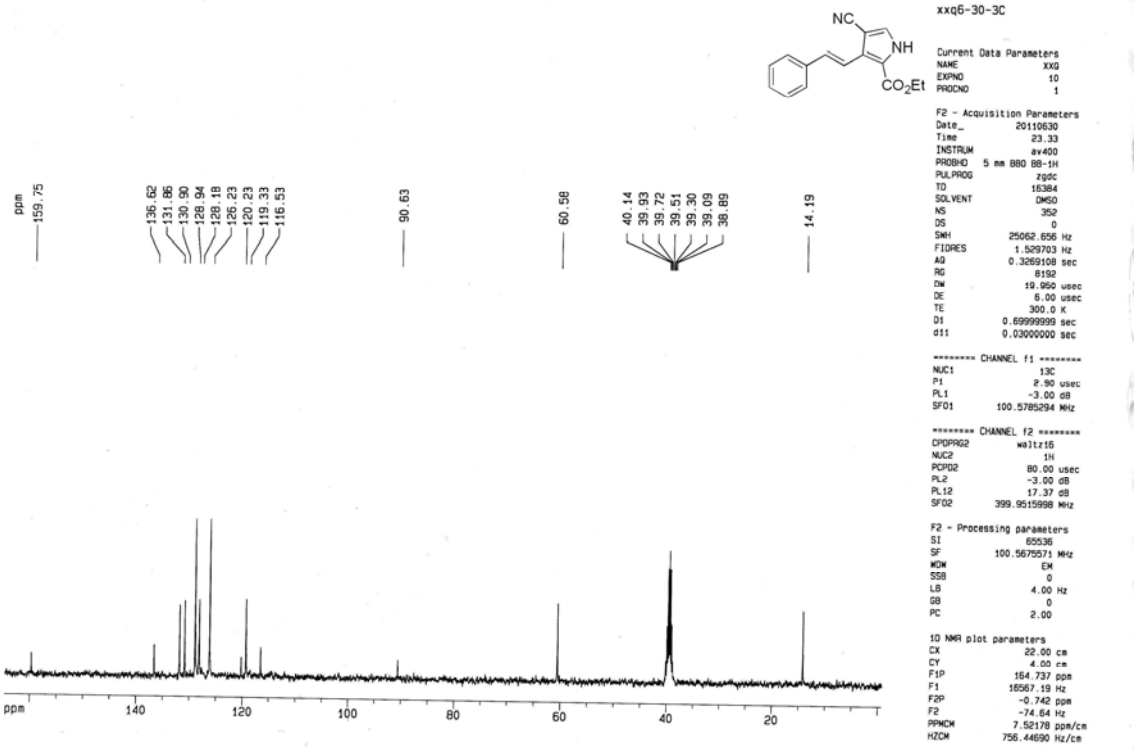
4e


ppm
12.725
7.865
7.719
7.541
7.522
7.328
7.309
7.289
7.069
7.048
7.019
7.000
6.982
4.349
4.331
4.314
4.296
3.843
3.786
3.368
3.334
3.288
2.502
1.353
1.335
1.318
0.001
NC
NH
CO2Et
O
Integral
0.814
0.962
1.909
0.999
1.000
1.009
1.062
2.008
2.955
3.012
ppm
12
10
8
6
4
2
0
XXQ7-5-1
Current Data Parameters
NAME XXQ
EXPNO 13
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110705
Time 17.24
INSTRUM av400
PROBHD 5 mm BBO BB-1H
PULPROG zg
TD 16384
SOLVENT DMSO
NS 8
DS 0
SWH 5630.631 Hz
FIDRES 0.343666 Hz
AQ 1.4549491 sec
RG 32
DW 88.800 usec
DE 6.00 usec
TE 313.0 K
D1 10.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 8.60 usec
PL1 -2.00 dB
SFO1 399.9525442 MHz
F2 - Processing parameters
SI 65536
SF 399.9500022 MHz
WDW EM
SSB 0
LB 0.50 Hz
GB 0
PC 10.00
1D NMR plot parameters
CX 22.00 cm
CY 80.00 cm
F1P 13.058 ppm
F1 5222.66 Hz
F2P -0.299 ppm
F2 -119.39 Hz
PPMCM 0.60713 ppm/c
HZCM 242.82022 Hz/cm


NC
NH
CO2Et
O
ppm
159.80
156.69
131.90
129.46
129.02
126.01
125.32
120.81
119.99
119.45
116.52
111.63
90.45
60.52
55.65
40.13
39.92
39.71
39.50
39.29
39.08
38.87
14.21
ppm
160
140
120
100
80
60
40
20
XXQ7-5-1 (2hr)
Current Data Parameters
NAME XXQ
EXPNO 17
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110707
Time 19.12
INSTRUM av400
PROBHD 5 mm BBO BB-1H
PULPROG zgdc
TD 16384
SOLVENT DMSO
NS 6997
DS 0
SWH 25062.656 Hz
FIDRES 1.529703 Hz
AQ 0.3269108 sec
RG 8192
DW 19.950 usec
DE 6.00 usec
TE 300.0 K
D1 0.69999999 sec
d11 0.03000000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 2.90 usec
PL1 -3.00 dB
SFO1 100.5785294 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 17.37 dB
SFO2 399.9515998 MHz
F2 - Processing parameters
SI 65536
SF 100.5675578 MHz
WDW EM
SSB 0
LB 4.00 Hz
GB 0
PC 5.00
1D NMR plot parameters
CX 22.00 cm
CY 10.00 cm
F1P 182.327 ppm
F1 18336.23 Hz
F2P -3.021 ppm
F2 -303.77 Hz
PPMCM 8.42491 ppm/cm
HZCM 847.27240 Hz/cm

4f






```
xxq6-30-3C

Current Data Parameters
NAME                  XXQ
EXPNO                  10
PROCNO                  1

F2 - Acquisition Parameters
Date_              20110630
Time                  23.33
INSTRUM               av400
PROBHD  5 mm BB-1H
PULPROG               zgdc
TD                   16384
SOLVENT              DMSO
NS                     352
DS                       0
SWH                25062.656 Hz
FIDRES              1.529703 Hz
AQ                  0.3269108 sec
RG                      8192
DW                   19.950 usec
DE                    6.00 usec
TE                   300.0 K
D1                0.69999999 sec
d11               0.03000000 sec

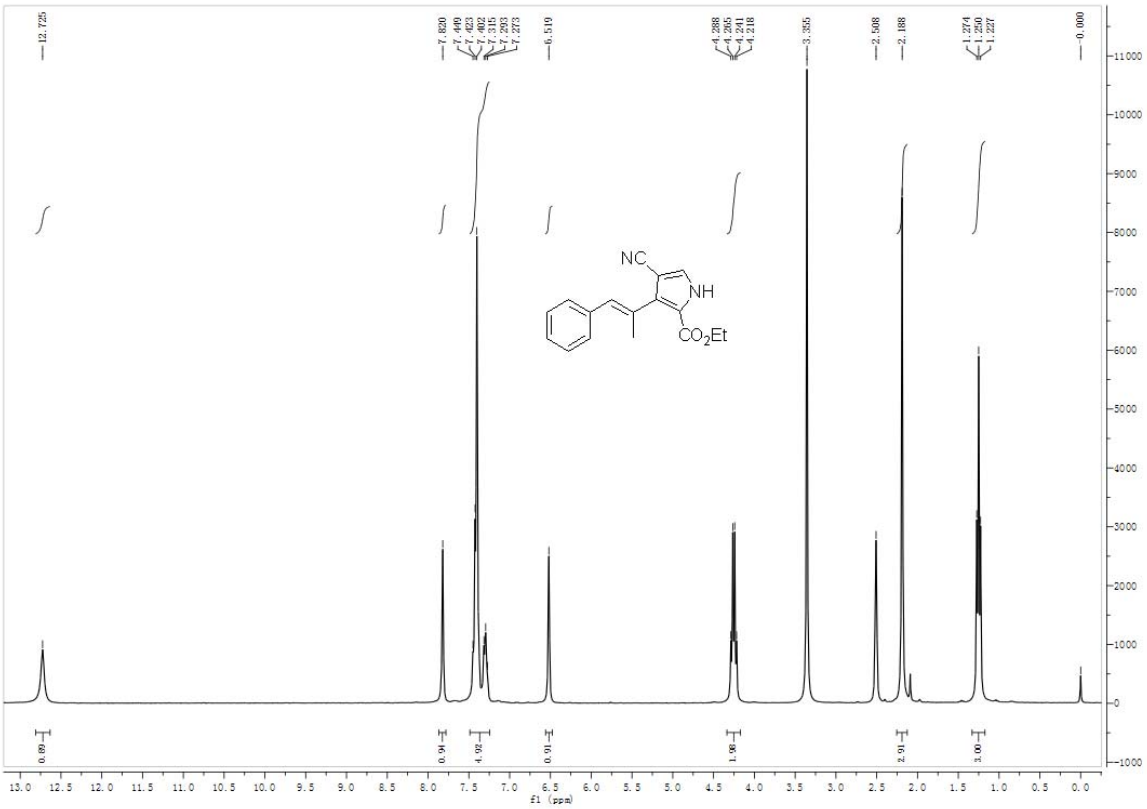
======== CHANNEL f1 ========
NUC1                    13C
P1                    2.90 usec
PL1                  -3.00 dB
SFO1           100.5785294 MHz

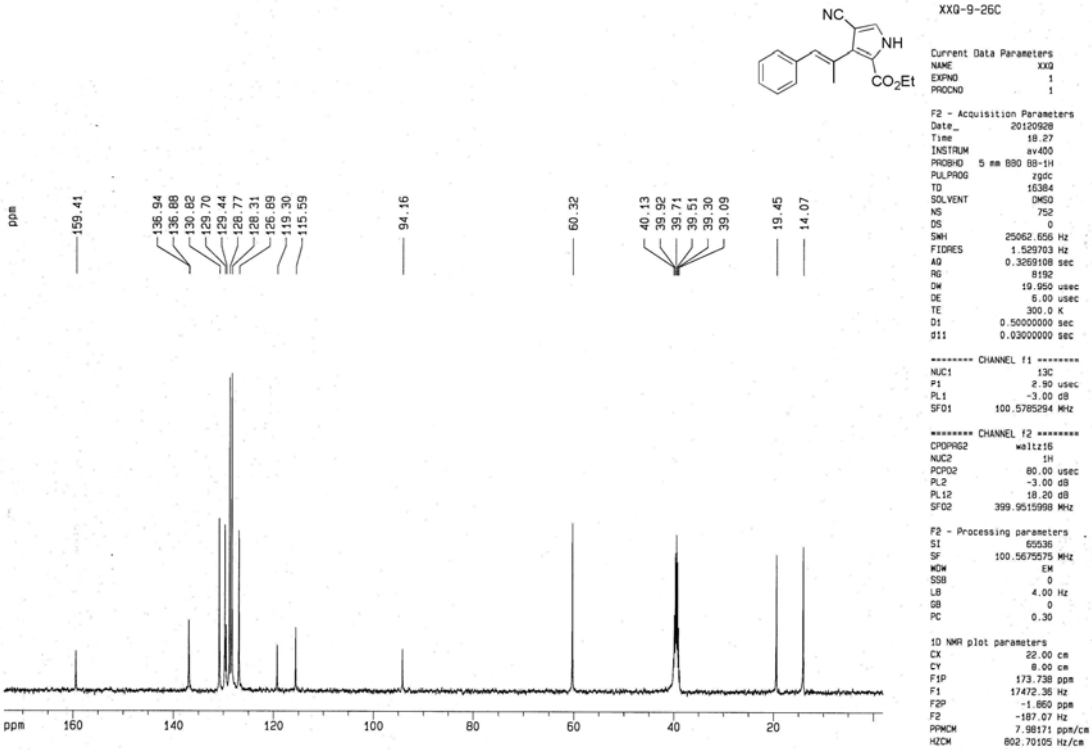
======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                    1H
PCPD2                80.00 usec
PL2                  -3.00 dB
PL12                 17.37 dB
SFO2           399.9515998 MHz

F2 - Processing parameters
SI                      65536
SF             100.5675571 MHz
WDW                     EM
SSB                      0
LB                    4.00 Hz
GB                       0
PC                    2.00

1D NMR plot parameters
CX                   22.00 cm
CY                    4.00 cm
F1P                 164.737 ppm
F1                16567.19 Hz
F2P                  -0.742 ppm
F2                  -74.64 Hz
PPMCM              7.52178 ppm/cm
HZCM             756.44690 Hz/cm
```

4g





XXQ-9-26C

Current Data Parameters
NAME XXQ
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120928
Time 18.27
INSTRUM av400
PROBHD 5 mm BBO BB-1H
PULPROG zgdc
TD 16384
SOLVENT DMSO
NS 752
DS 0
SWH 25062.656 Hz
FIDRES 1.529703 Hz
AQ 0.3269108 sec
RG 8192
DW 19.950 usec
DE 6.00 usec
TE 300.0 K
D1 0.50000000 sec
d11 0.03000000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 2.90 usec
PL1 -3.00 dB
SFO1 100.5785294 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 18.20 dB
SFO2 399.9515998 MHz

F2 - Processing parameters
SI 65536
SF 100.5675575 MHz
WDW EM
SSB 0
LB 4.00 Hz
GB 0
PC 0.30

1D NMR plot parameters
CX 22.00 cm
CY 8.00 cm
F1P 173.738 ppm
F1 17472.36 Hz
F2P -1.860 ppm
F2 -187.07 Hz
PPMCM 7.98171 ppm/cm
HZCM 802.70105 Hz/cm