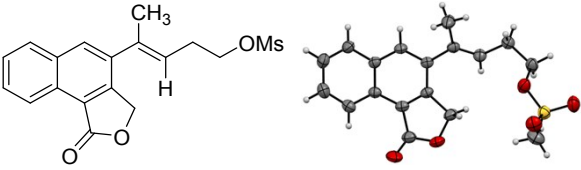
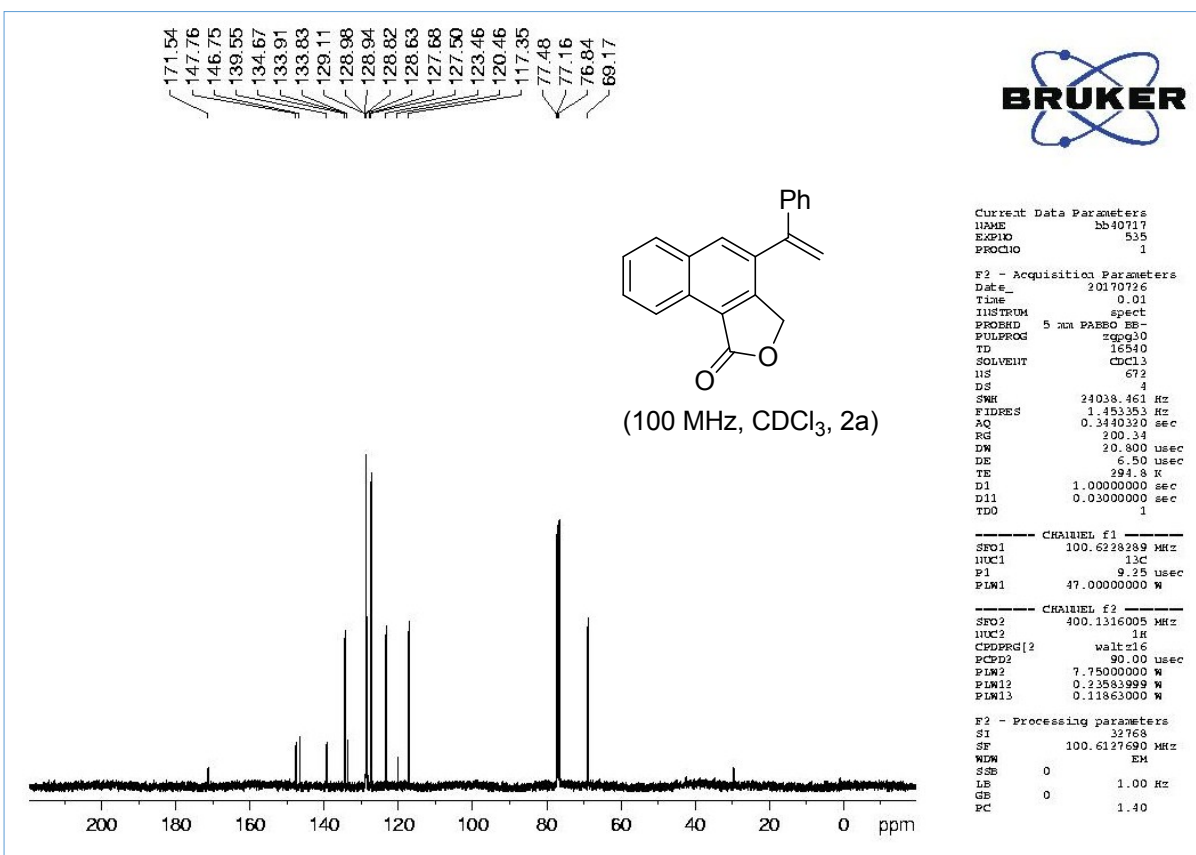
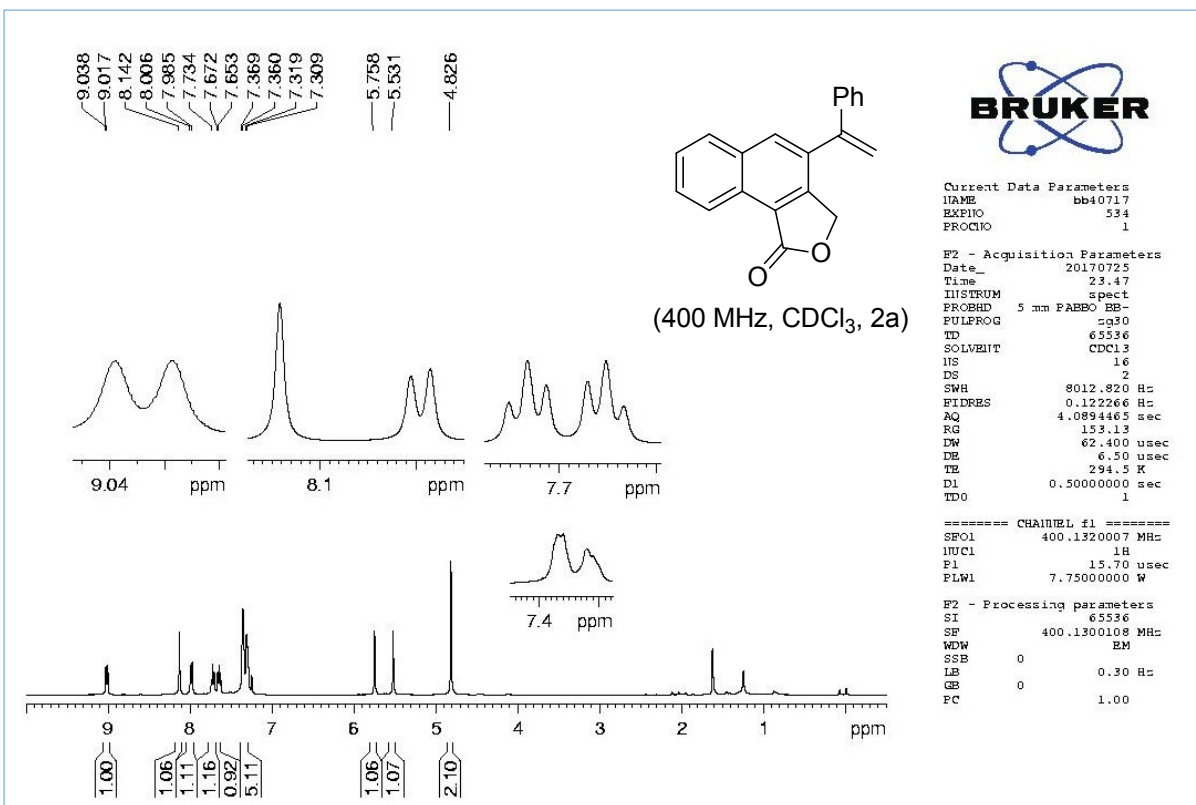
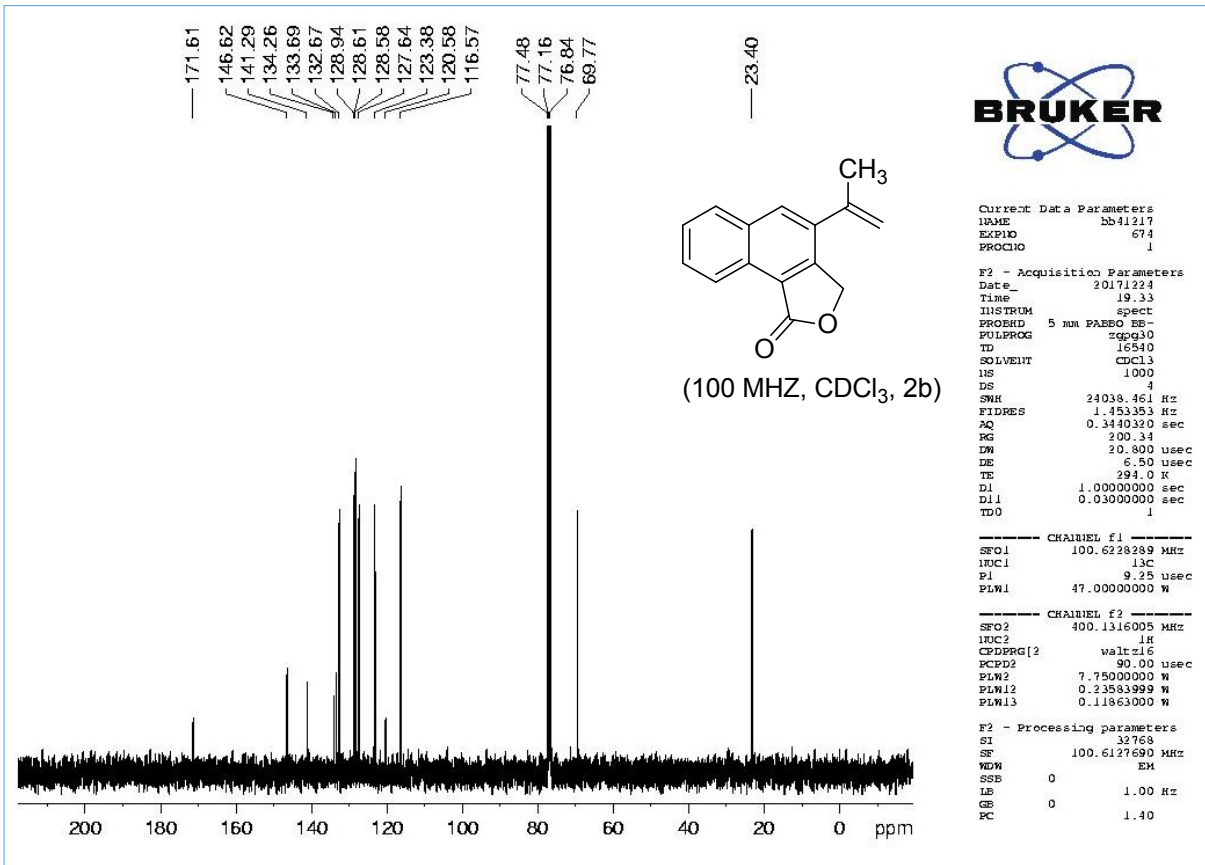
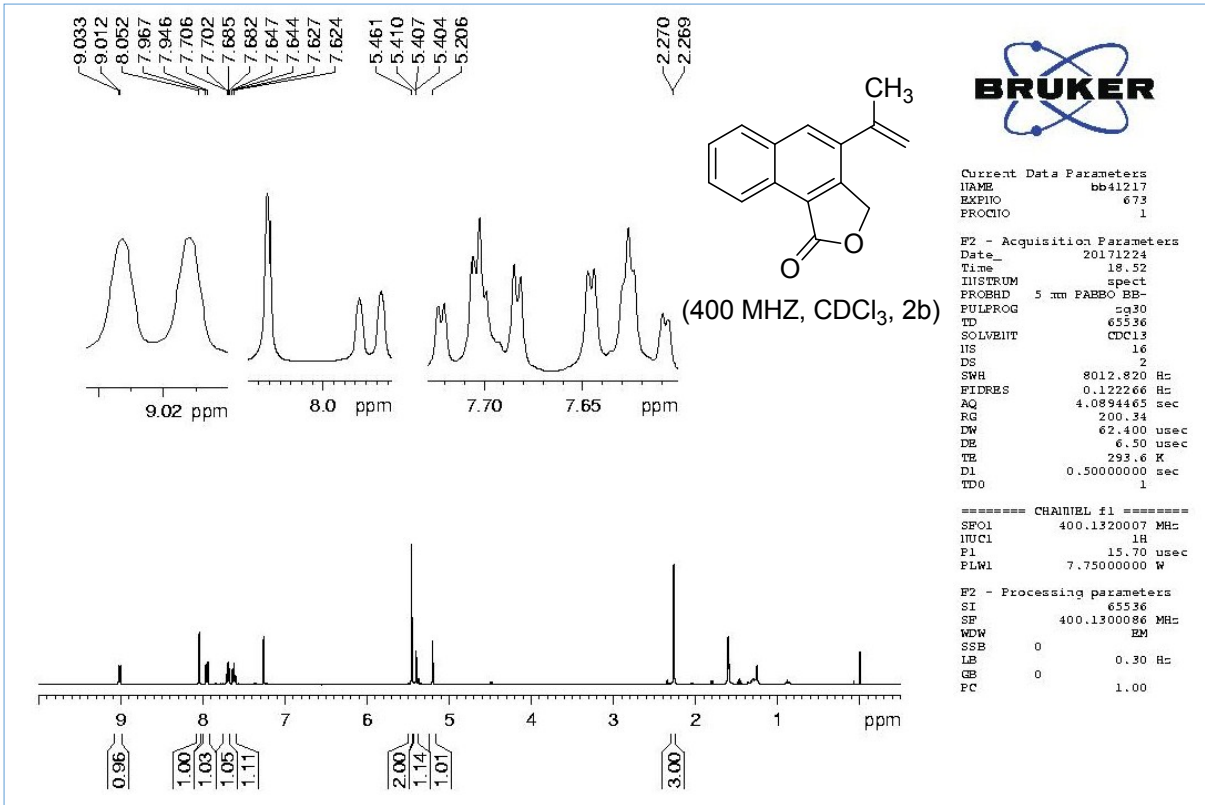


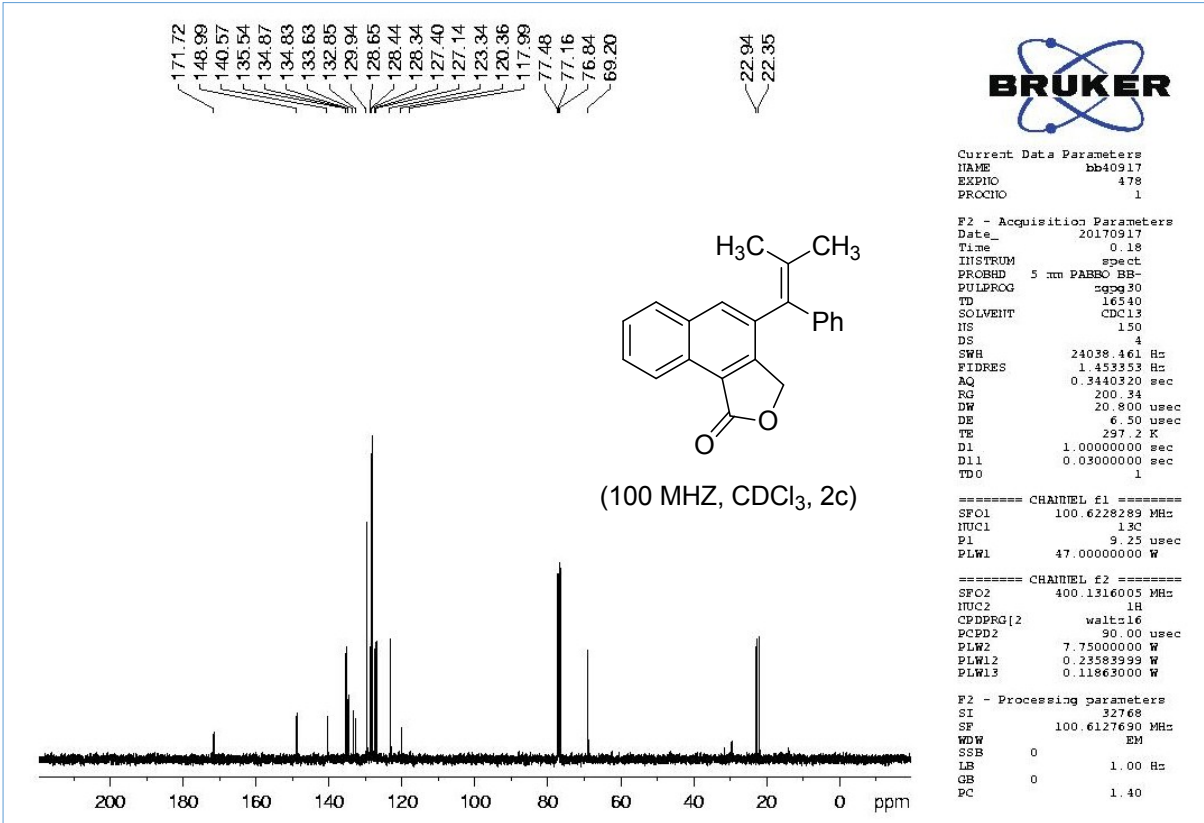
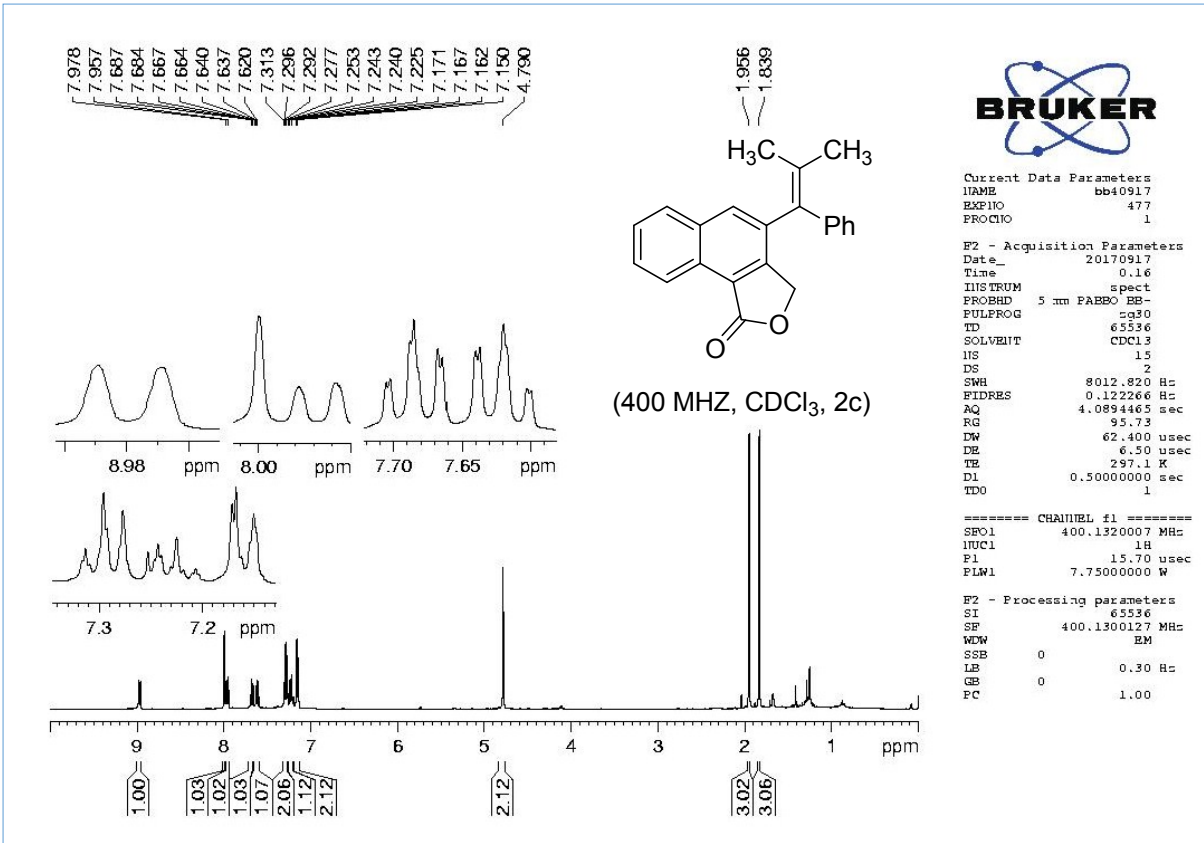
Acid Catalysed Rearrangement of Isobenzofurans to Angularly Fused Phthalides

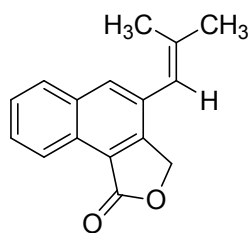
Crystallographic Data and Structure Refinements Summary for Compound **6f**

Molecular Structure (ORTEP Diagram)	
CCDC number	1846904
Formula	C ₁₈ H ₁₈ O ₅ S
Formula weight	346.38
Colour	yellow
Crystal morphology	orthogonalized
Temperature/K	296(2) K
Radiation	Mo k/a
Wavelength/Å	0.71073 Å
Crystal system	Triclinic
Space group	P-1
a (Å)	8.4865(4)
b (Å)	8.5936(4)
c (Å)	13.0039(6)
α (°)	71.285(2)
β (°)	82.909(2)
γ (°)	65.007(2)
Volume(Å ³)	814.03(7)
Z	2
Density (g/cm ³)	1.413
μ (1/mm)	0.224
F (000)	364
θ (min, max)	0.0548 and 0.1158
No. of unique reflns	3523
No. of parameters	220
R _{obs} , wR _{2_obs}	R1 = 0.0586, wR2 = 0.1266
Δρ _{min} , Δρ _{max} (eÅ ⁻³)	0.287 and -0.392
Goof	1.033

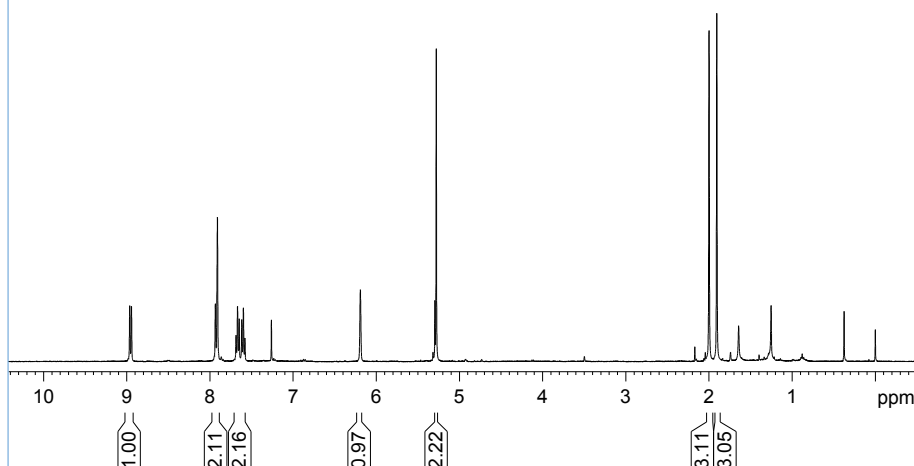








(400 MHz, CDCl₃, 2d)

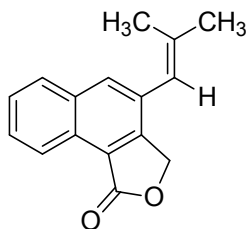


Current Data Parameters
NAME Desktop
EXPNO 619
PROCNO 1

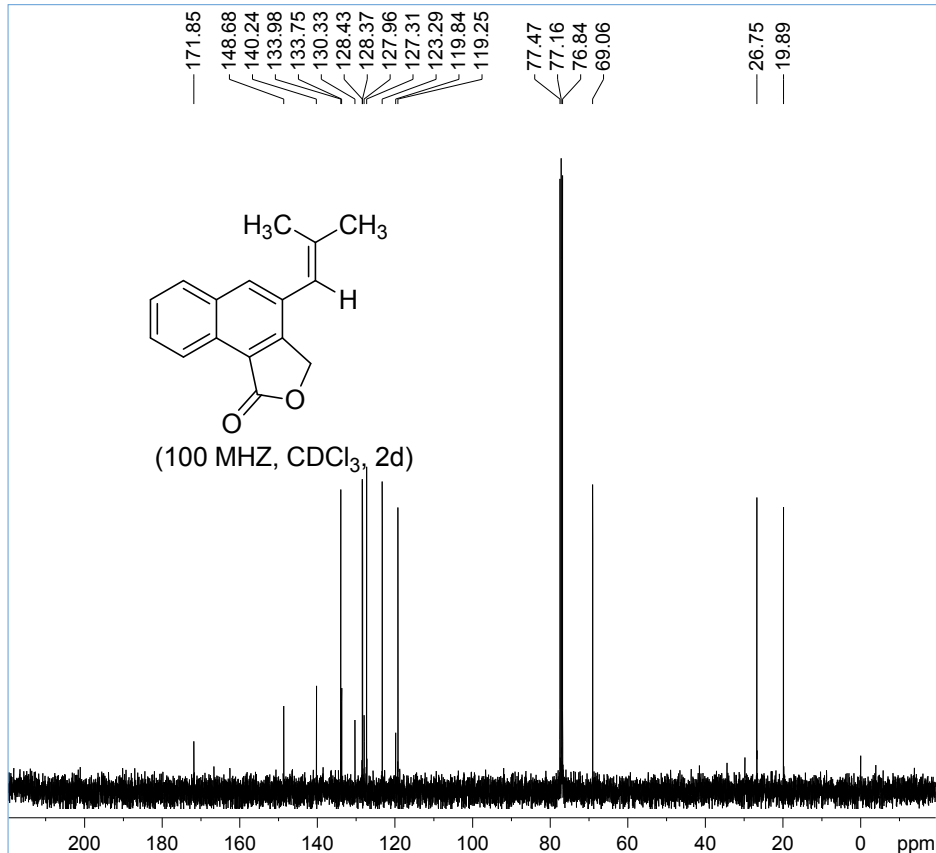
F2 - Acquisition Parameters
Date_ 20180724
Time_ 16.24
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 9
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 169.77
DW 62.400 usec
DE 6.50 usec
TE 295.4 K
D1 0.50000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1320007 MHz
NUC1 1H
P1 15.70 usec
PLW1 7.75000000 W

F2 - Processing parameters
SI 65536
SF 400.1300088 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



(100 MHz, CDCl₃, 2d)



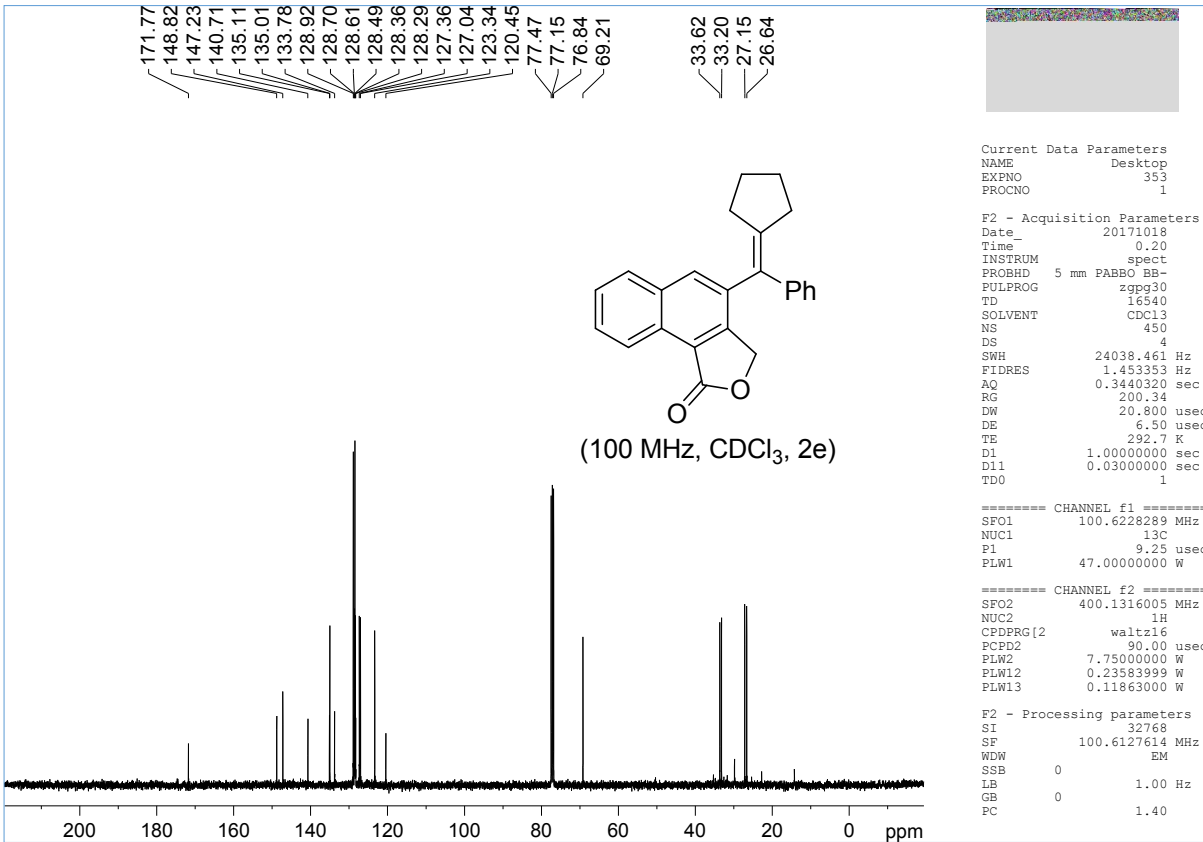
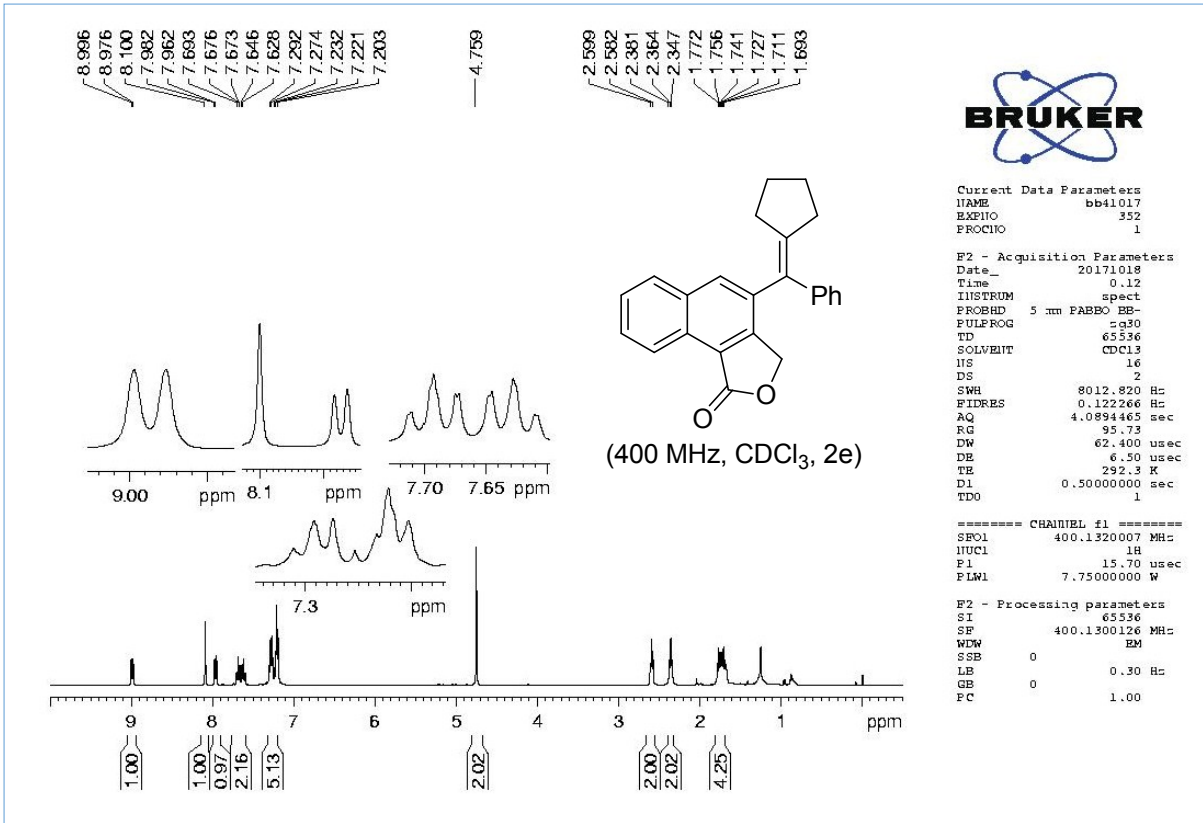
Current Data Parameters
NAME Desktop
EXPNO 620
PROCNO 1

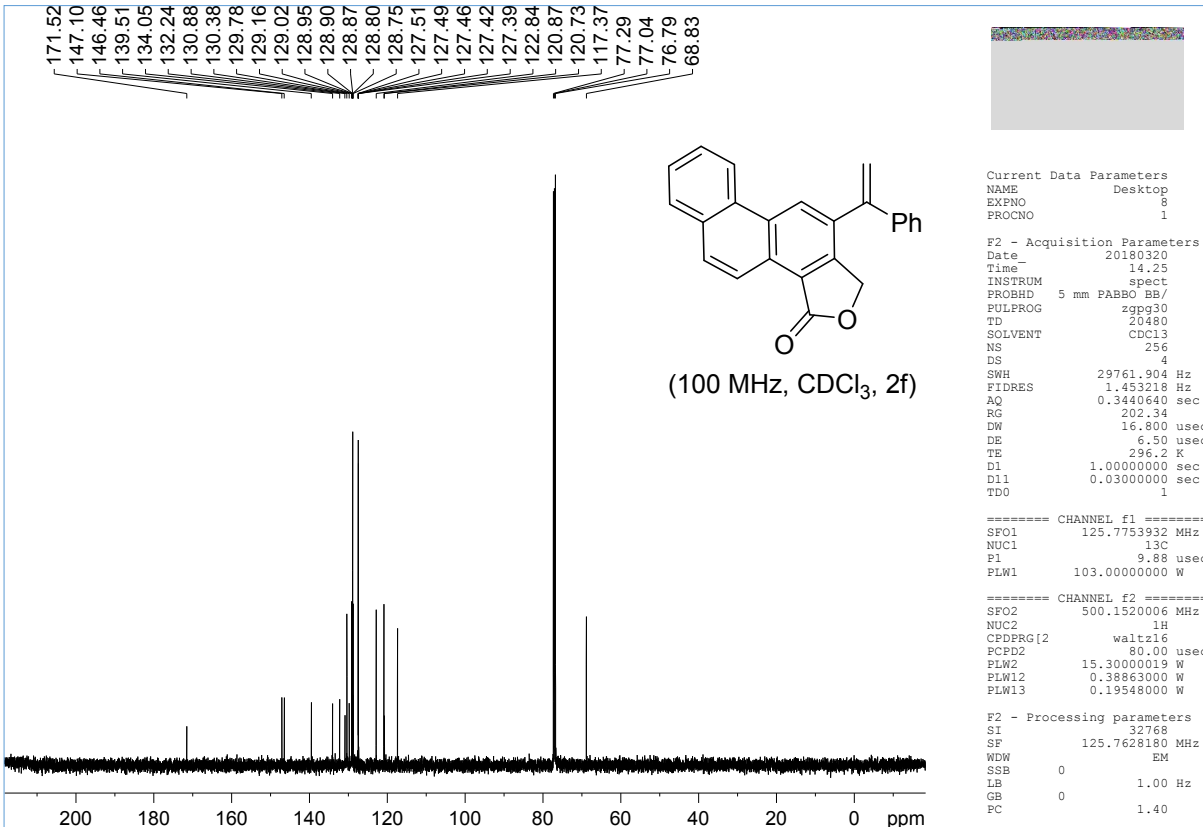
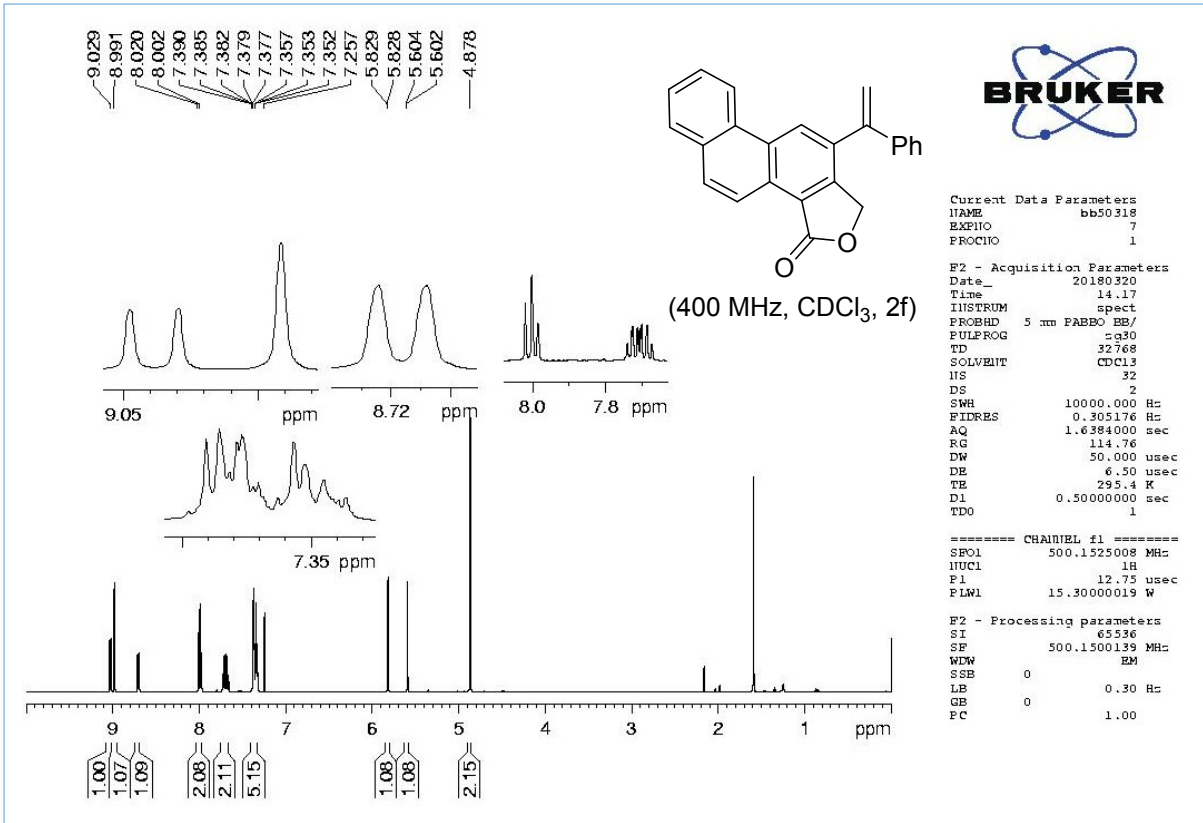
F2 - Acquisition Parameters
Date_ 20180724
Time_ 16.25
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 16540
SOLVENT CDCl3
NS 125
DS 4
SWH 24038.461 Hz
FIDRES 1.453353 Hz
AQ 0.3440320 sec
RG 200.34
DW 20.800 usec
DE 6.50 usec
TE 295.5 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

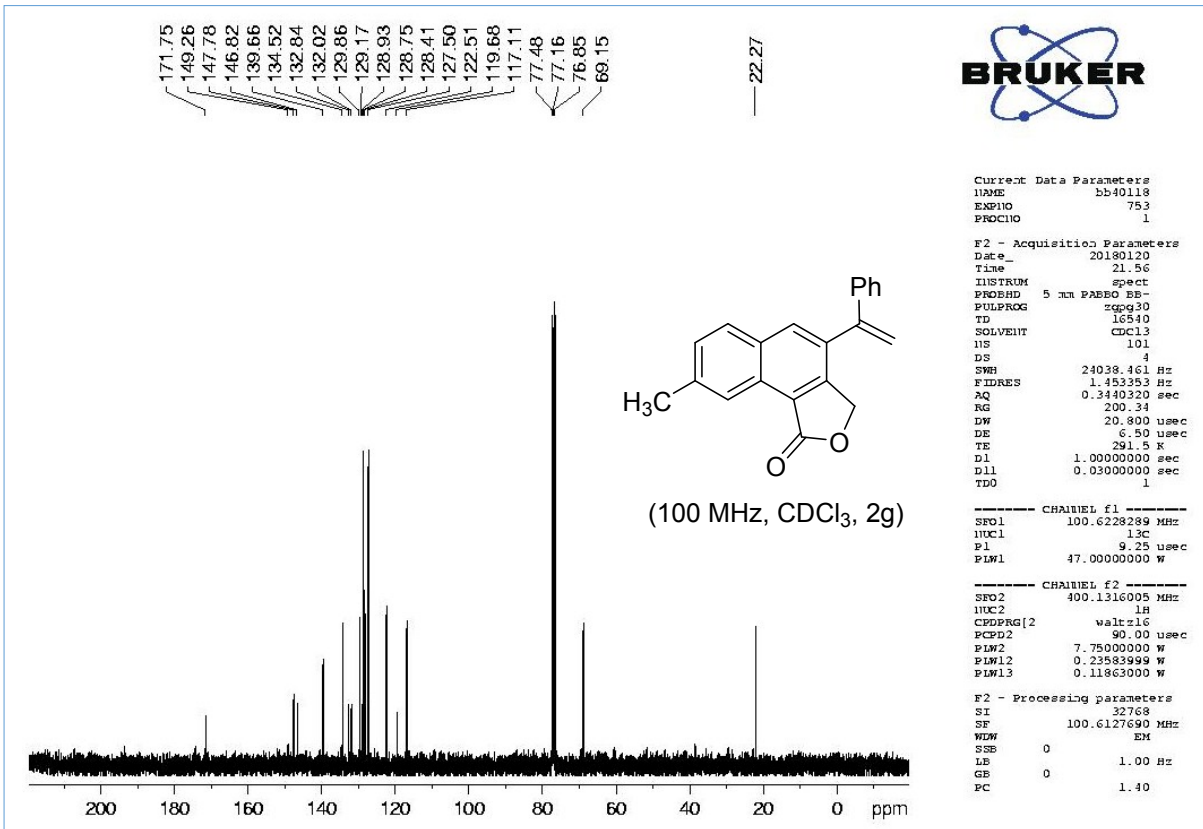
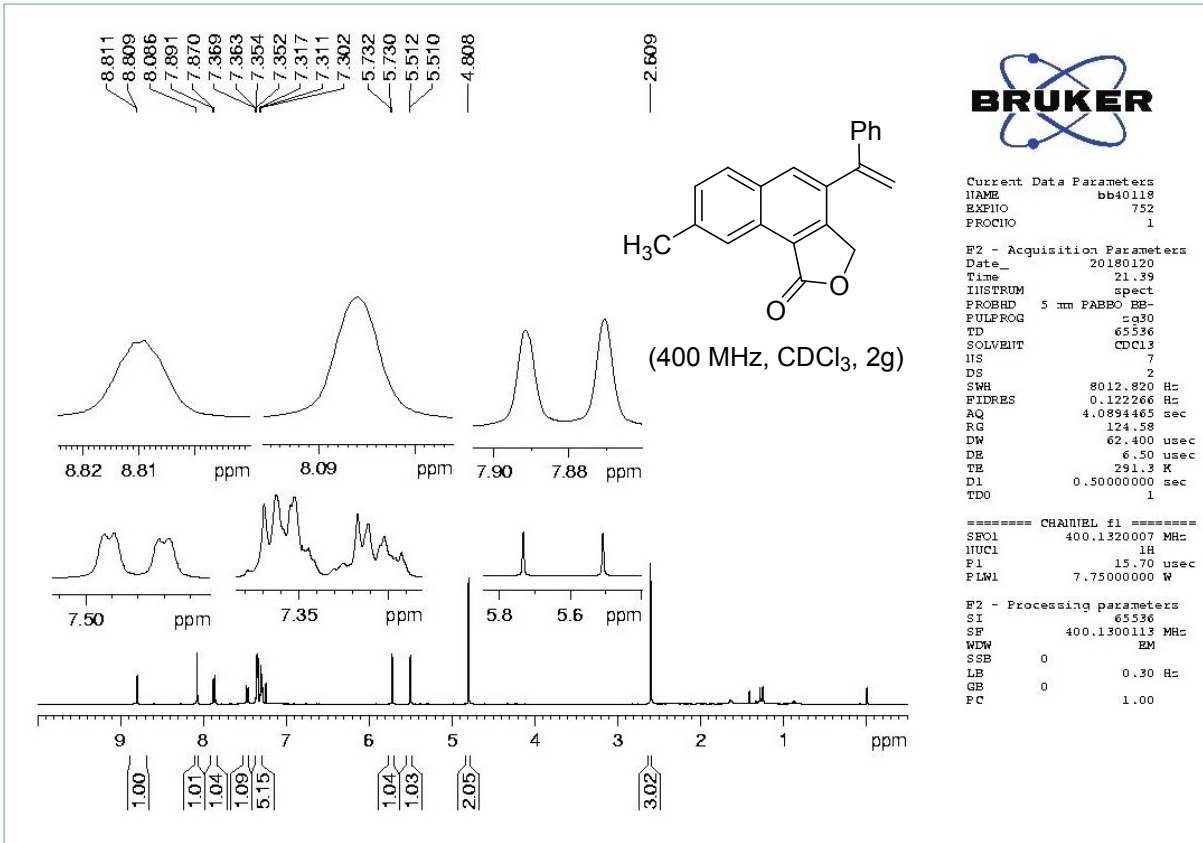
===== CHANNEL f1 =====
SFO1 100.6228289 MHz
NUC1 13C
P1 9.25 usec
PLW1 47.00000000 W

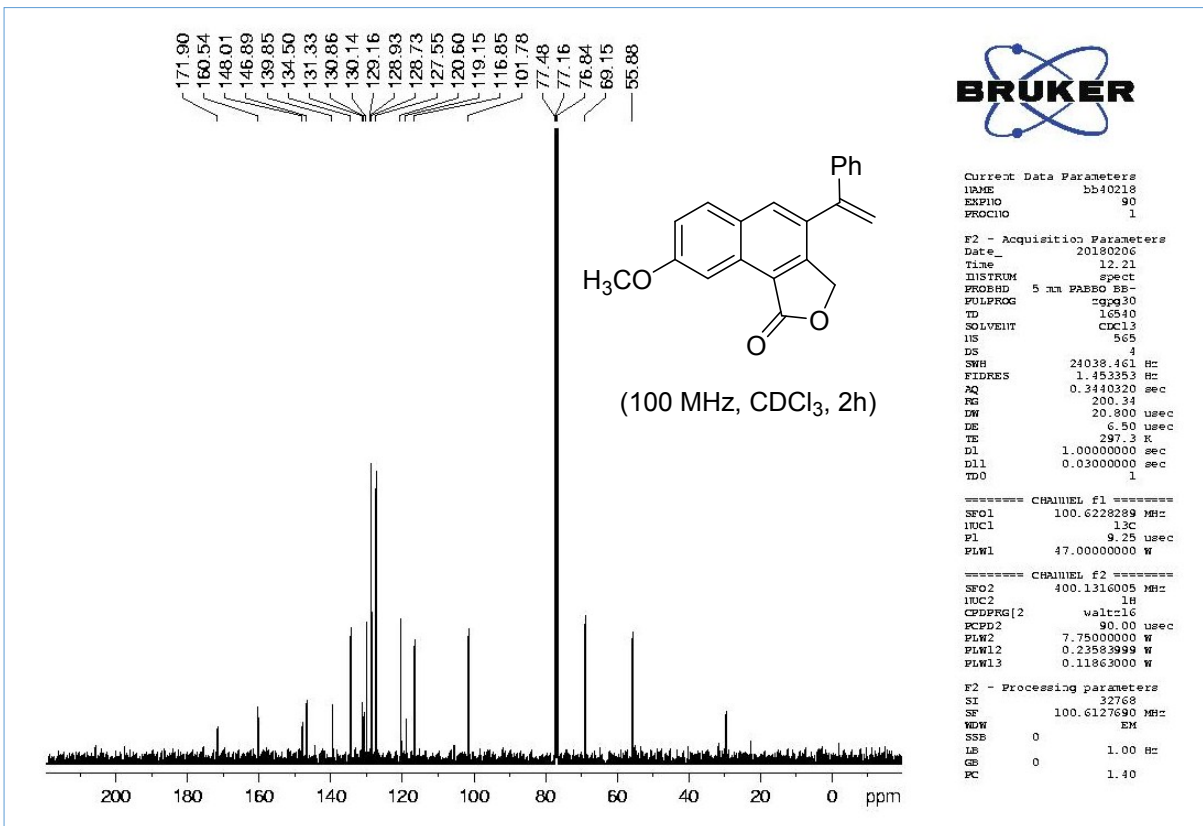
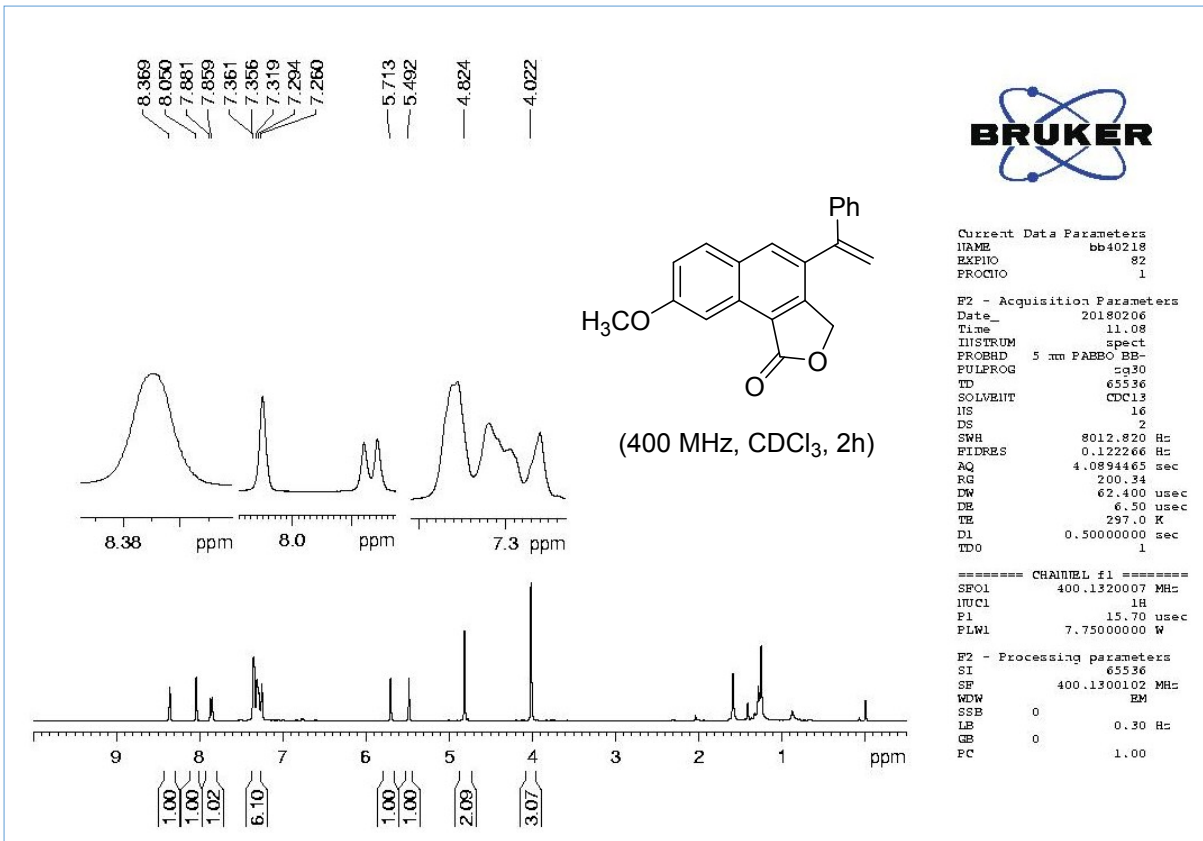
===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
PLW13 0.11863000 W

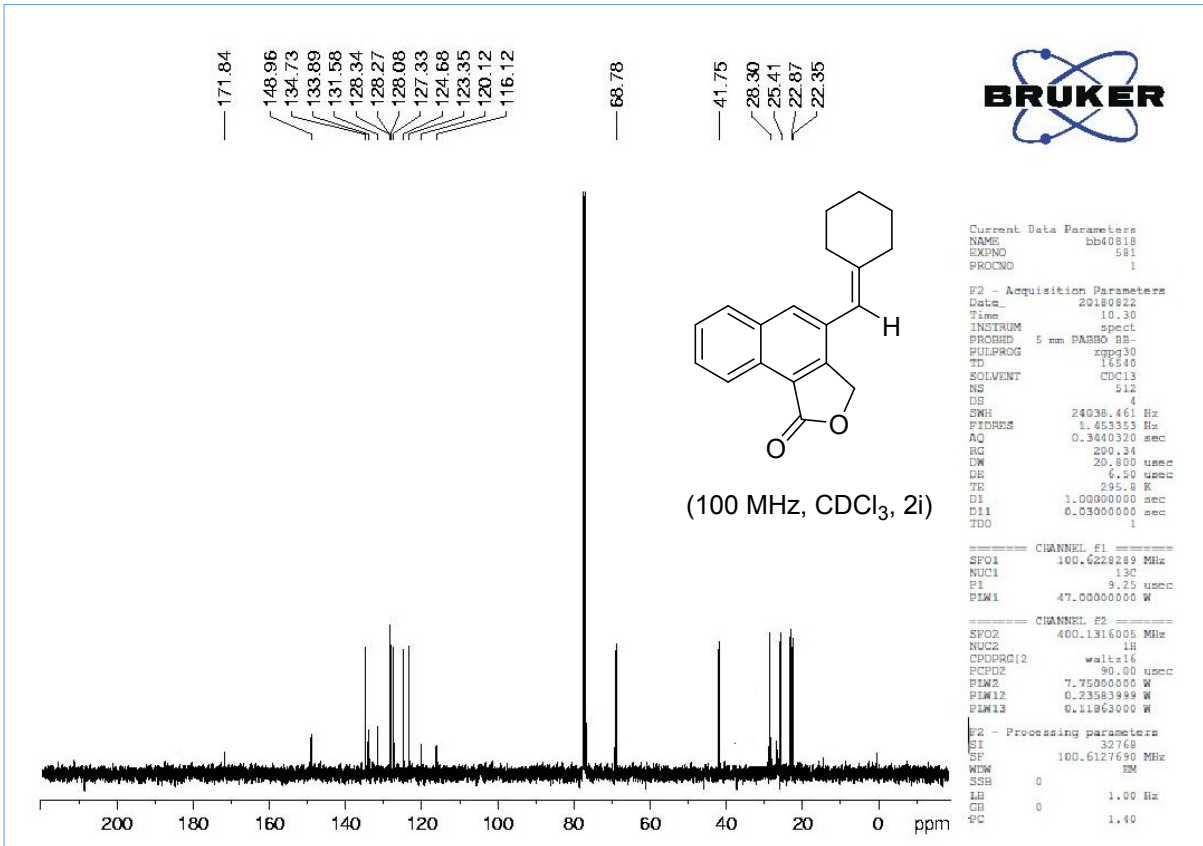
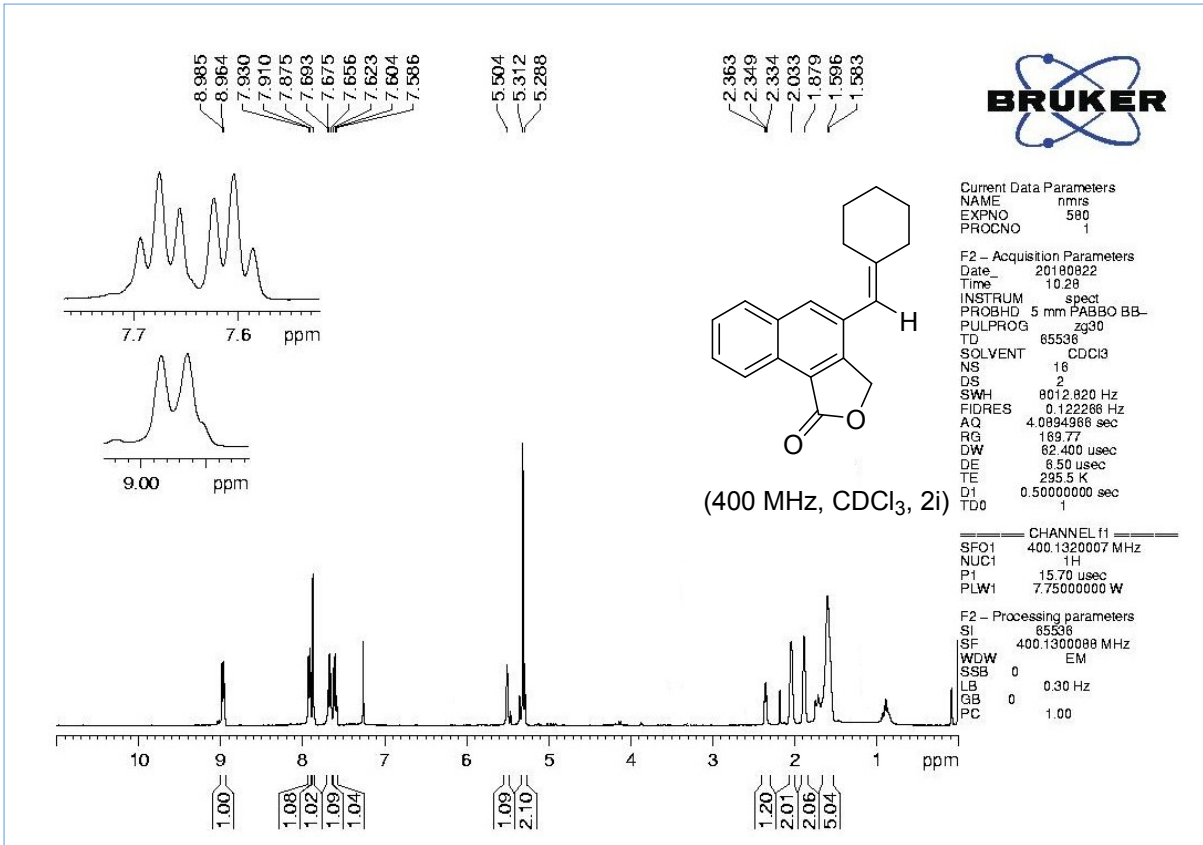
F2 - Processing parameters
SI 32768
SF 100.6127577 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

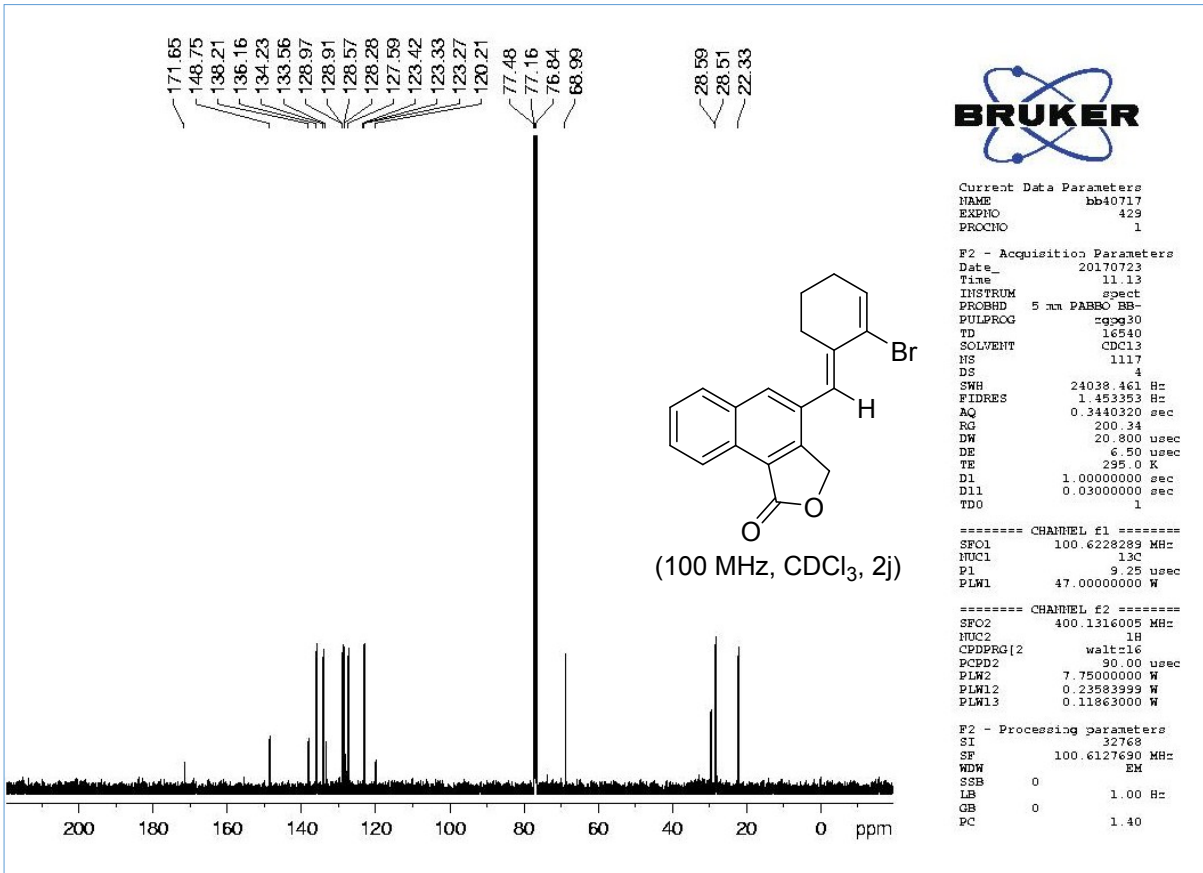
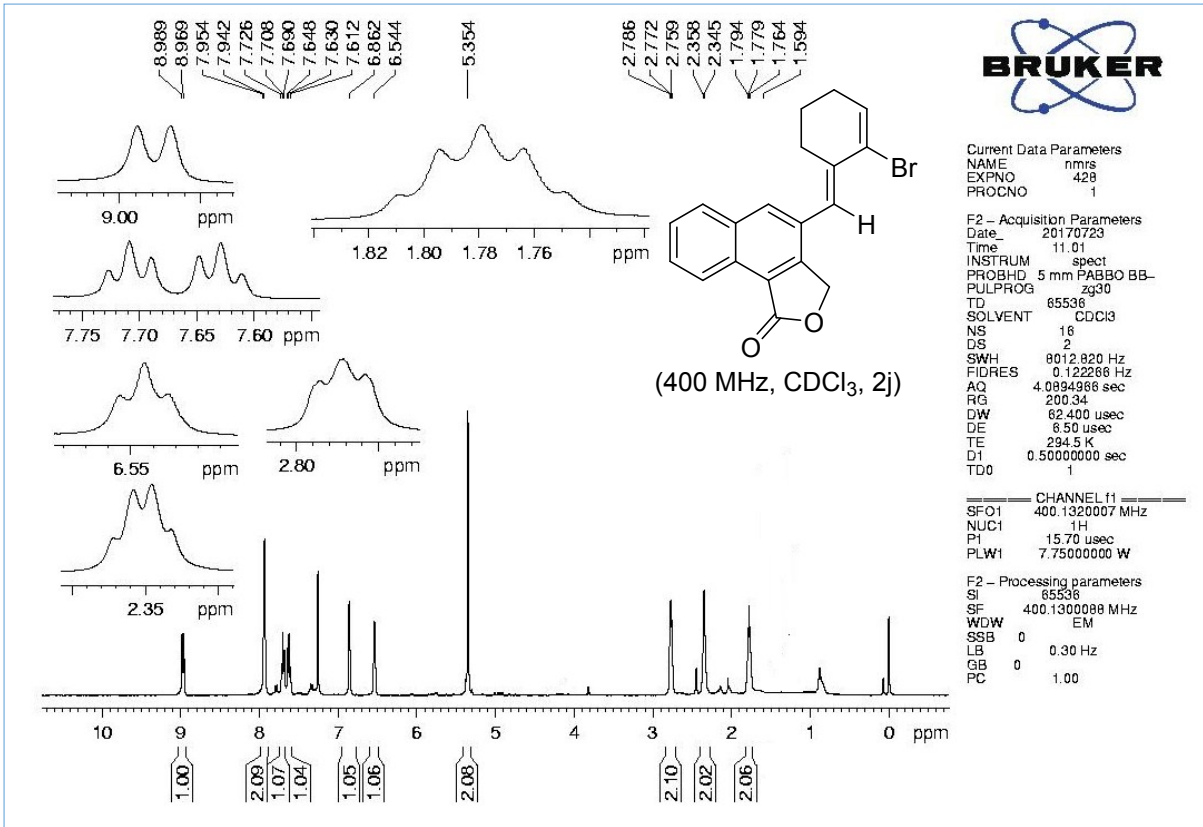


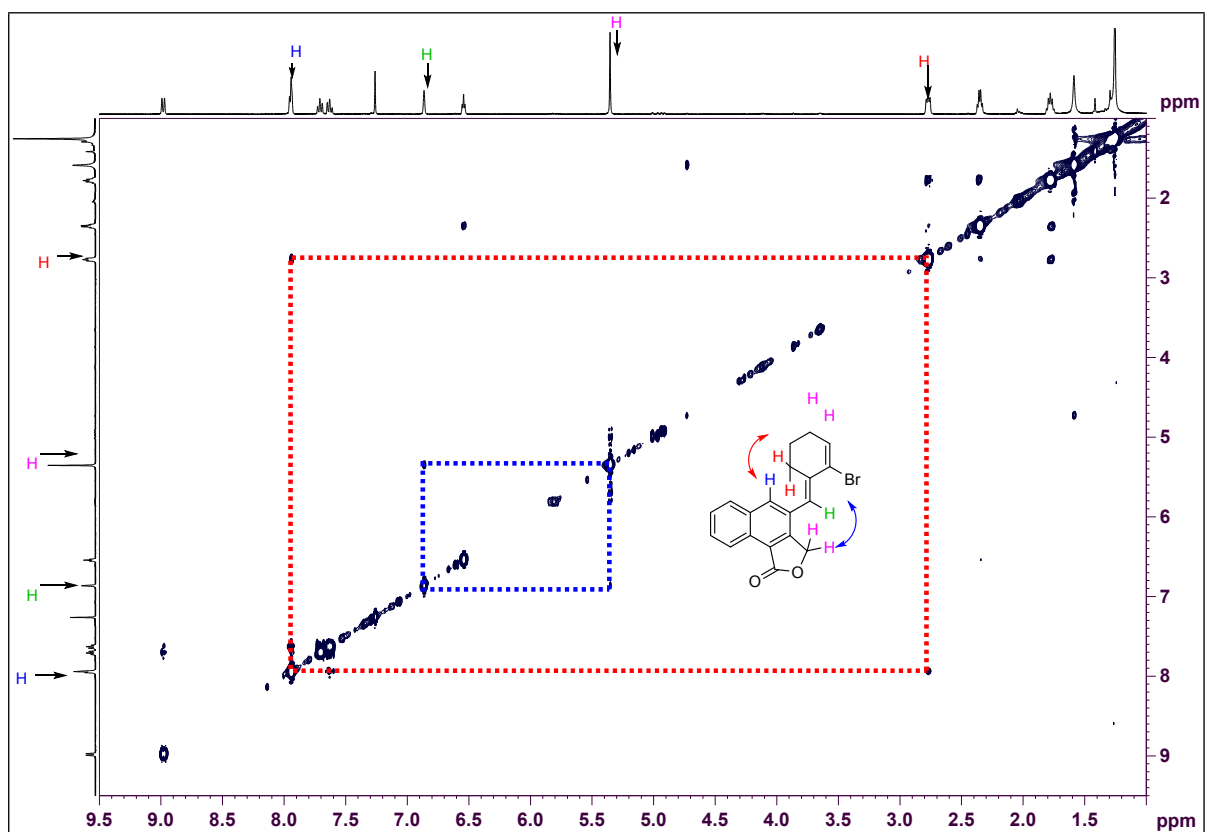




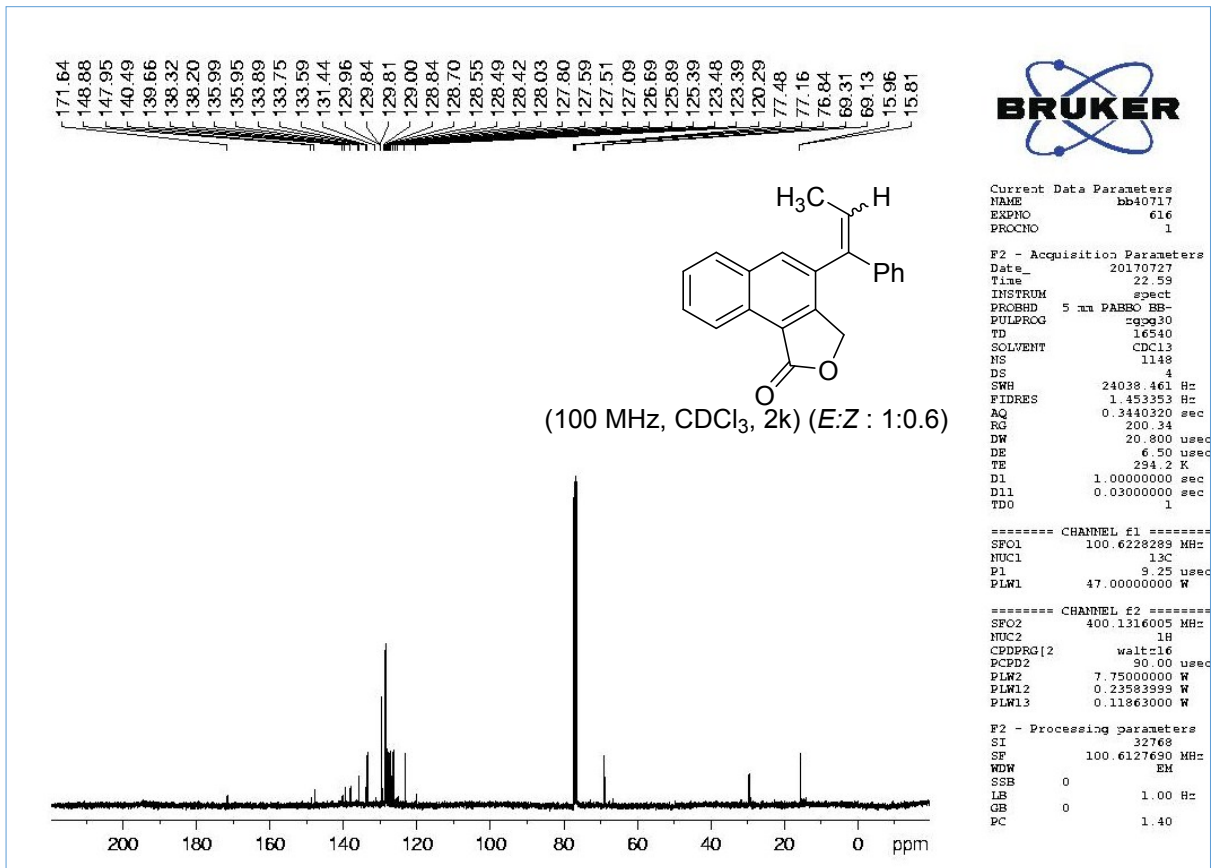
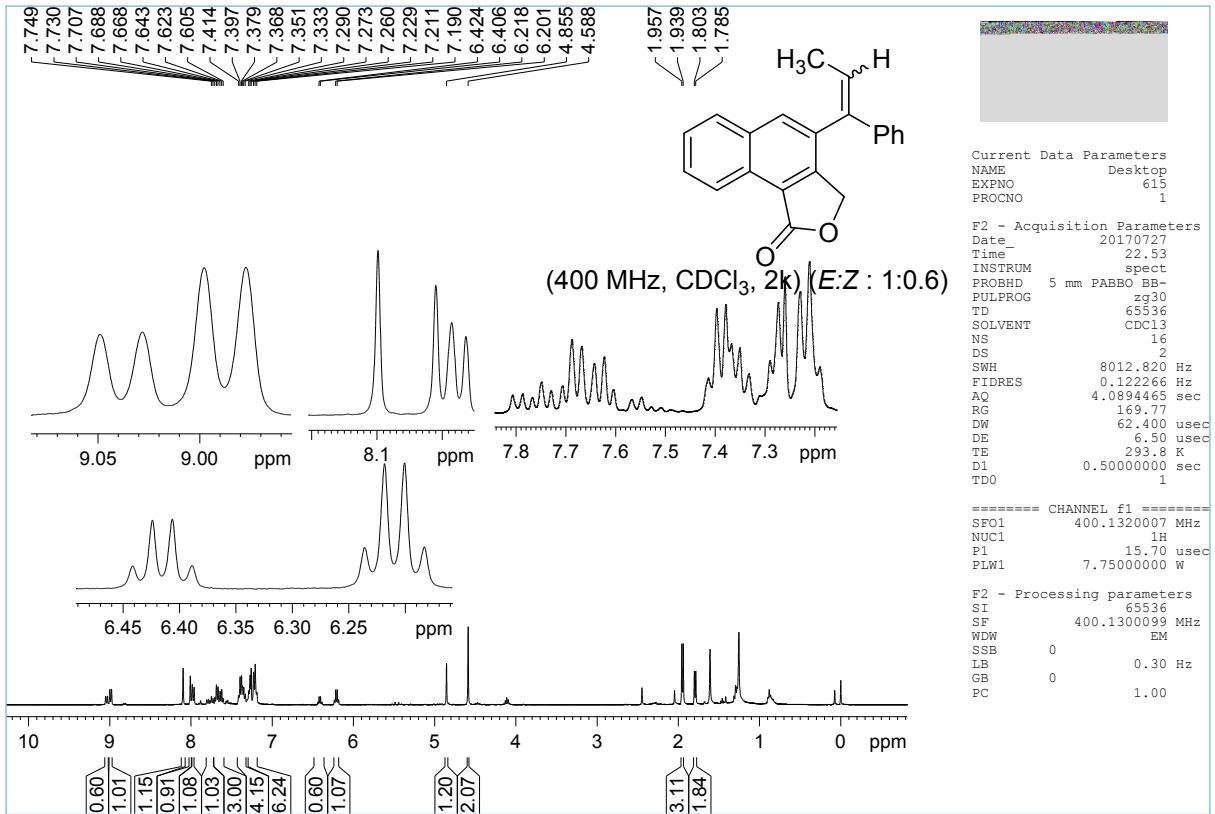


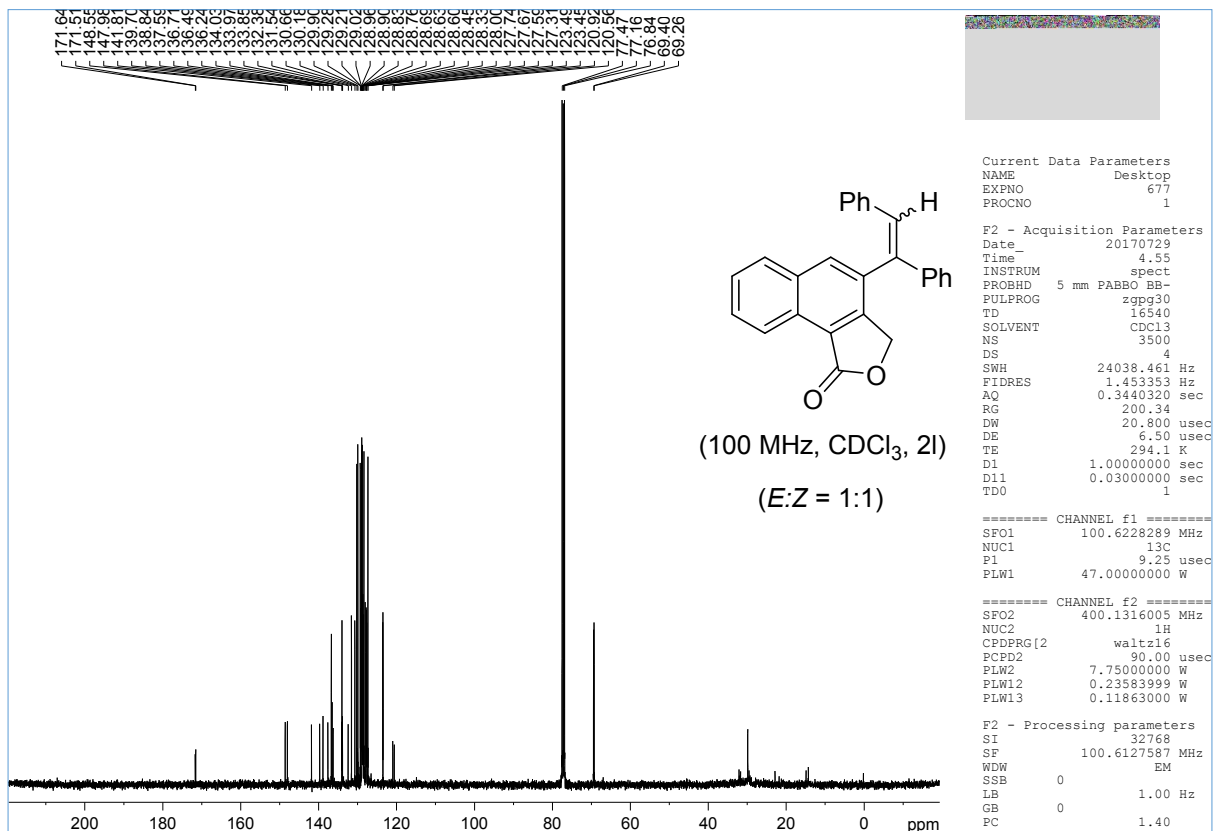
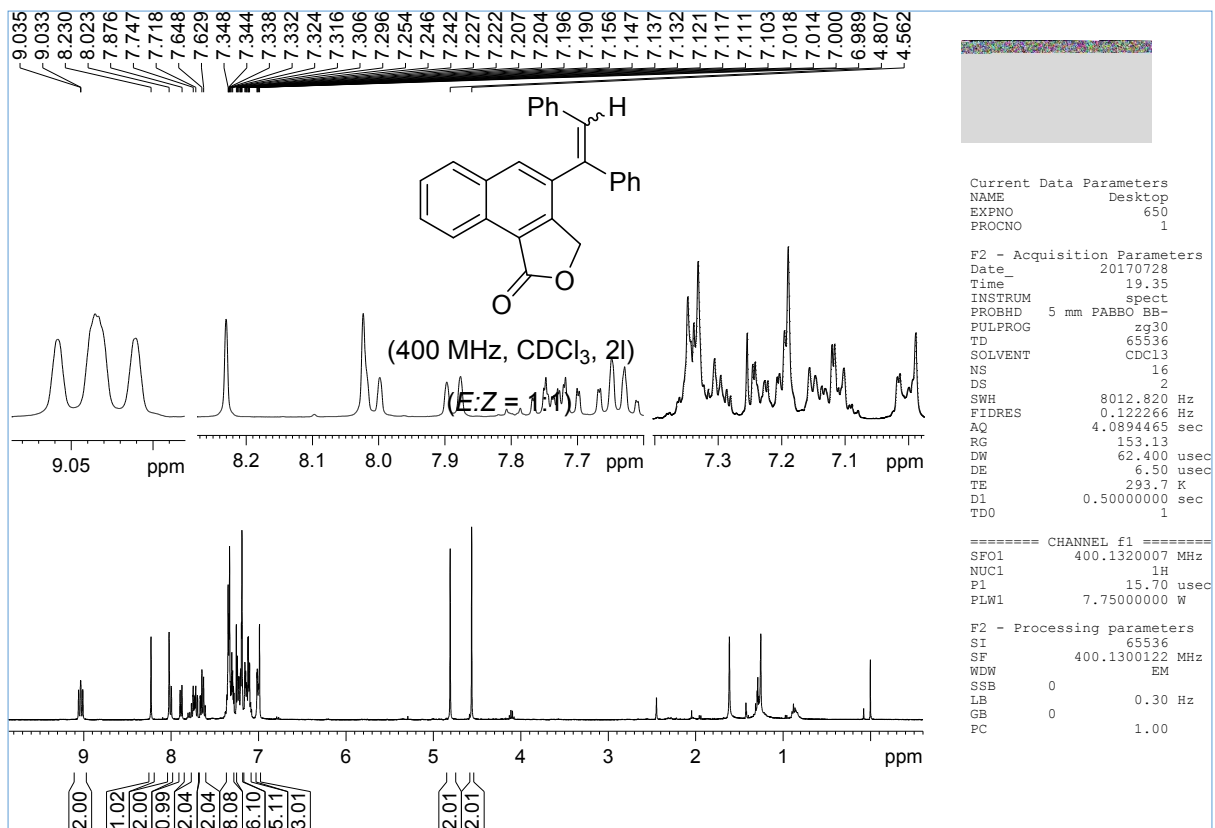


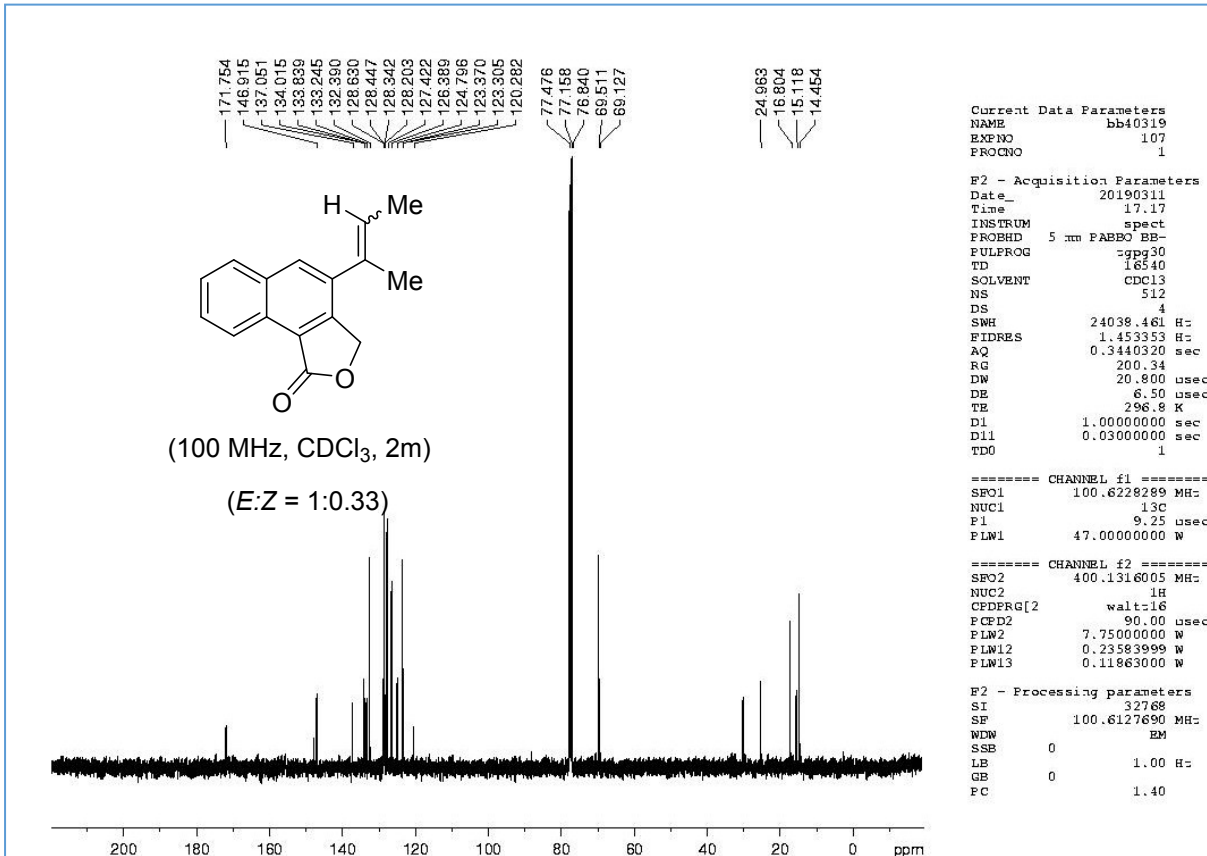
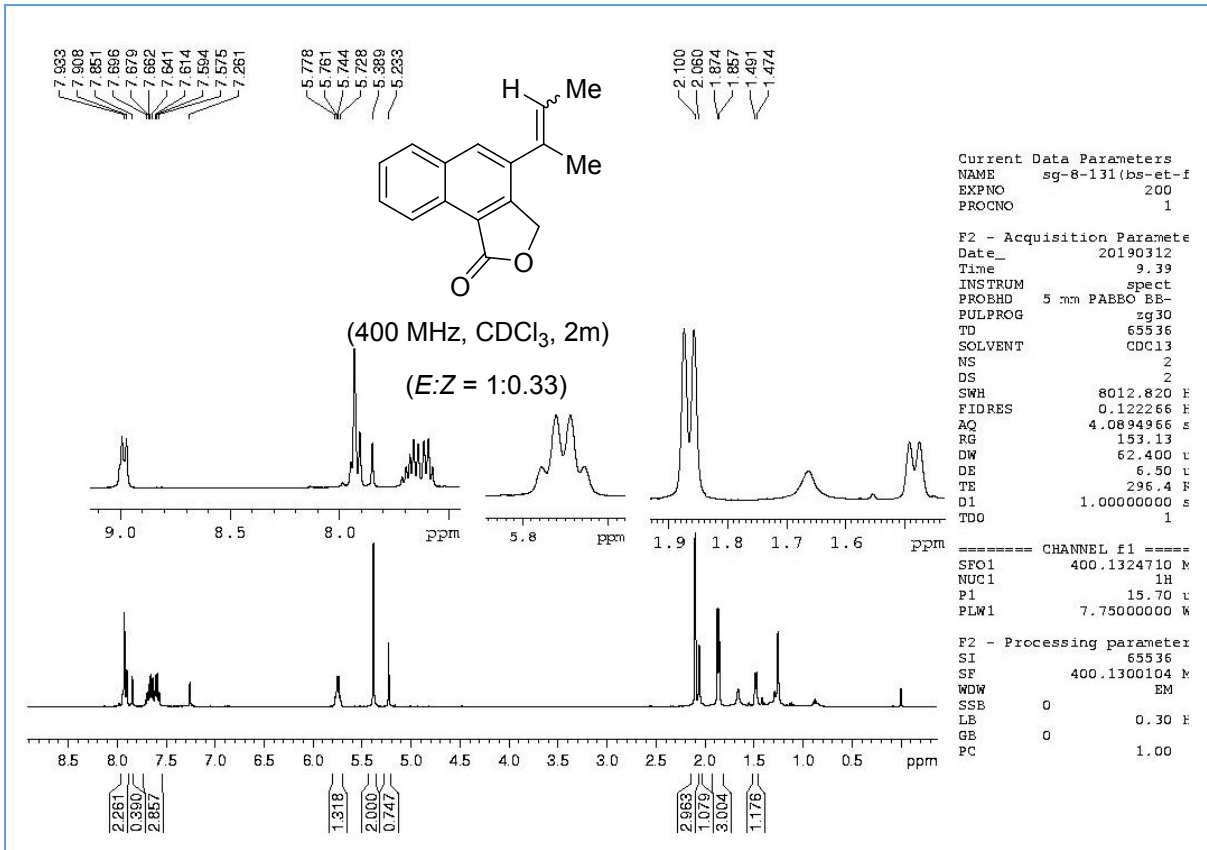


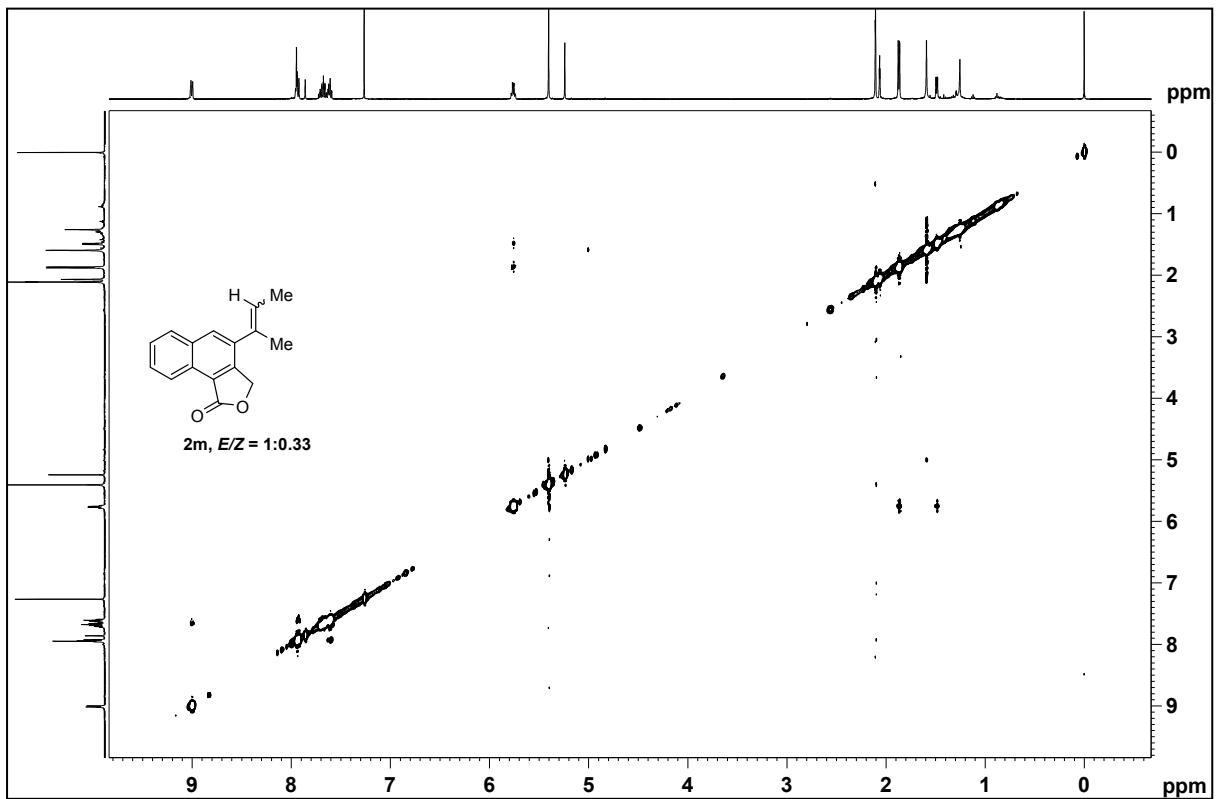
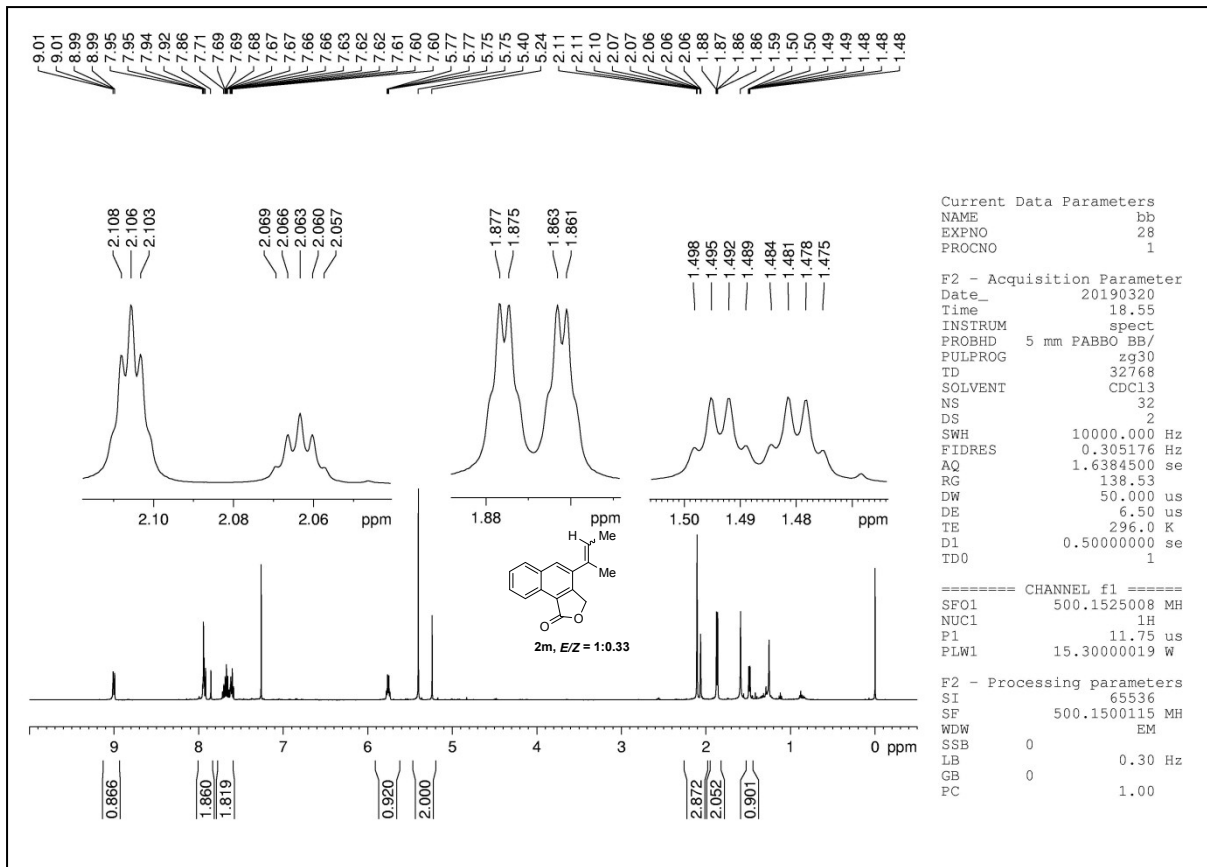


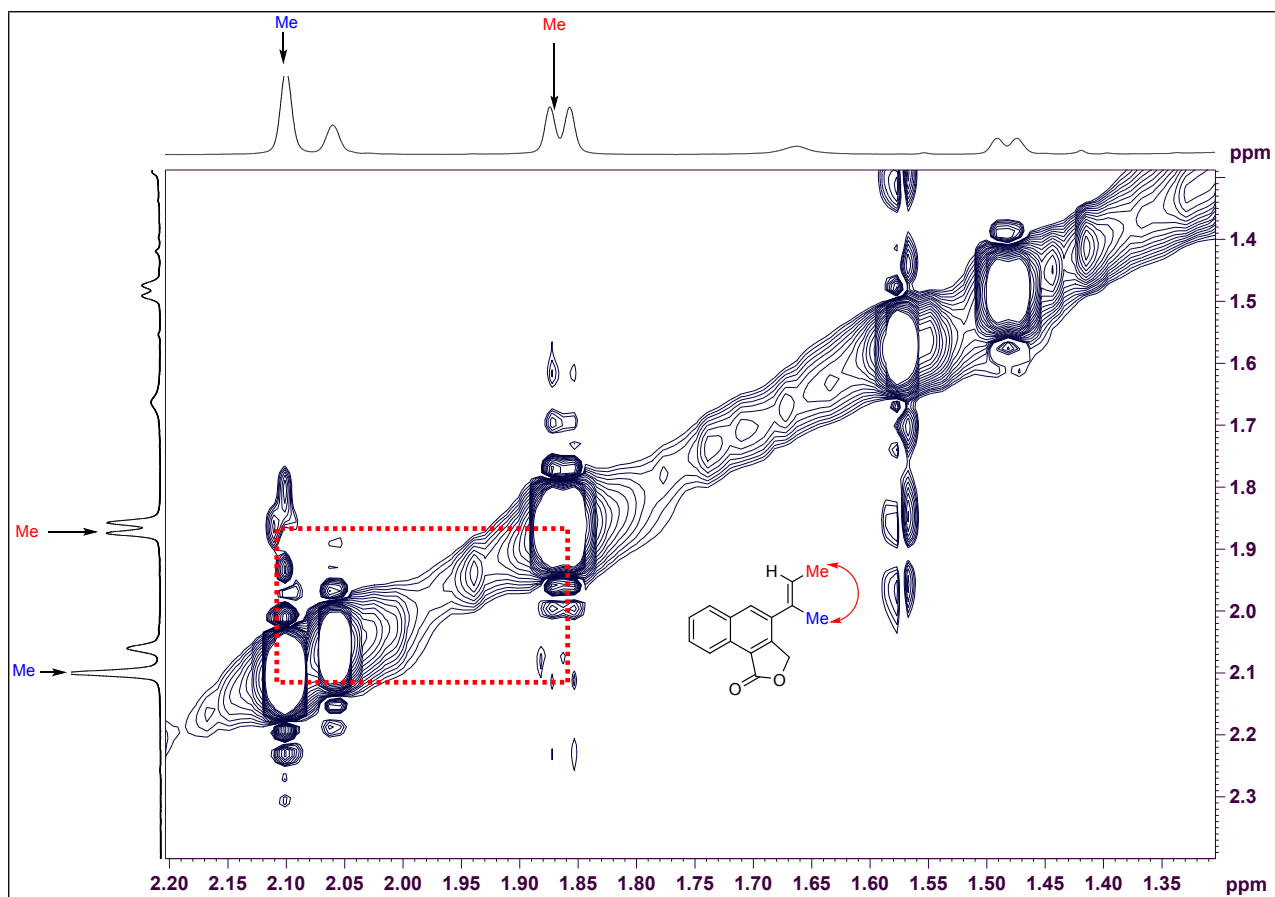
H¹-H¹ 2D NOESY (Nuclear Overhauser Effect Spectroscopy) of **2j** compound

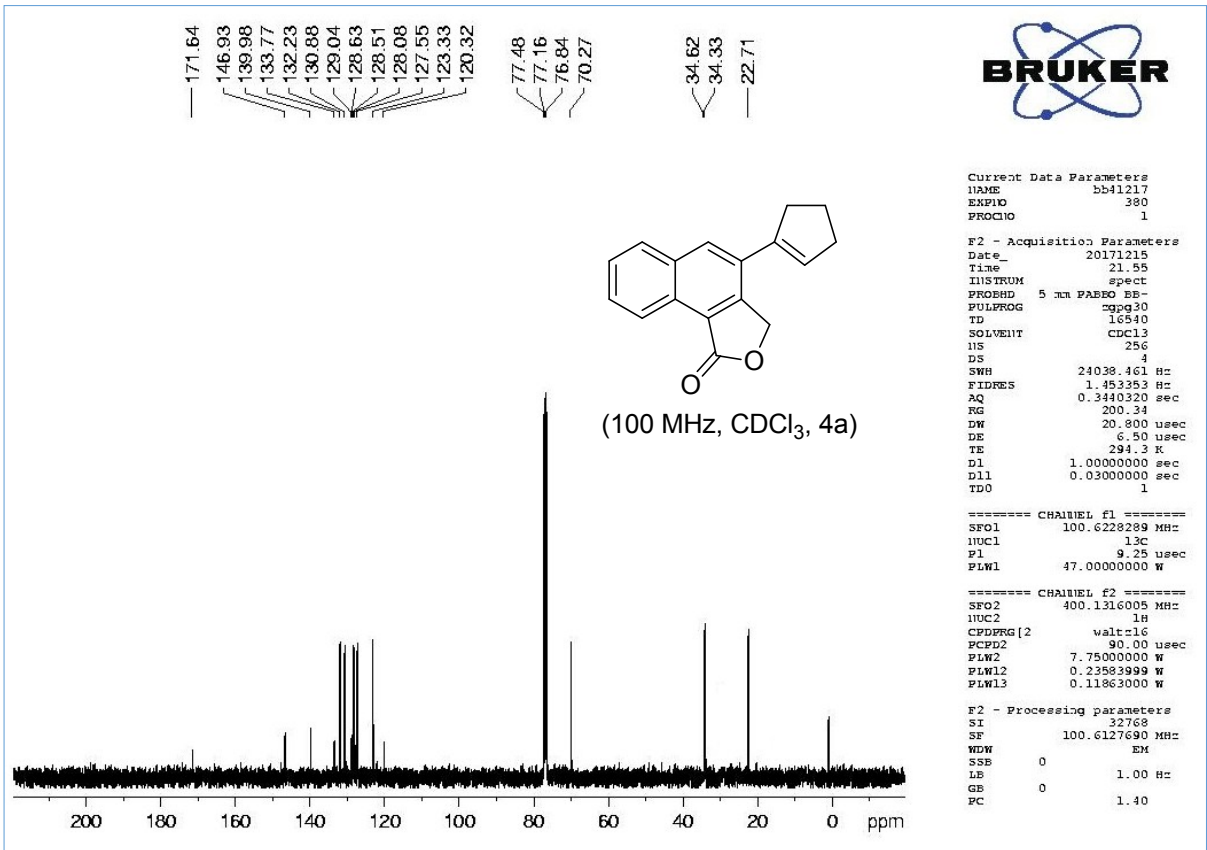
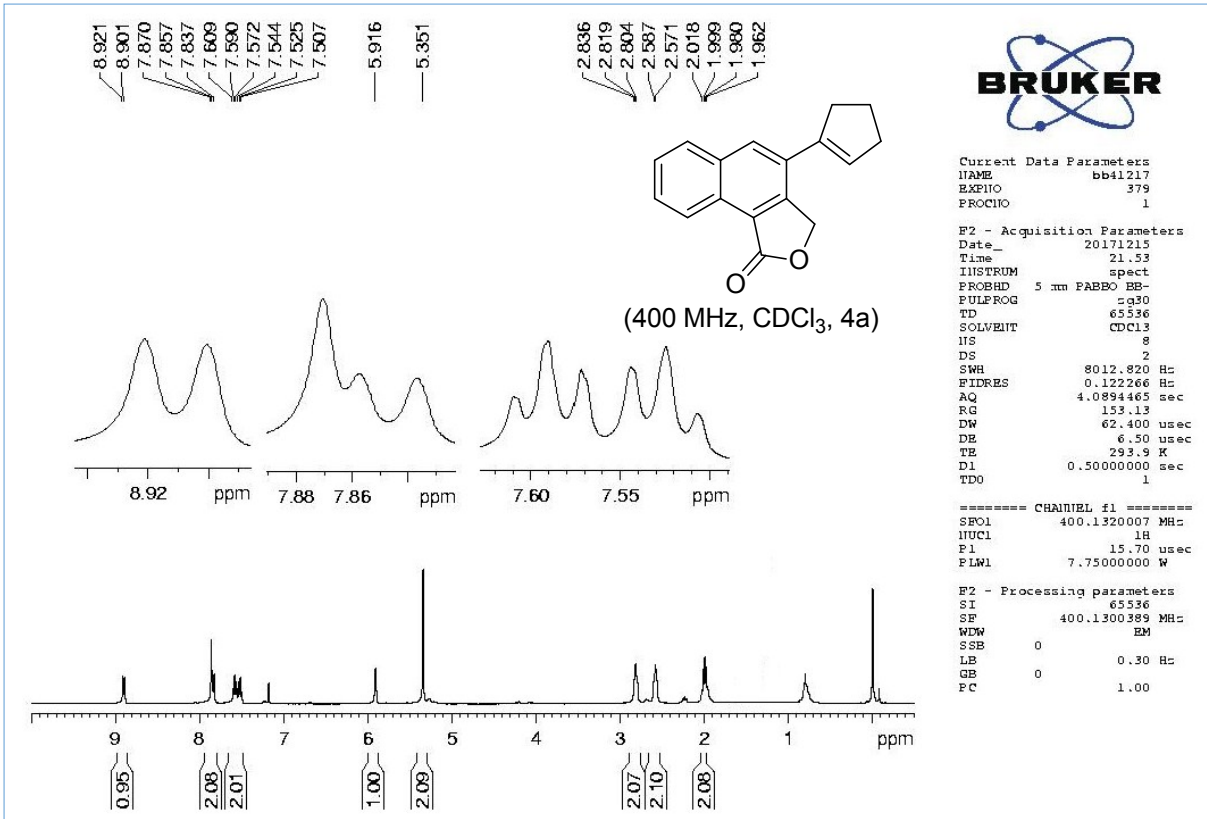


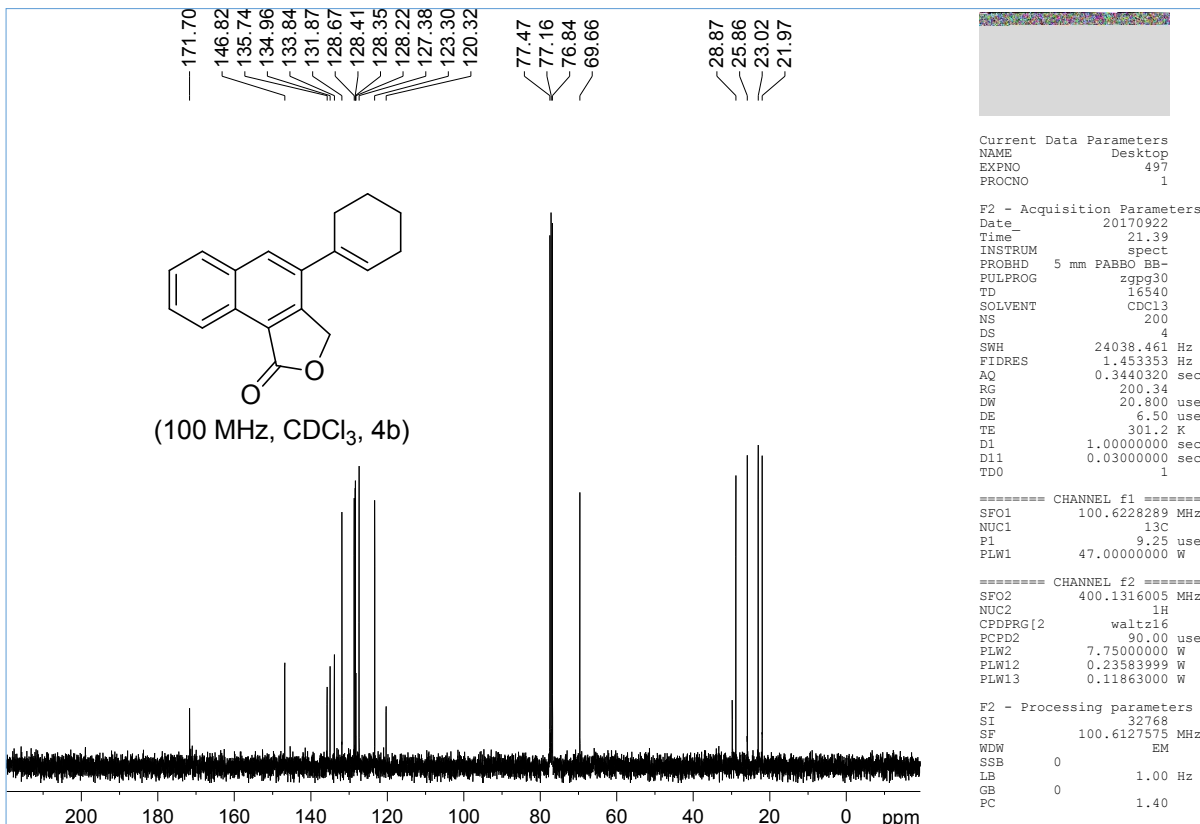
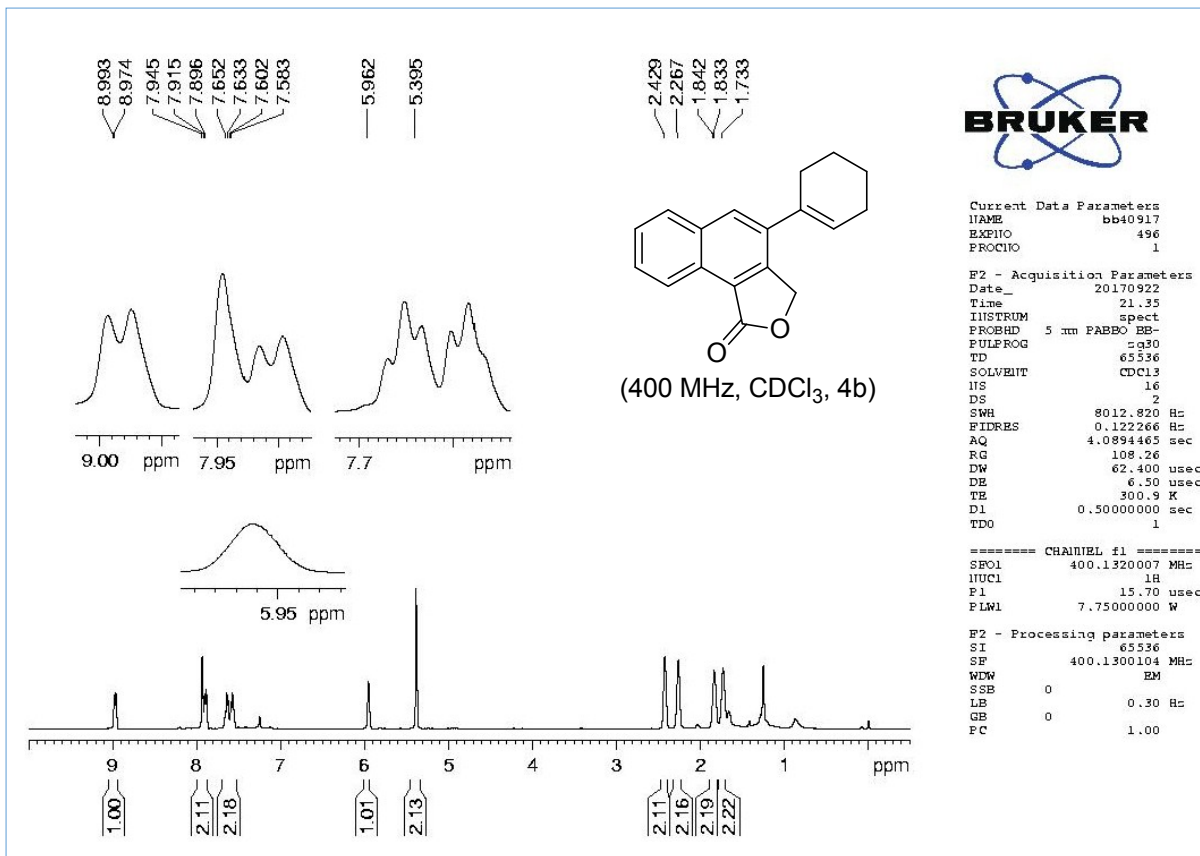


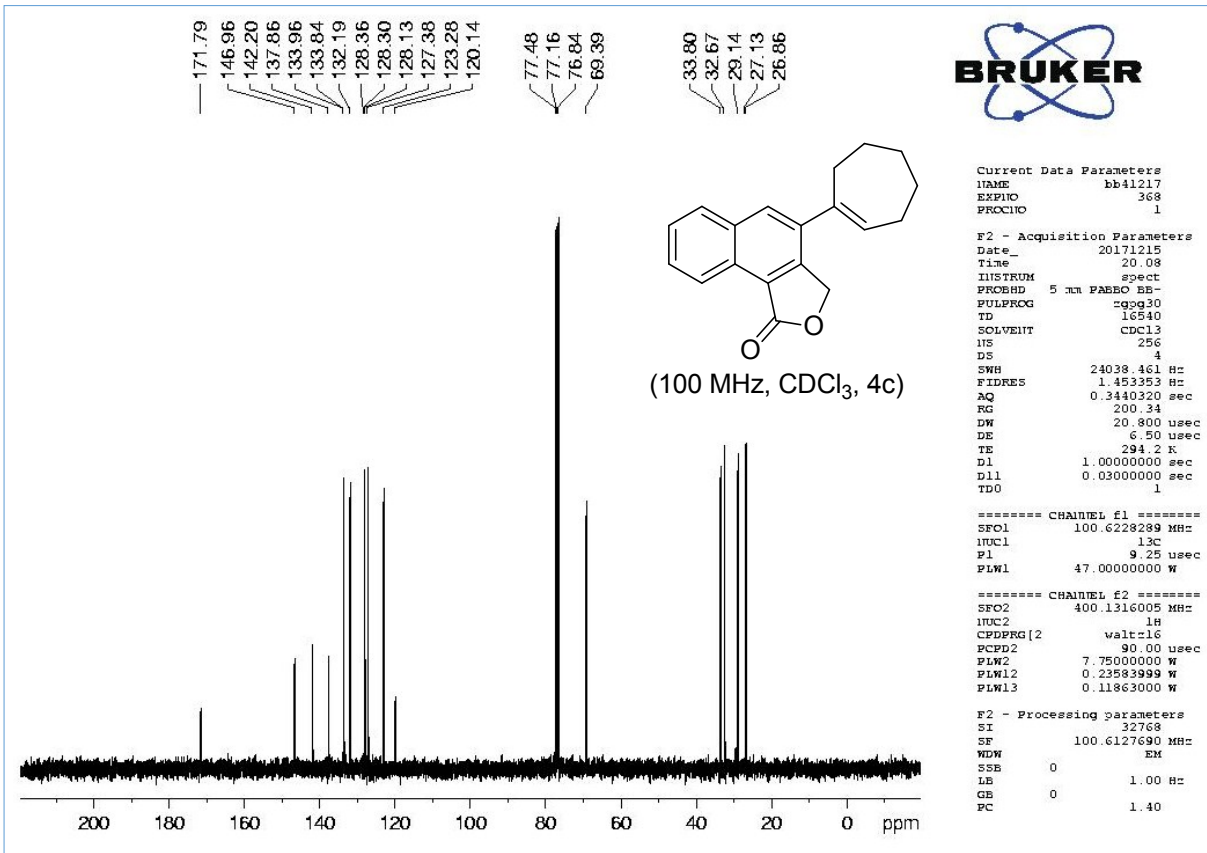
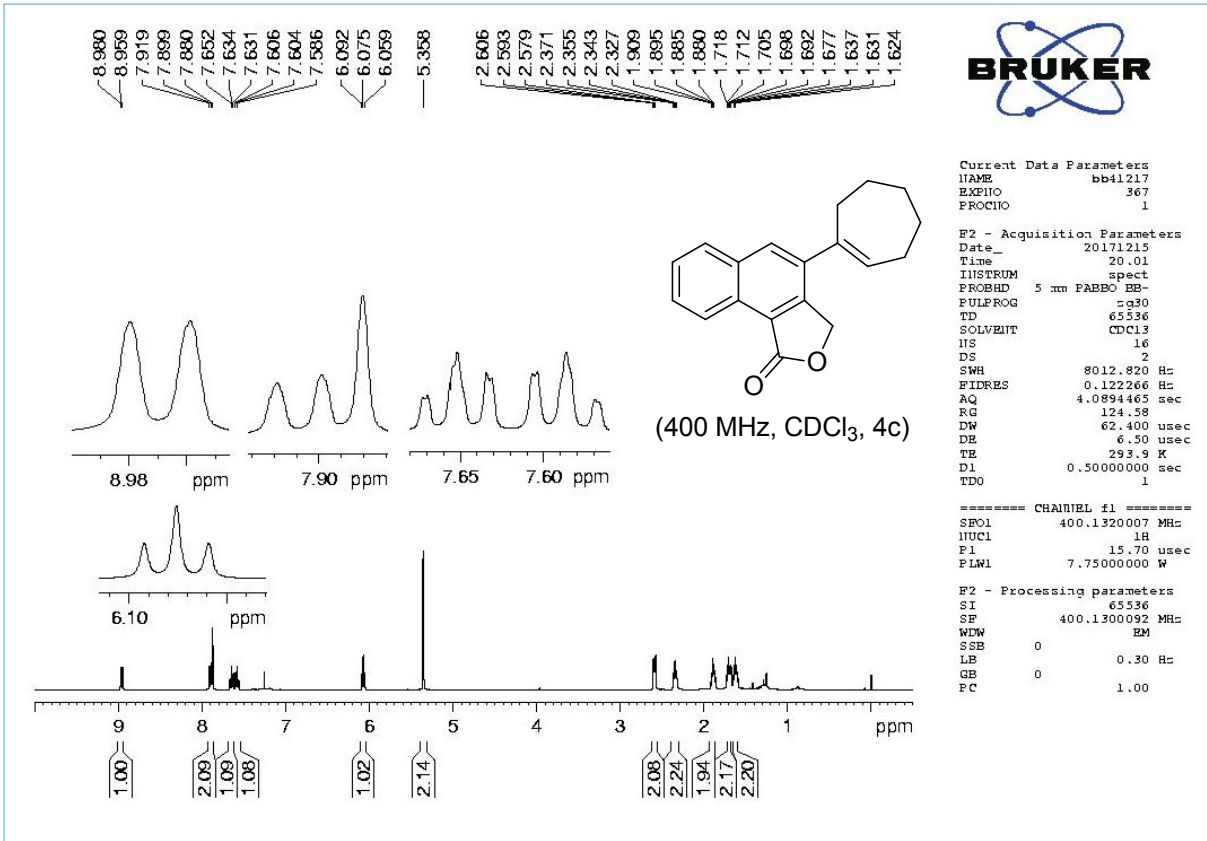


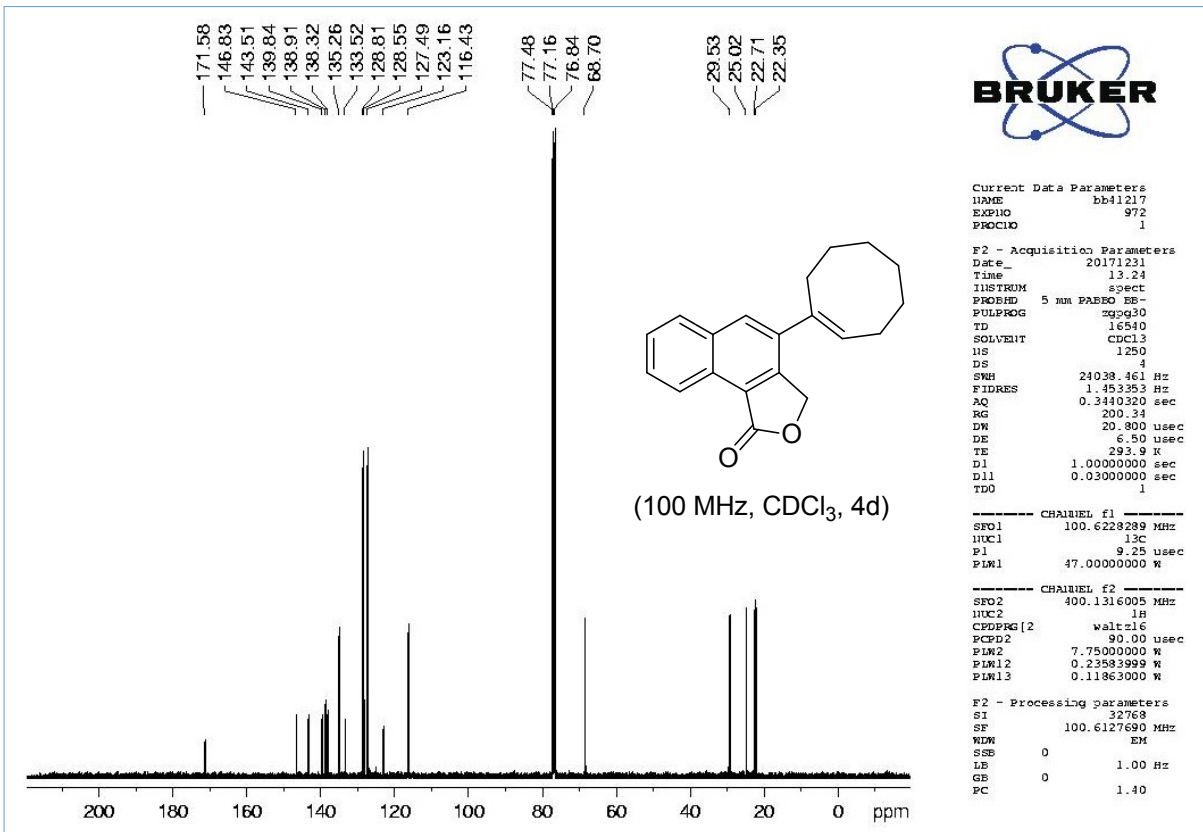
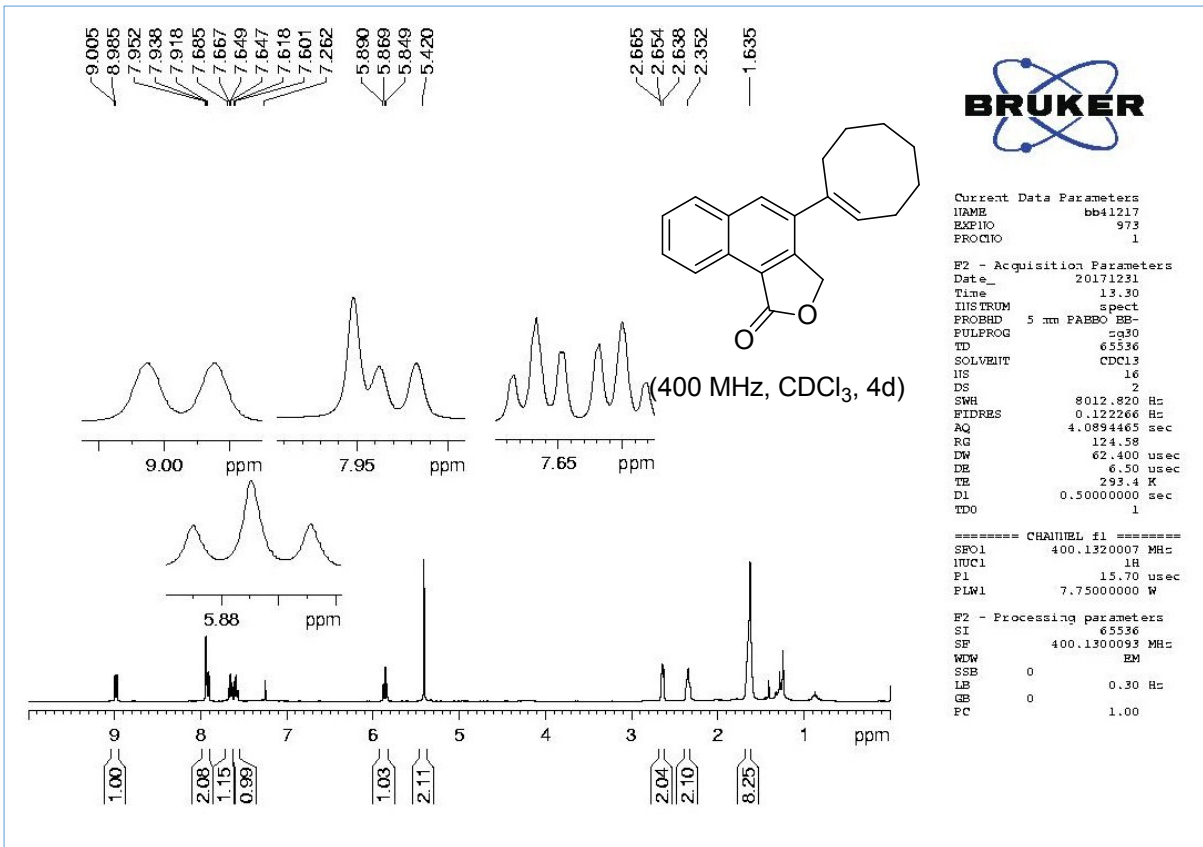


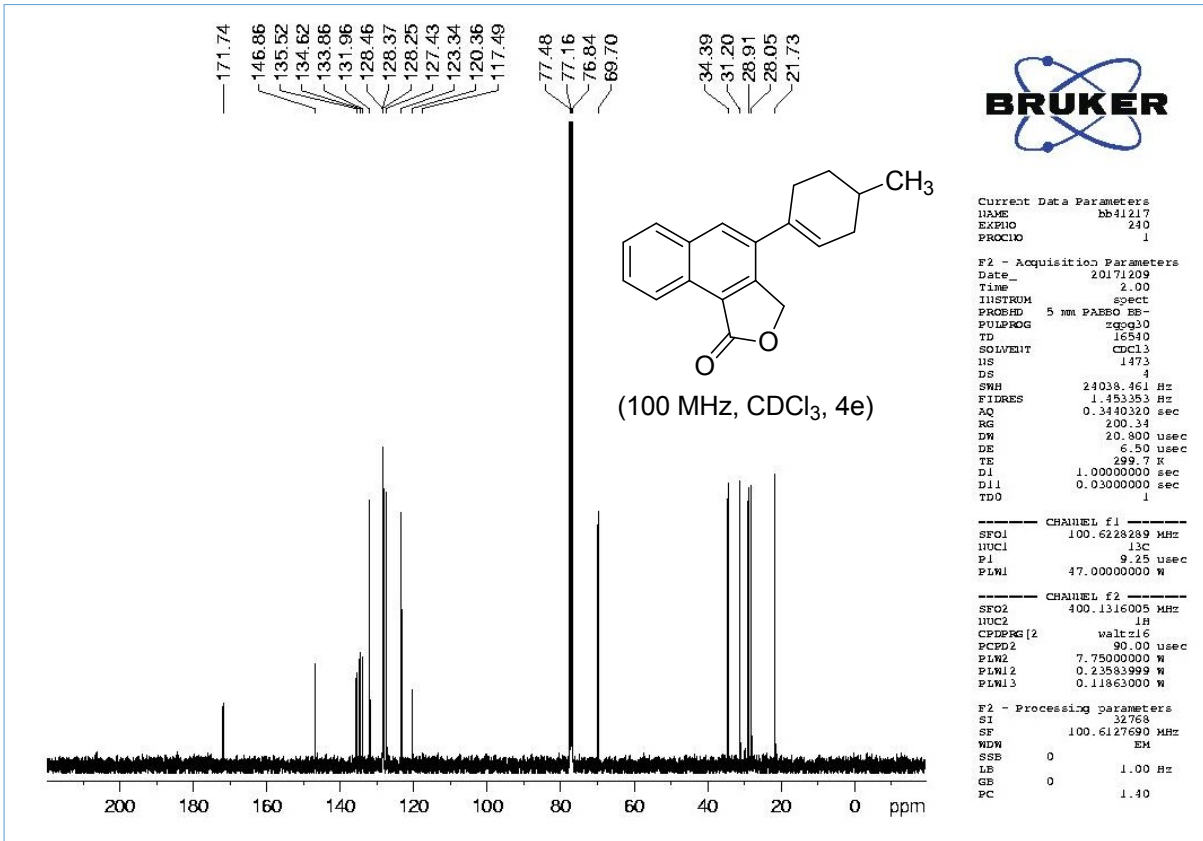
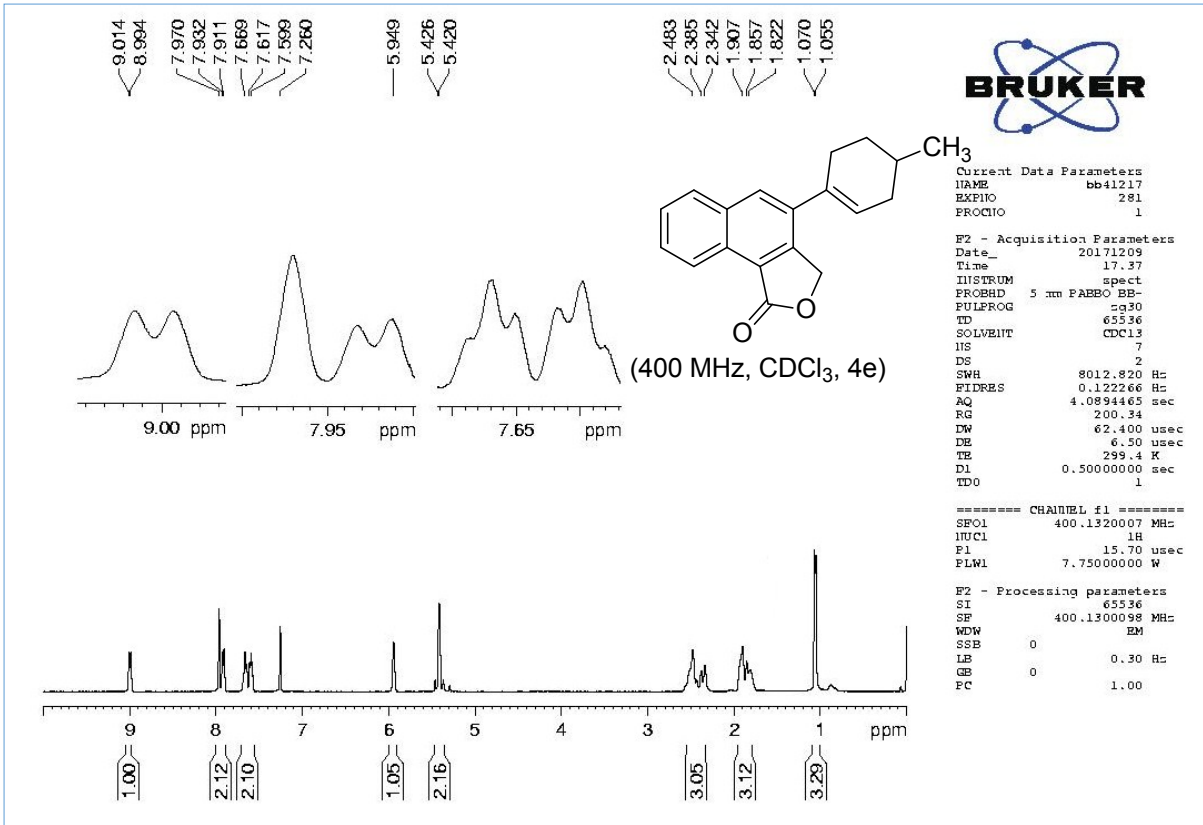


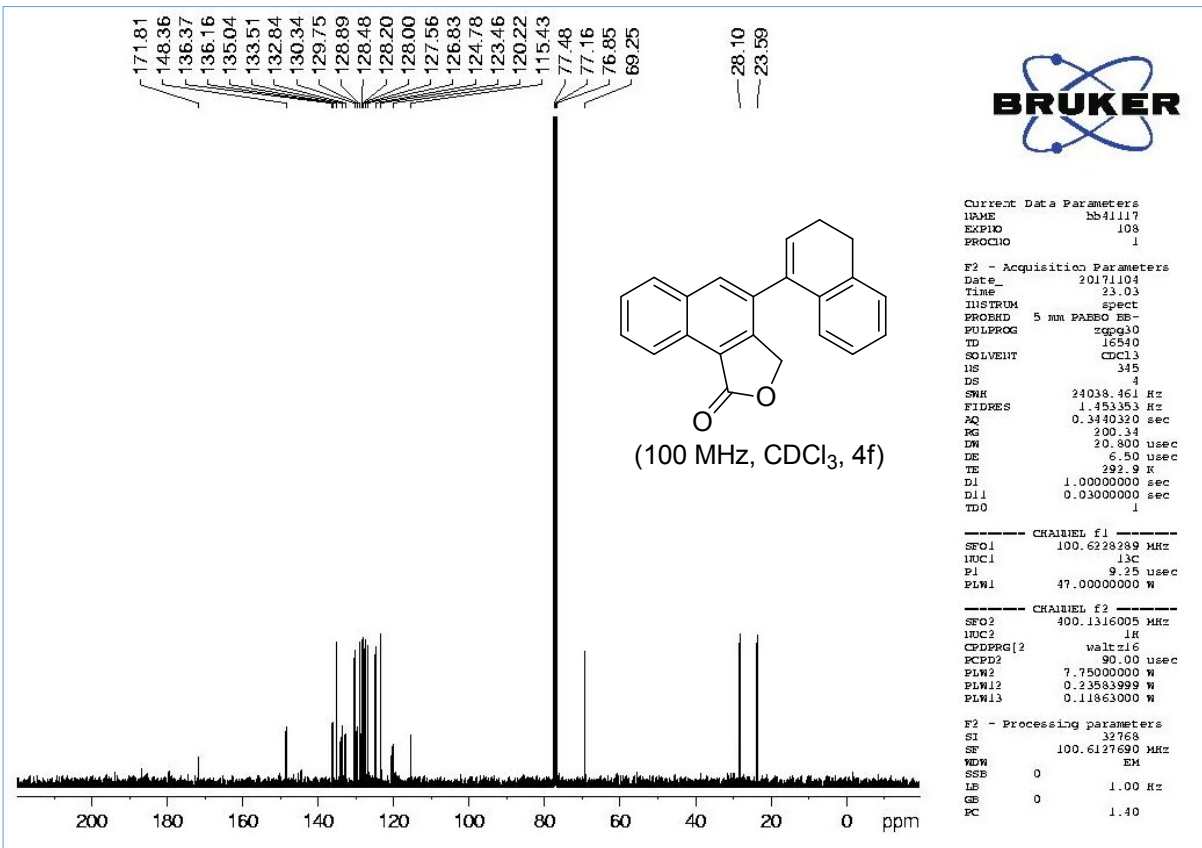
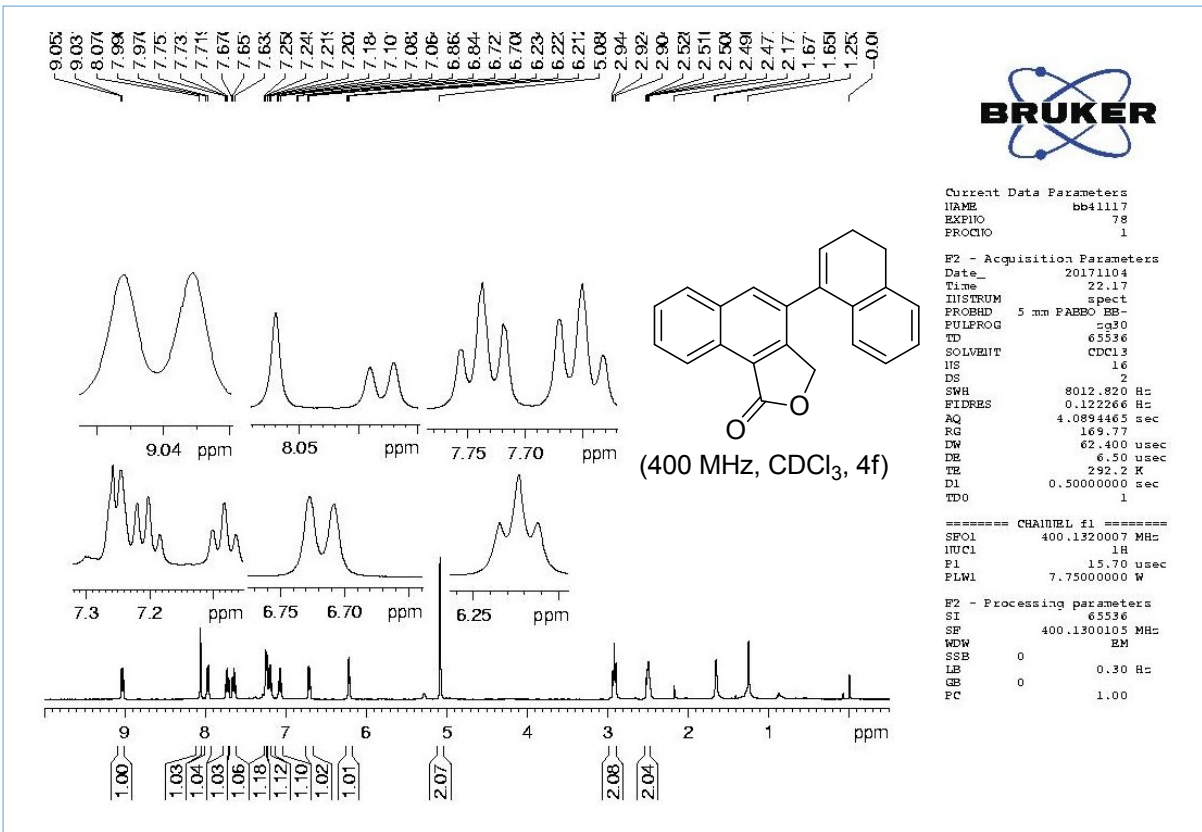


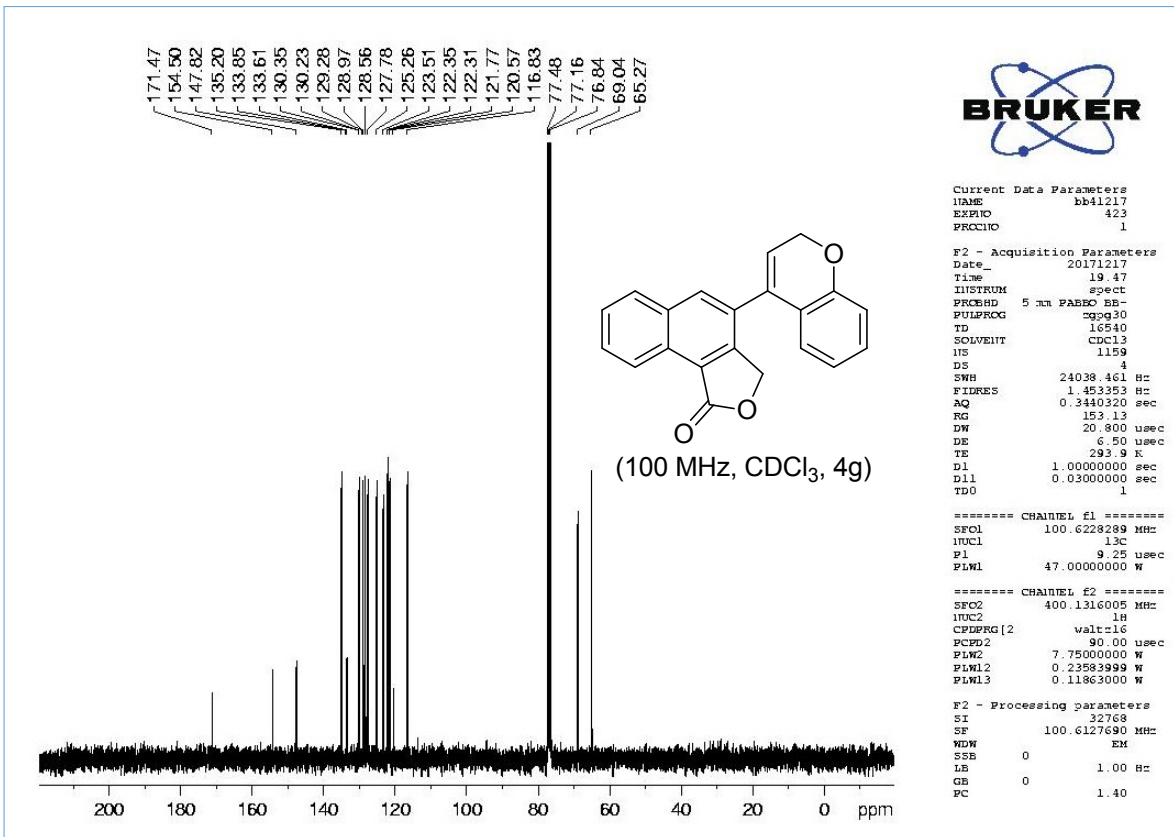
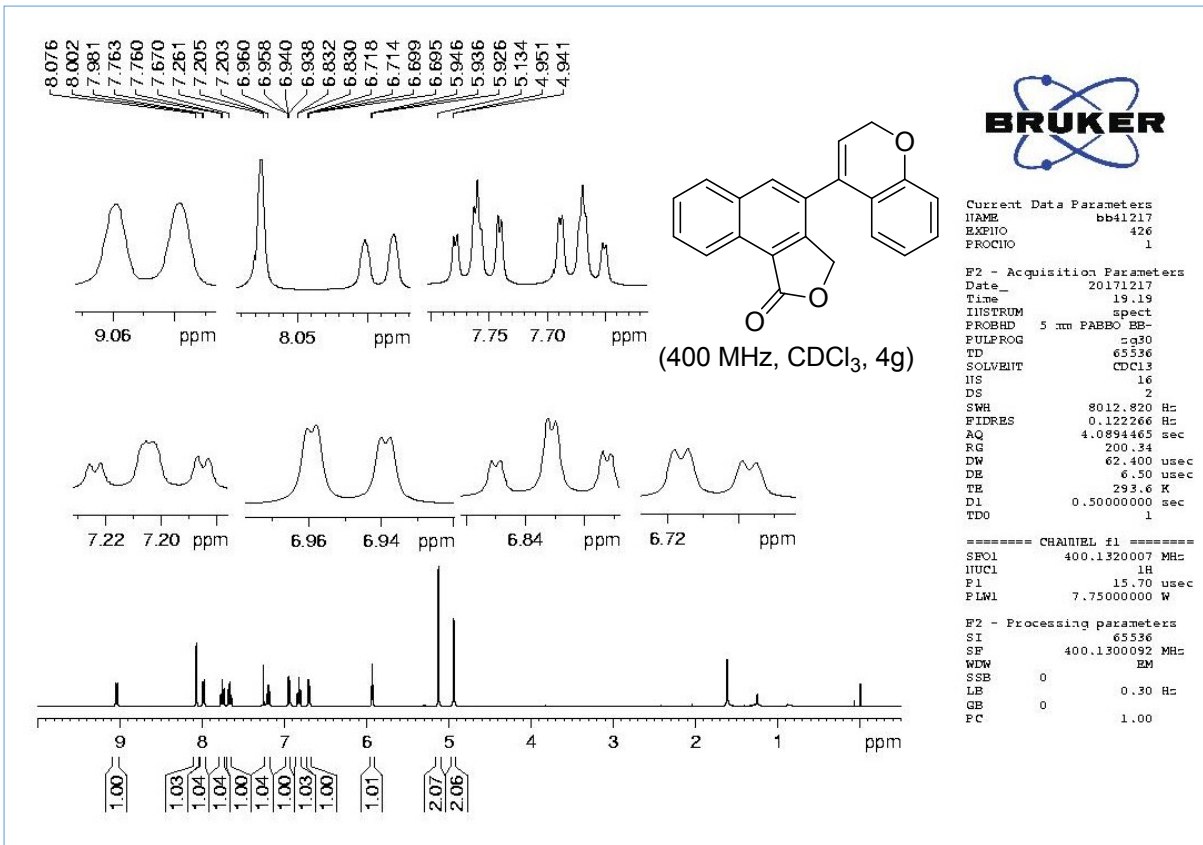


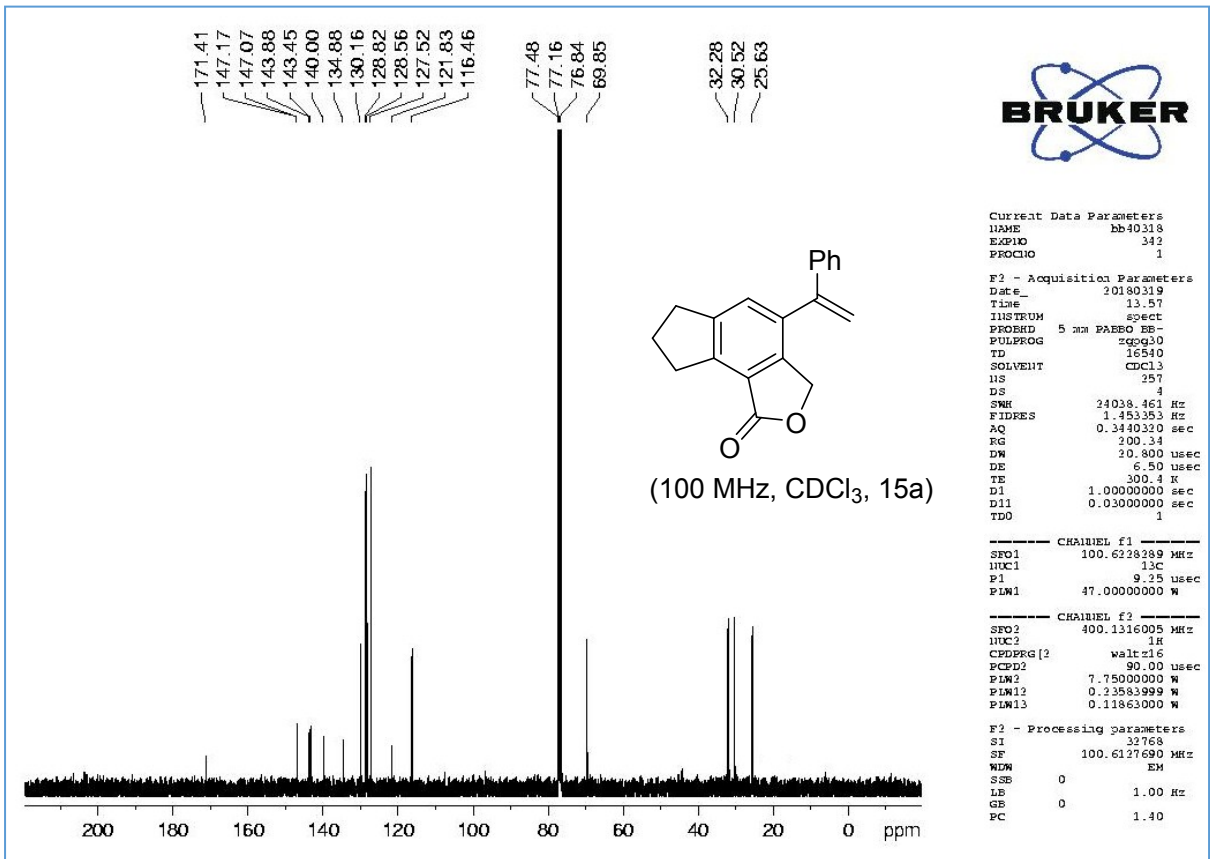
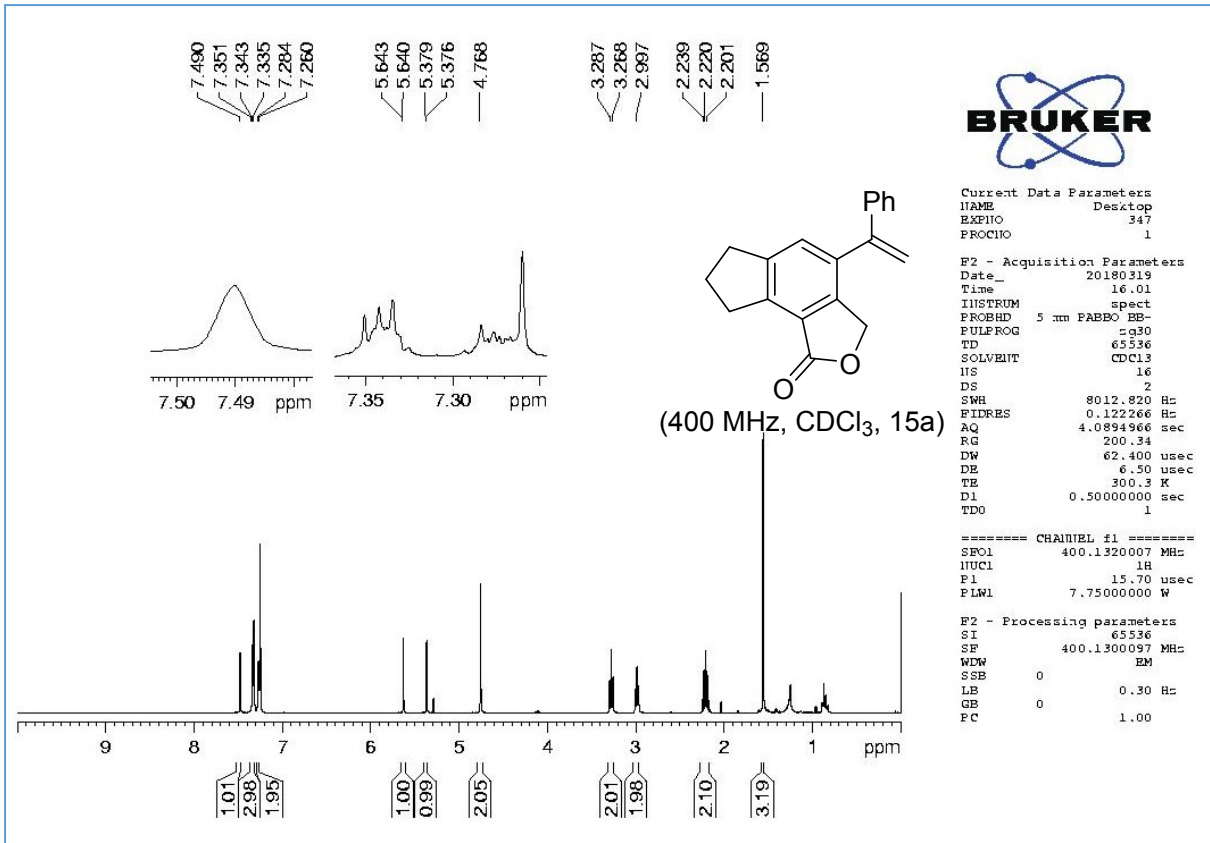


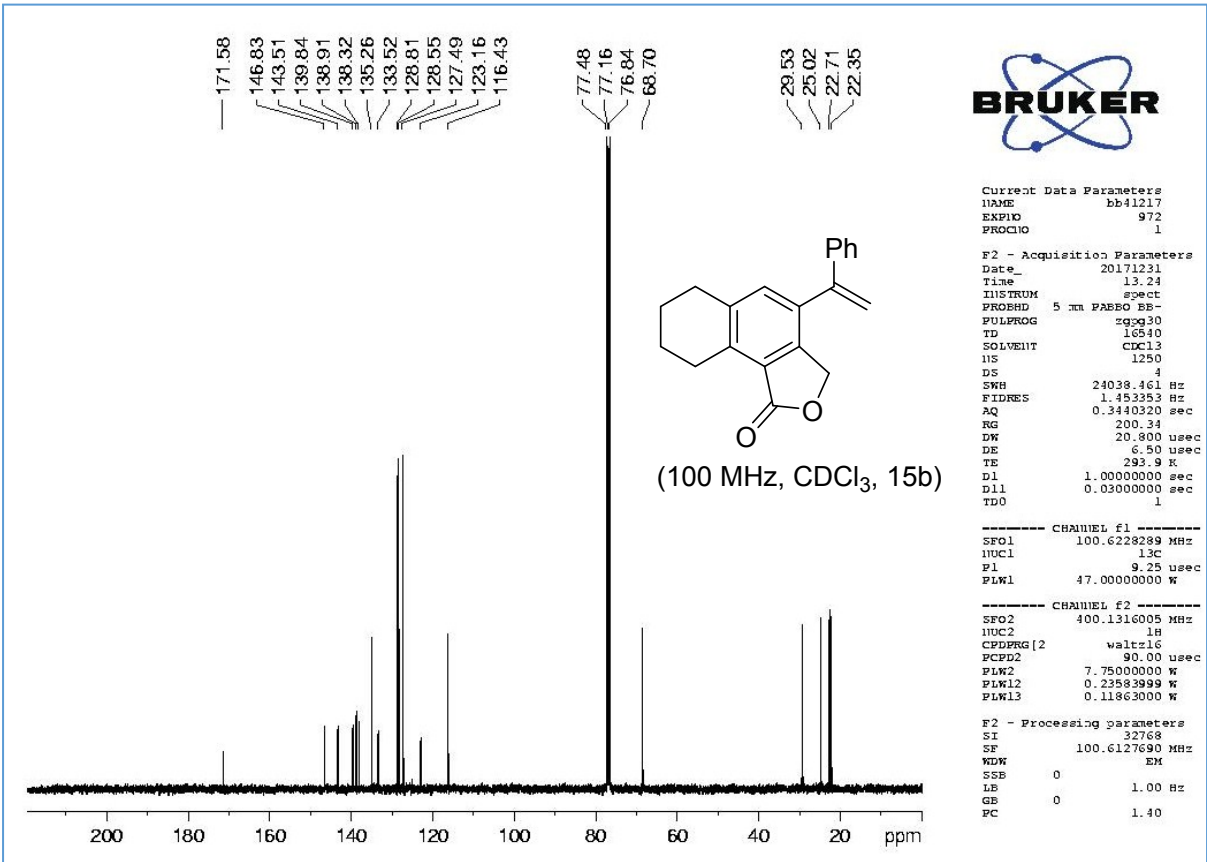
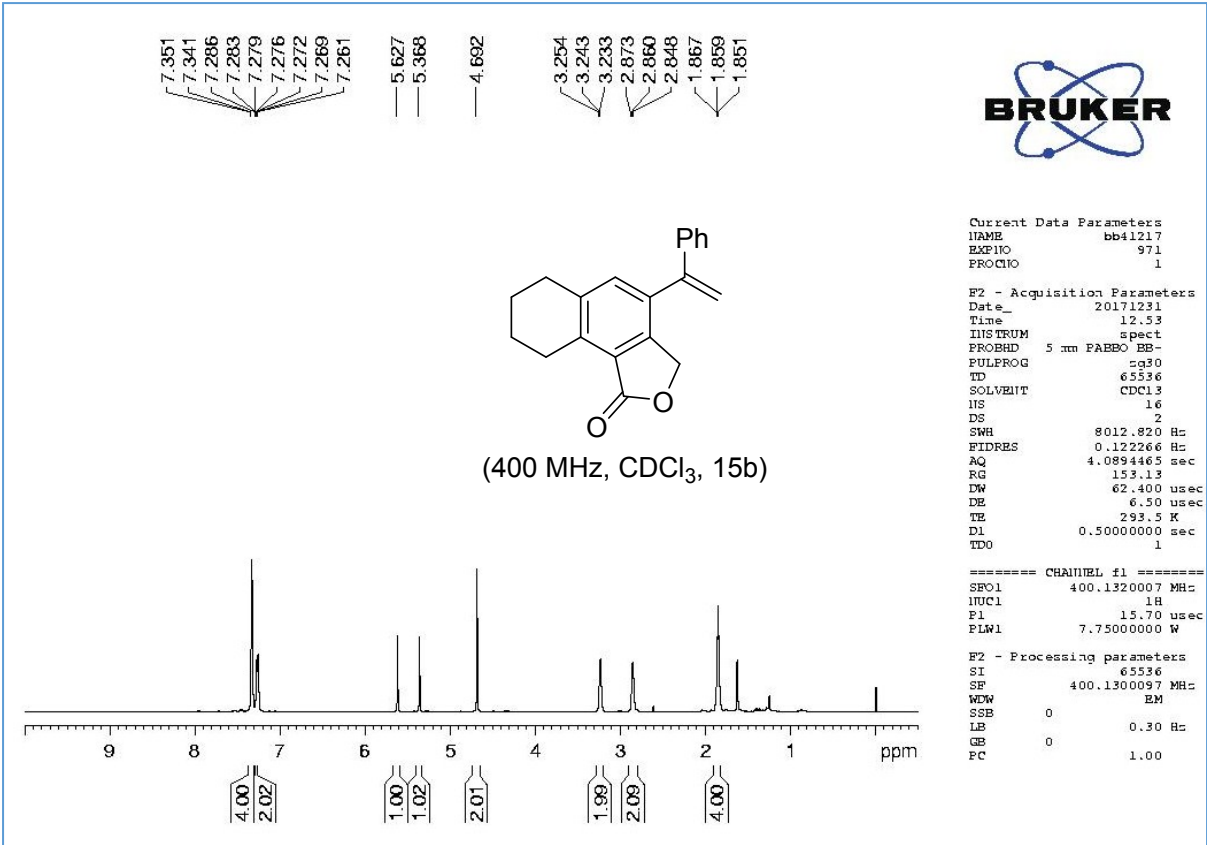


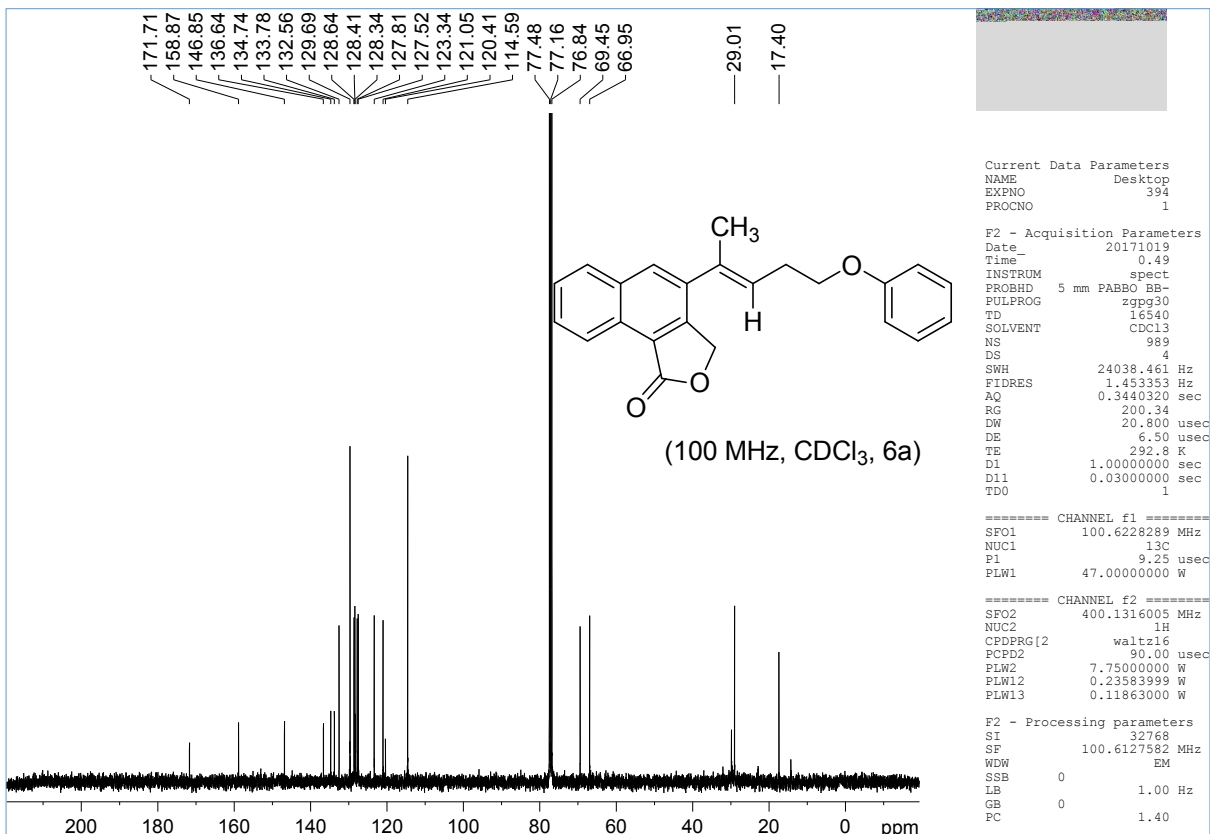
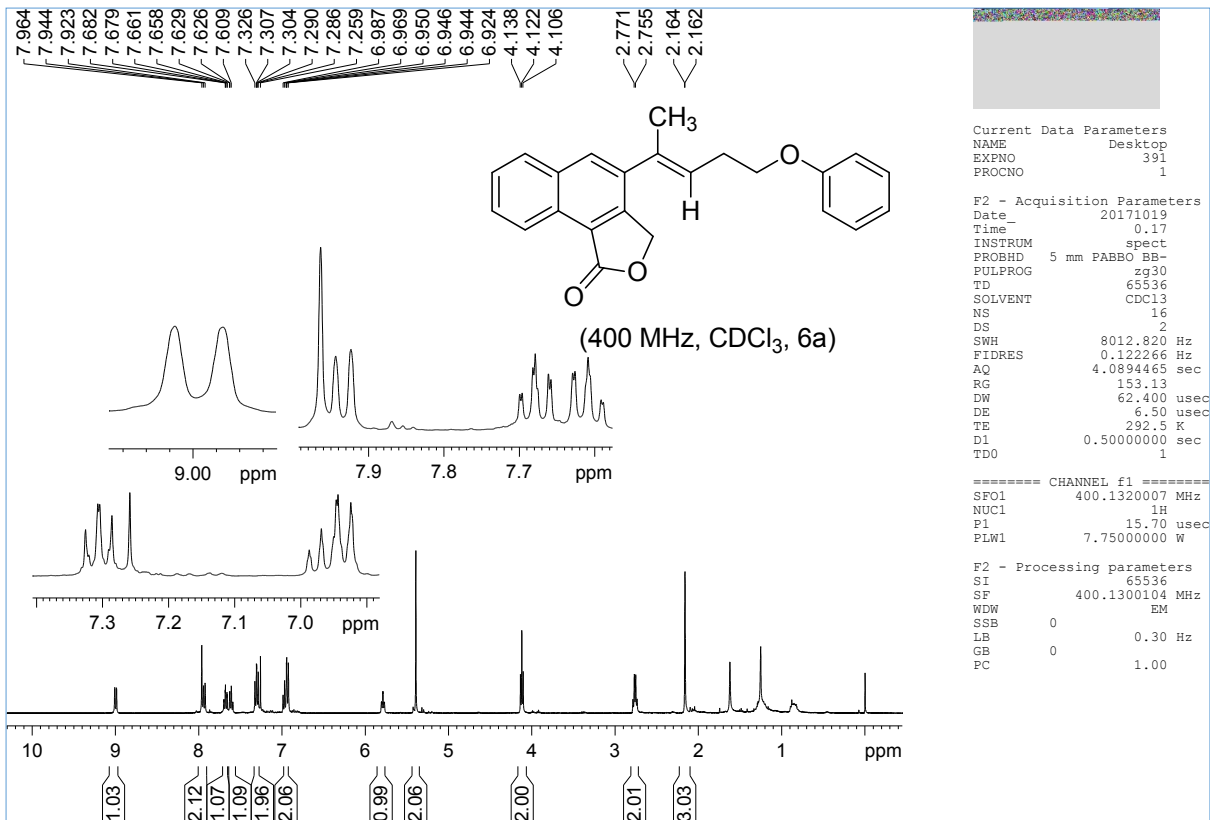


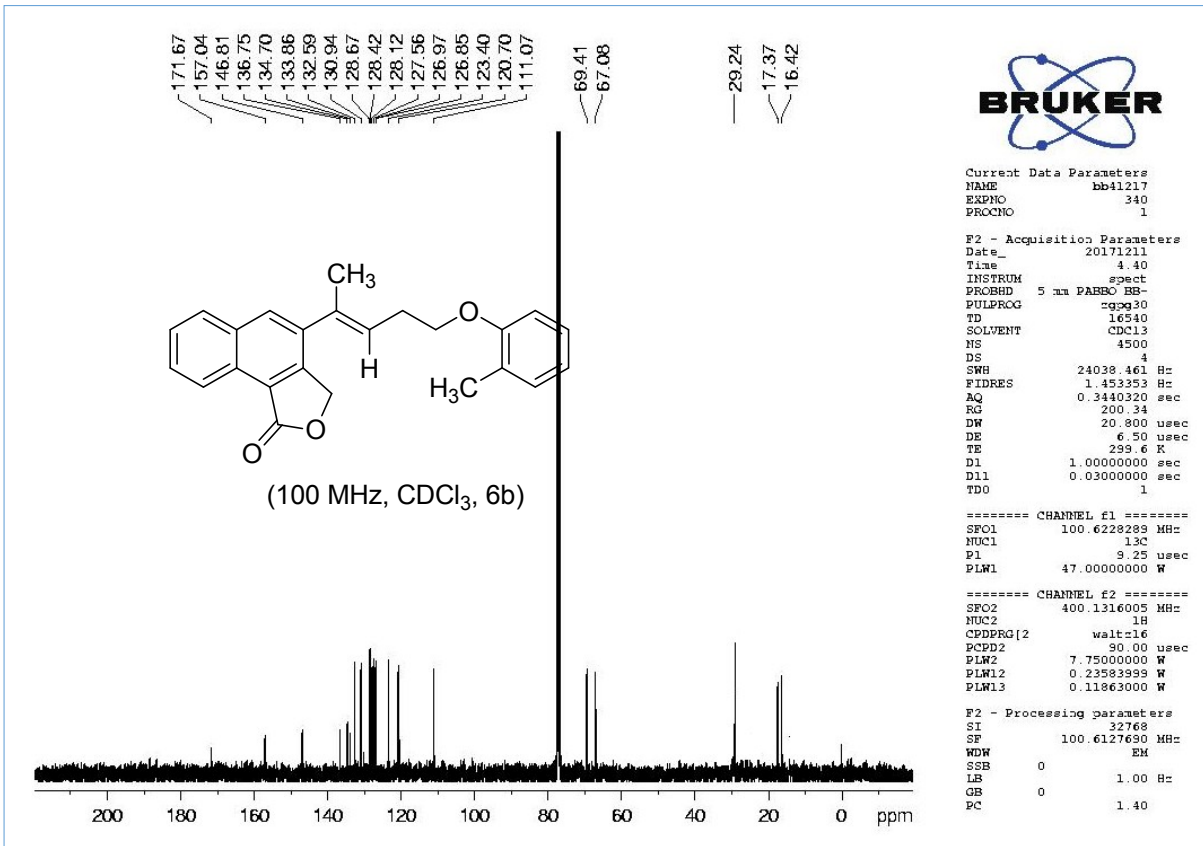
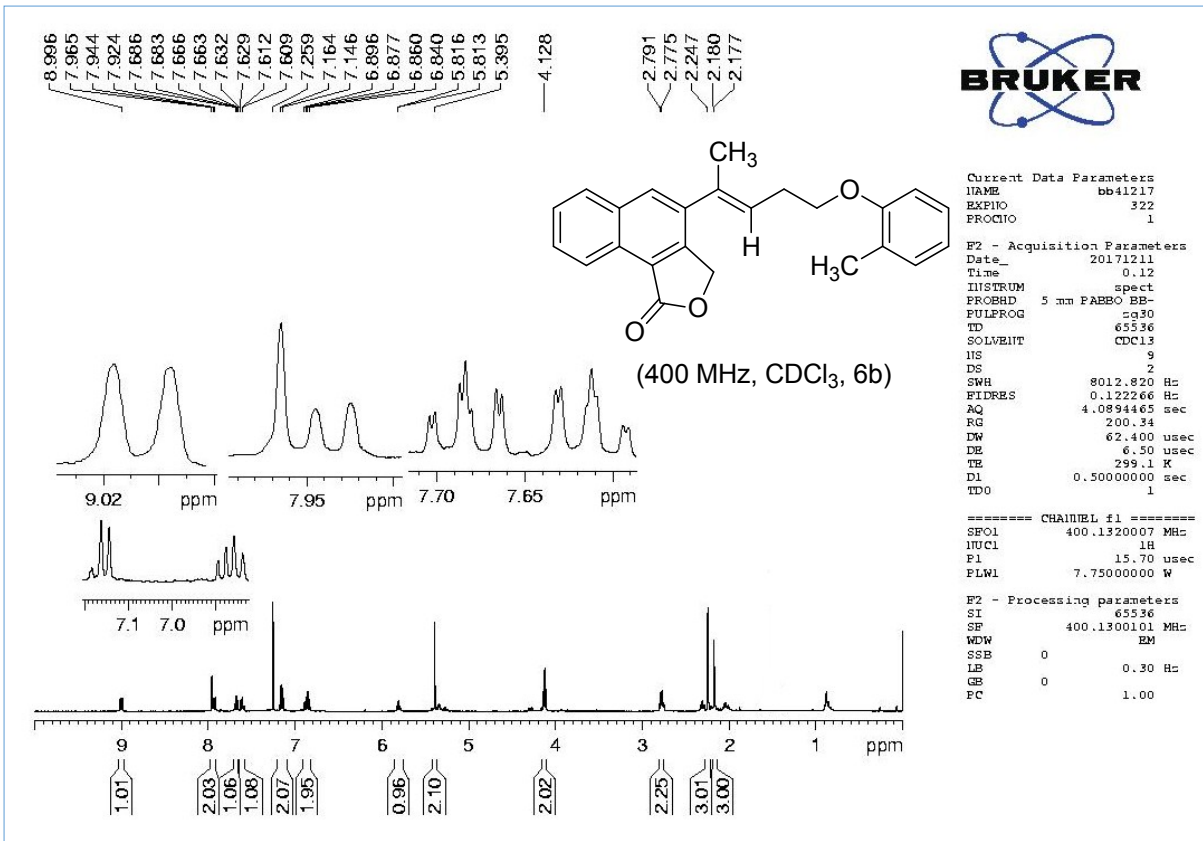










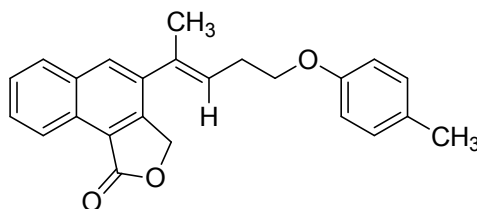


9.012
8.992
7.958
7.941
7.921
7.679
7.625
7.607
7.258
7.105
7.085
6.839
6.819
— 5.782
— 5.390
4.107
4.092
4.077
2.298
2.156

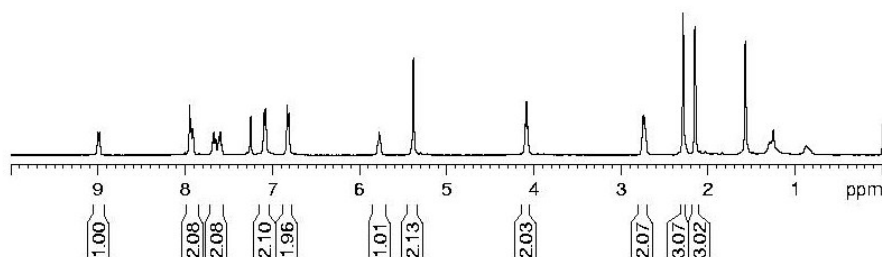


Current Data Parameters
NAME bb41217
EXPNO 241
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171209
Time 1.20
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65336
SOLVENT CDCl3
NS 12
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 200.34
DW 62.400 usec
DE 6.50 usec
TE 299.2 K
D1 0.50000000 sec
TDO 1



(400 MHz, CDCl₃, 6c)



===== CHANNEL f1 =====
SF01 400.1320007 MHz
NUC1 1H
P1 15.70 usec
PLW1 7.75000000 W

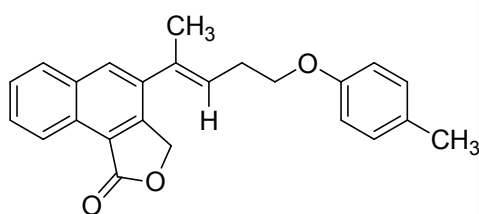
F2 - Processing parameters
SI 65336
SF 400.1300105 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

171.69
156.82
146.88
136.73
134.68
133.84
132.56
131.86
130.35
130.14
128.65
128.41
127.95
127.53
123.40
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77.16
76.84
69.45
67.20
29.09
20.61
17.40

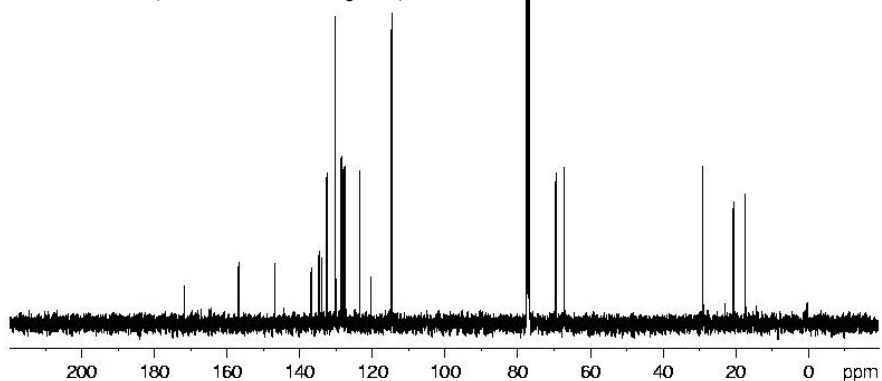


Current Data Parameters
NAME bb41217
EXPNO 242
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171209
Time 2.27
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 16540
SOLVENT CDCl3
NS 3000
DS 4
SWH 24038.461 Hz
FIDRES 1.453253 Hz
AQ 0.3440320 sec
RG 200.34
DW 20.800 usec
DE 6.50 usec
TE 299.7 K
D1 1.00000000 sec
D11 0.03000000 sec
TDO 1



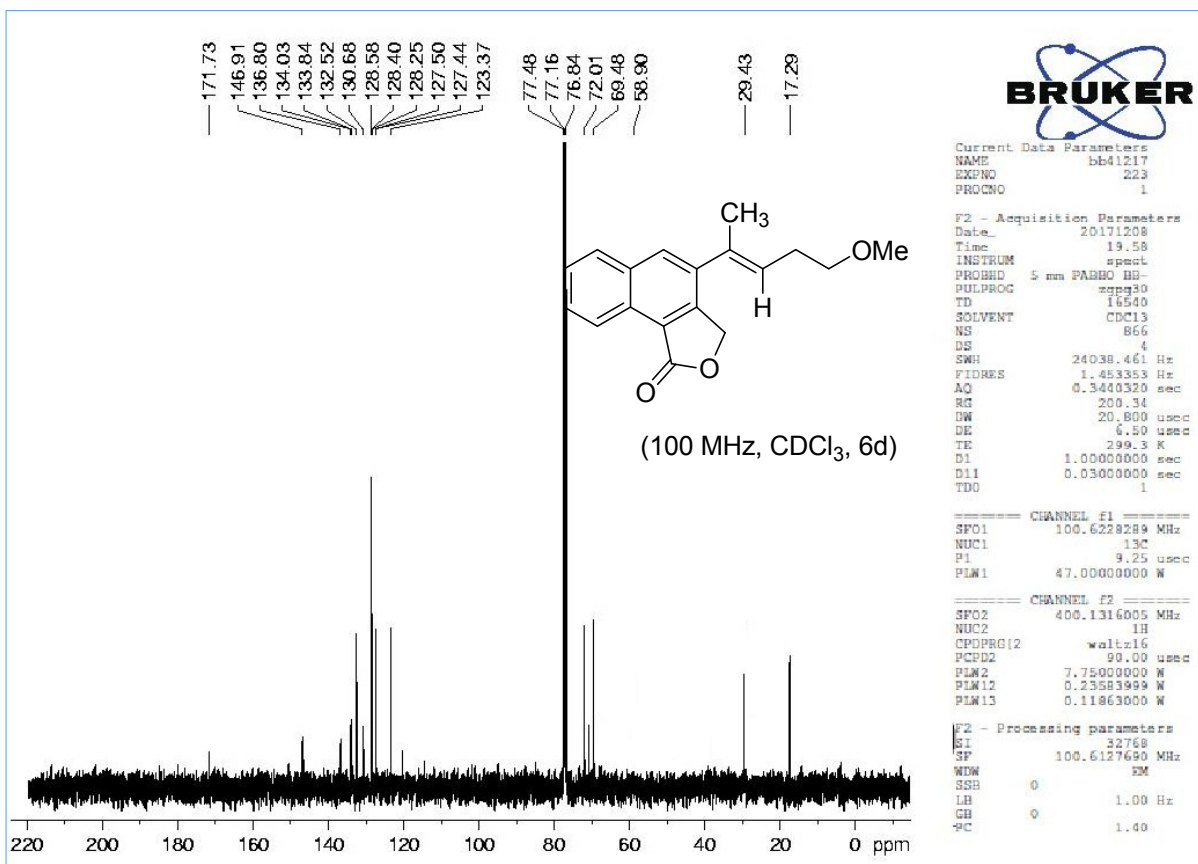
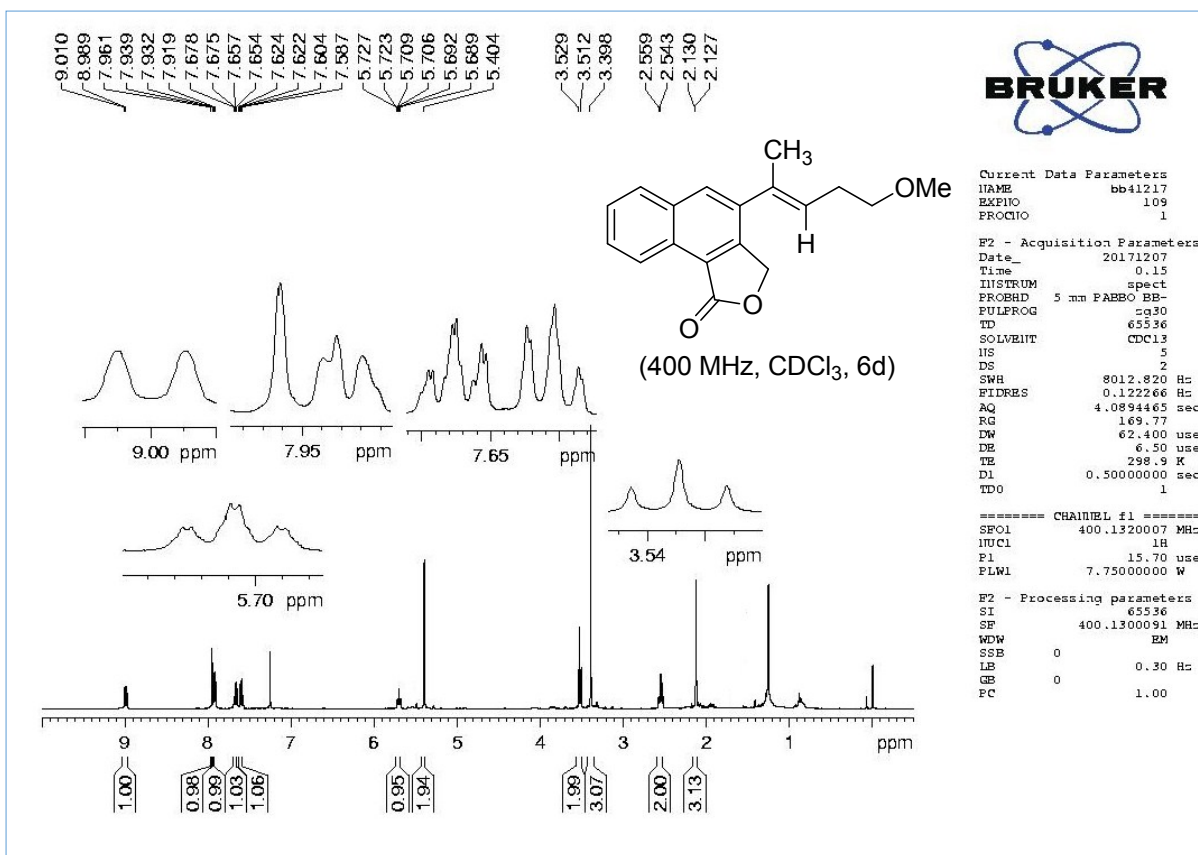
(100 MHz, CDCl₃, 6c)

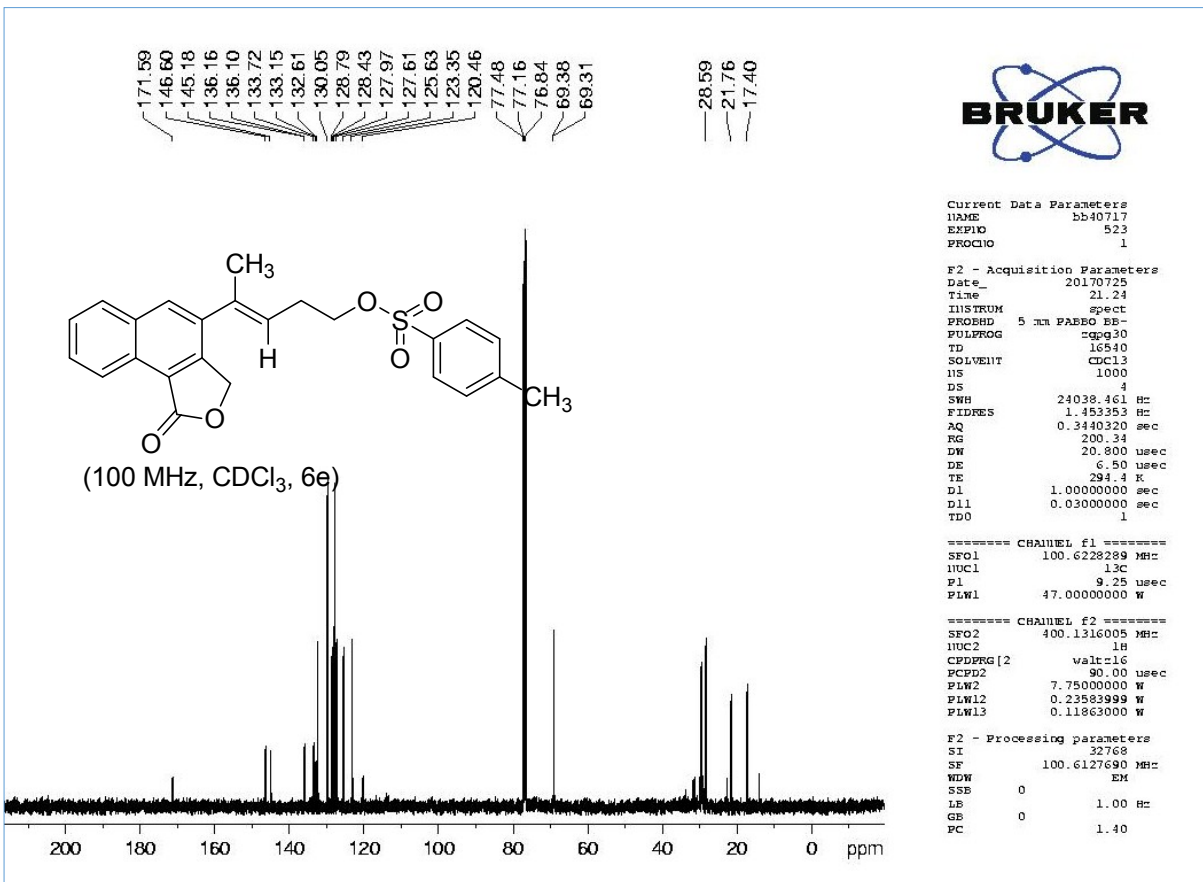
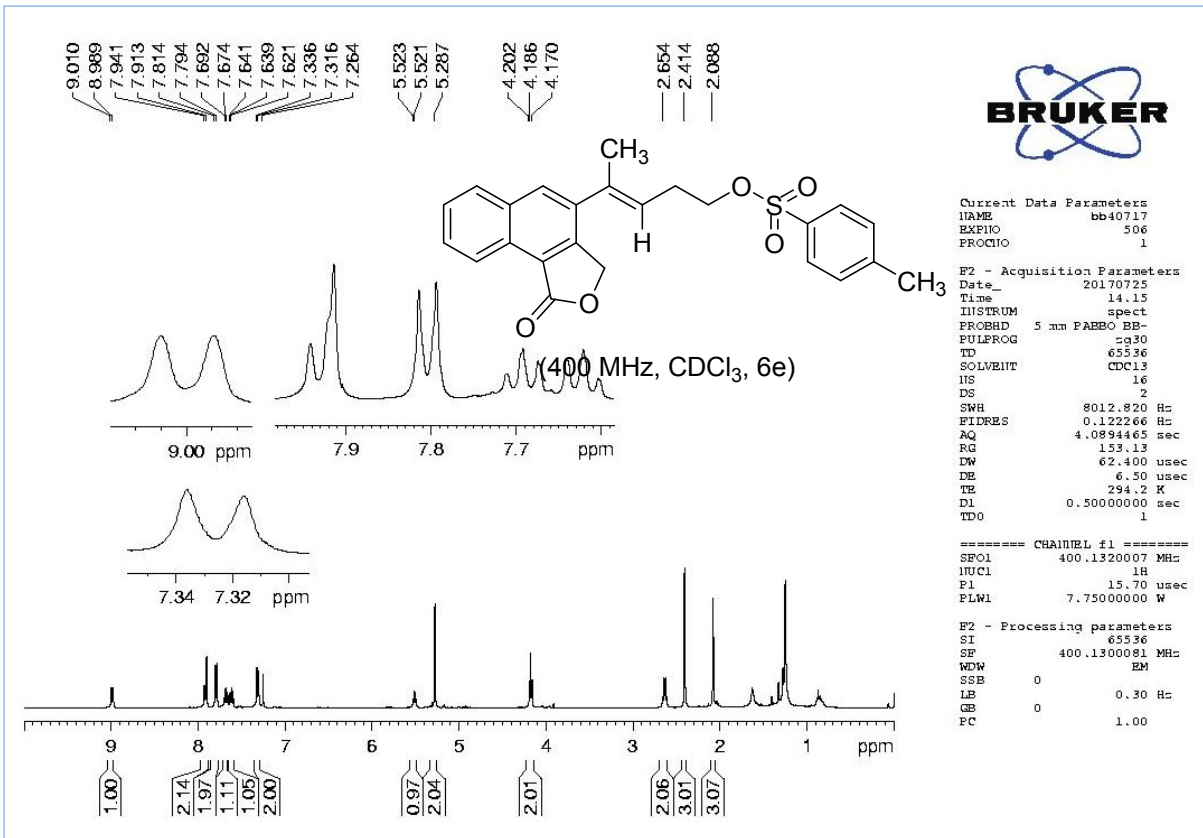


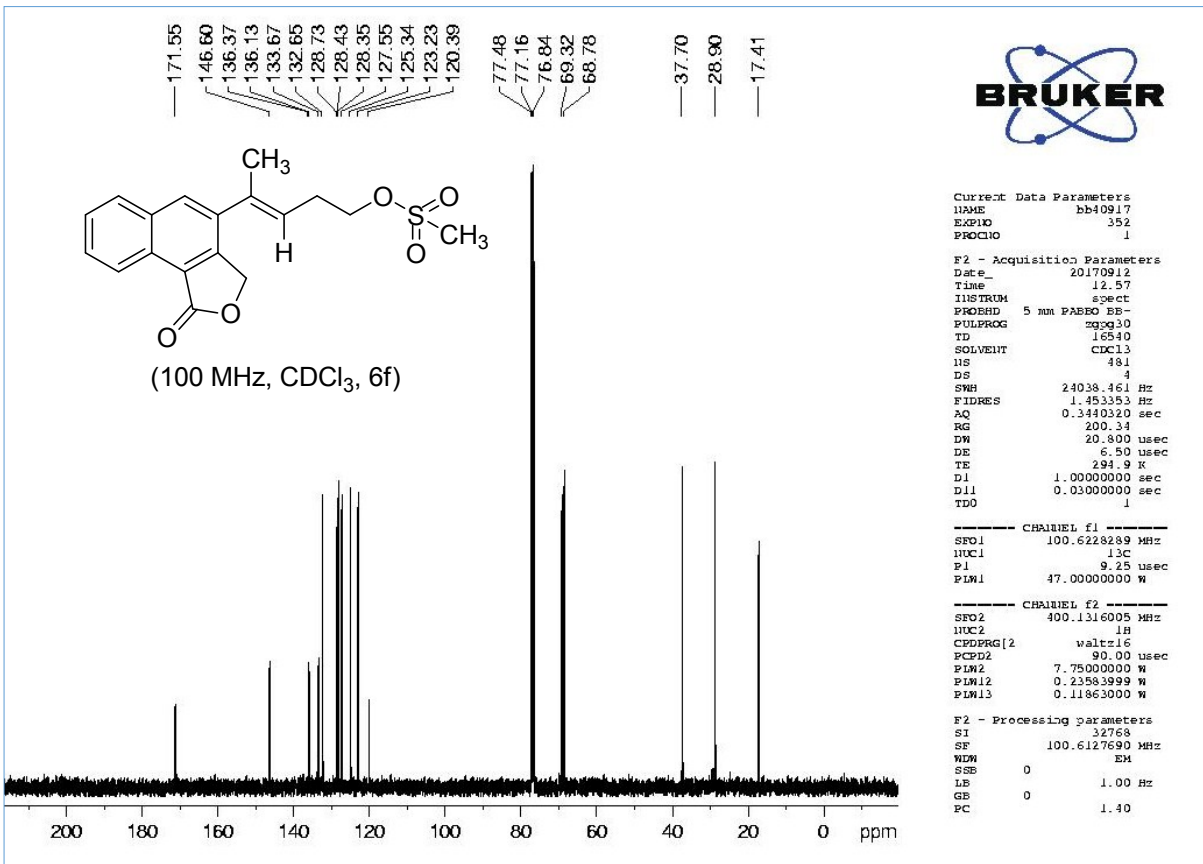
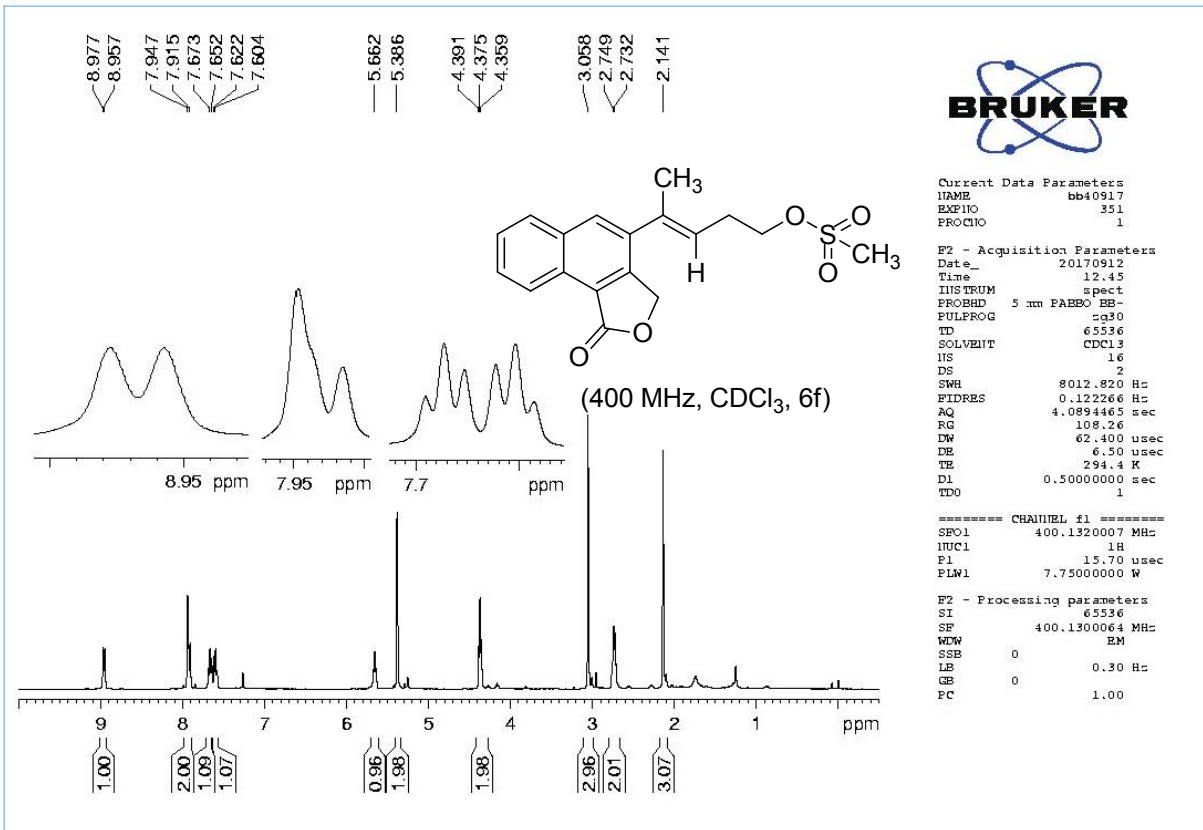
===== CHANNEL f1 =====
SF01 100.6228289 MHz
NUC1 13C
P1 9.25 usec
PLW1 47.00000000 W

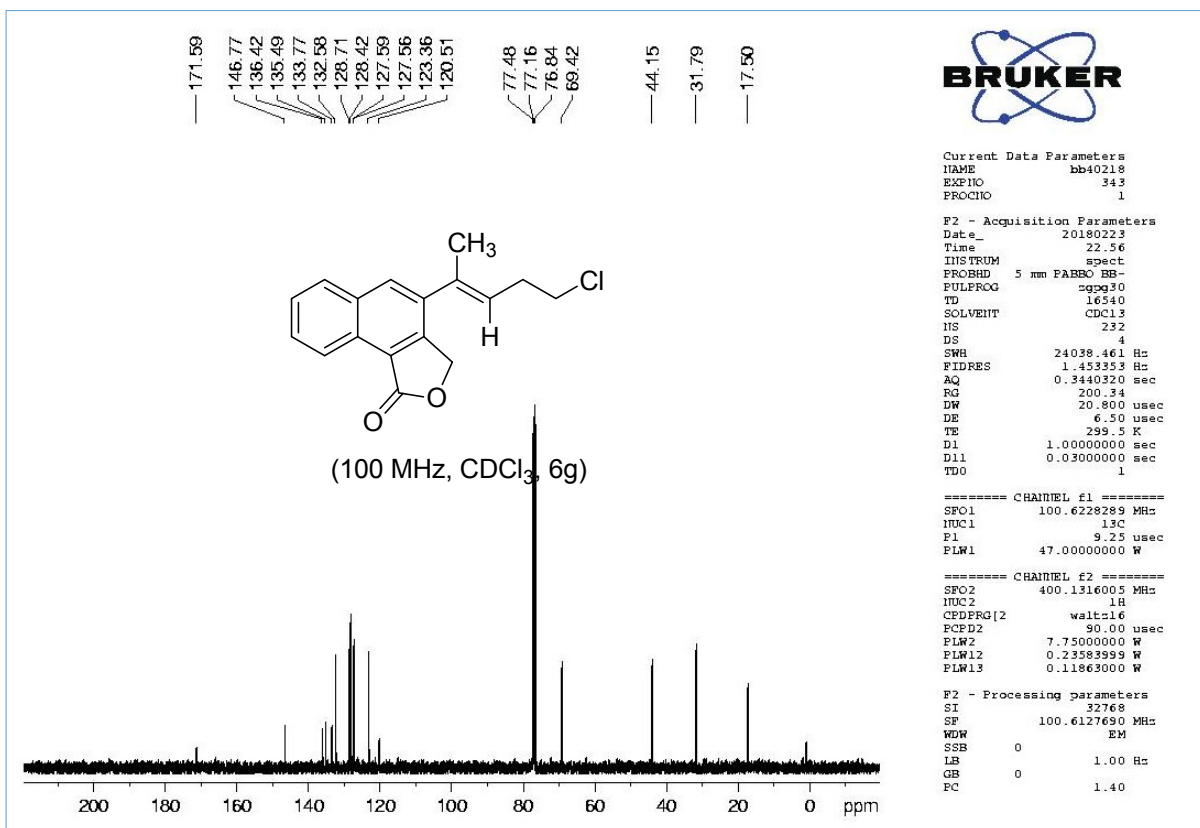
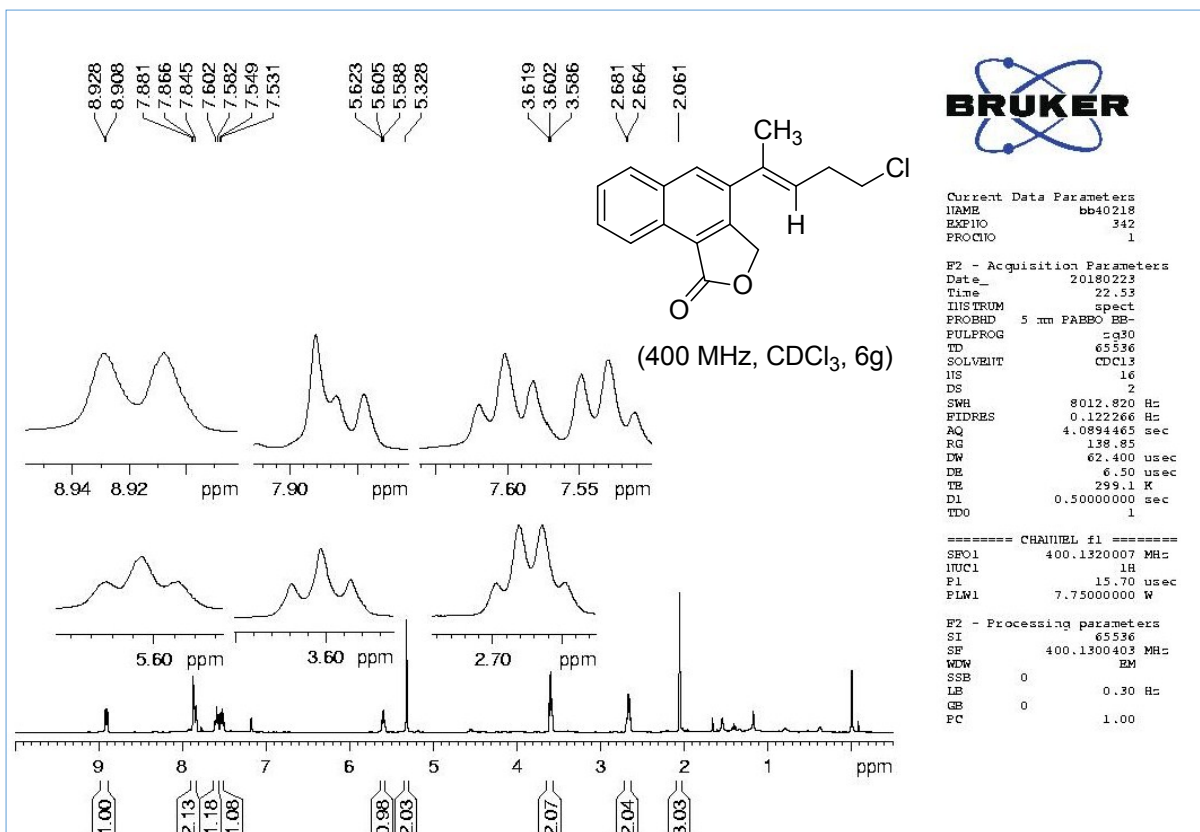
===== CHANNEL f2 =====
SF02 400.1316005 MHz
NUC2 1H
PCPD2 wait=16
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
PLW13 0.11863000 W

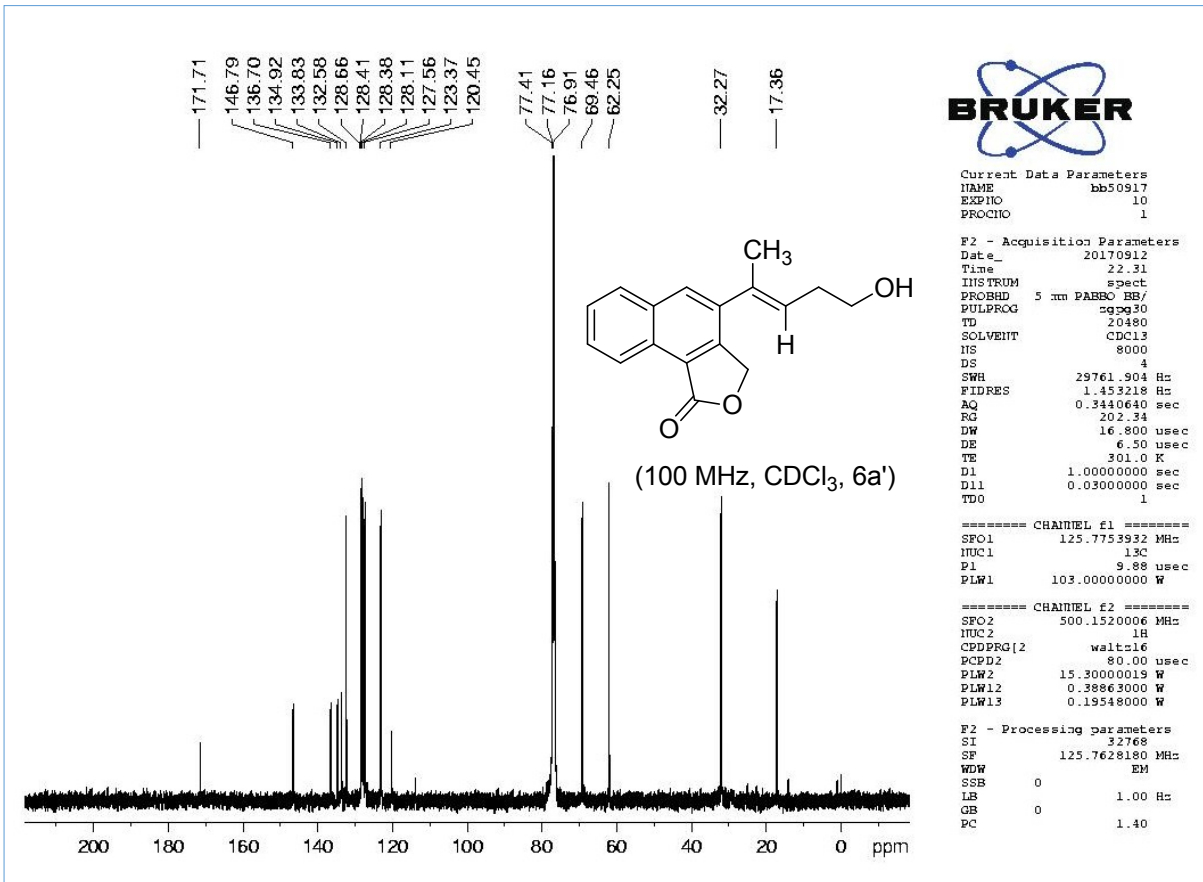
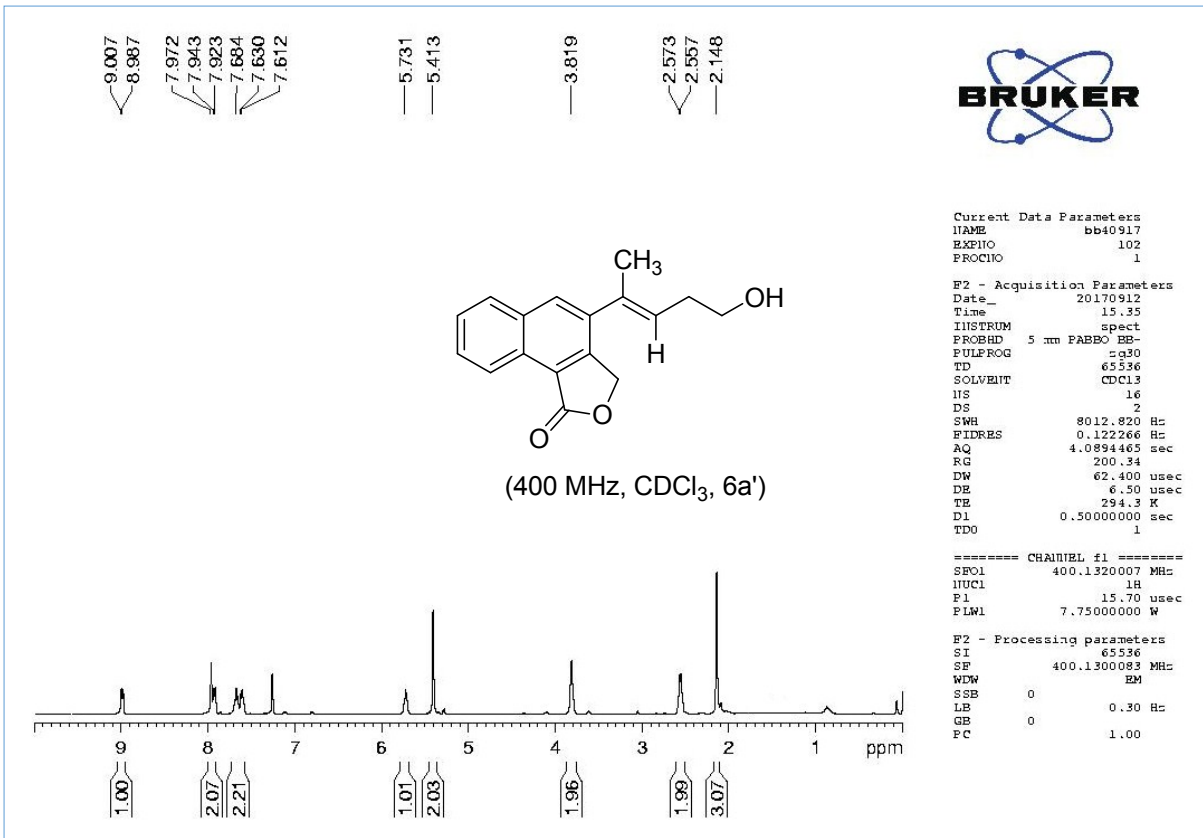
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

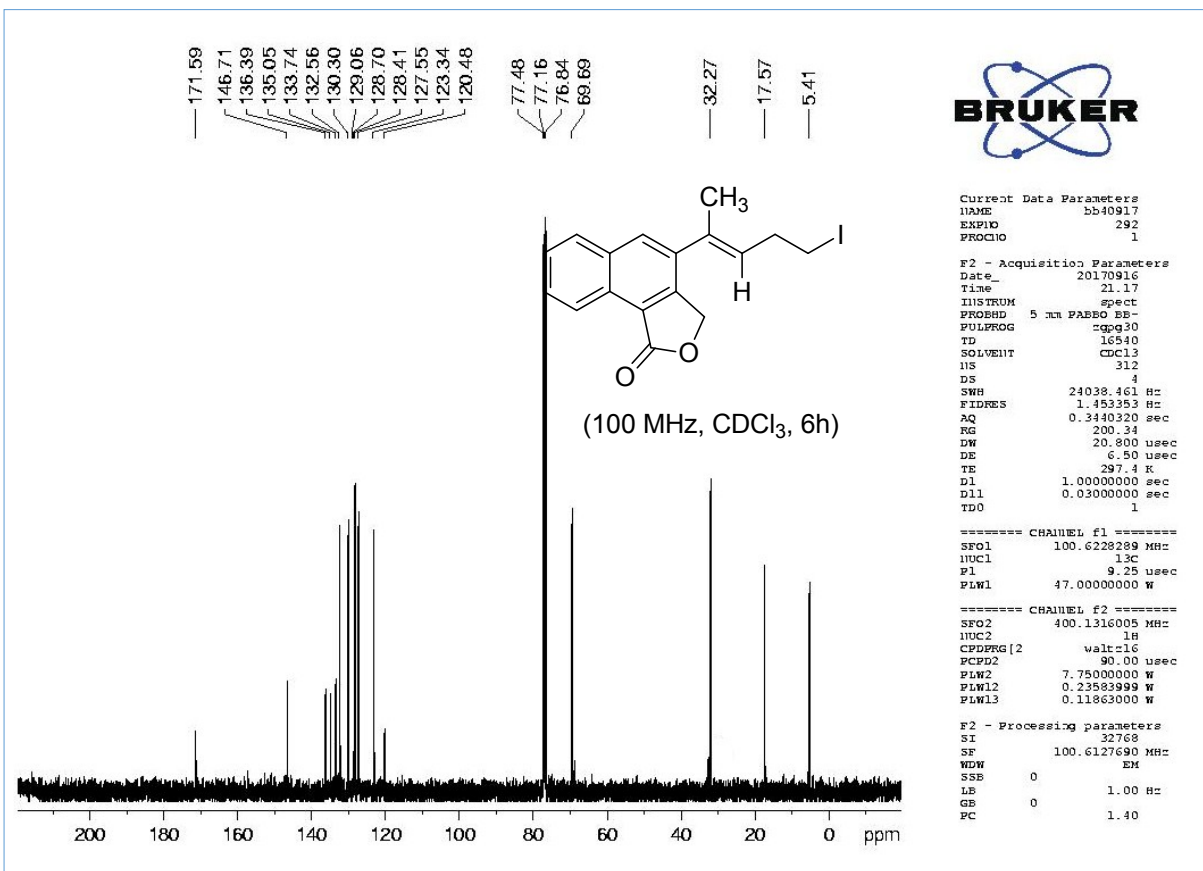
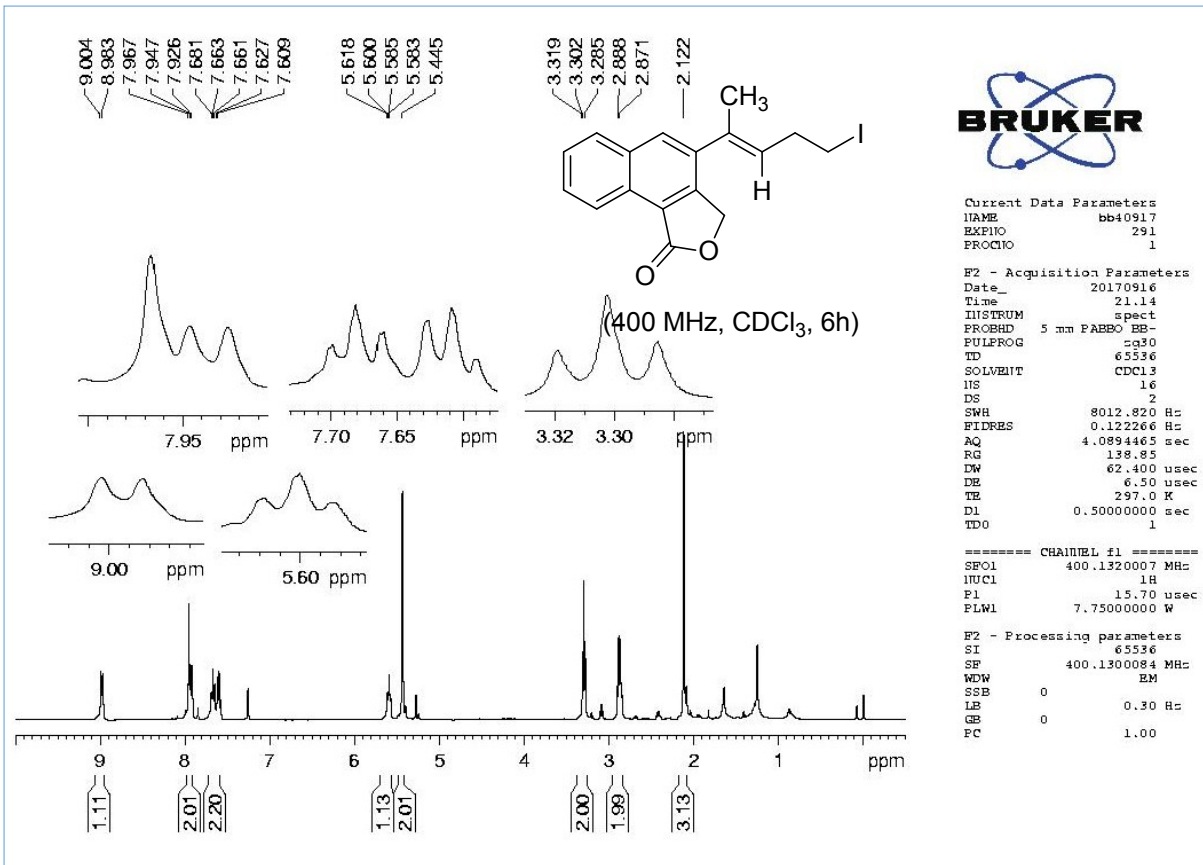


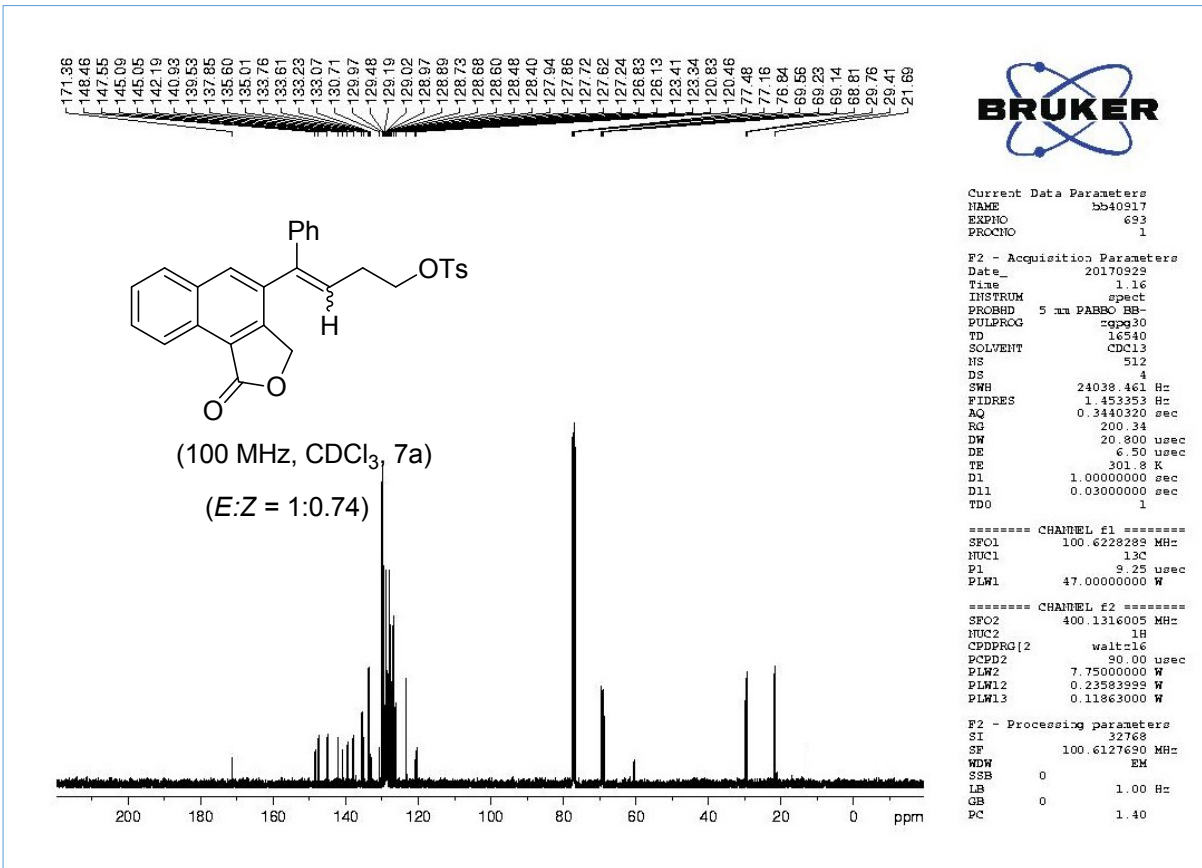
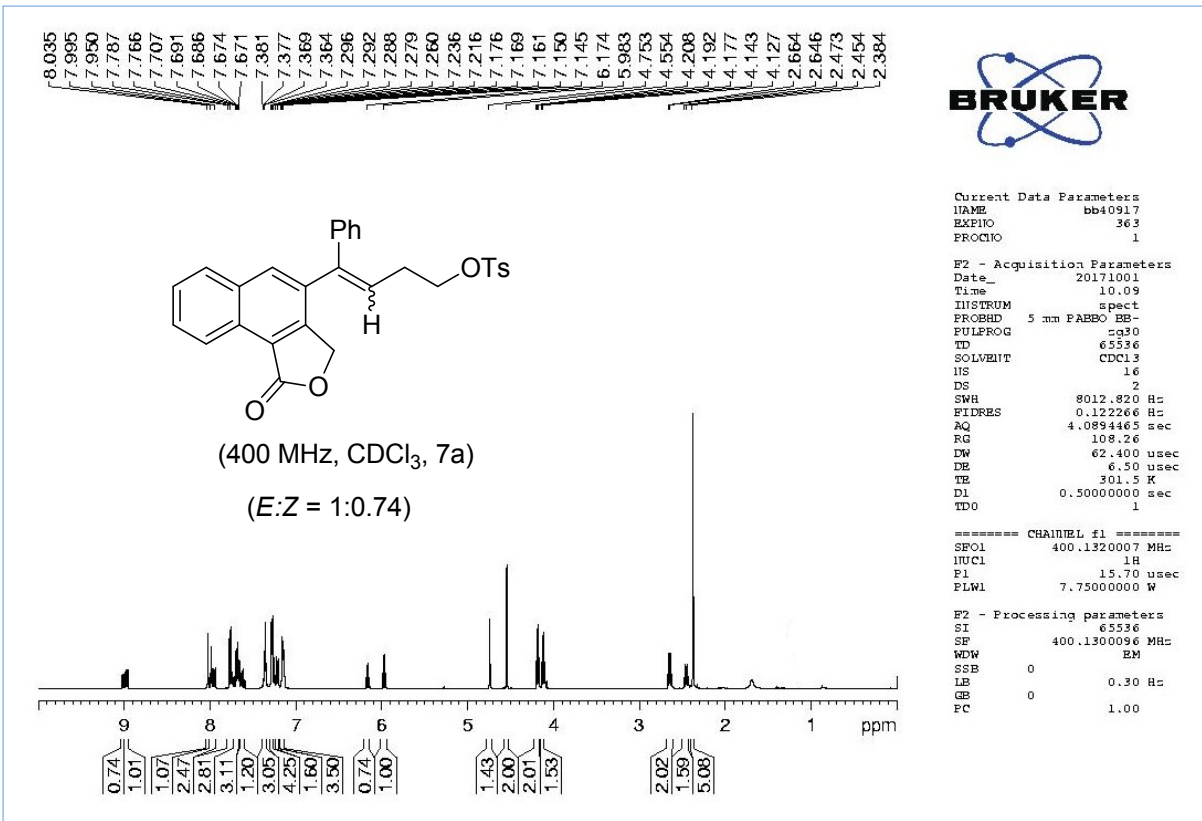




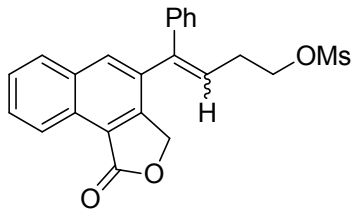




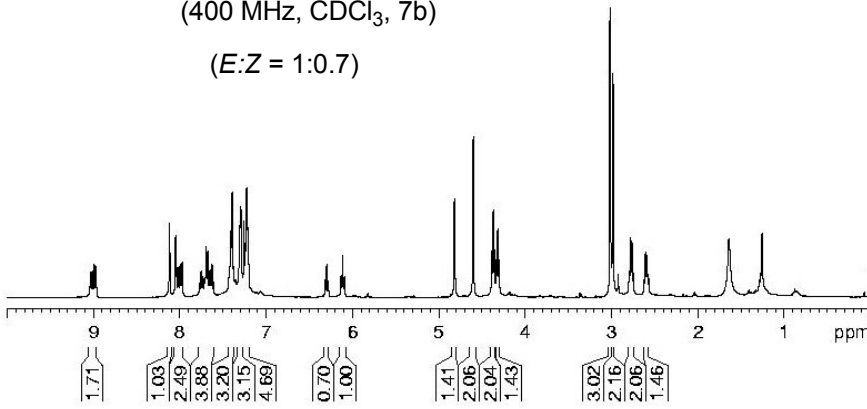




9.020
8.997
8.976
8.124
8.054
8.041
8.021
7.998
7.978
7.758
7.701
7.682
7.652
7.632
7.431
7.418
7.400
7.386
7.312
7.304
7.297
7.260
7.232
7.216
6.302
6.117
4.821
4.605
4.390
4.374
4.358
4.336
4.321
3.017
2.986
2.801
2.785
2.768
2.608
2.580



(400 MHz, CDCl₃, 7b)
(E:Z = 1:0.7)



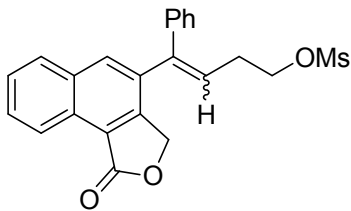
```
Current Data Parameters
NAME      bb40917
EXPNO     753
PROCNO    1

F2 - Acquisition Parameters
Date_     20171001
Time      10.32
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         16
DS         2
SWH        8012.820 Hz
FIDRES     0.122266 Hz
AQ         4.0894465 sec
RG         153.13
DW         62.400 usec
DE         6.50 usec
TE         301.1 K
D1         0.50000000 sec
TDO        1

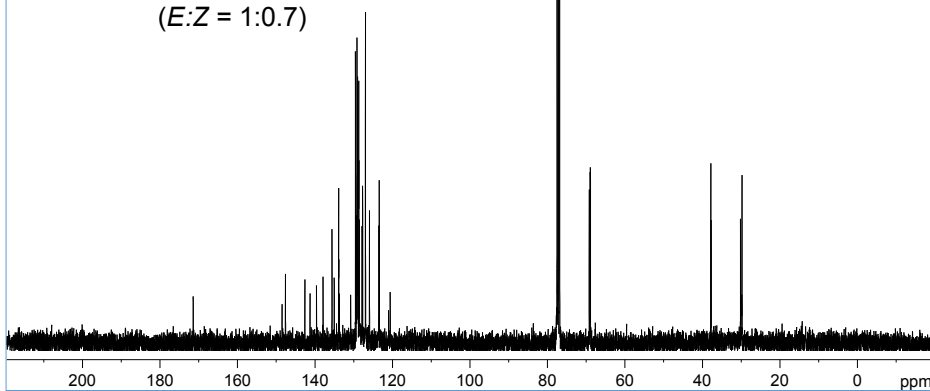
===== CHANNEL f1 =====
SFO1      400.1320007 MHz
NUC1      1H
P1        15.70 usec
PLW1      7.75000000 W

F2 - Processing parameters
SI         65536
SF         400.1300093 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
FC         1.00
```

171.39
148.46
147.59
142.57
141.24
139.57
137.89
135.58
133.00
133.86
133.67
130.76
129.52
129.29
129.13
129.05
128.99
128.87
128.82
128.67
128.63
128.52
128.52
127.82
127.67
126.94
125.90
123.49
123.39
120.96
120.56
77.48
77.16
76.84
68.92
68.87
37.79
37.71
30.13
29.74



(100 MHz, CDCl₃, 7b)
(E:Z = 1:0.7)



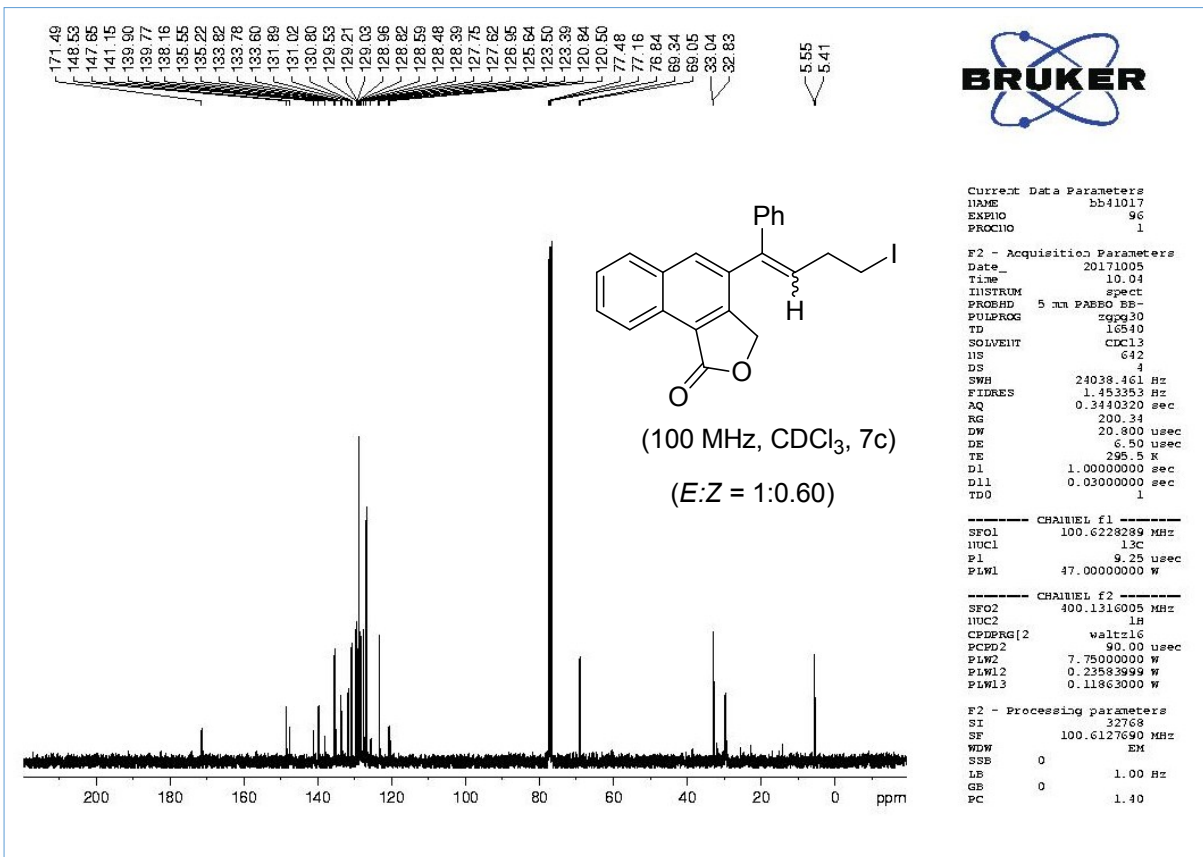
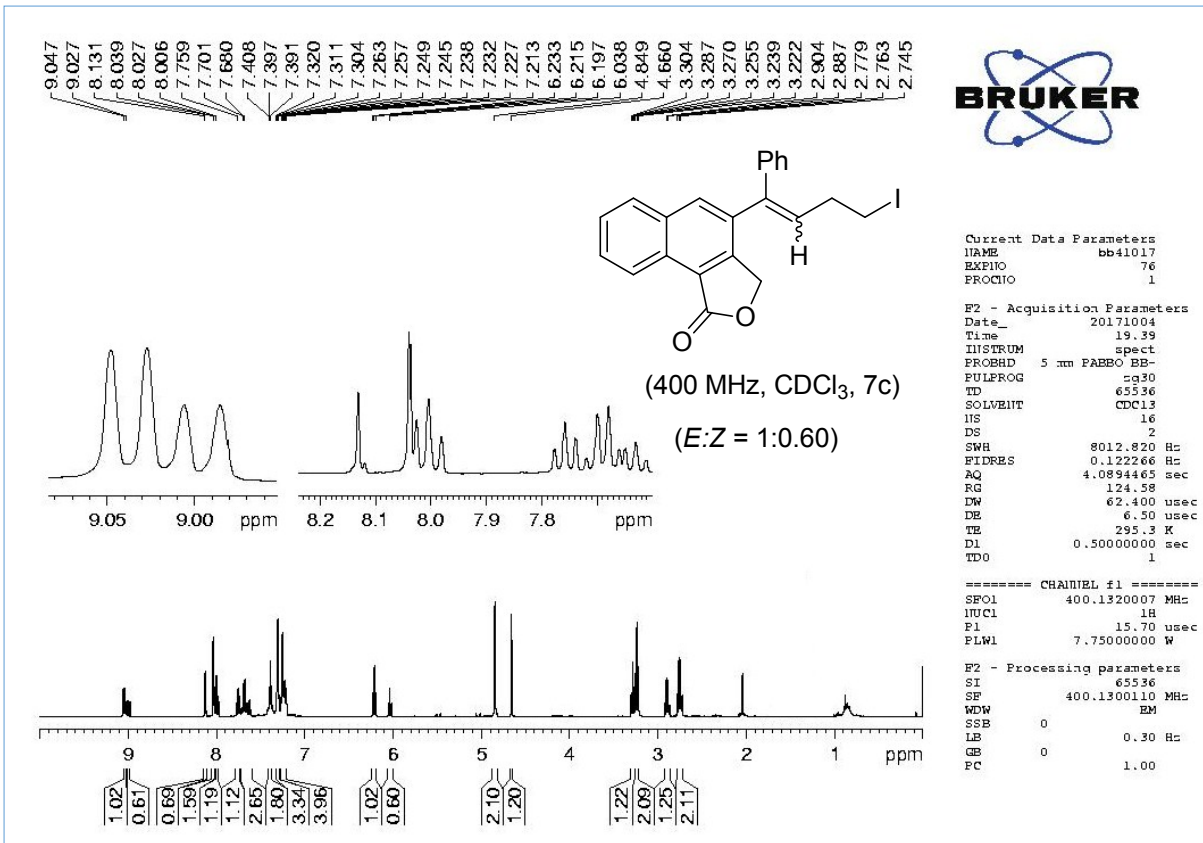
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Current Data Parameters
NAME      Desktop
EXPNO     754
PROCNO    1

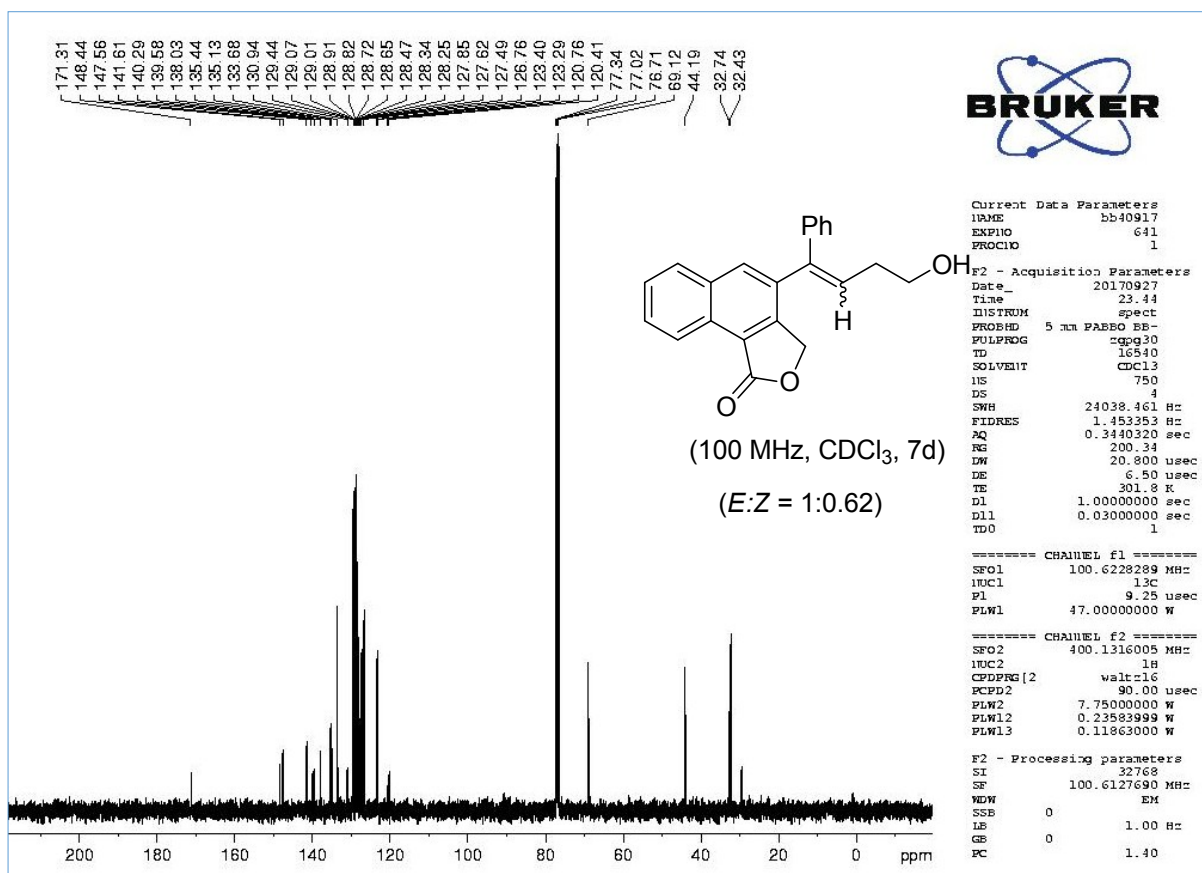
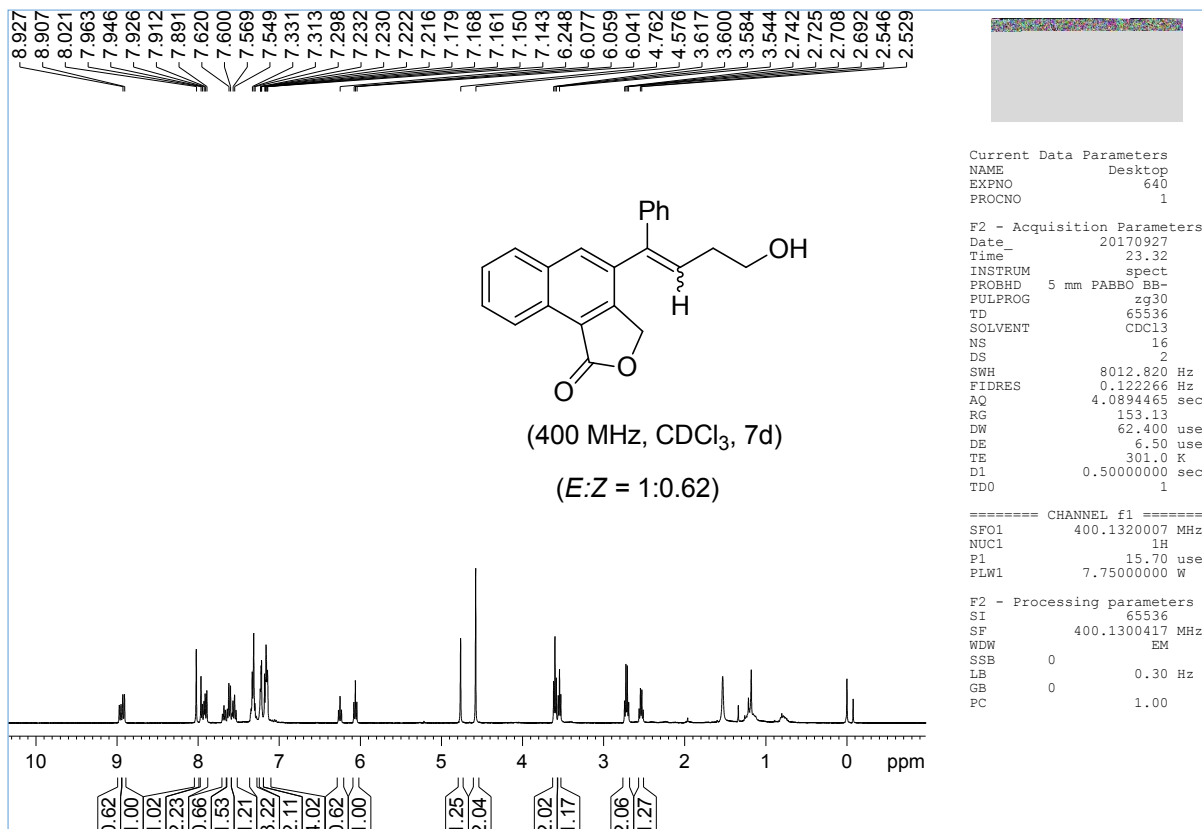
F2 - Acquisition Parameters
Date_     20171001
Time      10.36
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD         16540
SOLVENT   CDCl3
NS         1500
DS         4
SWH        24038.461 Hz
FIDRES     1.453353 Hz
AQ         0.3440320 sec
RG         200.34
DW         20.800 usec
DE         6.50 usec
TE         301.7 K
D1         1.00000000 sec
D11        0.03000000 sec
TDO        1

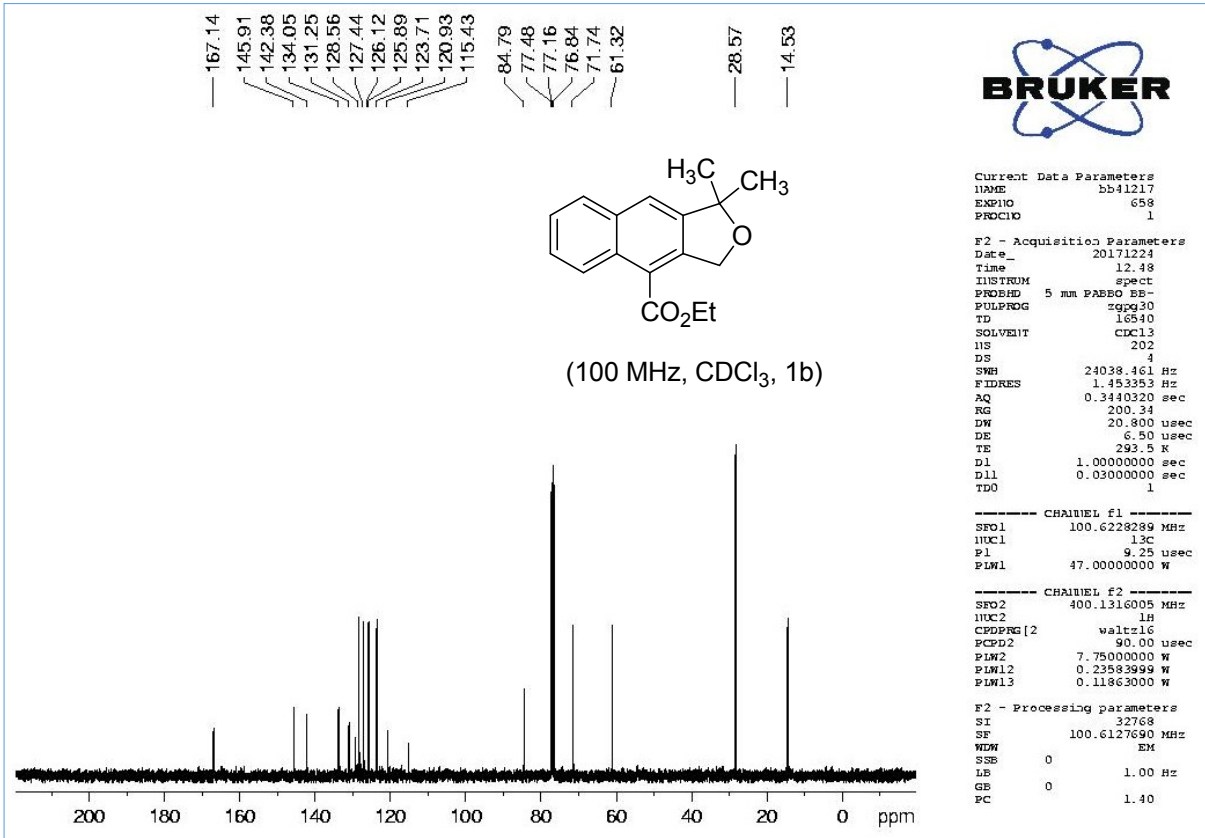
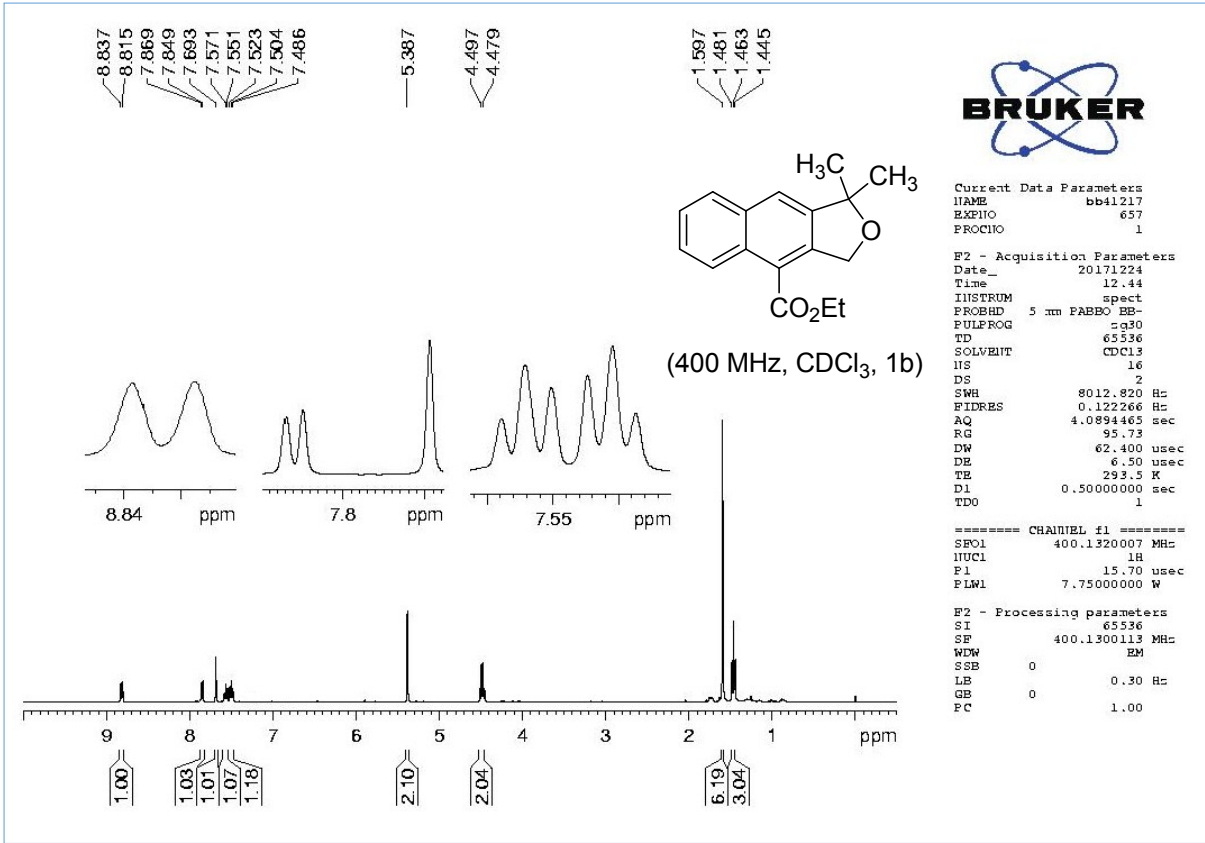
===== CHANNEL f1 =====
SFO1      100.6228289 MHz
NUC1      13C
P1         9.25 usec
PLW1      47.00000000 W

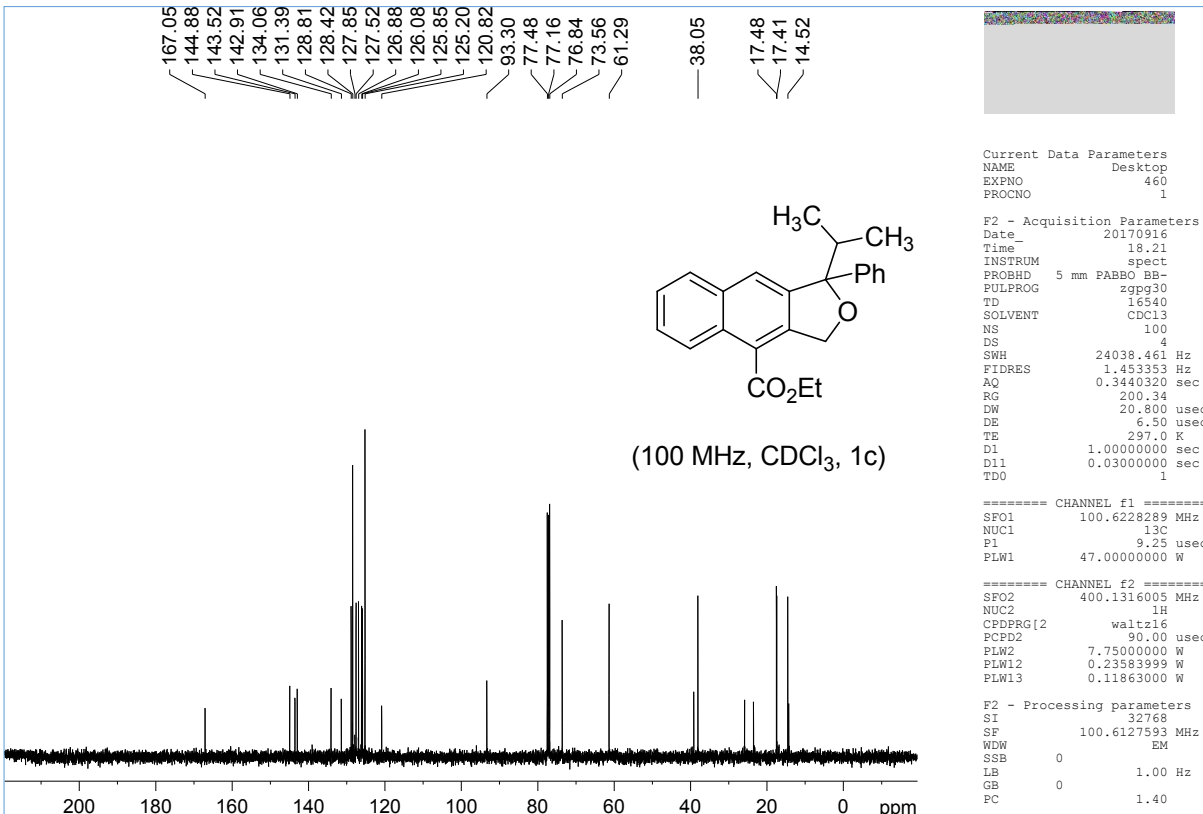
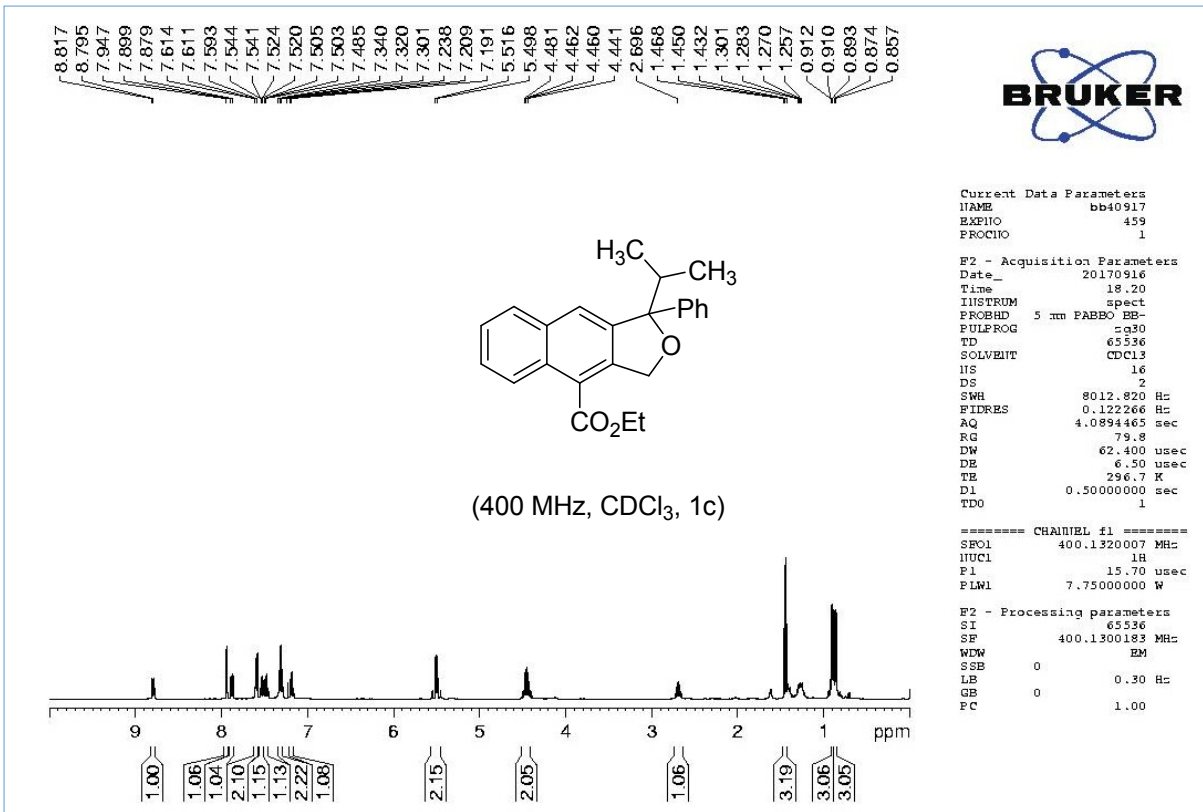
===== CHANNEL f2 =====
SFO2      400.1316005 MHz
NUC2      1H
CPDPRG[2] waltz16
PCPD2     90.00 usec
PLW2      7.75000000 W
PLW12     0.23583999 W
PLW13     0.11863000 W

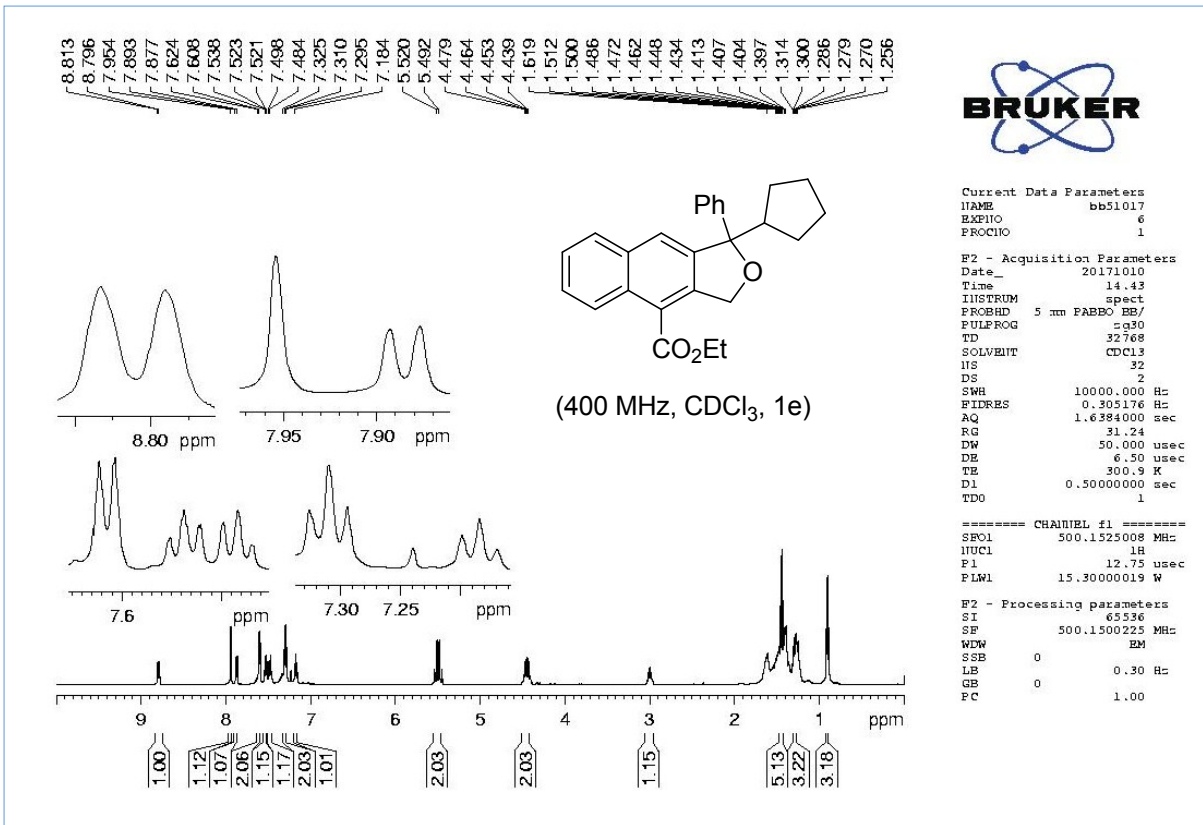
F2 - Processing parameters
SI         32768
SF         100.6127557 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
FC         1.40
```











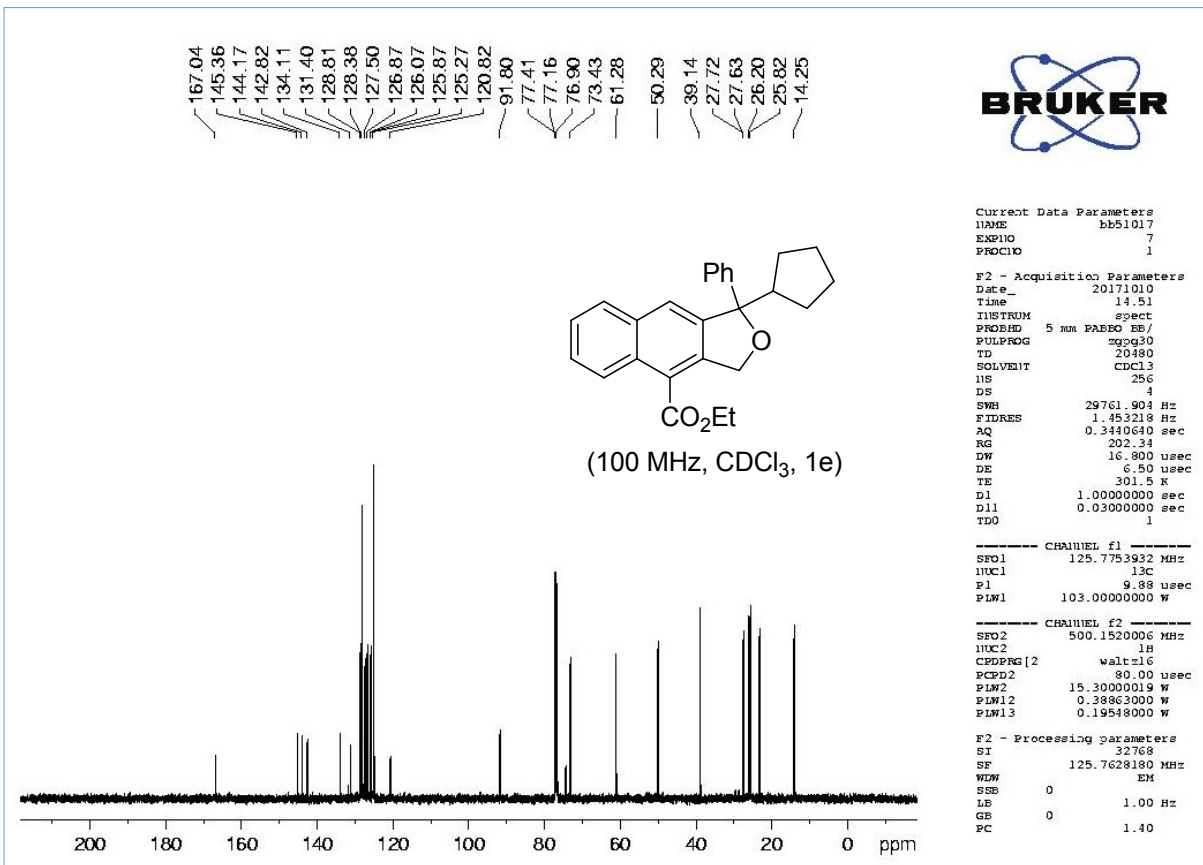
```

Current Data Parameters
NAME      bb51017
EXPNO     6
PROCNO    1

F2 - Acquisition Parameters
Date_     20171010
Time      14.43
INSTRUM   spect
PROBHD    5 mm FAPBO BB/
PULPROG   zg30
TD         32768
SOLVENT   CDCl3
NS         32
DS         2
SWH        10000.000 Hz
FIDRES     0.305176 Hz
AQ         1.6384000 sec
RG         31.24
DW         50.000 usec
DE         6.50 usec
TE         300.9 K
D1         0.50000000 sec
TDO        1

===== CHANNEL f1 =====
SFO1      500.1525008 MHz
NUC1       1H
P1         12.75 usec
PLW1      15.30000019 W

F2 - Processing parameters
SI         65536
SF         500.1500225 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
  
```



```

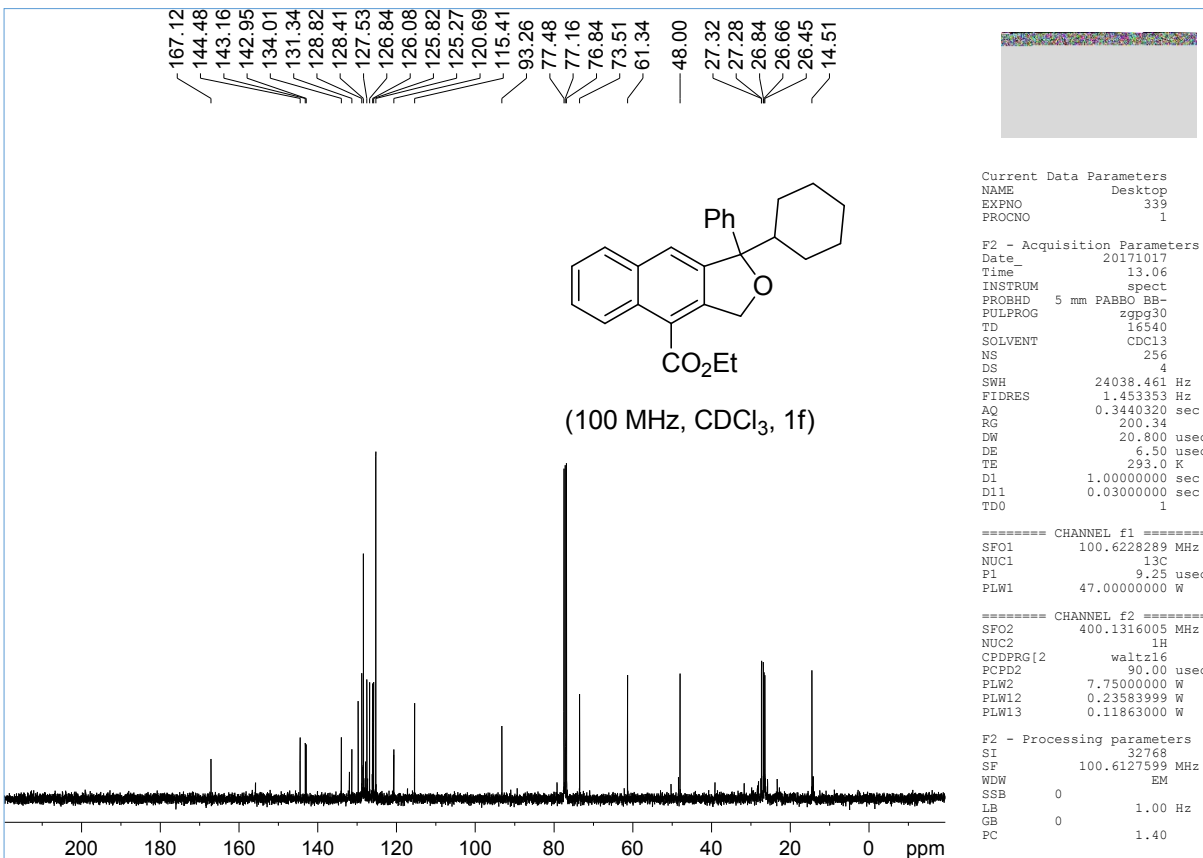
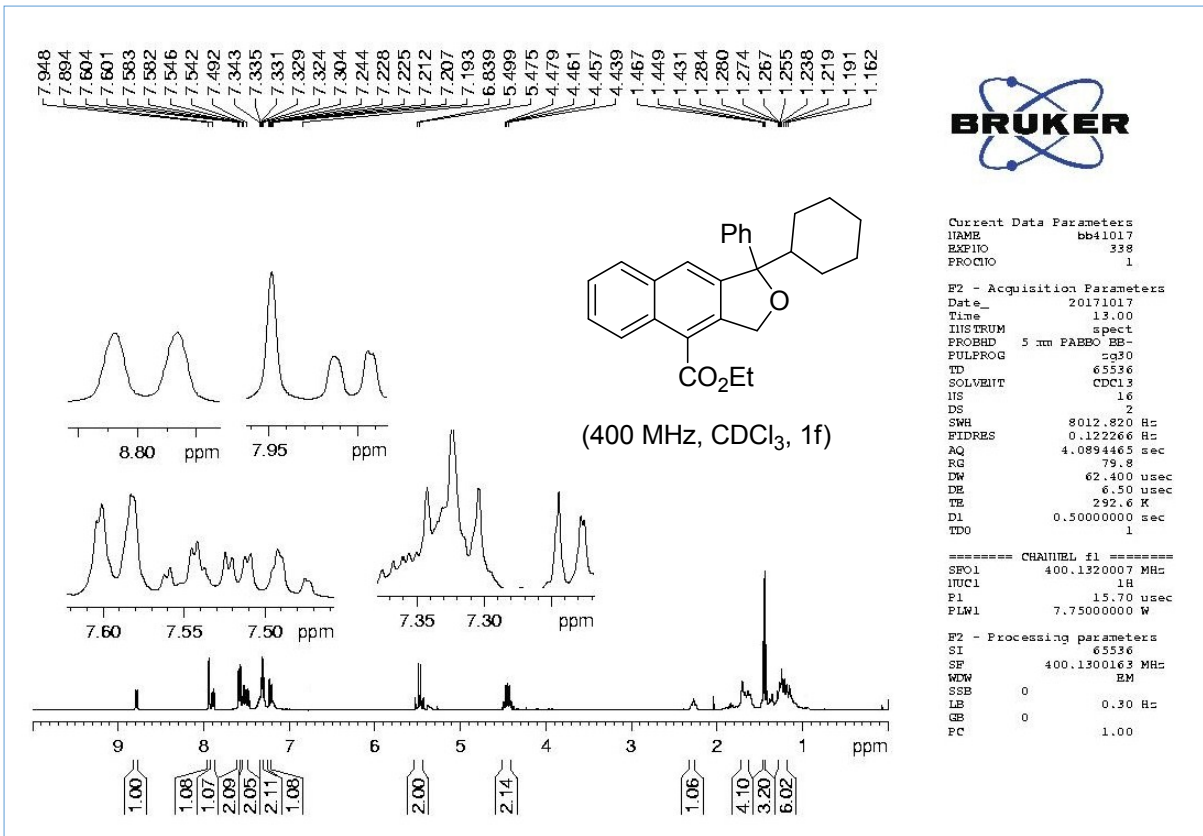
Current Data Parameters
NAME      bb51017
EXPNO     7
PROCNO    1

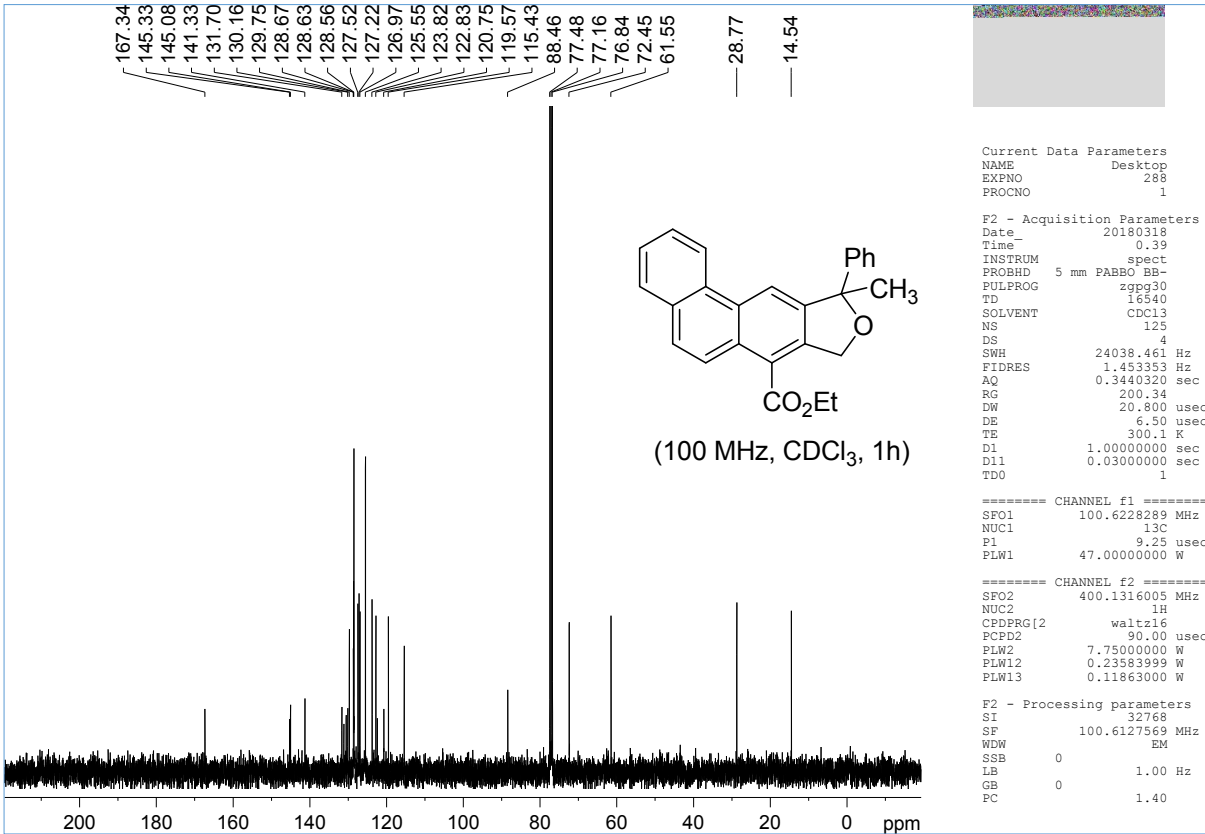
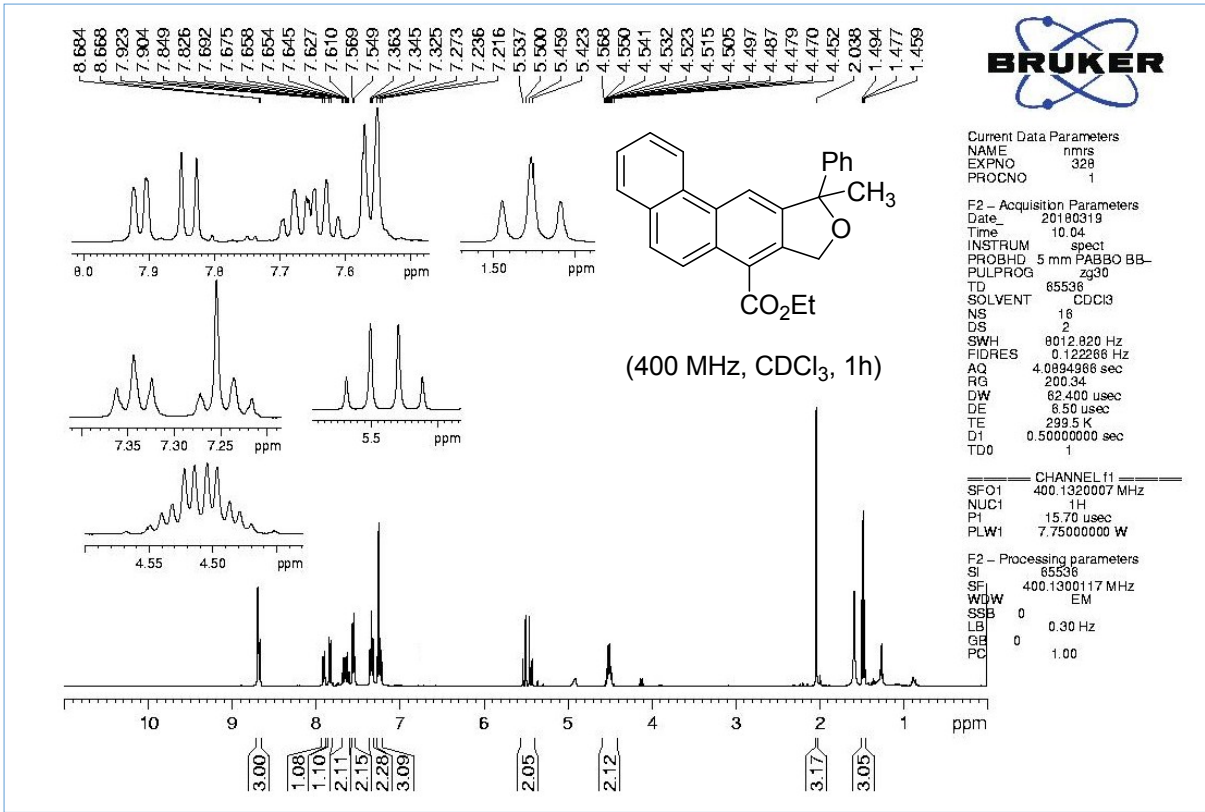
F2 - Acquisition Parameters
Date_     20171010
Time      14.51
INSTRUM   spect
PROBHD    5 mm FAPBO BB/
PULPROG   zgpg30
TD         20480
SOLVENT   CDCl3
NS         256
DS         4
SWH        29761.904 Hz
FIDRES     1.453218 Hz
AQ         0.3440640 sec
RG         202.34
DW         16.800 usec
DE         6.50 usec
TE         301.5 K
D1         1.00000000 sec
D11        0.03000000 sec
TDO        1

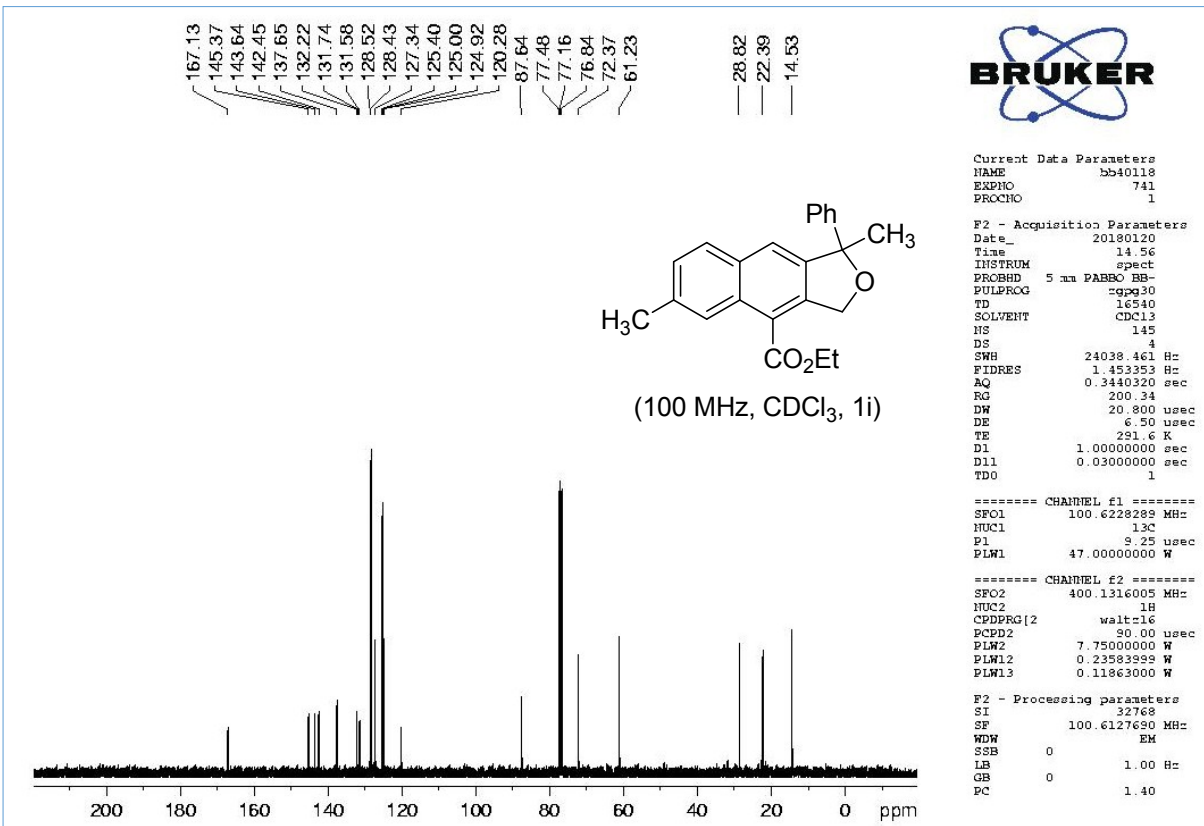
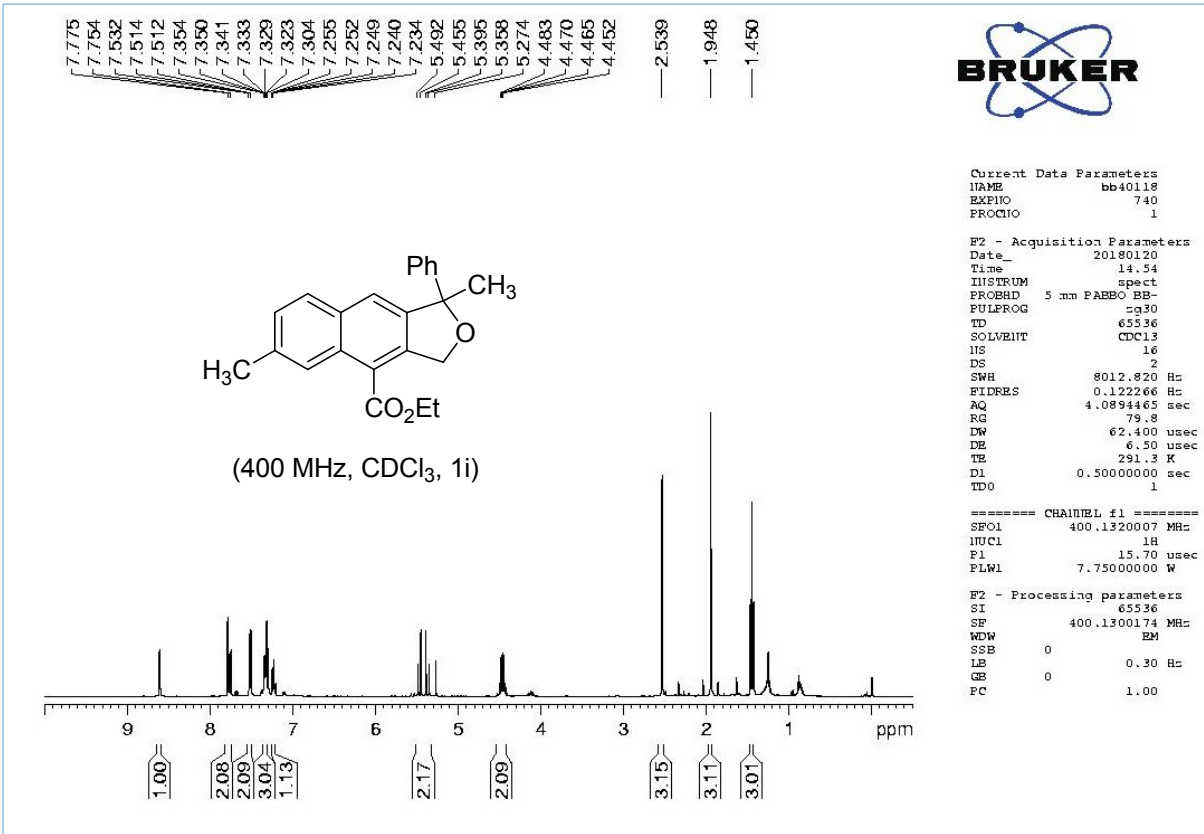
----- CHANNEL f1 -----
SFO1      125.7753932 MHz
NUC1       13C
P1         9.88 usec
PLW1      103.00000000 W

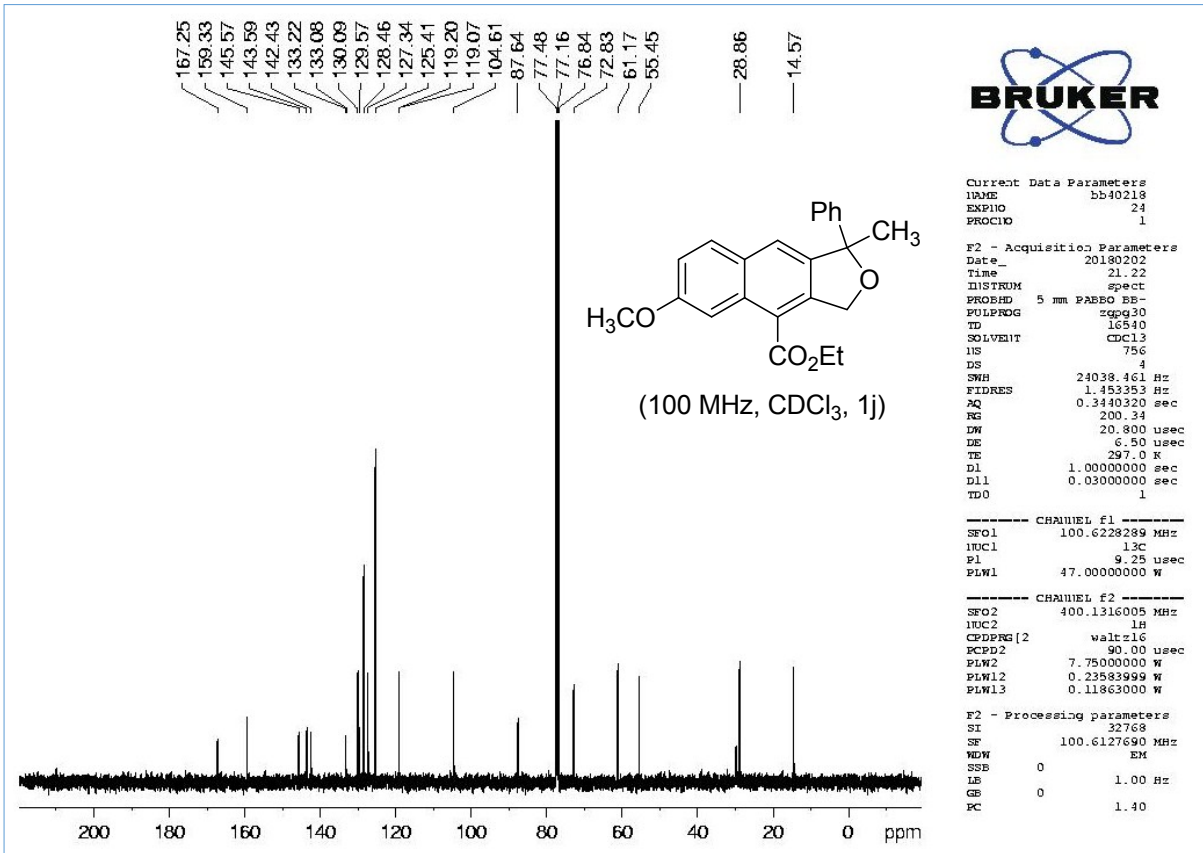
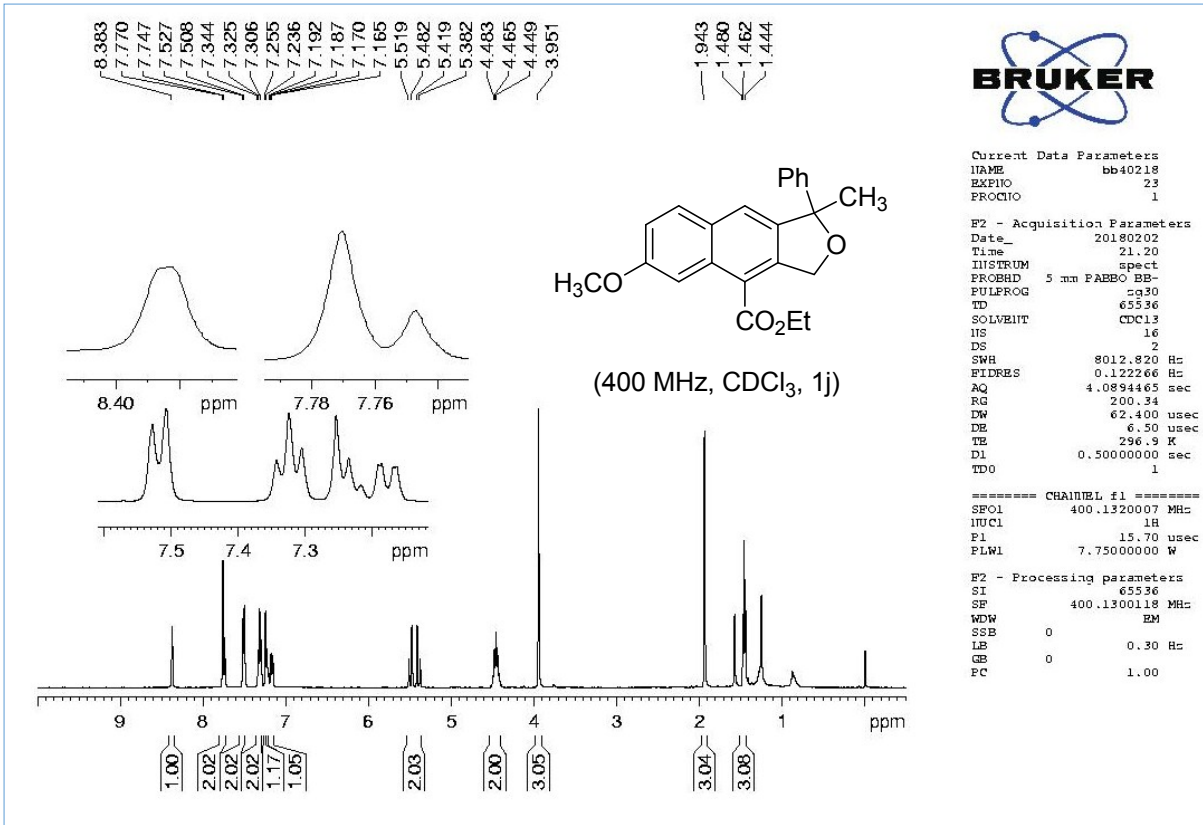
----- CHANNEL f2 -----
SFO2      500.1520006 MHz
NUC2       1H
CPDPRG[2] waltz16
PCPD2     80.00 usec
PLW2      15.30000019 W
PLW12     0.38863000 W
PLW13     0.19548000 W

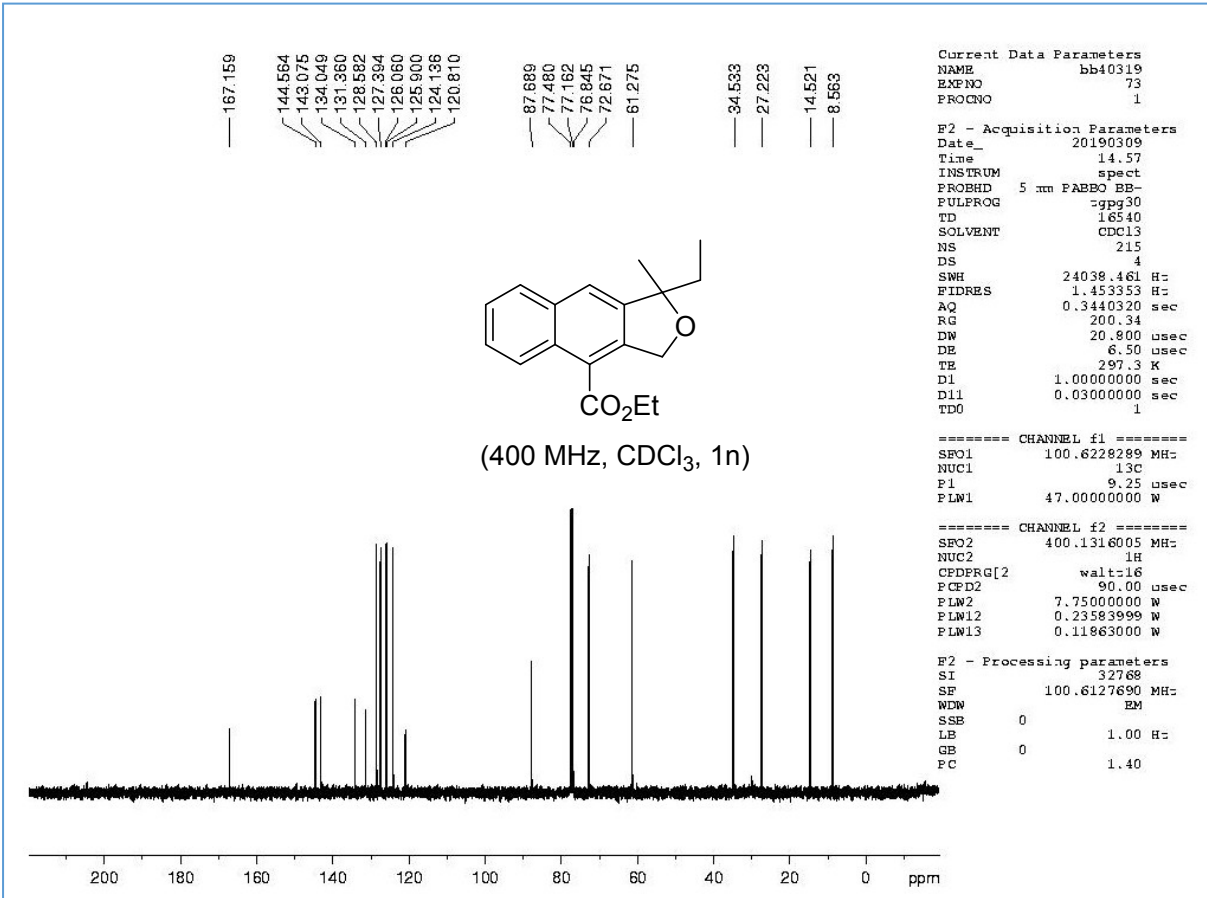
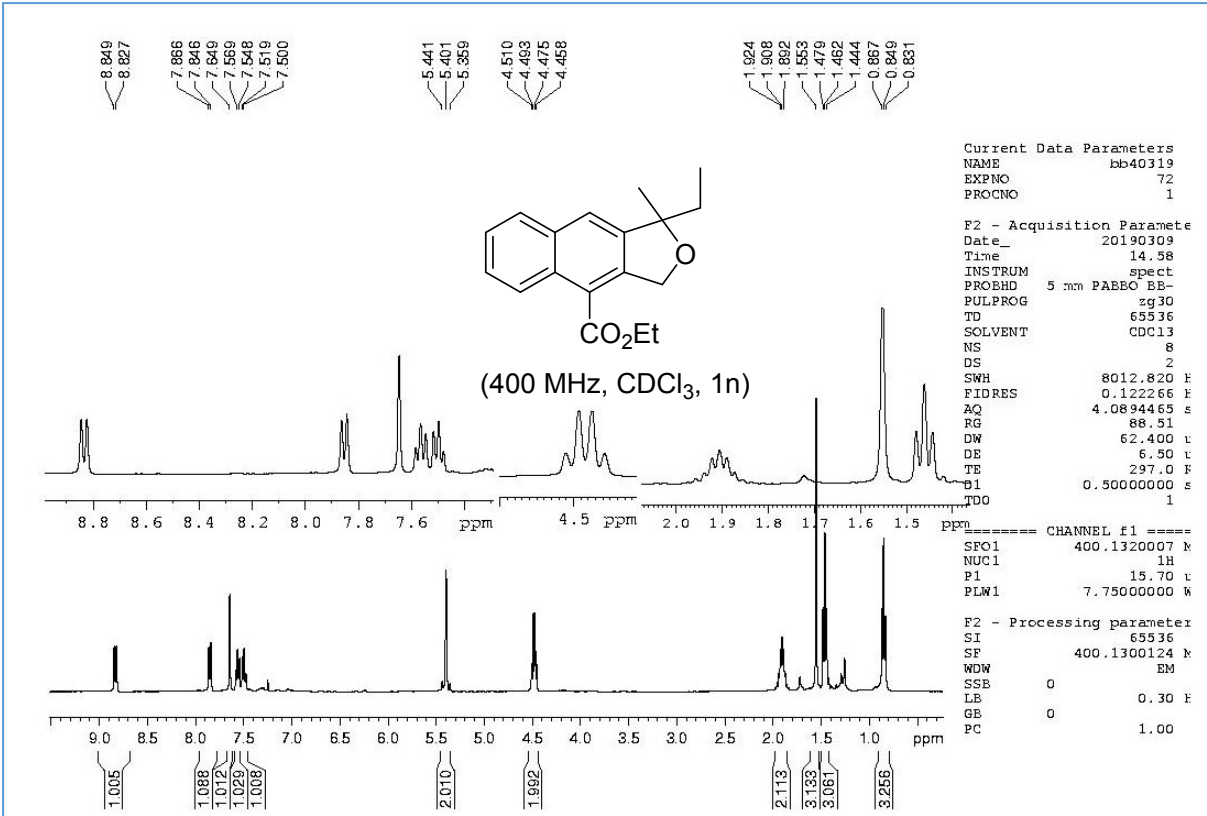
F2 - Processing parameters
SI         32768
SF         125.7628180 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
  
```

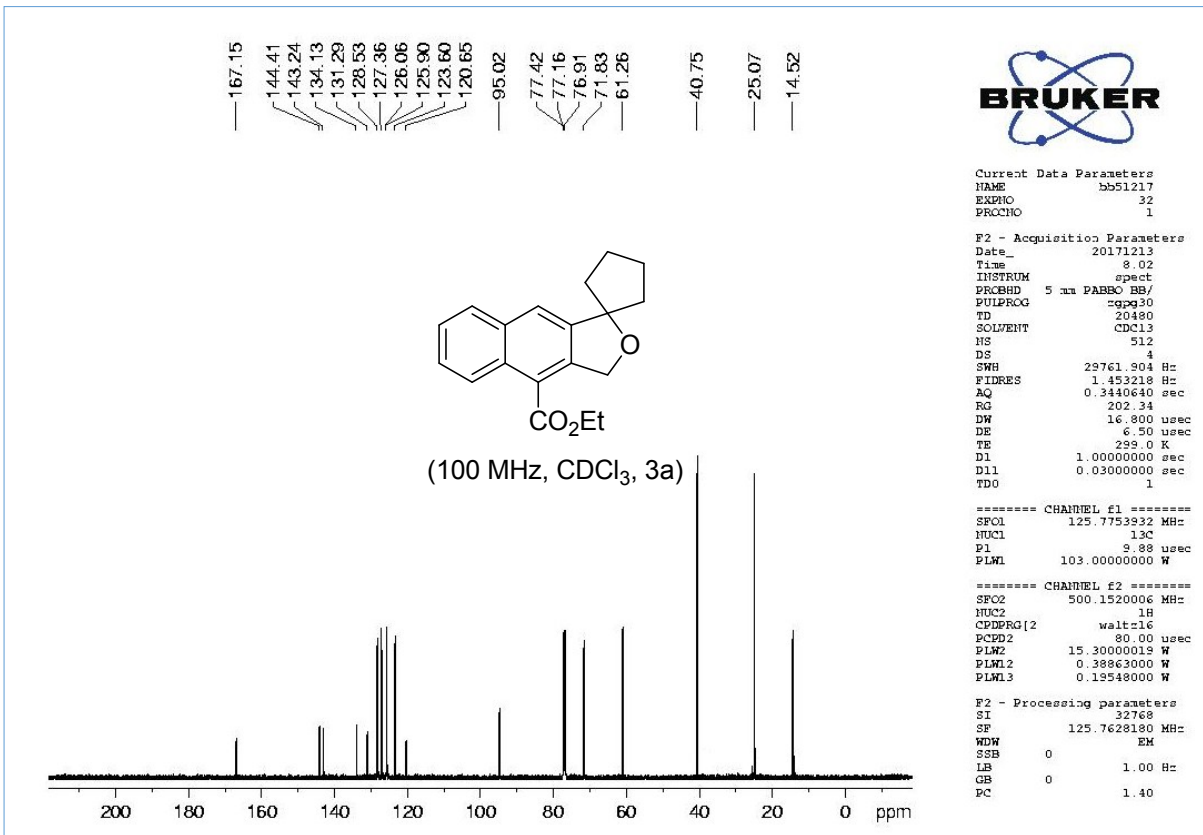
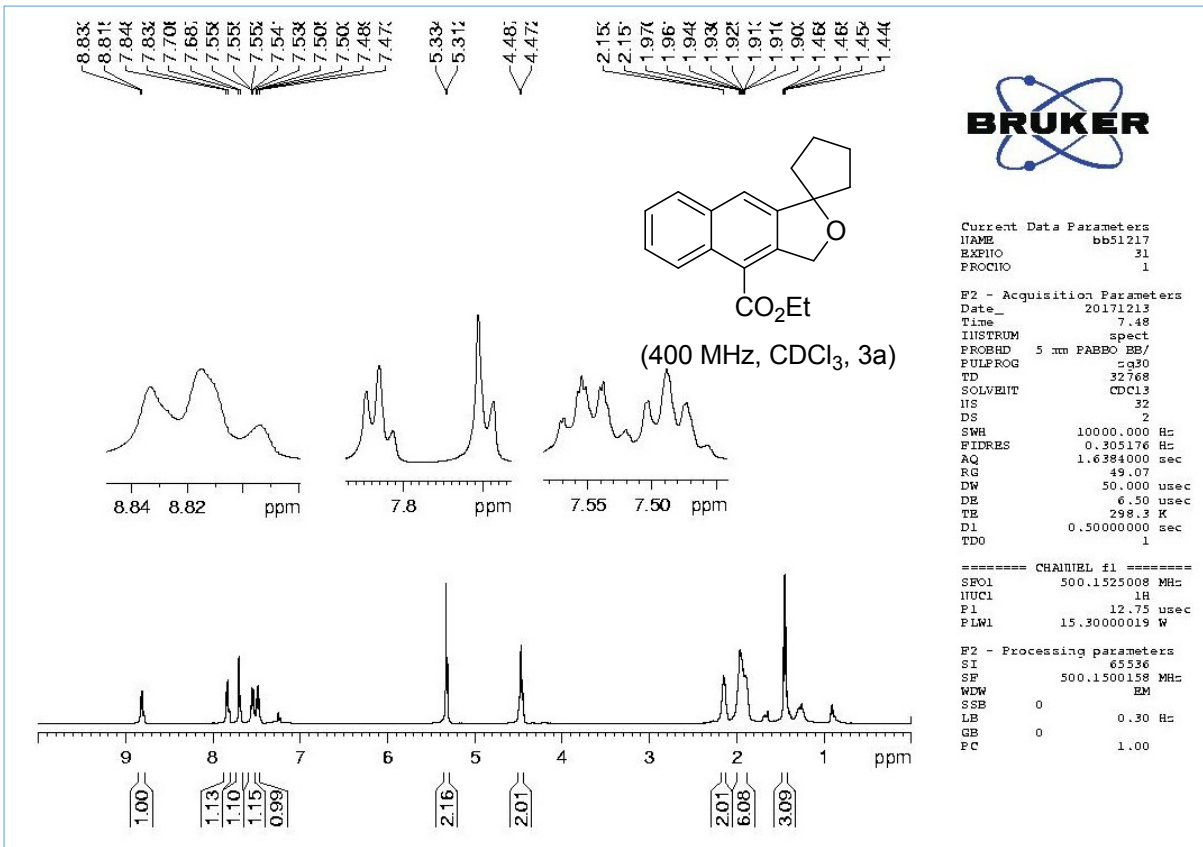


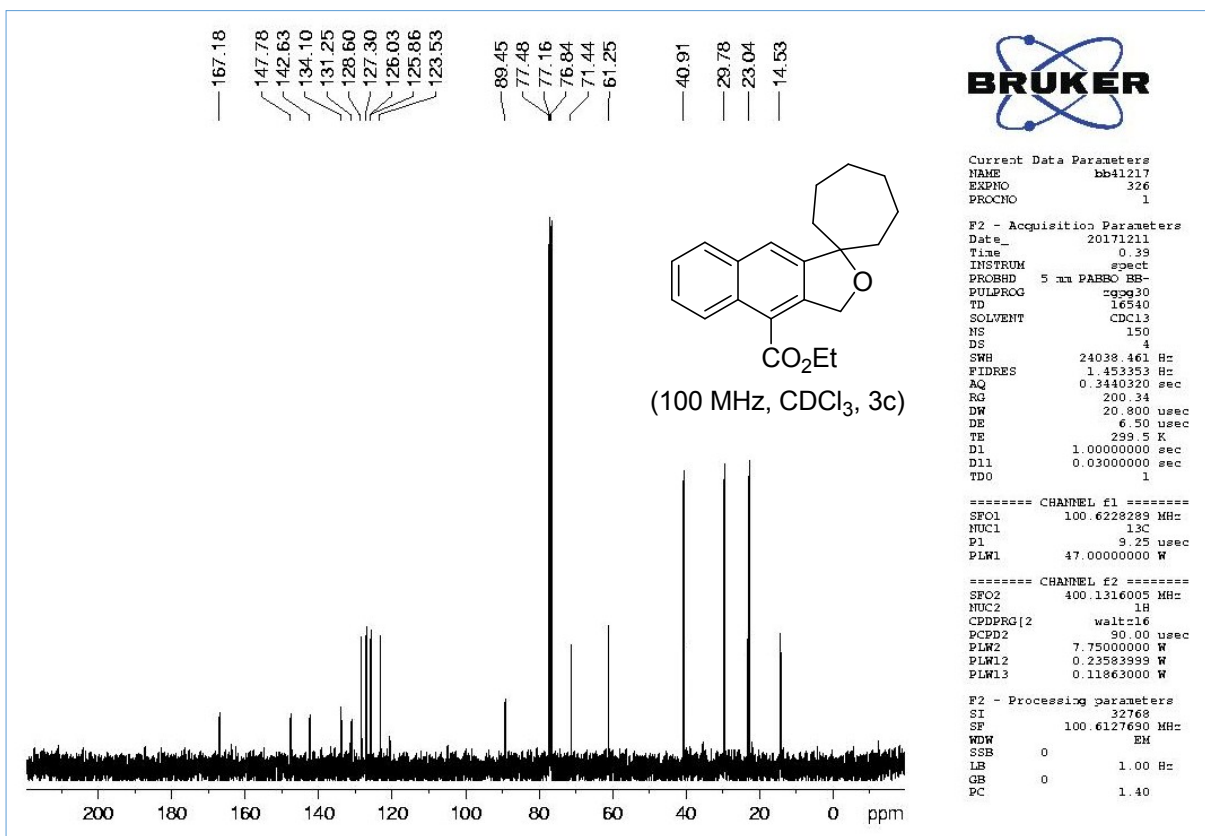
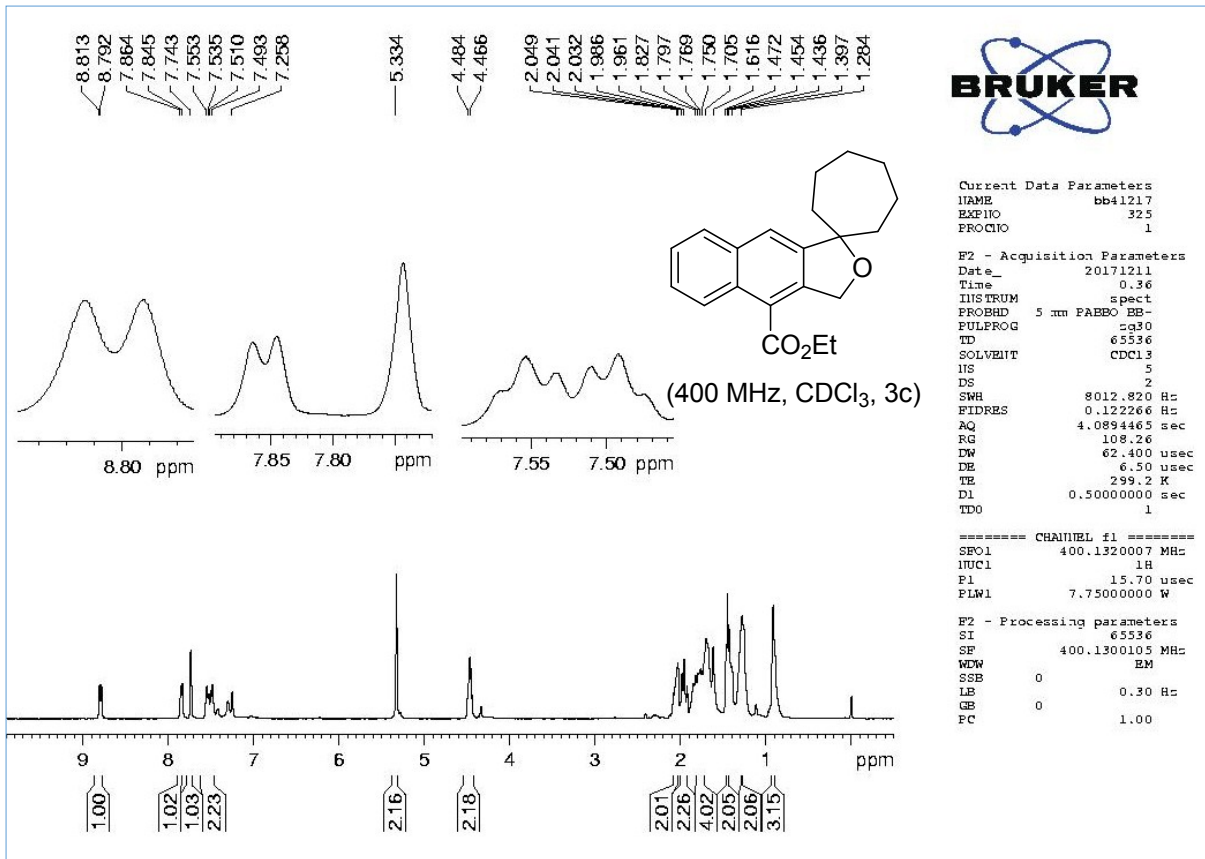


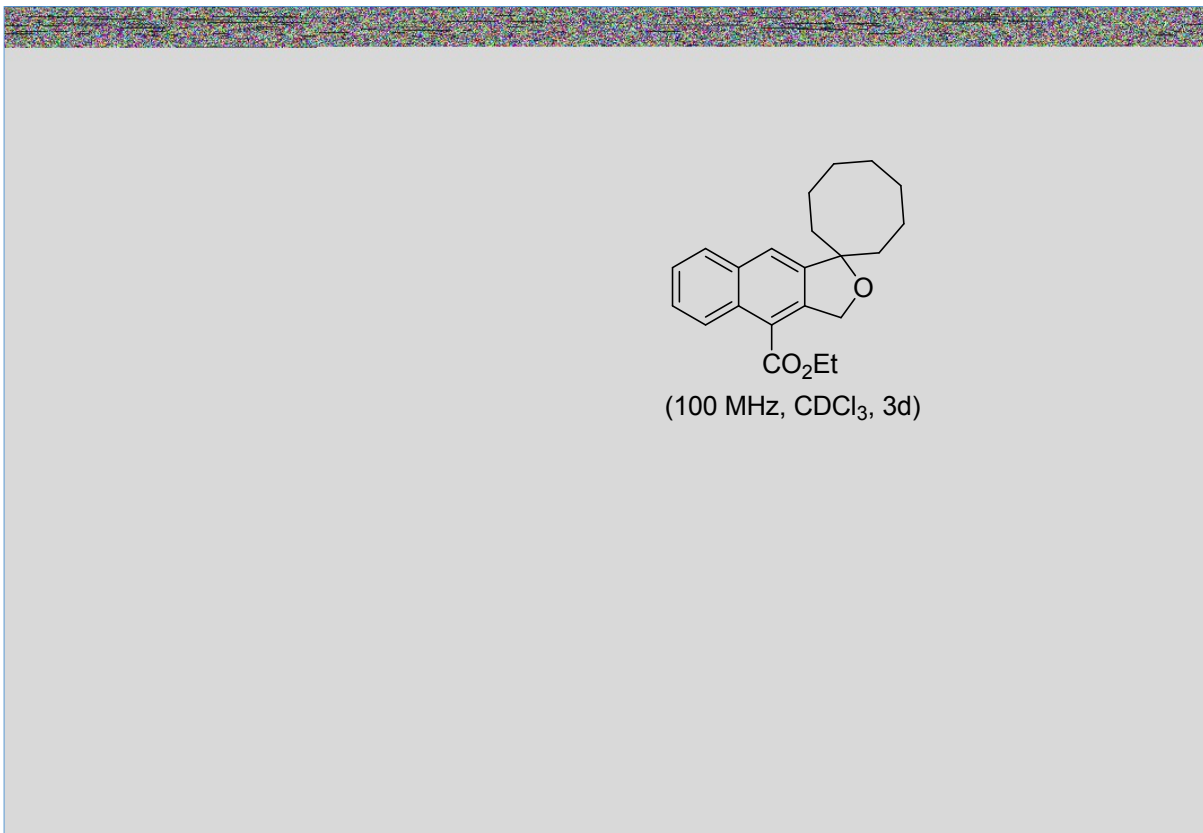
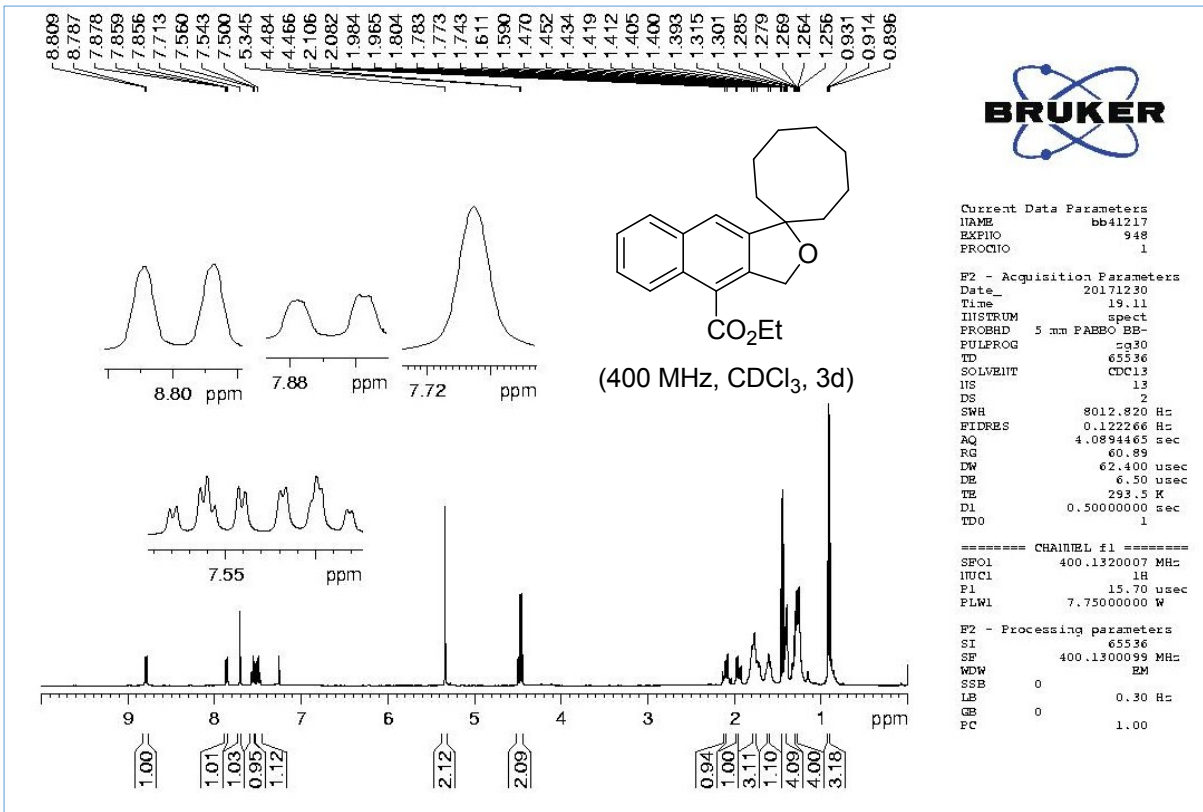


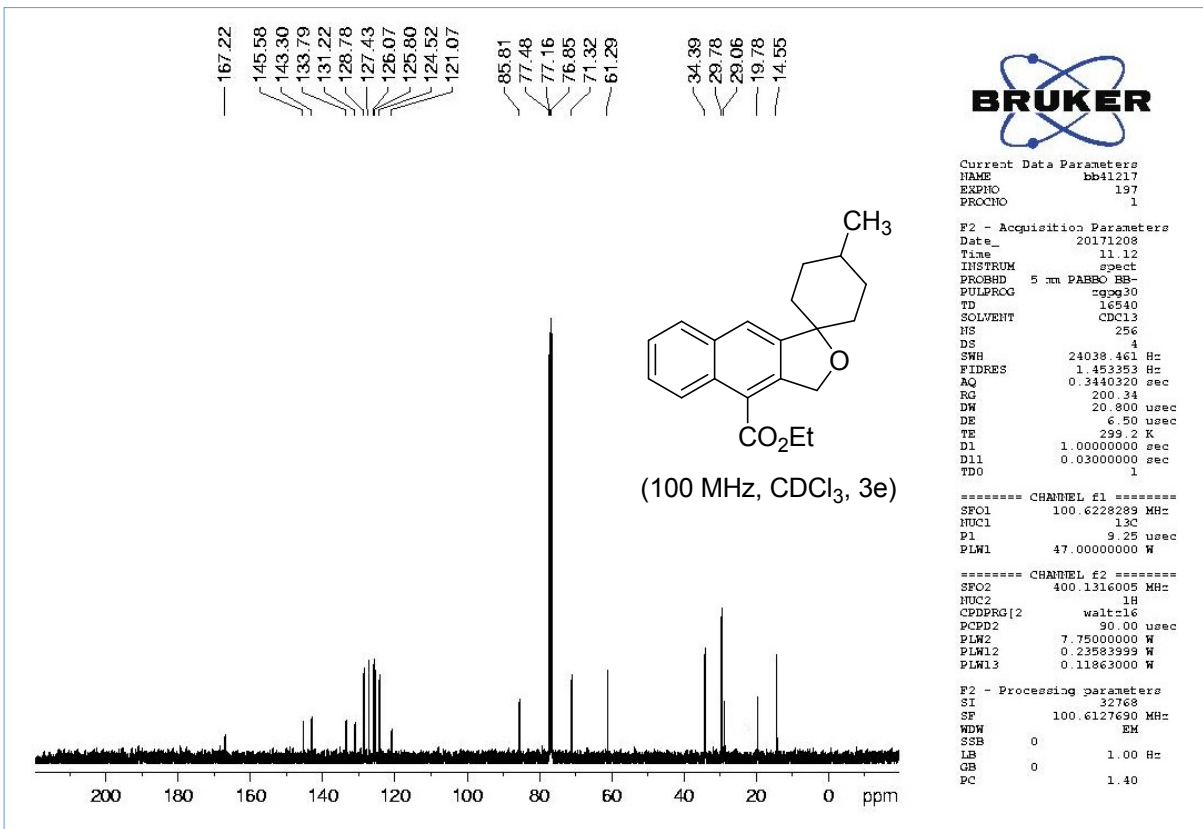
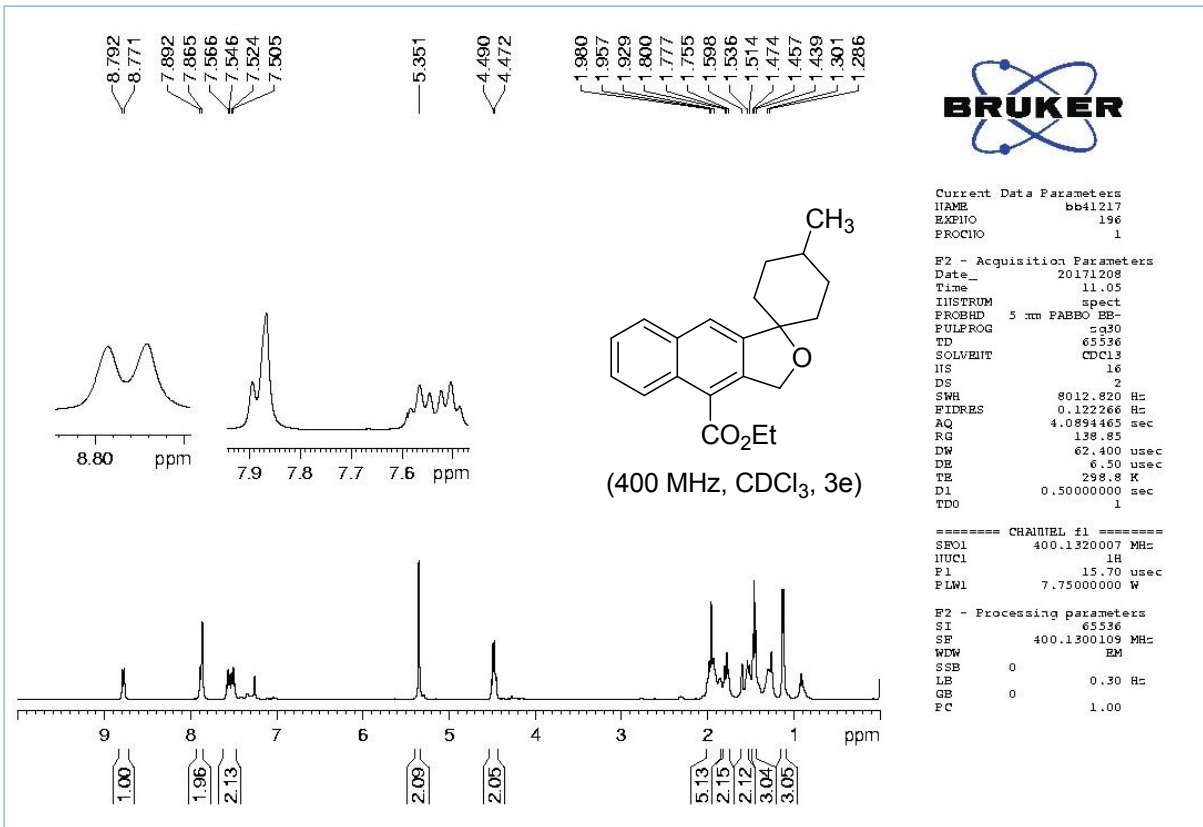


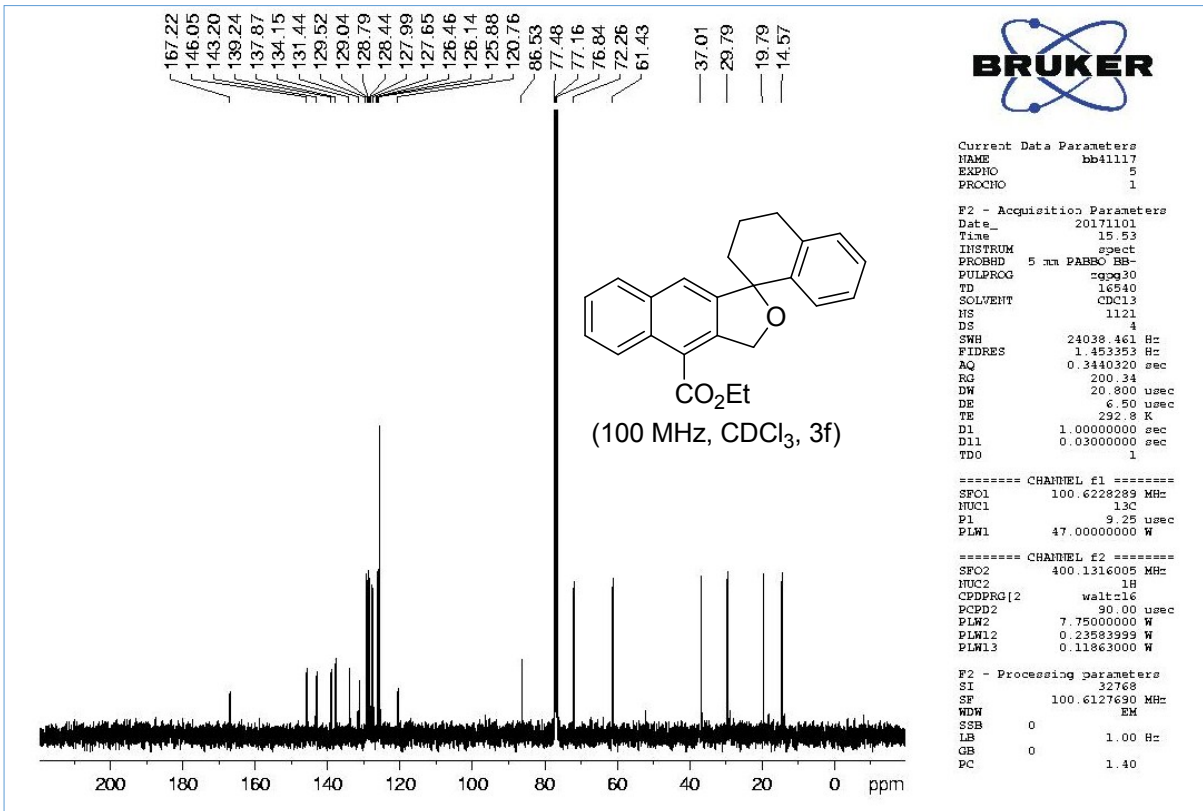
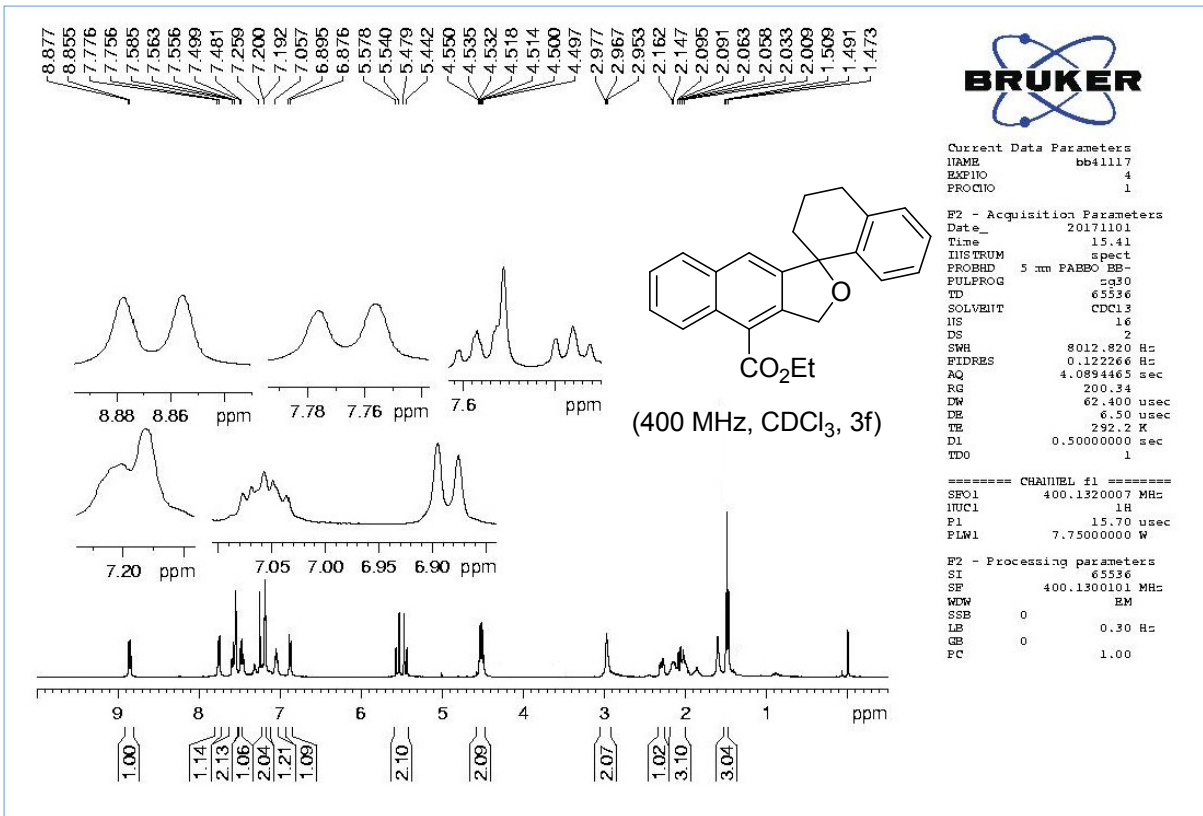


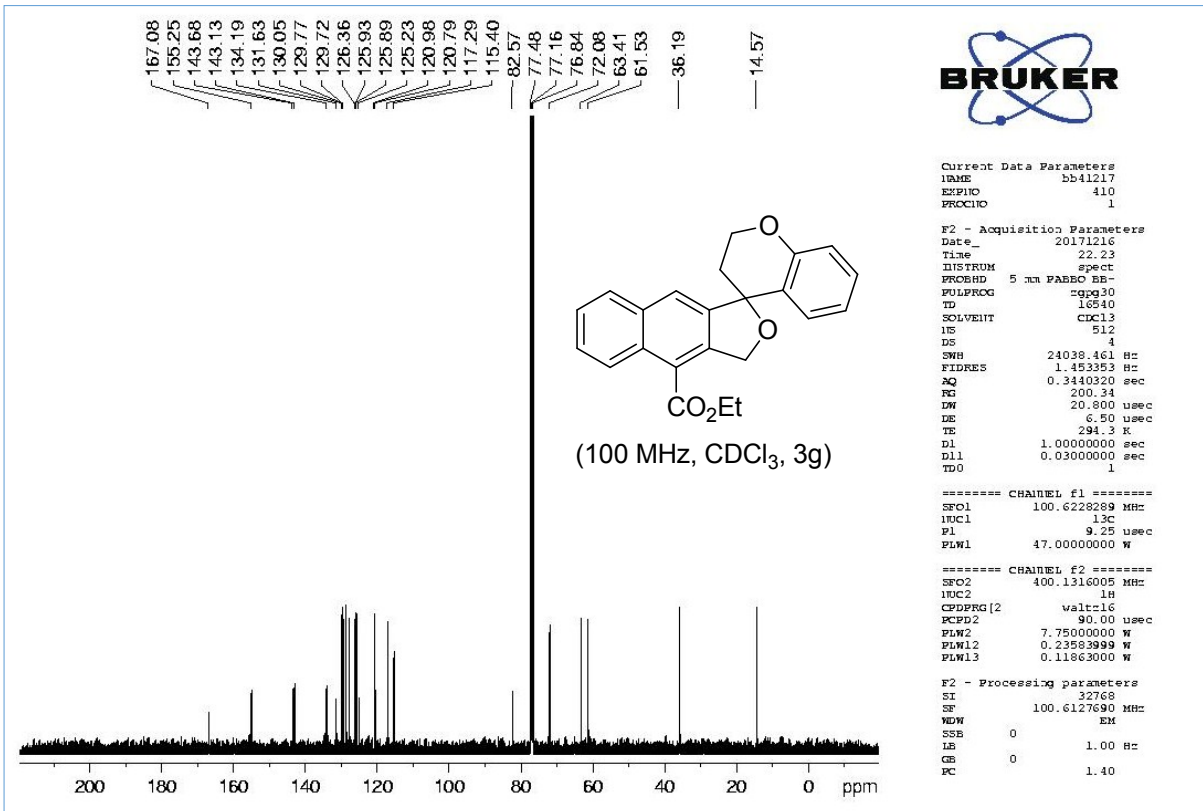
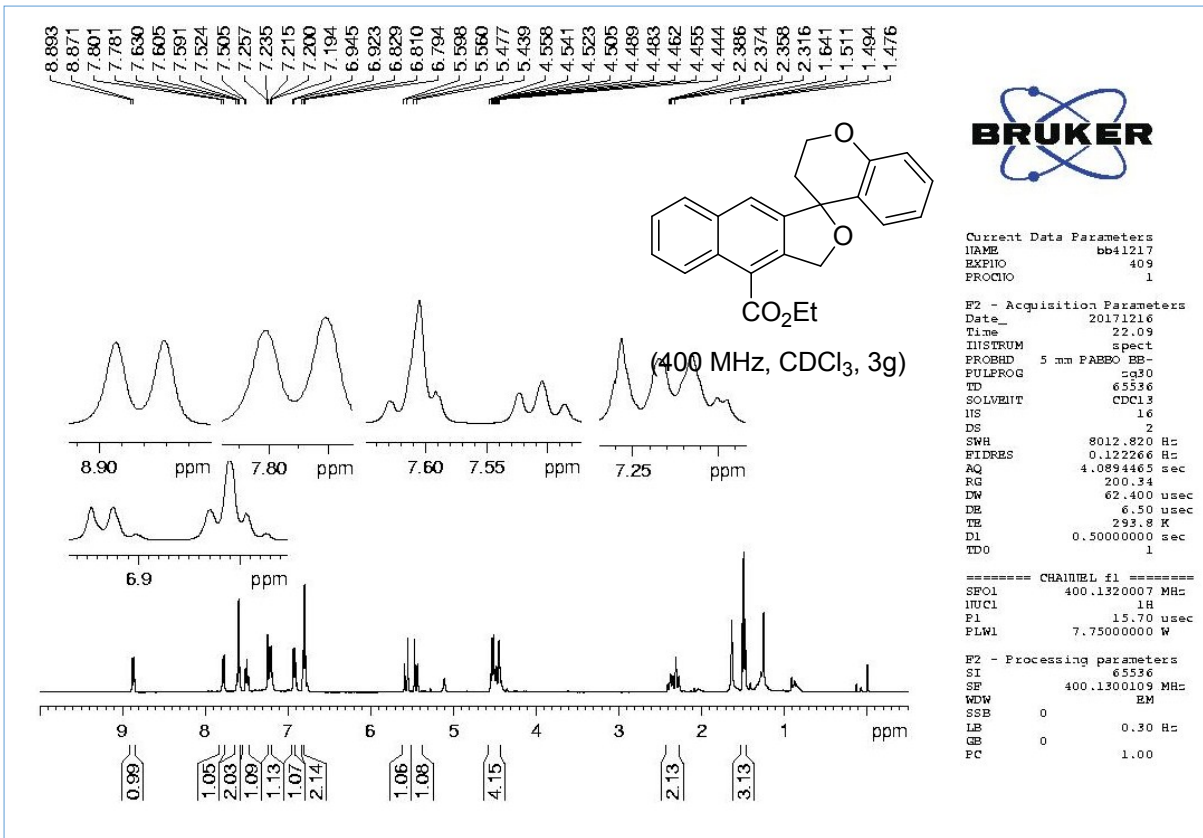


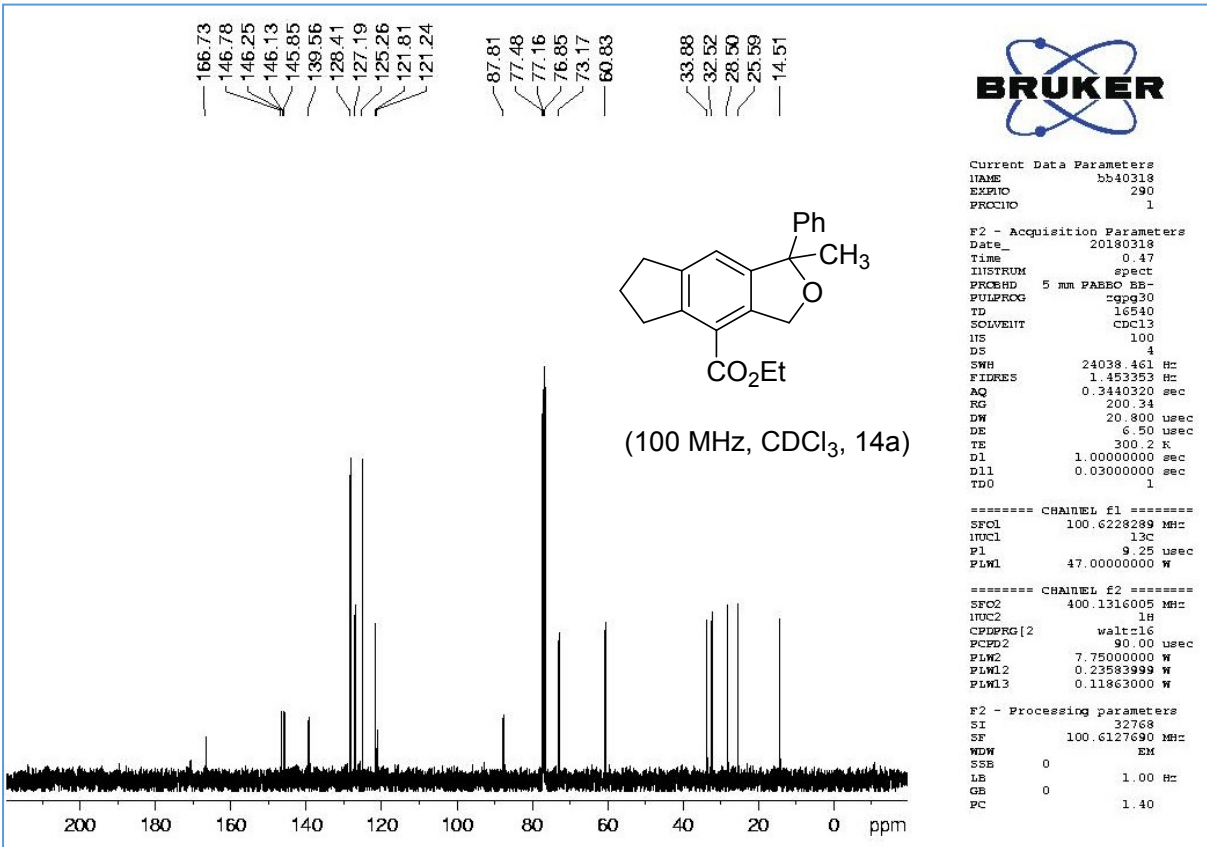
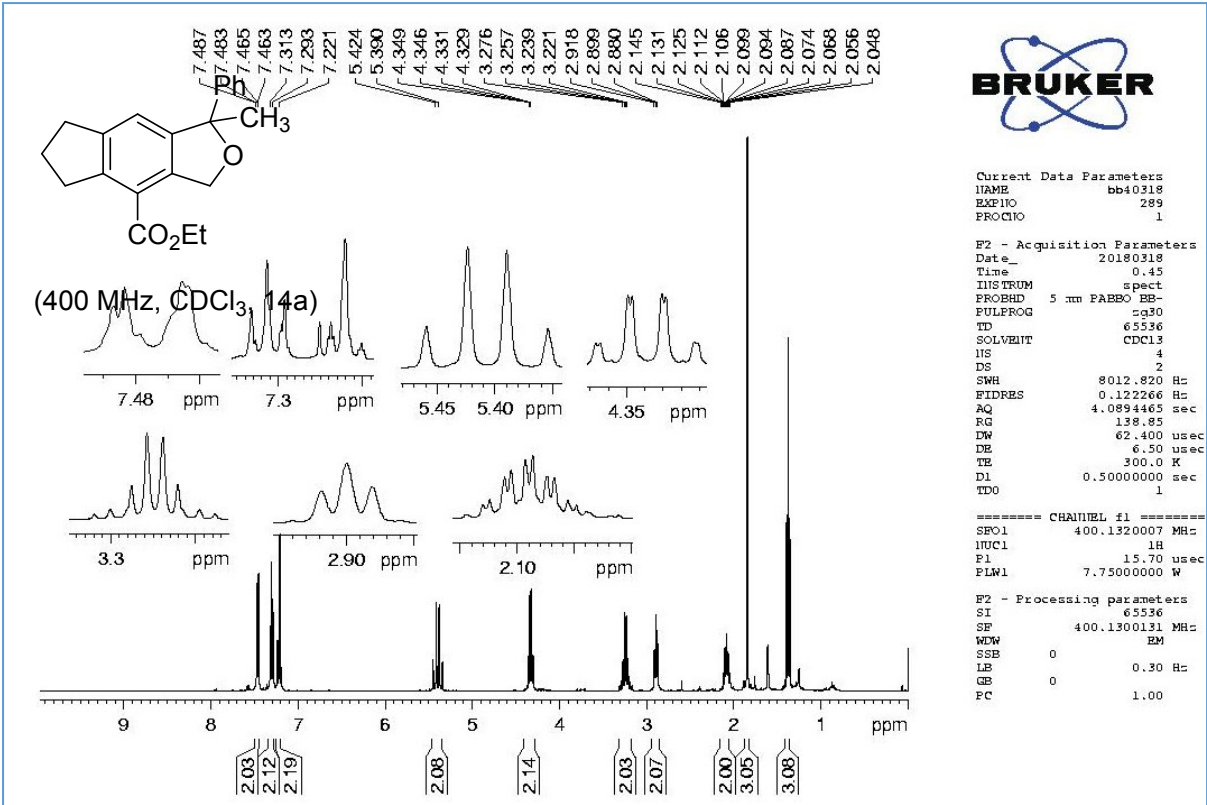


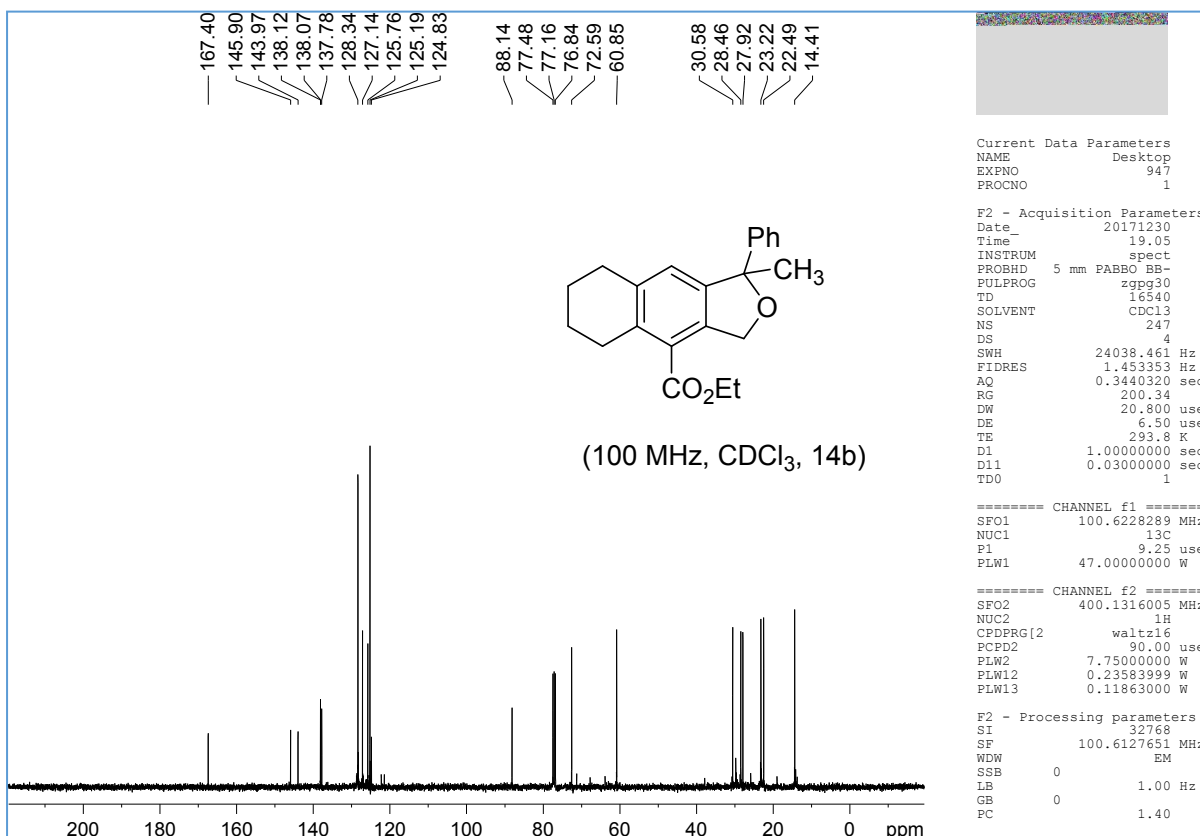
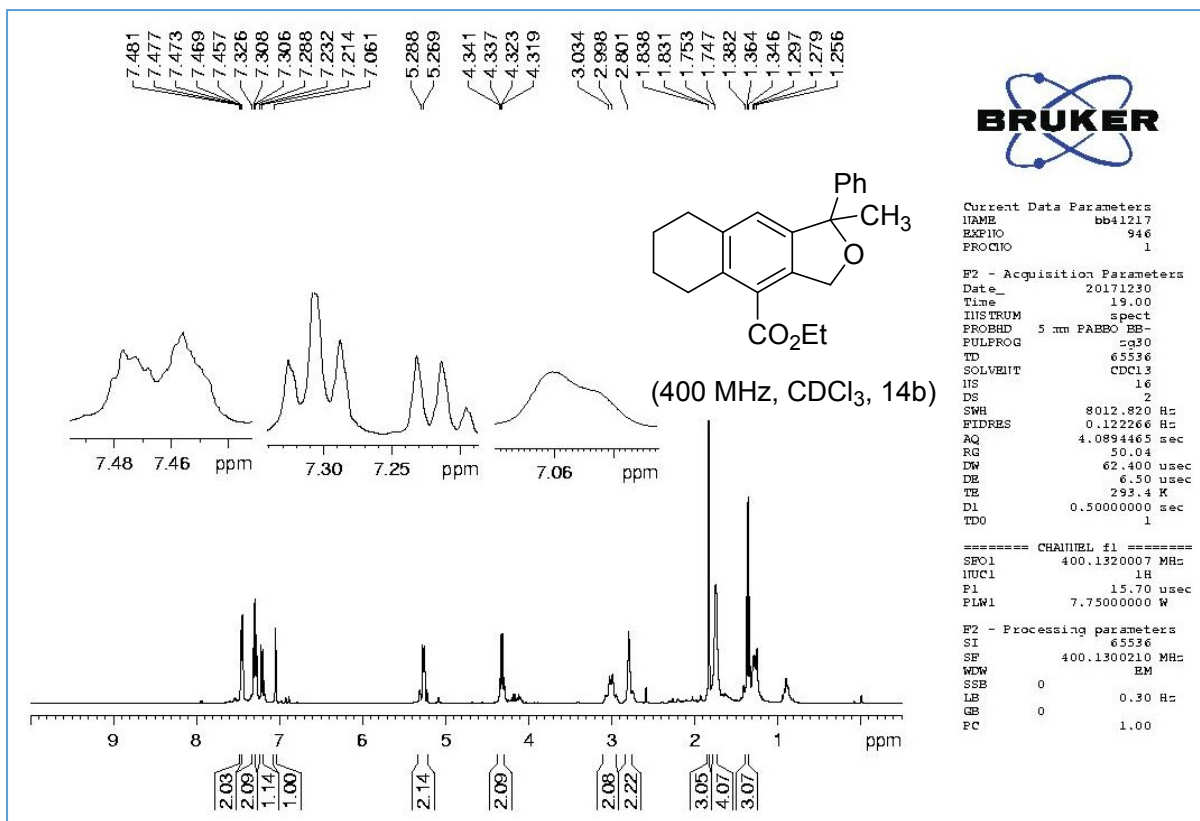


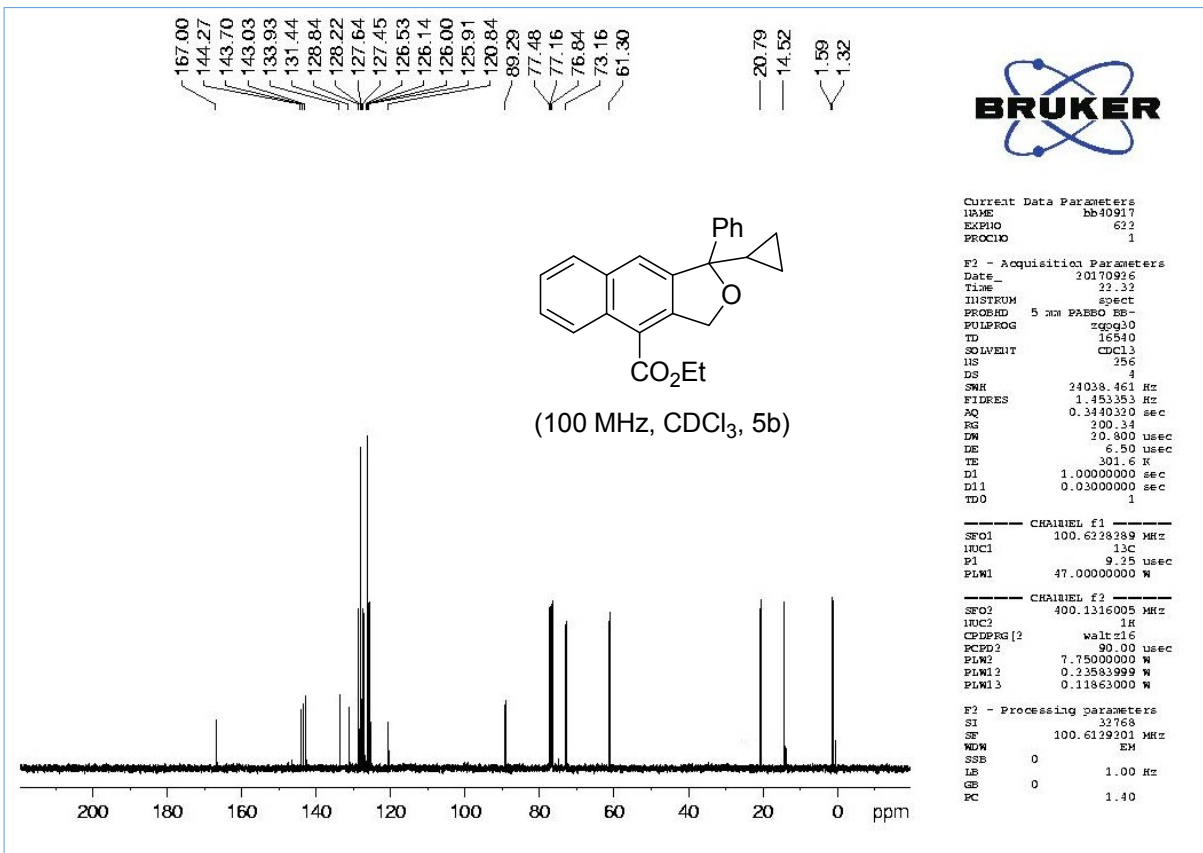
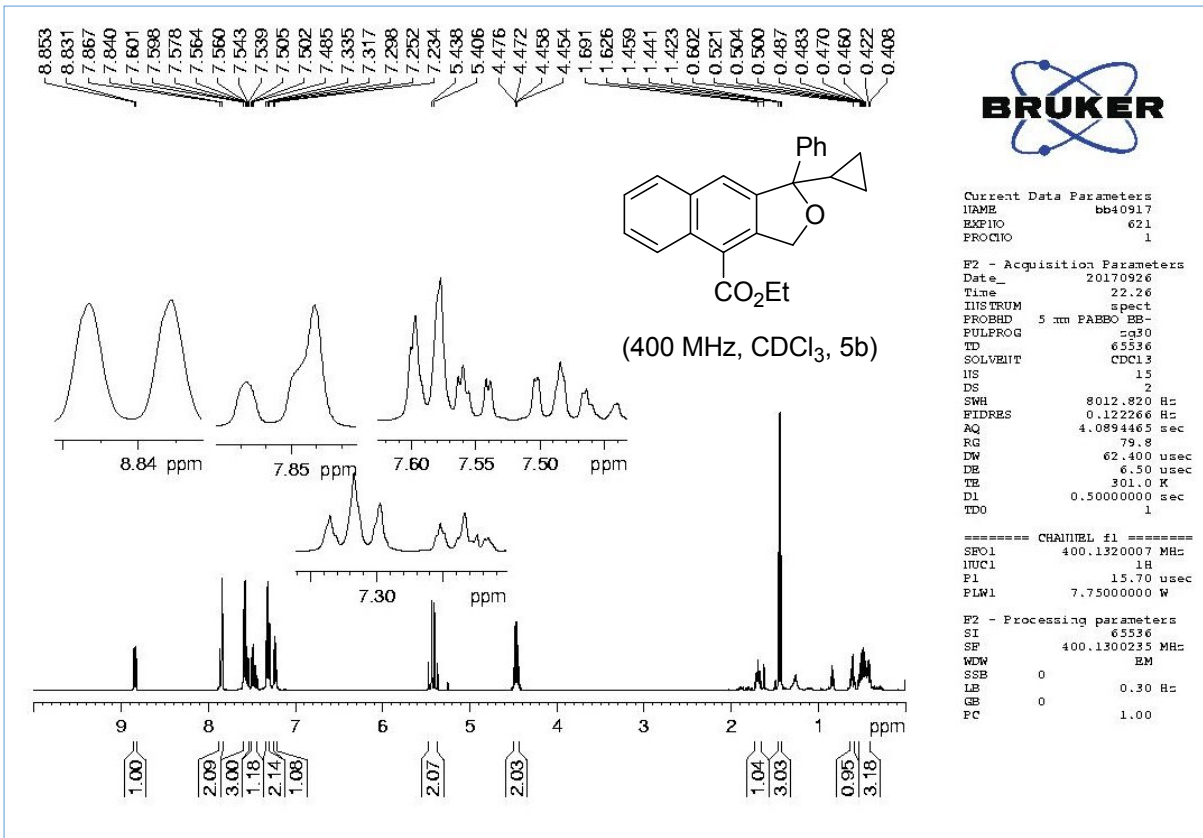


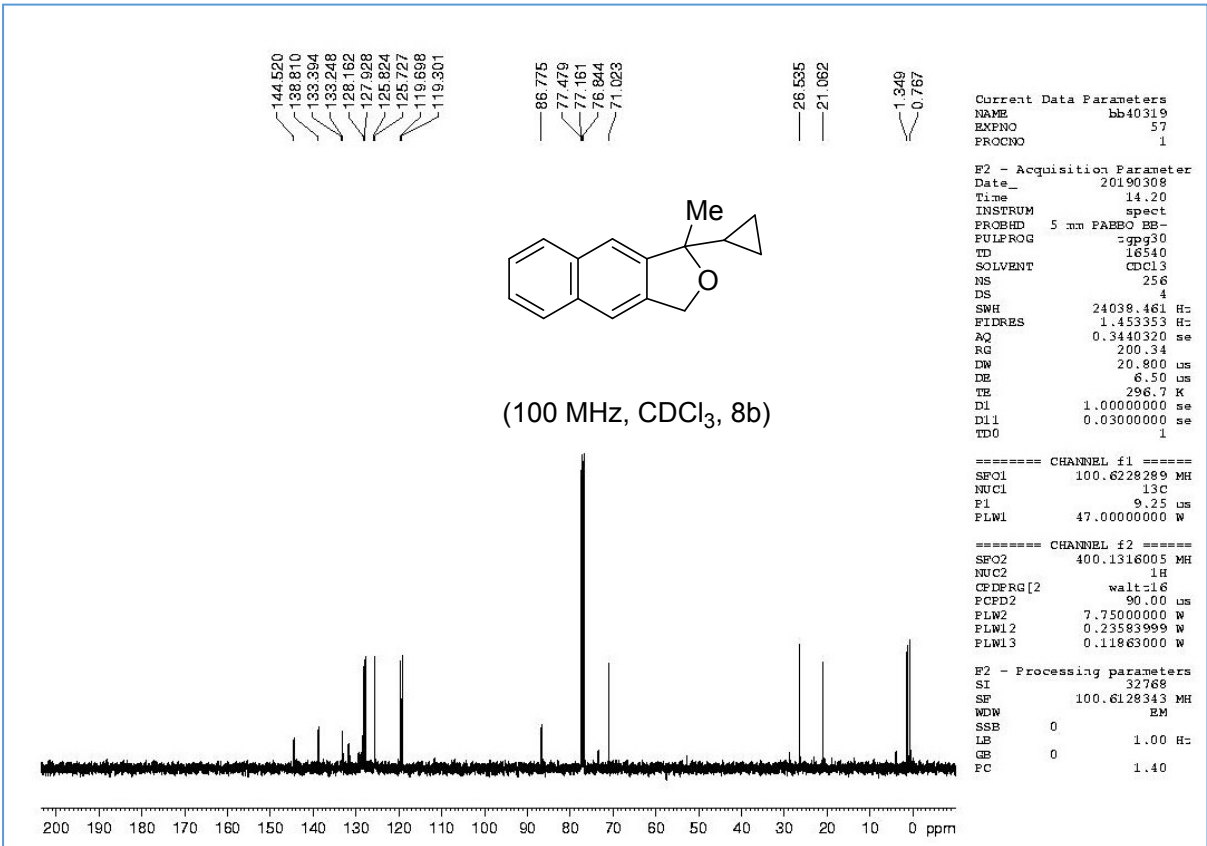
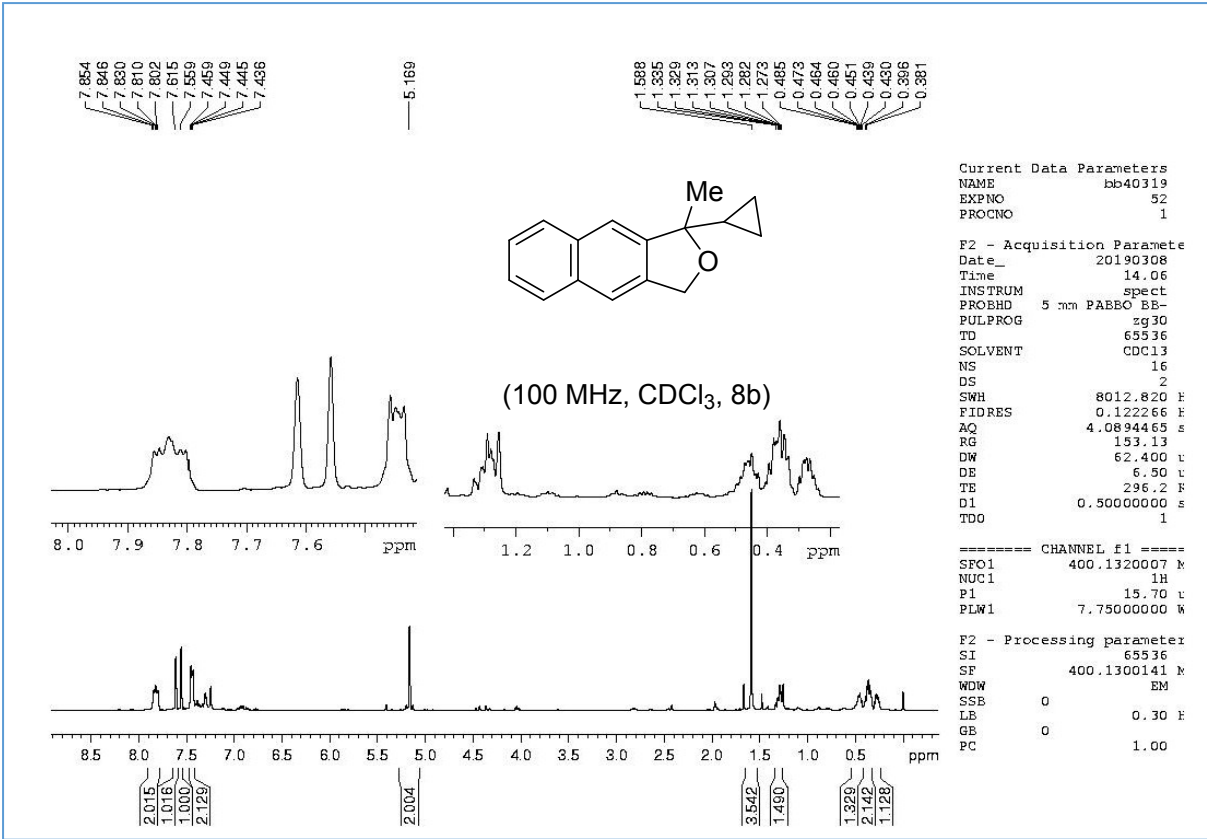


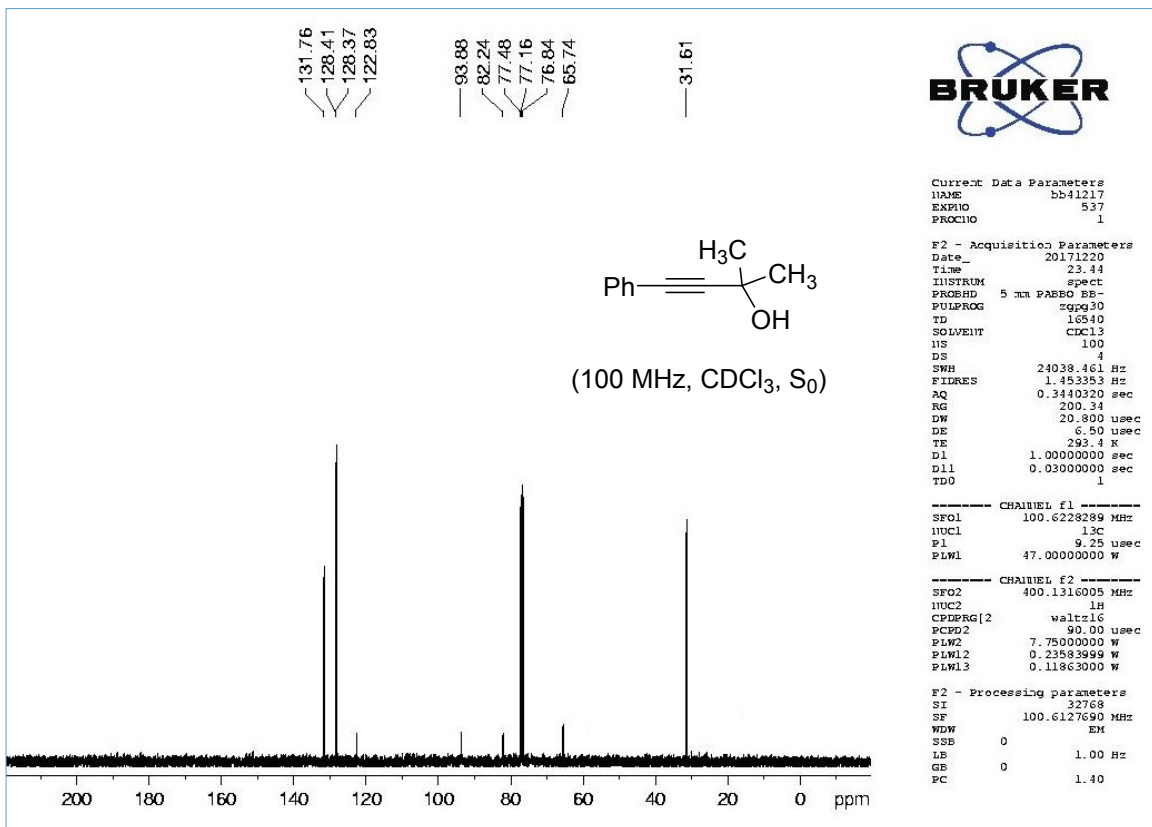
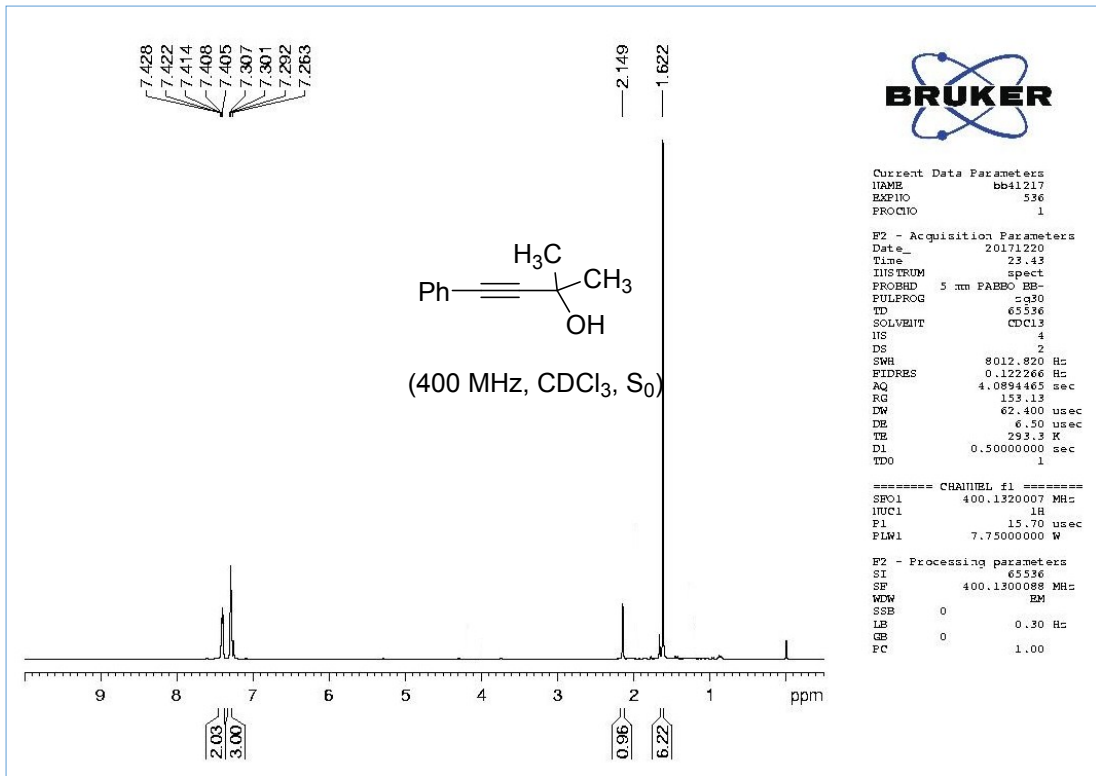


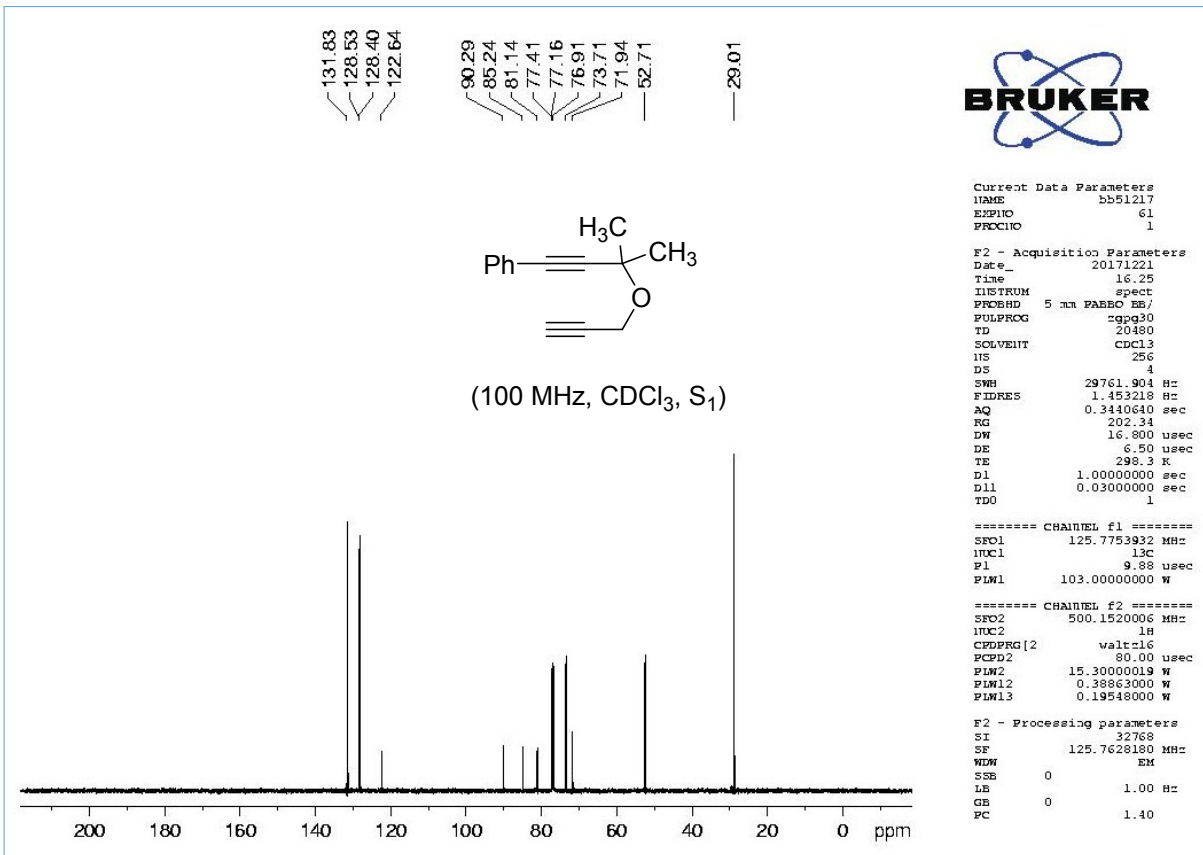
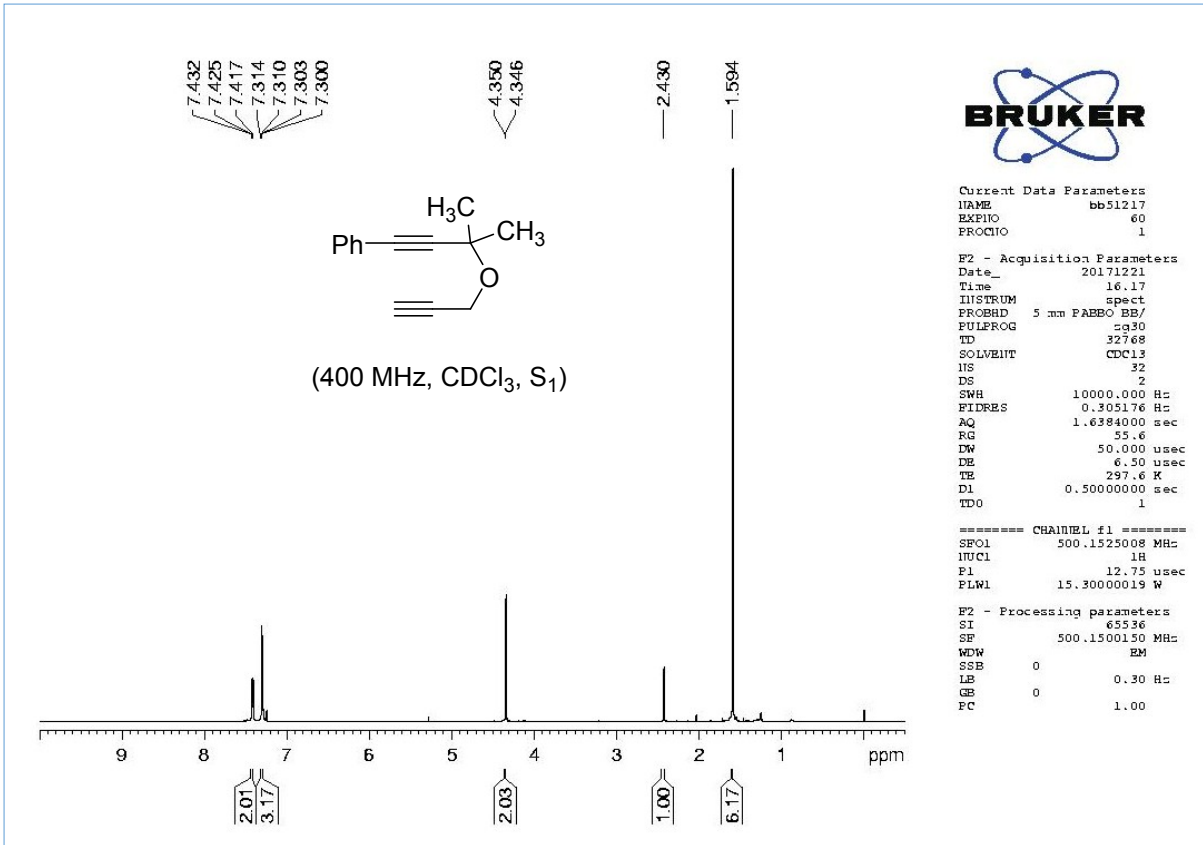


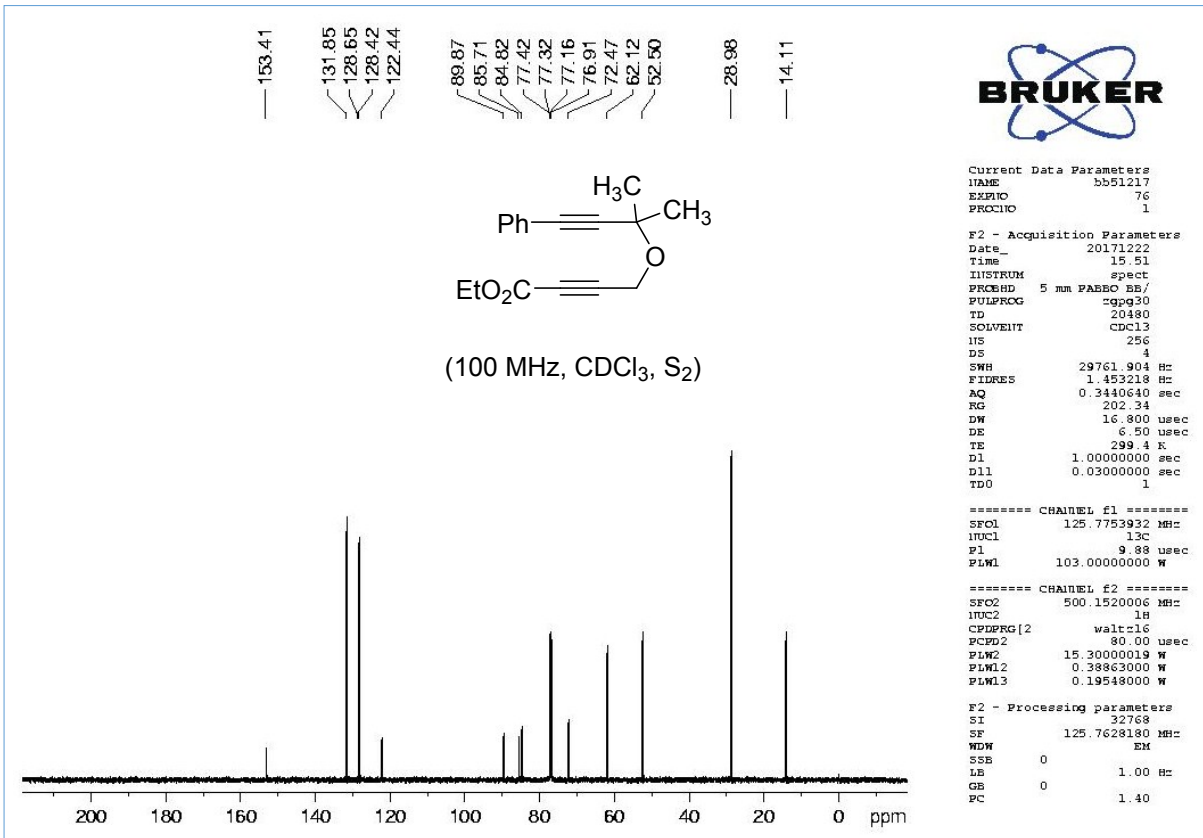
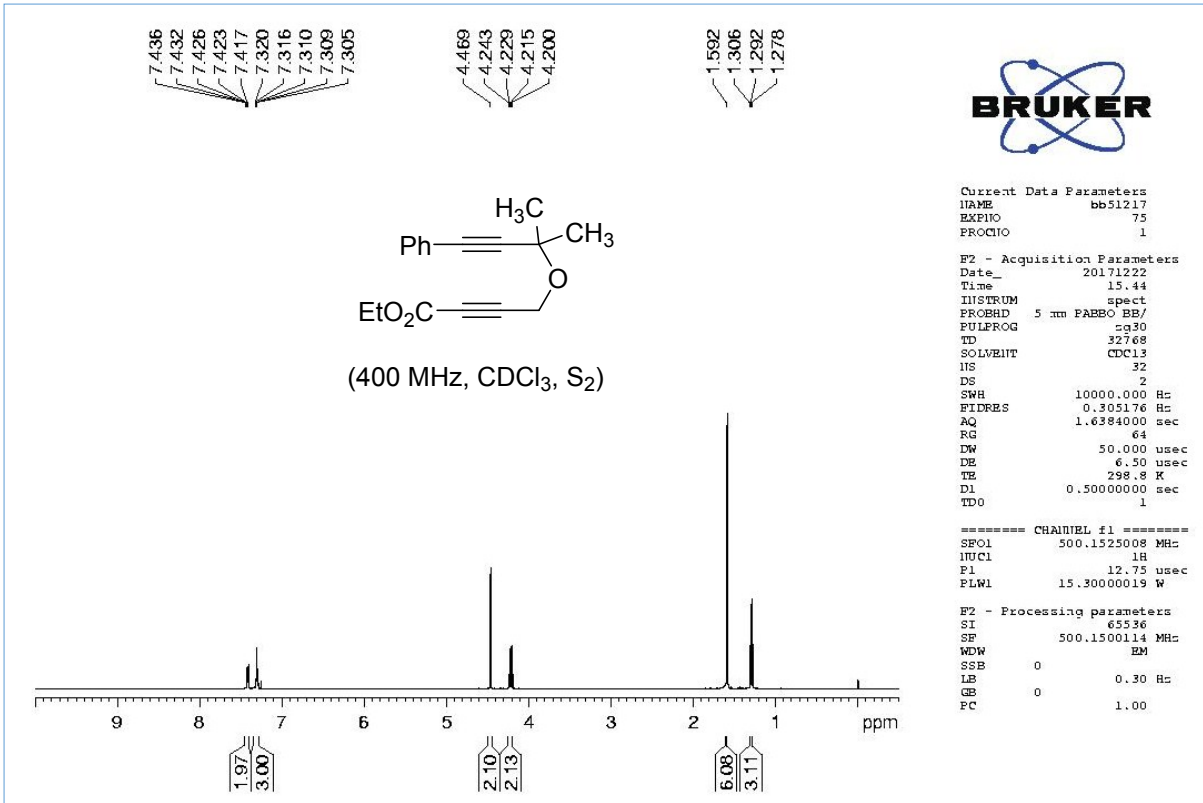


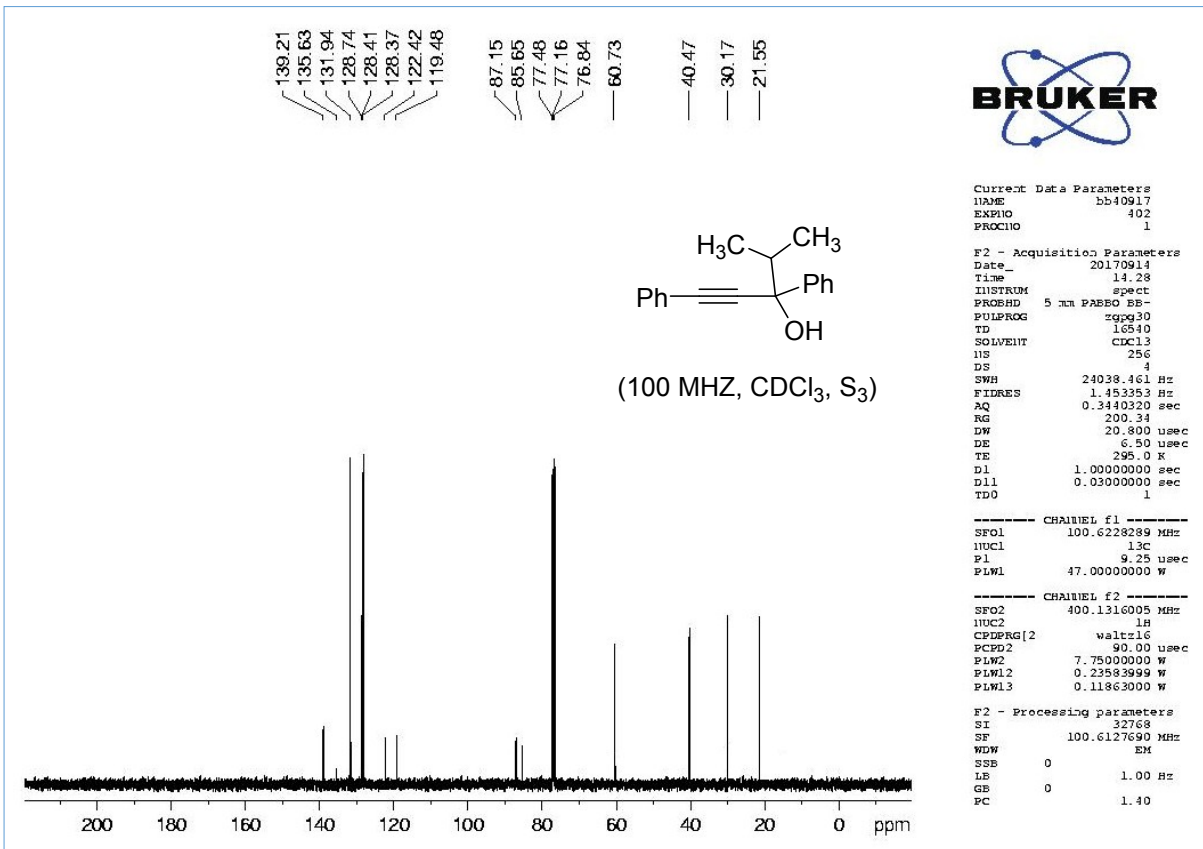
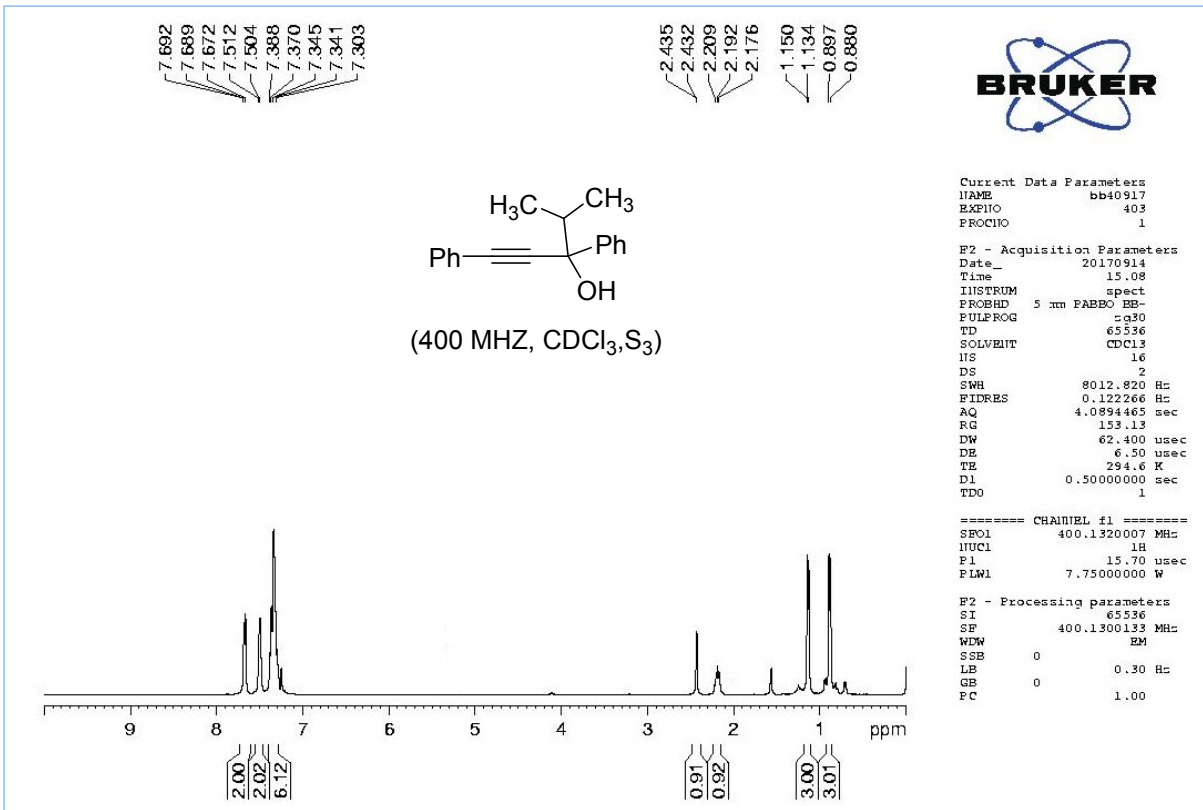


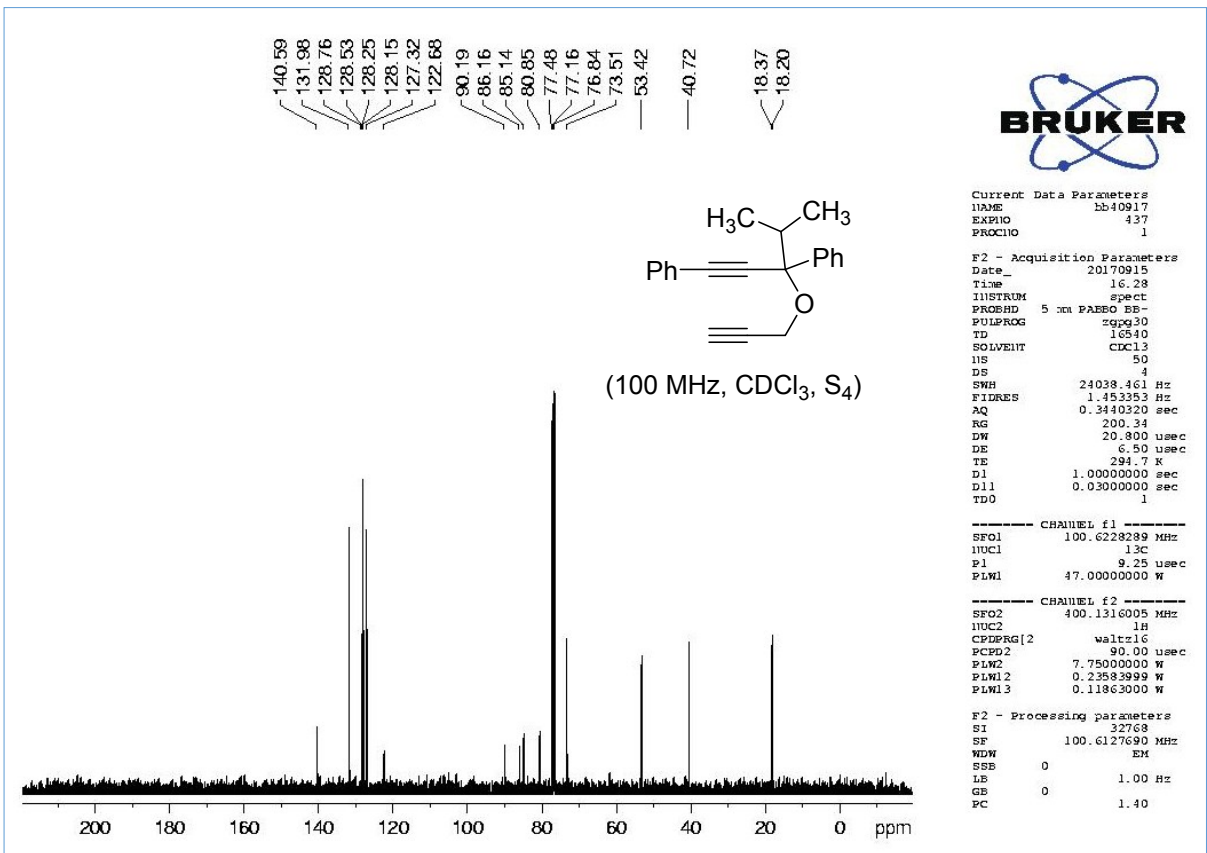
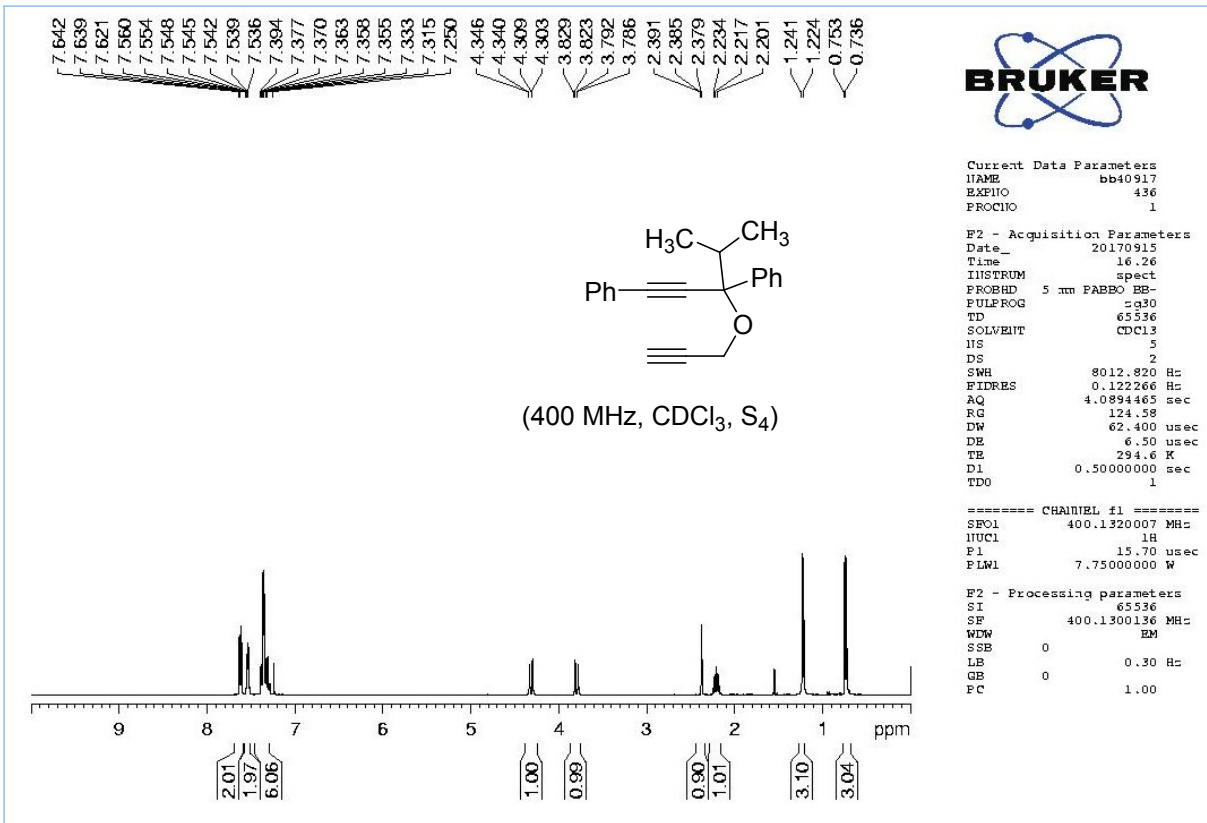


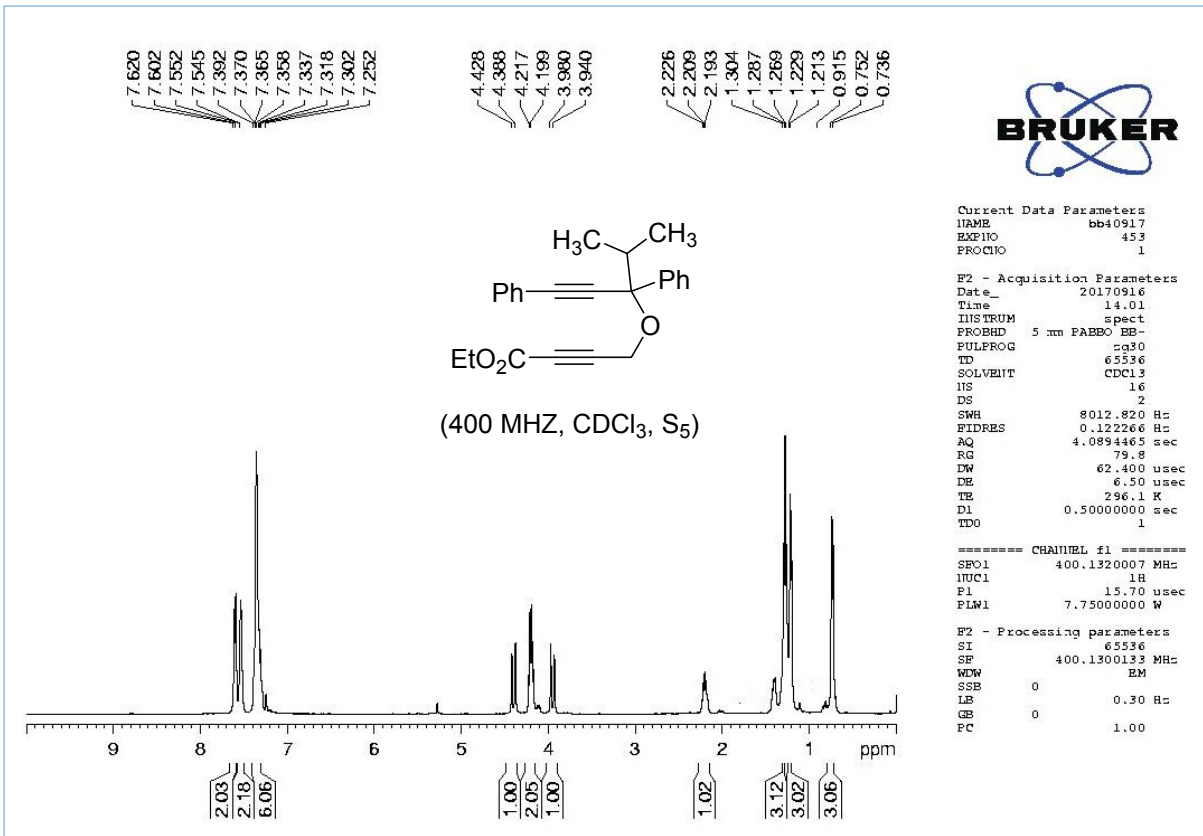










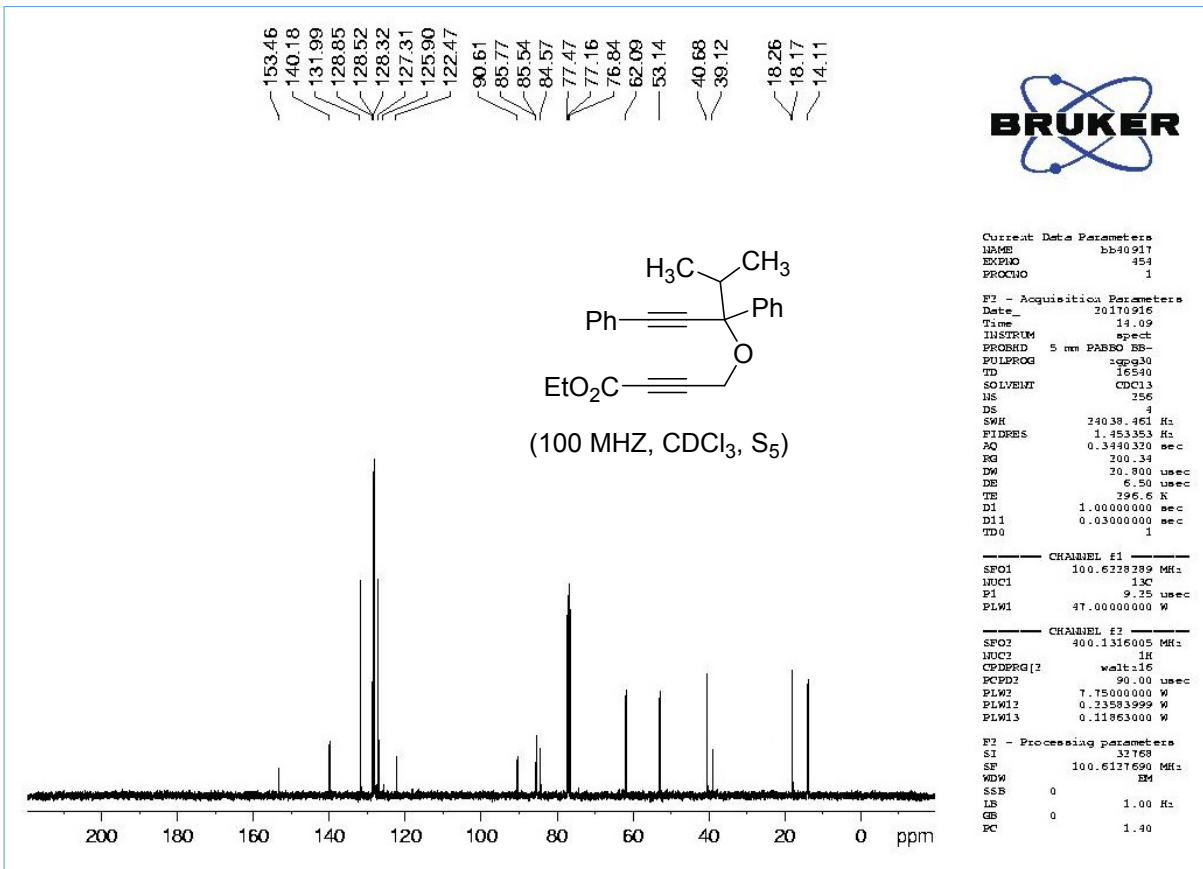


Current Data Parameters
 NAME bb40917
 EXPNO 453
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20170916
 Time 14.01
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 79.8
 DW 62.400 usec
 DE 6.50 usec
 TE 296.1 K
 D1 0.5000000 sec
 TDO 1

==== CHANNEL f1 =====
 SFO1 400.1320007 MHz
 NUCL1 1H
 P1 15.70 usec
 PLW1 7.7500000 W

F2 - Processing parameters
 SI 65536
 SF 400.1300139 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



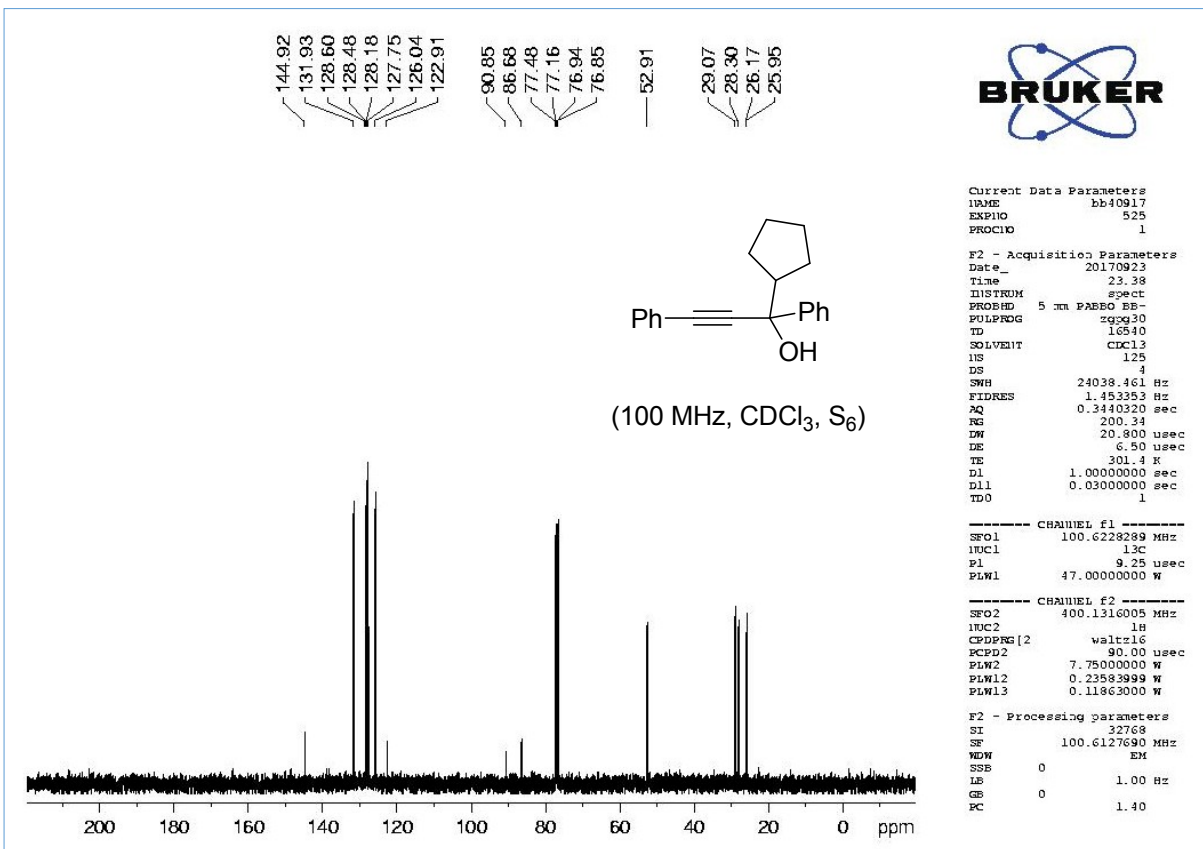
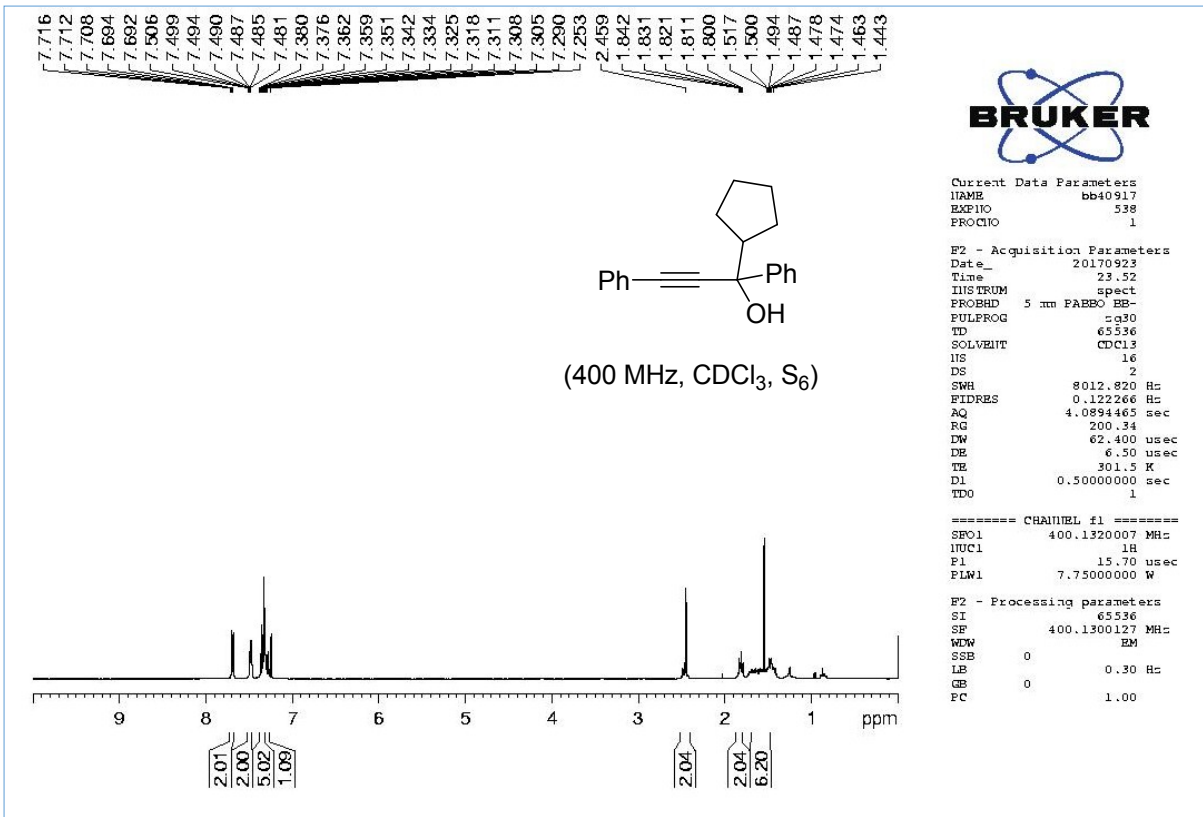
Current Data Parameters
 NAME bb40917
 EXPNO 454
 PROCNO 1

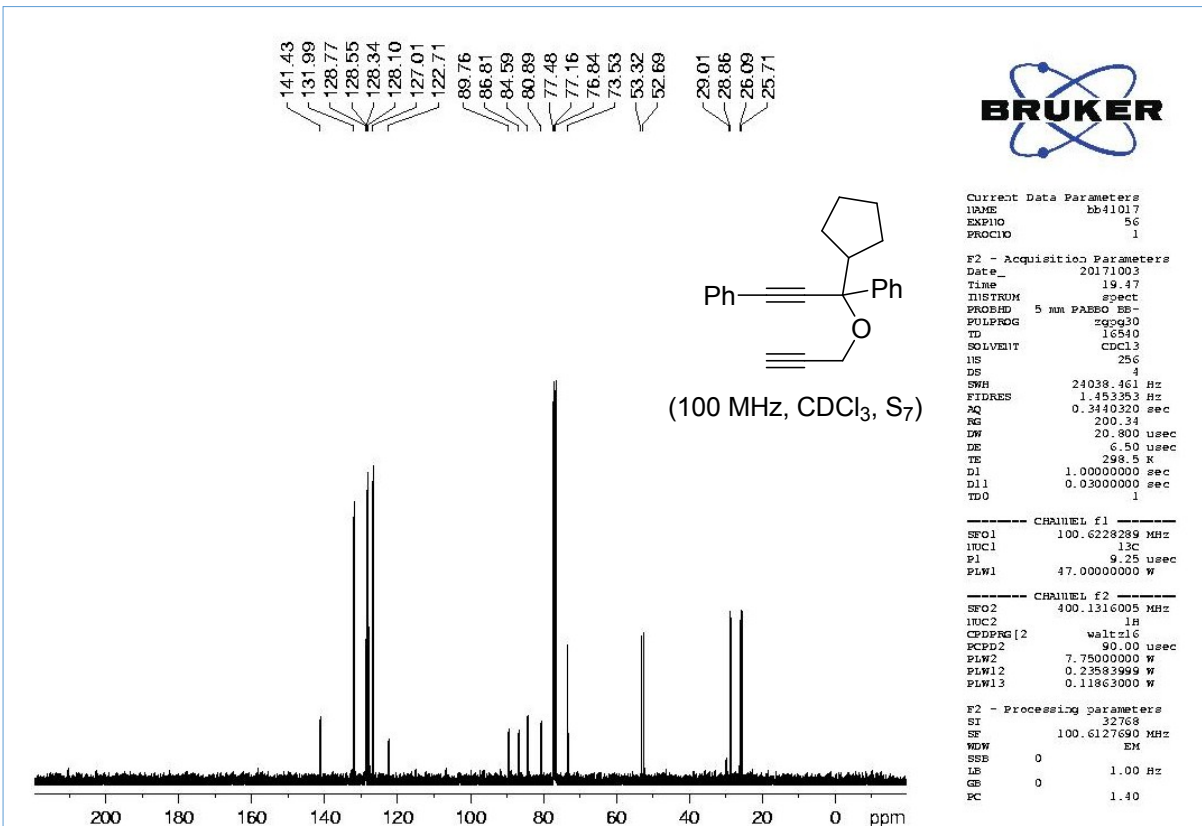
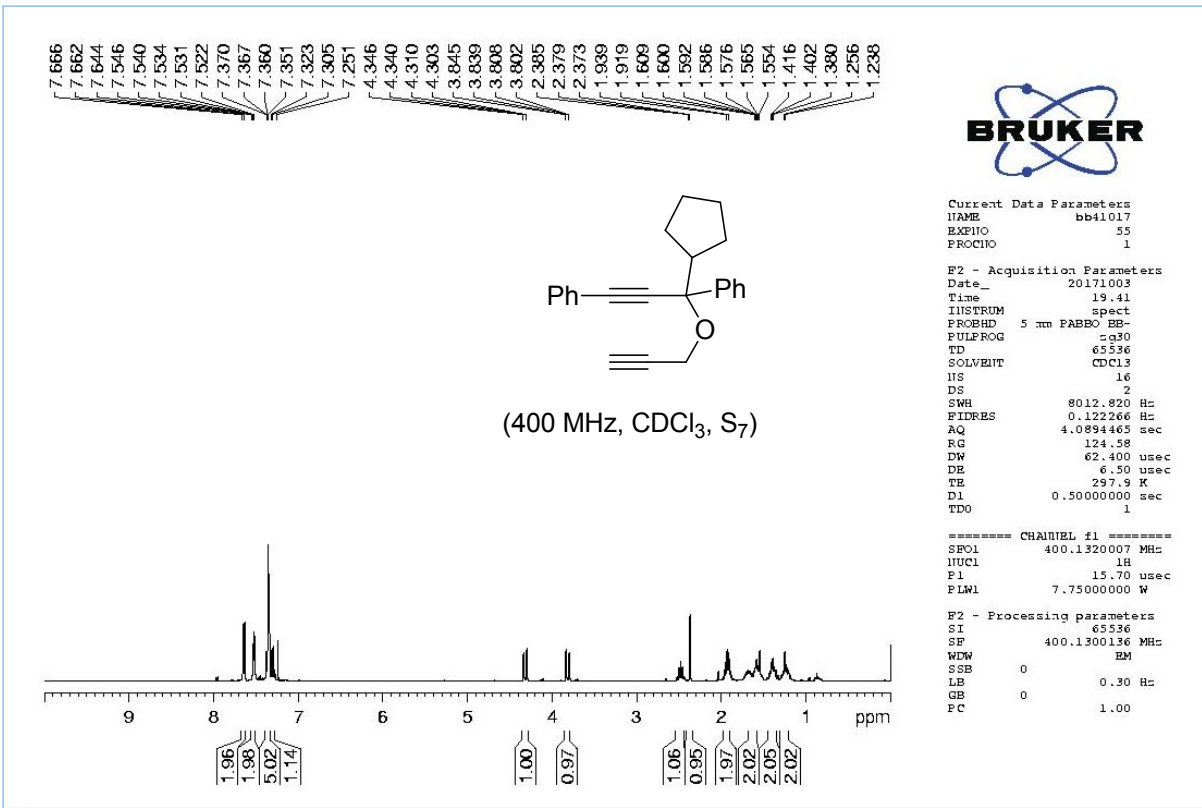
F2 - Acquisition Parameters
 Date_ 20170916
 Time 14.09
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 16540
 SOLVENT CDCl3
 NS 256
 DS 4
 SWH 24039.461 Hz
 FIDRES 1.453353 Hz
 AQ 0.3440320 sec
 RG 200.34
 DW 70.800 usec
 DE 6.50 usec
 TE 296.6 K
 D1 1.0000000 sec
 D11 0.0300000 sec
 TDO 1

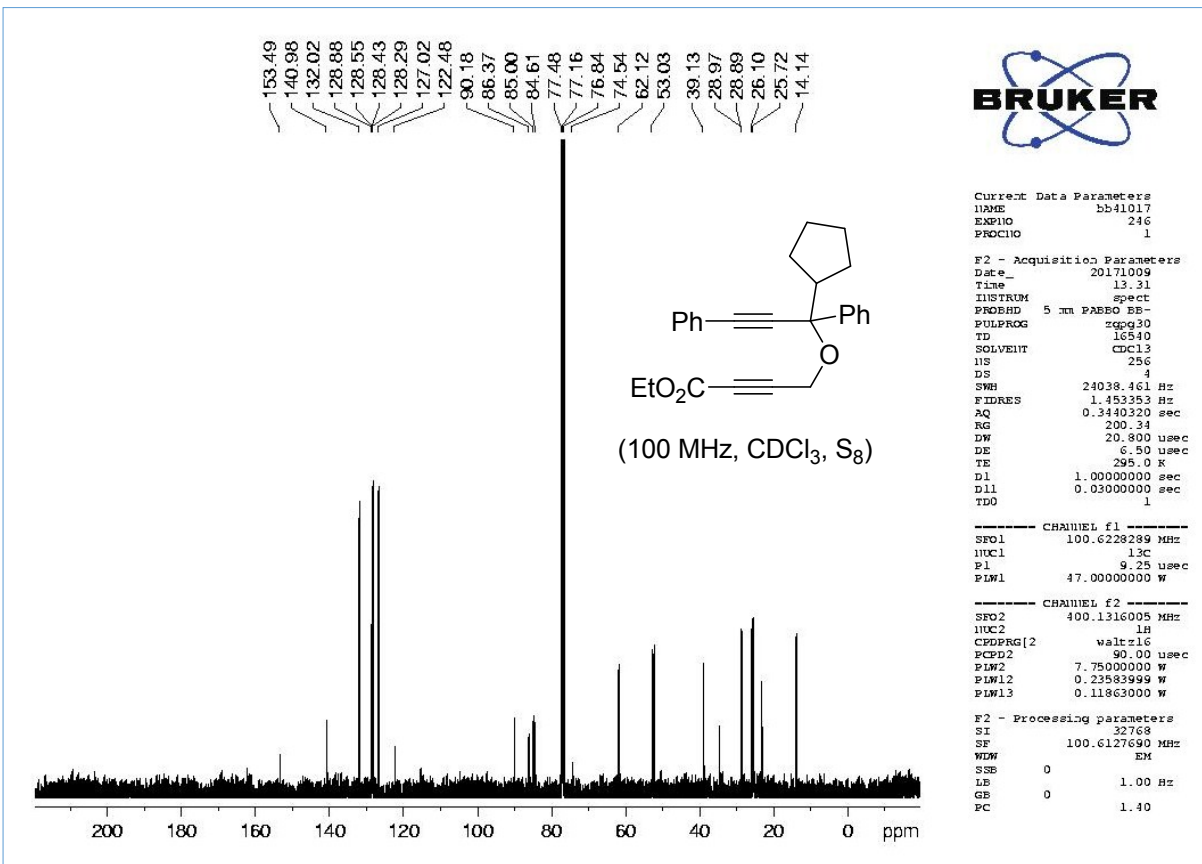
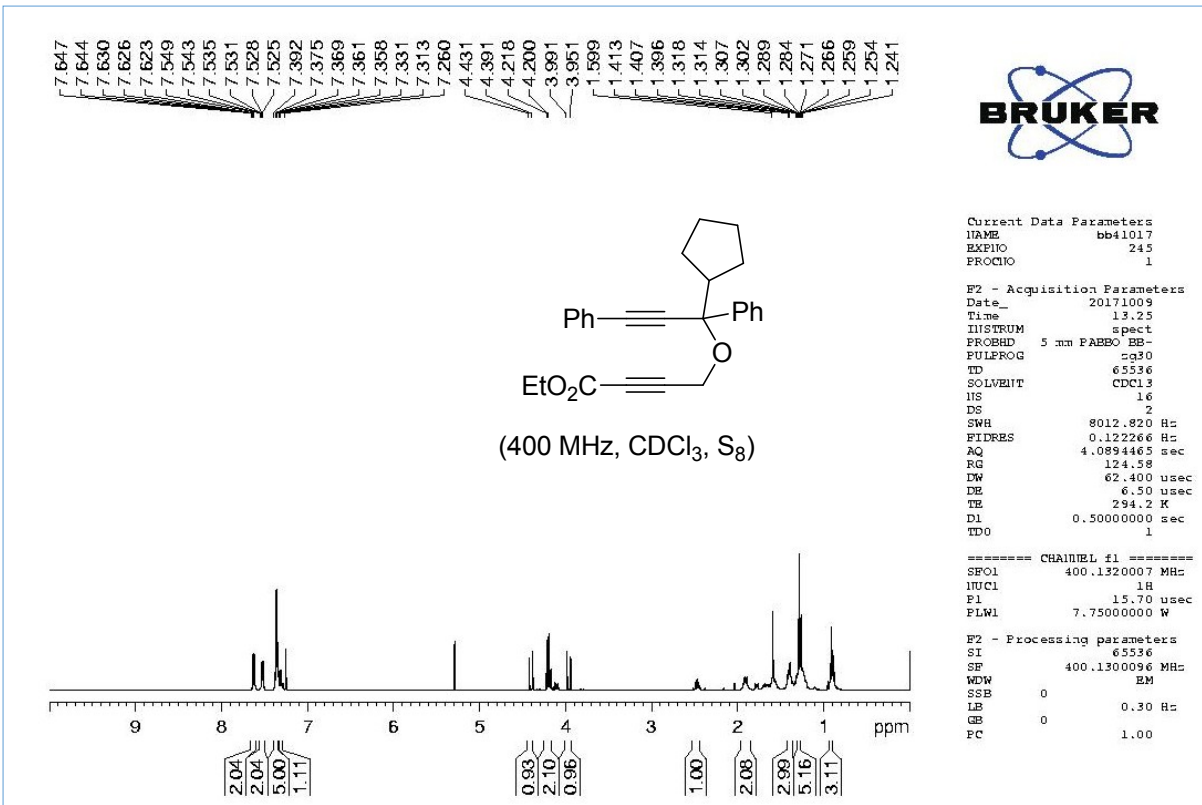
==== CHANNEL f1 =====
 SFO1 100.6238289 MHz
 NUCL1 13C
 P1 9.25 usec
 PLW1 47.0000000 W

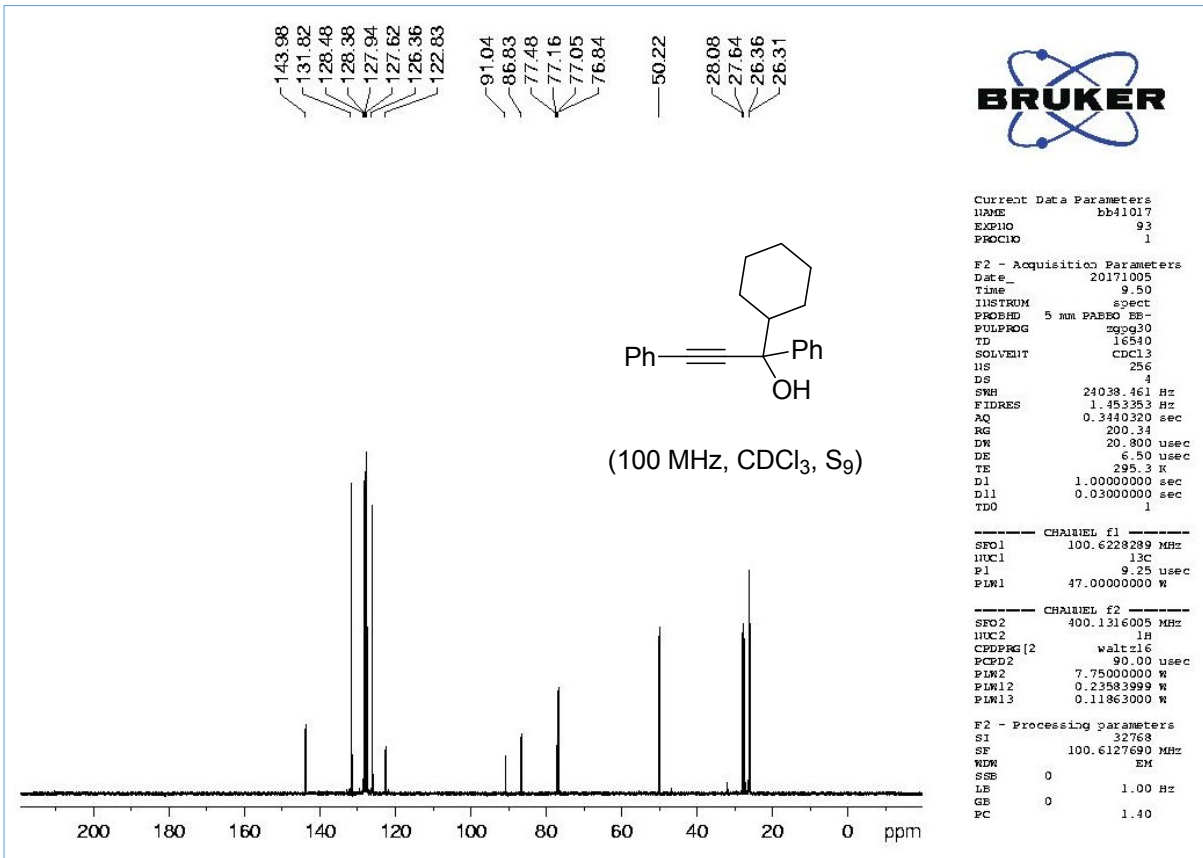
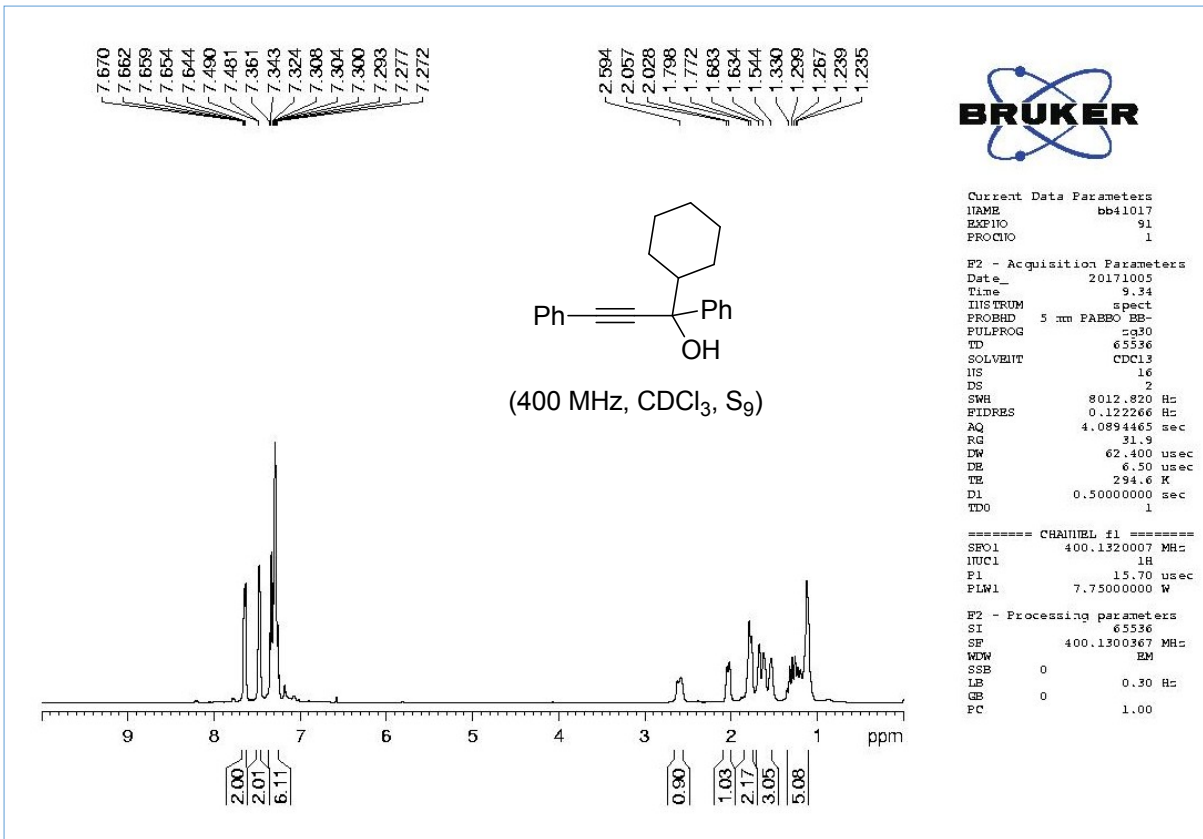
==== CHANNEL f2 =====
 SFO2 400.1316005 MHz
 NUCL2 1H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 7.7500000 W
 PLW12 0.23583999 W
 PLW13 0.11863000 W

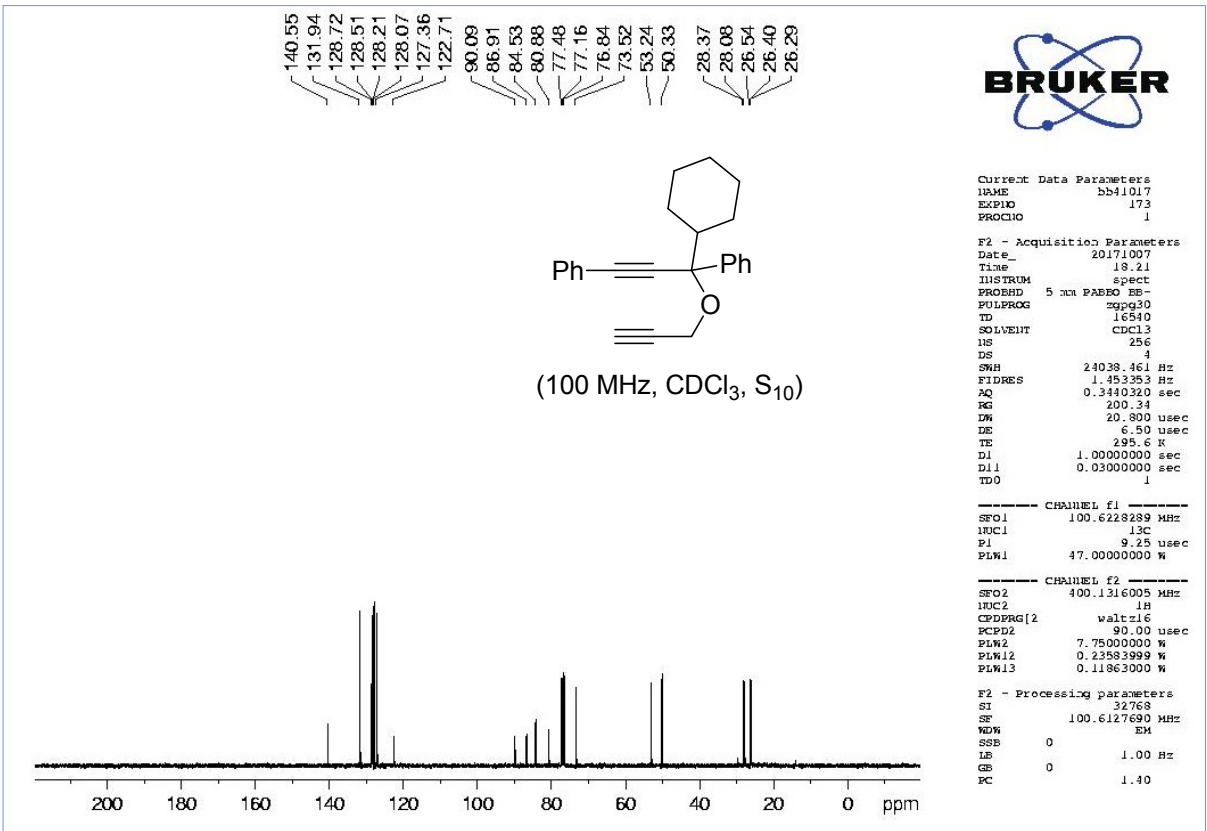
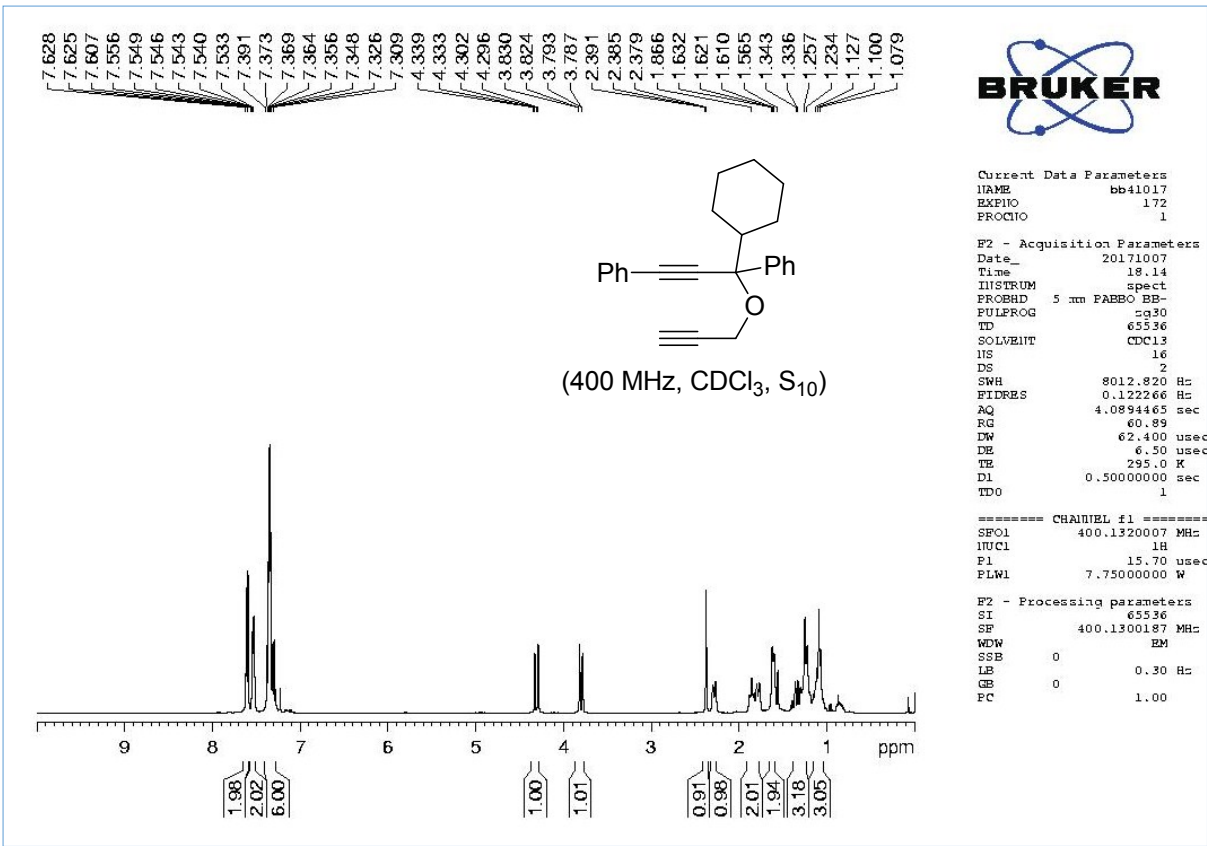
F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

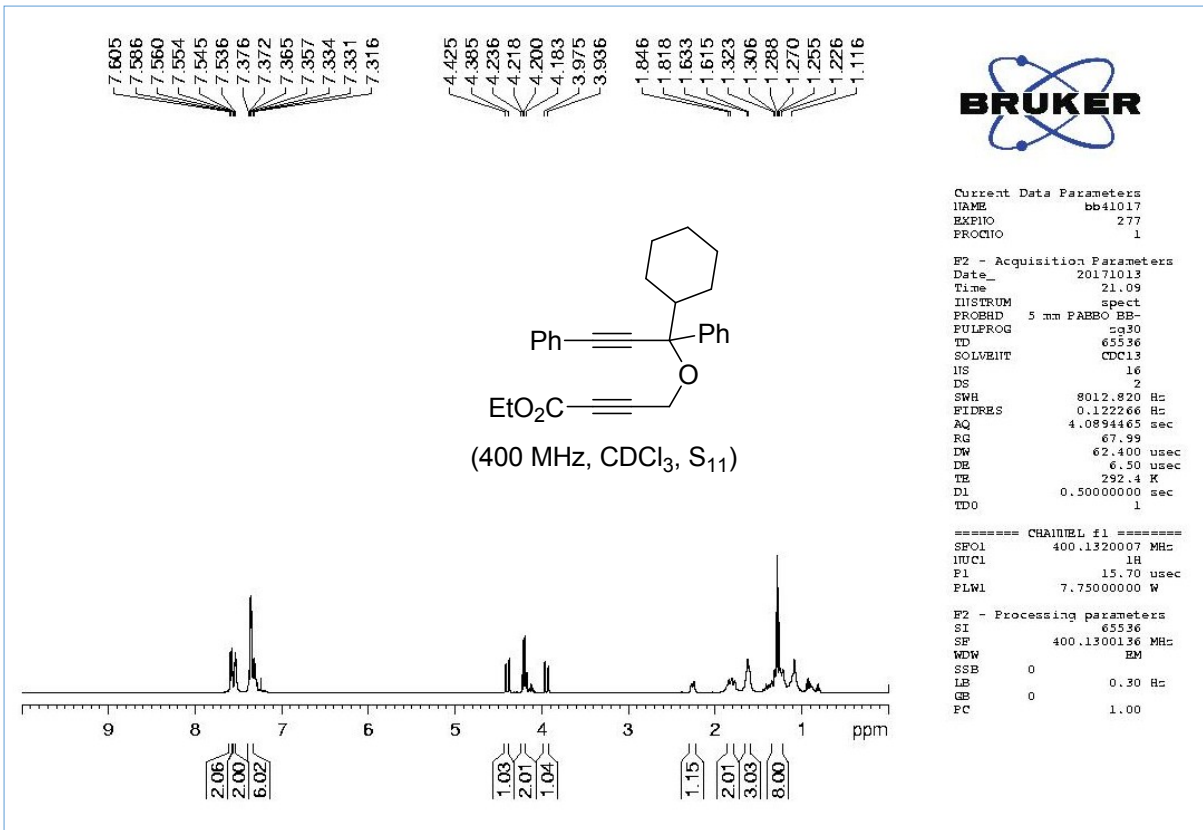










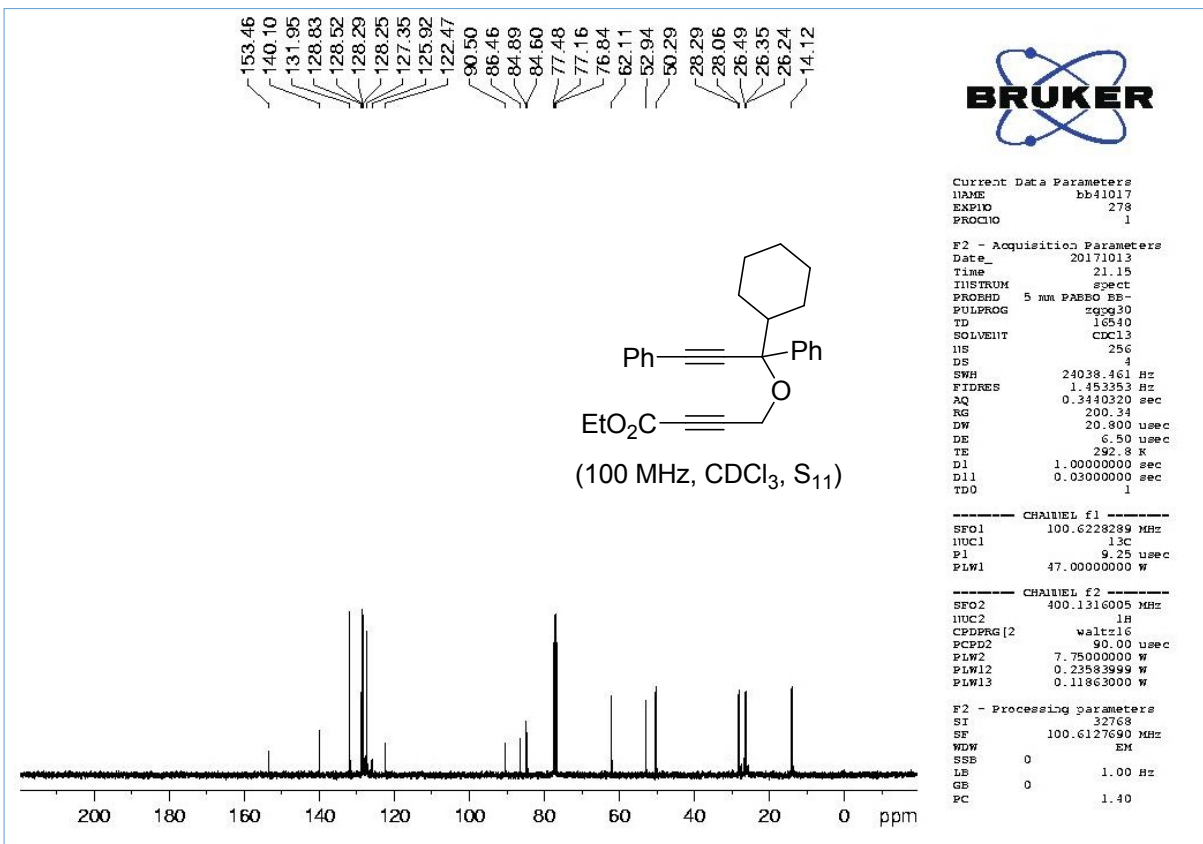


Current Data Parameters
 NAME bb41017
 EXPNO 277
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20171013
 Time 21.09
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 67.99
 DW 62.400 usec
 DE 6.50 usec
 TE 292.4 K
 D1 0.50000000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 400.1320007 MHz
 NUC1 1H
 P1 15.70 usec
 PLW1 7.75000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1300136 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 FC 1.00



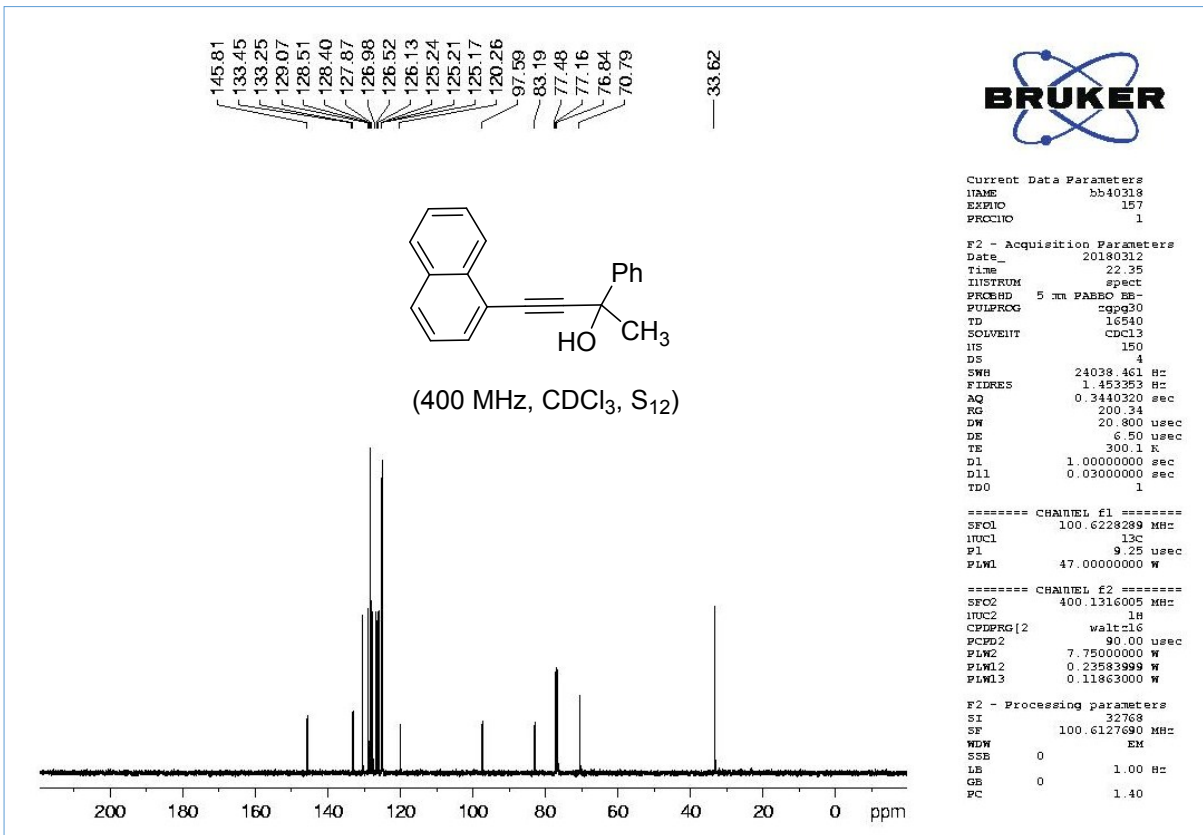
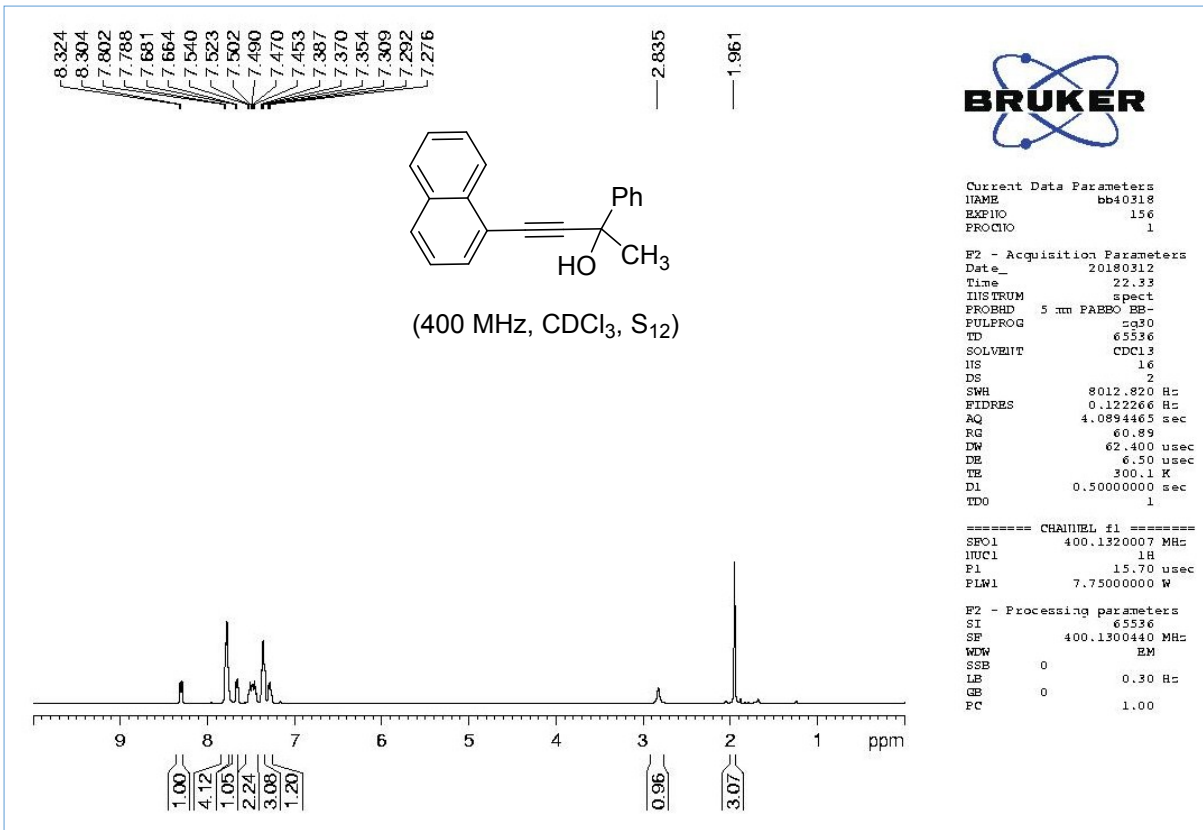
Current Data Parameters
 NAME bb41017
 EXPNO 277
 PROCNO 1

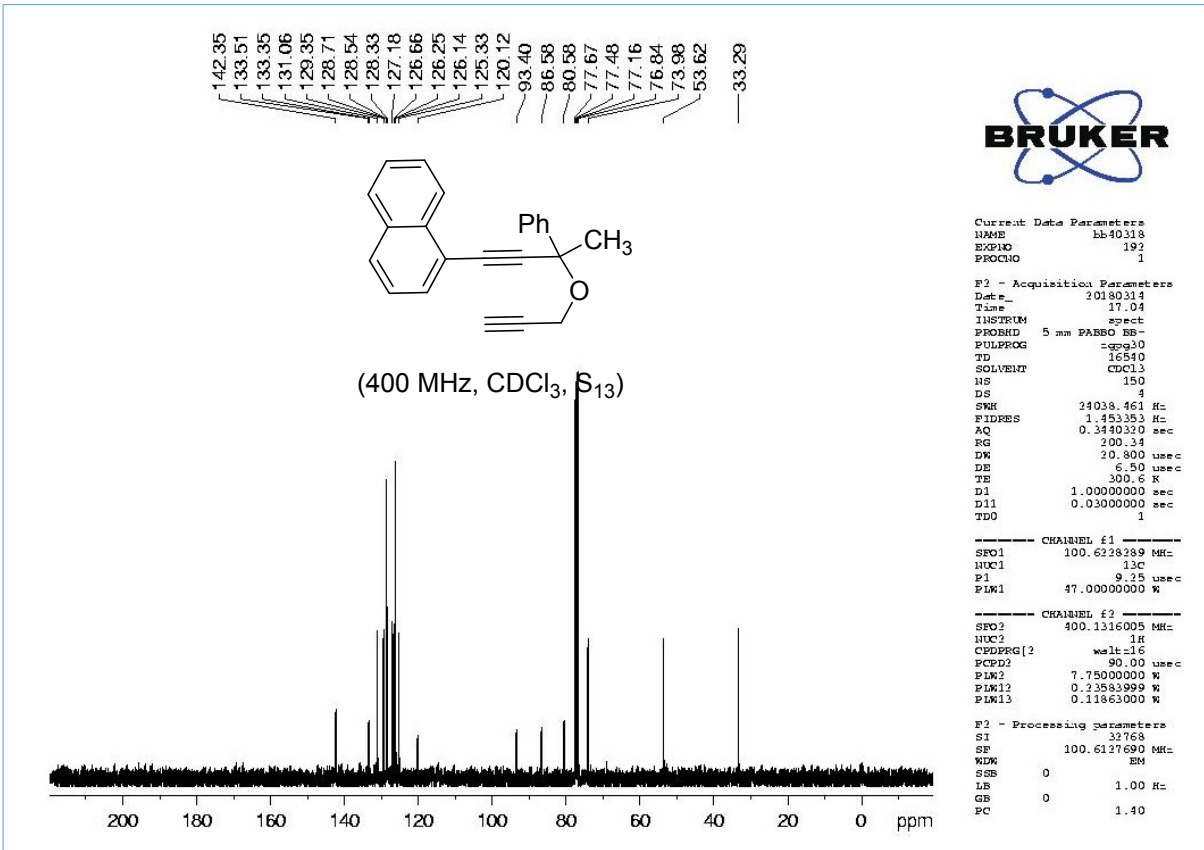
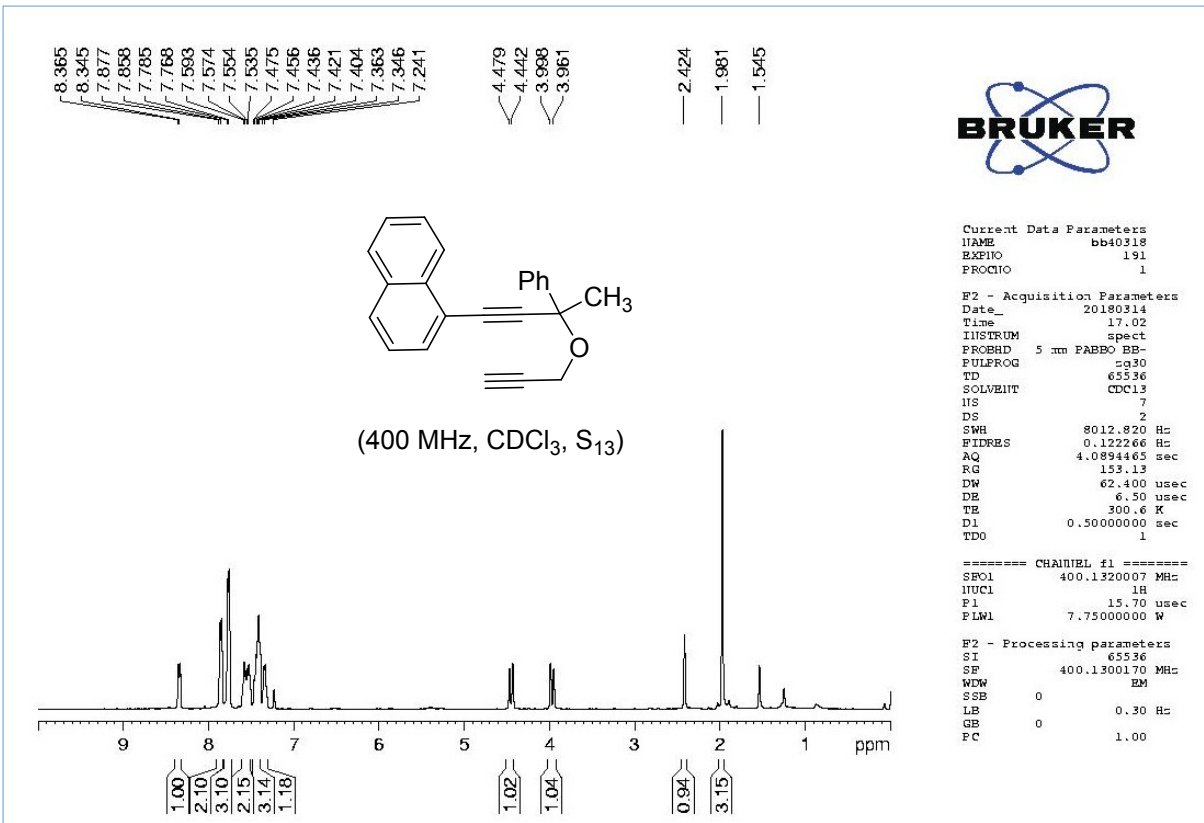
F2 - Acquisition Parameters
 Date_ 20171013
 Time 21.15
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 16540
 SOLVENT CDC13
 NS 256
 DS 4
 SWH 24038.461 Hz
 FIDRES 1.453353 Hz
 AQ 0.3440320 sec
 RG 200.34
 DW 20.800 usec
 DE 6.50 usec
 TE 292.8 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TDO 1

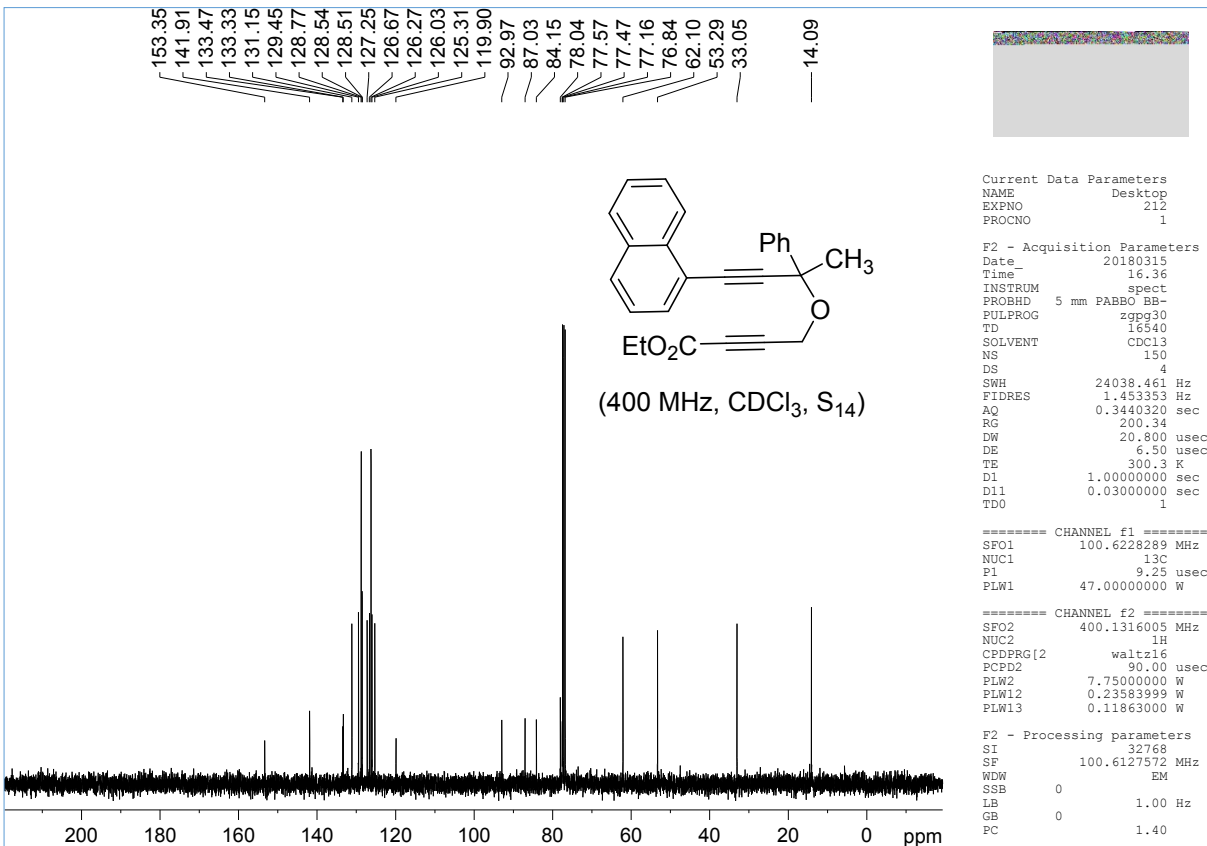
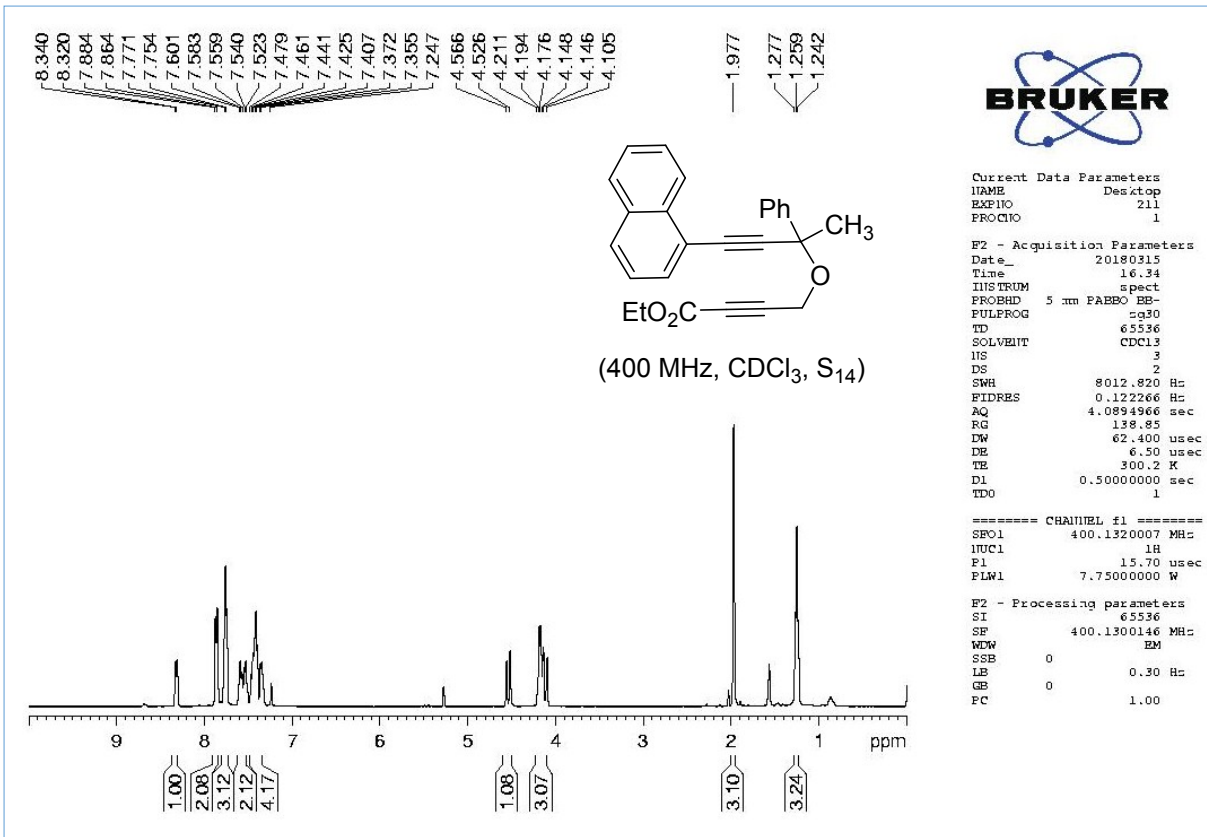
----- CHANNEL f1 -----
 SFO1 100.6228289 MHz
 NUC1 13C
 P1 9.25 usec
 PLW1 47.00000000 W

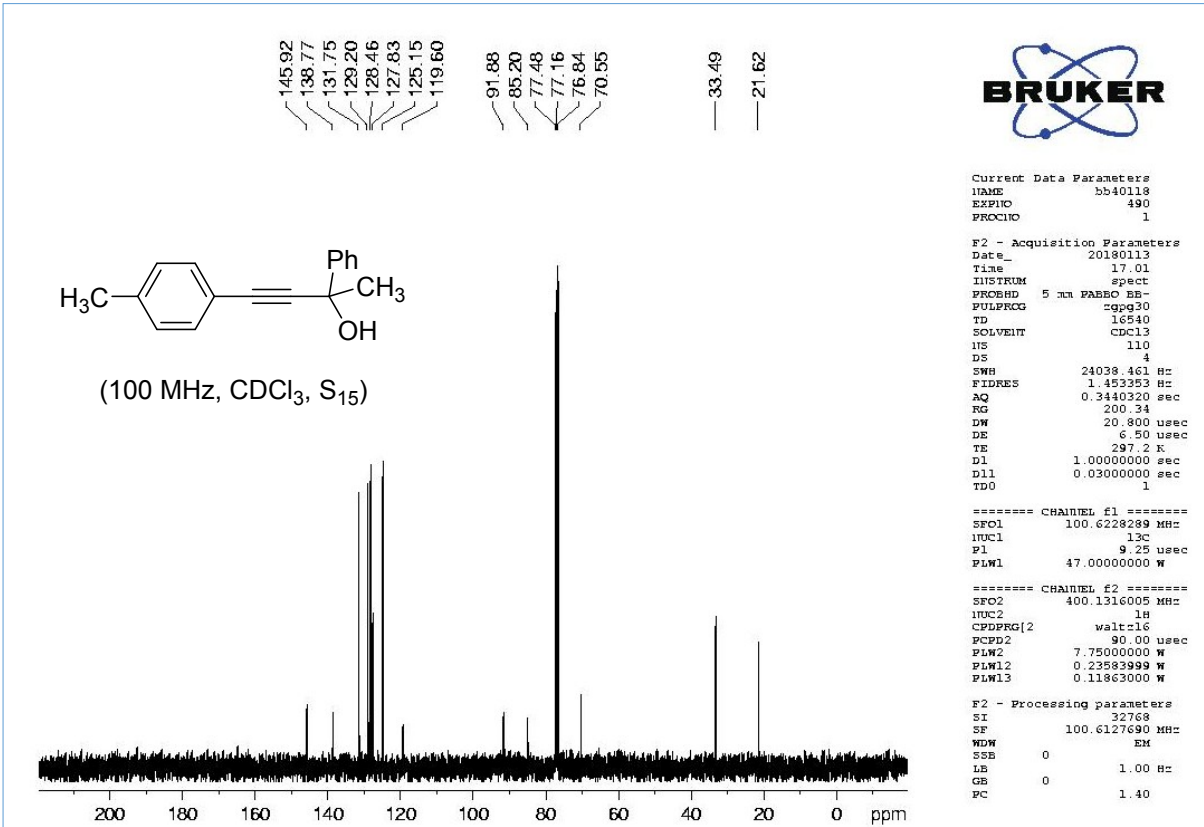
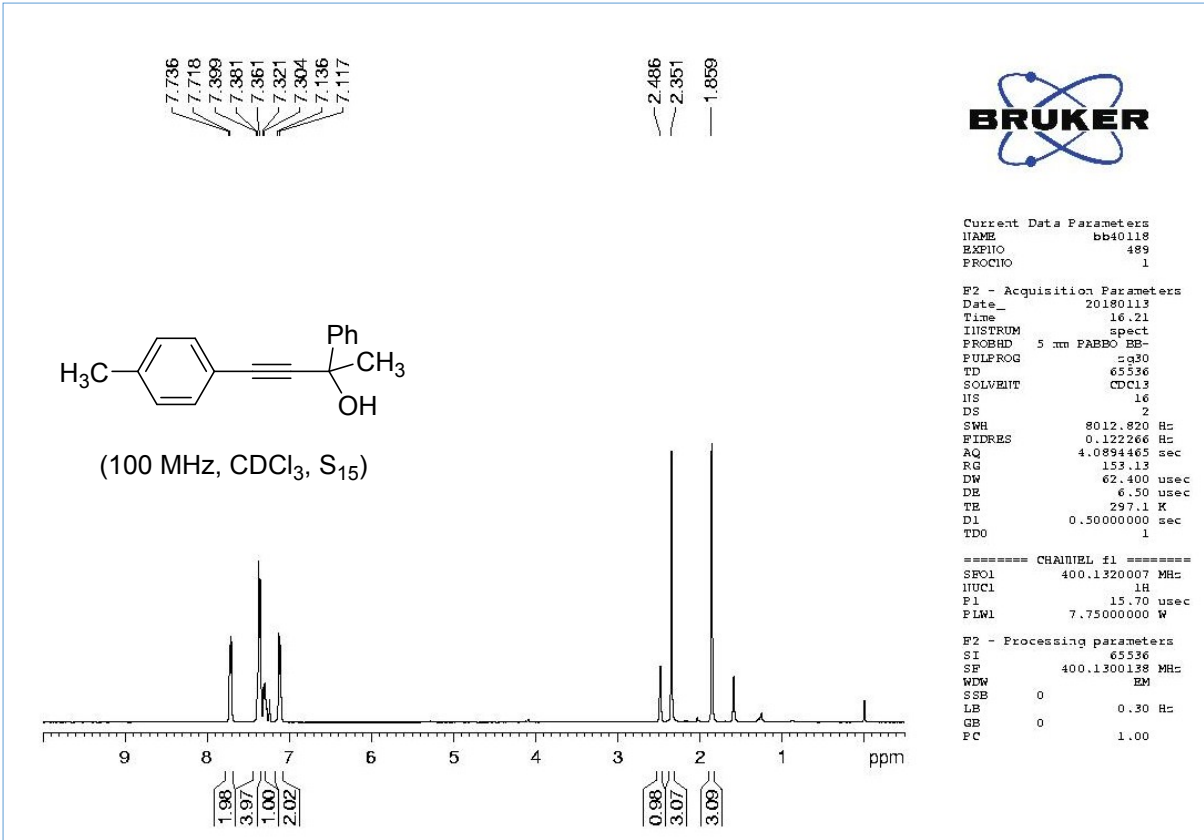
----- CHANNEL f2 -----
 SFO2 400.1316005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 7.75000000 W
 PLW12 0.23583999 W
 PLW13 0.11863000 W

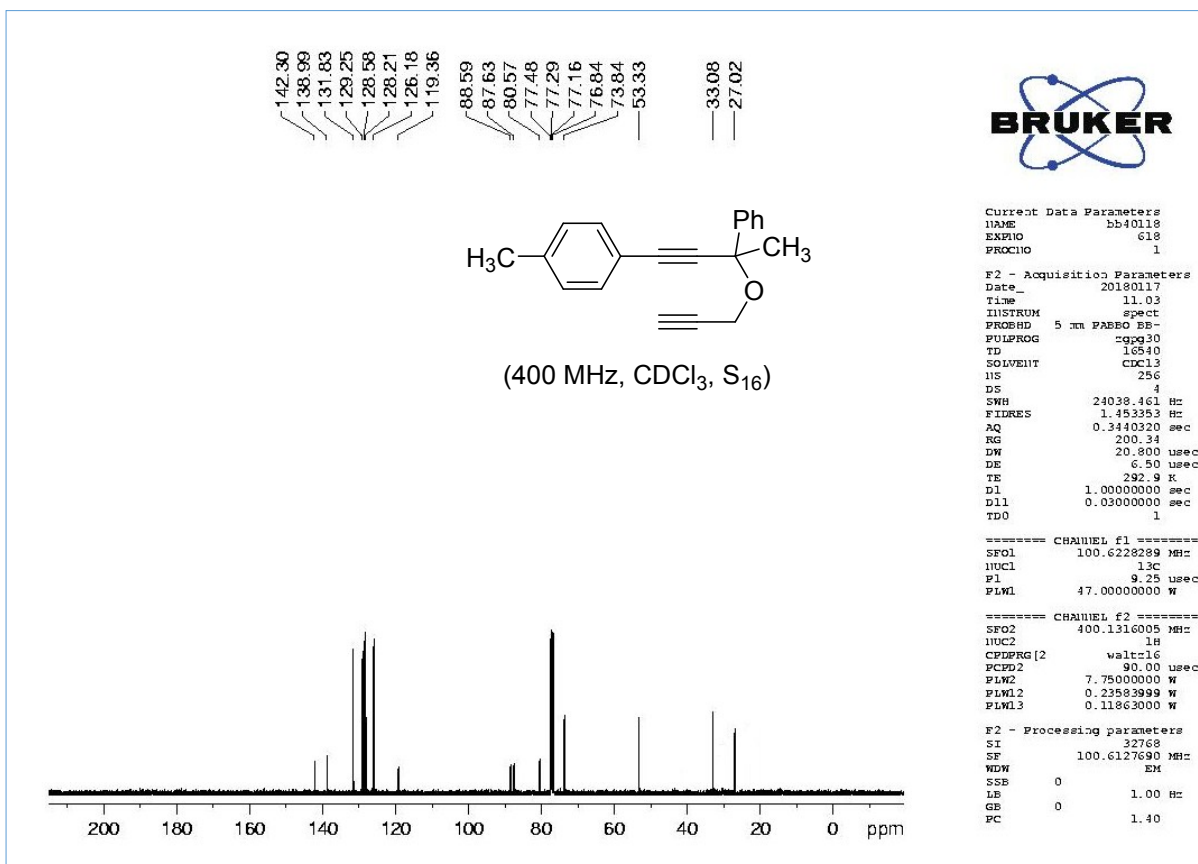
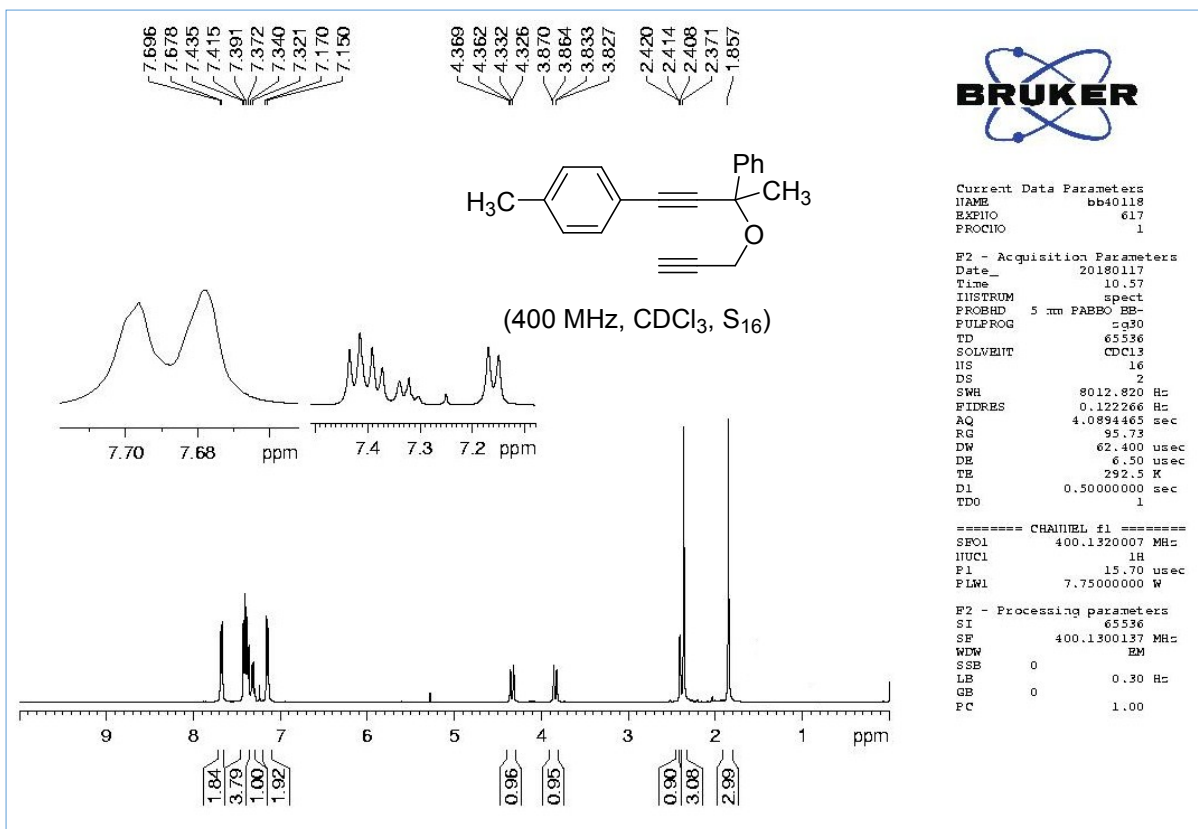
F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

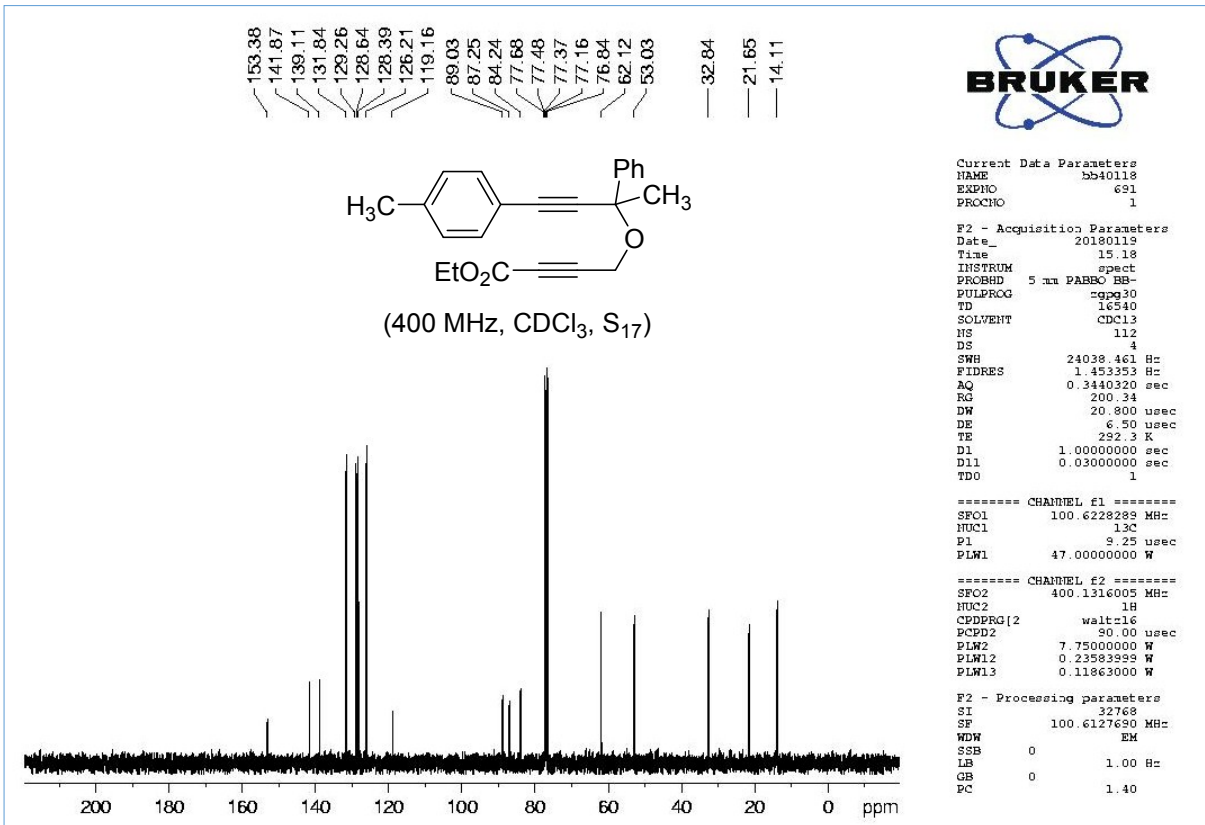
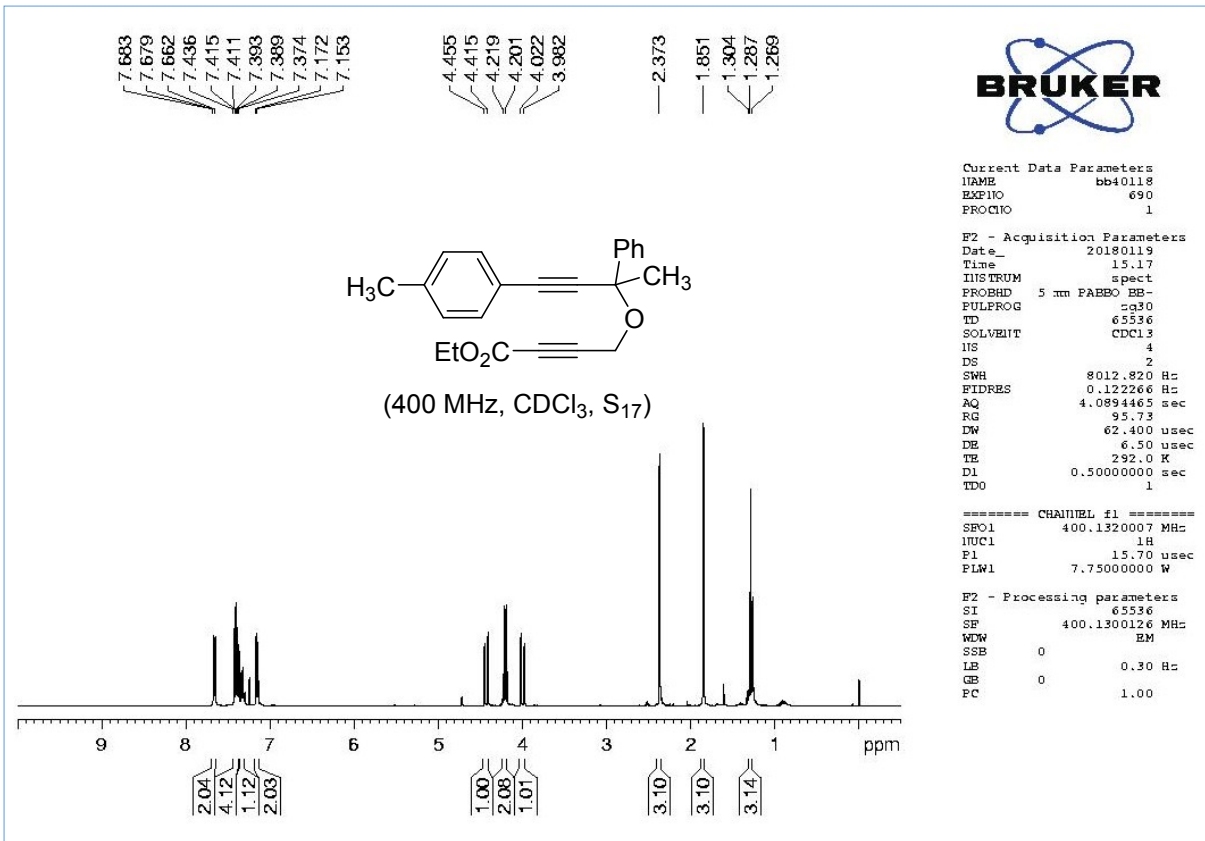


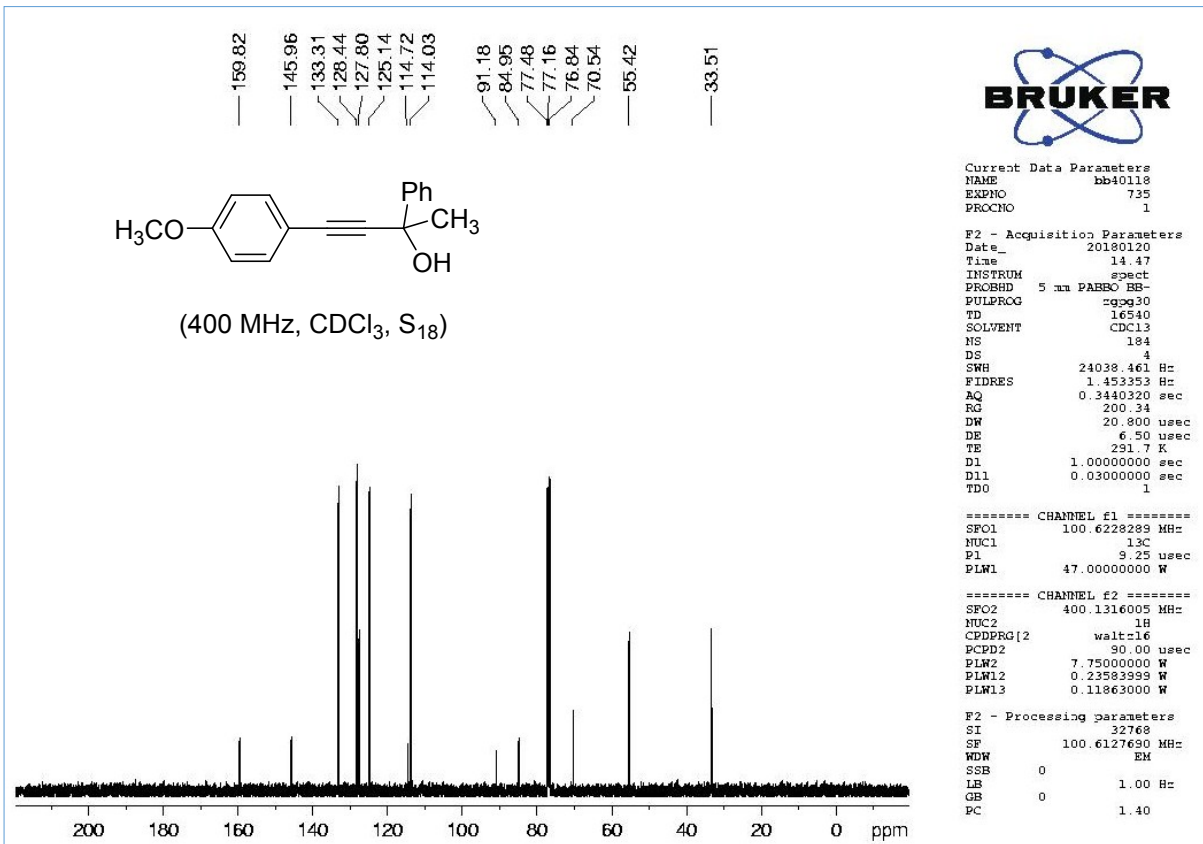
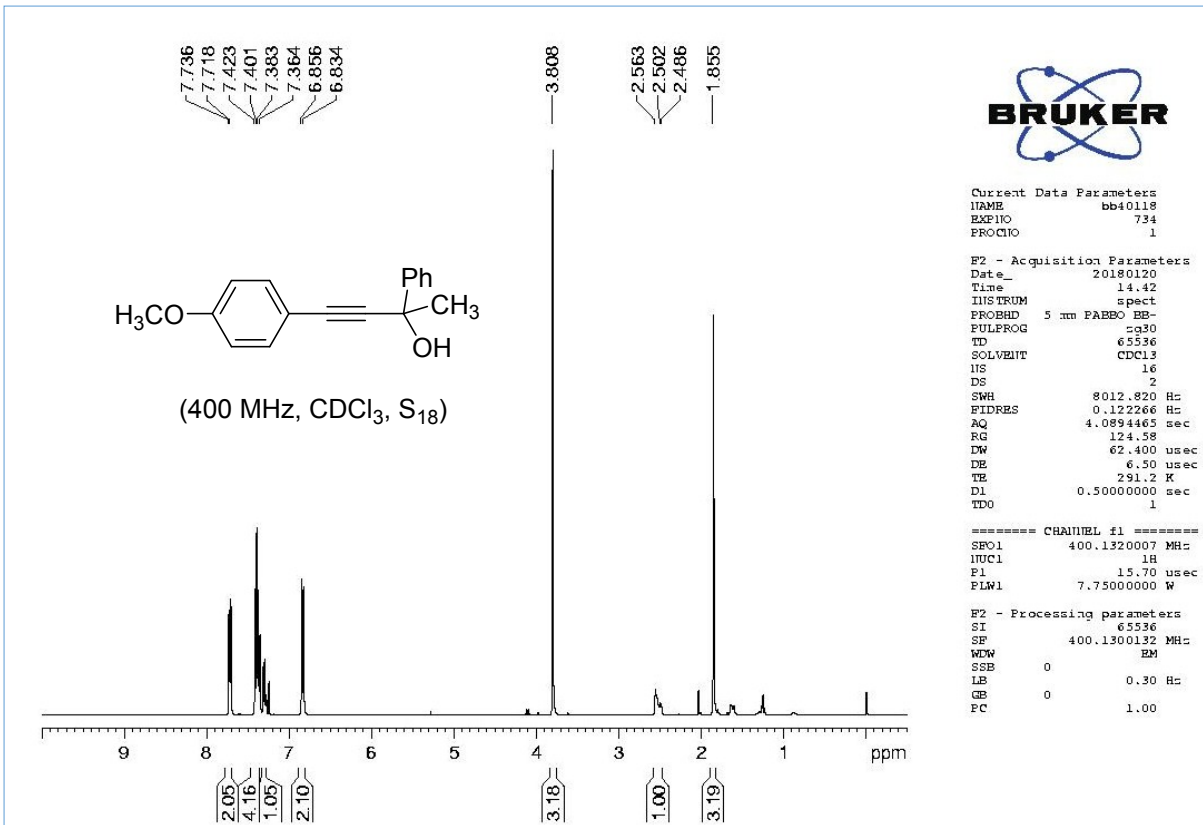


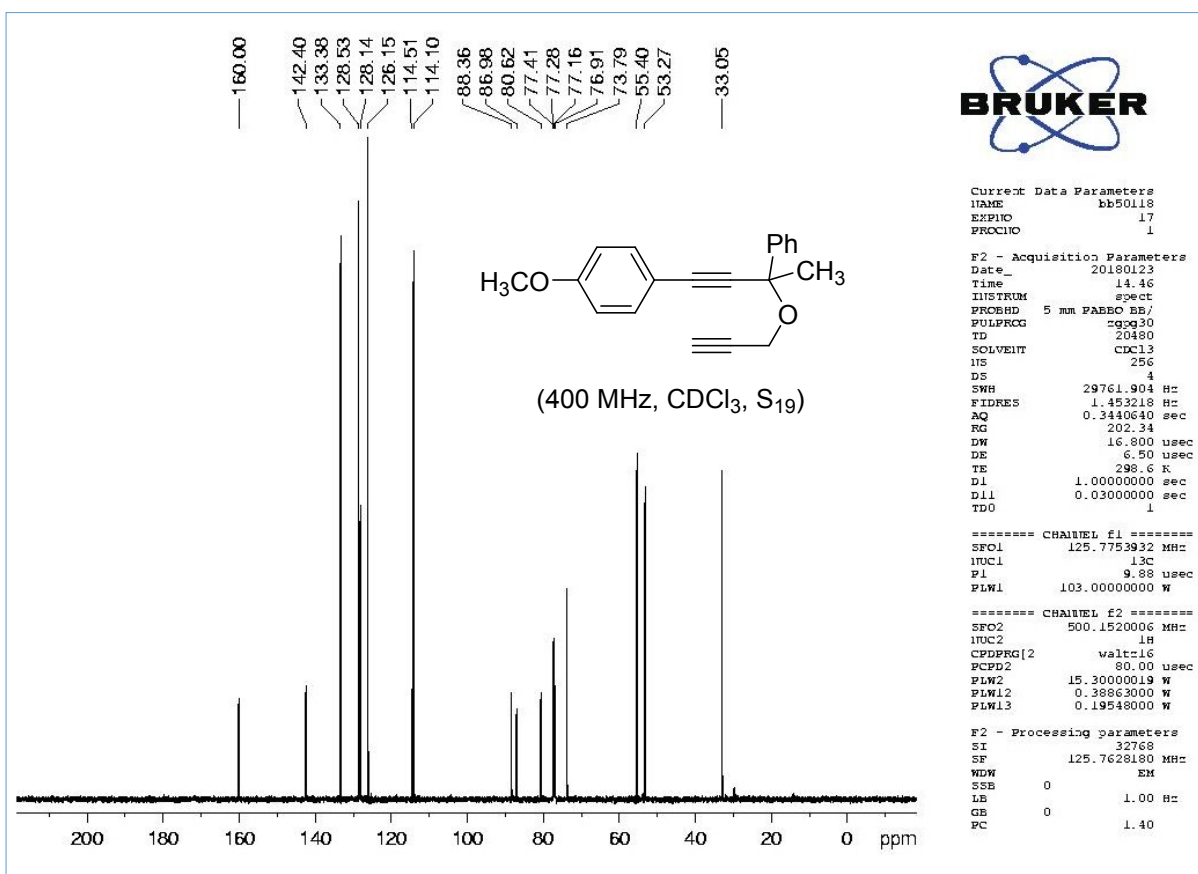
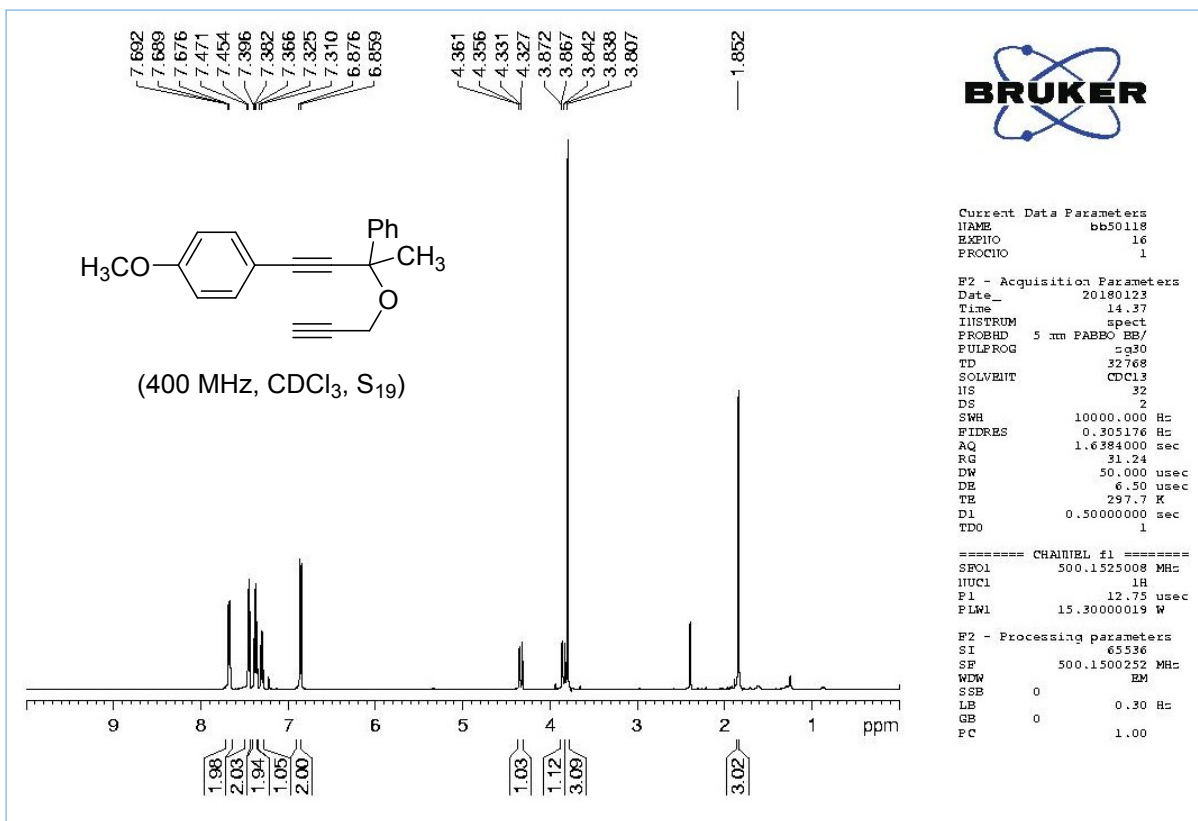


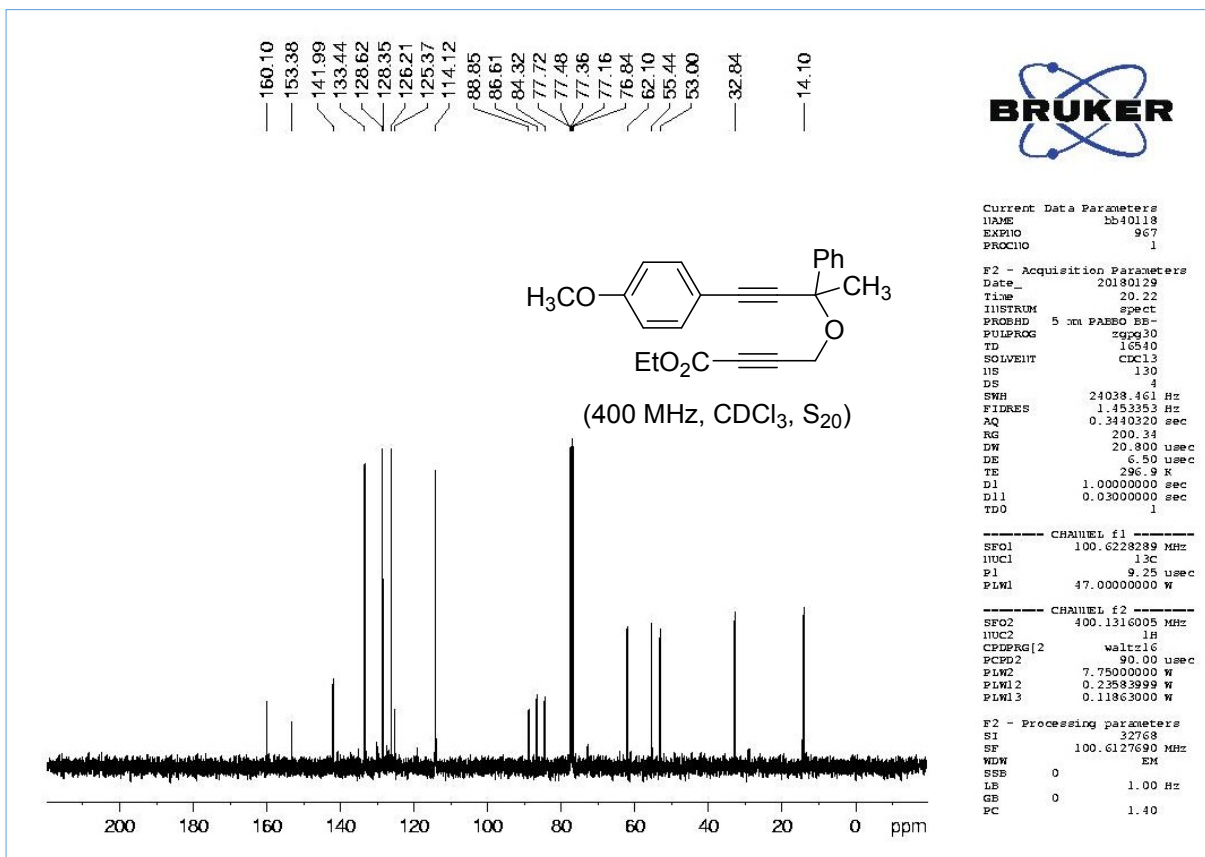
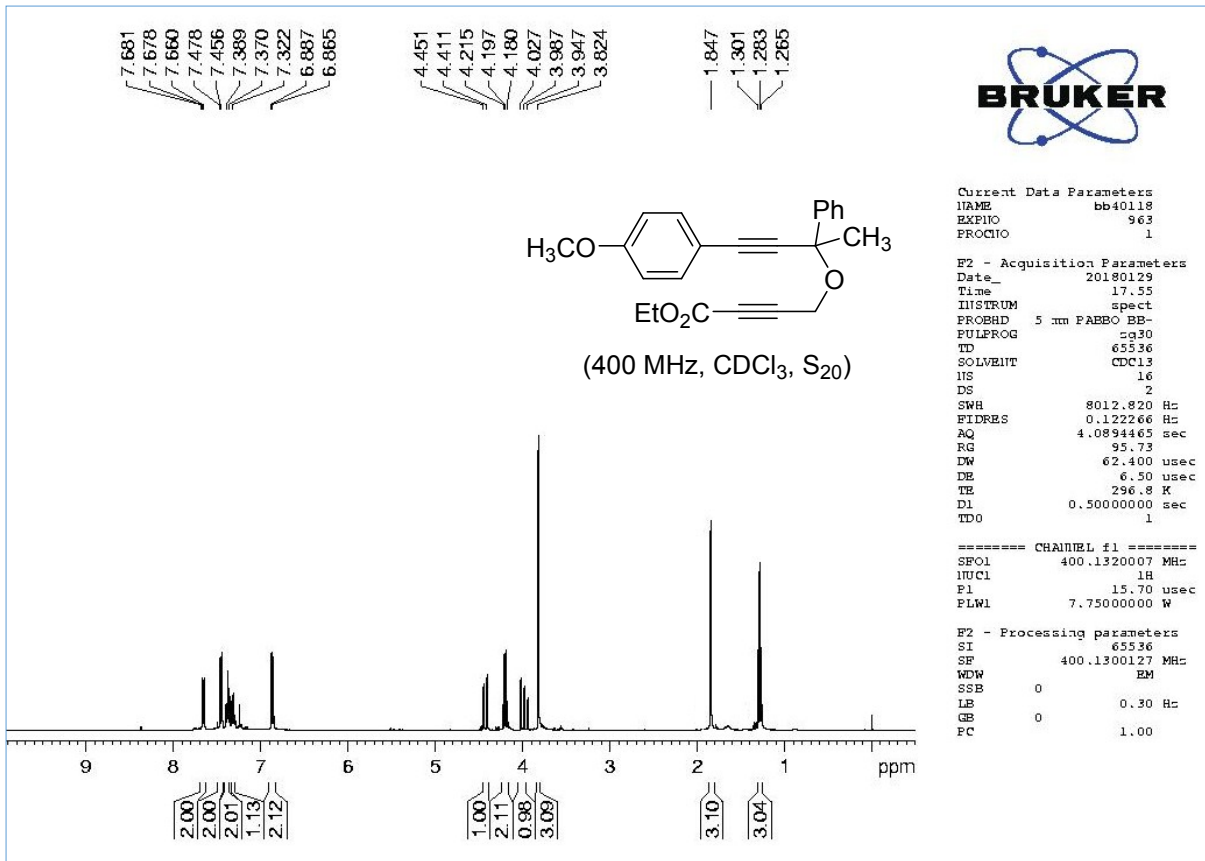


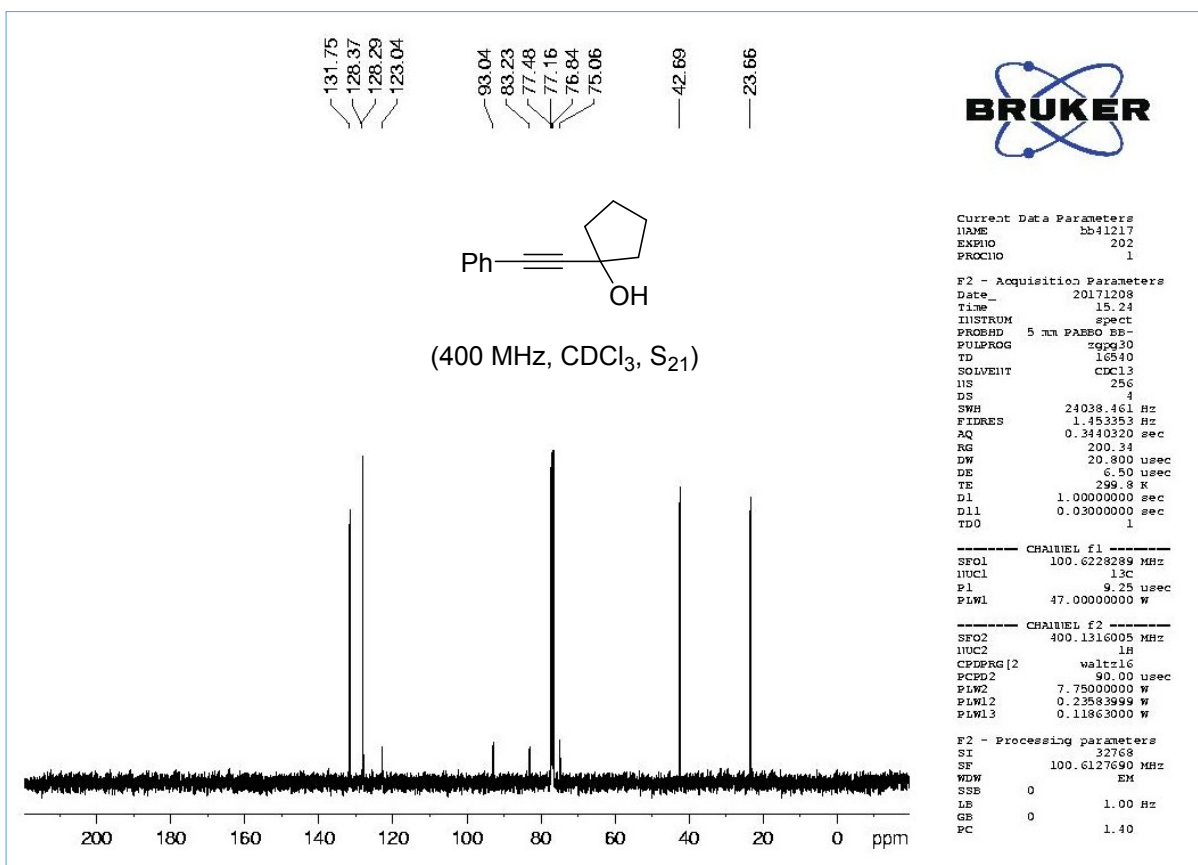
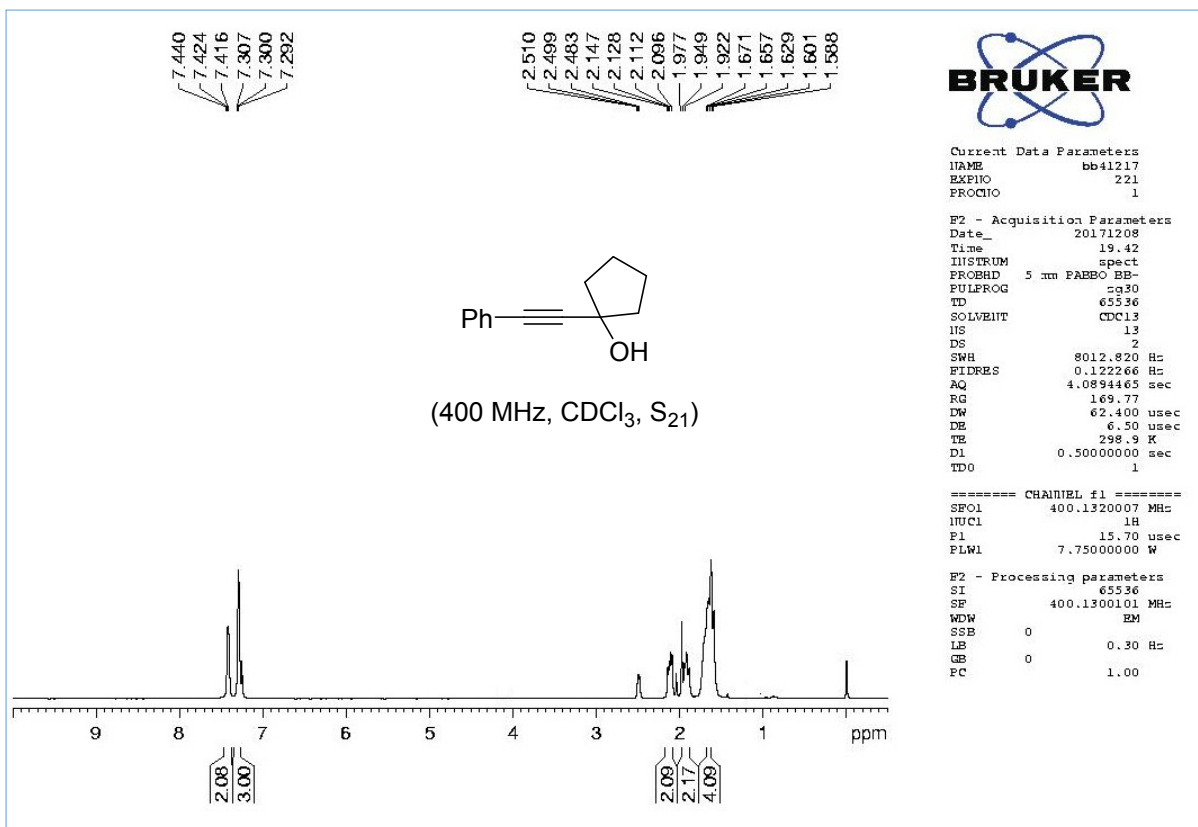


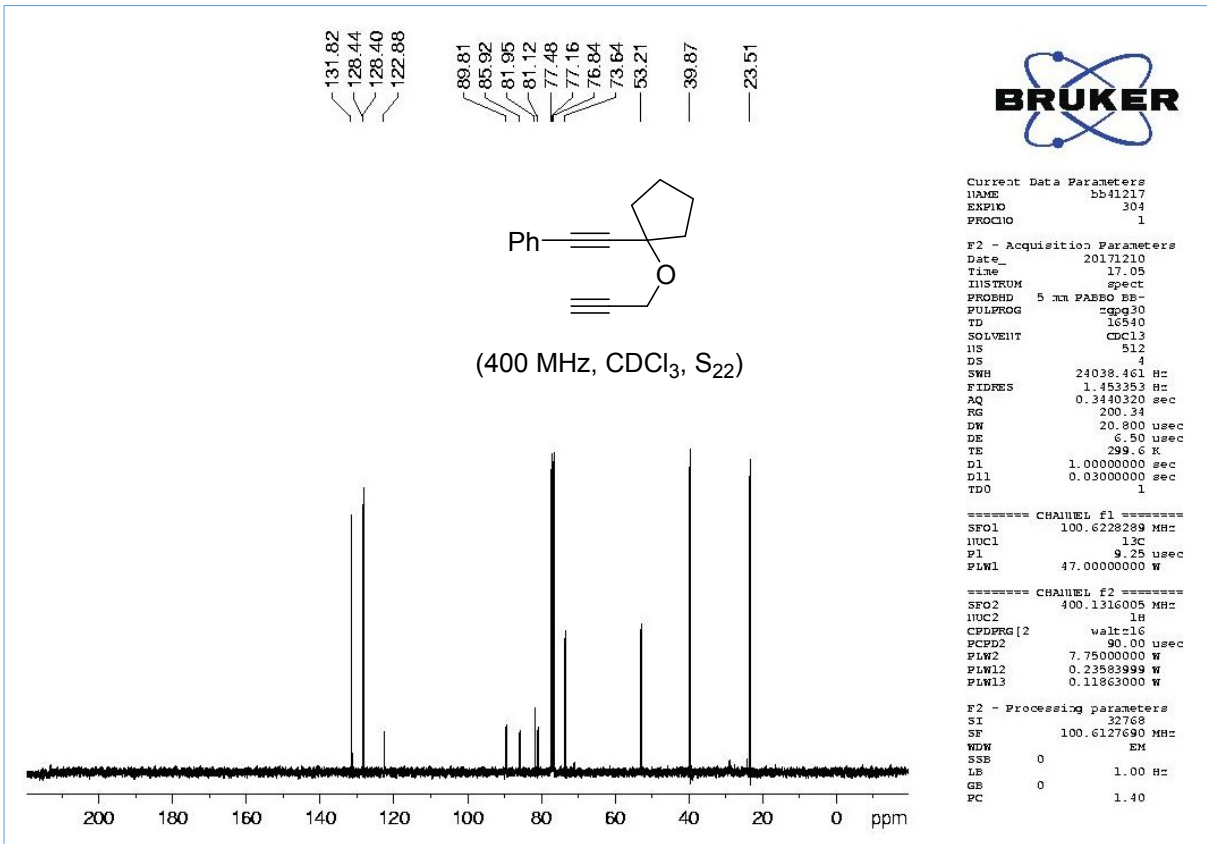
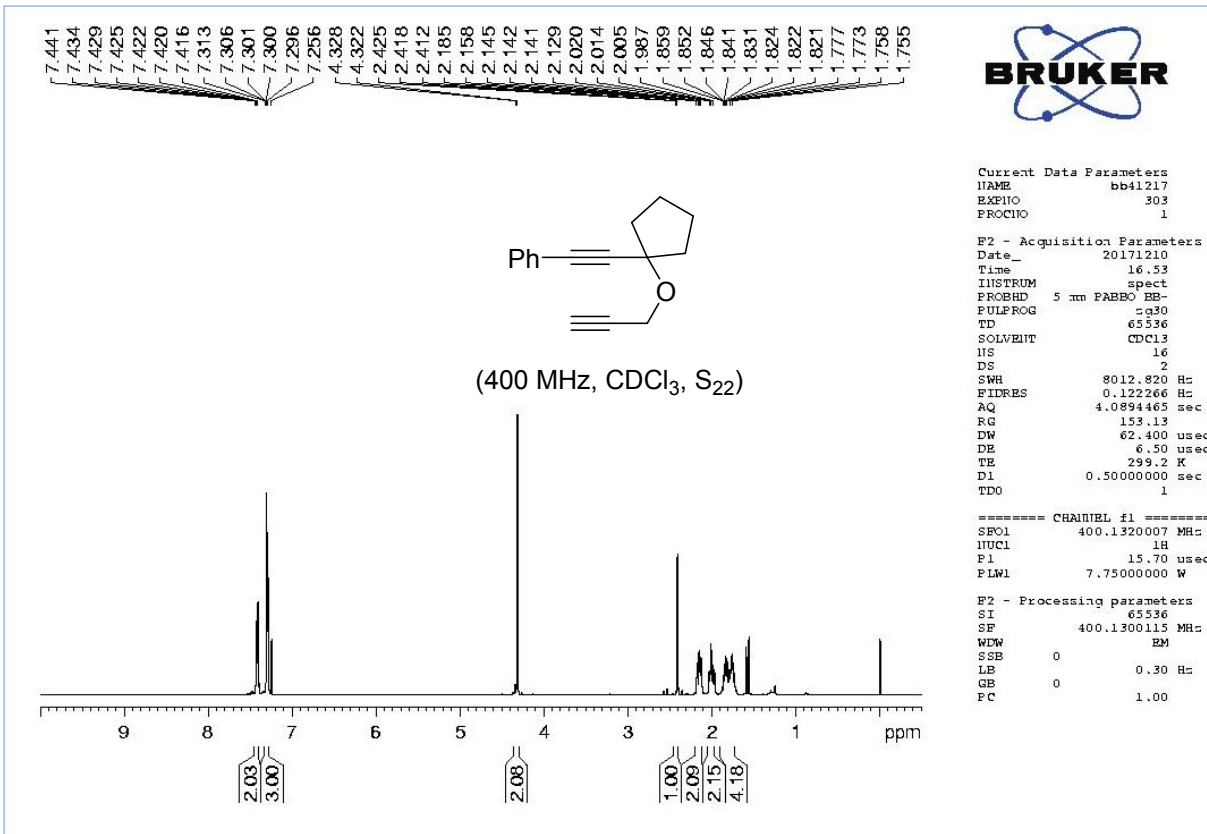


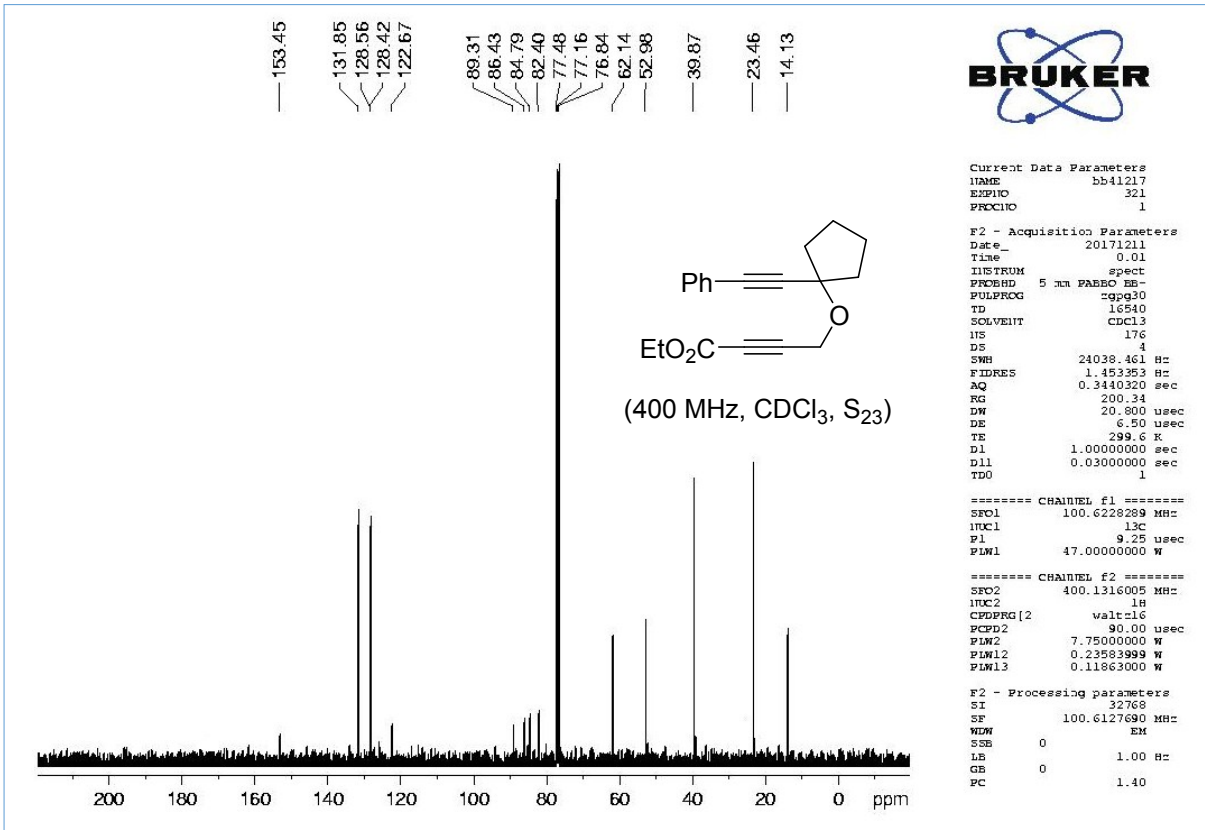
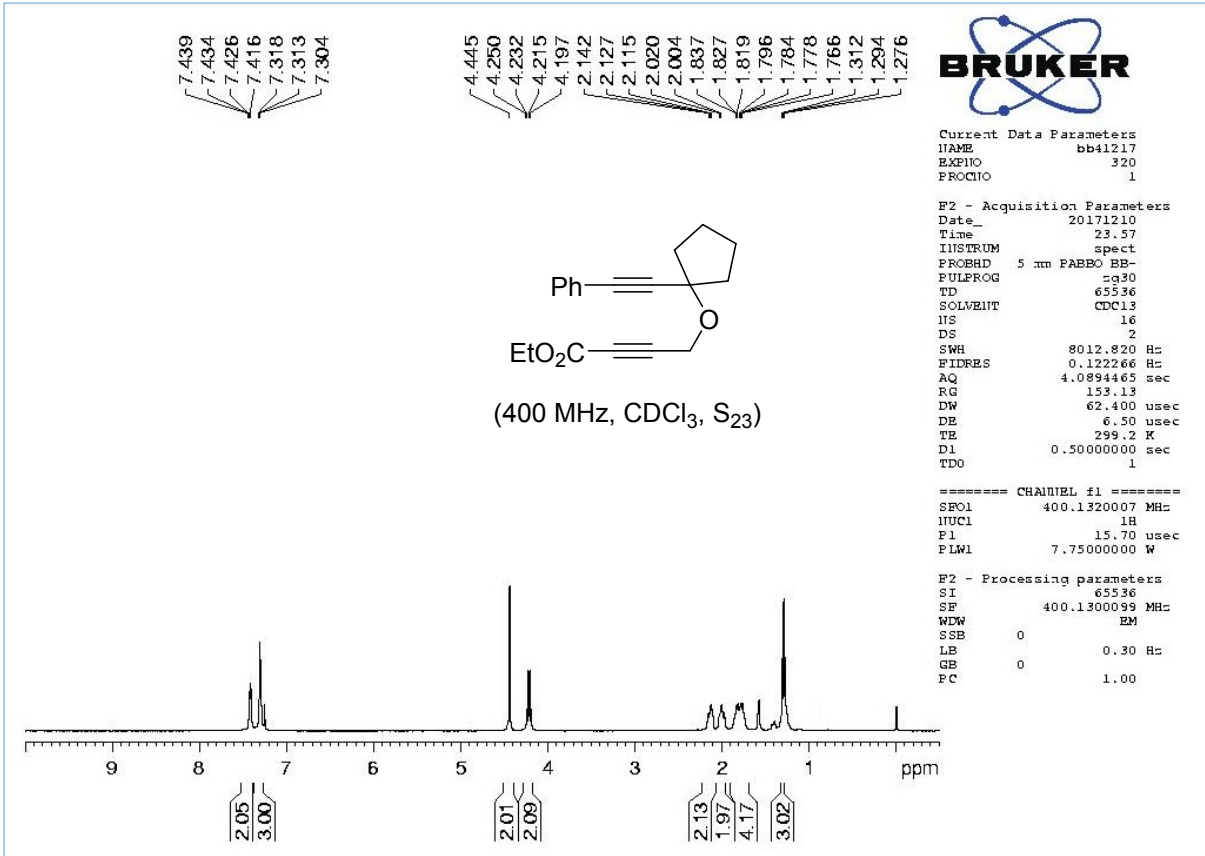


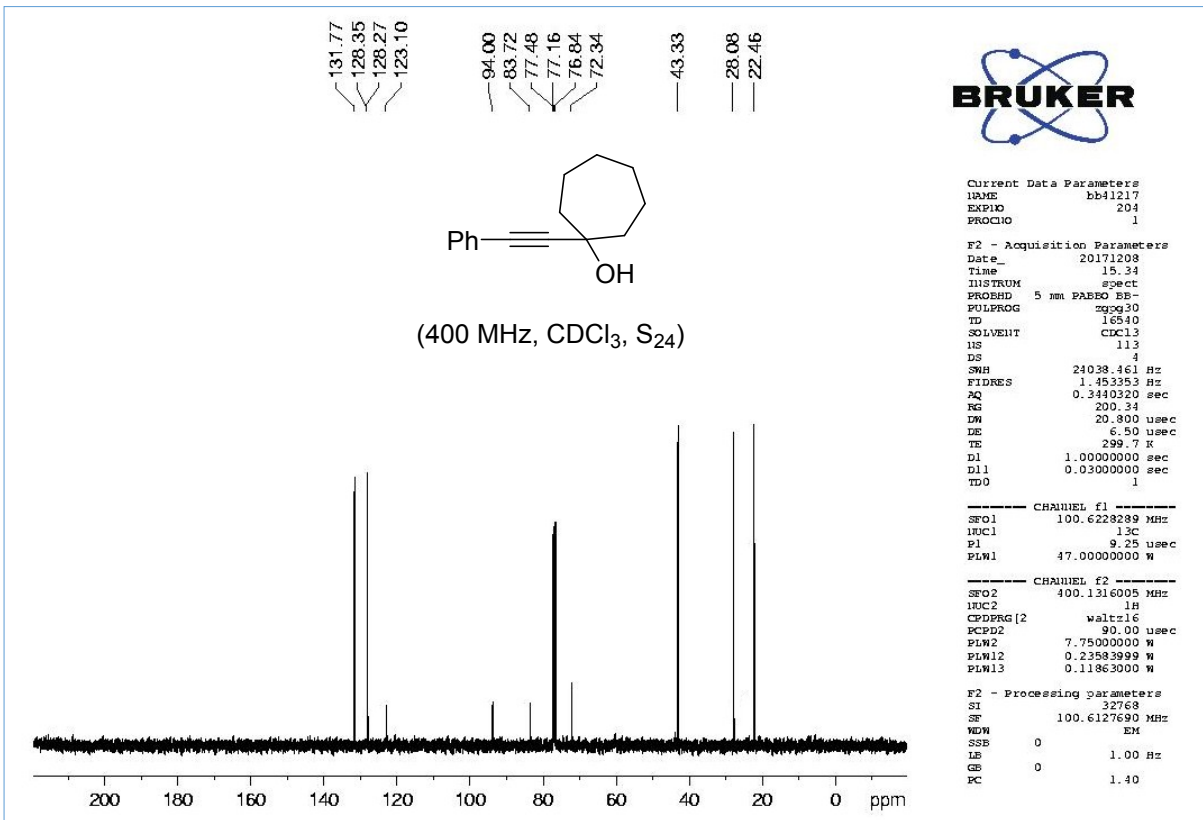
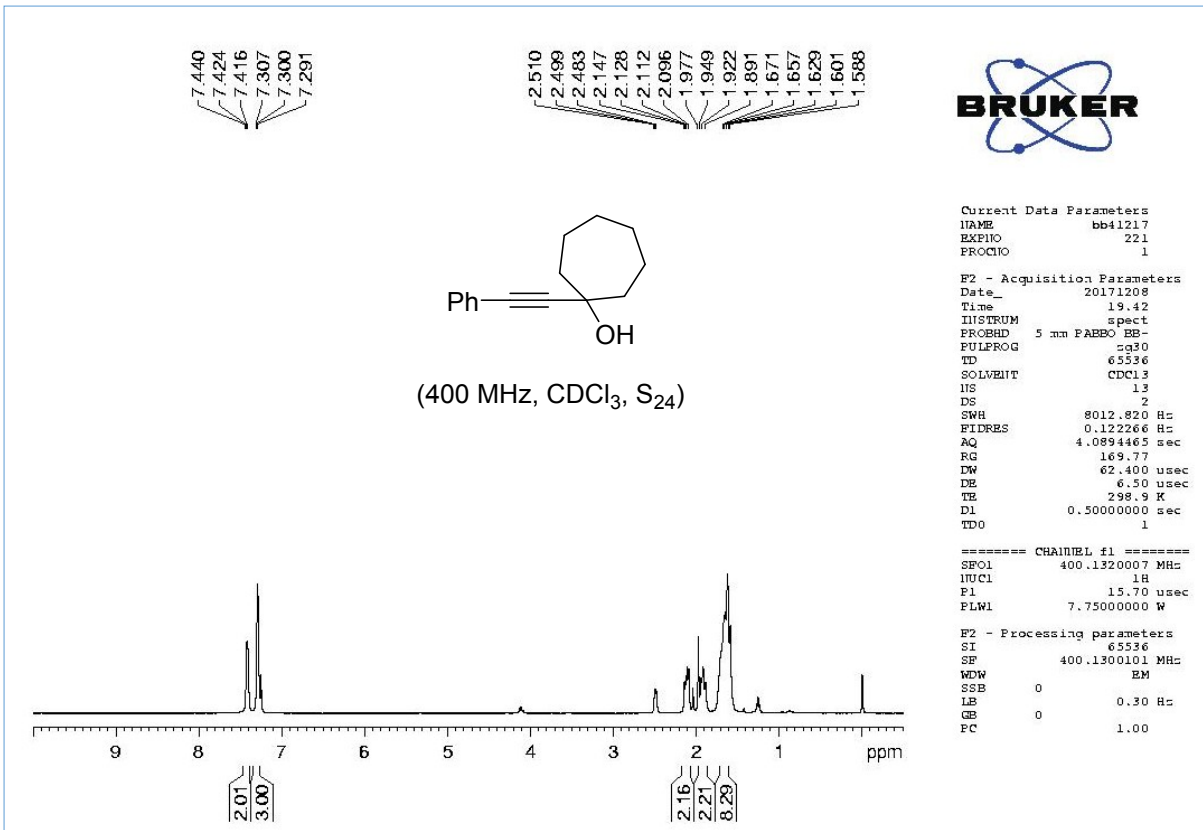


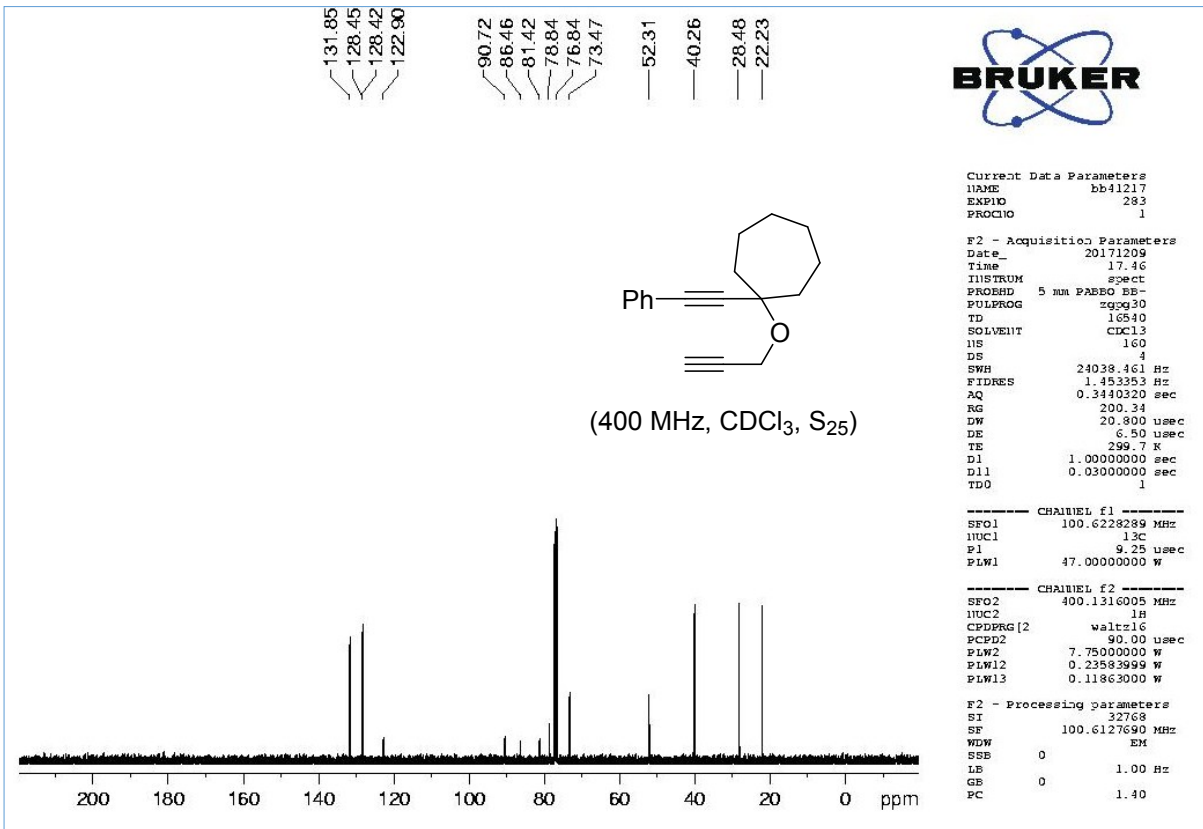
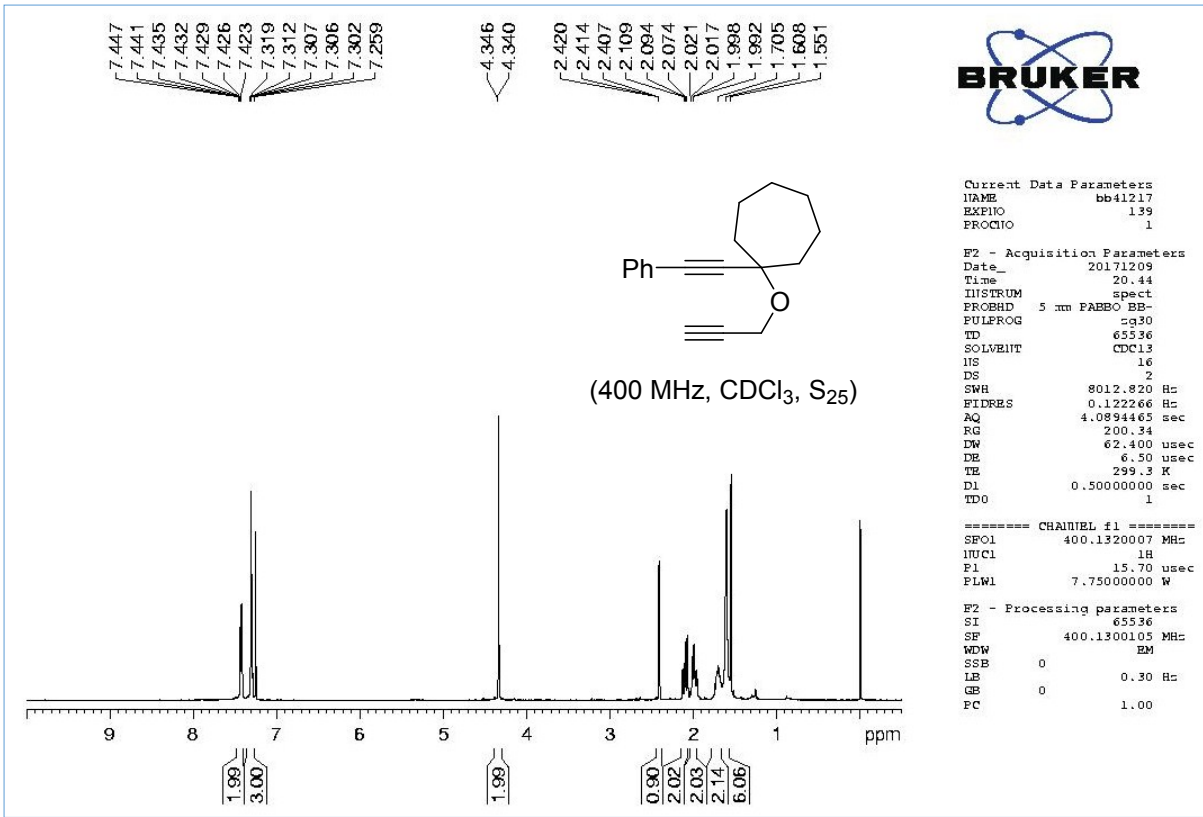


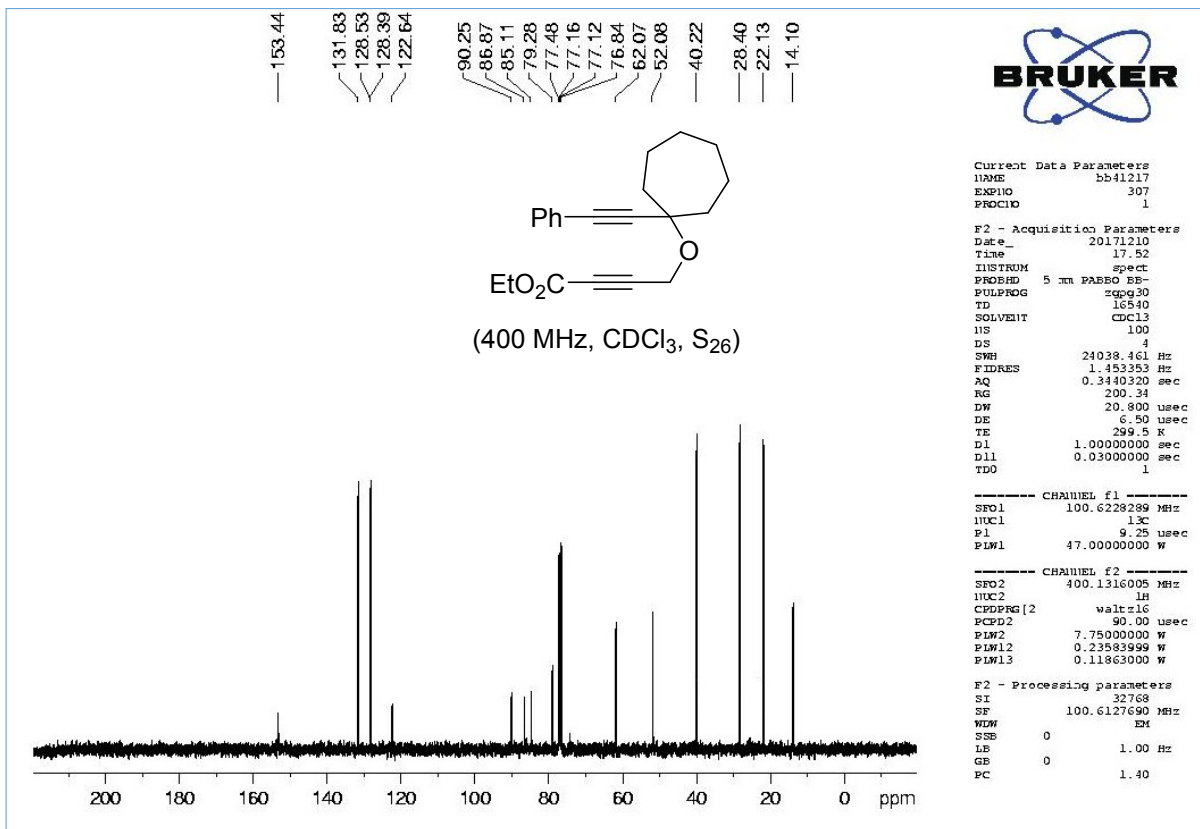
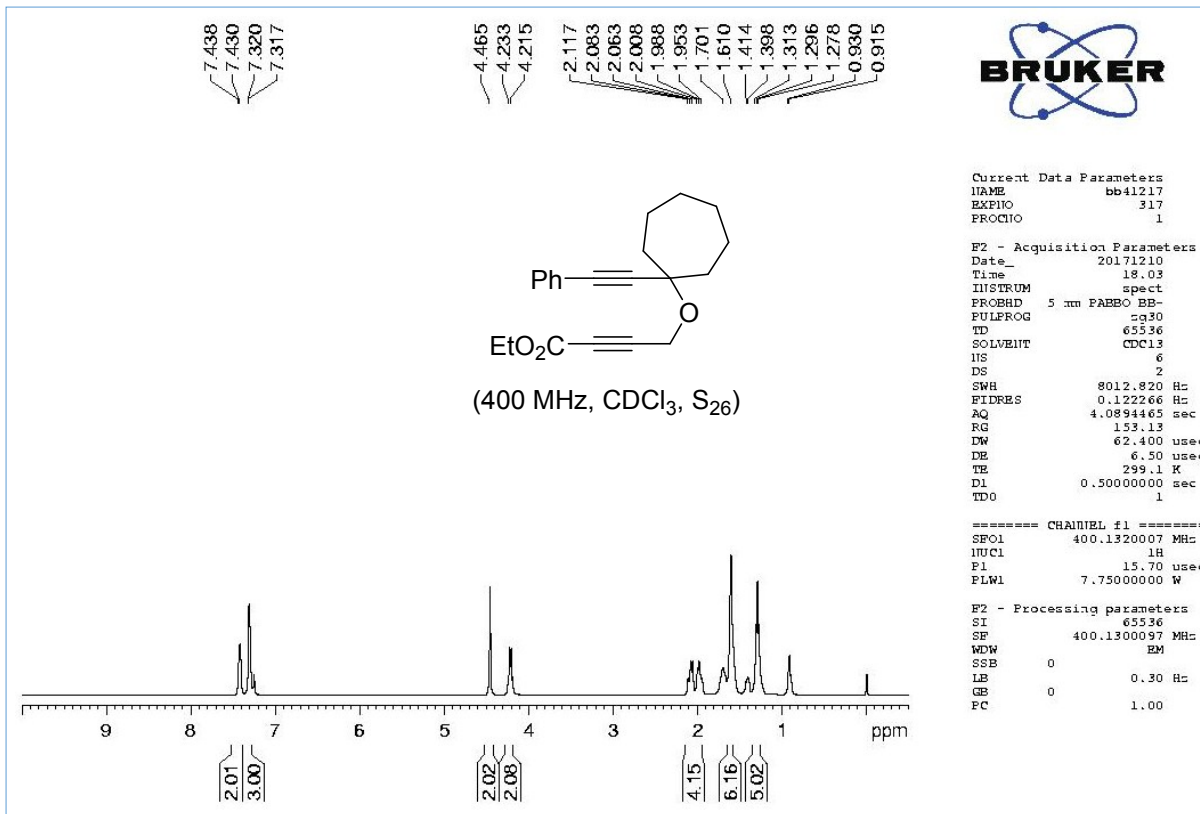


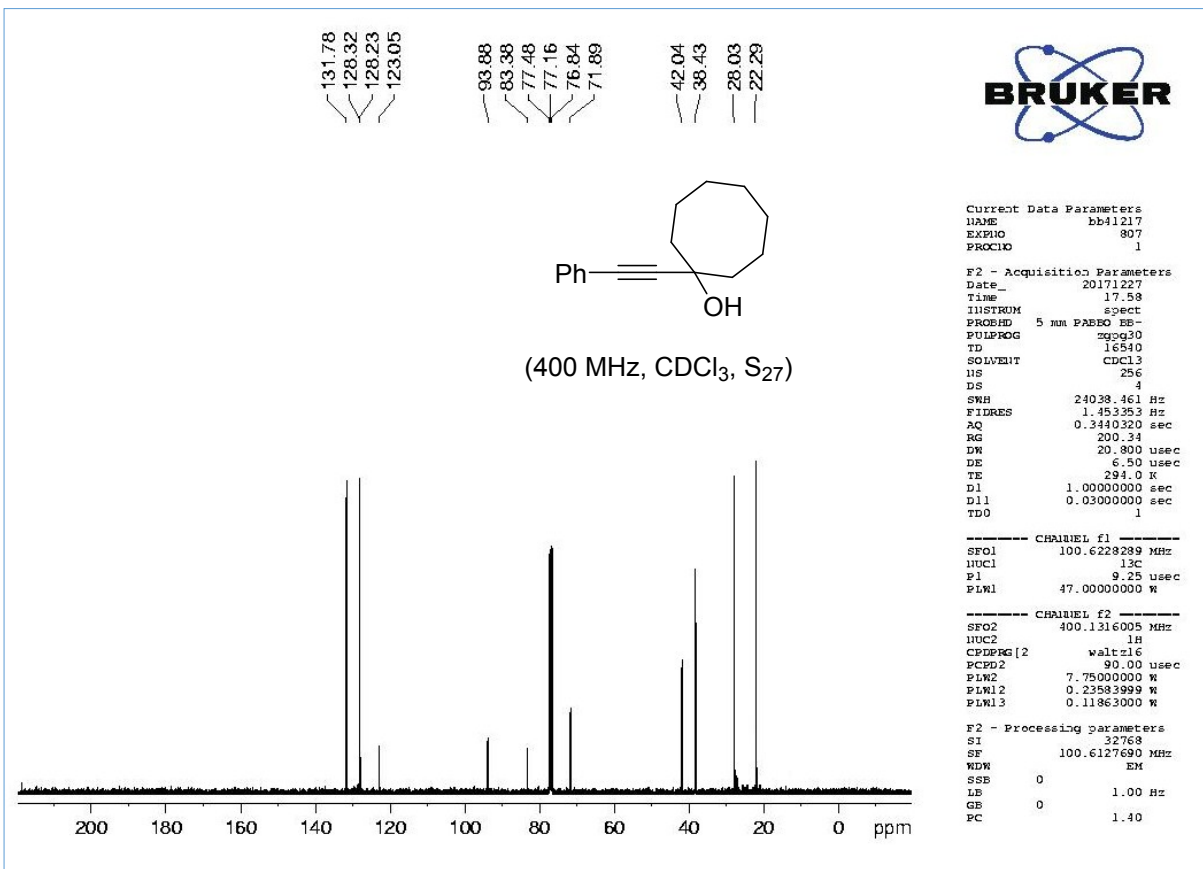
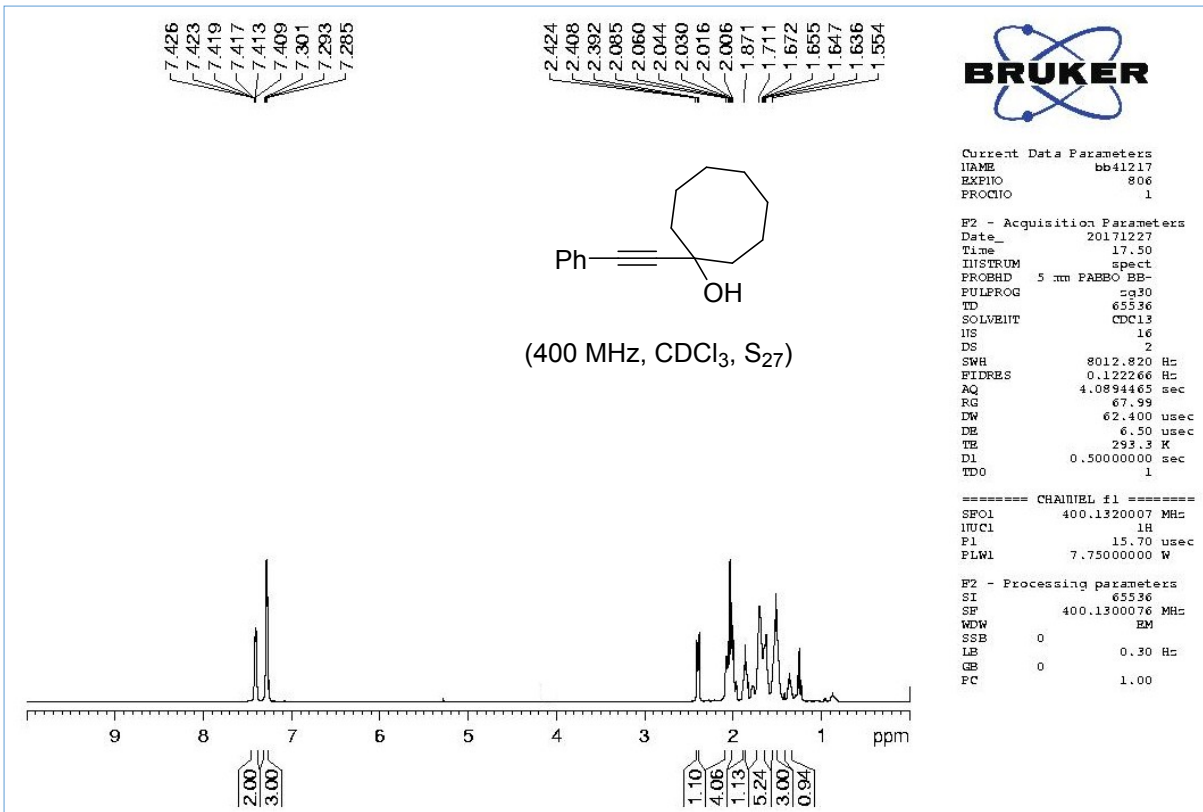


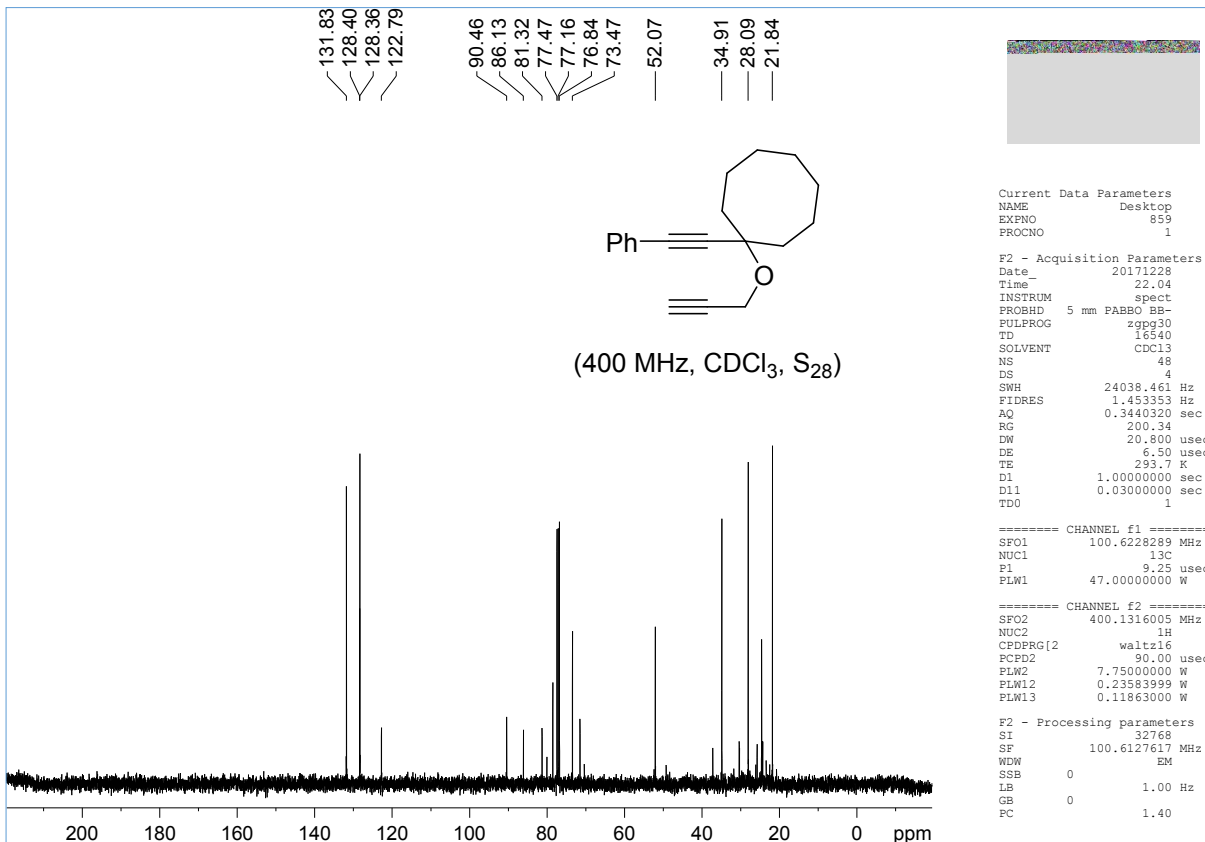
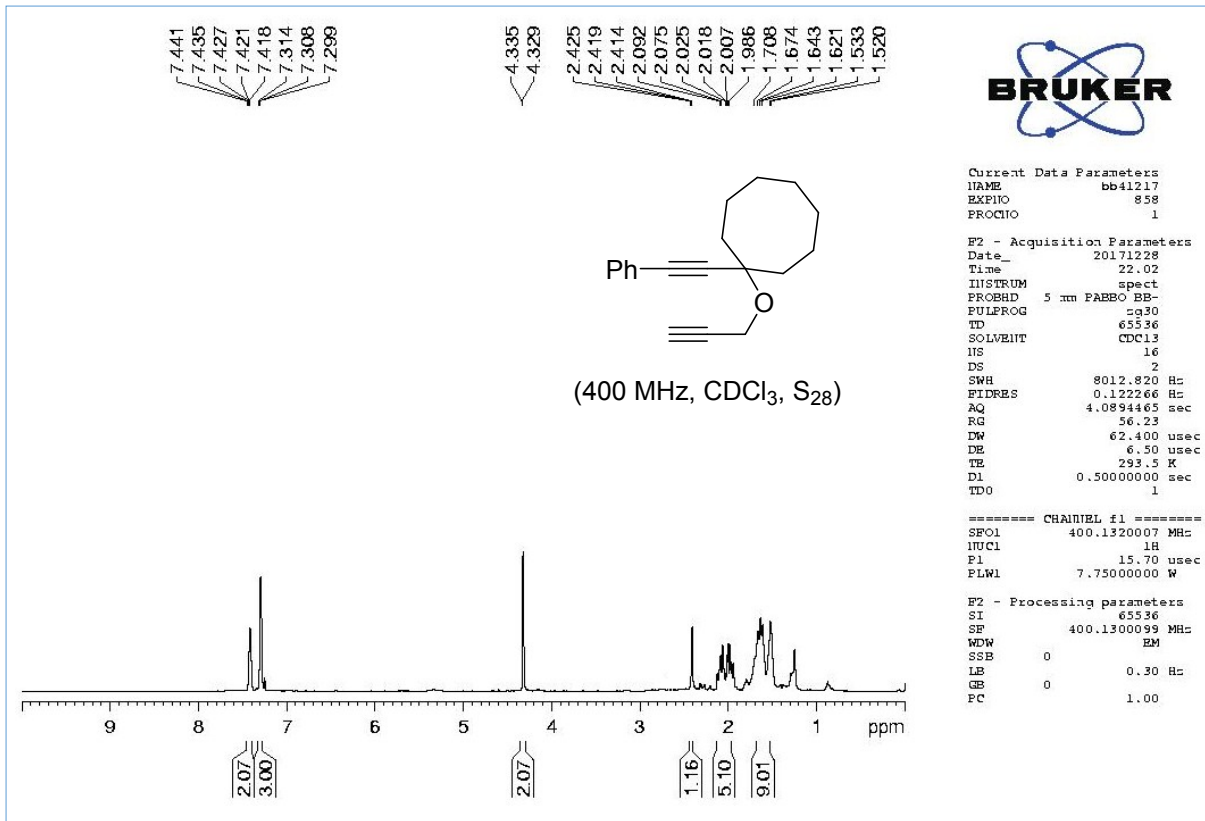


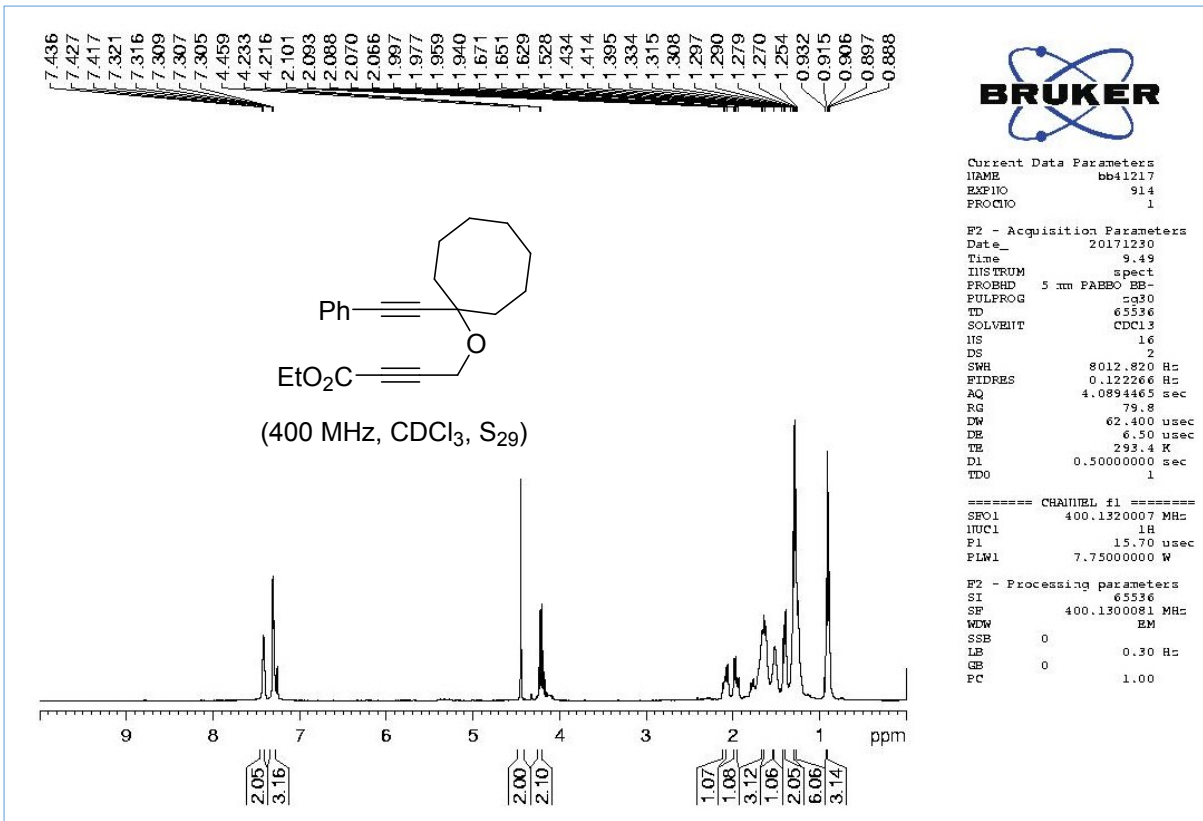










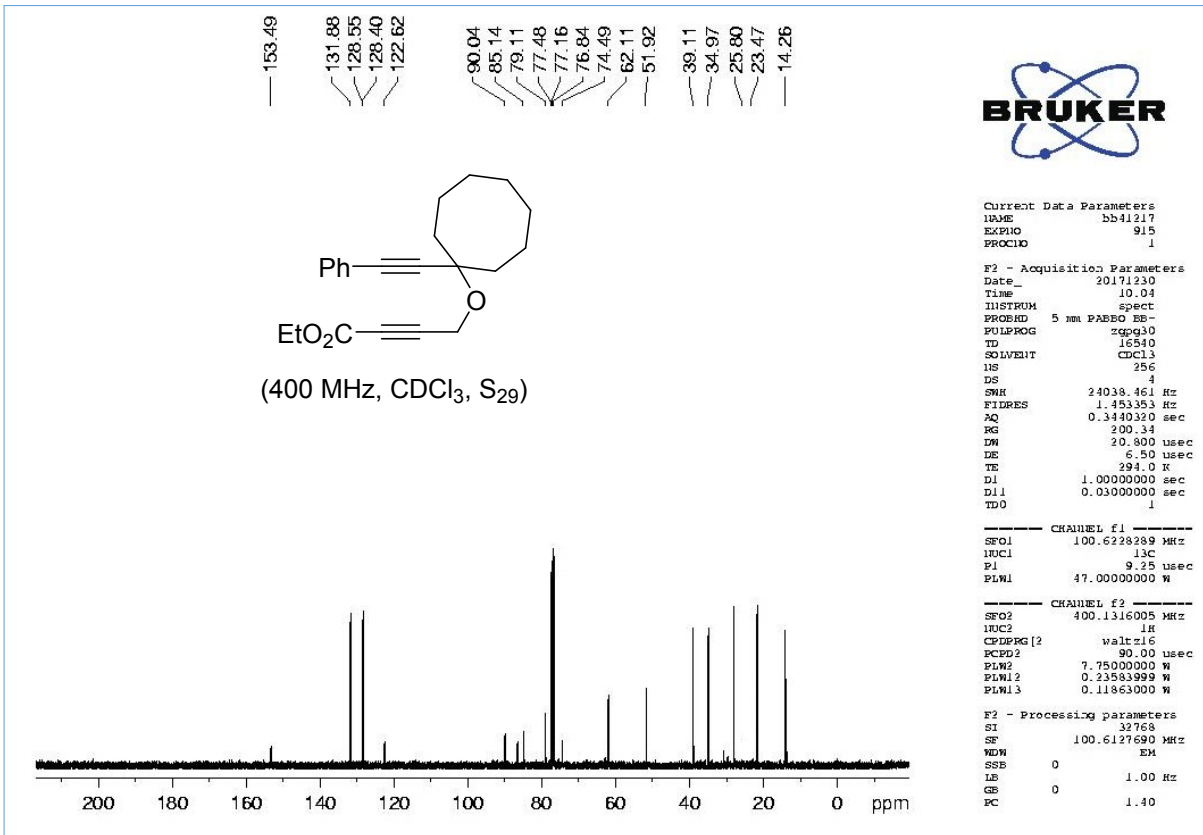


Current Data Parameters
NAME bb41217
EXPNO 914
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171230
Time 9.49
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 79.8
DM 62.400 usec
DE 6.50 usec
TE 293.4 K
D1 0.5000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1320007 MHz
NUC1 1H
P1 15.70 usec
PLW1 7.75000000 W

F2 - Processing parameters
SI 65536
SF 400.1300081 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



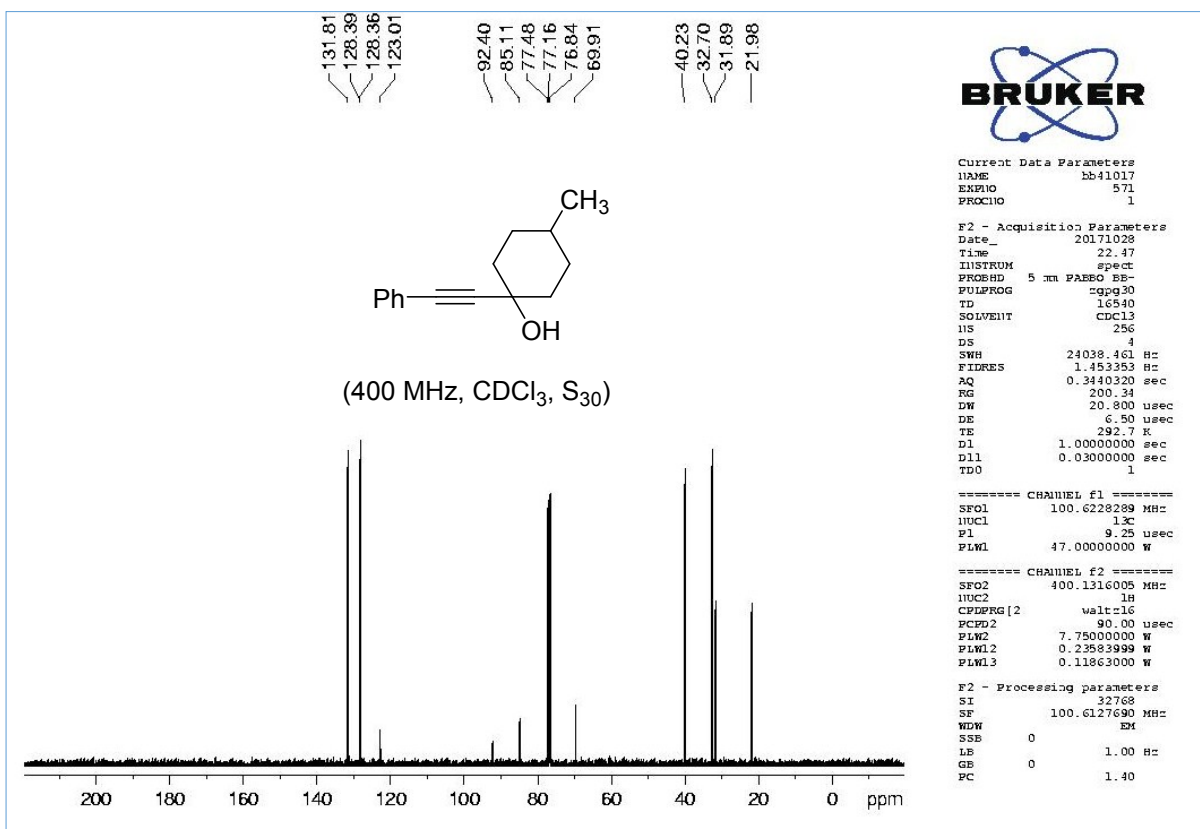
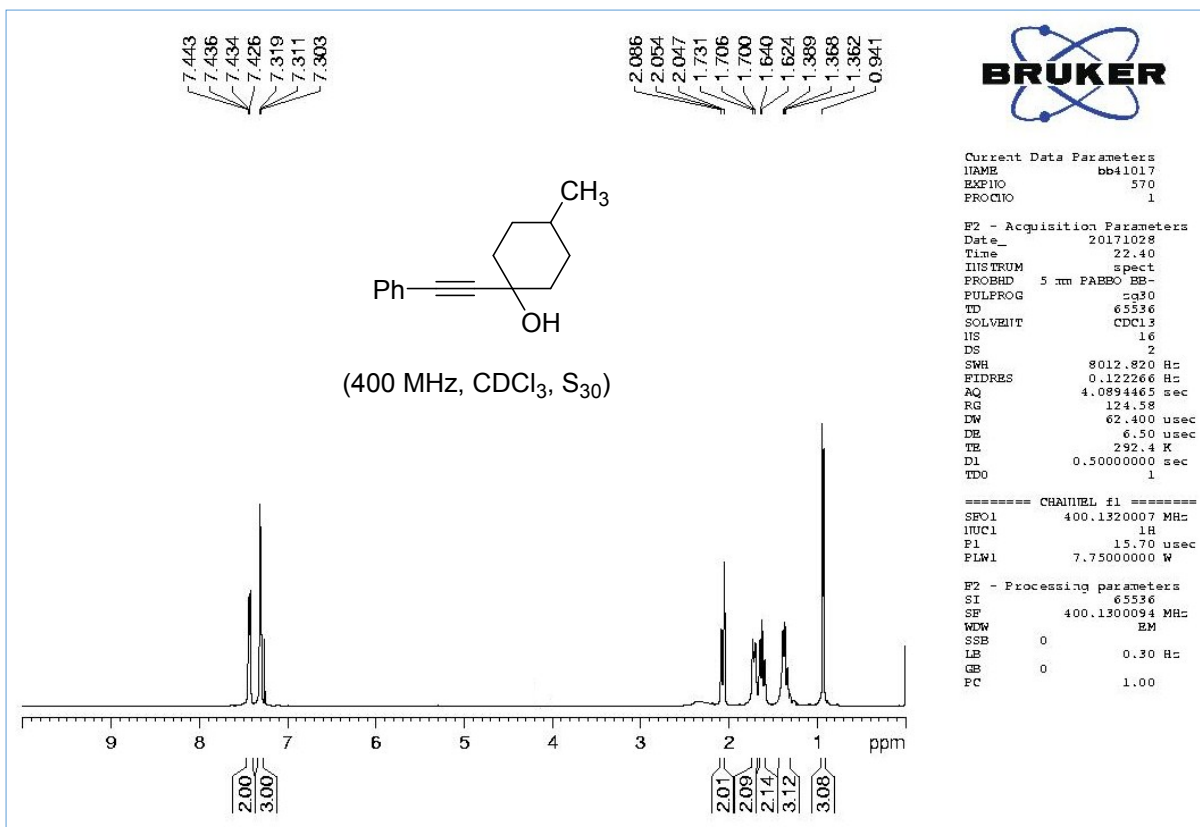
Current Data Parameters
NAME bb41217
EXPNO 915
PROCNO 1

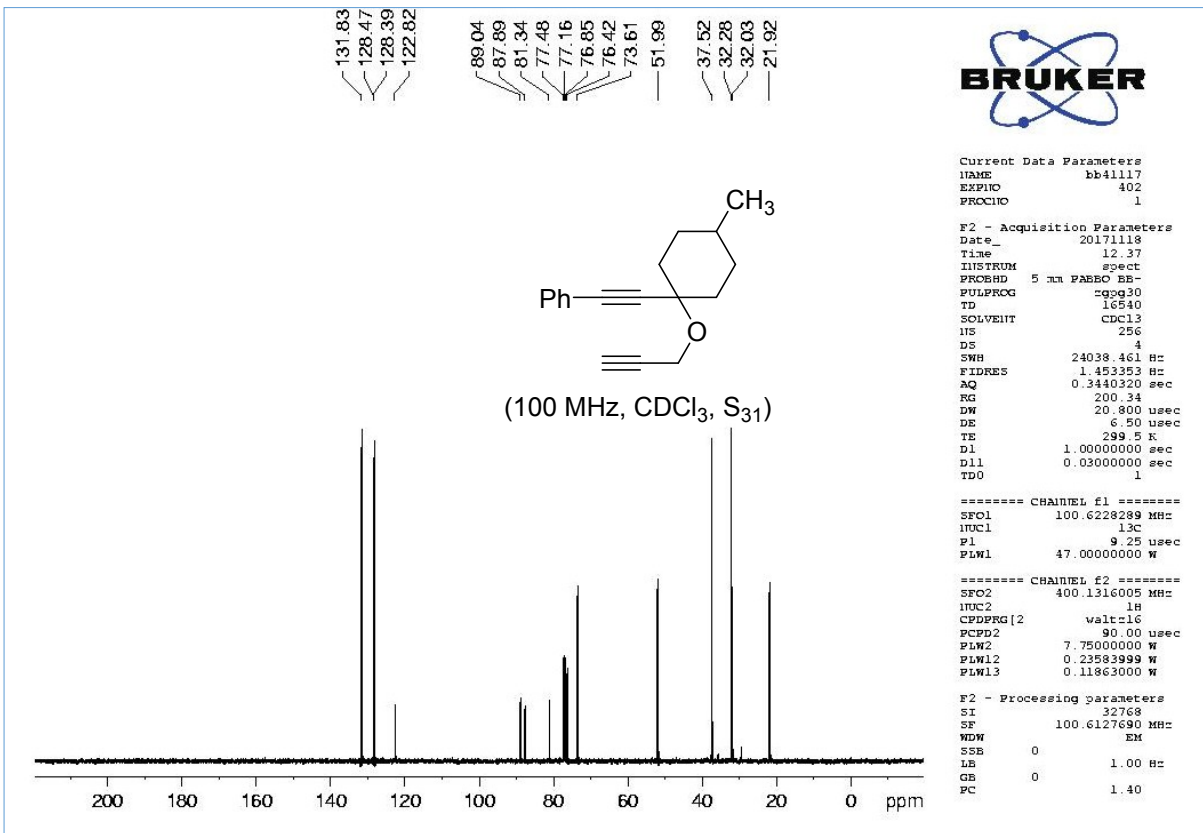
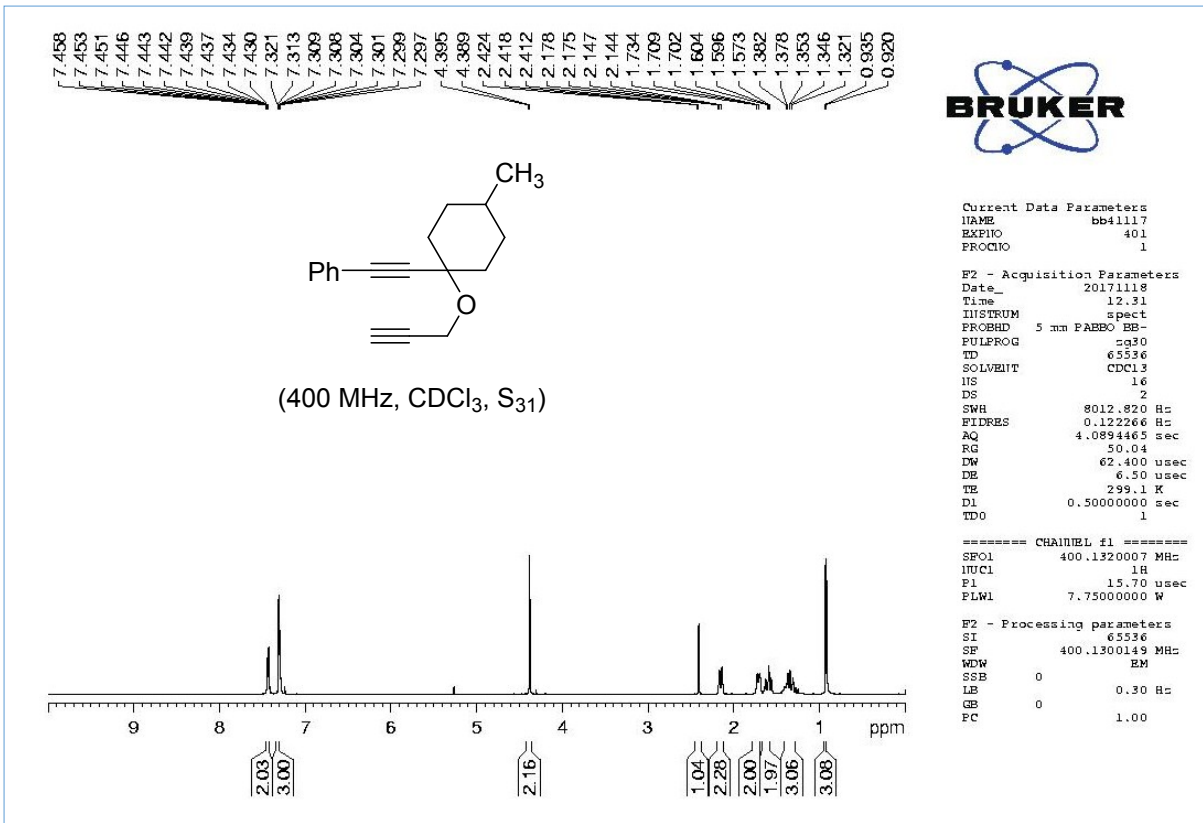
F2 - Acquisition Parameters
Date_ 20171230
Time 10.04
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 16540
SOLVENT CDCl₃
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 1.453353 Hz
AQ 0.3440320 sec
RG 200.34
DM 20.800 usec
DE 6.50 usec
TE 294.0 K
D1 1.0000000 sec
D11 0.0300000 sec
TD0 1

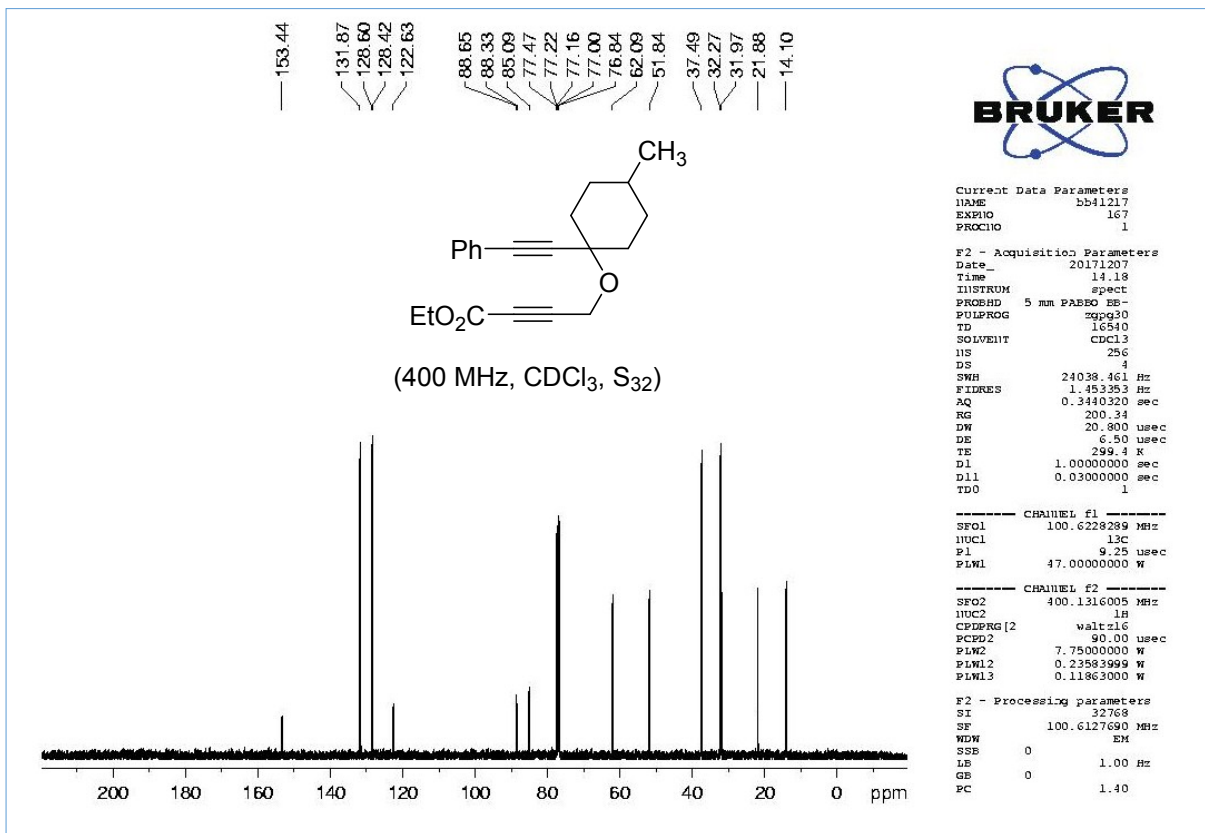
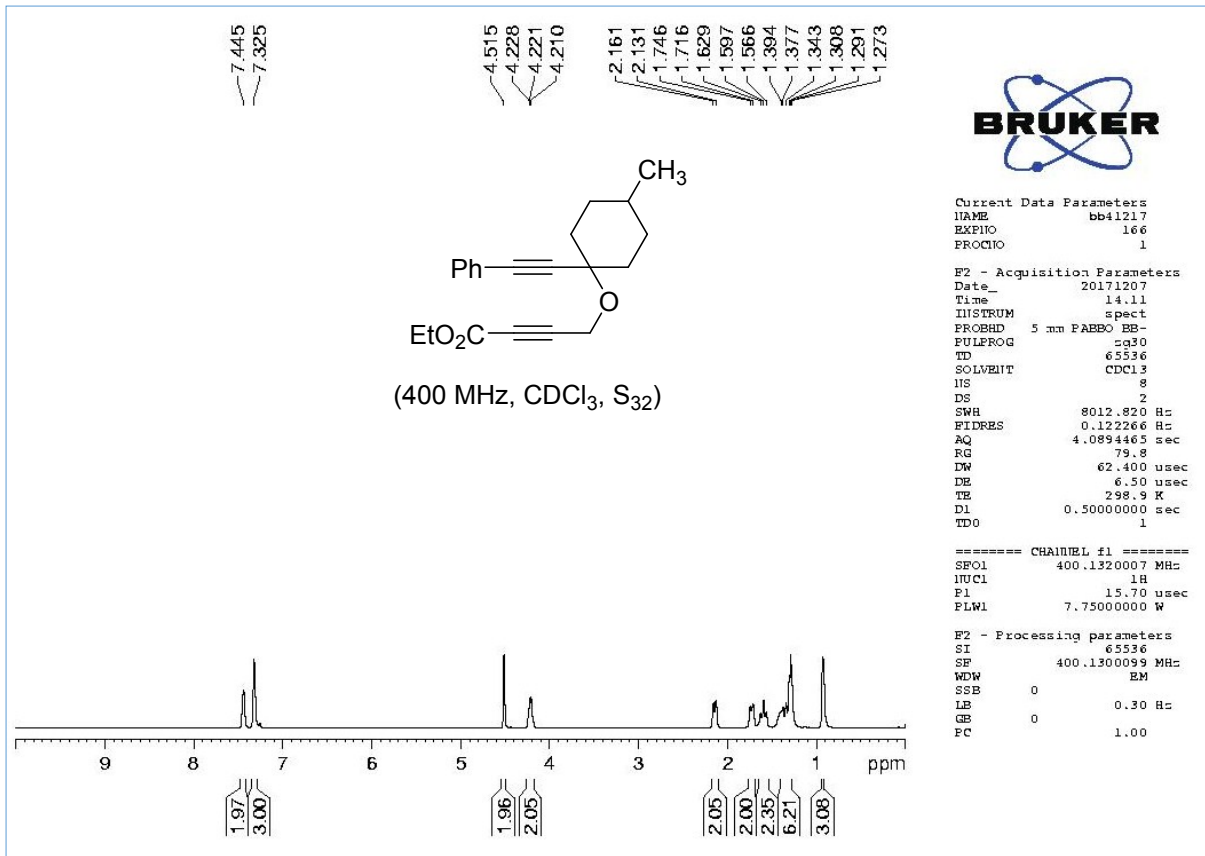
==== CHANNEL f1 =====
SFO1 100.6228289 MHz
NUC1 13C
P1 9.25 usec
PLW1 47.0000000 W

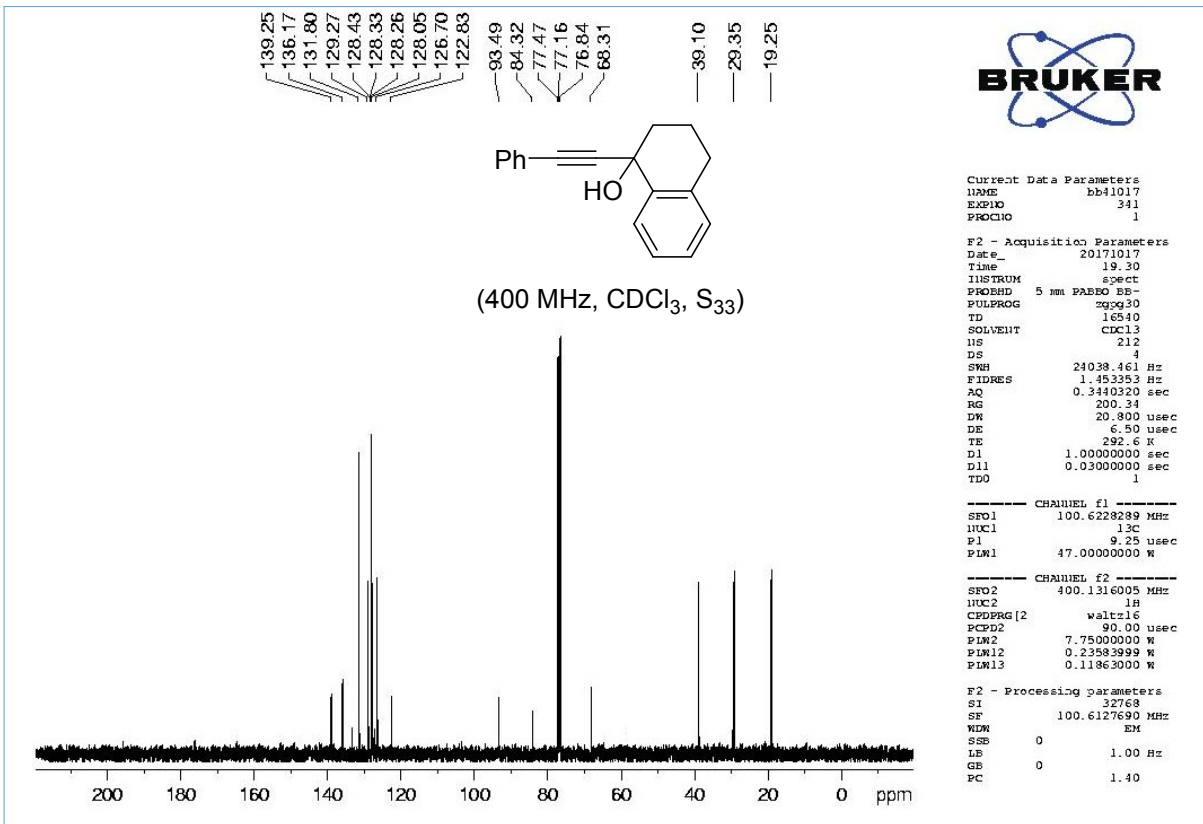
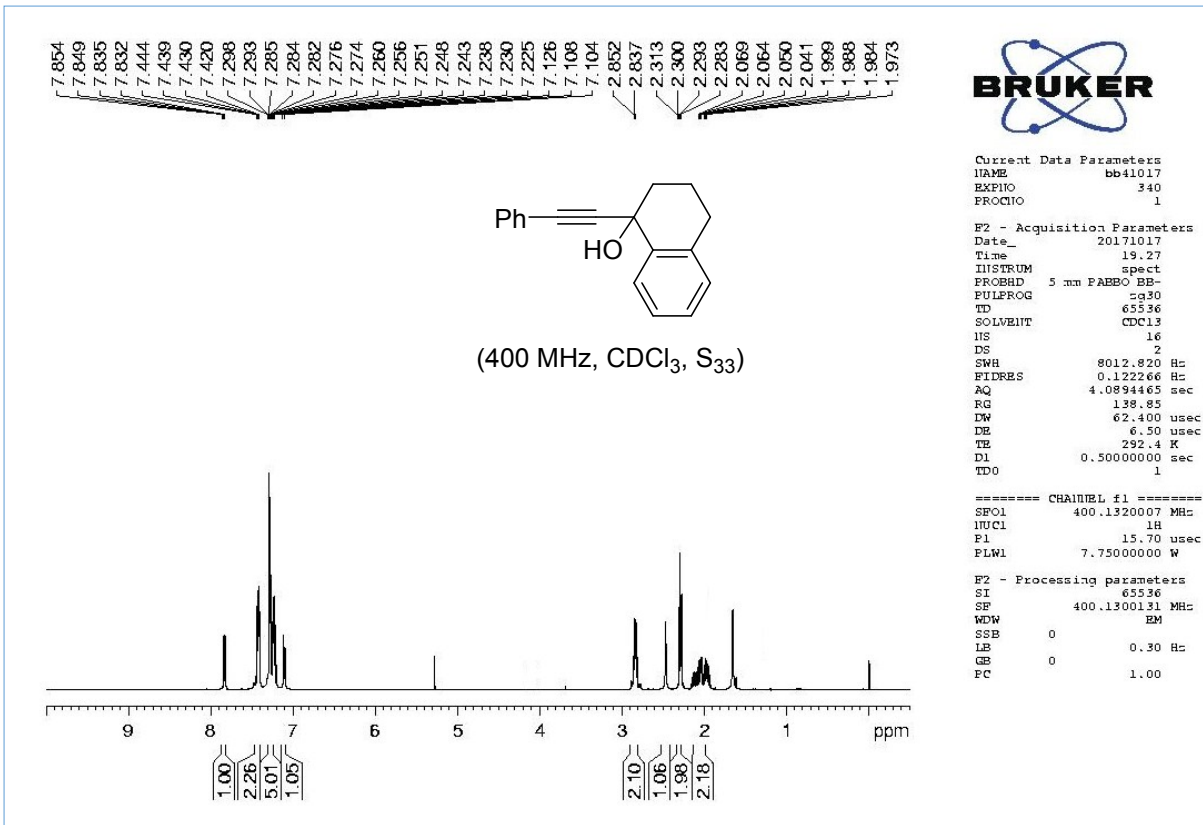
==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
PLW13 0.11863000 W

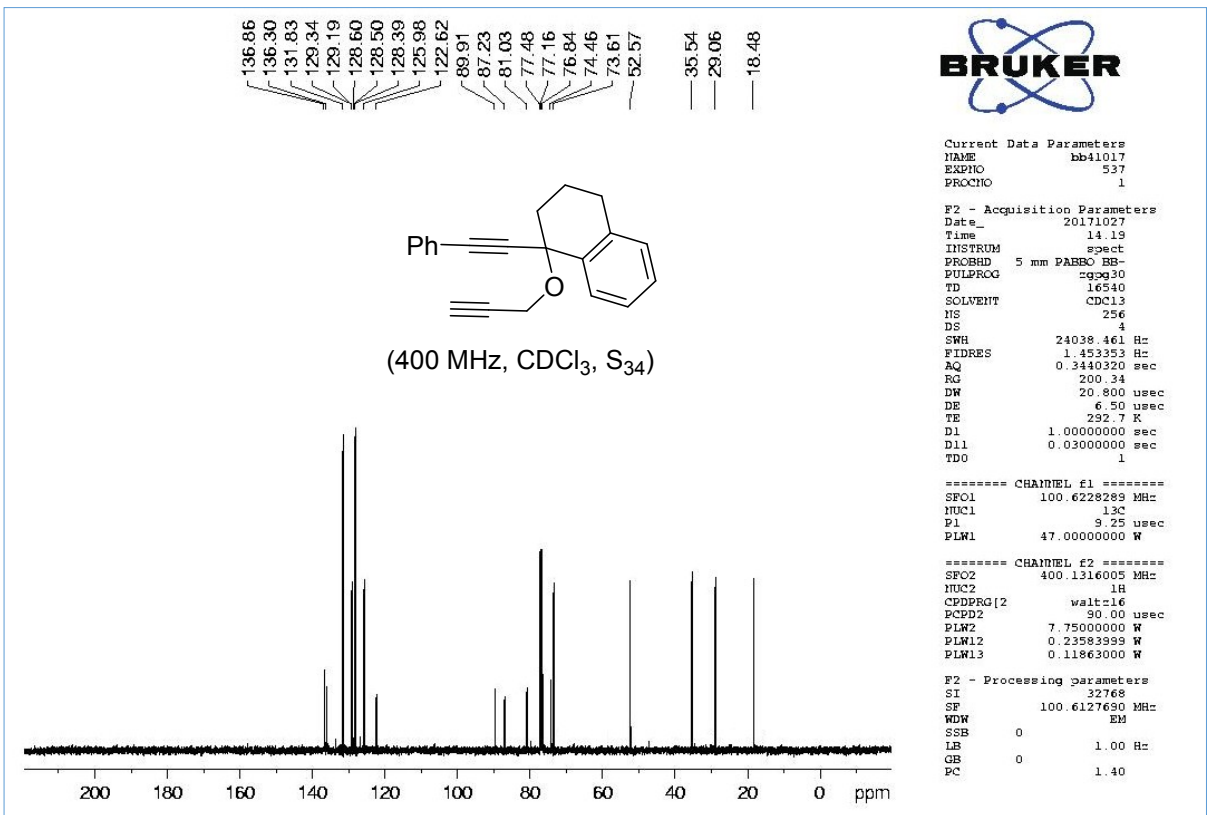
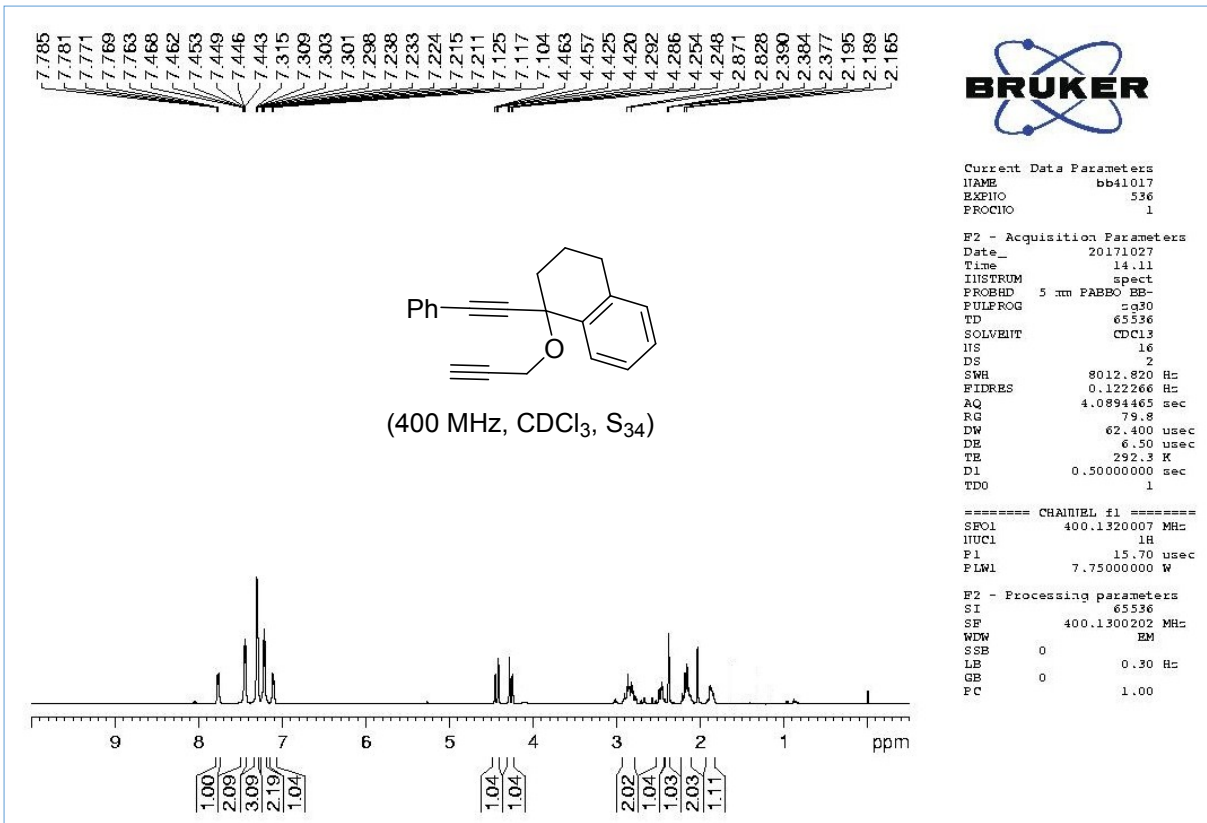
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

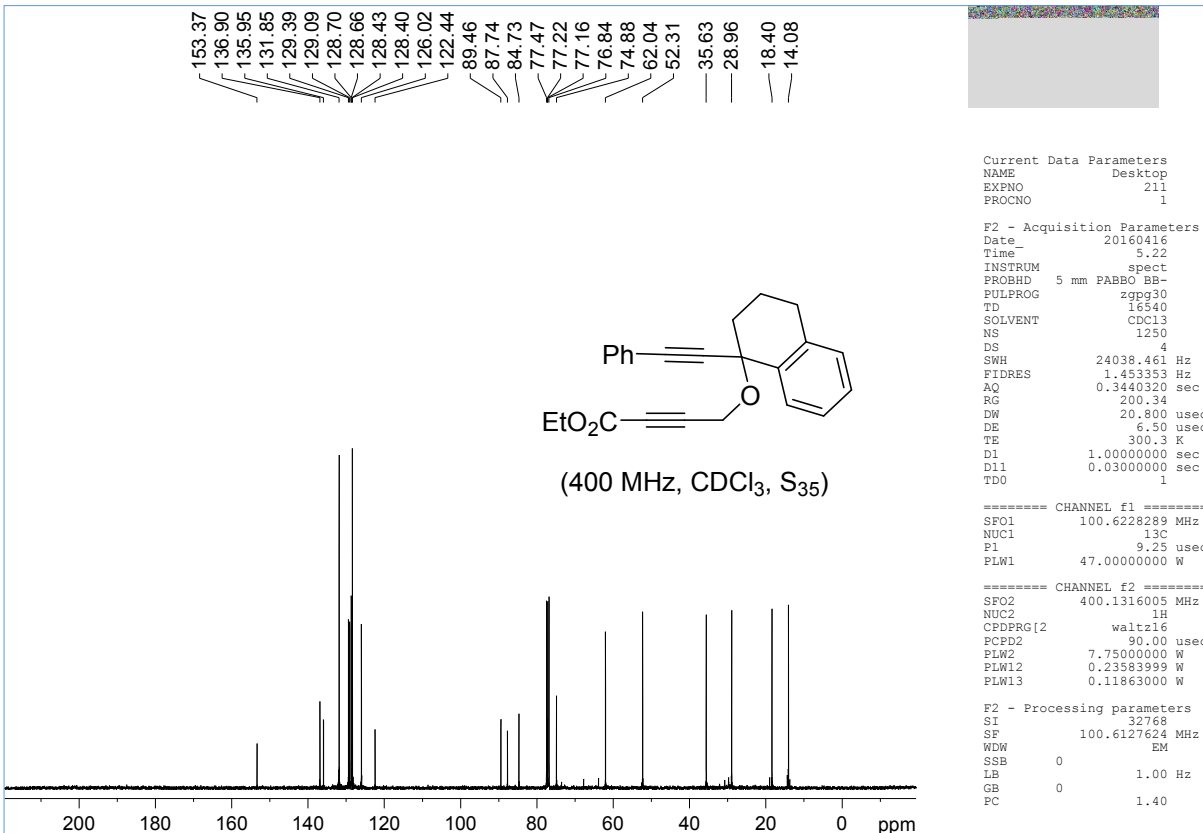
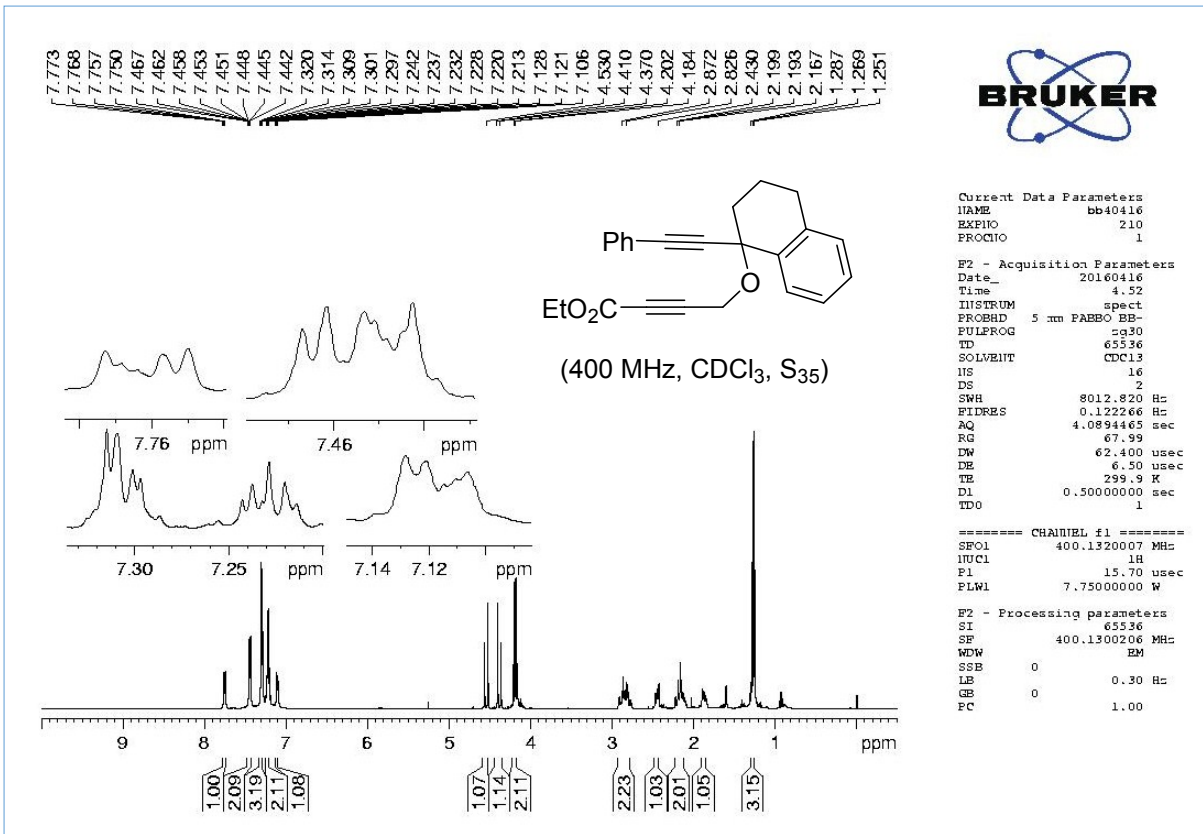


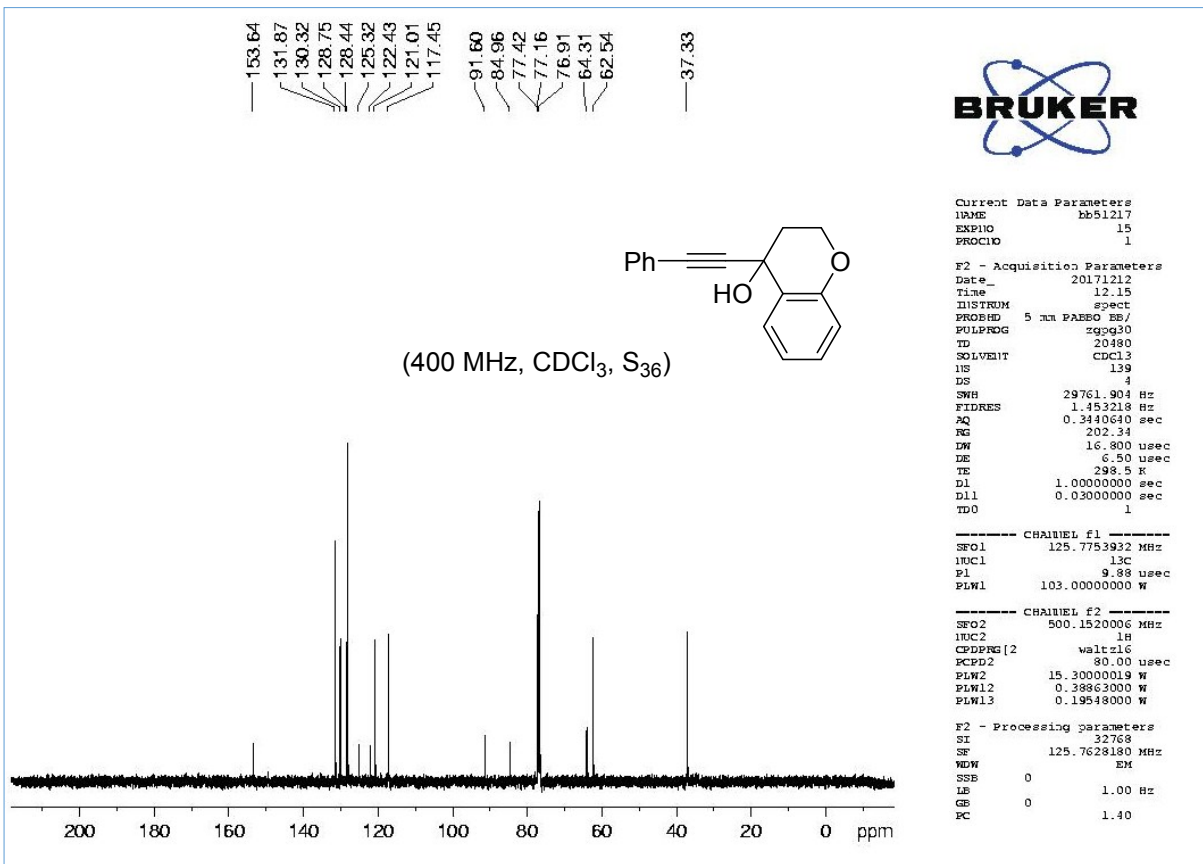
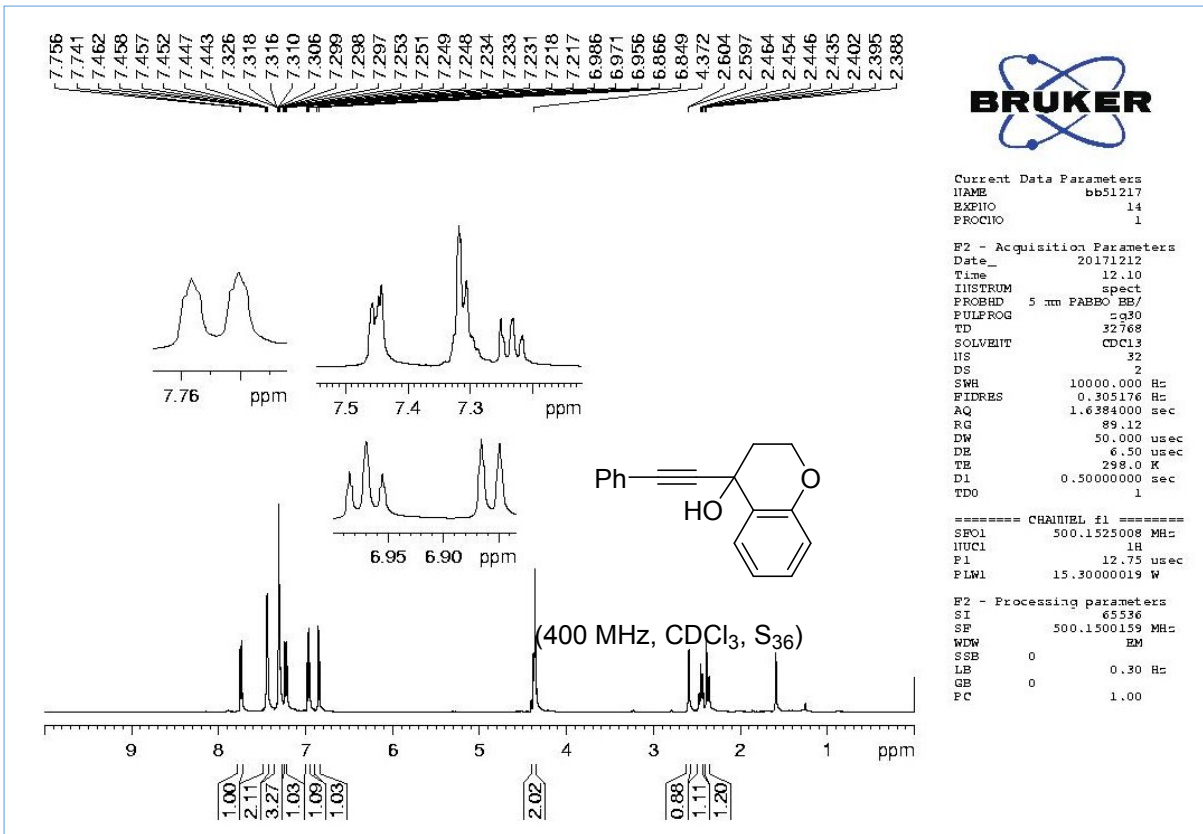










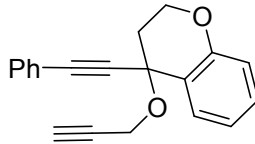


7.659
7.656
7.644
7.641
7.488
7.484
7.481
7.479
7.474
7.469
7.340
7.338
7.326
7.251
7.248
6.947
6.931
6.871
6.854
4.527
4.522
4.497
4.492
4.488
4.486
4.337
4.236
4.231
4.206
4.201
2.556
2.553
2.528
2.428
2.412
2.404
2.391
2.386
2.384
2.381

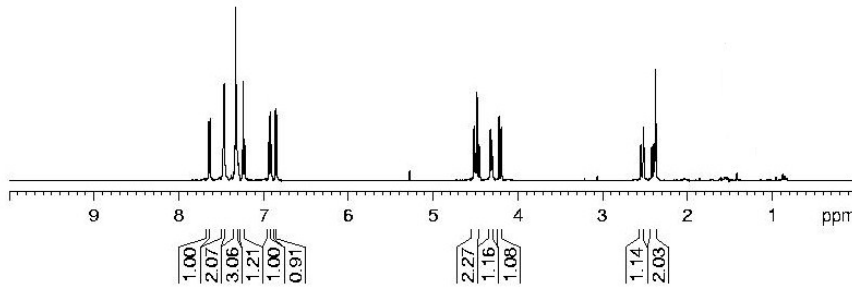


Current Data Parameters
NAME bb51217
EXPTO 33
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171213
Time 15.11
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 1.6384000 sec
RG 89.12
DW 50.000 usec
DE 6.50 usec
TE 298.0 K
D1 0.50000000 sec
TDO 1



(400 MHz, CDCl₃, S₃₇)



----- CHANNEL f1 -----
SFO1 500.1525008 MHz
NUC1 1H
P1 12.75 usec
PLW1 15.30000019 W

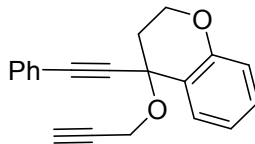
F2 - Processing parameters
SI 65536
SF 500.1500161 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

154.05
131.94
130.68
129.86
128.92
128.50
122.24
121.31
120.03
117.54
87.99
87.62
80.63
77.42
77.16
76.91
73.86
70.13
62.04
52.60
34.94

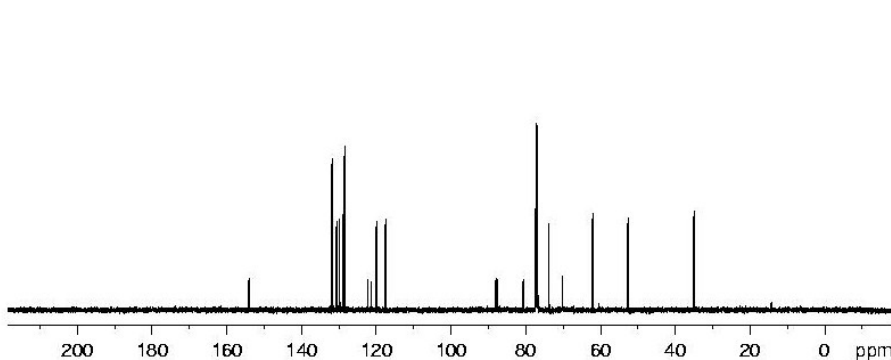


Current Data Parameters
NAME bb51217
EXPTO 34
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171213
Time 15.19
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 30480
SOLVENT CDCl3
NS 256
DS 4
SWH 29761.904 Hz
FIDRES 1.453218 Hz
AQ 0.3440640 sec
RG 202.34
DW 16.800 usec
DE 6.50 usec
TE 298.9 K
D1 1.00000000 sec
D11 0.03000000 sec
TDO 1



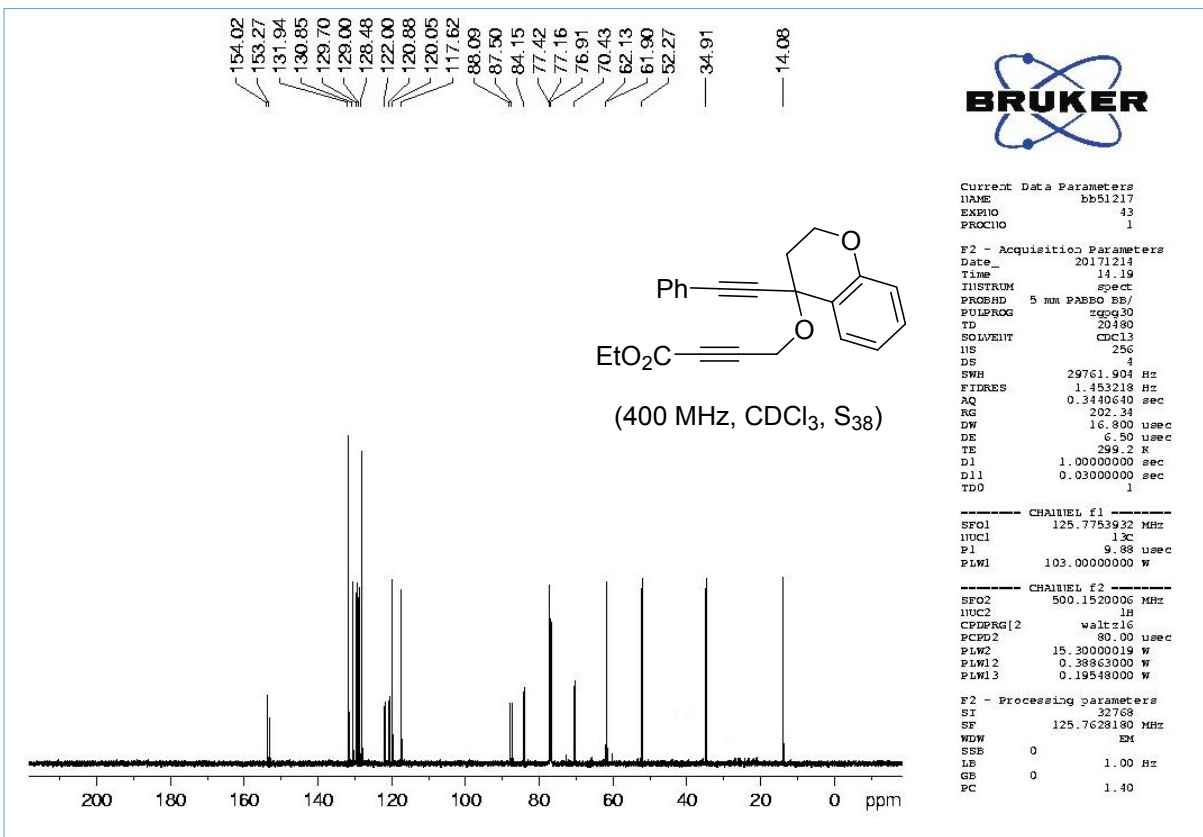
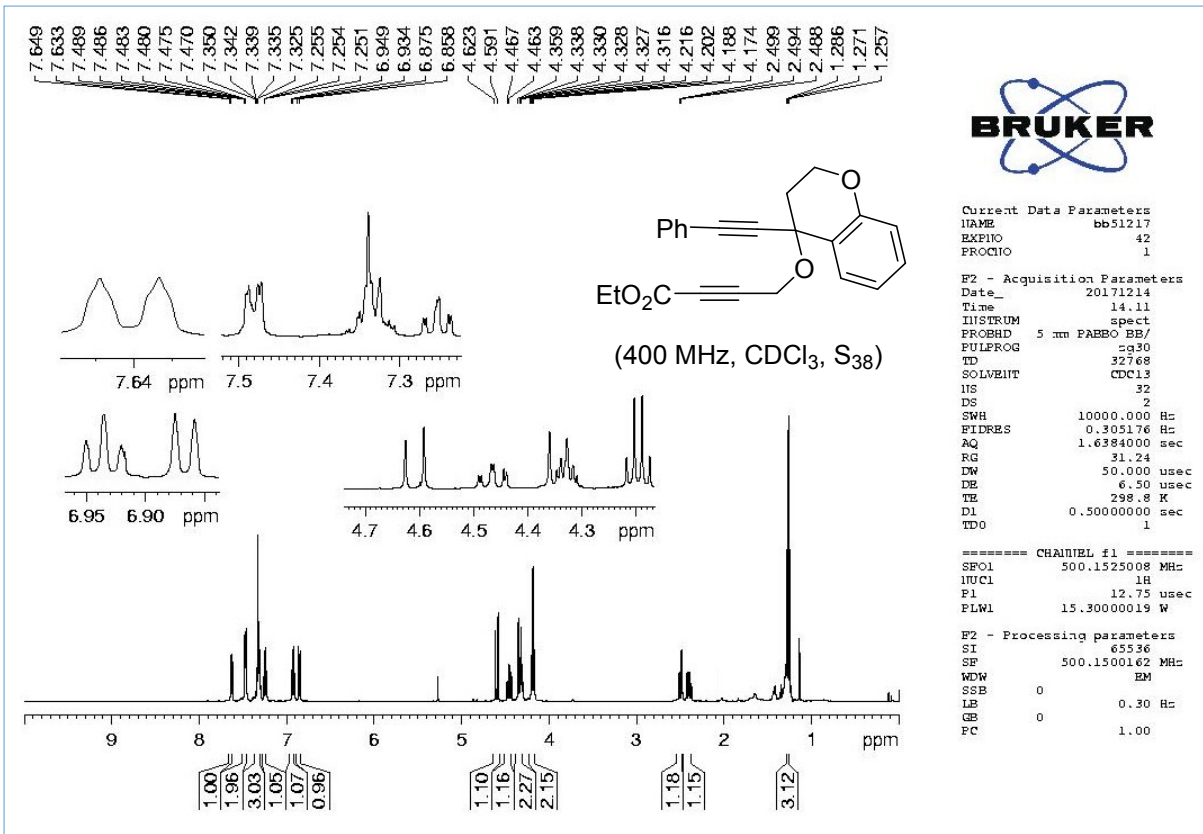
(400 MHz, CDCl₃, S₃₇)

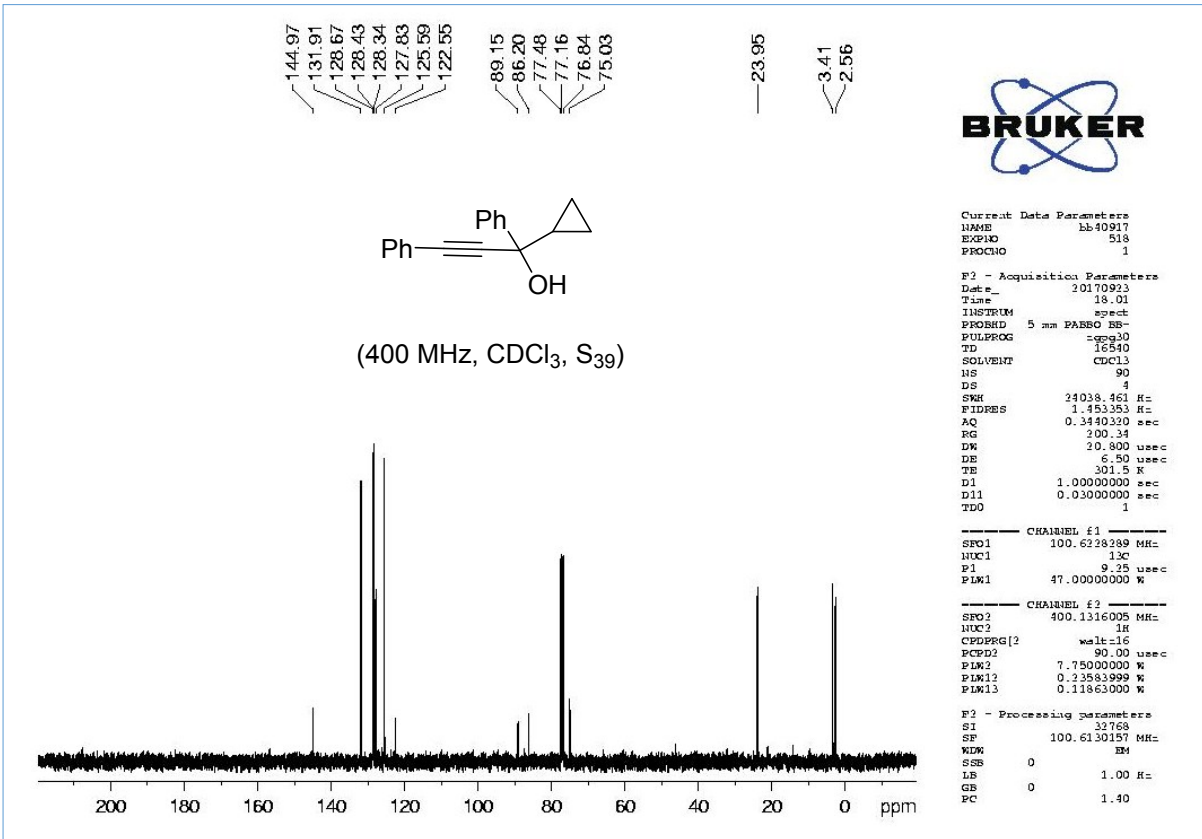
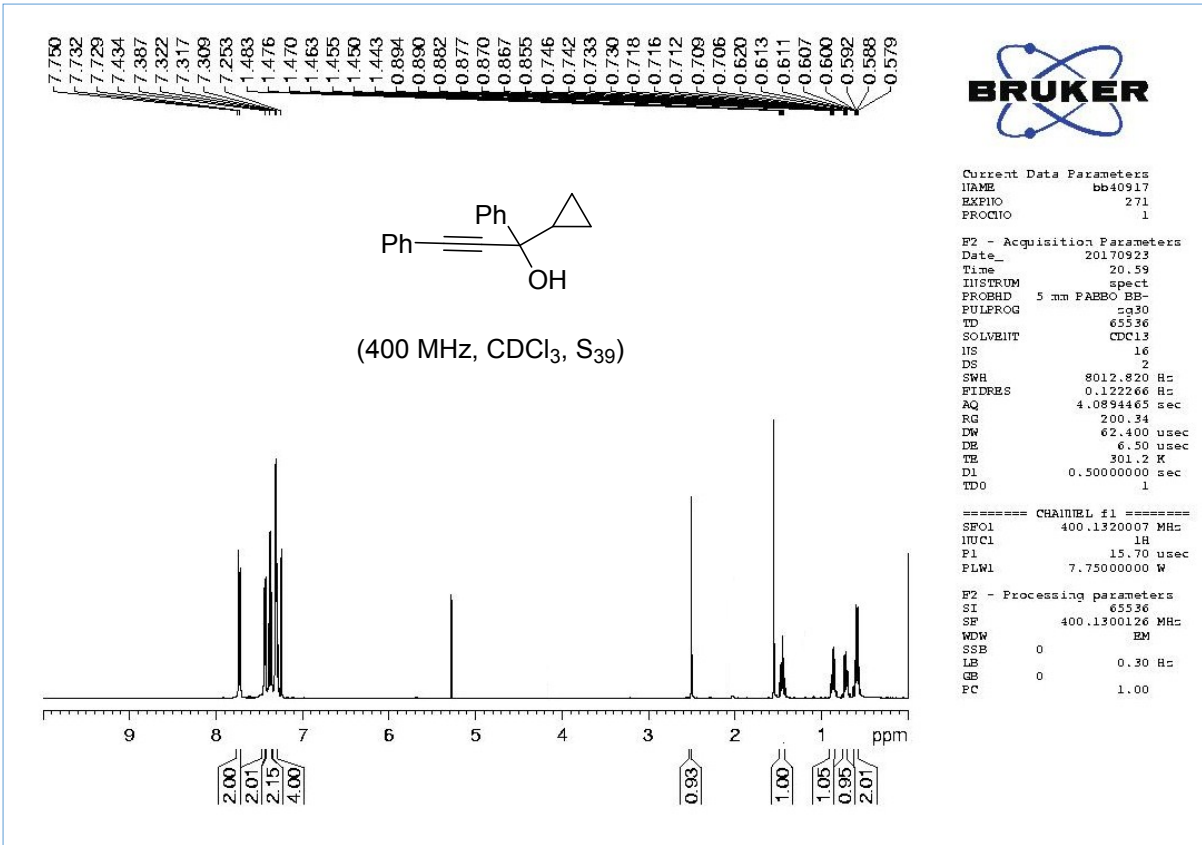


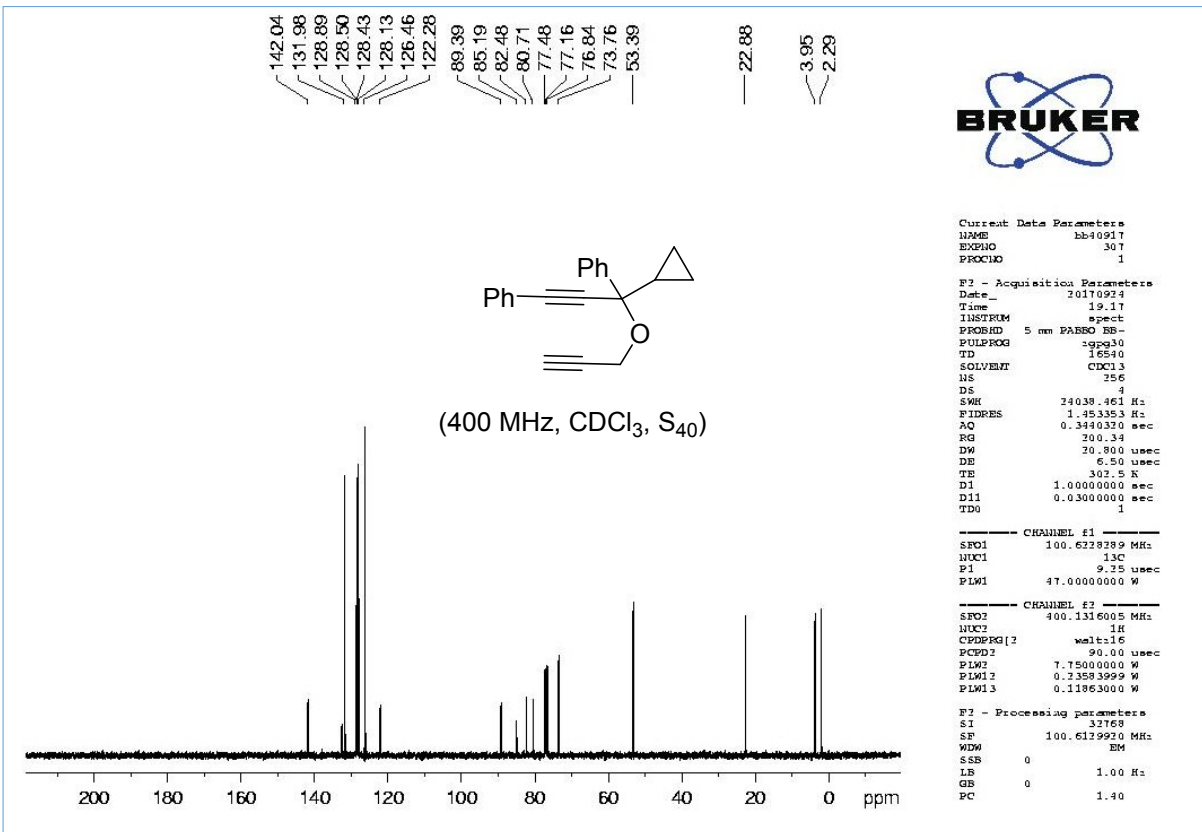
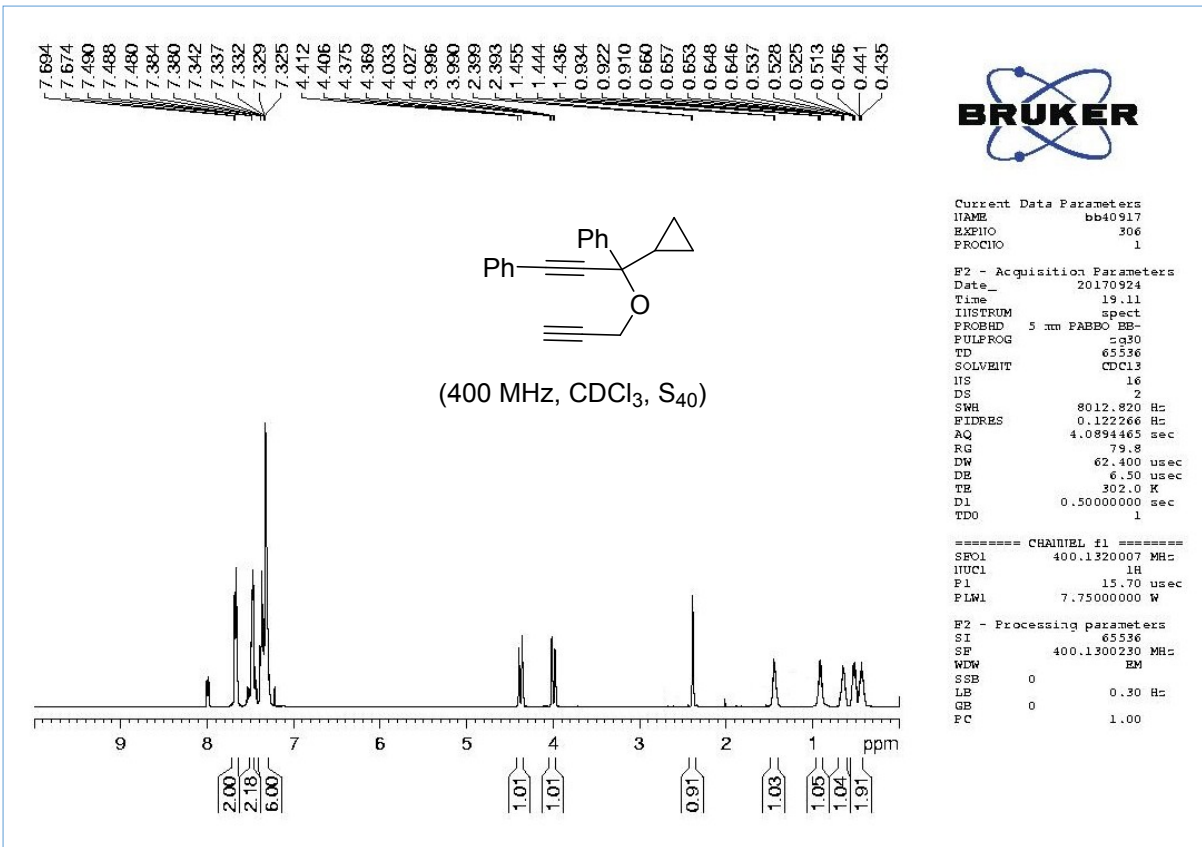
----- CHANNEL f1 -----
SFO1 125.7753932 MHz
NUC1 13C
P1 9.88 usec
PLW1 103.00000000 W

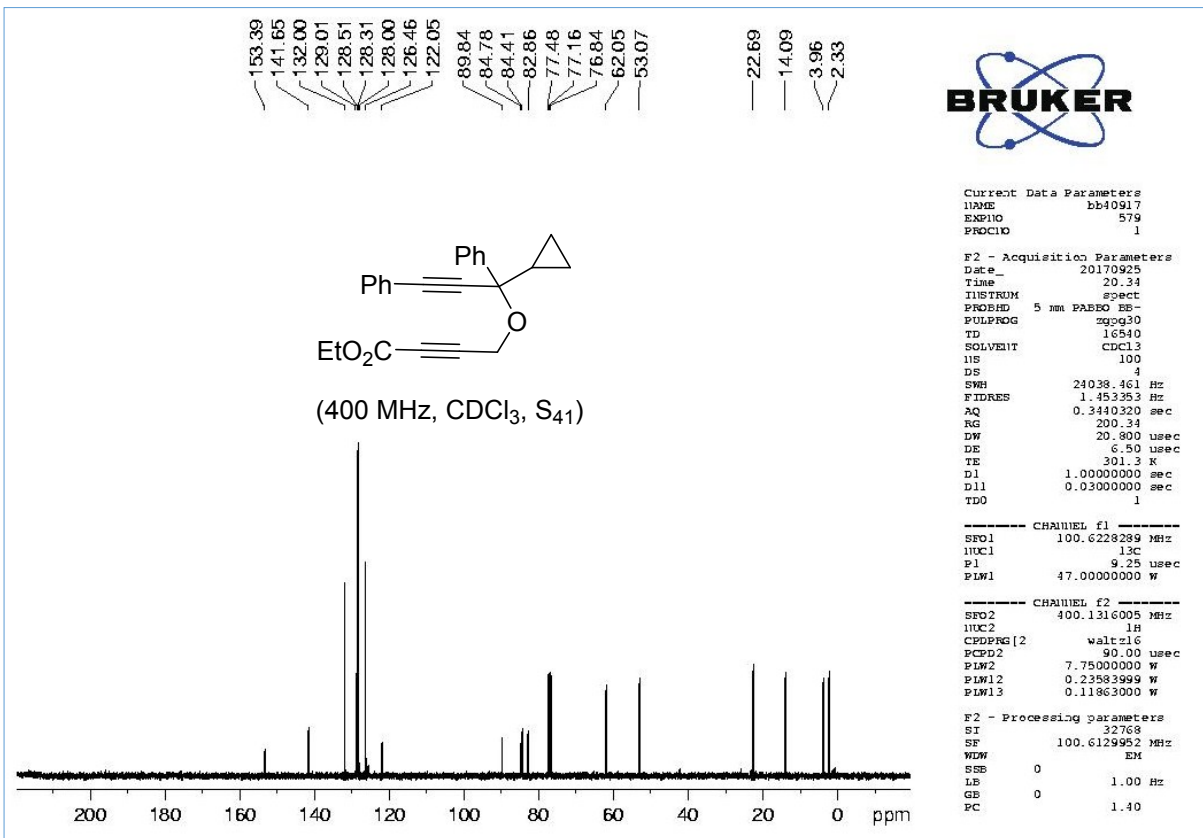
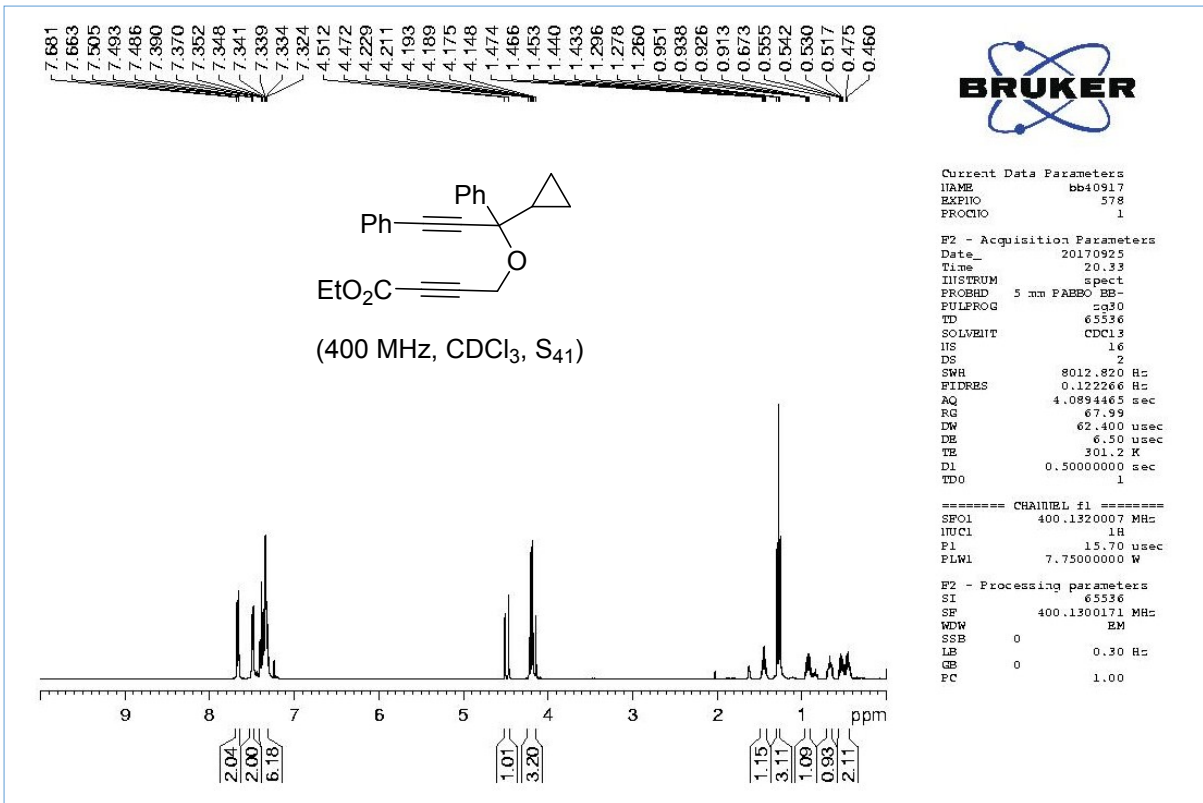
----- CHANNEL f2 -----
SFO2 500.1520005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 15.30000019 W
PLW12 0.38863000 W
PLW13 0.19548000 W

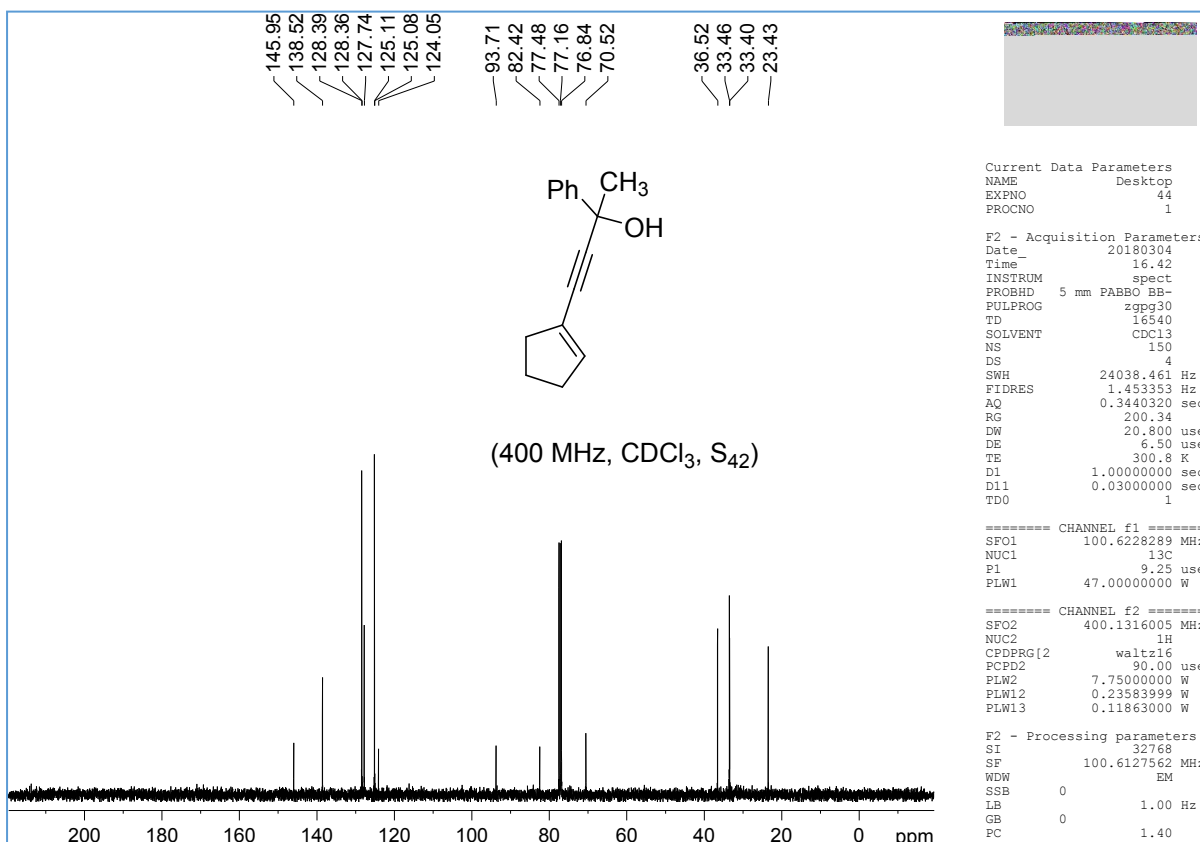
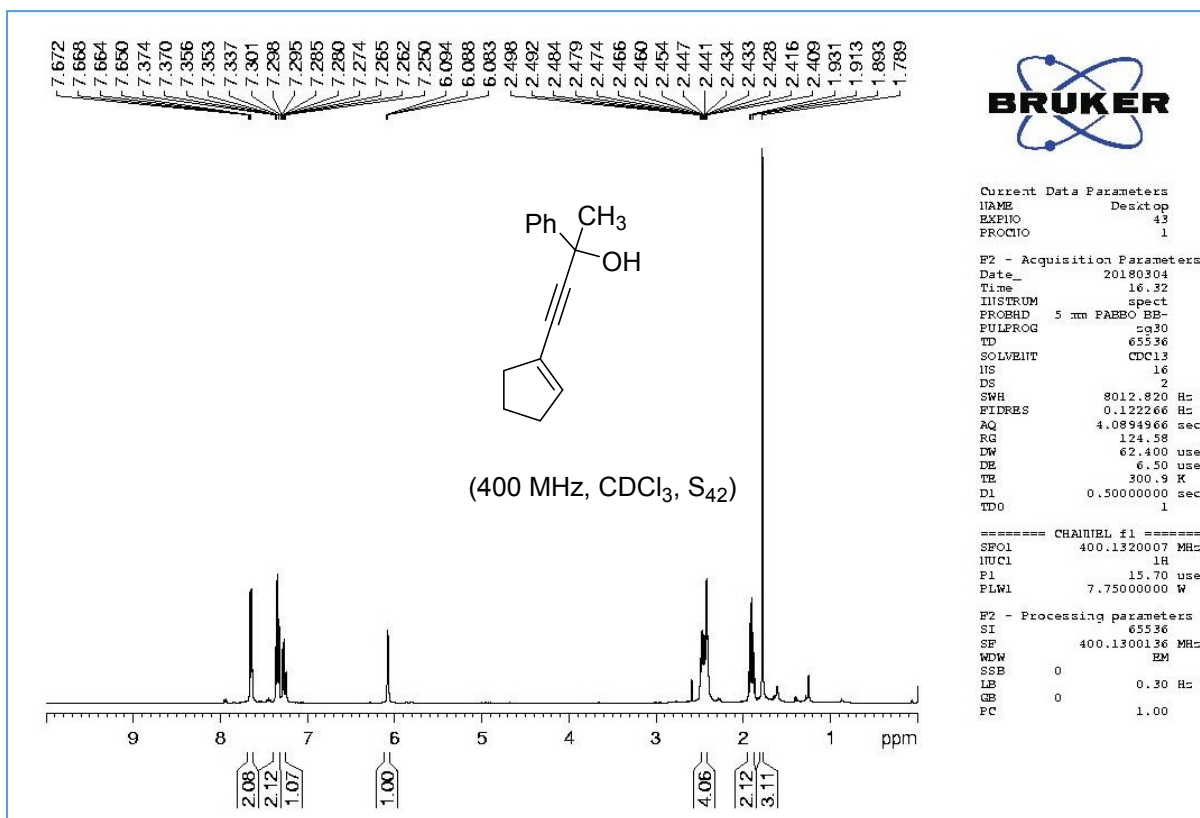
F2 - Processing parameters
SI 32768
SF 125.7628180 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

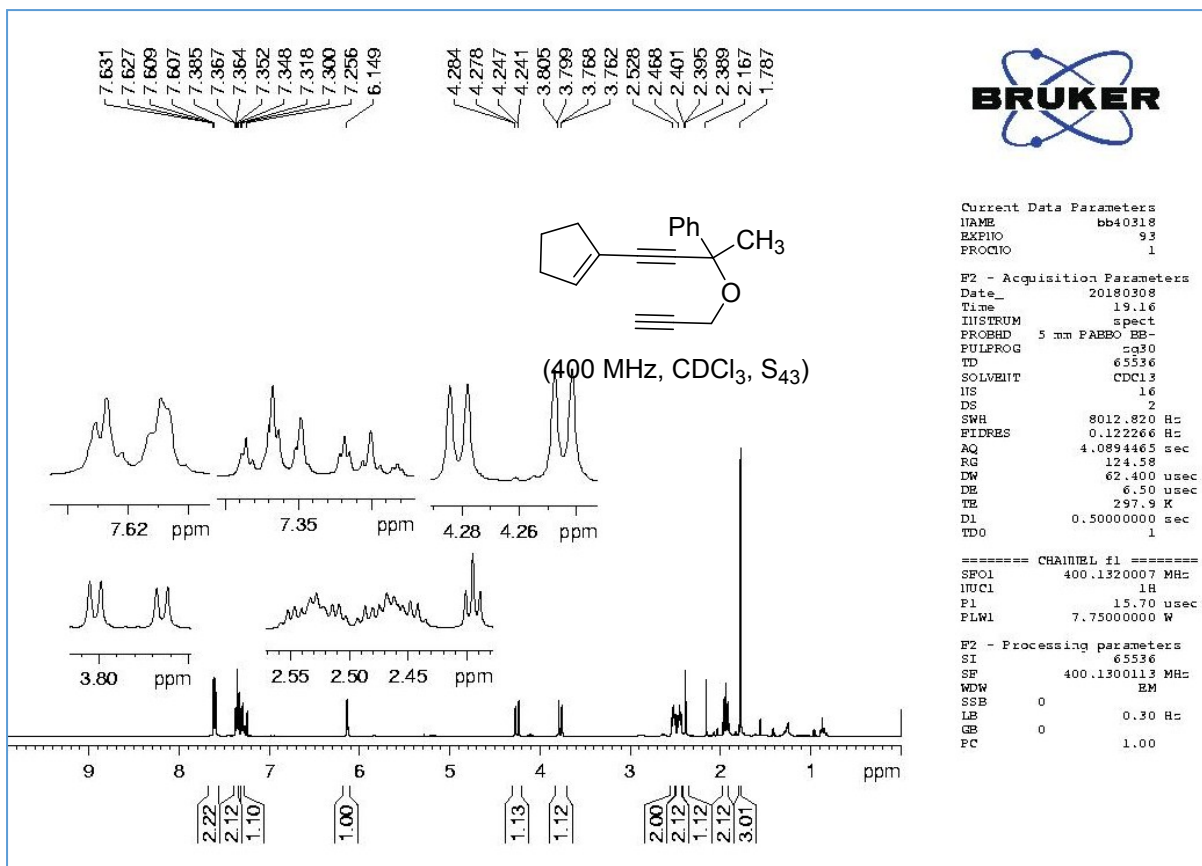










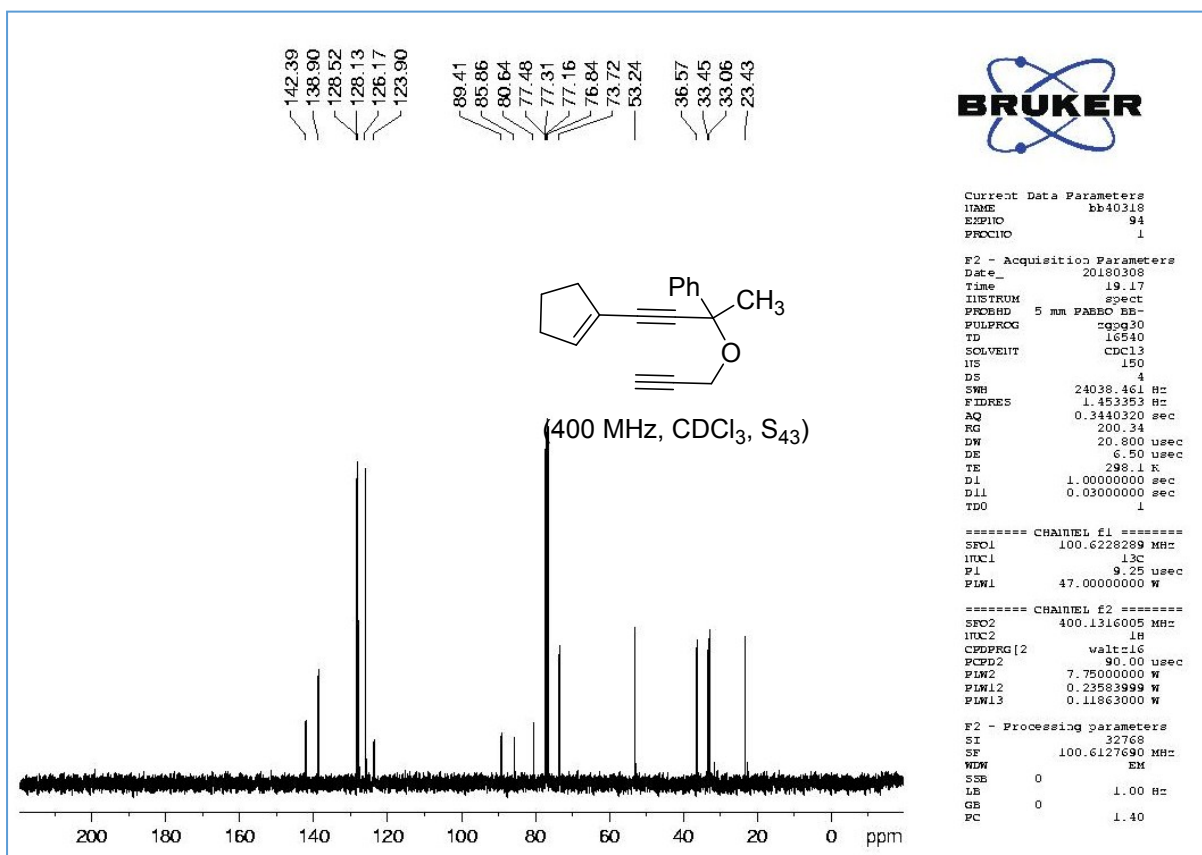


Current Data Parameters
 NAME bb40318
 EXPNO 93
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180308
 Time 19.16
 INSTRUM spect
 PROBHD 5 mm FAPBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 124.58
 DW 62.400 usec
 DE 6.50 usec
 TE 297.9 K
 D1 0.50000000 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 400.1320007 MHz
 NUCL1 1H
 P1 15.70 usec
 PLW1 7.75000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1300113 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



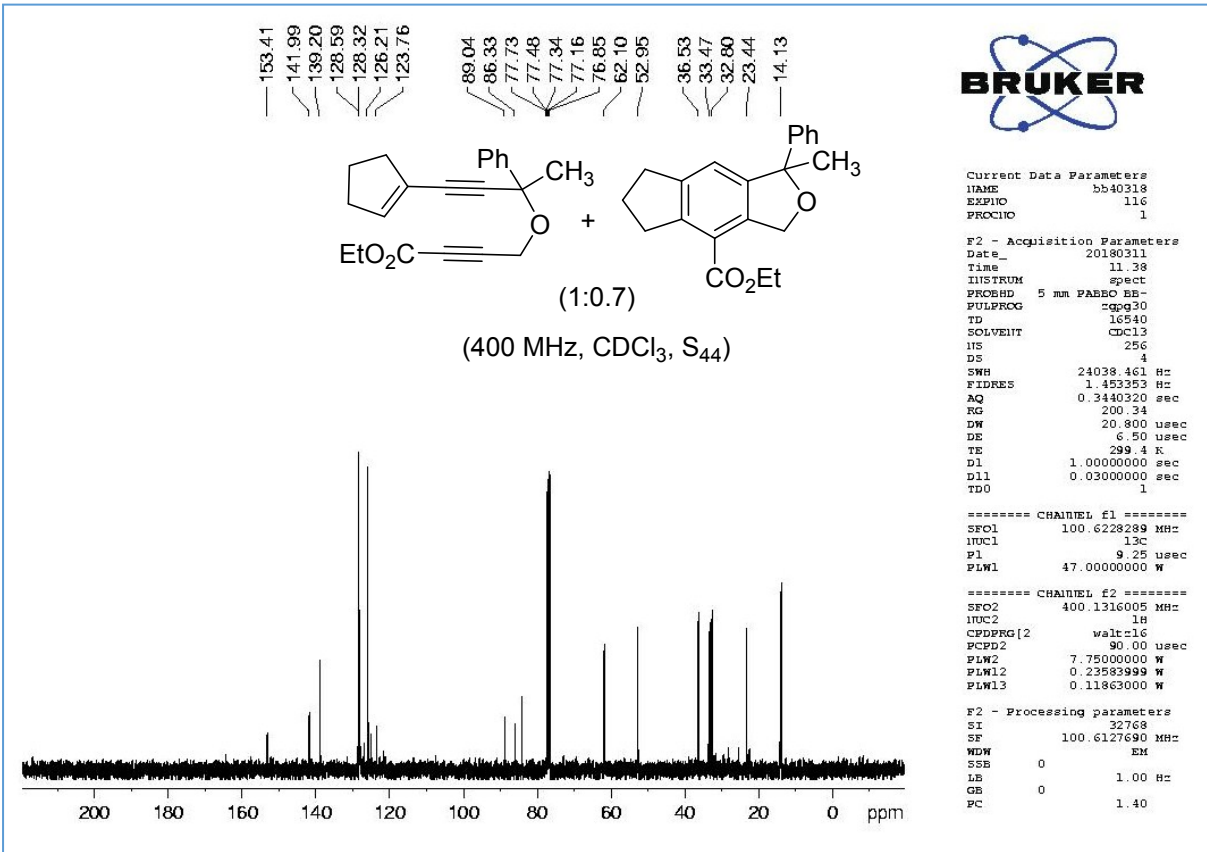
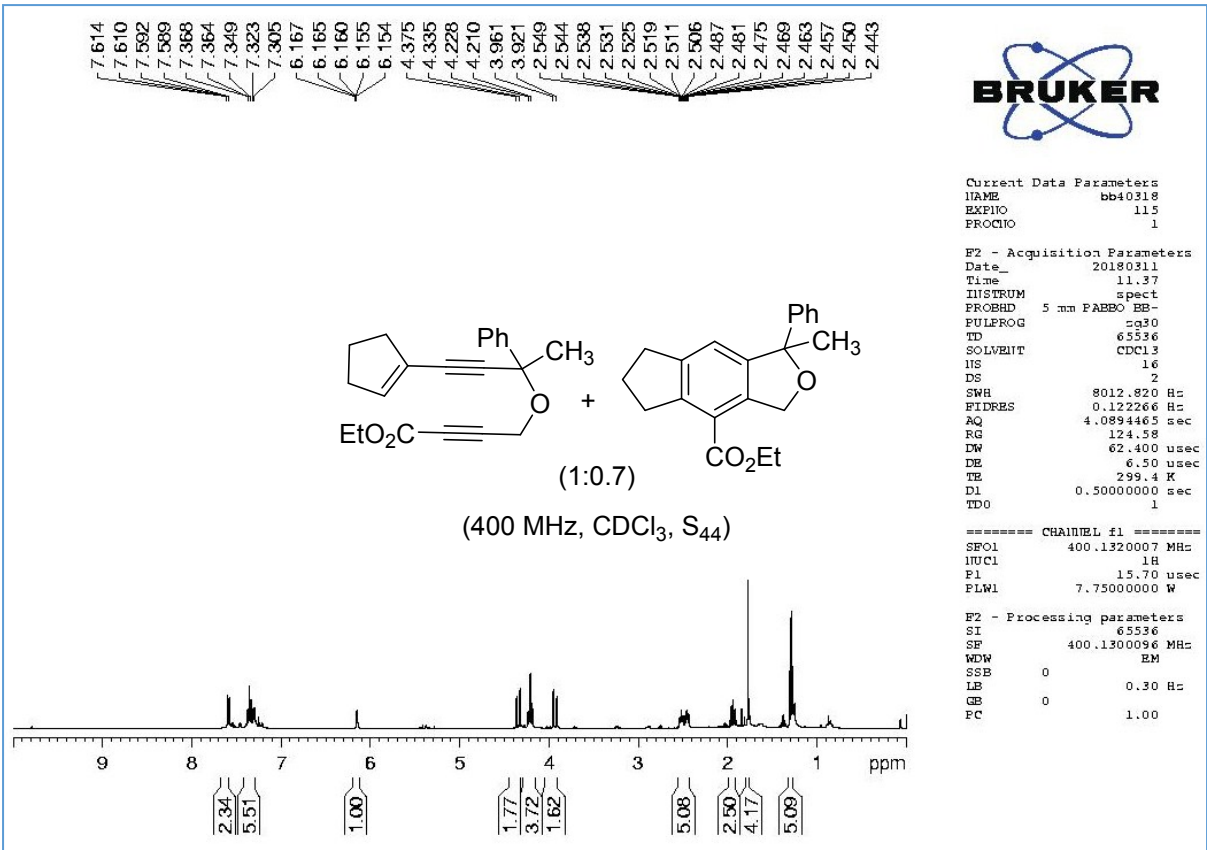
Current Data Parameters
 NAME bb40318
 EXPNO 94
 PROCNO 1

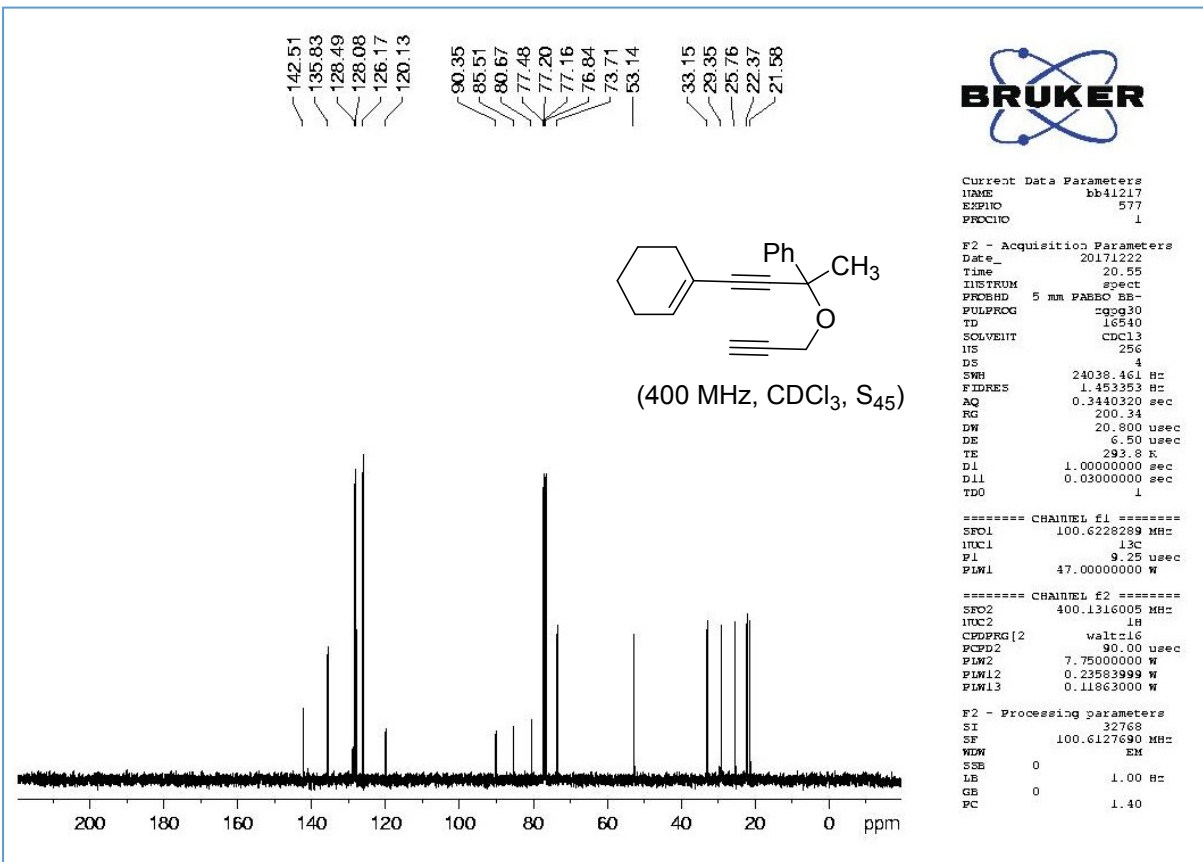
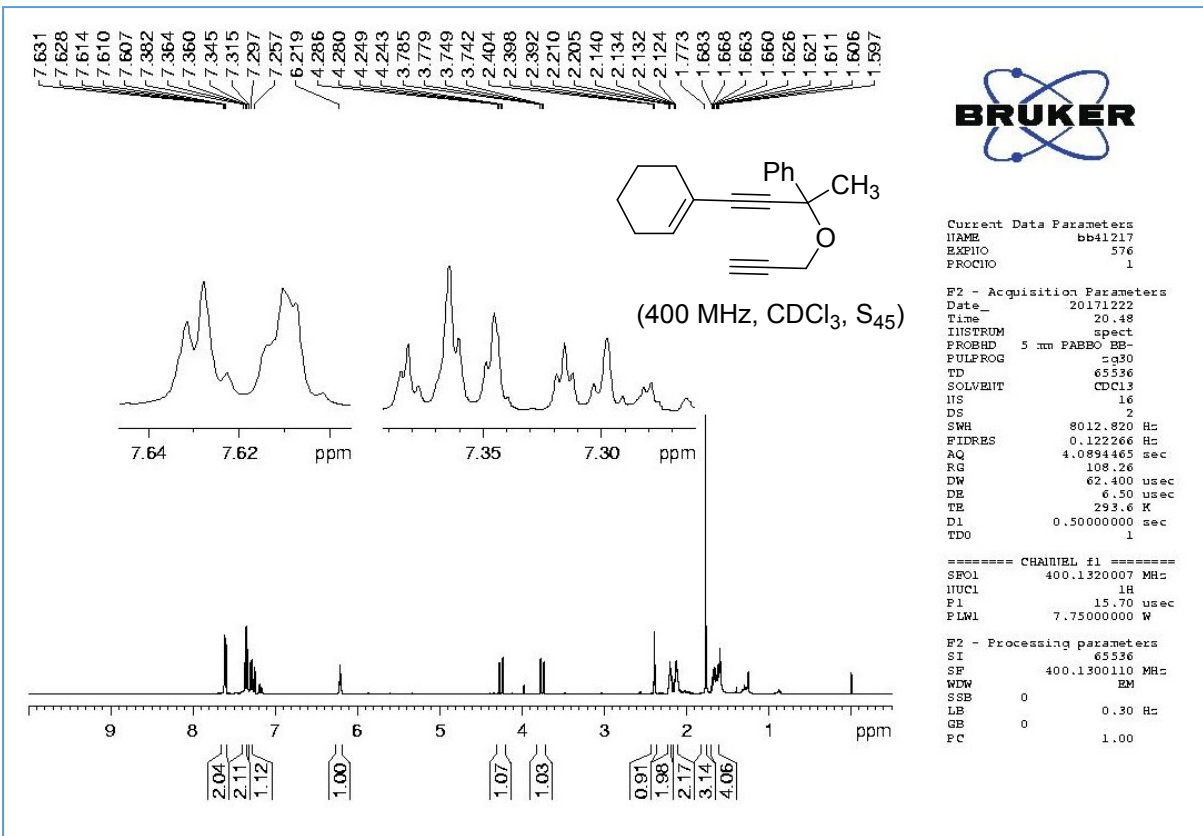
F2 - Acquisition Parameters
 Date_ 20180308
 Time 19.17
 INSTRUM spect
 PROBHD 5 mm FAPBO BB-
 PULPROG zgpg30
 TD 16640
 SOLVENT CDCl3
 NS 150
 DS 4
 SWH 24038.461 Hz
 FIDRES 1.453353 Hz
 AQ 0.3440320 sec
 RG 200.34
 DW 20.800 usec
 DE 6.50 usec
 TE 298.1 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 100.6228289 MHz
 NUCL1 13C
 P1 9.25 usec
 PLW1 47.00000000 W

==== CHANNEL f2 =====
 SFO2 400.1316005 MHz
 NUCL2 1H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 7.75000000 W
 PLW12 0.23583999 W
 PLW13 0.11863000 W

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40





7.479
7.476
7.458
7.456
7.365
7.346
7.337
7.319
7.316
7.303
7.299
7.259
7.061
5.295
5.283
5.263
4.348
4.343
4.339
4.330
4.326
4.228
4.211
3.941
3.901
2.813
2.205
2.200
2.141
2.135
2.132
2.125
2.120
1.839
1.768
1.391
1.373
1.355
1.297
1.279

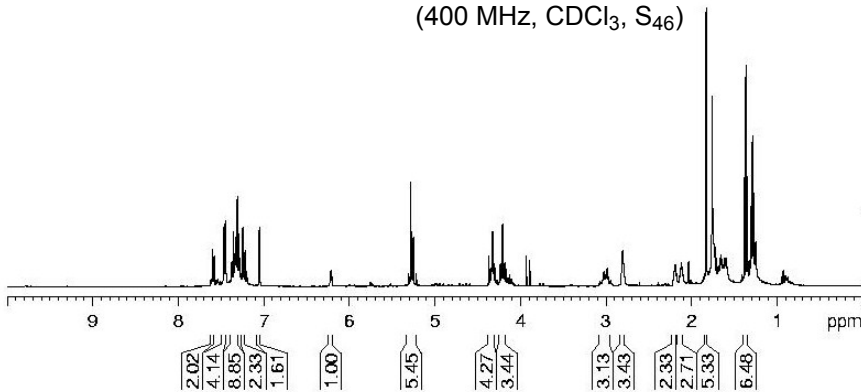
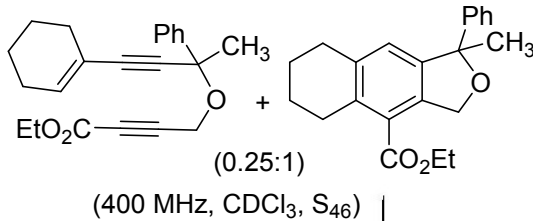


Current Data Parameters
NAME bb41217
EXPHO 912
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171230
Time 9.37
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
HS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 124.58
DW 62.400 usec
DE 6.50 usec
TE 293.6 K
D1 0.5000000 sec
TDO 1

===== CHANNEL f1 =====
SFO1 400.1320007 MHz
NUC1 1H
P1 15.70 usec
PLW1 7.75000000 W

F2 - Processing parameters
SI 65536
SF 400.1300104 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



167.49
145.95
144.01
138.19
138.10
137.84
136.11
128.56
128.40
127.20
126.21
125.82
125.25
88.20
77.48
77.16
76.84
72.64
62.12
60.92
53.57
52.86
30.64
28.50
27.97
23.26
22.54
14.46



Current Data Parameters
NAME bb41217
EXPHO 926
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171230
Time 13.45
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 16540
SOLVENT CDCl3
HS 750
DS 4
SWH 24038.461 Hz
FIDRES 1.453353 Hz
AQ 0.3440320 sec
RG 200.34
DW 20.800 usec
DE 6.50 usec
TE 293.9 K
D1 1.0000000 sec
D11 0.0300000 sec
TDO 1

===== CHANNEL f1 =====
SFO1 100.6228299 MHz
NUC1 13C
P1 9.25 usec
PLW1 47.00000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
PLW13 0.11863000 W

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

