Electronic Supplementary Material (ESI) for RSC Advances

Supplemetary Information

Ruthenium catalysed one-pot synthesis of S-allyl and cinnamyl dithiocarbamates using allyl and cinnamyl acetates in water

Sabir Ahammed, Amit Saha, and Brindaban C. Ranu*

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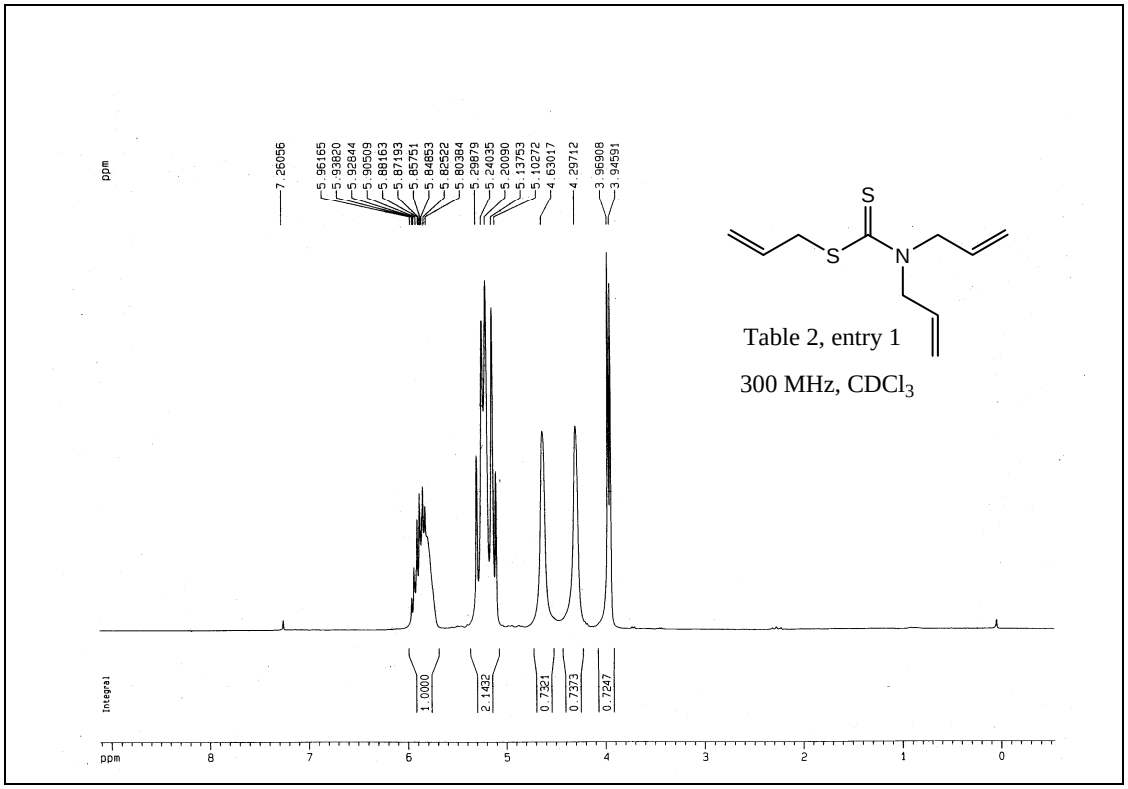
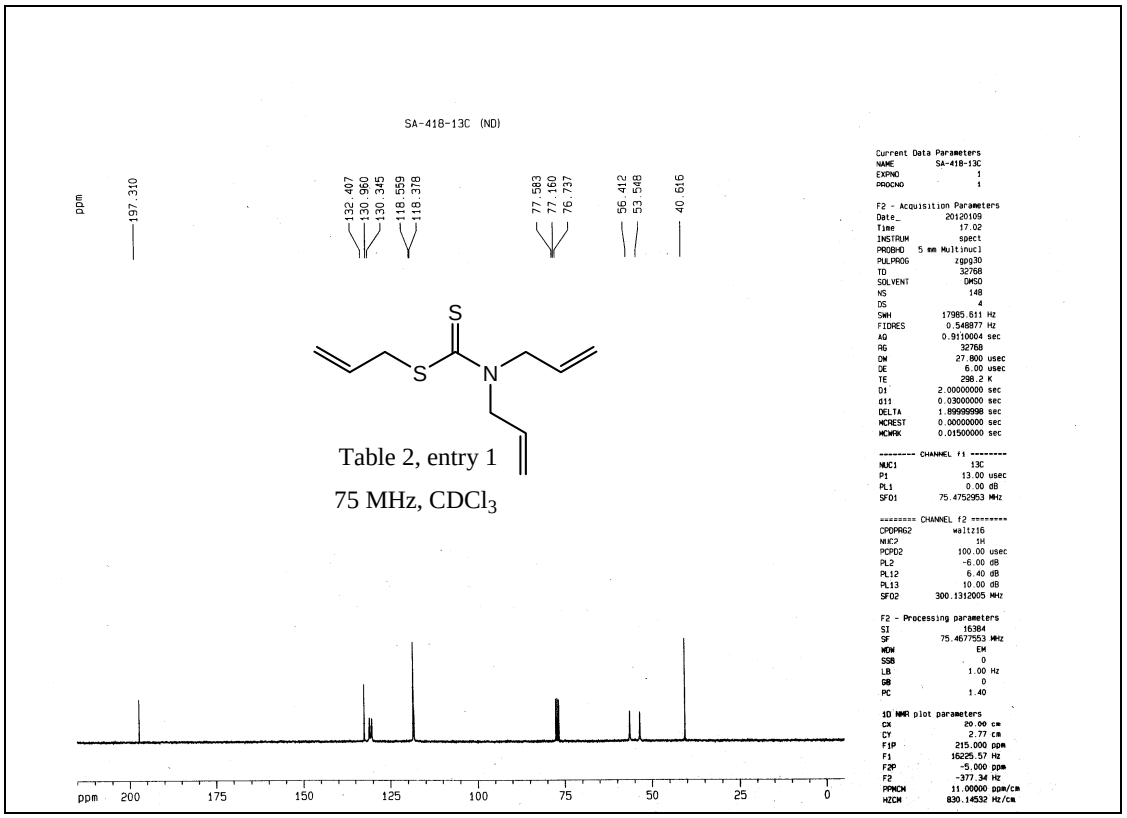

ppm
7.26056
5.96165
5.93820
5.92844
5.90509
5.88163
5.87193
5.85751
5.84853
5.82522
5.80384
5.29879
5.24035
5.20090
5.13753
5.10272
4.63017
4.29712
3.96908
3.94591
Integral
1.0000
2.1432
0.7321
0.7373
0.7247
ppm
8
7
6
5
4
3
2
1
0
S
S
N
Table 2, entry 1
300 MHz, CDCl3


SA-418-13C (ND)
ppm
197.310
132.407
130.960
130.345
118.559
118.378
77.583
77.160
76.737
56.412
53.548
40.616
S
S
N
Table 2, entry 1
75 MHz, CDCl3
ppm
200
175
150
125
100
75
50
25
0
Current Data Parameters
NAME SA-418-13C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120109
Time 17.02
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 148
DS 4
SWH 17985.611 Hz
FIDRES 0.548877 Hz
AQ 0.9110004 sec
RG 32768
DW 27.800 usec
DE 6.00 usec
TE 298.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 13C
P1 13.00 usec
PL1 0.00 dB
SFO1 75.4752953 MHz
-------- CHANNEL f2 --------
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -6.00 dB
PL12 6.40 dB
PL13 10.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 16384
SF 75.4677553 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 2.77 cm
F1P 215.000 ppm
F1 16225.57 Hz
F2P -5.000 ppm
F2 -377.34 Hz
PPMCM 11.00000 ppm/cm
HZCM 830.14532 Hz/cm

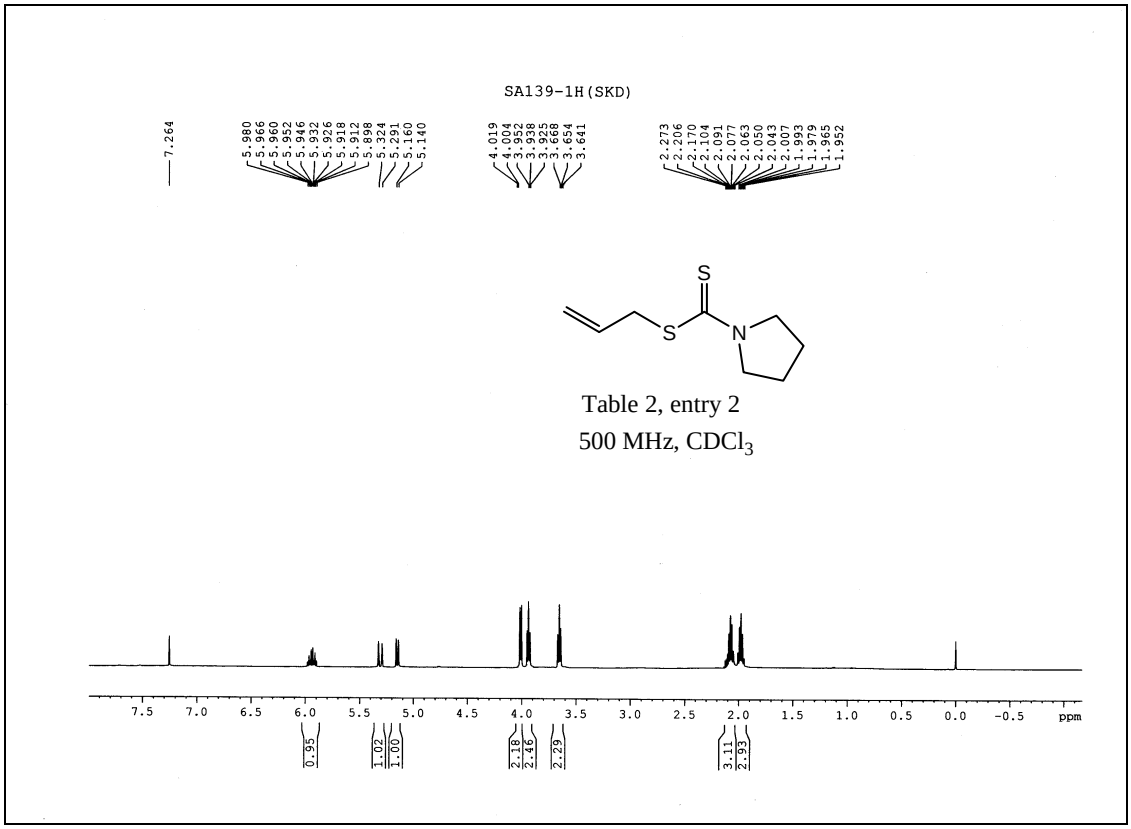


Table 2, entry 2

500 MHz, $CDCl_3$

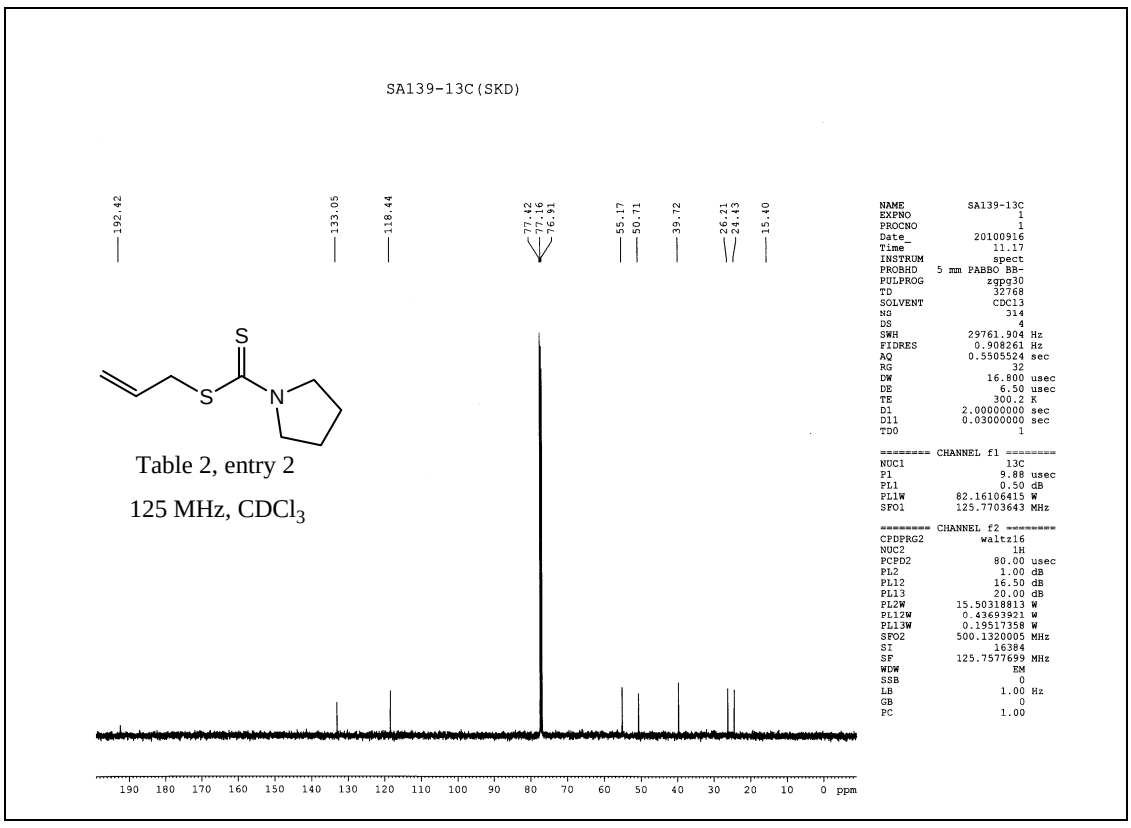
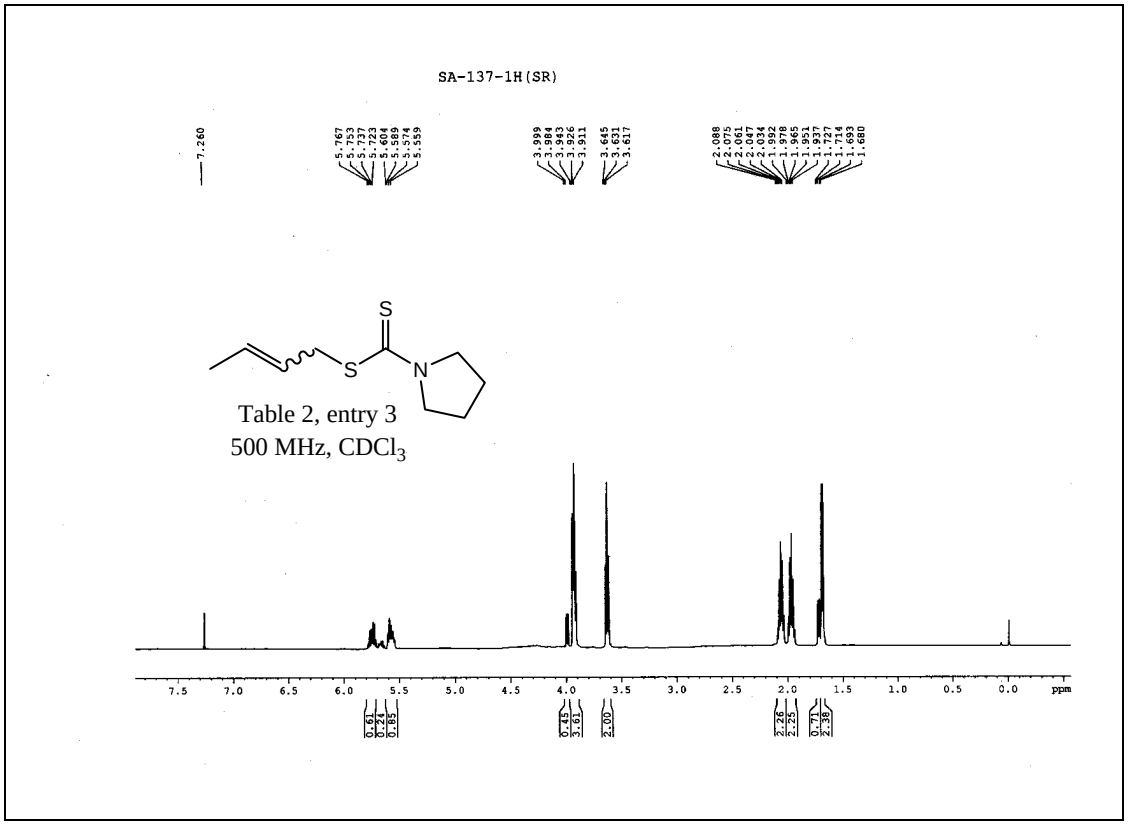
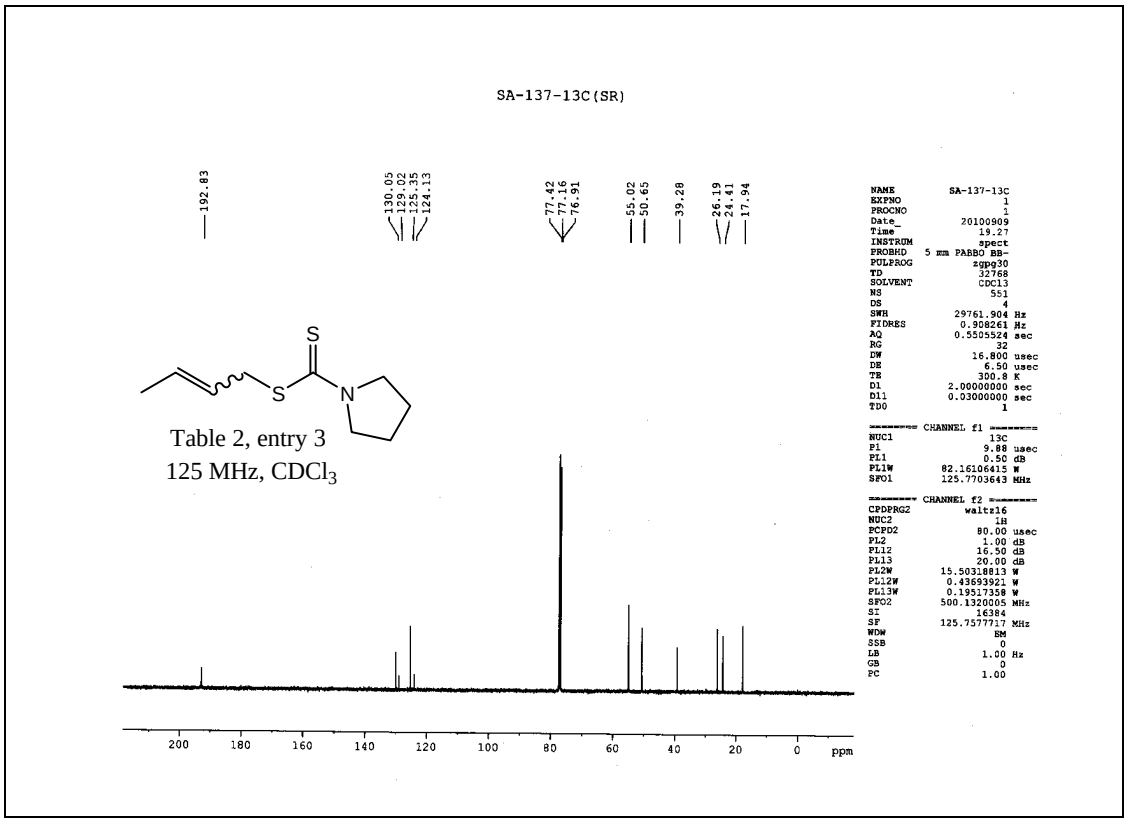


Table 2, entry 2

125 MHz, $CDCl_3$


SA-137-1H(SR)
7.260
5.767
5.753
5.737
5.723
5.604
5.589
5.574
5.559
3.999
3.984
3.965
3.926
3.911
3.645
3.631
3.617
2.088
2.075
2.061
2.047
2.034
1.992
1.978
1.965
1.951
1.937
1.727
1.711
1.693
1.680
S
S
N
Table 2, entry 3
500 MHz, CDCl3
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
ppm
0.61
0.24
0.89
0.45
3.61
2.00
2.26
2.25
0.71
2.36


SA-137-13C(SR)
192.83
130.05
129.02
125.35
124.13
77.42
77.16
76.91
55.02
50.65
39.28
26.19
24.41
17.94
S
S
N
Table 2, entry 3
125 MHz, CDCl3
NAME SA-137-13C
EXPNO 1
PROCNO 1
Date_ 20100909
Time 19.27
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 551
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 0.5505524 sec
RG 32
DW 16.800 usec
DE 6.50 usec
TE 300.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
CHANNEL f1
NUC1 13C
P1 9.88 usec
PL1 0.50 dB
PL1W 82.16106415 W
SFO1 125.7703643 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 16.50 dB
PL13 20.00 dB
PL2W 15.50318813 W
PL12W 0.43693921 W
PL13W 0.19517358 W
SFO2 500.1320005 MHz
SI 16384
SF 125.7577717 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
200
180
160
140
120
100
80
60
40
20
0
ppm

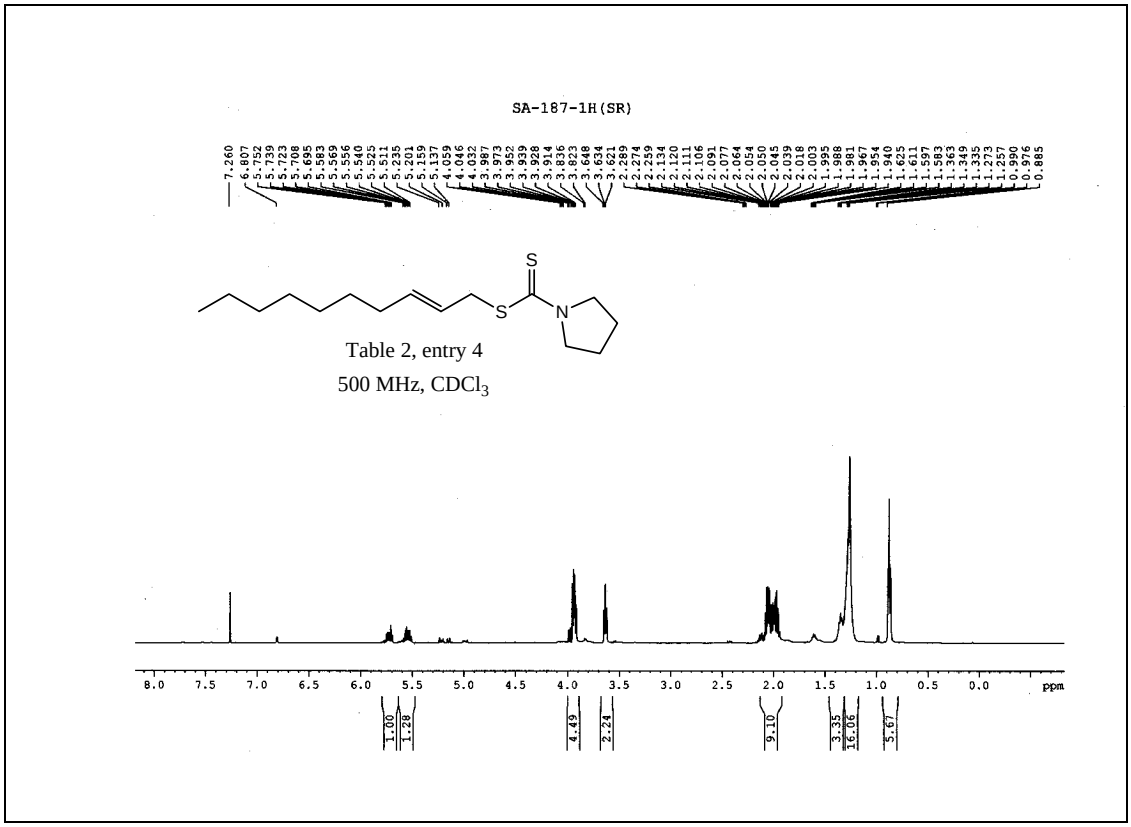


Table 2, entry 4

500 MHz, $CDCl_3$

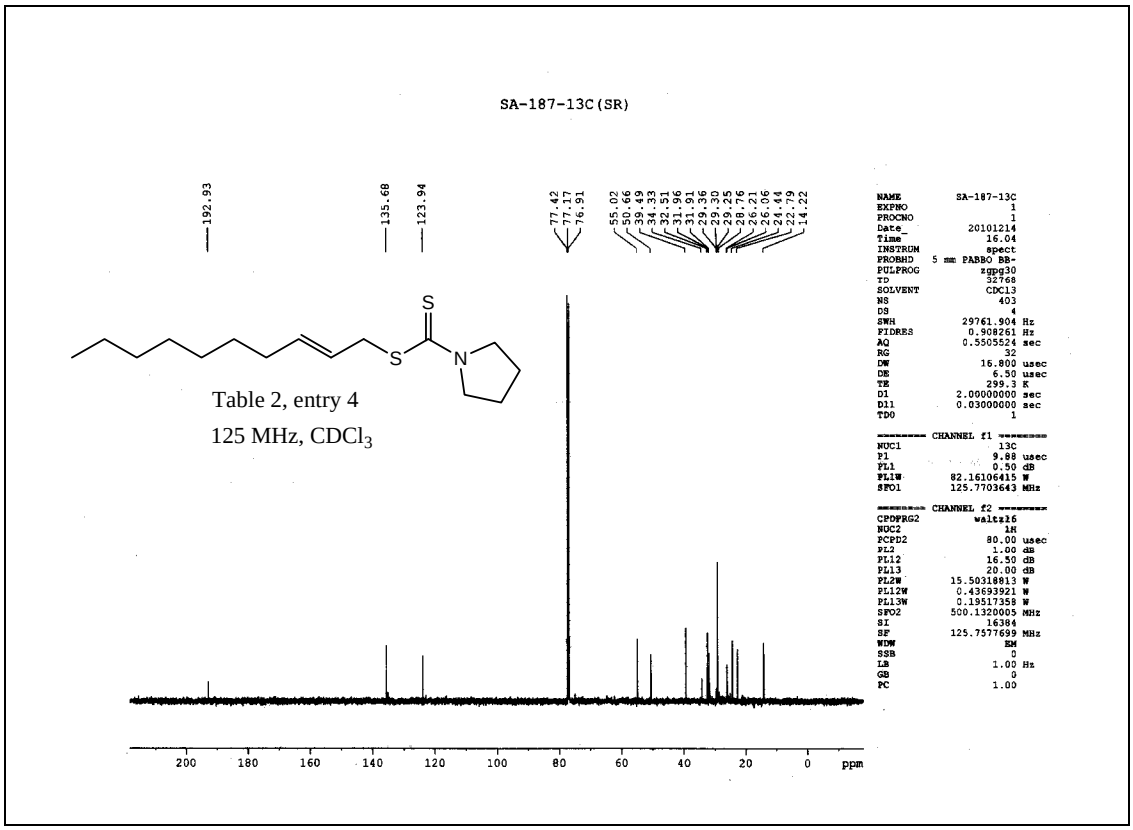


Table 2, entry 4

125 MHz, $CDCl_3$

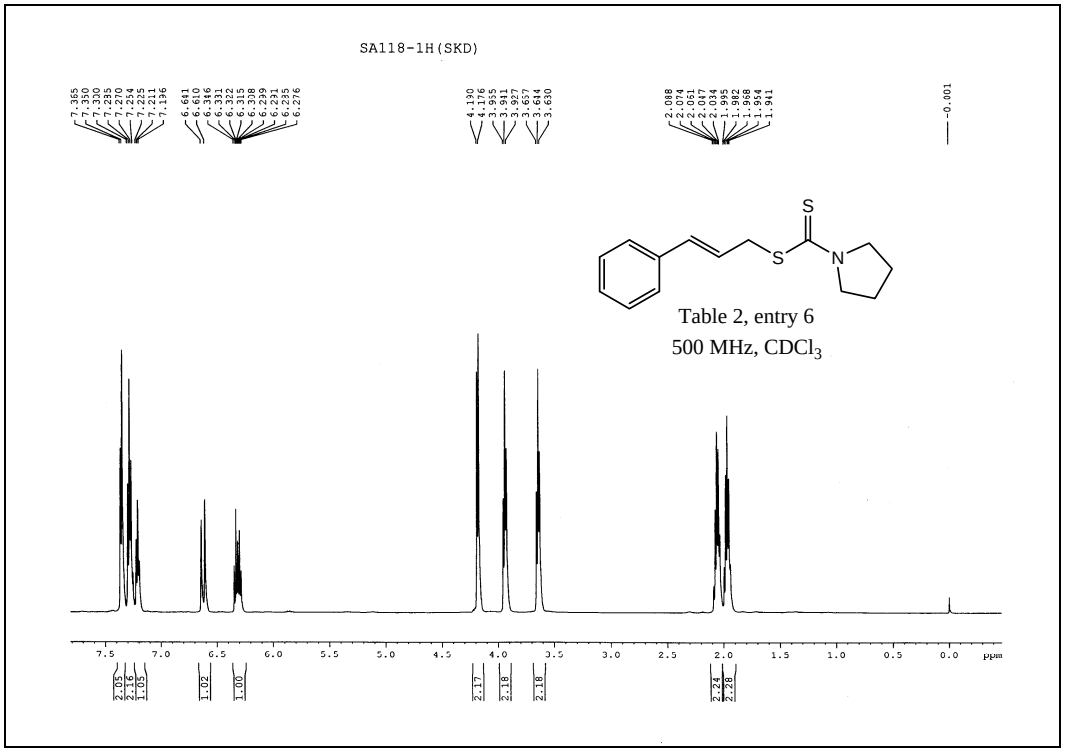


Table 2, entry 6
500 MHz, $CDCl_3$

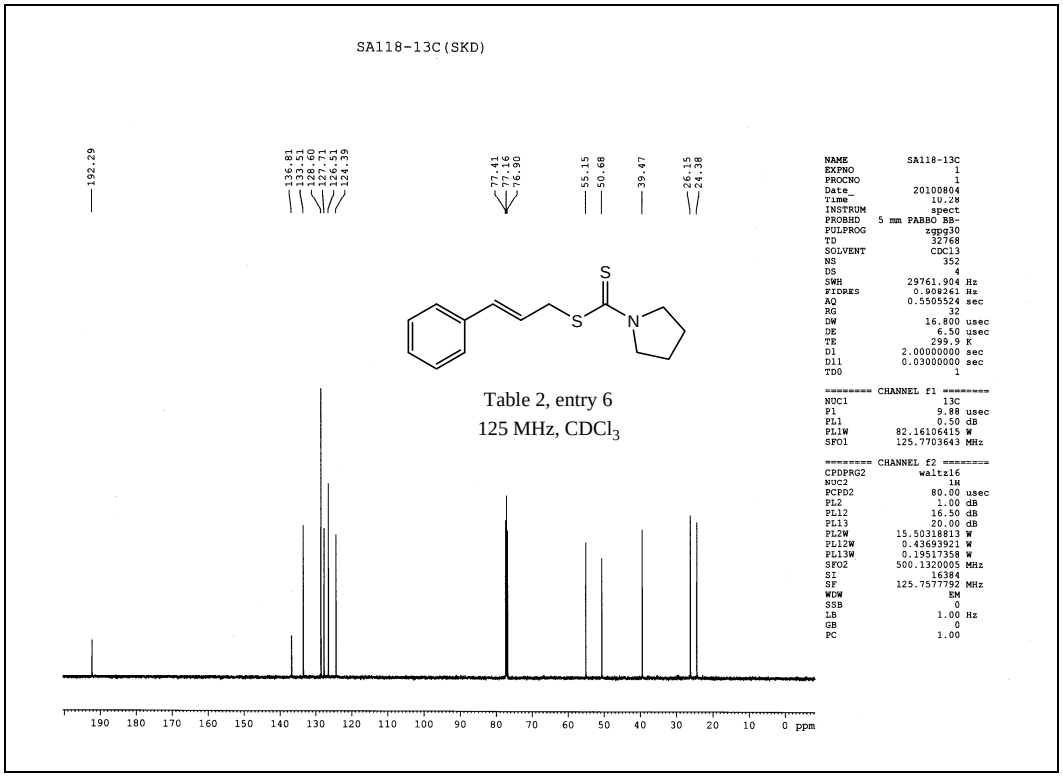


Table 2, entry 6
125 MHz, $CDCl_3$

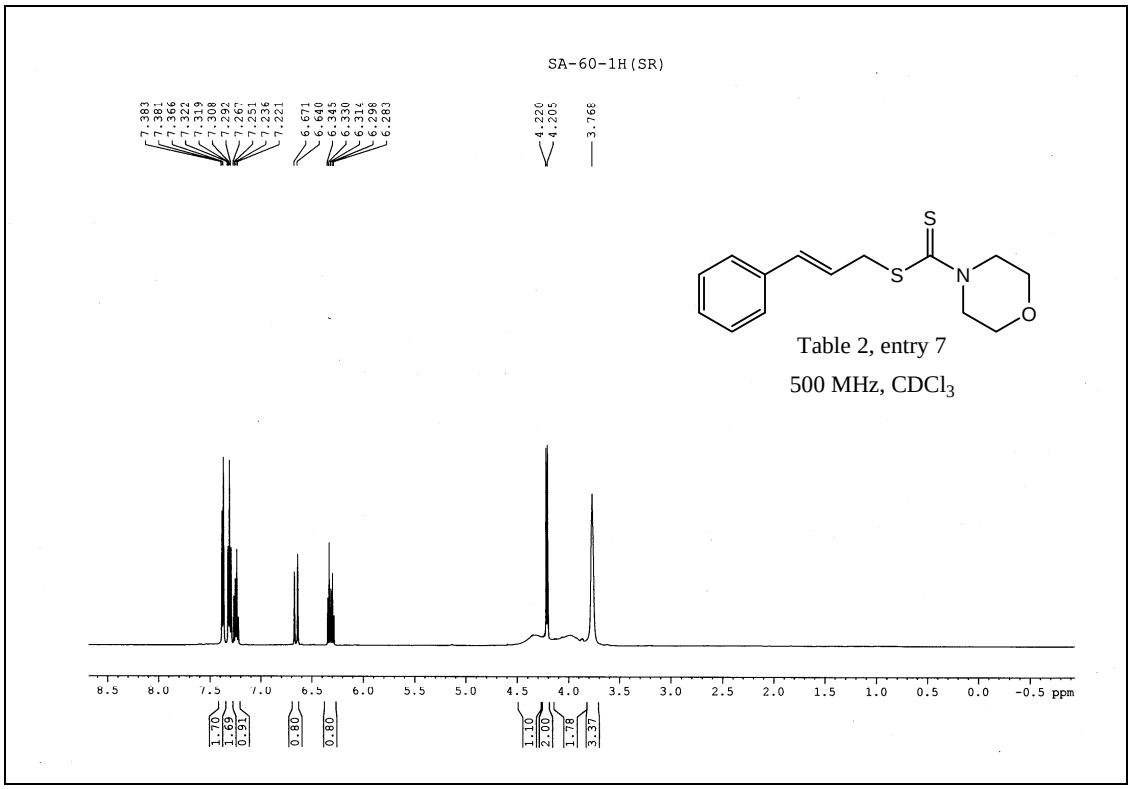


Table 2, entry 7

500 MHz, $CDCl_3$

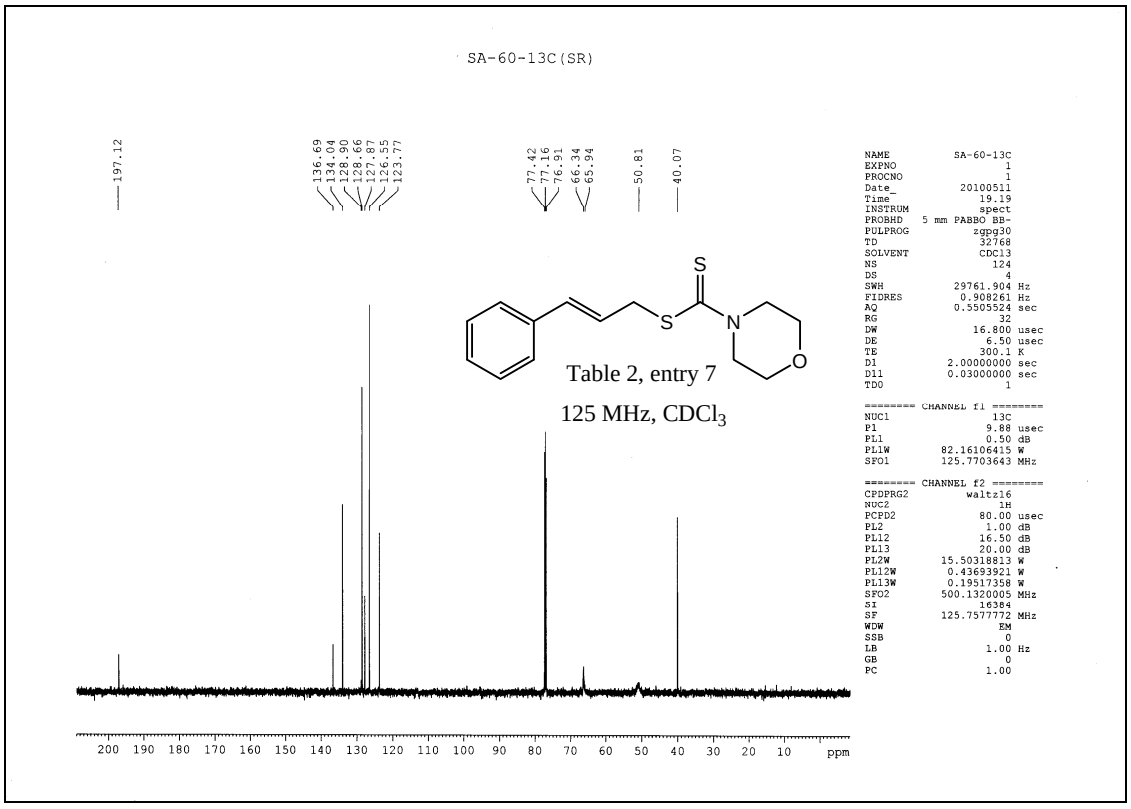
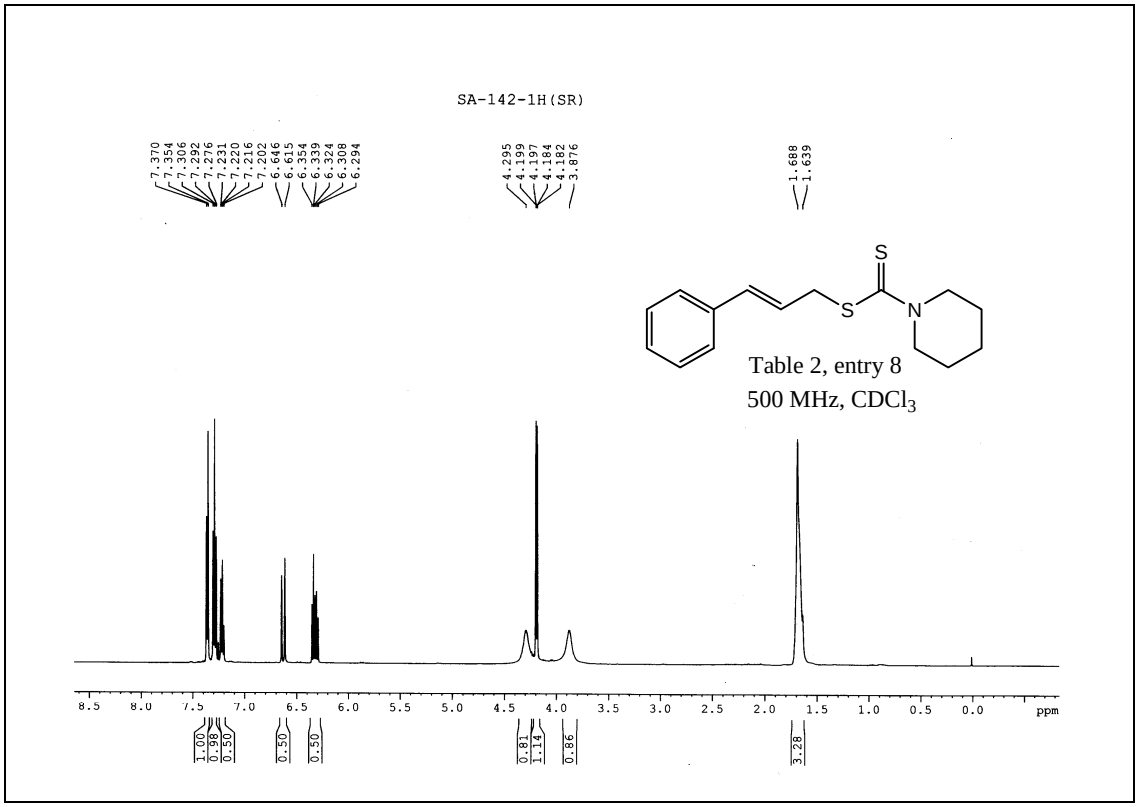
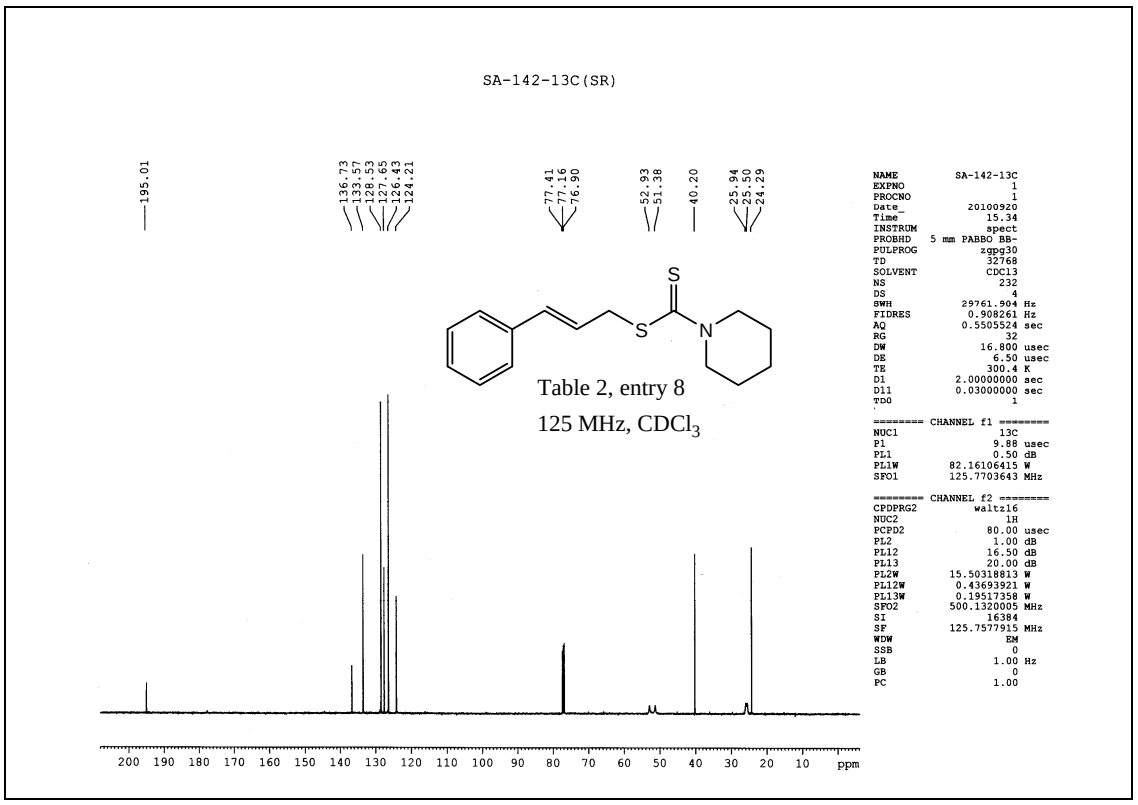
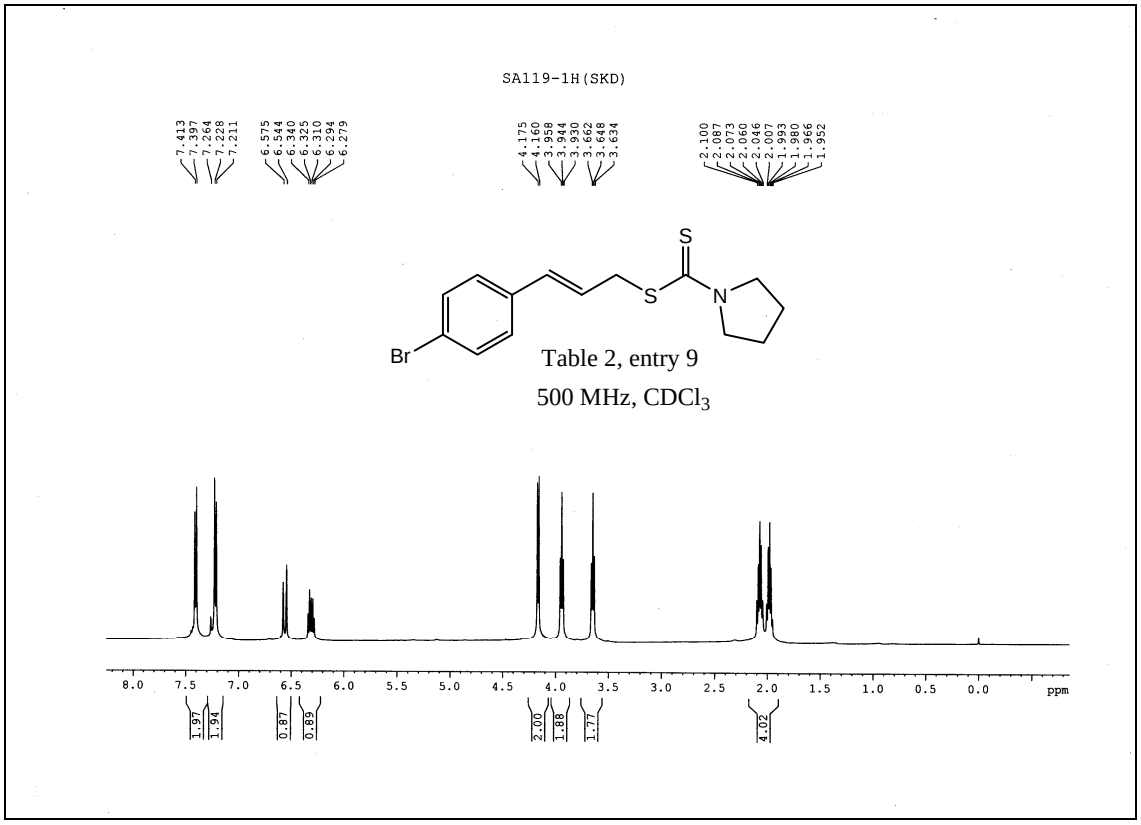


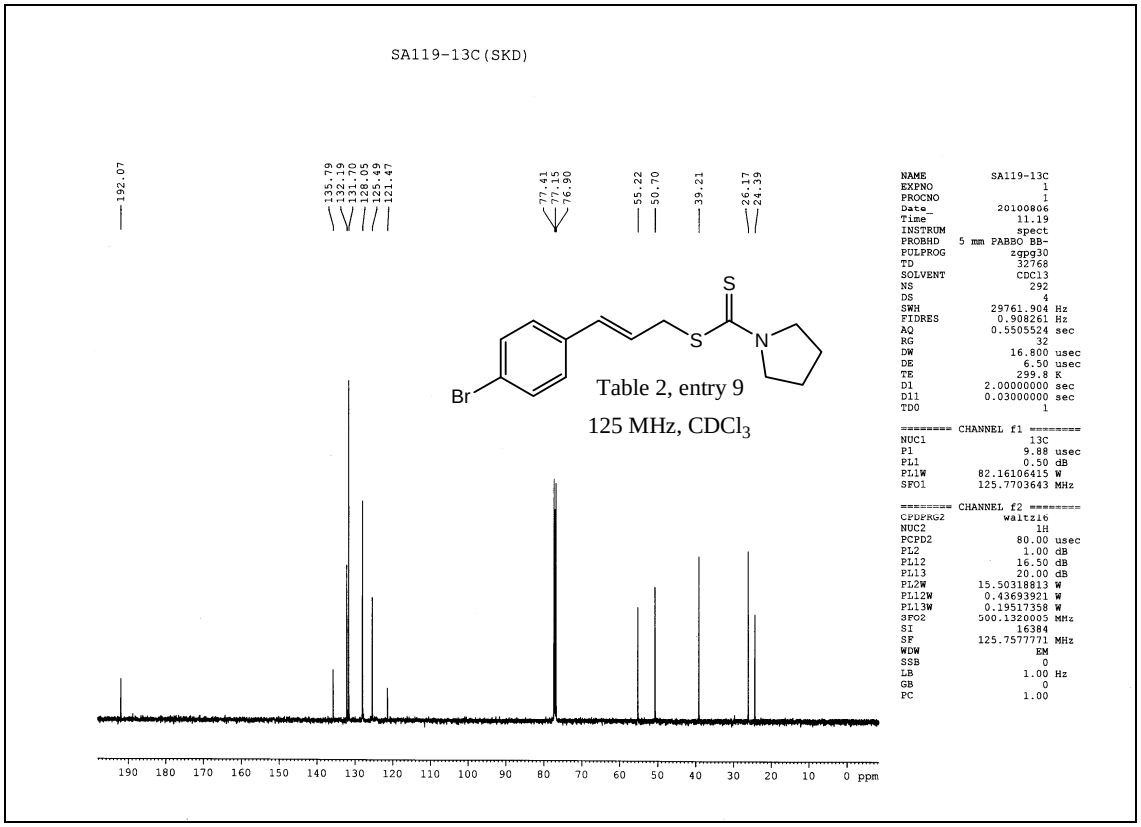
Table 2, entry 7

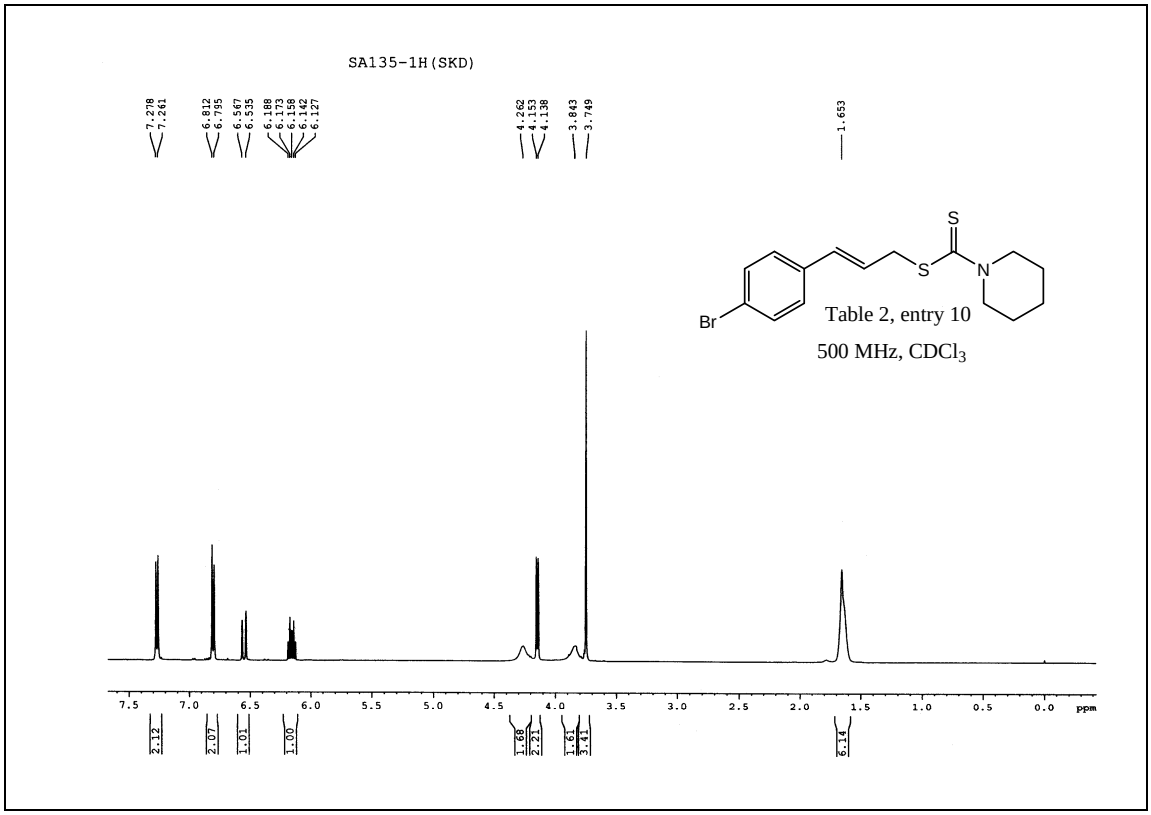
125 MHz, $CDCl_3$

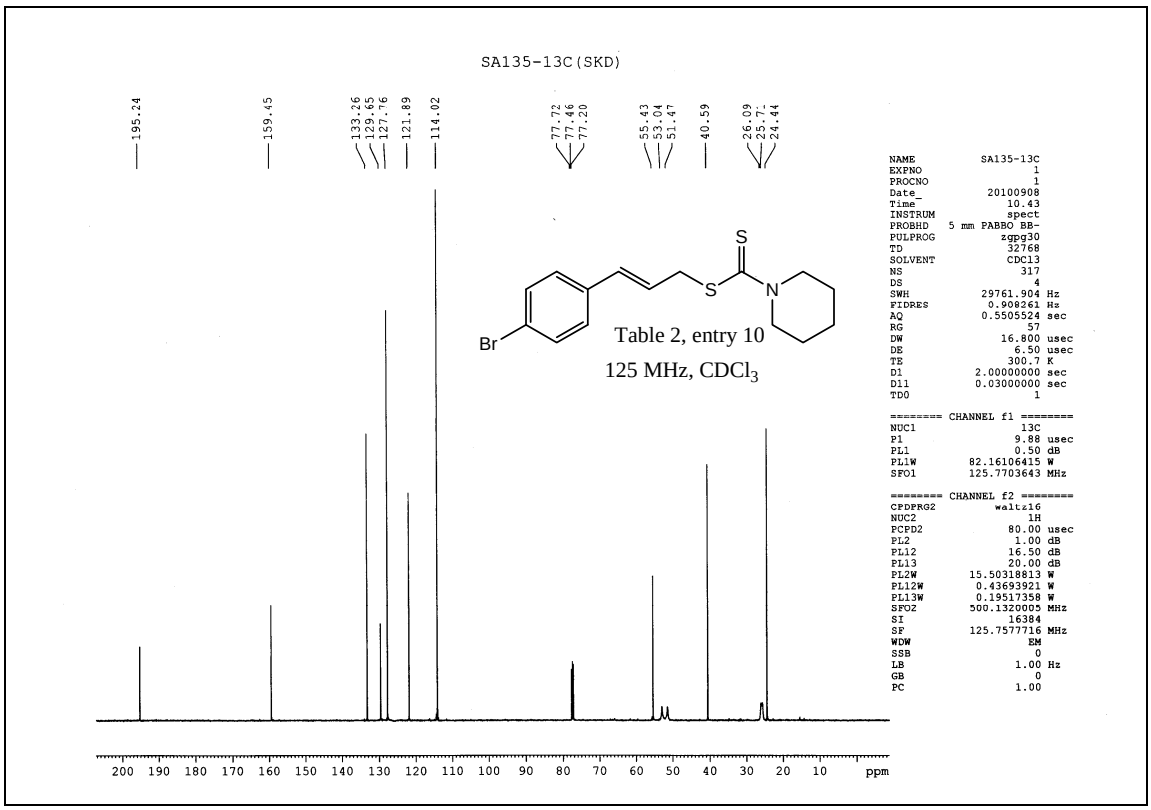

SA-142-1H(SR)
7.370
7.354
7.336
7.292
7.276
7.231
7.220
7.216
7.202
6.646
6.615
6.354
6.339
6.324
6.308
6.294
4.295
4.199
4.197
4.184
4.182
3.876
1.688
1.639
S
S
N
Table 2, entry 8
500 MHz, CDCl3
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.00
0.98
0.50
0.50
0.50
0.81
1.14
0.86
3.28

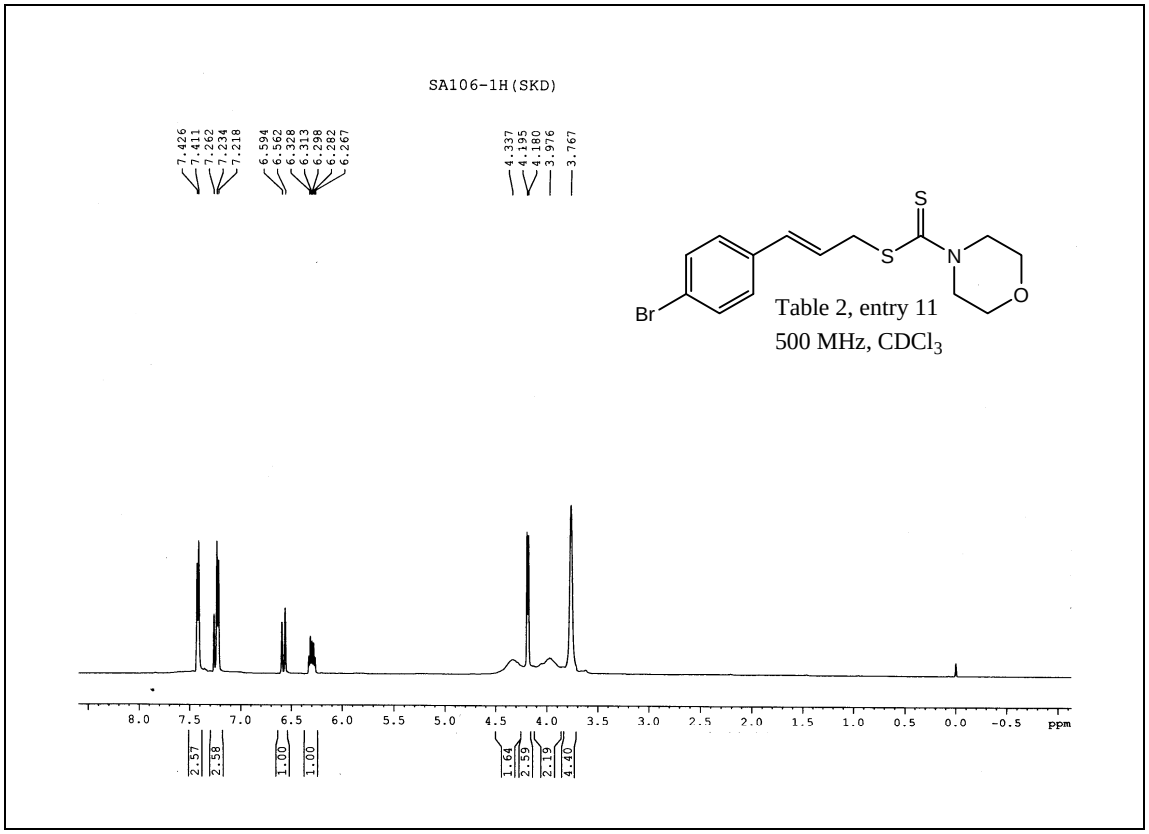

SA-142-13C(SR)
195.01
136.73
133.57
128.53
127.65
126.43
124.21
77.41
77.16
76.90
52.93
51.38
40.20
25.94
25.50
24.29
S
S
N
Table 2, entry 8
125 MHz, CDCl3
NAME SA-142-13C
EXPNO 1
PROCNO 1
Date_ 20100920
Time 15.34
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 232
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 0.5505524 sec
RG 32
DW 16.800 usec
DE 6.50 usec
TE 300.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.88 usec
PL1 0.50 dB
PL1W 82.16106415 W
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 16.50 dB
PL13 20.00 dB
PL2W 15.50318813 W
PL12W 0.43693921 W
PL13W 0.19517358 W
SFO2 500.1320005 MHz
SI 16384
SF 125.7577915 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

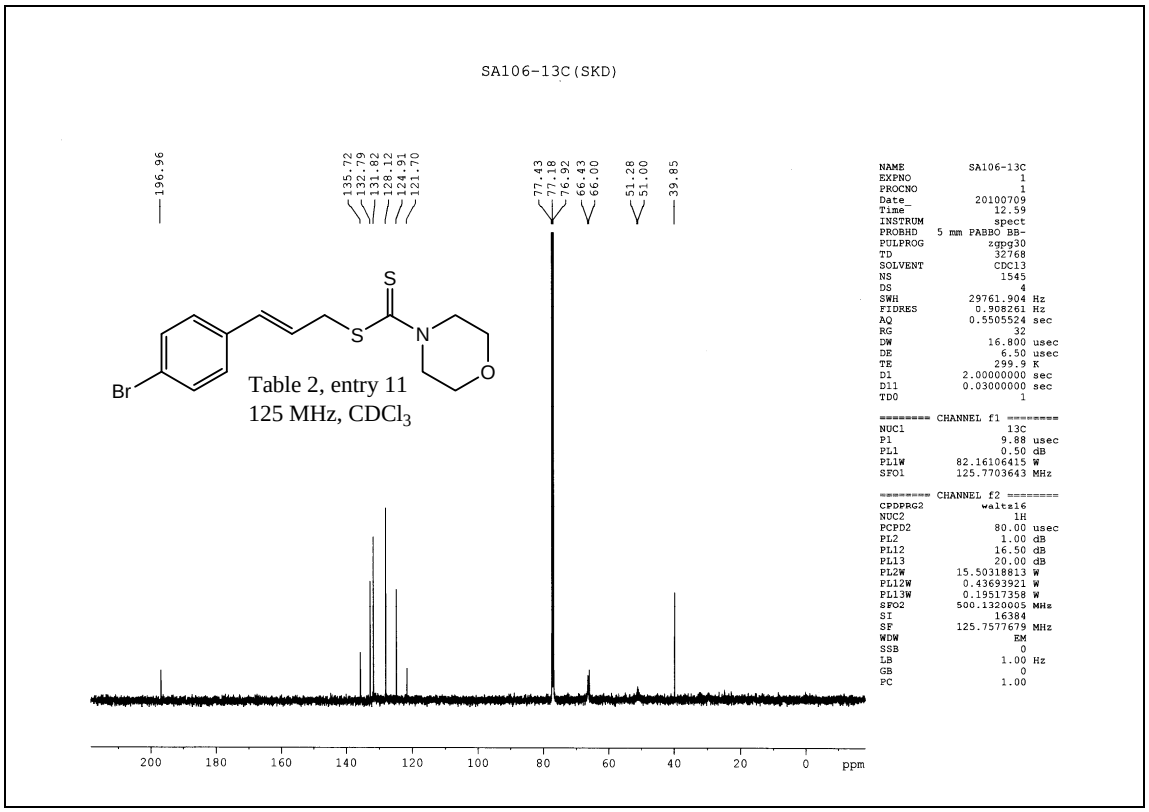

SA119-1H(SKD)
7.413
7.397
7.264
7.228
7.211
6.575
6.544
6.340
6.325
6.310
6.294
6.279
4.175
4.160
3.958
3.944
3.930
3.662
3.648
3.634
2.100
2.087
2.073
2.060
2.046
2.007
1.993
1.980
1.966
1.952
S
S
N
Br
Table 2, entry 9
500 MHz, CDCl3
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.97
1.94
0.87
0.89
2.00
1.88
1.77
4.02

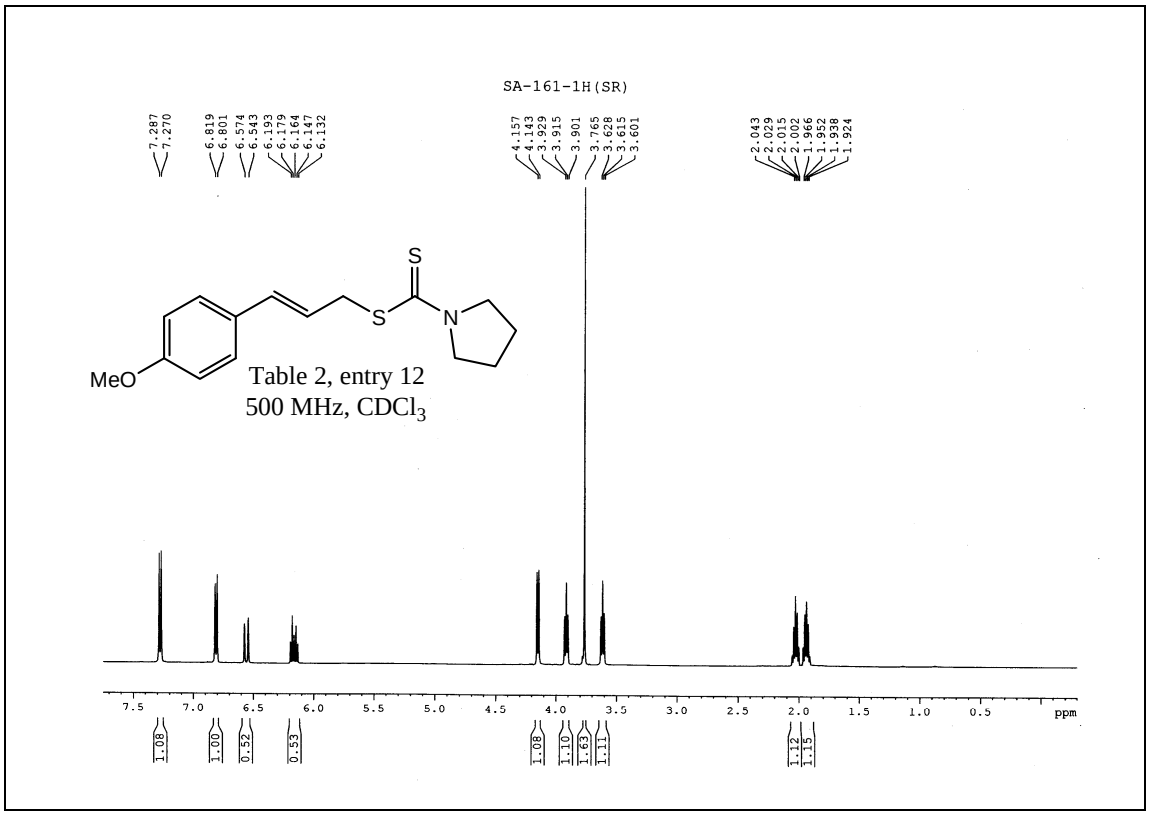

SA119-13C(SKD)
192.07
135.79
132.19
131.70
128.65
121.49
121.47
77.41
77.15
76.90
55.22
50.70
39.21
26.17
24.39
S
S
N
Br
Table 2, entry 9
125 MHz, CDCl3
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm
NAME SA119-13C
EXPNO 1
PROCNO 1
Date_ 20100806
Time 11.19
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 292
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 0.5505524 sec
RG 32
DW 16.800 usec
DE 6.50 usec
TE 299.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.88 usec
PL1 0.50 dB
PL1W 82.16106415 W
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 16.50 dB
PL13 20.00 dB
PL2W 15.50318813 W
PL12W 0.43693921 W
PL13W 0.19517358 W
SFO2 500.1320005 MHz
SI 16384
SF 125.7577771 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

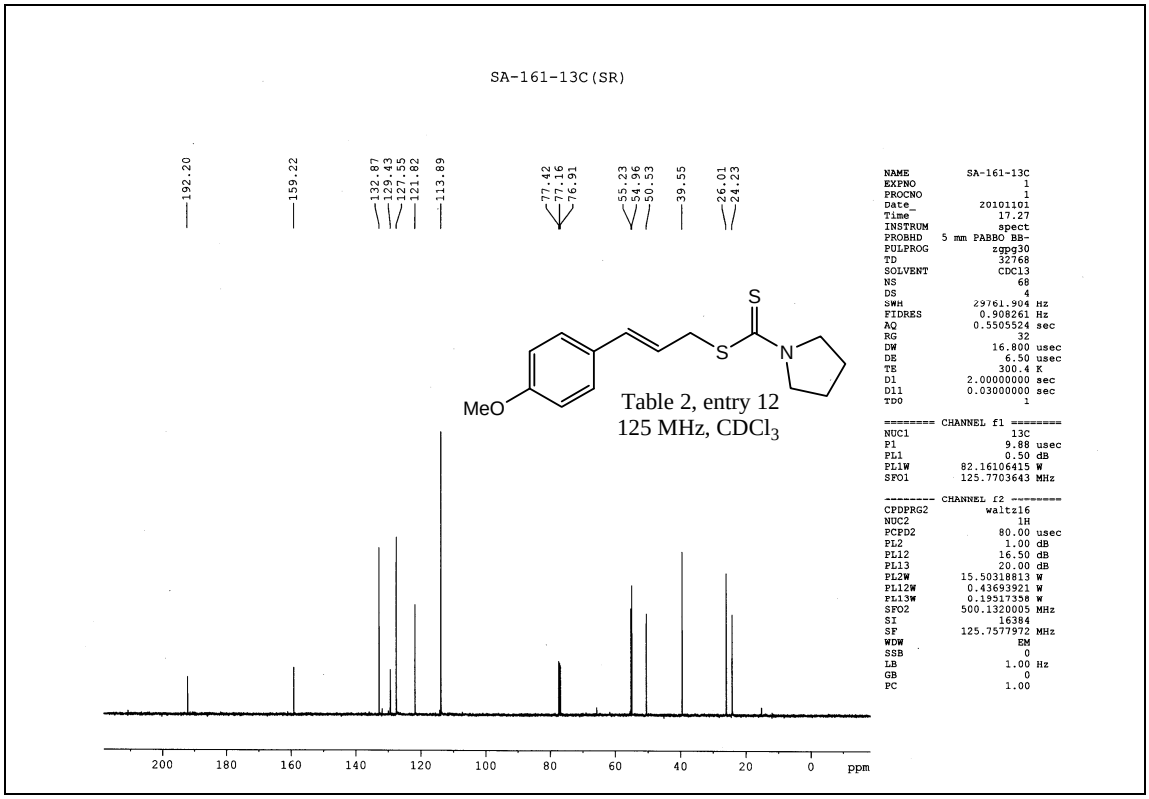

SA135-1H(SKD)
7.278
7.261
6.812
6.795
6.567
6.535
6.188
6.173
6.158
6.142
6.127
4.262
4.153
4.138
3.843
3.749
1.653
S
S
N
Br
Table 2, entry 10
500 MHz, CDCl3
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
2.12
2.07
1.01
1.00
1.68
2.21
1.61
3.41
6.14

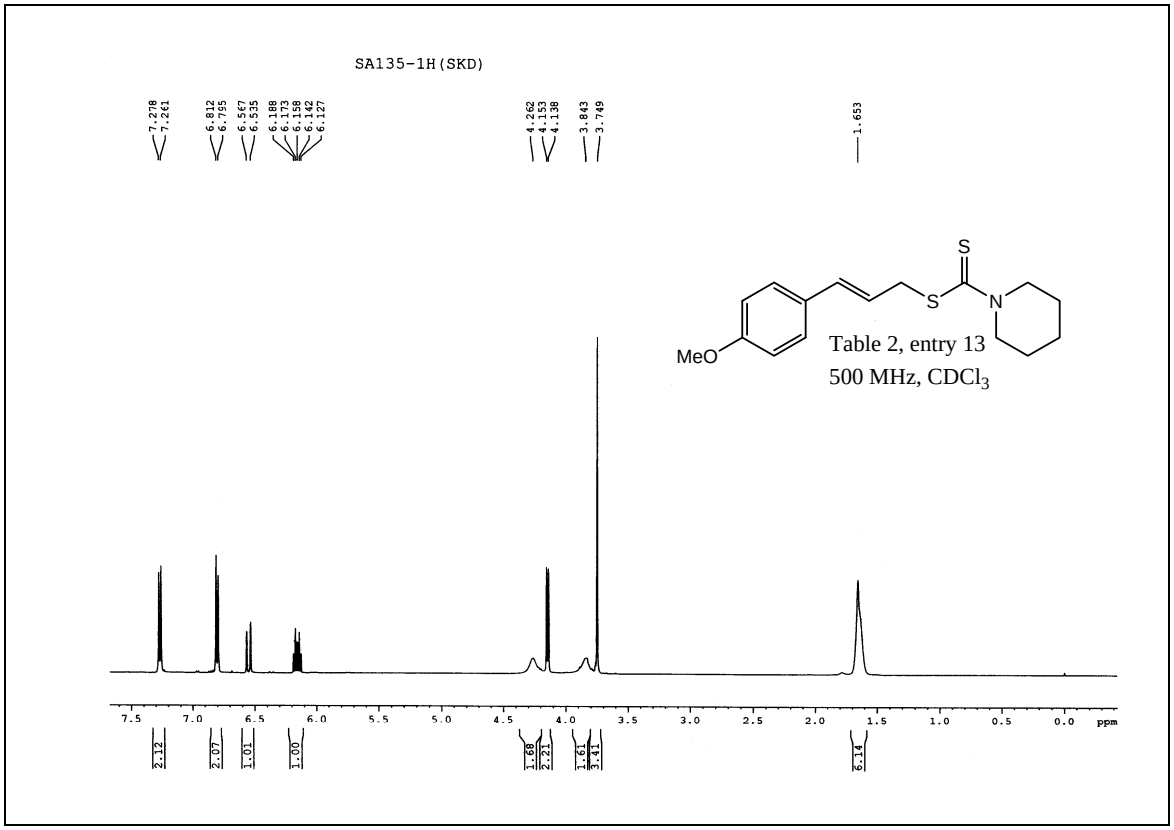

SA135-13C(SKD)
195.24
159.45
133.26
129.65
127.76
121.89
114.02
77.72
77.46
77.20
55.43
53.04
51.47
40.59
26.09
25.7
24.44
S
S
N
Br
Table 2, entry 10
125 MHz, CDCl3
NAME SA135-13C
EXPNO 1
PROCNO 1
Date_ 20100908
Time 10.43
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 317
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 0.5505524 sec
RG 57
DW 16.800 usec
DE 6.50 usec
TE 300.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.88 usec
PL1 0.50 dB
PL1W 82.16106415 W
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 16.50 dB
PL13 20.00 dB
PL2W 15.50318813 W
PL12W 0.43693921 W
PL13W 0.19517358 W
SFO2 500.1320005 MHz
SI 16384
SF 125.7577716 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

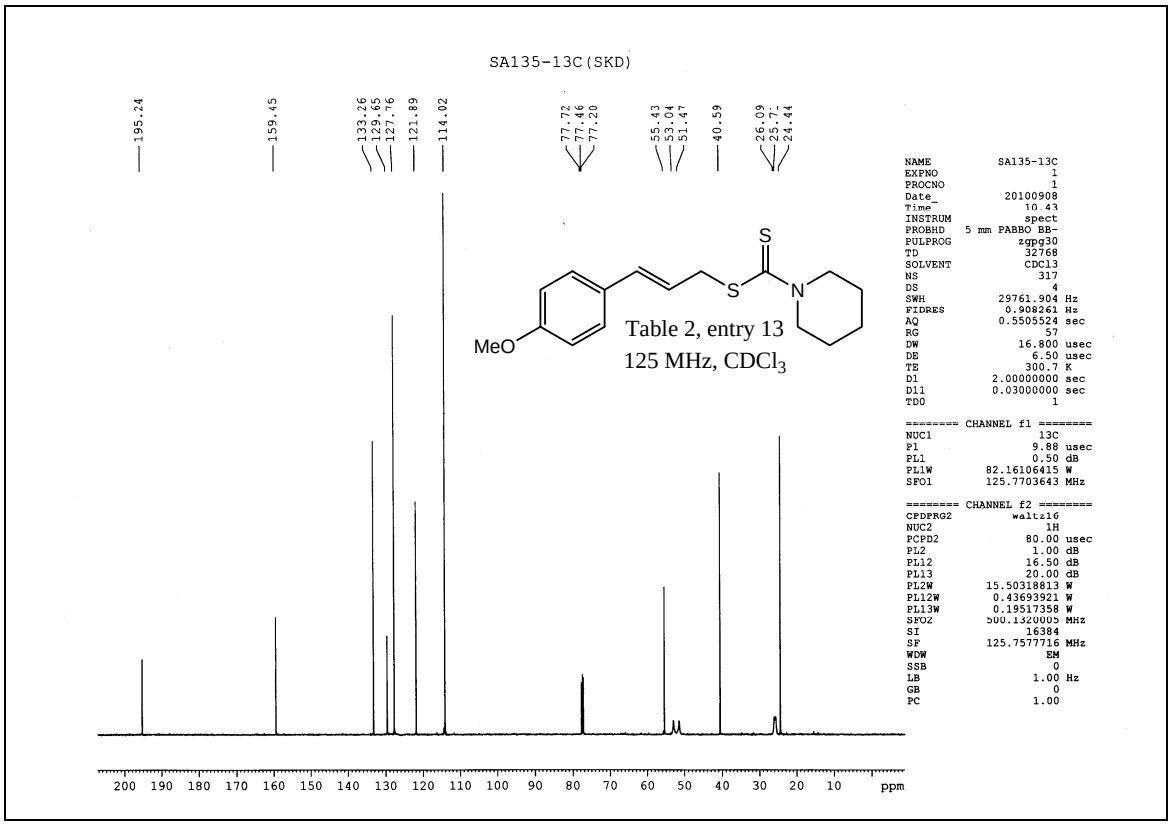

SA106-1H(SKD)
7.426
7.411
7.262
7.234
7.218
6.594
6.562
6.328
6.313
6.298
6.282
6.267
4.337
4.195
4.180
3.976
3.767
S
S
N
O
Br
Table 2, entry 11
500 MHz, CDCl3
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
ppm
2.57
2.58
1.00
1.00
1.64
2.59
2.19
4.40


SA106-13C(SKD)
196.96
135.72
132.79
131.82
128.12
124.91
121.70
77.43
77.18
76.92
66.43
66.00
51.28
51.00
39.85
S
S
N
O
Br
Table 2, entry 11
125 MHz, CDCl3
200
180
160
140
120
100
80
60
40
20
0
ppm
NAME SA106-13c
EXPNO 1
PROCNO 1
Date_ 20100709
Time_ 12.59
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 1545
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 0.5505524 sec
RG 32
DW 16.800 usec
DE 6.50 usec
TE 299.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.88 usec
PL1 0.50 dB
PL1W 82.16106415 W
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 16.50 dB
PL13 20.00 dB
PL2W 15.50318813 W
PL12W 0.43693921 W
PL13W 0.19517358 W
SFO2 500.1320005 MHz
SI 16384
SF 125.7577679 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00


SA-161-1H(SR)
7.287
7.270
6.819
6.801
6.574
6.543
6.193
6.179
6.164
6.147
6.132
4.157
4.143
3.929
3.915
3.901
3.765
3.628
3.615
3.601
2.043
2.029
2.015
2.002
1.966
1.952
1.938
1.924
S
S
N
MeO
Table 2, entry 12
500 MHz, CDCl3
ppm
1.08
1.00
0.52
0.53
1.08
1.10
1.63
1.11
1.12
1.15


SA-161-13C(SR)
192.20
159.22
132.87
129.43
127.55
121.82
113.89
77.42
77.16
76.91
55.23
54.96
50.53
39.55
26.01
24.23
S
S
N
MeO
Table 2, entry 12
125 MHz, CDCl3
ppm
NAME SA-161-13C
EXPNO 1
PROCNO 1
Date_ 20101101
Time 17.27
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 68
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 0.5505524 sec
RG 32
DW 16.800 usec
DE 6.50 usec
TE 300.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.88 usec
PL1 0.50 dB
PL1W 82.16106415 W
SFO1 125.7703643 MHz
-------- CHANNEL f2 --------
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 16.50 dB
PL13 20.00 dB
PL2W 15.50318813 W
PL12W 0.43693921 W
PL13W 0.19517358 W
SFO2 500.1320005 MHz
SI 16384
SF 125.7577972 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00


SA135-1H(SKD)
7.278
7.261
6.812
6.795
6.567
6.535
6.188
6.173
6.158
6.142
6.127
4.262
4.153
4.138
3.843
3.749
1.653
S
S
N
MeO
Table 2, entry 13
500 MHz, CDCl3
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
ppm
2.12
2.07
1.01
1.00
1.68
2.21
1.61
3.41
6.14


SA135-13C(SKD)
195.24
159.45
133.26
129.65
127.76
121.89
114.02
77.72
77.46
77.20
55.43
53.04
51.47
40.59
26.09
25.71
24.44
S
S
N
MeO
Table 2, entry 13
125 MHz, CDCl3
NAME SA135-13C
EXPNO 1
PROCNO 1
Date_ 20100908
Time_ 10.43
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 317
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 0.5505524 sec
RG 57
DW 16.800 usec
DE 6.50 usec
TE 300.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.88 usec
PL1 0.50 dB
PL1W 82.16106415 W
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 16.50 dB
PL13 20.00 dB
PL2W 15.50318813 W
PL12W 0.43693921 W
PL13W 0.19517358 W
SFO2 500.1320005 MHz
SI 16384
SF 125.7577716 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

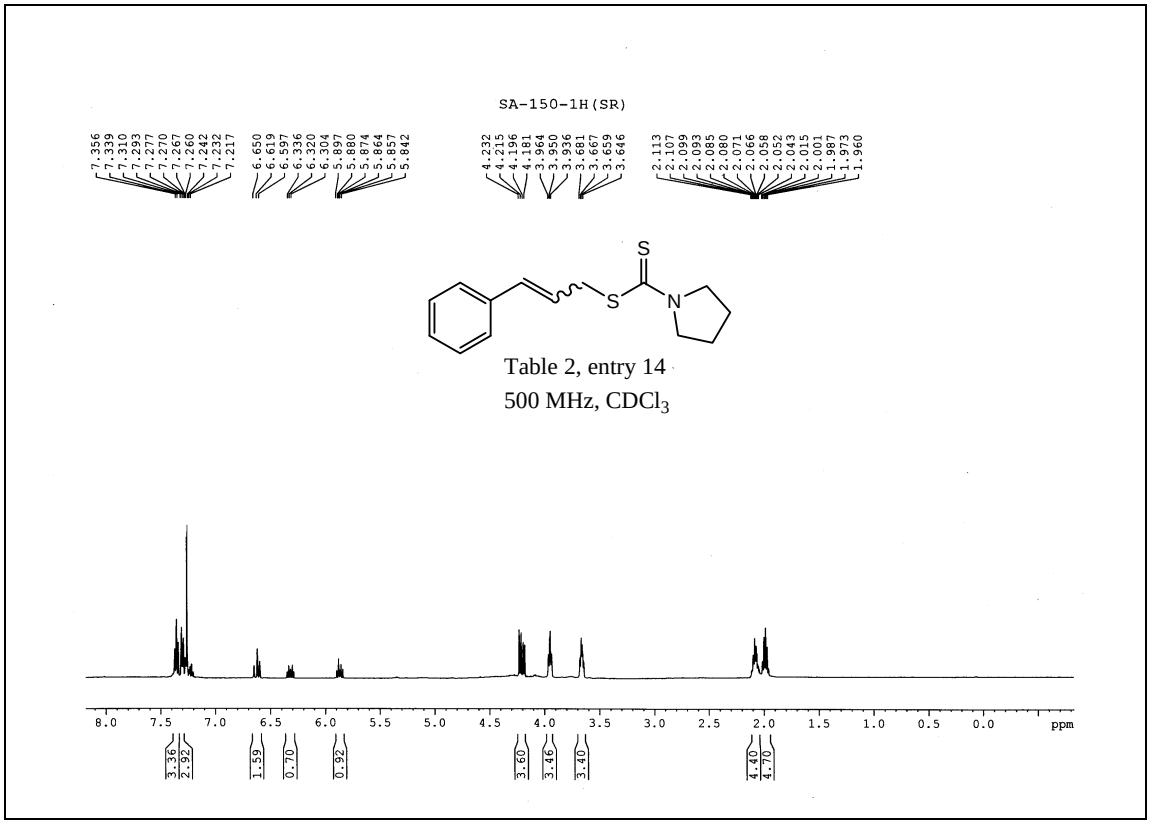


Table 2, entry 14
500 MHz, $CDCl_3$

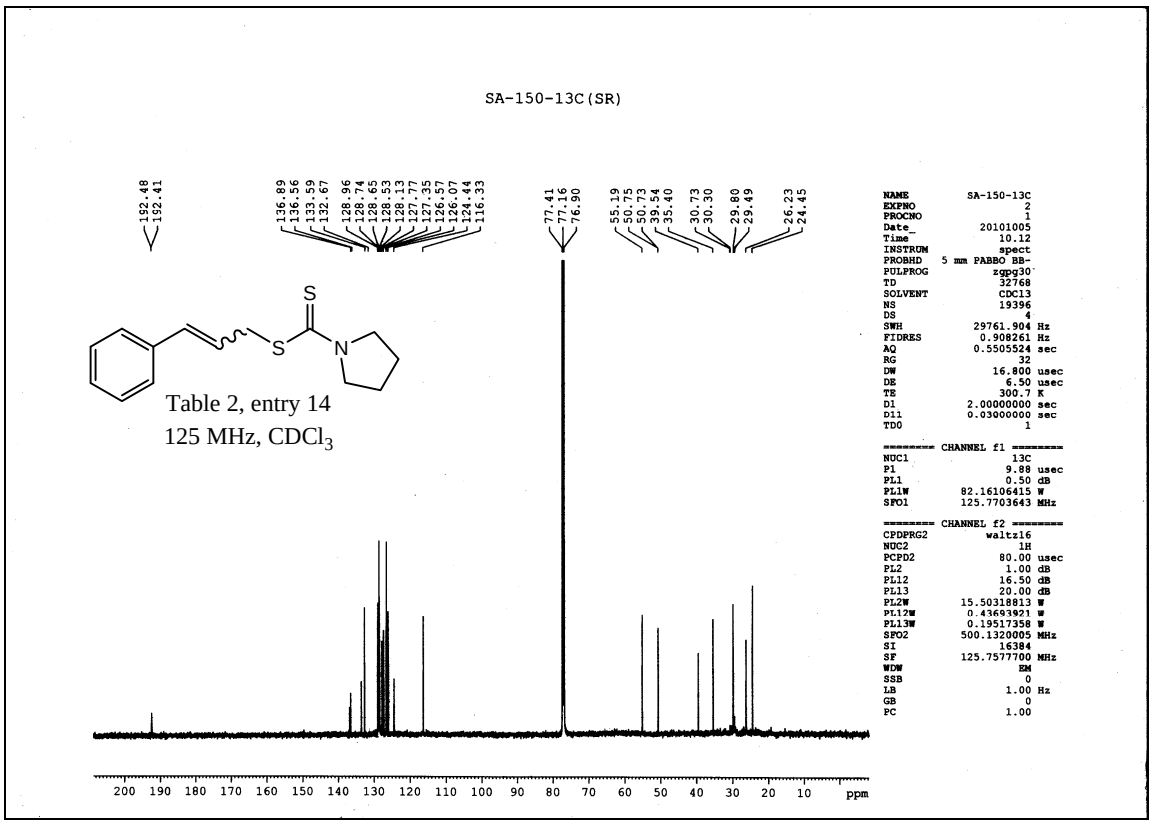
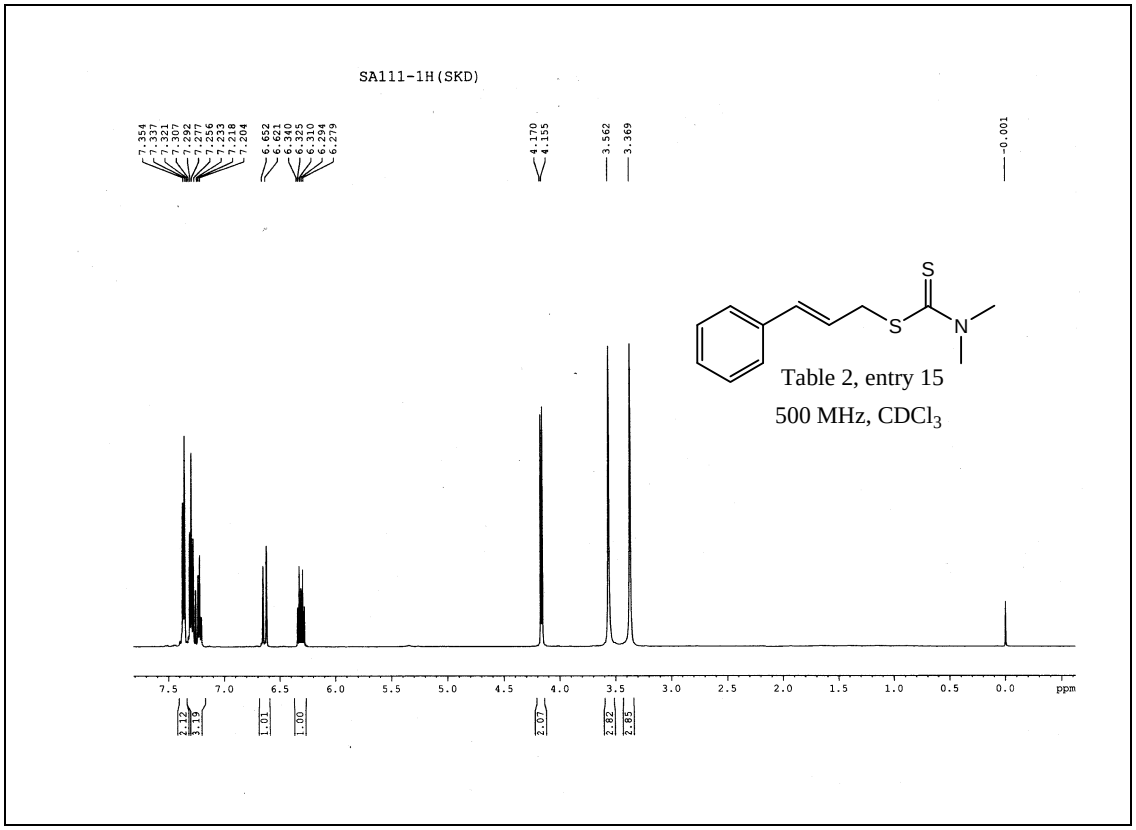
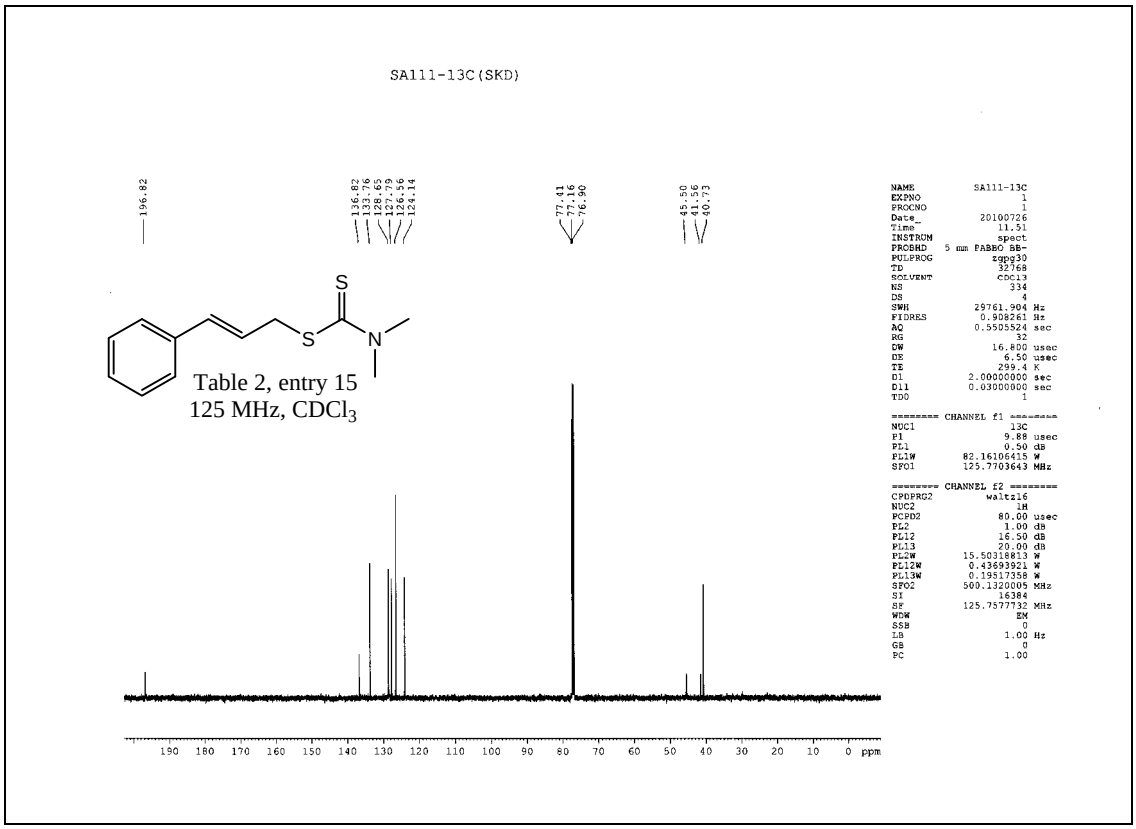
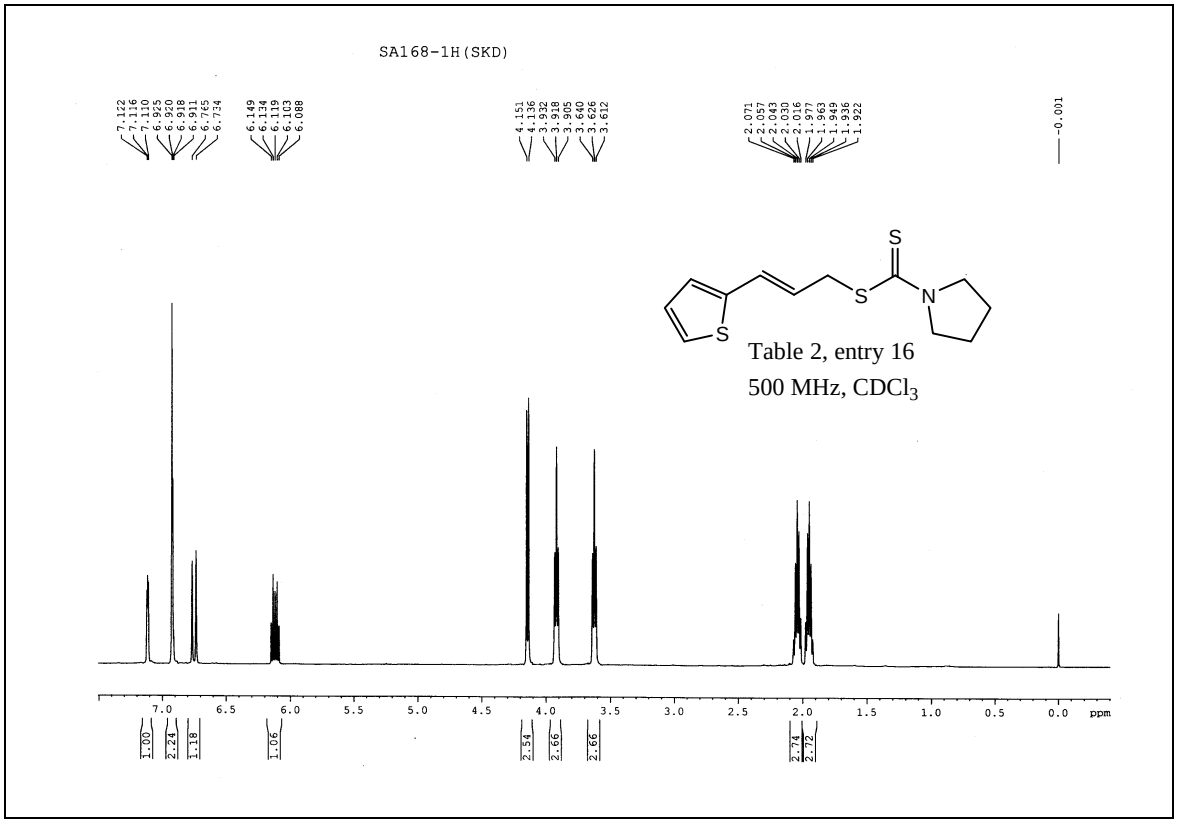
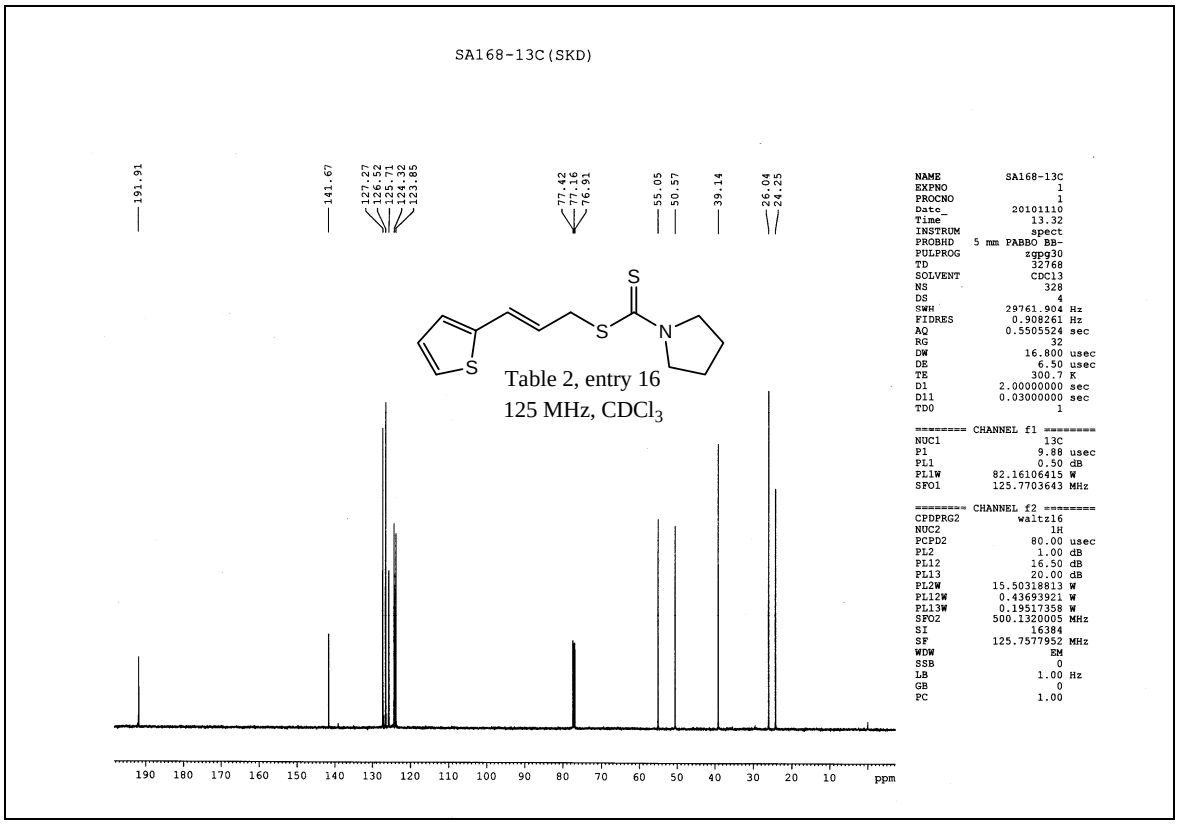


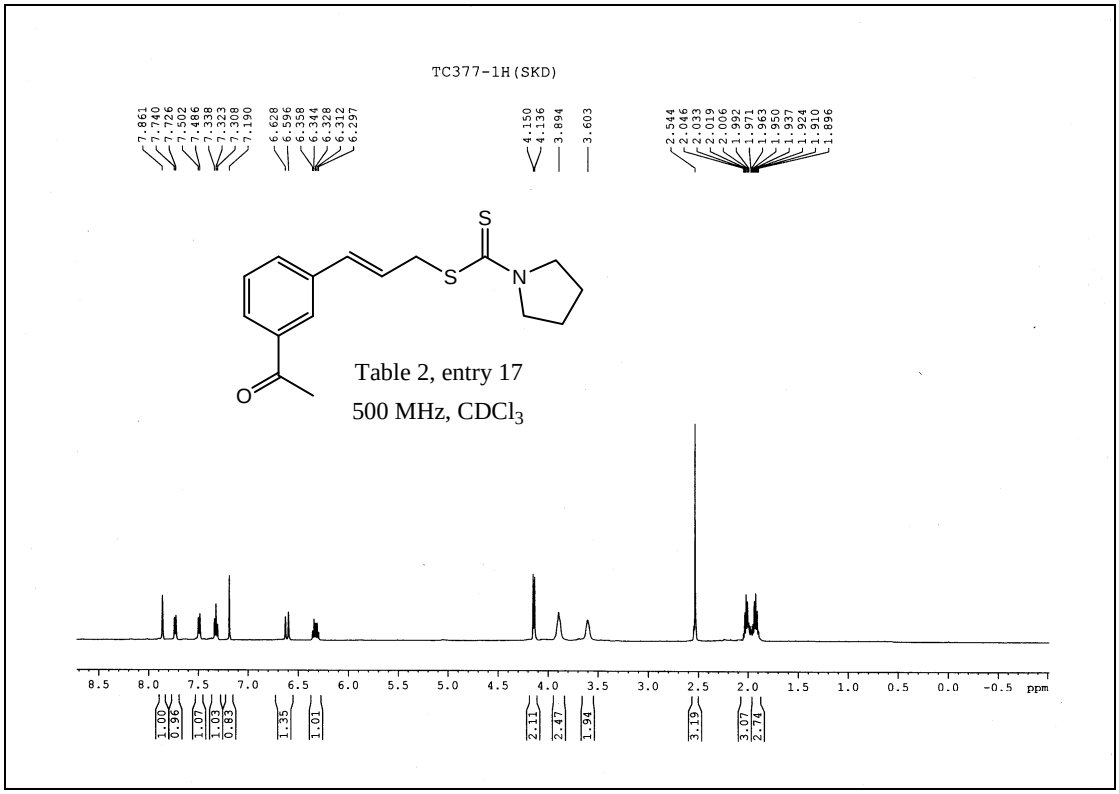
Table 2, entry 14
125 MHz, $CDCl_3$

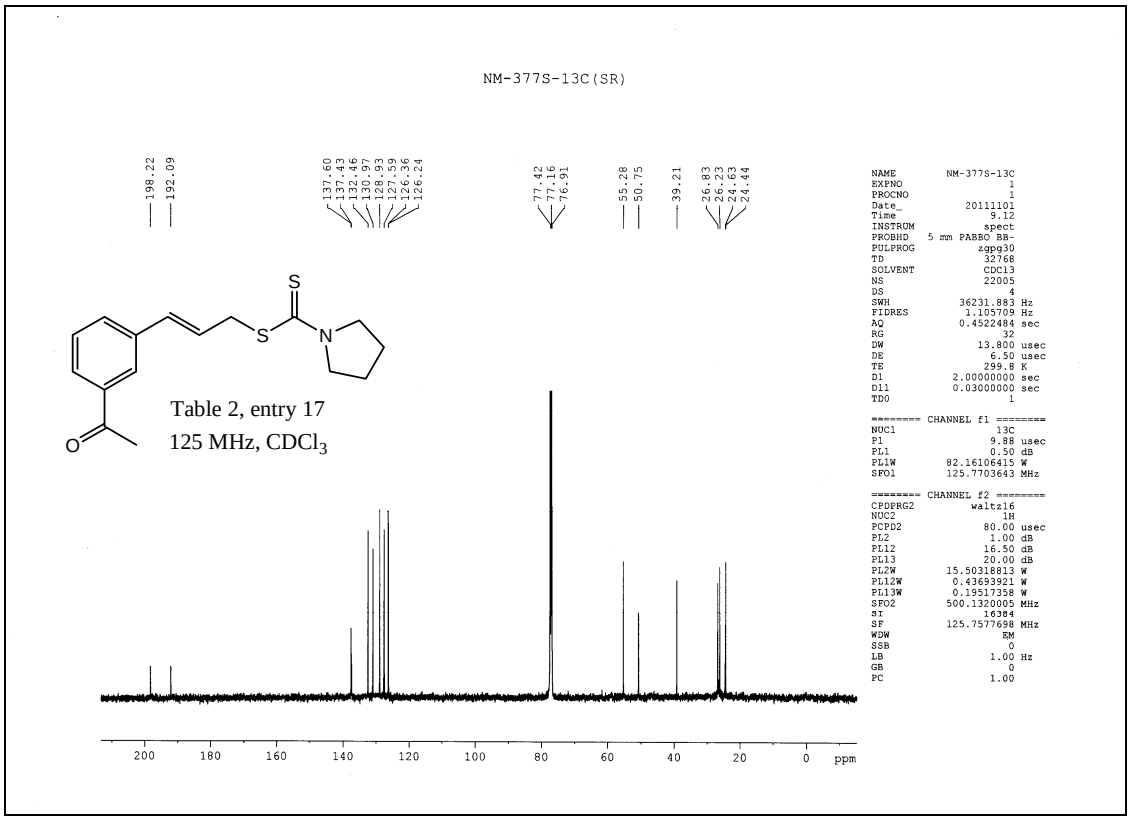

SA111-1H(SKD)
7.354
7.337
7.321
7.307
7.292
7.277
7.256
7.233
7.218
7.204
6.652
6.621
6.340
6.325
6.310
6.294
6.279
4.170
4.155
3.562
3.369
-0.001
S
S
N
Table 2, entry 15
500 MHz, CDCl3
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
2.12
2.10
2.15
1.01
1.00
2.07
2.82
2.85


SA111-13C(SKD)
196.82
136.82
133.76
128.65
127.75
126.56
124.14
77.41
77.16
76.90
45.50
41.56
40.73
S
S
N
Table 2, entry 15
125 MHz, CDCl3
NAME SA111-13C
EXPNO 1
PROCNO 1
Date_ 20100726
Time 11.51
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 334
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 0.5505524 sec
RG 32
DW 16.800 usec
DE 6.50 usec
TE 299.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.88 usec
PL1 0.50 dB
PL1W 82.16106415 W
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 16.50 dB
PL13 20.00 dB
PL2W 15.50318813 W
PL12W 0.43693921 W
PL13W 0.19517358 W
SFO2 500.1320005 MHz
SI 16384
SF 125.7577732 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


SA168-1H(SKD)
7.122
7.116
7.110
6.925
6.920
6.918
6.911
6.765
6.734
6.149
6.134
6.119
6.103
6.088
4.151
4.136
3.932
3.918
3.905
3.640
3.626
3.612
2.071
2.057
2.043
2.030
2.016
1.977
1.963
1.949
1.936
1.922
-0.001
S
S
N
S
Table 2, entry 16
500 MHz, CDCl3
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
ppm
1.00
2.24
1.18
1.06
2.54
2.66
2.66
2.74
2.72


SA168-13C(SKD)
191.91
141.67
127.27
126.52
125.71
124.32
123.85
77.42
77.16
76.91
55.05
50.57
39.14
26.04
24.25
S
S
N
S
Table 2, entry 16
125 MHz, CDCl3
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm
NAME SA168-13C
EXPNO 1
PROCNO 1
Date_ 20101110
Time 13.32
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 328
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 0.5505524 sec
RG 32
DW 16.800 usec
DE 6.50 usec
TE 300.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.88 usec
PL1 0.50 dB
PL1W 82.16106415 W
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 16.50 dB
PL13 20.00 dB
PL2W 15.50318813 W
PL12W 0.43693921 W
PL13W 0.19517358 W
SFO2 500.1320005 MHz
SI 16384
SF 125.7577952 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00


TC377-1H(SKD)
7.861
7.740
7.726
7.592
7.486
7.338
7.323
7.308
7.190
6.628
6.596
6.358
6.344
6.328
6.312
6.297
4.150
4.136
3.894
3.603
2.544
2.046
2.033
2.019
2.006
1.992
1.971
1.963
1.950
1.937
1.924
1.910
1.896
S
S
N
O
Table 2, entry 17
500 MHz, CDCl3
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
-0.5
ppm
1.00
0.96
1.07
1.03
0.83
1.35
1.01
2.11
2.47
1.94
3.19
3.07
2.74


NM-377S-13C(SR)
198.22
192.09
137.60
137.43
132.46
130.97
128.93
127.39
126.36
126.24
77.42
77.16
76.91
55.28
50.75
39.21
26.83
26.23
24.63
24.44
S
S
N
O
Table 2, entry 17
125 MHz, CDCl3
NAME NM-377S-13C
EXPNO 1
PROCNO 1
Date_ 20111101
Time_ 9.12
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 22005
DS 4
SWH 36231.883 Hz
FIDRES 1.105709 Hz
AQ 0.4522484 sec
RG 32
DW 13.800 usec
DE 6.50 usec
TE 299.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.88 usec
PL1 0.50 dB
PL1W 82.16106415 W
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 16.50 dB
PL13 20.00 dB
PL2W 15.50318813 W
PL12W 0.43693921 W
PL13W 0.19517358 W
SFO2 500.1320005 MHz
SI 16384
SF 125.7577698 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
200
180
160
140
120
100
80
60
40
20
0
ppm

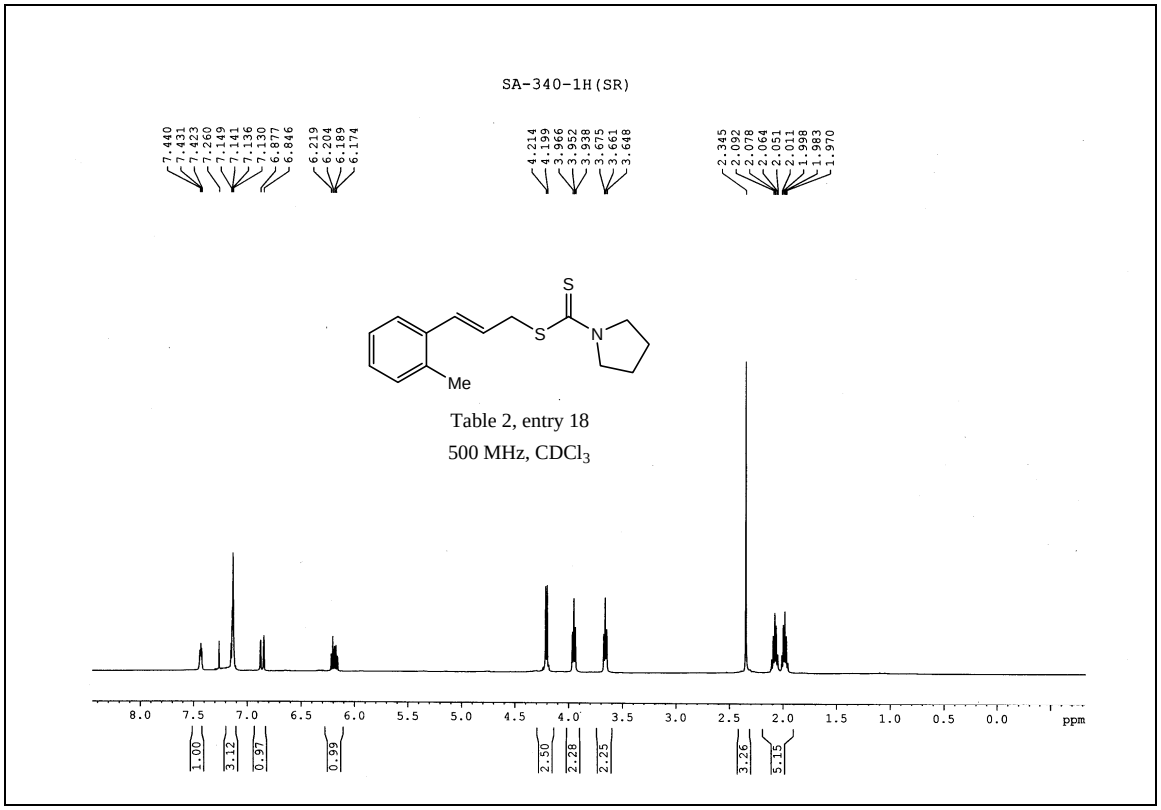


Table 2, entry 18

500 MHz, $CDCl_3$

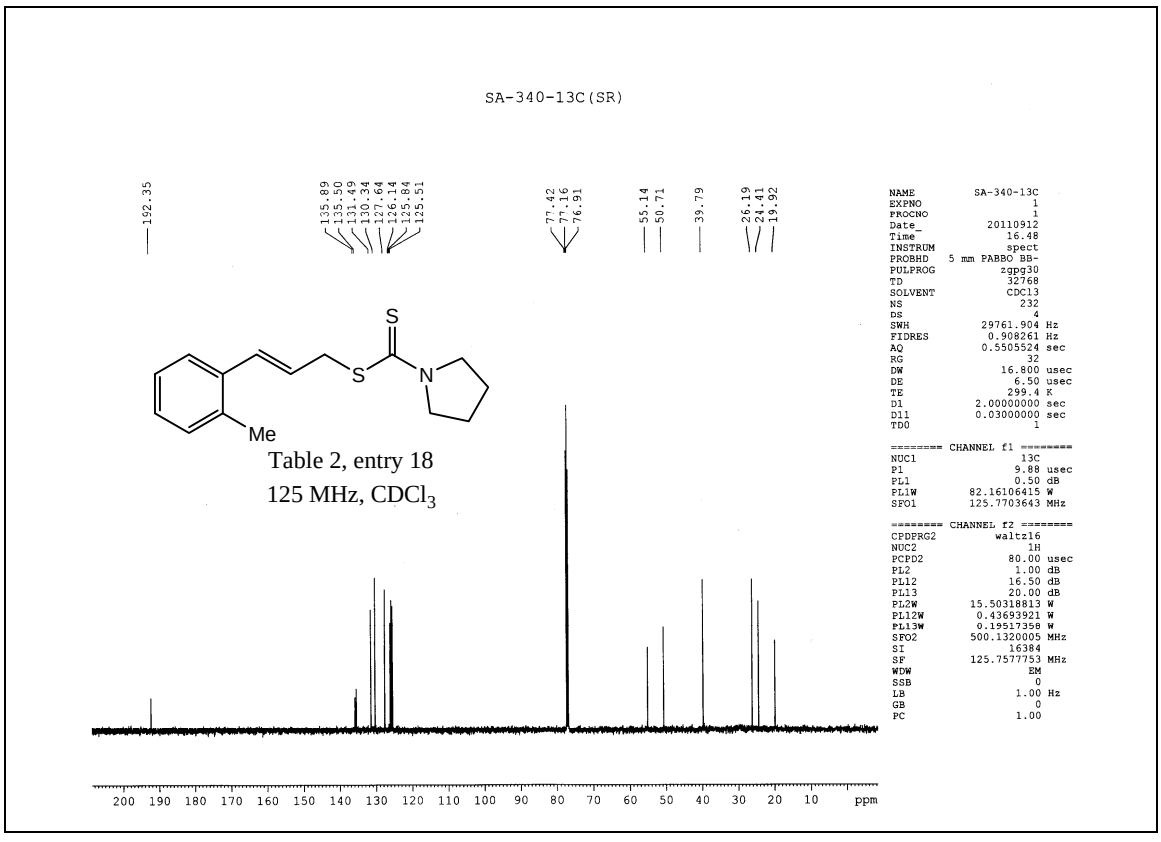
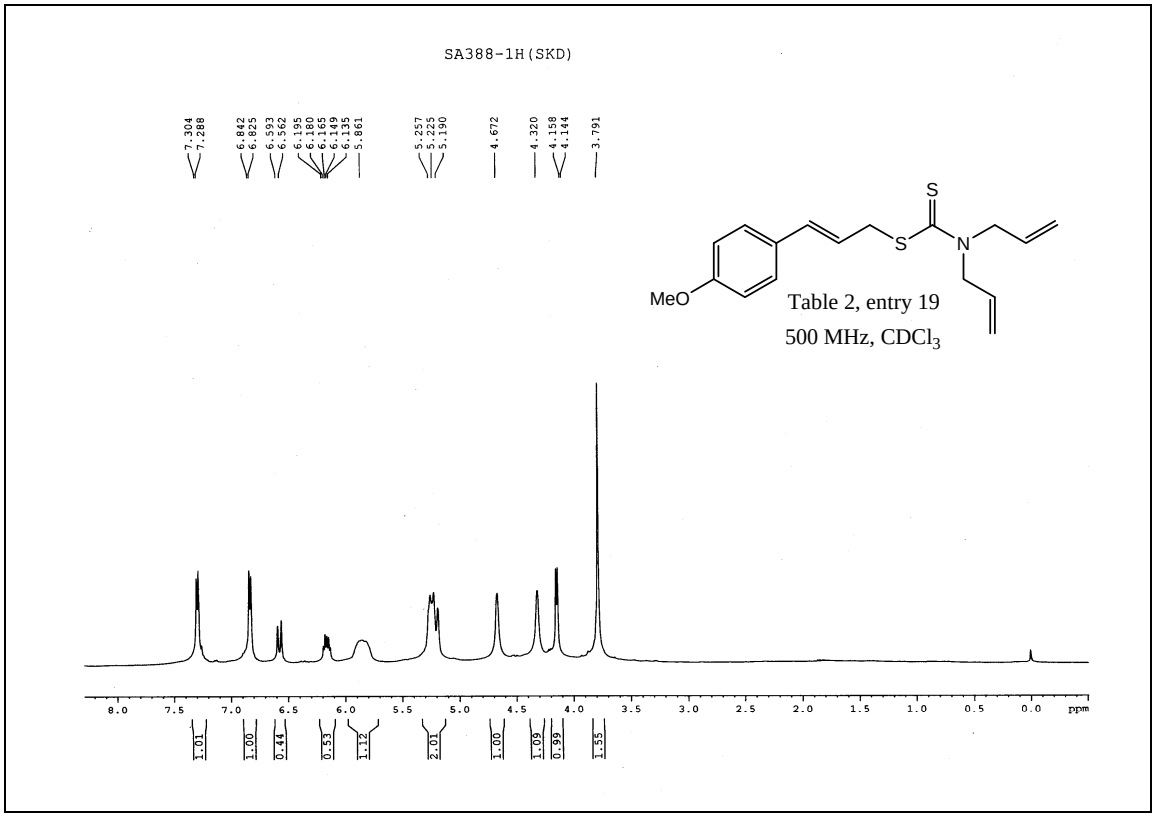
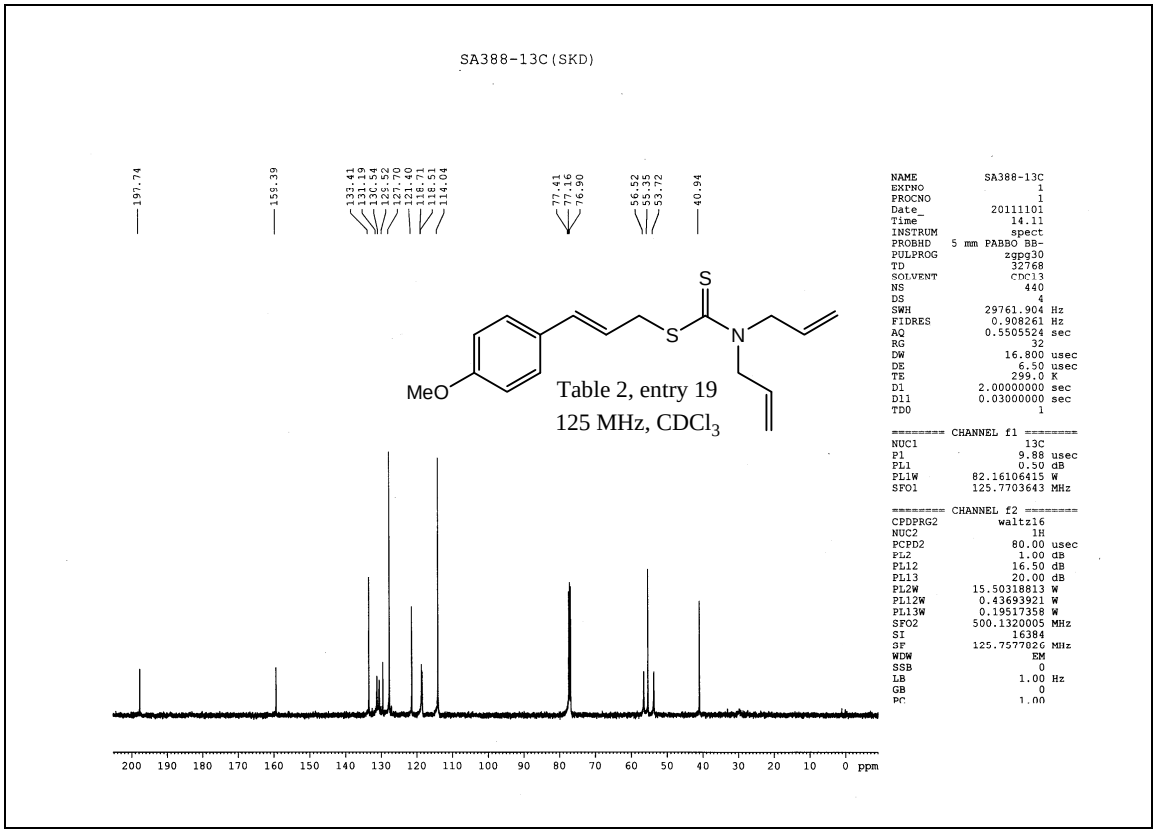
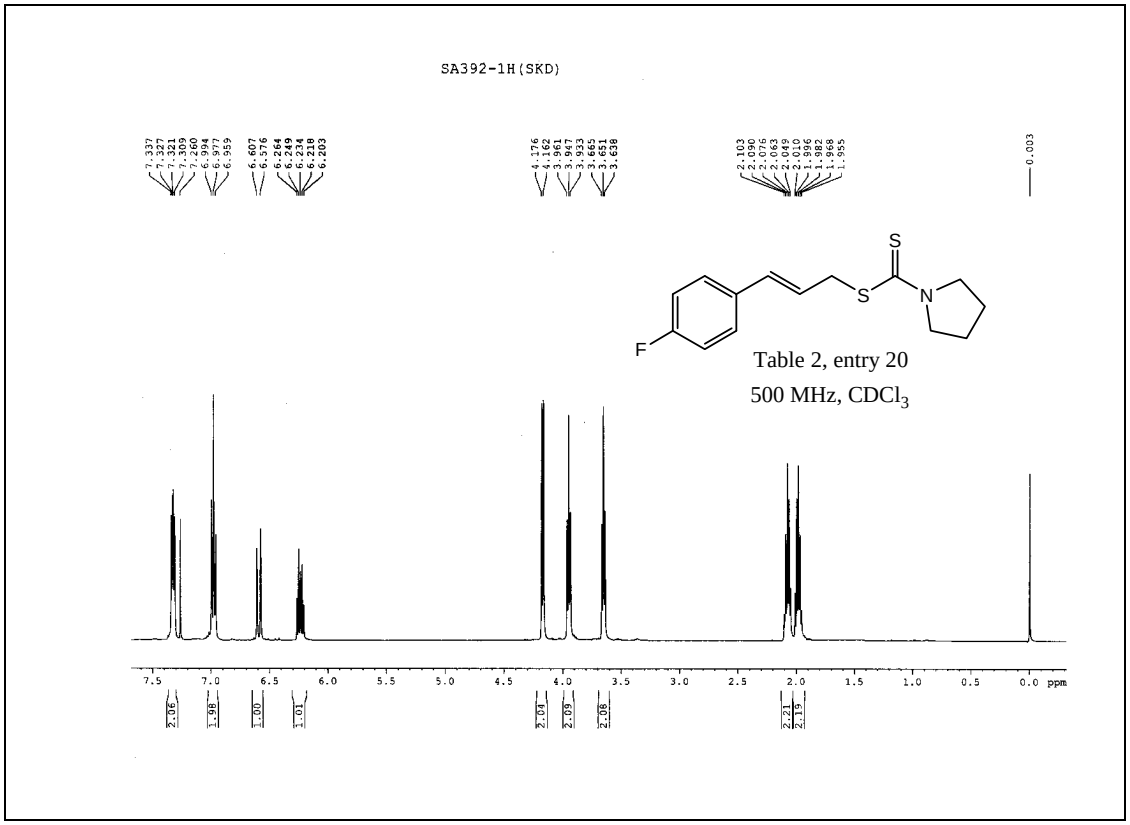


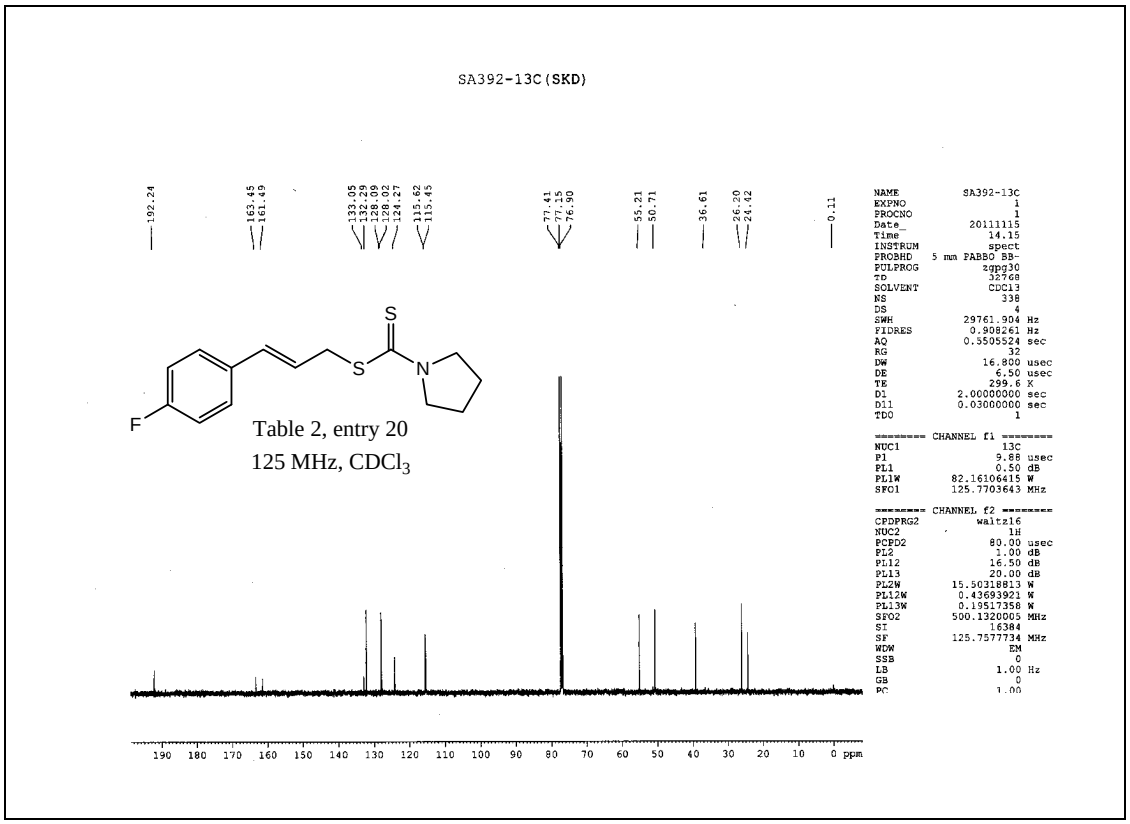
Table 2, entry 18

125 MHz, $CDCl_3$


SA388-1H(SKD)
7.304
7.288
6.842
6.825
6.593
6.562
6.195
6.180
6.165
6.149
6.135
5.861
5.257
5.225
5.190
4.672
4.320
4.158
4.144
3.791
S
S
N
MeO
Table 2, entry 19
500 MHz, CDCl3
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
ppm
1.01
1.00
0.44
0.53
1.12
2.01
1.00
1.09
0.99
1.55


SA388-13C(SKD)
197.74
159.39
133.41
131.19
130.54
129.52
127.70
121.40
118.71
118.51
114.04
77.41
77.16
76.90
56.52
55.35
53.72
40.94
S
S
N
MeO
Table 2, entry 19
125 MHz, CDCl3
NAME SA388-13C
EXPNO 1
PROCNO 1
Date_ 20111101
Time 14.11
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 440
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 0.5505524 sec
RG 32
DW 16.800 usec
DE 6.50 usec
TE 299.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.88 usec
PL1 0.50 dB
PL1W 82.16106415 W
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 16.50 dB
PL13 20.00 dB
PL2W 15.50318813 W
PL12W 0.43693921 W
PL13W 0.19517358 W
SFO2 500.1320005 MHz
SI 16384
SF 125.7577026 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm


SA392-1H(SKD)
7.337
7.327
7.321
7.260
6.994
6.977
6.959
6.607
6.576
6.264
6.249
6.234
6.218
6.203
4.176
4.162
3.961
3.947
3.933
3.665
3.651
3.638
2.103
2.090
2.076
2.063
2.049
2.036
1.996
1.982
1.968
1.955
0.003
S
S
N
F
Table 2, entry 20
500 MHz, CDCl3
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 ppm
2.06
1.98
1.00
1.01
2.04
2.09
2.08
2.21
2.19


SA392-13C(SKD)
192.24
163.45
161.49
133.05
132.98
128.09
128.02
124.27
115.62
115.45
77.41
77.15
76.90
55.21
50.71
36.61
26.20
24.42
0.11
S
S
N
F
Table 2, entry 20
125 MHz, CDCl3
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm
NAME SA392-13C
EXPNO 1
PROCNO 1
Date_ 20111115
Time 14.15
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 338
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 0.5505524 sec
RG 32
DW 16.800 usec
DE 6.50 usec
TE 299.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.88 usec
PL1 0.50 dB
PL1W 82.16106415 W
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 16.50 dB
PL13 20.00 dB
PL2W 15.50318813 W
PL12W 0.43693921 W
PL13W 0.19517358 W
SFO2 500.1320005 MHz
SI 16384
SF 125.7577734 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

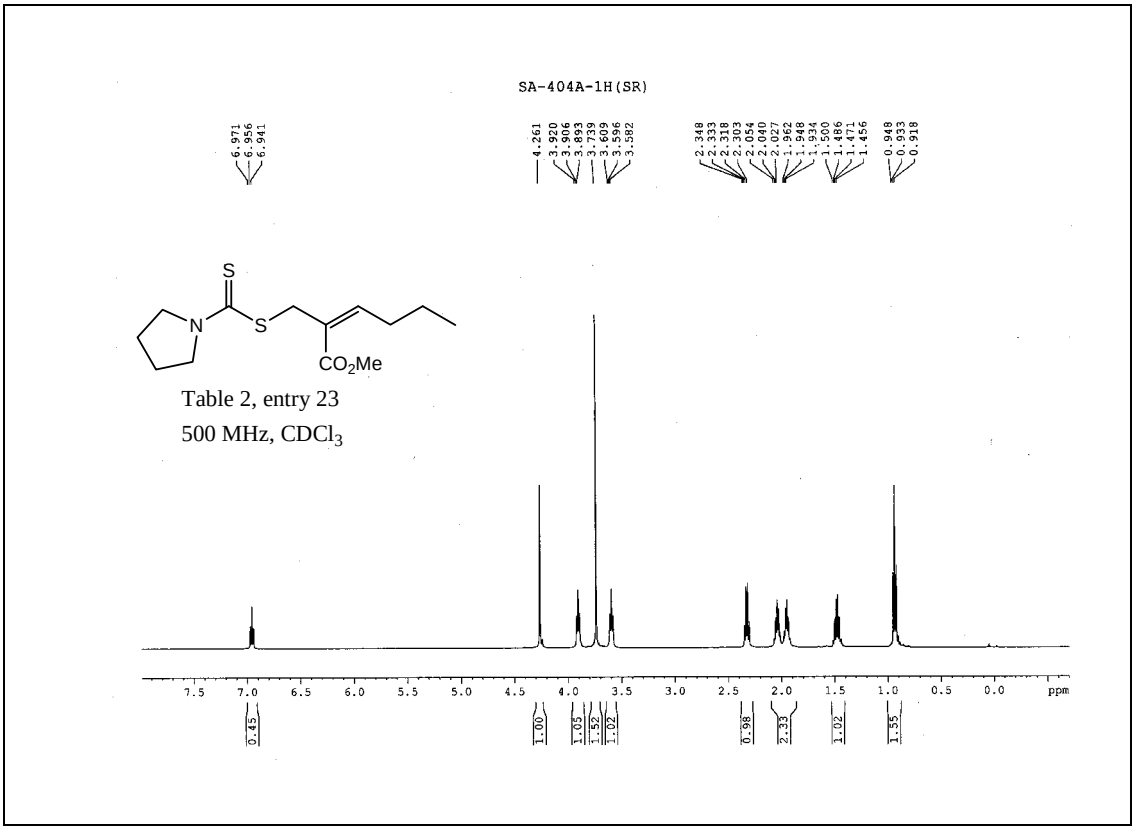


Table 2, entry 23

500 MHz, $CDCl_3$

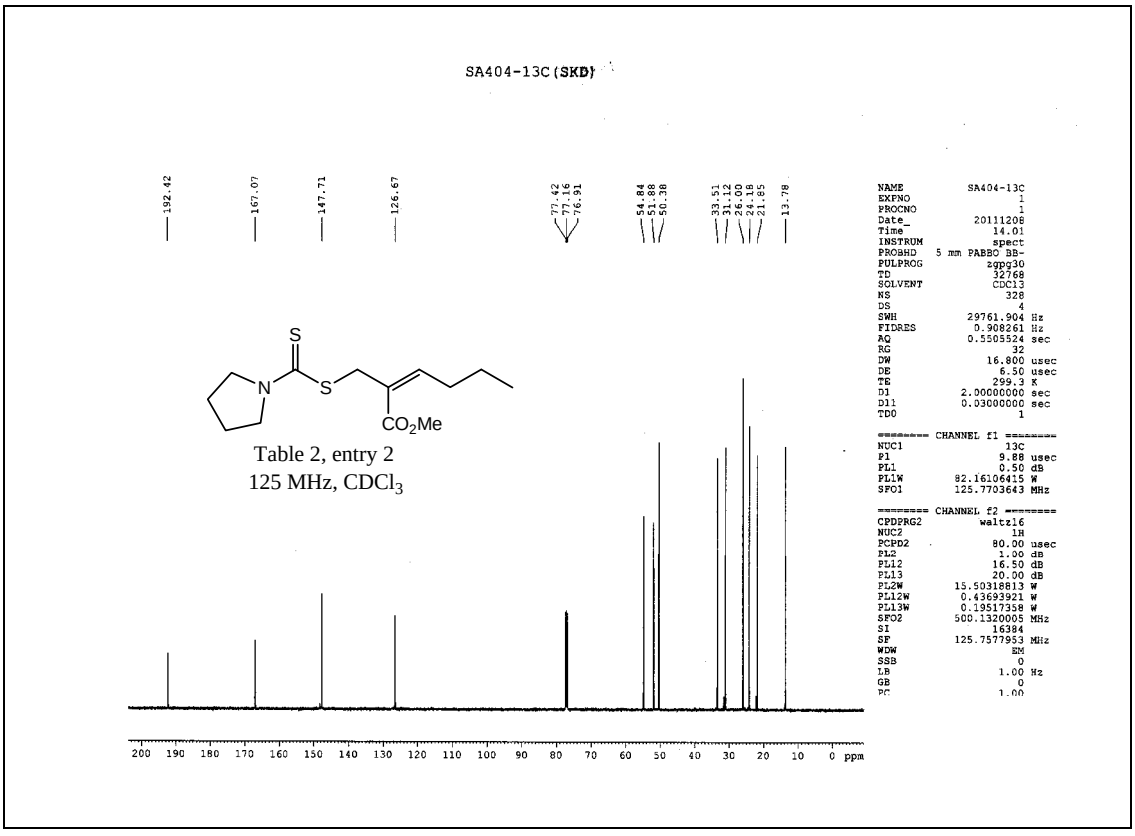
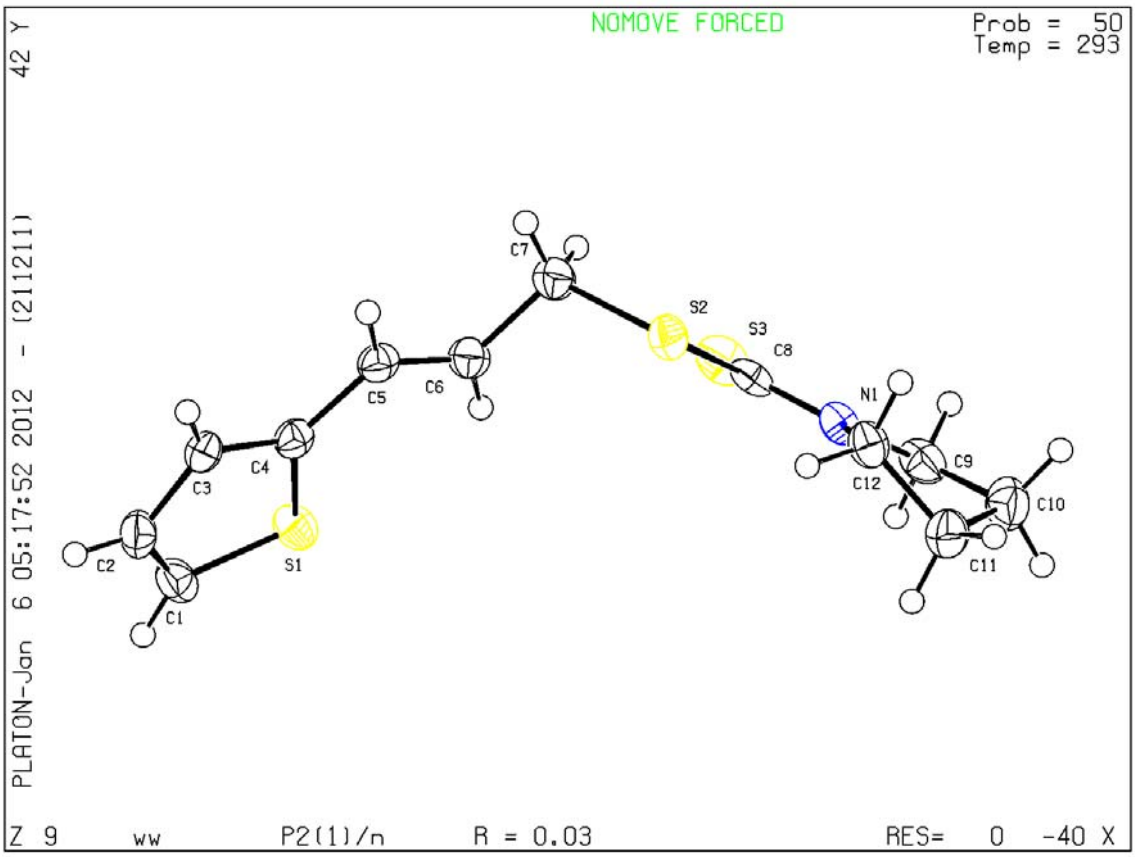


Table 2, entry 2

125 MHz, $CDCl_3$

2. X-Ray Structure of 2p.

(*E*)-3-(Thiophen-2-yl)allyl pyrrolidine-1-carbodithioate, (Table 2, entry 16). (The CCDC deposition number: CCDC 861311).



Bond precision:	C-C = 0.0024 A	Wavelength=0.71073	
Cell:	a=7.7884(5)	b=5.9160(4)	c=28.2073(19)
	alpha=90	beta=95.261(1)	gamma=90
Temperature:	293 K		
	Calculated	Reported	
Volume	1294.21(15)	1294.21(15)	
Space group	P 21/n P2(1)/n		
Hall group	-P 2yn	?	
Moiety formula	C12 H15 N S3	?	
Sum formula	C12 H15 N S3	C12 H15 N S3	
Mr	269.46	269.43	

Dx,g cm-3	1.383	1.383
Z	4	4
Mu (mm-1)	0.545	0.545
F000	568.0	568.0
F000’	569.61	
h,k,lmax	9,7,33	9,7,33
Nref	2272	2272
Tmin,Tmax	0.907,0.947	0.908,0.947
Tmin’	0.907	

Correction method= MULTI-SCAN

Data completeness= 1.000 Theta(max)= 25.000

R(reflections)= 0.0280(2032) wR2(reflections)= 0.0743(2272)

S = 1.069 Npar= 145

The following ALERTS were generated. Each ALERT has the format **test-name_ALERT_alert-type_alert-level**.

Click on the hyperlinks for more details of the test.

Alert level G

PLAT005_ALERT_5_G No _iucr_refine_instructions_details in CIF .... ?

PLAT128_ALERT_4_G Alternate Setting of Space-group P21/c P21/n

PLAT199_ALERT_1_G Check the Reported _cell_measurement_temperature 293 K

PLAT200_ALERT_1_G Check the Reported _diffrn_ambient_temperature 293 K

0 **ALERT level A** = Most likely a serious problem - resolve or explain

0 **ALERT level B** = A potentially serious problem, consider carefully

0 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

4 **ALERT level G** = General information/check it is not something unexpected

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

0 ALERT type 2 Indicator that the structure model may be wrong or deficient

0 ALERT type 3 Indicator that the structure quality may be low

1 ALERT type 4 Improvement, methodology, query or suggestion

1 ALERT type 5 Informative message, check