Supporting Information

Copper nanoparticles catalysed phenyl-selenylation of aryl iodides and vinyl bromides in water under ligand free condition

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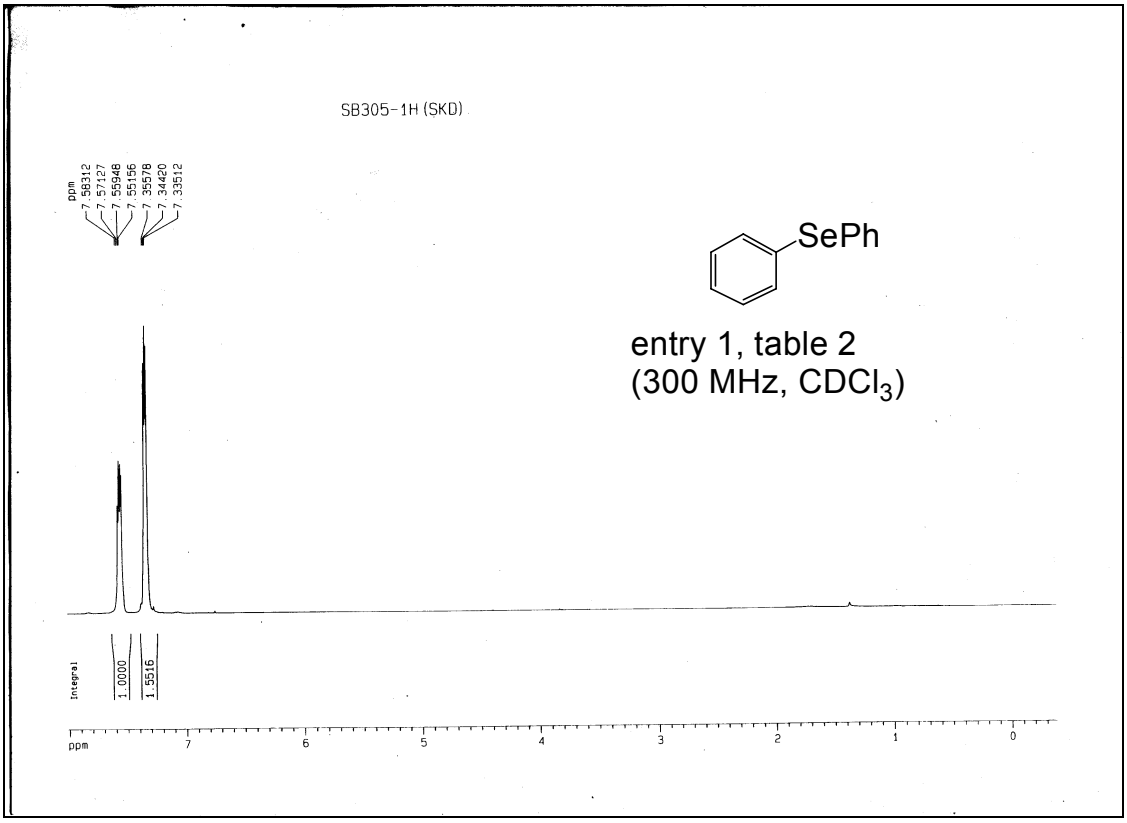
Copies of ^{1}H and ^{13}C NMR spectra of all products in Table 2 2-16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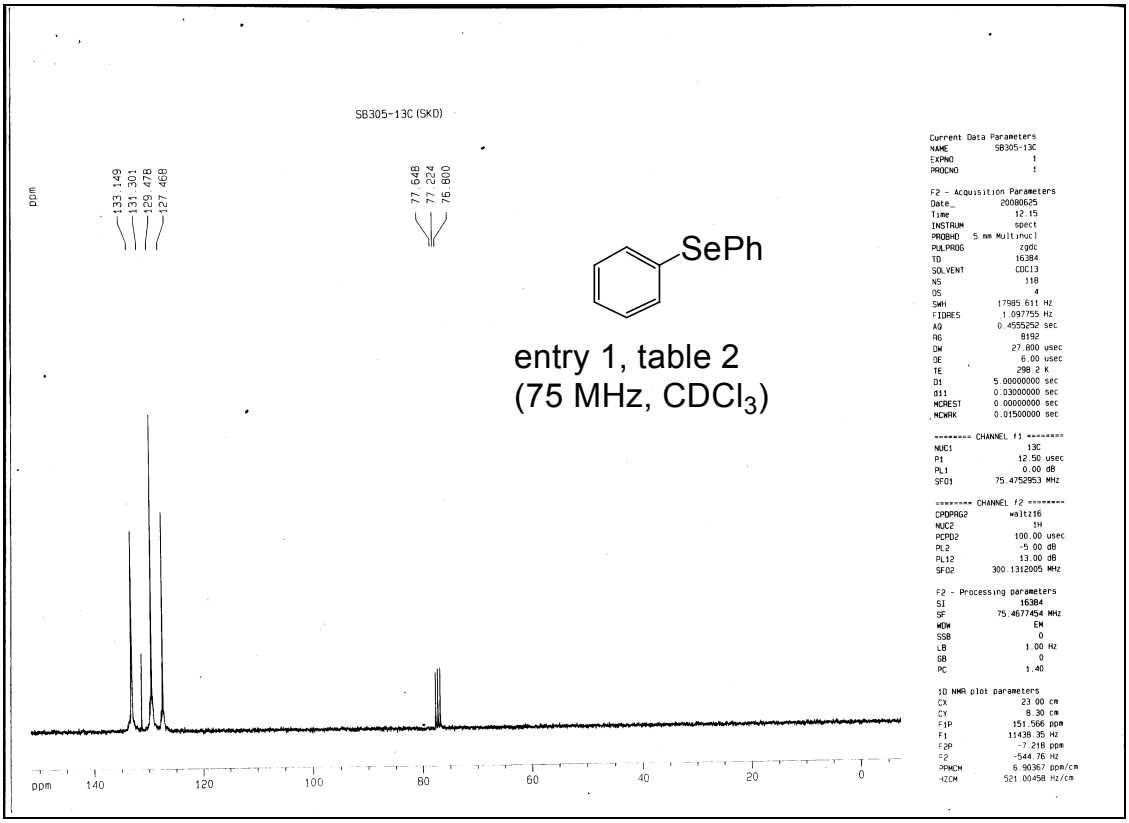
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MCWRK 0.01500000 sec
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SFO1 75.4752953 MHz
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PL12 13.00 dB
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LB 1.00 Hz
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PC 1.40
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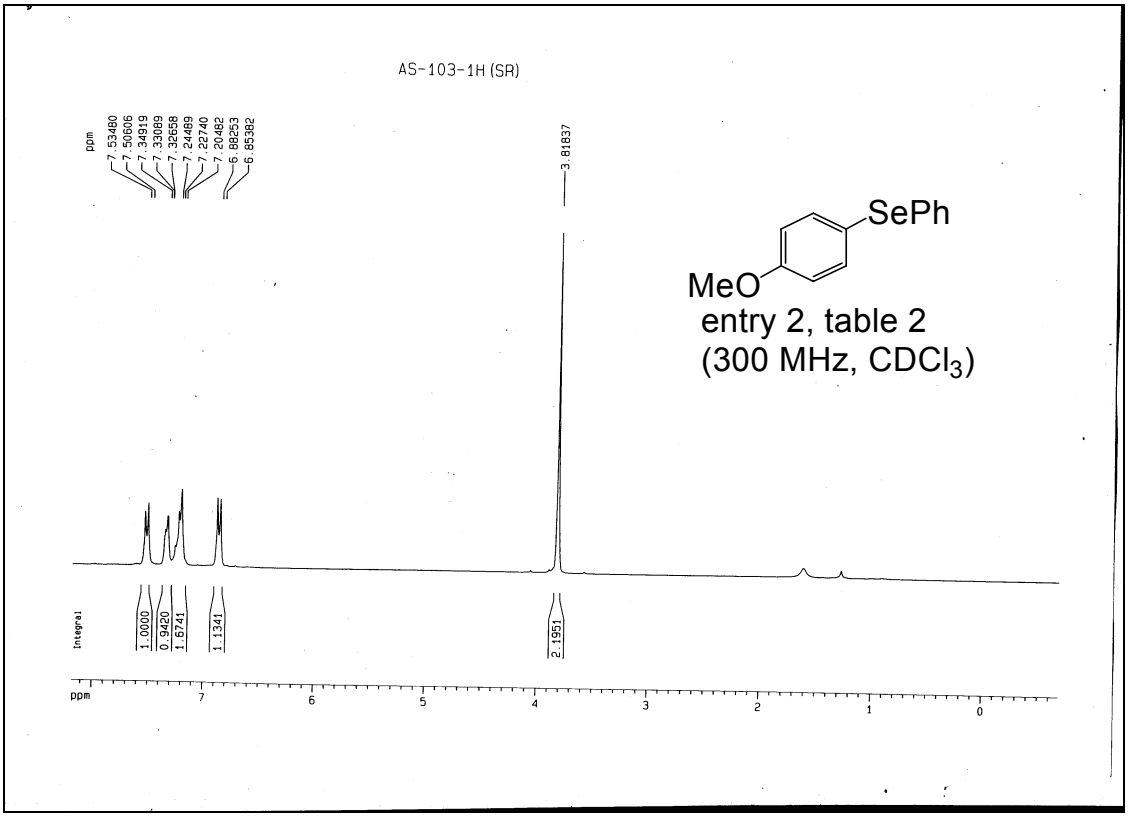
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SePh
MeO
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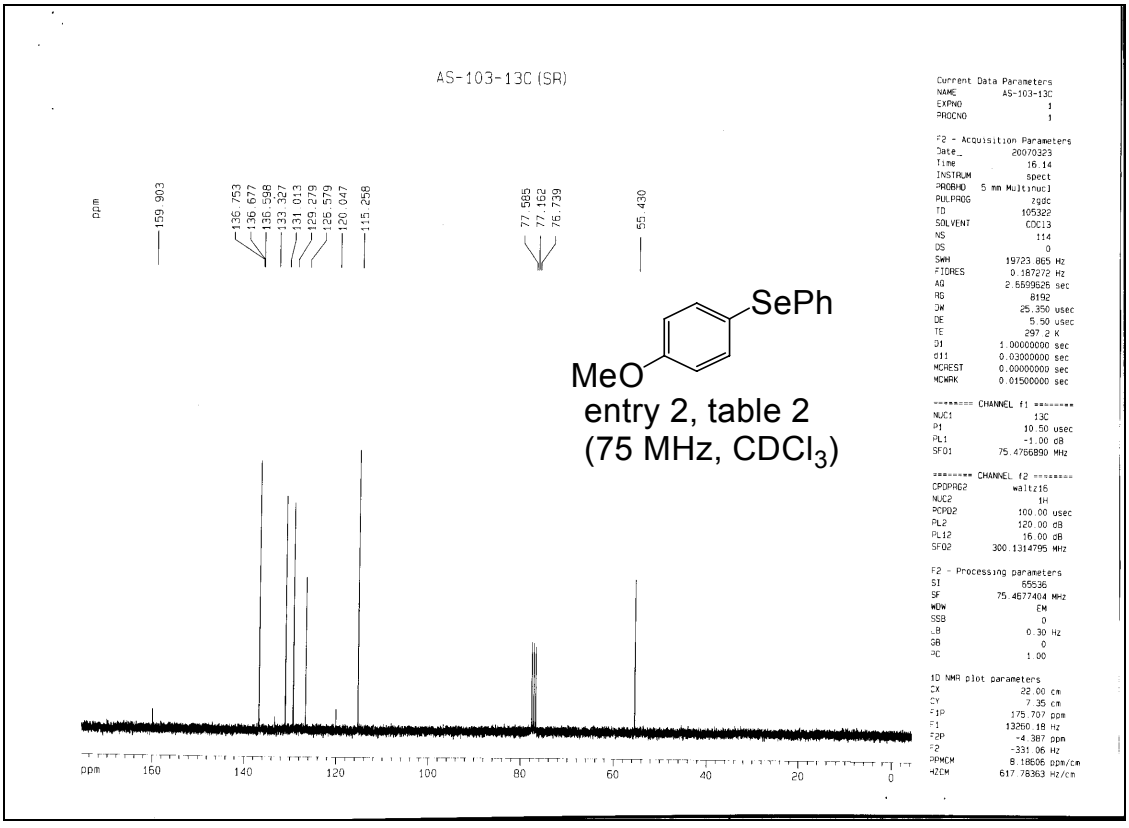
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76.739
55.430
SePh
MeO
entry 2, table 2
(75 MHz, CDCl3)
ppm
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140
120
100
80
60
40
20
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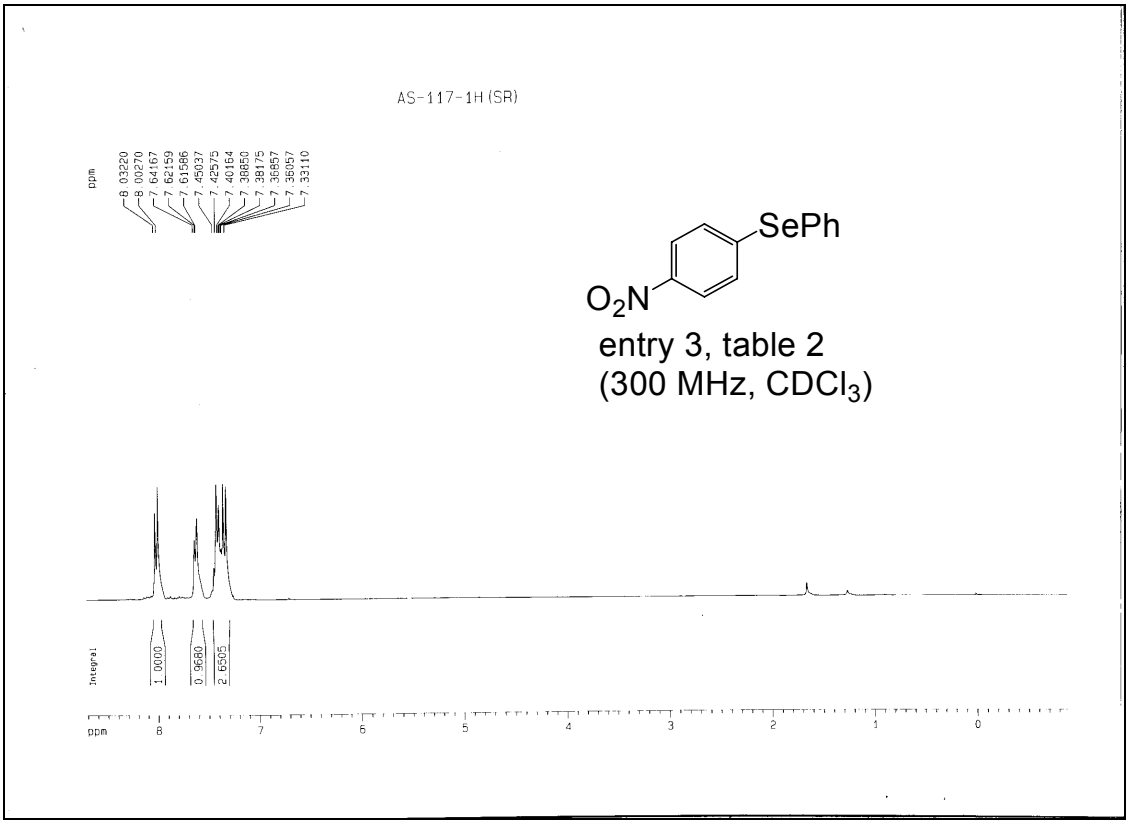
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7.62159
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7.38175
7.36857
7.36057
7.33110
SePh
O_2N
entry 3, table 2
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ppm
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7
6
5
4
3
2
1
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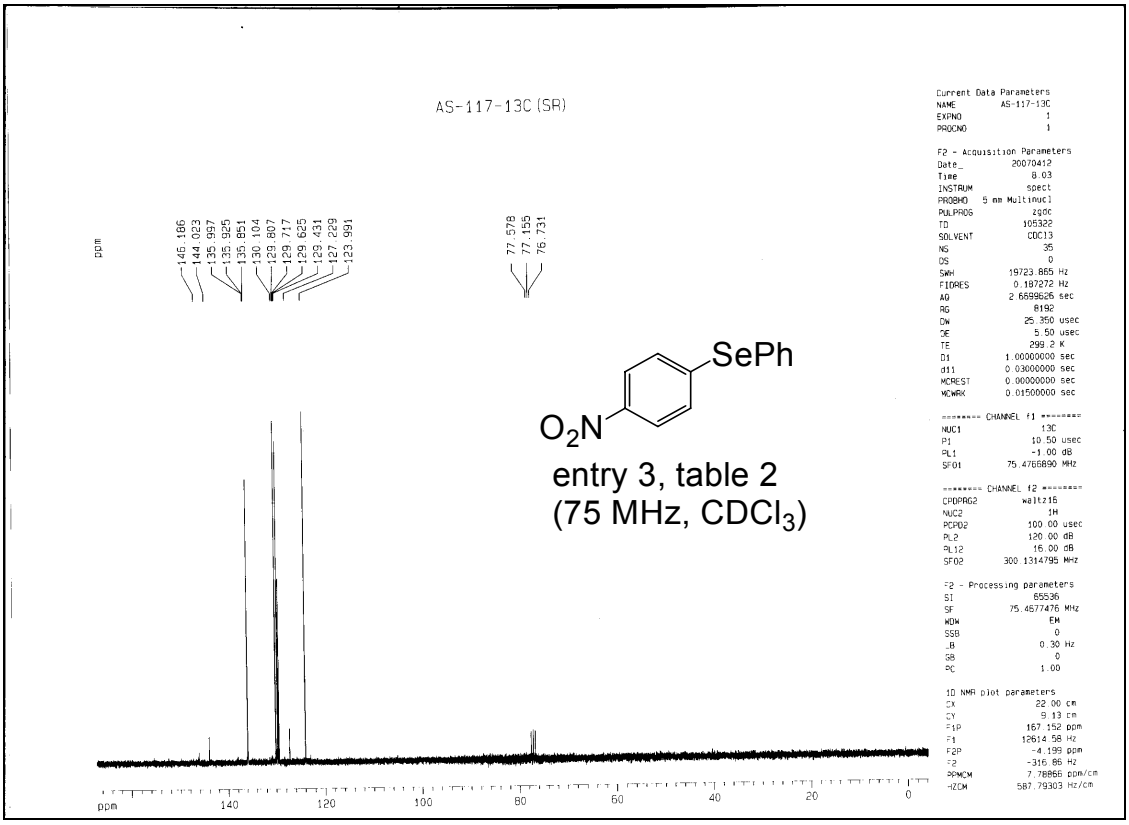
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129.431
127.229
123.991
77.578
77.155
76.731
SePh
O_2N
entry 3, table 2
(75 MHz, $CDCl_3$)
ppm
140
120
100
80
60
40
20
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======== CHANNEL f2 ========
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NUC2 1H
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LB 0.30 Hz
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PC 1.00
1D NMR plot parameters
CX 22.00 cm
CY 9.13 cm
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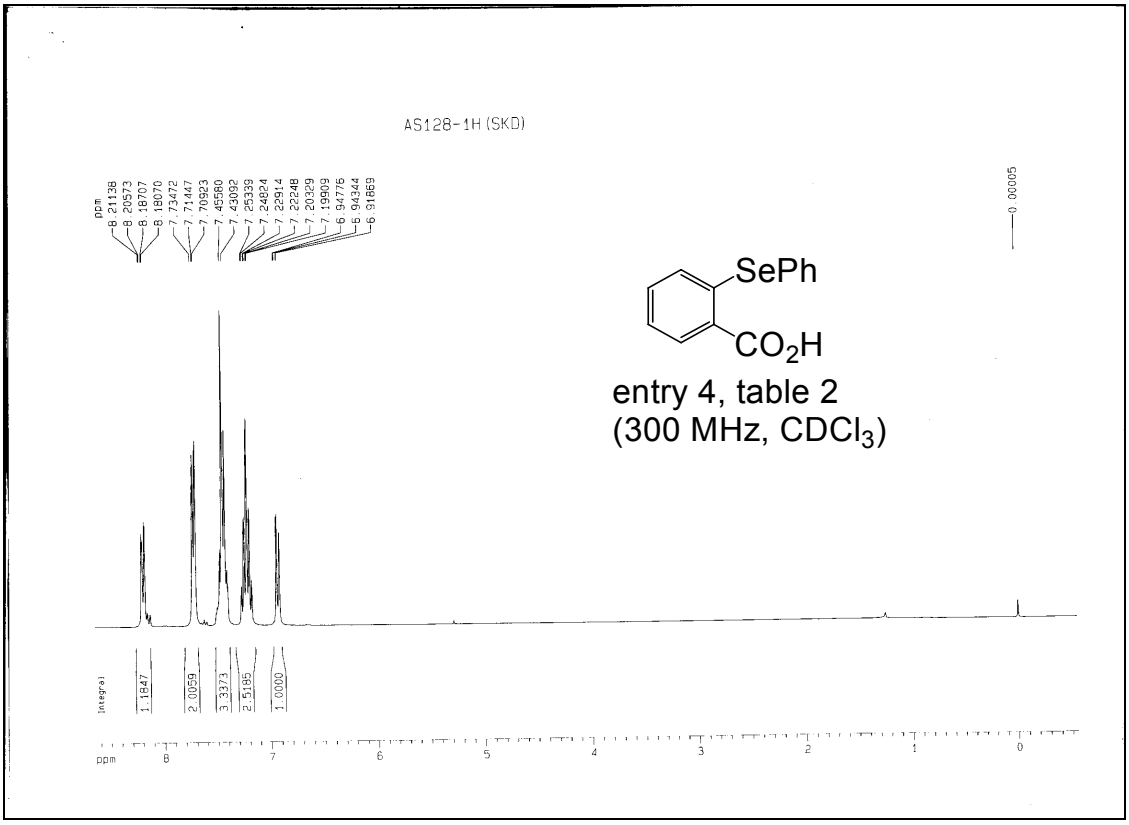
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7.43092
7.25339
7.24824
7.22914
7.22248
7.20329
7.19909
6.94776
6.94344
6.91869
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CO_2H
entry 4, table 2
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ppm
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6
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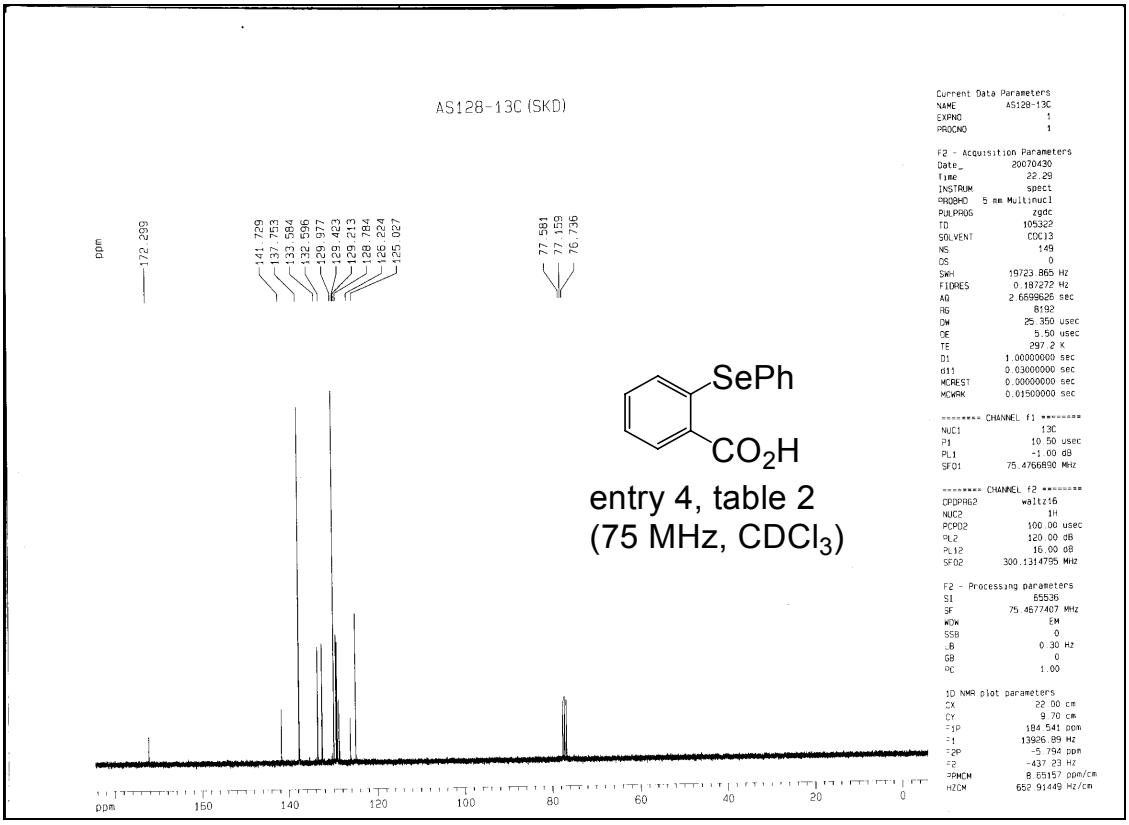
3
2
1
0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77.581
77.159
76.736
SePh
CO_2H
entry 4, table 2
(75 MHz, $CDCl_3$)
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140
120
100
80
60
40
20
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NUC1 13C
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SFO1 75.4766890 MHz
======== CHANNEL f2 ========
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NUC2 1H
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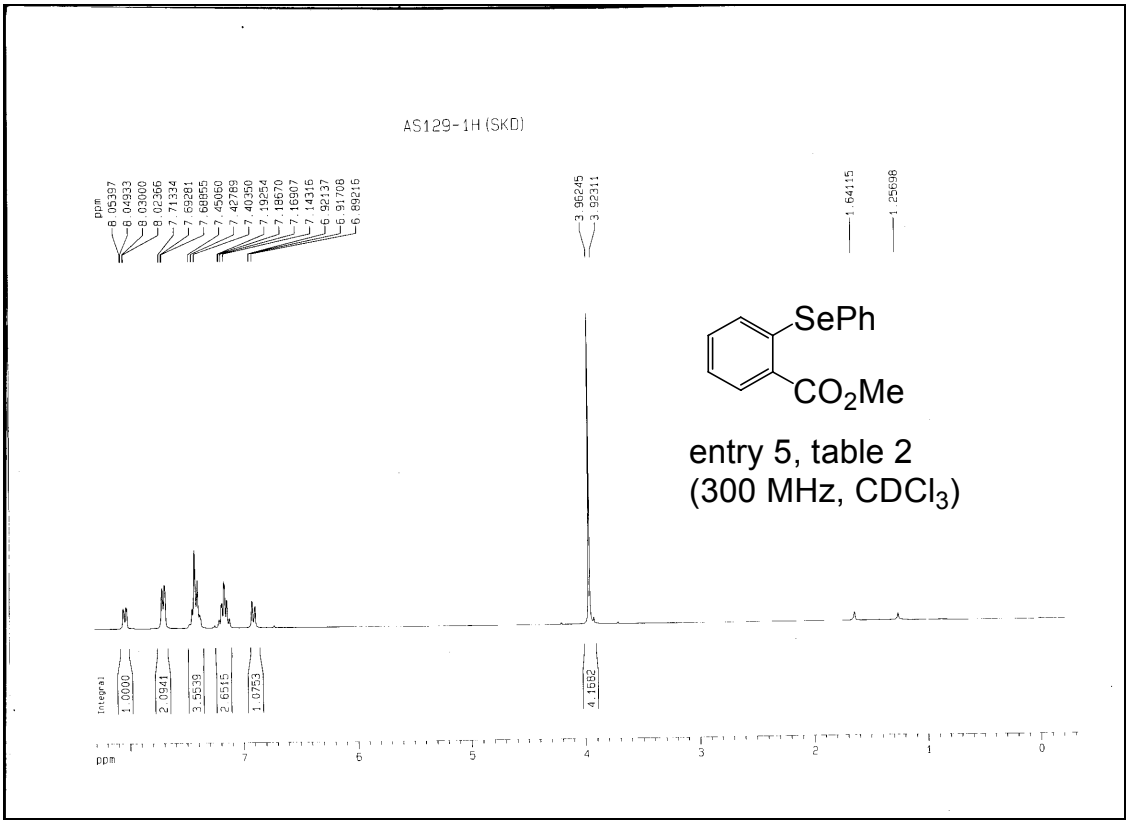
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7.40350
7.19254
7.18670
7.1690
7.14316
6.92137
6.91708
6.89216
3.96245
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1.64115
1.25698
SePh
CO2Me
entry 5, table 2
(300 MHz, CDCl3)
Integral
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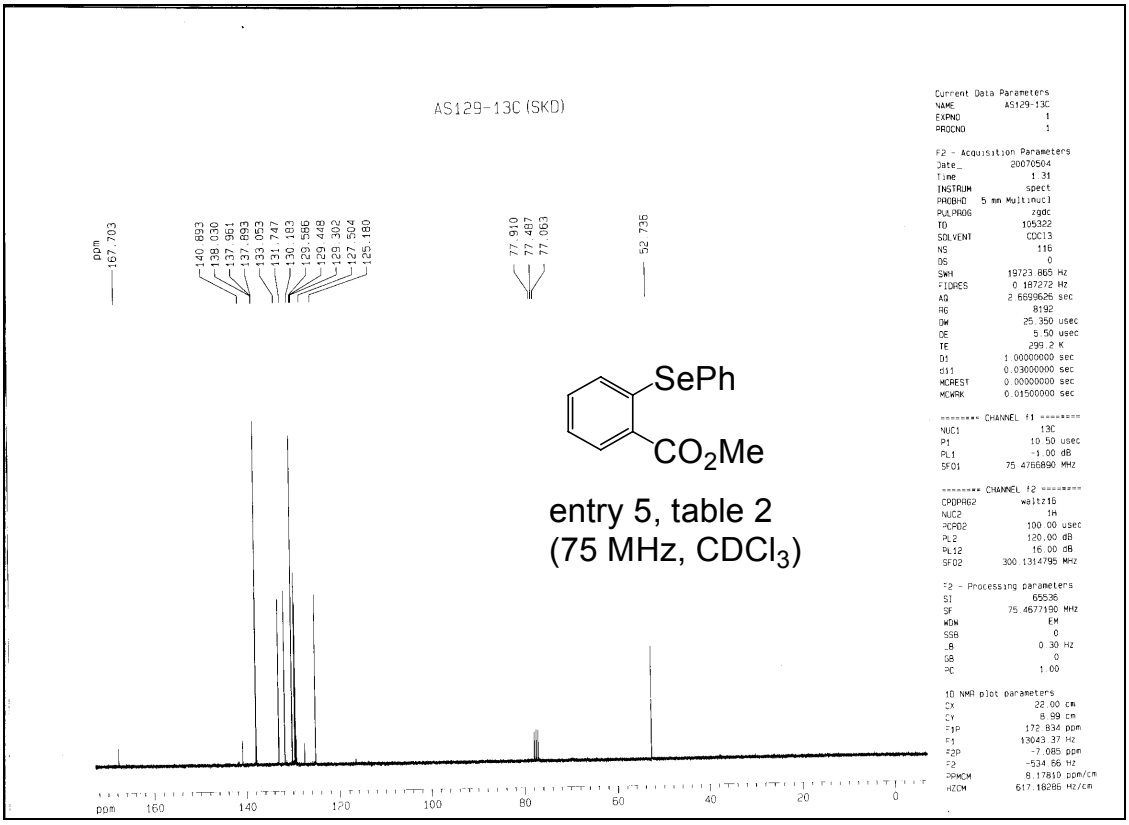
AS129-13C (SKD)
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129.448
129.302
127.504
125.180
77.910
77.487
77.063
52.736
SePh
CO2Me
entry 5, table 2
(75 MHz, CDCl3)
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140
120
100
80
60
40
20
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PROCNO 1
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PULPROG zgdc
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SOLVENT CDCl3
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d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
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NUC1 13C
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SFO1 75.4766890 MHz
======== CHANNEL f2 ========
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NUC2 1H
PCPD2 100.00 usec
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PL12 16.00 dB
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CY 8.99 cm
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F2P -7.085 ppm
F2 -534.66 Hz
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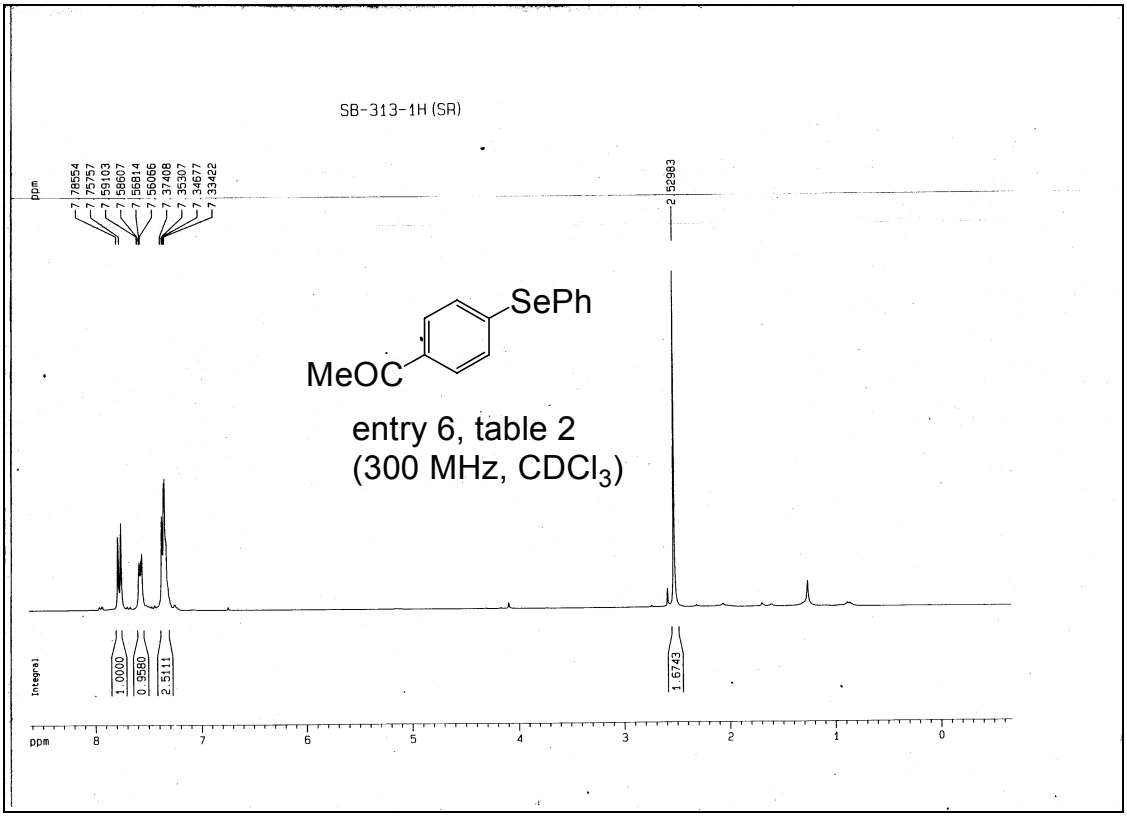
HZCM 617.1828 Hz/cm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7.34677
7.33422
2.52983
SePh
MeOC
entry 6, table 2
(300 MHz, CDCl3)
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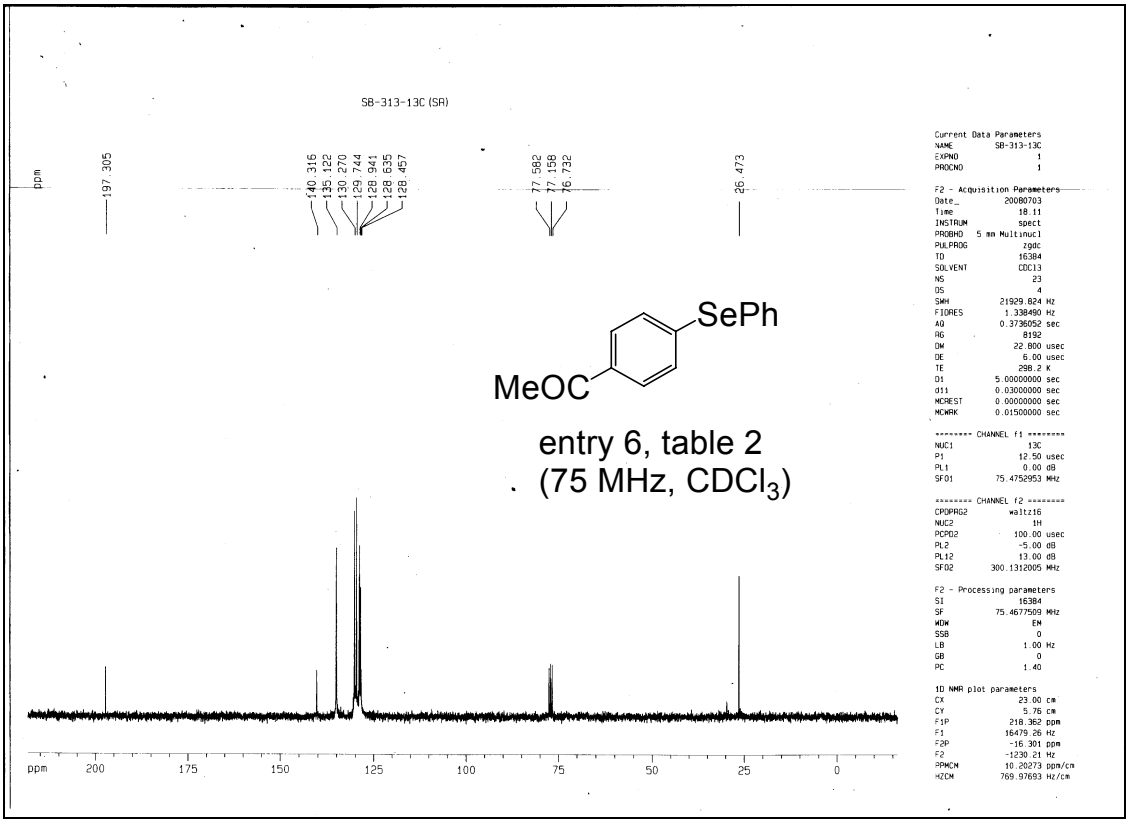
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135.122
130.270
129.744
128.941
128.635
128.457
77.582
77.158
76.732
26.473
SePh
MeOC
entry 6, table 2
(75 MHz, CDCl3)
ppm
200
175
150
125
100
75
50
25
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F2 - Acquisition Parameters
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PULPROG zgdc
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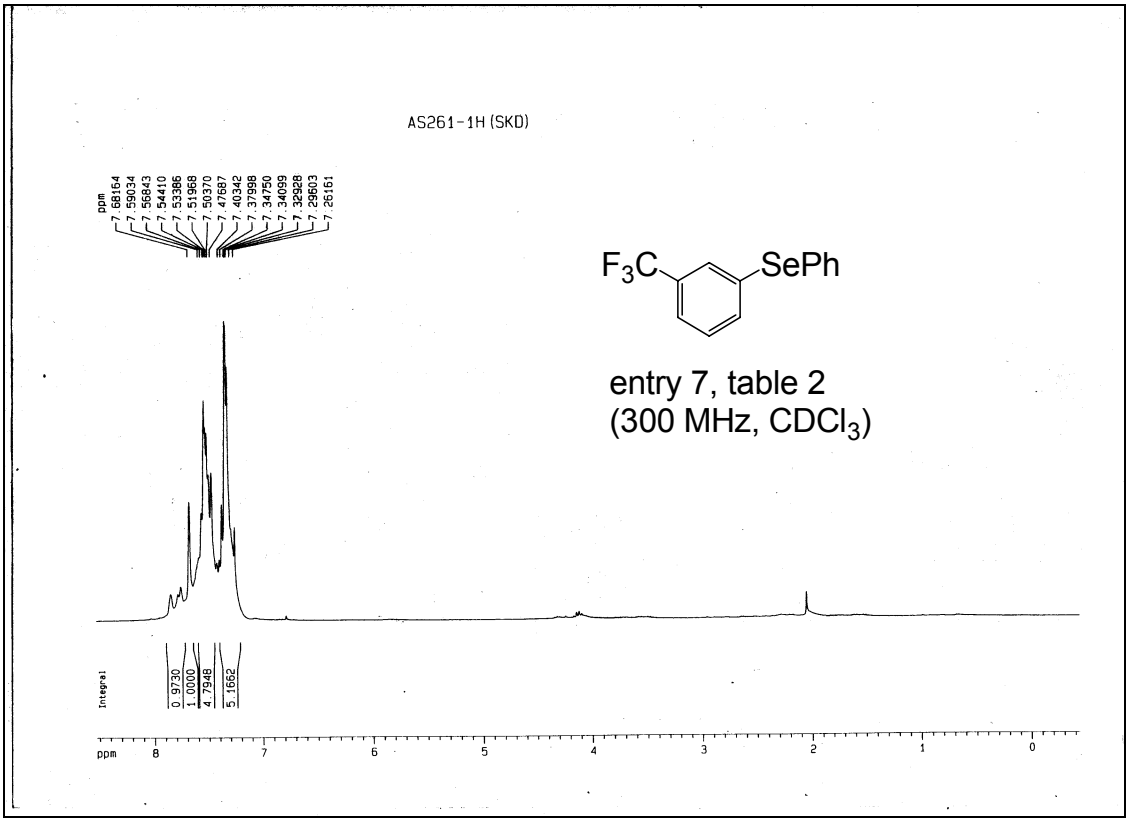
SWH 21929.824 Hz
FIDRES 1.338490 Hz
AQ 0.3736052 sec
RG 8192
DW 22.800 usec
DE 6.00 usec
TE 298.2 K
D1 5.00000000 sec
D11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 12.50 usec
PL1 0.00 dB
SFO1 75.4752953 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -5.00 dB
PL12 13.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 16384
SF 75.4677509 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 23.00 cm
CY 5.76 cm
F1P 218.362 ppm
F1 16479.26 Hz
F2P -16.301 ppm
F2 -1230.21 Hz
PPMCM 10.20273 ppm/cm
HZCM 769.97693 Hz/cm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7.56843
7.54410
7.53386
7.51968
7.50370
7.47687
7.40342
7.37998
7.34750
7.34099
7.32928
7.29603
7.26161
F3C
SePh
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(300 MHz, CDCl3)
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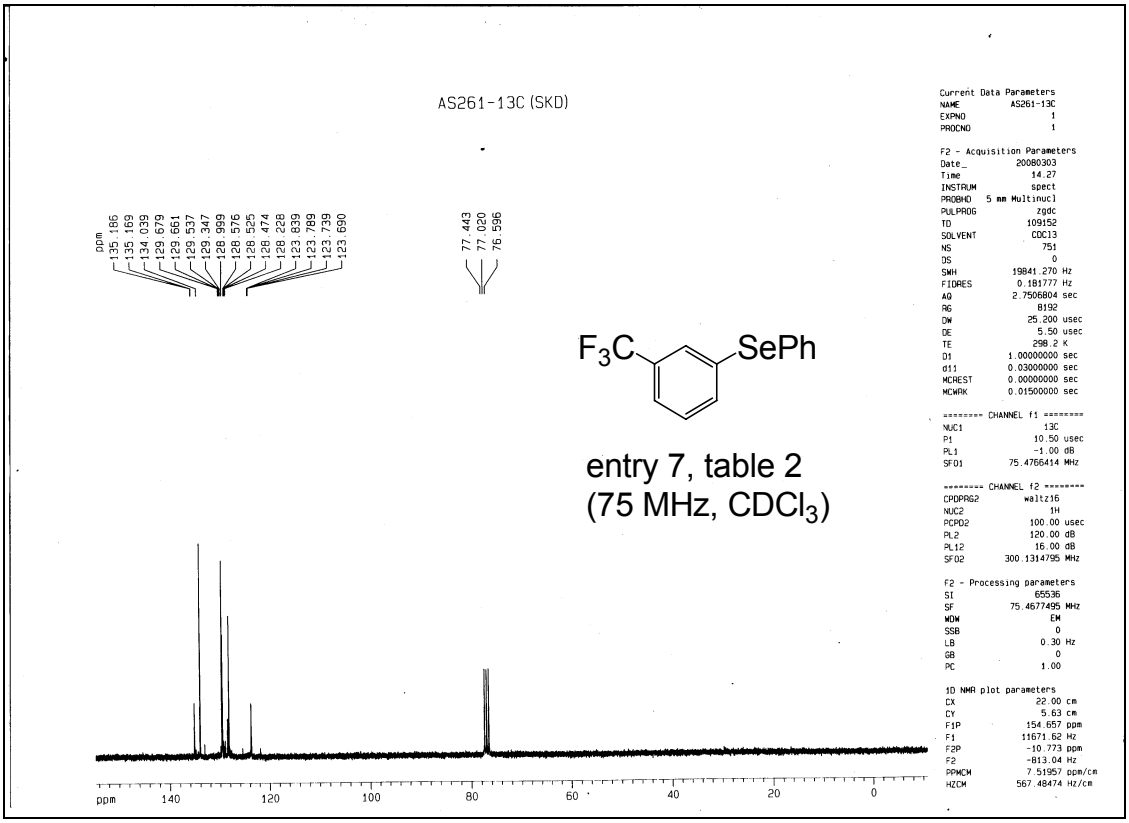
ppm 8 7 6 5 4 3 2 1 0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135.169
134.039
129.679
129.661
129.537
129.347
128.999
128.576
128.525
128.474
128.228
123.839
123.789
123.739
123.690
77.443
77.020
76.596
F3C
SePh
entry 7, table 2
(75 MHz, CDCl3)
ppm 140 120 100 80 60 40 20 0
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NAME AS261-13C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
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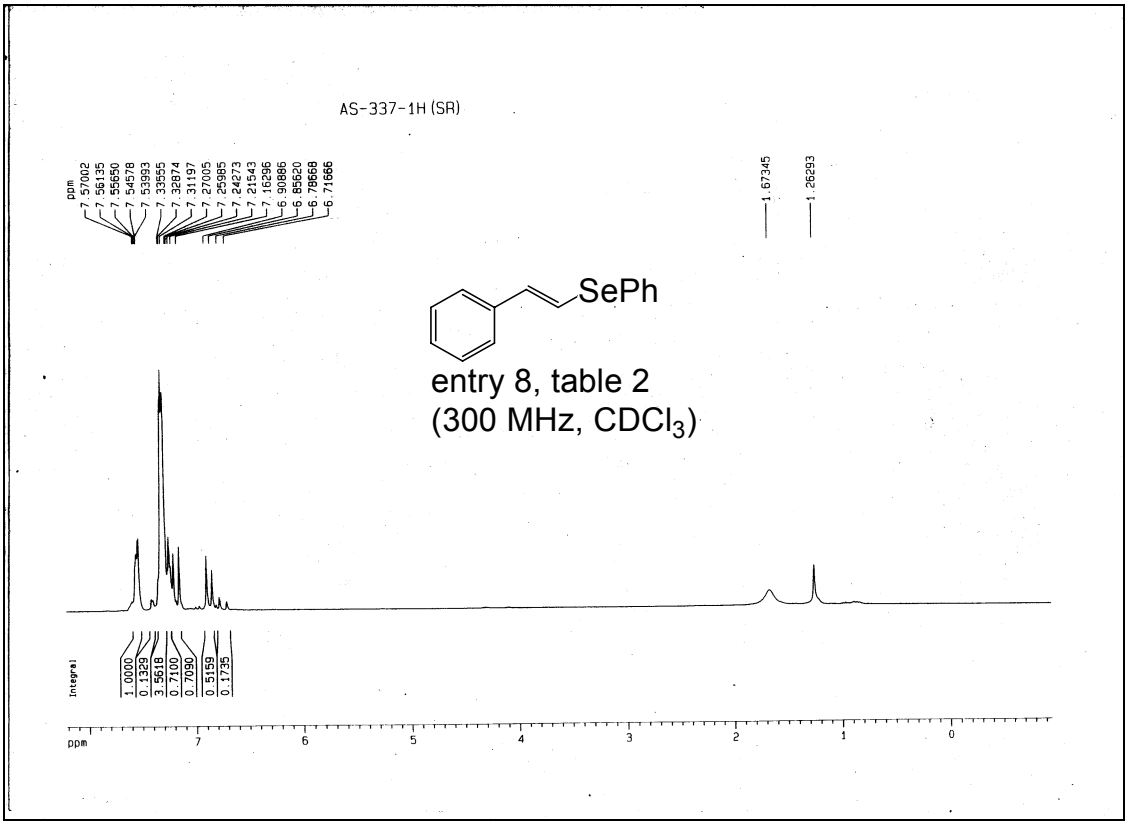
PROBHD 5 mm Multinucl
PULPROG zgdc
TD 109152
SOLVENT CDCl3
NS 751
DS 0
SWH 19841.270 Hz
FIDRES 0.181777 Hz
AQ 2.7506804 sec
RG 8192
DW 25.200 usec
DE 5.50 usec
TE 298.2 K
D1 1.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 -1.00 dB
SFO1 75.4766414 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 16.00 dB
SFO2 300.1314795 MHz
F2 - Processing parameters
SI 65536
SF 75.4677495 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 22.00 cm
CY 5.63 cm
F1P 154.657 ppm
F1 11671.62 Hz
F2P -10.773 ppm
F2 -813.04 Hz
PPMCM 7.51957 ppm/cm
HZCM 567.48474 Hz/cm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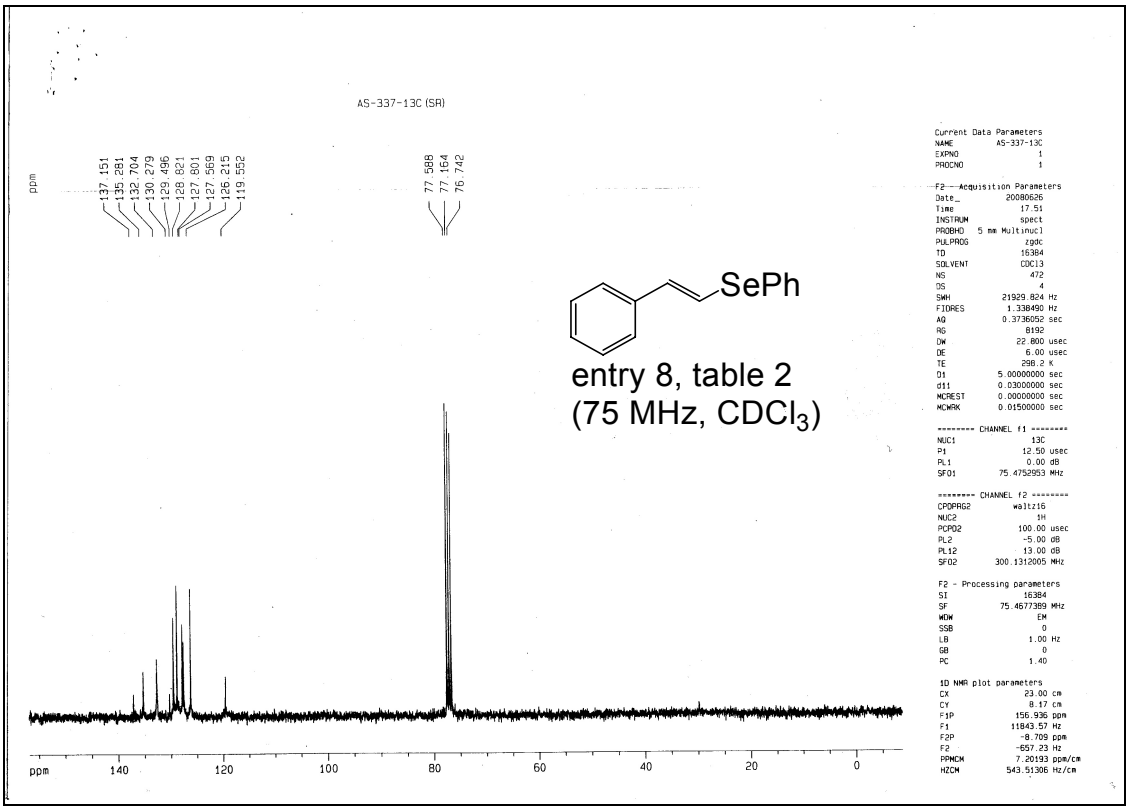
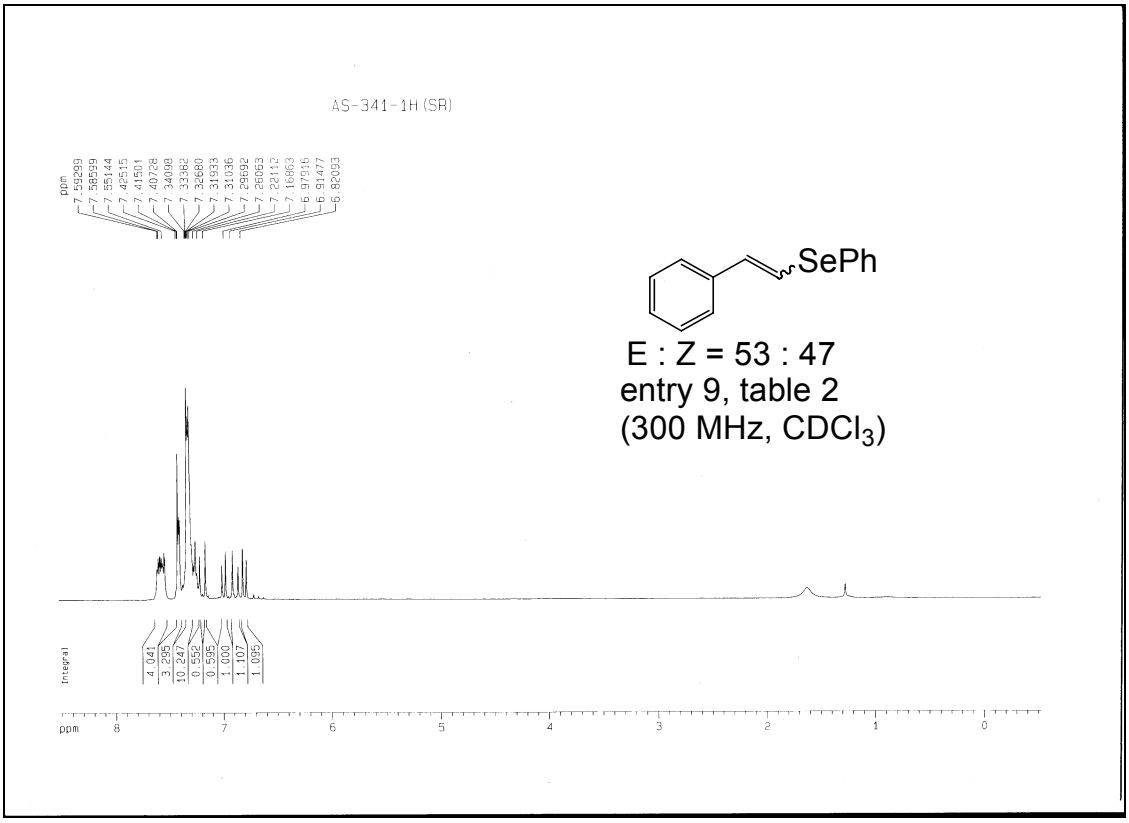
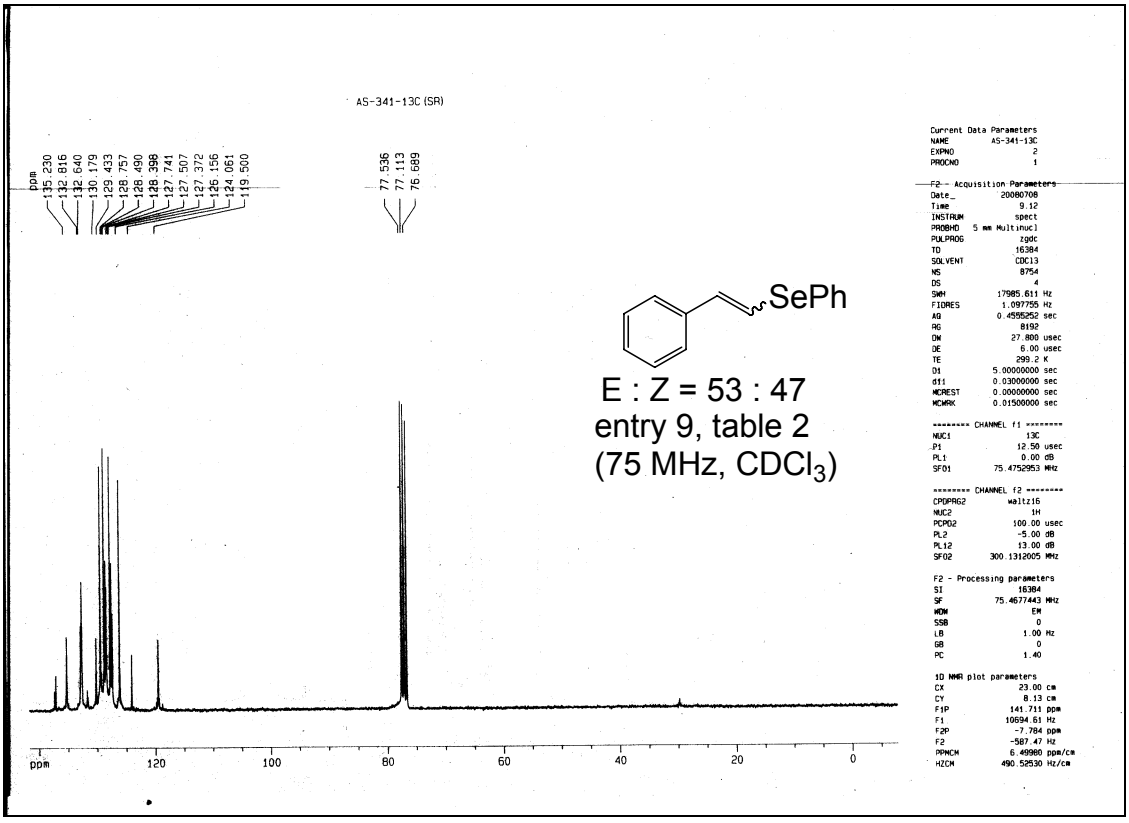
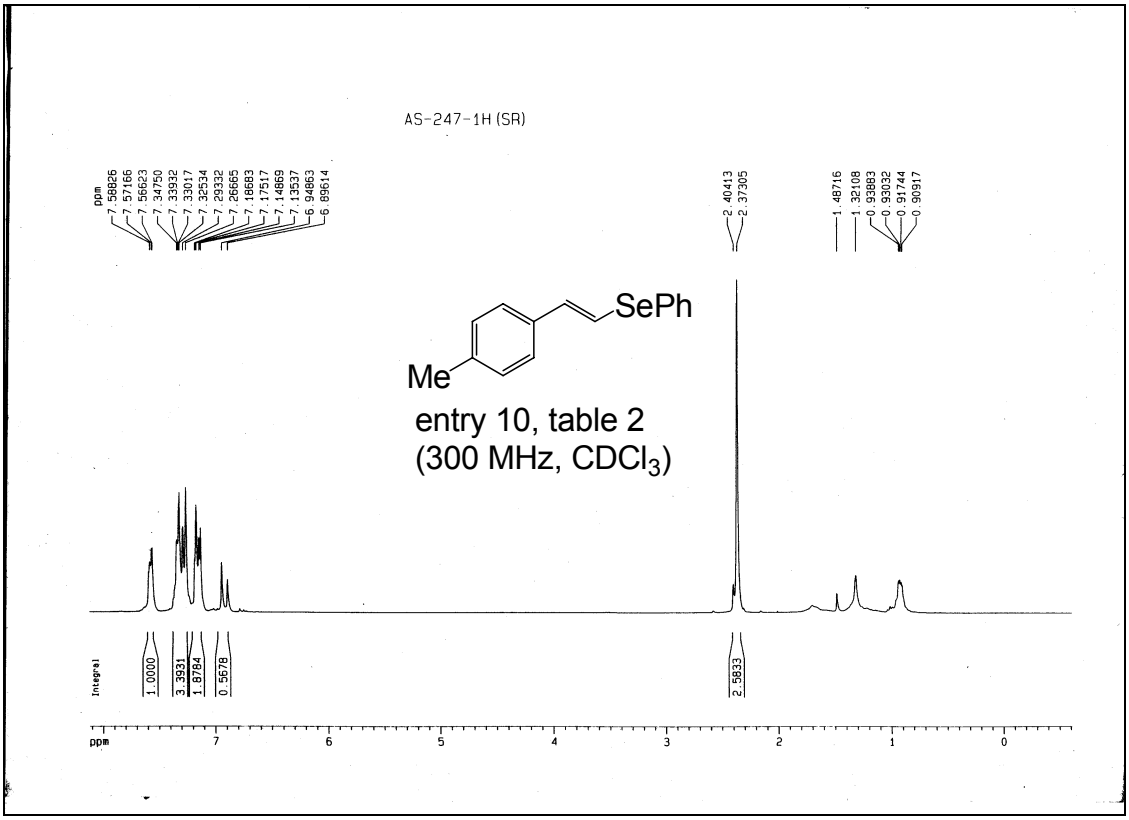
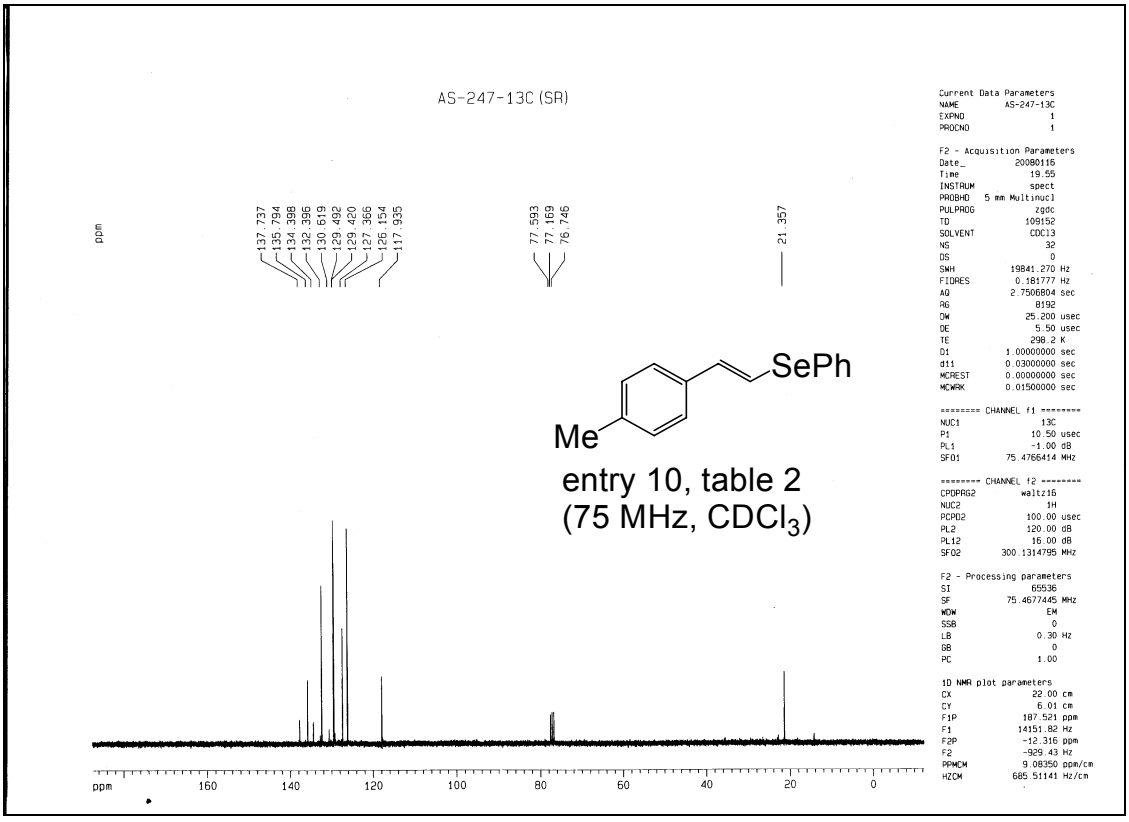
7.55650
7.54578
7.53993
7.33555
7.32874
7.31197
7.27005
7.25985
7.24273
7.21543
7.16296
6.90886
6.85620
6.78668
6.71666
1.67345
1.26293
SePh
entry 8, table 2
(300 MHz, CDCl3)
Integral
1.0000
0.1329
3.5618
0.7100
0.7090
0.5159
0.1735
ppm
7
6
5
4
3
2
1
0

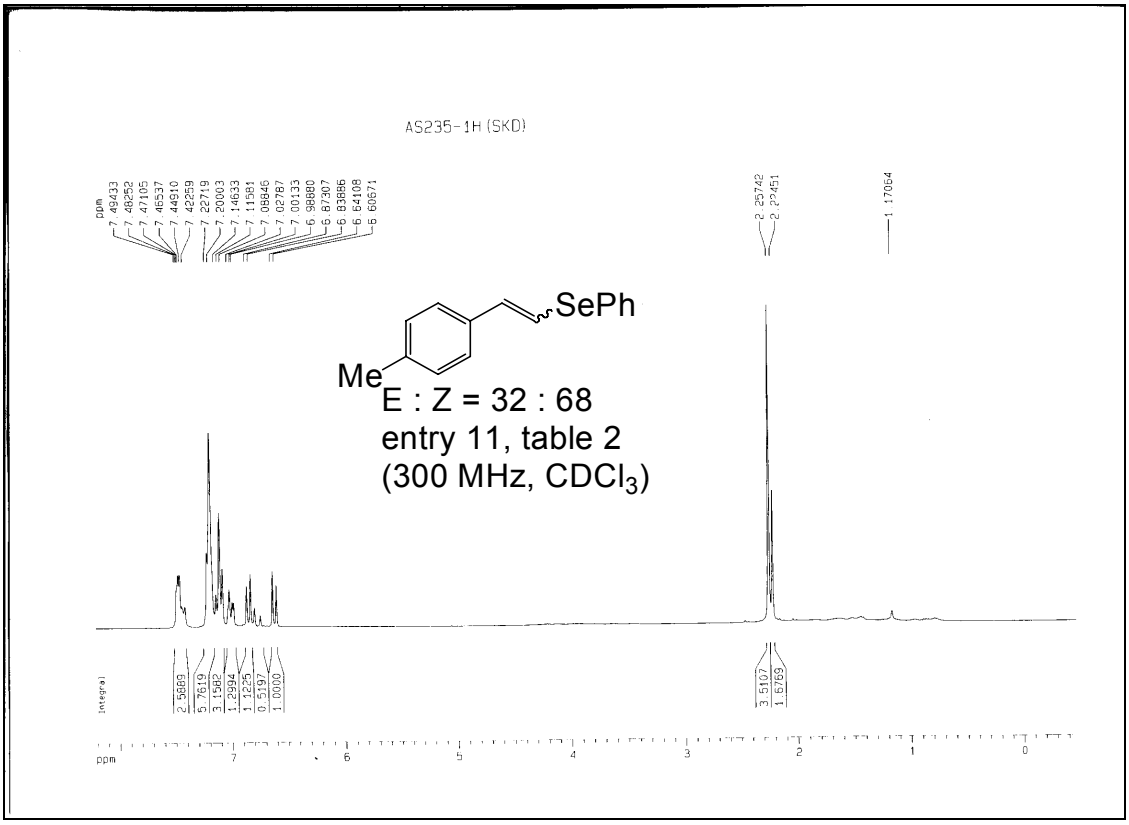

AS-337-13C (SR)
ppm
137.151
135.281
132.704
130.279
129.496
128.821
127.801
127.569
126.215
119.552
77.588
77.164
76.742
SePh
entry 8, table 2
(75 MHz, CDCl3)
ppm
140
120
100
80
60
40
20
0
Current Data Parameters
NAME AS-337-13C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20080626
Time 17.51
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgdc
TD 16384
SOLVENT CDCl3
NS 472
DS 4
SWH 21929.824 Hz
FIDRES 1.338490 Hz
AQ 0.3736052 sec
RG 8192
DW 22.800 usec
DE 6.00 usec
TE 298.2 K
D1 5.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 12.50 usec
PL1 0.00 dB
SFO1 75.4752953 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -5.00 dB
PL12 13.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 16384
SF 75.4677389 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 23.00 cm
CY 8.17 cm
F1P 156.936 ppm
F1 11843.57 Hz
F2P -8.709 ppm
F2 -657.23 Hz
PPMCM 7.20193 ppm/cm
HZCM 543.51306 Hz/cm

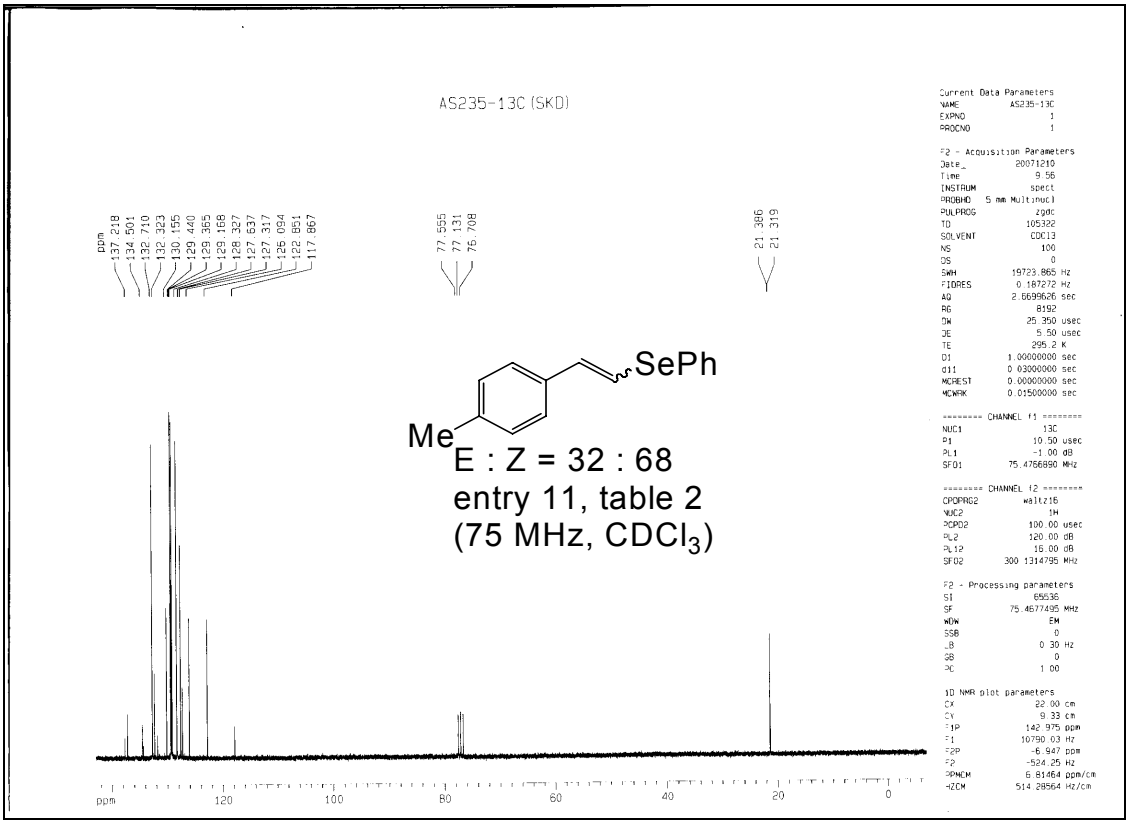

AS-341-1H (SR)
ppm
7.50299
7.50599
7.55144
7.42515
7.41501
7.40728
7.34098
7.33362
7.32680
7.31933
7.31036
7.29692
7.26063
7.22112
7.16863
6.97916
6.91477
6.82093
SePh
E : Z = 53 : 47
entry 9, table 2
(300 MHz, CDCl3)
Integral
4.041
3.295
10.247
0.552
0.595
1.000
1.107
1.095
ppm 8 7 6 5 4 3 2 1 0

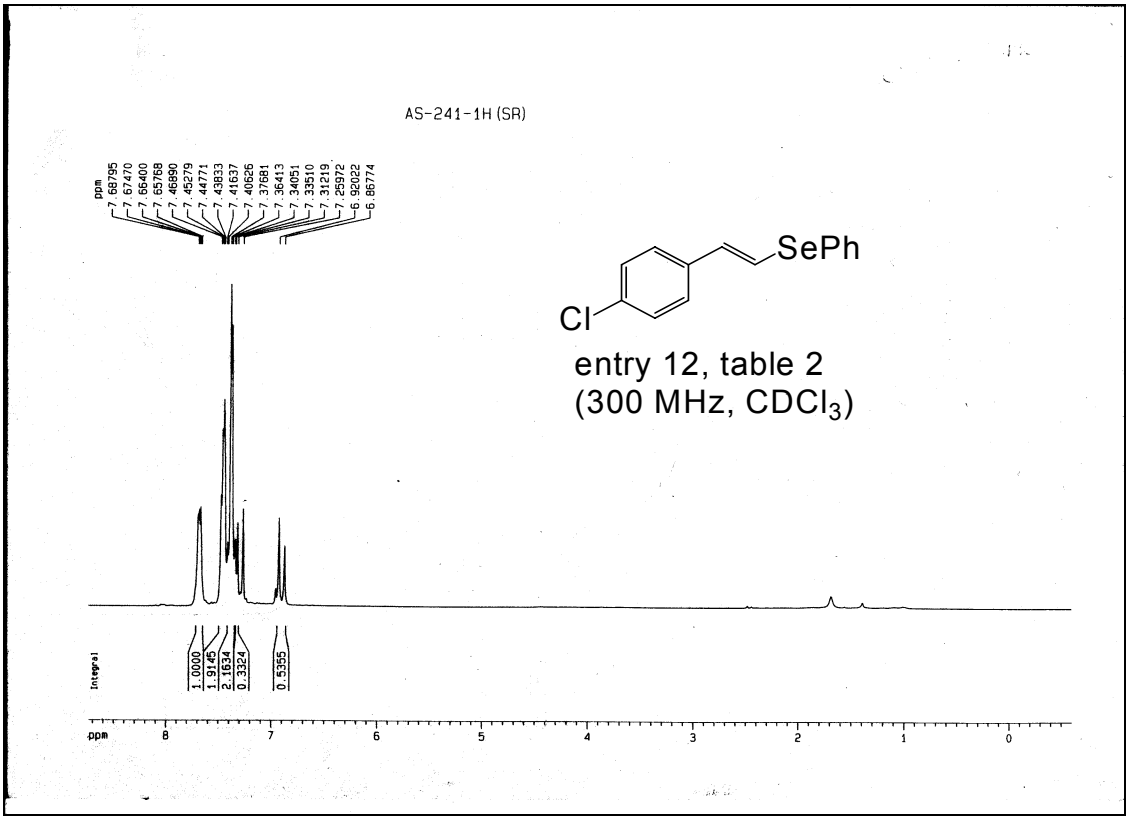

AS-341-13C (SR)
ppm
135.230
132.816
132.640
130.179
129.433
128.757
128.490
128.398
127.741
127.507
127.372
126.156
124.061
119.500
77.536
77.113
76.689
SePh
E : Z = 53 : 47
entry 9, table 2
(75 MHz, CDCl3)
ppm 120 100 80 60 40 20 0
Current Data Parameters
NAME AS-341-13C
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20080708
Time 9.12
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgdc
TD 16384
SOLVENT CDCl3
NS 8754
DS 4
SWH 17985.611 Hz
FIDRES 1.097755 Hz
AQ 0.4595252 sec
RG 8192
DW 27.800 usec
DE 6.00 usec
TE 299.2 K
D1 5.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 13C
P1 12.50 usec
PL1 0.00 dB
SFO1 75.4752953 MHz
-------- CHANNEL f2 --------
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -5.00 dB
PL12 13.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 16384
SF 75.4677443 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 23.00 cm
CY 8.13 cm
F1P 141.711 ppm
F1 10694.61 Hz
F2P -7.784 ppm
F2 -587.47 Hz
PPMCM 6.49980 ppm/cm
HZCM 490.52530 Hz/cm

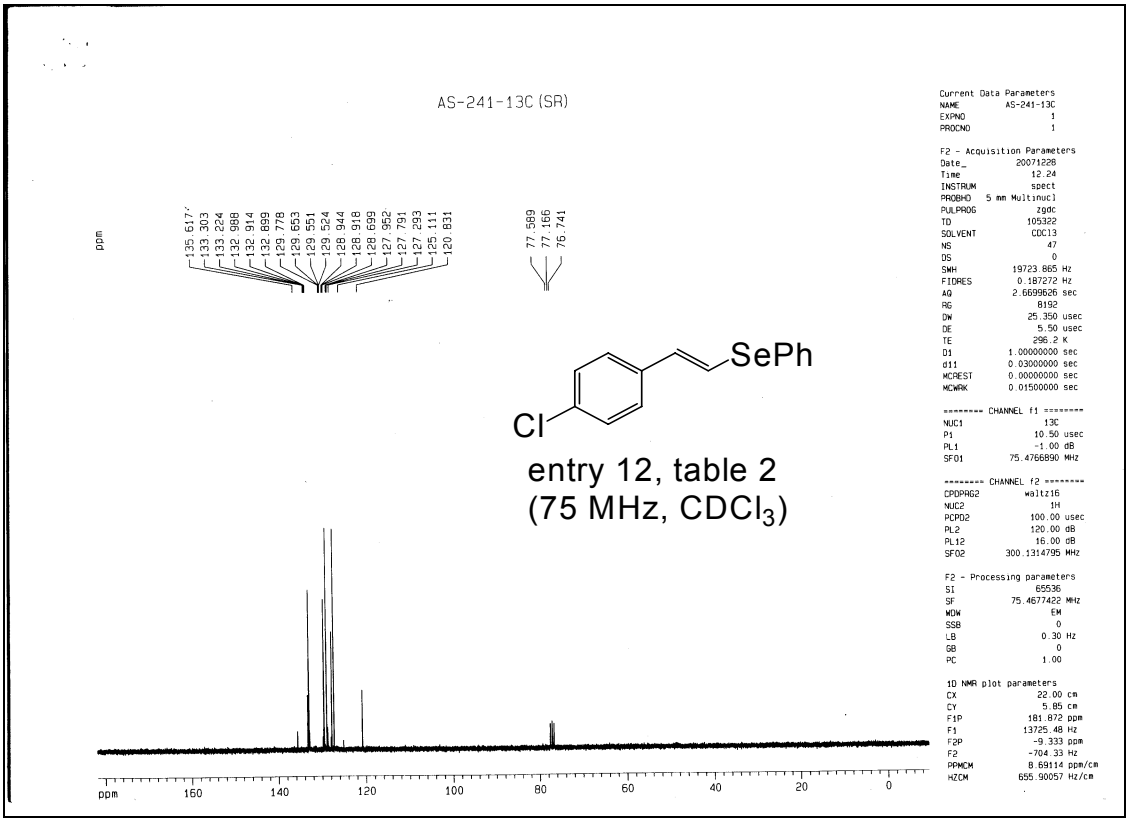

AS-247-1H (SR)
ppm
7.58826
7.57166
7.56623
7.34750
7.33932
7.33017
7.32534
7.29332
7.26665
7.18683
7.17517
7.14869
7.13537
6.94863
6.89614
2.40413
2.37305
1.48716
1.32108
0.93883
0.93032
0.91744
0.90917
SePh
Me
entry 10, table 2
(300 MHz, CDCl3)
Integral
1.0000
3.3931
1.8784
0.5678
2.5833
ppm
7
6
5
4
3
2
1
0

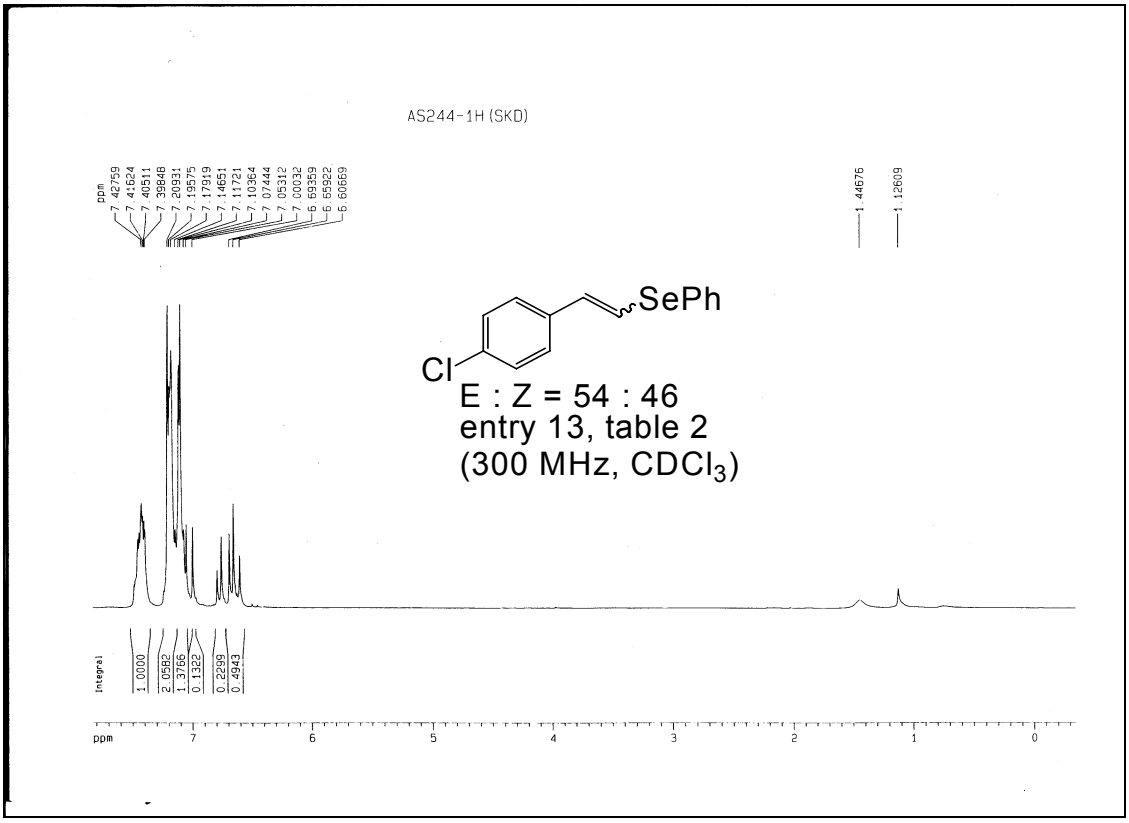

AS-247-13C (SR)
ppm
137.737
135.794
134.398
132.395
130.619
129.492
129.420
127.366
126.154
117.935
77.593
77.169
76.746
21.357
SePh
Me
entry 10, table 2
(75 MHz, CDCl3)
ppm
160
140
120
100
80
60
40
20
0
Current Data Parameters
NAME AS-247-13C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20080116
Time 19.55
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgdc
TD 109152
SOLVENT CDCl3
NS 32
DS 0
SWH 19841.270 Hz
FIDRES 0.181777 Hz
AQ 2.7506804 sec
RG 8192
DW 25.200 usec
DE 5.50 usec
TE 298.2 K
D1 1.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 -1.00 dB
SFO1 75.4766414 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 16.00 dB
SFO2 300.1314795 MHz
F2 - Processing parameters
SI 65536
SF 75.4677445 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 22.00 cm
CY 6.01 cm
F1P 187.521 ppm
F1 14151.82 Hz
F2P -12.316 ppm
F2 -929.43 Hz
PPMCM 9.08350 ppm/cm
HZCM 685.51141 Hz/cm

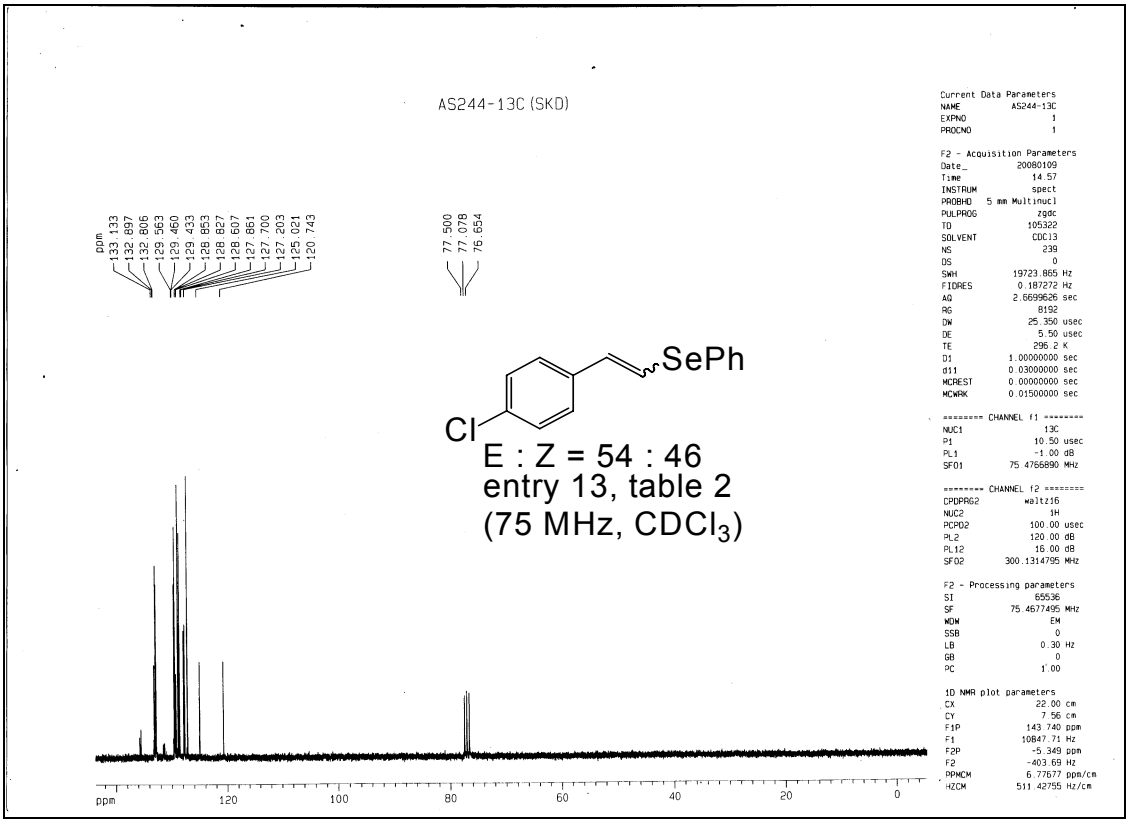

AS235-1H (SKD)
ppm
7.49433
7.48252
7.47105
7.46537
7.44510
7.42259
7.22719
7.20003
7.14633
7.11581
7.08846
7.02787
7.00133
6.98880
6.87307
6.83886
6.64108
6.60671
2.25742
2.22451
1.17064
SePh
Me
E : Z = 32 : 68
entry 11, table 2
(300 MHz, CDCl3)
Integral
2.5889
5.7619
3.1582
1.2994
1.1225
0.5197
1.0000
3.5107
1.6769
ppm
7
6
5
4
3
2
1
0

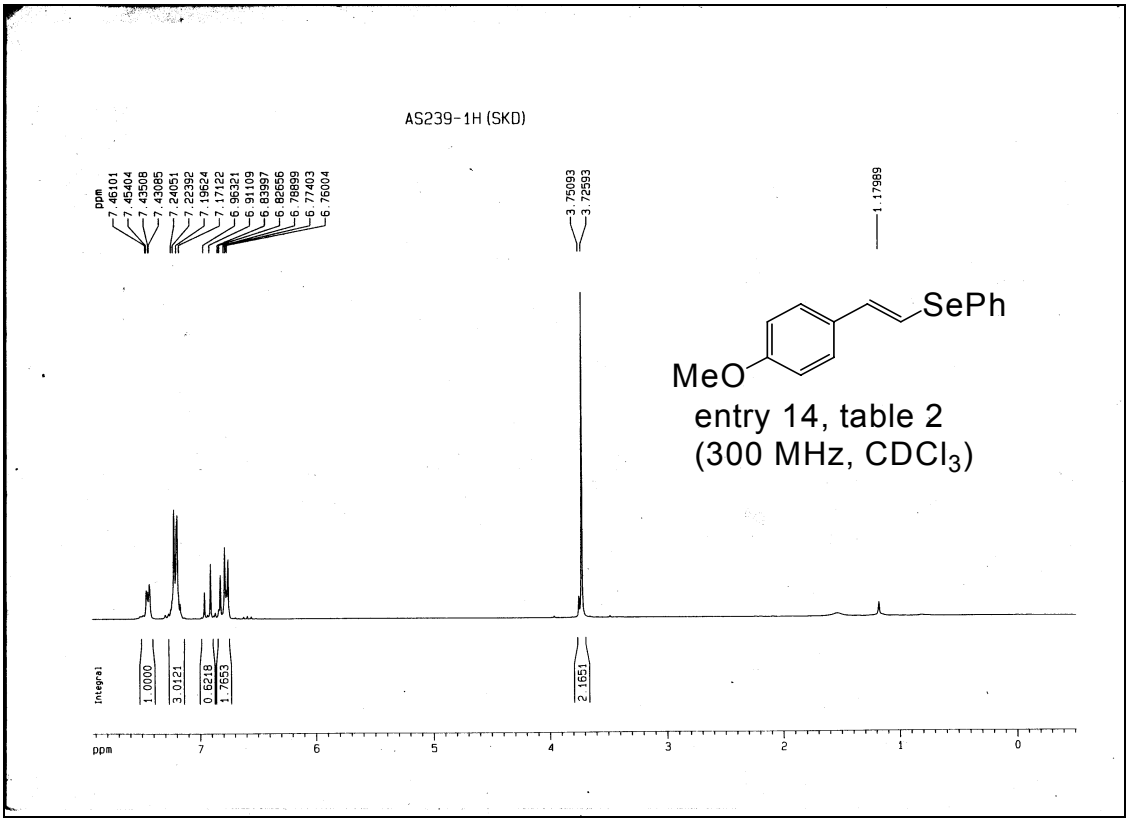

AS235-13C (SKD)
ppm
137.218
134.501
132.710
132.323
130.155
129.440
129.365
129.168
128.327
127.637
127.317
126.094
122.851
117.867
77.555
77.131
75.708
21.386
21.319
SePh
Me
E : Z = 32 : 68
entry 11, table 2
(75 MHz, CDCl3)
ppm
120
100
80
60
40
20
0
Current Data Parameters
NAME AS235-13C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20071210
Time 9.56
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg
TD 105322
SOLVENT CDCl3
NS 100
DS 0
SWH 19723.865 Hz
FIDRES 0.187272 Hz
AQ 2.6699626 sec
RG 8192
DW 25.350 usec
DE 5.50 usec
TE 295.2 K
D1 1.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 -1.00 dB
SFO1 75.4766890 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 16.00 dB
SFO2 300.1314795 MHz
F2 - Processing parameters
SI 65536
SF 75.4677495 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 22.00 cm
CY 9.33 cm
F1P 142.975 ppm
F1 10790.03 Hz
F2P -6.947 ppm
F2 -524.25 Hz
PPMCM 6.81464 ppm/cm
HZCM 514.28564 Hz/cm

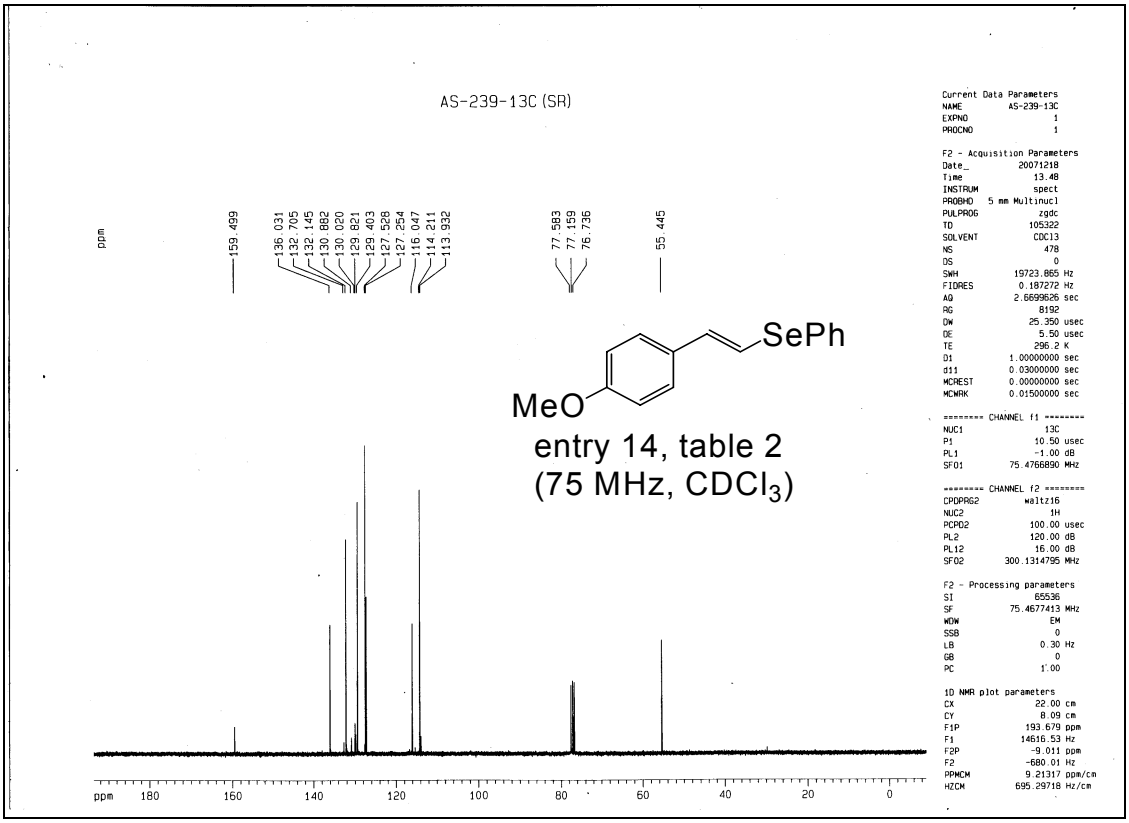

AS-241-1H (SR)
ppm
7.68795
7.67470
7.66400
7.65768
7.46890
7.45279
7.44771
7.43833
7.41637
7.40626
7.37681
7.36413
7.34051
7.33510
7.31219
7.25972
6.92022
6.86774
SePh
Cl
entry 12, table 2
(300 MHz, CDCl3)
Integral
1.0000
1.9145
2.1634
0.3324
0.5355
ppm
8
7
6
5
4
3
2
1
0

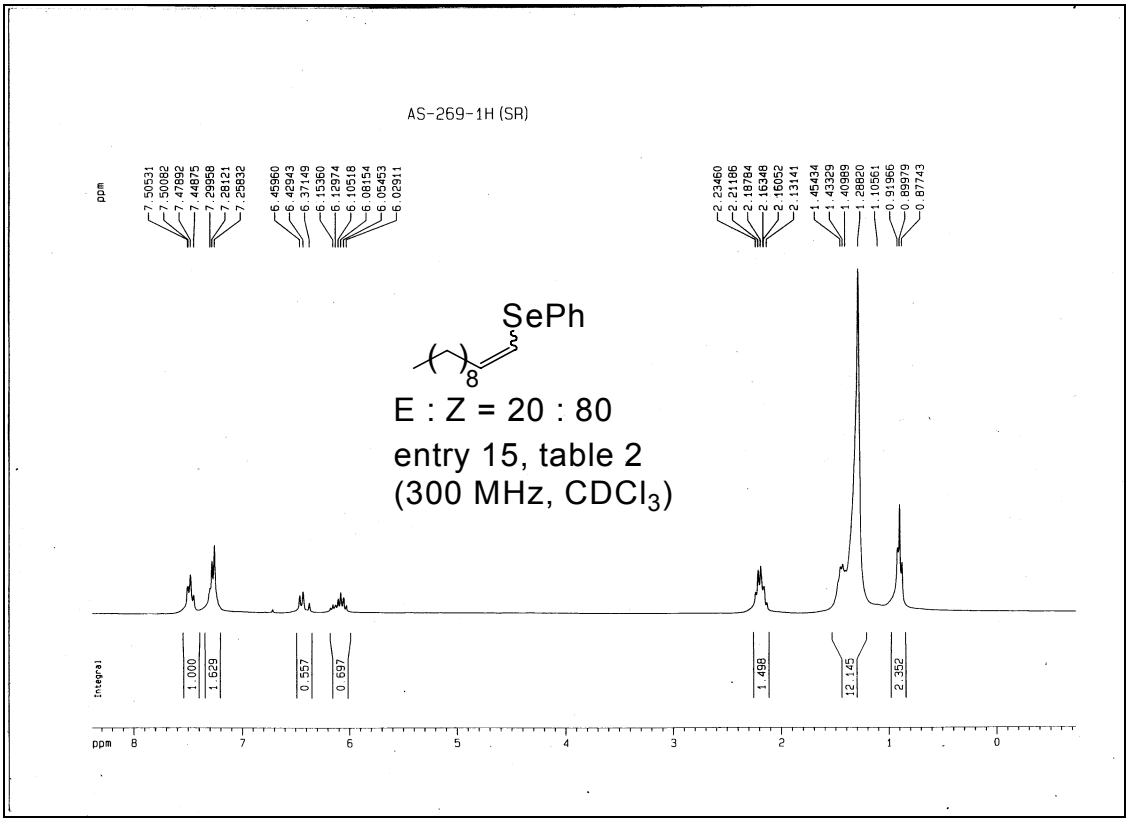

AS-241-13C (SR)
ppm
135.617
133.303
133.224
132.988
132.914
132.899
129.778
129.653
129.551
129.524
128.944
128.918
128.699
127.952
127.791
127.293
125.111
120.831
77.589
77.166
76.741
SePh
Cl
entry 12, table 2
(75 MHz, CDCl3)
ppm
160
140
120
100
80
60
40
20
0
Current Data Parameters
NAME AS-241-13C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20071228
Time 12.24
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgdc
TD 105322
SOLVENT CDCl3
NS 47
DS 0
SWH 19723.865 Hz
FIDRES 0.187272 Hz
AQ 2.6699626 sec
RG 8192
DW 25.350 usec
DE 5.50 usec
TE 296.2 K
D1 1.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 -1.00 dB
SFO1 75.4766890 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 16.00 dB
SFO2 300.1314795 MHz
F2 - Processing parameters
SI 65536
SF 75.4677422 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 22.00 cm
CY 5.85 cm
F1P 181.872 ppm
F1 13725.48 Hz
F2P -9.333 ppm
F2 -704.33 Hz
PPMCM 8.69114 ppm/cm
HZCM 655.90057 Hz/cm

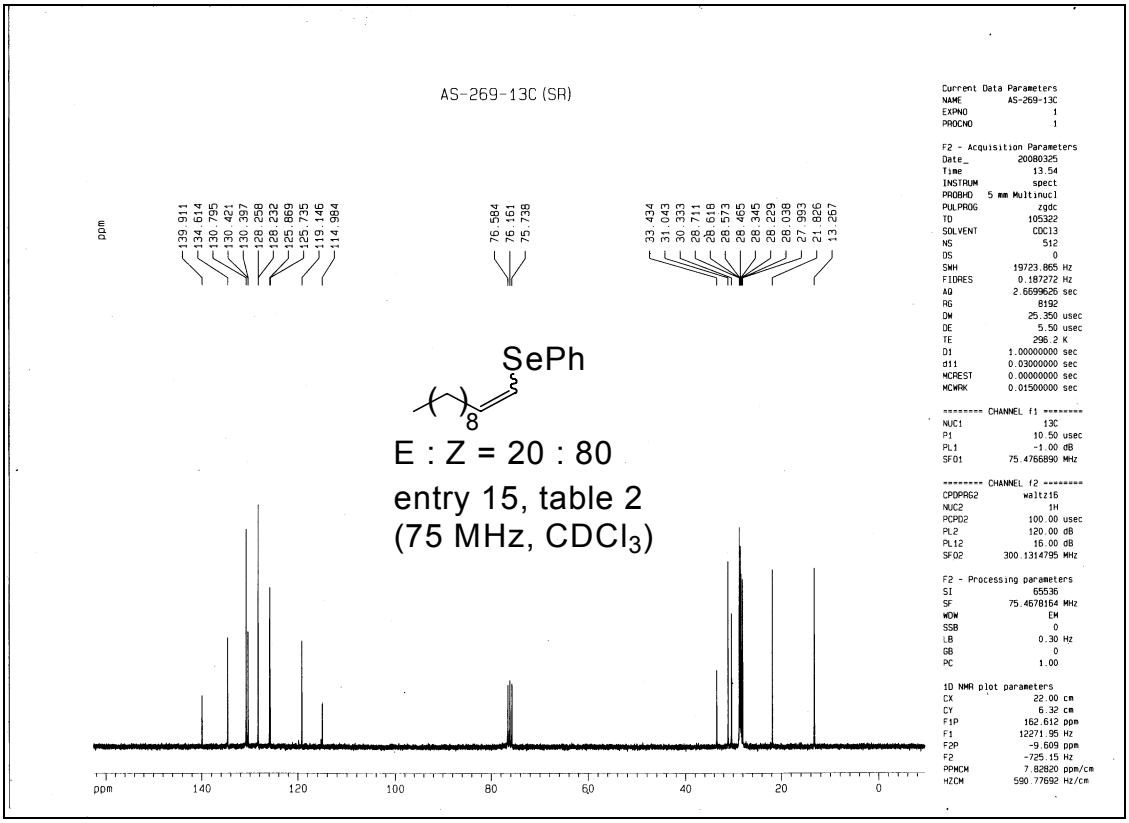

AS244-1H (SKD)
ppm
7.42759
7.41624
7.40511
7.39846
7.20931
7.19575
7.17919
7.14651
7.11721
7.10364
7.07444
7.05312
7.00032
6.69359
6.65922
6.60669
1.44676
1.12609
SePh
Cl
E : Z = 54 : 46
entry 13, table 2
(300 MHz, CDCl3)
Integral
1.0000
2.0582
1.3766
0.1322
0.2299
0.4943
ppm
7
6
5
4
3
2
1
0


AS244-13C (SKD)
ppm
133.133
132.897
132.806
129.563
129.460
128.433
128.853
128.827
128.607
127.861
127.700
127.203
125.021
120.743
77.500
77.078
76.654
SePh
Cl
E : Z = 54 : 46
entry 13, table 2
(75 MHz, CDCl3)
ppm
120
100
80
60
40
20
0
Current Data Parameters
NAME AS244-13C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20080109
Time 14.57
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgdc
TD 105322
SOLVENT CDCl3
NS 239
DS 0
SWH 19723.865 Hz
FIDRES 0.187272 Hz
AQ 2.6699626 sec
RG 8192
DW 25.350 usec
DE 5.50 usec
TE 296.2 K
D1 1.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 -1.00 dB
SFO1 75.4766890 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 16.00 dB
SFO2 300.1314795 MHz
F2 - Processing parameters
SI 65536
SF 75.4677495 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 22.00 cm
CY 7.56 cm
F1P 143.740 ppm
F1 10847.71 Hz
F2P -5.349 ppm
F2 -403.69 Hz
PPMCM 6.77677 ppm/cm
HZCM 511.42755 Hz/cm


AS239-1H (SKD)
ppm
7.46101
7.45404
7.43508
7.43085
7.24051
7.22392
7.19624
7.17122
6.96321
6.91109
6.83997
6.82656
6.78899
6.77403
6.76004
3.75093
3.72593
1.17989
SePh
MeO
entry 14, table 2
(300 MHz, CDCl3)
Integral
1.0000
3.0121
0.6218
1.7653
2.1651
ppm
7
6
5
4
3
2
1
0


AS-239-13C (SR)
ppm
159.499
136.031
132.705
132.145
130.882
130.020
129.821
129.403
127.528
127.254
116.047
114.211
113.932
77.583
77.159
76.736
55.445
SePh
MeO
entry 14, table 2
(75 MHz, CDCl3)
ppm
180
160
140
120
100
80
60
40
20
0
Current Data Parameters
NAME AS-239-13C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20071218
Time 13.48
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgdc
TD 105322
SOLVENT CDCl3
NS 478
DS 0
SWH 19723.865 Hz
FIDRES 0.187272 Hz
AQ 2.6699626 sec
RG 8192
DW 25.350 usec
DE 5.50 usec
TE 296.2 K
D1 1.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 -1.00 dB
SFO1 75.4766890 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 16.00 dB
SFO2 300.1314795 MHz
F2 - Processing parameters
SI 65536
SF 75.4677413 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 22.00 cm
CY 8.09 cm
F1P 193.679 ppm
F1 14616.53 Hz
F2P -9.011 ppm
F2 -680.01 Hz
PPMCM 9.21317 ppm/cm
HZCM 695.29718 Hz/cm


AS-269-1H (SR)
ppm
7.50531
7.50082
7.47892
7.44875
7.29958
7.28121
7.25832
6.45960
6.42943
6.37149
6.15360
6.12974
6.10518
6.08154
6.05453
6.02911
2.23460
2.21186
2.18784
2.16348
2.16052
2.13141
1.45434
1.43329
1.40989
1.28820
1.10561
0.91966
0.89979
0.87743
SePh
8
E : Z = 20 : 80
entry 15, table 2
(300 MHz, CDCl3)
Integral
1.000
1.629
0.557
0.697
1.498
12.145
2.352
ppm 8 7 6 5 4 3 2 1 0


AS-269-13C (SR)
ppm
139.911
134.614
130.795
130.421
130.397
128.258
128.232
125.869
125.735
119.146
114.984
76.584
76.161
75.738
33.434
31.043
30.333
28.711
28.618
28.573
28.465
28.345
28.229
28.038
27.993
21.826
13.267
SePh
8
E : Z = 20 : 80
entry 15, table 2
(75 MHz, CDCl3)
ppm 140 120 100 80 60 40 20 0
Current Data Parameters
NAME AS-269-13C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20080325
Time 13.54
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgdc
TD 105322
SOLVENT CDCl3
NS 512
DS 0
SWH 19723.865 Hz
FIDRES 0.187272 Hz
AQ 2.6699626 sec
RG 8192
DW 25.350 usec
DE 5.50 usec
TE 296.2 K
D1 1.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 -1.00 dB
SF01 75.4766890 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 16.00 dB
SF02 300.1314795 MHz
F2 - Processing parameters
SI 65536
SF 75.4678164 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 22.00 cm
CY 6.32 cm
F1P 162.612 ppm
F1 12271.95 Hz
F2P -9.609 ppm
F2 -725.15 Hz
PPMCM 7.82820 ppm/cm
HZCM 590.77692 Hz/cm