Development of an Asymmetric Trimethylenemethane Cycloaddition Reaction: Application in the Enantioselective Synthesis of Highly Substituted Carbocycles

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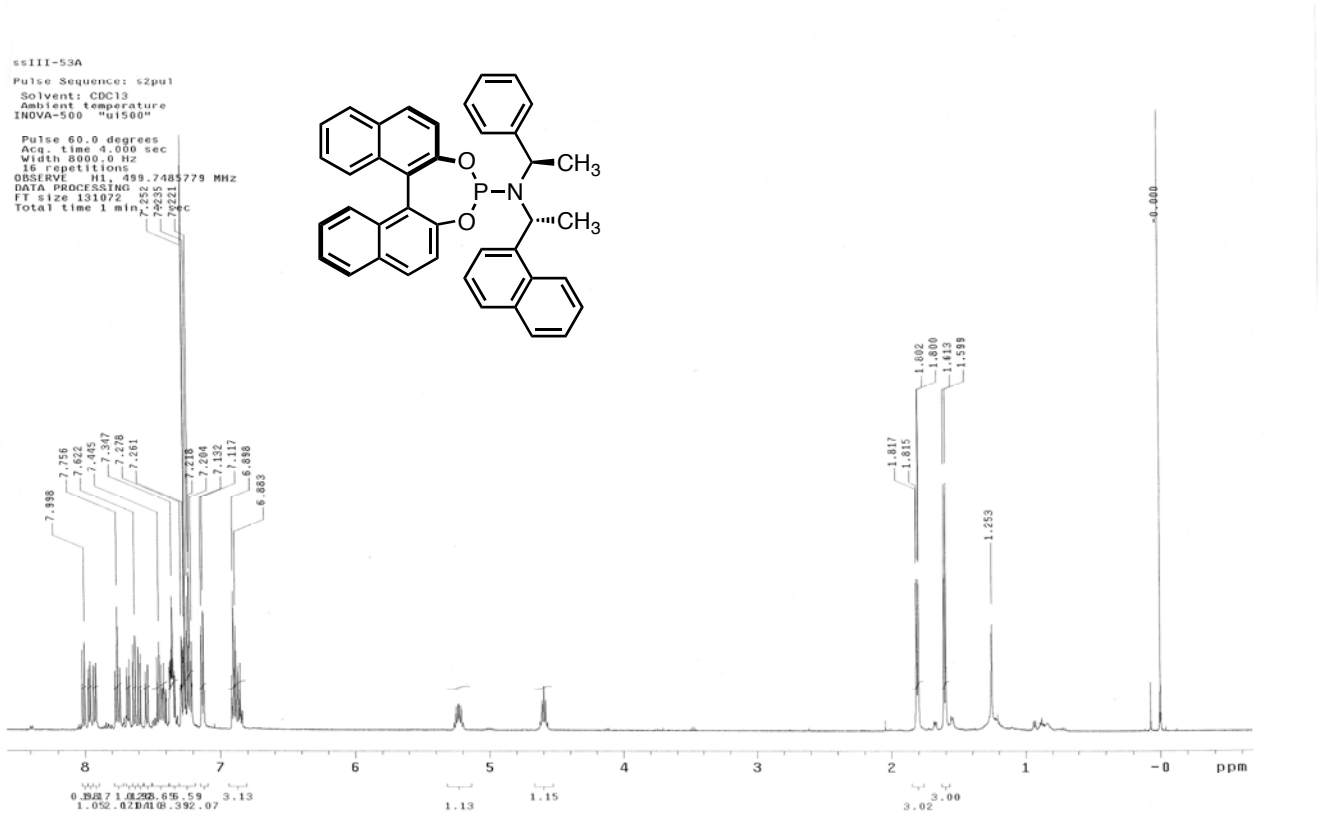
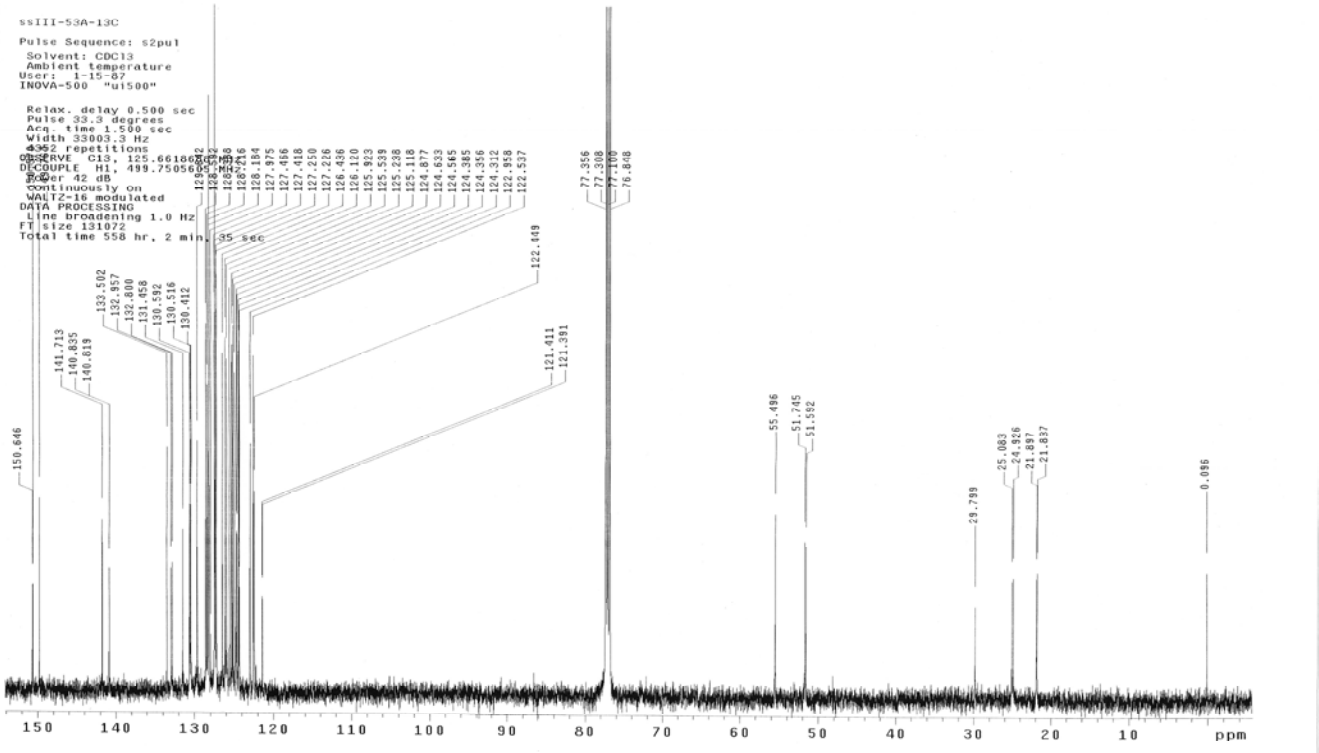
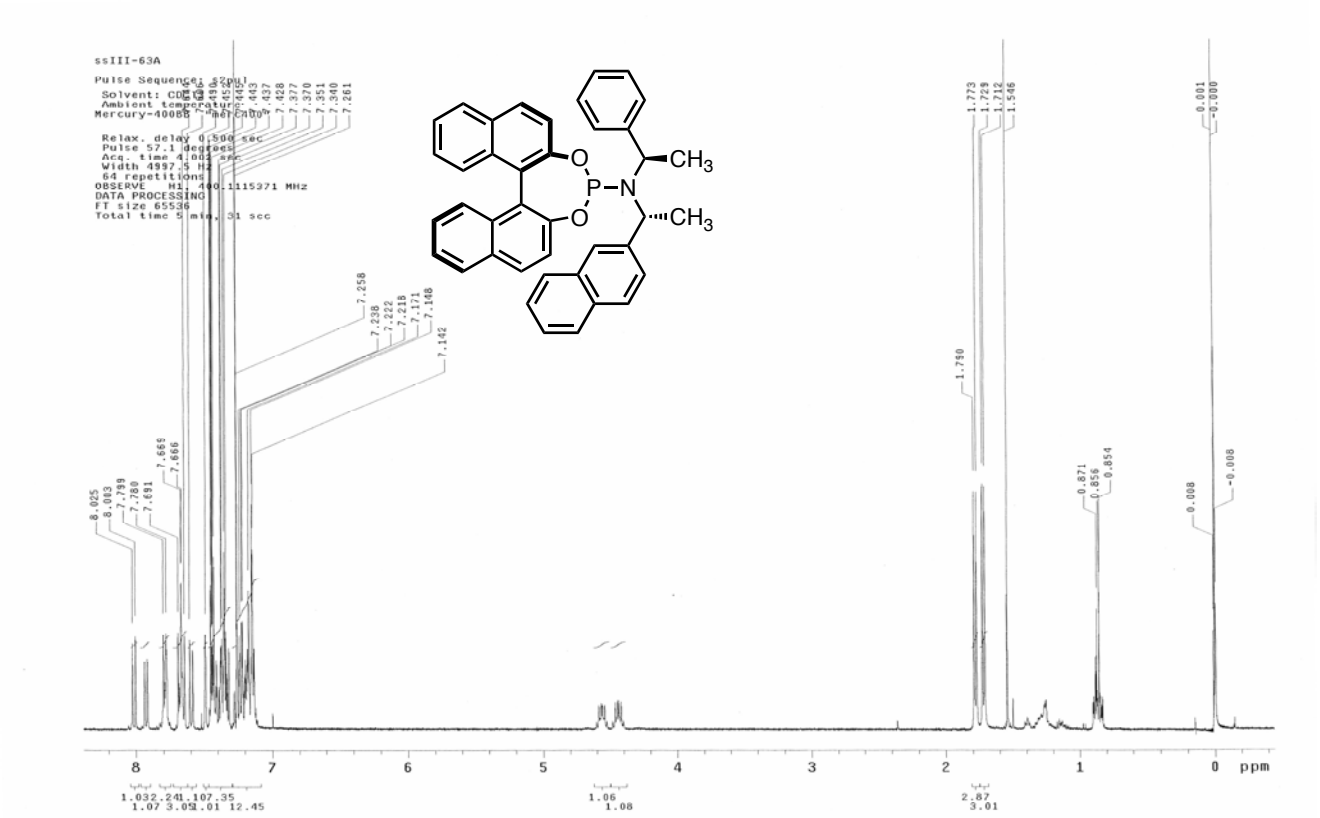
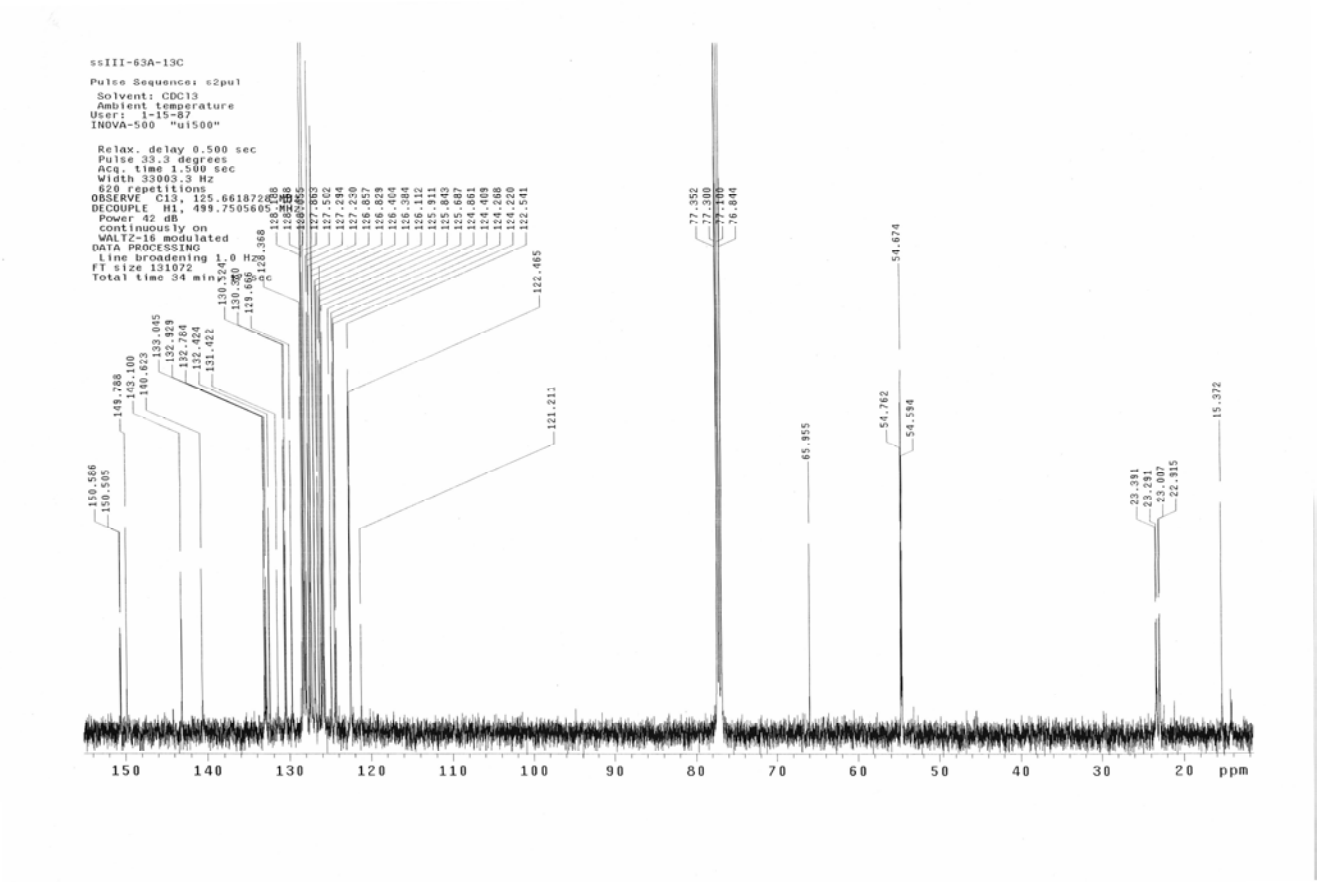
Supporting Information

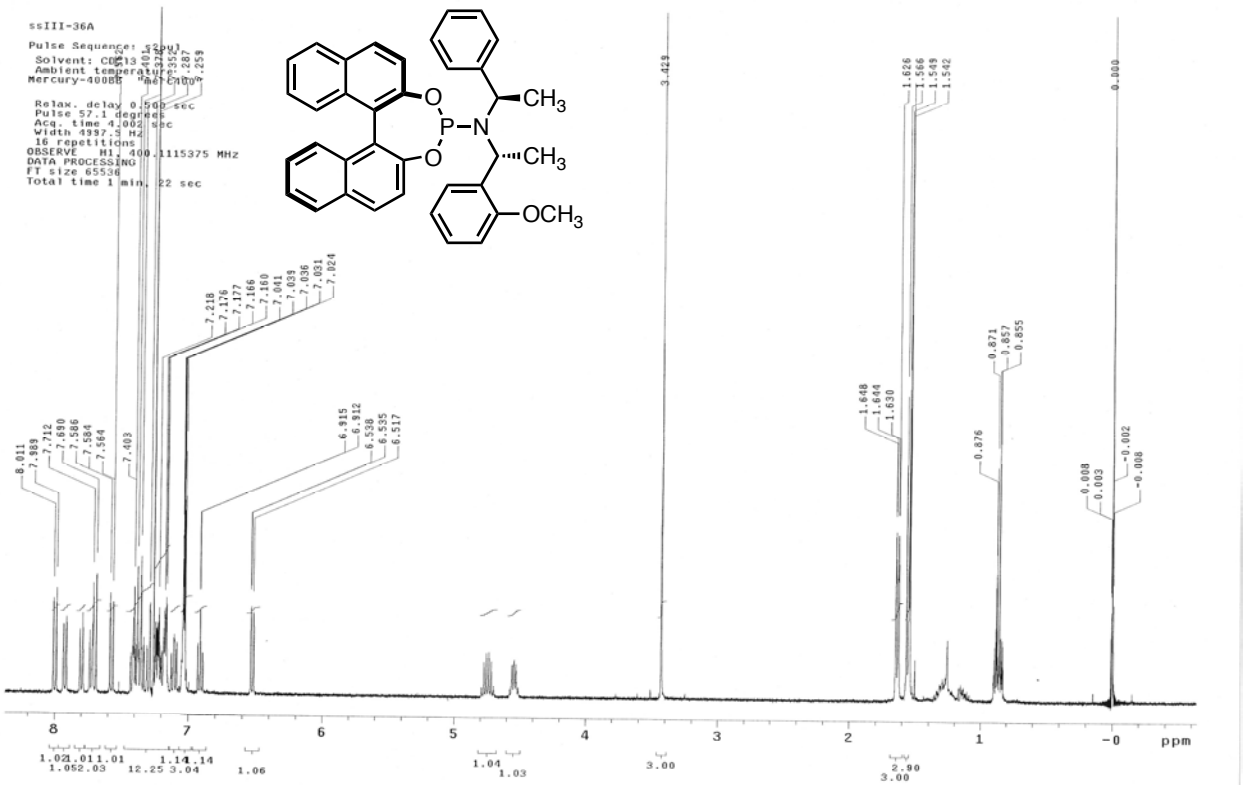
Selected Spectra

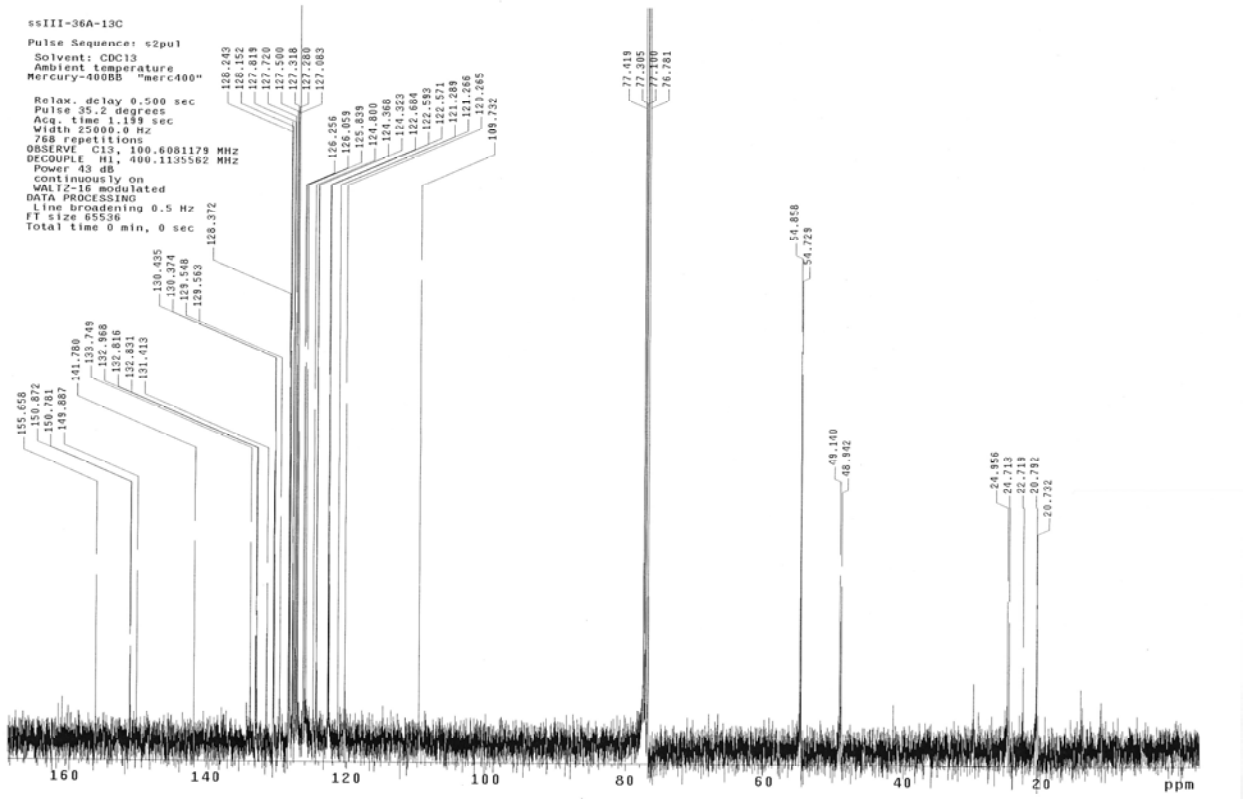

ssIII-53A
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
INOVA-500 "ui500"
Pulse 60.0 degrees
Acq. time 4.000 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.7485779 MHz
DATA PROCESSING
FT size 131072
Total time 1 min
O
P
N
O
CH3
CH3
ppm

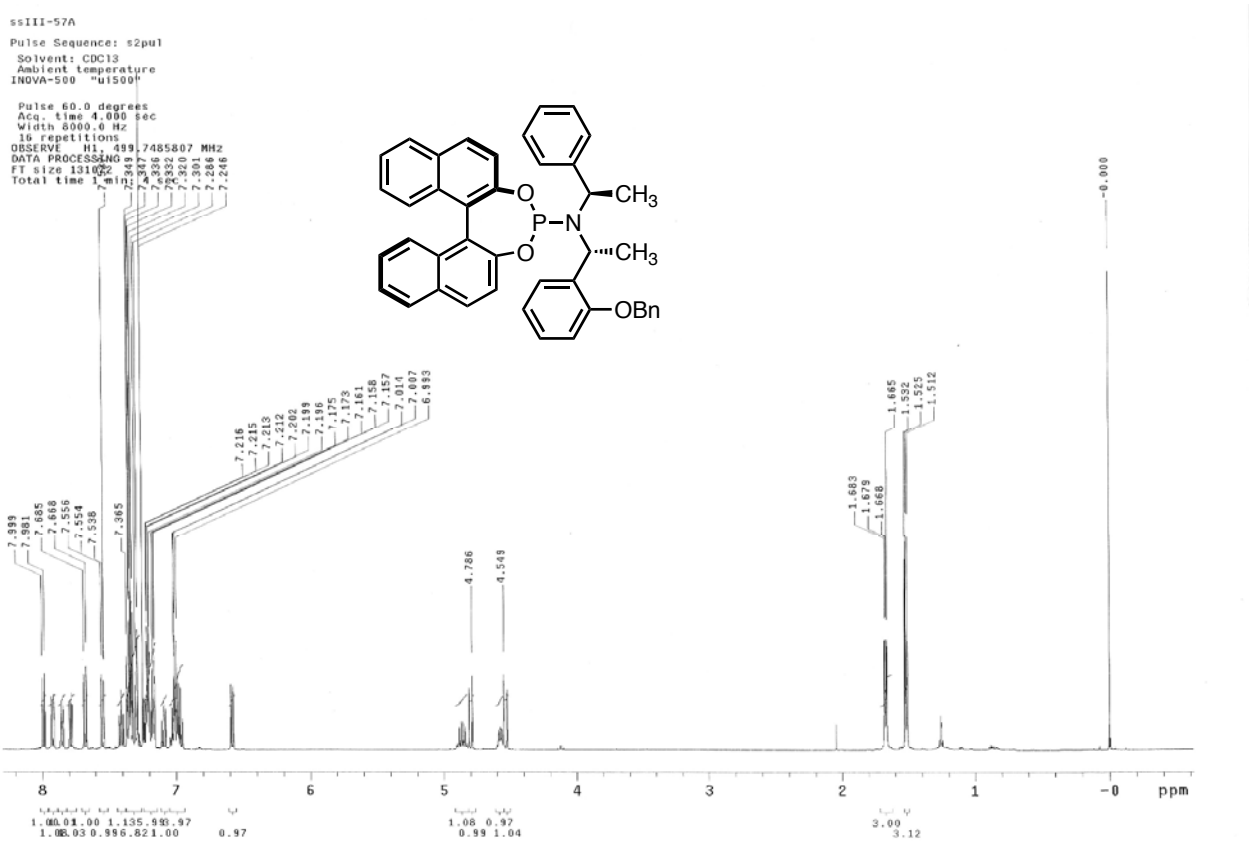

ssIII-53A-13C
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-15-87
INOVA-500 "ui500"
Relax. delay 0.500 sec
Pulse 33.3 degrees
Acq. time 1.500 sec
Width 33003.3 Hz
4352 repetitions
DECOUPLE H1, 499.7505605 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 558 hr, 2 min, 35 sec
ppm

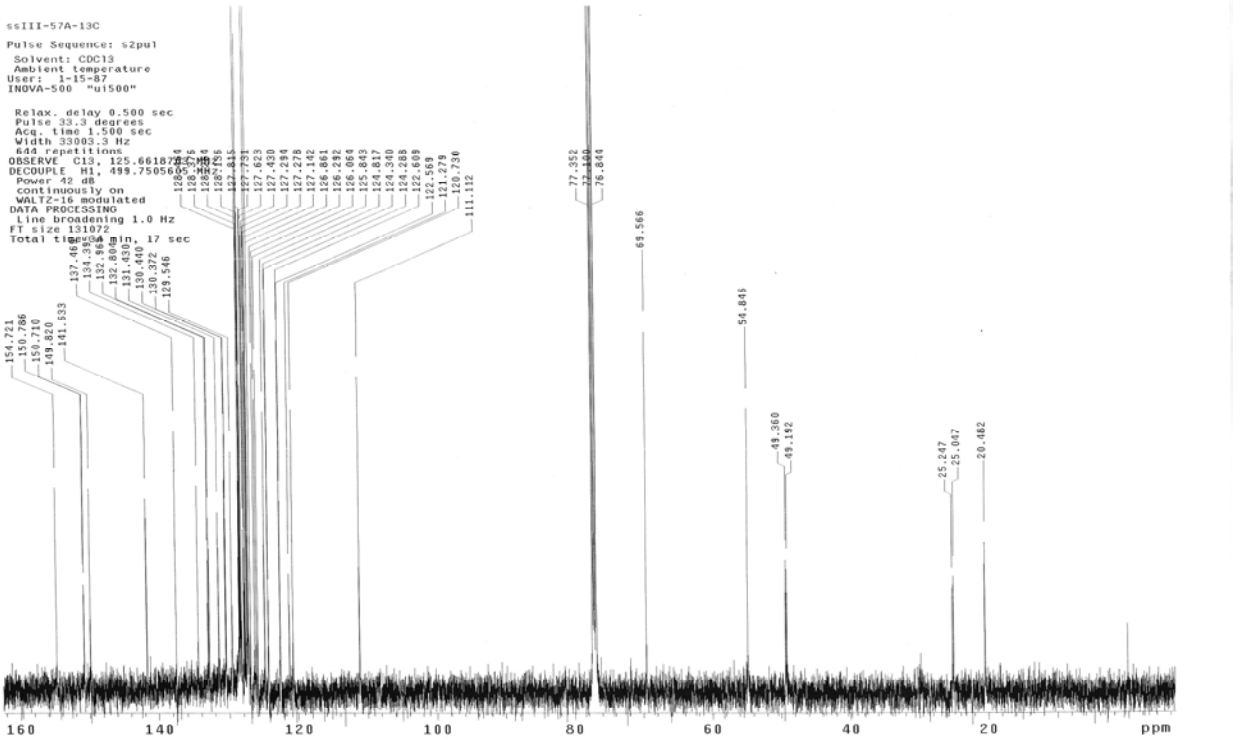

ssIII-63A
Relax. delay 0.500 sec
Pulse 57.1 degrees
Acq. time 4.001 sec
Width 4997.5 Hz
64 repetitions
OBSERVE H1, 400.1115371 MHz
DATA PROCESSING
FT size 65536
Total time 5 min, 31 scc
O
P
N
CH3
CH3
ppm

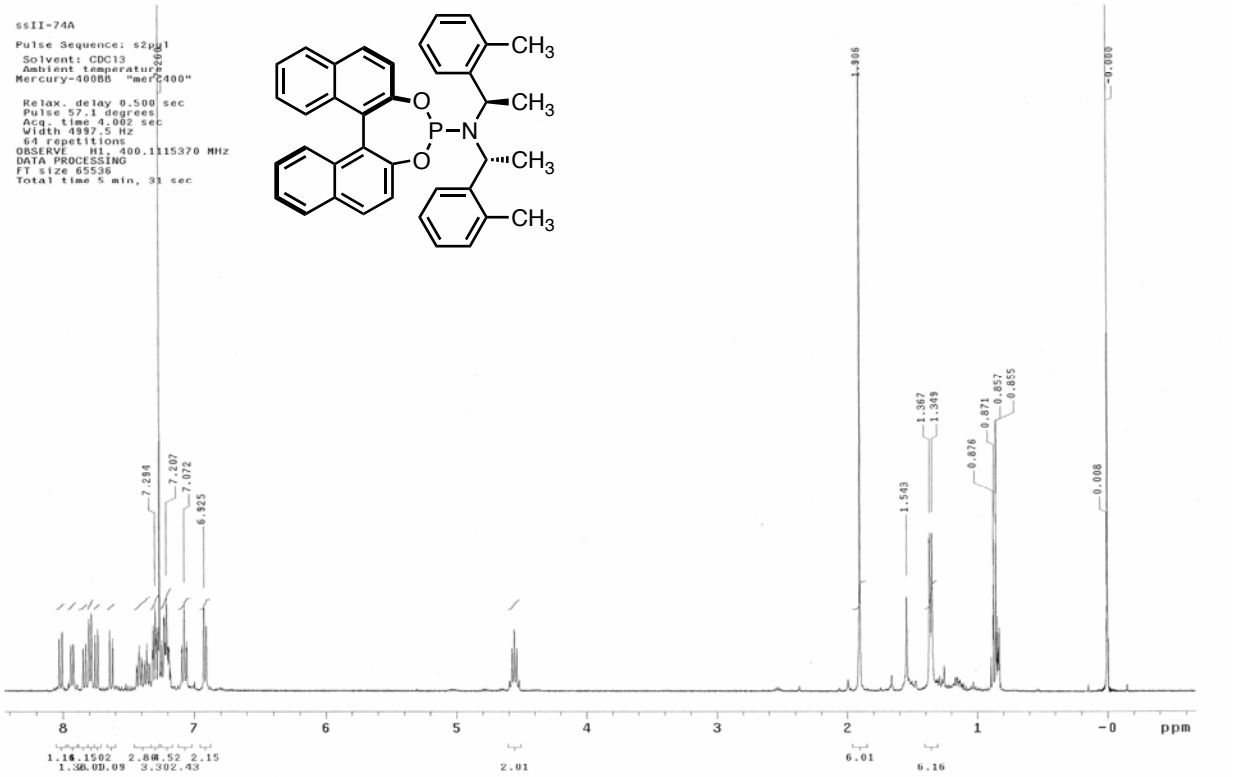

ssIII-63A-13C
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-15-07
INOVA-500 "ui500"
Relax. delay 0.500 sec
Pulse 33.3 degrees
Acq. time 1.500 sec
Width 33003.3 Hz
620 repetitions
OBSERVE C13, 125.6618728 MHz
DECOUPLE H1, 499.7505605 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 34 min, 24 sec
ppm

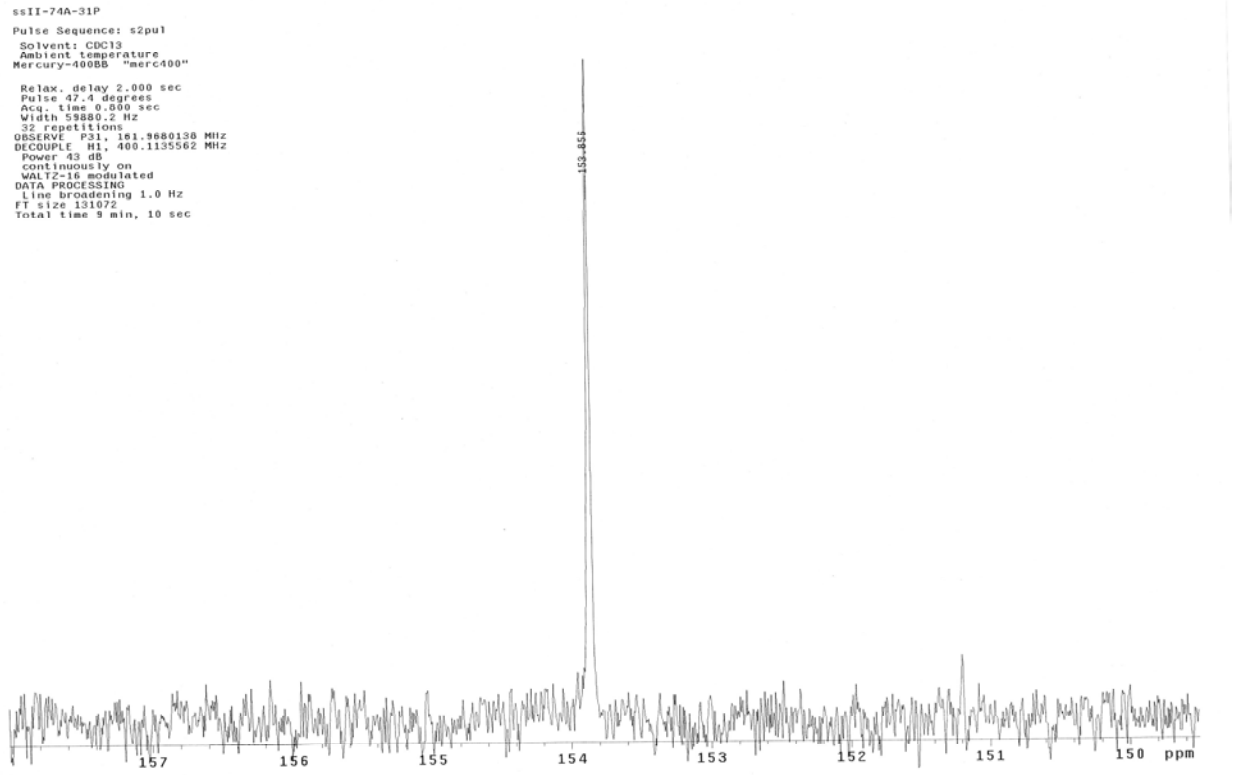

ssIII-36A
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "merc400"
Relax. delay 0.500 sec
Pulse 57.1 degrees
Acq. time 4.002 sec
Width 4997.3 Hz
16 repetitions
OBSERVE H1, 400.1115375 MHz
DATA PROCESSING
FT size 65536
Total time 1 min, 22 sec
O
P
N
O
CH3
CH3
OCH3
8.011
7.988
7.712
7.690
7.686
7.584
7.564
7.403
7.218
7.176
7.177
7.166
7.160
7.041
7.039
7.036
7.031
7.024
6.915
6.912
6.538
6.535
6.517
3.429
1.648
1.644
1.630
1.626
1.566
1.549
1.542
0.876
0.871
0.857
0.855
0.008
0.003
0.000
-0.002
-0.006
8
7
6
5
4
3
2
1
-0
ppm
1.02 1.01 1.01
1.05 2.03
1.14 1.14
12.25 3.04
1.06
1.04
1.03
3.00
2.90
3.00

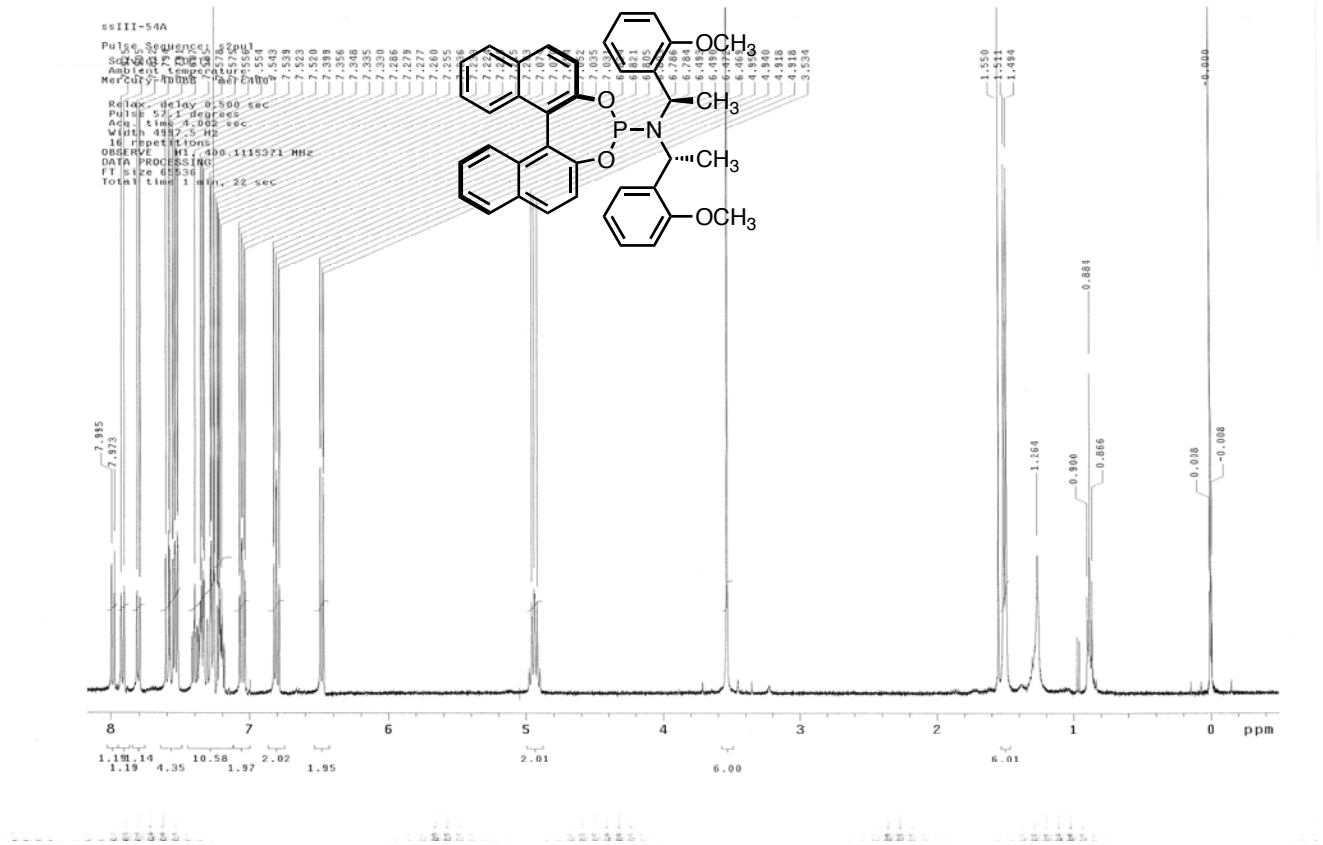

ssIII-36A-13C
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "merc400"
Relax. delay 0.500 sec
Pulse 35.2 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
768 repetitions
OBSERVE C13, 100.6081179 MHz
DECOUPLE H1, 400.1135562 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 0 min, 0 sec
128.243
128.152
127.819
127.720
127.500
127.318
127.280
127.083
126.256
126.059
125.839
124.800
124.368
124.323
122.684
122.593
122.571
121.288
121.266
120.265
109.732
128.372
130.435
130.374
129.548
129.563
155.658
150.872
150.761
149.887
141.780
133.748
132.868
132.616
132.431
131.413
77.419
77.305
77.100
76.781
54.858
54.729
49.140
48.942
24.956
24.713
22.719
20.792
20.732
160
140
120
100
80
60
40
20
ppm

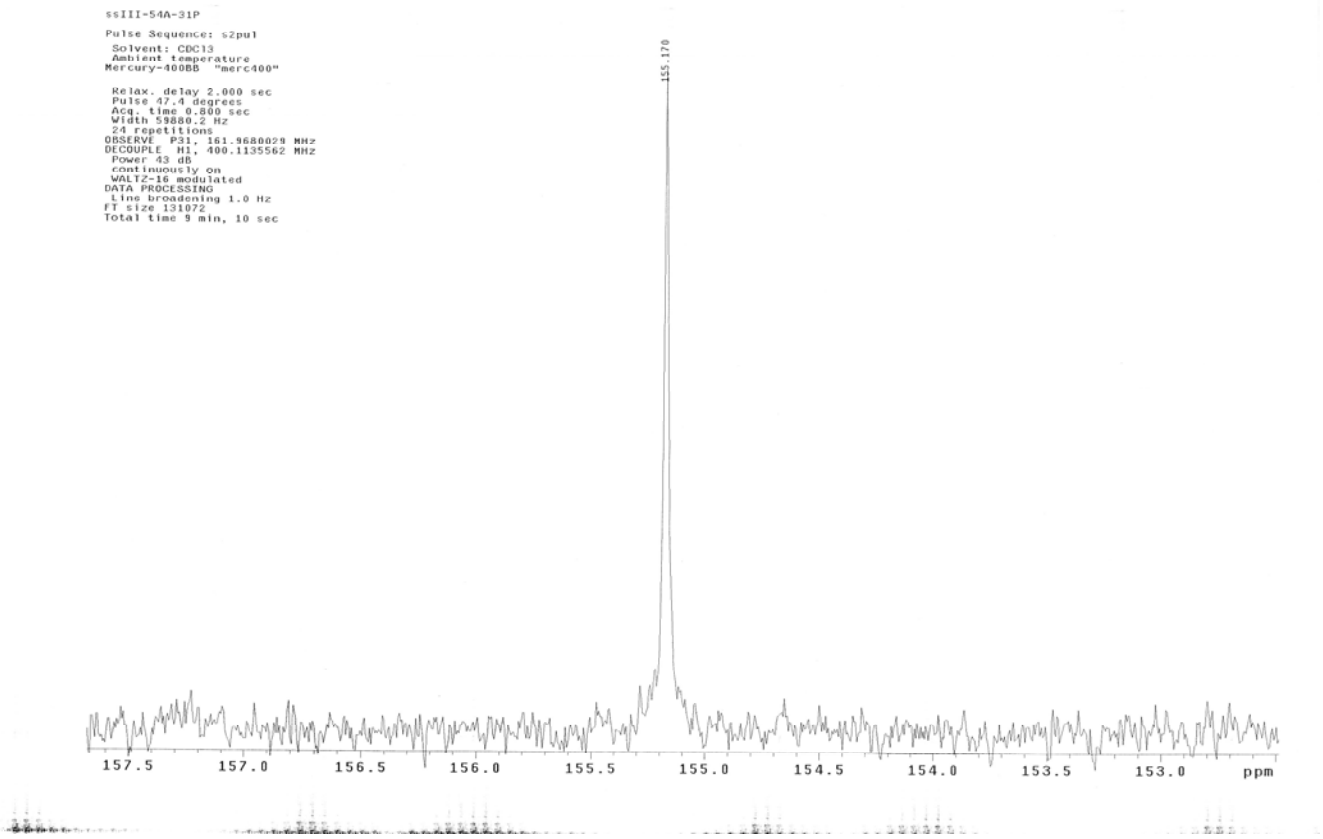

ssIII-57A
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
INOVA-500 "ui500"
Pulse 60.0 degrees
Acq. time 4.000 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.7485807 MHz
DATA PROCESSING
FT size 131072
Total time 1 min
CH3
CH3
OBn
ppm

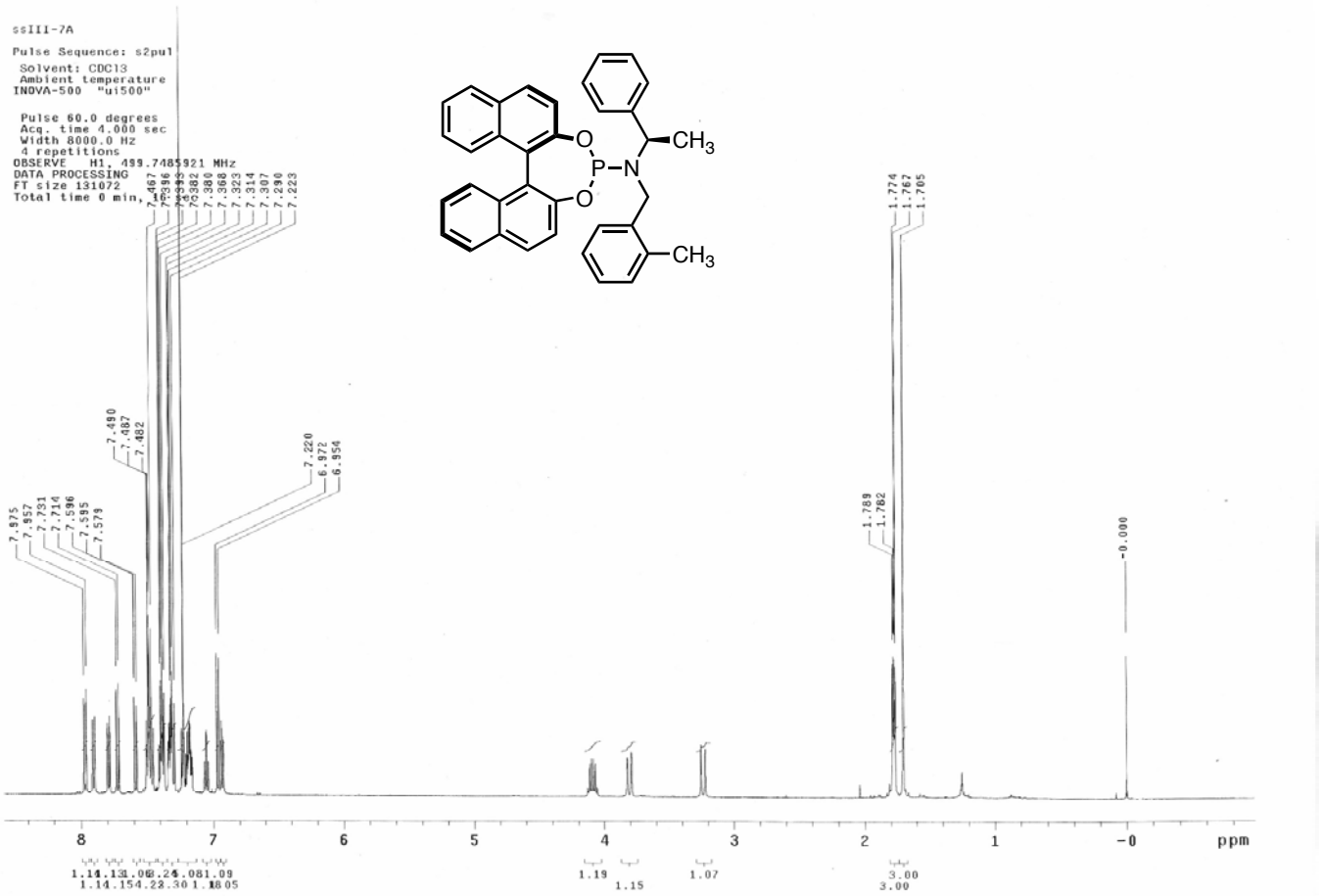

ssIII-57A-13C
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-15-07
INOVA-500 "ui500"
Relax. delay 0.500 sec
Pulse 33.3 degrees
Acq. time 1.500 sec
Width 33003.3 Hz
644 repetitions
DECOUPLE H1, 499.7505605 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
ppm

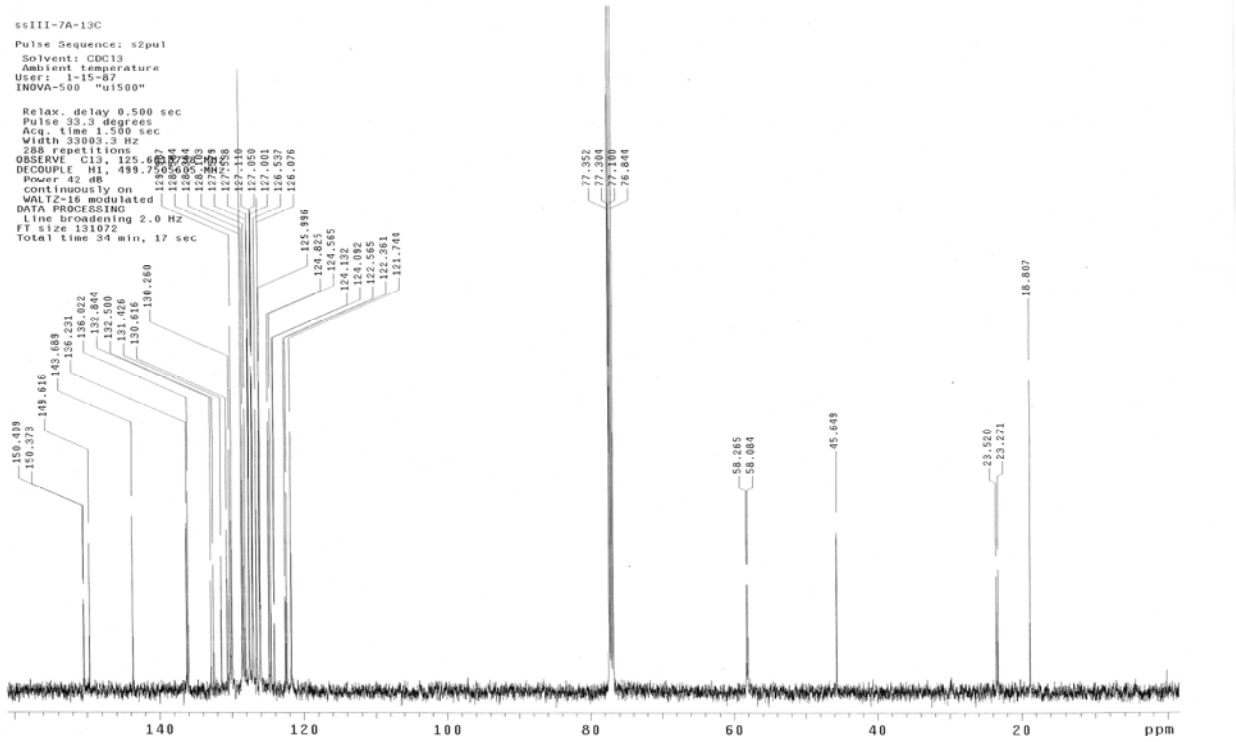

ssII-74A
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "merc400"
Relax. delay 0.500 sec
Pulse 57.1 degrees
Acq. time 4.002 sec
Width 4997.5 Hz
64 repetitions
OBSERVE H1, 400.1115370 MHz
DATA PROCESSING
FT size 65536
Total time 5 min, 31 sec
CH3
CH3
CH3
CH3
O
P
N
O
7.284
7.207
7.072
6.925
1.906
1.543
1.367
1.349
0.876
0.871
0.857
0.855
0.000
0.008
8
7
6
5
4
3
2
1
-0
ppm
1.16
1.15
2.80
2.52
2.15
1.38
8.00
3.09
3.30
2.43
2.01
6.01
6.16

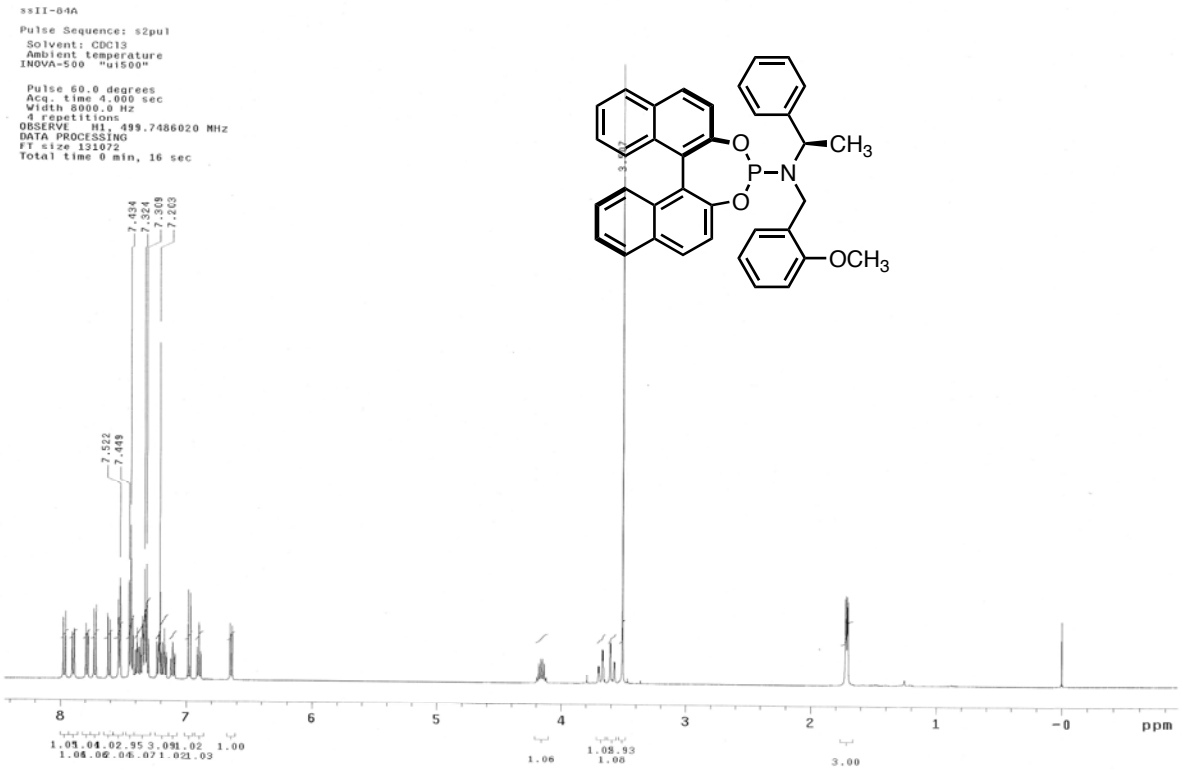

ssII-74A-31P
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "merc400"
Relax. delay 2.000 sec
Pulse 47.4 degrees
Acq. time 0.000 sec
Width 59880.2 Hz
32 repetitions
OBSERVE P31, 161.9680130 MHz
DECOUPLE H1, 400.1135562 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 9 min, 10 sec
153.851
157
156
155
154
153
152
151
150
ppm

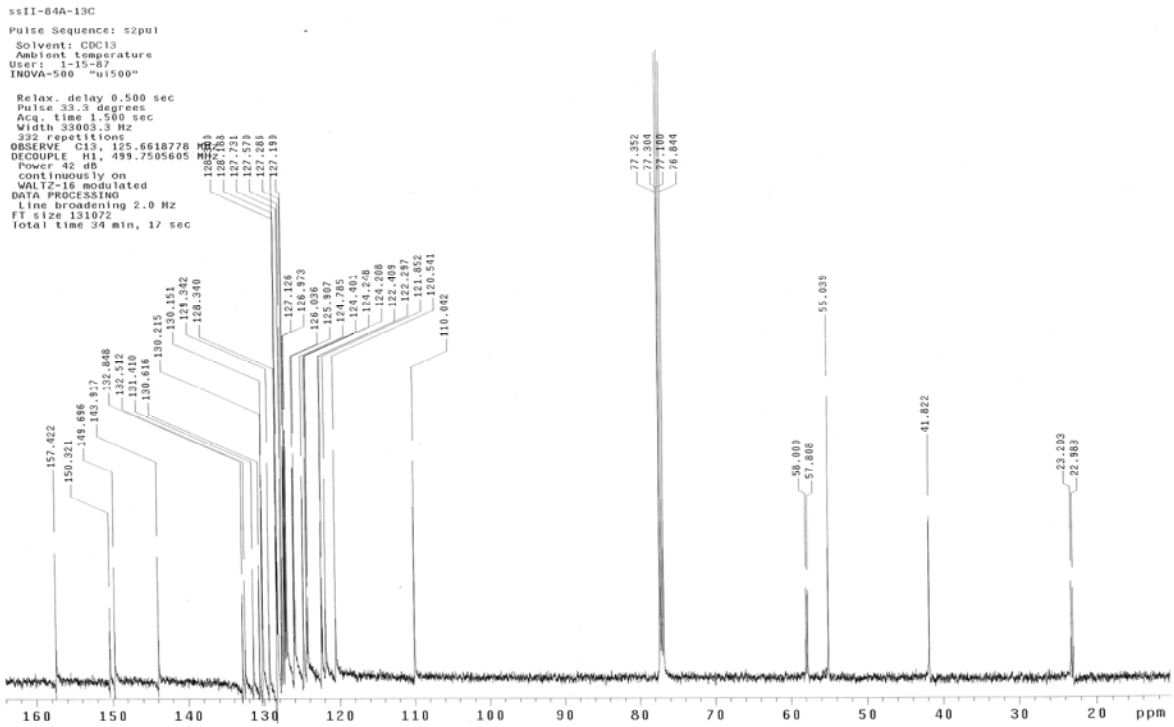

ssIII-54A
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "merc400"
Relax. delay 0.500 sec
Pulse 57.1 degrees
Acq. time 4.002 sec
Width 4987.5 Hz
16 repetitions
OBSERVE H1, 400.1115371 MHz
DATA PROCESSING
FT size 65536
Total time 1 min, 22 sec
OCH3
CH3
P
N
O
CH3
OCH3
ppm

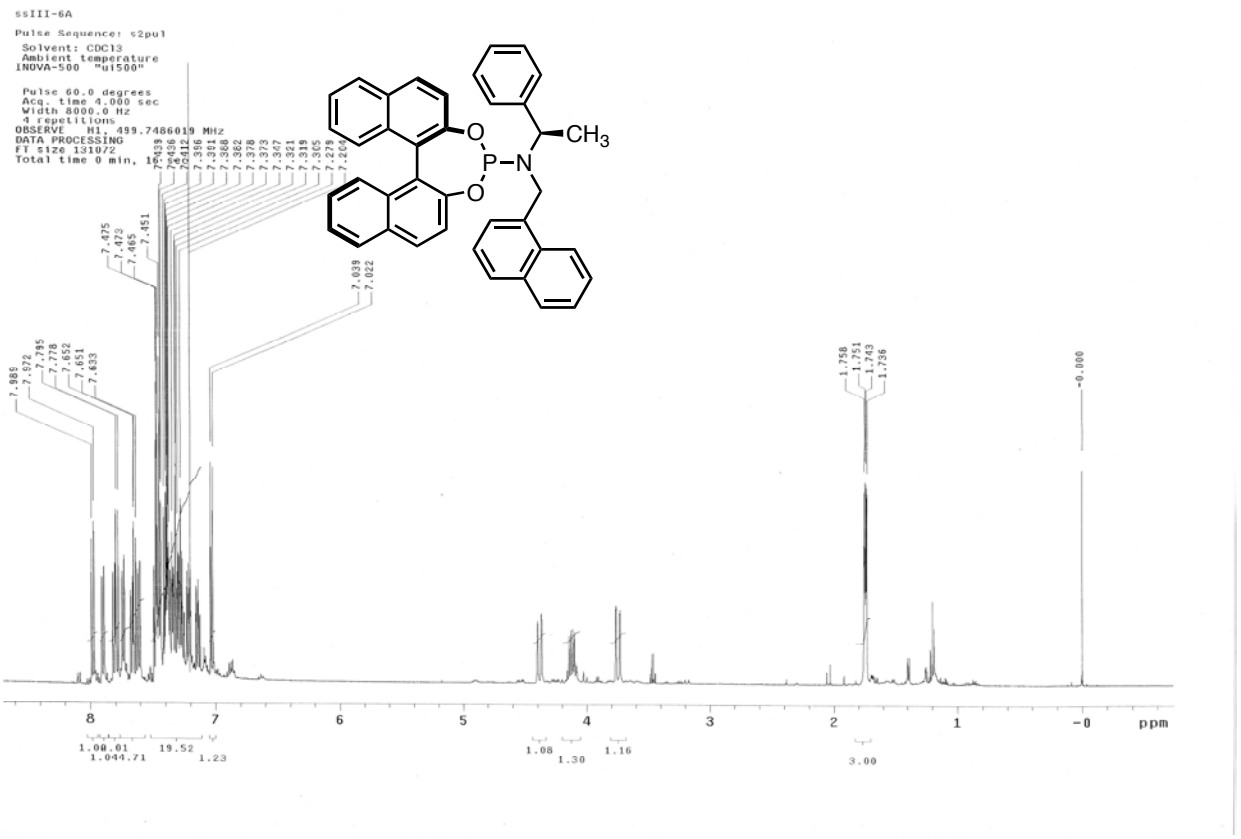

ssIII-54A-31P
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "merc400"
Relax. delay 2.000 sec
Pulse 47.4 degrees
Acq. time 0.800 sec
Width 59880.2 Hz
24 repetitions
OBSERVE P31, 161.9680029 MHz
DECOUPLE H1, 400.1135562 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 9 min, 10 sec
155.170
ppm

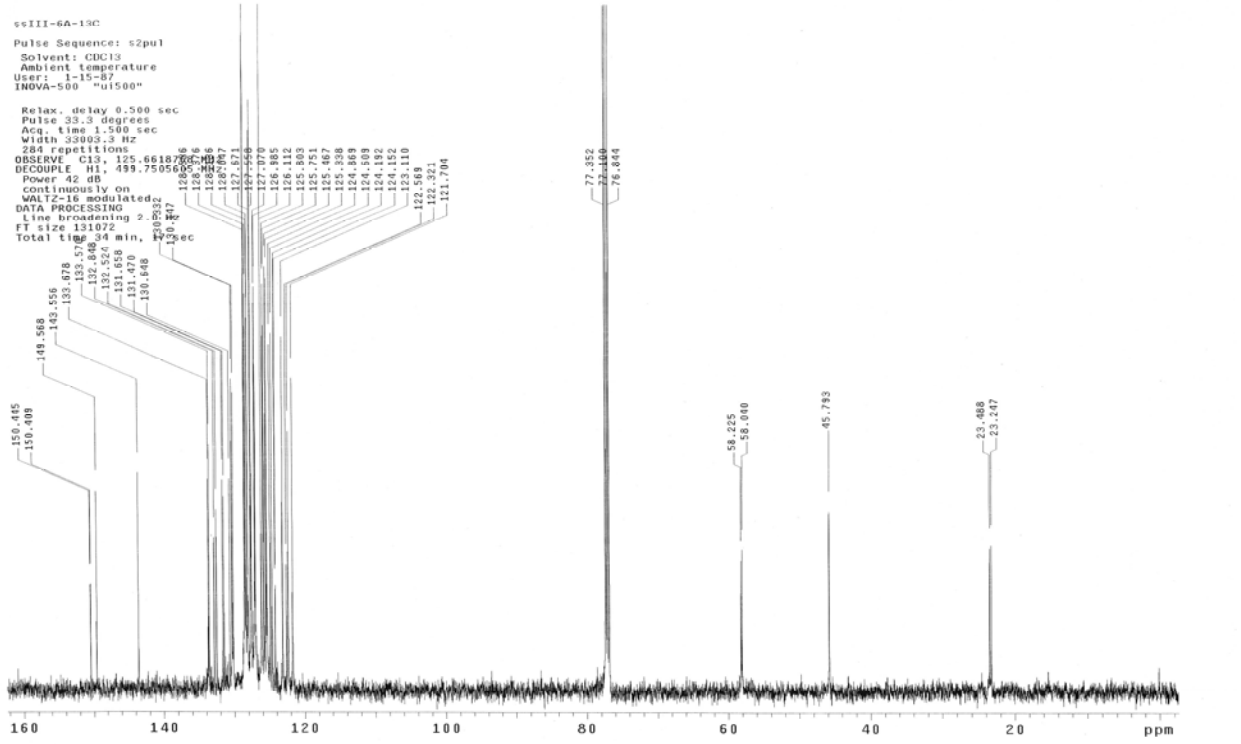

ssIII-7A
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
INOVA-500 "ui500"
Pulse 60.0 degrees
Acq. time 4.000 sec
Width 8000.0 Hz
4 repetitions
OBSERVE H1, 499.7485921 MHz
DATA PROCESSING
FT size 131072
Total time 0 min, 17 sec
CH3
CH3
ppm

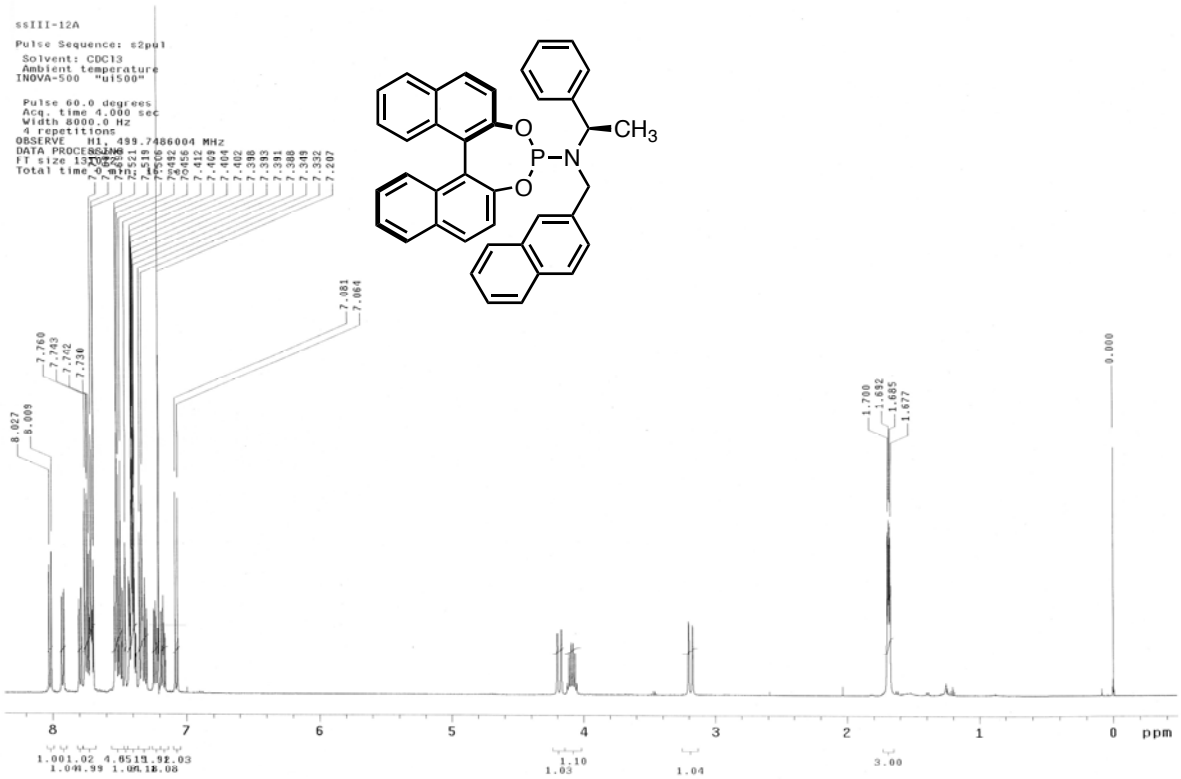

ssIII-7A-13C
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-15-87
INOVA-500 "ui500"
Relax. delay 0.500 sec
Pulse 33.3 degrees
Acq. time 1.500 sec
Width 33003.3 Hz
288 repetitions
DECOUPLE H1, 499.7505605 MHz
Power 42 dB
continuously On
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 131072
Total time 34 min, 17 sec
ppm

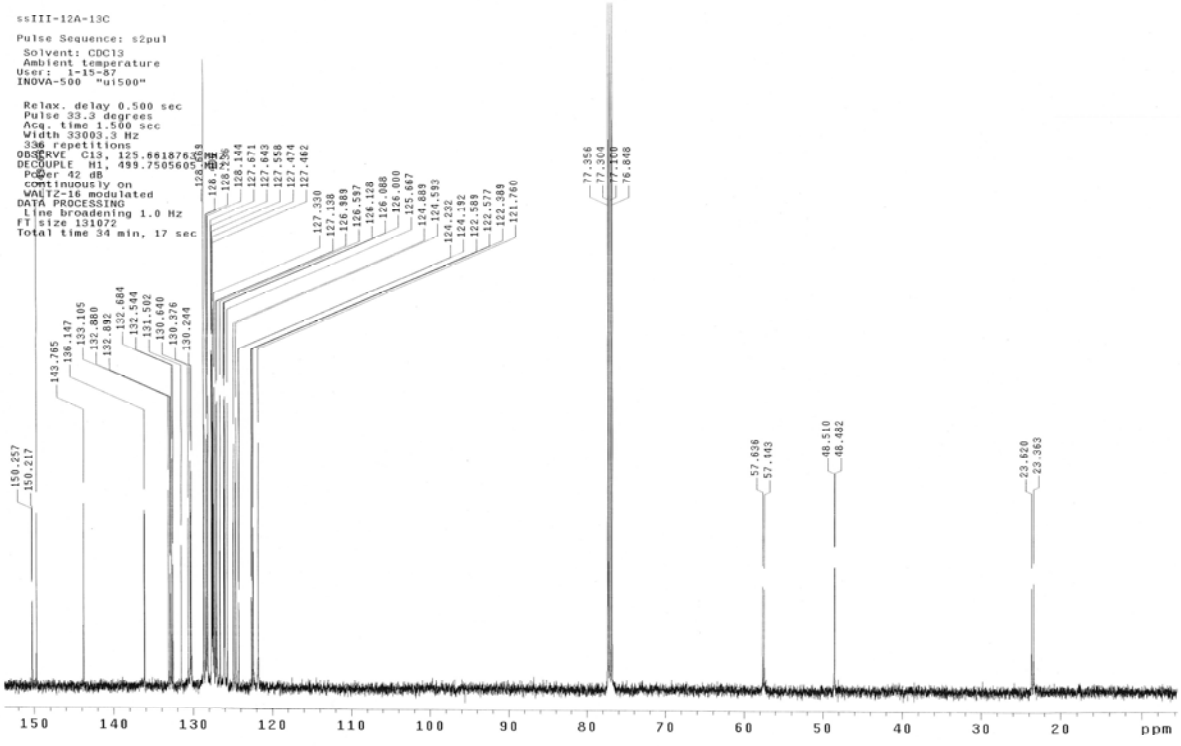

ssII-84A
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
INOVA-500 "ui500"
Pulse 60.0 degrees
Acq. time 4.000 sec
Width 8000.0 Hz
4 repetitions
OBSERVE H1, 499.7486020 MHz
DATA PROCESSING
FT size 131072
Total time 0 min, 16 sec
7.434
7.324
7.309
7.263
7.522
7.449
CH3
O
P
N
O
OCH3
8
7
6
5
4
3
2
1
-0
ppm
1.00
1.04
2.04
2.95
3.09
1.02
1.00
1.06
1.08
1.93
1.08
3.00

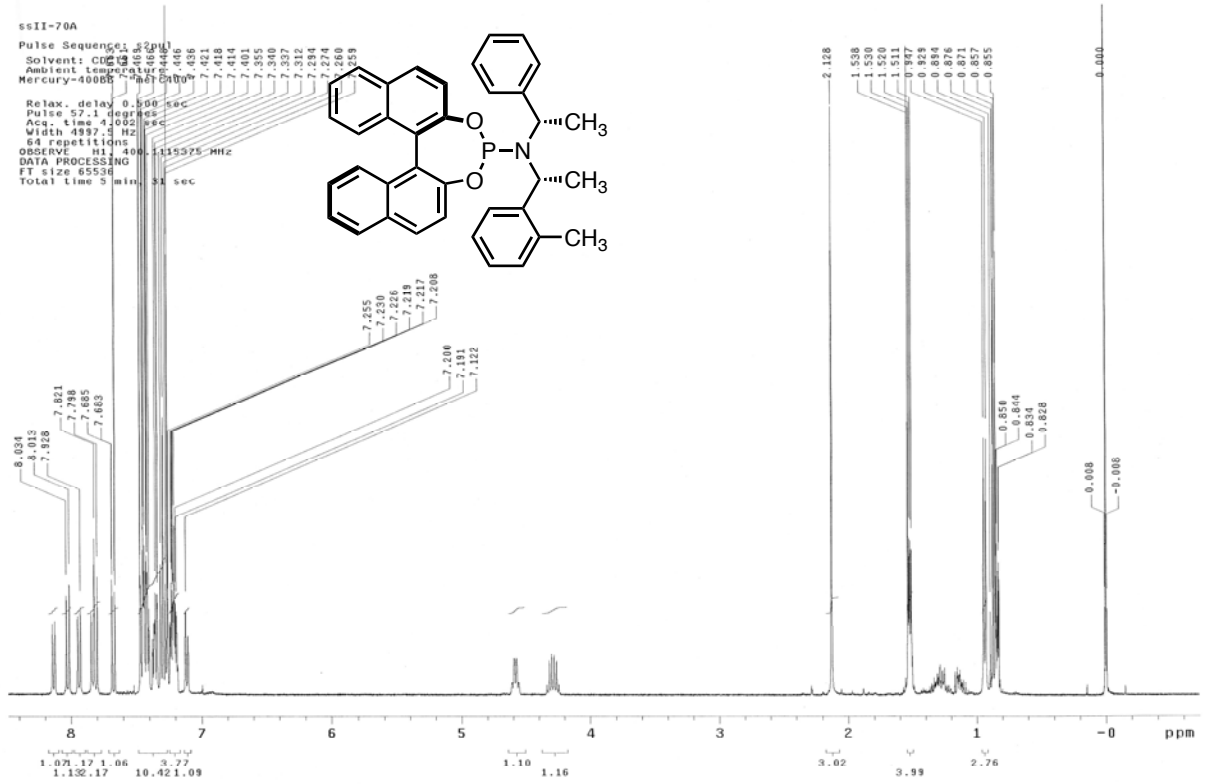

ssII-84A-13C
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-15-87
INOVA-500 "ui500"
Relax. delay 0.500 sec
Pulse 33.3 degrees
Acq. time 1.500 sec
Width 33003.3 Hz
332 repetitions
OBSERVE C13, 125.6618778 MHz
DECOUPLE H1, 499.7505605 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 131072
Total time 34 min, 17 sec
157.422
150.321
149.696
143.917
132.848
132.512
131.410
130.616
130.215
130.151
128.340
127.126
126.973
126.036
125.907
124.785
124.401
124.208
122.409
122.297
121.852
120.541
110.042
77.352
77.304
77.100
76.844
58.003
57.808
55.039
41.822
23.203
22.983
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

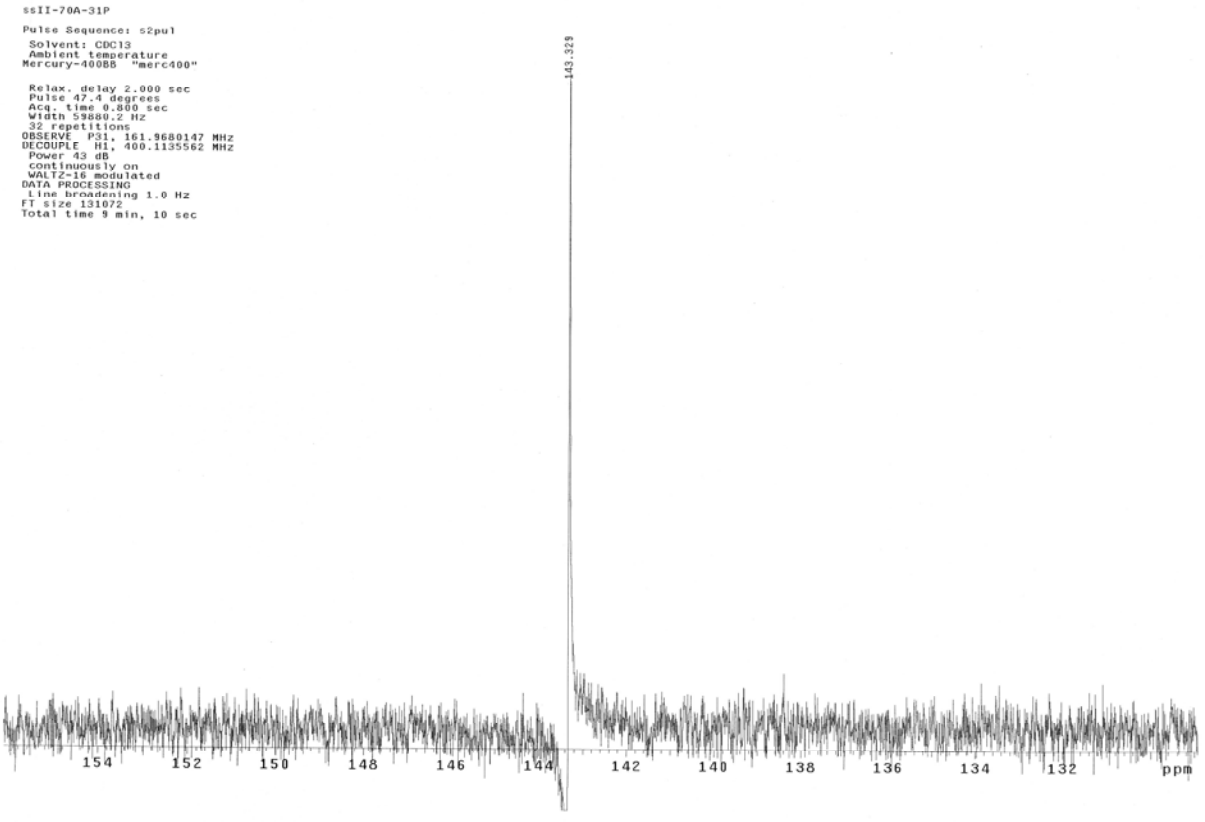

ssIII-6A
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
INOVA-500 "ui500"
Pulse 60.0 degrees
Acq. time 4.000 sec
Width 8000.0 Hz
4 repetitions
OBSERVE H1, 499.7486019 MHz
DATA PROCESSING
FT size 1310/2
Total time 0 min, 16 sec
CH3
ppm

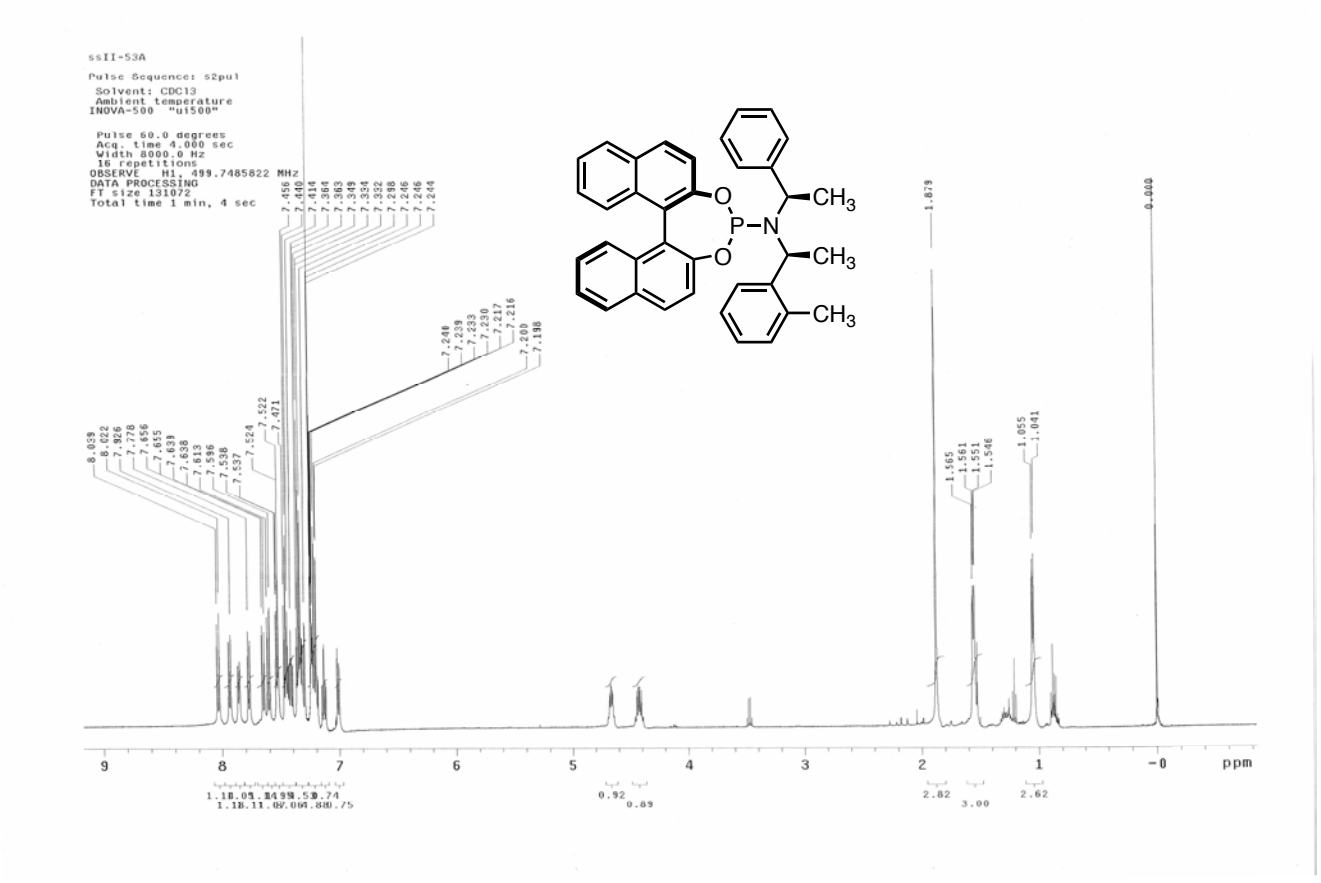

ssIII-6A-13C
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-15-87
INOVA-500 "ui500"
Relax. delay 0.500 sec
Pulse 33.3 degrees
Acq. time 1.500 sec
Width 33803.3 Hz
284 repetitions
OBSERVE C13, 125.6618706 MHz
DECOUPLE H1, 499.7505605 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 131072
Total time 34 min, 17 sec
ppm

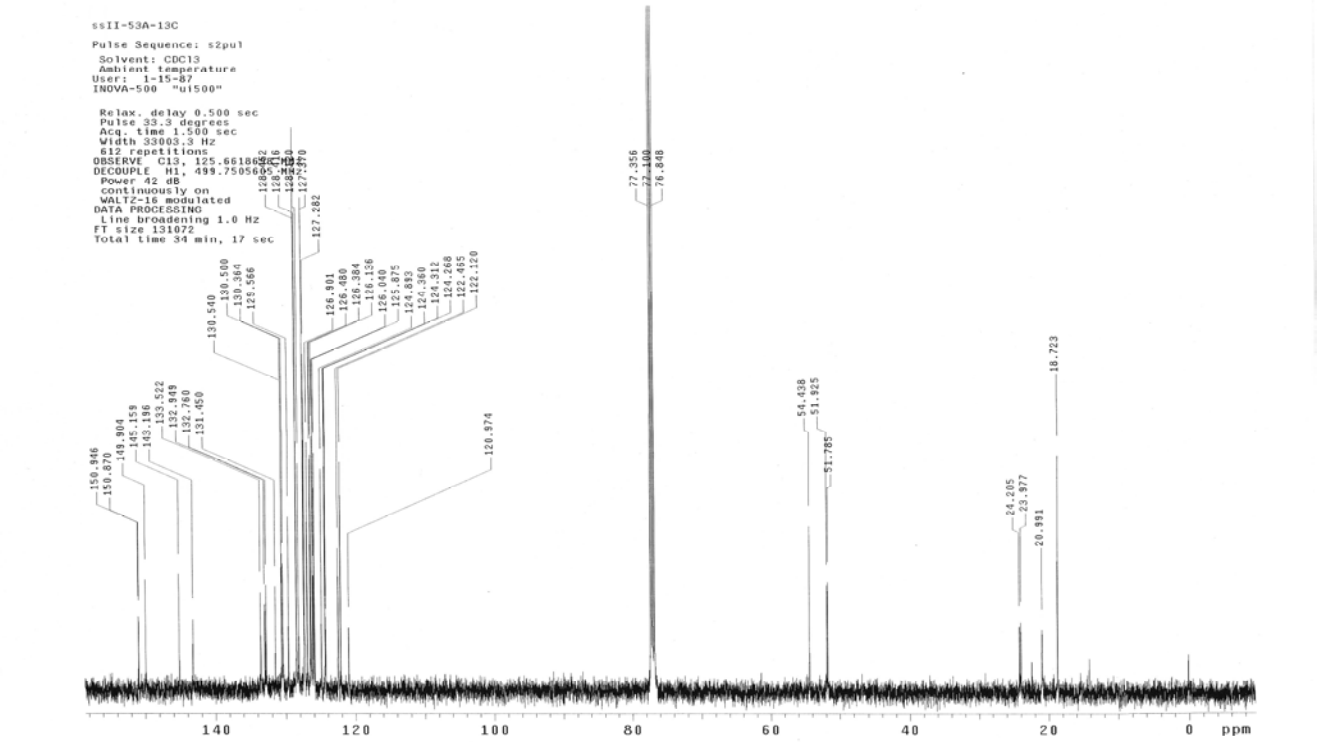

ssIII-12A
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
INOVA-500 "ui500"
Pulse 60.0 degrees
Acq. time 4.000 sec
Width 8000.0 Hz
4 repetitions
OBSERVE H1, 499.7486004 MHz
DATA PROCESSING
FT size 131072
Total time 0 min
O
P
N
CH3
ppm

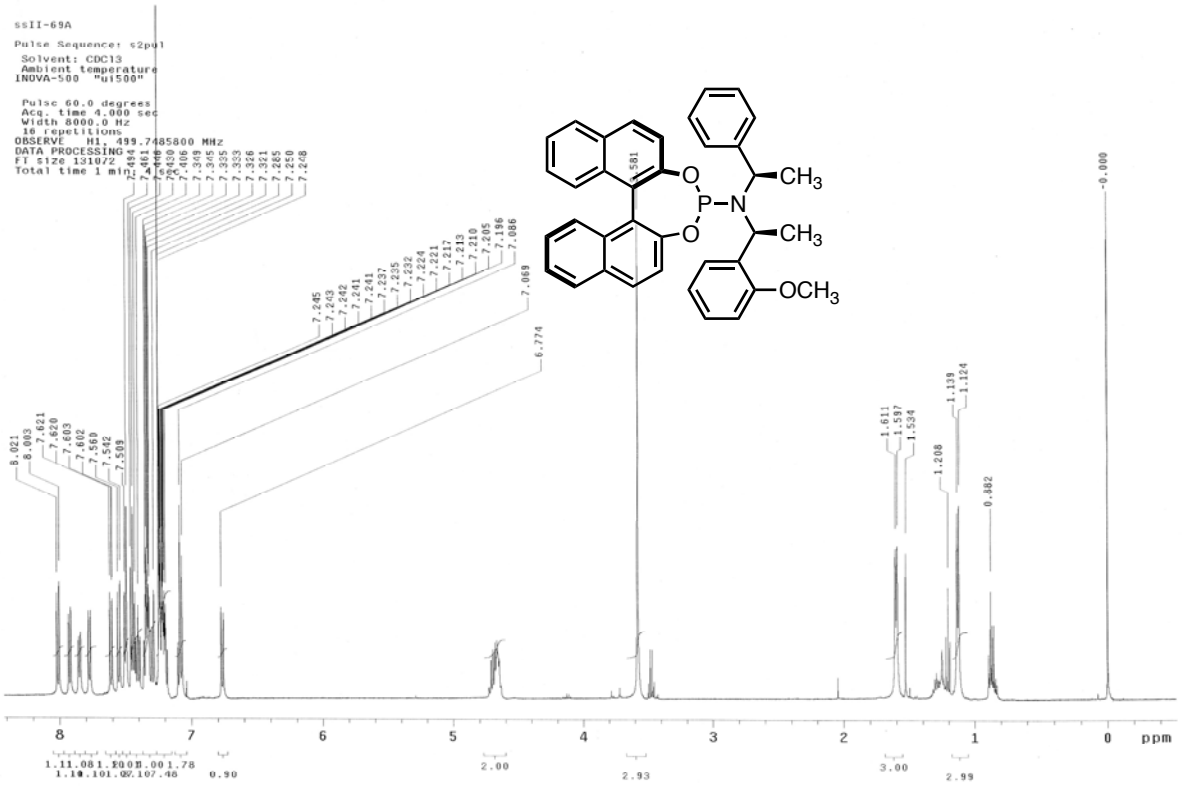

ssIII-12A-13C
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-15-87
INOVA-500 "ui500"
Relax. delay 0.500 sec
Pulse 33.3 degrees
Acq. time 1.500 sec
Width 33003.3 Hz
336 repetitions
DECOUPLE H1, 499.7505605 MHz
Power 42 dB
Continuously On
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 34 min, 17 sec
ppm

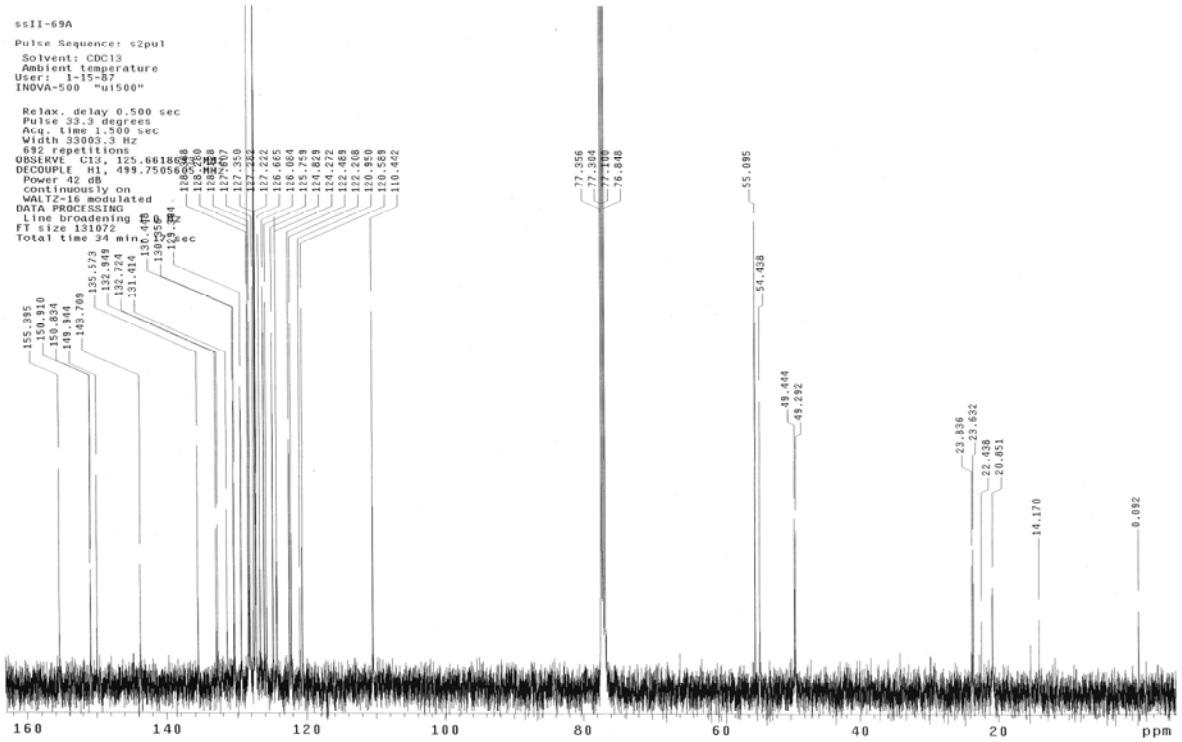

ssII-70A
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "merc400"
Relax. delay 0.500 sec
Pulse 57.1 degrees
Acq. time 4.002 sec
Width 4997.5 Hz
64 repetitions
OBSERVE H1, 400.1115375 MHz
DATA PROCESSING
FT size 65536
Total time 5 min, 31 sec
O
P
N
O
O
CH3
CH3
CH3
8.034
8.013
7.828
7.821
7.798
7.685
7.663
7.255
7.230
7.226
7.219
7.217
7.208
7.200
7.191
7.122
2.128
1.538
1.530
1.520
1.511
0.927
0.884
0.876
0.871
0.857
0.855
0.850
0.844
0.834
0.828
0.000
0.008
-0.006
8
7
6
5
4
3
2
1
-0
ppm
1.07
1.17
1.06
1.13
2.17
3.77
10.42
1.09
1.10
1.16
3.02
3.99
2.76

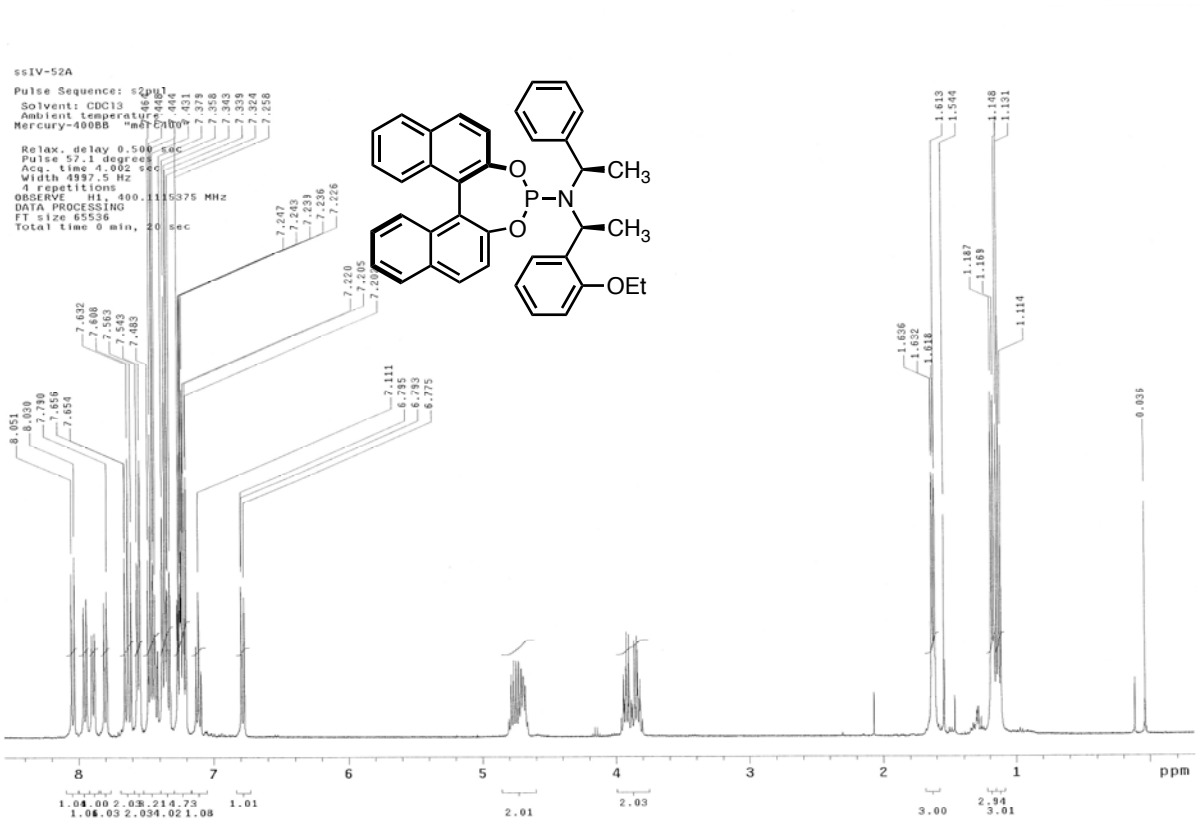

ssII-70A-31P
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "merc400"
Relax. delay 2.000 sec
Pulse 47.4 degrees
Acq. time 0.800 sec
Width 59880.2 Hz
32 repetitions
OBSERVE P31, 161.9680147 MHz
DECOUPLE H1, 400.1135562 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 9 min, 10 sec
143.329
154
152
150
148
146
144
142
140
138
136
134
132
ppm

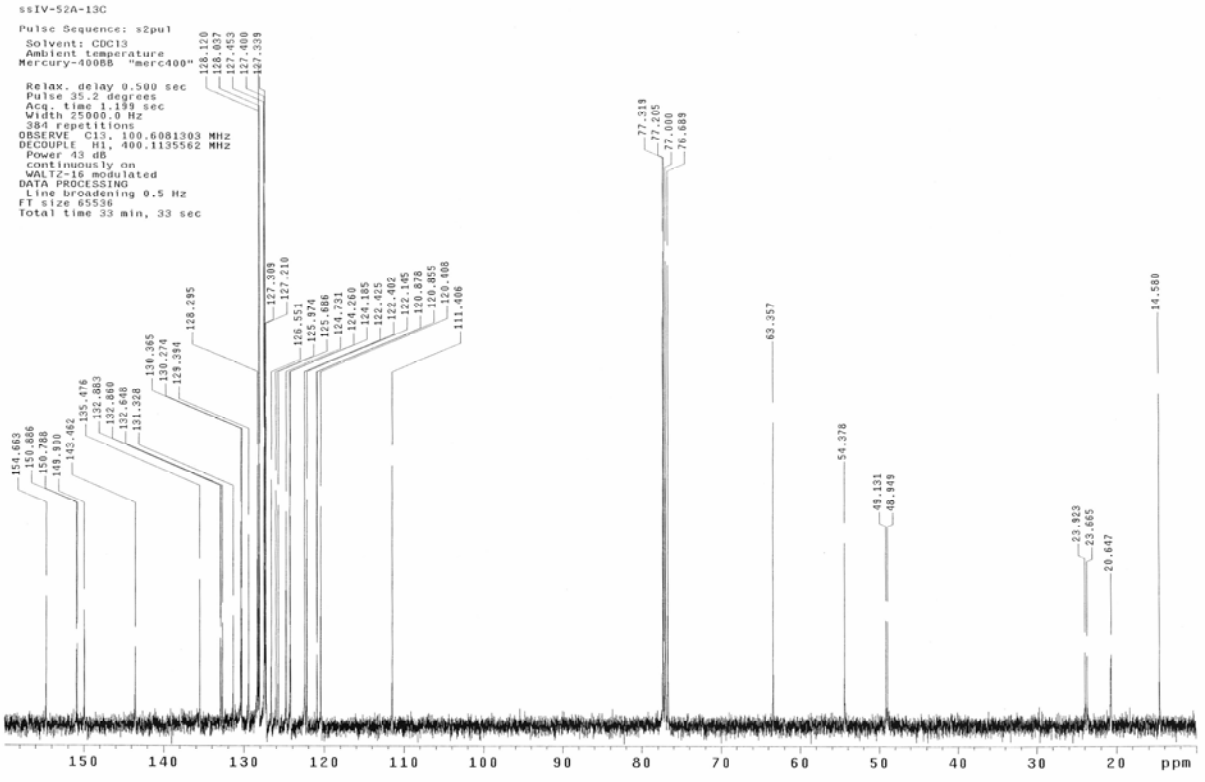

ssII-53A
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
INOVA-500 "ui500"
Pulse 60.0 degrees
Acq. time 4.000 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.7485822 MHz
DATA PROCESSING
FT size 131072
Total time 1 min, 4 sec
O
P
N
O
CH3
CH3
CH3
ppm

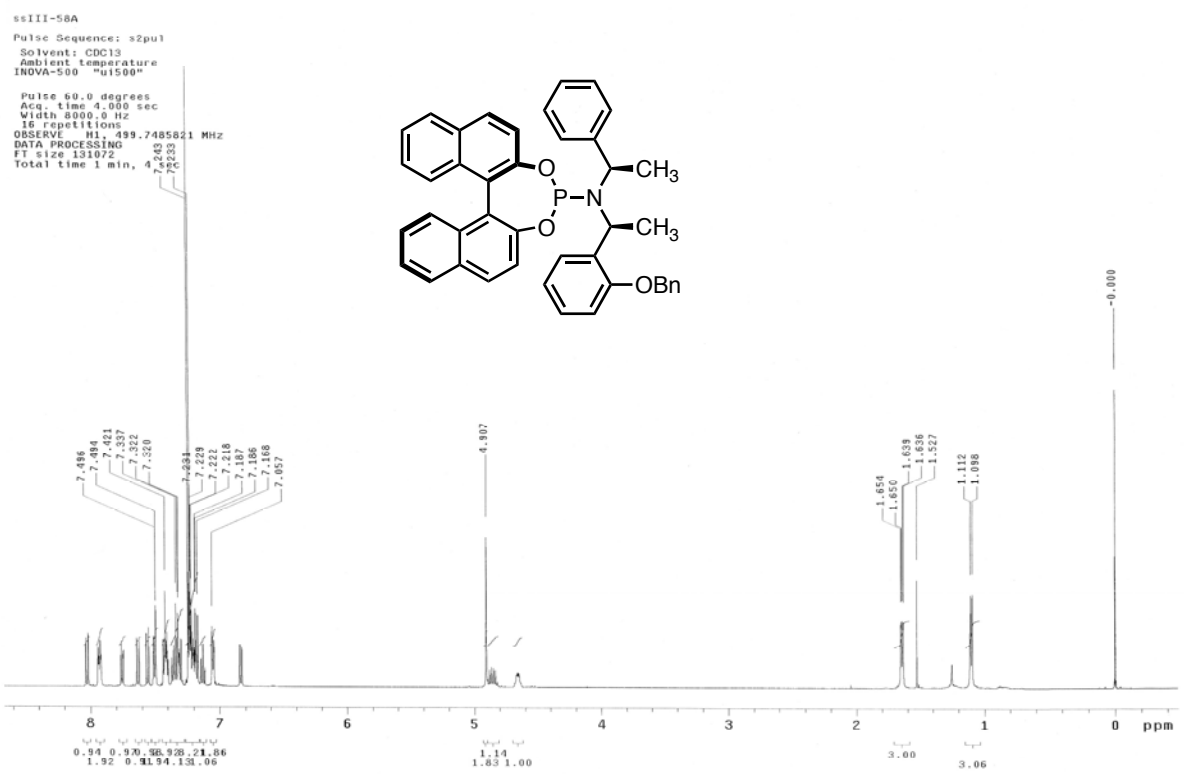

ssII-53A-13C
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-15-87
INOVA-500 "ui500"
Relax. delay 0.500 sec
Pulse 33.3 degrees
Acq. time 1.500 sec
Width 33003.3 Hz
612 repetitions
DECOUPLE H1, 499.7505605 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 34 min, 17 sec
ppm

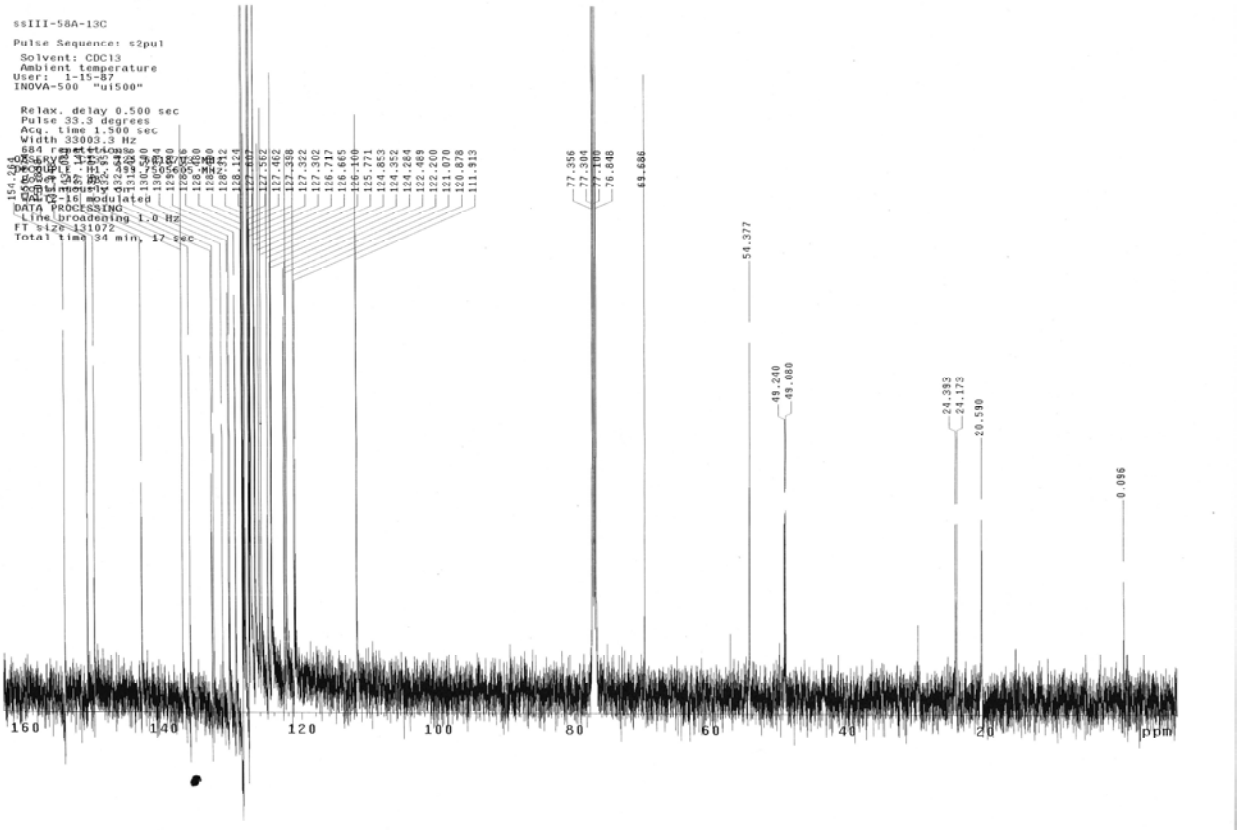

ssII-69A
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
INOVA-500 "ui500"
Pulse 60.0 degrees
Acq. time 4.000 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.7485800 MHz
DATA PROCESSING
FT size 131072
Total time 1 min
O
P
N
O
CH3
CH3
OCH3
ppm

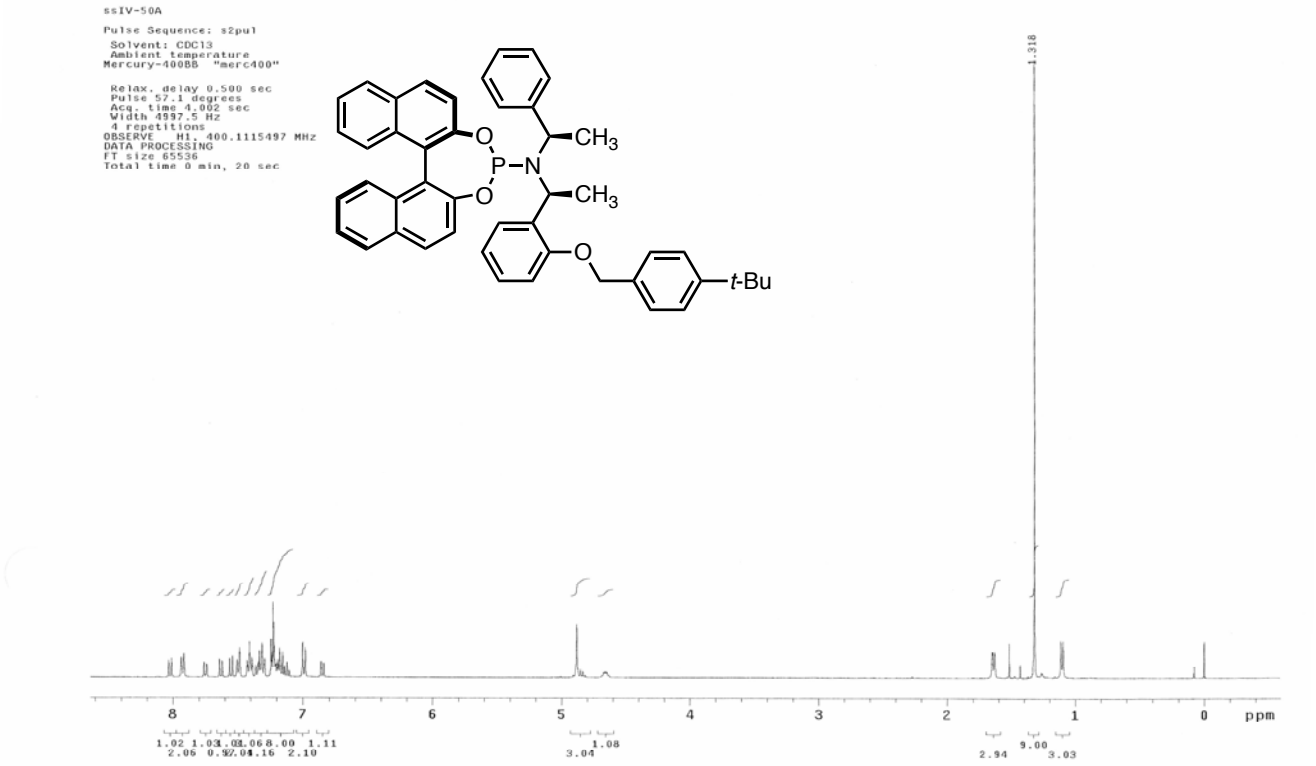

ssII-69A
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: I-15-87
INOVA-500 "ui500"
Relax. delay 0.500 sec
Pulse 33.3 degrees
Acq. time 1.500 sec
Width 33003.3 Hz
692 repetitions
OBSERVE C13, 125.6618648 MHz
DECOUPLE H1, 499.7505605 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 10.0 Hz
FT size 131072
Total time 34 min, 13 sec
ppm

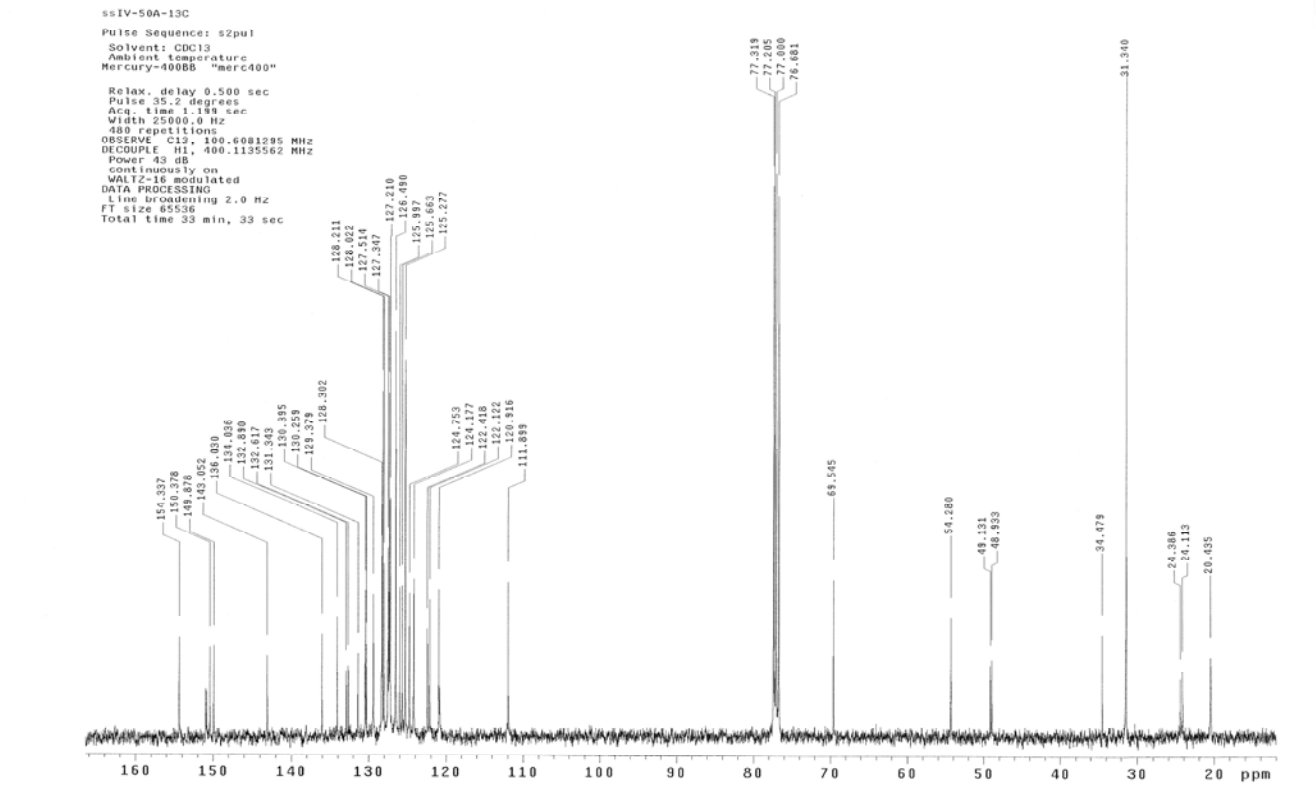

ssIV-52A
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "merc400"
Relax. delay 0.500 sec
Pulse 57.1 degrees
Acq. time 4.002 sec
Width 4997.5 Hz
4 repetitions
OBSERVE H1, 400.1135375 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 20 sec
O
P
N
O
CH3
CH3
OEt
ppm

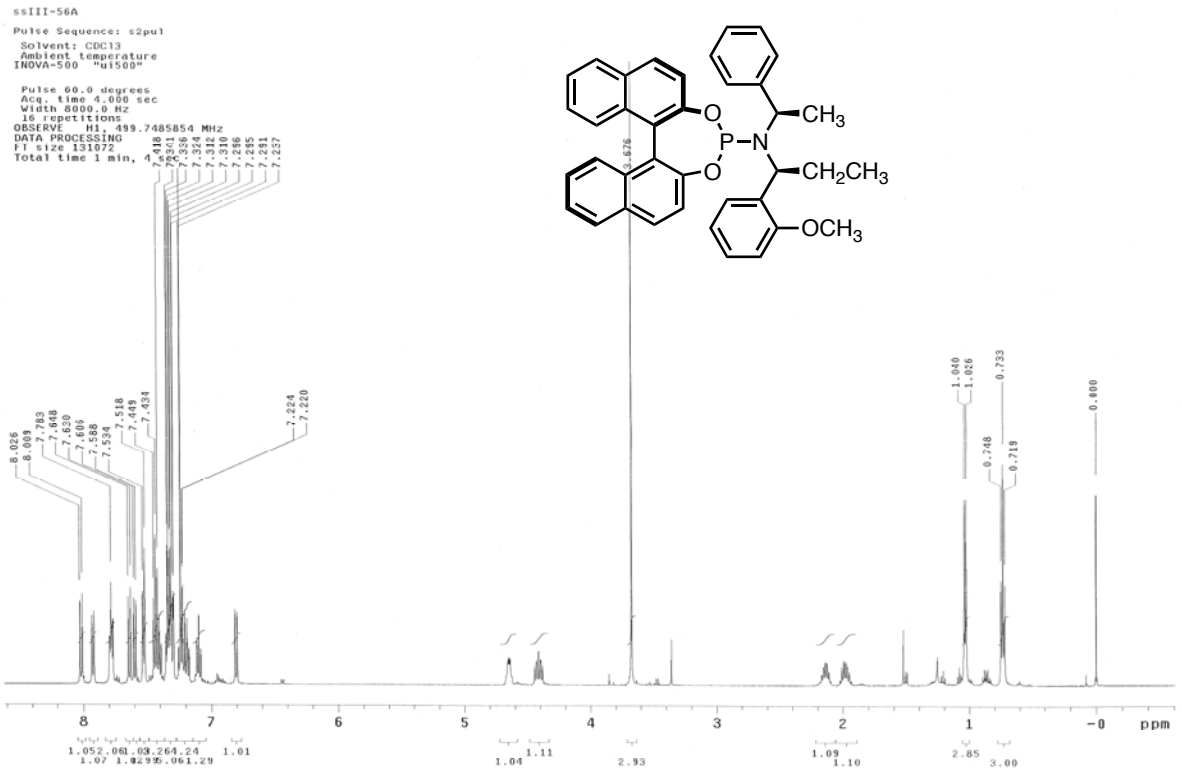

ssIV-52A-13C
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "merc400"
Relax. delay 0.500 sec
Pulse 35.2 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
384 repetitions
OBSERVE C13, 100.6081303 MHz
DECOUPLE H1, 400.1135562 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 33 min, 33 sec
ppm

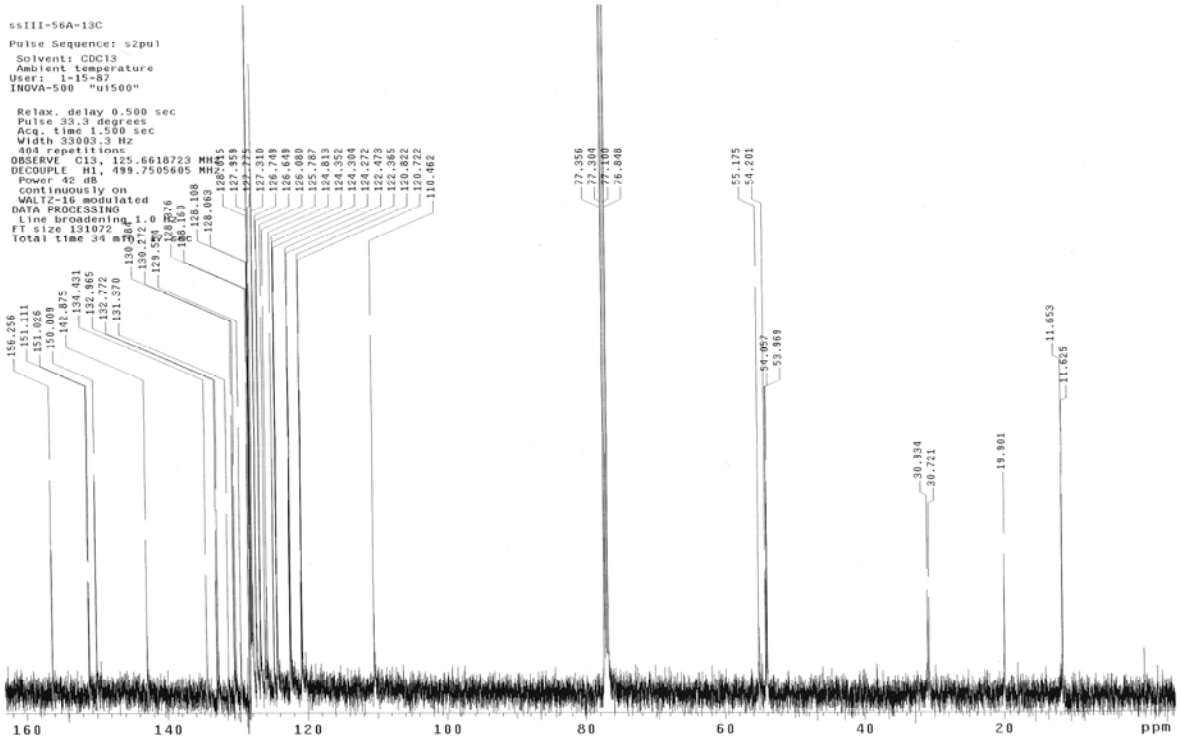

ssIII-58A
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
INOVA-500 "u1500"
Pulse 60.0 degrees
Acq. time 4.000 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.7485821 MHz
DATA PROCESSING
FT size 131072
Total time 1 min, 4 sec
CH3
CH3
OBn
ppm

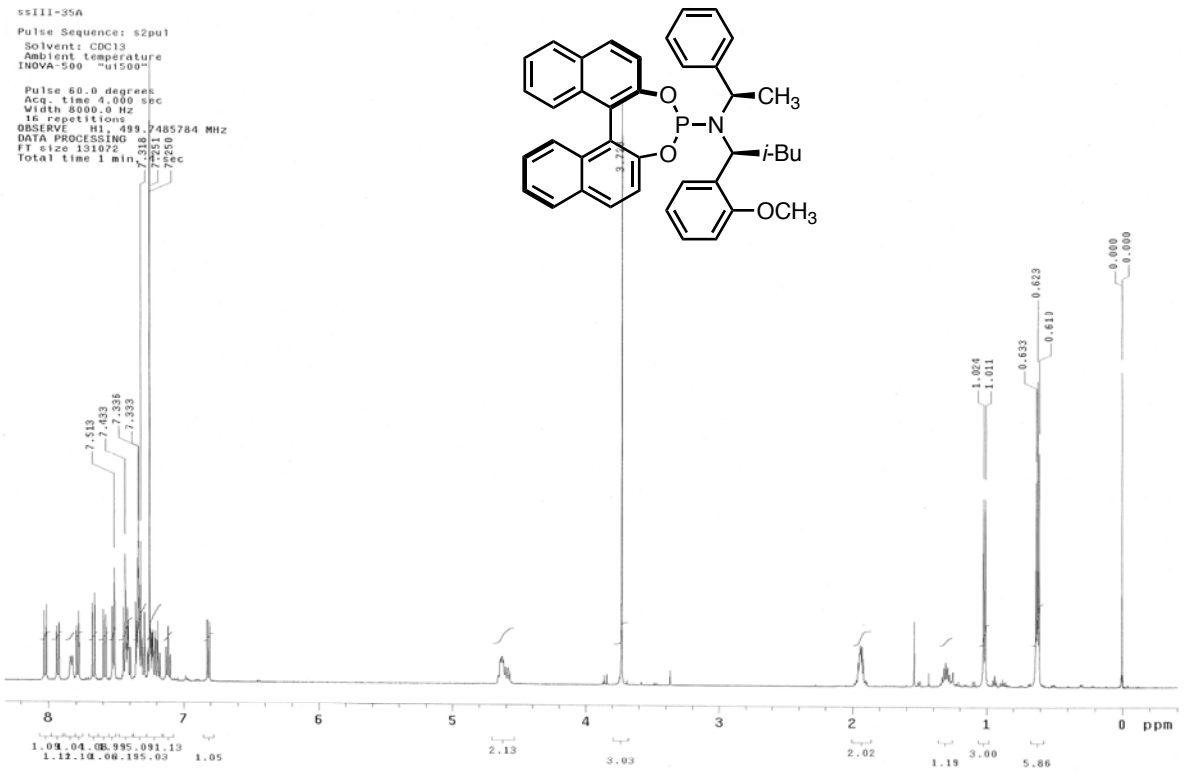

ssIII-58A-13C
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-15-87
INOVA-500 "u1500"
Relax. delay 0.500 sec
Pulse 33.3 degrees
Acq. time 1.500 sec
Width 33003.3 Hz
684 repetitions
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 34 min, 17 sec
ppm

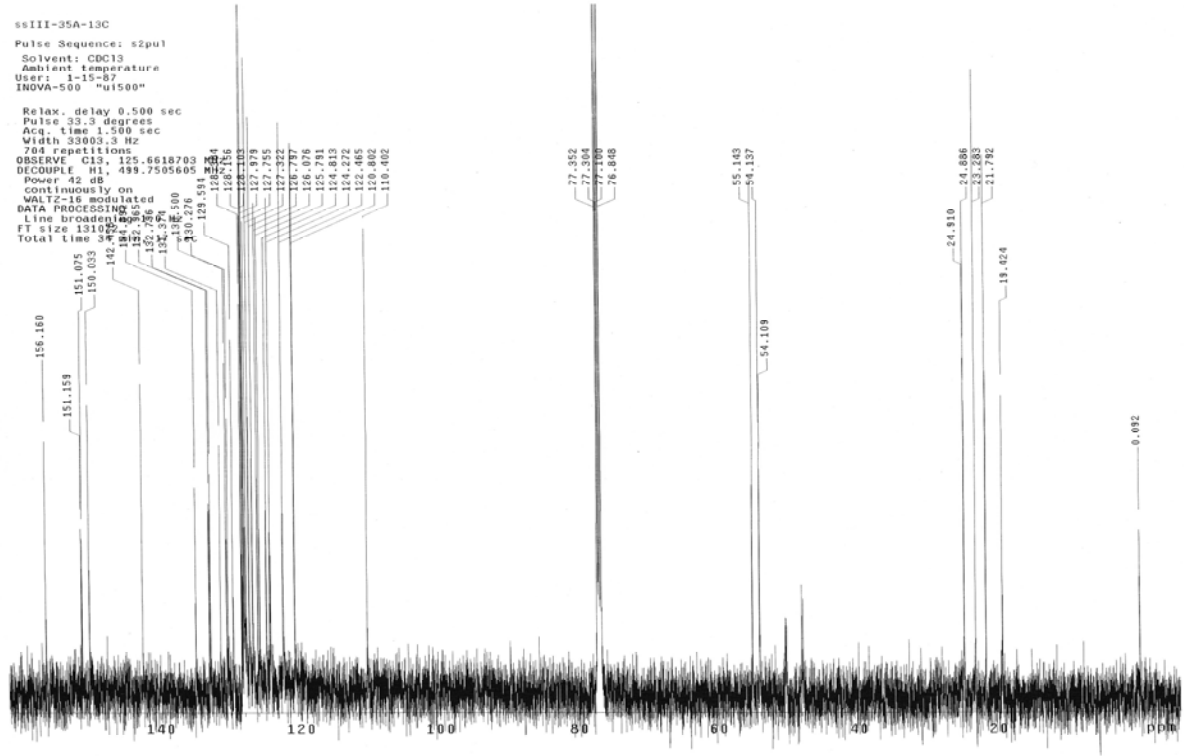

ssIV-50A
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "merc400"
Relax. delay 0.500 sec
Pulse 57.1 degrees
Acq. time 4.002 sec
Width 4997.5 Hz
4 repetitions
OBSERVE H1, 400.1115497 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 20 sec
O
P
N
O
CH3
CH3
O
t-Bu
1.318
8
7
6
5
4
3
2
1
0
ppm
1.02 1.03 1.06 8.00 1.11
2.06 0.92 4.16 2.10
1.08
3.04
2.94
9.00
3.03

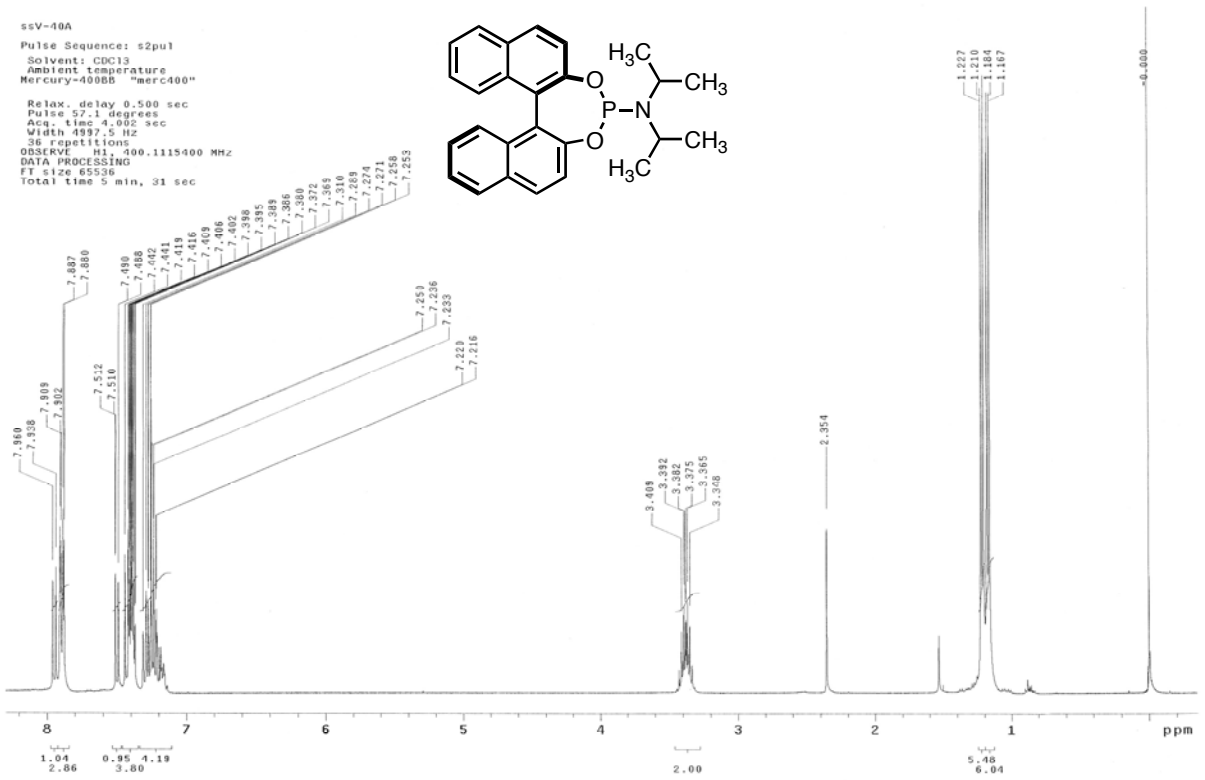

ssIV-50A-13C
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "merc400"
Relax. delay 0.500 sec
Pulse 35.2 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
480 repetitions
OBSERVE C13, 100.6081295 MHz
DECOUPLE H1, 400.1135562 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 65536
Total time 33 min, 33 sec
77.319
77.205
77.000
76.681
31.340
69.545
54.280
49.131
48.933
34.479
24.086
24.113
20.435
150.337
150.378
149.878
143.052
136.030
134.036
132.890
132.617
131.343
130.395
130.259
129.379
128.302
128.211
128.022
127.514
127.347
127.210
126.490
125.937
125.663
125.277
124.753
124.177
122.418
122.122
120.916
111.899
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

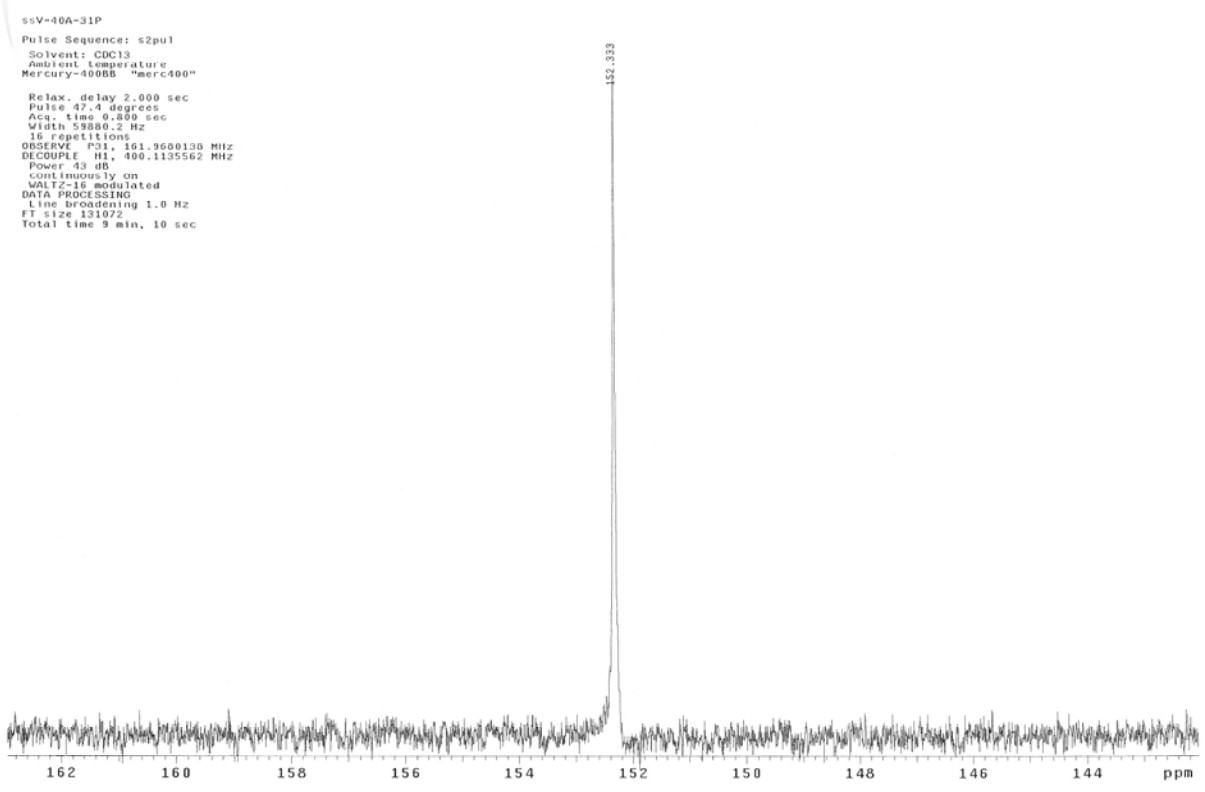

ssIII-56A
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
INOVA-500 "ui500"
Pulse 60.0 degrees
Acq. time 4.000 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.7485854 MHz
DATA PROCESSING
FT size 131072
Total time 1 min, 4 s
CH3
CH2CH3
OCH3
ppm

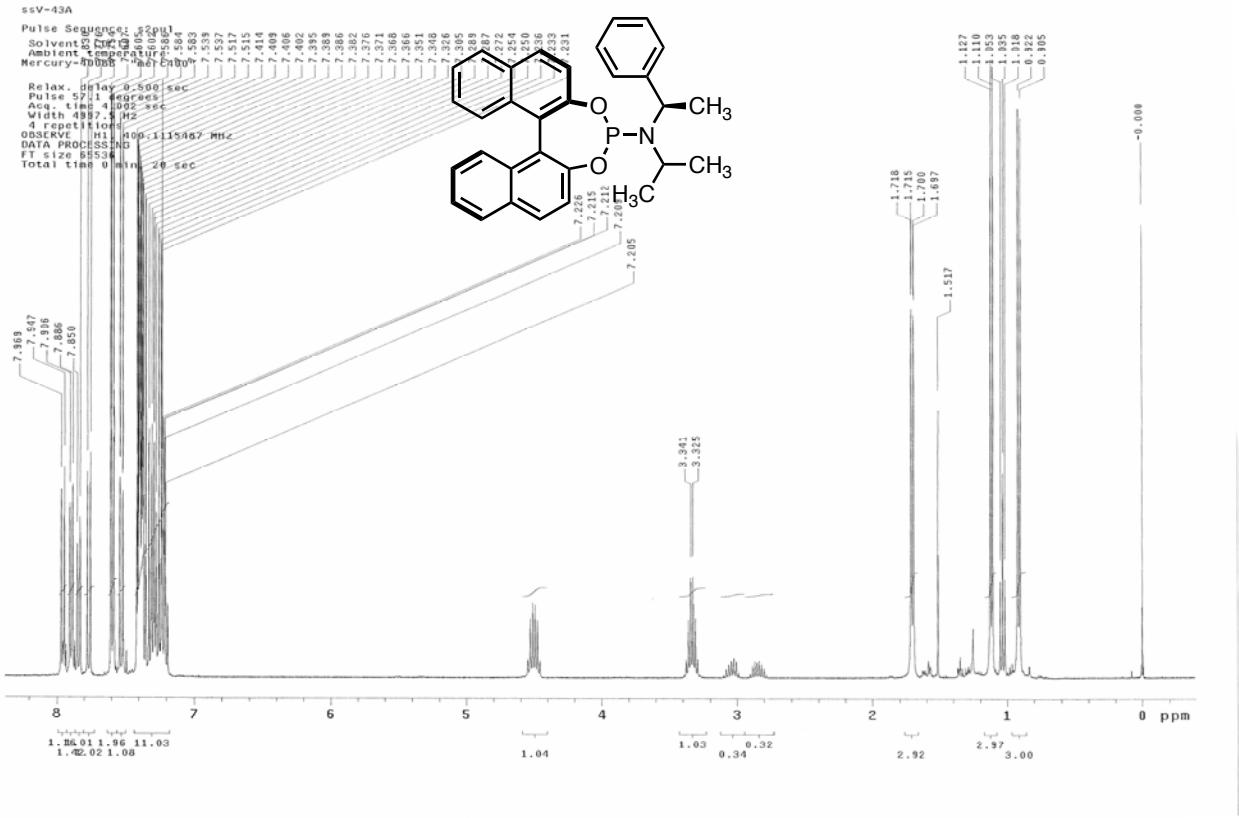

ssIII-56A-13C
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
INOVA-500 "ui500"
Relax. delay 0.500 sec
Pulse 33.3 degrees
Acq. time 1.500 sec
Width 33003.3 Hz
404 repetitions
OBSERVE C13, 125.6618723 MHz
DECOUPLE H1, 499.7505605 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 34 min
ppm

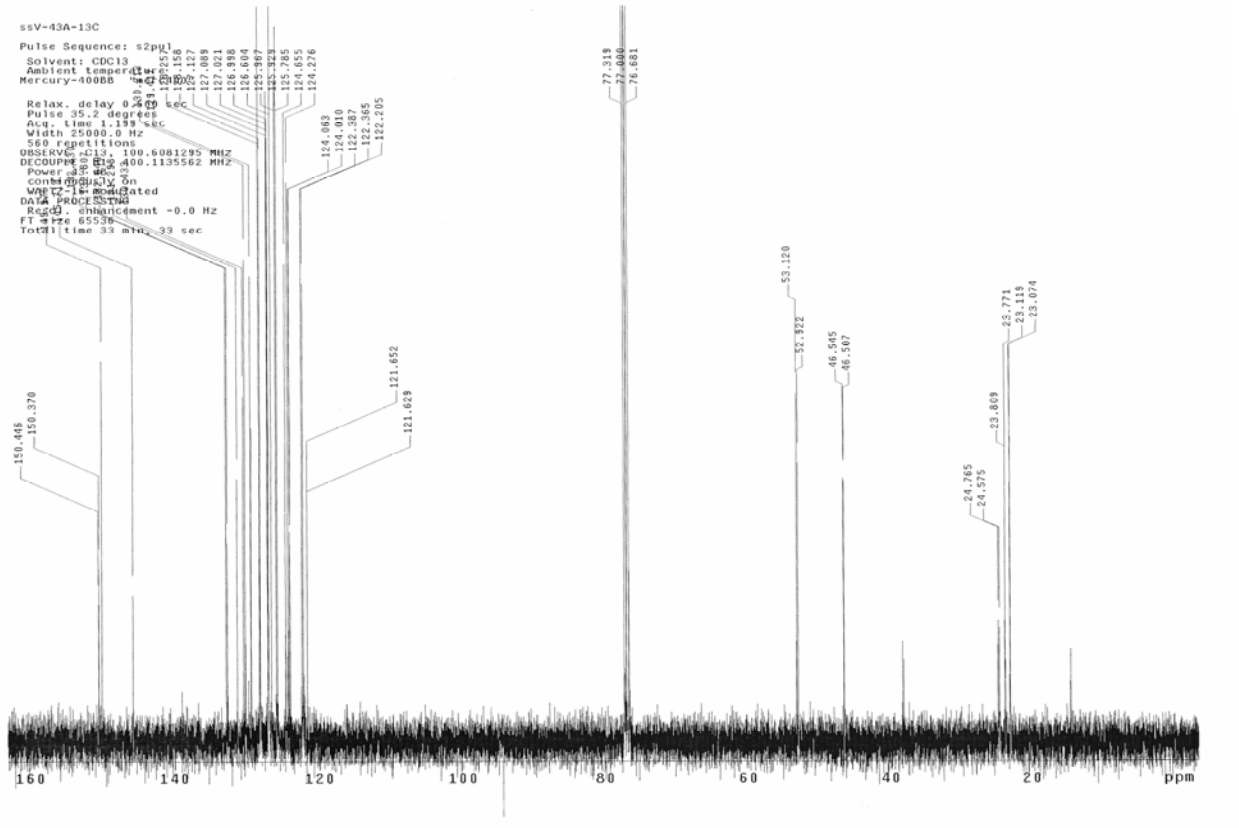

ssIII-35A
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
INOVA-500 "u1500"
Pulse 60.0 degrees
Acq. time 4.000 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.7485784 MHz
DATA PROCESSING
FT size 131072
Total time 1 min, 5 sec
O
P
N
O
CH3
i-Bu
OCH3
ppm

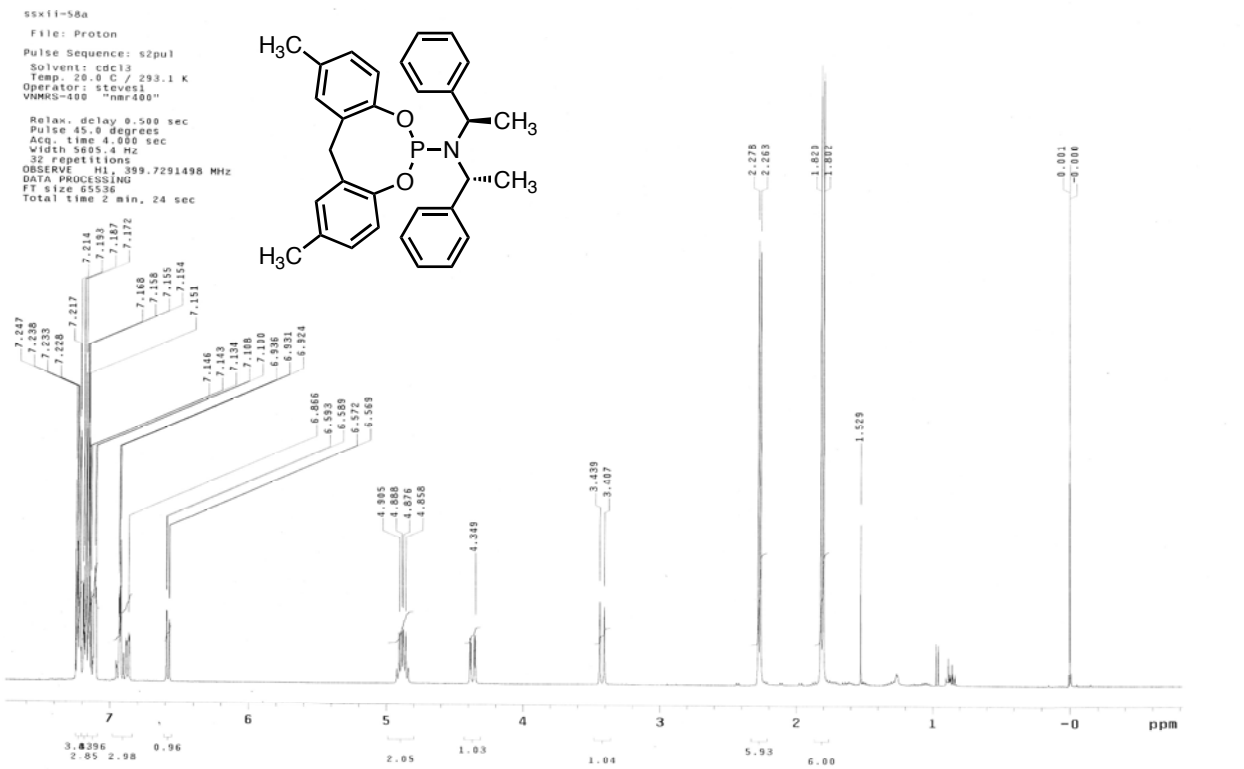

ssIII-35A-13C
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-15-87
INOVA-500 "u1500"
Relax. delay 0.500 sec
Pulse 33.3 degrees
Acq. time 1.500 sec
Width 33003.3 Hz
704 repetitions
OBSERVE C13, 125.6618703 MHz
DECOUPLE H1, 499.7505605 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening
FT size 131072
Total time 34 min
ppm

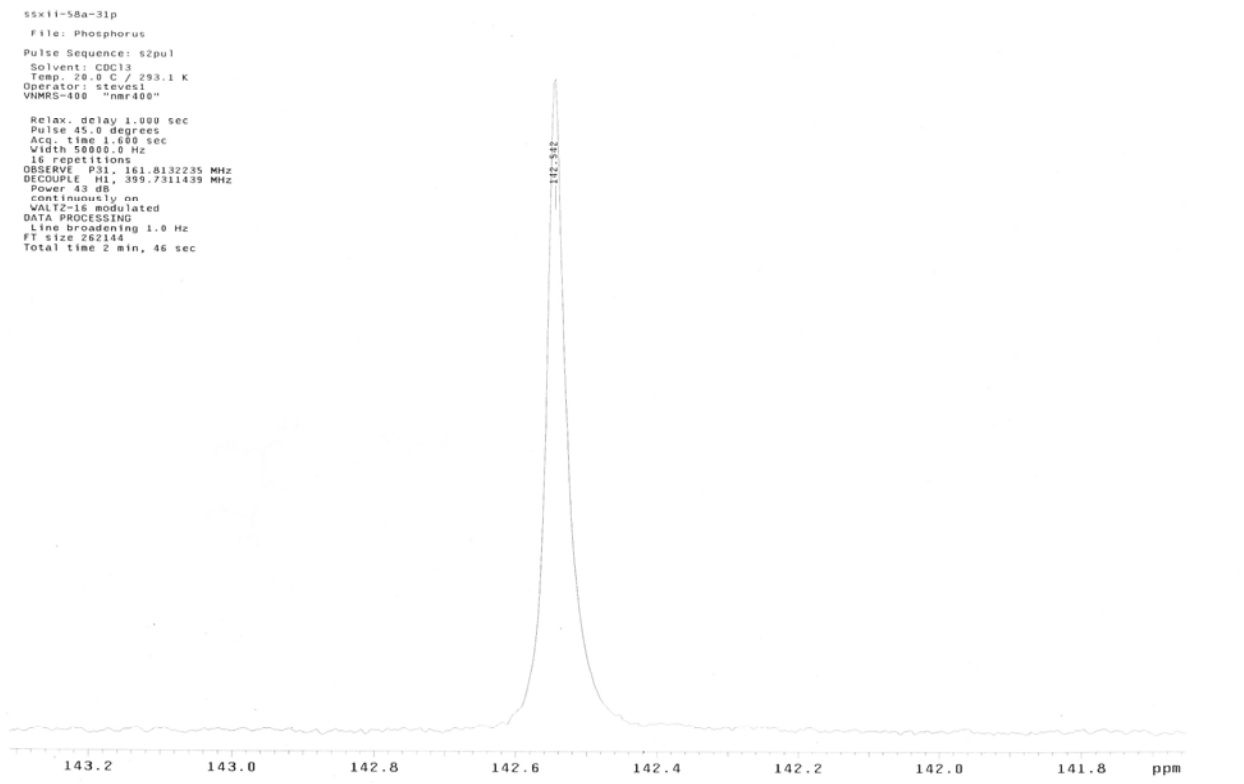

ssV-40A
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "merc400"
Relax. delay 0.500 sec
Pulse 57.1 degrees
Acq. time 4.002 sec
Width 4997.5 Hz
36 repetitions
OBSERVE H1, 400.1115400 MHz
DATA PROCESSING
FT size 65536
Total time 5 min, 31 sec
ppm

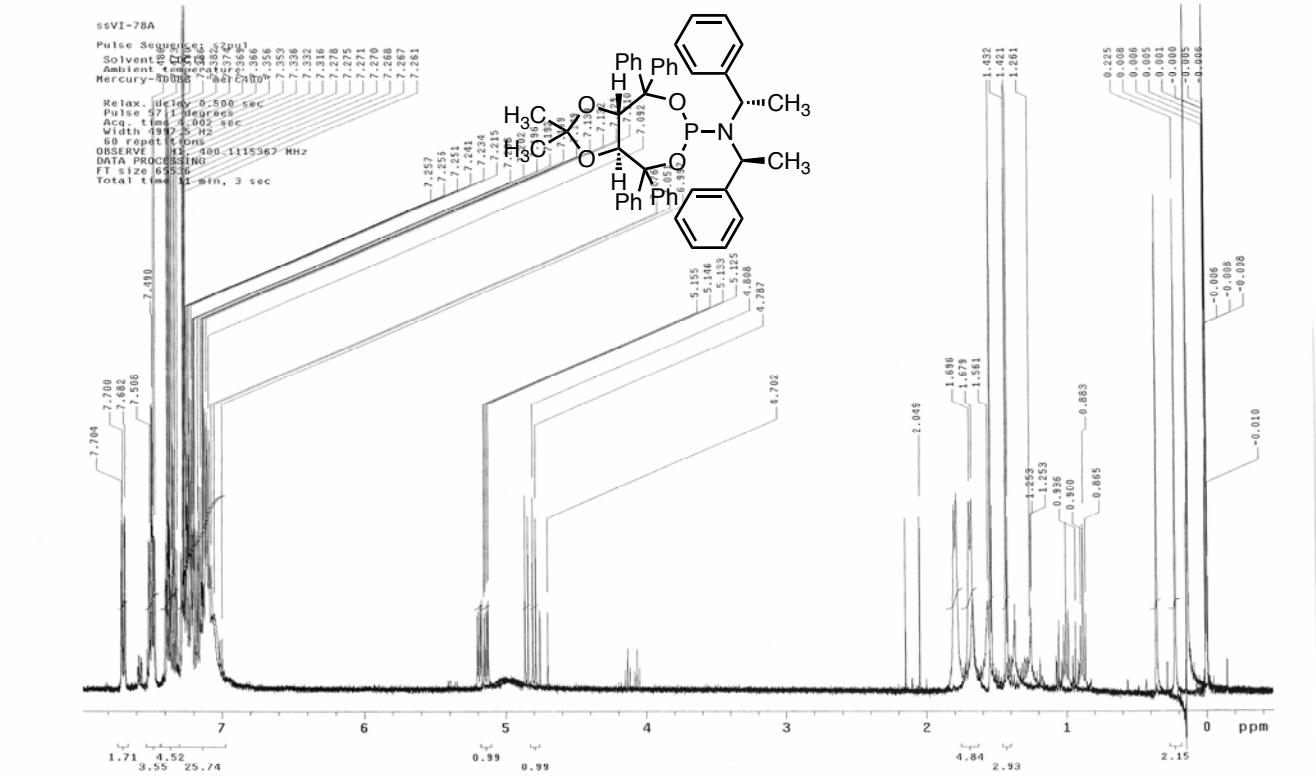

ssV-40A-31P
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "merc400"
Relax. delay 2.000 sec
Pulse 47.4 degrees
Acq. time 0.800 sec
Width 59880.2 Hz
16 repetitions
OBSERVE P31, 161.9600138 MHz
DECOUPLE H1, 400.1135562 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 9 min, 10 sec
152.333
ppm

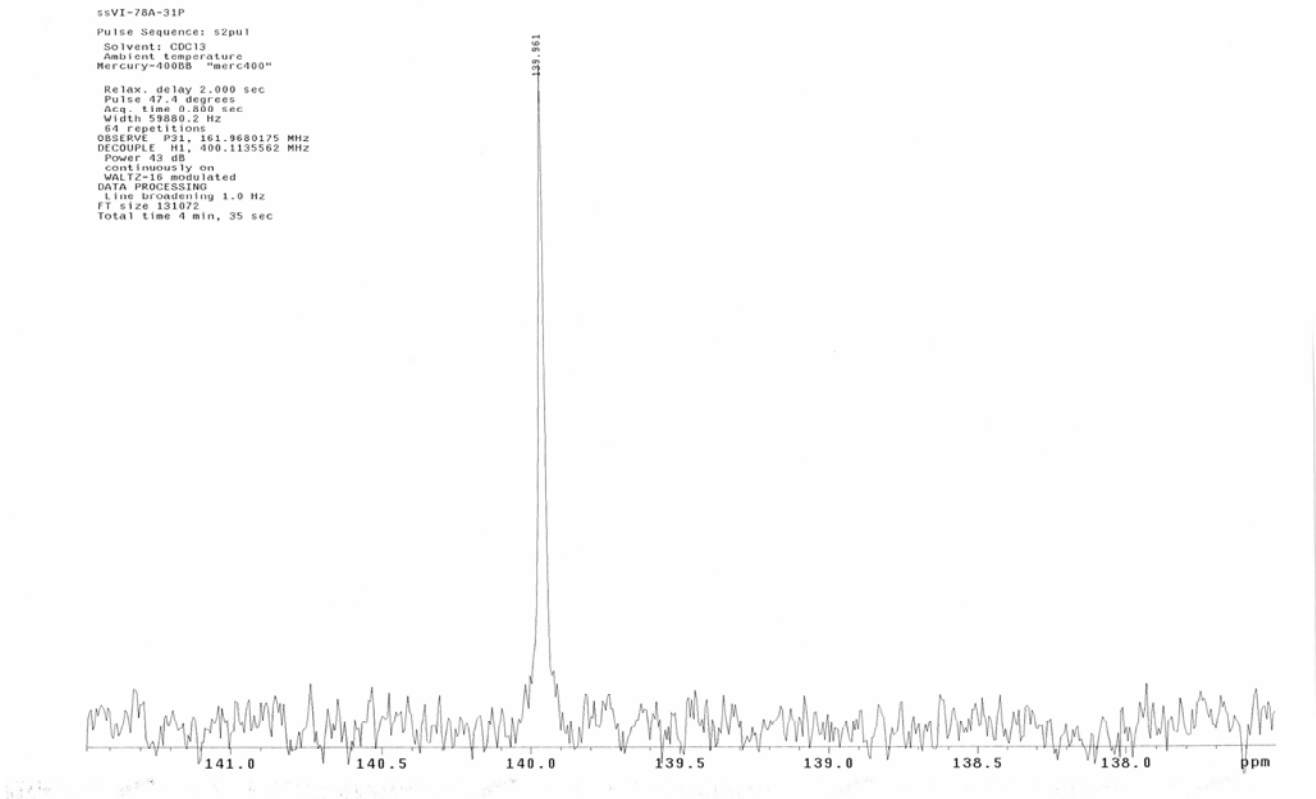

ssV-43A
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "heptane"
Relax. delay 0.500 sec
Pulse 57.1 degrees
Acq. time 4.092 sec
Width 4997.5 Hz
4 repetitions
OBSERVE H1, 400.1115467 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 20 sec
O
P
N
O
O
CH3
CH3
H3C
7.968
7.547
7.916
7.866
7.850
7.226
7.215
7.212
7.205
3.341
3.325
1.718
1.715
1.700
1.697
1.517
1.127
1.110
1.053
1.035
1.018
0.322
0.305
-0.000
8
7
6
5
4
3
2
1
0 ppm
1.00
1.01
1.96
11.03
1.42
2.02
1.08
1.04
1.03
0.34
0.32
2.92
2.97
3.00

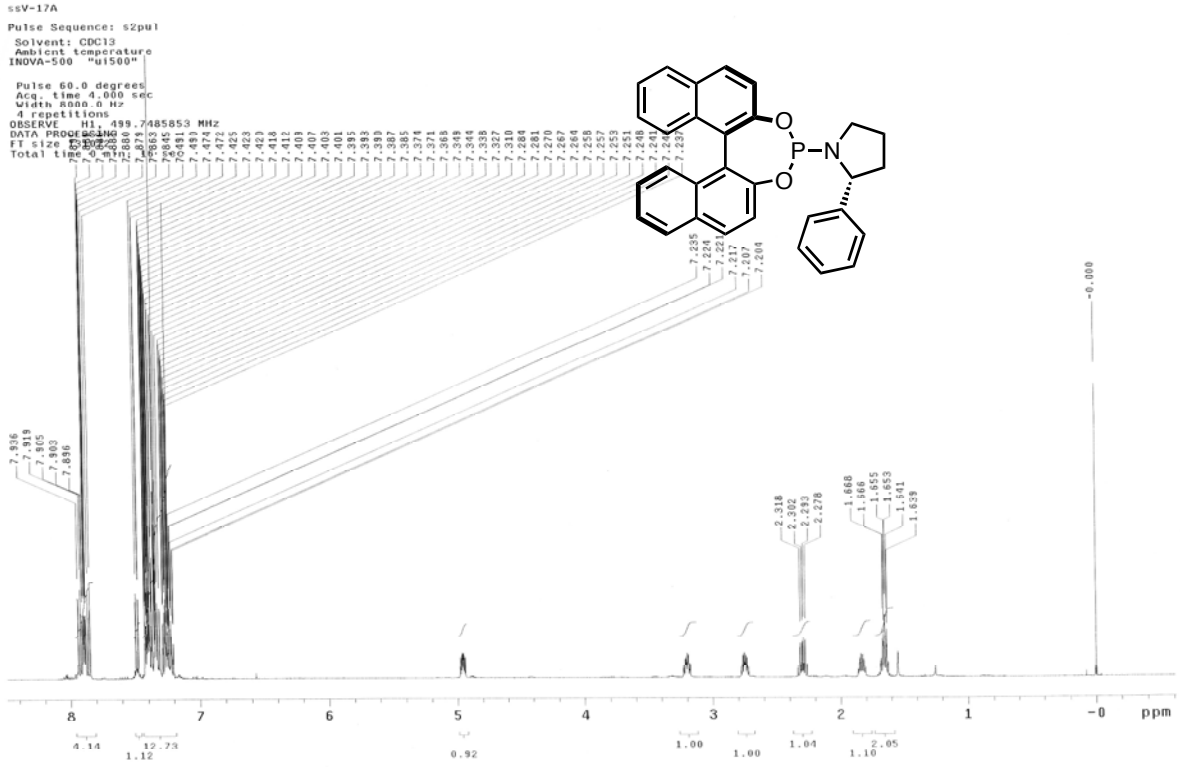

ssV-43A-13C
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB
Relax. delay 0.400 sec
Pulse 35.2 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
560 repetitions
OBSERVE C13, 100.6081295 MHZ
DECOUPLE H1, 400.1135562 MHZ
Power 35 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Resol. enhancement -0.0 Hz
FT size 65536
Total time 33 min, 33 sec
150.446
150.370
121.652
121.629
124.063
124.010
123.387
122.565
122.205
125.329
125.785
124.655
124.276
127.089
127.021
126.998
126.604
125.967
77.319
77.000
76.681
53.120
52.922
46.545
46.507
24.765
24.575
23.869
23.771
23.119
23.074
160
140
120
100
80
60
40
20
ppm

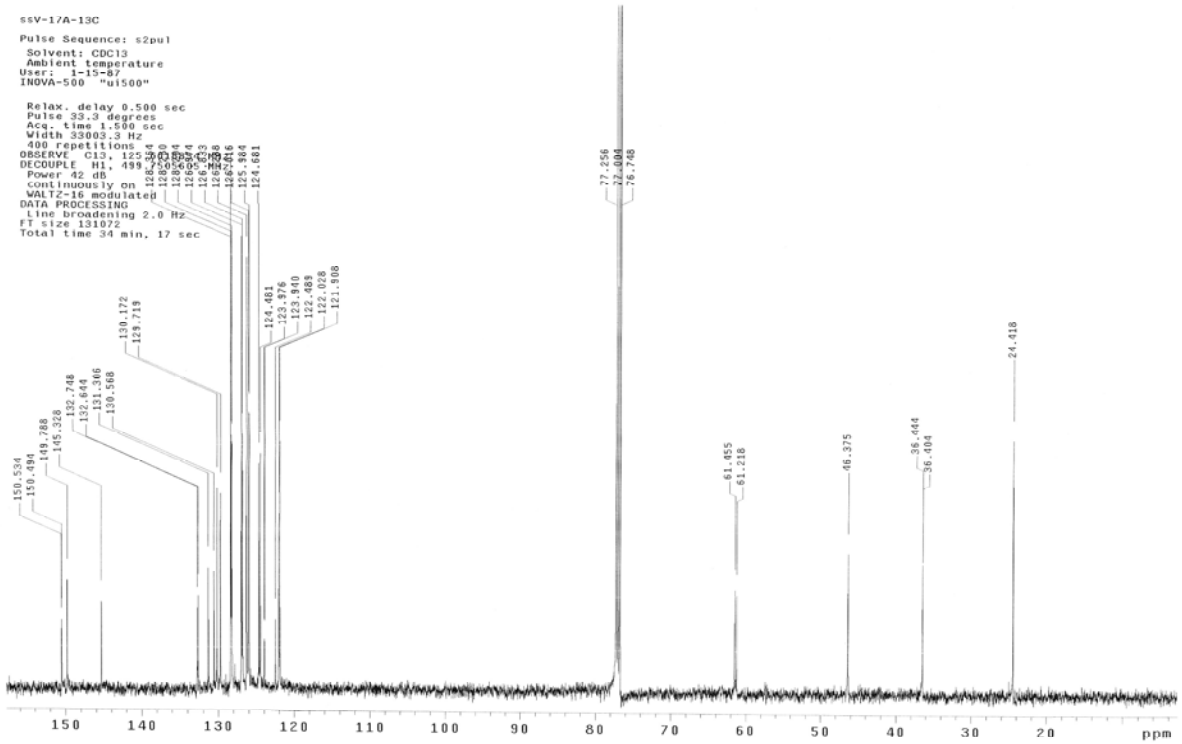

ssxii-58a
File: Proton
Pulse Sequence: s2pul
Solvent: cdcl3
Temp. 28.0 C / 293.1 K
Operator: stevesl
VNMRS-400 "nmr400"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 4.000 sec
Width 5605.4 Hz
32 repetitions
OBSERVE H1, 399.7291498 MHz
DATA PROCESSING
FT size 655360
Total time 2 min, 24 sec
H3C
CH3
CH3
H3C
O
P
N
O
ppm

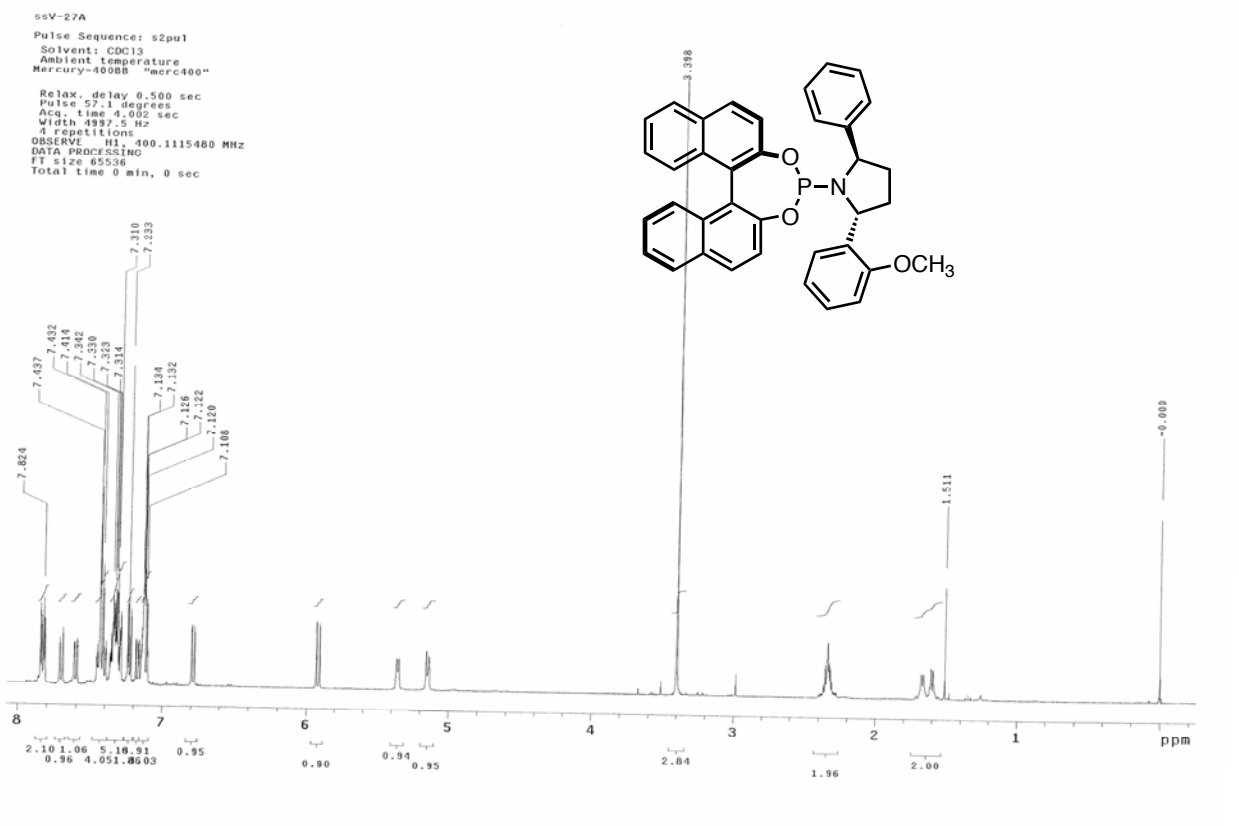

ssxii-58a-31p
File: Phosphorus
Pulse Sequence: s2pul
Solvent: CDCl3
Temp. 28.0 C / 293.1 K
Operator: stevesl
VNMRS-400 "nmr400"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.600 sec
Width 50000.0 Hz
16 repetitions
OBSERVE P31, 161.8132235 MHz
DECOUPLE H1, 399.7311439 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 262144
Total time 2 min, 46 sec
142.542
ppm

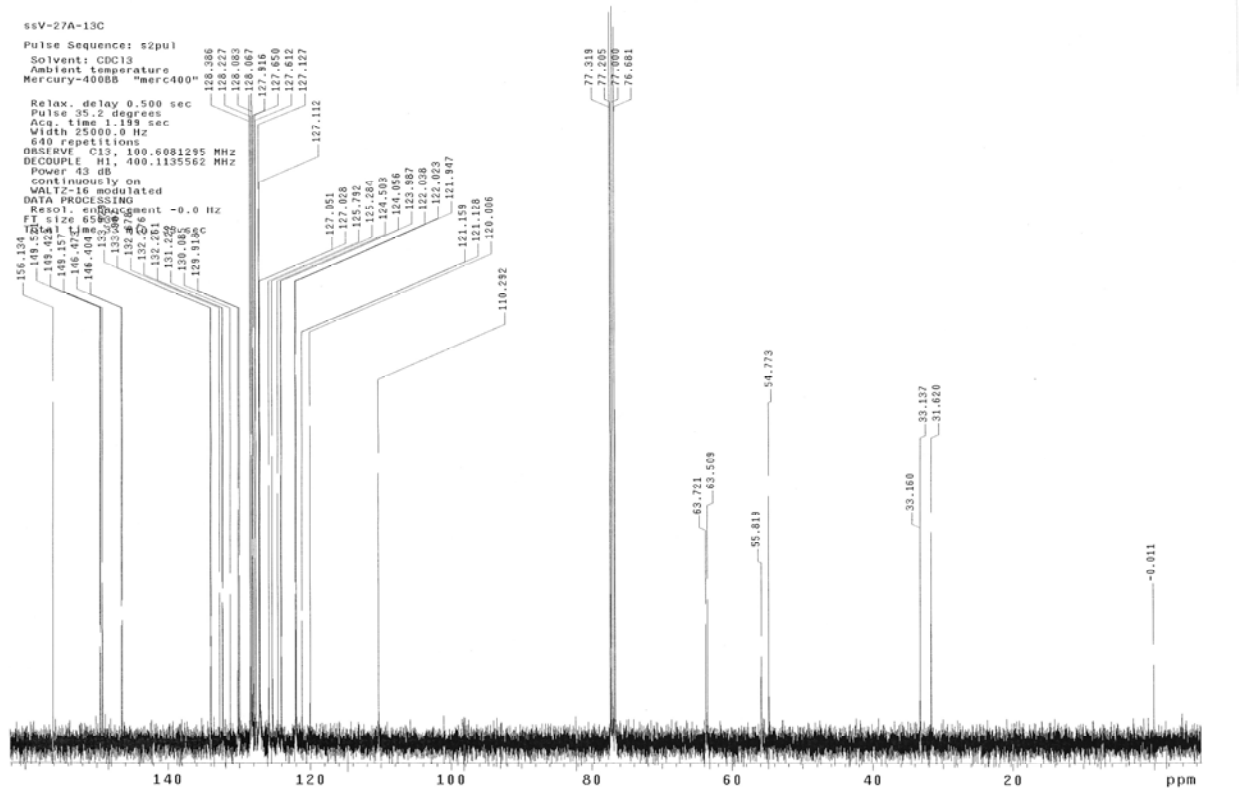

ssVI-78A
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "merc400"
Relax. delay 0.500 sec
Pulse 57.1 degrees
Acq. time 4.002 sec
Width 4997.5 Hz
60 repetitions
OBSERVE H1, 400.1115367 MHz
DATA PROCESSING
FT size 65536
Total time 11 min, 3 sec
Ph
H
O
P–N
CH3
H3C
ppm
1.71
4.52
3.55
25.74
0.99
0.99
4.84
2.93
2.15

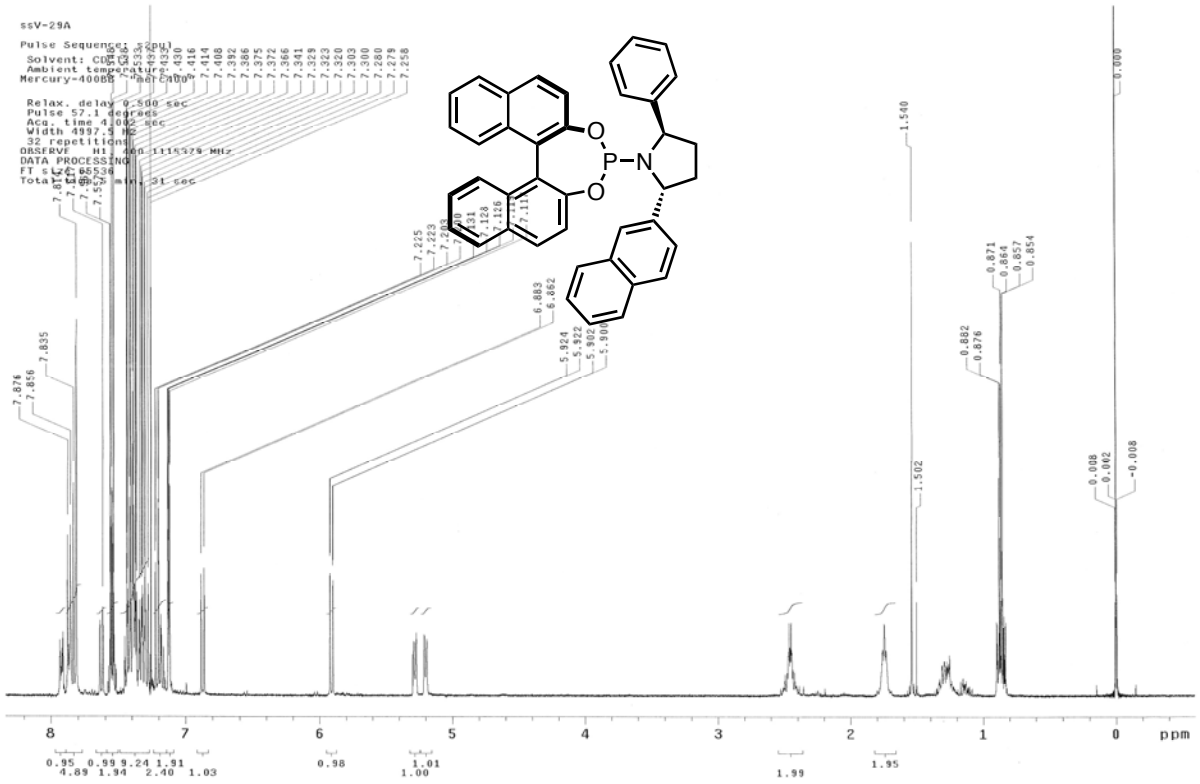

ssVI-78A-31P
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "merc400"
Relax. delay 2.000 sec
Pulse 47.4 degrees
Acq. time 0.800 sec
Width 59880.2 Hz
64 repetitions
OBSERVE P31, 161.9680175 MHz
DECOUPLE H1, 400.1135562 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 4 min, 35 sec
139.961
141.0
140.5
140.0
139.5
139.0
138.5
138.0
ppm

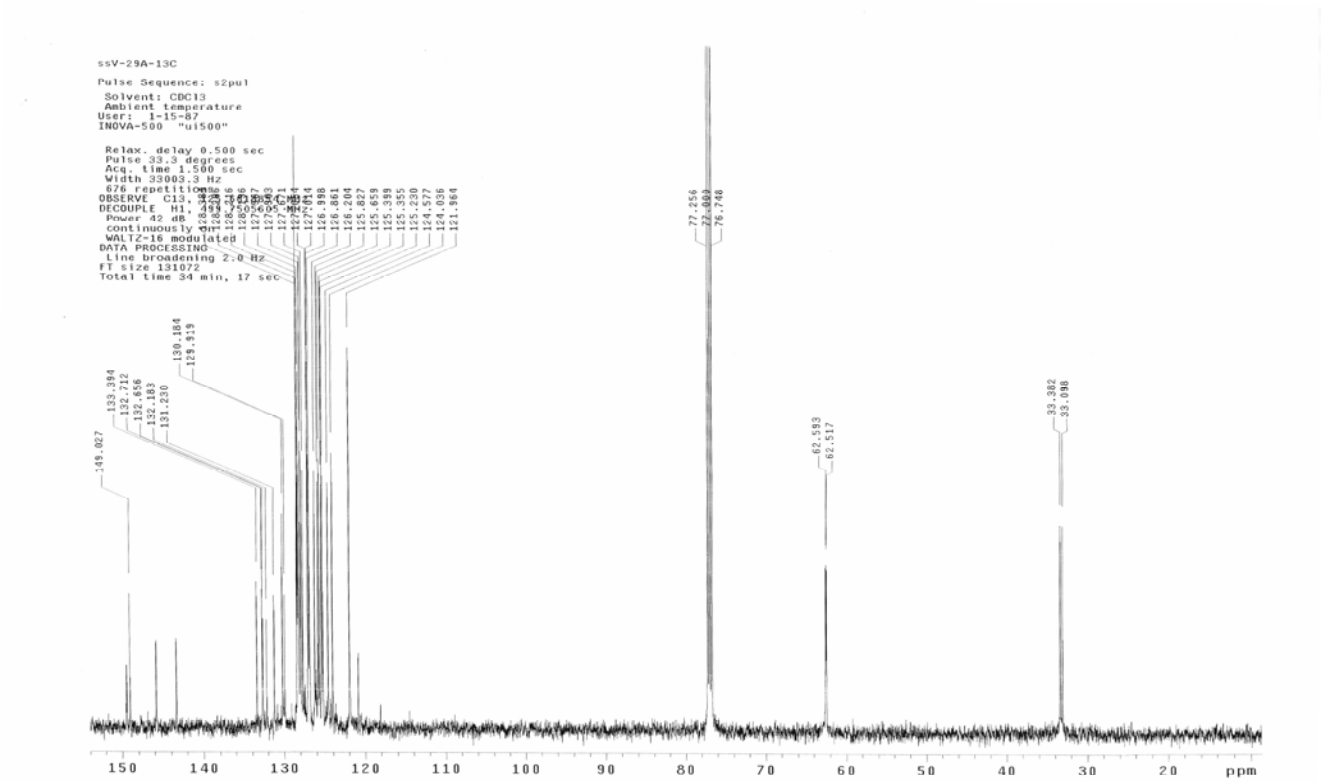

ssV-17A
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
INOVA-500 "ui500"
Pulse 60.0 degrees
Acq. time 4.000 sec
Width 8000.0 Hz
4 repetitions
OBSERVE H1, 499.7485853 MHz
DATA PROCESSING
FT size 131072
Total time 9 min, 16 sec
O
P
N
O
ppm

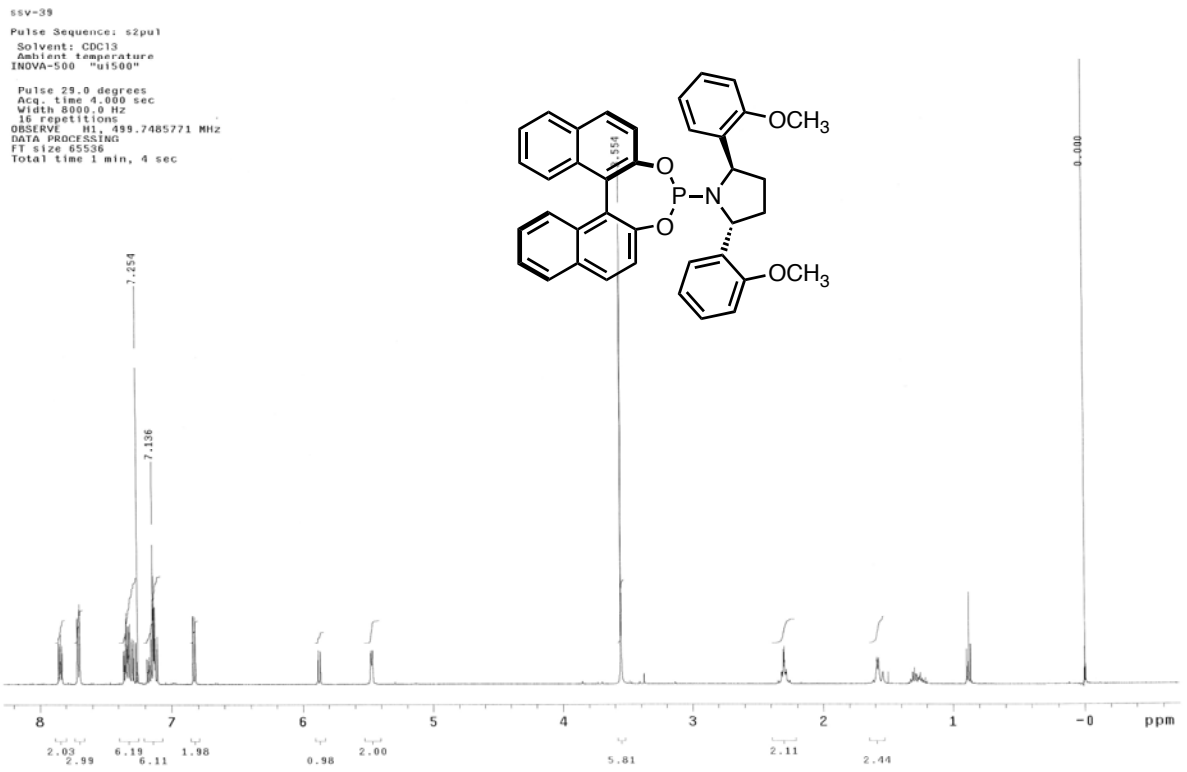

ssV-17A-13C
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-15-87
INOVA-500 "ui500"
Relax. delay 0.500 sec
Pulse 33.3 degrees
Acq. time 1.500 sec
Width 33003.3 Hz
400 repetitions
OBSERVE C13, 125
DECOUPLE H1, 499
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 131072
Total time 34 min, 17 sec
ppm

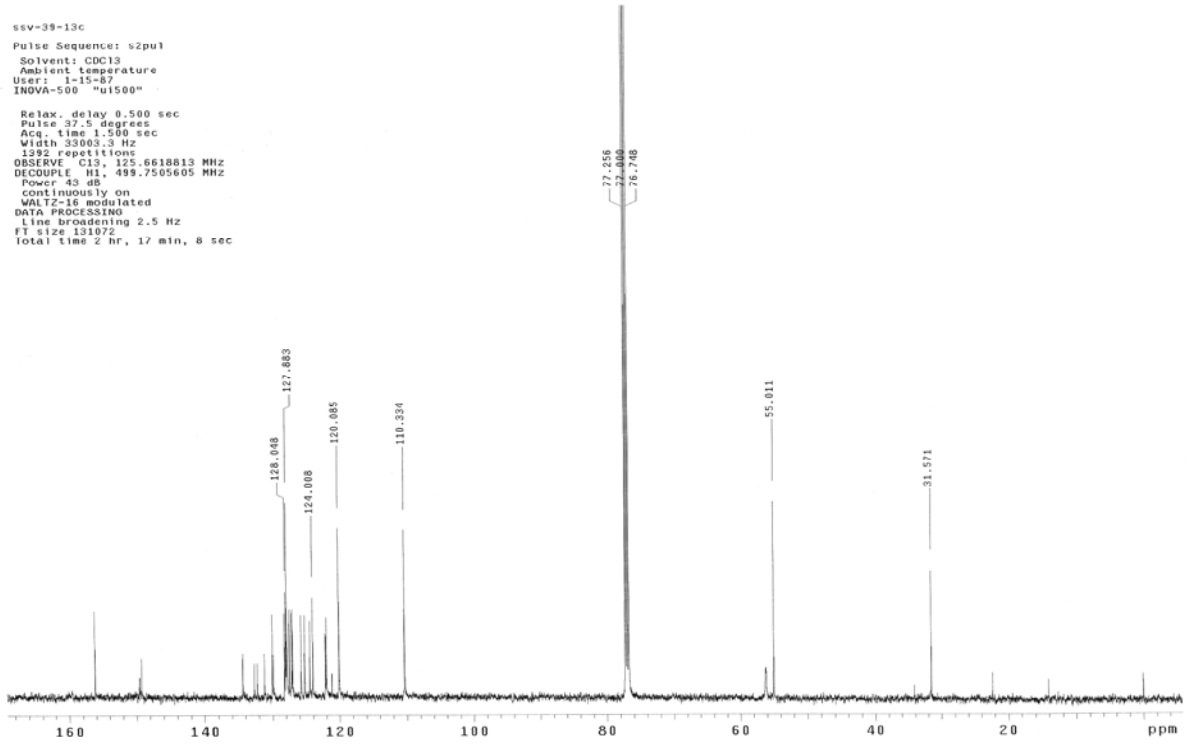

ssV-27A
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "merc400"
Relax. delay 0.500 sec
Pulse 57.1 degrees
Acq. time 4.002 sec
Width 4997.5 Hz
4 repetitions
OBSERVE H1, 400.1115480 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 0 sec
OCH3
ppm

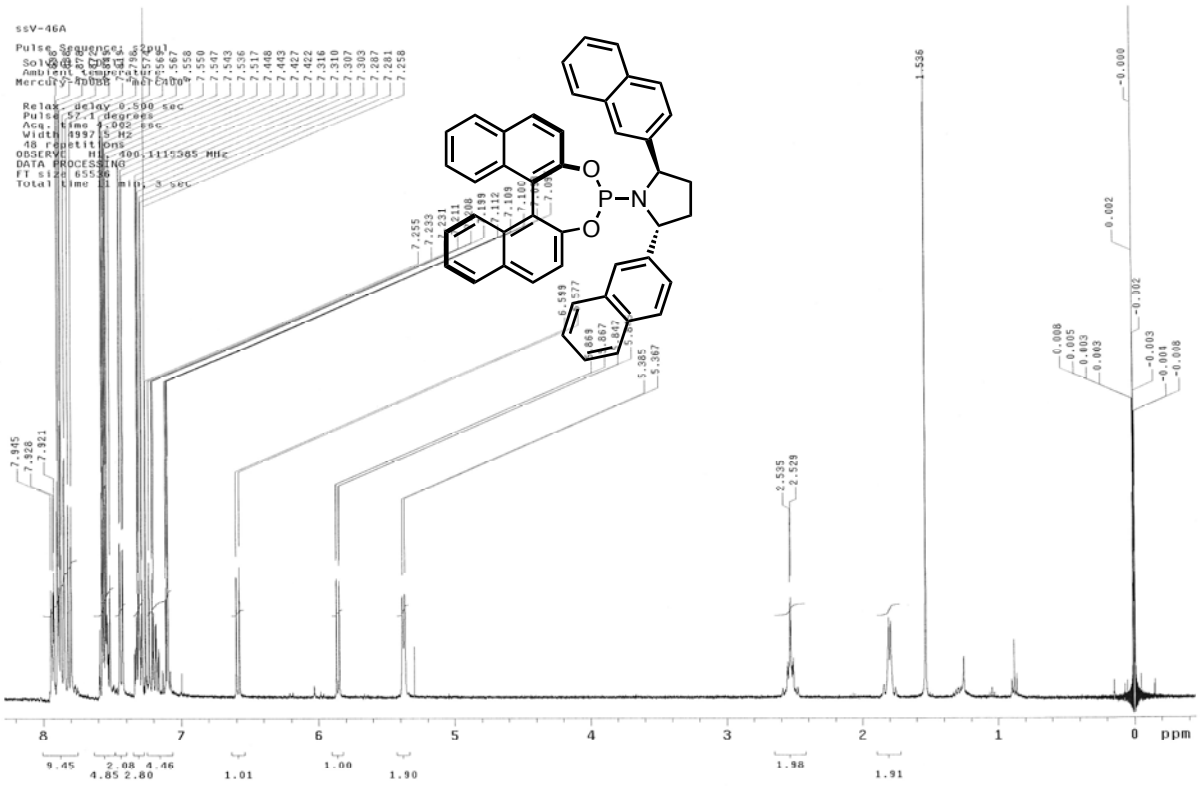

ssV-27A-13C
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "merc400"
Relax. delay 0.500 sec
Pulse 35.2 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
640 repetitions
OBSERVE C13, 100.6081295 MHz
DECOUPLE H1, 400.1135562 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
ppm

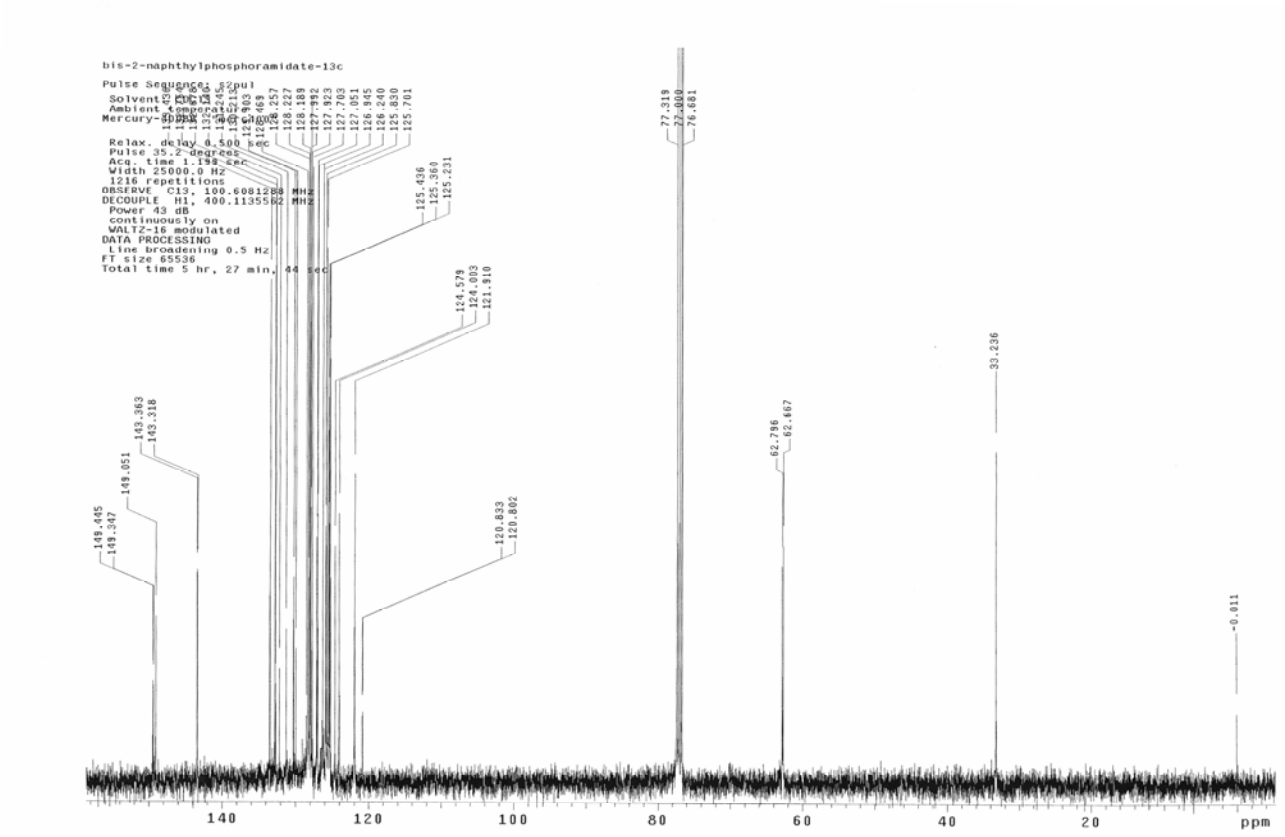

ssV-29A
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "hercl400"
Relax. delay 0.500 sec
Pulse 57.1 degrees
Acq. time 4.002 sec
Width 4997.5 Hz
32 repetitions
OBSERVE H1, 399.8116579 MHz
DATA PROCESSING
FT size 65536
Total time 3 min, 31 sec
ppm

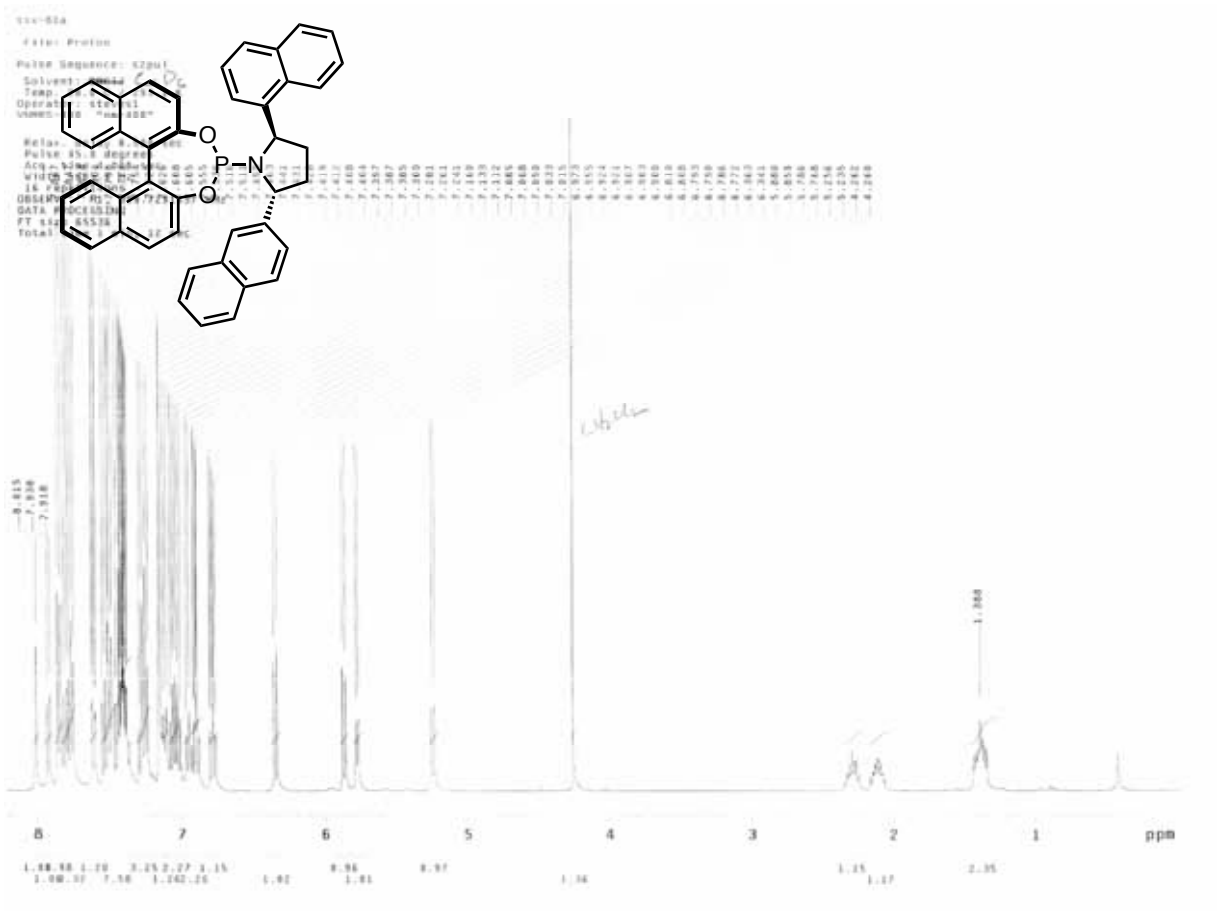

ssV-29A-13C
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-15-87
INOVA-500 "ui500"
Relax. delay 0.500 sec
Pulse 33.3 degrees
Acq. time 1.500 sec
Width 33003.3 Hz
876 repetitions
DECOUPLE H1,
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 131072
Total time 34 min, 17 sec
ppm

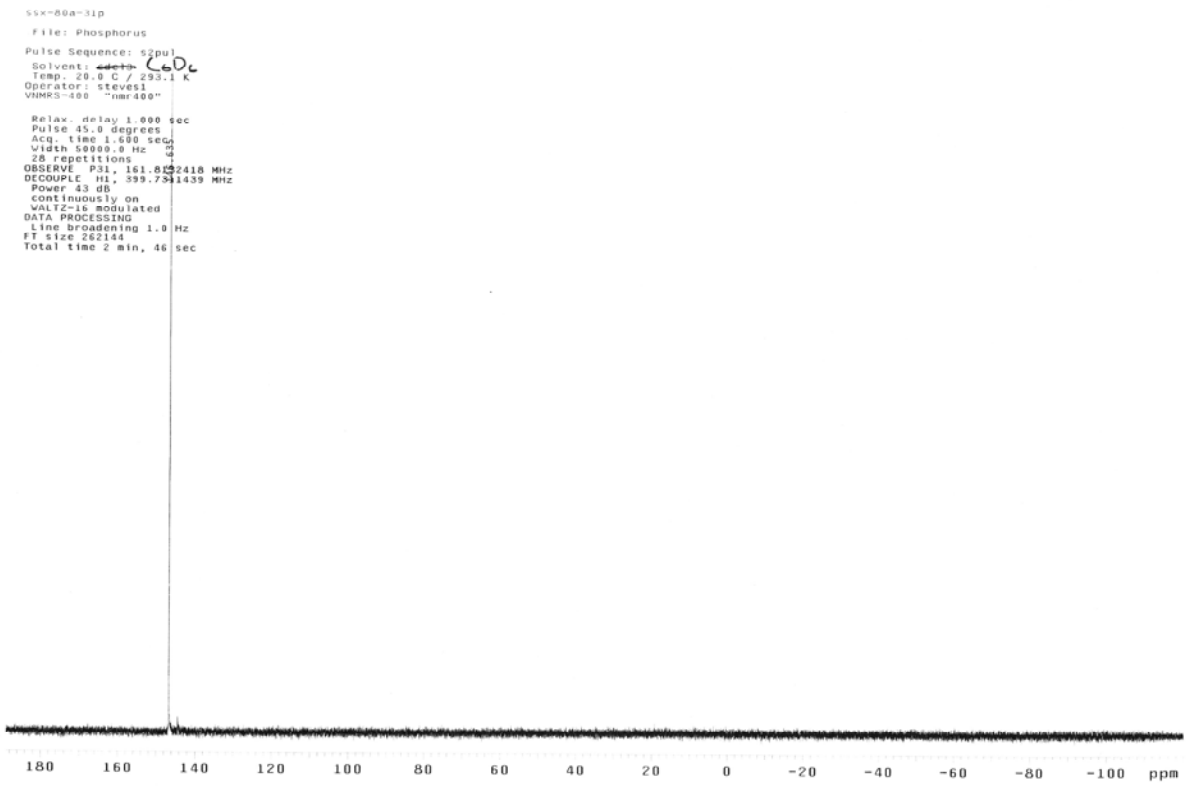

ssv-39
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
INOVA-500 "ui500"
Pulse 29.0 degrees
Acq. time 4.000 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.7485771 MHz
DATA PROCESSING
FT size 65536
Total time 1 min, 4 sec
OCH3
OCH3
P
N
O
O
7.254
7.136
5.554
0.000
ppm
2.03
2.99
6.19
6.11
1.98
0.98
2.00
5.81
2.11
2.44

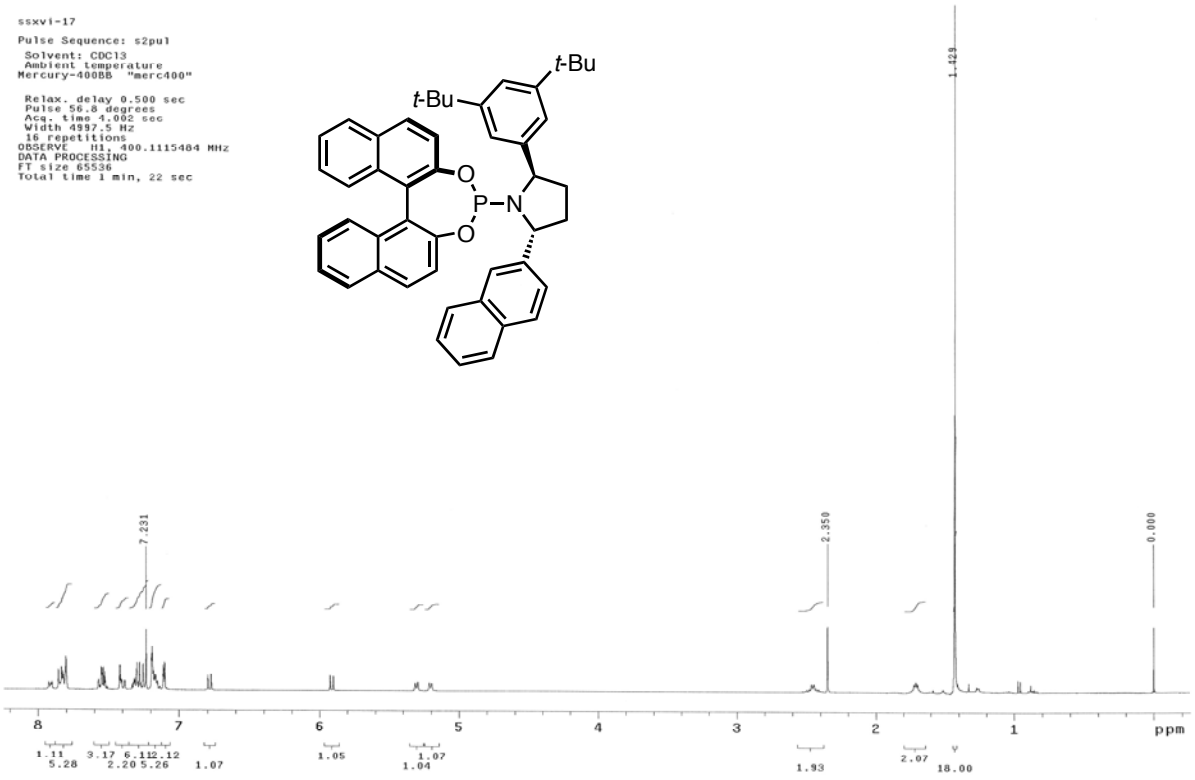

ssv-39-13c
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-15-87
INOVA-500 "ui500"
Relax. delay 0.500 sec
Pulse 37.5 degrees
Acq. time 1.500 sec
Width 33003.3 Hz
1392 repetitions
OBSERVE C13, 125.6618813 MHz
DECOUPLE H1, 499.7505605 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.5 Hz
FT size 131072
Total time 2 hr, 17 min, 8 sec
77.256
77.000
76.748
127.883
128.048
124.008
120.085
110.334
55.011
31.571
ppm

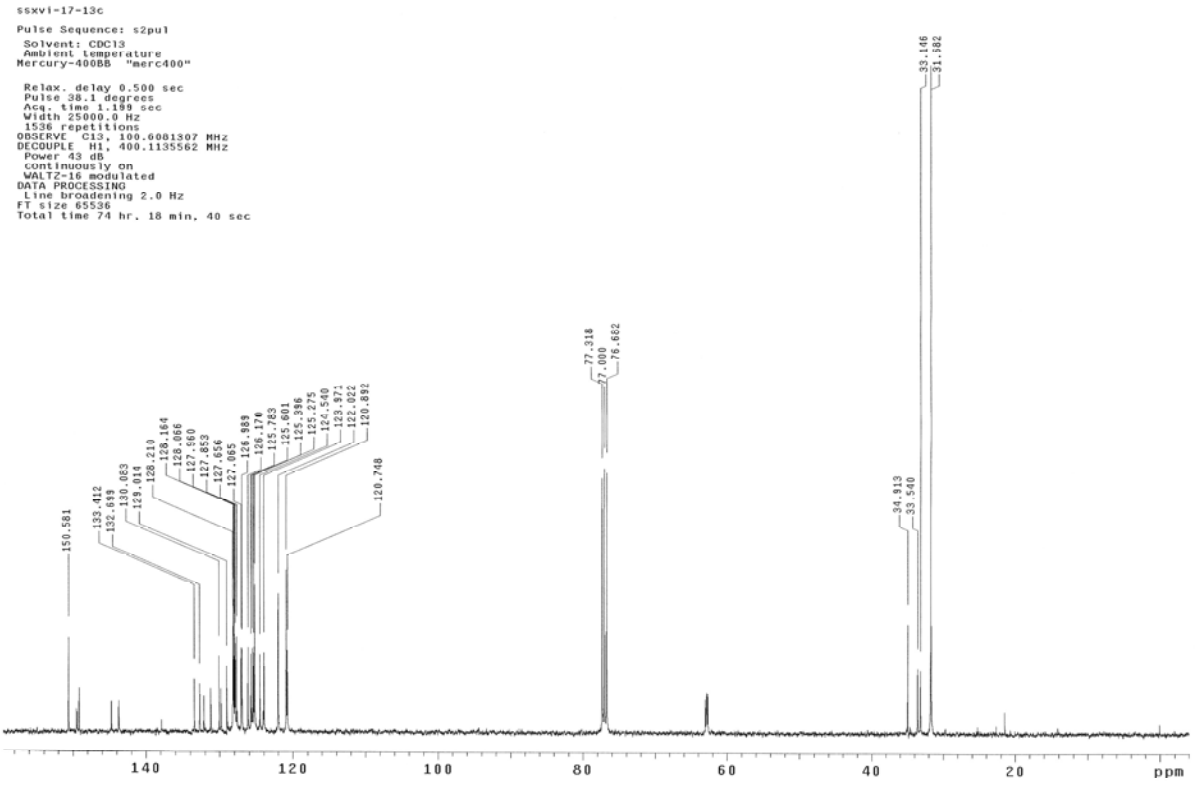

ssV-46A
Relax. delay 0.500 sec
Pulse 57.1 degrees
Acq. time 4.002 sec
Width 4997.5 Hz
48 repetitions
OBSERVE H1, 400.1115585 MHz
DATA PROCESSING
FT size 65536
Total time 11 min, 3 sec
7.945
7.928
7.921
7.255
7.233
7.211
7.199
7.112
7.109
7.106
7.008
6.559
6.577
6.869
6.867
6.842
5.385
5.367
2.535
2.529
1.536
0.000
0.002
-0.302
0.008
0.005
0.003
0.003
-0.003
-0.004
-0.008
8
7
6
5
4
3
2
1
0
ppm
9.45
2.08
4.46
4.85
2.80
1.01
1.00
1.90
1.98
1.91

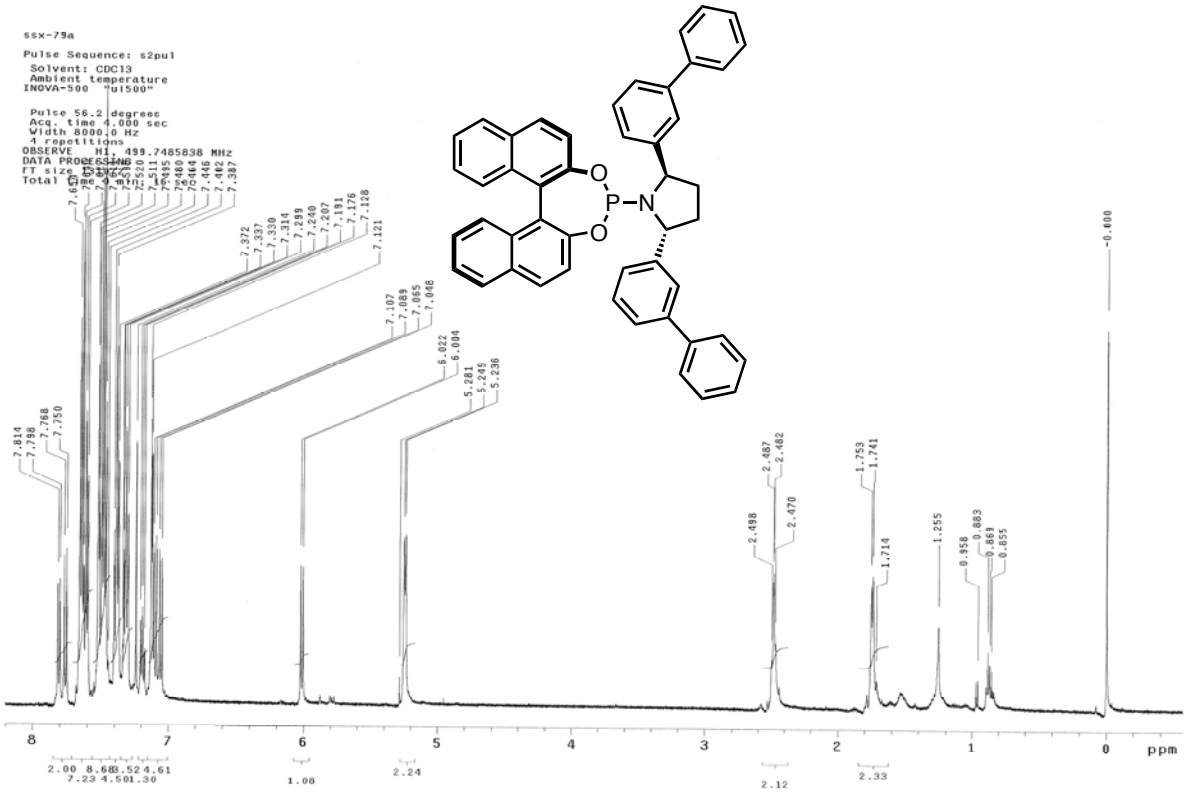

bis-2-naphthylphosphoramidate-13c
Relax. delay 0.500 sec
Pulse 35.2 degrees
Acq. time 1.198 sec
Width 25000.0 Hz
1216 repetitions
OBSERVE C13, 100.6081288 MHz
DECOUPLE H1, 400.1135562 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 5 hr, 27 min, 44 sec
149.445
149.347
149.051
143.363
143.318
128.468
128.257
128.227
128.189
127.492
127.423
127.703
127.051
126.945
126.240
125.830
125.701
125.436
125.360
125.231
124.579
124.003
121.910
120.833
120.802
77.319
77.000
76.681
62.796
62.667
33.236
-0.011
140
120
100
80
60
40
20
ppm

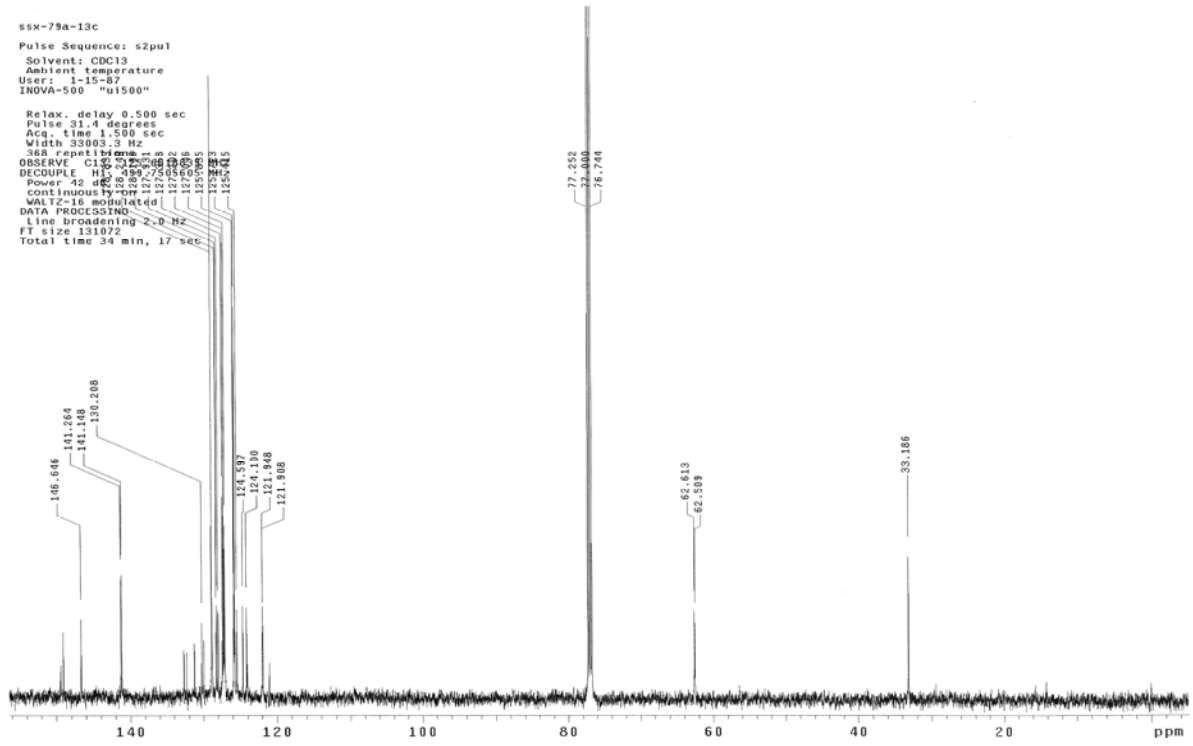

8
7
6
5
4
3
2
1
ppm

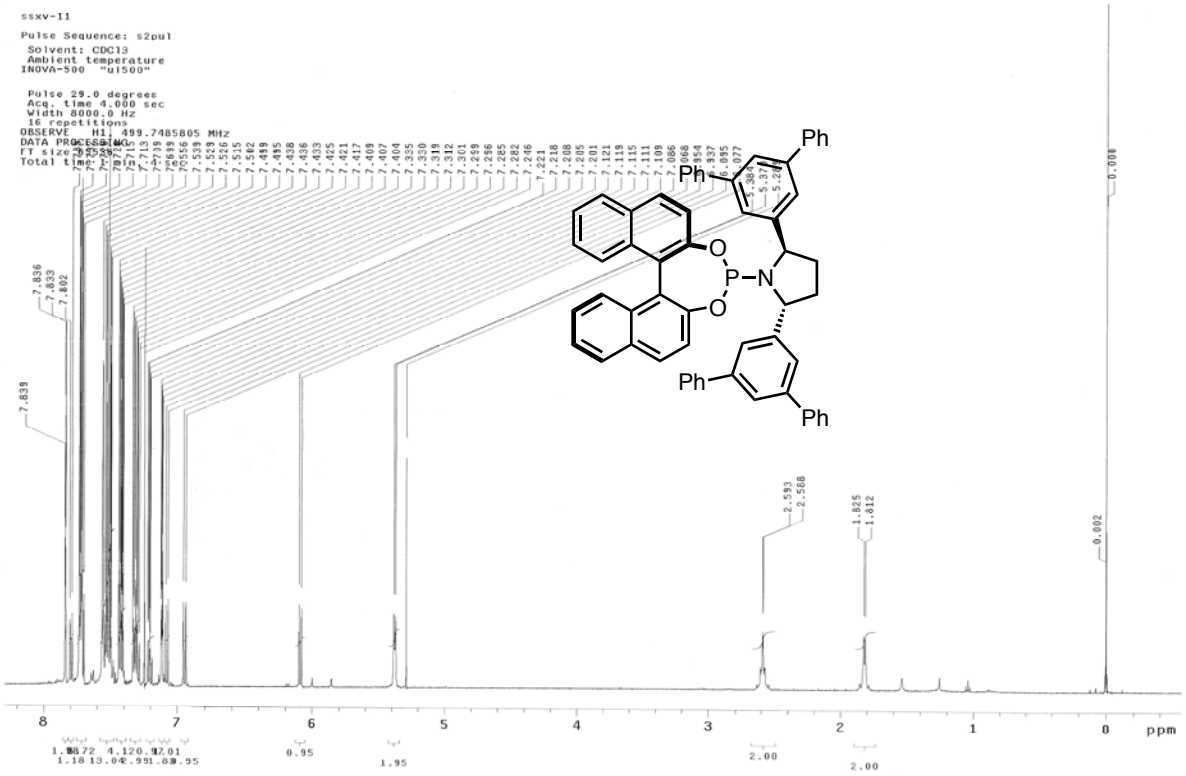

ssx-80a-31p
File: Phosphorus
Pulse Sequence: s2pul
Solvent: C6D6
Temp. 20.0 C / 293.1 K
Operator: steves1
VNMRS-400 "nmr400"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.600 sec
Width 50000.0 Hz
28 repetitions
DECOUPLE H1, 399.7
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 262144
Total time 2 min, 46 sec
180
160
140
120
100
80
60
40
20
0
-20
-40
-60
-80
-100
ppm

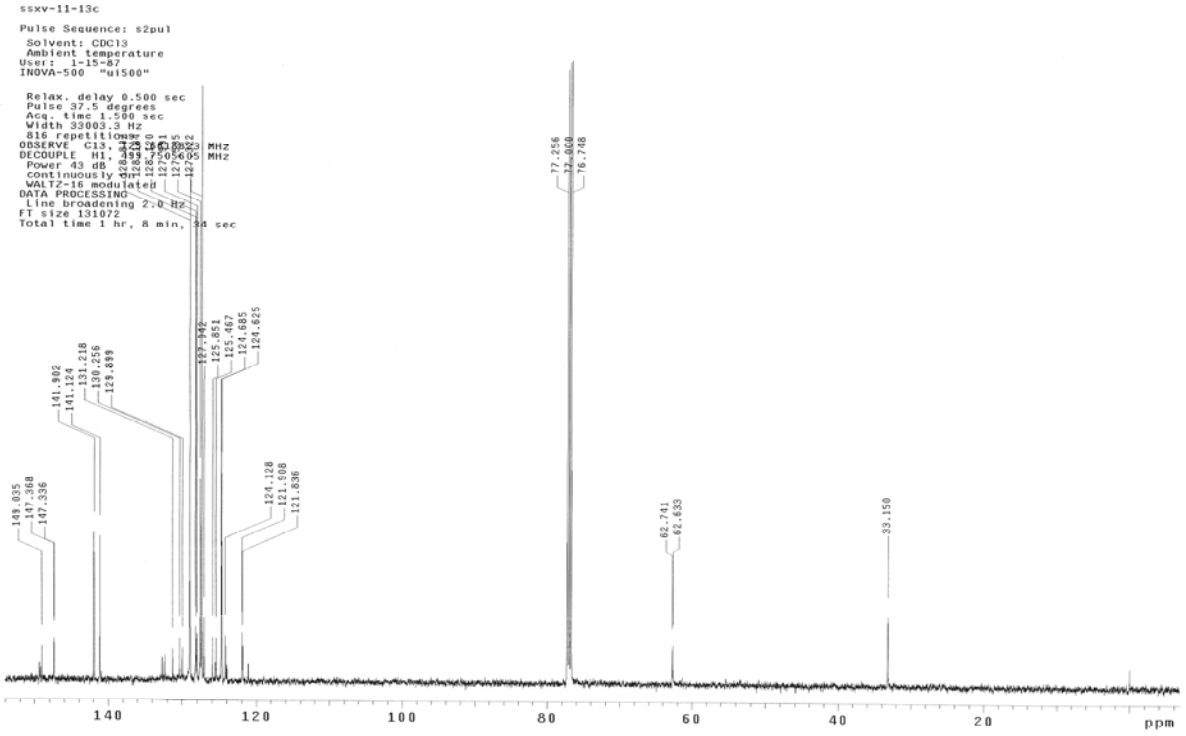

ssxvi-17
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "merc400"
Relax. delay 0.500 sec
Pulse 56.8 degrees
Acq. time 4.002 sec
Width 4997.5 Hz
16 repetitions
OBSERVE H1, 400.1115484 MHz
DATA PROCESSING
FT size 65536
Total time 1 min, 22 sec
t-Bu
t-Bu
O
P
N
O
7.231
2.350
1.428
0.000
8
7
6
5
4
3
2
1
ppm
1.11
5.28
3.17
2.20
6.11
5.26
2.12
1.07
1.05
1.07
1.04
1.93
2.07
18.00

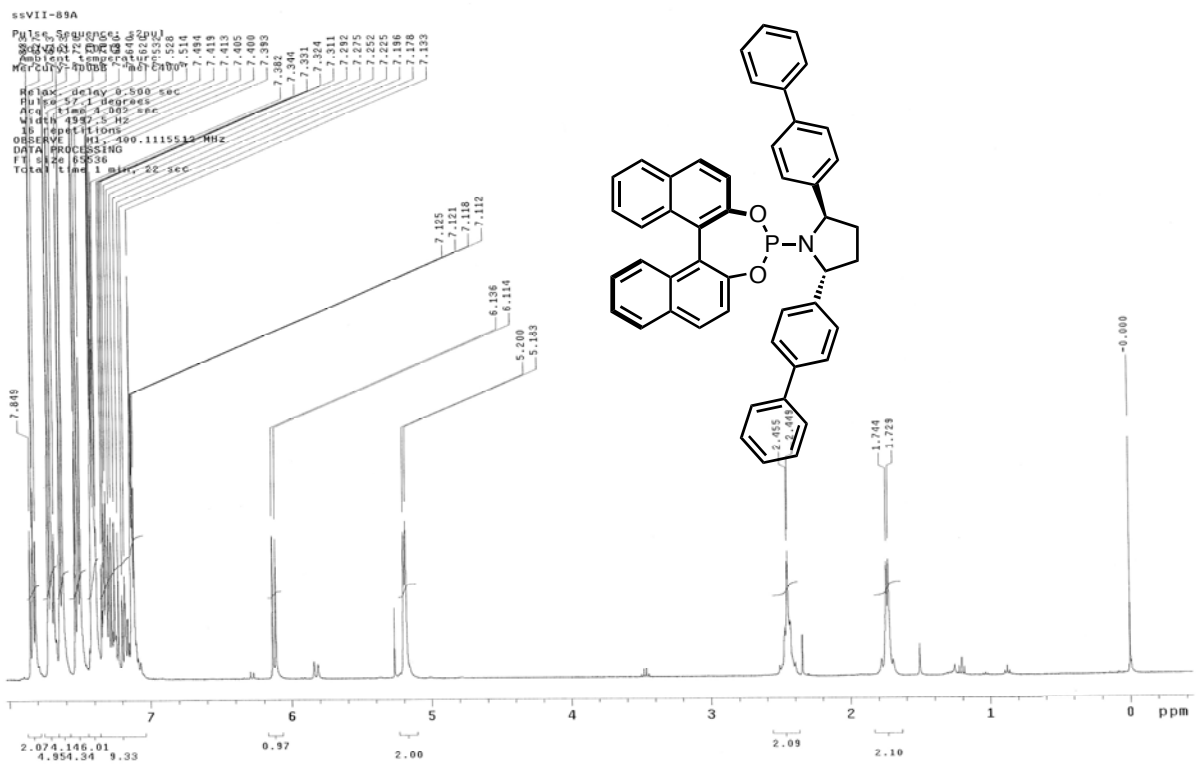

ssxvi-17-13c
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "merc400"
Relax. delay 0.500 sec
Pulse 38.1 degrees
Acq. time 1.189 sec
Width 25000.0 Hz
1536 repetitions
OBSERVE C13, 100.6081307 MHz
DECOUPLE H1, 400.1135562 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 65536
Total time 74 hr, 18 min, 40 sec
33.146
31.182
77.318
77.000
76.662
34.913
33.540
150.581
133.412
132.699
130.083
129.014
128.210
128.164
128.066
127.860
127.853
127.656
127.065
126.989
126.170
125.763
125.601
125.396
125.276
125.060
123.871
122.022
120.892
120.748
140
120
100
80
60
40
20
ppm

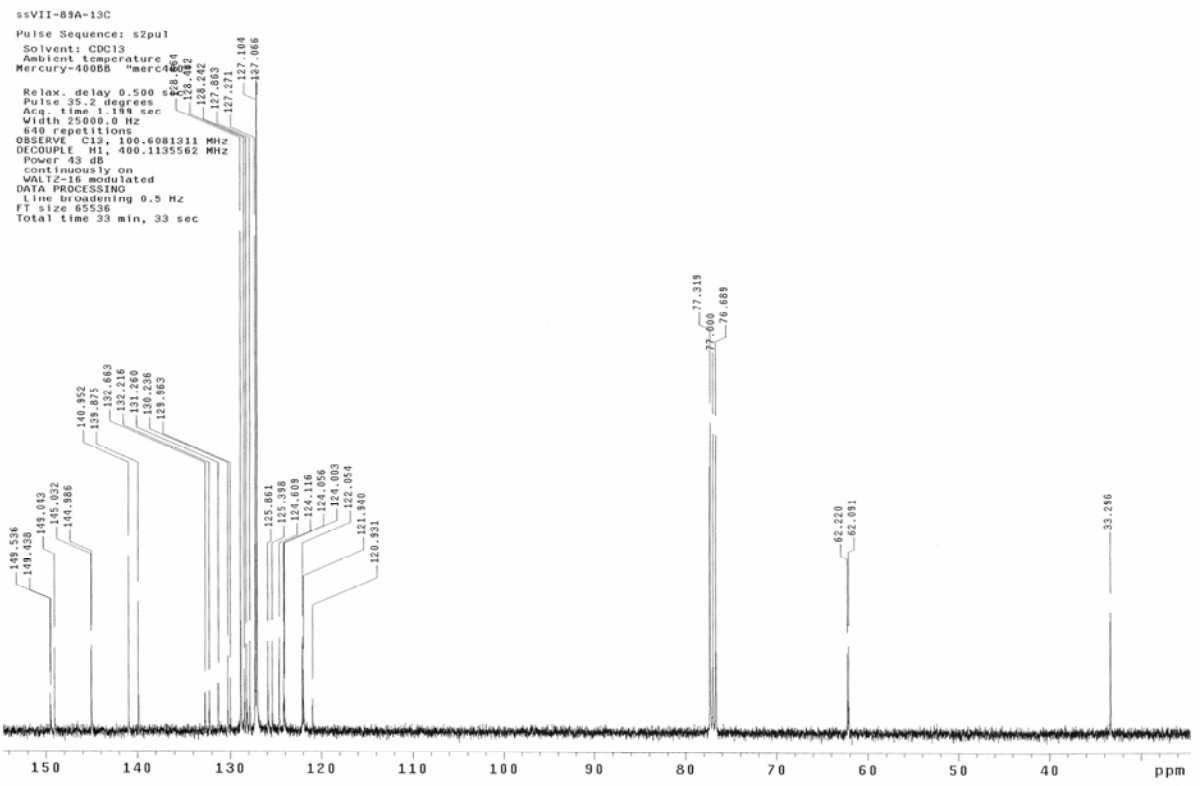

ssx-79a
Pulse Sequence: s2pul
Solvent: CDC13
Ambient temperature
INOVA-500 "ui500"
Pulse 56.2 degrees
Acq. time 4.000 sec
Width 8000.0 Hz
4 repetitions
OBSERVE H1, 499.7485838 MHz
DATA PROCESSING
FT size 65536
Total time 3 min, 16 sec
7.814
7.798
7.768
7.750
7.372
7.337
7.330
7.314
7.299
7.240
7.203
7.191
7.176
7.128
7.121
7.107
7.089
7.065
7.048
6.022
6.004
5.281
5.245
5.236
2.498
2.487
2.482
2.470
1.753
1.741
1.714
1.255
0.958
0.883
0.869
0.855
0.000
8
7
6
5
4
3
2
1
0
ppm
2.00 8.68 8.52 4.61
7.23 4.50 1.30
1.08
2.24
2.12
2.33
O
P
N
O

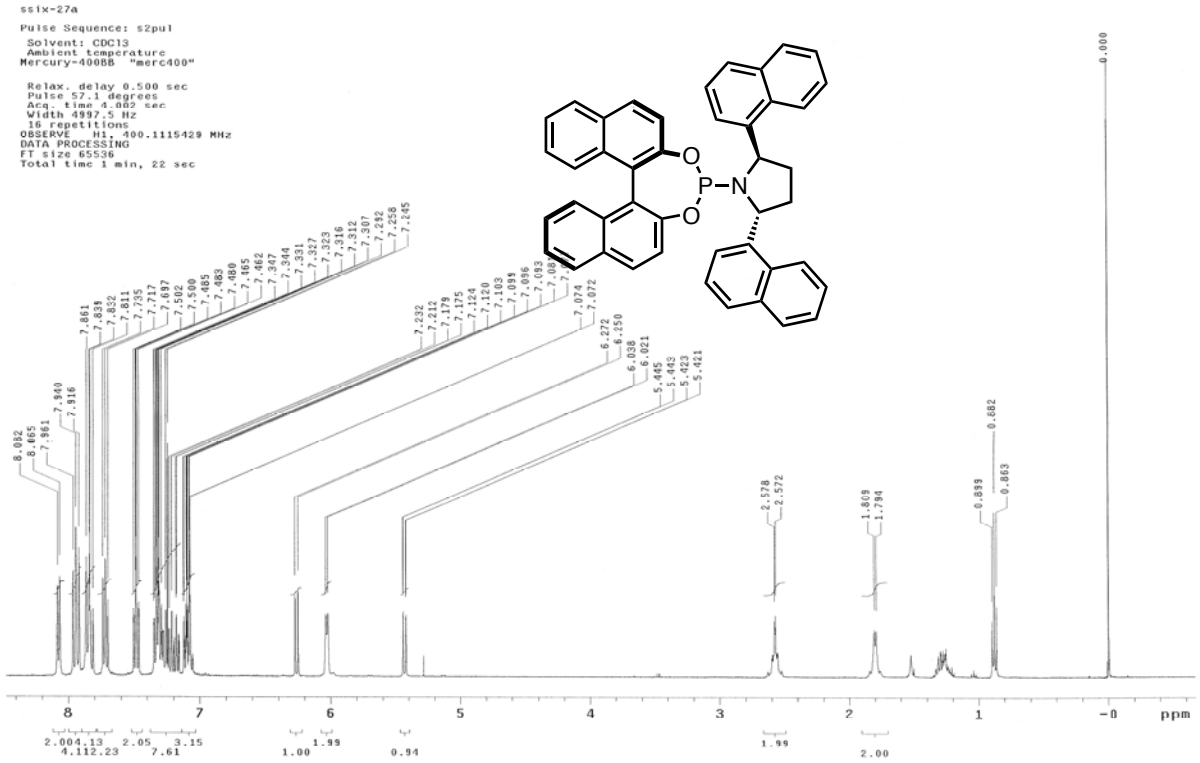

ssx-79a-13c
Pulse Sequence: s2pul
Solvent: CDC13
Ambient temperature
User: 1-15-87
INOVA-500 "ui500"
Relax. delay 0.500 sec
Pulse 31.4 degrees
Acq. time 1.500 sec
Width 33003.3 Hz
368 repetitions
OBSERVE C13
DECOUPLE H1
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 131072
Total time 34 min, 17 sec
146.646
141.264
141.148
130.208
124.597
124.130
121.948
121.908
77.252
77.000
76.744
62.613
62.509
33.186
140
120
100
80
60
40
20
ppm

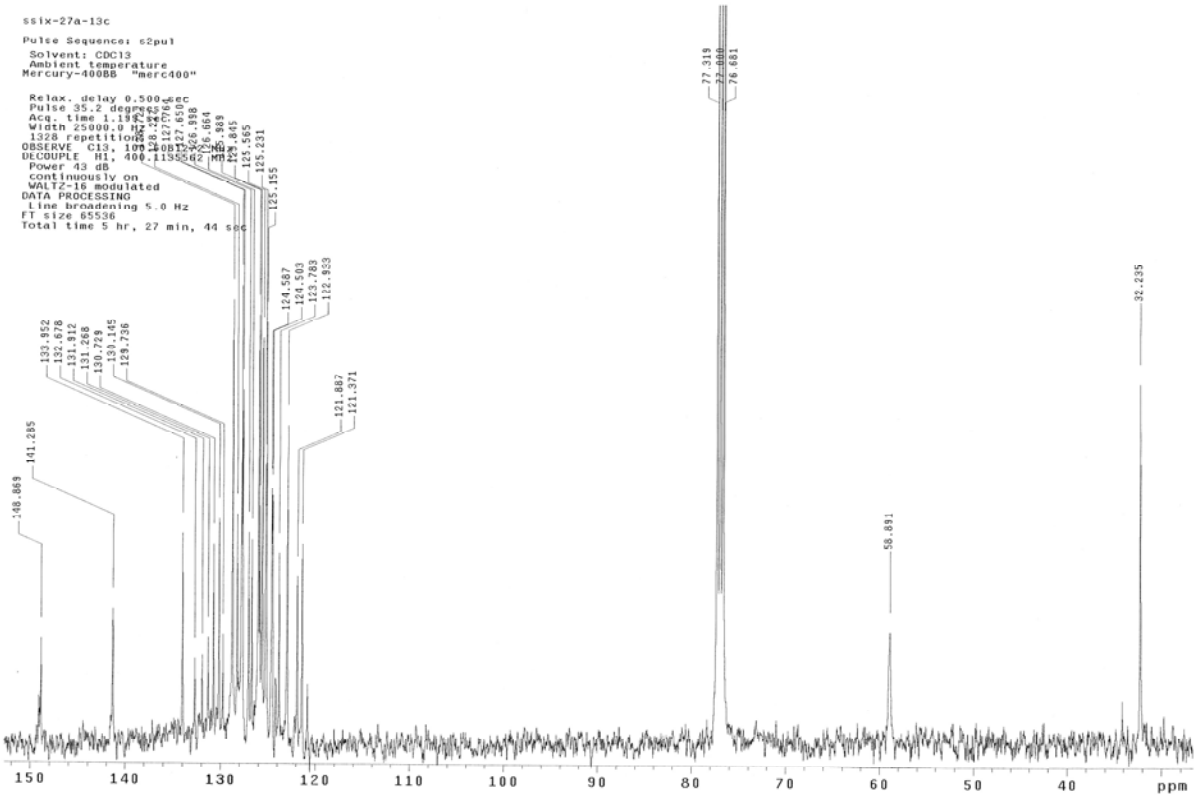

ssxv-11
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
INOVA-500 "u1500"
Pulse 29.0 degrees
Acq. time 4.000 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.7485805 MHz
DATA PROCESSING
FT size 131072
Total time
Ph
Ph
O
P
N
O
Ph
Ph
ppm

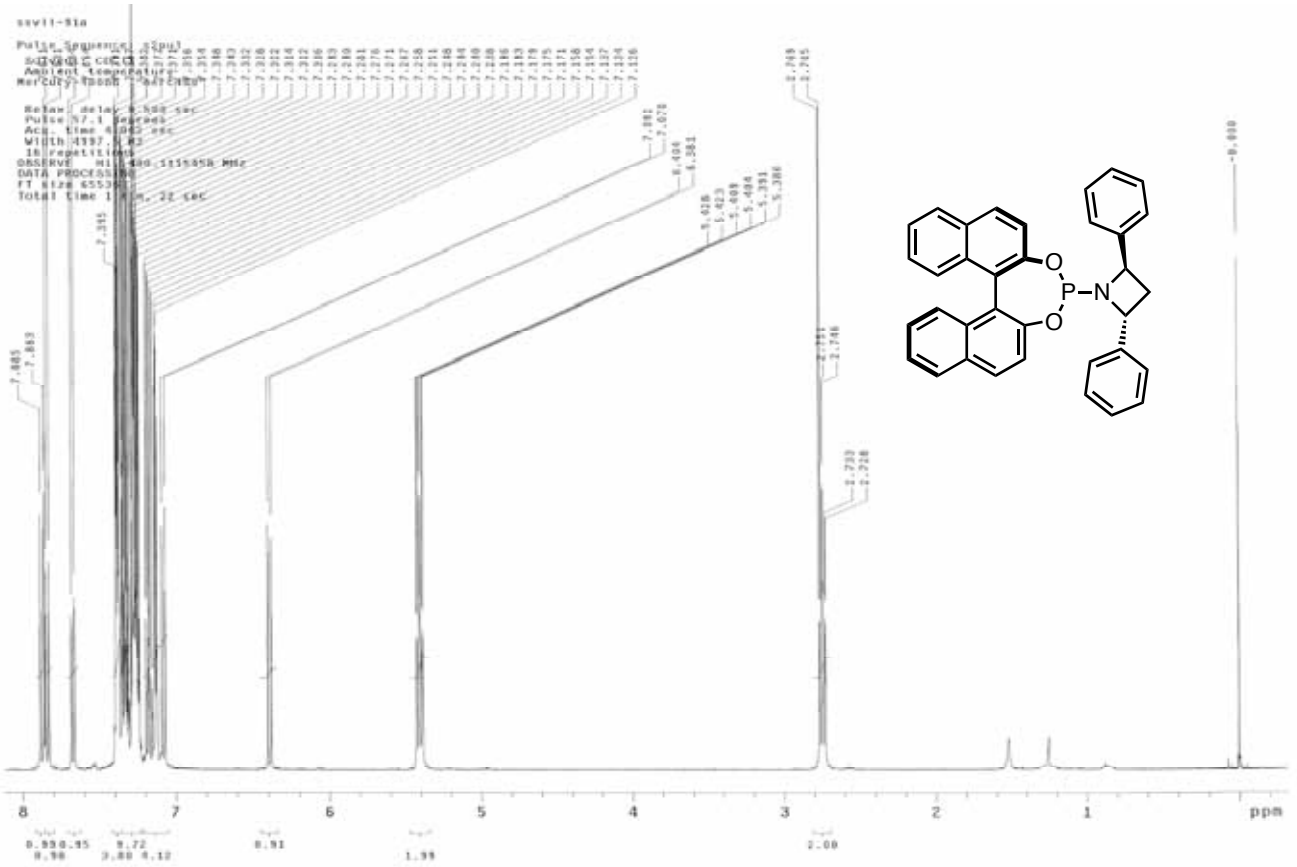

ssxv-11-13c
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-15-87
INOVA-500 "u1500"
Relax. delay 0.500 sec
Pulse 37.5 degrees
Acq. time 1.500 sec
Width 33003.3 Hz
816 repetitions
OBSERVE C13,
DECOUPLE H1,
Power 43 dB
continuously
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 131072
Total time 1 hr, 8 min,
77.256
77.060
76.748
62.741
62.633
33.150
ppm

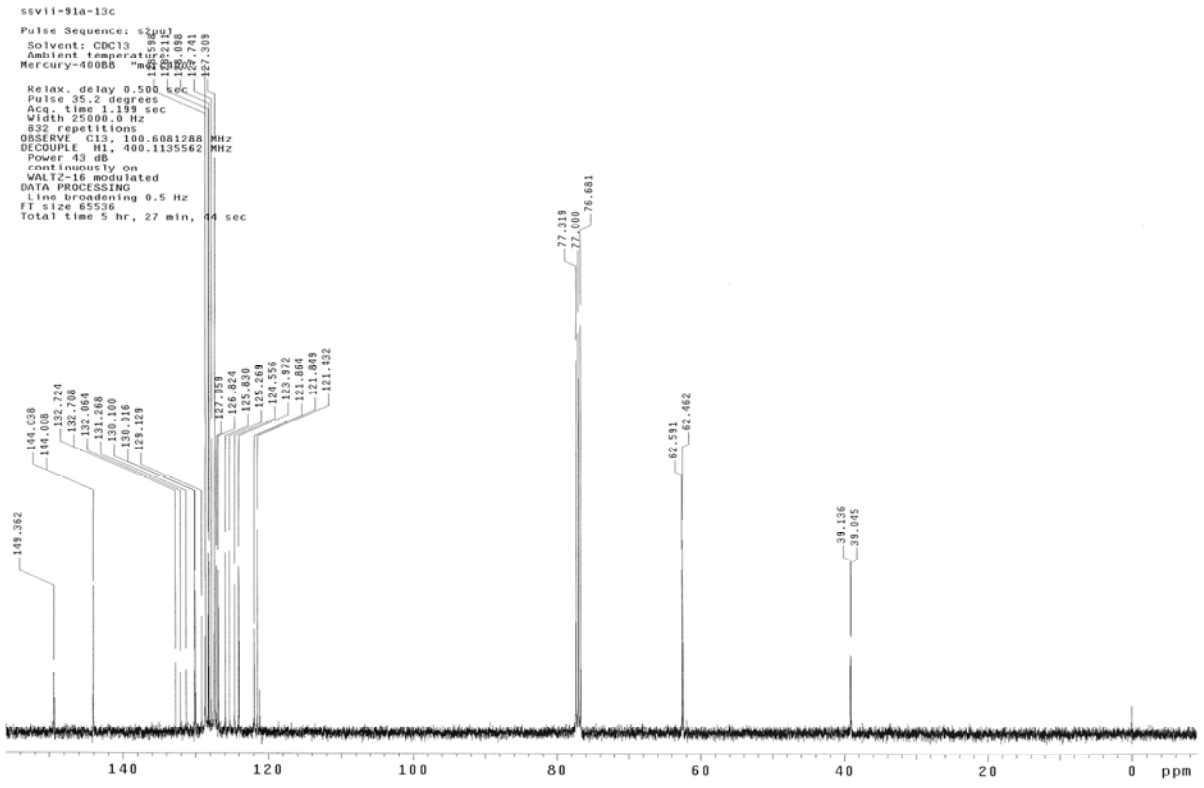

ssVII-89A
Relax. delay 0.500 sec
Pulse 57.1 degrees
Acq. time 4.005 sec
Width 4992.5 Hz
16 repetitions
OBSERVE H1, 400.1115512 MHz
DATA PROCESSING
FT size 65536
Total time 1 min, 22 sec
7.849
7.425
7.121
7.118
7.112
6.136
6.114
5.200
5.183
2.455
2.449
1.744
1.729
0.000
O
P
N
O
7
6
5
4
3
2
1
0
ppm
2.074.146.01
4.954.34
9.33
0.97
2.00
2.09
2.10

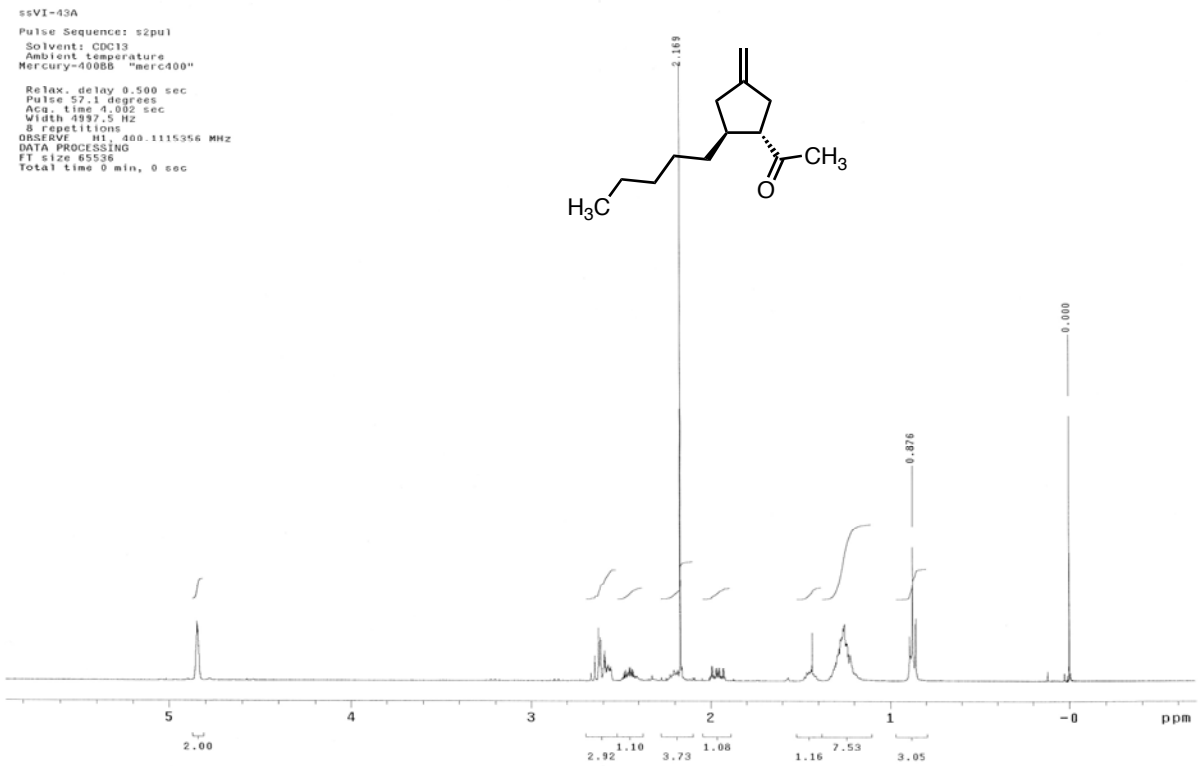

ssVII-89A-13C
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "merc400"
Relax. delay 0.500 sec
Pulse 35.2 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
640 repetitions
OBSERVE C13, 100.6081311 MHz
DECOUPLE H1, 400.1135562 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 33 min, 33 sec
149.536
149.438
149.043
145.032
144.986
140.952
139.875
132.663
132.216
131.260
131.206
129.663
128.464
128.402
128.242
127.863
127.271
127.104
127.066
125.861
125.398
124.609
124.116
124.056
124.003
122.054
121.940
120.931
77.319
77.000
76.680
62.220
62.091
33.256
150
140
130
120
110
100
90
80
70
60
50
40
ppm

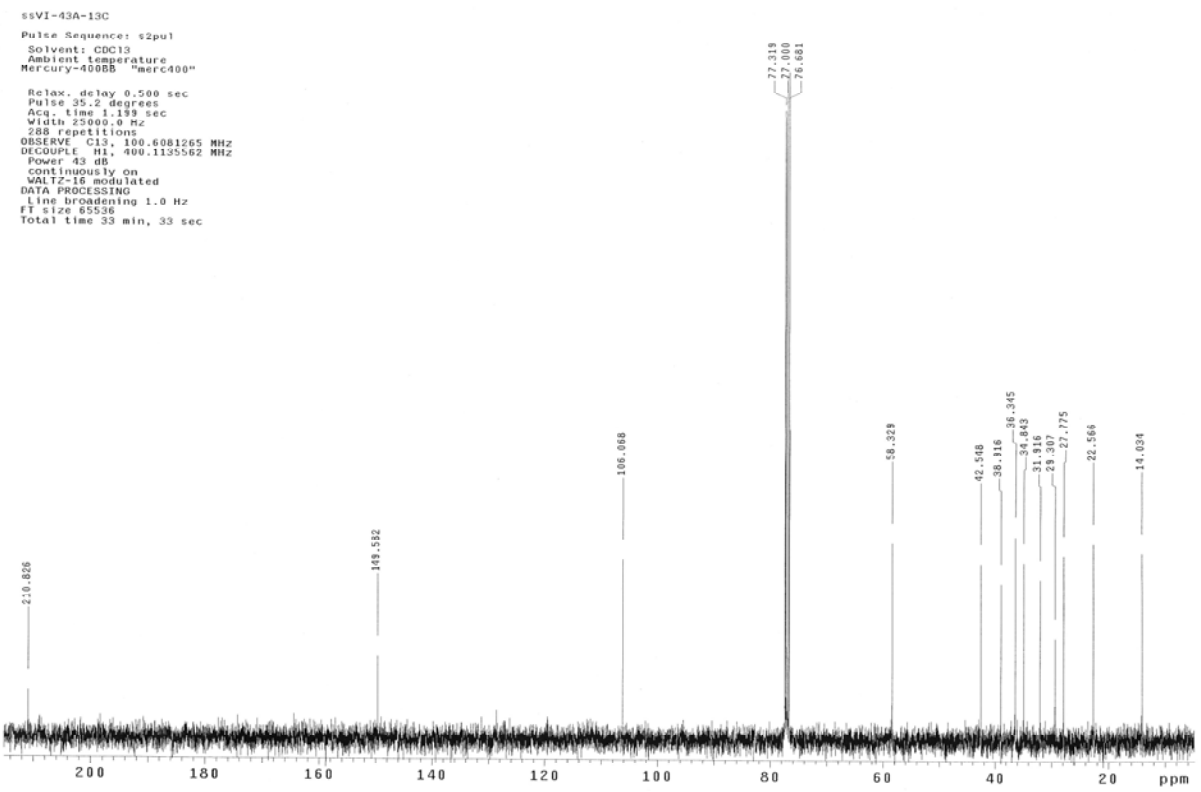

ssix-27a
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "merc400"
Relax. delay 0.500 sec
Pulse 57.1 degrees
Acq. time 4.002 sec
Width 4997.5 Hz
16 repetitions
OBSERVE H1, 400.1115429 MHz
DATA PROCESSING
FT size 65536
Total time 1 min, 22 sec
O
P
N
O
ppm

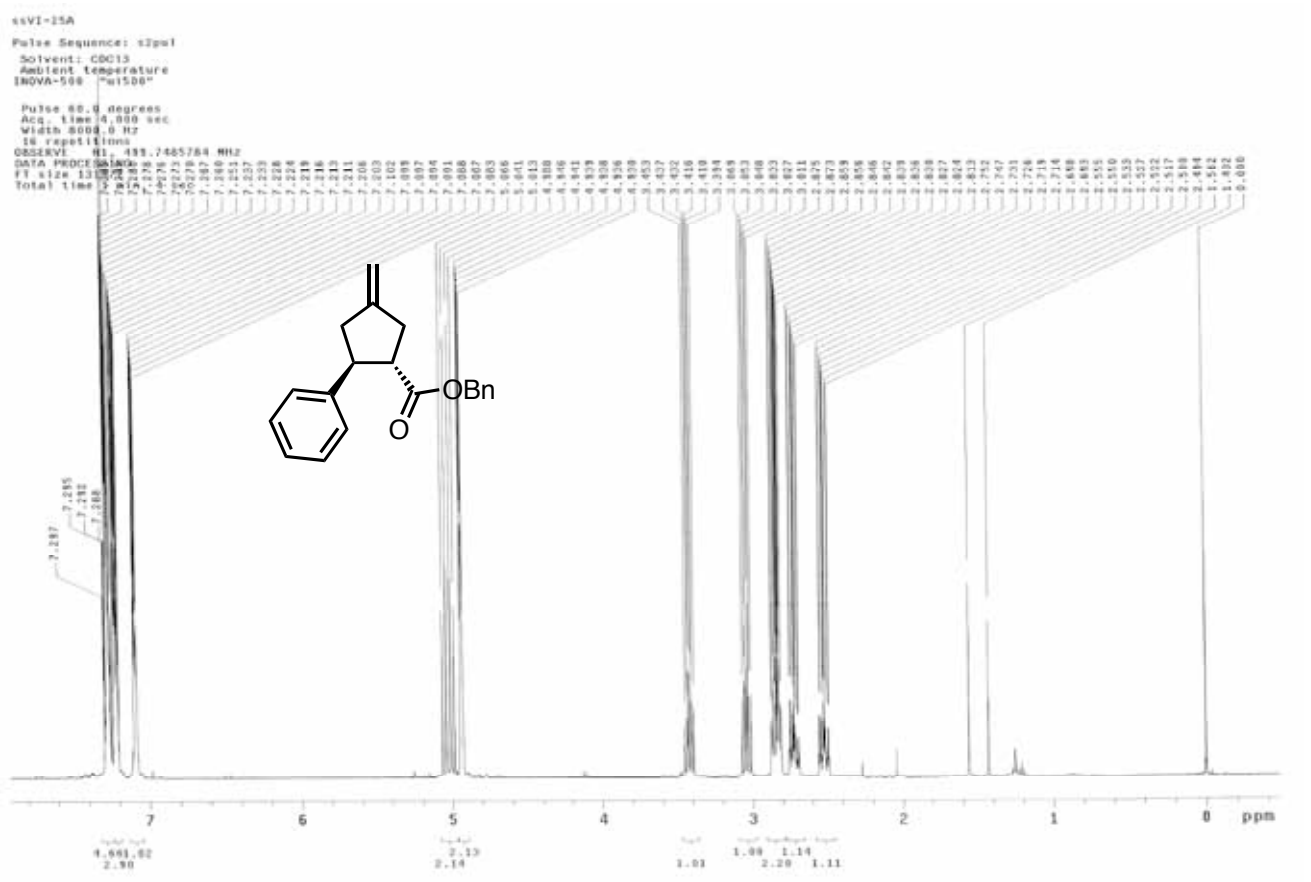

ssix-27a-13c
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "merc400"
Relax. delay 0.500 sec
Pulse 35.2 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
1328 repetitions
OBSERVE C13, 100.6281
DECOUPLE H1, 400.1135562 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 5.0 Hz
FT size 65536
Total time 5 hr, 27 min, 44 sec
ppm

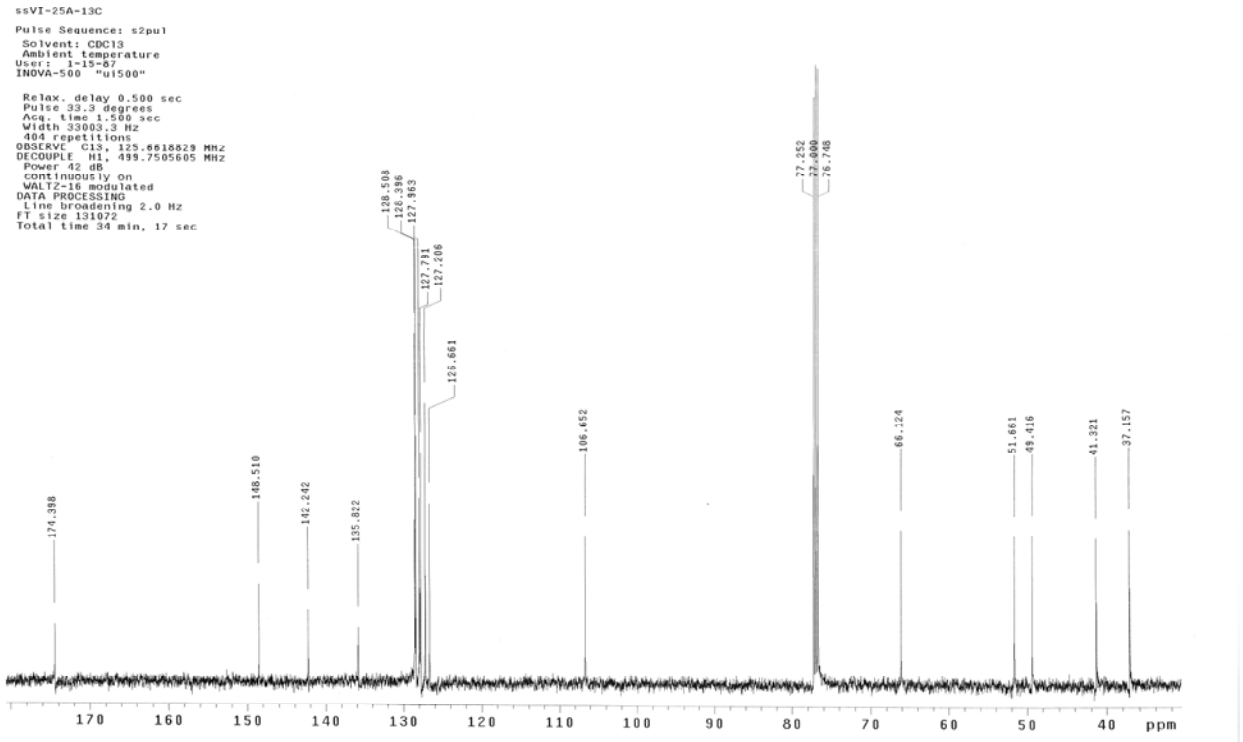

ssvii-91a
ppm

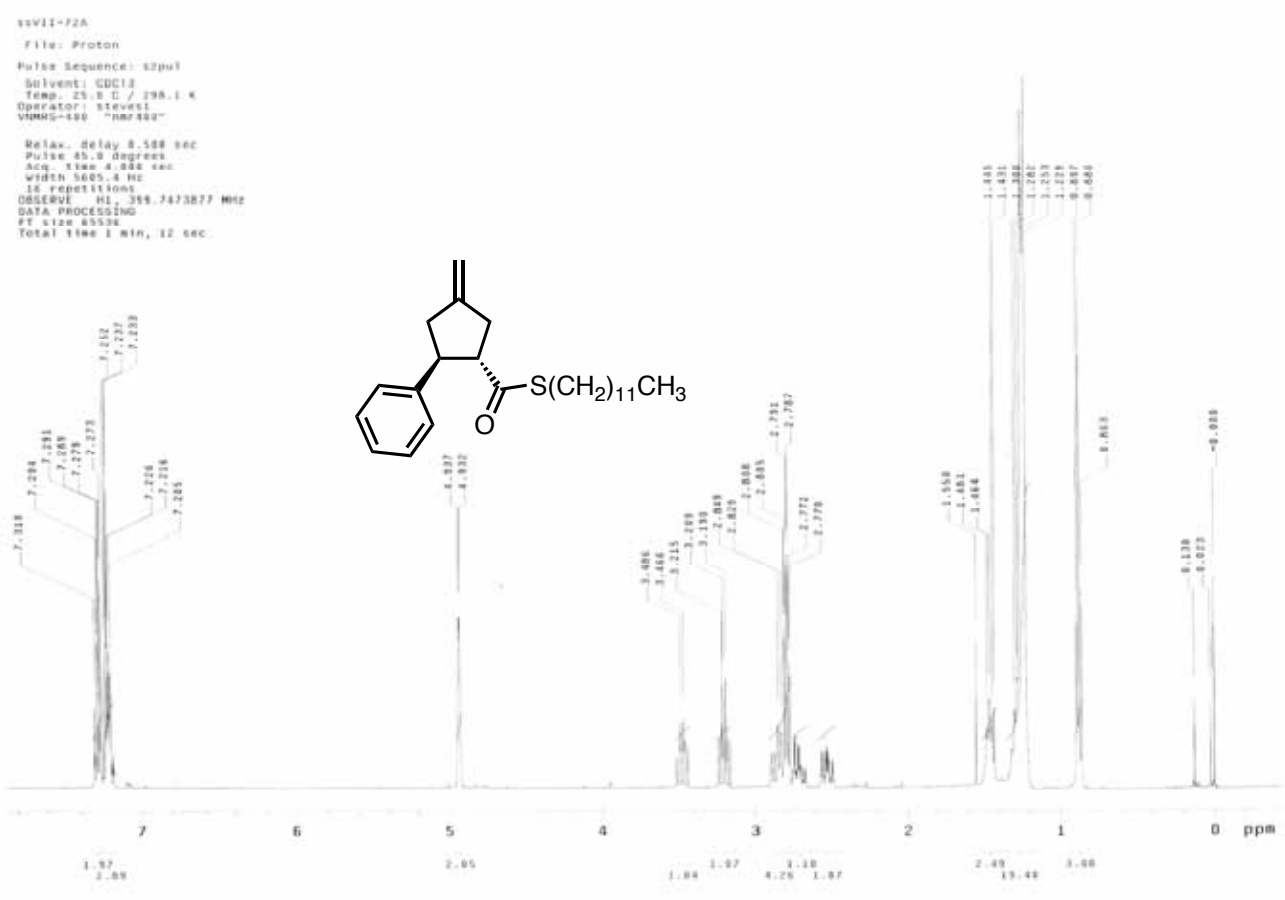

ssvii-91a-13c
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "mercury"
Relax. delay 0.500 sec
Pulse 35.2 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
832 repetitions
OBSERVE C13, 100.6081288 MHz
DECOUPLE H1, 400.1135562 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 5 hr, 27 min, 44 sec
ppm

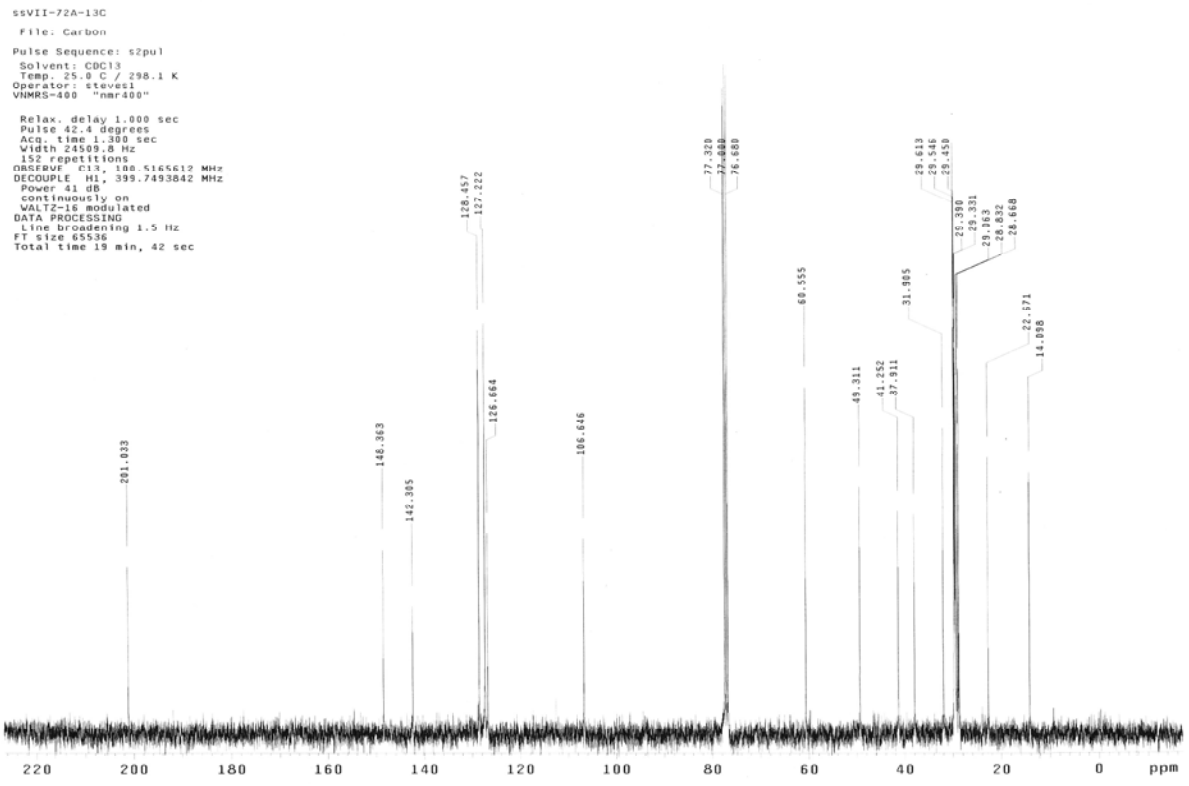

ssVI-43A
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "merc400"
Relax. delay 0.500 sec
Pulse 52.1 degrees
Acq. time 4.002 sec
Width 4997.5 Hz
8 repetitions
OBSERVE H1, 400.1115356 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 0 sec
2.169
0.876
0.000
CH3
O
H3C
5
4
3
2
1
-0
ppm
2.00
2.92
1.10
3.73
1.08
1.16
7.53
3.05

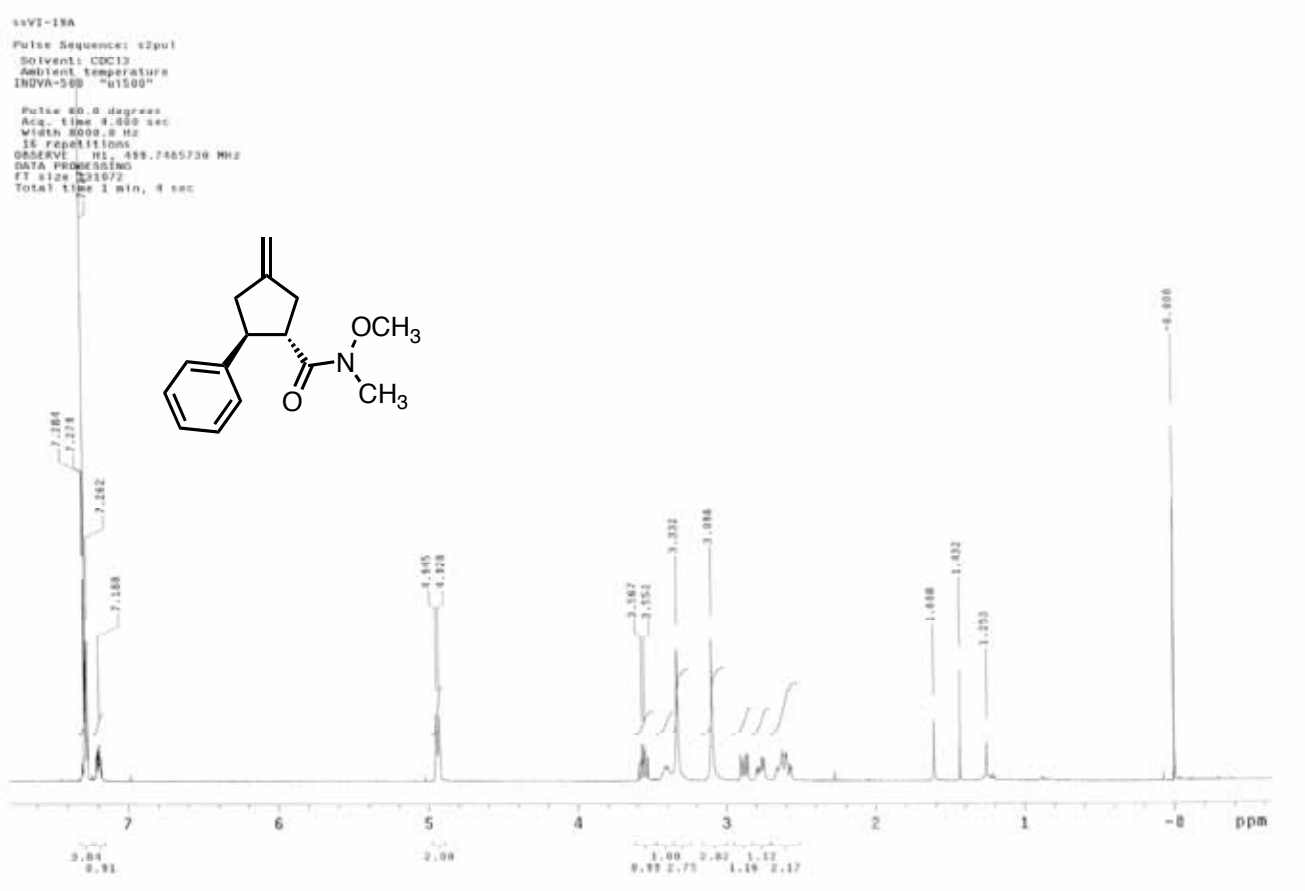

ssVI-43A-13C
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "merc400"
Relax. delay 0.500 sec
Pulse 35.2 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
288 repetitions
OBSERVE C13, 100.6081265 MHz
DECOUPLE H1, 400.1135562 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 33 min, 33 sec
77.319
77.000
76.681
210.826
149.582
106.068
58.329
42.548
38.816
36.345
34.843
31.916
29.307
27.175
22.566
14.034
200
180
160
140
120
100
80
60
40
20
ppm

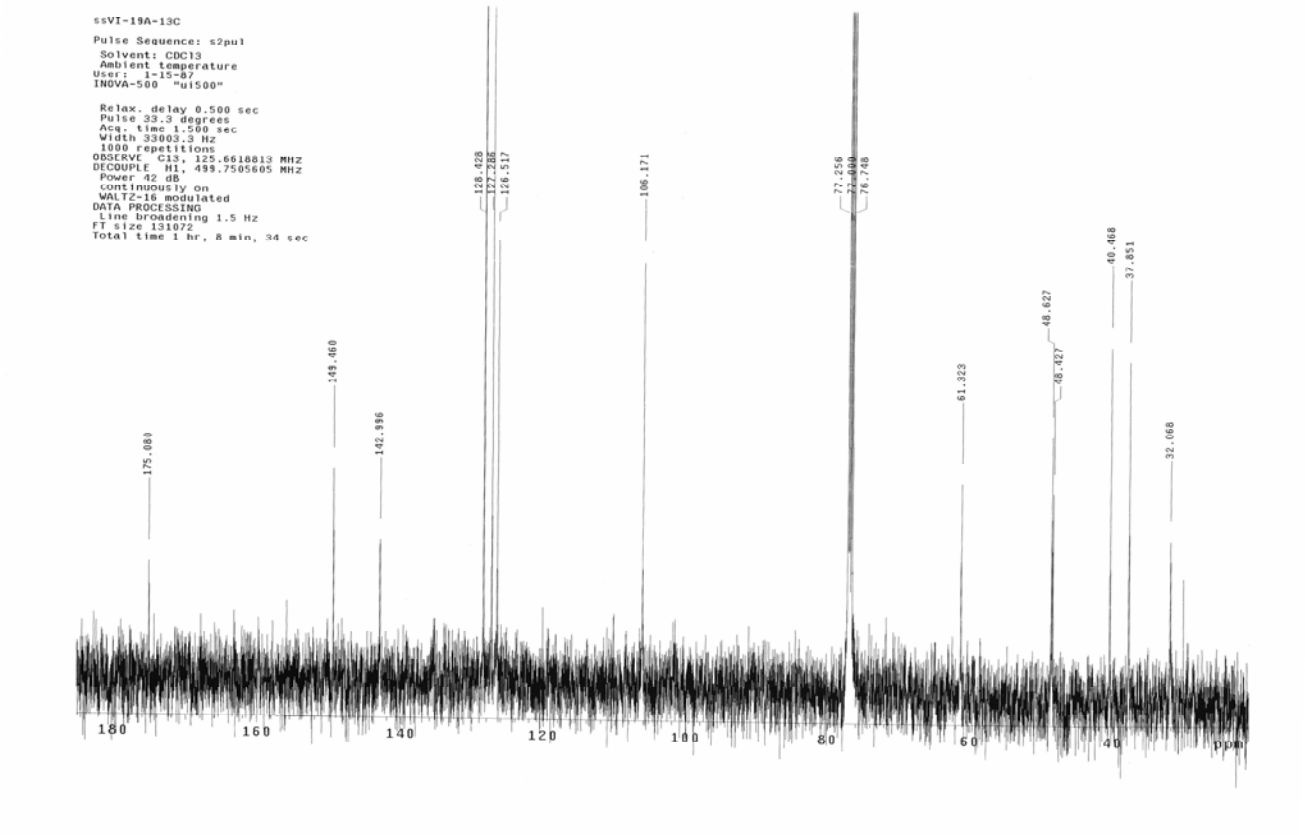

ssVI-15A
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
INOVA-500 "ui500"
Pulse 60.0 degrees
Acq. time 4.000 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.7485784 MHz
DATA PROCESSING
FT size 131072
Total time 2 min, 8 sec
OBn
O
ppm

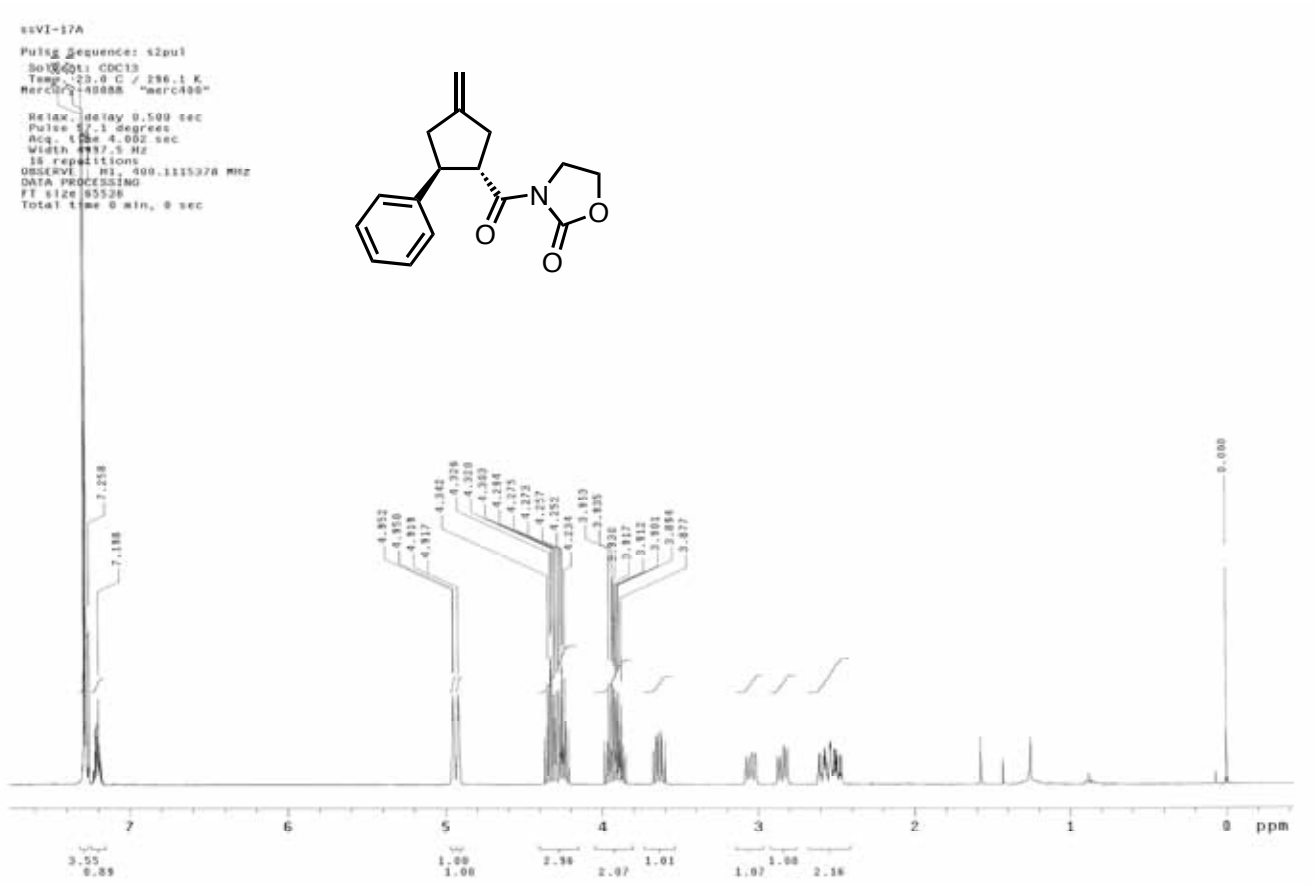

ssVI-25A-13C
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-15-87
INOVA-500 "ui500"
Relax. delay 0.500 sec
Pulse 33.3 degrees
Acq. time 1.500 sec
Width 33003.3 Hz
404 repetitions
OBSERVE C13, 125.6618829 MHz
DECOUPLE H1, 499.7505605 MHz
Power 42 dB
continuously On
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 131072
Total time 34 min, 17 sec
128.508
128.396
127.983
127.711
127.206
126.661
106.652
77.252
77.000
76.748
66.124
51.661
49.416
41.321
37.157
174.398
148.510
142.242
135.822
ppm

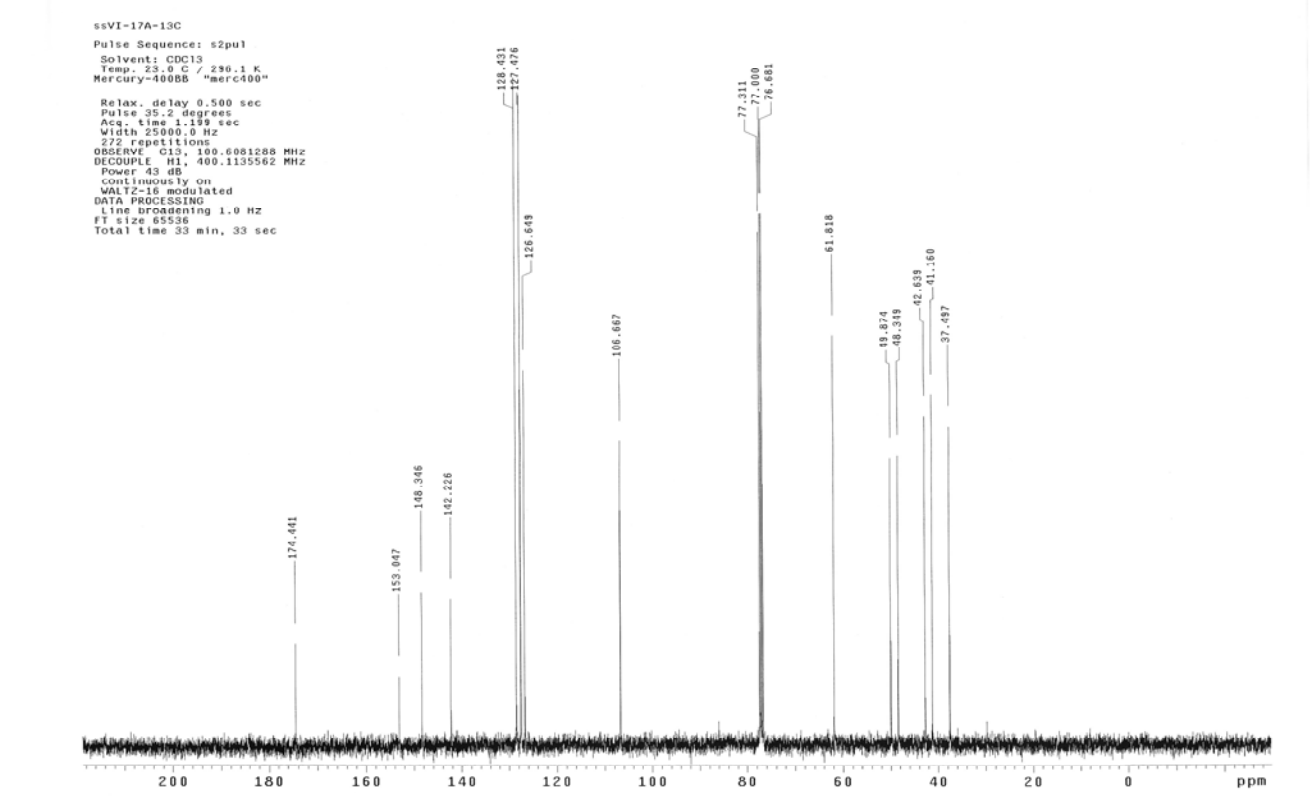

ssVII-72A
File: Proton
Pulse Sequence: s2pul
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
Operator: stevesl
VNMRS-400 "nmr400"
Relax. delay 8.588 sec
Pulse 45.0 degrees
Acq. time 4.848 sec
Width 5605.4 Hz
16 repetitions
OBSERVE H1, 399.7473877 MHz
DATA PROCESSING
FT size 65536
Total time 1 min, 12 sec
S(CH2)11CH3
O
7
6
5
4
3
2
1
0
ppm

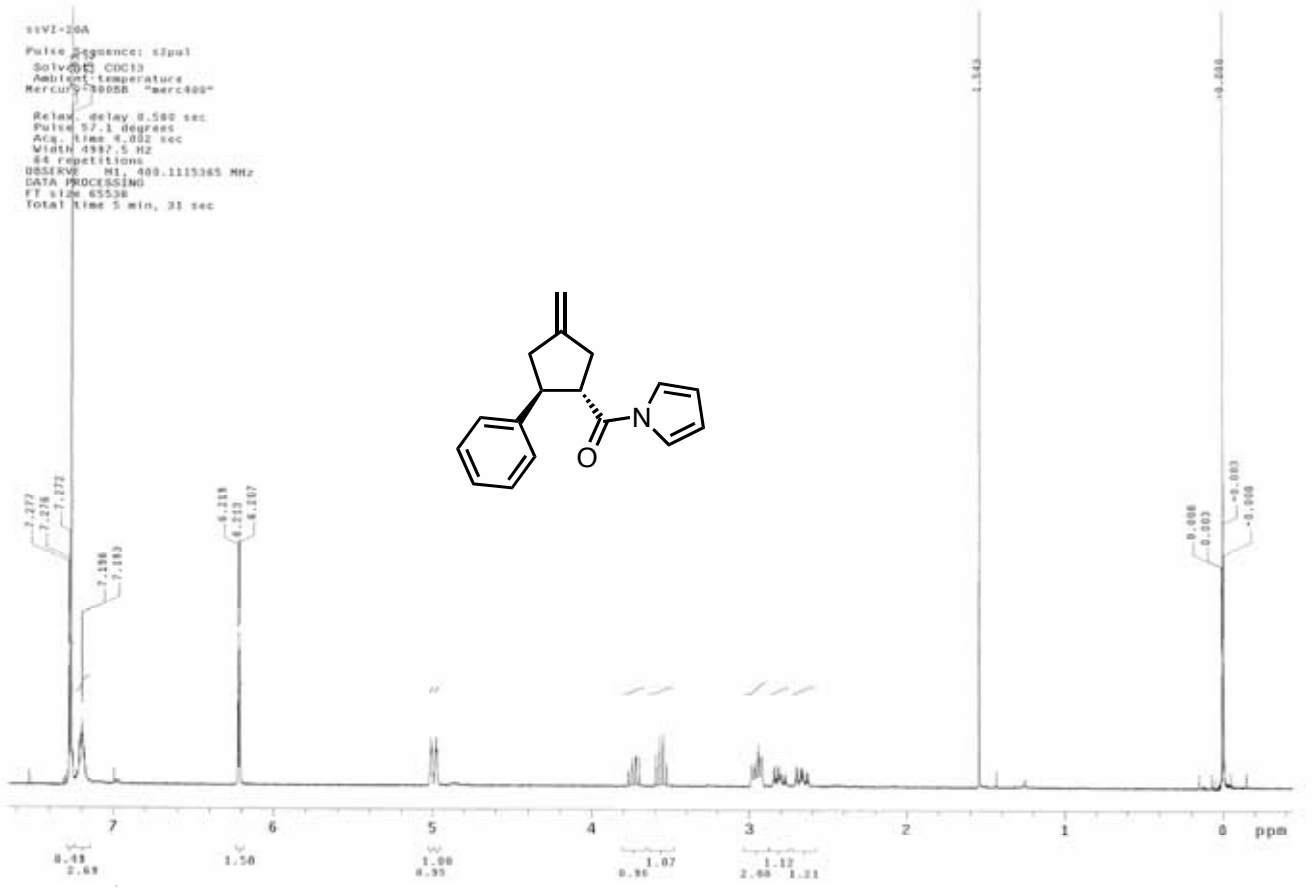

ssVII-72A-13C
File: Carbon
Pulse Sequence: s2pul
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
Operator: stevesl
VNMRS-400 "nmr400"
Relax. delay 1.000 sec
Pulse 42.4 degrees
Acq. time 1.300 sec
Width 24509.8 Hz
152 repetitions
OBSERVE C13, 100.5165612 MHz
DECOUPLE H1, 399.7493842 MHz
Power 41 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 65536
Total time 19 min, 42 sec
201.033
148.383
142.305
128.457
127.222
126.664
106.646
77.320
76.680
60.555
49.311
41.252
37.911
31.985
29.613
29.546
29.450
29.390
29.331
29.163
28.832
28.668
22.671
14.098
220
200
180
160
140
120
100
80
60
40
20
0
ppm

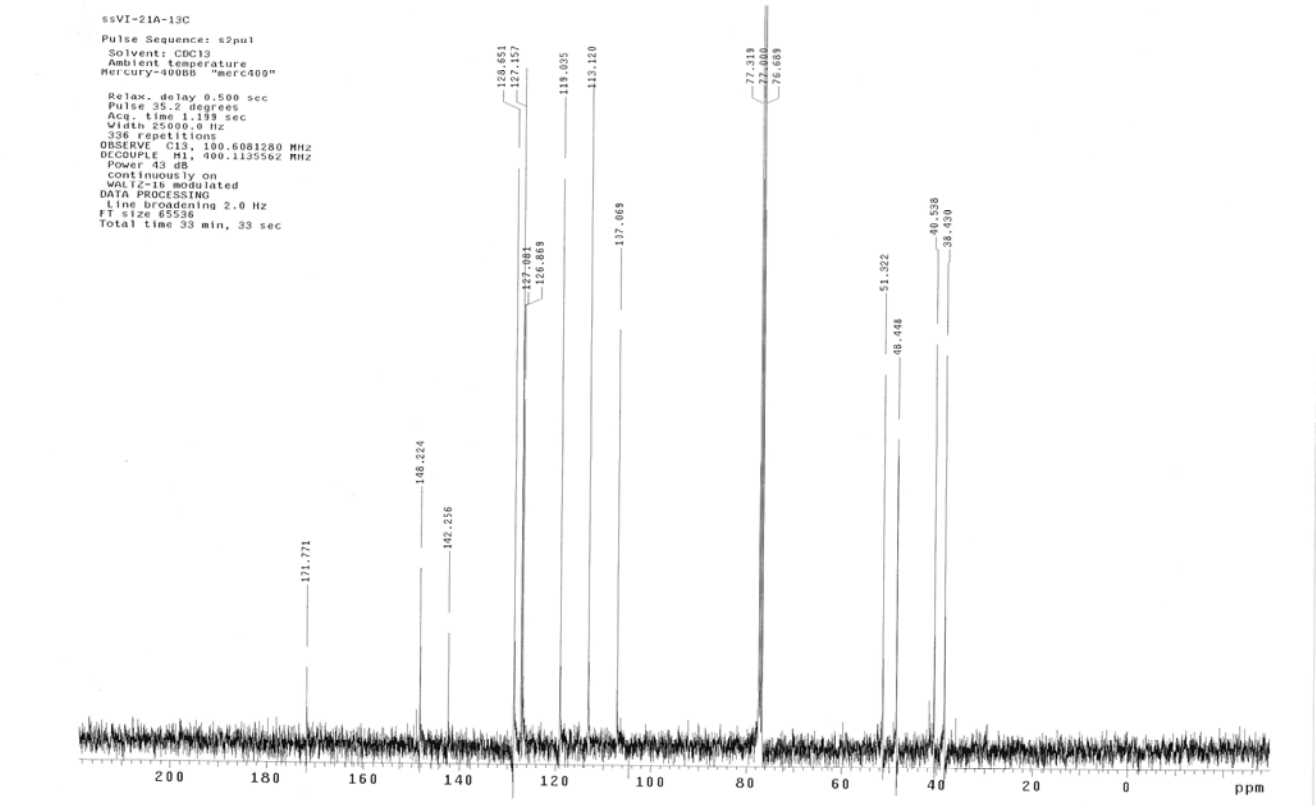

ssVI-19A
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
INOVA-500 "ui500"
Pulse 60.0 degrees
Acq. time 4.000 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.7465730 MHz
DATA PROCESSING
FT size 131072
Total time 1 min, 4 sec
OCH3
N
CH3
O
ppm

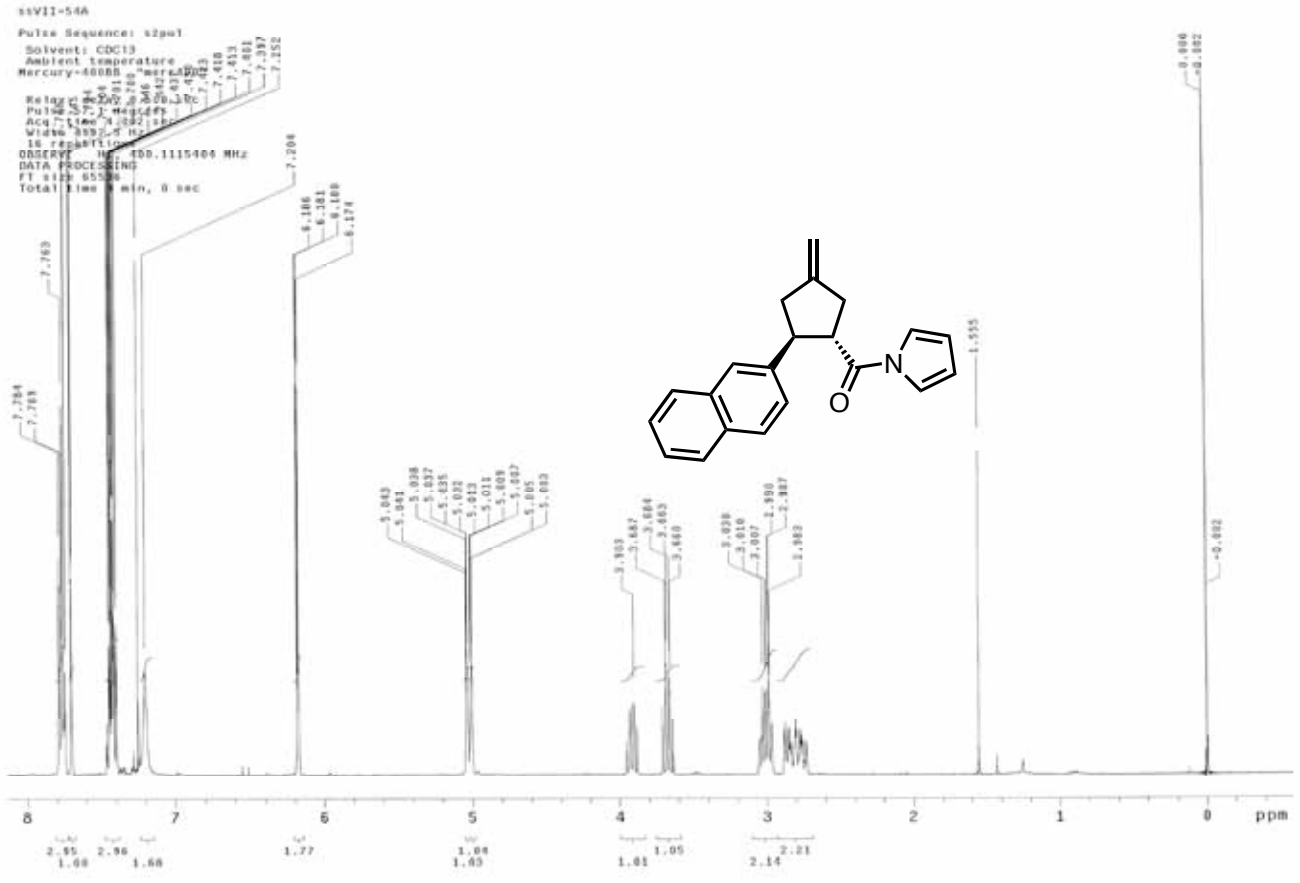

ssVI-19A-13C
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-15-07
INOVA-500 "ui500"
Relax. delay 0.500 sec
Pulse 33.3 degrees
Acq. time 1.500 sec
Width 33003.3 Hz
1000 repetitions
OBSERVE C13, 125.6618813 MHz
DECOUPLE H1, 499.7505605 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 1 hr, 8 min, 34 sec
ppm

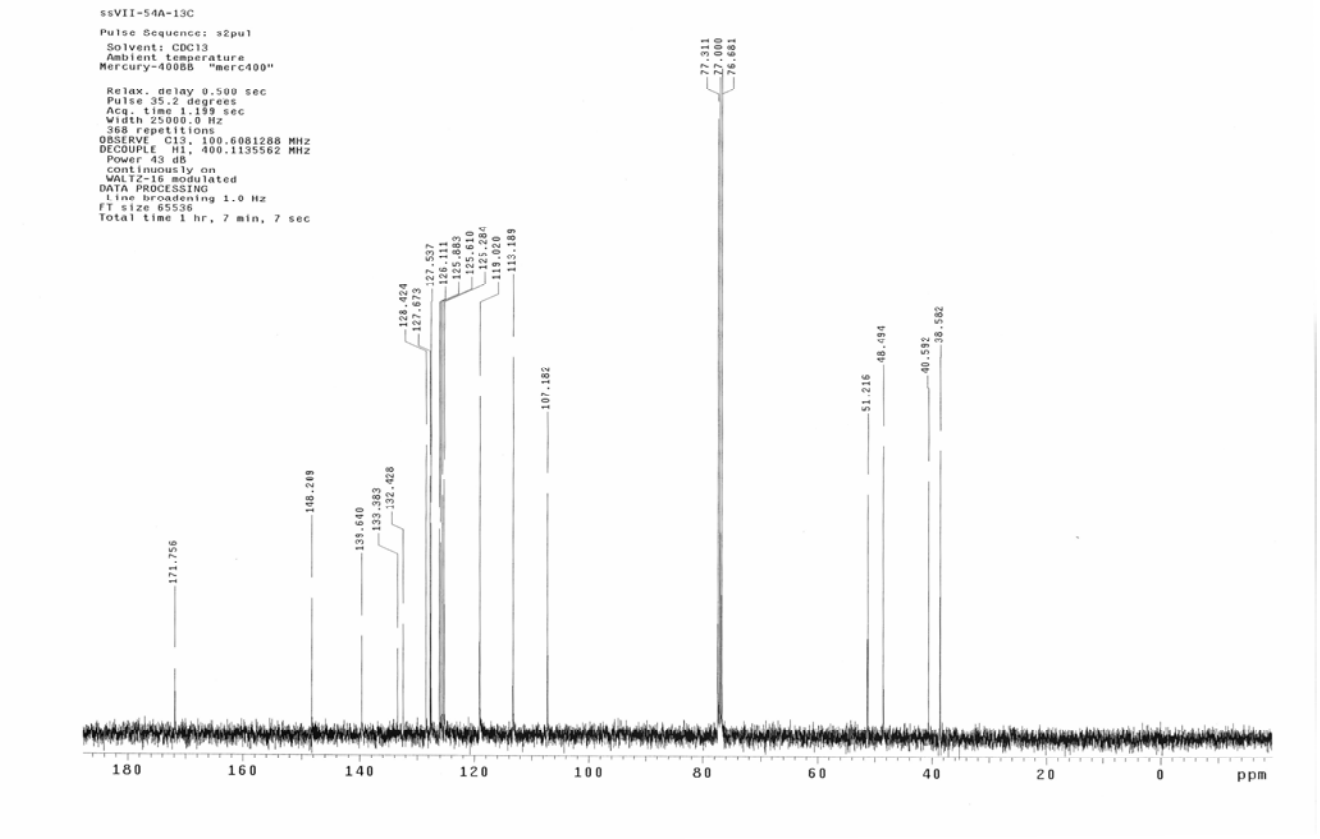

ssVI-17A
Pulse Sequence: s2pul
Solvent: CDC13
Temp. 23.0 C / 296.1 K
Mercury-400BB "merc400"
Relax. delay 0.500 sec
Pulse 57.1 degrees
Acq. time 4.002 sec
Width 4997.5 Hz
16 repetitions
OBSERVE H1, 400.1115378 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 0 sec
7.258
7.188
0.000
ppm
3.55
0.89
1.00
1.00
2.96
2.07
1.01
1.07
1.08
2.16

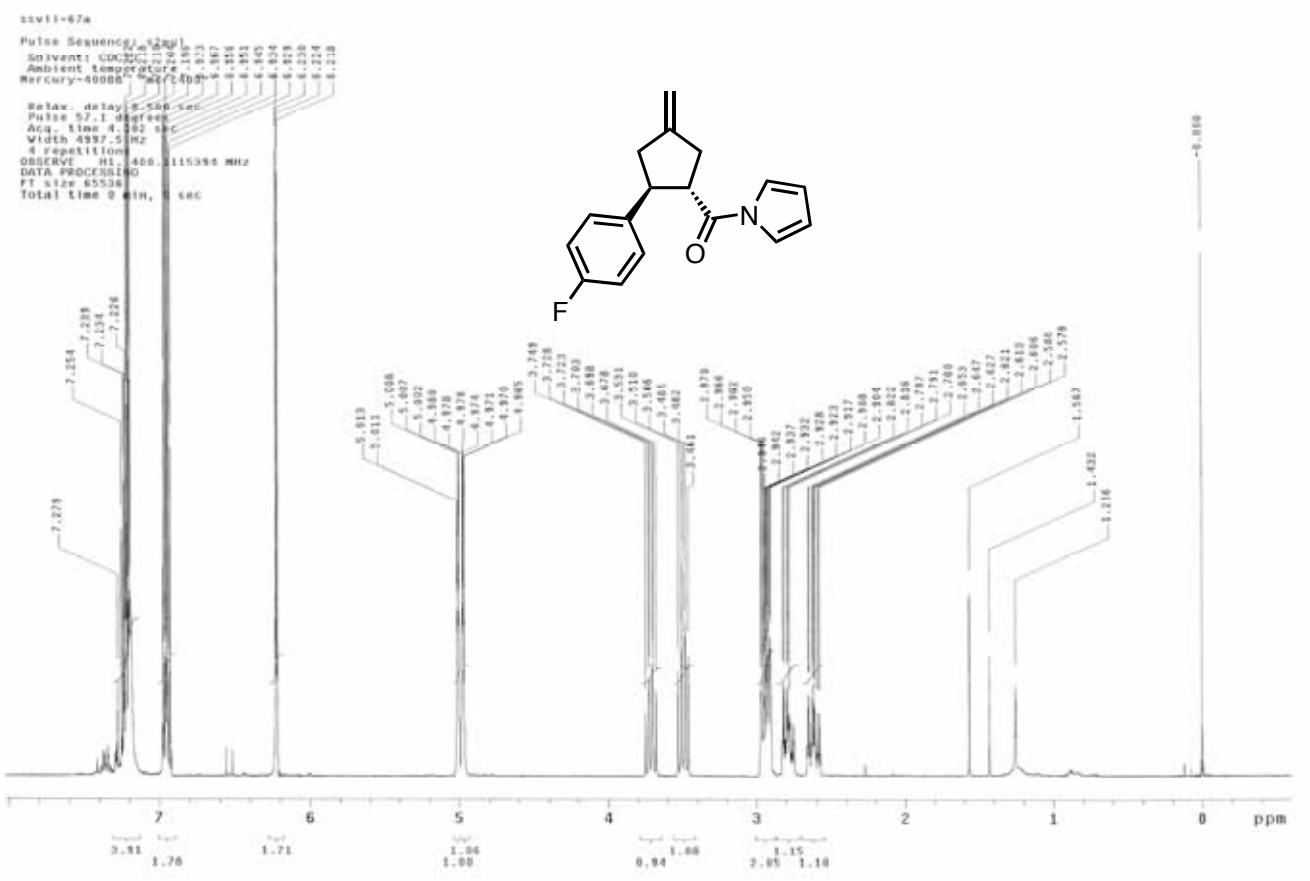

ssVI-17A-13C
Pulse Sequence: s2pul
Solvent: CDC13
Temp. 23.0 C / 230.1 K
Mercury-400BB "merc400"
Relax. delay 0.500 sec
Pulse 35.2 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
272 repetitions
OBSERVE C13, 100.6081288 MHz
DECOUPLE H1, 400.1135562 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 33 min, 33 sec
174.441
153.047
148.346
142.226
128.431
127.476
126.649
106.667
77.311
77.000
76.681
61.818
49.874
49.339
42.639
41.160
37.497
200
180
160
140
120
100
80
60
40
20
0
ppm

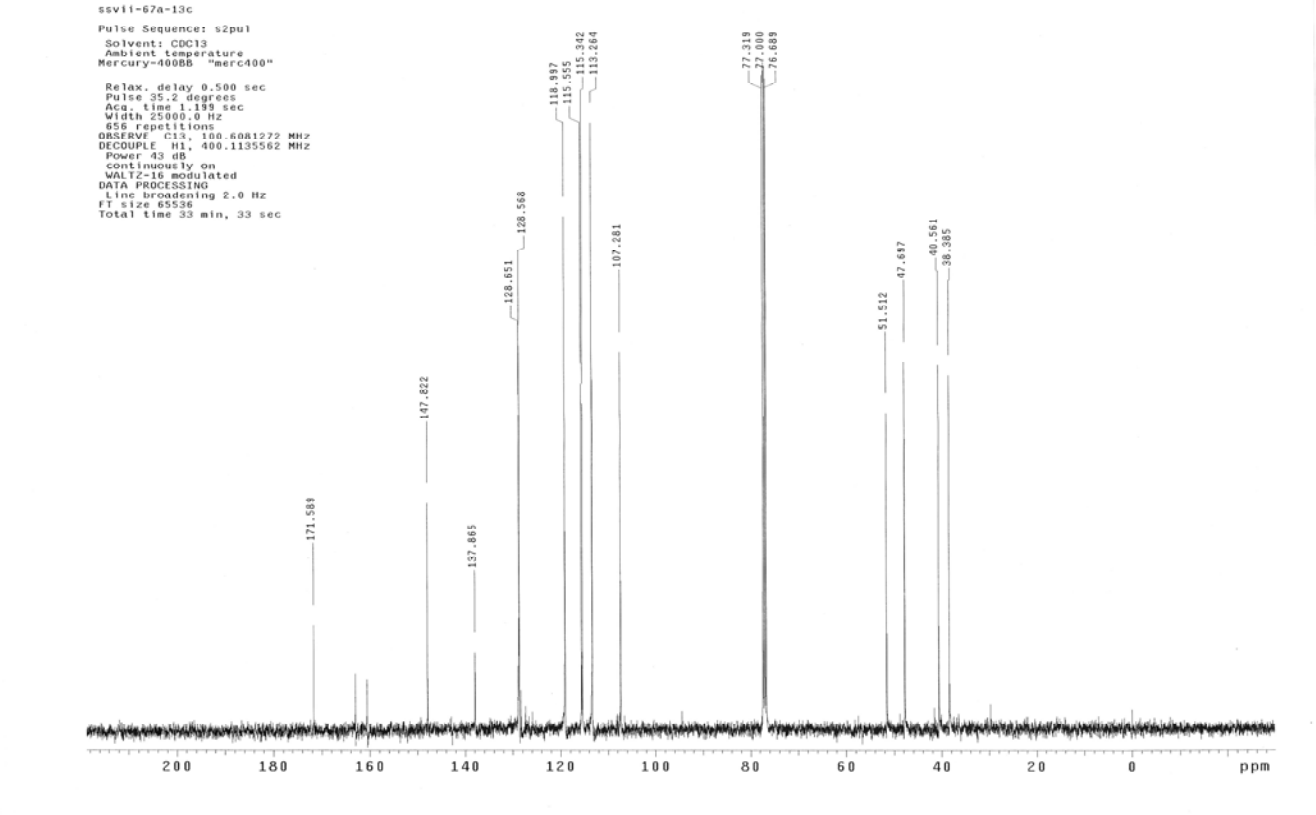

ssVI-20A
Pulse Sequence: s1pul
Solvent: CDCl3
Ambient temperature
Mercury-300BB "merc400"
Relax. delay 0.500 sec
Pulse 57.1 degrees
Acq. time 4.002 sec
Width 4997.5 Hz
44 repetitions
OBSERVE H1, 400.1115365 MHz
DATA PROCESSING
FT size 65536
Total time 5 min, 31 sec
N
O
ppm

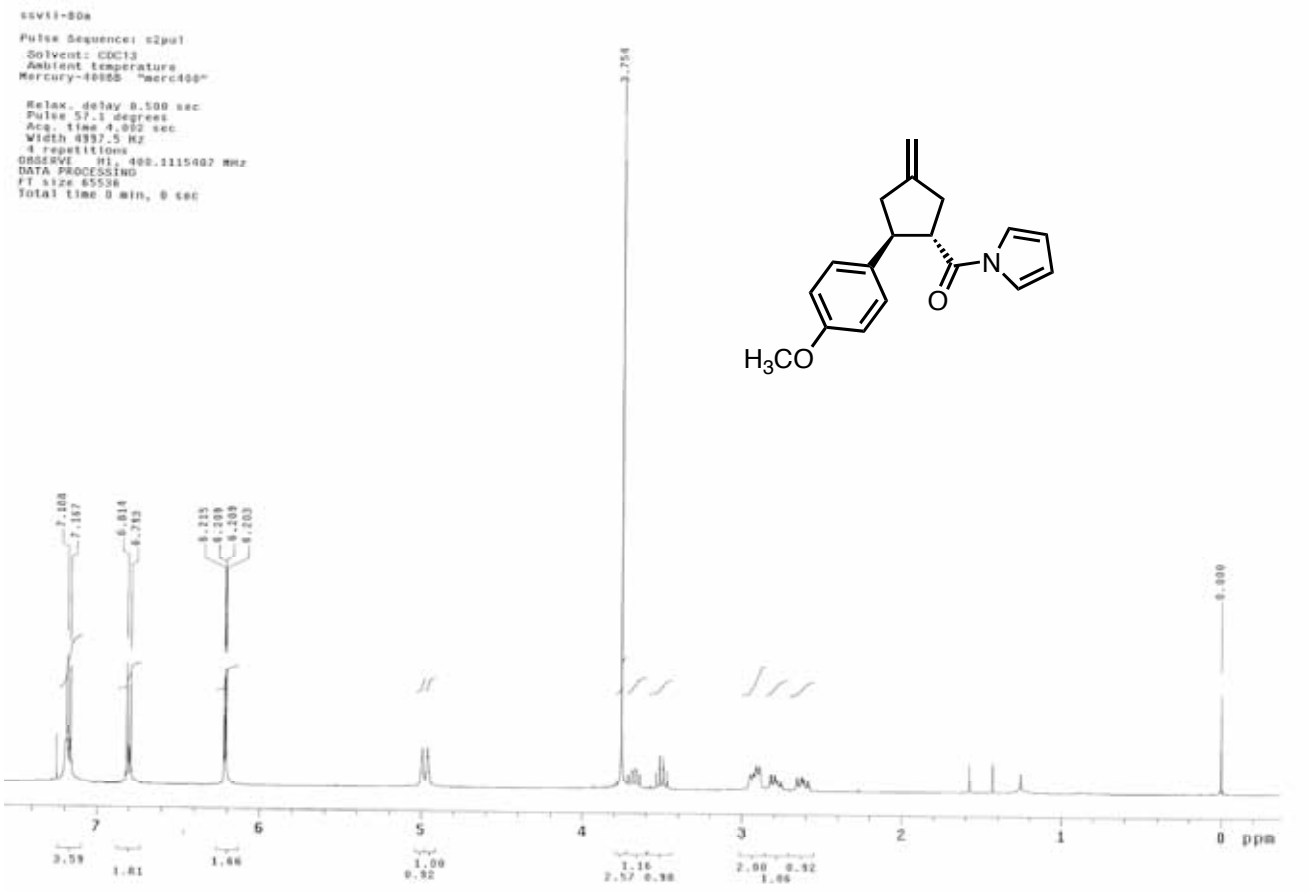

ssVI-21A-13C
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "merc400"
Relax. delay 0.500 sec
Pulse 35.2 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
336 repetitions
OBSERVE C13, 100.6081280 MHz
DECOUPLE H1, 400.1135562 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 65536
Total time 33 min, 33 sec
ppm

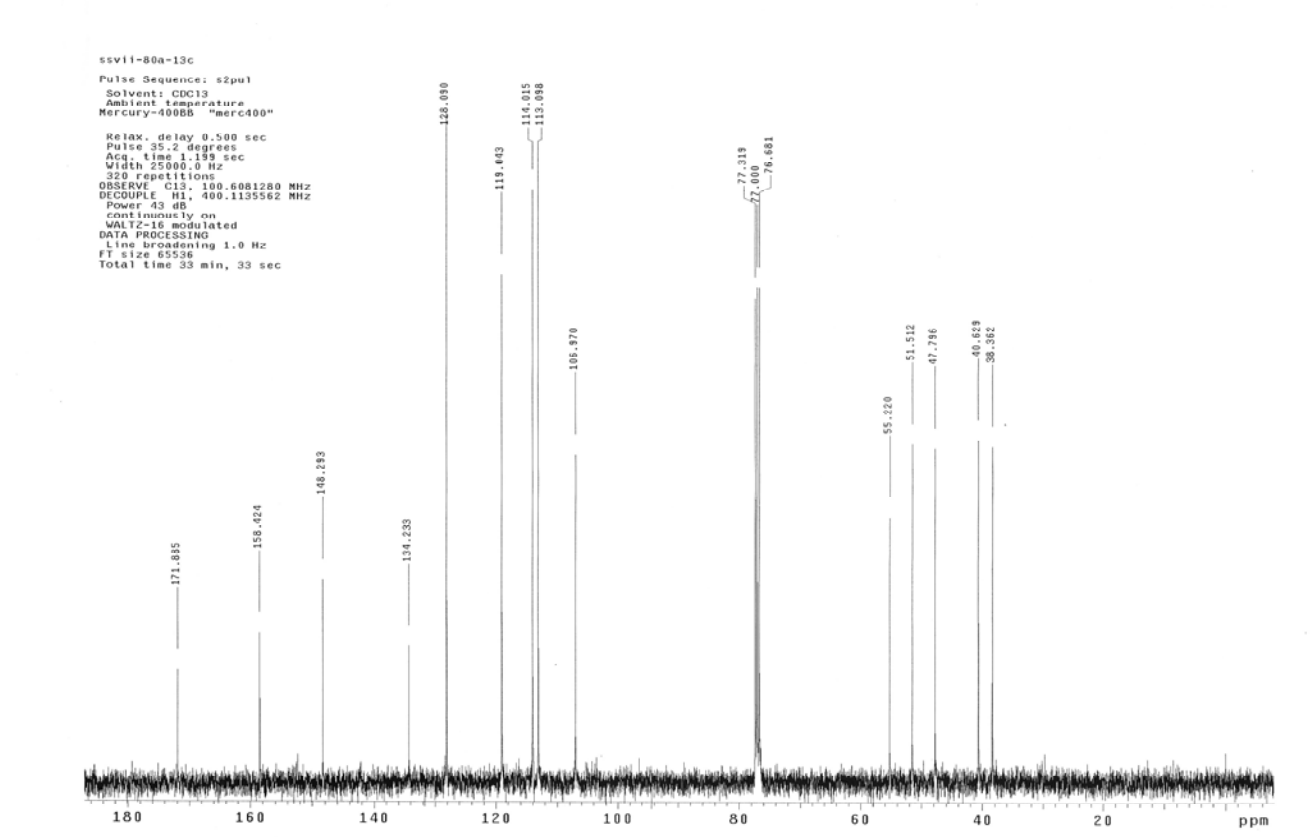

ssVII-54A
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "merc400"
ppm

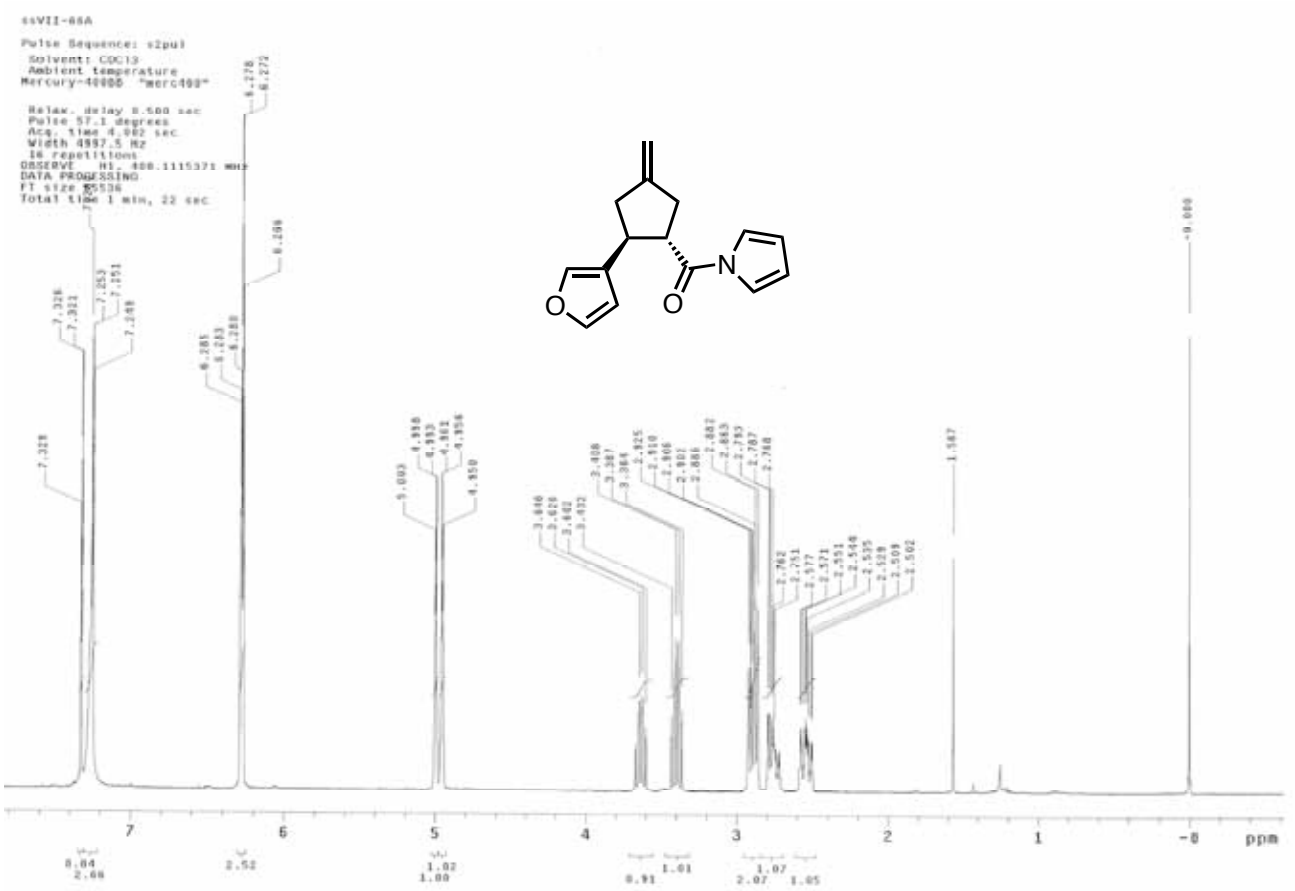

ssVII-54A-13C
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "merc400"
Relax. delay 0.500 sec
Pulse 35.2 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
368 repetitions
OBSERVE C13, 100.6081288 MHz
DECOUPLE H1, 400.1135562 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 1 hr, 7 min, 7 sec
ppm

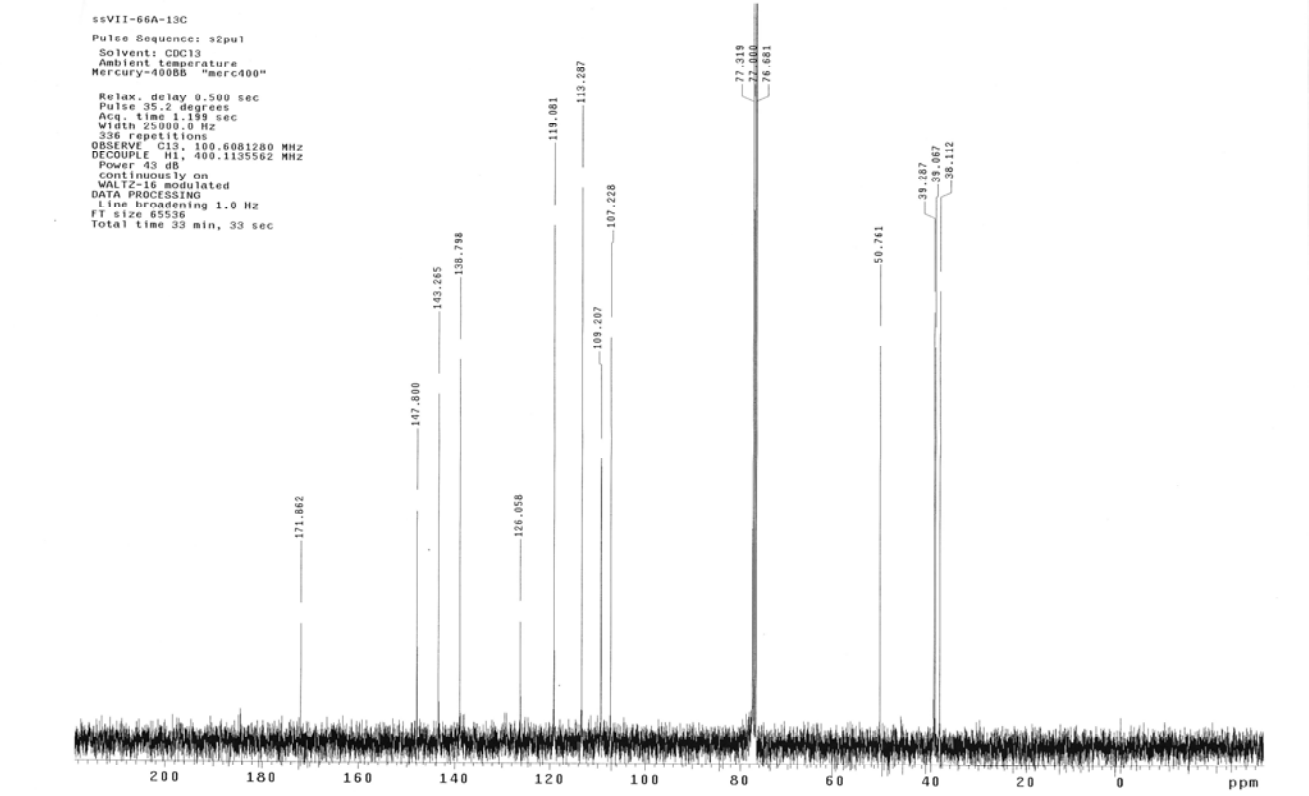

ssvii-67a
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "merc400"
Relax. delay 0.500 sec
Pulse 57.1 degrees
Acq. time 4.092 sec
Width 4997.5 Hz
4 repetitions
OBSERVE H1, 400.1115396 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 1 sec
F
O
N
ppm

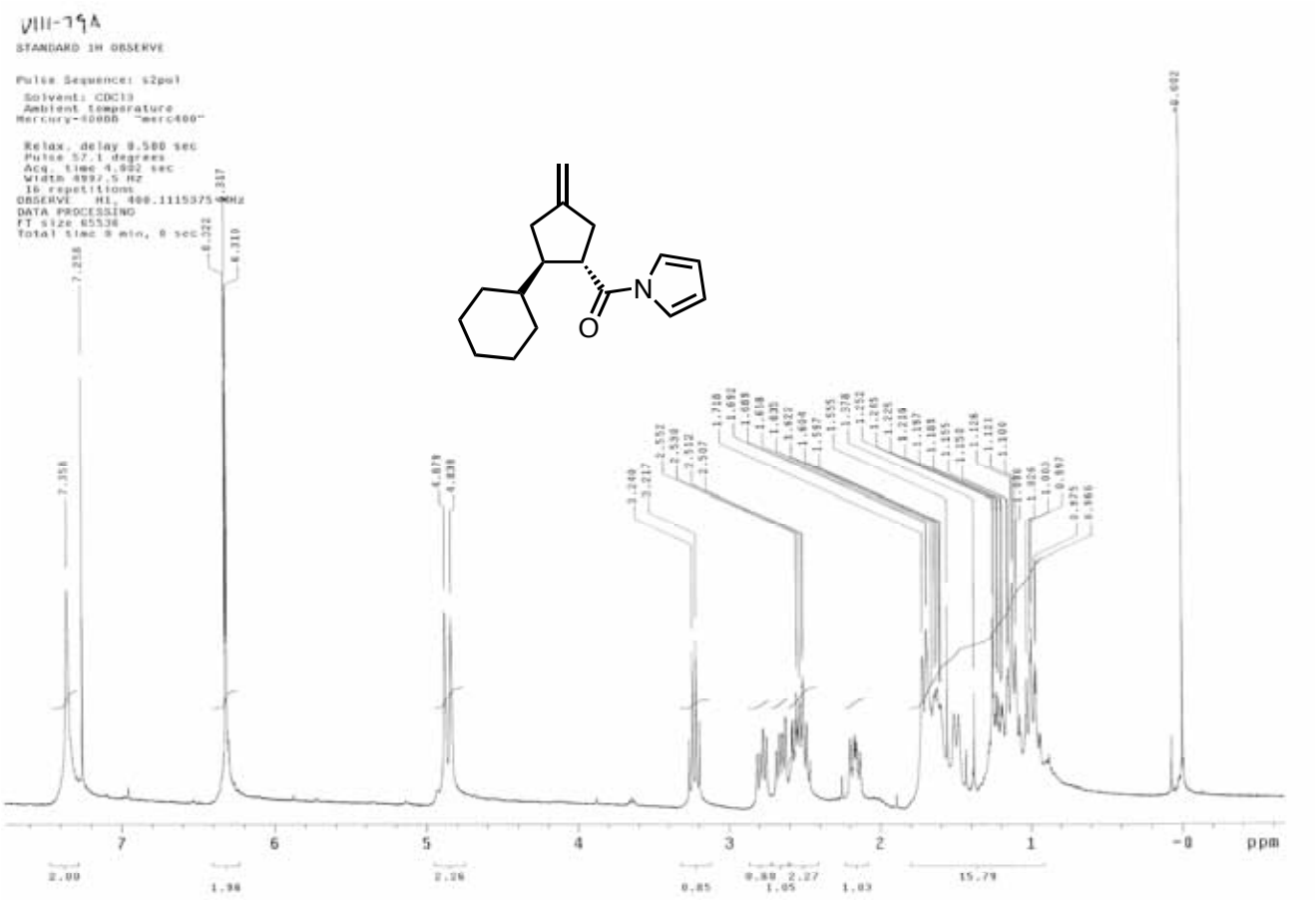

ssvii-67a-13c
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "merc400"
Relax. delay 0.500 sec
Pulse 35.2 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
656 repetitions
OBSERVE C13, 100.6081272 MHz
DECOUPLE H1, 400.1135562 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 65536
Total time 33 min, 33 sec
171.589
147.822
137.865
128.651
128.568
118.997
115.555
115.342
113.264
107.281
77.319
77.000
76.689
51.512
47.697
40.561
30.385
ppm

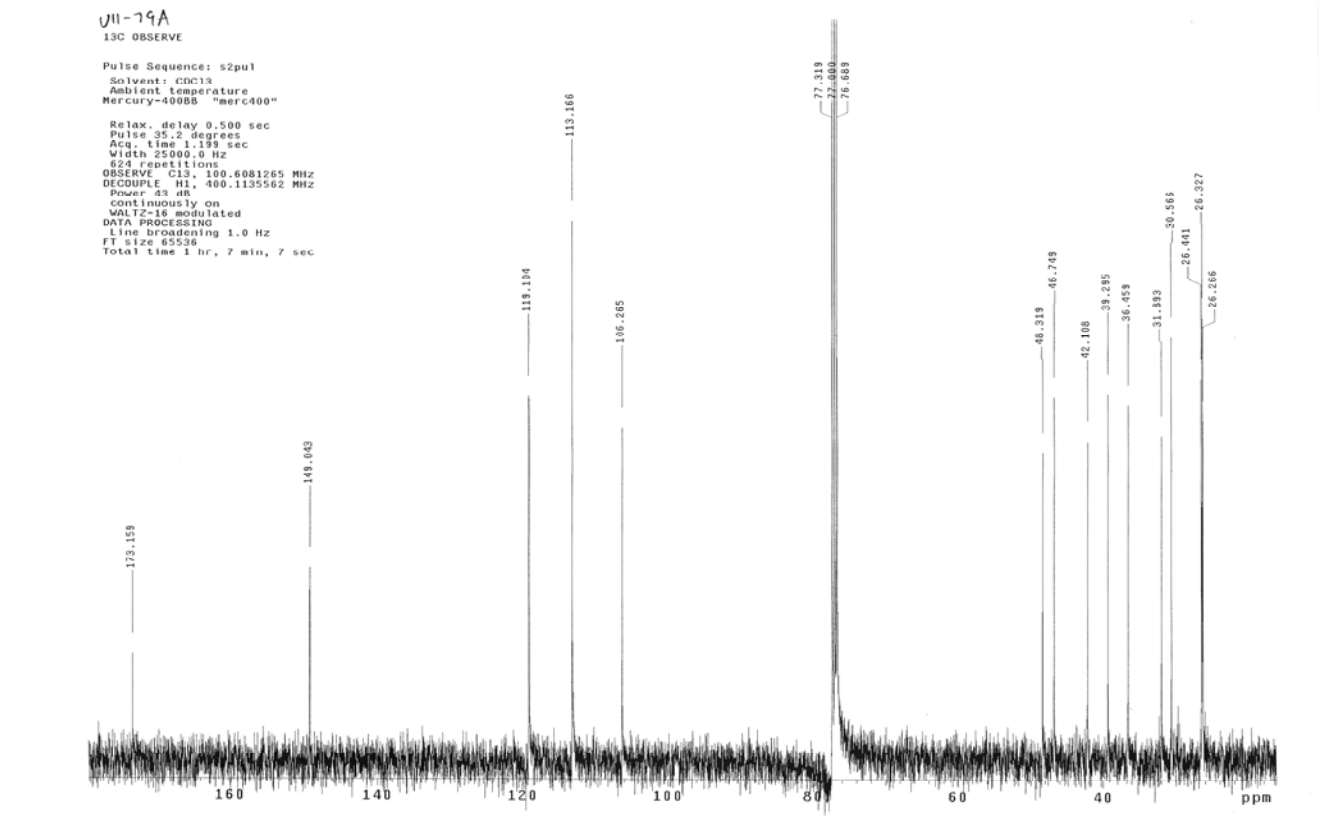

ssvii-80a
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "merc400"
Relax. delay 0.500 sec
Pulse 57.1 degrees
Acq. time 4.002 sec
Width 4997.5 Hz
4 repetitions
OBSERVE H1, 400.1115402 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 0 sec
7.188
7.167
6.814
6.793
3.754
0.000
3.59
1.81
1.66
1.00
0.92
1.16
2.57
0.98
2.00
0.92
1.66
ppm
H3CO
O
N

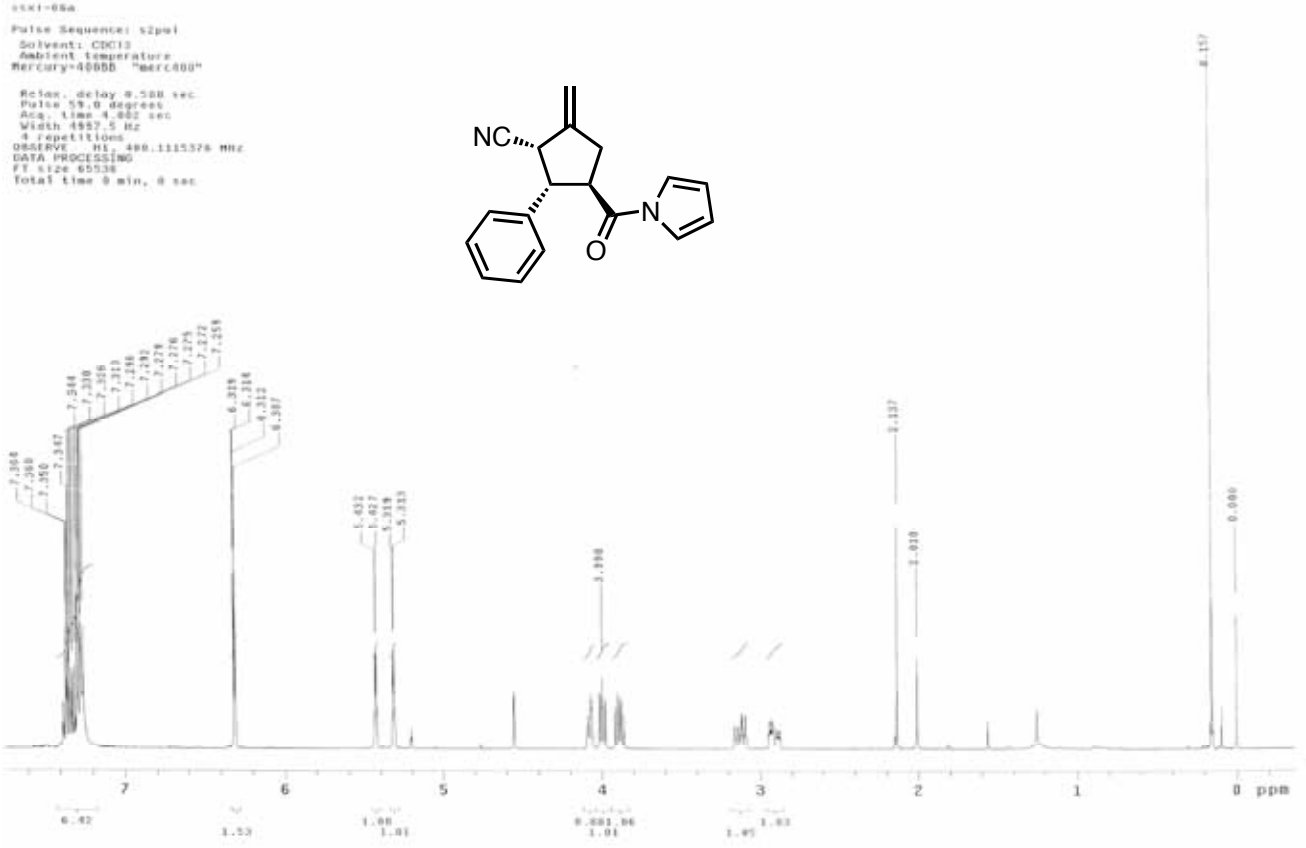

ssvii-80a-13c
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "merc400"
Relax. delay 0.500 sec
Pulse 35.2 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
320 repetitions
OBSERVE C13, 100.6081280 MHz
DECOUPLE H1, 400.1135562 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 33 min, 33 sec
171.885
158.424
148.293
134.233
120.090
119.443
114.015
113.098
105.970
77.319
77.000
76.681
55.220
51.512
47.796
40.629
38.362
ppm

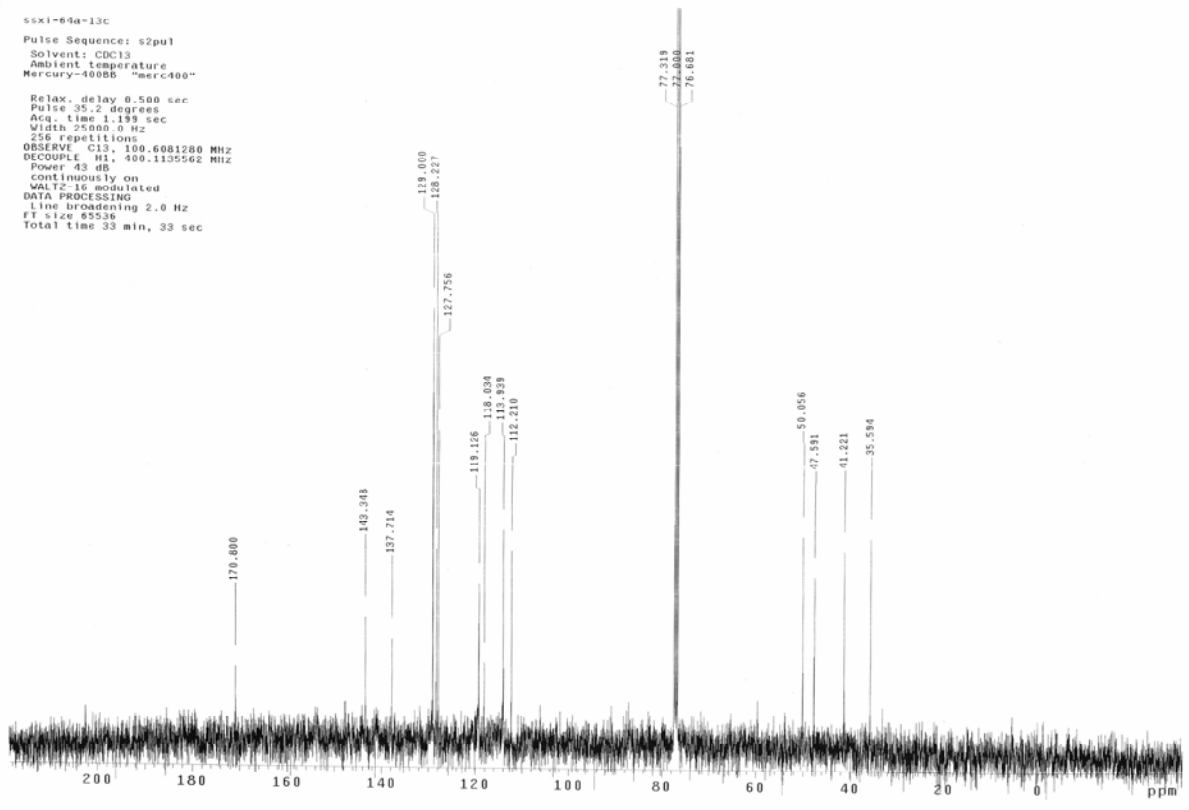

ssVII-66A
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "merc400"
Relax. delay 0.500 sec
Pulse 57.1 degrees
Acq. time 4.002 sec
Width 4987.5 Hz
16 repetitions
OBSERVE H1, 400.1115371 MHz
DATA PROCESSING
FT size 65536
Total time 1 min, 22 sec
O
O
N
ppm

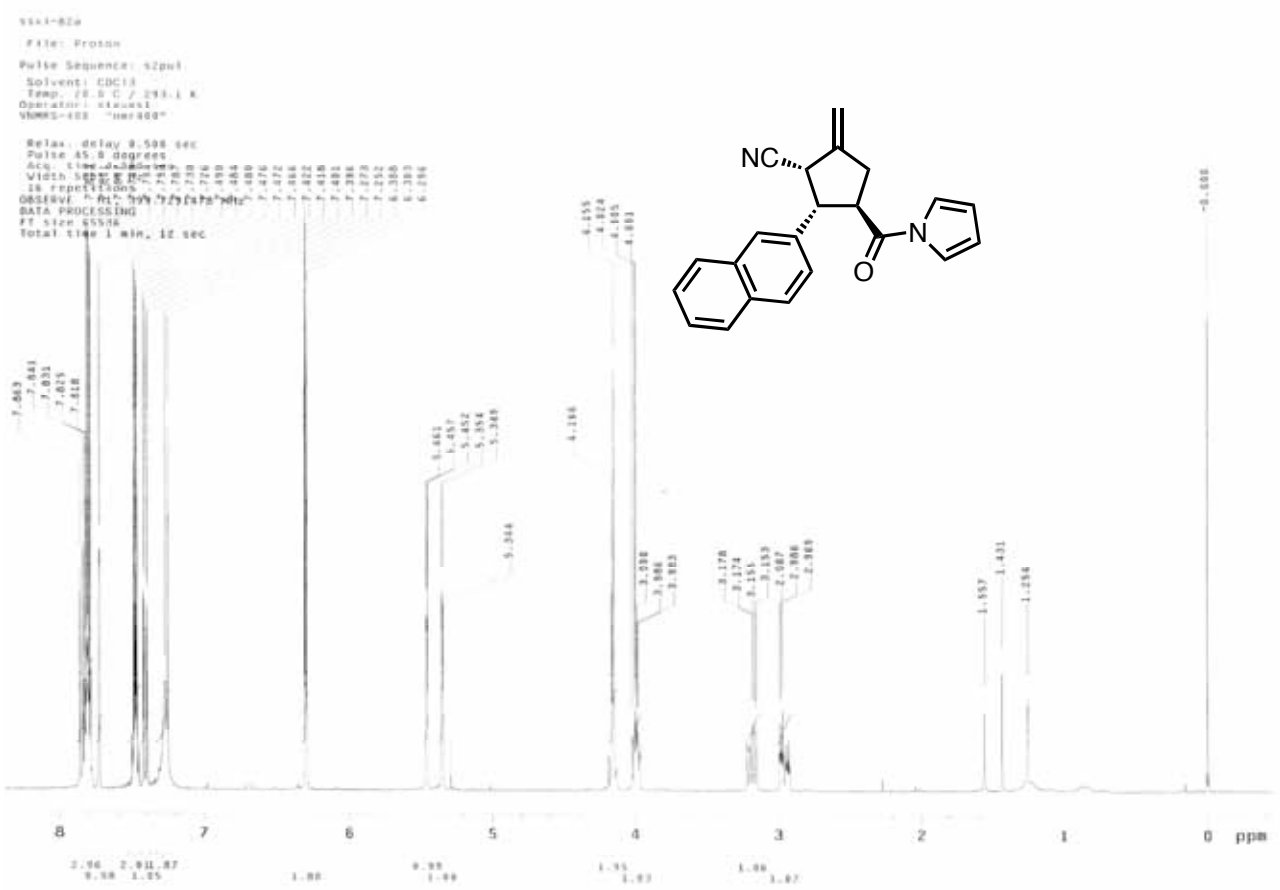

ssVII-66A-13C
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "merc400"
Relax. delay 0.500 sec
Pulse 35.2 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
336 repetitions
OBSERVE C13, 100.6081280 MHz
DECOUPLE H1, 400.1135562 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
line broadening 1.0 Hz
FT size 65536
Total time 33 min, 33 sec
171.862
147.800
143.265
138.798
126.058
119.081
113.287
109.207
107.228
77.319
77.000
76.681
50.761
39.287
39.067
38.112
ppm

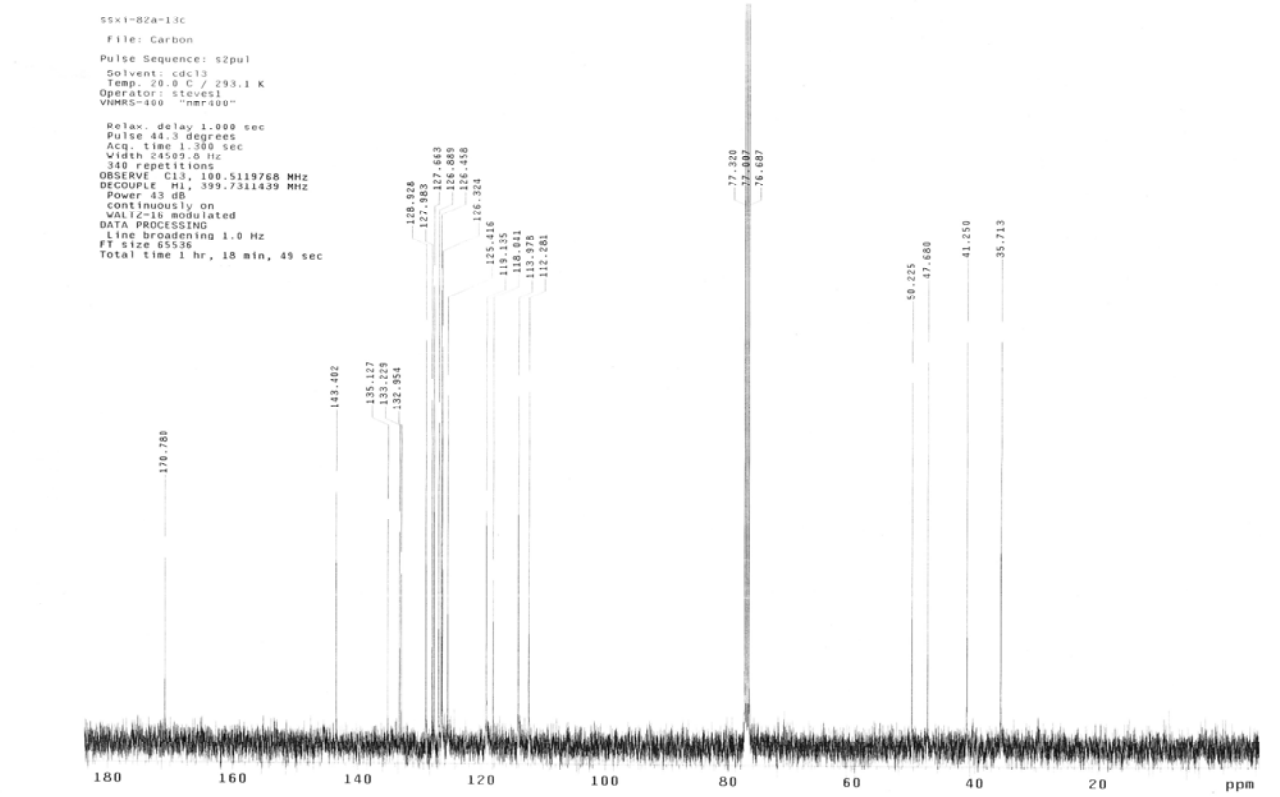

VIII-79A
STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "merc400"
Relax. delay 0.500 sec
Pulse 57.1 degrees
Acq. time 4.002 sec
Width 4997.5 Hz
16 repetitions
OBSERVE H1, 400.1115375 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 0 sec
ppm

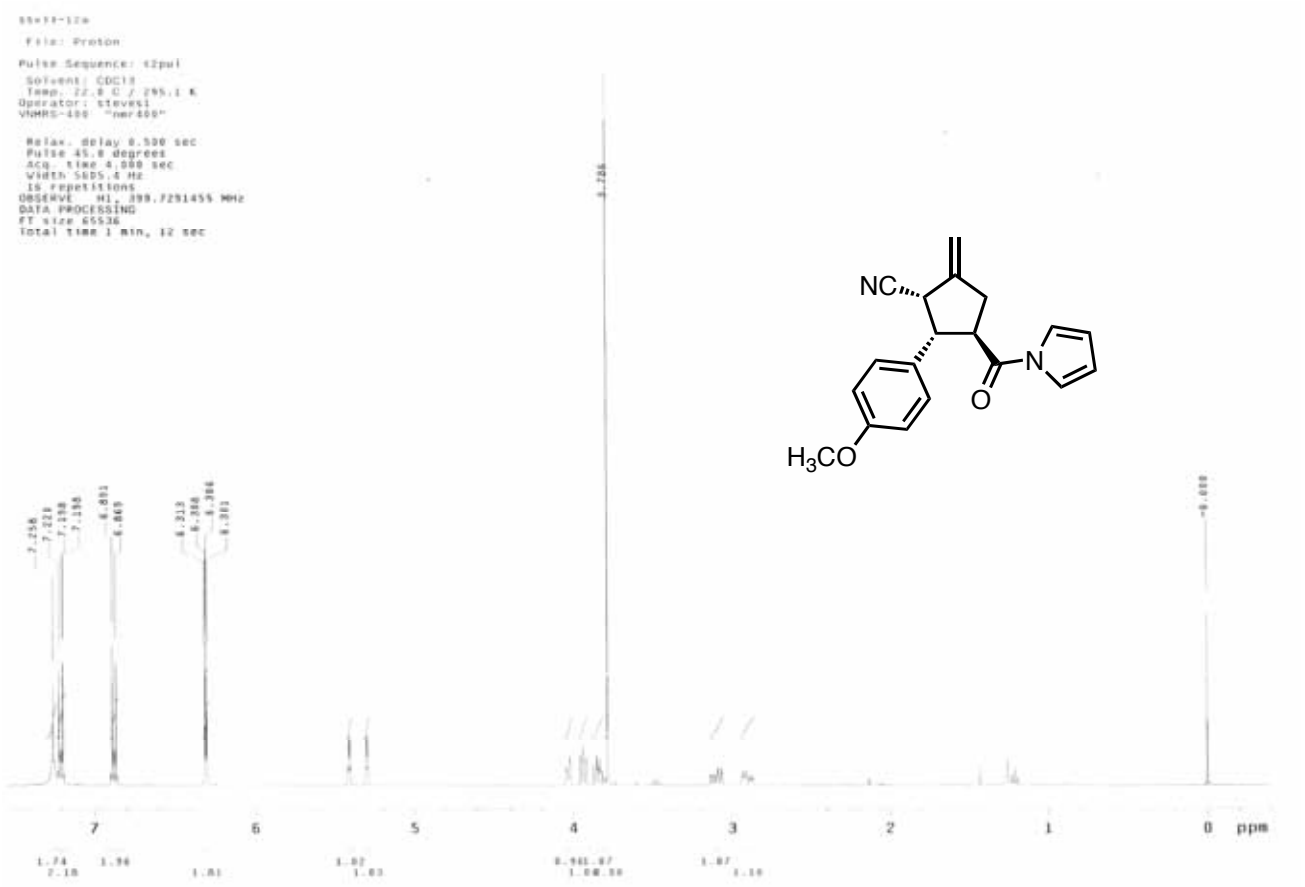

VII-79A
13C OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "merc400"
Relax. delay 0.500 sec
Pulse 35.2 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
624 repetitions
OBSERVE C13, 100.6081265 MHz
DECOUPLE H1, 400.1135562 MHz
Power 45 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 1 hr, 7 min, 7 sec
ppm

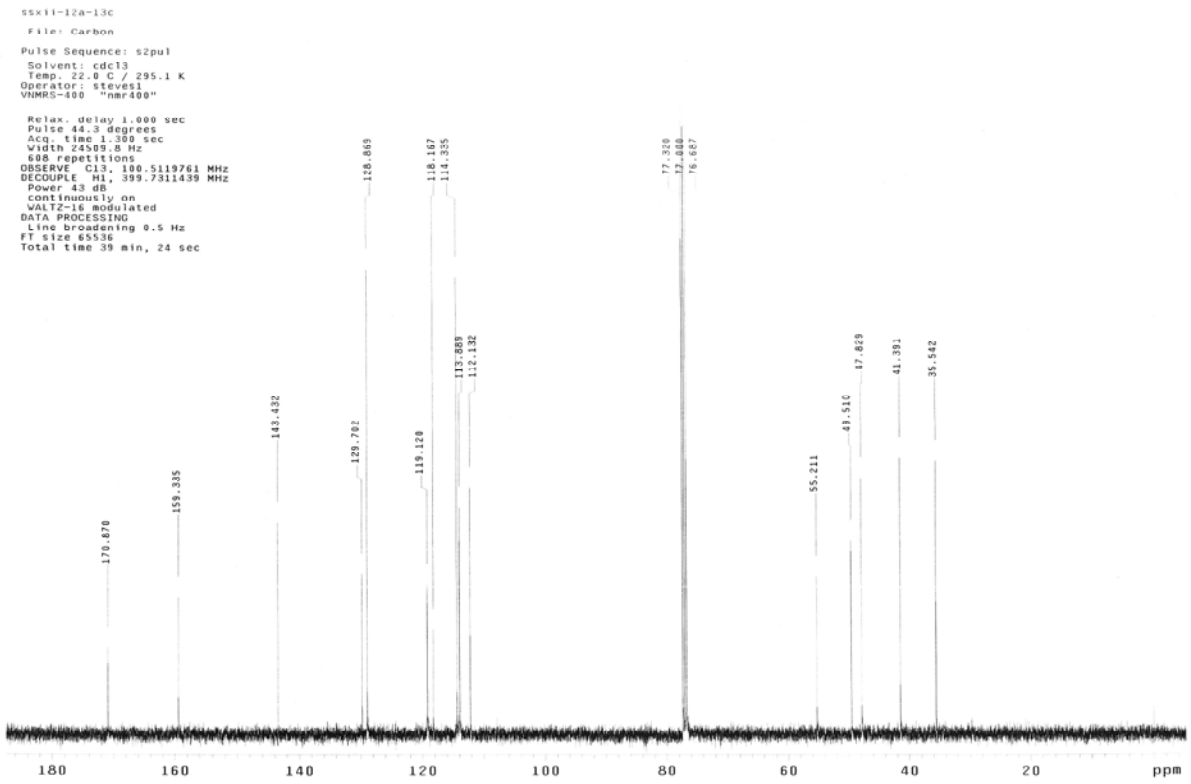

ssxi-65a
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "merc400"
Relax. delay 0.500 sec
Pulse 59.0 degrees
Acq. time 4.002 sec
Width 4987.5 Hz
4 repetitions
OBSERVE H1, 400.1115376 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 0 sec
NC
N
O
ppm

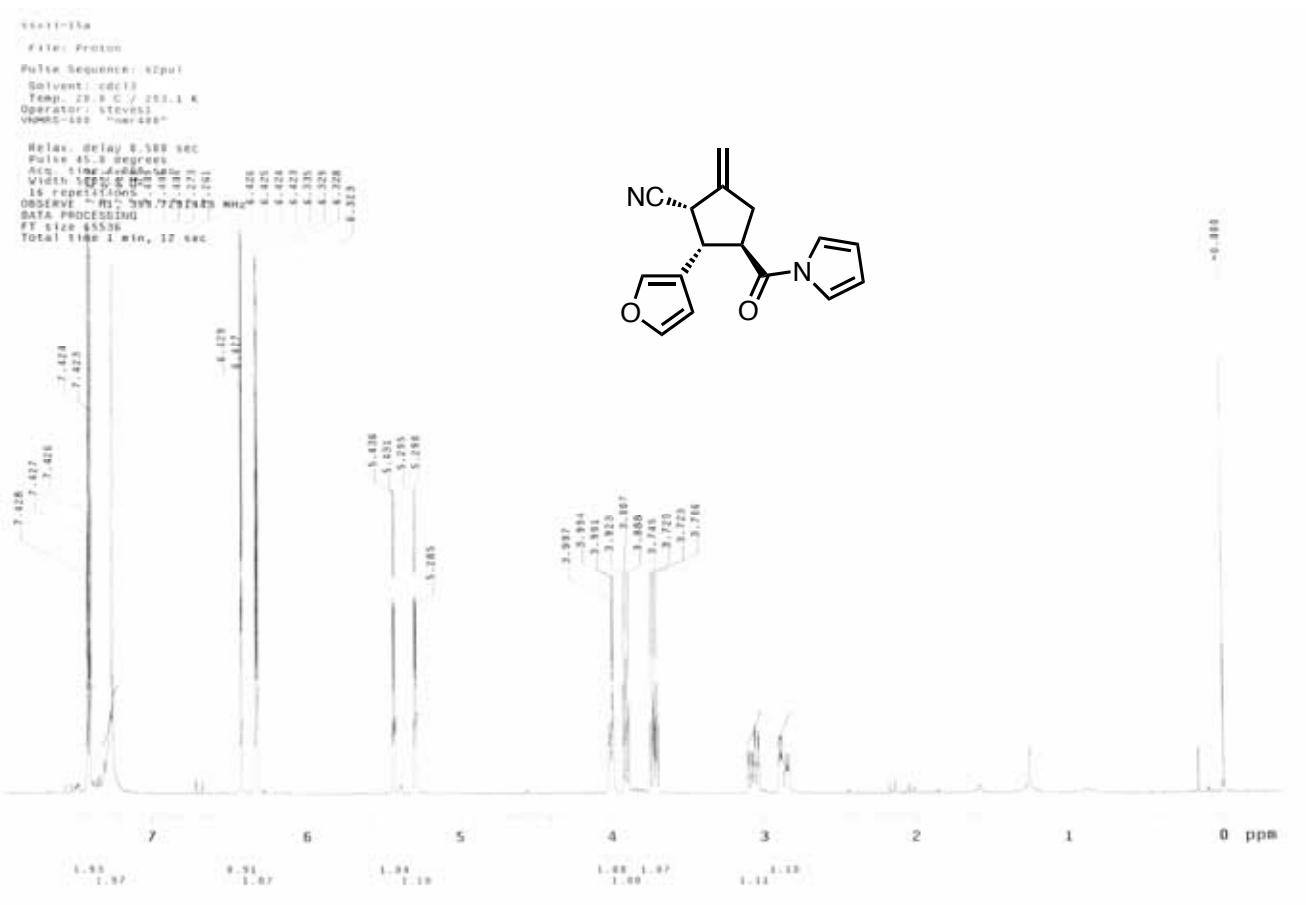

ssxi-64a-13c
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "merc400"
Relax. delay 0.500 sec
Pulse 35.2 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
256 repetitions
OBSERVE C13, 100.6081280 MHz
DECOUPLE H1, 400.1135562 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
line broadening 2.0 Hz
FT size 65536
Total time 33 min, 33 sec
170.800
143.348
137.714
129.000
128.227
127.756
119.126
118.034
113.939
112.210
77.319
77.000
76.681
50.056
47.591
41.221
35.594
ppm

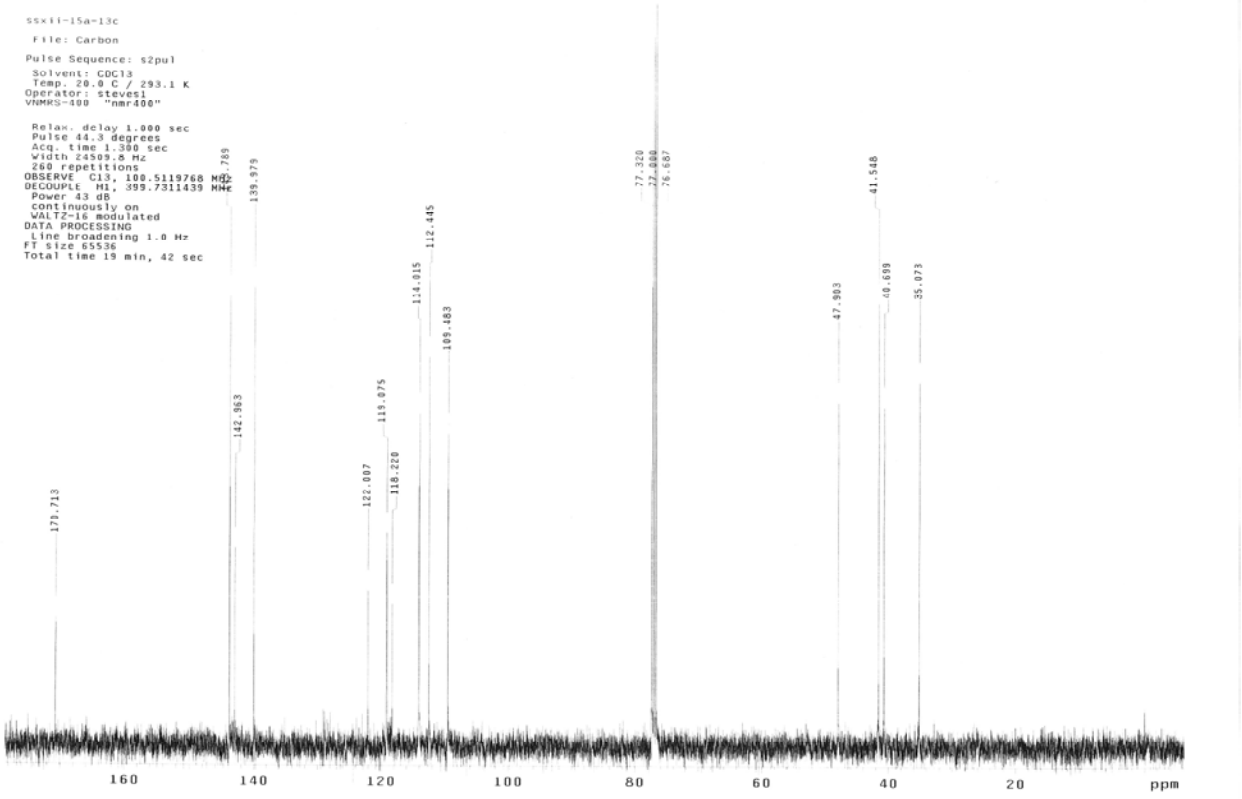

NC
N
O
ppm

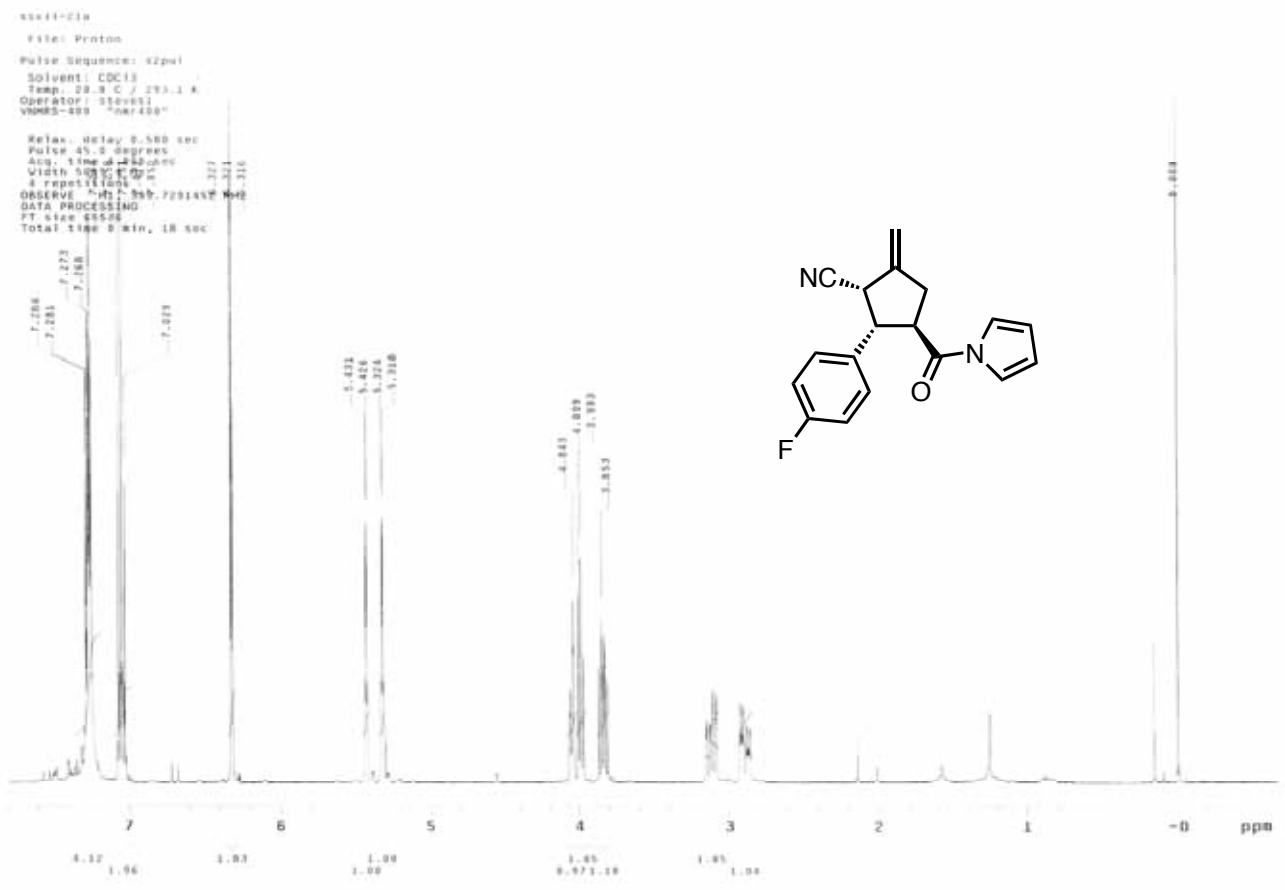

ppm

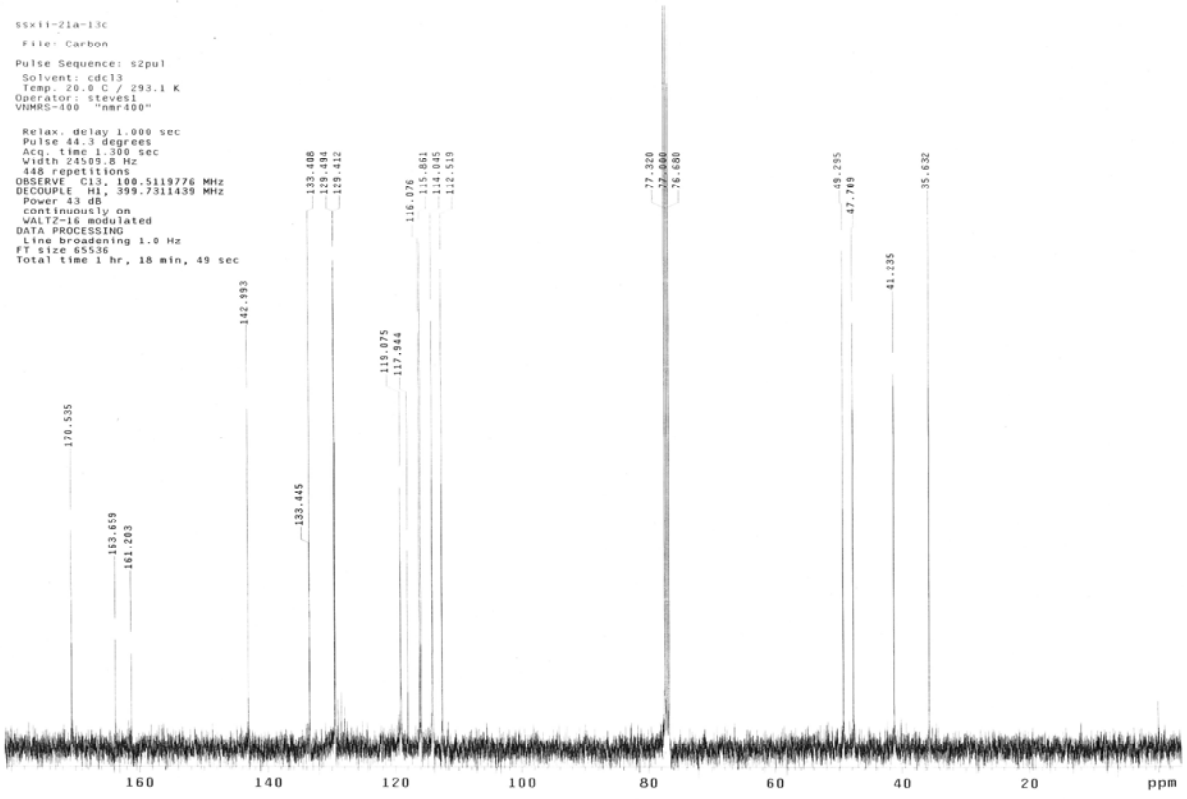

NC
N
O
H_3CO
7
6
5
4
3
2
1
0
ppm

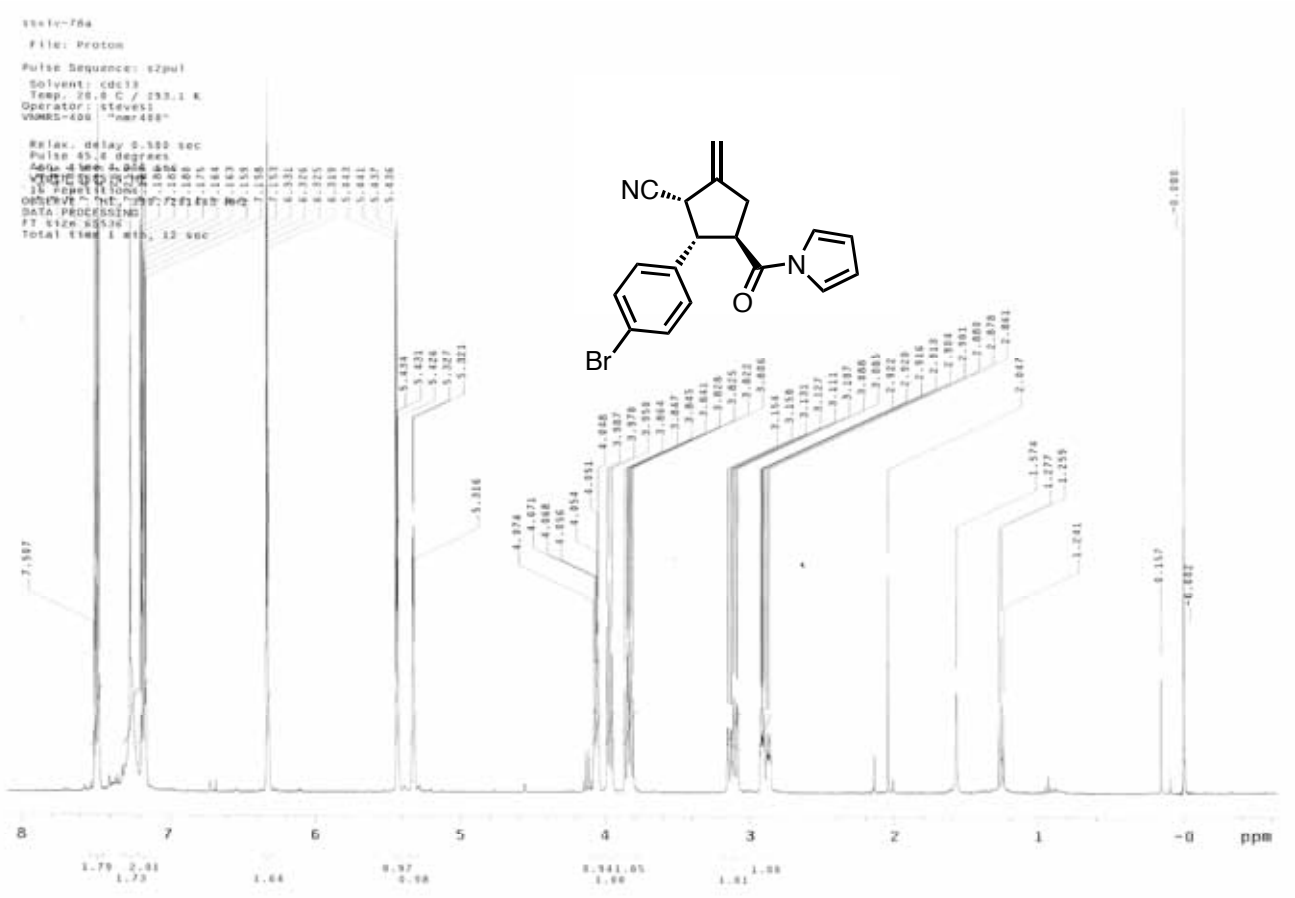

ssxii-12a-13c
File: Carbon
Pulse Sequence: s2pul
Solvent: cdcl3
Temp. 22.0 C / 295.1 K
Operator: stevesl
VNMRS-400 "nmr400"
Relax. delay 1.000 sec
Pulse 44.3 degrees
Acq. time 1.300 sec
Width 24509.8 Hz
608 repetitions
OBSERVE C13, 100.5119761 MHz
DECOUPLE H1, 399.7311439 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 39 min, 24 sec
170.870
159.335
143.432
129.702
128.669
119.120
118.167
114.335
113.888
112.132
77.320
77.000
76.687
55.211
49.516
47.829
41.391
35.542
180
160
140
120
100
80
60
40
20
ppm

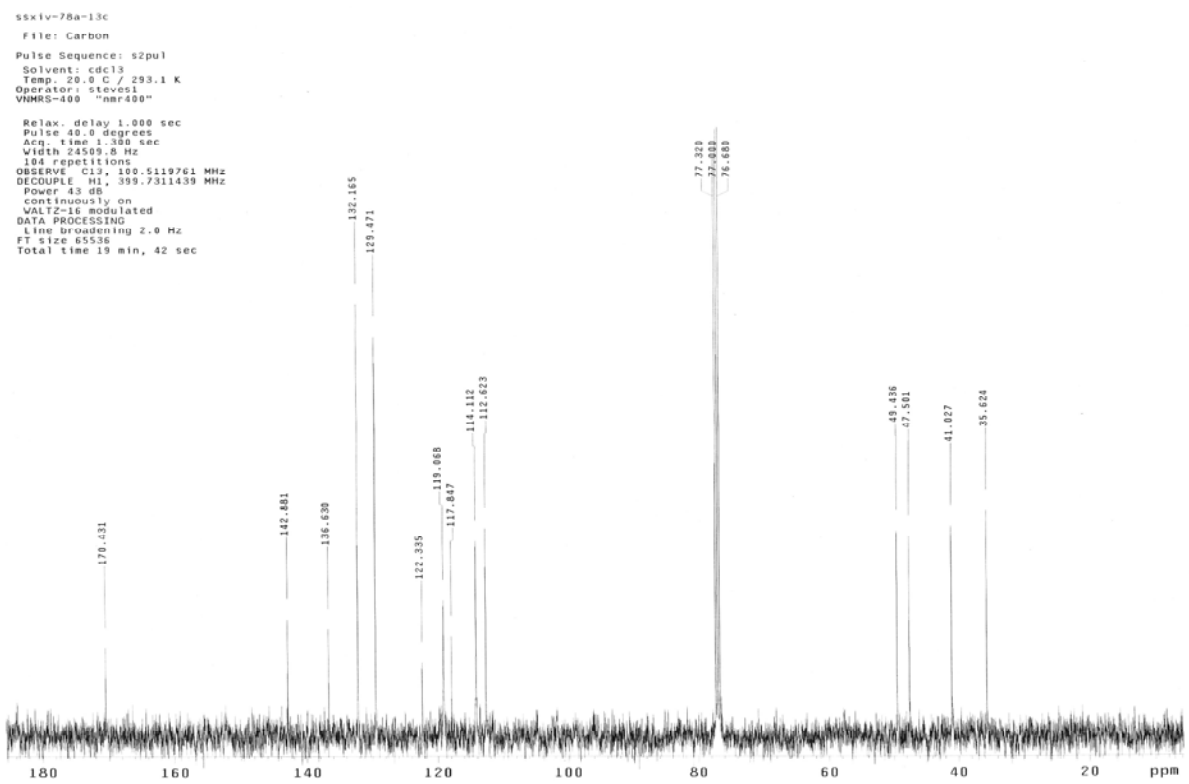

NC
O
O
N
7
6
5
4
3
2
1
0 ppm

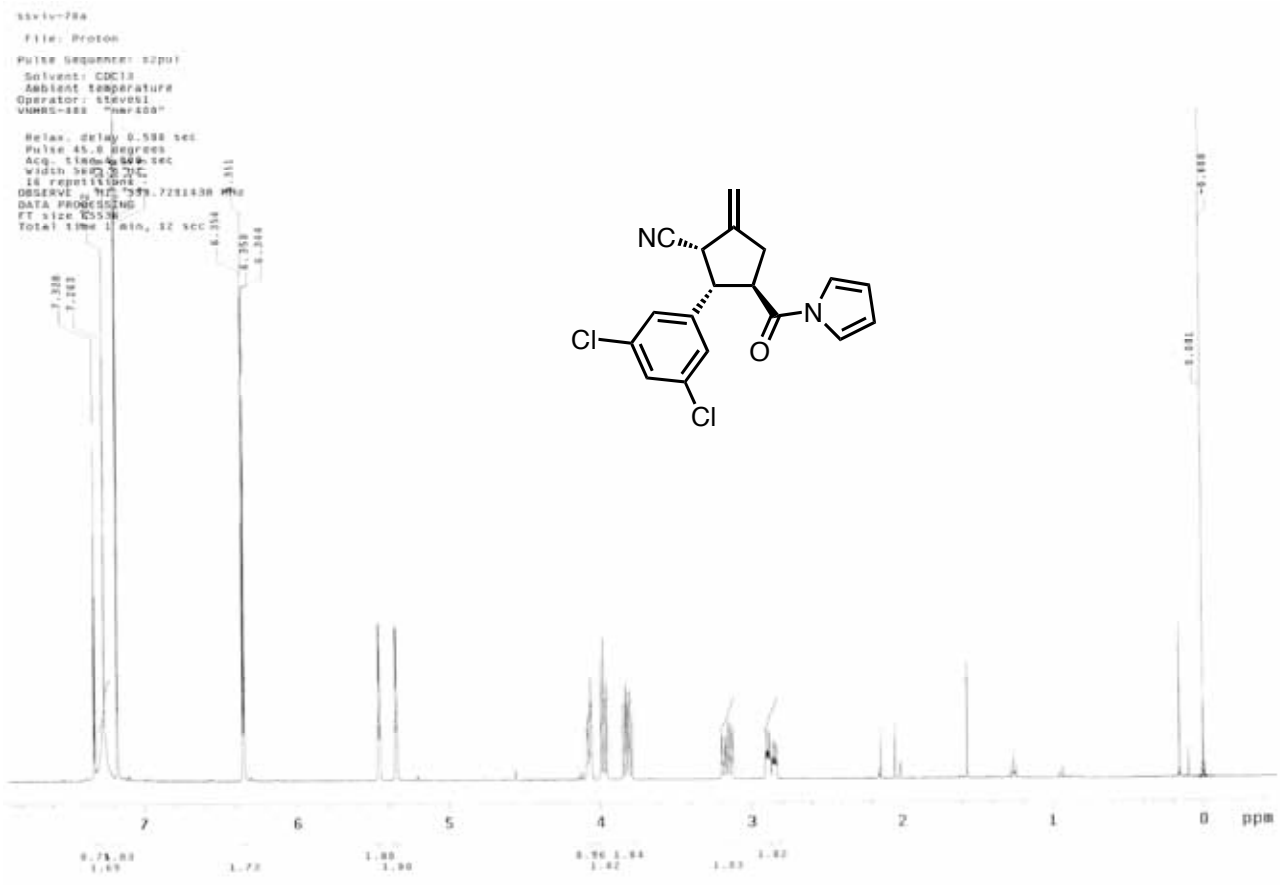

160
140
120
100
80
60
40
20
ppm

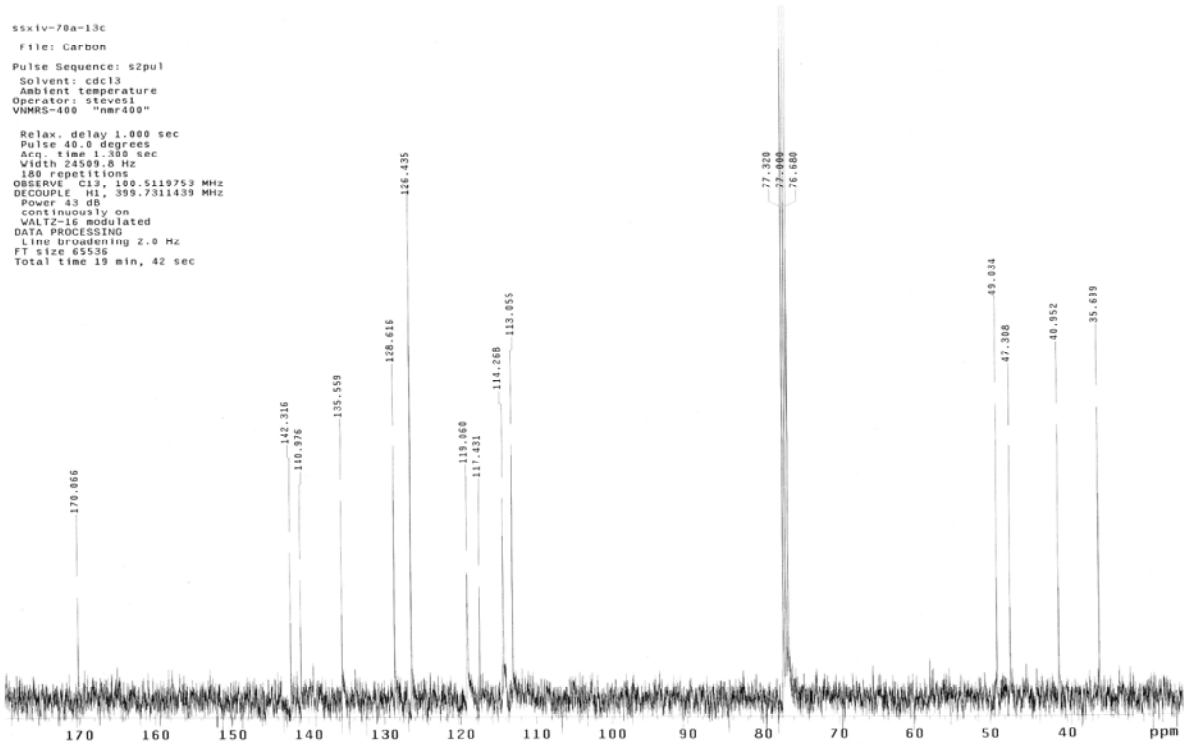

File: Proton
Pulse Sequence: s2pul
Solvent: CDCl3
Temp. 20.0 C / 293.1 K
Operator: stevesl
VNMRS-400 "nmr400"
Relax. delay 0.500 sec
Pulse 45.0 degrees
4 repetitions
DATA PROCESSING
FT size 65536
Total time 0 min, 18 sec
NC
N
O
F
7
6
5
4
3
2
1
-0
ppm

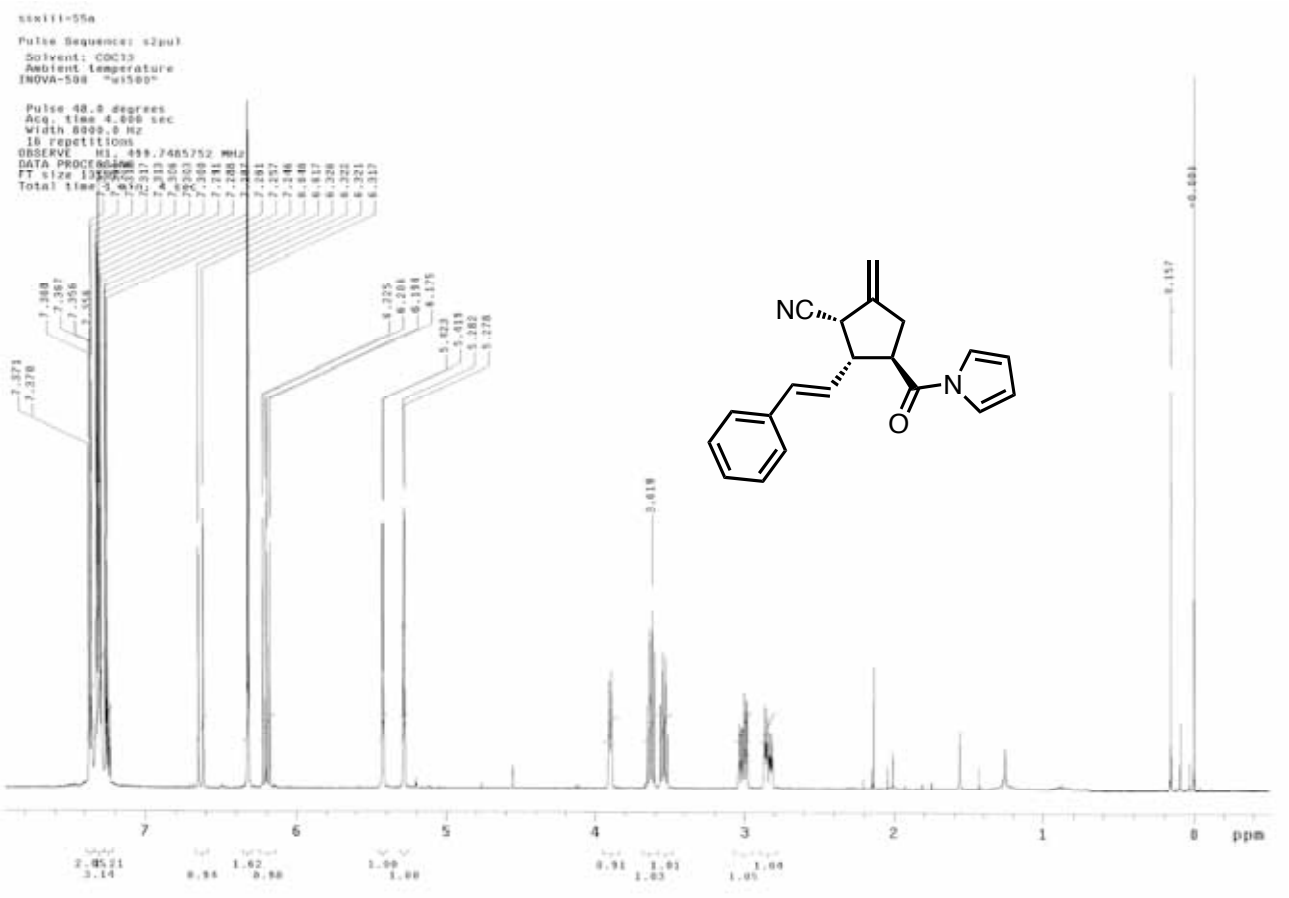

File: Carbon
Pulse Sequence: s2pul
Solvent: cdcl3
Temp. 20.0 C / 293.1 K
Operator: stevesl
VNMRS-400 "nmr400"
Relax. delay 1.000 sec
Pulse 44.3 degrees
Acq. time 1.300 sec
Width 24509.8 Hz
448 repetitions
OBSERVE C13, 100.5119776 MHz
DECOUPLE H1, 399.7311439 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 1 hr, 18 min, 49 sec
170.535
163.659
161.203
142.993
133.445
133.408
129.494
129.412
119.075
117.944
116.076
115.861
114.045
112.519
77.320
77.000
76.680
49.295
47.769
41.235
35.632
160
140
120
100
80
60
40
20
ppm

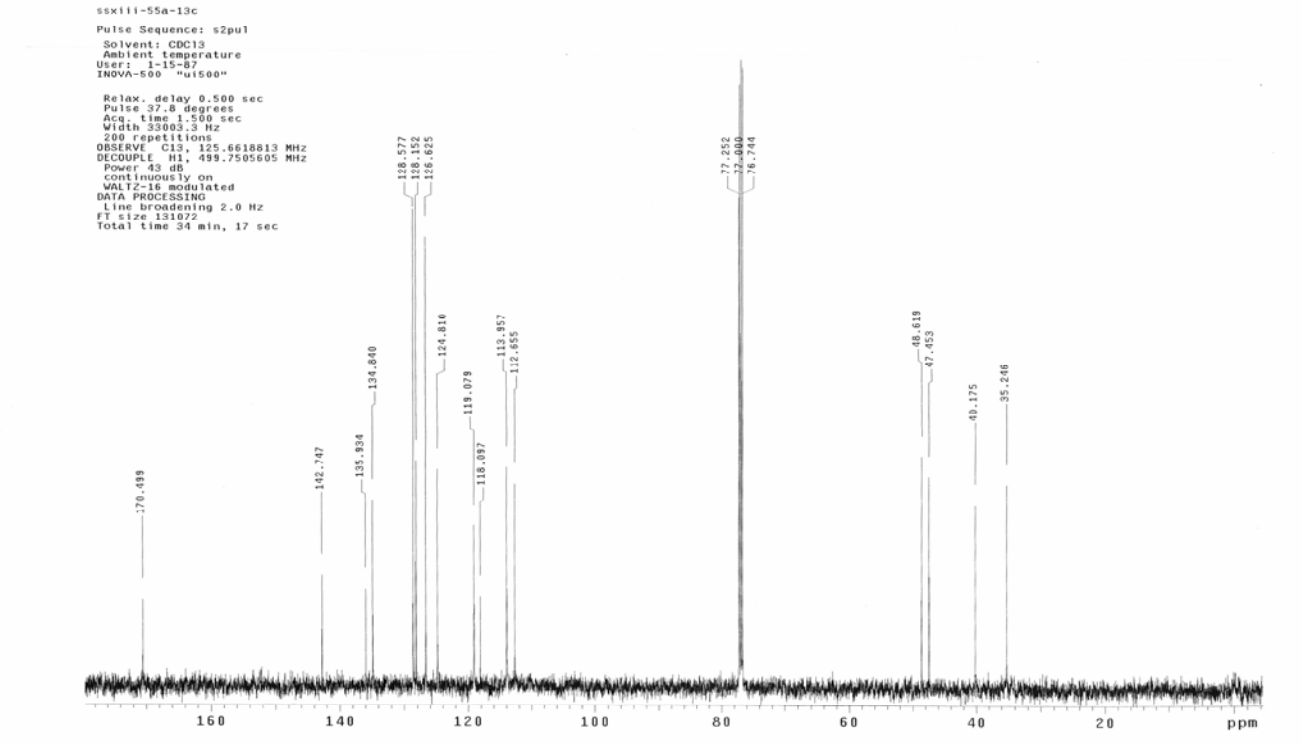

NC
O
N
Br
8
7
6
5
4
3
2
1
-0
ppm

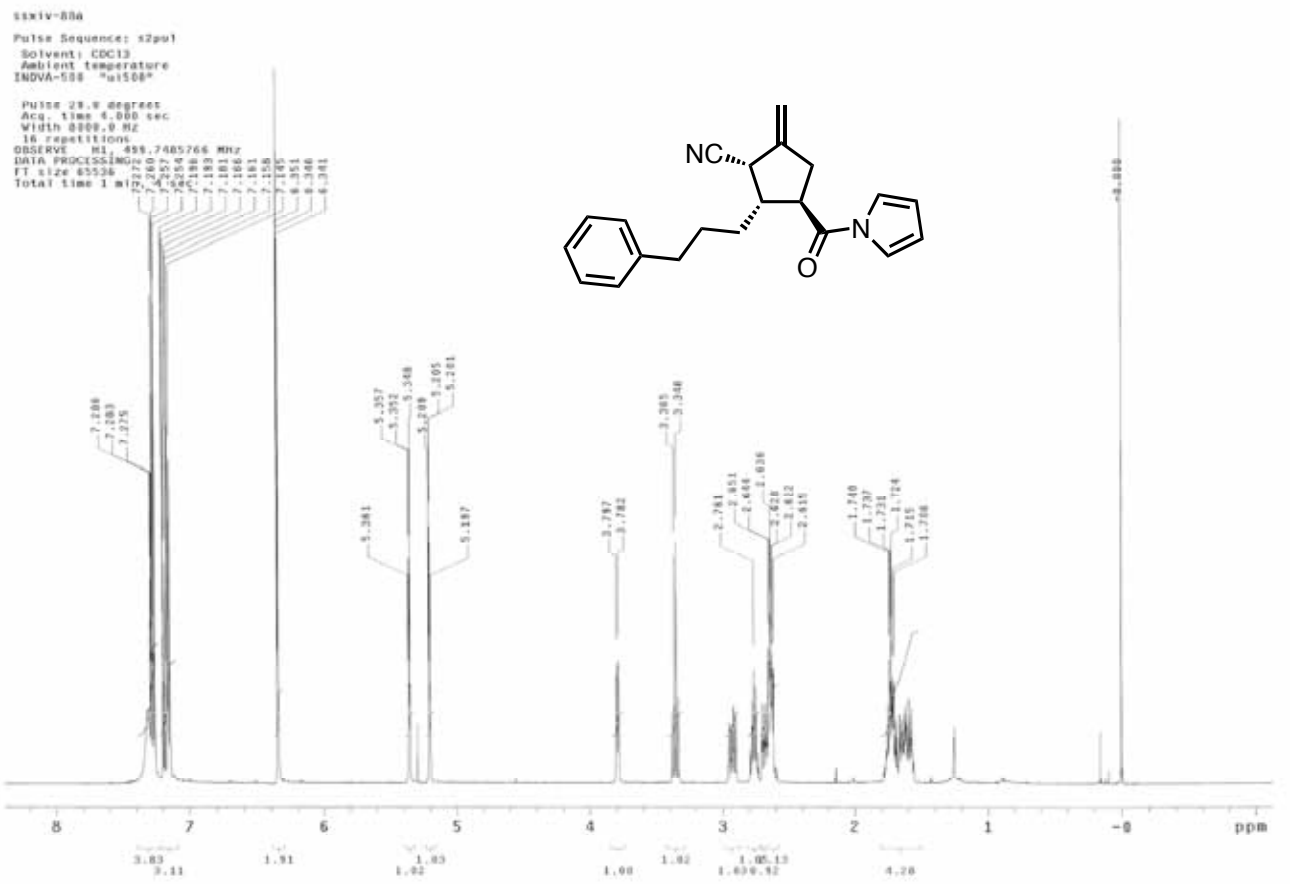

ssxiv-78a-13c
File: Carbon
Pulse Sequence: s2pul
Solvent: cdcl3
Temp. 20.0 C / 293.1 K
Operator: stevesi
VNMRS-400 "nmr400"
Relax. delay 1.000 sec
Pulse 40.0 degrees
Acq. time 1.380 sec
Width 24509.8 Hz
104 repetitions
OBSERVE C13, 100.5119761 MHz
DECOUPLE H1, 399.7311439 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 65536
Total time 19 min, 42 sec
180
160
140
120
100
80
60
40
20
ppm

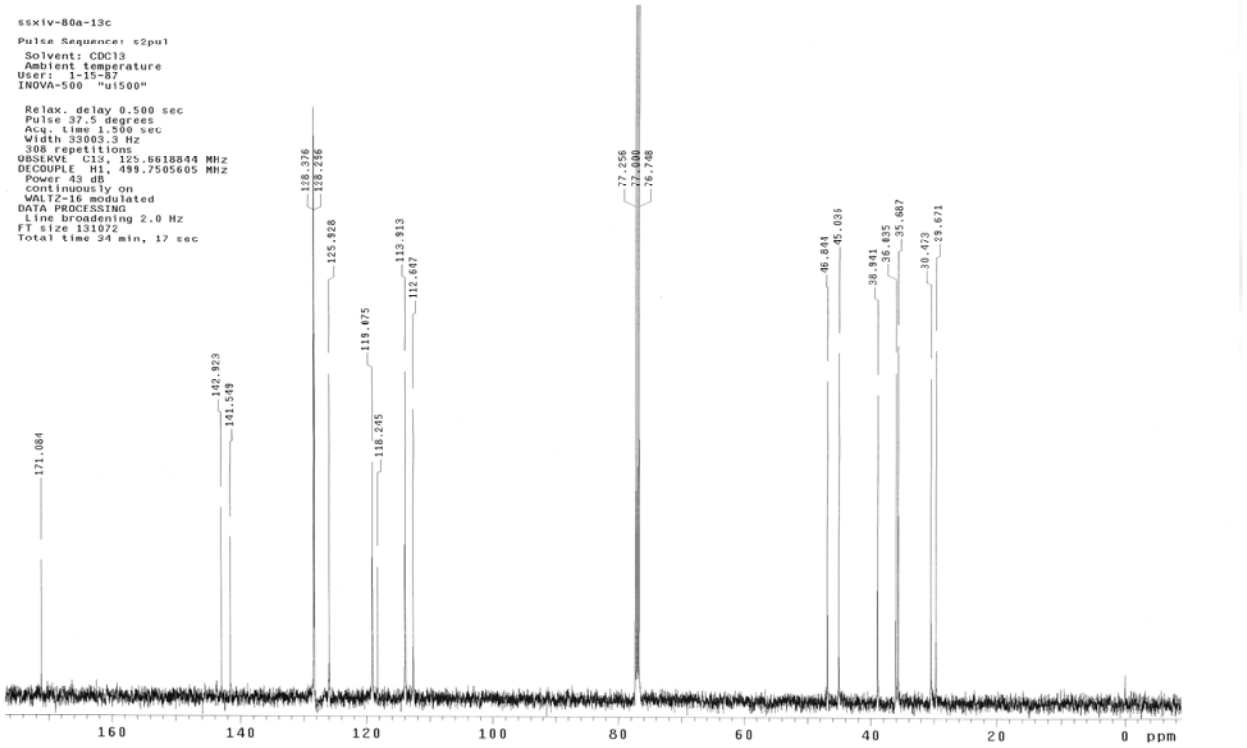

NC
Cl
Cl
O
N
7
6
5
4
3
2
1
0
ppm

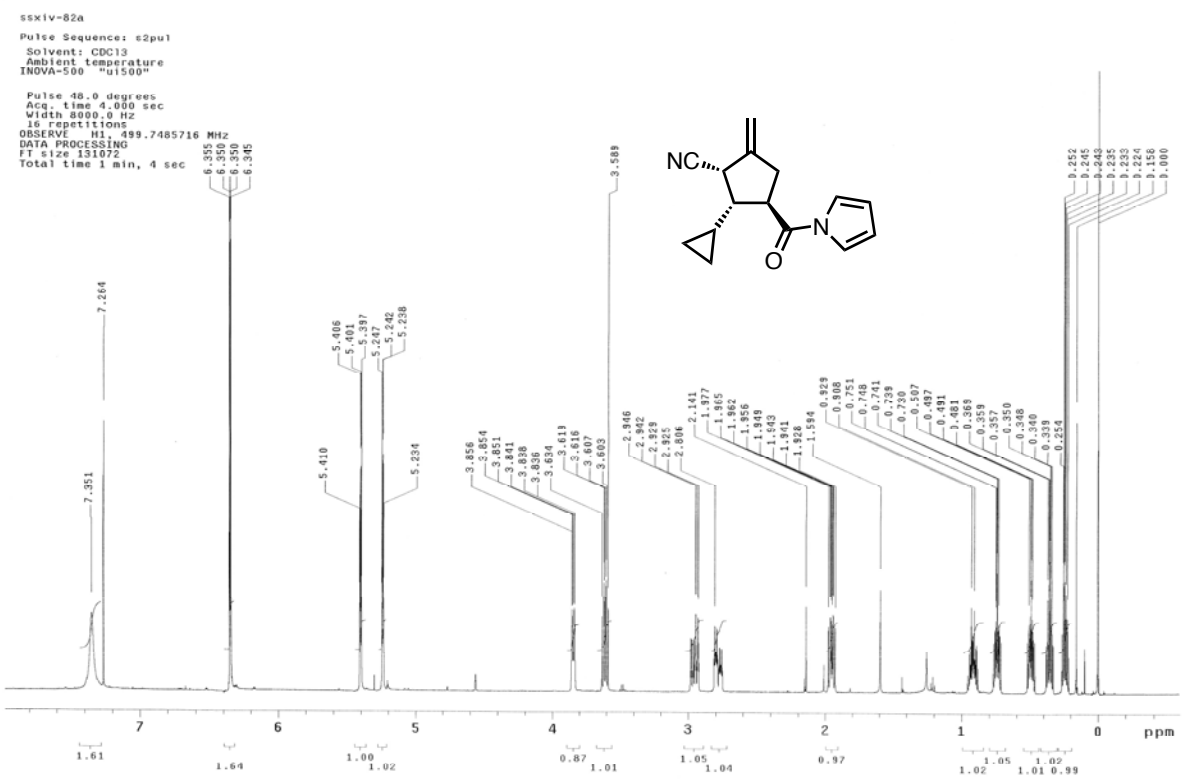

ssxiv-70a-13c
File: Carbon
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
Operator: steves1
VNMRS-400 "nmr400"
Relax. delay 1.000 sec
Pulse 40.0 degrees
Acq. time 1.300 sec
Width 24509.8 Hz
180 repetitions
OBSERVE C13, 100.5119753 MHz
DECOUPLE H1, 399.7311439 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 65536
Total time 19 min, 42 sec
170.066
142.316
110.976
135.559
128.616
126.435
119.060
117.431
114.268
113.055
77.320
77.000
76.680
49.034
47.308
40.952
35.639
170
160
150
140
130
120
110
100
90
80
70
60
50
40
ppm

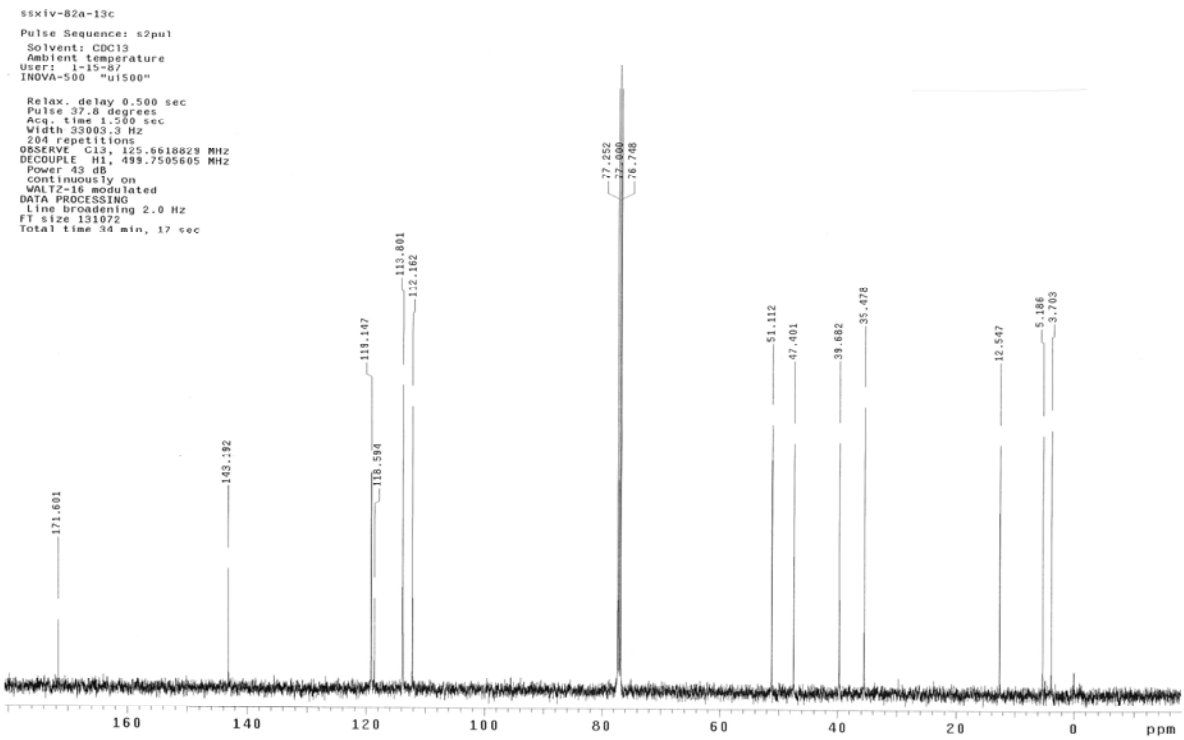

ssxiii-55a
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
INOVA-500 "ui500"
Pulse 48.0 degrees
Acq. time 4.000 sec
width 8000.0 Hz
16 repetitions
NC
N
O
ppm


ssxiii-55a-13c
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
INOVA-500 "ui500"
Relax. delay 0.500 sec
Pulse 37.8 degrees
Acq. time 1.500 sec
Width 33003.3 Hz
200 repetitions
OBSERVE C13, 125.6618813 MHz
DECOUPLE H1, 499.7505605 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 131072
Total time 34 min, 17 sec
ppm


ssxiv-88a
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
INOVA-500 "ui500"
Pulse 28.9 degrees
Acq. time 4.000 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.7485766 MHz
DATA PROCESSING
FT size 65536
Total time 1 min, 4 sec
NC
N
O
ppm


ssxiv-88a-13c
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-15-87
INOVA-500 "ui500"
Relax. delay 0.500 sec
Pulse 37.5 degrees
Acq. time 1.500 sec
Width 33003.3 Hz
308 repetitions
OBSERVE C13, 125.6618844 MHz
DECOUPLE H1, 499.7505605 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 131072
Total time 34 min, 17 sec
171.084
142.923
141.549
128.376
128.256
125.828
119.675
118.245
113.913
112.647
77.256
77.000
76.748
46.844
45.036
38.941
36.435
35.687
30.473
29.671
ppm


ssxiv-82a
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
INOVA-500 "ui500"
Pulse 48.0 degrees
Acq. time 4.000 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.7485716 MHz
DATA PROCESSING
FT size 131072
Total time 1 min, 4 sec
NC
N
O
ppm


ssxiv-82a-13c
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: l-15-87
INOVA-500 "ui500"
Relax. delay 0.500 sec
Pulse 37.8 degrees
Acq. time 1.500 sec
Width 33003.3 Hz
204 repetitions
OBSERVE C13, 125.6618829 MHz
DECOUPLE H1, 499.7505605 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
line broadening 2.0 Hz
FT size 131072
Total time 34 min, 17 sec
ppm