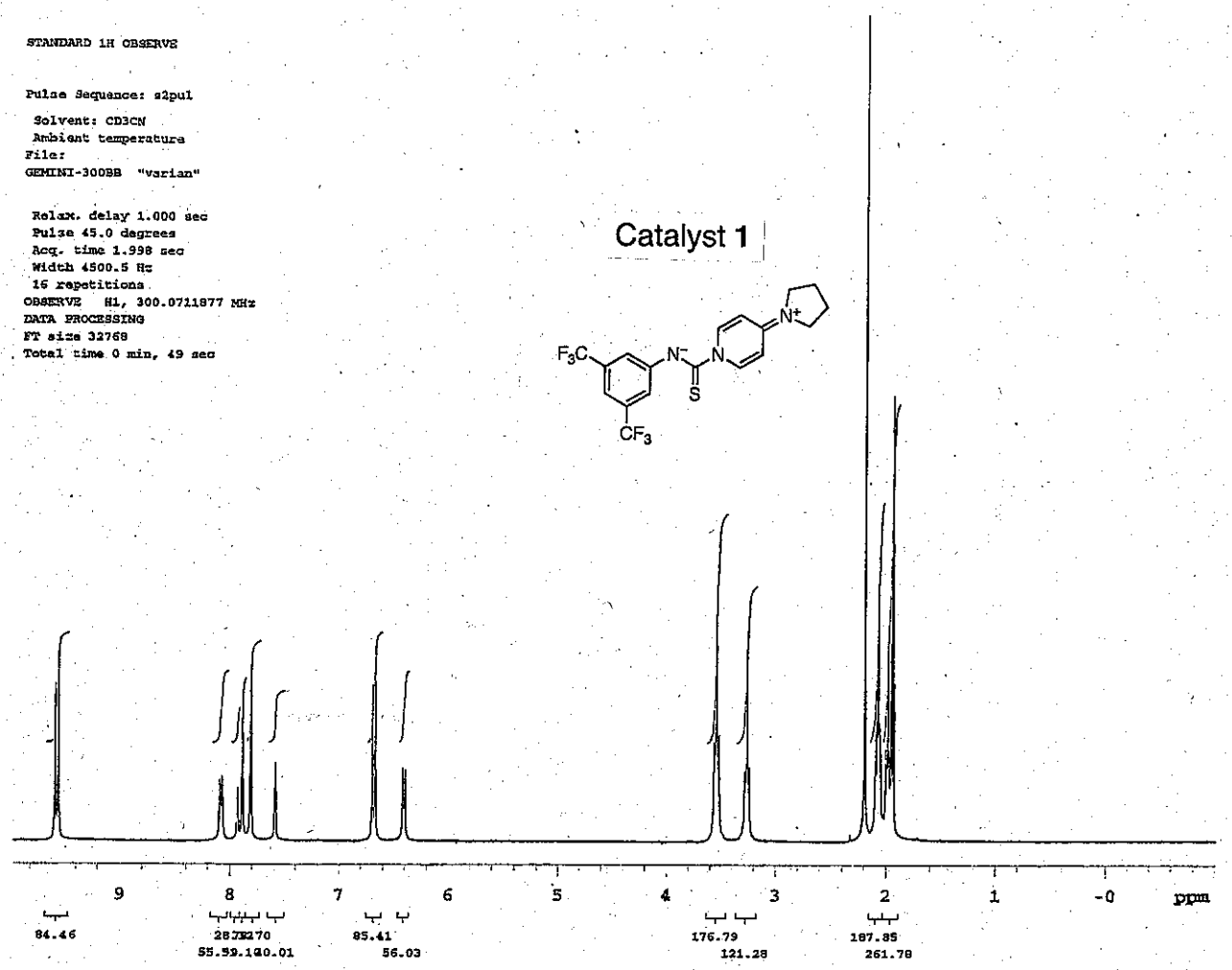
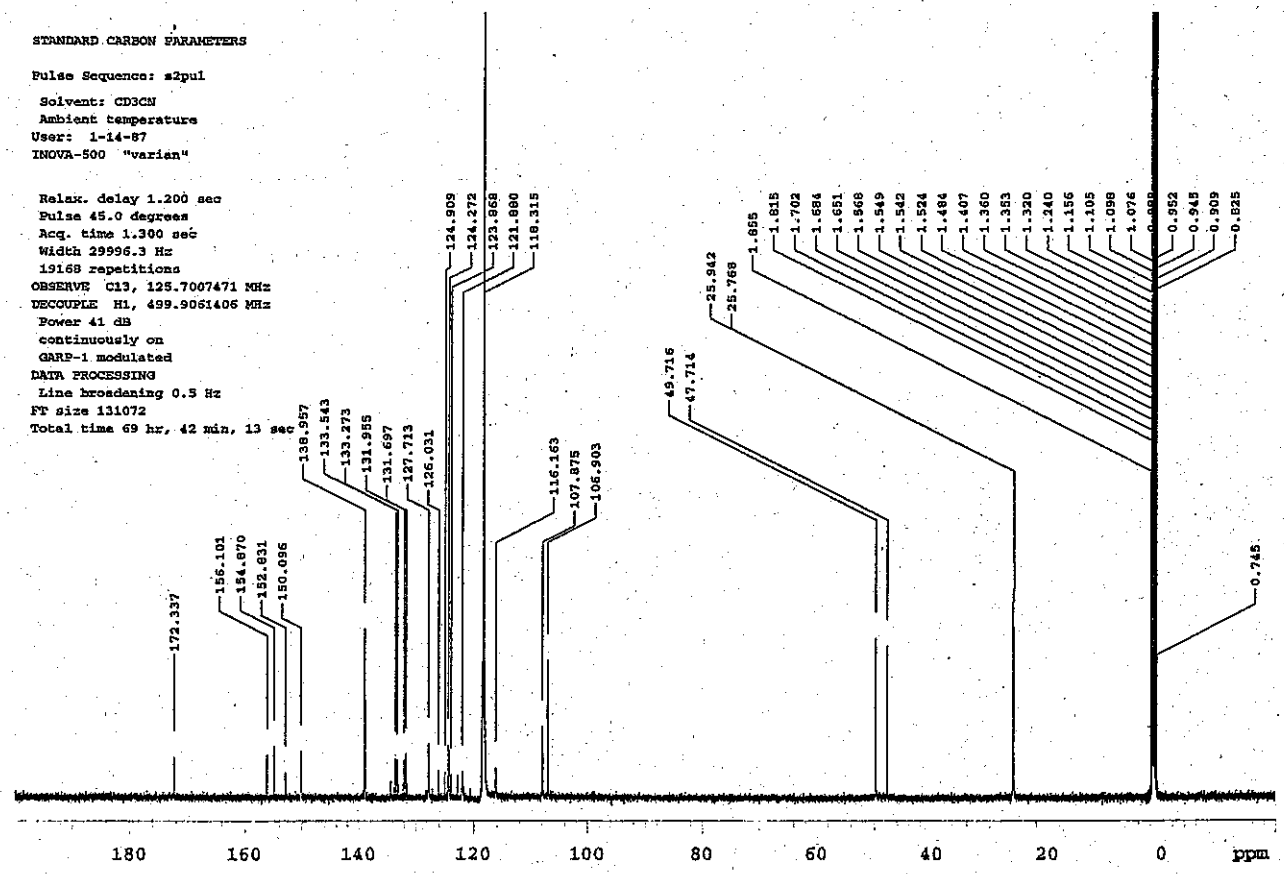
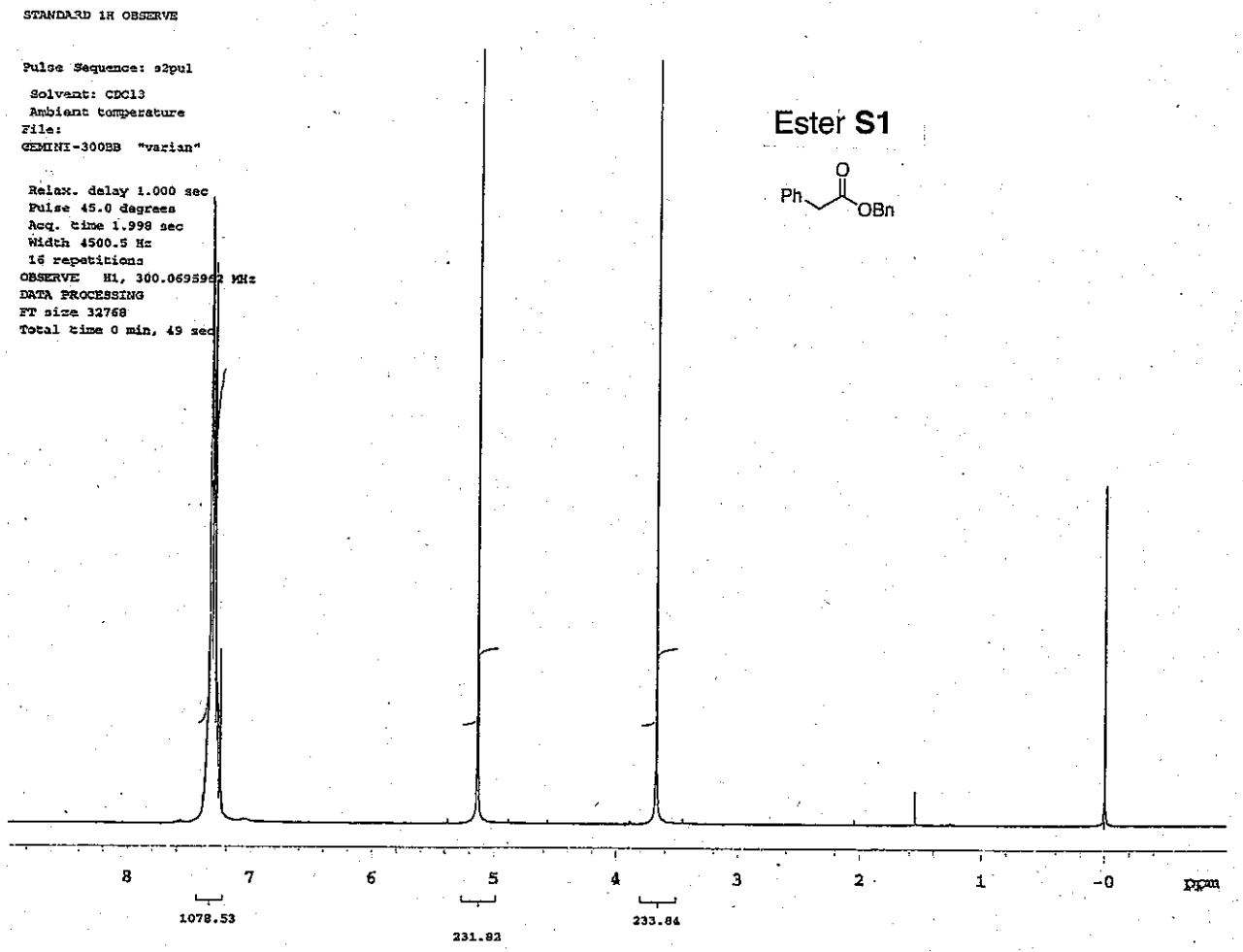
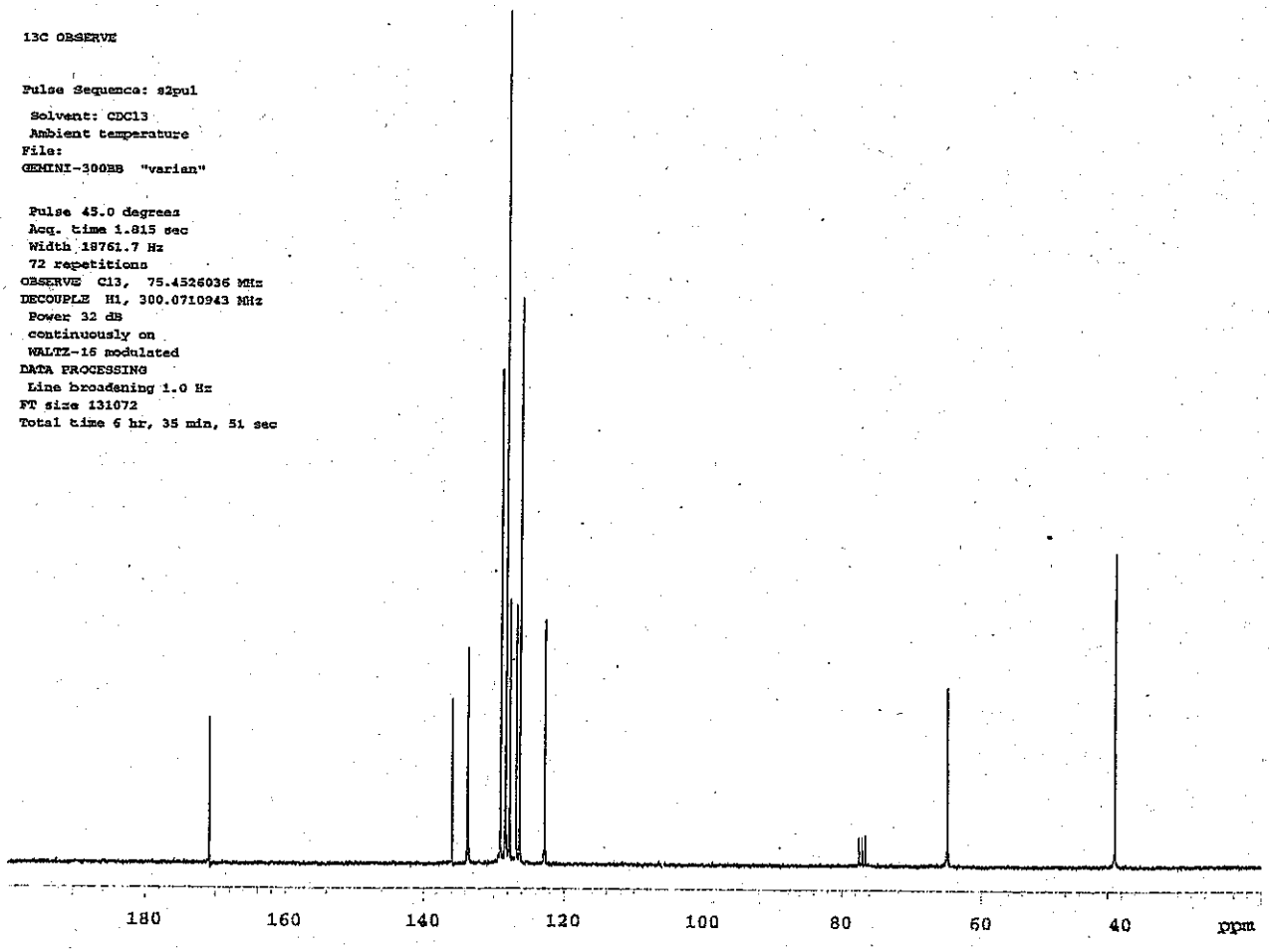
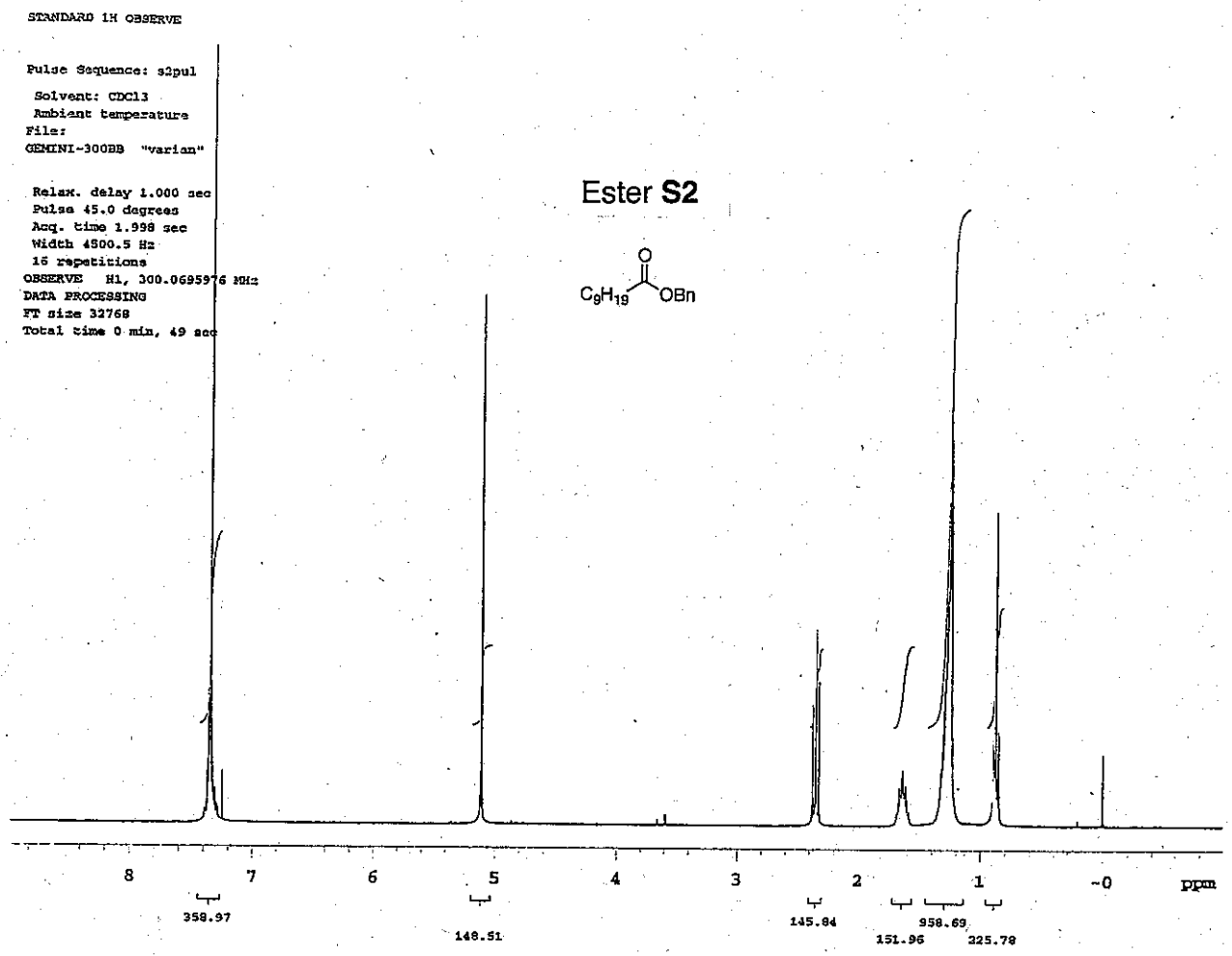
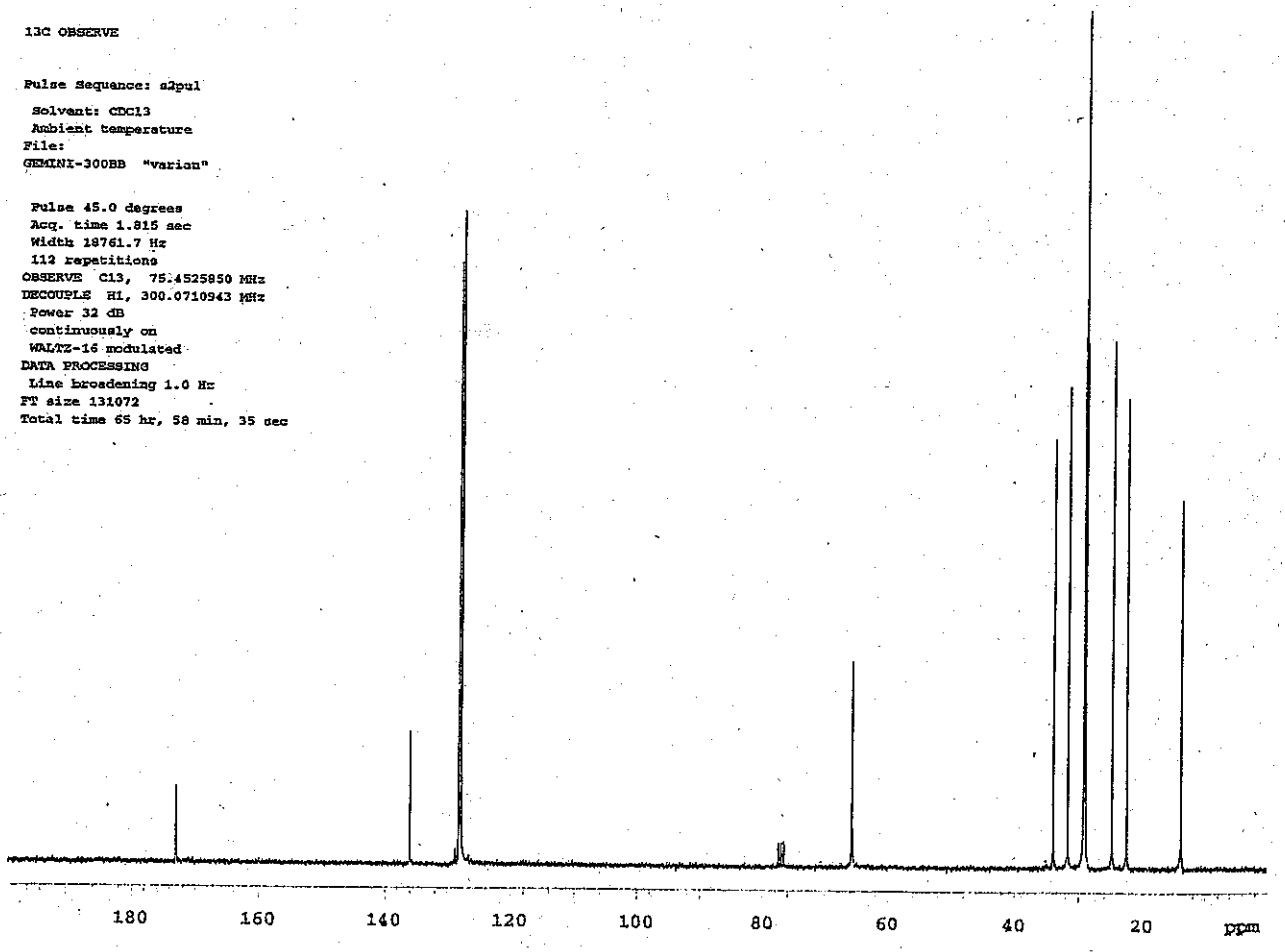

STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CD3CN
Ambient temperature
File:
GEMINI-300BB "varian"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.998 sec
Width 4500.5 Hz
16 repetitions
OBSERVE H1, 300.0711877 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 49 sec
Catalyst 1
F3C
CF3
N
S
N+
9
8
7
6
5
4
3
2
1
-0
ppm
84.46
55.59
140.01
85.41
56.03
176.79
121.28
187.85
261.78

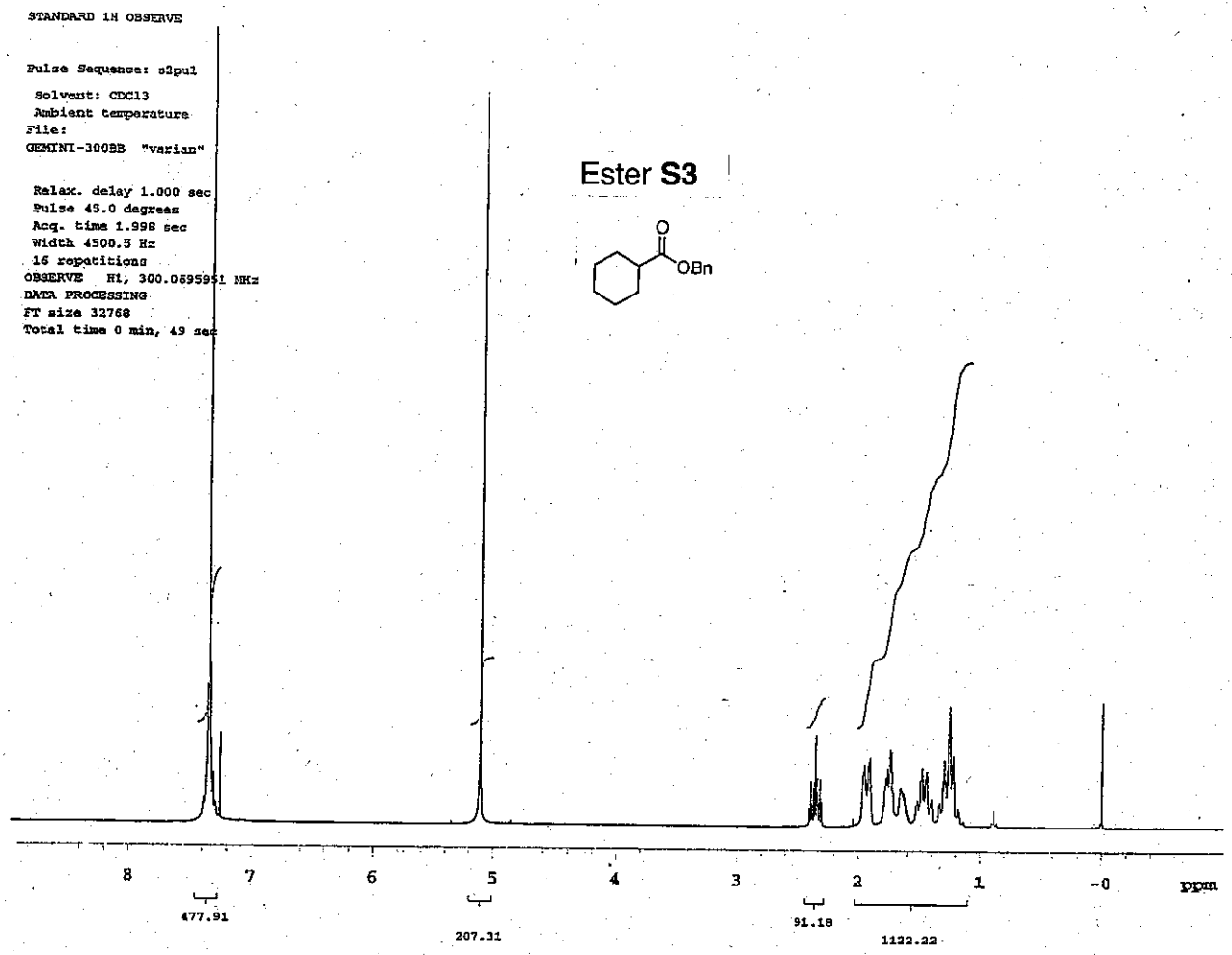

STANDARD CARBON PARAMETERS
Pulse Sequence: s2pul
Solvent: CD3CN
Ambient temperature
User: 1-14-87
INOVA-500 "varian"
Relax. delay 1.200 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 29996.3 Hz
19168 repetitions
OBSERVE C13, 125.7007471 MHz
DECOUPLE H1, 499.9061406 MHz
Power 41 dB
continuously on
GARP-1 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 69 hr, 42 min, 13 sec
172.337
156.101
154.870
152.631
150.096
138.957
133.543
133.273
131.985
131.697
127.713
126.031
124.909
124.272
123.868
121.880
118.315
116.163
107.875
106.903
49.716
47.714
25.942
25.768
1.865
1.815
1.702
1.684
1.651
1.568
1.549
1.542
1.524
1.484
1.407
1.360
1.353
1.330
1.240
1.156
1.105
1.098
1.076
0.952
0.945
0.909
0.825
0.745
180
160
140
120
100
80
60
40
20
0
ppm

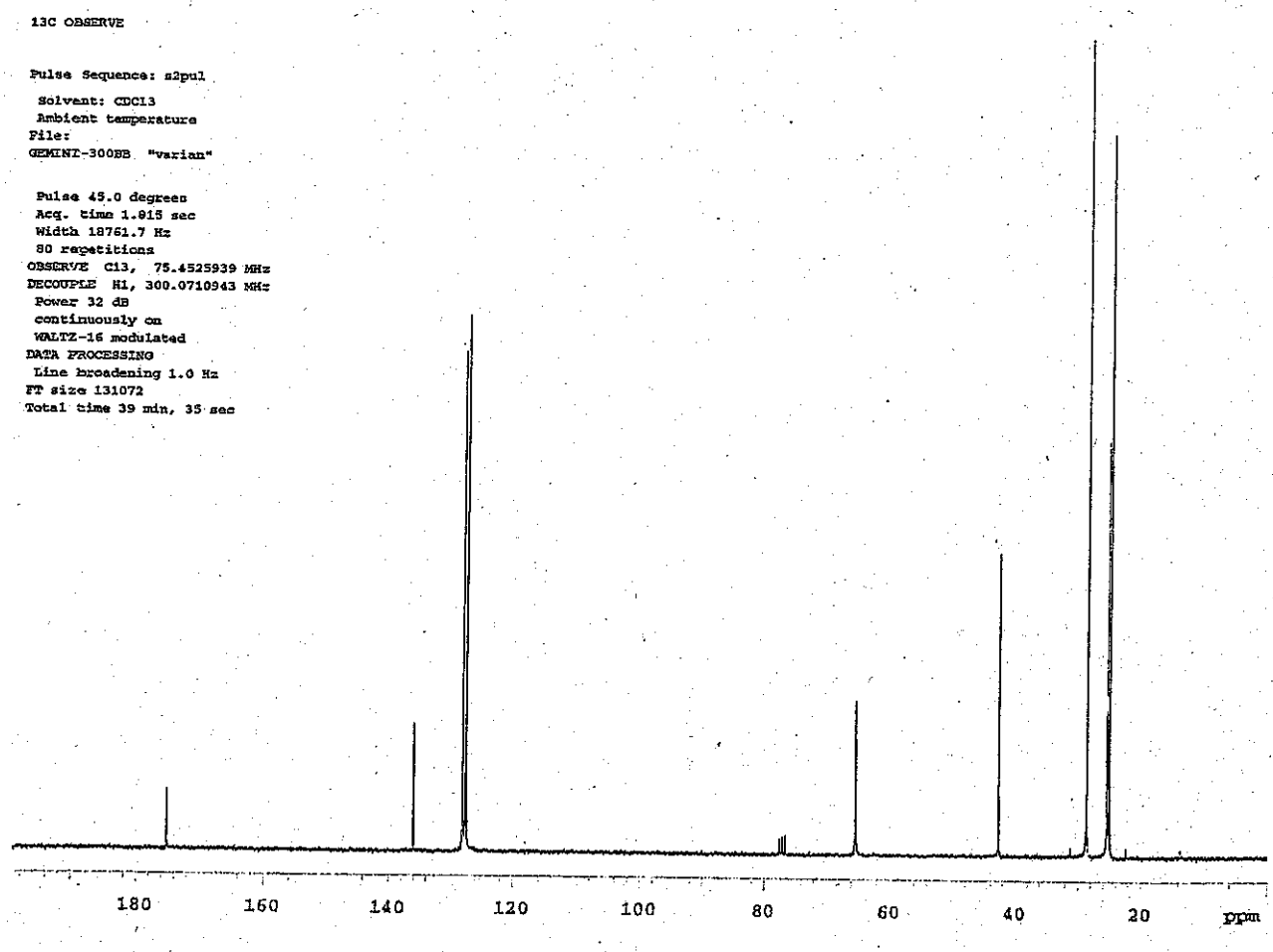

STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File:
GEMINI-300BB "varian"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.998 sec
Width 4500.5 Hz
16 repetitions
OBSERVE H1, 300.0695962 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 49 sec
Ester S1
Ph
O
OBn
8
7
6
5
4
3
2
1
-0
ppm
1078.53
231.82
233.84

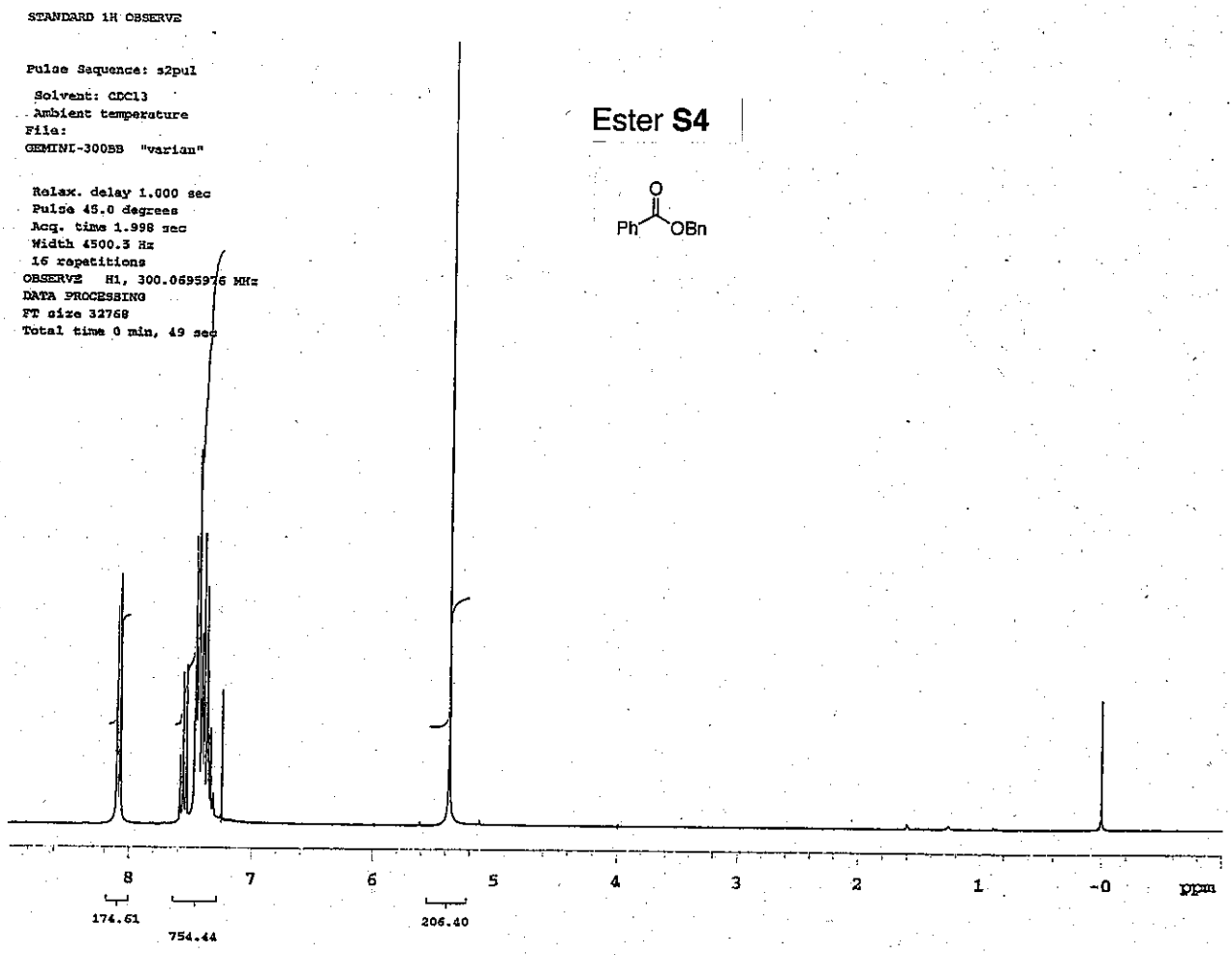

13C OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File:
GEMINI-300BB "varian"
Pulse 45.0 degrees
Acq. time 1.815 sec
Width 18761.7 Hz
72 repetitions
OBSERVE C13, 75.4526036 MHz
DECOUPLE H1, 300.0710943 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 6 hr, 35 min, 51 sec
180
160
140
120
100
80
60
40
ppm

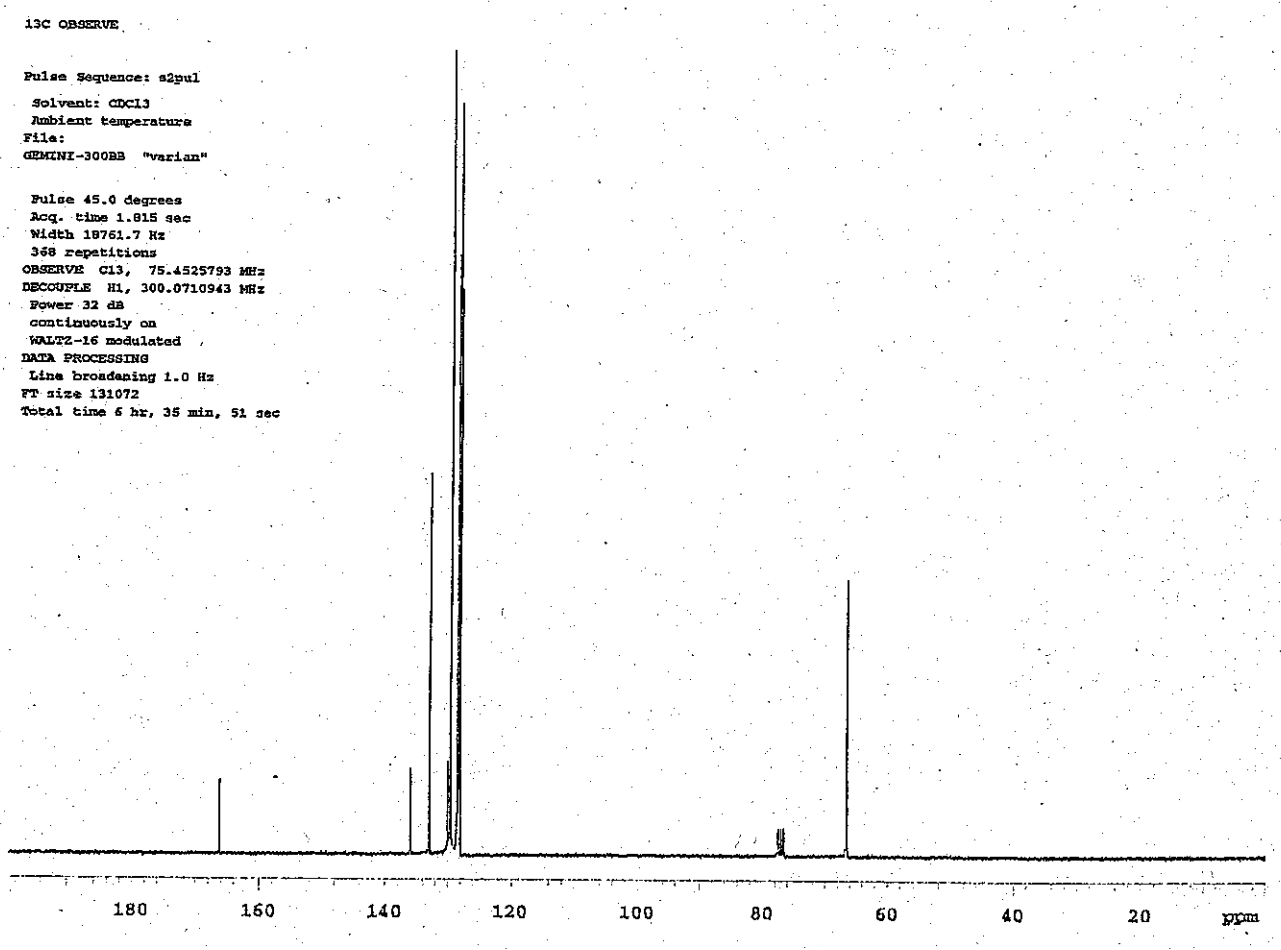

STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File:
GEMINI-300BB "varian"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.998 sec
Width 4500.5 Hz
16 repetitions
OBSERVE H1, 300.0695976 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 49 sec
Ester S2
C9H19
OBn
8
7
6
5
4
3
2
1
~0
ppm
358.97
148.51
145.84
151.96
958.69
225.78

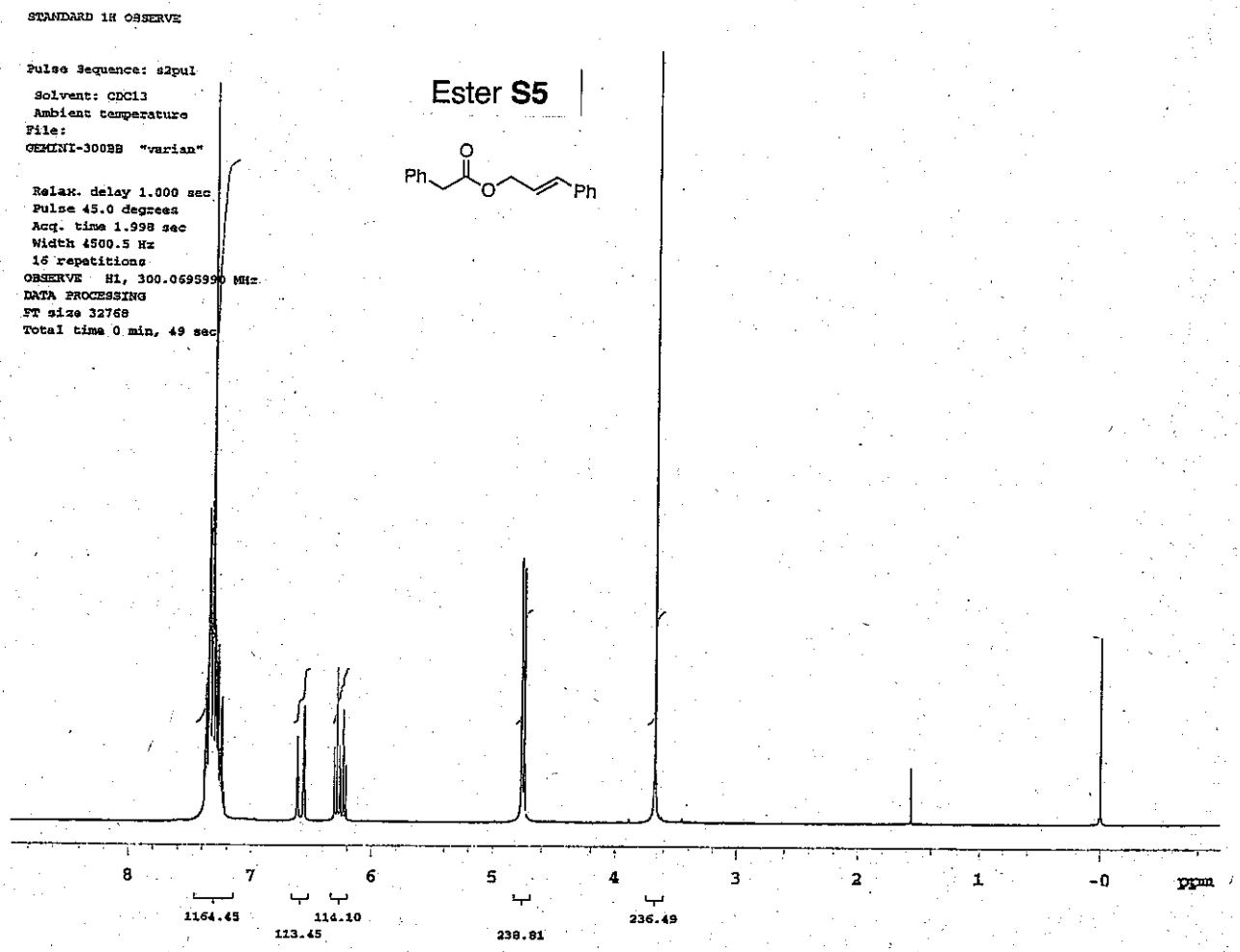

13C OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File:
GEMINI-300BB "varian"
Pulse 45.0 degrees
Acq. time 1.815 sec
Width 18761.7 Hz
112 repetitions
OBSERVE C13, 75.4525850 MHz
DECOUPLE H1, 300.0710943 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 65 hr, 58 min, 35 sec
180
160
140
120
100
80
60
40
20
ppm

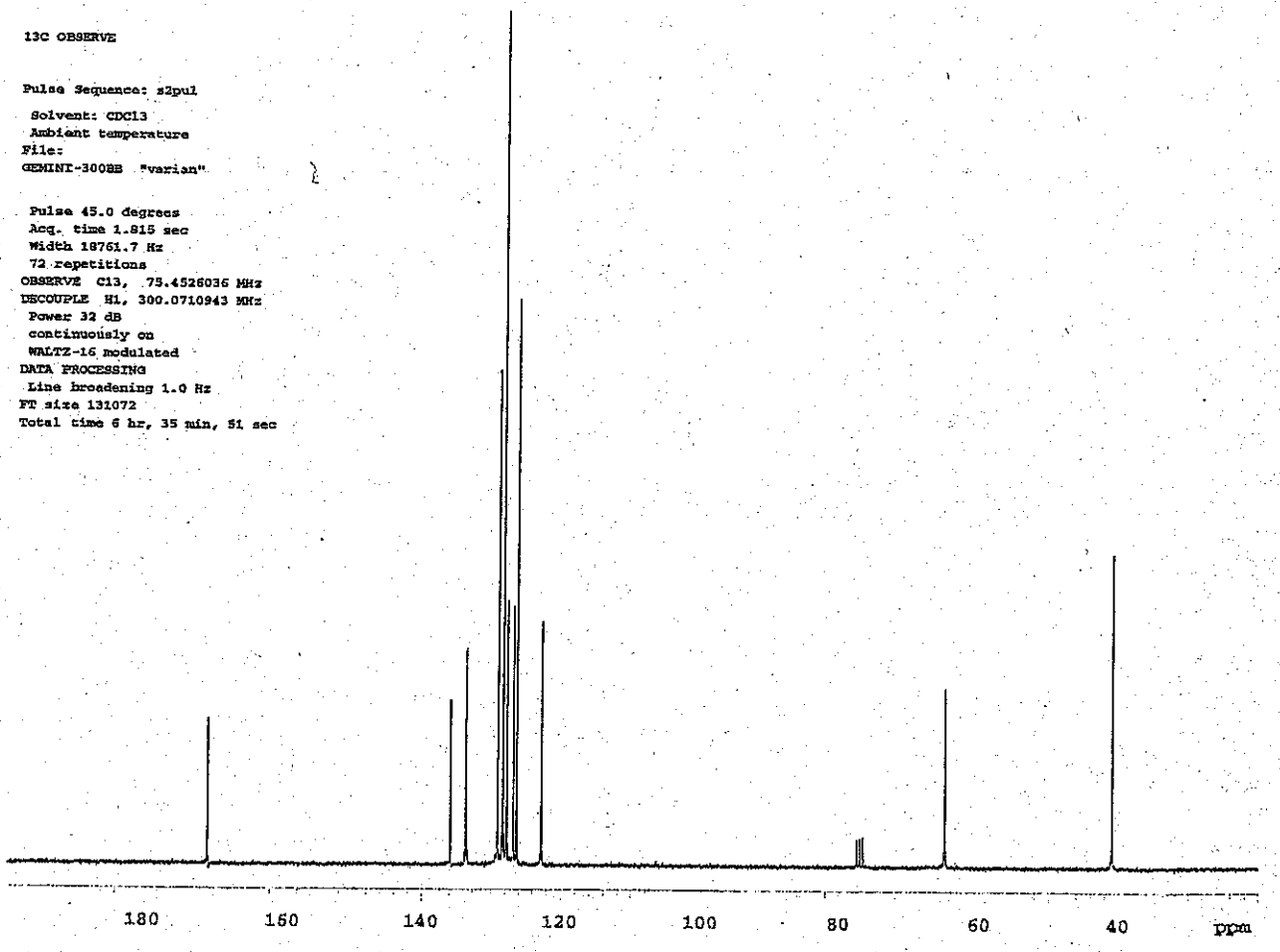

STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File:
GEMINI-300BB "varian"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.998 sec
Width 4500.5 Hz
16 repetitions
OBSERVE H1, 300.0595951 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 49 sec
Ester S3
OBn
8
7
6
5
4
3
2
1
-0
ppm
477.91
207.31
91.18
1122.22


13C OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File:
GEMINI-300BB "varian"
Pulse 45.0 degrees
Acq. time 1.915 sec
Width 18761.7 Hz
80 repetitions
OBSERVE C13, 75.4525939 MHz
DECOUPLE H1, 300.0710943 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 39 min, 35 sec
180
160
140
120
100
80
60
40
20
ppm


STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File:
GEMINI-300BB "varian"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.998 sec
Width 4500.3 Hz
16 repetitions
OBSERVE H1, 300.0695976 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 49 sec
Ester S4
Ph
O
OBn
8
7
6
5
4
3
2
1
-0
ppm
174.61
754.44
206.40


13C OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File:
GEMINI-300BB "varian"
Pulse 45.0 degrees
Acq. time 1.815 sec
Width 18761.7 Hz
368 repetitions
OBSERVE C13, 75.4525793 MHz
DECOUPLE H1, 300.0710943 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 6 hr, 35 min, 51 sec
180
160
140
120
100
80
60
40
20
ppm


STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File:
GEMINI-300BB "varian"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.998 sec
Width 4500.5 Hz
16 repetitions
OBSERVE H1, 300.0695990 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 49 sec
Ester S5
Ph
O
O
Ph
8
7
6
5
4
3
2
1
-0
ppm
1164.45
113.45
114.10
238.81
236.49

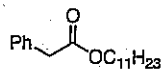

13C OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File:
GEMINI-300BB "varian"
Pulse 45.0 degrees
Acq. time 1.815 sec
Width 18761.7 Hz
72 repetitions
OBSERVE C13, 75.4526036 MHz
DECOUPLE H1, 300.0710943 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 6 hr, 35 min, 51 sec
180
160
140
120
100
80
60
40
ppm

STANDARD 1H OBSERVE

Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File:
GEMINI-300BB "varian"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.998 sec
Width 4500.5 Hz
16 repetitions
OBSERVE H1, 300.0695924 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 49 sec

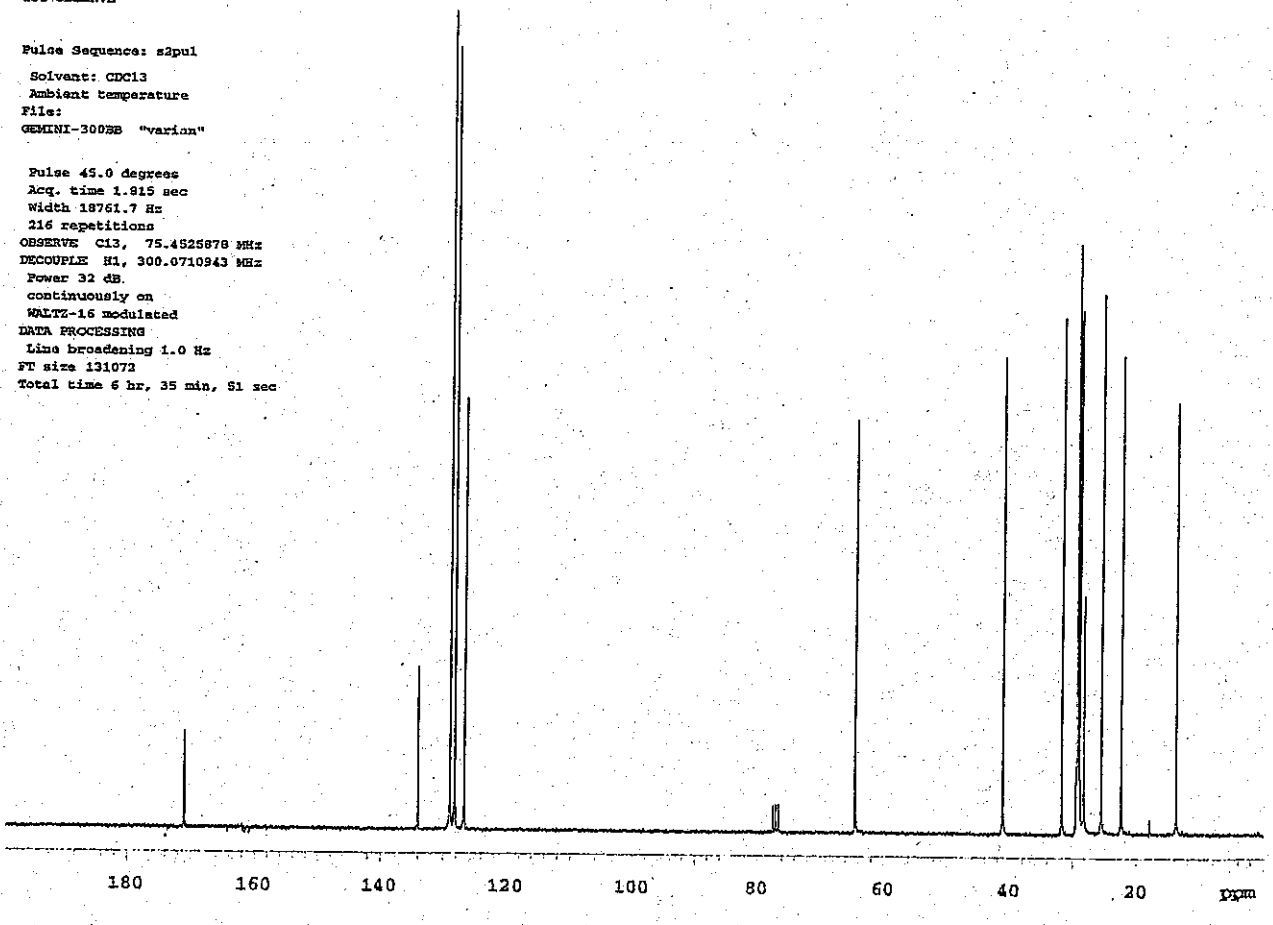
Ester **S6**

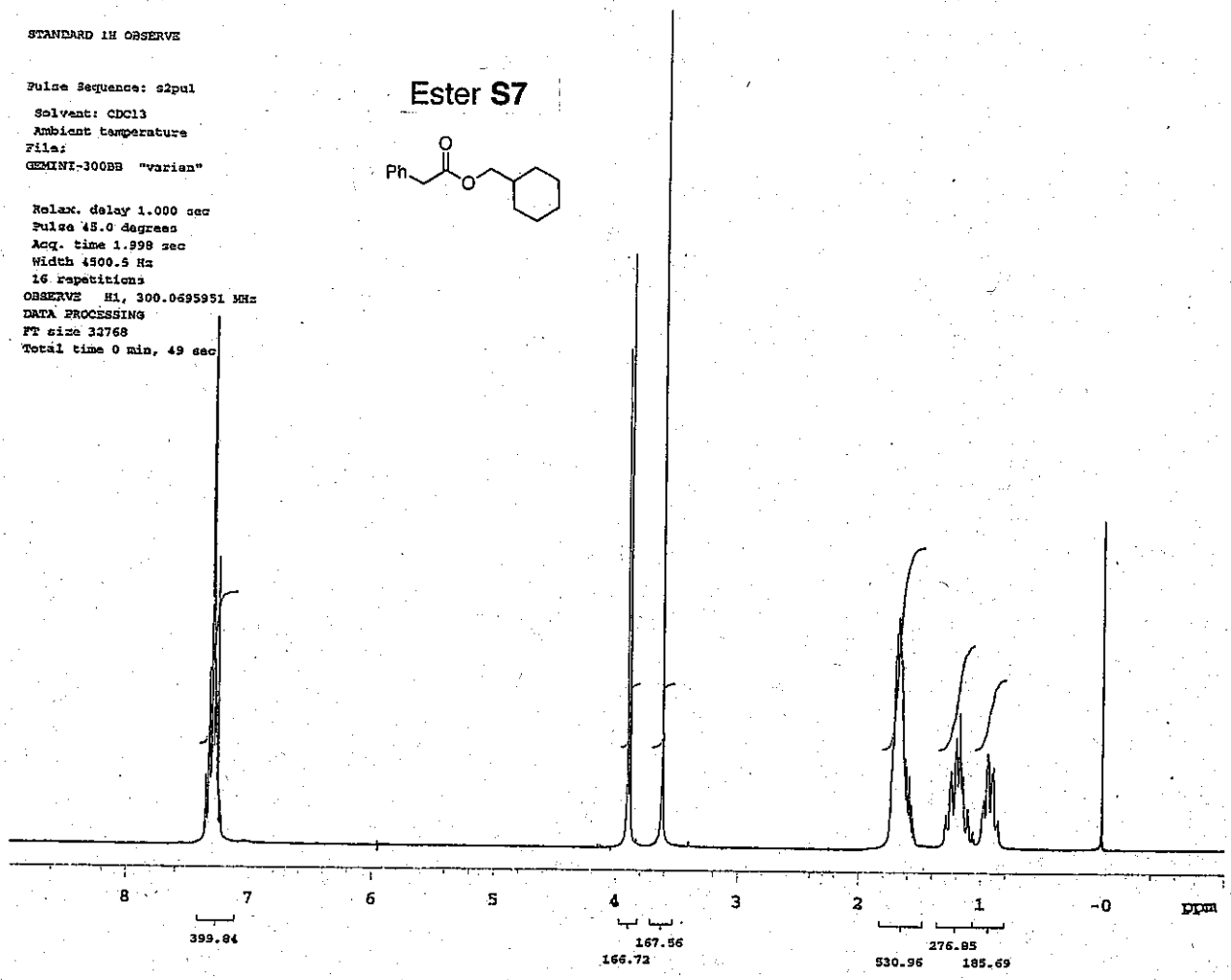


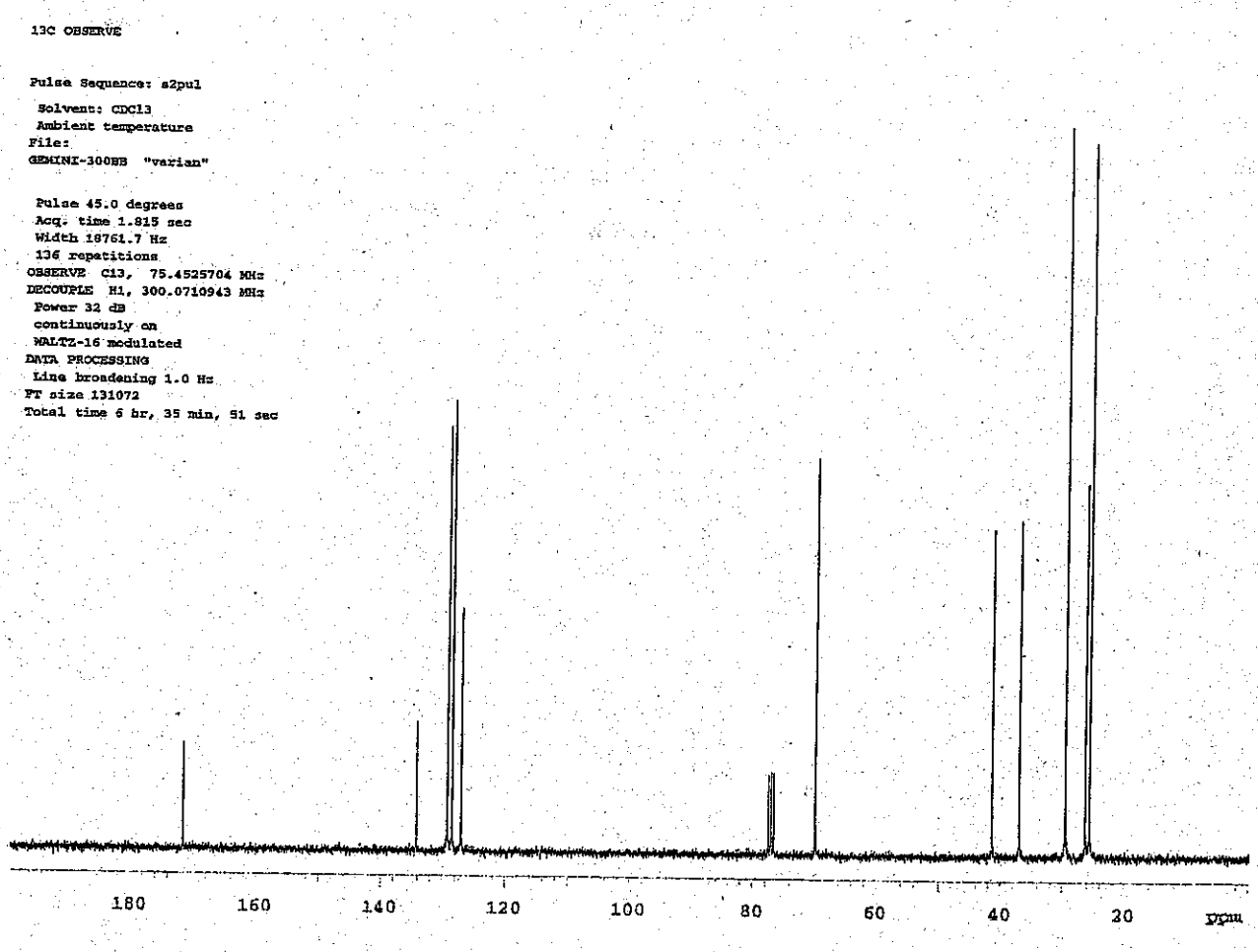
13C OBSERVE

Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File:
GEMINI-300BB "varian"

Pulse 45.0 degrees
Acq. time 1.815 sec
Width 18761.7 Hz
216 repetitions
OBSERVE C13, 75.4525878 MHz
DECOUPLE H1, 300.0710943 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 6 hr, 35 min, 51 sec




STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File:
GEMINI-300BB "varian"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.998 sec
Width 4500.5 Hz
16 repetitions
OBSERVE H1, 300.0695951 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 49 sec
Ester S7
Ph
O
O
8
7
6
5
4
3
2
1
-0
ppm
399.84
167.56
166.72
276.85
530.96
185.69

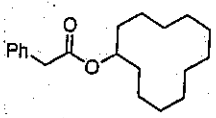

13C OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File:
GEMINI-300BB "varian"
Pulse 45.0 degrees
Acq. time 1.815 sec
Width 19761.7 Hz
136 repetitions
OBSERVE C13, 75.4525704 MHz
DECOUPLE H1, 300.0710943 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 6 hr, 35 min, 51 sec
180
160
140
120
100
80
60
40
20
ppm

STANDARD 1H OBSERVE

Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File:
GEMINI-300BB "varian"

Relax. delay 1.000 sec
Pulse 10.6 degrees
Acq. time 1.998 sec
Width 4500.5 Hz
16 repetitions
OBSERVE H1, 300.0696058 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 49 sec

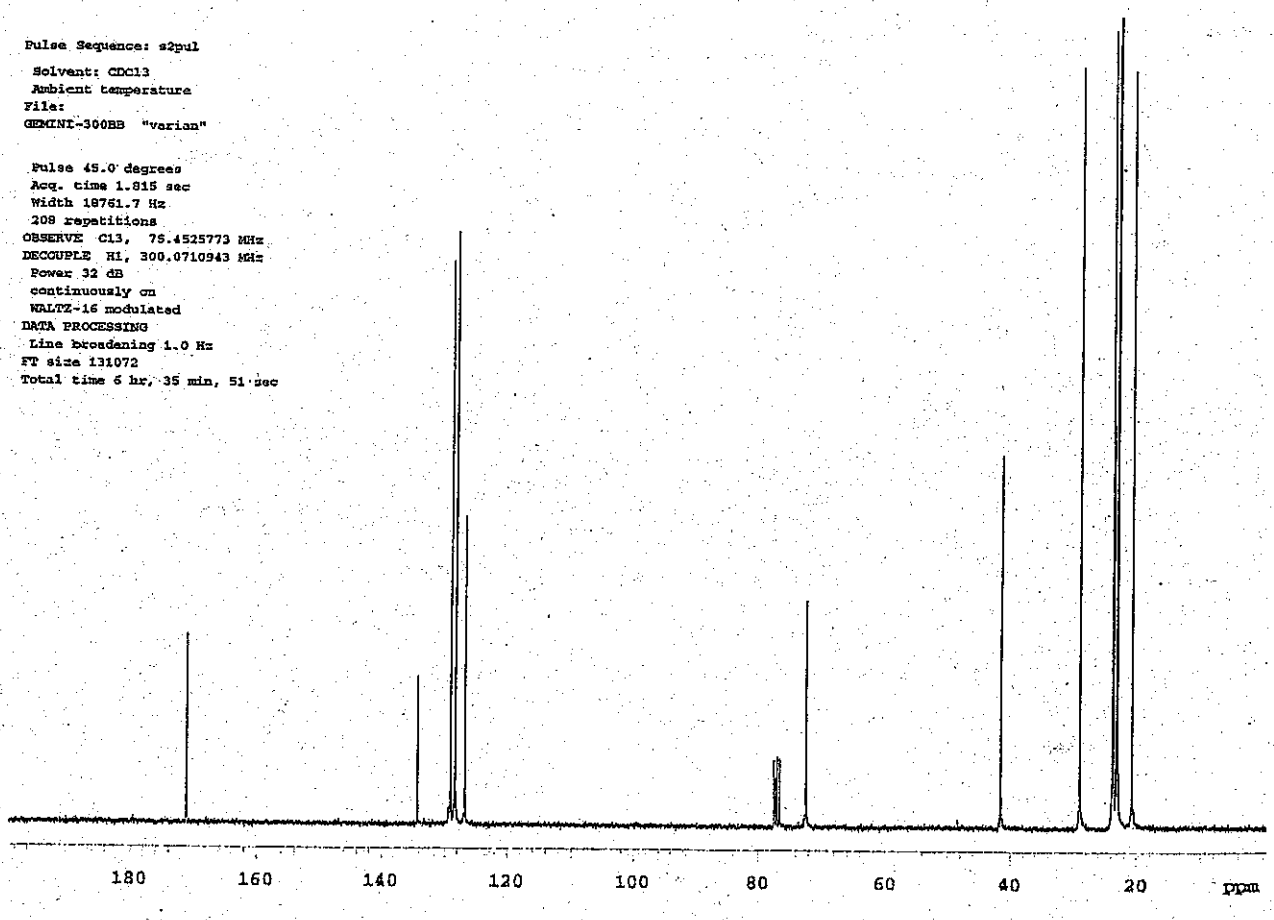
Ester **S8**



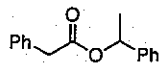
13C OBSERVE

Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File:
GEMINI-300BB "varian"

Pulse 45.0 degrees
Acq. time 1.815 sec
Width 18761.7 Hz
208 repetitions
OBSERVE C13, 75.4525773 MHz
DECOUPLE H1, 300.0710943 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 6 hr, 35 min, 51 sec



Ester **S9**



STANDARD 1H OBSERVE

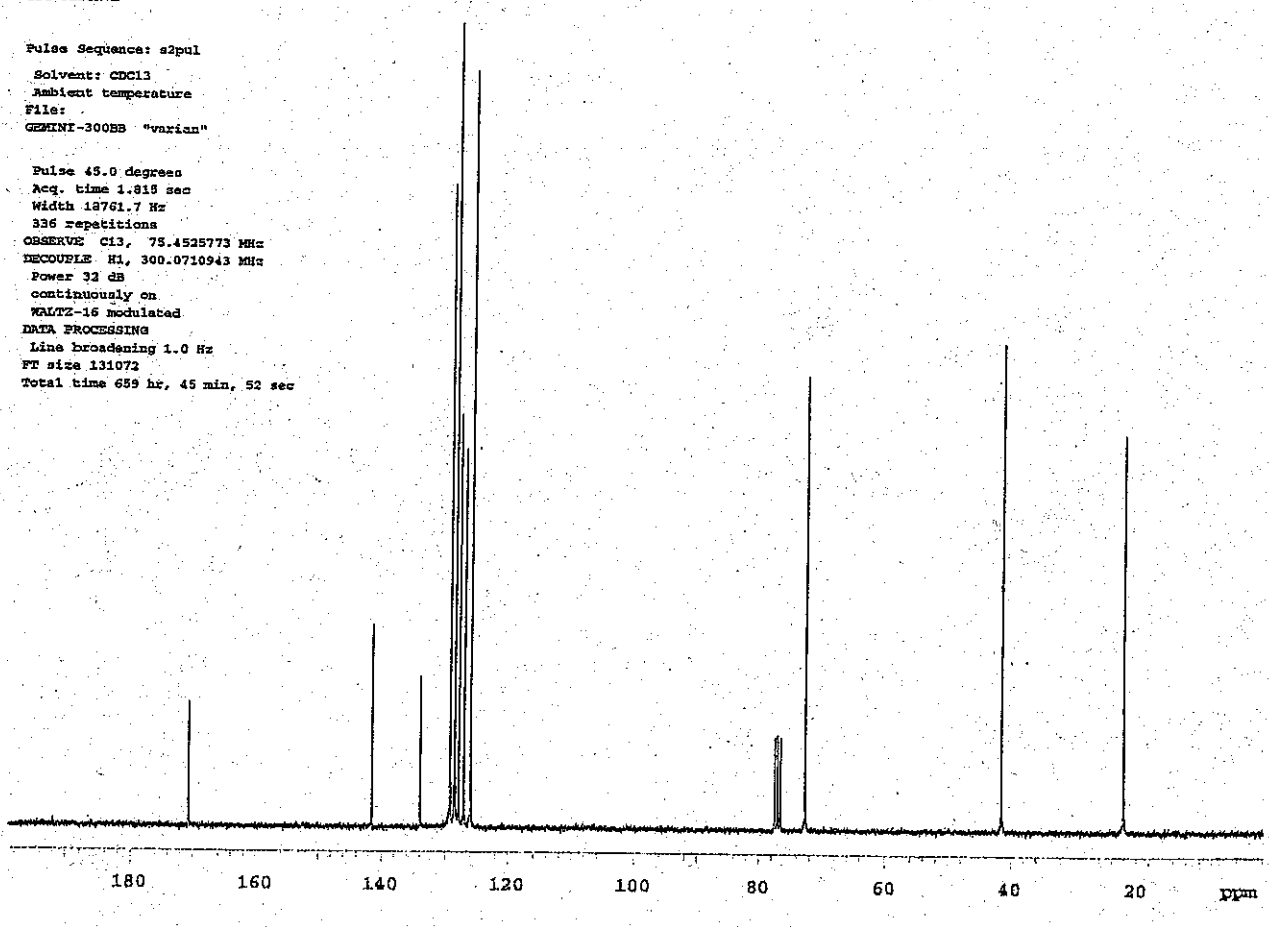
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File:
GEMINI-300BB "varian"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.998 sec
Width 4500.5 Hz
16 repetitions
OBSERVE H1, 300.0695992 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 49 sec

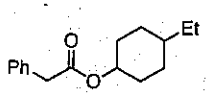
13C OBSERVE

Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File:
GEMINI-300BB "varian"

Pulse 45.0 degrees
Acq. time 1.815 sec
Width 18761.7 Hz
336 repetitions
OBSERVE C13, 75.4525773 MHz
DECOUPLE H1, 300.0710943 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 659 hr, 45 min, 52 sec



Ester **S10**



STANDARD 1H OBSERVE

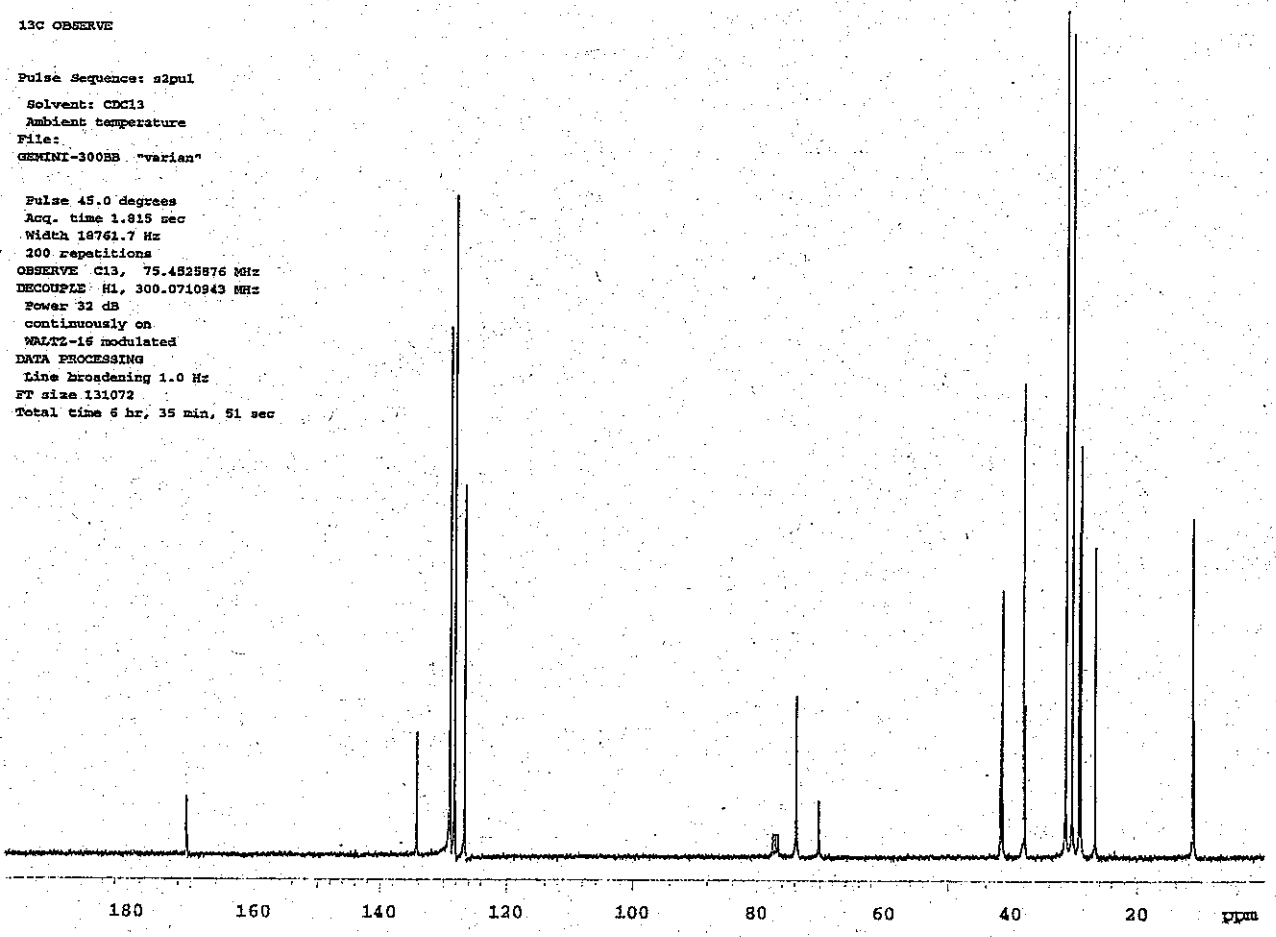
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File:
GEMINI-300BB "varian"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.998 sec
Width 4500.5 Hz
16 repetitions
OBSERVE H1, 300.0695951 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 49 sec

13C OBSERVE

Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File:
GEMINI-300BB "varian"

Pulse 45.0 degrees
Acq. time 1.815 sec
Width 18761.7 Hz
200 repetitions
OBSERVE C13, 75.4525876 MHz
DECOUPLE H1, 300.0710943 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 6 hr, 35 min, 51 sec



STANDARD 1H OBSERVE

Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

File:

GEMINI-300BB "varian"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.998 sec

Width 4500.5 Hz

16 repetitions

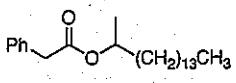
OBSERVE H1, 300.0695940 MHz

DATA PROCESSING

FT size 32768

Total time 0 min, 49 sec

Ester **S11**



13C OBSERVE

Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

File:

GEMINI-300BB "varian"

Pulse 45.0 degrees

Acq. time 1.815 sec

Width 18761.7 Hz

168 repetitions

OBSERVE C13, 75.4525732 MHz

DECOUPLE H1, 300.0710943 MHz

Power 32 dB

continuously on

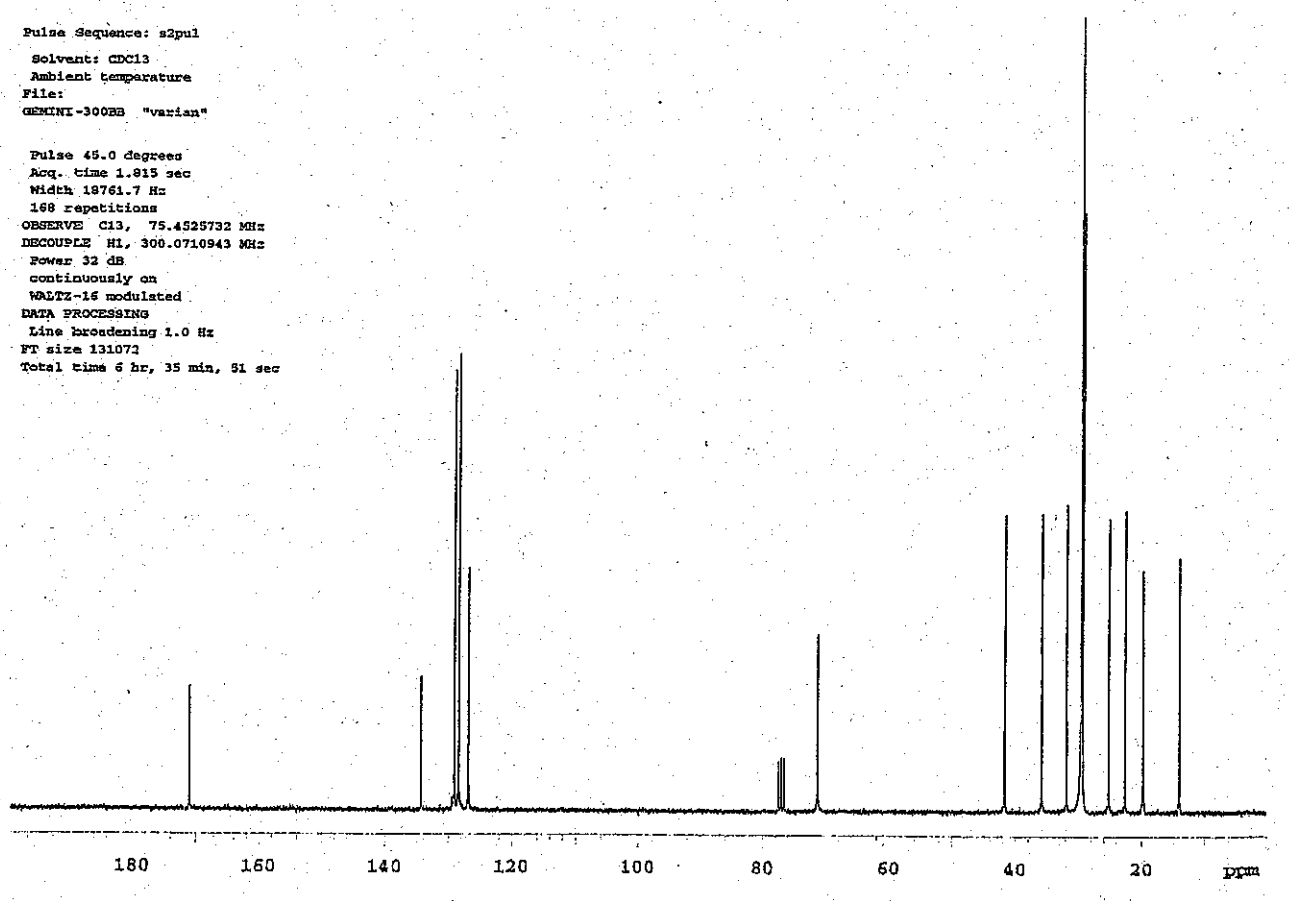
WALTZ-16 modulated

DATA PROCESSING

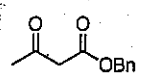
Line broadening 1.0 Hz

FT size 131072

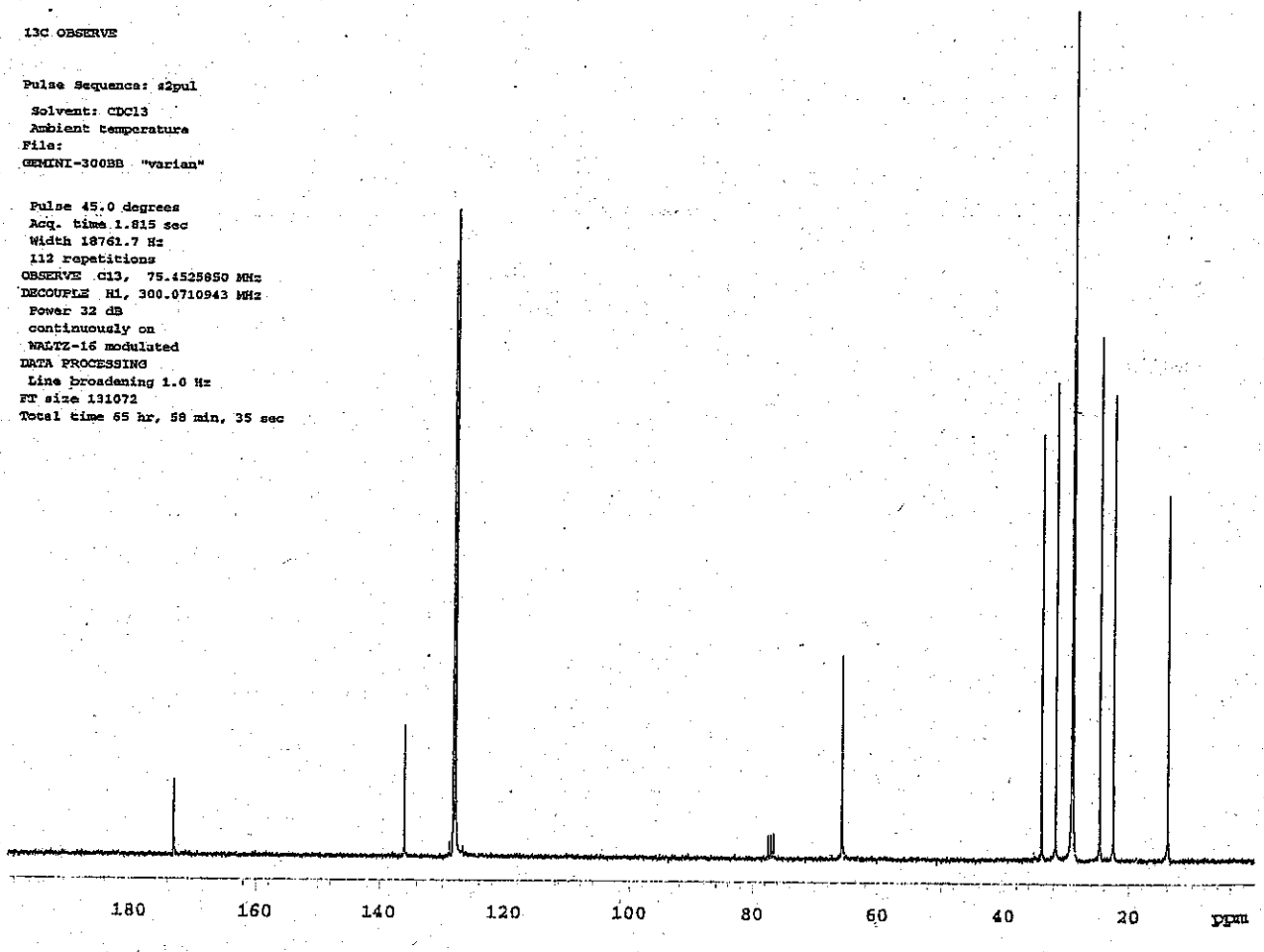
Total time 6 hr, 35 min, 51 sec

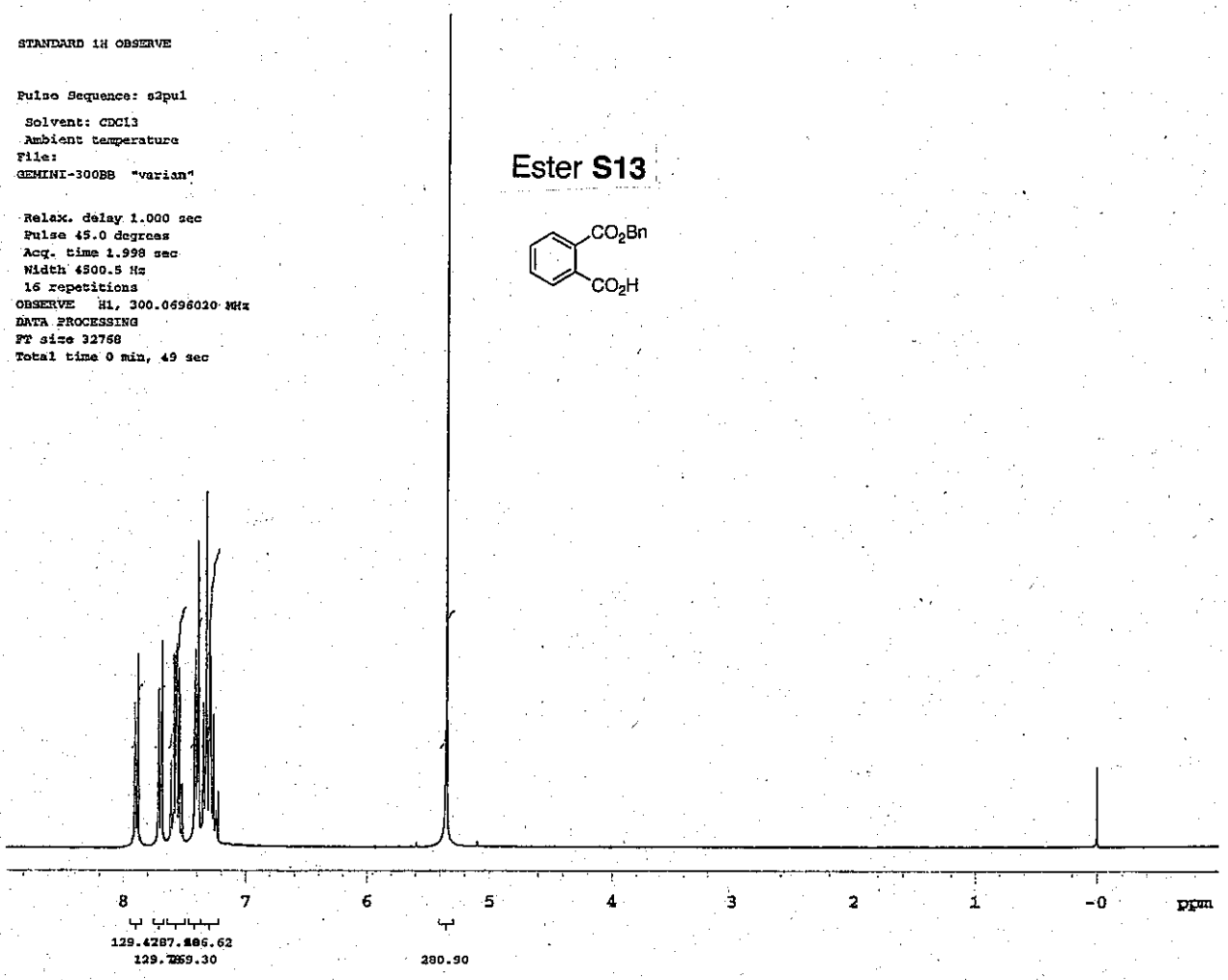


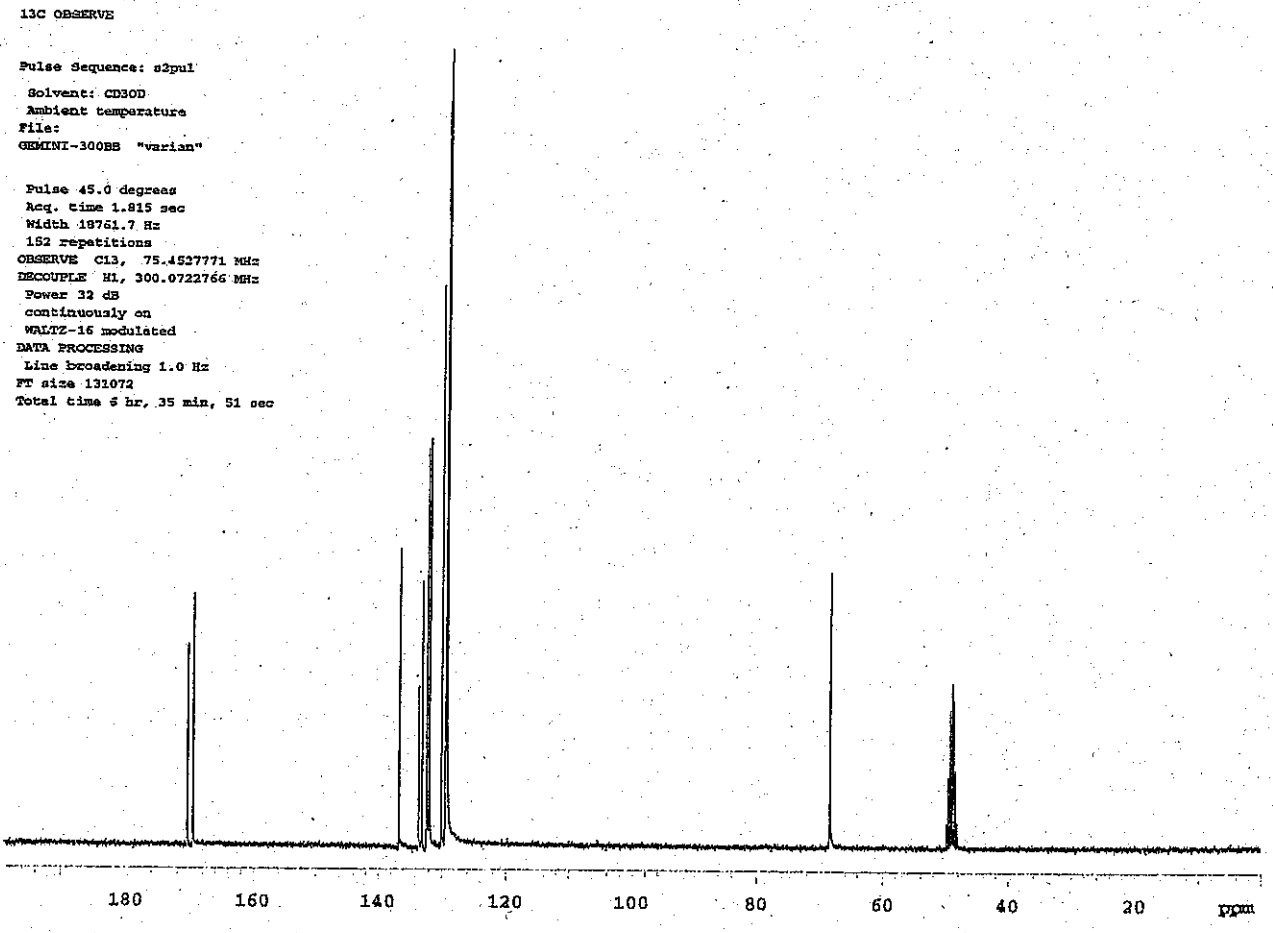
Ester **S12**


O
O
OBn

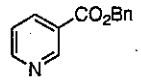
STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File:
GEMINI-300BB "varian"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.998 sec
Width 4500.5 Hz
16 repetitions
OBSERVE H1, 300.0695937 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 49 sec
8
7
6
5
4
3
2
1
-0
ppm
575.22
239.70
213.35
312.15


13C OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File:
GEMINI-300BB "varian"
Pulse 45.0 degrees
Acq. time 1.815 sec
Width 18761.7 Hz
112 repetitions
OBSERVE C13, 75.4525850 MHz
DECOUPLE H1, 300.0710943 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 65 hr, 58 min, 35 sec
180
160
140
120
100
80
60
40
20
ppm


STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File:
GEMINI-300BB "varian"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.998 sec
Width 4500.5 Hz
16 repetitions
OBSERVE H1, 300.0696020 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 49 sec
Ester S13
CO2Bn
CO2H
8
7
6
5
4
3
2
1
-0
ppm
129.4287.806.62
129.7259.30
280.90


13C OBSERVE
Pulse Sequence: s2pul
Solvent: CD3OD
Ambient temperature
File:
GEMINI-300BB "varian"
Pulse 45.0 degrees
Acq. time 1.815 sec
Width 19761.7 Hz
152 repetitions
OBSERVE C13, 75.4527771 MHz
DECOUPLE H1, 300.0722766 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 5 hr, 35 min, 51 sec
180
160
140
120
100
80
60
40
20
ppm

Ester **S14**




```
STANDARD 1H OBSERVE

Pulse Sequence: s2pul
 Solvent: CDCl3
 Ambient temperature
File:
GEMINI-300BB  "varian"

 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 1.998 sec
 Width 4500.5 Hz
 16 repetitions
OBSERVE   H1, 300.0695921 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 49 sec
```



```
13C OBSERVE

Pulse Sequence: s2pul
 Solvent: CDCl3
 Ambient temperature
File:
GEMINI-300BB  "varian"

 Pulse 45.0 degrees
 Acq. time 1.815 sec
 Width 18761.7 Hz
 224 repetitions
OBSERVE   C13,  75.4525810 MHz
DECOUPLE  H1, 300.0710943 MHz
 Power 32 dB
 continuously on
 WALTZ-16 modulated
DATA PROCESSING
 Line broadening 1.0 Hz
FT size 131072
Total time 6 hr, 35 min, 51 sec
```

