Electronic Supplementary Material (ESI) for RSC Advances

Microwave-Assisted Synthesis of Hydro-pyridine Derivatives and Study of the DPPH$^{\bullet}$-scavenging Activity

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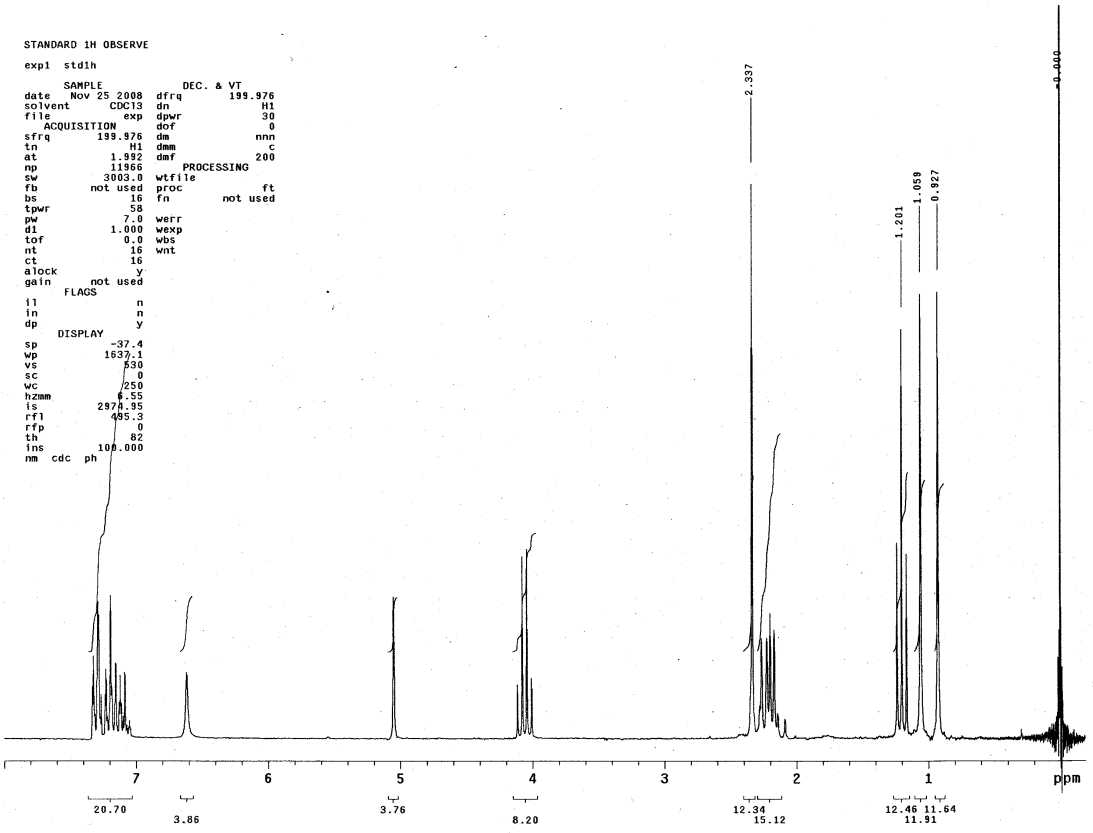
Supporting Information

^{1}H and ^{13}C-NMR of compounds:

General: All reagents were purchased in the higher quality available and were used without further purification. Thin-layer chromatography (TLC) was performed on silica gel F_{254} plates (Merck). All compounds were detected using UV light. Melting points were obtained on an Electrothermal 88629 apparatus and were uncorrected. Infrared spectra (FTIR) were recorded on a Perkin Elmer FT-IR 1600 spectrophotometer with a KBr disk. ^{1}H and ^{13}C nuclear magnetic resonance spectra at 200 Hz and 50.289 Hz, respectively, were recorded on a Varian Mercury 200 MHz Spectrometer in $CDCl_3$ and DMSO-d_6 with TMS as internal standard. The chemical shifts are expressed as δ values in parts per million (ppm) and the coupling constants (*J*) are given in hertz (Hz). Electrospray ionization mass apectra (ESI-MS) were obtained with an ion trap, and the intensities were reported as a percentage relative to the base peak after the corresponding *m/z* value. HRMS were obtained in an Agilent LCTOF, a high resolution TOF analyzer with Windows XP based OS and APCI/ESI ionization. The purity was obtained on a High Pressure Liquid Chromatograph 1090 series II, column HPC-18. Microwave equipment was a self-tuning single mode CEM Discover™ Focused Synthesizer. All the spectrophotometric data were acquired using an Spectronic® 20Genesys™.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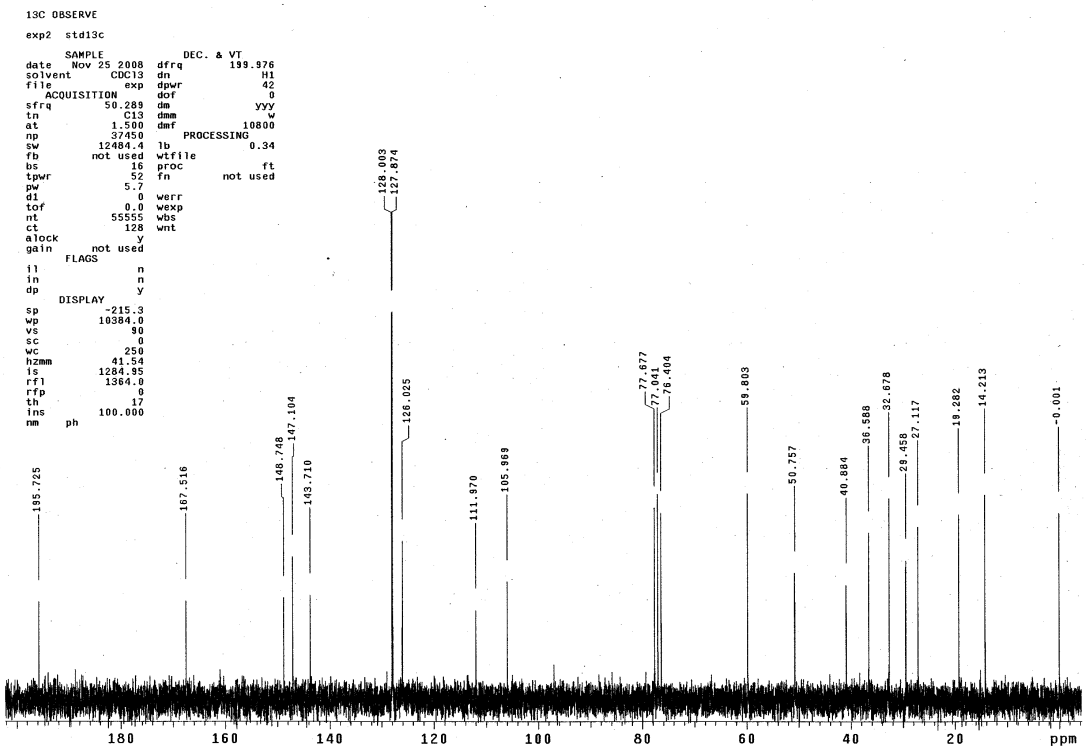
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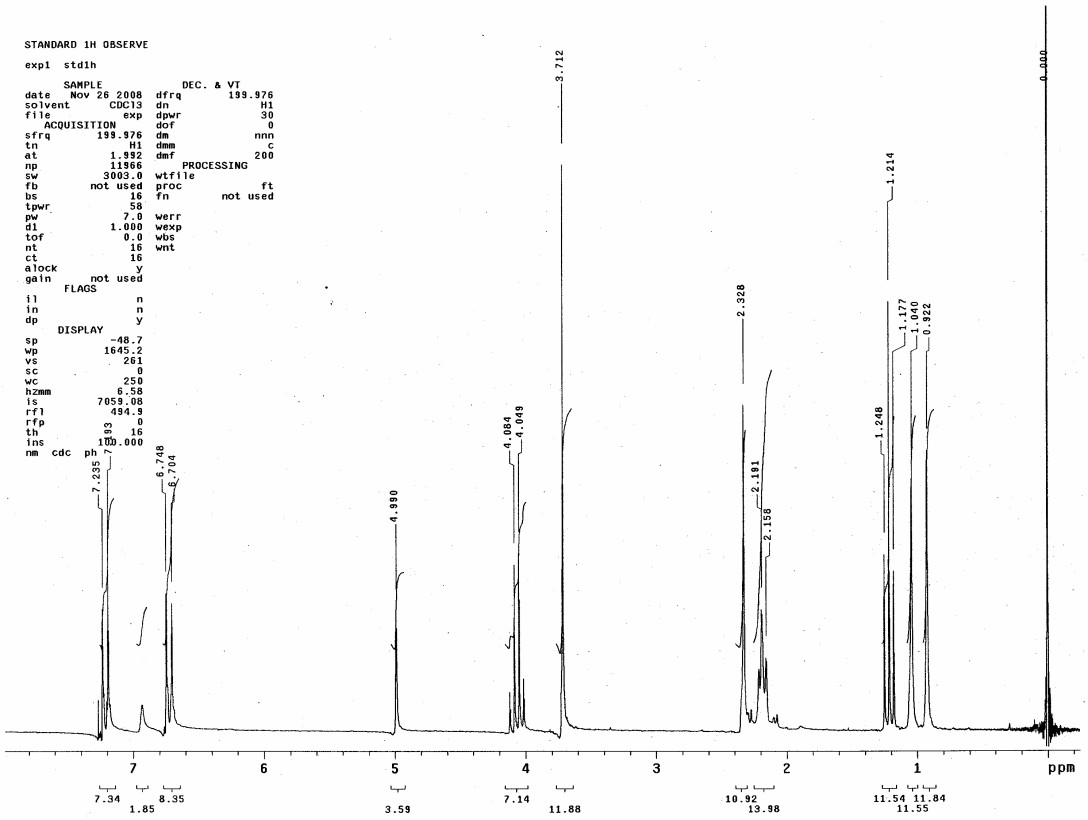

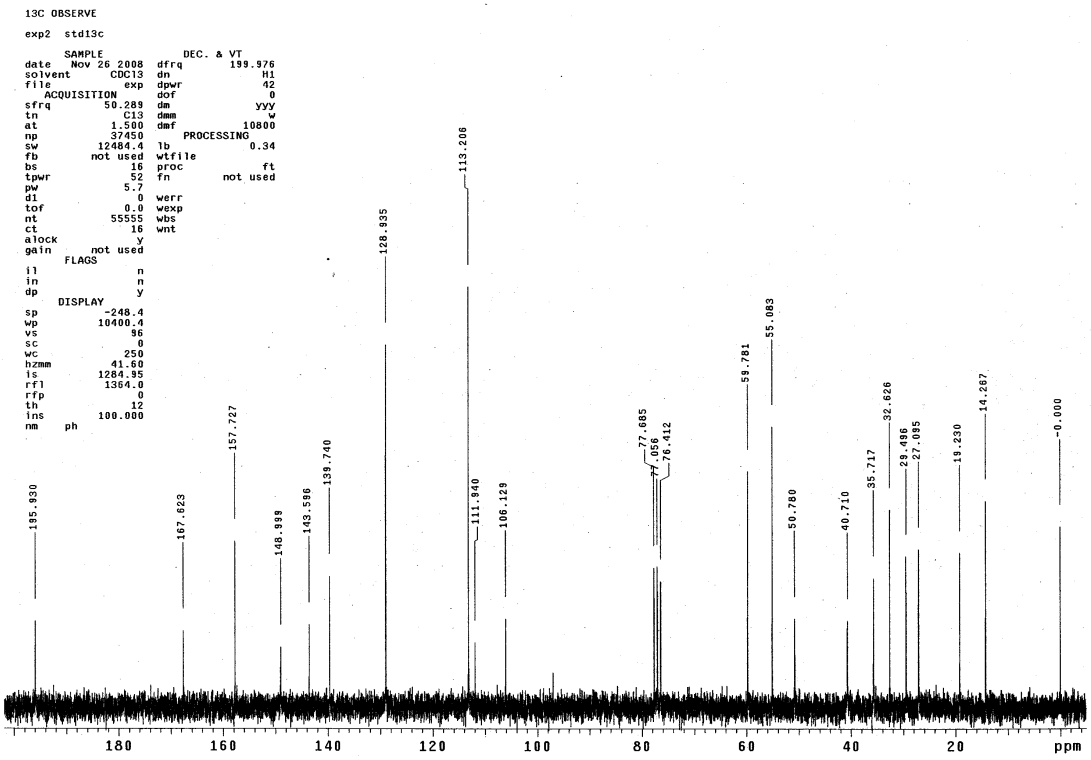

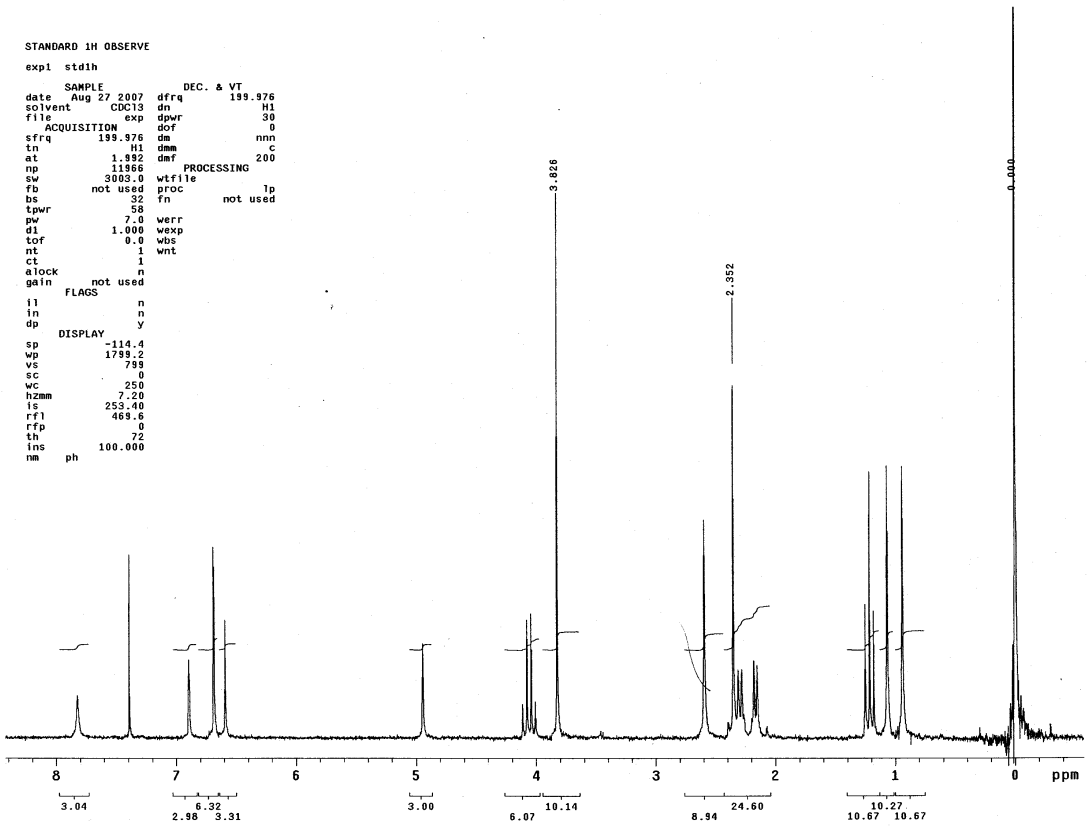

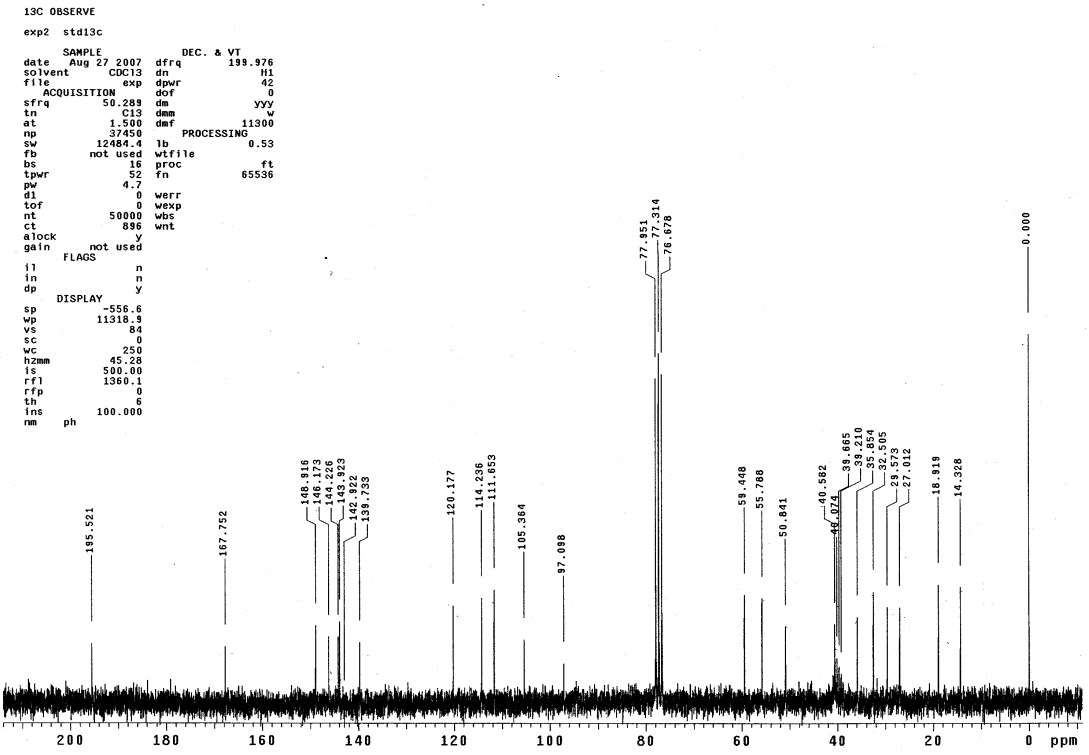

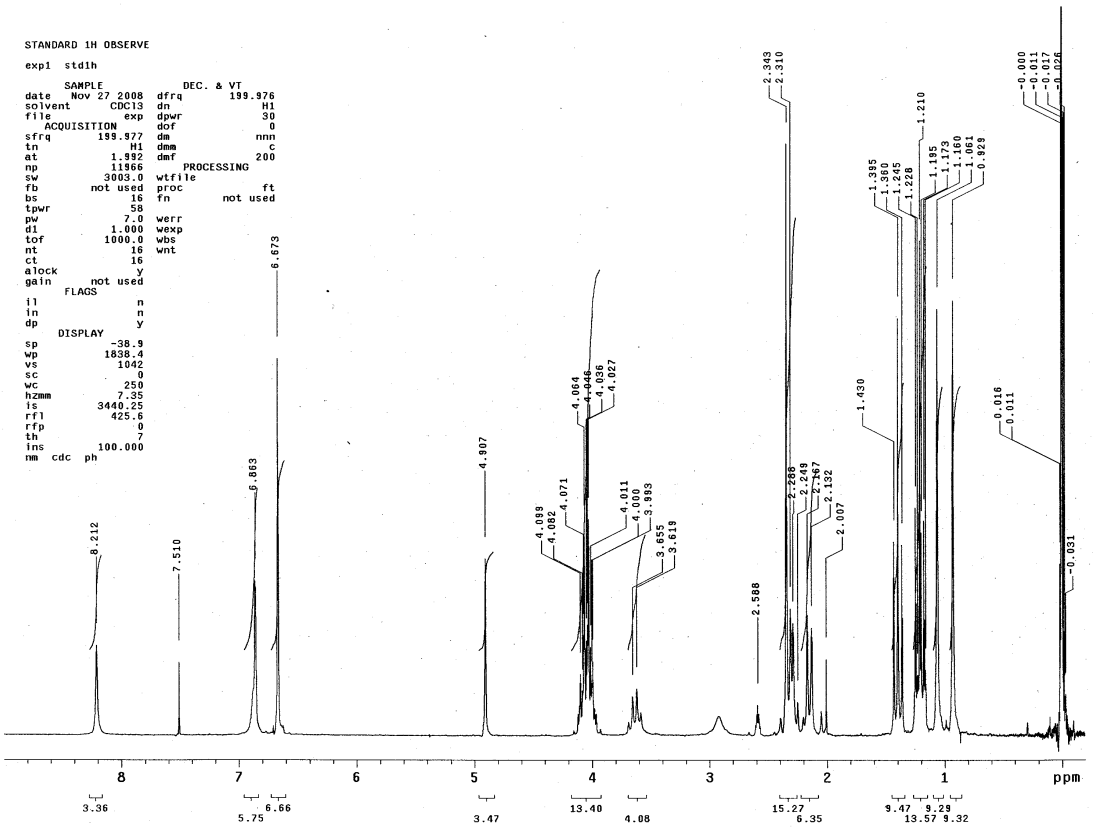
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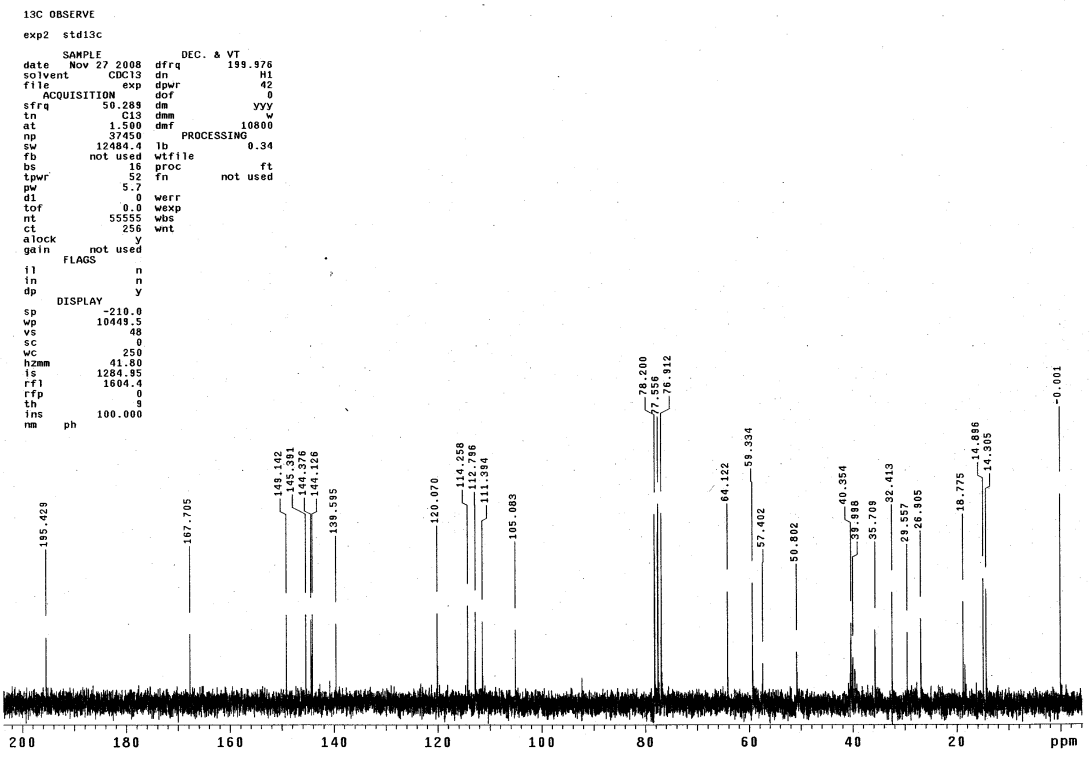
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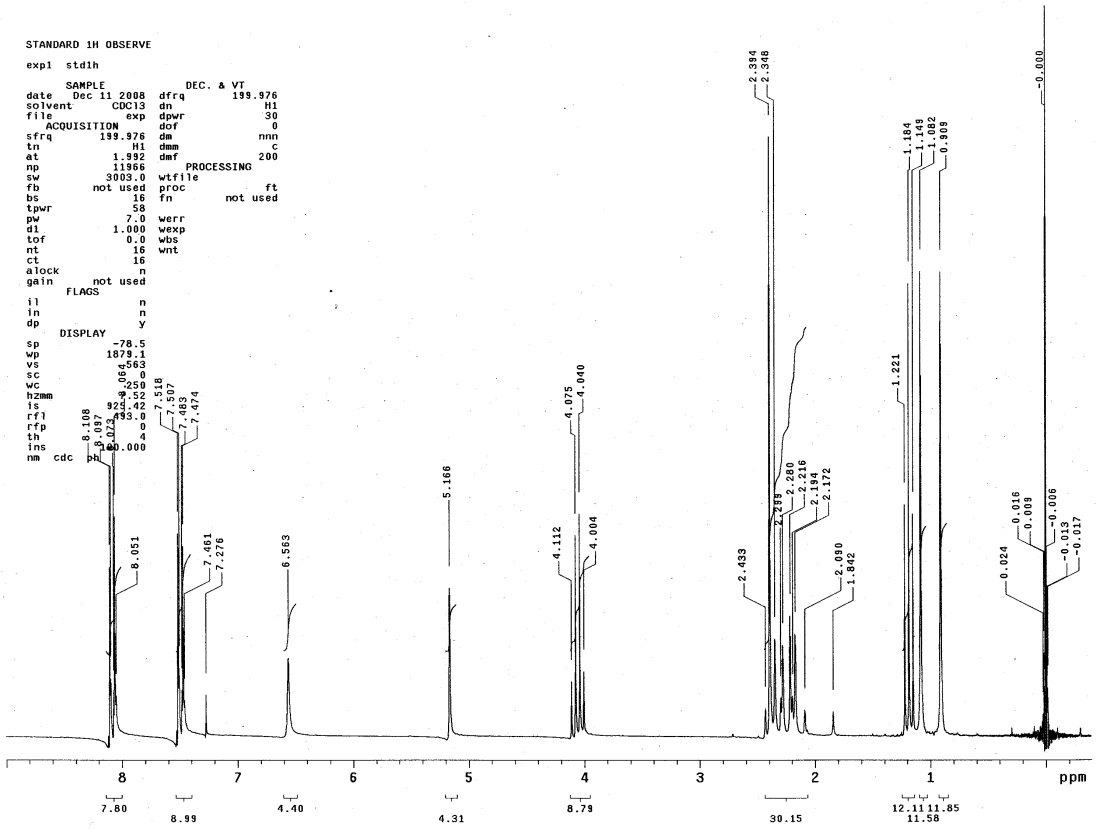
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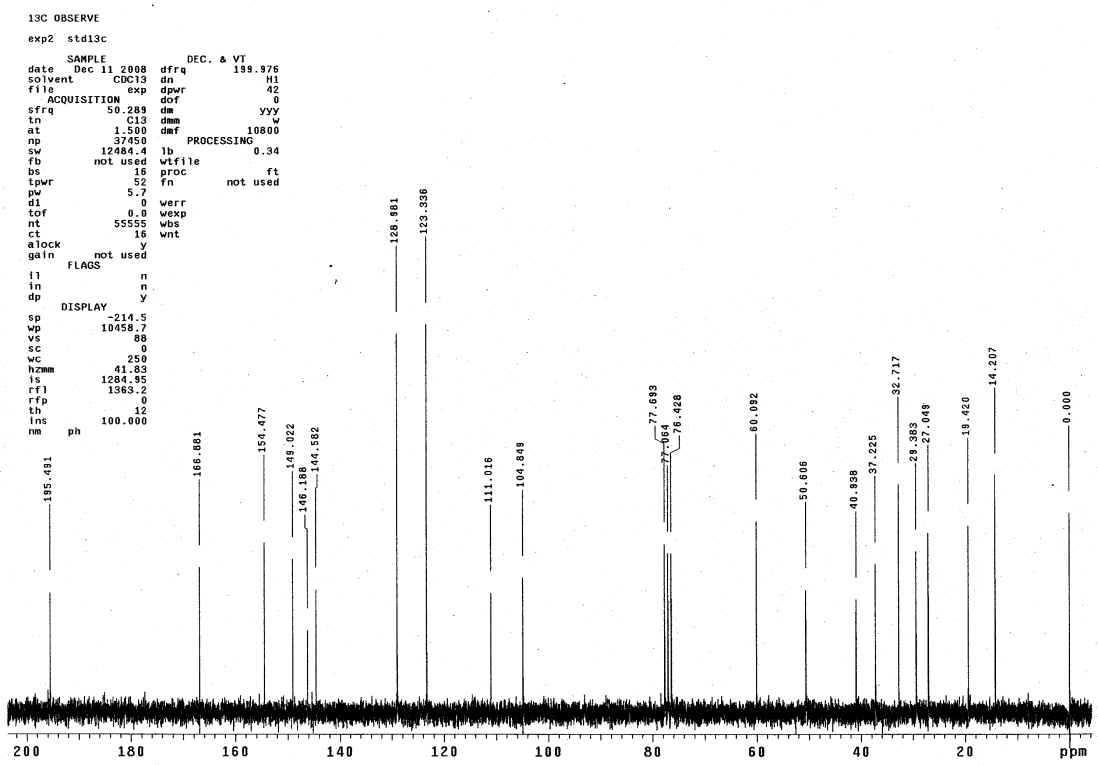
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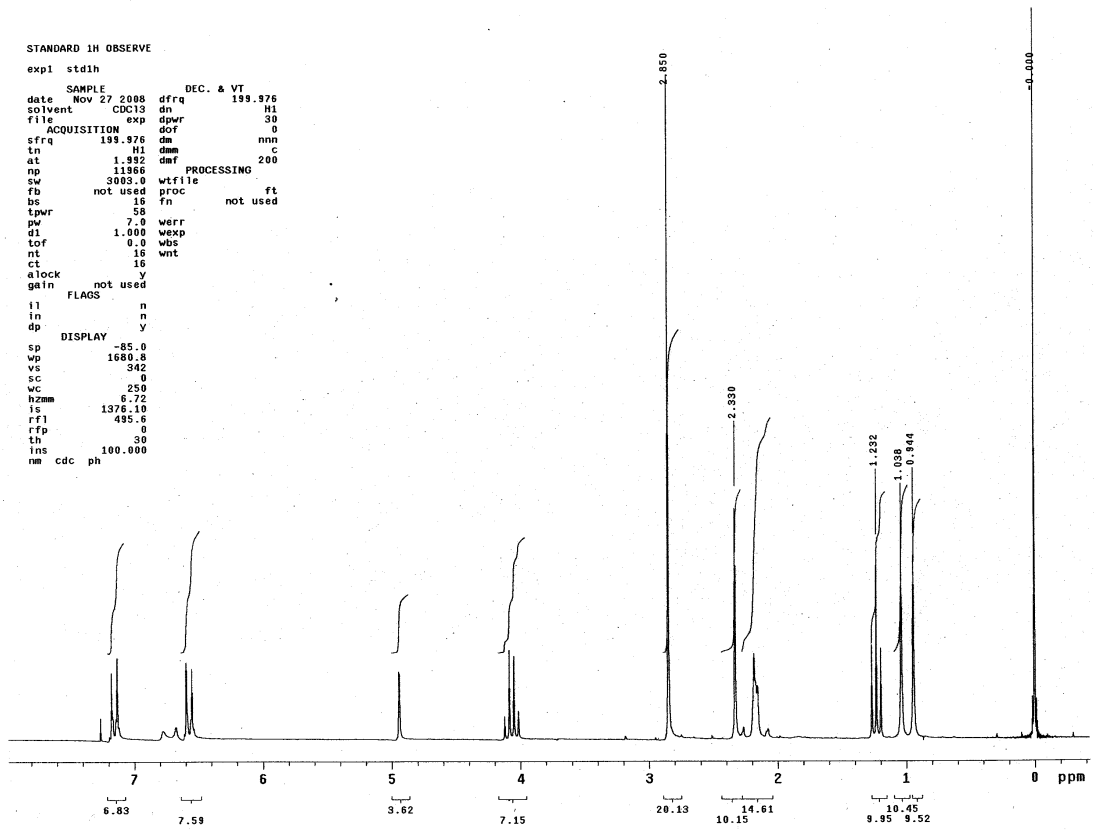

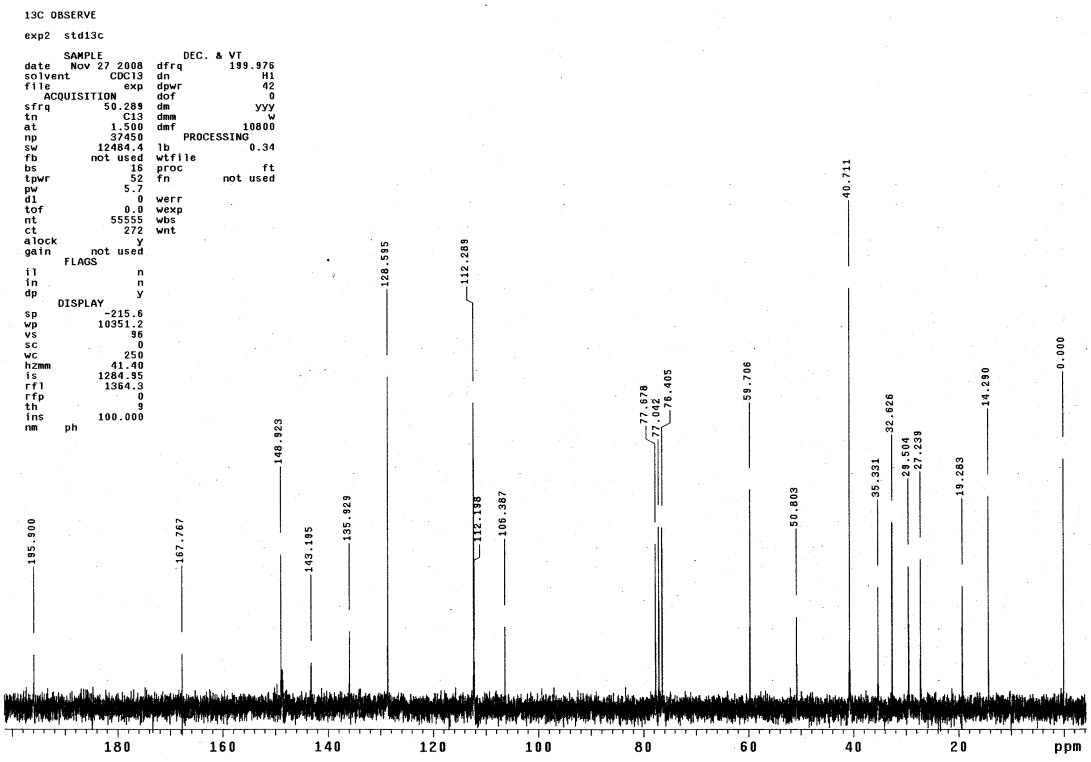

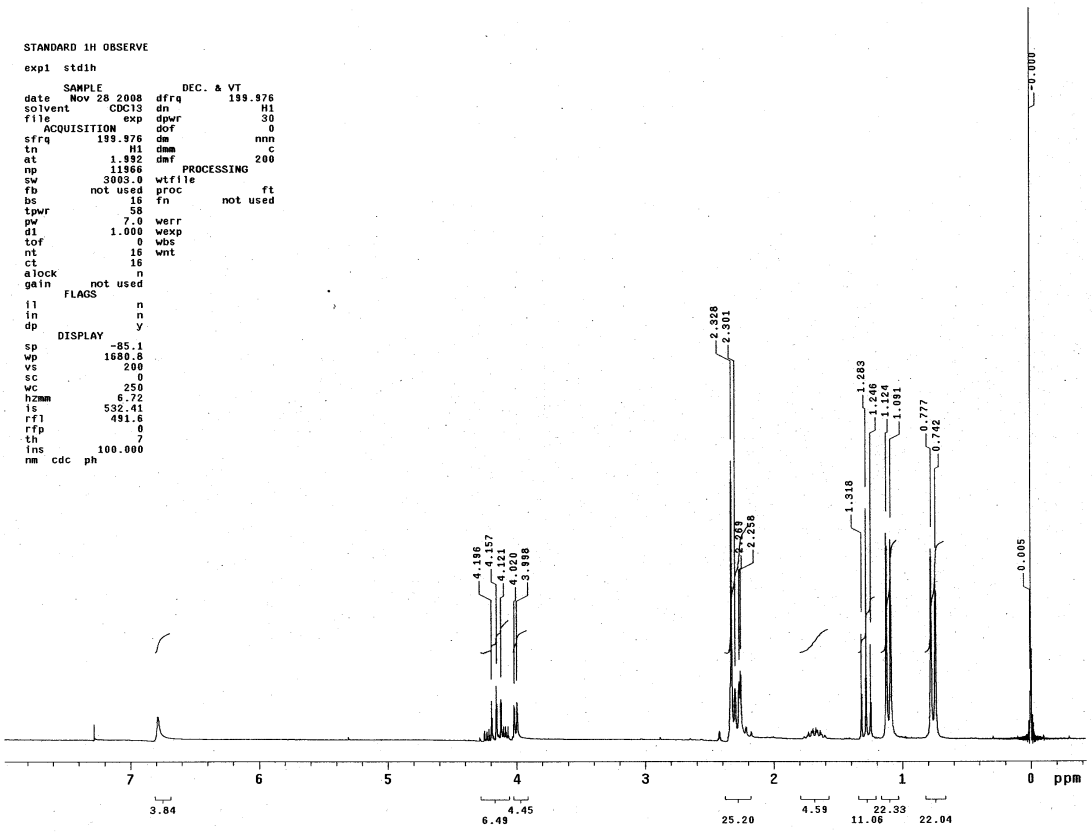
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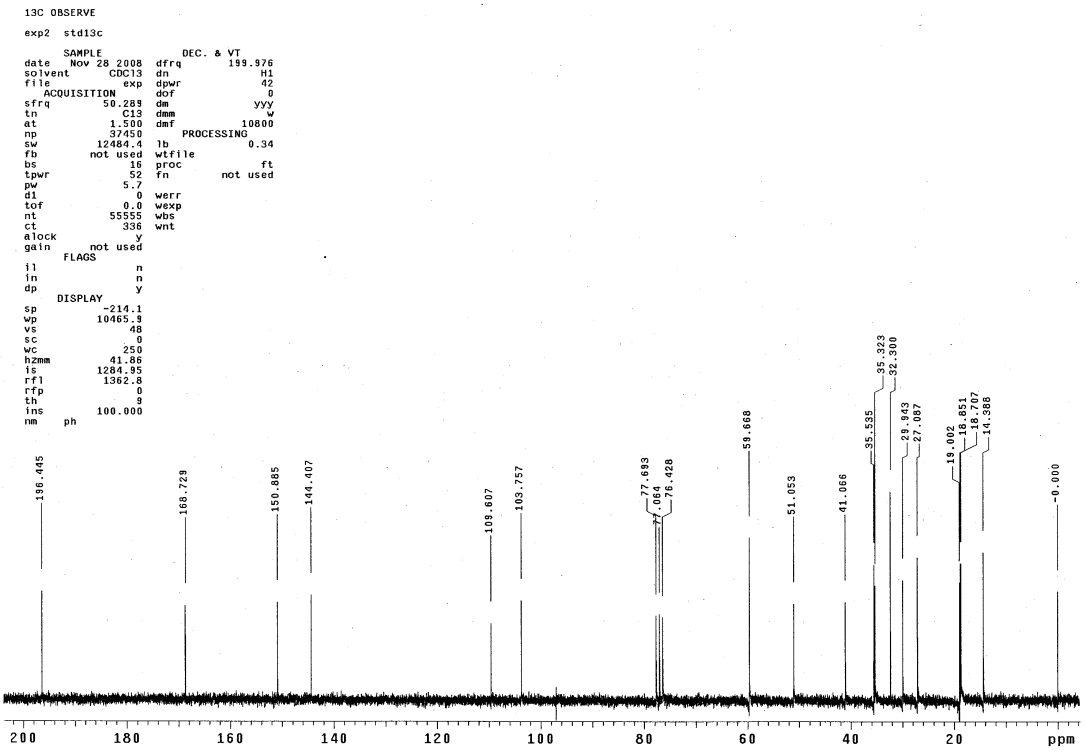
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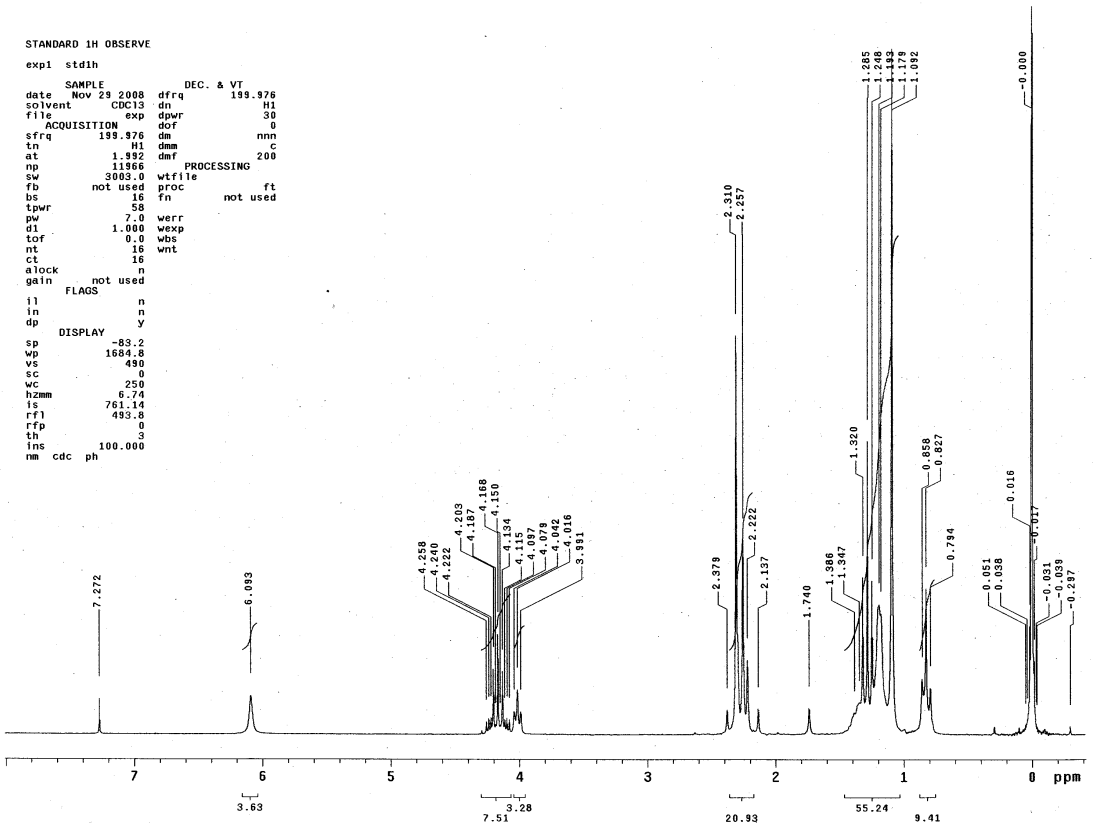
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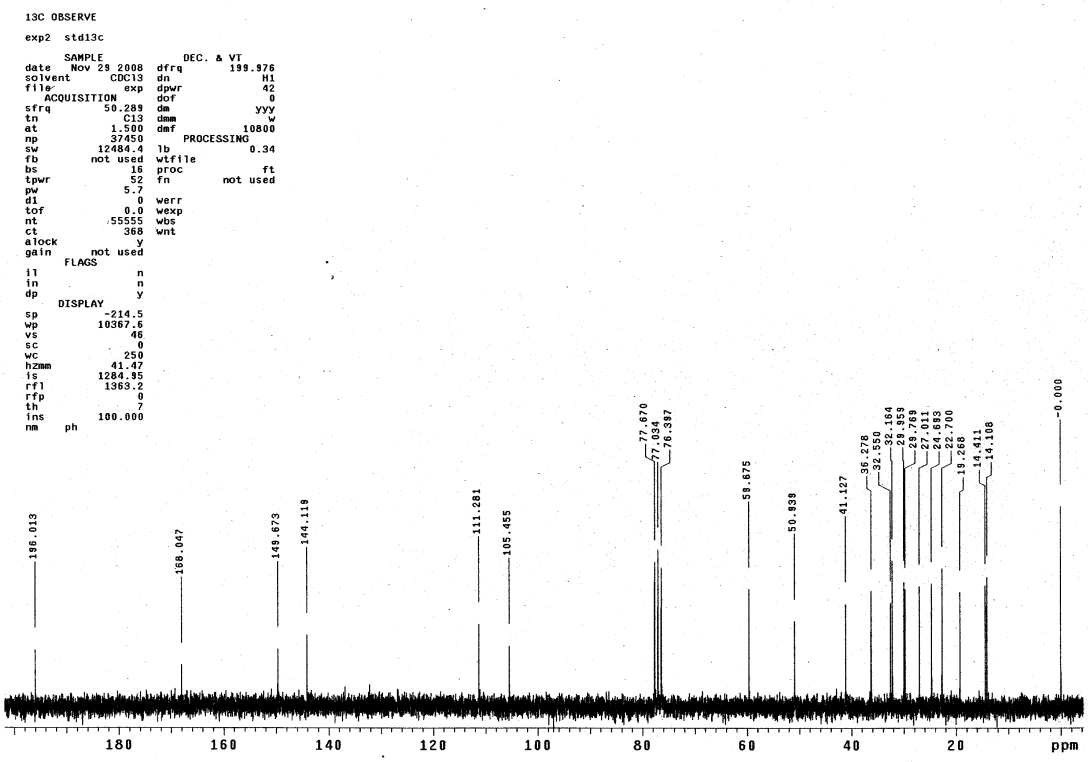
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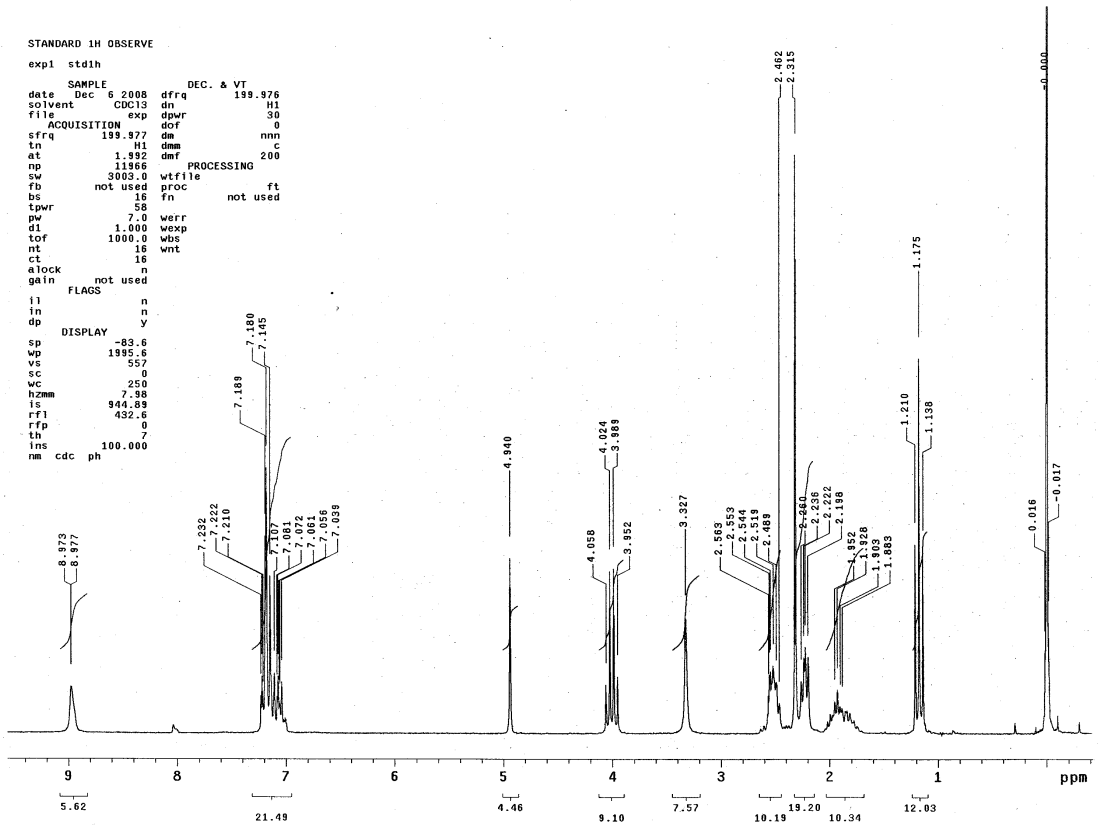
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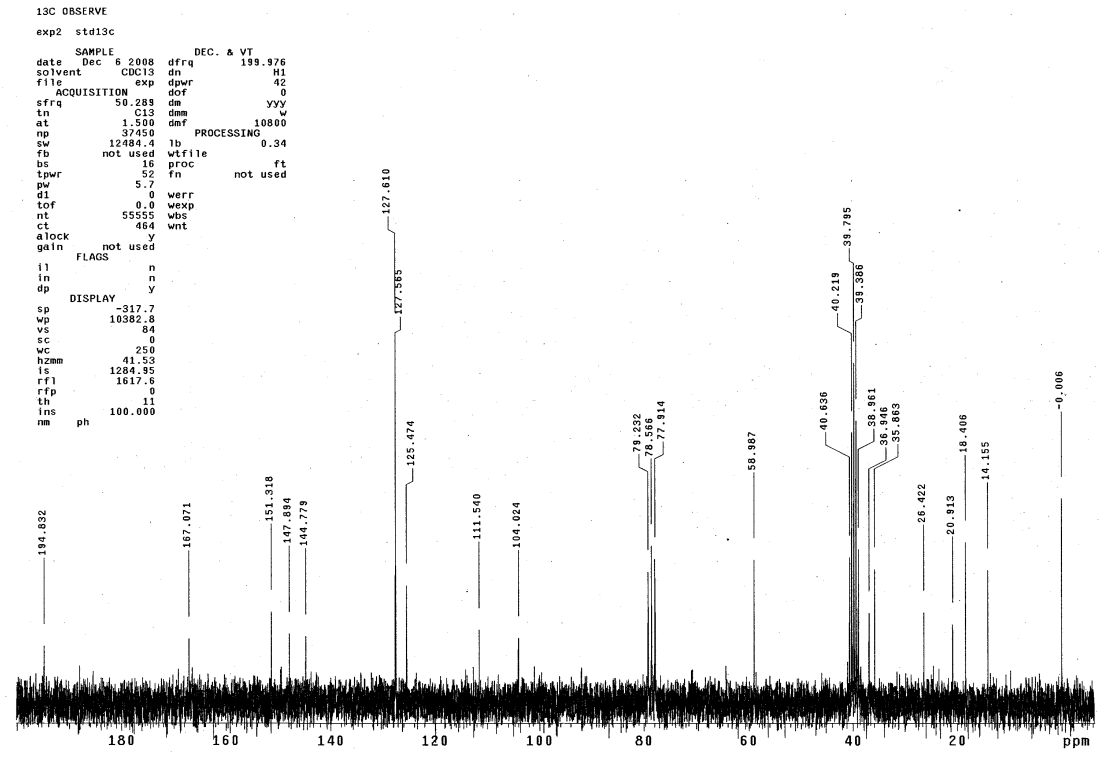
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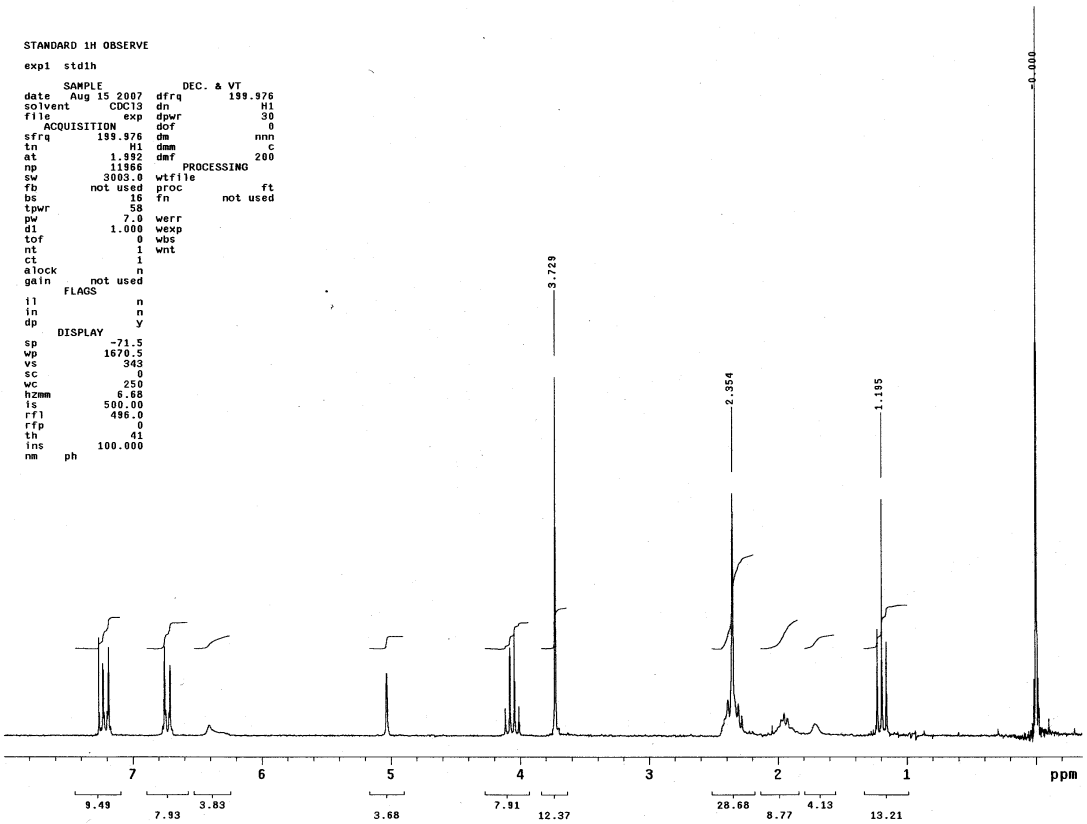
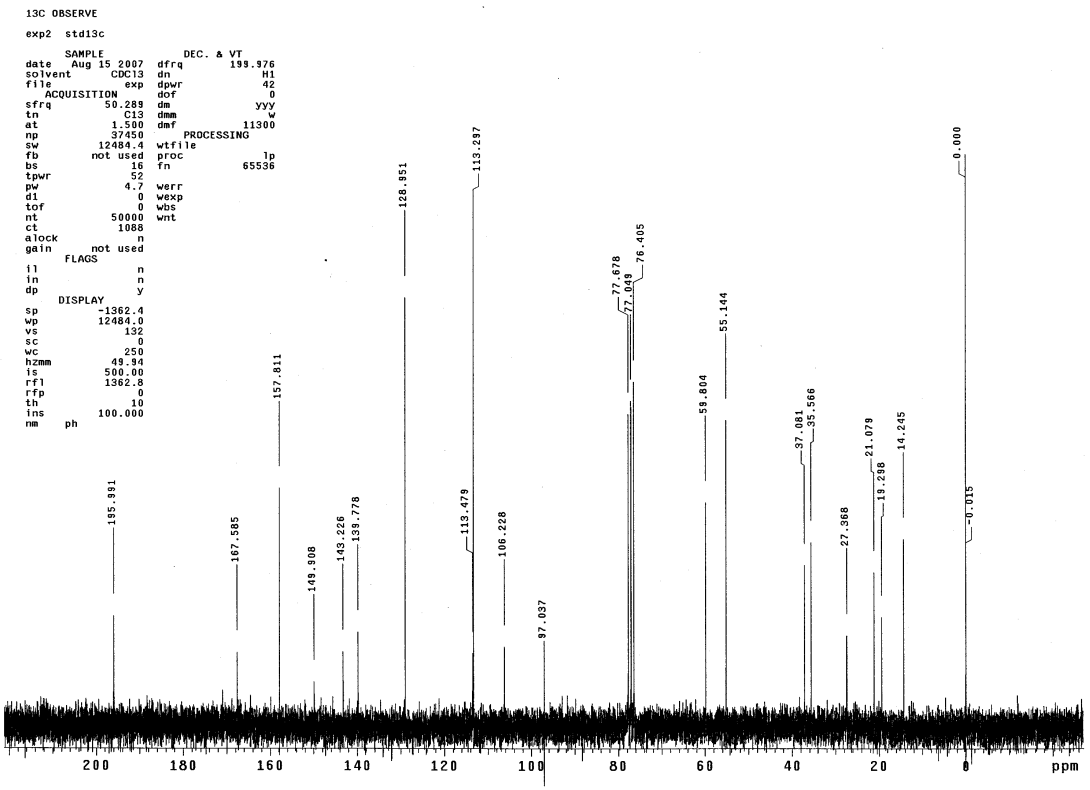
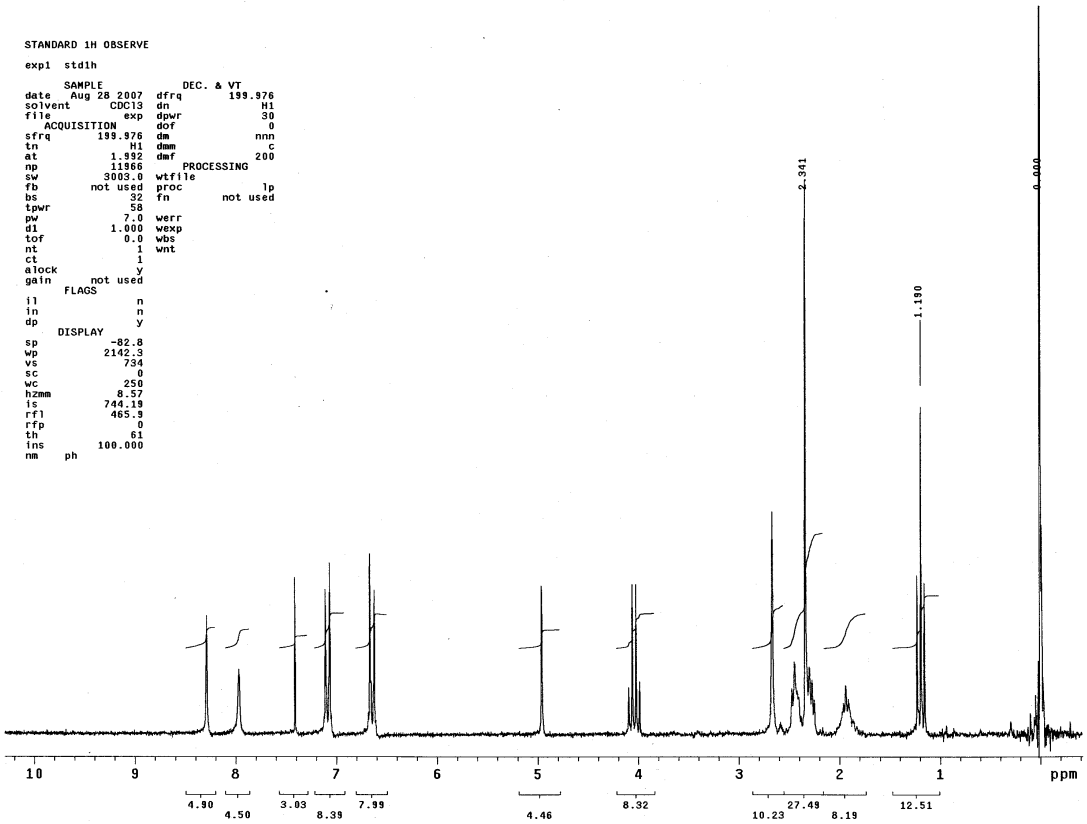
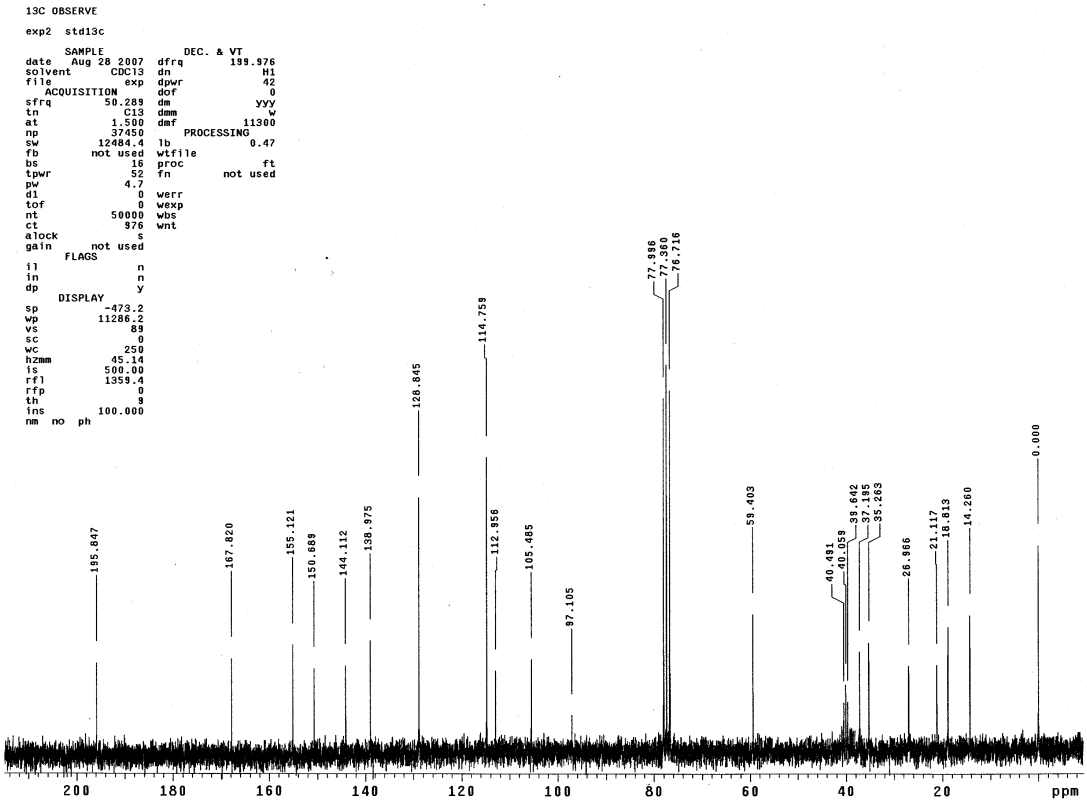
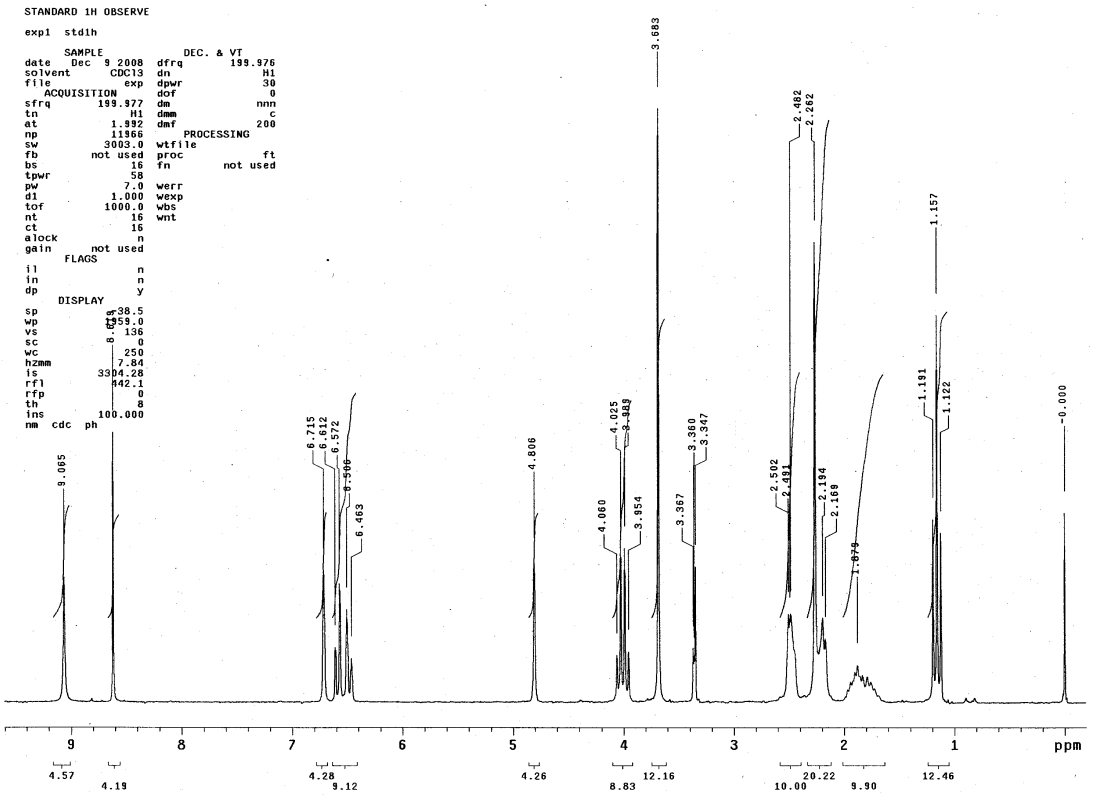
hzmm 41.53
is 1284.95
rfl 1617.6
rfp 0
th 11
ins 100.000
nm ph
DEC. & VT
dfrq 199.976
dn H1
dpwr 42
dof 0
dm yyy
dmm w
dmf 10800
PROCESSING
lb 0.34
wtfile
proc ft
fn not used
werr
wexp
wbs
wnt
194.832
167.071
151.318
147.884
144.779
127.610
127.585
125.474
111.540
104.024
79.232
78.568
77.914
58.987
40.636
40.219
39.795
39.388
38.961
38.946
35.863
26.422
20.913
18.406
14.155
-0.006
ppm

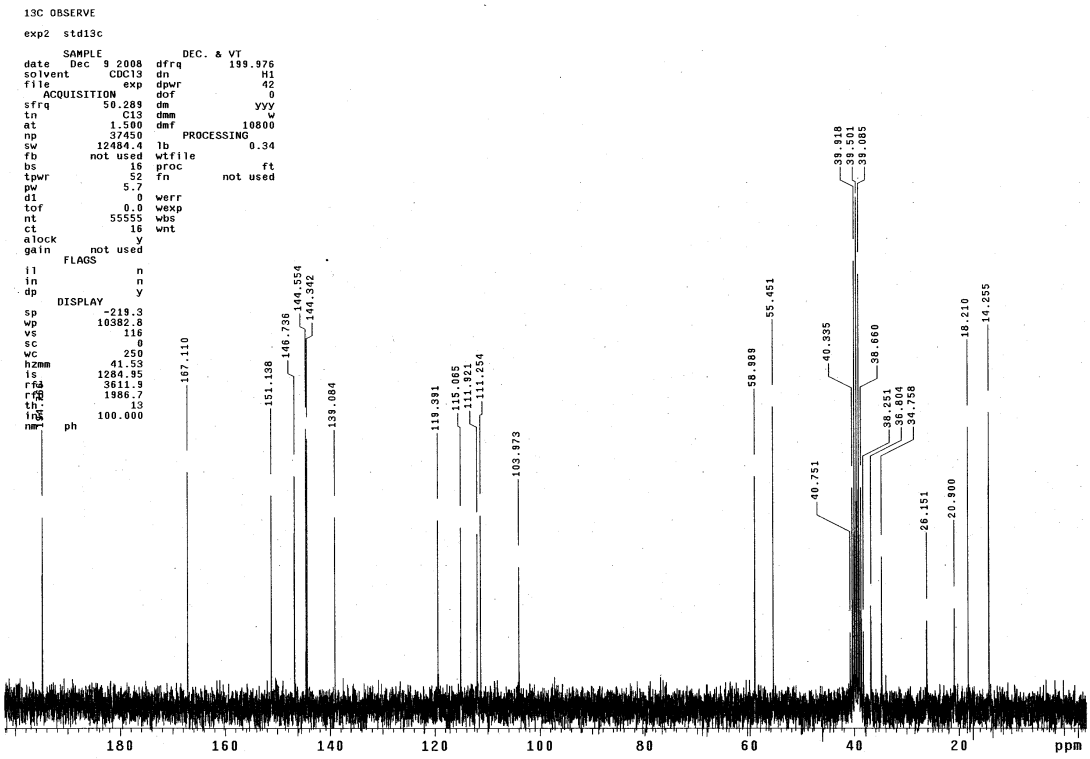


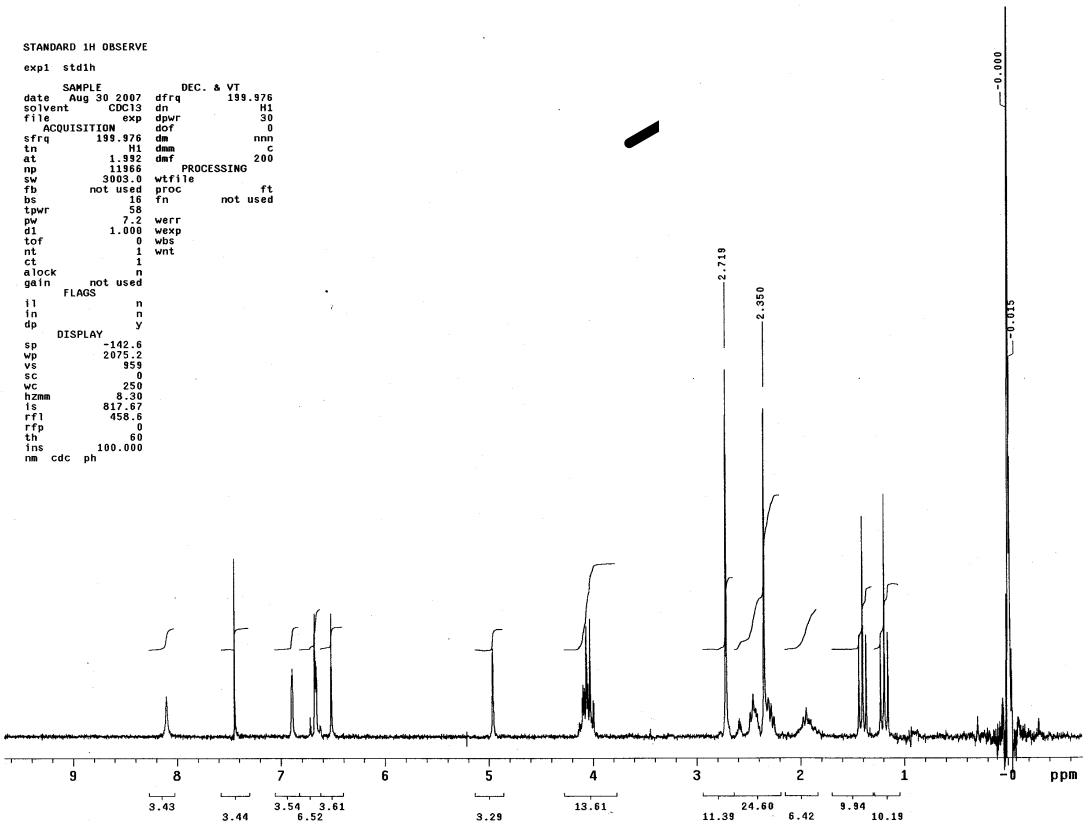


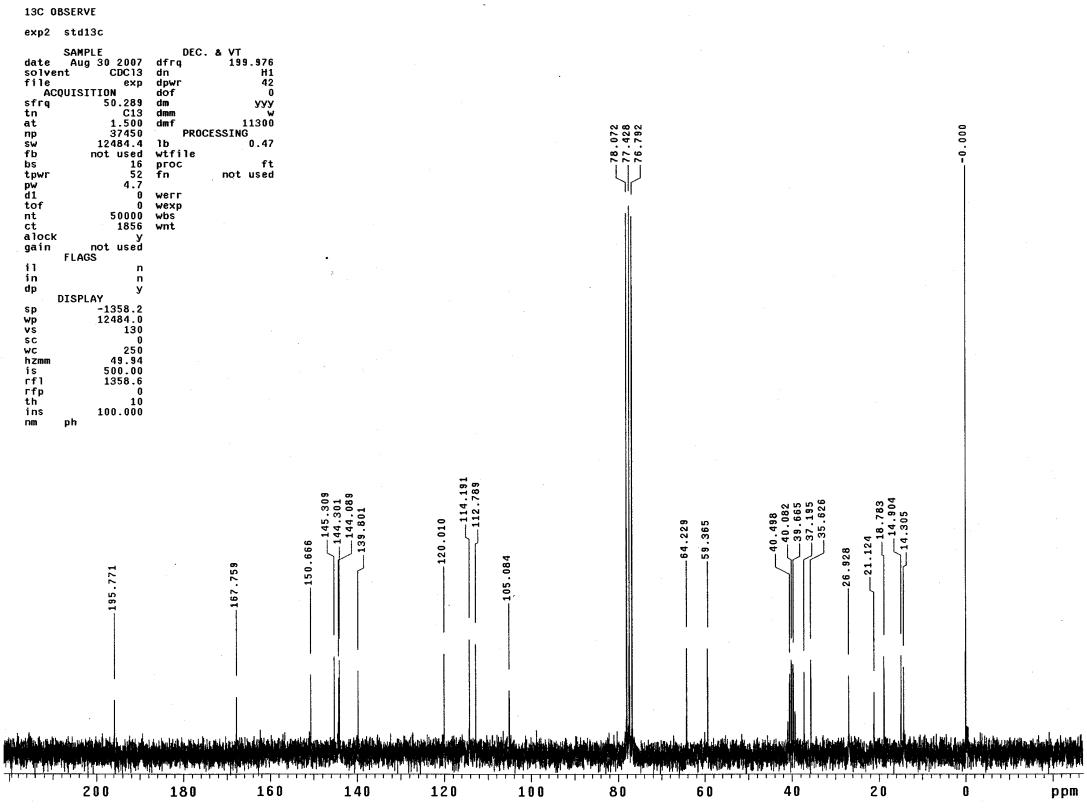


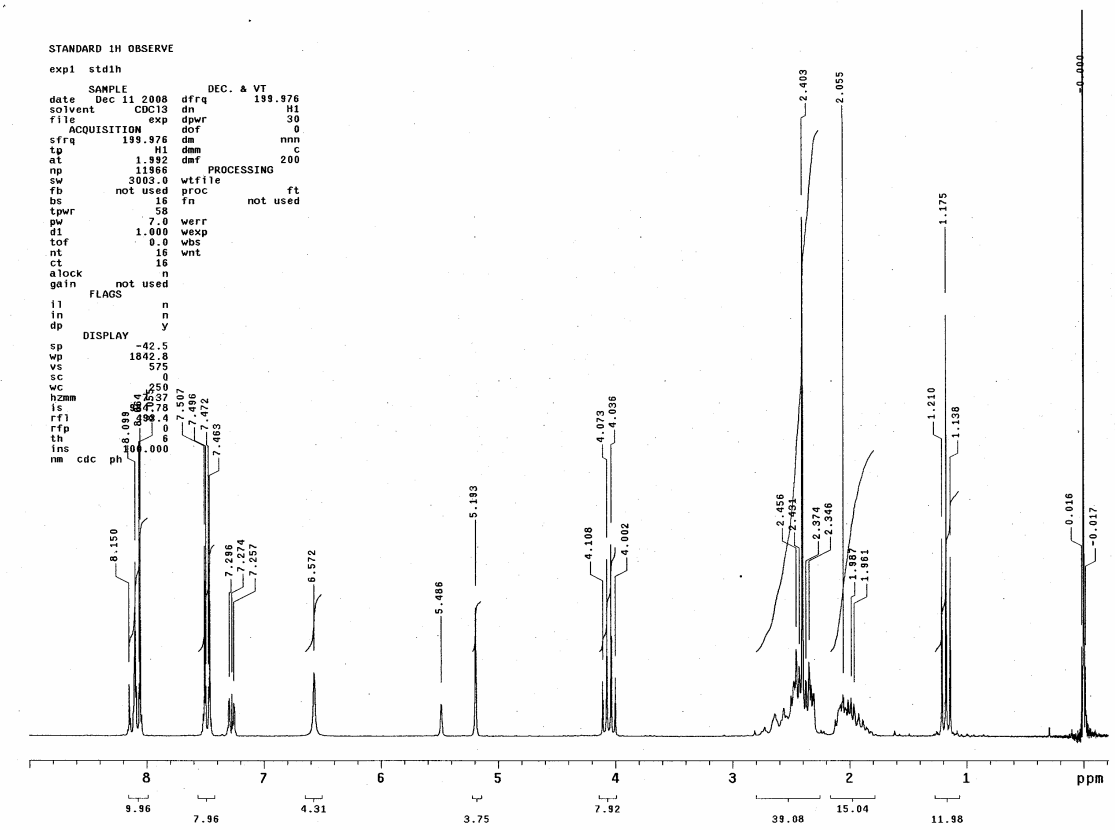


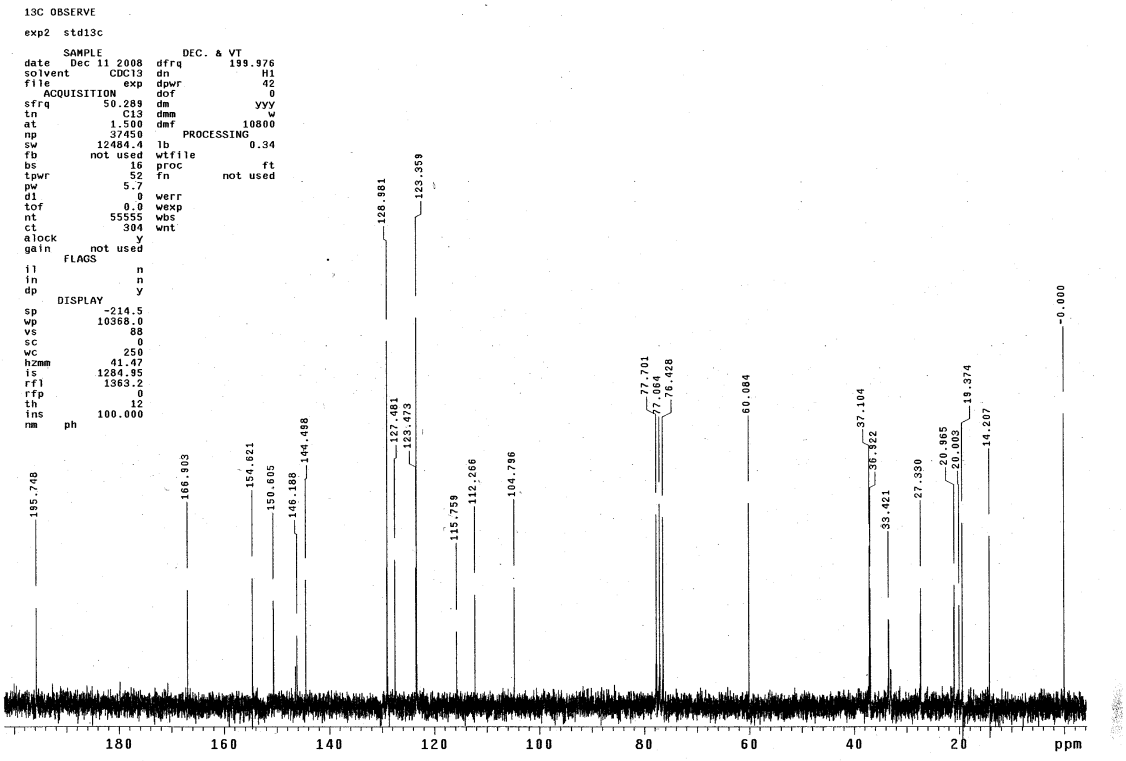

STANDARD 1H OBSERVE
exp1 std1h
SAMPLE
date Dec 9 2008
solvent CDCl3
file exp
ACQUISITION
sfrq 199.977
tn H1
at 1.992
np 11866
sw 3003.0
fb not used
bs 16
tpwr 58
pw 7.0
d1 1.000
tof 1000.0
nt 16
ct 16
alock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -38.5
wp 1959.0
vs 1.136
sc 0
wc 250
hzmm 7.84
is 3304.28
rfl 442.1
rfp 0
th 8
ins 100.000
nm cdc ph
DEC. & VT
dfrq 199.976
dn H1
dpwr 30
dof 0
dm nnn
dmm c
dmf 200
PROCESSING
wtfile
proc ft
fn not used
werr
wexp
wbs
wnt
9.065
6.715
6.612
6.572
6.506
6.463
4.806
4.060
4.025
3.989
3.954
3.683
3.367
3.360
3.347
2.502
2.491
2.482
2.262
2.194
2.168
1.674
1.191
1.157
1.122
-0.000
ppm
4.57
4.19
4.28
9.12
4.26
8.83
12.16
10.00
20.22
9.90
12.46

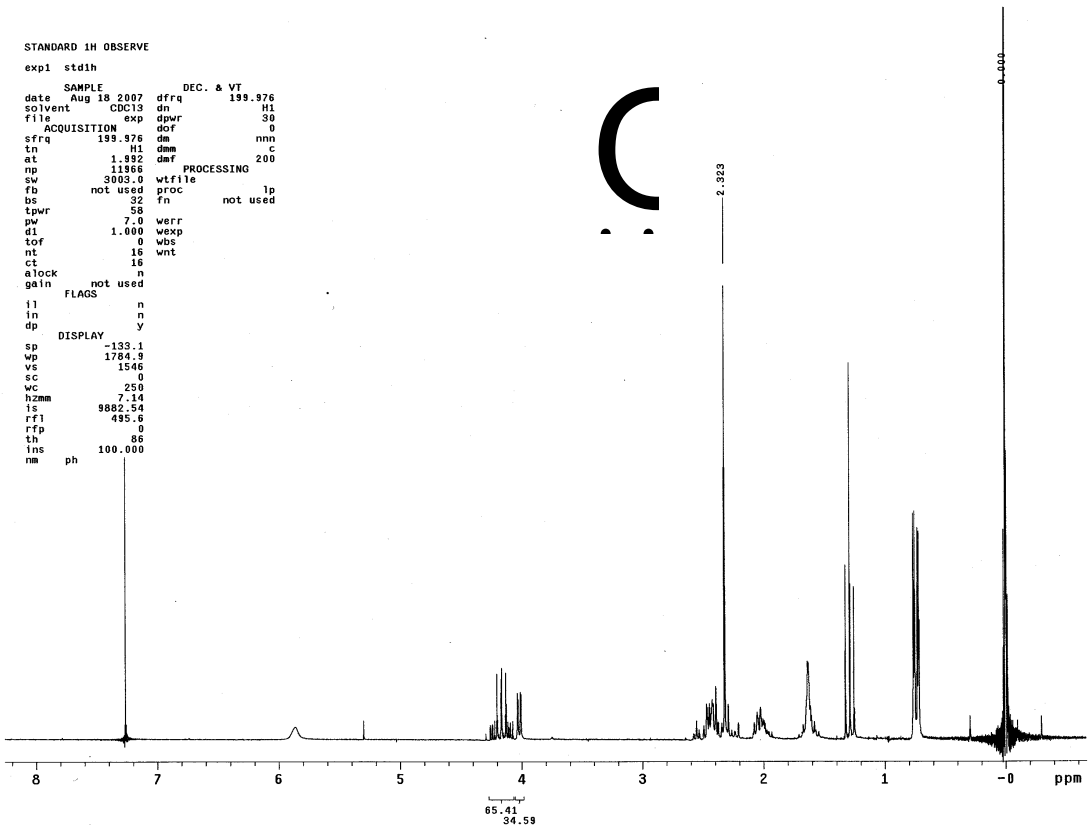

13C OBSERVE
exp2 std13c
SAMPLE
date Dec 9 2008
solvent CDCl3
file exp
ACQUISITION
sfrq 50.289
tn C13
at 1.500
np 37450
sw 12484.4
fb not used
bs 16
tpwr 52
pw 5.7
d1 0
tof 0.0
nt 55555
ct 16
alock y
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -219.3
wp 10382.8
vs 116
sc 0
wc 250
hzmm 41.53
is 1284.95
rfl 3611.9
rfp 1986.7
th 13
ins 100.000
nm ph
DEC. & VT
dfrq 199.976
dn H1
dpwr 42
dof 0
dm yyy
dmm w
dmf 10800
PROCESSING
lb 0.34
wtfile
proc ft
fn not used
werr
wexp
wbs
wnt
167.110
151.138
146.736
144.554
144.342
139.084
119.381
115.065
111.921
111.254
103.973
58.988
55.451
40.751
40.335
39.918
39.501
39.085
38.660
38.251
36.804
34.758
26.151
20.900
18.210
14.255
ppm

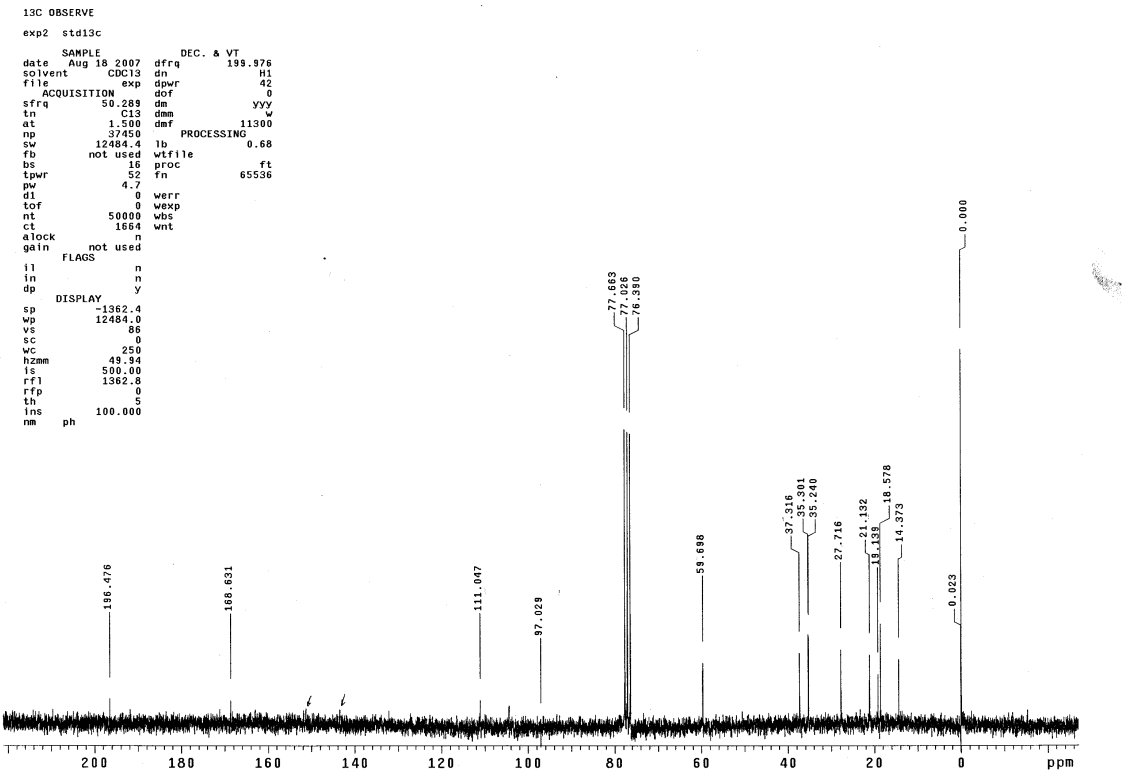

STANDARD 1H OBSERVE
exp1 std1h
SAMPLE
date Aug 30 2007
solvent CDCl3
file exp
ACQUISITION
sfrq 199.976
tn H1
at 1.992
np 11966
sw 3003.0
fb not used
bs 16
tpwr 58
pw 7.2
d1 1.000
tof 0
nt 1
ct 1
alock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -142.6
wp 2075.2
vs 959
sc 0
wc 250
hzmm 8.30
is 817.67
rfl 458.6
rfp 0
th 60
ins 100.000
nm cdc ph
DEC. & VT
dfrq 199.976
dn H1
dpwr 30
dof 0
dm nnn
dmm c
dmf 200
PROCESSING
wtfile
proc ft
fn not used
werr
wexp
wbs
wnt
2.719
2.350
-0.000
-0.015
ppm
3.43
3.44
3.54
3.61
6.52
3.29
13.61
11.39
24.60
6.42
9.94
10.19

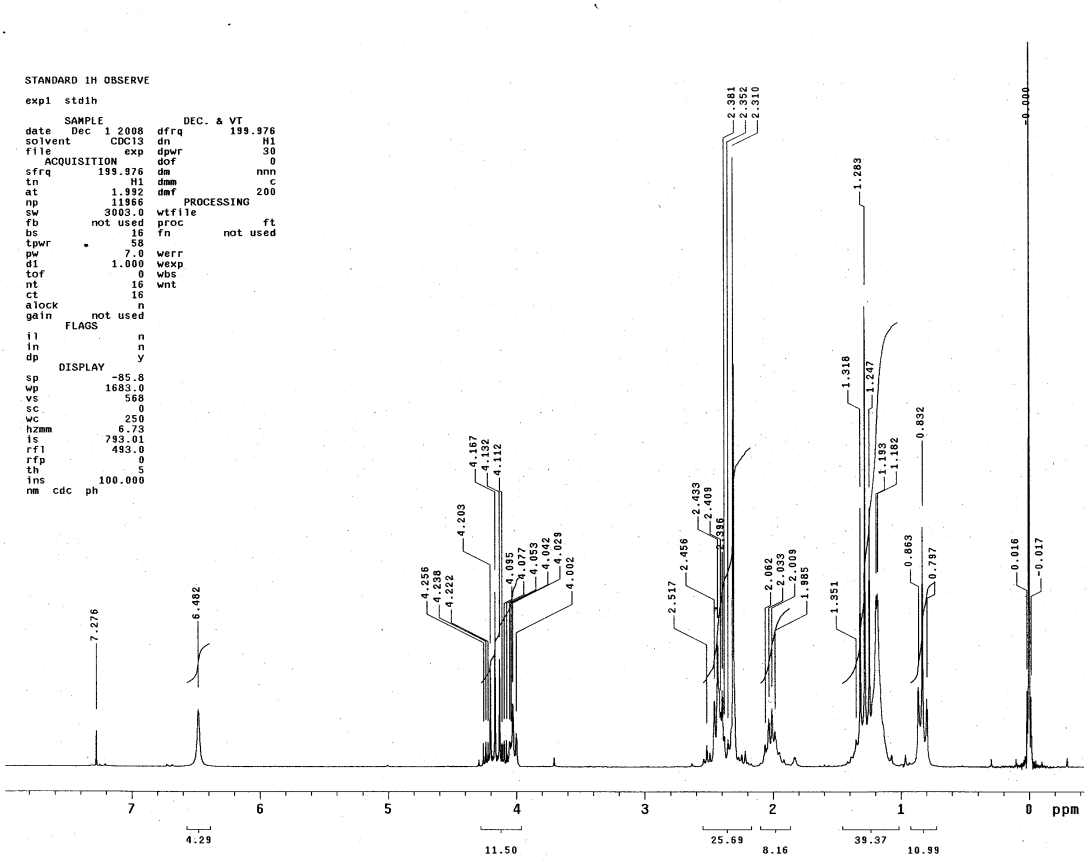

13C OBSERVE
exp2 std13c
SAMPLE
date Aug 30 2007
solvent CDCl3
file exp
ACQUISITION
sfrq 50.289
tn C13
at 1.500
np 37450
sw 12484.4
fb not used
bs 16
tpwr 52
pw 4.7
d1 0
tof 0
nt 50000
ct 1856
alock y
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -1358.2
wp 12484.0
vs 130
sc 0
wc 250
hzmm 49.94
is 500.00
rfl 1358.6
rfp 0
th 10
ins 100.000
nm ph
DEC. & VT
dfrq 199.976
dn H1
dpwr 42
dof 0
dm yyy
dmm w
dmf 11300
PROCESSING
lb 0.47
wtfile
proc ft
fn not used
werr
wexp
wbs
wnt
78.072
77.428
76.792
-0.000
195.771
167.759
150.666
145.309
144.301
144.088
139.801
120.010
114.181
112.789
105.084
64.229
59.365
40.498
40.082
39.665
37.185
35.826
26.928
21.124
18.788
14.904
14.305
ppm

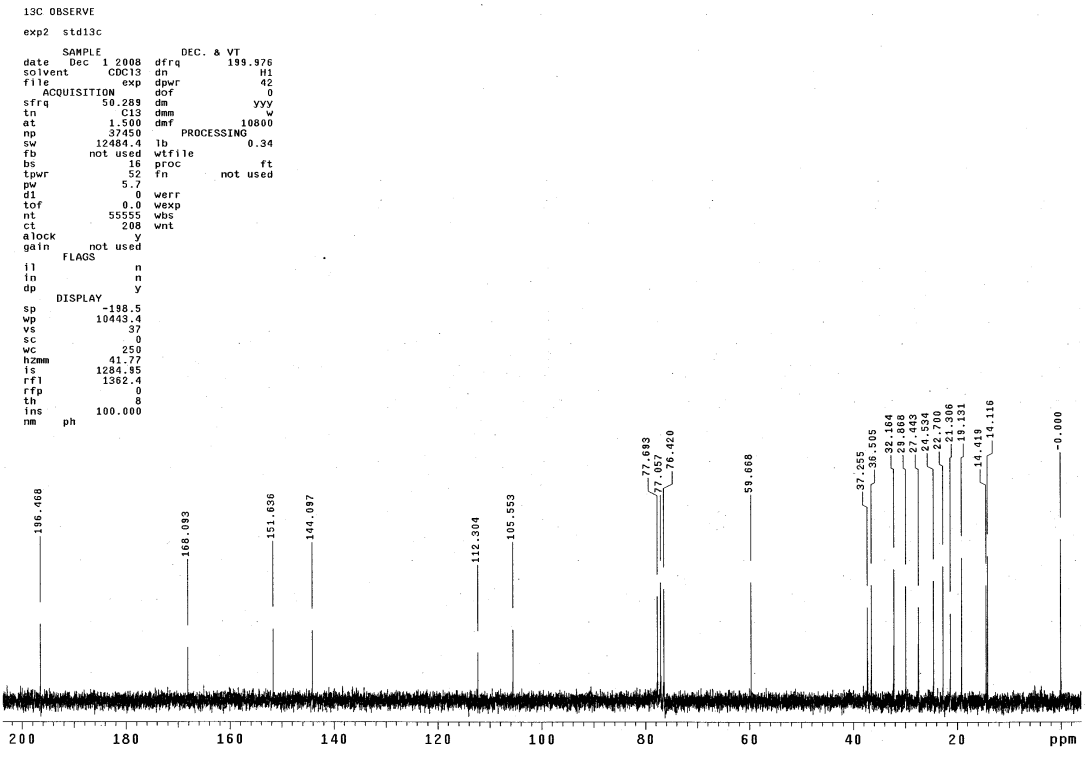

STANDARD 1H OBSERVE
exp1 stdih
SAMPLE
date Dec 11 2008
solvent CDCl3
file exp
ACQUISITION
sfrq 199.976
tn H1
at 1.992
np 11966
sw 3003.0
fb not used
bs 16
tpwr 58
pw 7.0
d1 1.000
tof 0.0
nt 16
ct 16
alock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -42.5
wp 1842.8
vs 575
sc 0
wc 250
hzmm 92.37
is 184.78
rfl 93.4
rfp 0
th 6
ins 100.000
nm cdc ph
DEC. & VT
dfrq 199.976
dn H1
dpwr 30
dof 0
dm nnn
dmm c
dmf 200
PROCESSING
wtfile
proc ft
fn not used
werr
wexp
wbs
wnt
8.150
8.099
7.507
7.496
7.472
7.463
7.298
7.274
7.257
6.572
5.488
5.193
4.108
4.073
4.036
4.002
2.456
2.431
2.403
2.374
2.346
2.055
1.987
1.961
1.210
1.175
1.138
0.016
-0.000
-0.017
8
7
6
5
4
3
2
1
ppm
9.96
7.96
4.31
3.75
7.92
39.08
15.04
11.98

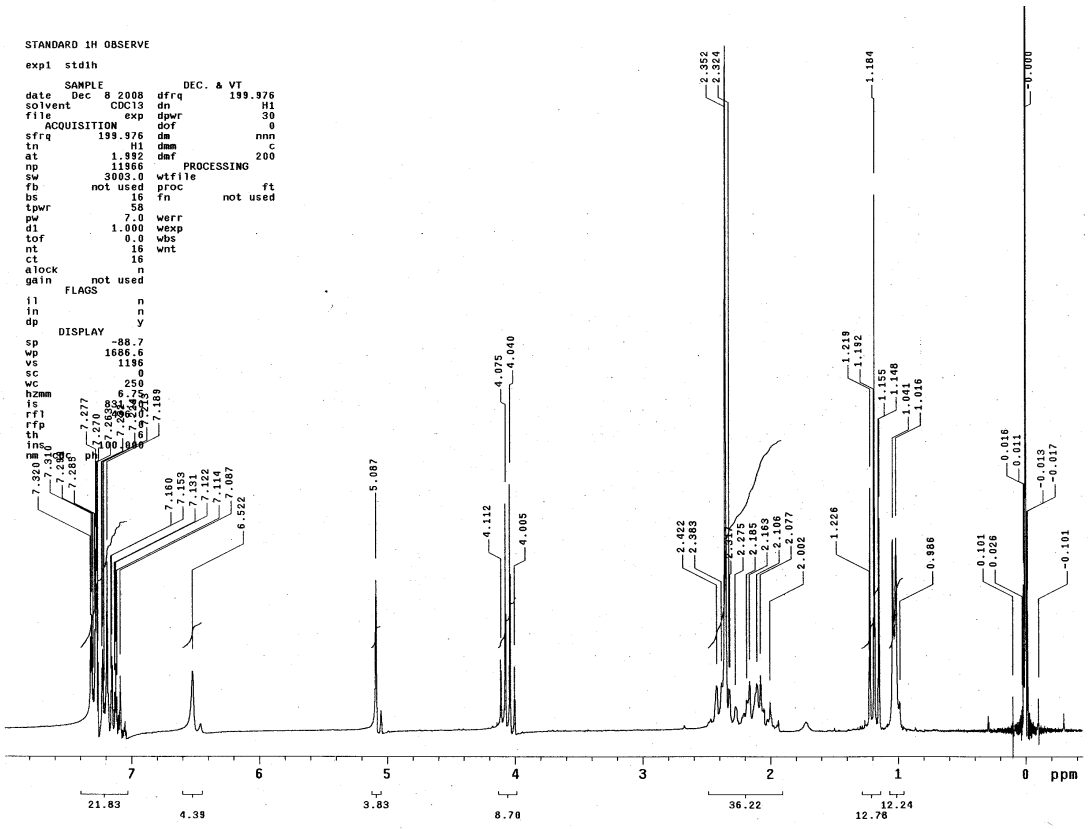

13C OBSERVE
exp2 stdi3c
SAMPLE
date Dec 11 2008
solvent CDCl3
file exp
ACQUISITION
sfrq 50.289
tn C13
at 1.500
np 37450
sw 12484.4
fb not used
bs 16
tpwr 52
pw 5.7
d1 0
tof 0.0
nt 55555
ct 304
alock y
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -214.5
wp 10368.0
vs 88
sc 0
wc 250
hzmm 41.47
is 1284.95
rfl 1363.2
rfp 0
th 12
ins 100.000
nm ph
DEC. & VT
dfrq 199.976
dn H1
dpwr 42
dof 0
dm yyy
dmm w
dmf 10800
PROCESSING
lb 0.34
wtfile
proc ft
fn not used
werr
wexp
wbs
wnt
195.748
166.903
154.621
150.605
146.188
144.488
128.981
127.481
123.473
123.359
115.759
112.266
104.786
77.701
77.064
76.428
60.084
37.104
36.922
33.421
27.330
20.965
20.003
19.374
14.207
-0.000
180
160
140
120
100
80
60
40
20
ppm

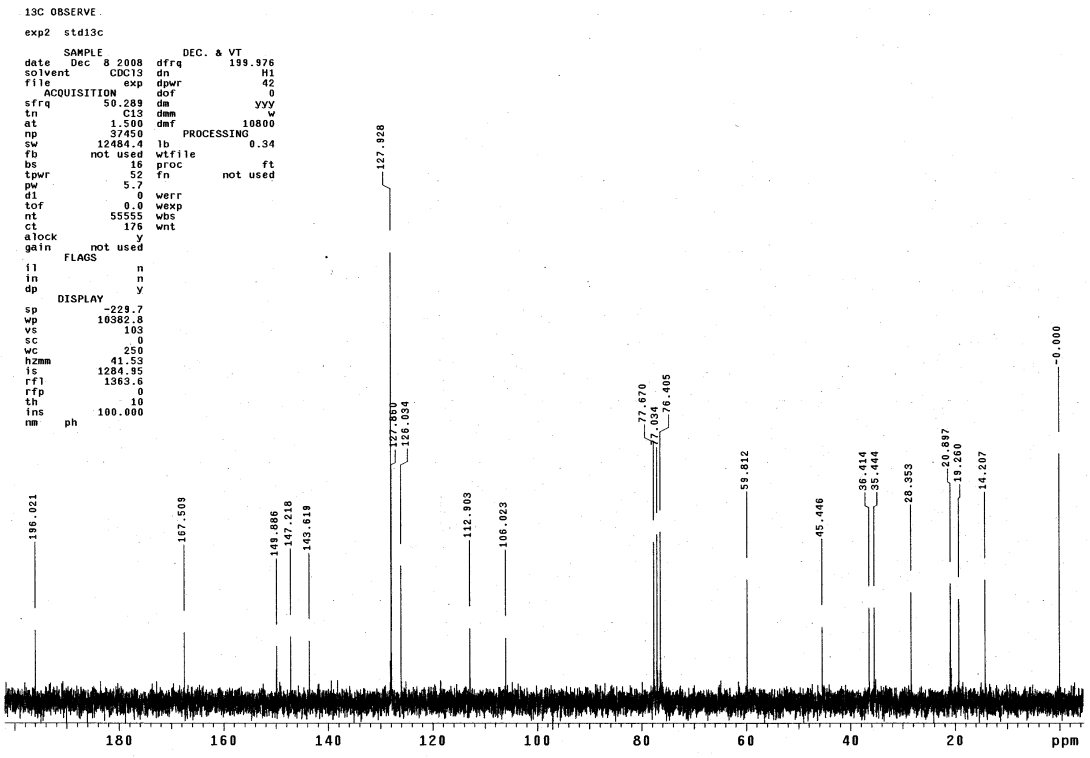

STANDARD 1H OBSERVE
exp1 std1h
SAMPLE
date Aug 18 2007
solvent CDCl3
file exp
ACQUISITION
sfrq 199.976
tn H1
at 1.992
np 11966
sw 3003.0
fb not used
bs 32
tpwr 58
pw 7.0
d1 1.000
tof 0
nt 16
ct 16
alock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -133.1
wp 1784.9
vs 1546
sc 0
wc 250
hzmm 7.14
is 9882.54
rfl 495.6
rfp 0
th 86
ins 100.000
nm ph
DEC. & VT
dfrq 199.976
dn H1
dpwr 30
dof 0
dm nnn
dmm c
dmf 200
PROCESSING
wtfile
proc lp
fn not used
werr
wexp
wbs
wnt
2.323
0.000
8
7
6
5
4
3
2
1
-0
ppm
65.41
34.59

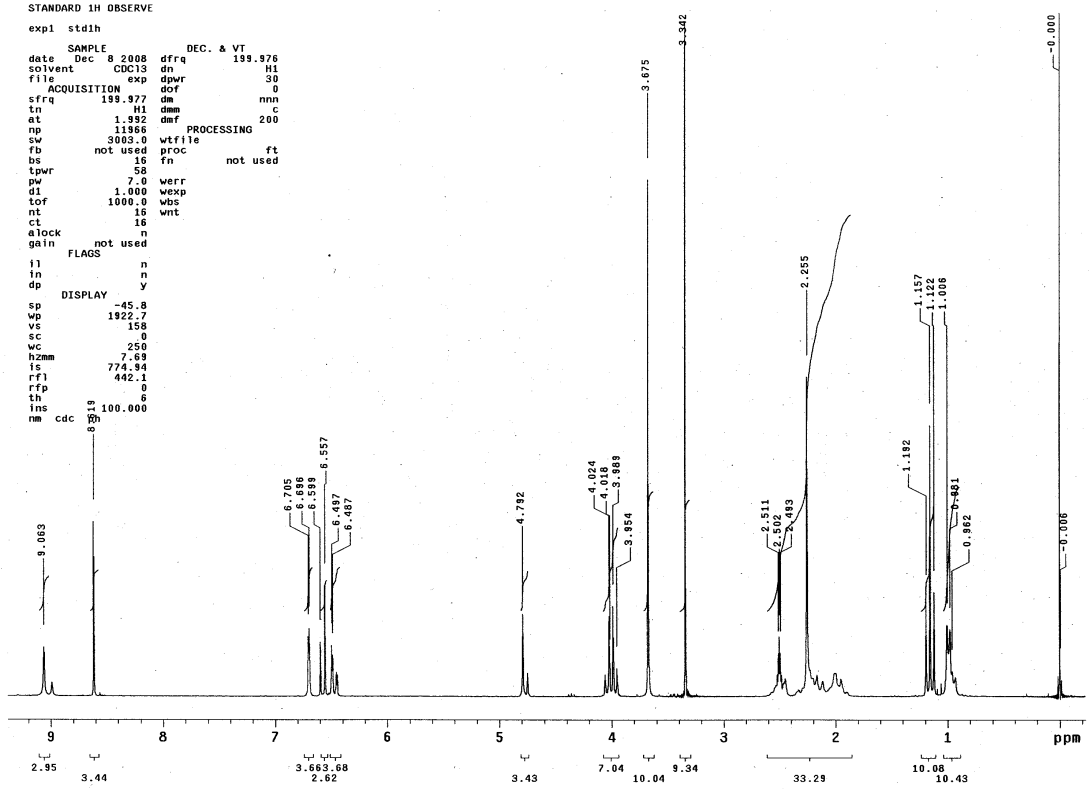

13C OBSERVE
exp2 std13c
SAMPLE
date Aug 18 2007
solvent CDCl3
file exp
ACQUISITION
sfrq 50.289
tn C13
at 1.500
np 37450
sw 12484.4
fb not used
bs 16
tpwr 52
pw 4.7
d1 0
tof 0
nt 50000
ct 1664
alock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -1362.4
wp 12484.0
vs 86
sc 0
wc 250
hzmm 49.94
is 500.00
rfl 1362.8
rfp 0
th 5
ins 100.000
nm ph
DEC. & VT
dfrq 199.976
dn H1
dpwr 42
dof 0
dm yyy
dmm w
dmf 11300
PROCESSING
lb 0.68
wtfile
proc ft
fn 65536
werr
wexp
wbs
wnt
196.476
168.631
111.047
97.029
77.663
77.026
76.390
59.698
37.316
35.301
35.240
27.716
21.132
19.139
18.578
14.373
0.023
0.000
200
180
160
140
120
100
80
60
40
20
0
ppm

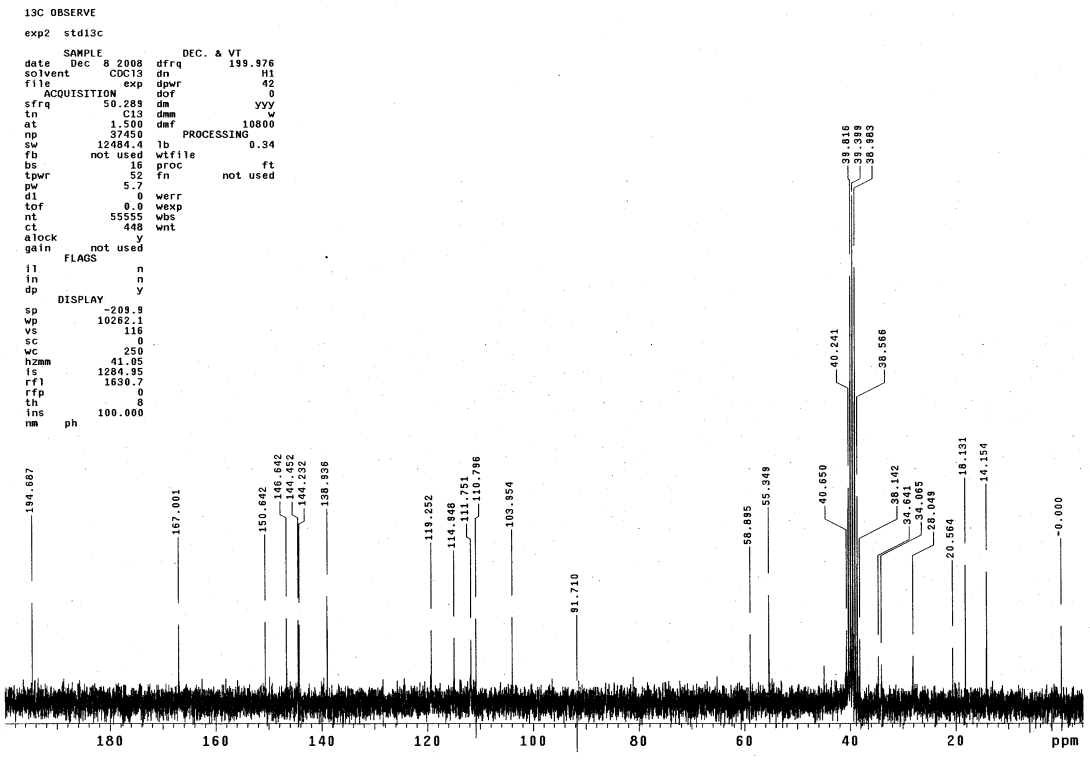

STANDARD 1H OBSERVE
exp1 stdih
SAMPLE
date Dec 1 2008
solvent CDCl3
file exp
ACQUISITION
sfrq 199.976
tn H1
at 1.992
np 11966
sw 3003.0
fb not used
bs 16
tpwr 58
pw 7.0
d1 1.000
tof 0
nt 16
ct 16
alock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -85.8
wp 1683.0
vs 568
sc 0
wc 250
hzmm 6.73
is 793.01
rfl 493.0
rfp 0
th 5
ins 100.000
nm cdc ph
DEC. & VT
dfrq 199.976
dn H1
dpwr 30
dof 0
dm nnn
dmm c
dmf 200
PROCESSING
wtfile
proc ft
fn not used
werr
wexp
wbs
wnt
7.276
6.482
4.256
4.238
4.222
4.203
4.167
4.132
4.112
4.095
4.077
4.053
4.042
4.029
4.002
2.517
2.456
2.433
2.409
2.381
2.352
2.310
2.062
2.033
2.009
1.985
1.951
1.918
1.283
1.247
1.193
1.182
0.863
0.832
0.797
0.016
0.000
-0.017
7
6
5
4
3
2
1
0
ppm
4.29
11.50
25.69
8.16
39.37
10.99

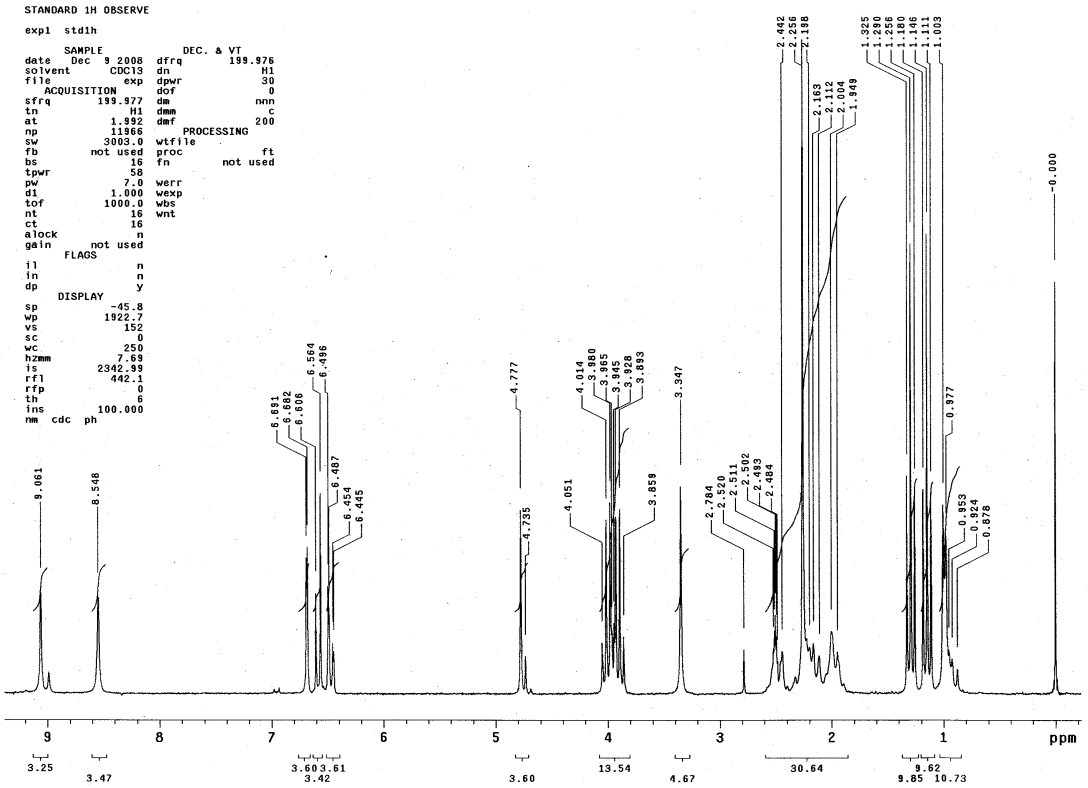

13C OBSERVE
exp2 stdi3c
SAMPLE
date Dec 1 2008
solvent CDCl3
file exp
ACQUISITION
sfrq 50.289
tn C13
at 1.500
np 37450
sw 12484.4
fb not used
bs 16
tpwr 52
pw 5.7
d1 0
tof 0.0
nt 55555
ct 208
alock y
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -198.5
wp 10443.4
vs 37
sc 0
wc 250
hzmm 41.77
is 1284.95
rfl 1362.4
rfp 0
th 8
ins 100.000
nm ph
DEC. & VT
dfrq 199.976
dn H1
dpwr 42
dof 0
dm yyy
dmm w
dmf 10800
PROCESSING
lb 0.34
wtfile
proc ft
fn not used
werr
wexp
wbs
wnt
196.468
168.093
151.636
144.097
112.304
105.553
77.693
77.057
76.420
59.668
37.255
36.505
32.164
29.868
27.443
24.534
22.700
21.306
19.131
14.419
14.116
-0.000
200
180
160
140
120
100
80
60
40
20
ppm

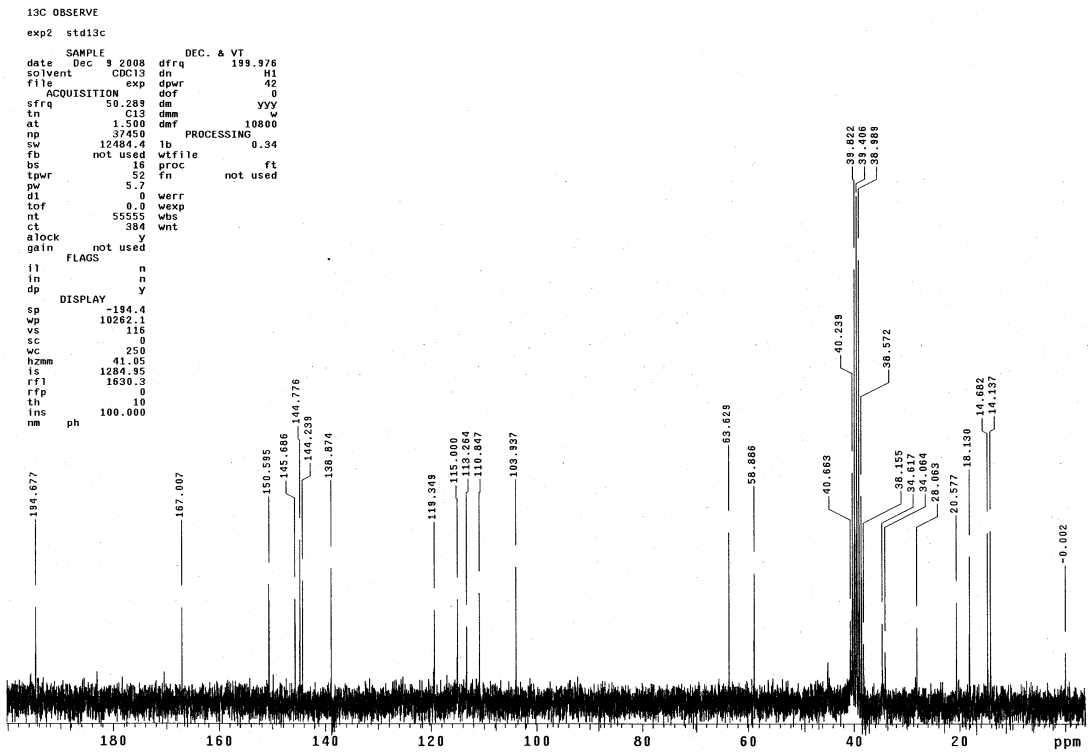


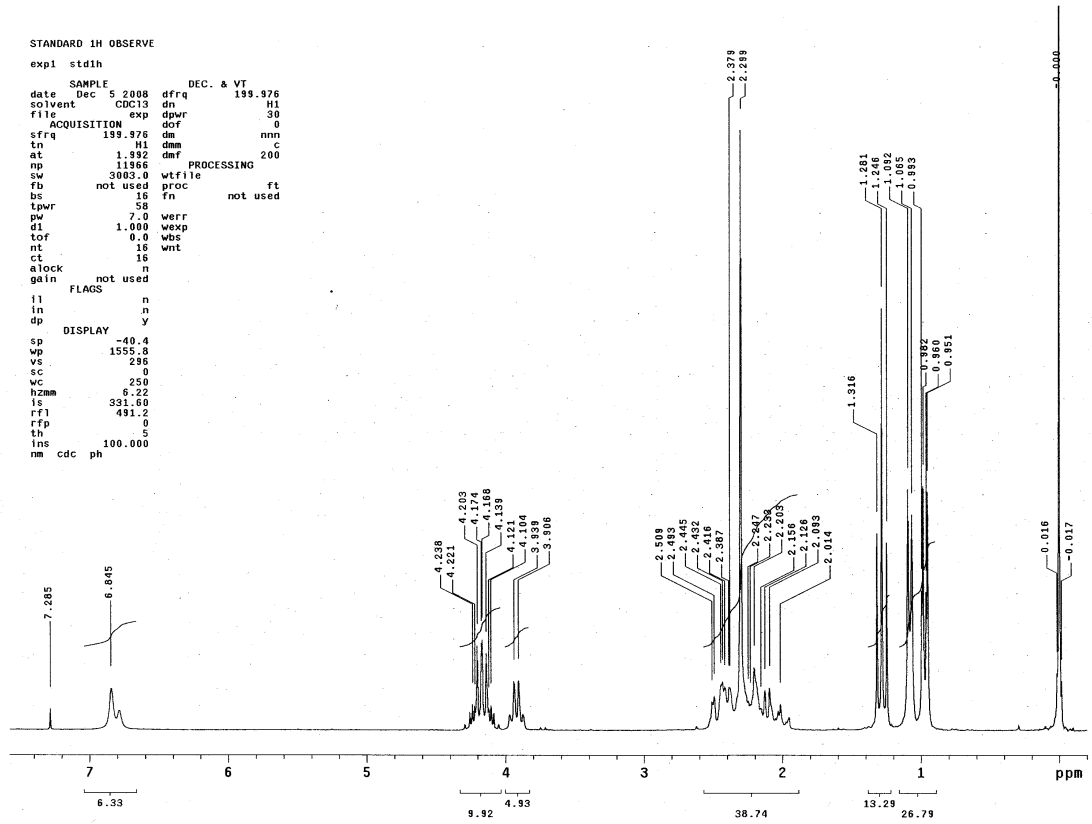


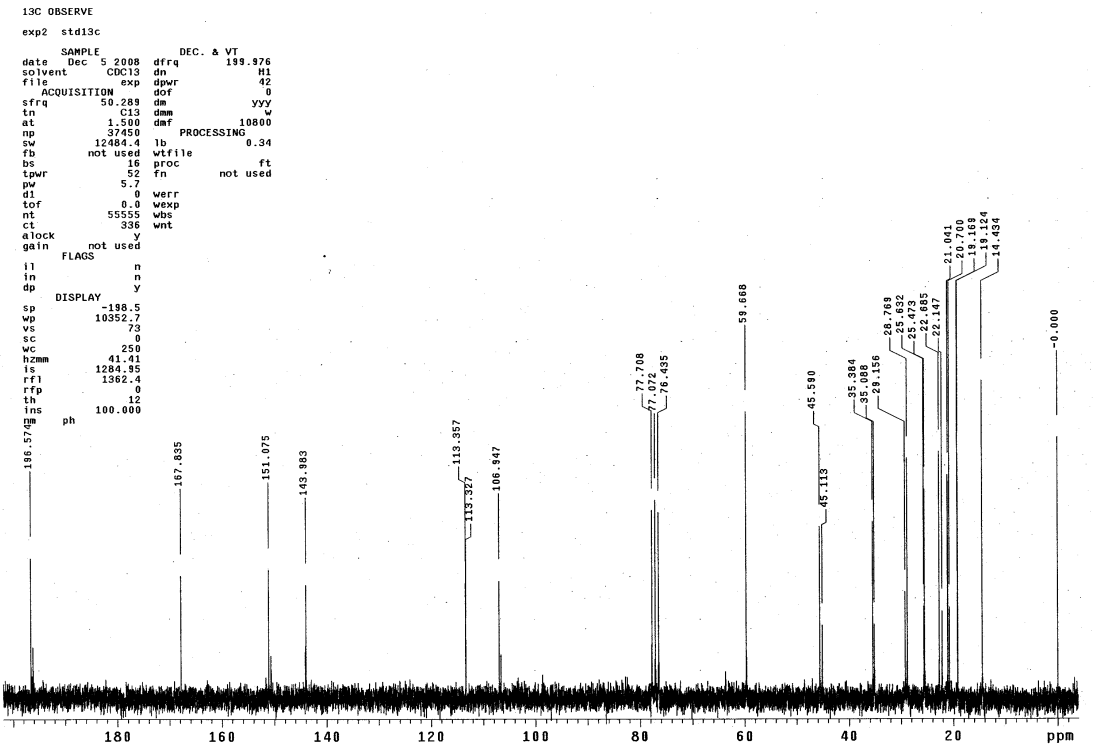

STANDARD 1H OBSERVE
exp1 std1h
SAMPLE
date Dec 8 2008
solvent CDCl3
file exp
ACQUISITION
sfrq 199.977
tn H1
at 1.992
np 11966
sw 3003.0
fb not used
bs 16
tpwr 58
pw 7.0
d1 1.000
tof 1000.0
nt 16
ct 16
alock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -45.8
wp 1922.7
vs 158
sc 0
wc 250
hzmm 7.69
is 774.94
rfl 442.1
rfp 0
th 6
ins 100.000
nm cdc ph
DEC. & VT
dfrq 199.976
dn H1
dpwr 30
dof 0
dm nnn
dmm c
dmf 200
PROCESSING
wtfile
proc ft
fn not used
werr
wexp
wbs
wnt
9.063
8.819
6.705
6.686
6.599
6.557
6.497
6.487
4.792
4.024
4.018
3.988
3.954
3.675
3.342
2.511
2.502
2.493
2.255
1.192
1.157
1.122
1.006
0.981
0.962
0.000
0.006
ppm
2.95
3.44
3.663.68
2.62
3.43
7.04
10.04
9.34
33.29
10.08
10.43

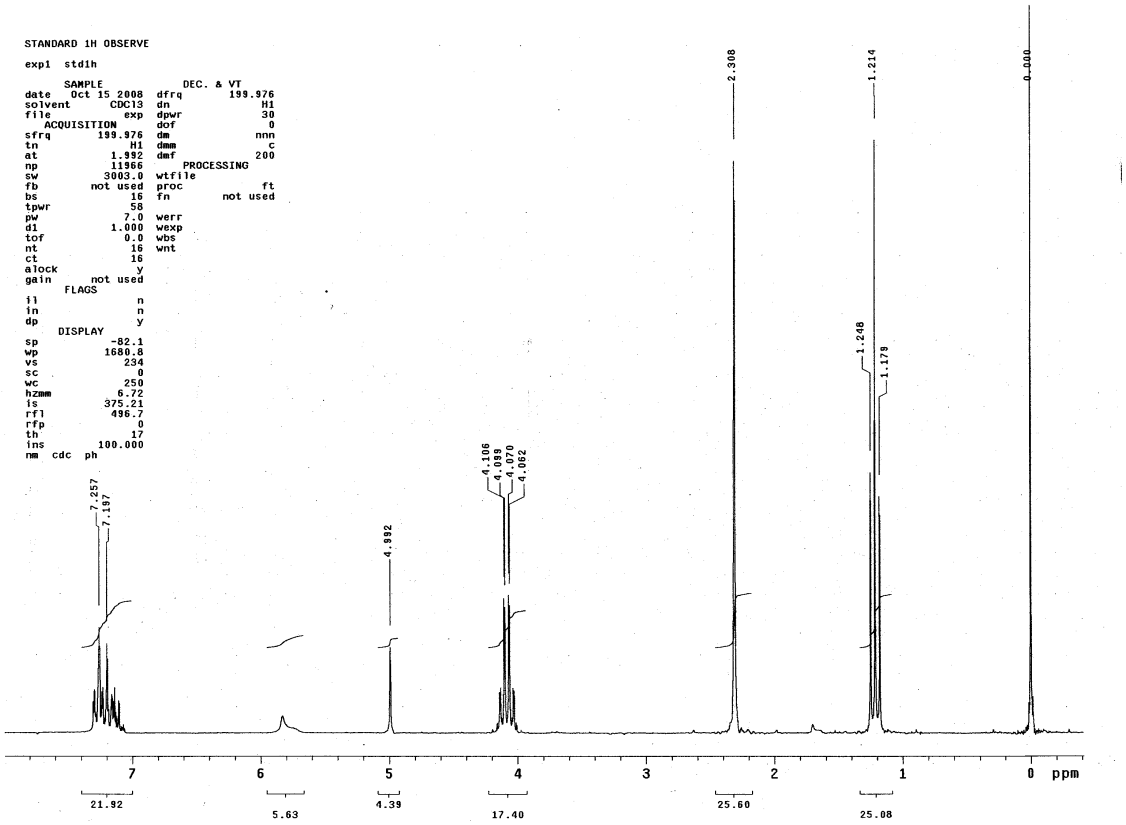

13C OBSERVE
exp2 std13c
SAMPLE
date Dec 8 2008
solvent CDCl3
file exp
ACQUISITION
sfrq 50.289
tn C13
at 1.500
np 37450
sw 12484.4
fb not used
bs 16
tpwr 52
pw 5.7
d1 0
tof 0.0
nt 55555
ct 448
alock y
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -209.9
wp 10262.1
vs 116
sc 0
wc 250
hzmm 41.05
is 1284.95
rfl 1630.7
rfp 0
th 8
ins 100.000
nm ph
DEC. & VT
dfrq 199.976
dn H1
dpwr 42
dof 0
dm yyy
dmm w
dmf 10800
PROCESSING
lb 0.34
wtfile
proc ft
fn not used
werr
wexp
wbs
wnt
194.687
167.001
150.642
146.642
146.452
144.232
138.936
119.252
114.948
111.751
110.796
103.954
91.710
58.895
55.349
40.650
40.241
39.816
39.389
38.983
38.566
38.142
34.641
34.065
28.049
20.564
18.131
14.154
-0.000
180
160
140
120
100
80
60
40
20
ppm

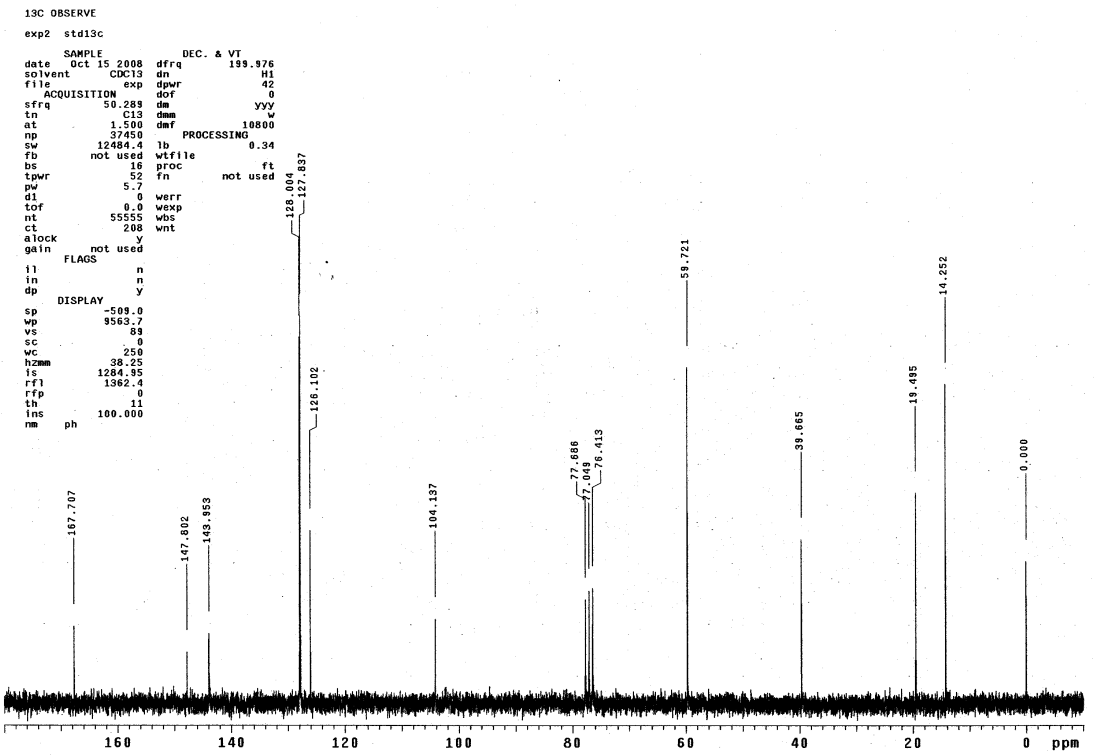

STANDARD 1H OBSERVE
exp1 std1h
SAMPLE
date Dec 9 2008
solvent CDCl3
file exp
ACQUISITION
sfrq 199.977
tn H1
at 1.992
np 11966
sw 3003.0
fb not used
bs 16
tpwr 58
pw 7.0
d1 1.000
tof 1000.0
nt 16
ct 16
alock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -45.8
wp 1922.7
vs 152
sc 0
wc 250
hzmm 7.69
is 2342.99
rfl 442.1
rfp 0
th 6
ins 100.000
nm cdc ph
DEC. & VT
dfrq 199.976
dn H1
dpwr 30
dof 0
dm nnn
dmm c
dmf 200
PROCESSING
wtfile
proc ft
fn not used
werr
wexp
wbs
wnt
9.061
8.548
6.691
6.682
6.606
6.564
6.486
6.487
6.454
6.445
4.777
4.735
4.051
4.014
3.980
3.965
3.945
3.928
3.893
3.859
3.347
2.784
2.520
2.511
2.502
2.493
2.484
2.442
2.256
2.198
2.163
2.112
2.004
1.949
1.925
1.300
1.256
1.180
1.146
1.111
1.003
0.977
0.853
0.824
0.878
-0.000
ppm
3.25
3.47
3.60
3.61
3.42
3.60
13.54
4.67
30.64
9.62
9.85
10.73

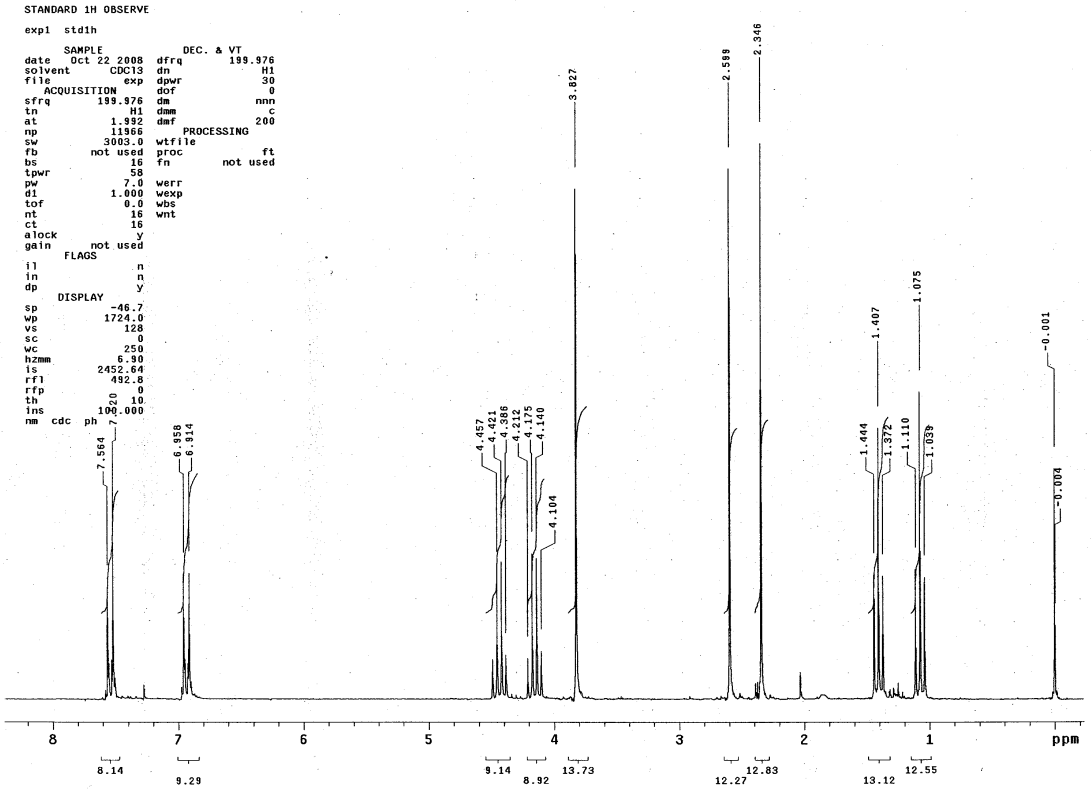

13C OBSERVE
exp2 std13c
SAMPLE
date Dec 9 2008
solvent CDCl3
file exp
ACQUISITION
sfrq 50.289
tn C13
at 1.500
np 37450
sw 12484.4
fb not used
bs 16
tpwr 52
pw 5.7
d1 0
tof 0.0
nt 55555
ct 384
alock y
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -194.4
wp 10262.1
vs 116
sc 0
wc 250
hzmm 41.05
is 1284.95
rfl 1630.3
rfp 0
th 10
ins 100.000
nm ph
DEC. & VT
dfrq 199.976
dn H1
dpwr 42
dof 0
dm yyy
dmm w
dmf 10800
PROCESSING
lb 0.34
wtfile
proc ft
fn not used
werr
wexp
wbs
wnt
194.677
167.007
150.595
145.686
144.776
144.239
138.874
119.349
115.000
113.264
110.847
103.337
63.629
58.886
40.663
40.239
39.822
39.406
38.989
38.572
38.155
34.617
34.084
26.068
20.577
18.130
14.682
14.137
-0.002
ppm

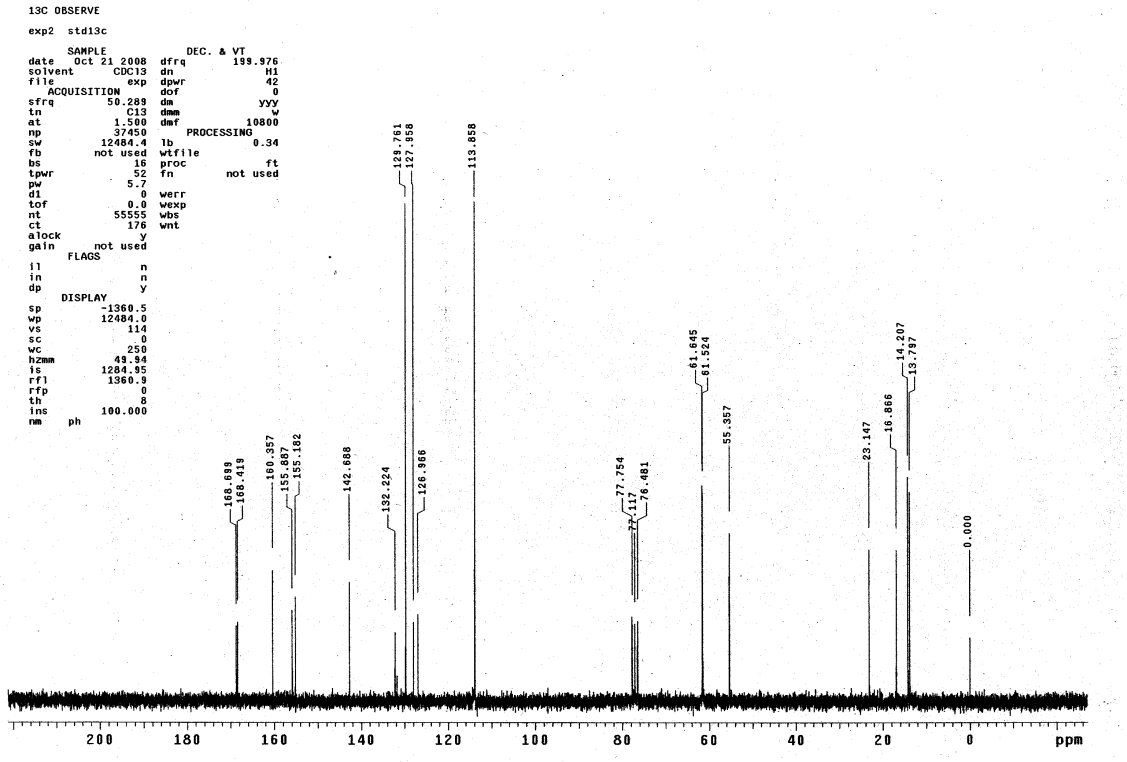

STANDARD 1H OBSERVE
exp1 std1h
SAMPLE
date Dec 5 2008
solvent CDCl3
file exp
ACQUISITION
sfrq 199.976
tn H1
at 1.992
np 11866
sw 3003.0
fb not used
bs 16
tpwr 58
pw 7.0
d1 1.000
tof 0.0
nt 16
ct 16
alock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -40.4
wp 1555.8
vs 296
sc 0
wc 250
hzmm 6.22
is 331.60
rfl 491.2
rfp 0
th 5
ins 100.000
nm cdc ph
DEC. & VT
dfrq 199.976
dn H1
dpwr 30
dof 0
dm nnn
dmm c
dmf 200
PROCESSING
wtfile
proc ft
fn not used
werr
wexp
wbs
wnt
7.285
6.845
4.238
4.221
4.203
4.174
4.168
4.139
4.121
4.104
4.100
3.938
3.906
2.509
2.493
2.445
2.432
2.416
2.387
2.379
2.299
2.247
2.232
2.203
2.156
2.126
2.093
2.014
1.316
1.281
1.246
1.092
1.055
0.993
0.982
0.960
0.951
0.016
-0.000
-0.017
7
6
5
4
3
2
1
ppm
6.33
9.92
4.93
38.74
13.29
26.79

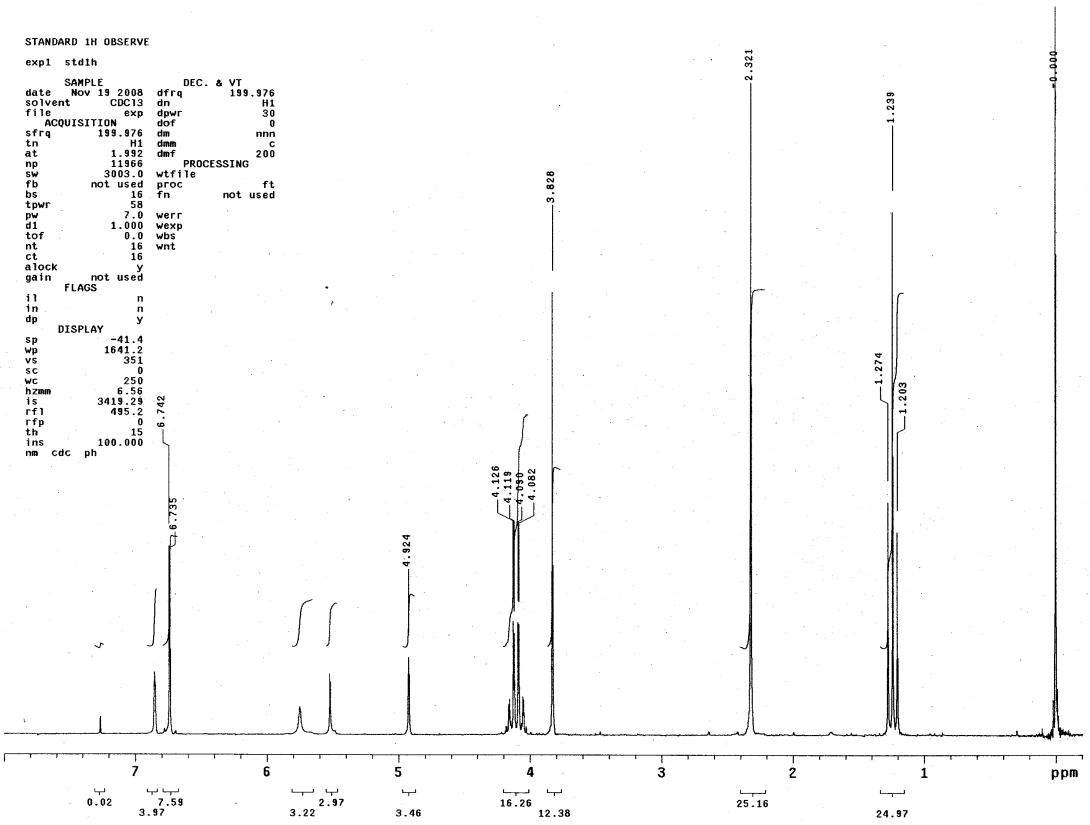

13C OBSERVE
exp2 std13c
SAMPLE
date Dec 5 2008
solvent CDCl3
file exp
ACQUISITION
sfrq 50.289
tn C13
at 1.500
np 37450
sw 12484.4
fb not used
bs 16
tpwr 52
pw 5.7
d1 0
tof 0.0
nt 55555
ct 336
alock y
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -198.5
wp 10352.7
vs 73
sc 0
wc 250
hzmm 41.41
is 1284.95
rfl 1362.4
rfp 0
th 12
ins 100.000
nm ph
DEC. & VT
dfrq 199.976
dn H1
dpwr 42
dof 0
dm yyy
dmm w
dmf 10800
PROCESSING
lb 0.34
wtfile
proc ft
fn not used
werr
wexp
wbs
wnt
186.574
167.835
151.075
143.983
113.357
113.327
106.947
77.708
77.072
76.435
59.668
45.590
45.113
35.384
35.088
29.156
28.769
25.692
25.473
22.685
22.147
21.041
20.700
19.169
19.124
14.434
-0.000
180
160
140
120
100
80
60
40
20
ppm

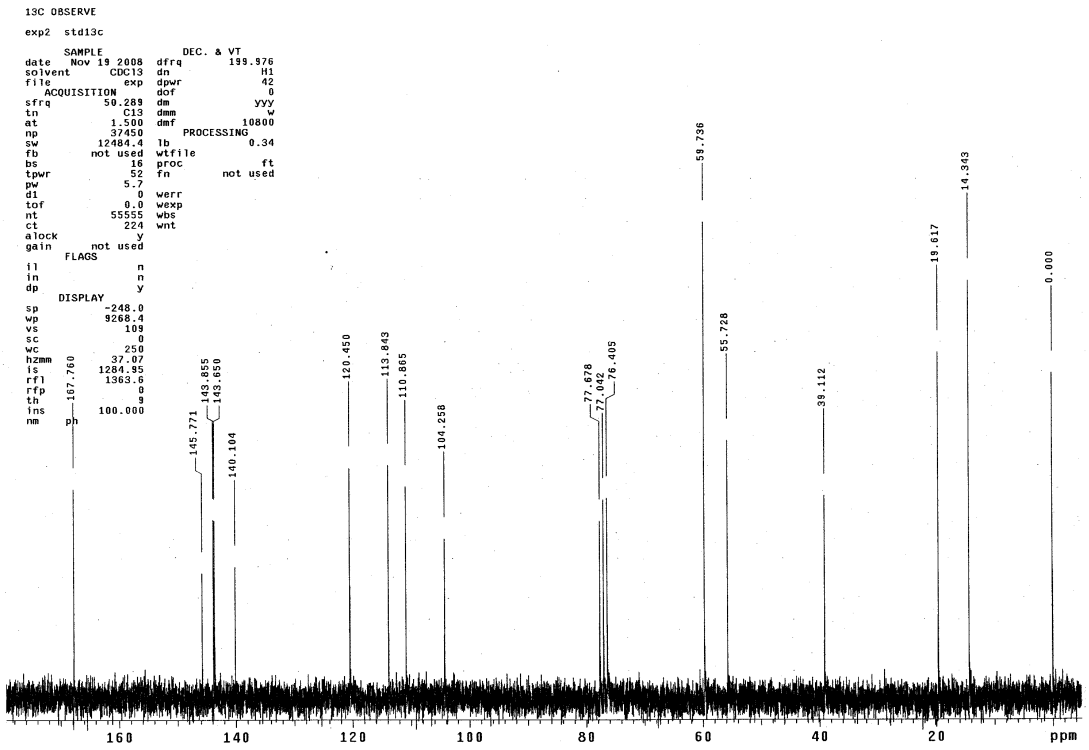

STANDARD 1H OBSERVE
exp1 std1h
SAMPLE
date Oct 15 2008
solvent CDCl3
file exp
ACQUISITION
sfrq 199.976
tn H1
at 1.992
np 11966
sw 3003.0
fb not used
bs 16
tpwr 58
pw 7.0
d1 1.000
tof 0.0
nt 16
ct 16
alock y
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -82.1
wp 1680.8
vs 234
sc 0
wc 250
hzmm 6.72
is 375.21
rfl 496.7
rfp 0
th 17
ins 100.000
nm cdc ph
DEC. & VT
dfrq 199.976
dn H1
dpwr 30
dof 0
dm nnn
dmm c
dmf 200
PROCESSING
wtfile
proc ft
fn not used
werr
wexp
wbs
wnt
7.257
7.197
4.992
4.106
4.099
4.070
4.062
2.308
1.248
1.214
1.179
0.000
7
6
5
4
3
2
1
0 ppm
21.92
5.63
4.39
17.40
25.60
25.08

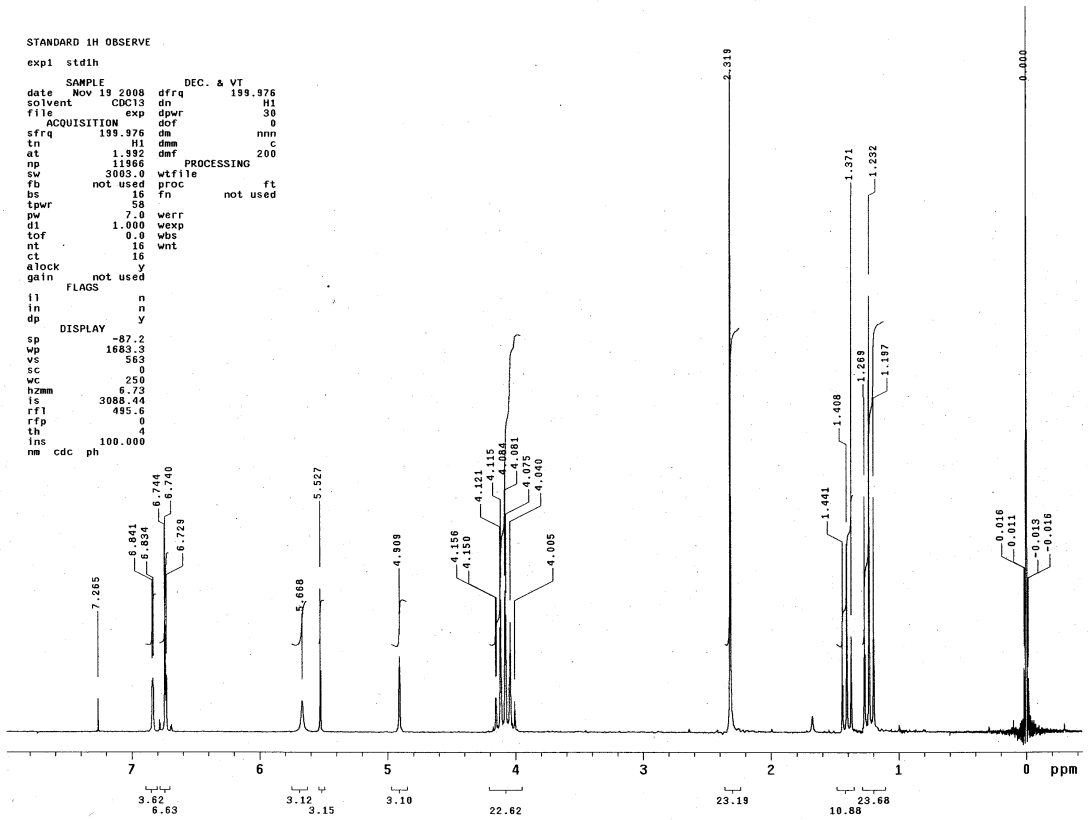

13C OBSERVE
exp2 std13c
SAMPLE
date Oct 15 2008
solvent CDCl3
file exp
ACQUISITION
sfrq 50.289
tn C13
at 1.500
np 37450
sw 12484.4
fb not used
bs 16
tpwr 52
pw 5.7
d1 0
tof 0.0
nt 55555
ct 208
alock y
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -509.0
wp 9563.7
vs 89
sc 0
wc 250
hzmm 38.25
is 1284.95
rfl 1362.4
rfp 0
th 11
ins 100.000
nm ph
DEC. & VT
dfrq 199.976
dn H1
dpwr 42
dof 0
dm yyy
dmm w
dmf 10800
PROCESSING
lb 0.34
wtfile
proc ft
fn not used
werr
wexp
wbs
wnt
167.707
147.802
143.953
128.004
127.837
126.102
104.137
77.686
77.049
76.413
59.721
39.665
19.495
14.252
0.000
160
140
120
100
80
60
40
20
0 ppm

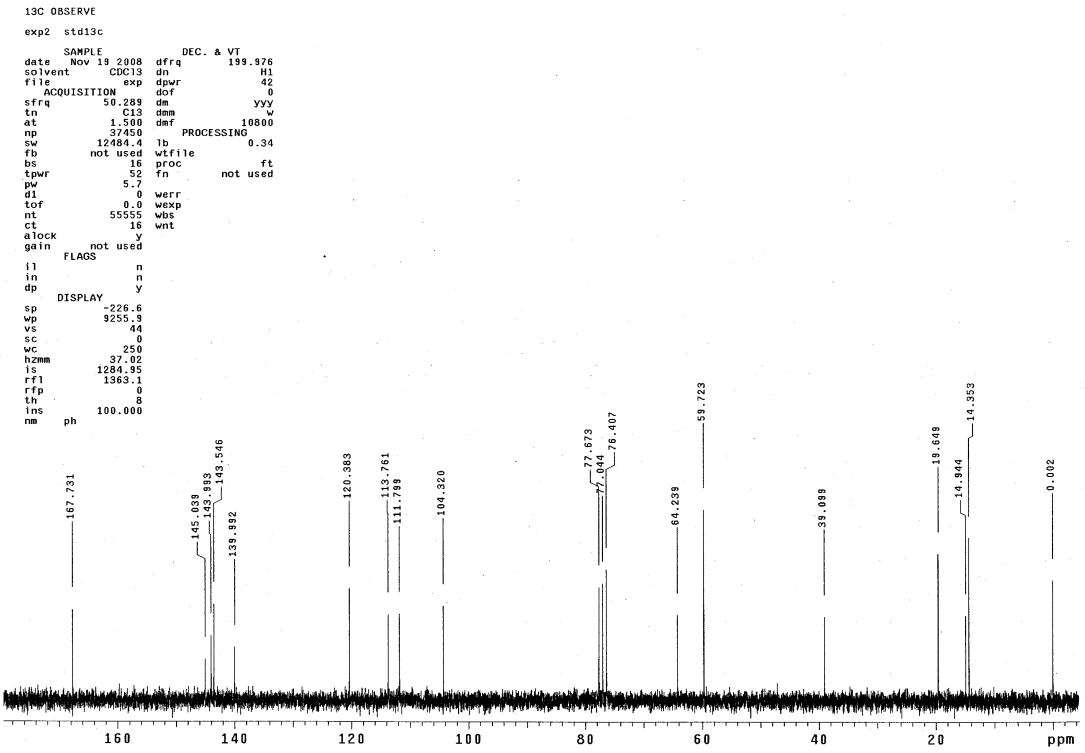

STANDARD 1H OBSERVE
exp1 std1h
SAMPLE
date Oct 22 2008
solvent CDCl3
file exp
ACQUISITION
sfrq 199.976
tn H1
at 1.992
np 11966
sw 3003.0
fb not used
bs 16
tpwr 58
pw 7.0
d1 1.000
tof 0.0
nt 16
ct 16
alock y
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -46.7
wp 1724.0
vs 128
sc 0
wc 250
hzmm 6.90
is 2452.64
rfl 492.8
rfp 0
th 10
ins 100.000
nm cdc ph
DEC. & VT
dfrq 199.976
dn H1
dpwr 30
dof 0
dm nnn
dmm c
dmf 200
PROCESSING
wtfile
proc ft
fn not used
werr
wexp
wbs
wnt
7.564
7.560
6.958
6.914
4.457
4.421
4.386
4.175
4.140
4.104
3.827
2.589
2.346
1.444
1.407
1.372
1.110
1.075
1.039
-0.001
-0.004
8
7
6
5
4
3
2
1
ppm
8.14
9.29
9.14
8.92
13.73
12.27
12.83
13.12
12.55

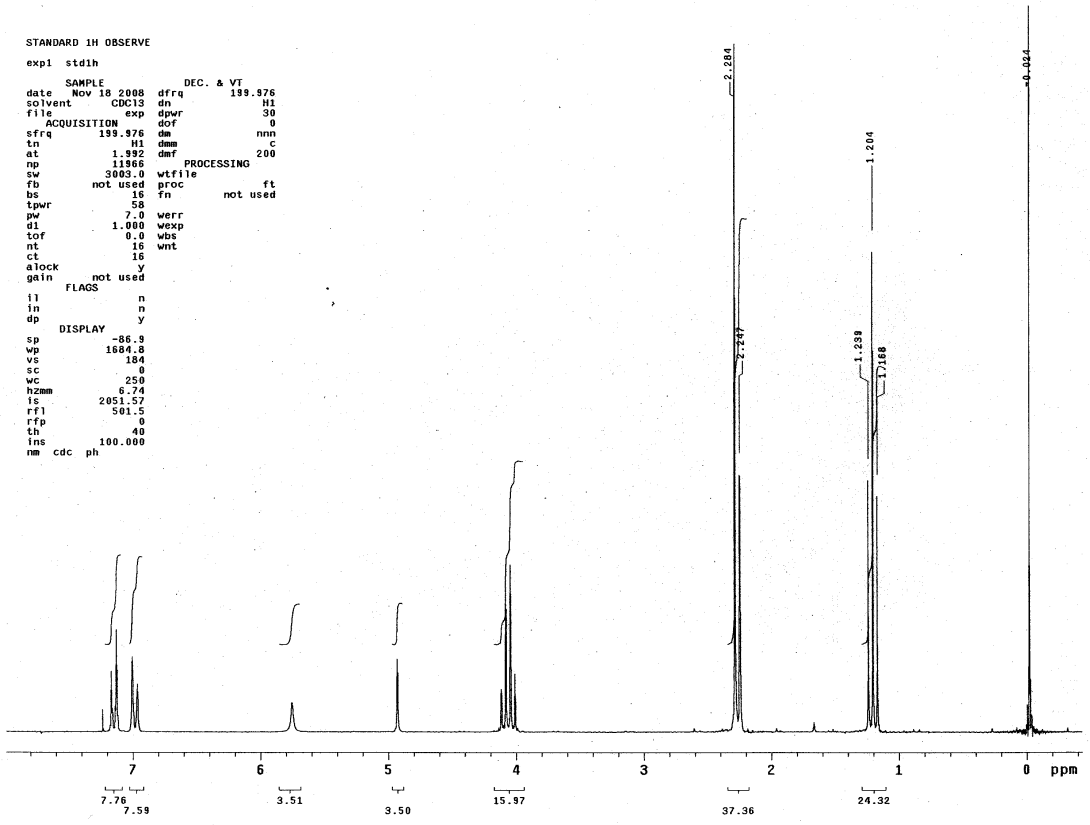

13C OBSERVE
exp2 std13c
SAMPLE
date Oct 21 2008
solvent CDCl3
file exp
ACQUISITION
sfrq 50.289
tn C13
at 1.500
np 37450
sw 12484.4
fb not used
bs 16
tpwr 52
pw 5.7
d1 0
tof 0.0
nt 55555
ct 176
alock y
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -1360.5
wp 12484.0
vs 114
sc 0
wc 250
hzmm 49.94
is 1284.95
rfl 1360.9
rfp 0
th 8
ins 100.000
nm ph
DEC. & VT
dfrq 199.976
dn H1
dpwr 42
dof 0
dm yyy
dmm w
dmf 10800
PROCESSING
lb 0.34
wtfile
proc ft
fn not used
werr
wexp
wbs
wnt
168.689
168.418
160.357
155.887
155.182
142.688
132.224
129.761
127.958
126.966
113.858
77.754
77.117
76.481
61.645
61.524
55.357
23.147
16.866
14.207
13.797
0.000
200
180
160
140
120
100
80
60
40
20
0
ppm

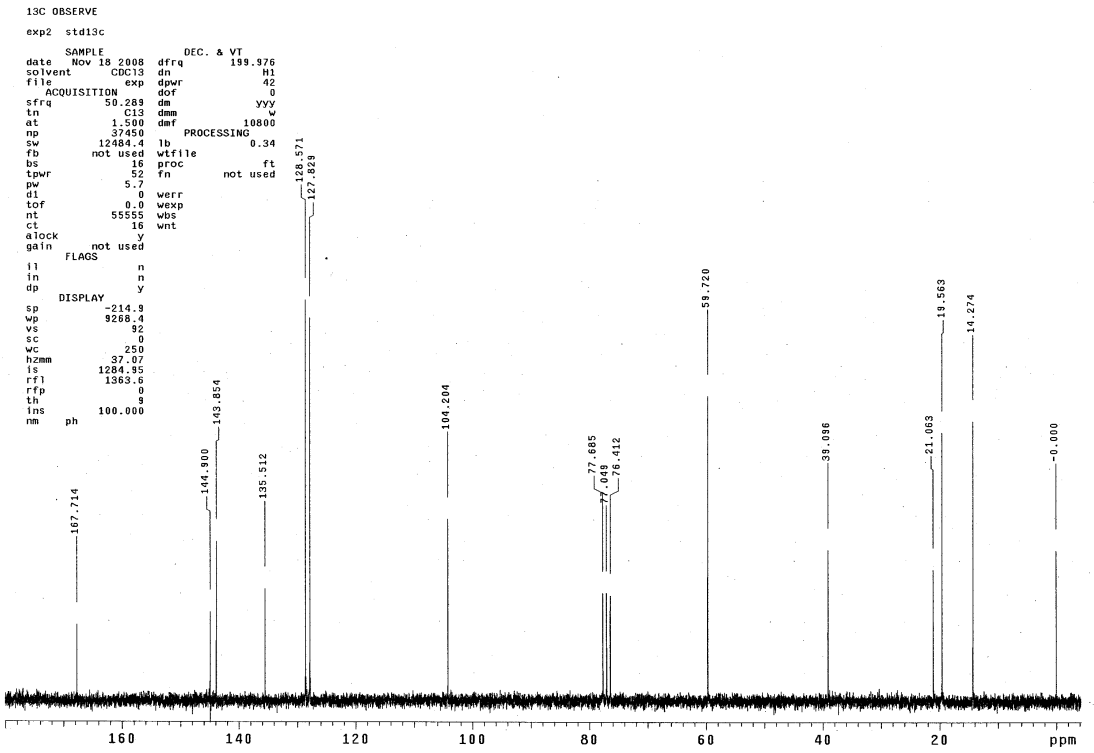

STANDARD 1H OBSERVE
exp1 std1h
SAMPLE
date Nov 19 2008
solvent CDCl3
file exp
ACQUISITION
sfrq 199.976
tn H1
at 1.992
np 11866
sw 3003.0
fb not used
bs 16
tpwr 58
pw 7.0
d1 1.000
tof 0.0
nt 16
ct 16
alock y
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -41.4
wp 1641.2
vs 351
sc 0
wc 250
hzmm 6.56
is 3419.29
rfl 495.2
rfp 0
th 15
ins 100.000
nm cdc ph
DEC. & VT
dfrq 199.976
dn H1
dpwr 30
dof 0
dm nnn
dmm c
dmf 200
PROCESSING
wtfile
proc ft
fn not used
werr
wexp
wbs
wnt
6.742
6.735
4.924
4.126
4.119
4.090
4.082
3.828
2.321
1.239
1.274
1.203
0.000
7
6
5
4
3
2
1
ppm
0.02
7.59
3.97
3.22
2.97
3.46
16.26
12.38
25.16
24.97

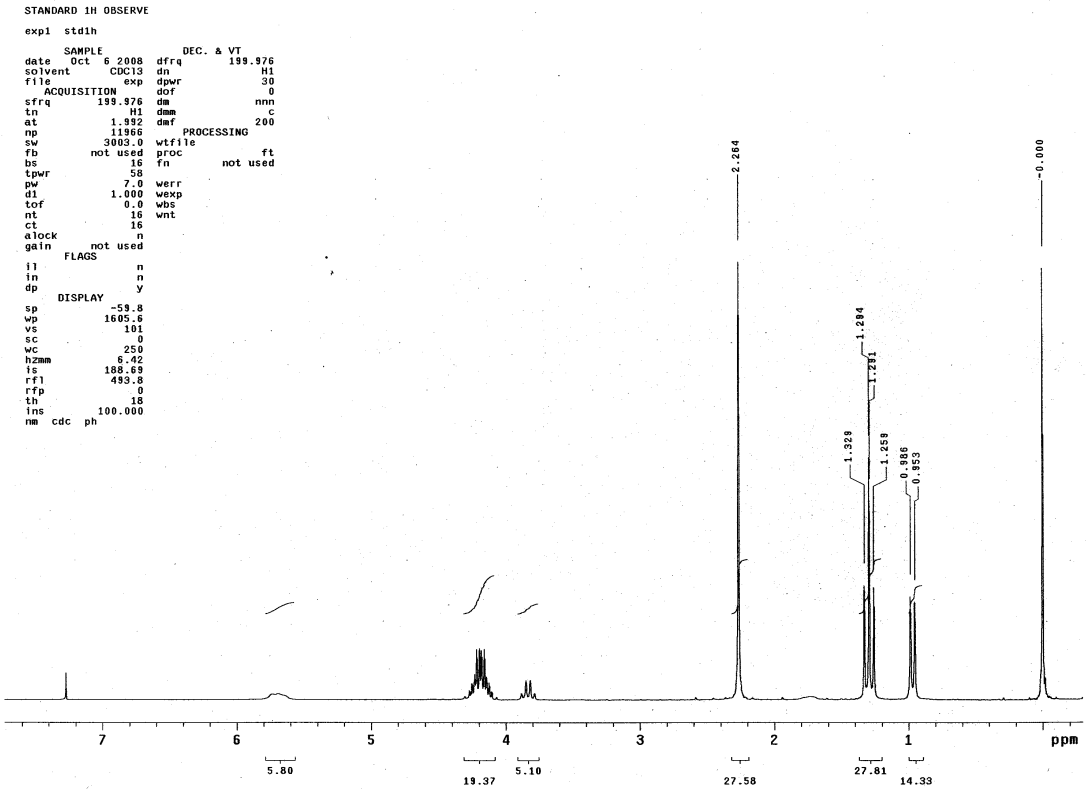

13C OBSERVE
exp2 std13c
SAMPLE
date Nov 19 2008
solvent CDCl3
file exp
ACQUISITION
sfrq 50.289
tn C13
at 1.500
np 37450
sw 12484.4
fb not used
bs 16
tpwr 52
pw 5.7
d1 0
tof 0.0
nt 55555
ct 224
alock y
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -248.0
wp 9268.4
vs 109
sc 0
wc 250
hzmm 37.07
is 1284.95
rfl 1363.6
rfp 0
th 9
ins 100.000
nm ph
DEC. & VT
dfrq 199.976
dn H1
dpwr 42
dof 0
dm yyy
dmm w
dmf 10800
PROCESSING
lb 0.34
wtfile
proc ft
fn not used
werr
wexp
wbs
wnt
167.760
145.771
143.855
143.650
140.104
120.450
113.843
110.865
104.258
77.678
77.042
76.405
59.736
55.728
39.112
19.617
14.343
0.000
160
140
120
100
80
60
40
20
ppm

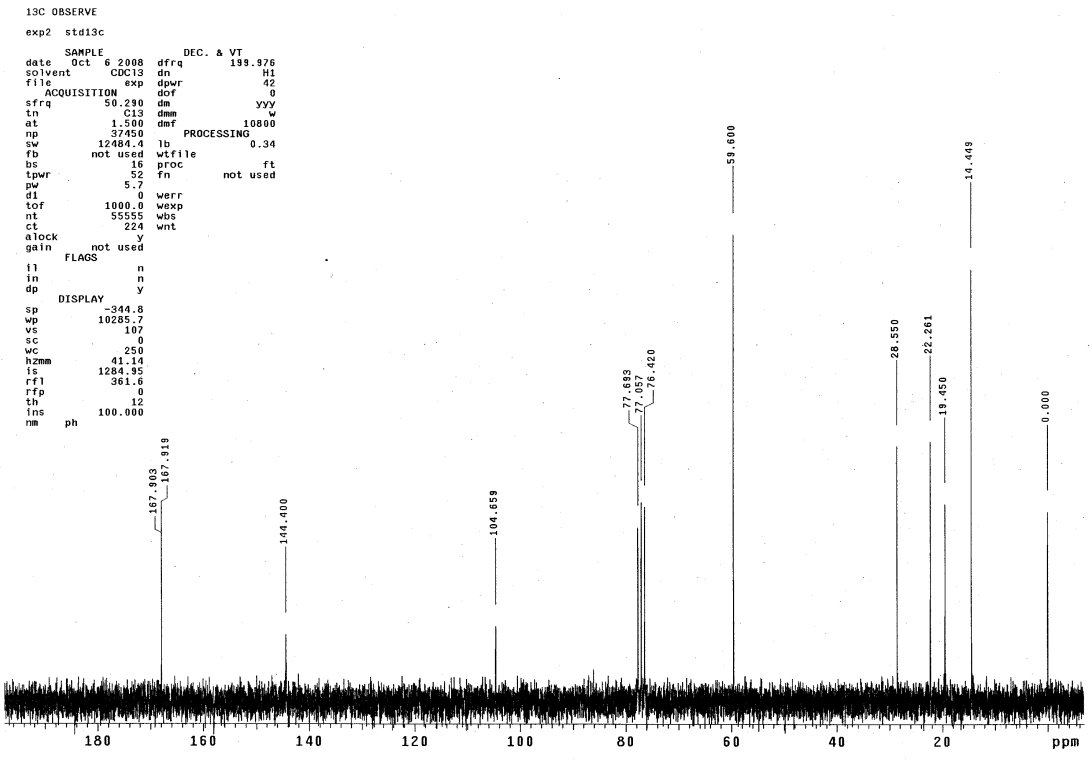

STANDARD 1H OBSERVE
exp1 std1h
SAMPLE
date Nov 19 2008
solvent CDCl3
file exp
ACQUISITION
sfrq 199.976
tn H1
at 1.992
np 11866
sw 3003.0
fb not used
bs 16
tpwr 58
pw 7.0
d1 1.000
tof 0.0
nt 16
ct 16
alock y
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -87.2
wp 1683.3
vs 563
sc 0
wc 250
hzmm 6.73
is 3088.44
rfl 495.6
rfp 0
th 4
ins 100.000
nm cdc ph
DEC. & VT
dfrq 199.976
dn H1
dpwr 30
dof 0
dm nnn
dmm c
dmf 200
PROCESSING
wtfile
proc ft
fn not used
werr
wexp
wbs
wnt
7.265
6.841
6.834
6.744
6.740
6.729
5.668
5.527
4.909
4.156
4.150
4.121
4.115
4.084
4.081
4.075
4.040
4.005
2.319
1.441
1.408
1.371
1.269
1.232
1.197
0.016
0.011
-0.013
-0.018
0.000
7
6
5
4
3
2
1
0
ppm
3.62
6.63
3.12
3.15
3.10
22.62
23.19
10.88
23.68

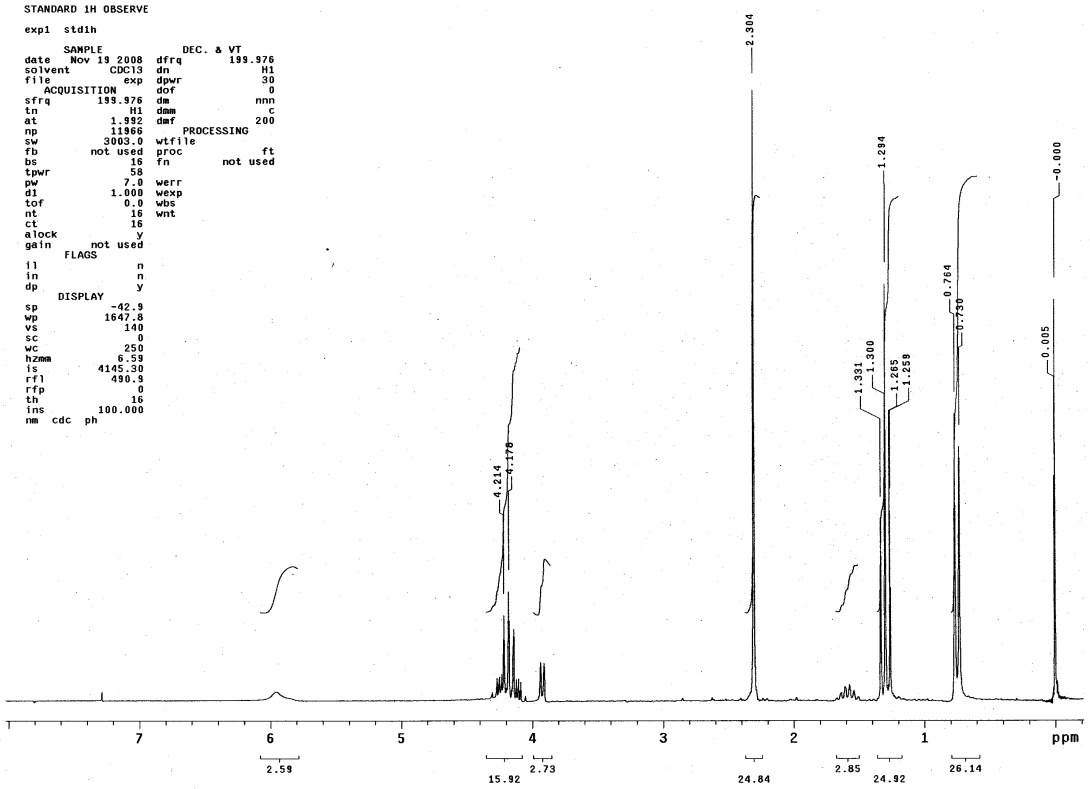

13C OBSERVE
exp2 std13c
SAMPLE
date Nov 19 2008
solvent CDCl3
file exp
ACQUISITION
sfrq 50.289
tn C13
at 1.500
np 37450
sw 12484.4
fb not used
bs 16
tpwr 52
pw 5.7
d1 0
tof 0.0
nt 55555
ct 16
alock y
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -226.6
wp 9255.9
vs 44
sc 0
wc 250
hzmm 37.02
is 1284.95
rfl 1363.1
rfp 0
th 8
ins 100.000
nm ph
DEC. & VT
dfrq 199.976
dn H1
dpwr 42
dof 0
dm yyy
dmm w
dmf 10800
PROCESSING
lb 0.34
wtfile
proc ft
fn not used
werr
wexp
wbs
wnt
167.731
145.039
143.893
143.546
139.892
120.383
113.761
111.799
104.320
77.673
77.044
76.407
64.239
59.723
39.009
19.649
14.944
14.353
0.002
160
140
120
100
80
60
40
20
ppm

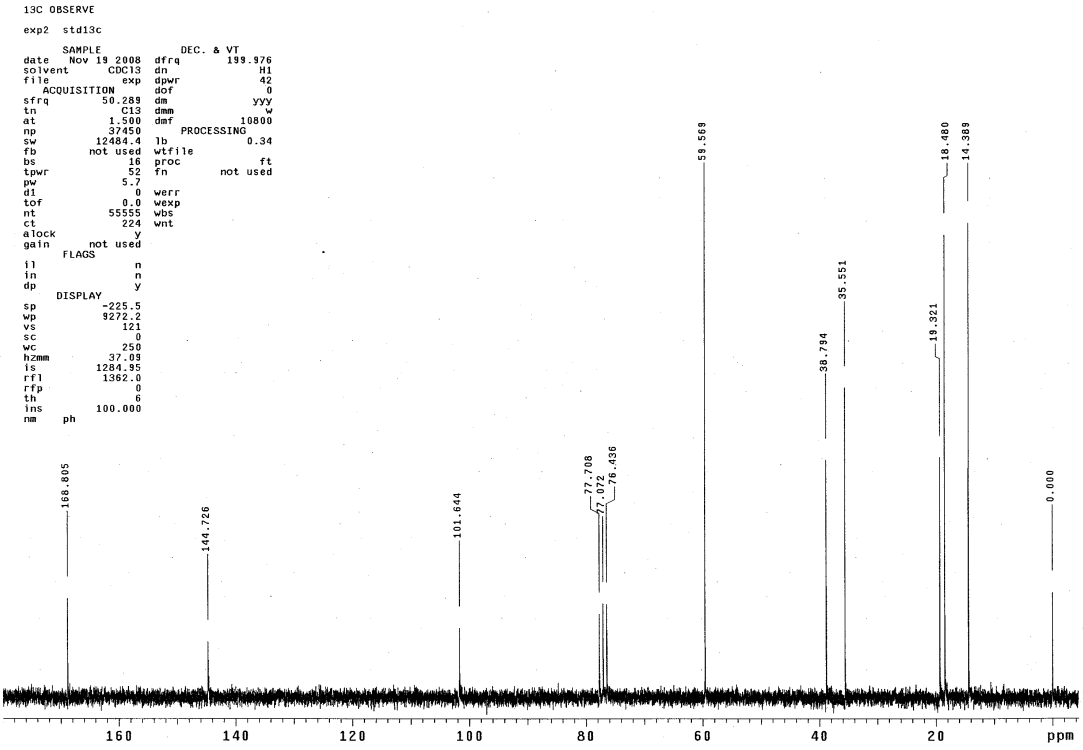

STANDARD 1H OBSERVE
exp1 std1h
SAMPLE
date Nov 18 2008
solvent CDCl3
file exp
ACQUISITION
sfrq 199.976
tn H1
at 1.992
np 11968
sw 3003.0
fb not used
bs 16
tpwr 58
pw 7.0
d1 1.000
tof 0.0
nt 16
ct 16
alock y
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -86.9
wp 1684.8
vs 184
sc 0
wc 250
hzmm 6.74
is 2051.57
rfl 501.5
rfp 0
th 40
ins 100.000
nm cdc ph
DEC. & VT
dfrq 199.976
dn H1
dpwr 30
dof 0
dm nnn
dmm c
dmf 200
PROCESSING
wtfile
proc ft
fn not used
werr
wexp
wbs
wnt
2.284
1.204
0.024
2.247
1.239
1.168
7
6
5
4
3
2
1
0
ppm
7.76
7.59
3.51
3.50
15.97
37.36
24.32

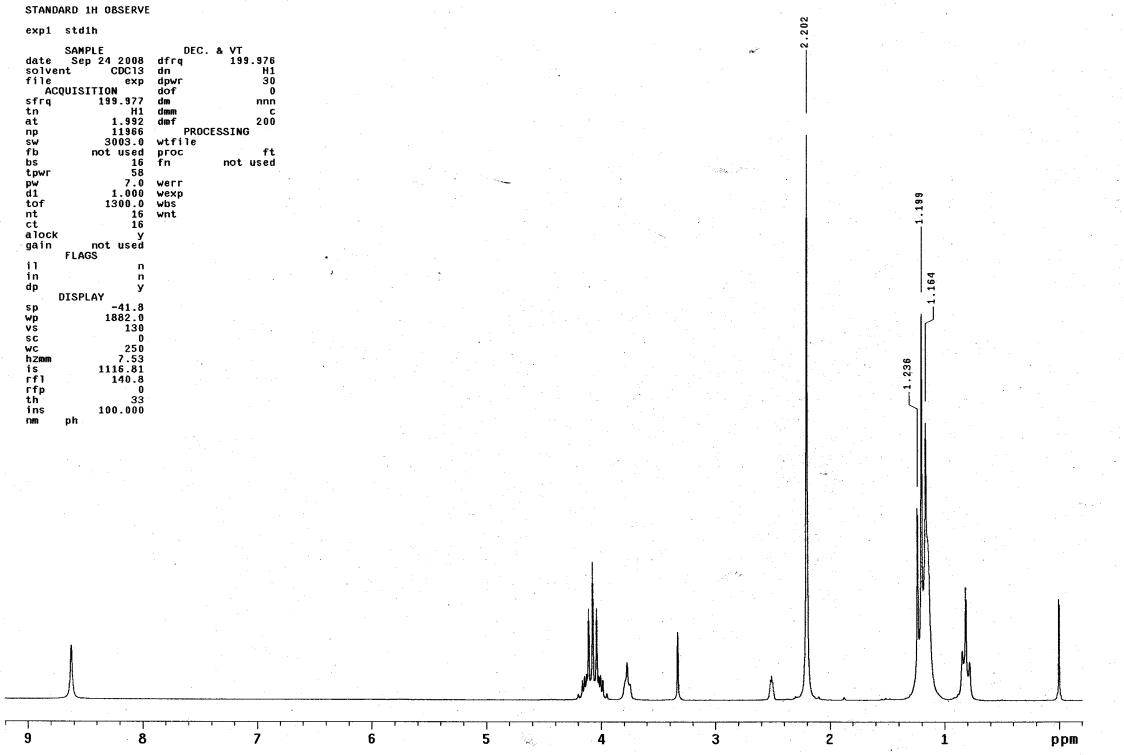

13C OBSERVE
exp2 std13c
SAMPLE
date Nov 18 2008
solvent CDCl3
file exp
ACQUISITION
sfrq 50.289
tn C13
at 1.500
np 37450
sw 12484.4
fb not used
bs 16
tpwr 52
pw 5.7
d1 0
tof 0.0
nt 55555
ct 16
alock y
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -214.9
wp 9268.4
vs 92
sc 0
wc 250
hzmm 37.07
is 1284.95
rfl 1363.6
rfp 0
th 9
ins 100.000
nm ph
DEC. & VT
dfrq 199.976
dn H1
dpwr 42
dof 0
dm yyy
dmm w
dmf 10800
PROCESSING
lb 0.34
wtfile
proc ft
fn not used
wexp
wbs
wnt
128.571
127.829
167.714
144.900
143.854
135.512
104.204
77.685
77.049
76.412
59.720
39.096
21.063
19.563
14.274
0.000
160
140
120
100
80
60
40
20
ppm

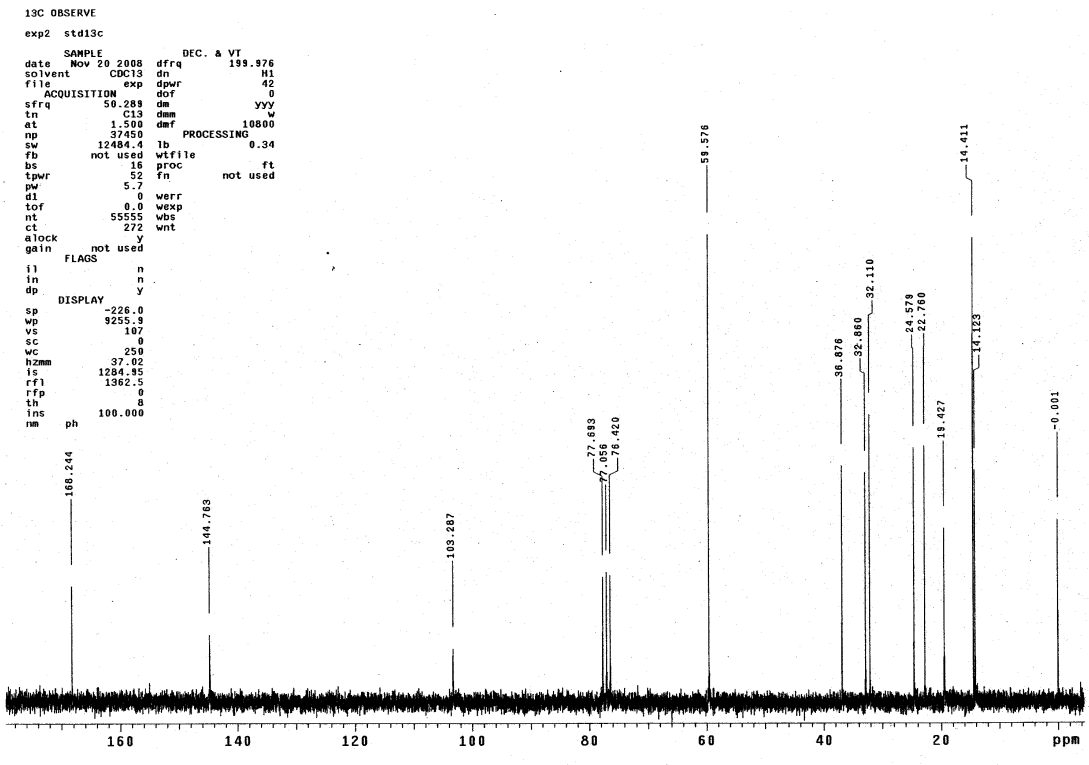

STANDARD 1H OBSERVE
exp1 std1h
SAMPLE
date Oct 6 2008
solvent CDCl3
file exp
ACQUISITION
sfrq 199.976
tn H1
at 1.992
np 11966
sw 3003.0
fb not used
bs 16
tpwr 58
pw 7.0
d1 1.000
tof 0.0
nt 16
ct 16
alock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -59.8
wp 1605.6
vs 101
sc 0
wc 250
hzmm 6.42
is 188.69
rfl 493.8
rfp 0
th 18
ins 100.000
nm cdc ph
DEC. & VT
dfrq 199.976
dn H1
dpwr 30
dof 0
dm nnn
dmm c
dmf 200
PROCESSING
wtfile
proc ft
fn not used
werr
wexp
wbs
wnt
2.264
1.284
1.281
1.329
1.259
0.986
0.953
0.000
7
6
5
4
3
2
1
ppm
5.80
19.37
5.10
27.58
27.81
14.33

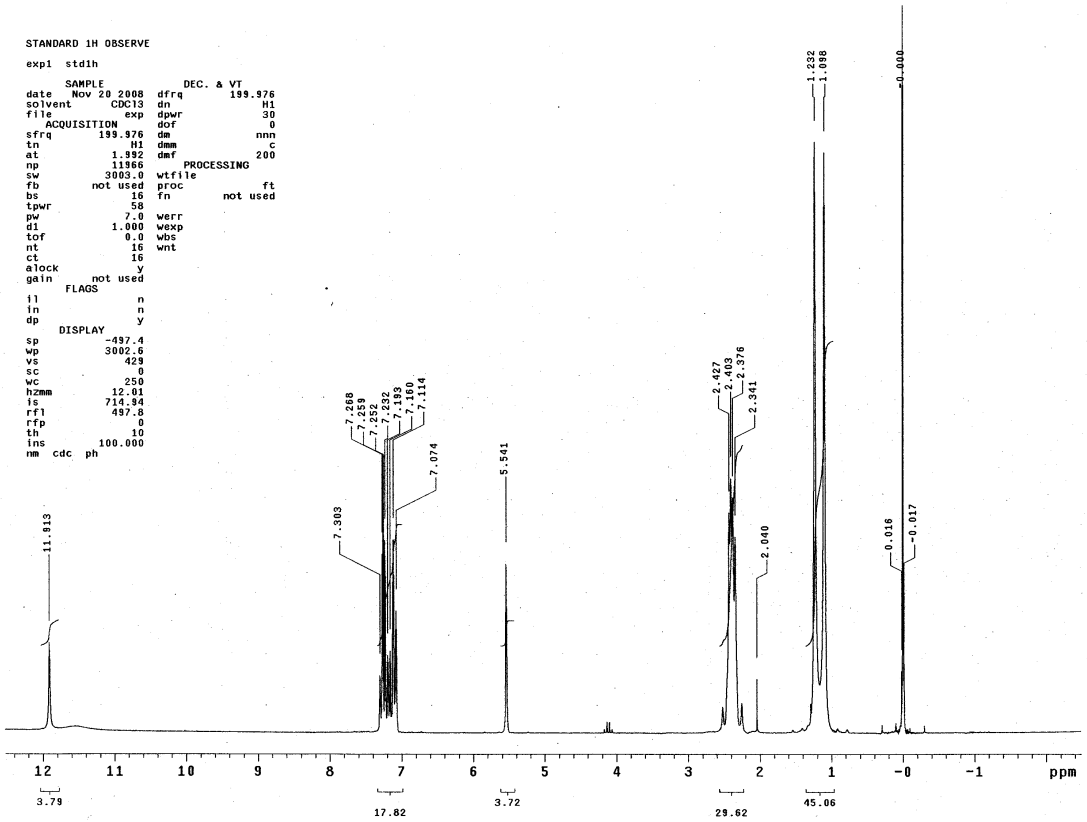

13C OBSERVE
exp2 std13c
SAMPLE
date Oct 6 2008
solvent CDCl3
file exp
ACQUISITION
sfrq 50.290
tn C13
at 1.500
np 37450
sw 12484.4
fb not used
bs 16
tpwr 52
pw 5.7
d1 0
tof 1000.0
nt 55555
ct 224
alock y
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -344.8
wp 10285.7
vs 107
sc 0
wc 250
hzmm 41.14
is 1284.95
rfl 361.6
rfp 0
th 12
ins 100.000
nm ph
DEC. & VT
dfrq 199.976
dn H1
dpwr 42
dof 0
dm yyy
dmm w
dmf 10800
PROCESSING
lb 0.34
wtfile
proc ft
fn not used
werr
wexp
wbs
wnt
167.903
167.919
144.400
104.659
77.683
77.057
76.420
59.600
28.550
22.261
19.450
14.449
0.000
180
160
140
120
100
80
60
40
20
ppm

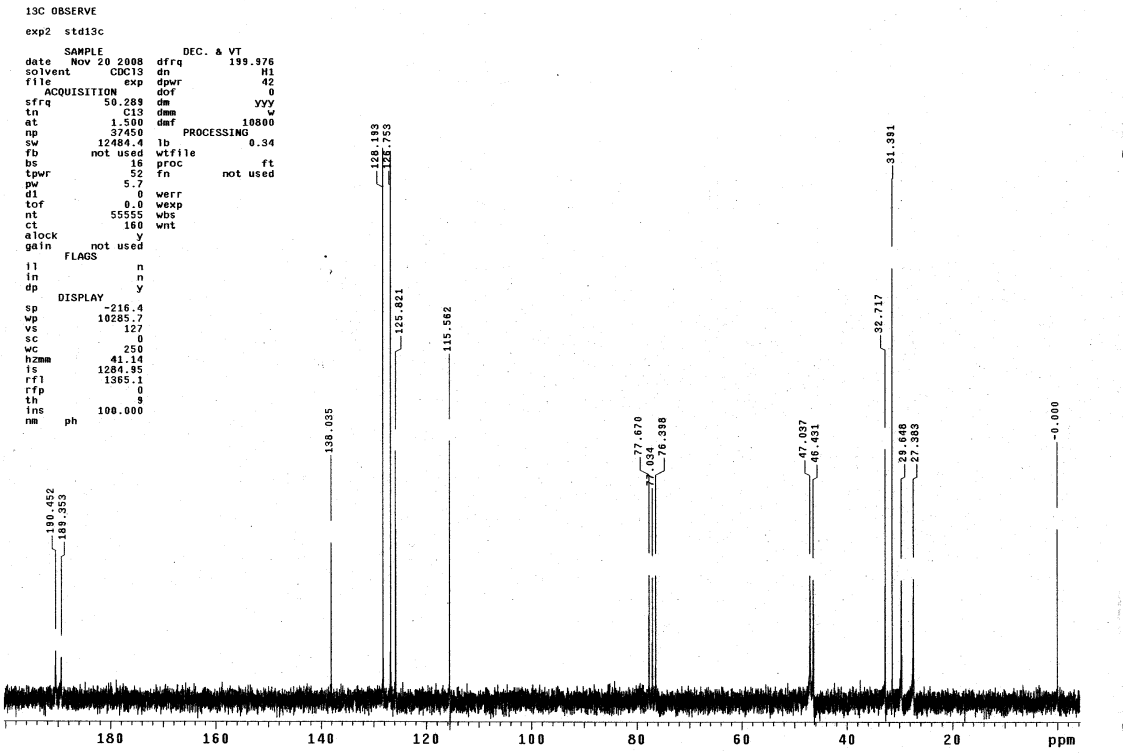

STANDARD 1H OBSERVE
exp1 std1h
SAMPLE
date Nov 19 2008
solvent CDCl3
file exp
ACQUISITION
sfrq 199.976
tn H1
at 1.992
np 11966
sw 3003.0
fb not used
bs 16
tpwr 58
pw 7.0
d1 1.000
tof 0.0
nt 16
ct 16
alock y
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -42.9
wp 1647.8
vs 140
sc 0
wc 250
hzmm 6.59
is 4145.30
rfl 490.9
rfp 0
th 16
ins 100.000
nm cdc ph
DEC. & VT
dfrq 199.976
dn H1
dpwr 30
dof 0
dm nnn
dmm c
dmf 200
PROCESSING
wtfile
proc ft
fn not used
werr
wexp
wbs
wnt
2.304
1.294
0.000
0.764
0.730
0.005
1.331
1.300
1.265
1.259
4.214
4.178
7
6
5
4
3
2
1
ppm
2.59
15.92
2.73
24.84
2.85
24.92
26.14

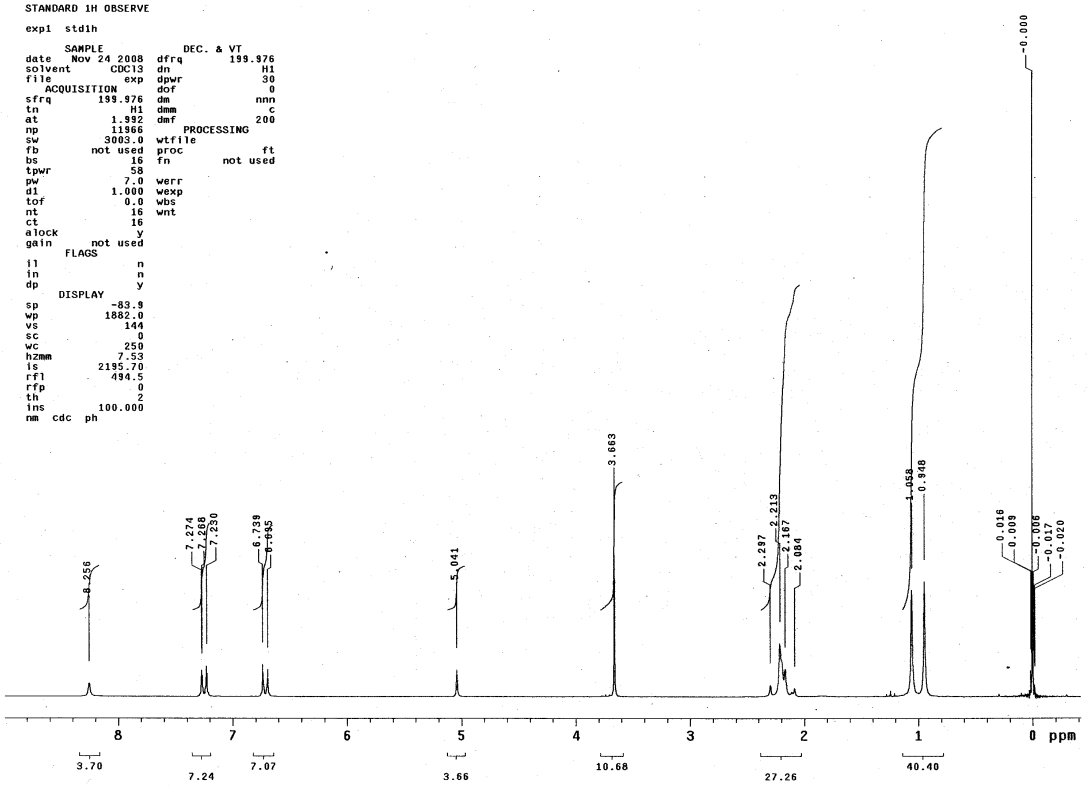

13C OBSERVE
exp2 std13c
SAMPLE
date Nov 19 2008
solvent CDCl3
file exp
ACQUISITION
sfrq 50.289
tn C13
at 1.500
np 37450
sw 12484.4
fb not used
bs 16
tpwr 52
pw 5.7
d1 0
tof 0.0
nt 55555
ct 224
alock y
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -225.5
wp 9272.2
vs 121
sc 0
wc 250
hzmm 37.09
is 1284.95
rfl 1362.0
rfp 0
th 6
ins 100.000
nm ph
DEC. & VT
dfrq 199.976
dn H1
dpwr 42
dof 0
dm yyy
dmm w
dmf 10800
PROCESSING
lb 0.34
wtfile
proc ft
fn not used
werr
wexp
wbs
wnt
59.569
18.480
14.389
35.551
38.794
19.321
168.805
144.726
101.644
77.708
77.072
76.436
0.000
160
140
120
100
80
60
40
20
ppm

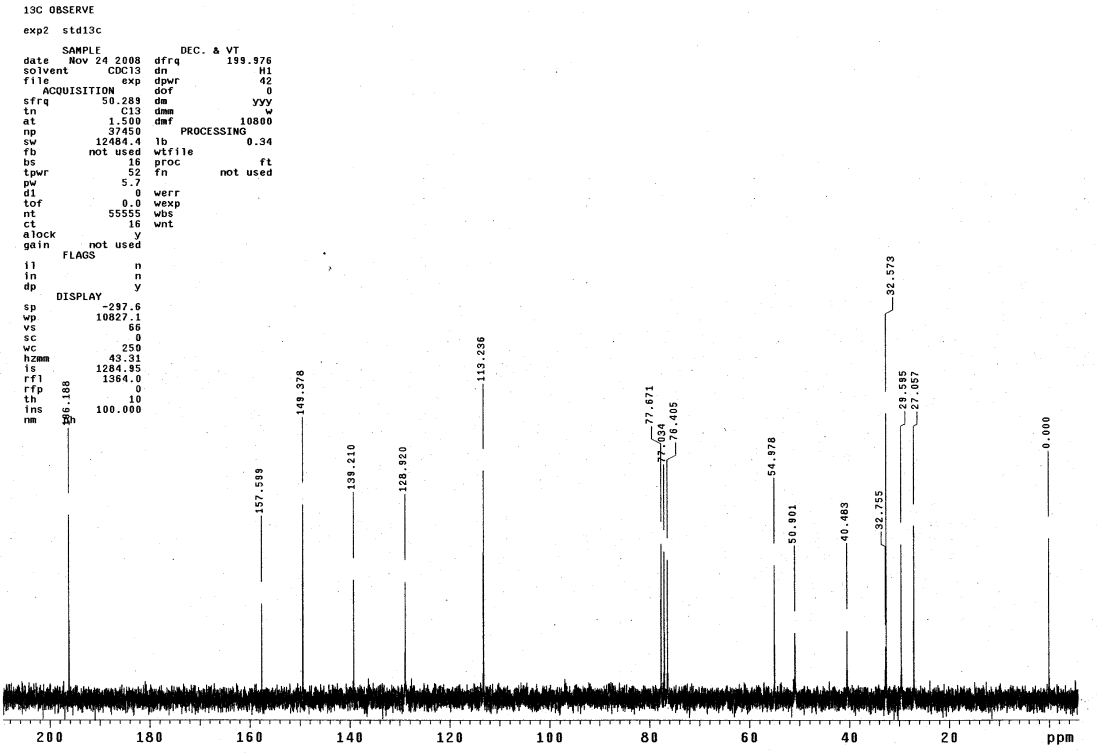


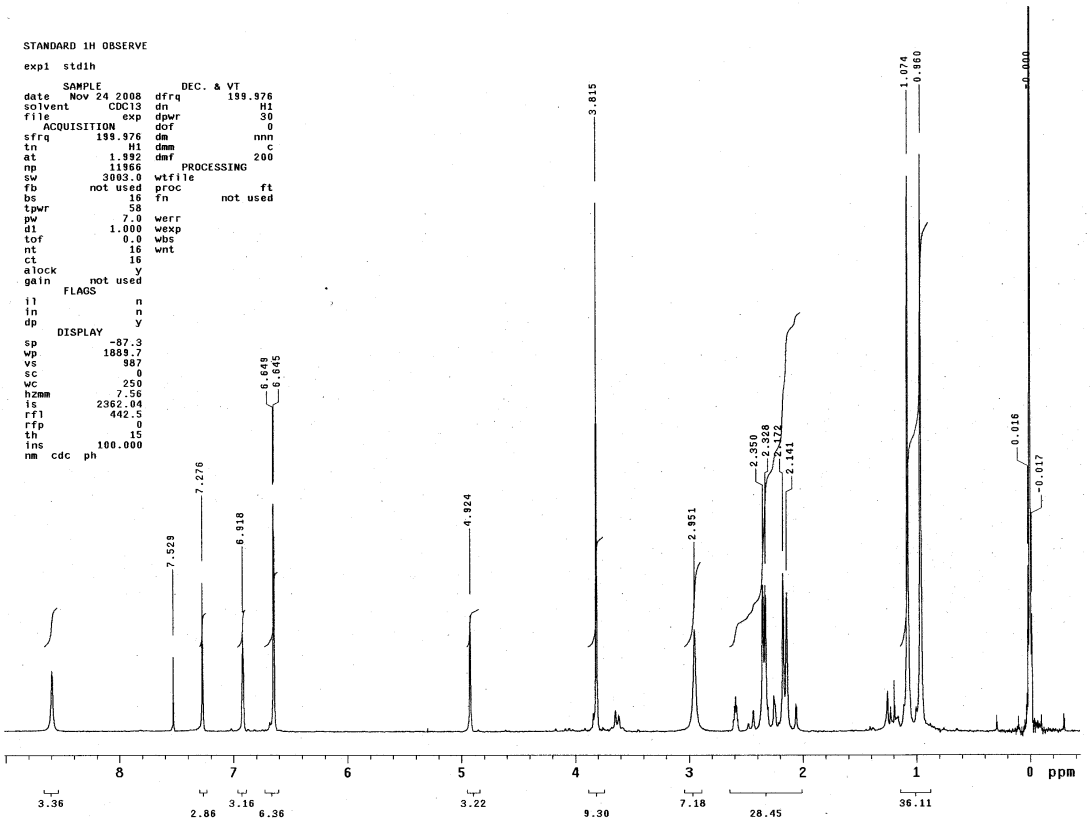


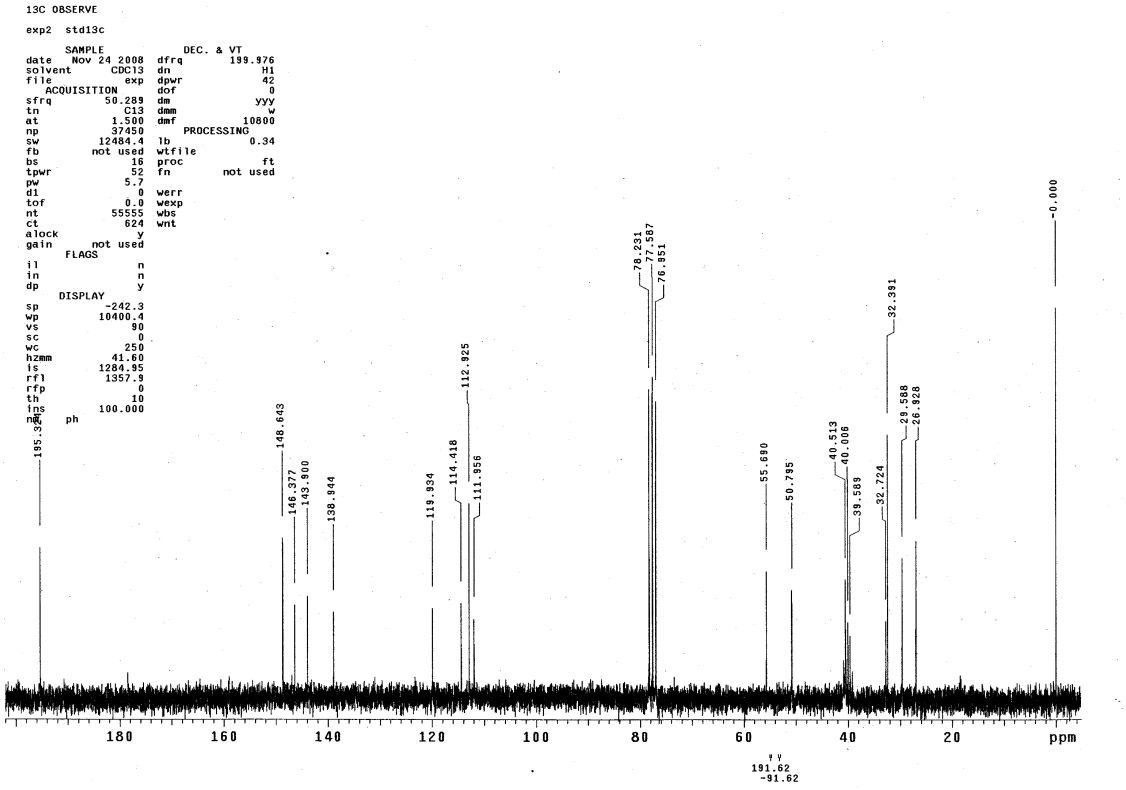


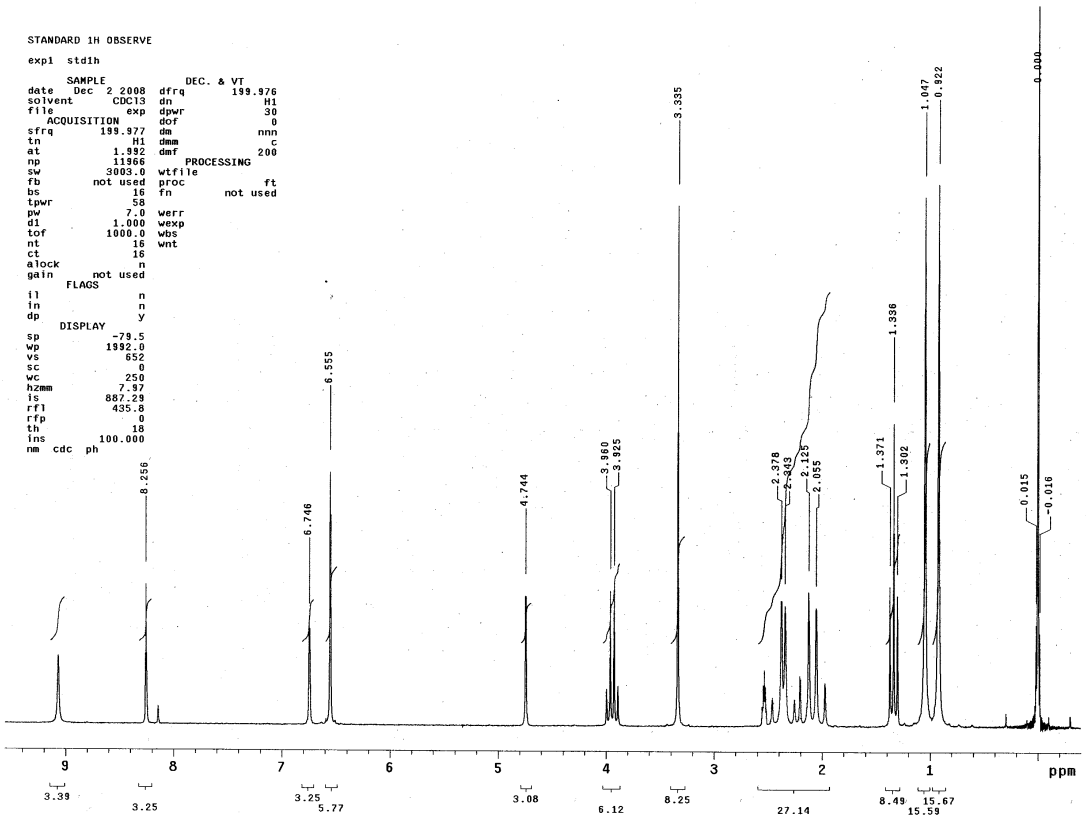


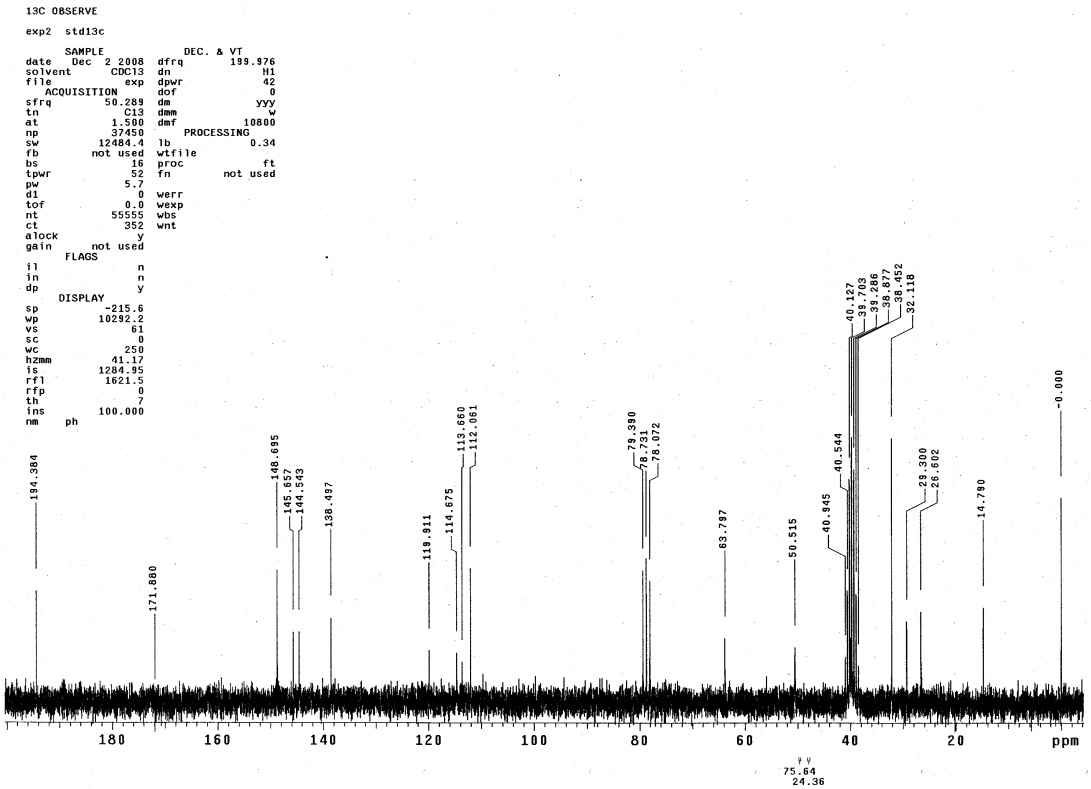


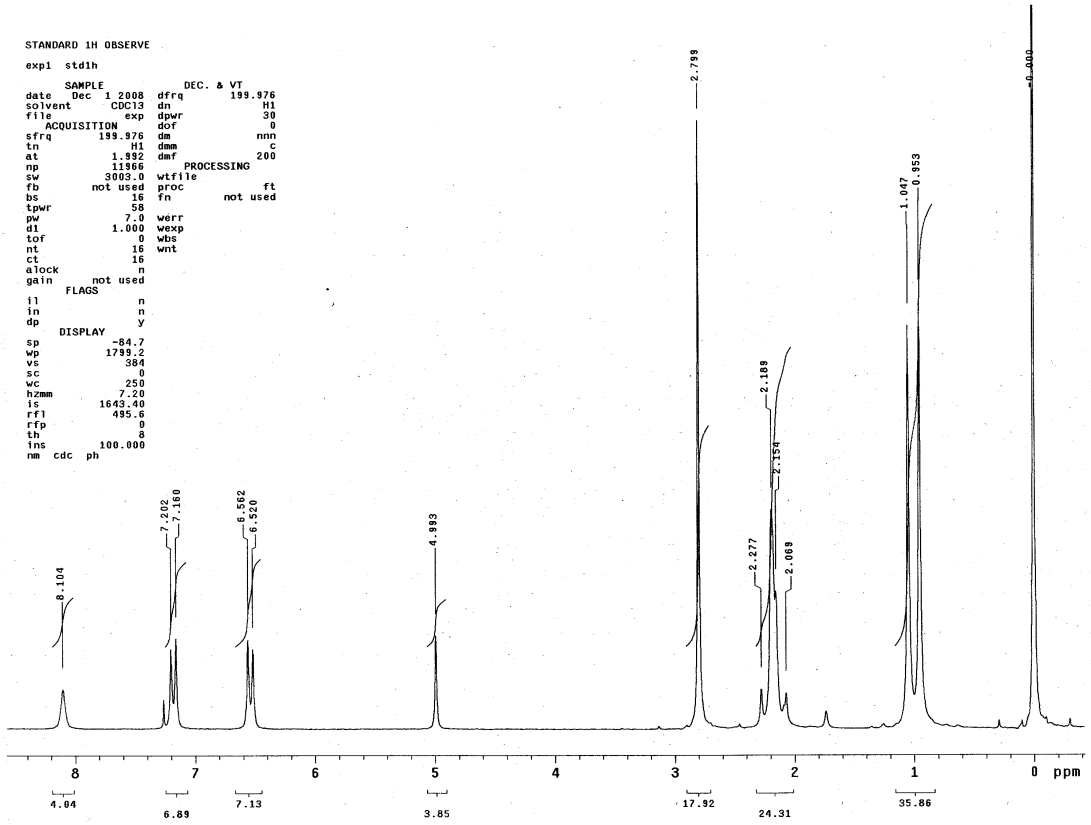


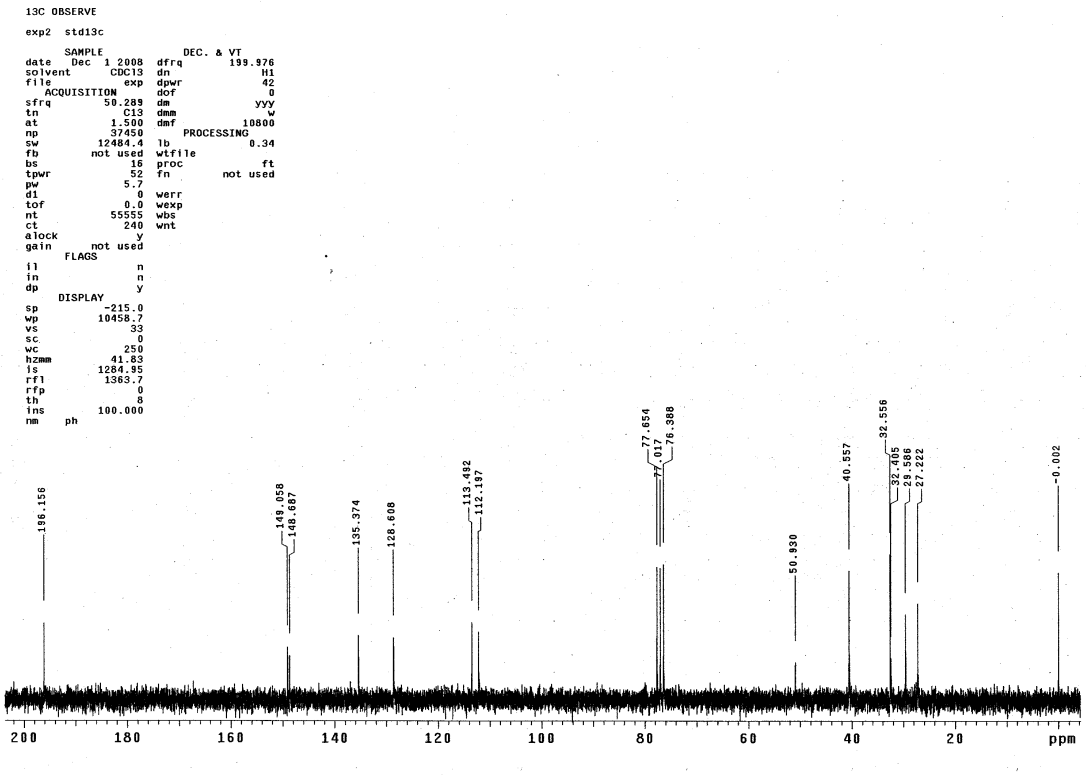

STANDARD 1H OBSERVE
exp1 std1h
SAMPLE
date Nov 24 2008
solvent CDCl3
file exp
ACQUISITION
sfrq 199.976
tn H1
at 1.992
np 11966
sw 3003.0
fb not used
bs 16
tpwr 58
pw 7.0
d1 1.000
tof 0.0
nt 16
ct 16
alock y
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -87.3
wp 1889.7
vs 987
sc 0
wc 250
hzmm 7.56
is 2362.04
rfl 442.5
rfp 0
th 15
ins 100.000
nm cdc ph
DEC. & VT
dfrq 199.976
dn H1
dpwr 30
dof 0
dm nnn
dmm c
dmf 200
PROCESSING
wtfile
proc ft
fn not used
werr
wexp
wbs
wnt
7.529
7.276
6.918
6.649
6.645
4.924
3.815
2.951
2.350
2.328
2.172
2.141
1.074
0.960
0.016
-0.000
-0.017
8
7
6
5
4
3
2
1
0 ppm
3.36
2.86
3.16
6.36
3.22
9.30
7.18
28.45
36.11

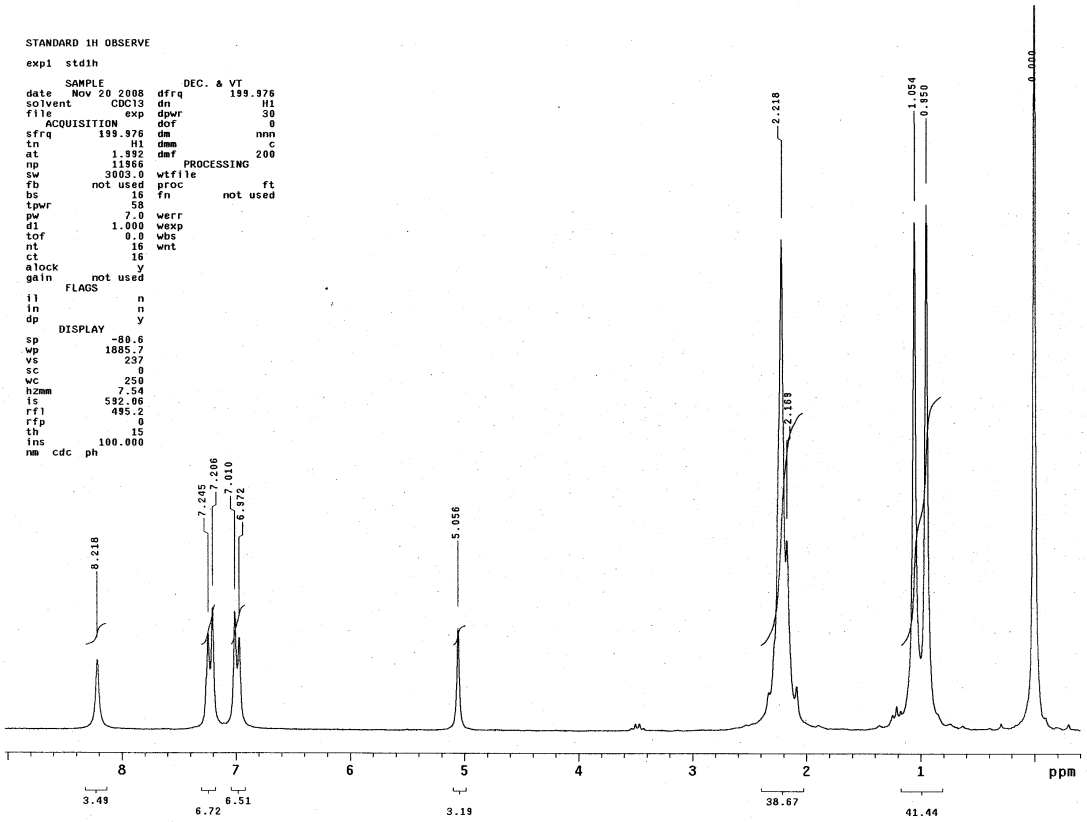

13C OBSERVE
exp2 std13c
SAMPLE
date Nov 24 2008
solvent CDCl3
file exp
ACQUISITION
sfrq 50.289
tn C13
at 1.500
np 37450
sw 12484.4
fb not used
bs 16
tpwr 52
pw 5.7
d1 0
tof 0.0
nt 55555
ct 624
alock y
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -242.3
wp 10400.4
vs 90
sc 0
wc 250
hzmm 41.60
is 1284.95
rfl 1357.9
rfp 0
th 10
ins 100.000
nm ph
DEC. & VT
dfrq 199.976
dn H1
dpwr 42
dof 0
dm yyy
dmm w
dmf 10800
PROCESSING
lb 0.34
wtfile
proc ft
fn not used
werr
wexp
wbs
wnt
195.3
148.643
146.377
143.900
138.944
119.934
114.418
112.925
111.956
78.231
77.587
76.951
55.690
50.795
40.513
40.006
39.589
32.724
32.391
29.588
26.928
-0.000
180
160
140
120
100
80
60
40
20
ppm
191.62
-91.62

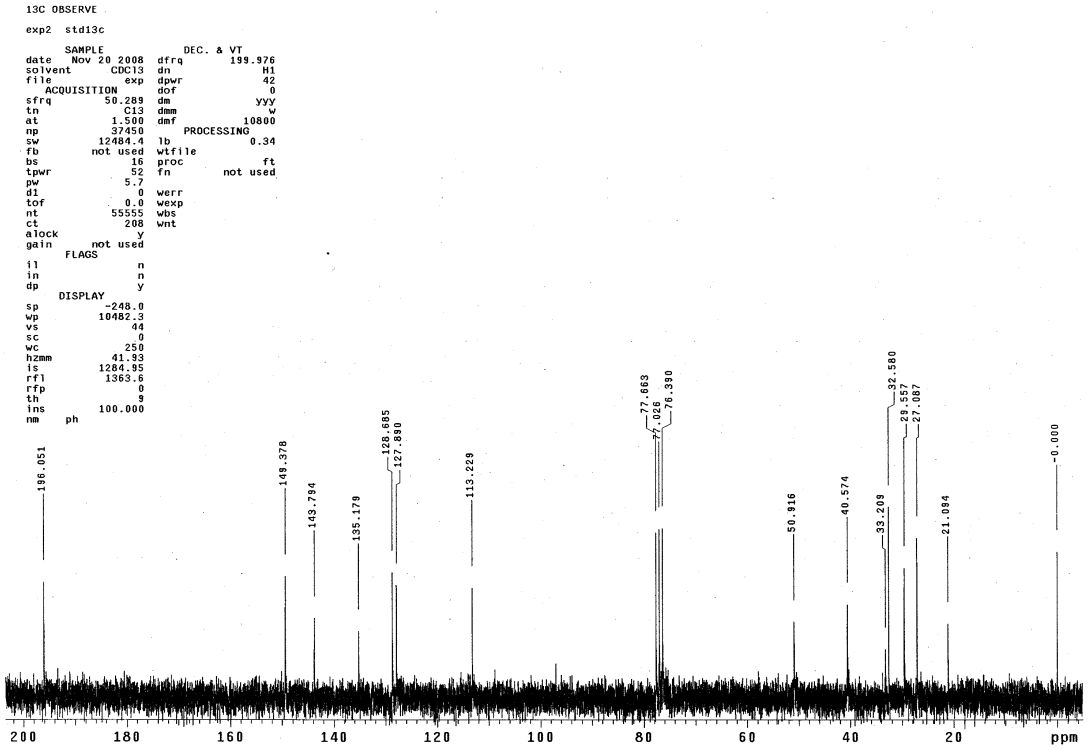

STANDARD 1H OBSERVE
exp1 std1h
SAMPLE
date Dec 2 2008
solvent CDCl3
file exp
ACQUISITION
sfrq 199.977
tn H1
at 1.992
np 11966
sw 3003.0
fb not used
bs 16
tpwr 58
pw 7.0
d1 1.000
tof 1000.0
nt 16
ct 16
alock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -79.5
wp 1892.0
vs 652
sc 0
wc 250
hzmm 7.97
is 887.29
rfl 435.8
rfp 0
th 18
ins 100.000
nm cdc ph
DEC. & VT
dfrq 199.976
dn H1
dpwr 30
dof 0
dm nnn
dmm c
dmf 200
PROCESSING
wtfile
proc ft
fn not used
werr
wexp
wbs
wnt
8.256
6.746
6.555
4.744
3.980
3.925
3.335
2.378
2.343
2.125
2.055
1.371
1.336
1.302
1.047
0.922
0.015
0.000
-0.016
ppm
3.39
3.25
3.25
5.77
3.08
6.12
8.25
27.14
8.49
15.67
15.59

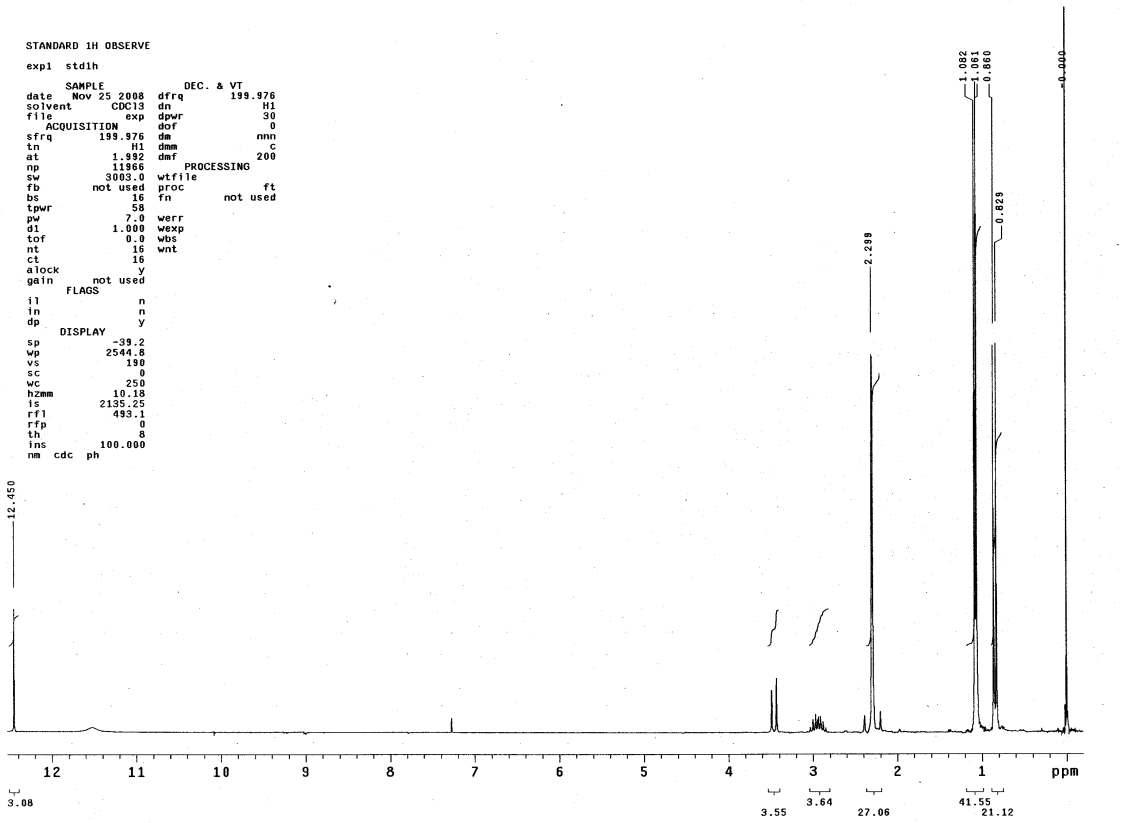

13C OBSERVE
exp2 std13c
SAMPLE
date Dec 2 2008
solvent CDCl3
file exp
ACQUISITION
sfrq 50.289
tn C13
at 1.500
np 37450
sw 12484.4
fb not used
bs 16
tpwr 52
pw 5.7
d1 0
tof 0.0
nt 55555
ct 352
alock y
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -215.6
wp 10292.2
vs 61
sc 0
wc 250
hzmm 41.17
is 1284.95
rfl 1621.5
rfp 0
th 7
ins 100.000
nm ph
DEC. & VT
dfrq 199.976
dn H1
dpwr 42
dof 0
dm yyy
dmm w
dmf 10800
PROCESSING
lb 0.34
wtfile
proc ft
fn not used
194.384
171.880
148.695
145.657
144.543
138.497
119.911
114.675
113.660
112.061
79.390
78.731
78.072
63.787
50.515
40.945
40.544
40.127
39.703
39.286
38.877
38.452
32.118
29.300
26.602
14.790
-0.000
ppm
75.64
24.36

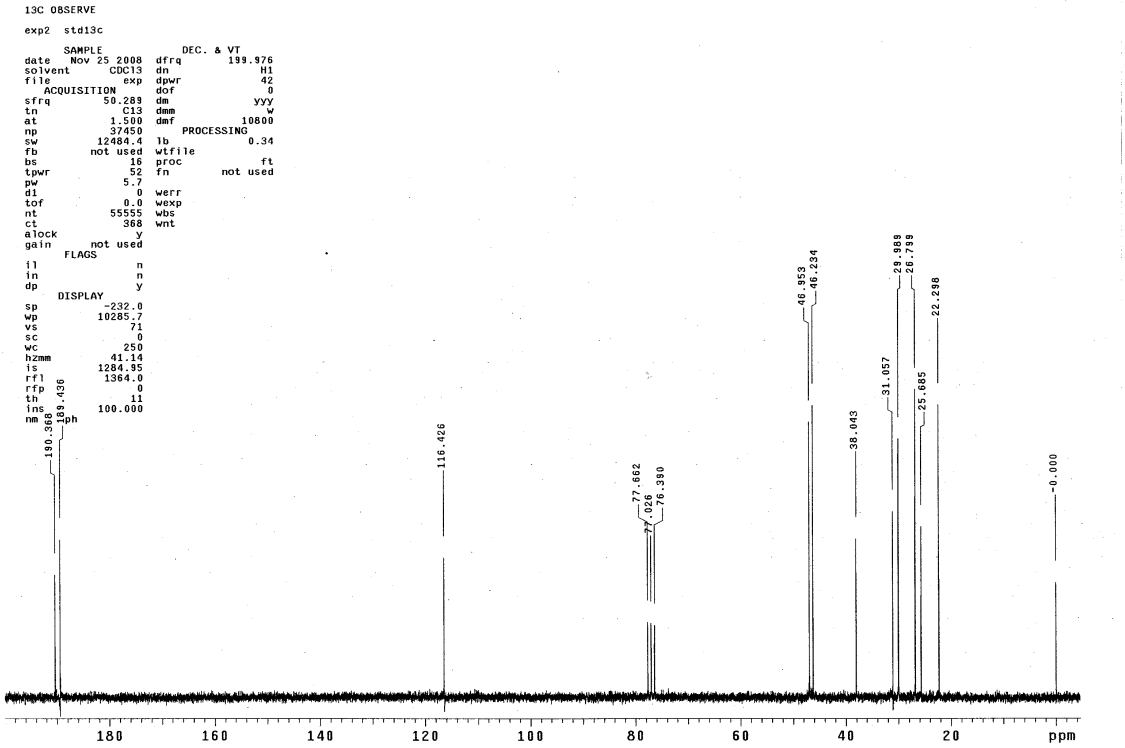


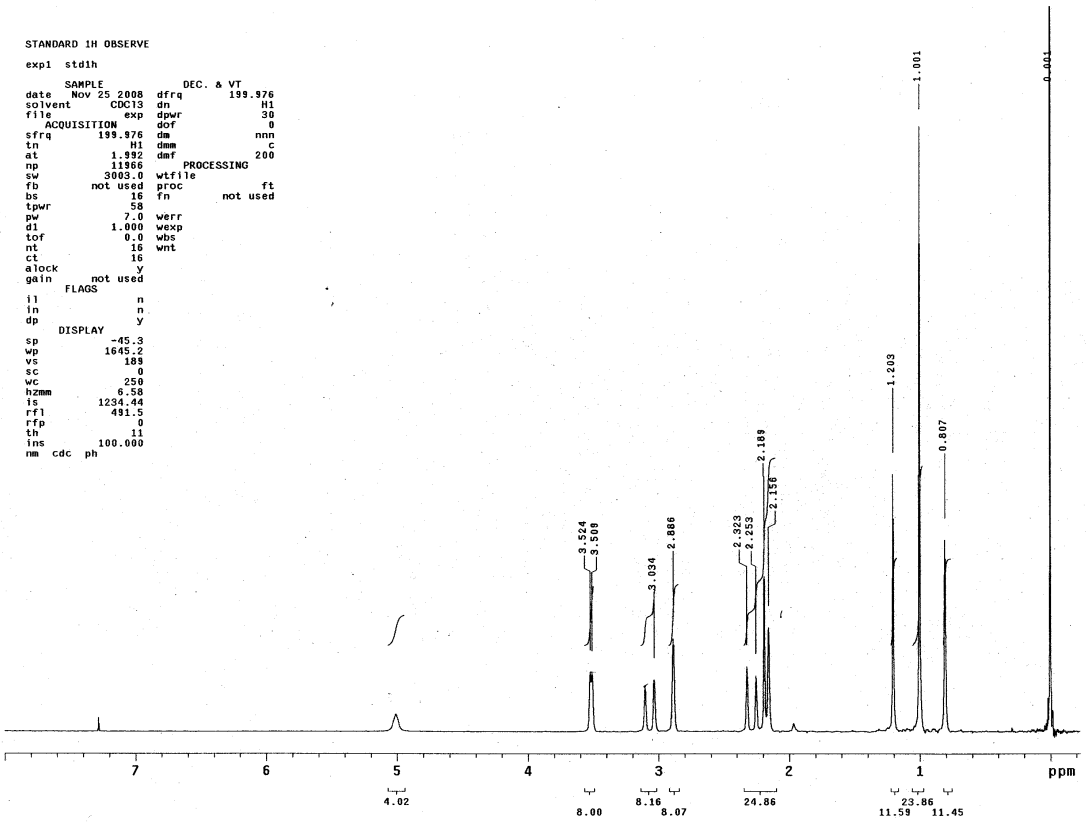


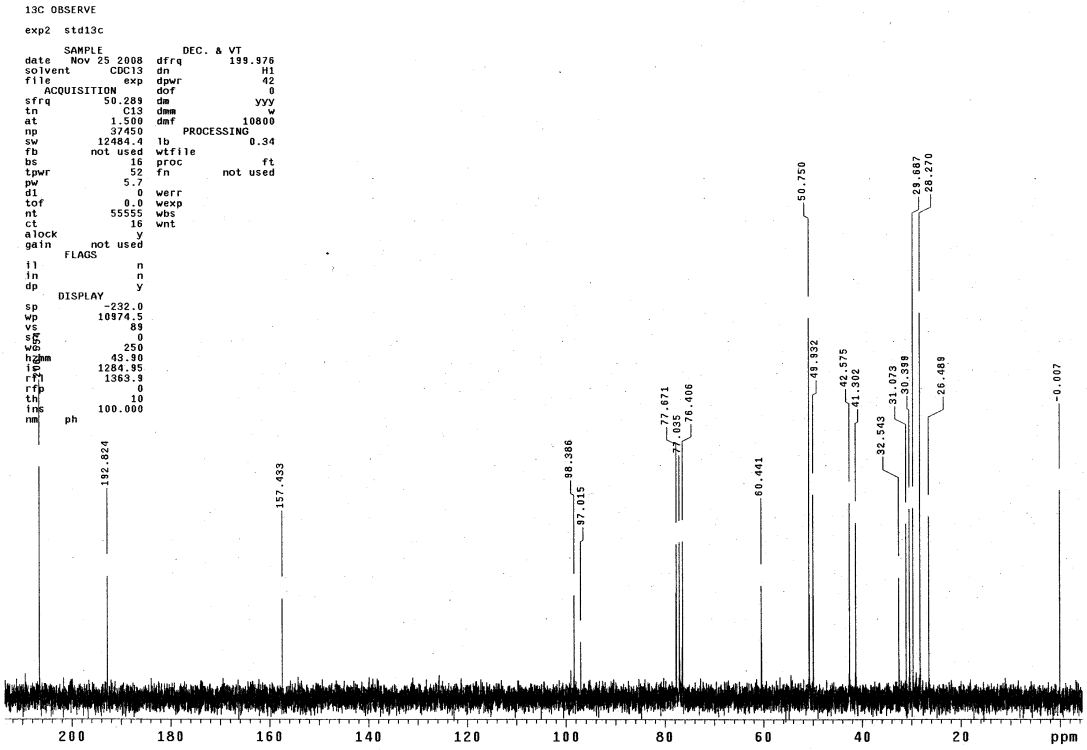

STANDARD 1H OBSERVE
exp1 std1h
SAMPLE
date Nov 20 2008
solvent CDCl3
file exp
ACQUISITION
sfrq 199.976
tn H1
at 1.992
np 11966
sw 3003.0
fb not used
bs 16
tpwr 58
pw 7.0
d1 1.000
tof 0.0
nt 16
ct 16
alock y
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -80.6
wp 1885.7
vs 237
sc 0
wc 250
hzmm 7.54
is 592.06
rfl 495.2
rfp 0
th 15
ins 100.000
nm cdc ph
DEC. & VT
dfrq 199.976
dn H1
dpwr 30
dof 0
dm nnn
dmm c
dmf 200
PROCESSING
wtfile
proc ft
fn not used
werr
wexp
wbs
wnt
8.218
7.245
7.206
7.010
6.972
5.056
2.218
2.169
1.054
0.950
0.000
8
7
6
5
4
3
2
1
ppm
3.49
6.72
6.51
3.19
38.67
41.44


13C OBSERVE
exp2 std13c
SAMPLE
date Nov 20 2008
solvent CDCl3
file exp
ACQUISITION
sfrq 50.289
tn C13
at 1.500
np 37450
sw 12484.4
fb not used
bs 16
tpwr 52
pw 5.7
d1 0
tof 0.0
nt 55555
ct 208
alock y
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -248.0
wp 10482.3
vs 44
sc 0
wc 250
hzmm 41.93
is 1284.95
rfl 1363.6
rfp 0
th 9
ins 100.000
nm ph
DEC. & VT
dfrq 199.976
dn H1
dpwr 42
dof 0
dm yyy
dmm w
dmf 10800
PROCESSING
lb 0.34
wtfile
proc ft
fn not used
werr
wexp
wbs
wnt
166.051
149.378
143.794
135.179
128.685
127.830
113.229
77.663
77.026
76.390
50.916
40.574
32.580
29.557
27.087
21.084
-0.000
200
180
160
140
120
100
80
60
40
20
ppm






STANDARD 1H OBSERVE
exp1 std1h
SAMPLE
date Nov 25 2008
solvent CDCl3
file exp
ACQUISITION
sfrq 199.976
tn H1
at 1.992
np 11966
sw 3003.0
fb not used
bs 16
tpwr 58
pw 7.0
d1 1.000
tof 0.0
nt 16
ct 16
alock y
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -45.3
wp 1645.2
vs 189
sc 0
wc 250
hzmm 8.58
is 1234.44
rfl 491.5
rfp 0
th 11
ins 100.000
nm cdc ph
DEC. & VT
dfrq 199.976
dn H1
dpwr 30
dof 0
dm nnn
dmm c
dmf 200
PROCESSING
wtfile
proc ft
fn not used
werr
wexp
wbs
wnt
3.524
3.508
3.034
2.886
2.323
2.253
2.189
2.156
1.203
1.001
0.807
0.001
7
6
5
4
3
2
1
ppm
4.02
8.00
8.16
8.07
24.86
11.59
23.86
11.45


13C OBSERVE
exp2 std13c
SAMPLE
date Nov 25 2008
solvent CDCl3
file exp
ACQUISITION
sfrq 50.289
tn C13
at 1.500
np 37450
sw 12484.4
fb not used
bs 16
tpwr 52
pw 5.7
d1 0
tof 0.0
nt 55555
ct 16
alock y
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -232.0
wp 10374.5
vs 89
sc 0
wc 250
hzmm 43.90
is 1284.95
rfl 1363.9
rfp 0
th 10
ins 100.000
nm ph
DEC. & VT
dfrq 199.976
dn H1
dpwr 42
dof 0
dm yyy
dmm w
dmf 10800
PROCESSING
lb 0.34
wtfile
proc ft
fn not used
werr
wexp
wbs
wnt
192.824
157.433
98.386
97.015
77.671
77.035
76.406
60.441
50.750
49.332
42.575
41.302
32.543
31.073
30.398
29.687
28.270
26.489
0.007
200
180
160
140
120
100
80
60
40
20
ppm