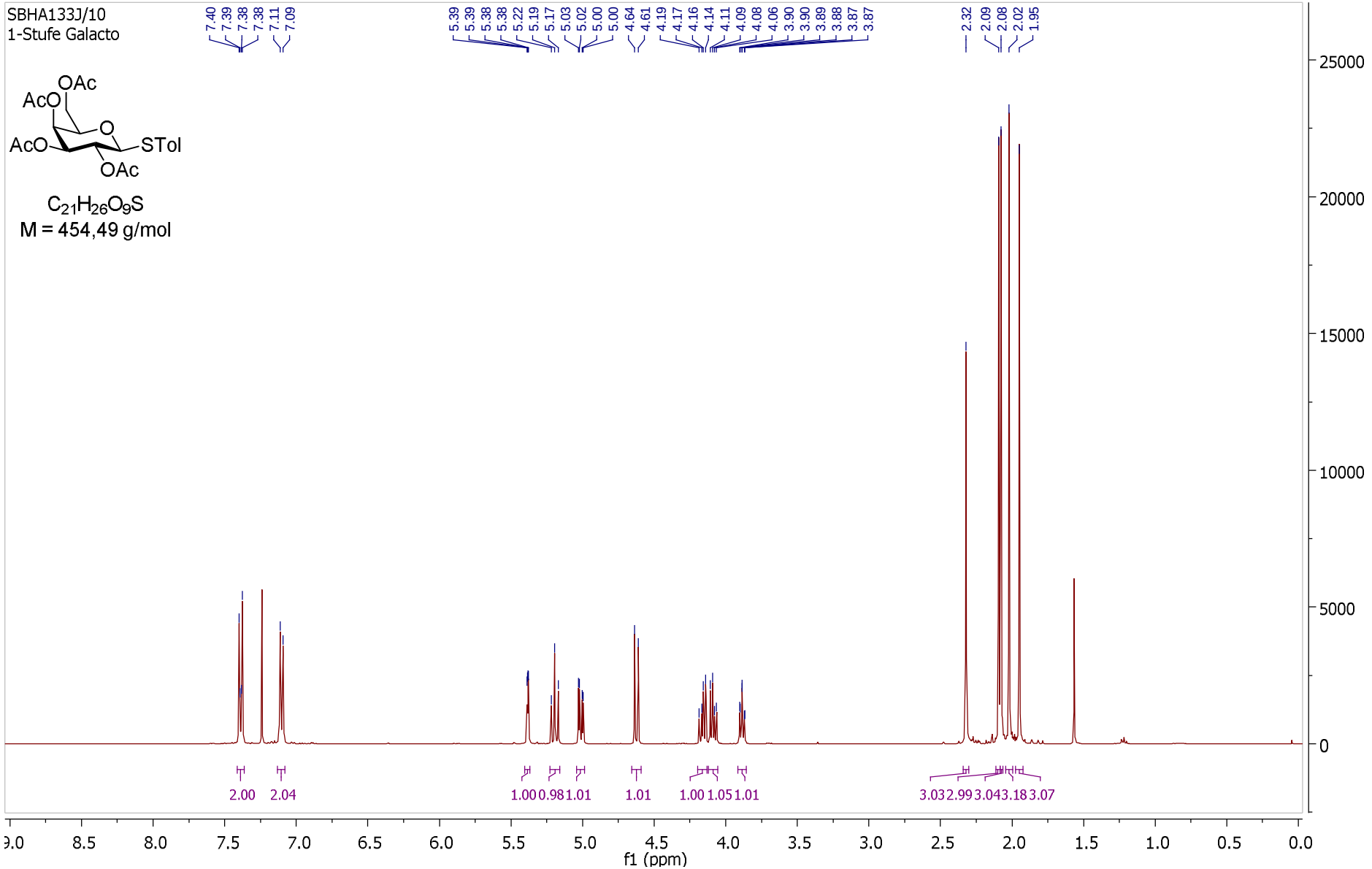
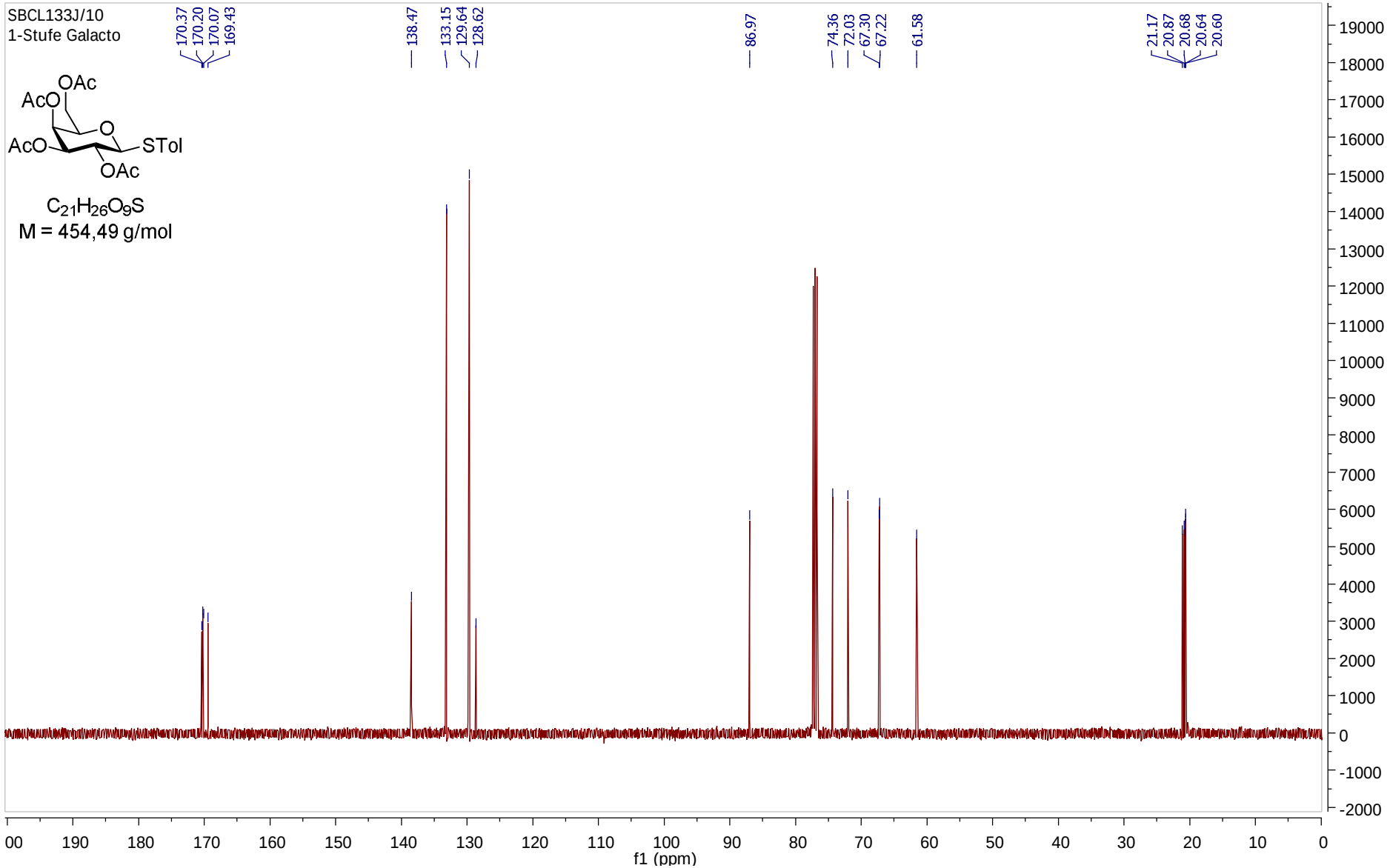
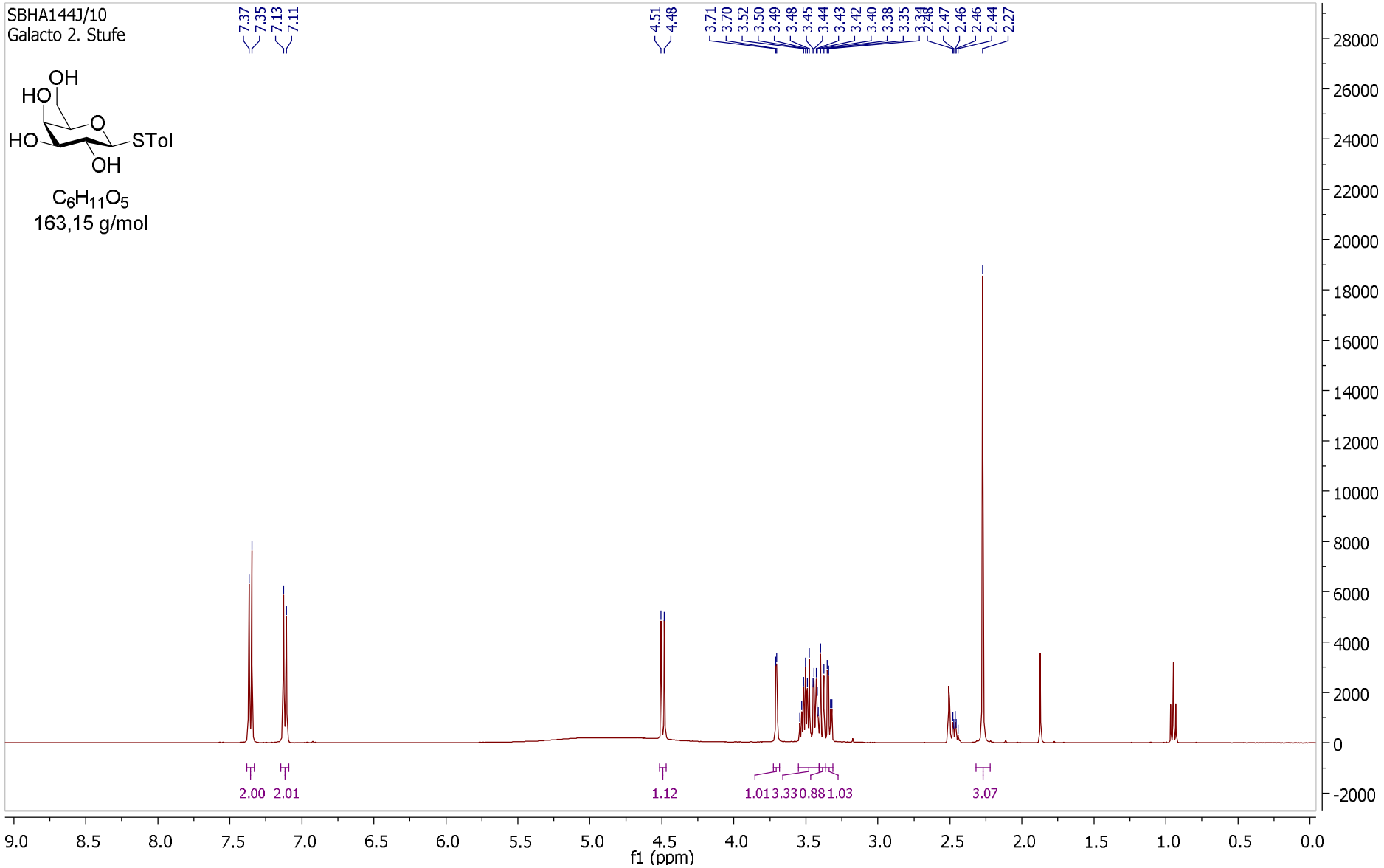
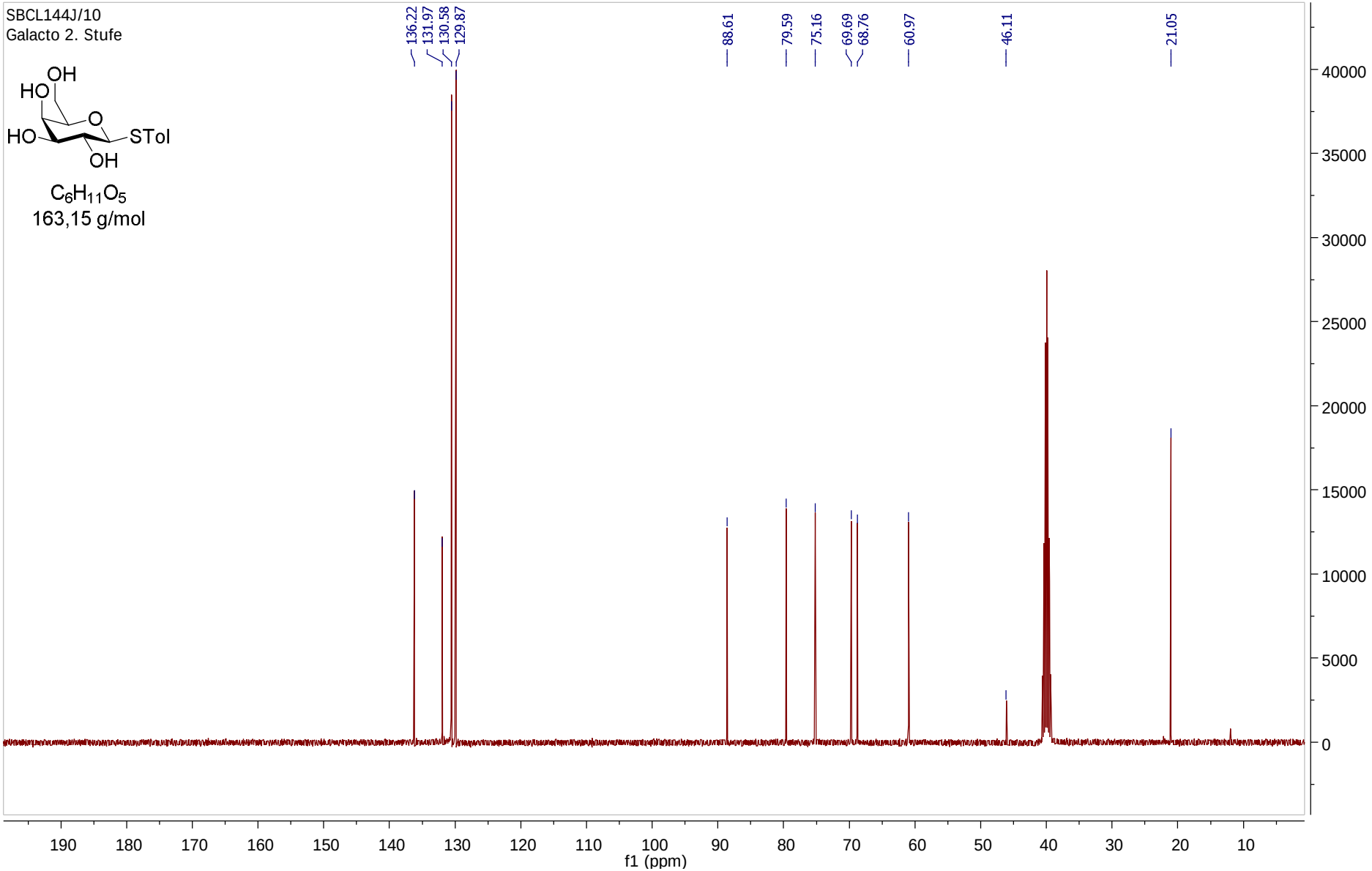
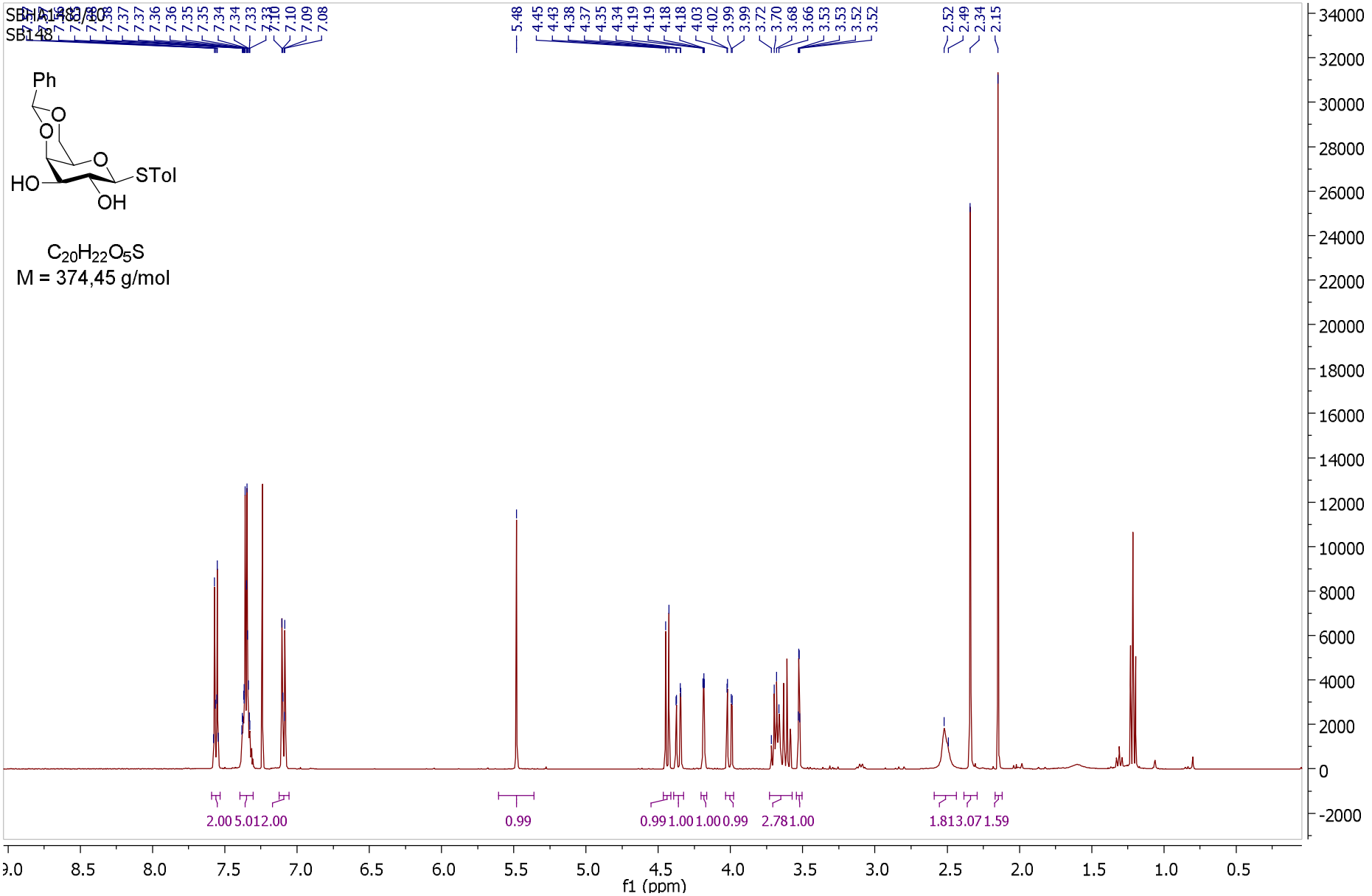
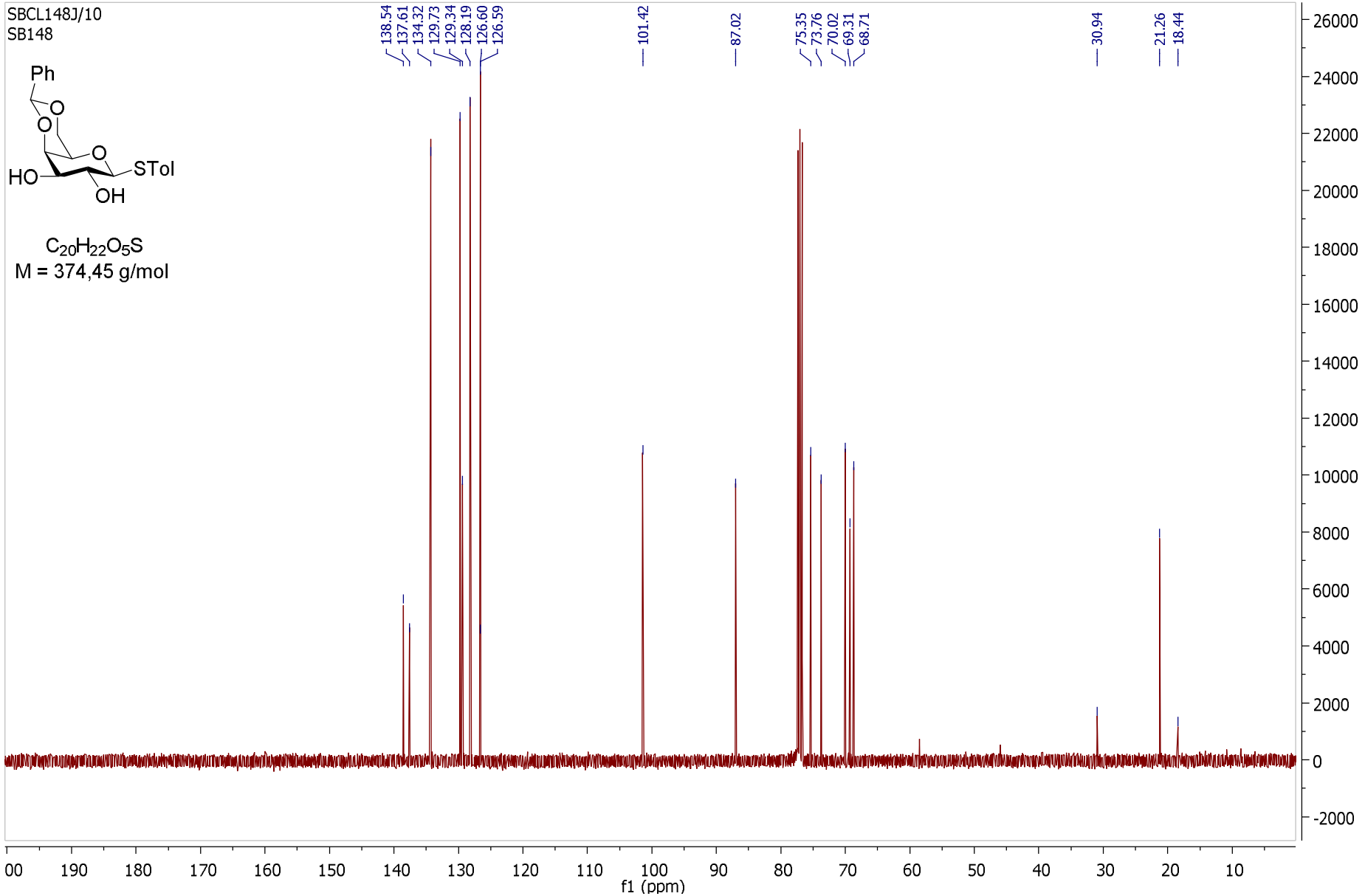

SBHA133J/10
1-Stufe Galacto
OAc
AcO
O
AcO
STol
OAc
$C_{21}H_{26}O_9S$
M = 454,49 g/mol
7.40 7.39 7.38 7.38 7.11 7.09
5.39 5.39 5.38 5.38 5.22 5.19 5.17 5.03 5.02 5.00 5.00 4.64 4.61 4.19 4.17 4.16 4.14 4.11 4.09 4.08 4.06 3.90 3.90 3.89 3.88 3.87 3.87
2.32 2.09 2.08 2.02 1.95
2.00 2.04
1.00 0.98 1.01
1.01
1.00 1.05 1.01
3.03 2.99 3.04 3.18 3.07
25000
20000
15000
10000
5000
0
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

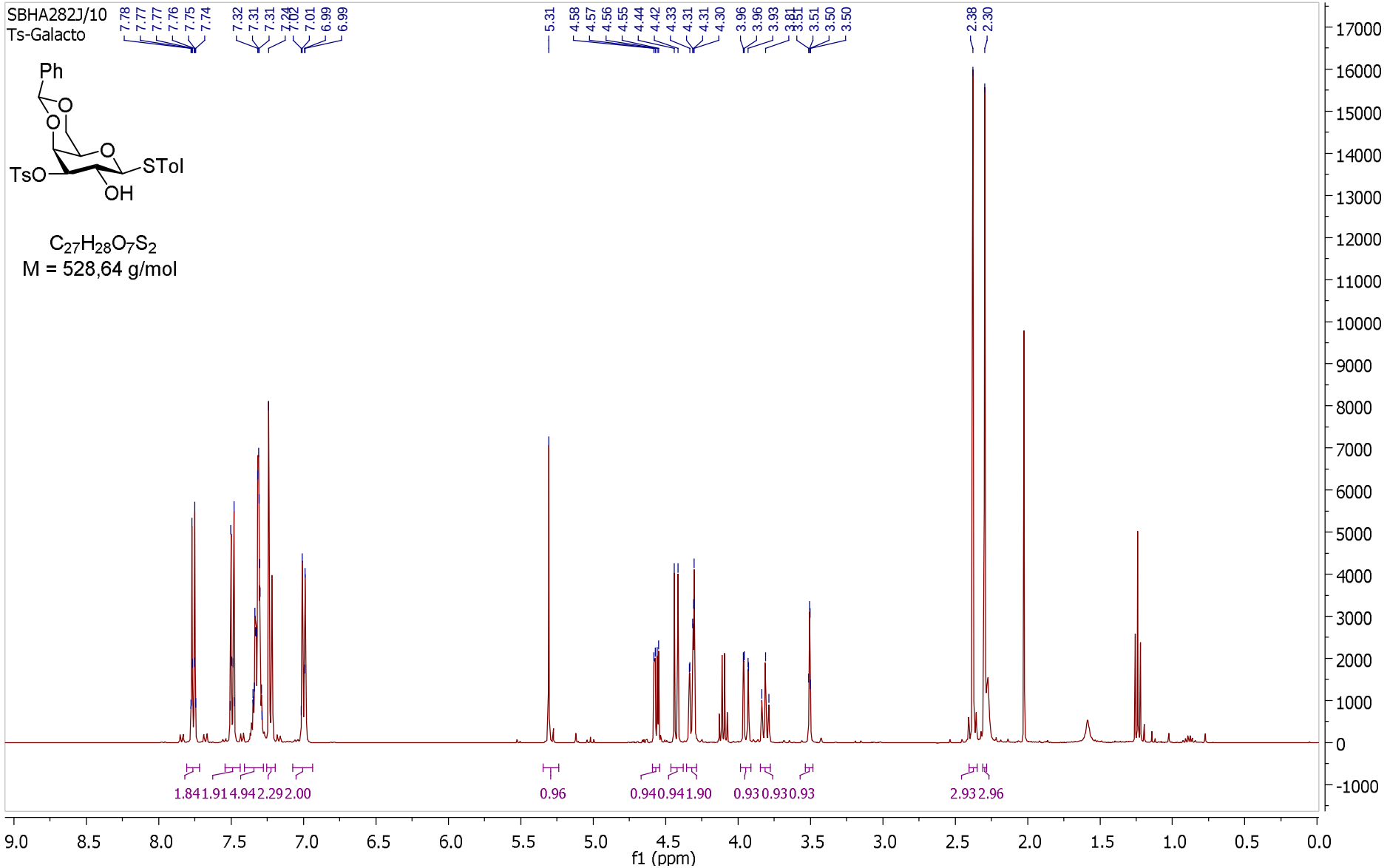

SBCL133J/10
1-Stufe Galacto
170.37
170.20
170.07
169.43
138.47
133.15
129.64
128.62
86.97
74.36
72.03
67.30
67.22
61.58
21.17
20.87
20.68
20.64
20.60
OAc
AcO
O
AcO
STol
OAc
C21H26O9S
M = 454,49 g/mol
19000
18000
17000
16000
15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
-2000
00
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

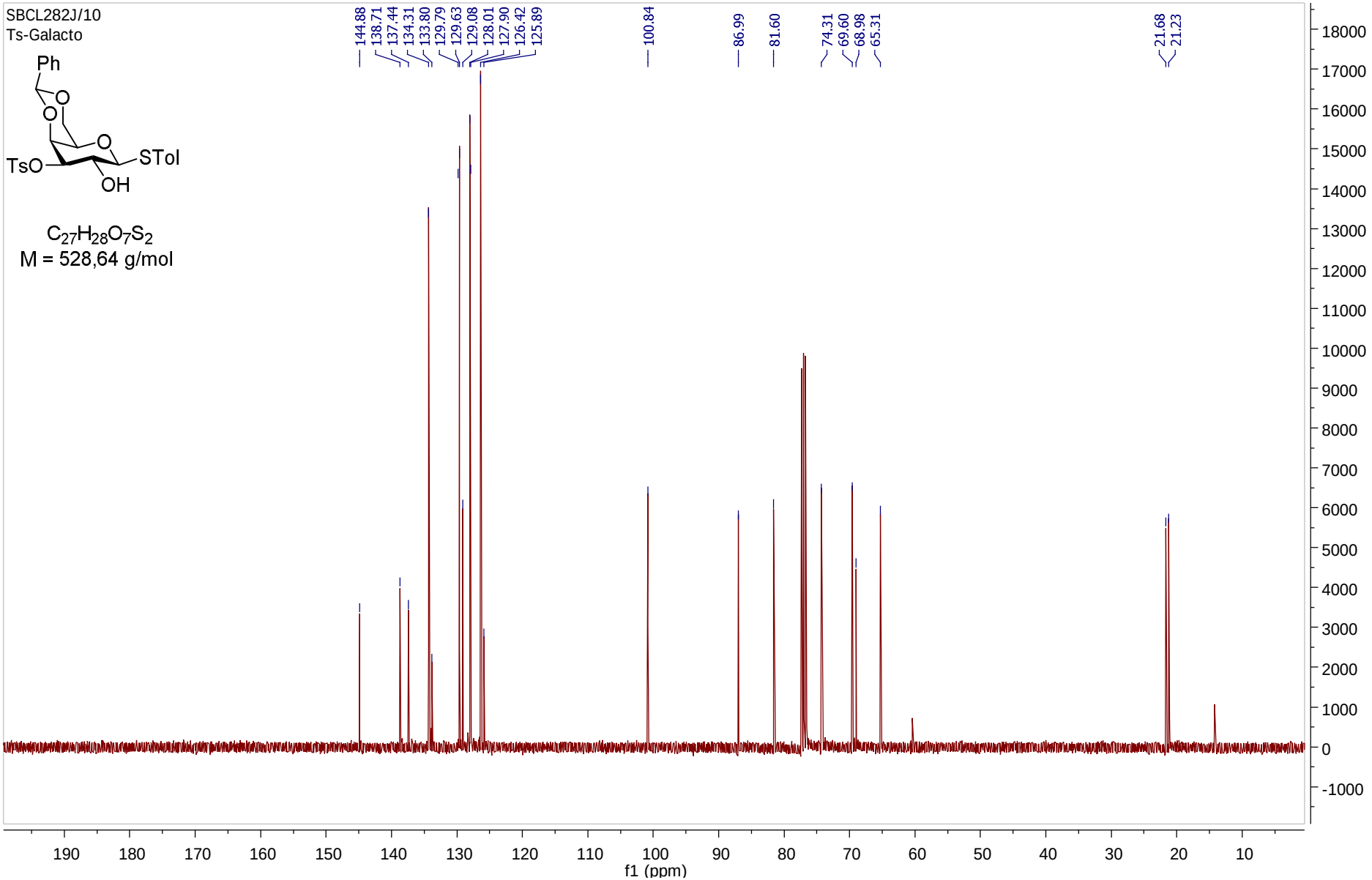

SBHA144J/10
Galacto 2. Stufe
OH
HO
O
HO
STol
OH
$C_6H_{11}O_5$
163,15 g/mol
7.37
7.35
7.13
7.11
4.51
4.48
3.71
3.70
3.52
3.50
3.49
3.48
3.45
3.44
3.43
3.42
3.40
3.38
3.35
2.47
2.46
2.46
2.44
2.27
2.00
2.01
1.12
1.01
3.33
0.88
1.03
3.07
f1 (ppm)

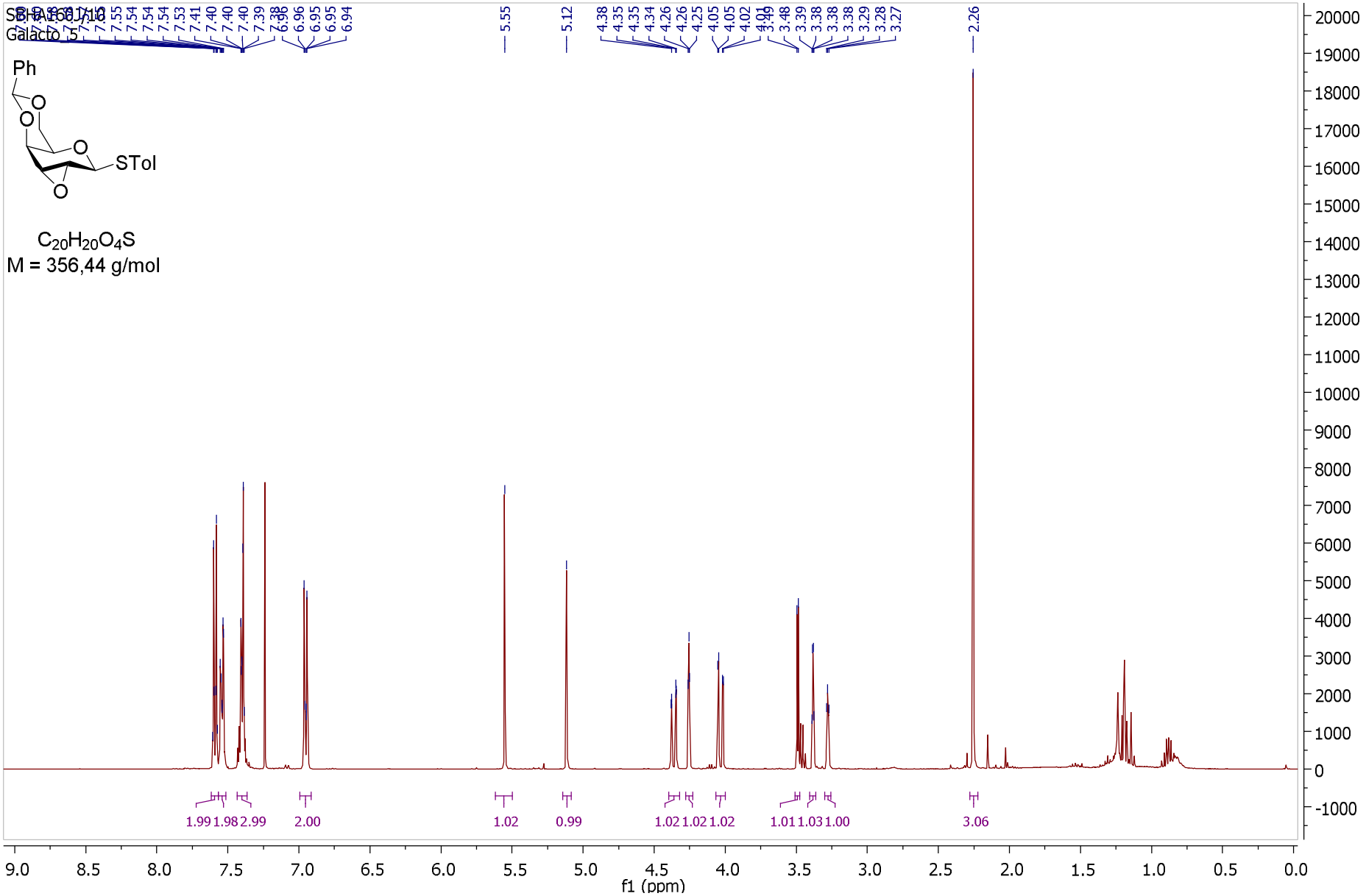

SBCL144J/10
Galacto 2. Stufe
OH
HO
O
HO
STol
OH
C6H11O5
163,15 g/mol
136.22
131.97
130.58
129.87
88.61
79.59
75.16
69.69
68.76
60.97
46.11
21.05
40000
35000
30000
25000
20000
15000
10000
5000
0
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

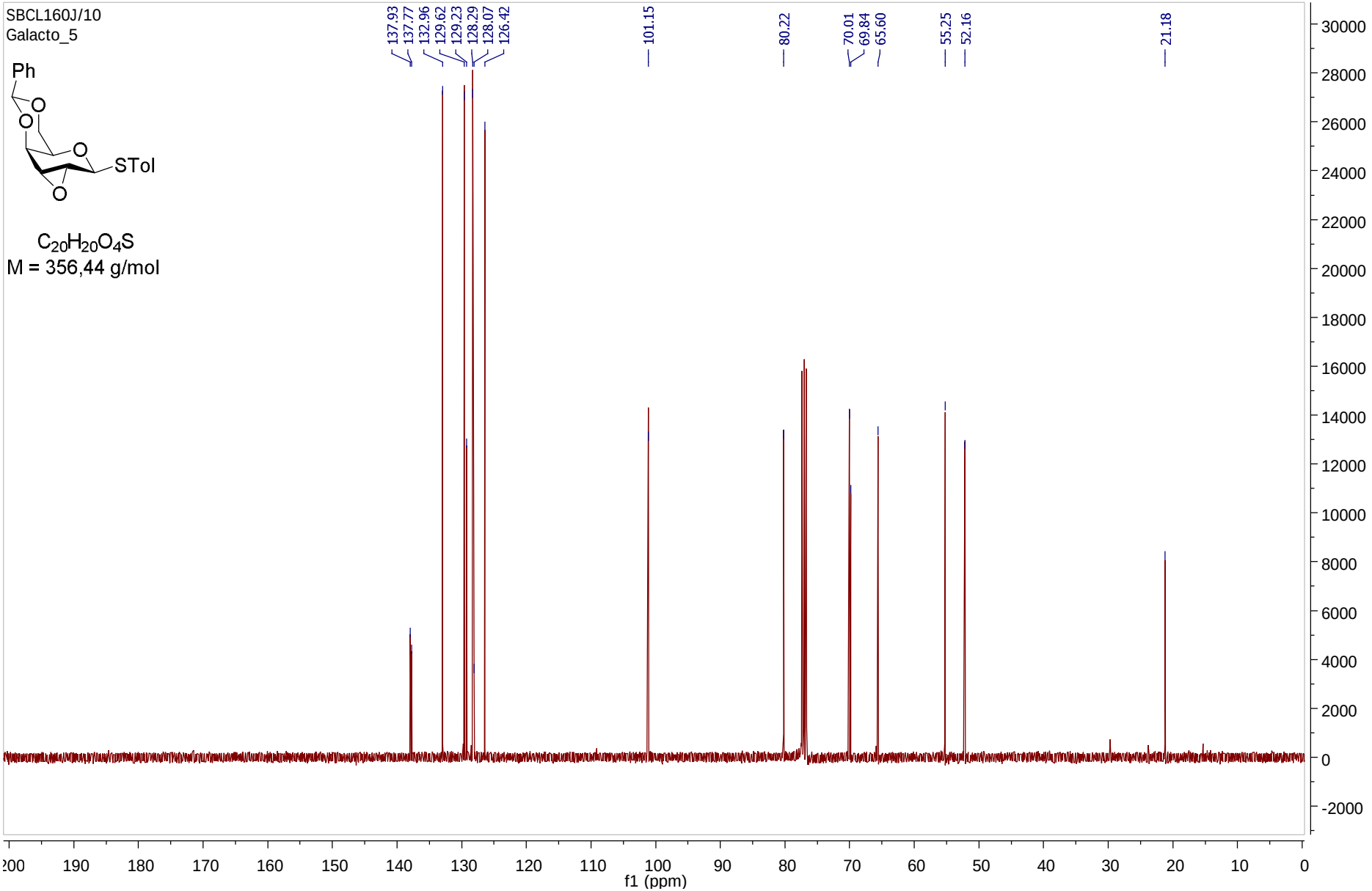

SBHA148/30
SB148
Ph
O
O
O
HO
OH
STol
$C_{20}H_{22}O_5S$
M = 374,45 g/mol
f1 (ppm)

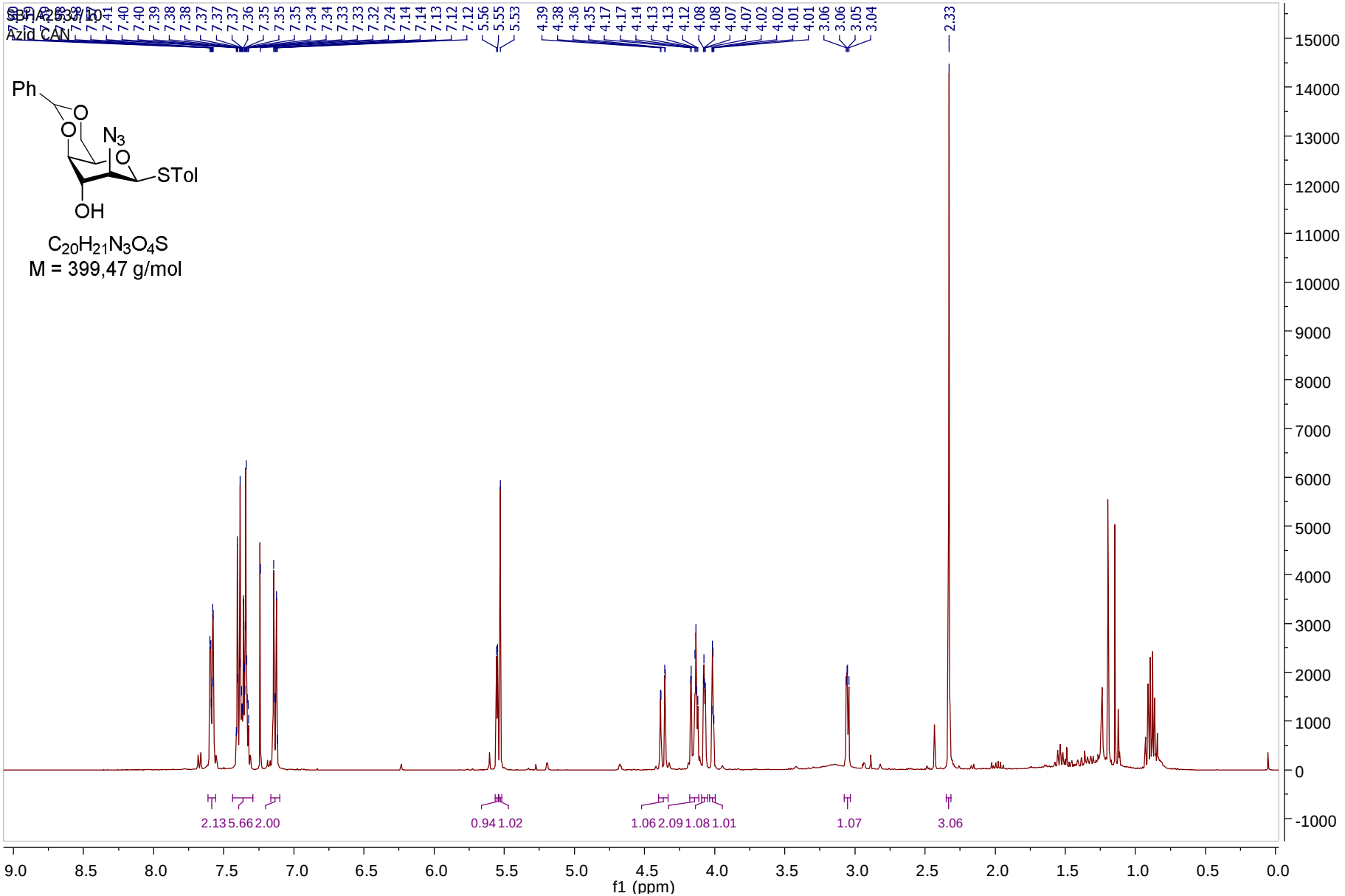

SBCL148J/10
SB148
Ph
O
O
O
HO
OH
STol
C20H22O5S
M = 374,45 g/mol
138.54
137.61
134.32
129.73
129.34
128.19
126.60
126.59
101.42
87.02
75.35
73.76
70.02
69.31
68.71
30.94
21.26
18.44
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
00
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

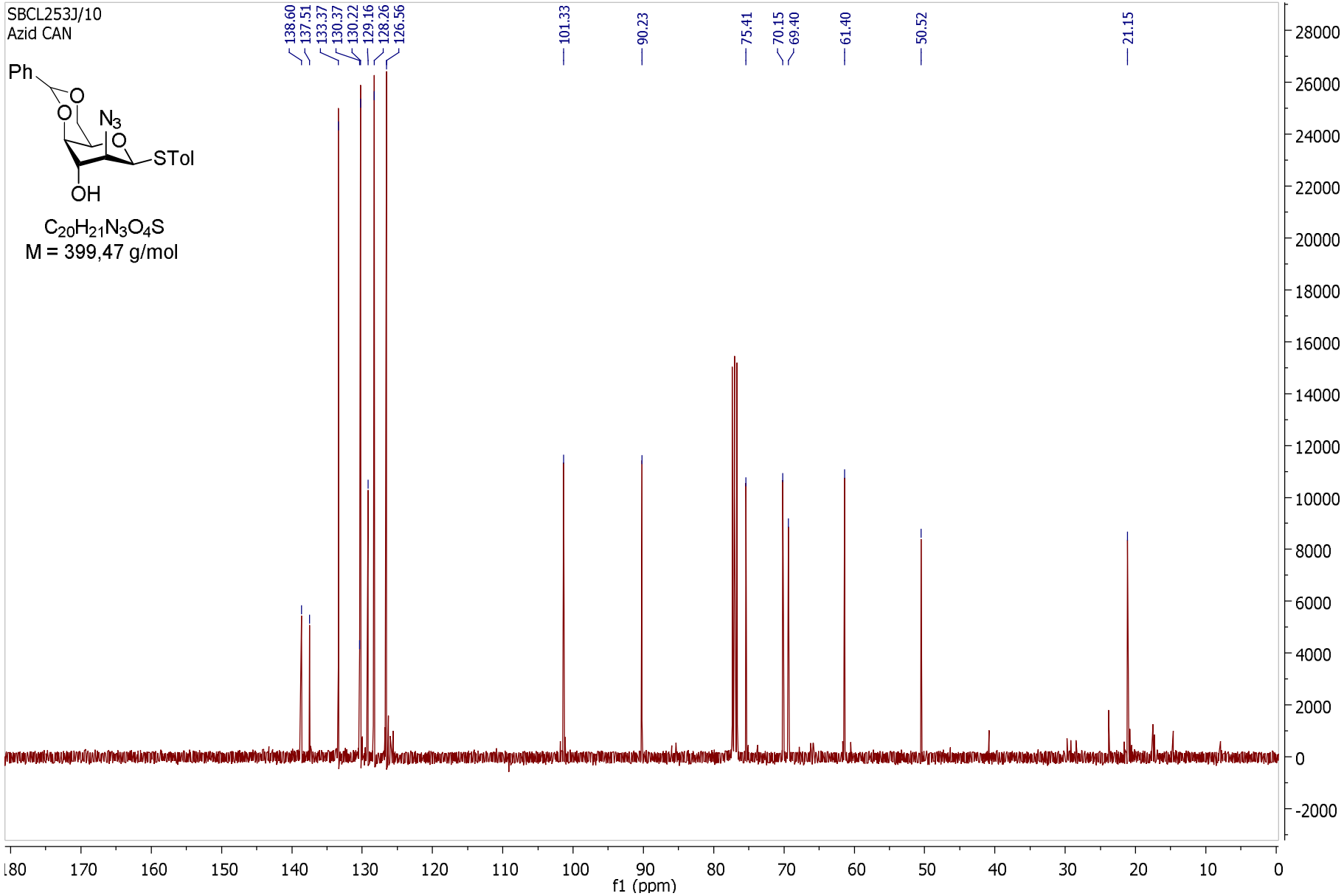

SBHA282J/10
Ts-Galacto
7.78 7.77 7.77 7.76 7.75 7.74 7.32 7.31 7.31 7.24 7.02 7.01 6.99 6.99
5.31
4.58 4.57 4.56 4.55 4.44 4.42 4.33 4.31 4.31 4.30
3.96 3.96 3.93 3.81 3.51 3.50 3.50
2.38 2.30
Ph
O
O
O
TsO
STol
OH
C27H28O7S2
M = 528,64 g/mol
1.84 1.91 4.94 2.29 2.00
0.96
0.94 0.94 1.90
0.93 0.93 0.93
2.93 2.96
17000 16000 15000 14000 13000 12000 11000 10000 9000 8000 7000 6000 5000 4000 3000 2000 1000 0 -1000
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

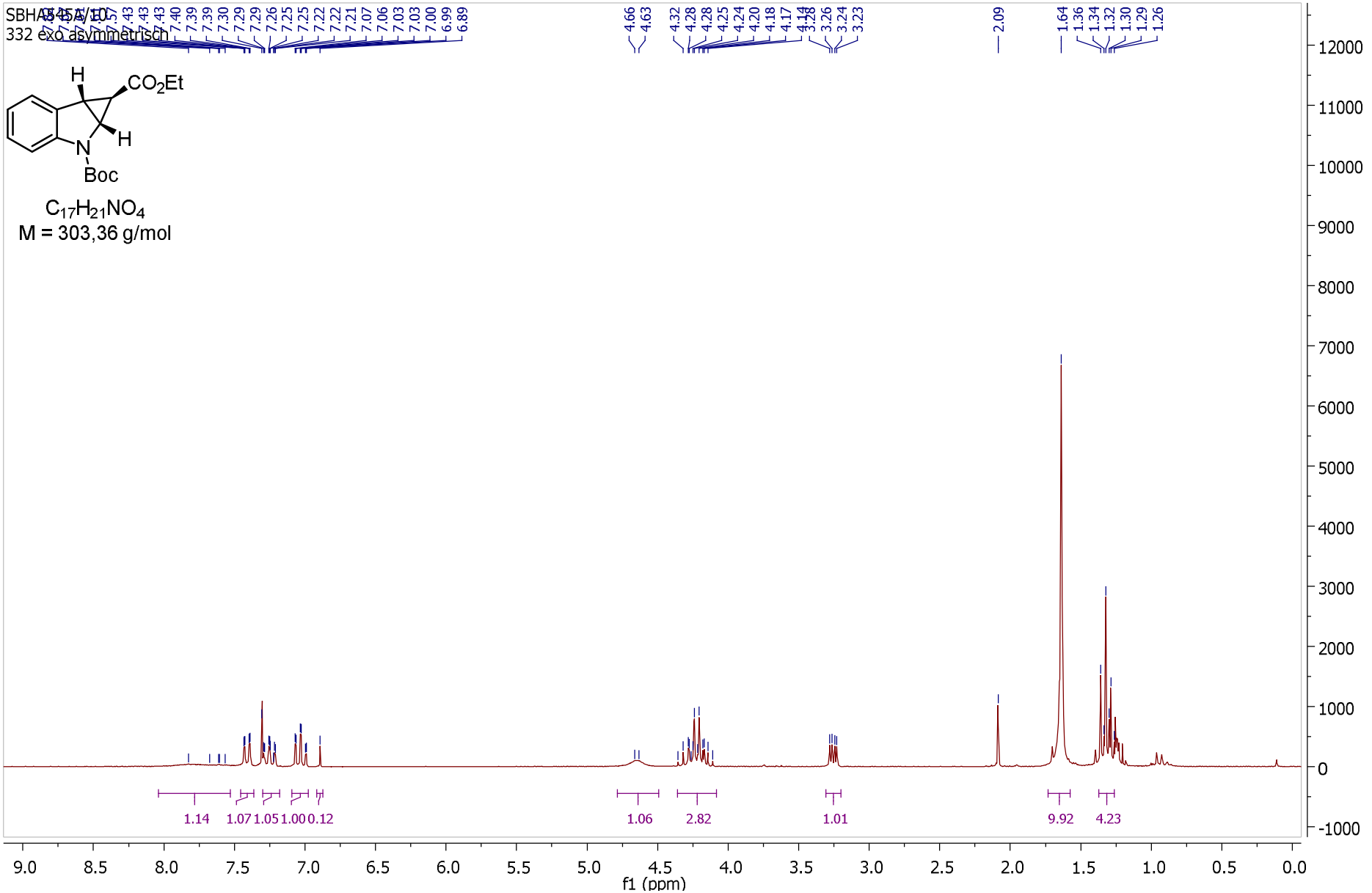

SBCL282J/10
Ts-Galacto
Ph
O
O
O
TsO
STol
OH
C27H28O7S2
M = 528,64 g/mol
144.88
138.71
137.44
134.31
133.80
129.79
129.63
129.08
128.01
127.90
126.42
125.89
100.84
86.99
81.60
74.31
69.60
68.98
65.31
21.68
21.23
18000
17000
16000
15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


Ph
O
O
O
O
STol
C20H20O4S
M = 356,44 g/mol
7.55
7.54
7.54
7.53
7.41
7.40
7.40
7.39
6.96
6.96
6.95
6.95
6.94
5.55
5.12
4.38
4.35
4.34
4.26
4.26
4.25
4.05
4.05
4.02
3.48
3.39
3.38
3.38
3.38
3.29
3.28
3.27
2.26
1.99 1.98 2.99
2.00
1.02
0.99
1.02 1.02 1.02
1.01 1.03 1.00
3.06
20000
19000
18000
17000
16000
15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

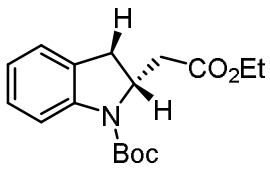

SBCL160J/10
Galacto_5
Ph
O
O
O
O
STol
C20H20O4S
M = 356,44 g/mol
137.93
137.77
132.96
129.62
129.23
128.29
128.07
126.42
101.15
80.22
70.01
69.84
65.60
55.25
52.16
21.18
30000
28000
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


SBHA2533/10
Azid CAN
Ph
O
O
N3
O
STol
OH
C20H21N3O4S
M = 399,47 g/mol
2.13 5.66 2.00
0.94 1.02
1.06 2.09 1.08 1.01
1.07
3.06
f1 (ppm)

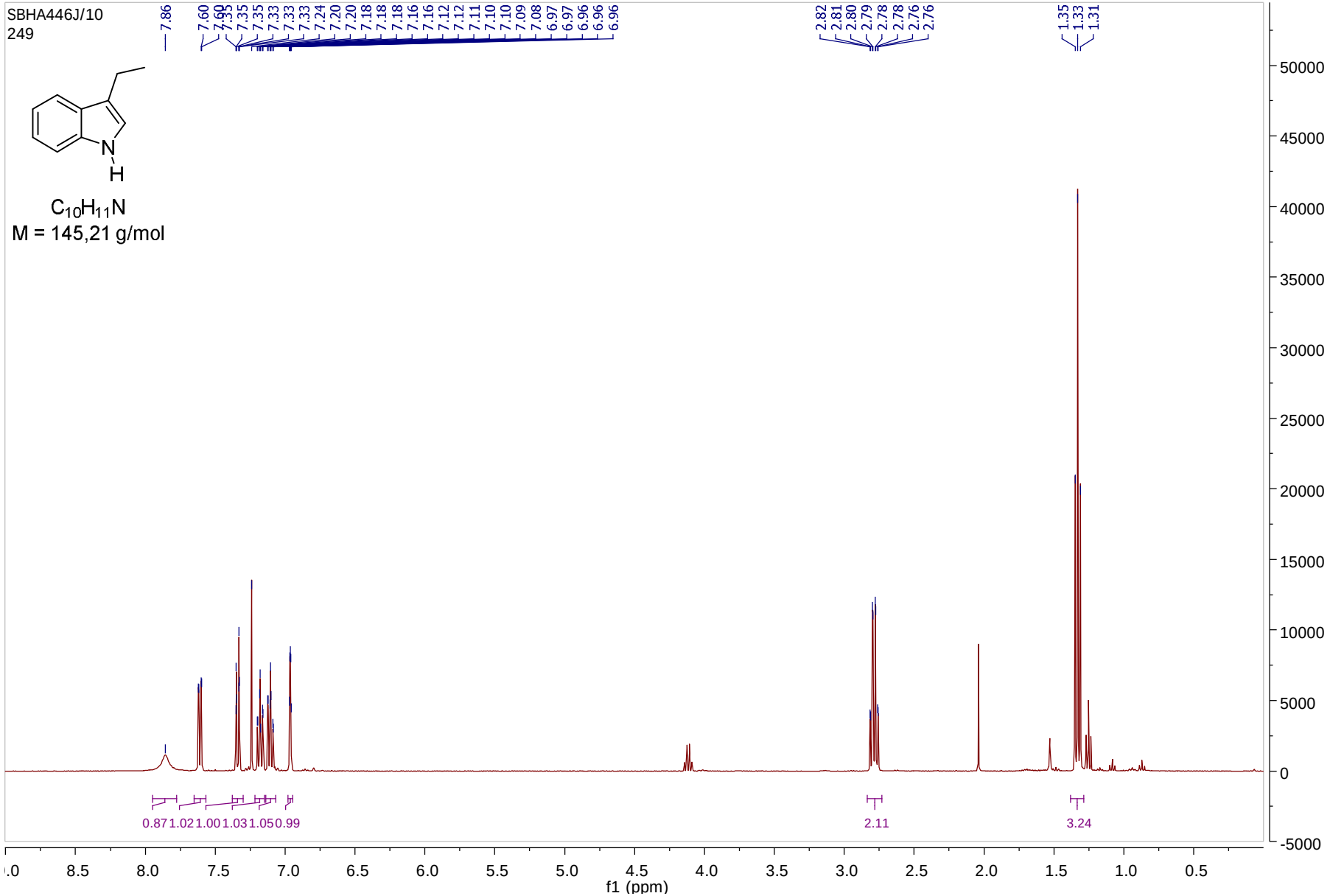

SBCL253J/10
Azid CAN
Ph
O
O
N3
O
STol
OH
C20H21N3O4S
M = 399,47 g/mol
138.60
137.51
133.37
130.37
130.22
129.16
128.26
126.56
101.33
90.23
75.41
70.15
69.40
61.40
50.52
21.15
28000
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

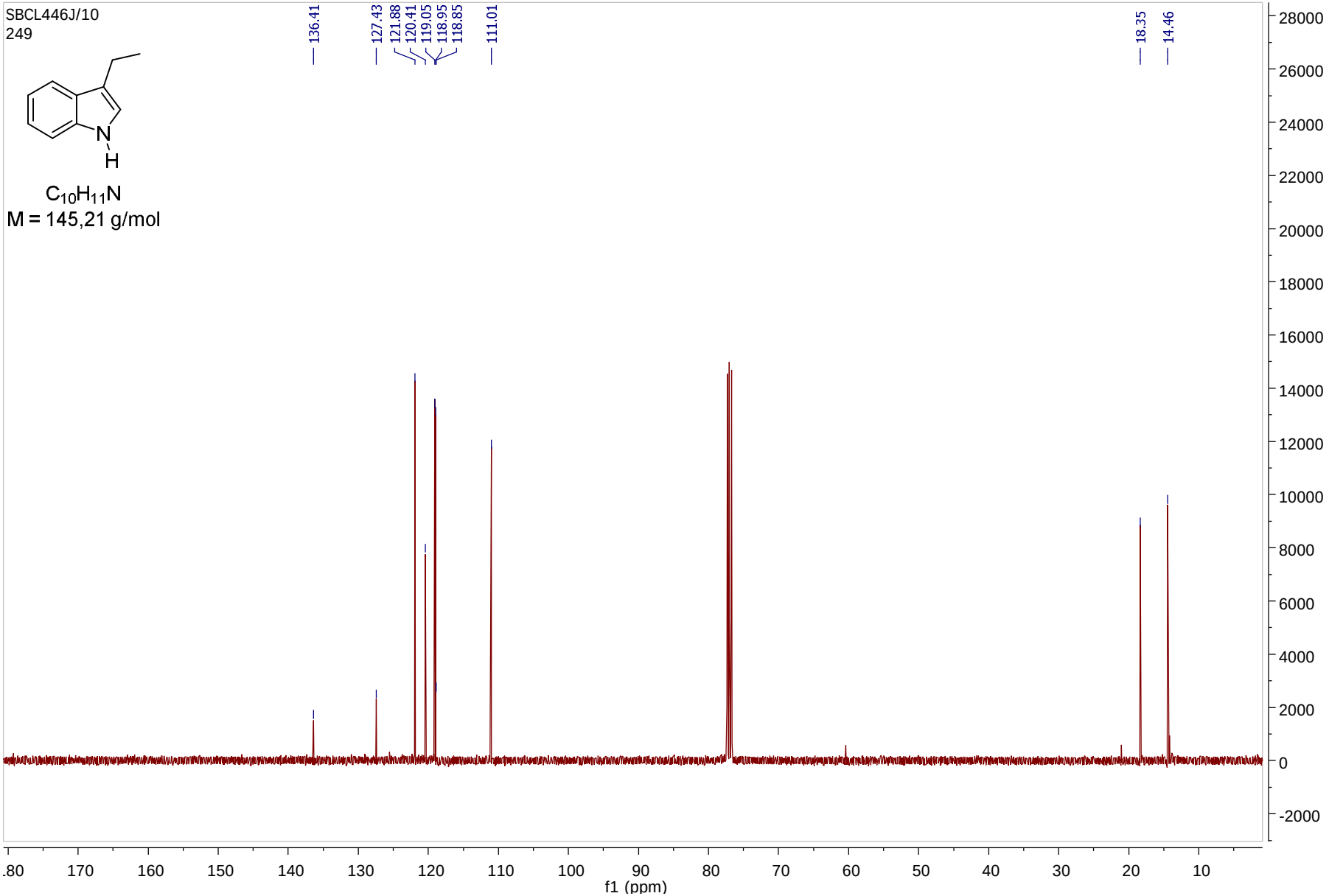

SBHA545A/1D
332 exo asymmetrisch
H
CO2Et
H
N
Boc
C17H21NO4
M = 303,36 g/mol
7.57 7.43 7.43 7.40 7.39 7.39 7.30 7.29 7.29 7.26 7.25 7.25 7.22 7.22 7.21 7.07 7.06 7.03 7.03 7.00 6.99 6.89
4.66 4.63 4.32 4.28 4.28 4.25 4.24 4.20 4.18 4.17 4.14 3.28 3.26 3.24 3.23
2.09
1.64 1.36 1.34 1.32 1.30 1.29 1.26
1.14 1.07 1.05 1.00 0.12
1.06 2.82 1.01 9.92 4.23
12000 11000 10000 9000 8000 7000 6000 5000 4000 3000 2000 1000 0 -1000
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

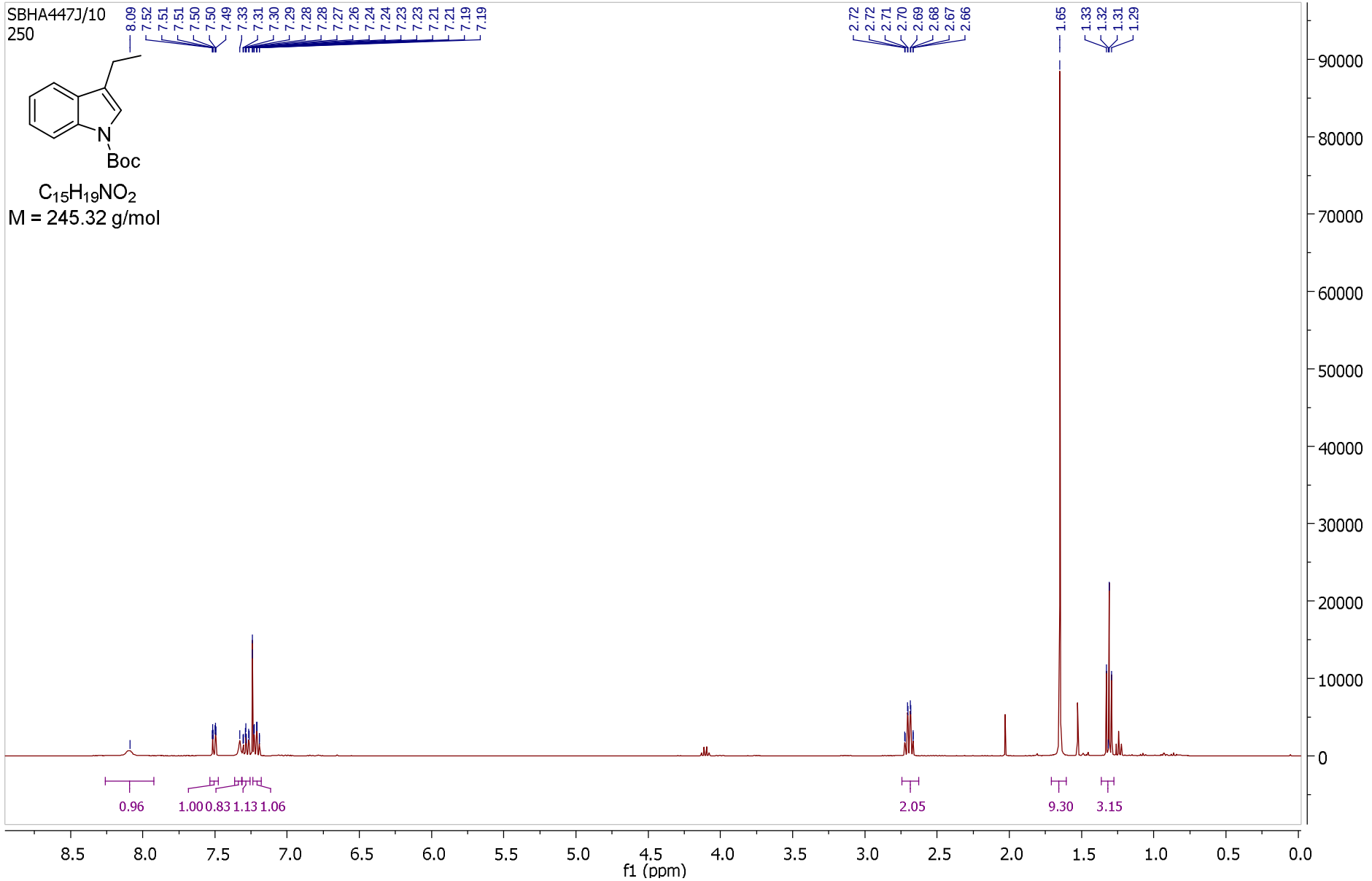
SBHA546A/10
333 Hydieren exo



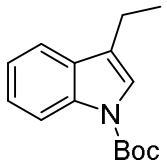
$C_{17}H_{23}NO_4$
M = 305,37 g/mol


SBHA446J/10
249
7.86
7.60
7.60
7.35
7.35
7.33
7.33
7.24
7.20
7.20
7.18
7.18
7.18
7.16
7.12
7.12
7.11
7.10
7.10
7.09
7.08
6.97
6.97
6.96
6.96
6.96
2.82
2.81
2.80
2.79
2.78
2.78
2.76
2.76
1.35
1.33
1.31
N
H
C10H11N
M = 145,21 g/mol
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
0.87
1.02
1.00
1.03
1.05
0.99
2.11
3.24
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

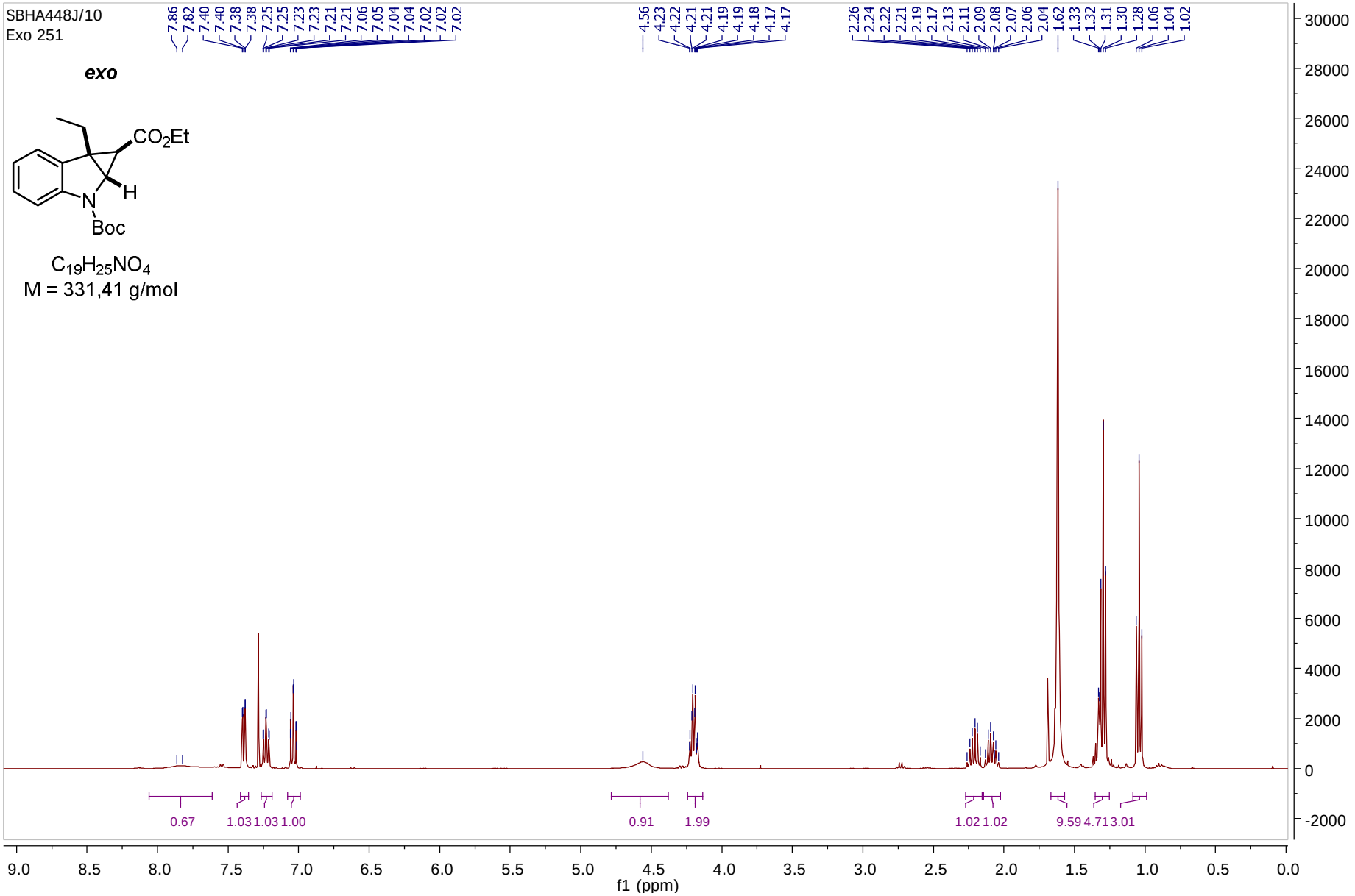

SBCL446J/10
249
136.41
127.43
121.88
120.41
119.05
118.95
118.85
111.01
18.35
14.46
N
H
$C_{10}H_{11}N$
M = 145,21 g/mol
28000
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

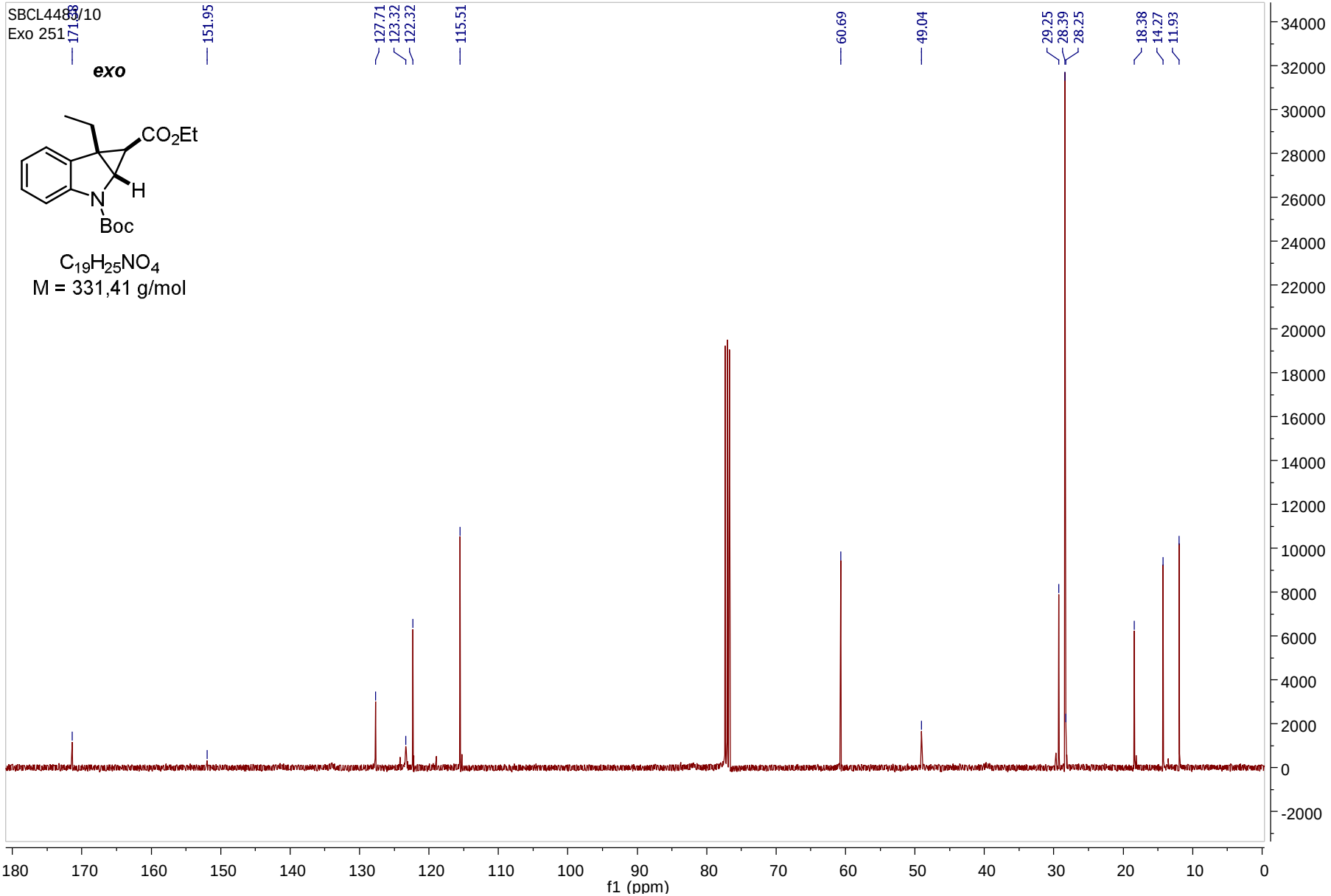

SBHA447J/10
250
8.09
7.52
7.51
7.51
7.50
7.50
7.49
7.33
7.31
7.30
7.29
7.28
7.28
7.27
7.26
7.24
7.24
7.23
7.23
7.21
7.21
7.19
7.19
2.72
2.72
2.71
2.70
2.69
2.68
2.67
2.66
1.65
1.33
1.32
1.31
1.29
N
Boc
C15H19NO2
M = 245.32 g/mol
0.96
1.00
0.83
1.13
1.06
2.05
9.30
3.15
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

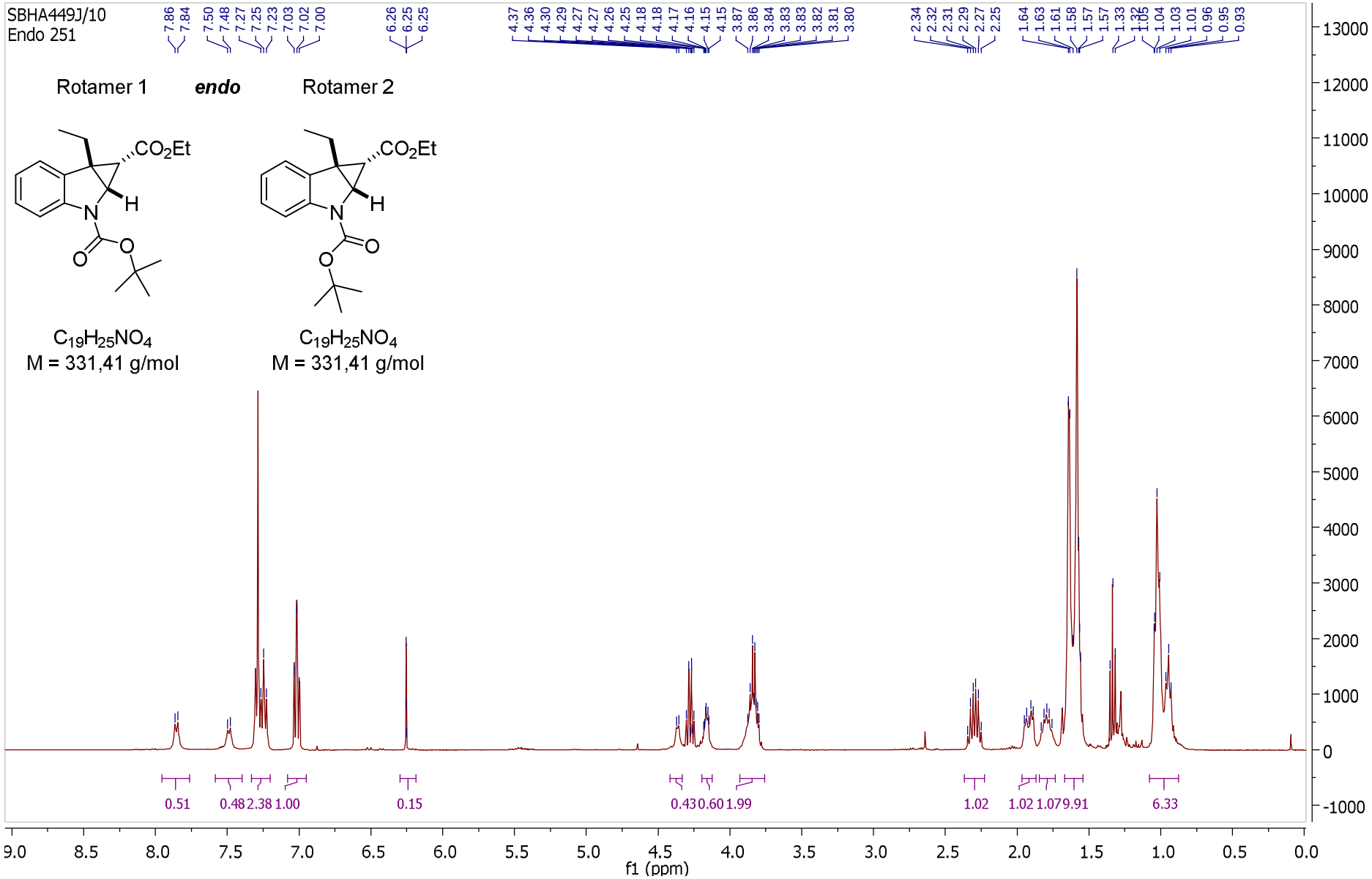
SBCL447J/10
250

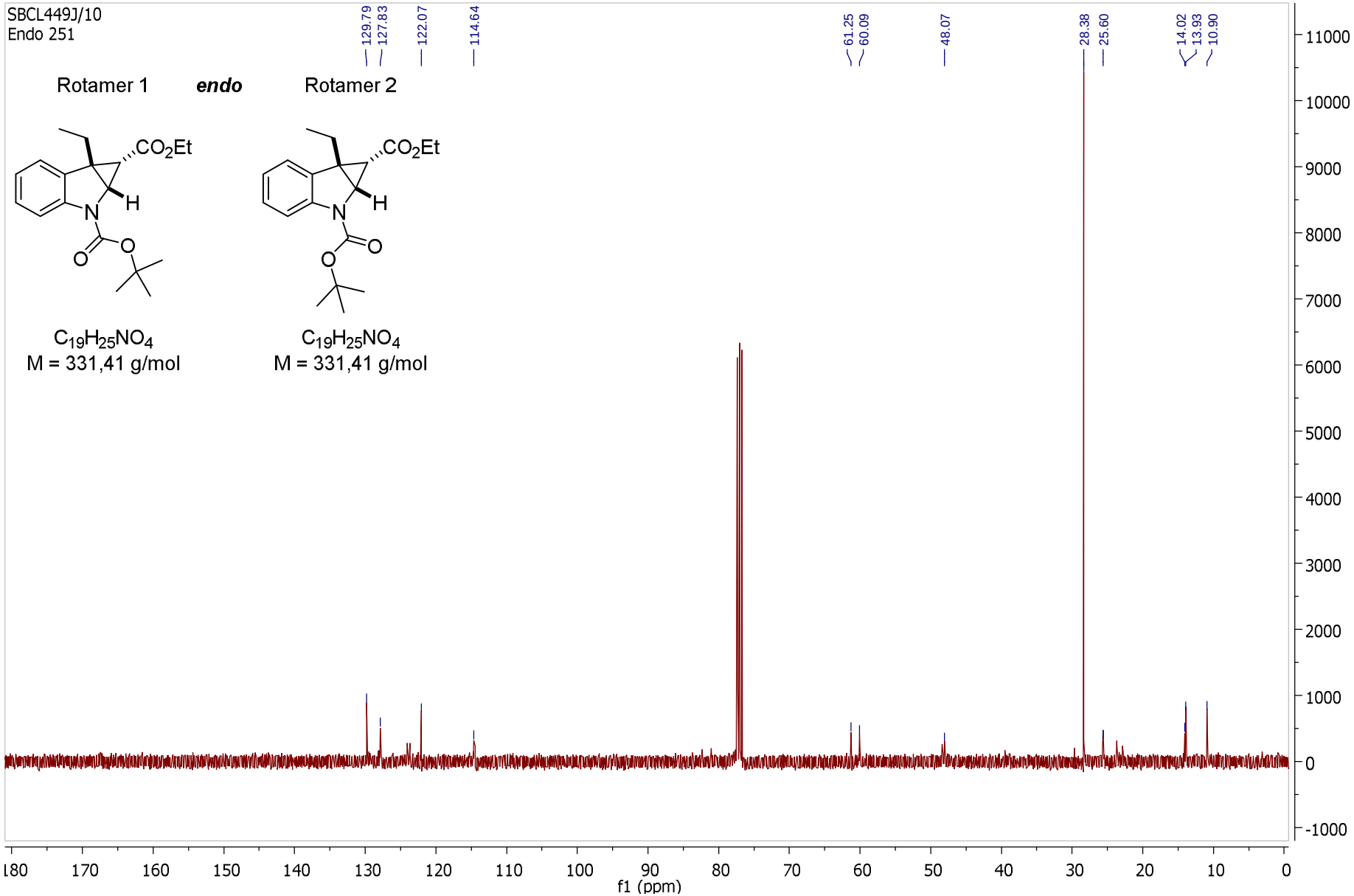


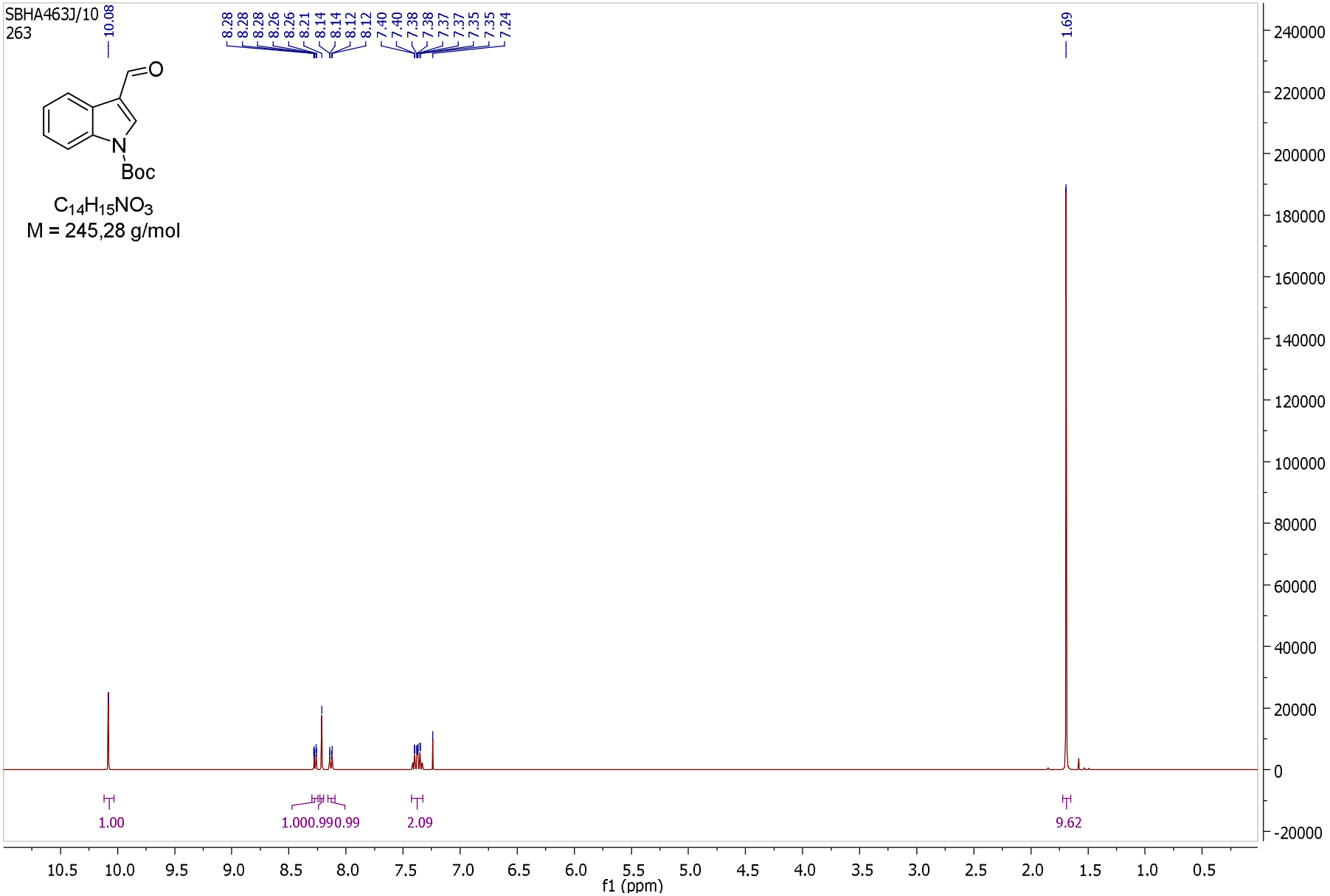
$C_{15}H_{19}NO_2$
M = 245.32 g/mol

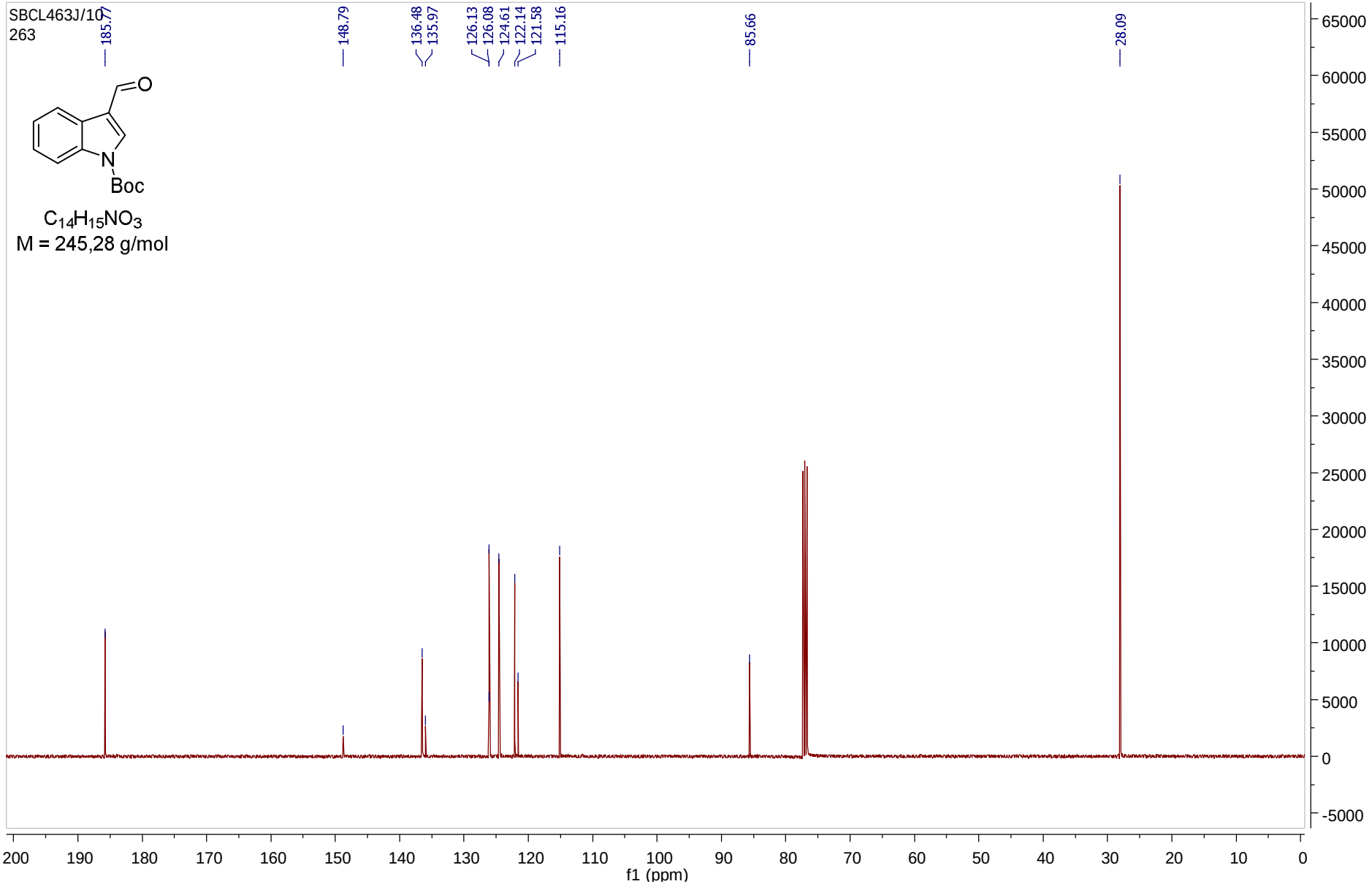

SBHA448J/10
Exo 251
exo
CO2Et
H
N
Boc
C19H25NO4
M = 331,41 g/mol
7.86 7.82 7.40 7.40 7.38 7.38 7.25 7.25 7.23 7.23 7.21 7.21 7.06 7.05 7.04 7.04 7.02 7.02 7.02
4.56 4.23 4.22 4.21 4.21 4.19 4.19 4.18 4.17 4.17
2.26 2.24 2.22 2.21 2.19 2.17 2.13 2.11 2.09 2.08 2.07 2.06 2.04 1.62 1.33 1.32 1.31 1.30 1.28 1.06 1.04 1.02
0.67 1.03 1.03 1.00 0.91 1.99 1.02 1.02 9.59 4.71 3.01
30000 28000 26000 24000 22000 20000 18000 16000 14000 12000 10000 8000 6000 4000 2000 0 -2000
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

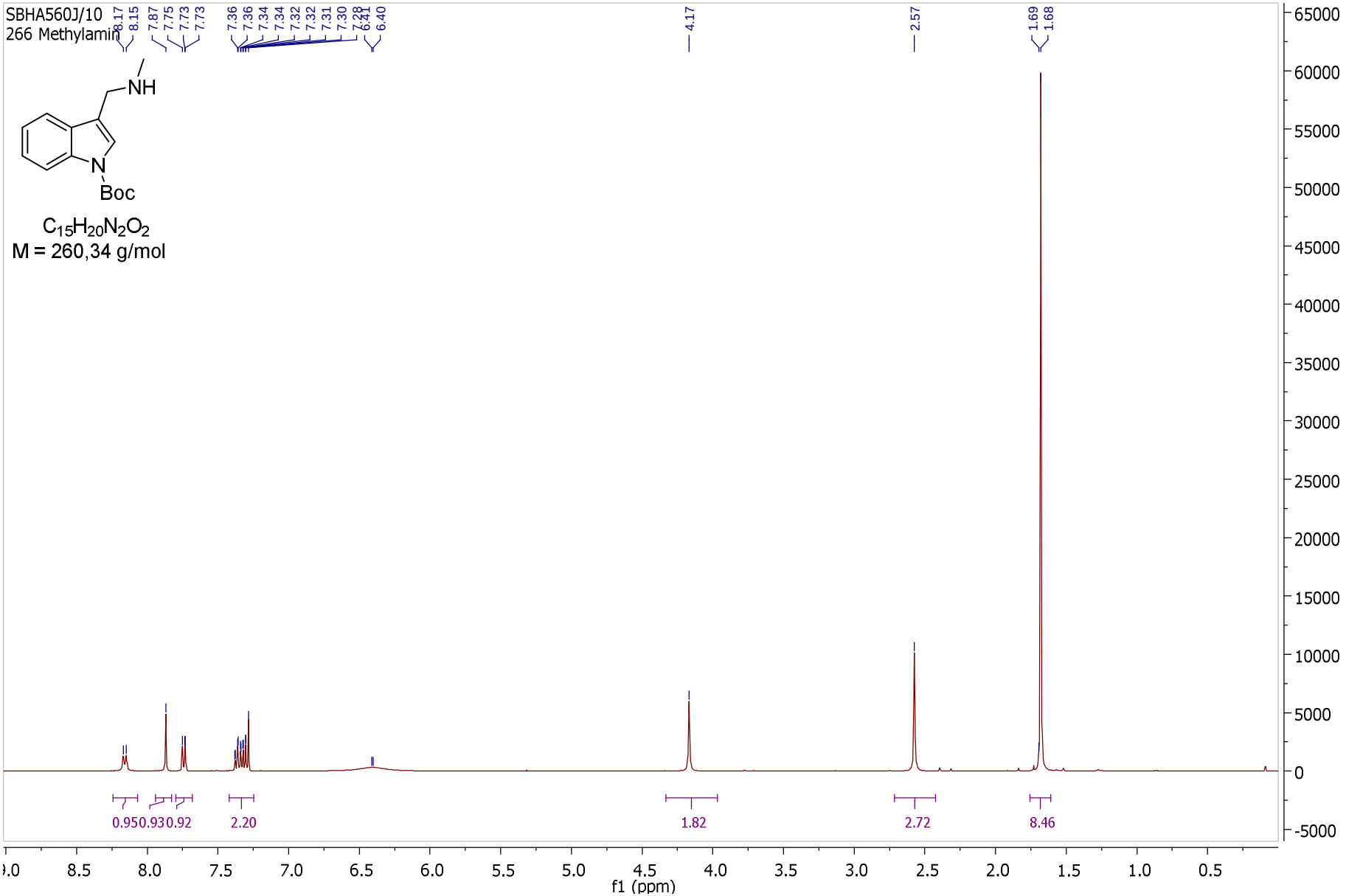

SBCL4483/10
Exo 251
171.38
151.95
127.71
123.32
122.32
115.51
60.69
49.04
29.25
28.39
28.25
18.38
14.27
11.93
exo
CO2Et
H
N
Boc
C19H25NO4
M = 331,41 g/mol
f1 (ppm)

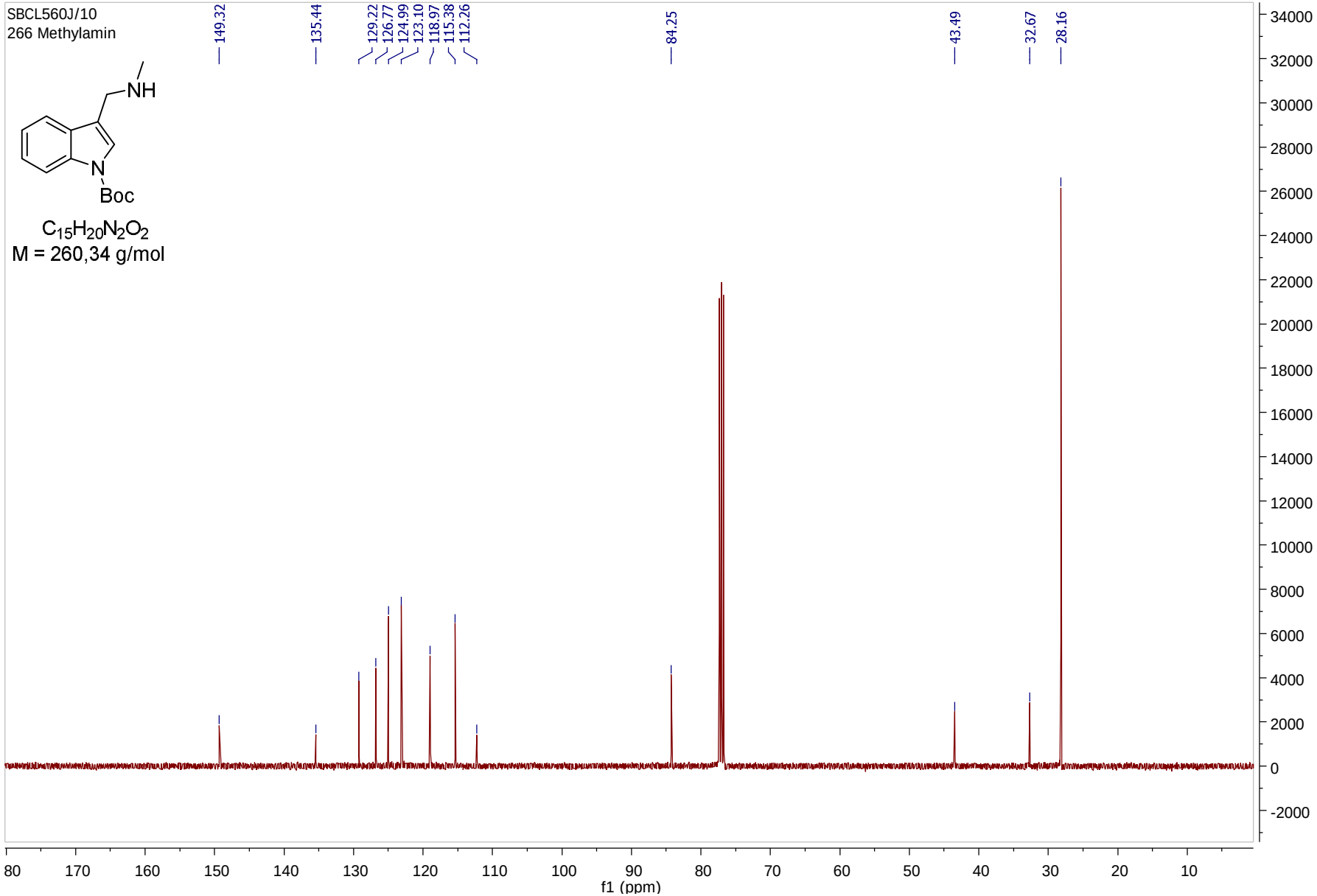

SBHA449J/10
Endo 251
Rotamer 1
endo
Rotamer 2
CO2Et
N
H
O
O
C19H25NO4
M = 331,41 g/mol
C19H25NO4
M = 331,41 g/mol
f1 (ppm)

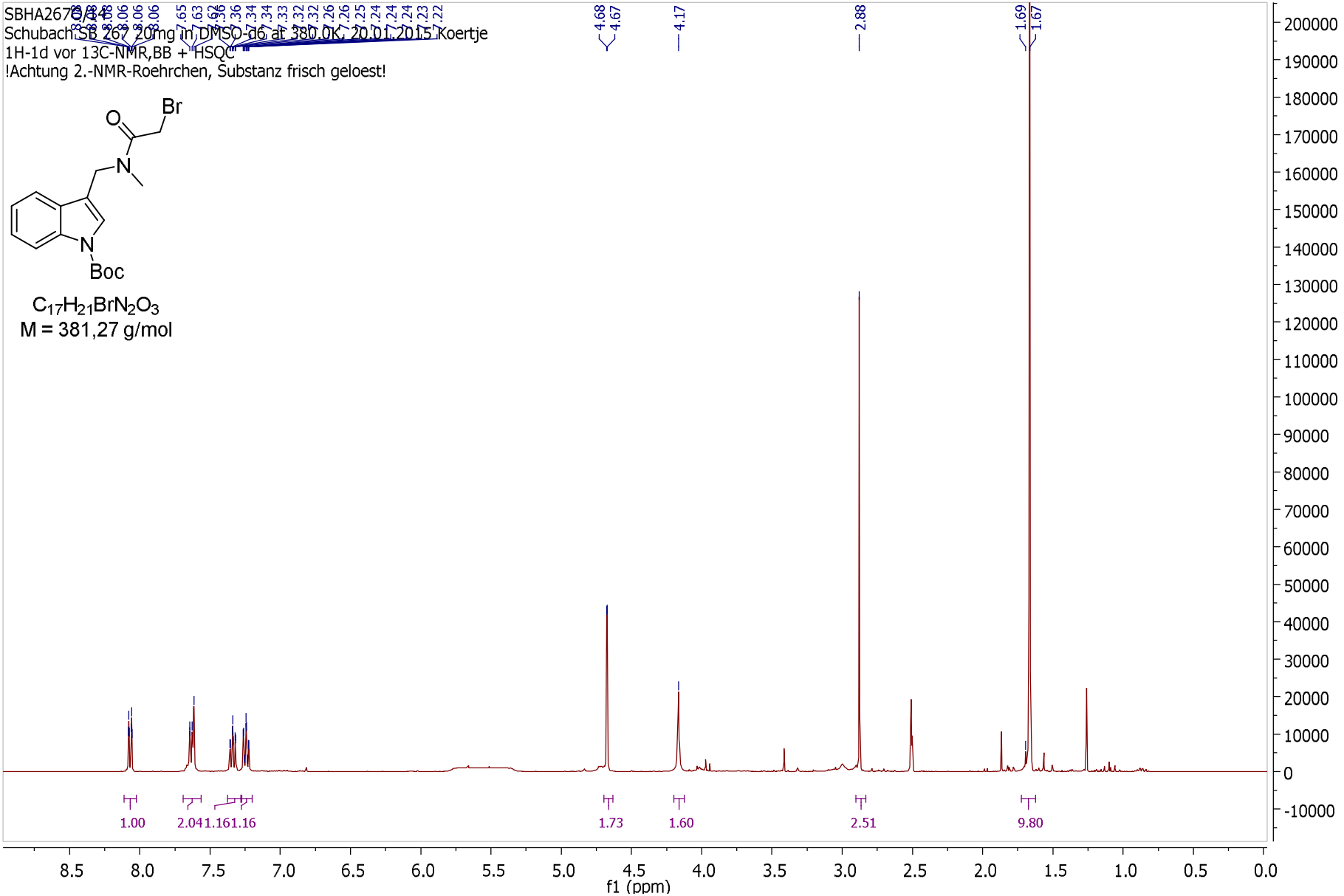

SBCL449J/10
Endo 251
129.79
127.83
122.07
114.64
61.25
60.09
48.07
28.38
25.60
14.02
13.93
10.90
Rotamer 1
endo
Rotamer 2
CO2Et
H
N
O
O
O
C19H25NO4
M = 331,41 g/mol
C19H25NO4
M = 331,41 g/mol
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

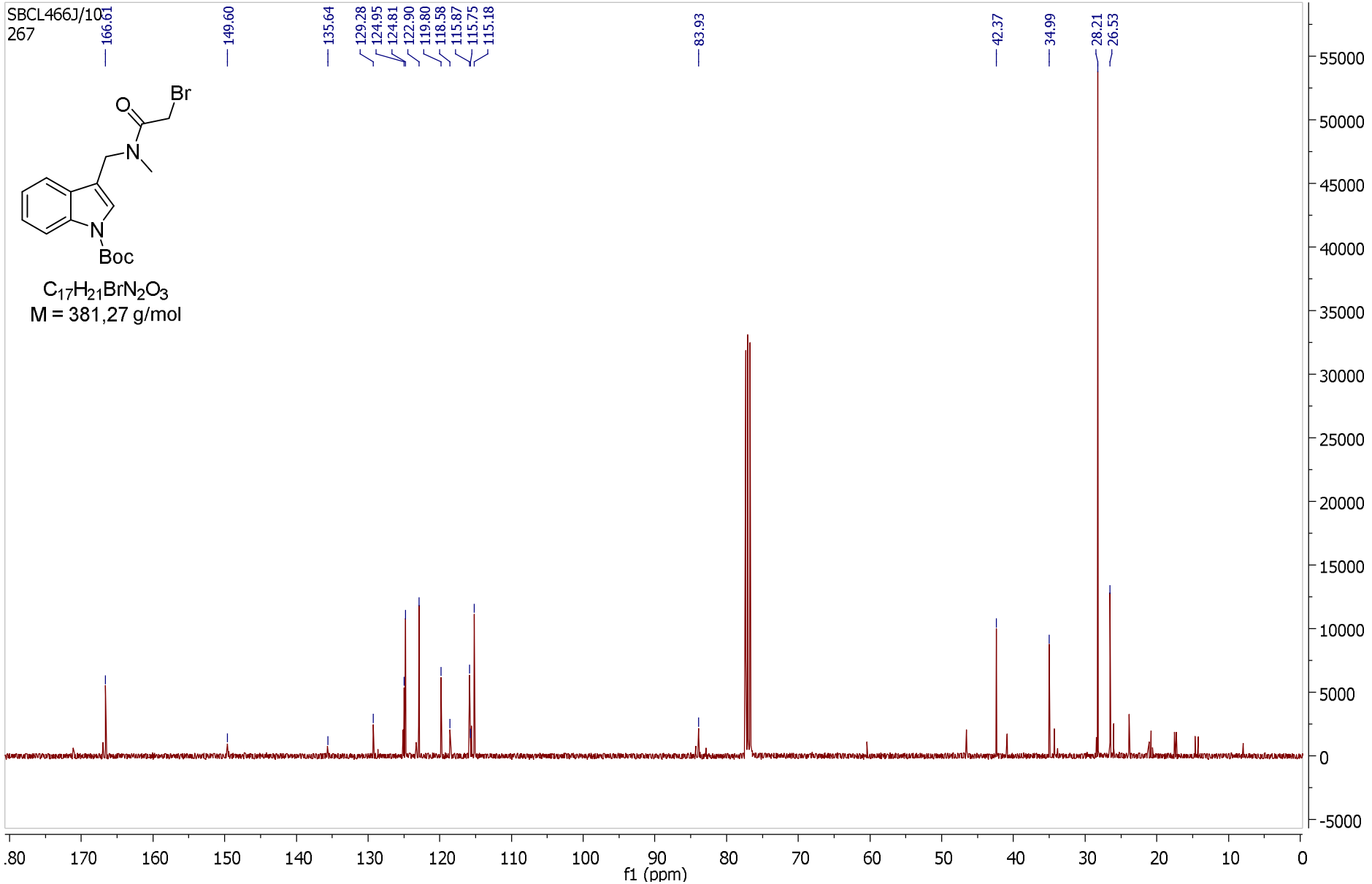

SBHA463J/10
263
10.08
8.28
8.28
8.28
8.26
8.26
8.21
8.14
8.14
8.12
8.12
7.40
7.40
7.38
7.38
7.37
7.37
7.35
7.35
7.24
1.69
O
N
Boc
C14H15NO3
M = 245,28 g/mol
1.00
1.00
0.99
0.99
2.09
9.62
240000
220000
200000
180000
160000
140000
120000
100000
80000
60000
40000
20000
0
-20000
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

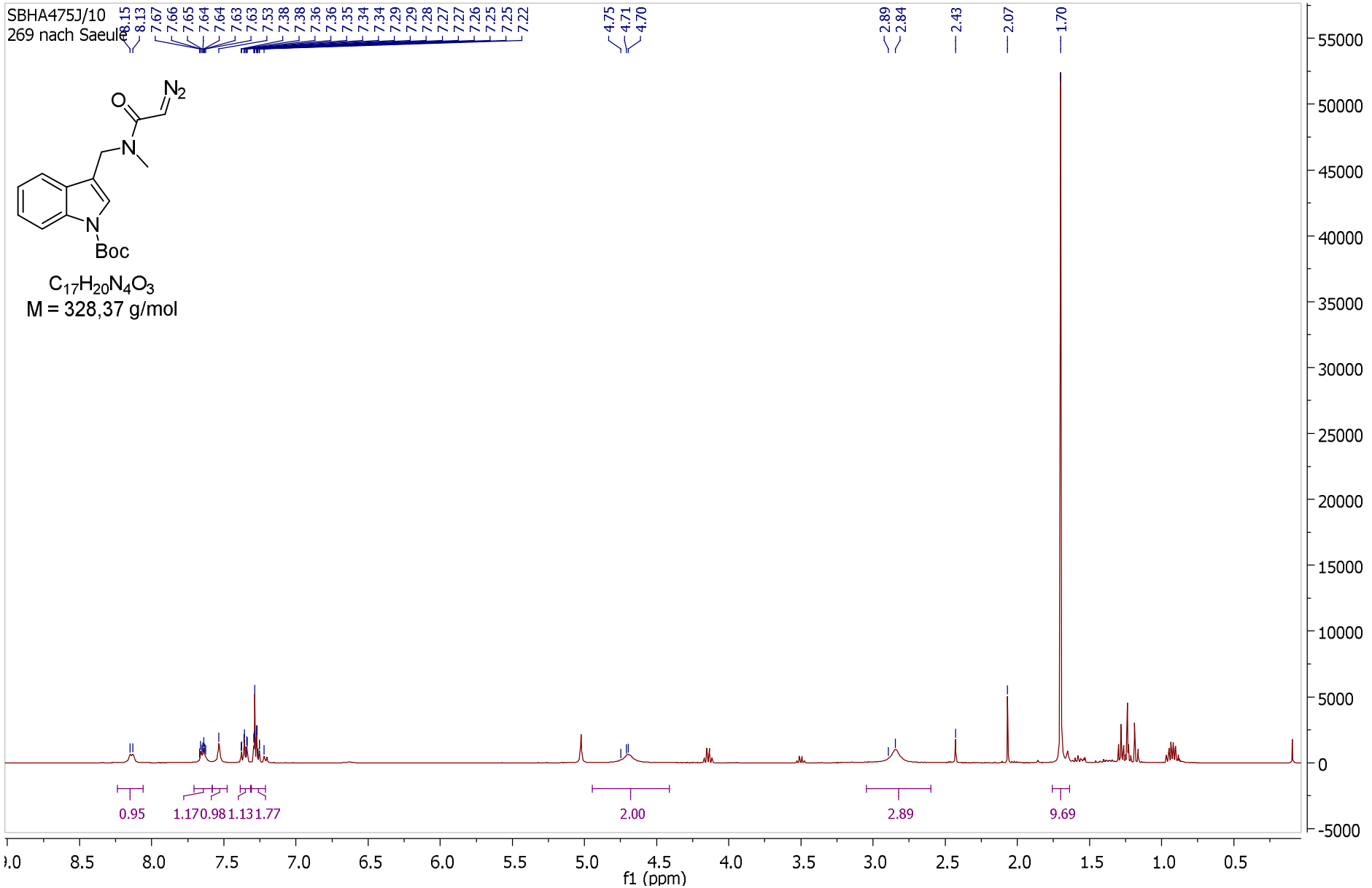

SBCL463J/10
263
185.77
148.79
136.48
135.97
126.13
126.08
124.61
122.14
121.58
115.16
85.66
28.09
O
N
Boc
C14H15NO3
M = 245,28 g/mol
65000
60000
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

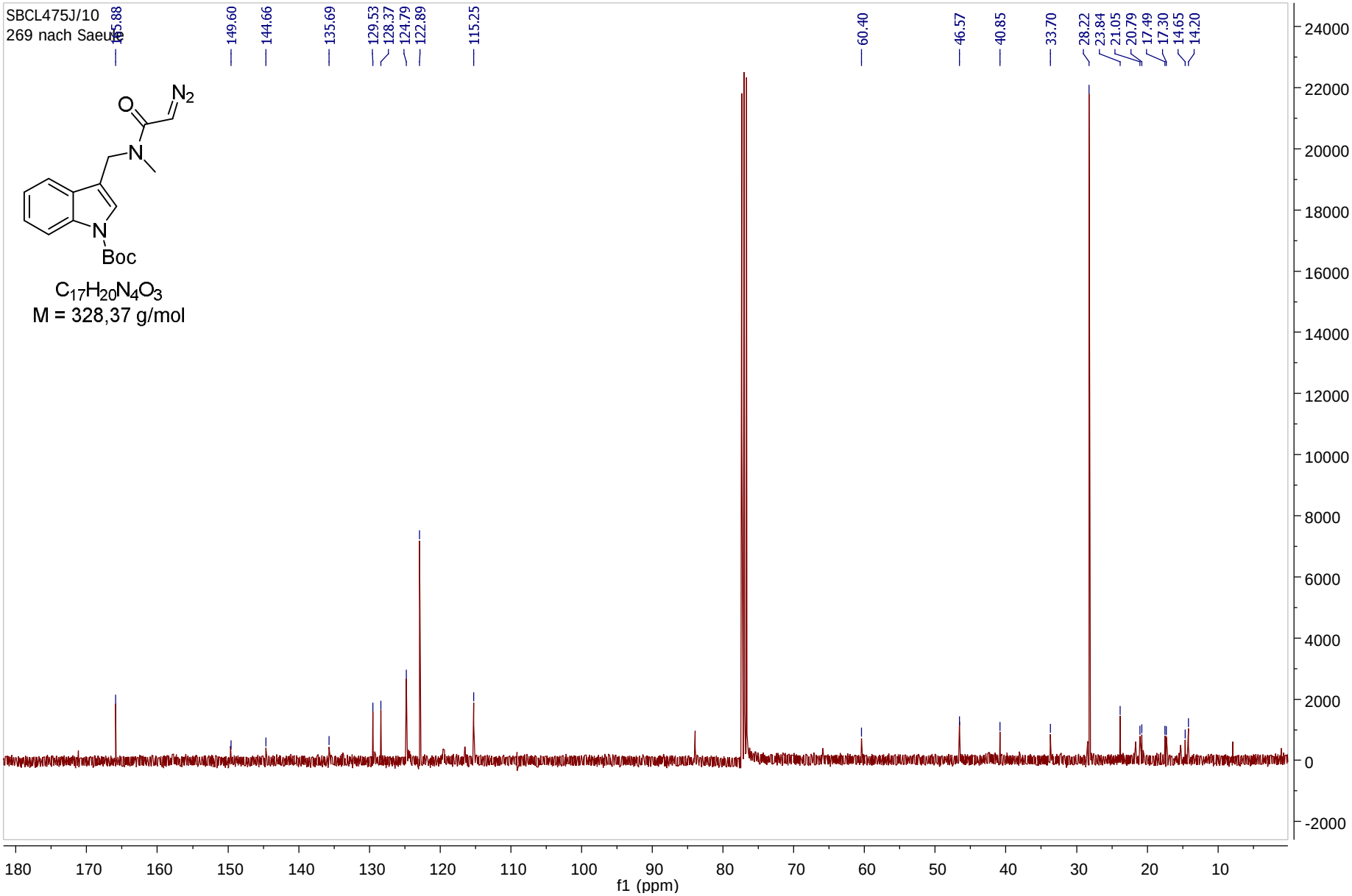

SBHA560J/10
266 Methylamin
8.17
8.15
7.87
7.75
7.73
7.73
7.36
7.36
7.34
7.34
7.32
7.32
7.31
7.30
7.28
6.41
6.40
4.17
2.57
1.69
1.68
NH
N
Boc
C15H20N2O2
M = 260,34 g/mol
0.95
0.93
0.92
2.20
1.82
2.72
8.46
65000
60000
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

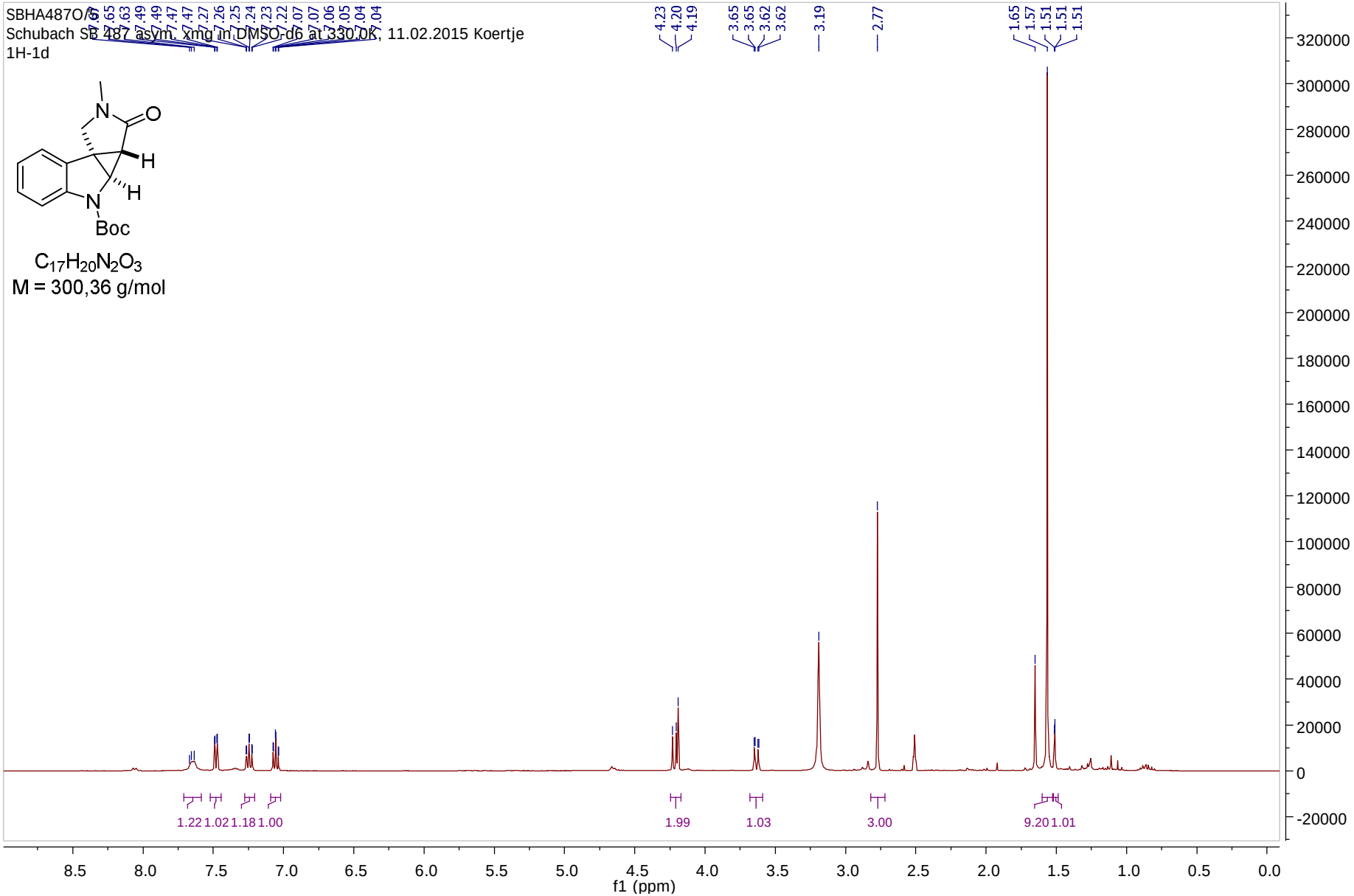

SBCL560J/10
266 Methylamin
149.32
135.44
129.22
126.77
124.99
123.10
118.97
115.38
112.26
84.25
43.49
32.67
28.16
NH
N
Boc
C15H20N2O2
M = 260,34 g/mol
34000
32000
30000
28000
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
80
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

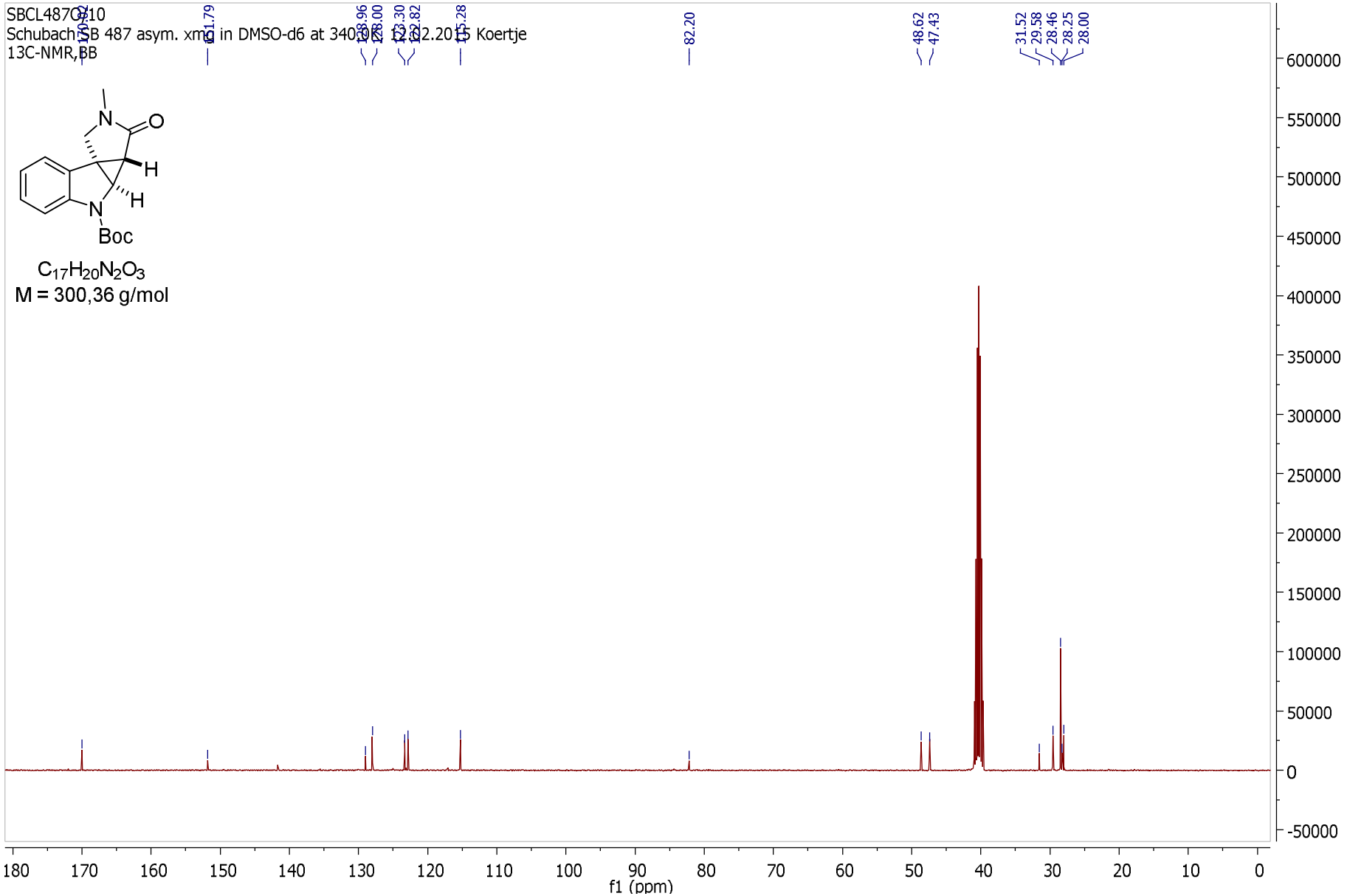

SBHA267/3/4
Schubach SB 267 20mg in DMSO-d6 at 380.0K, 20.01.2015 Koertje
1H-1d vor 13C-NMR,BB + HSQC
!Achtung 2.-NMR-Roehrchen, Substanz frisch geloest!
Br
O
N
N
Boc
C17H21BrN2O3
M = 381,27 g/mol
4.68
4.67
4.17
2.88
1.69
1.67
1.00
2.04
1.16
1.16
1.73
1.60
2.51
9.80
f1 (ppm)


SBCL466J/103
267
166.61
149.60
135.64
129.28
124.95
124.81
122.90
119.80
118.58
115.87
115.75
115.18
83.93
42.37
34.99
28.21
26.53
O
Br
N
N
Boc
C17H21BrN2O3
M = 381,27 g/mol
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
.80
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


SBHA475J/10
269 nach Saeule
8.15
8.13
7.67
7.66
7.65
7.64
7.64
7.63
7.63
7.53
7.38
7.38
7.36
7.36
7.35
7.34
7.34
7.29
7.29
7.28
7.27
7.27
7.26
7.25
7.25
7.22
4.75
4.71
4.70
2.89
2.84
2.43
2.07
1.70
O
N2
N
N
Boc
C17H20N4O3
M = 328,37 g/mol
0.95
1.17
0.98
1.13
1.77
2.00
2.89
9.69
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

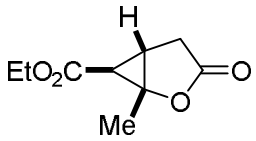

SBCL475J/10
269 nach Saeure
165.88
149.60
144.66
135.69
129.53
128.37
124.79
122.89
115.25
60.40
46.57
40.85
33.70
28.22
23.84
21.05
20.79
17.49
17.30
14.65
14.20
O
N2
N
N
Boc
C17H20N4O3
M = 328,37 g/mol
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


SBHA487O/5
Schubach SB 487 asym. xmg in DMSO-d6 at 330.0K, 11.02.2015 Koertje
1H-1d
7.65 7.63 7.49 7.49 7.47 7.47 7.27 7.26 7.25 7.24 7.23 7.22 7.07 7.07 7.06 7.05 7.04 7.04
4.23 4.20 4.19
3.65 3.65 3.62 3.62
3.19
2.77
1.65 1.57 1.51 1.51 1.51
N
O
H
H
N
Boc
C17H20N2O3
M = 300,36 g/mol
1.22 1.02 1.18 1.00
1.99
1.03
3.00
9.20 1.01
f1 (ppm)

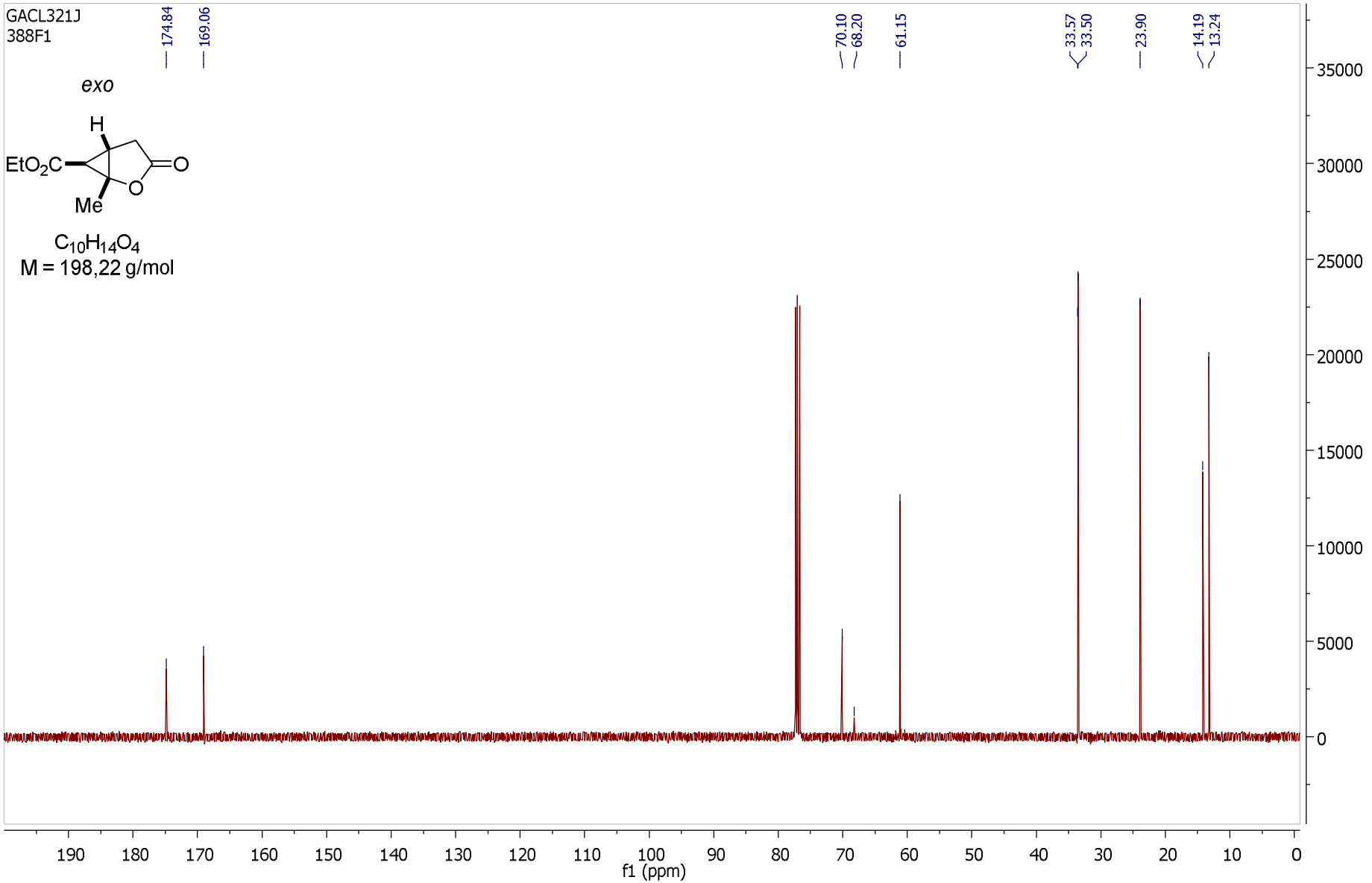

SBCL487G10
Schubach, SB 487 asym. xmod in DMSO-d6 at 340.0K, 12.02.2015 Koertje
13C-NMR, BB
170.92
161.79
128.96
128.00
123.30
122.82
115.28
82.20
48.62
47.43
31.52
29.58
28.46
28.25
28.00
O
N
H
H
N
Boc
C17H20N2O3
M = 300,36 g/mol
600000
550000
500000
450000
400000
350000
300000
250000
200000
150000
100000
50000
0
-50000
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

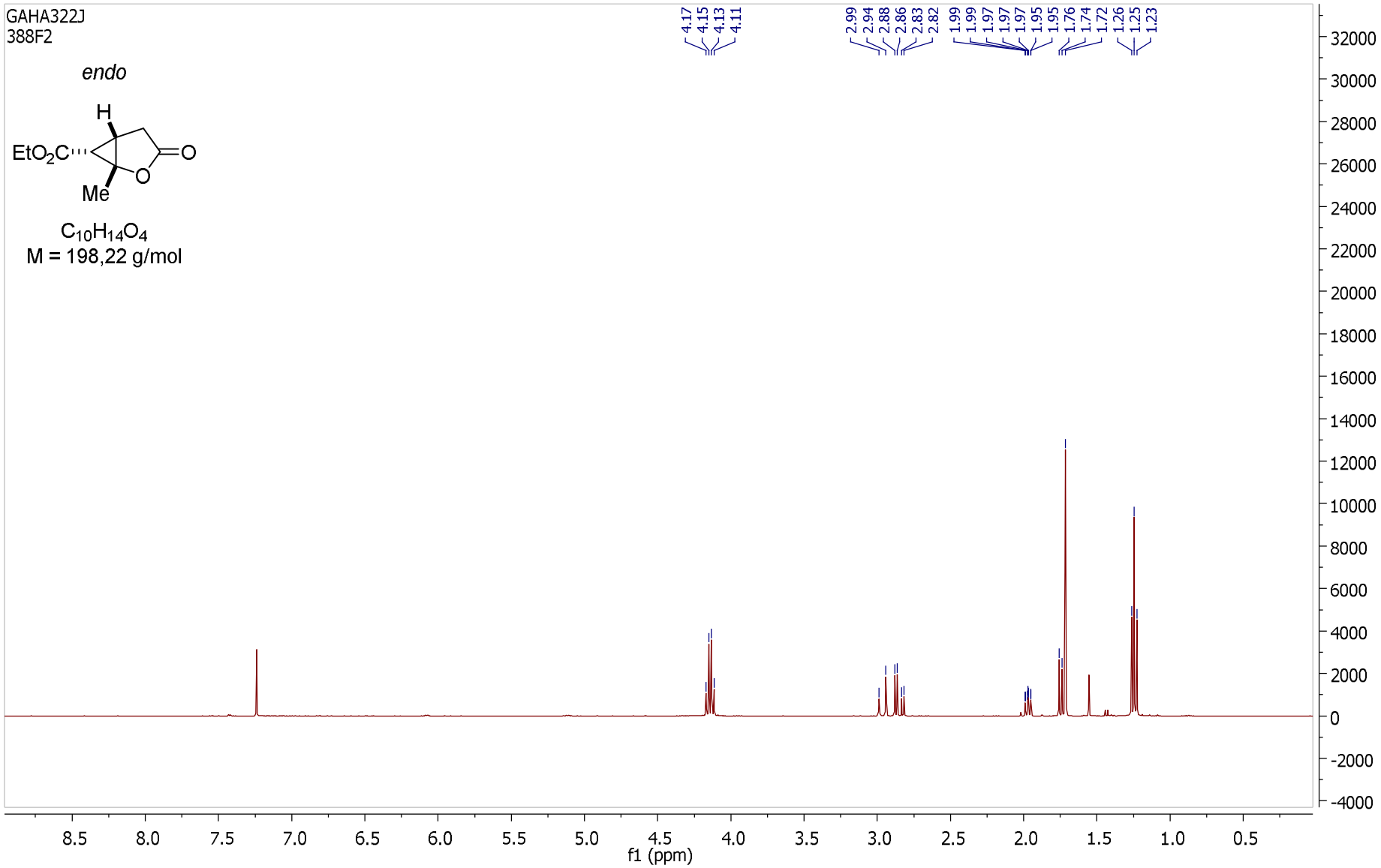
GAHA321J/10
388F1

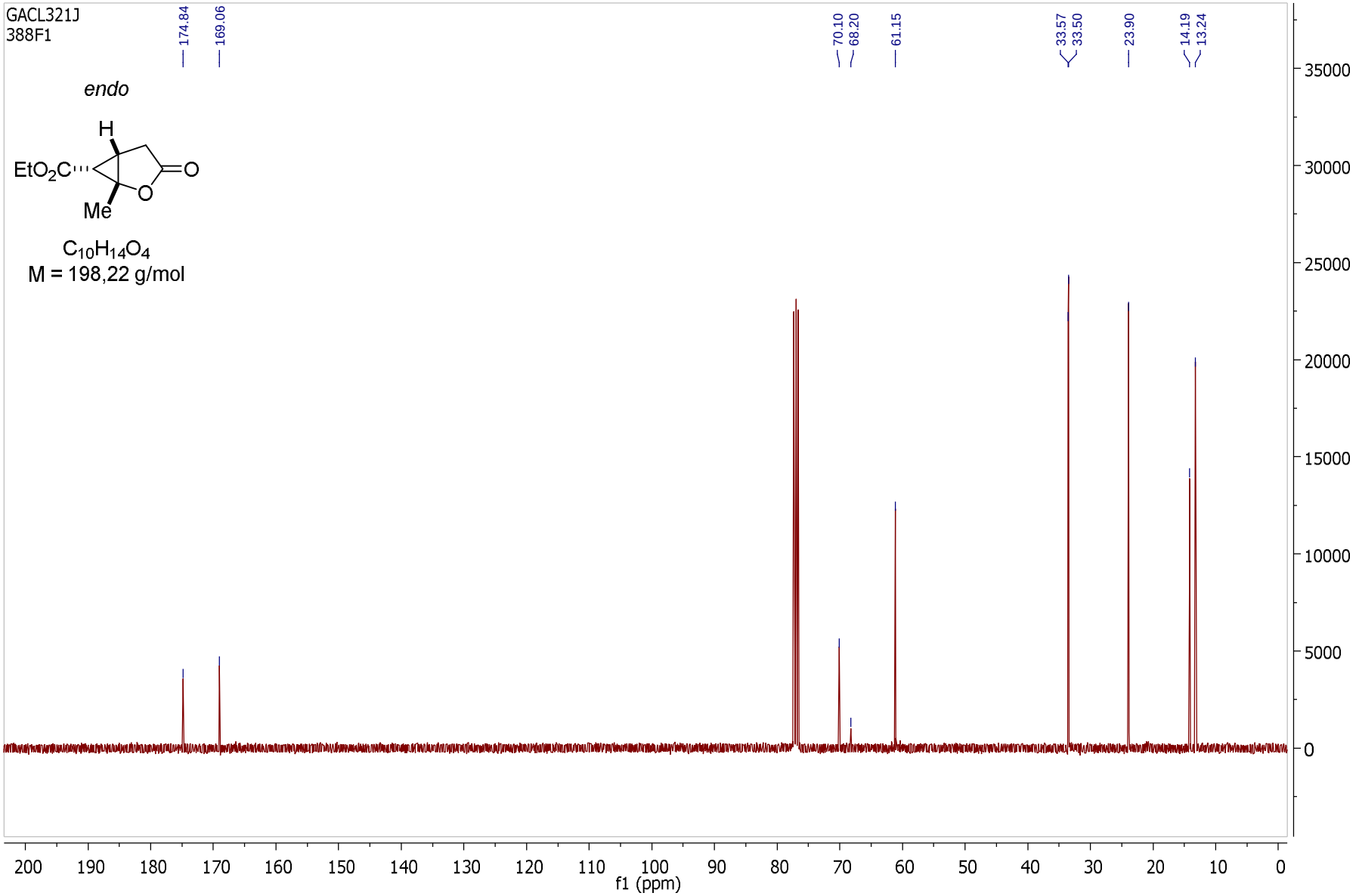
exo

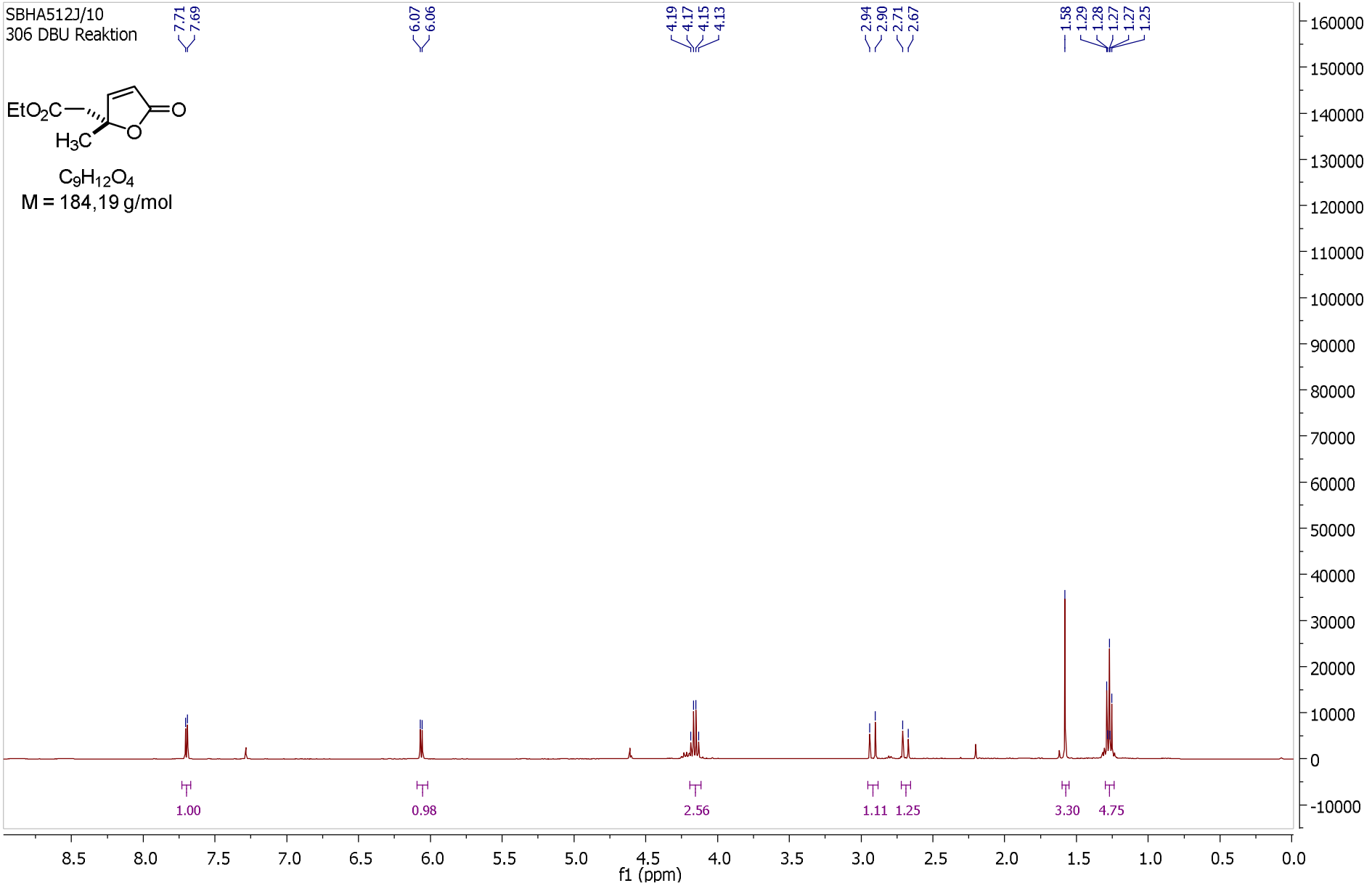


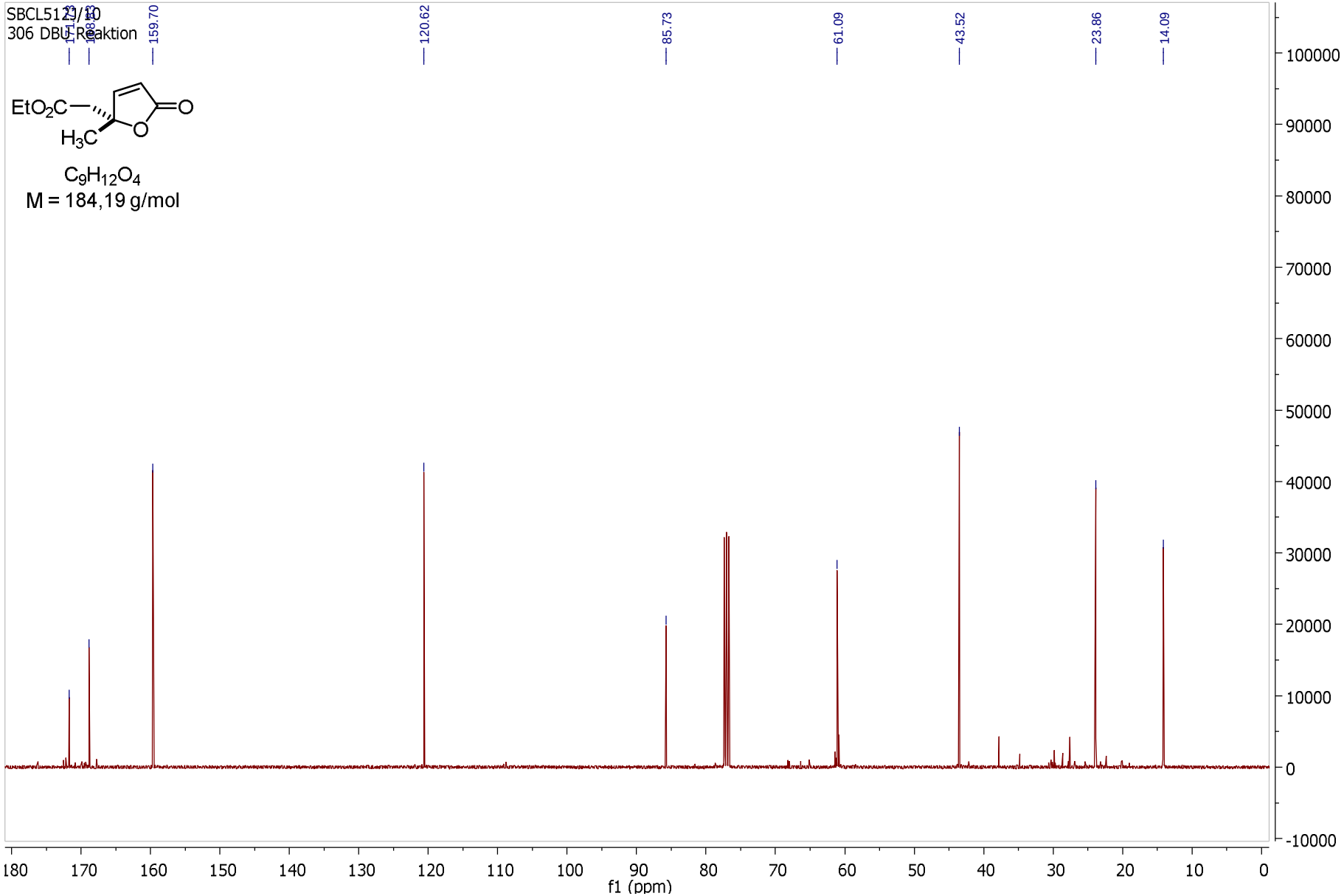
$C_{10}H_{14}O_4$
M = 198,22 g/mol

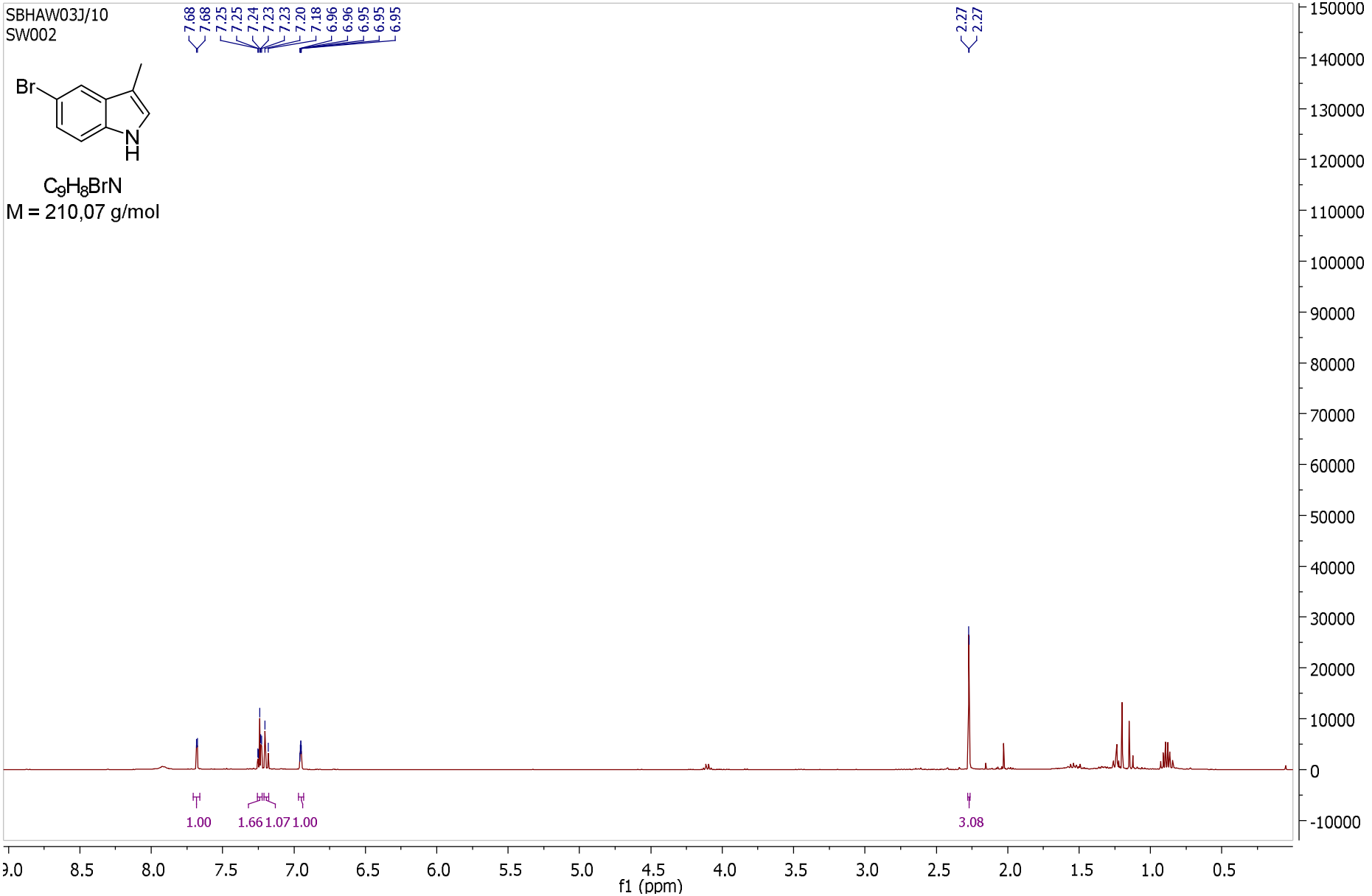

GACL321J
388F1
174.84
169.06
70.10
68.20
61.15
33.57
33.50
23.90
14.19
13.24
exo
H
EtO2C
O
O
Me
C10H14O4
M = 198,22 g/mol
35000
30000
25000
20000
15000
10000
5000
0
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

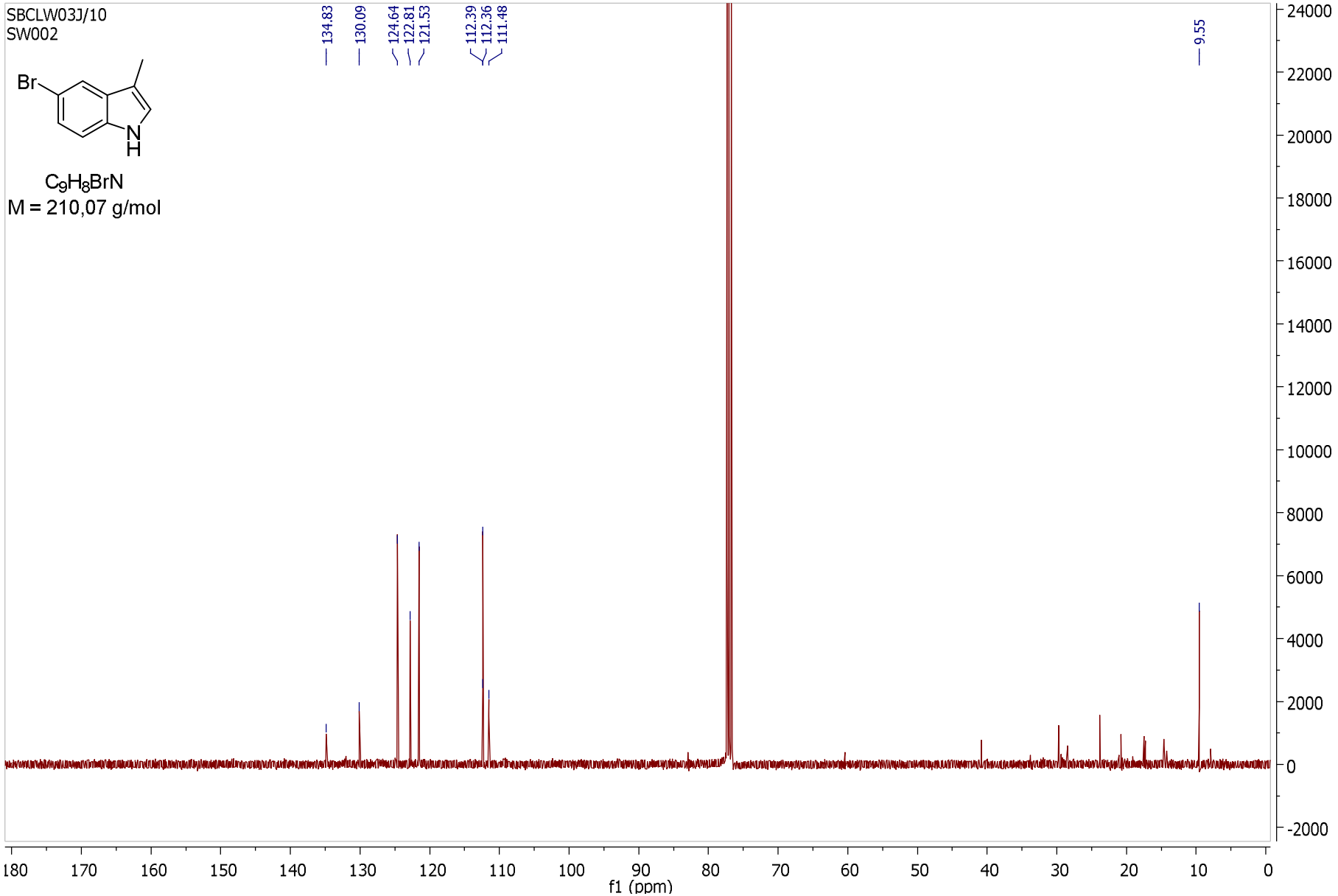

GAHA322J
388F2
endo
H
EtO2C
O
O
Me
C10H14O4
M = 198,22 g/mol
4.17
4.15
4.13
4.11
2.99
2.94
2.88
2.86
2.83
2.82
1.99
1.99
1.97
1.97
1.97
1.95
1.95
1.76
1.74
1.72
1.26
1.25
1.23
32000
30000
28000
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
-4000
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

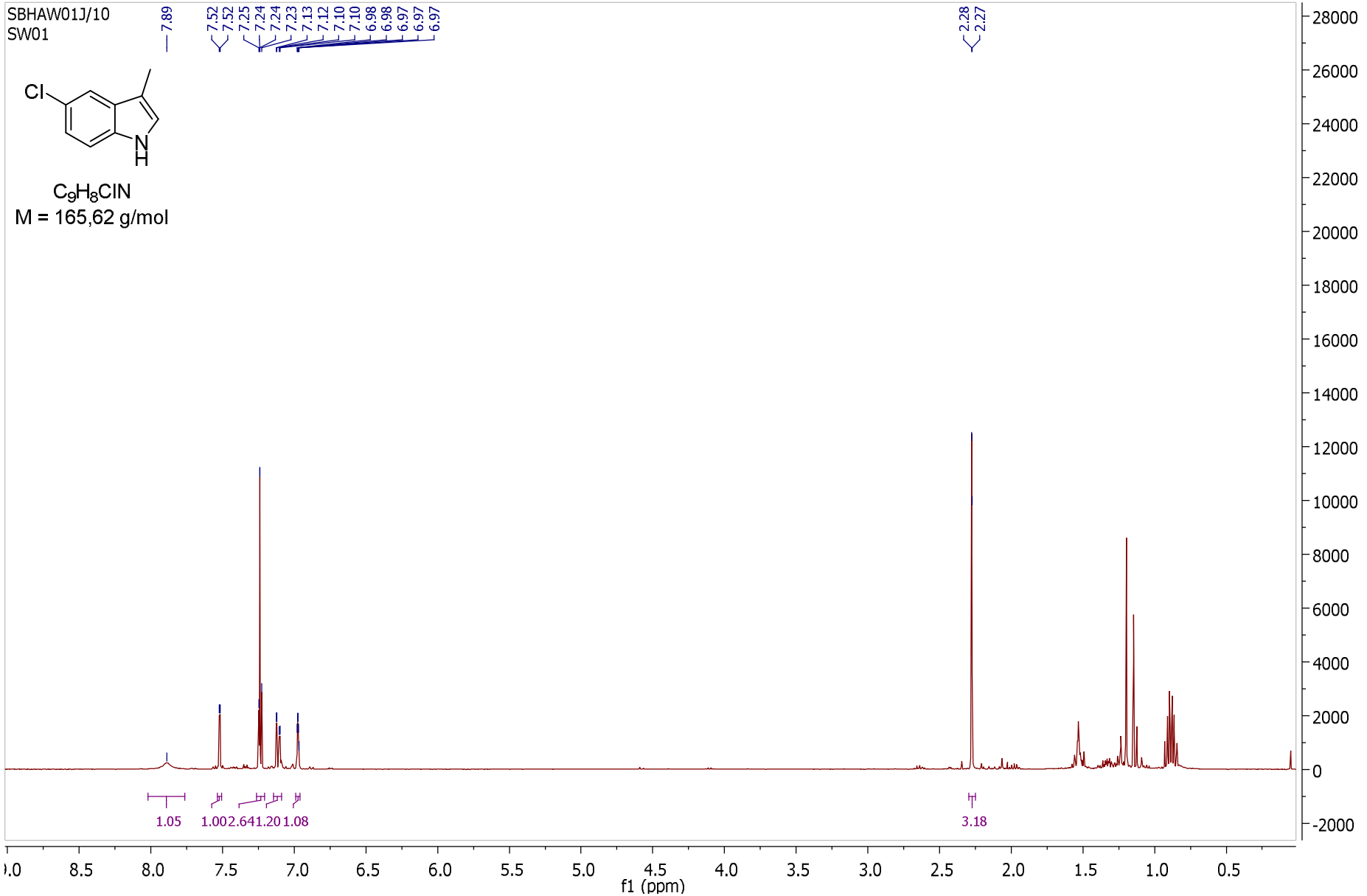

GACL321J
388F1
174.84
169.06
70.10
68.20
61.15
33.57
33.50
23.90
14.19
13.24
endo
H
EtO2C
O
O
Me
C10H14O4
M = 198,22 g/mol
35000
30000
25000
20000
15000
10000
5000
0
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

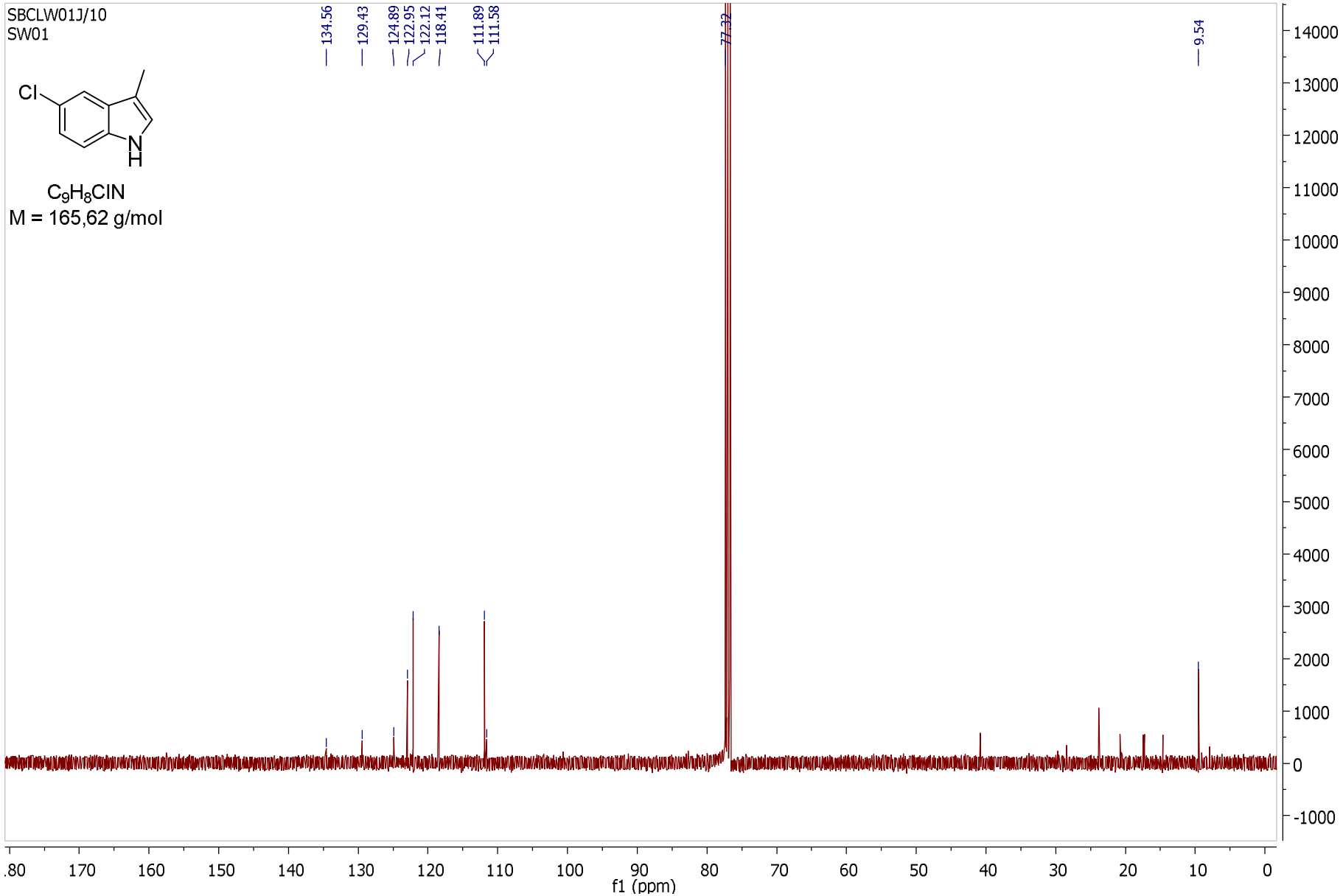

SBHA512J/10
306 DBU Reaktion
7.71
7.69
6.07
6.06
4.19
4.17
4.15
4.13
2.94
2.90
2.71
2.67
1.58
1.29
1.28
1.27
1.27
1.25
EtO2C
H3C
O
C9H12O4
M = 184,19 g/mol
1.00
0.98
2.56
1.11
1.25
3.30
4.75
f1 (ppm)

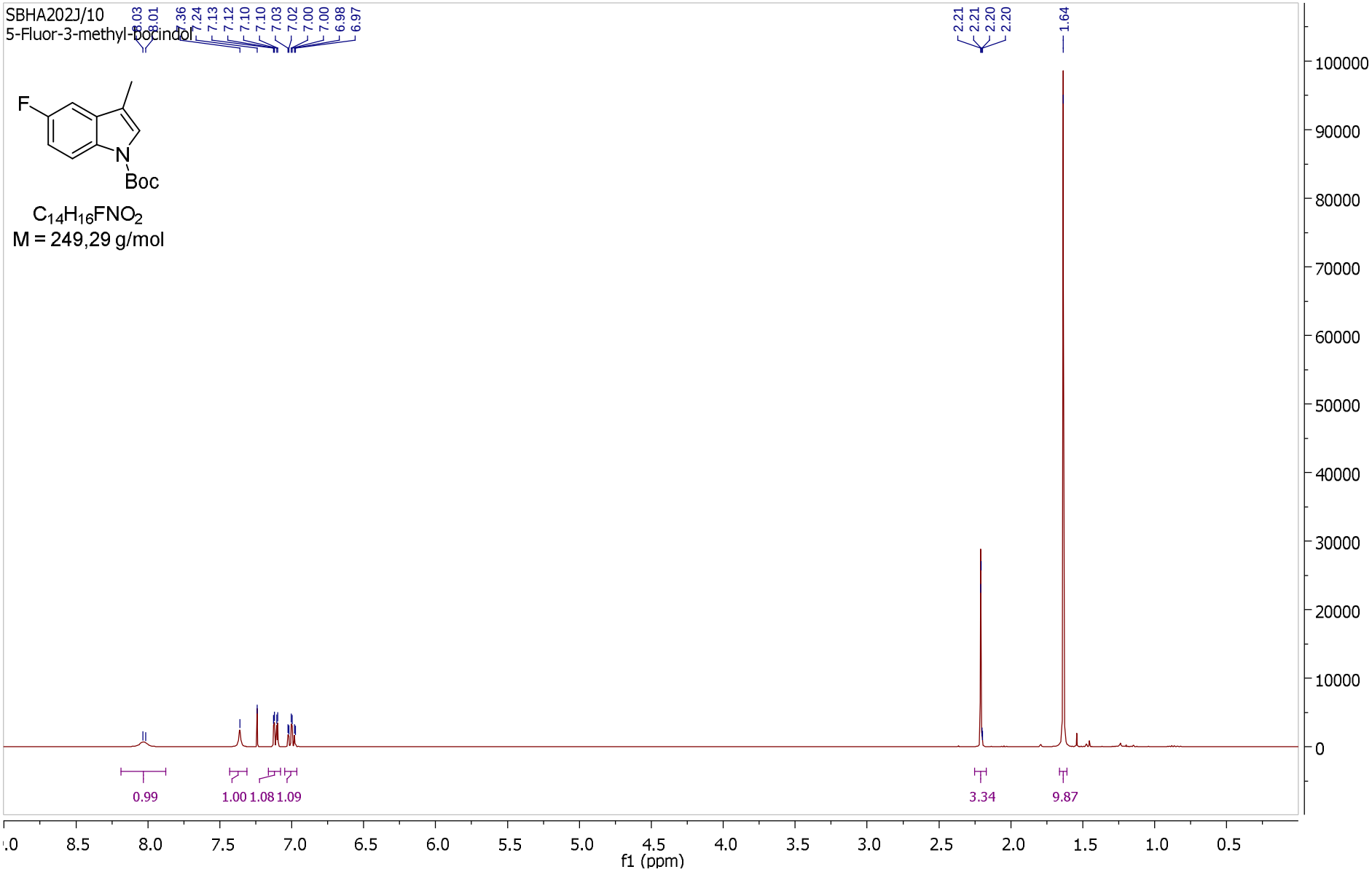

SBCL512/10
306 DBU Reaktion
169.70
120.62
85.73
61.09
43.52
23.86
14.09
EtO2C
H3C
O
C9H12O4
M = 184,19 g/mol
100000
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
-10000
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

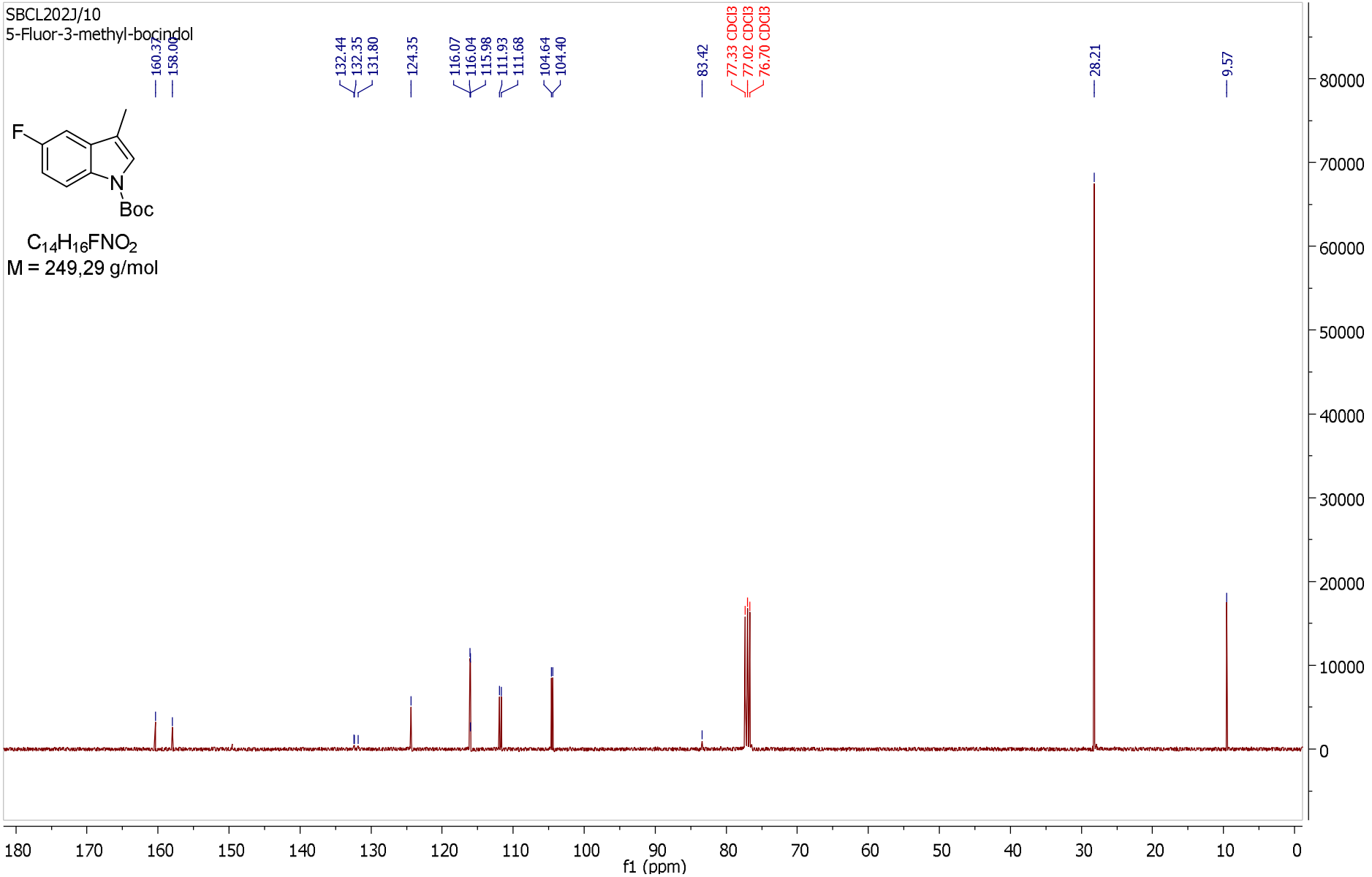

SBHAW03J/10
SW002
7.68
7.68
7.25
7.25
7.24
7.23
7.23
7.20
7.18
6.96
6.96
6.95
6.95
6.95
2.27
2.27
Br
N
H
C9H8BrN
M = 210,07 g/mol
1.00
1.66
1.07
1.00
3.08
150000
140000
130000
120000
110000
100000
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
-10000
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

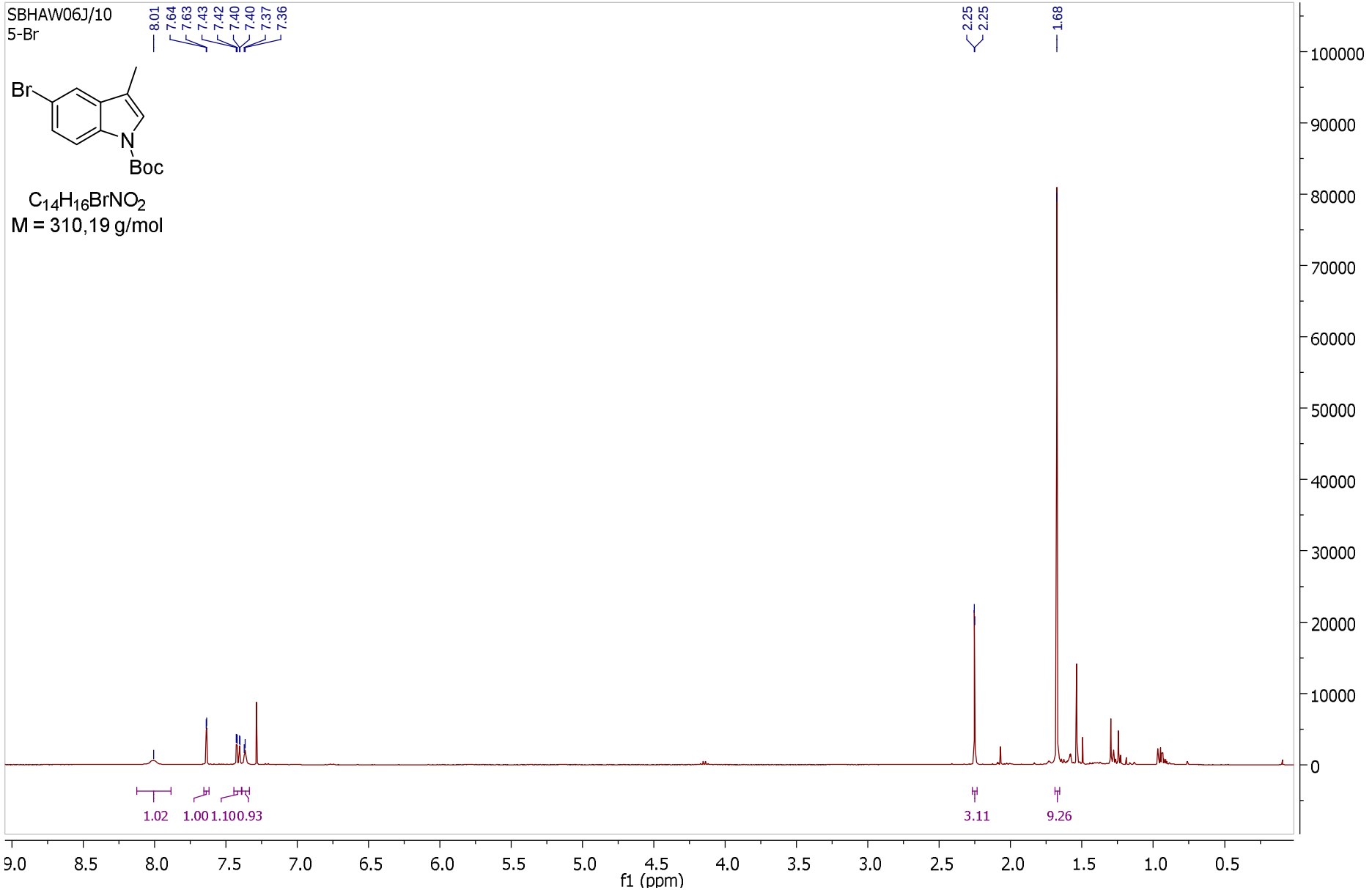

SBCLW03J/10
SW002
Br
N
H
C9H8BrN
M = 210,07 g/mol
134.83
130.09
124.64
122.81
121.53
112.39
112.36
111.48
9.55
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

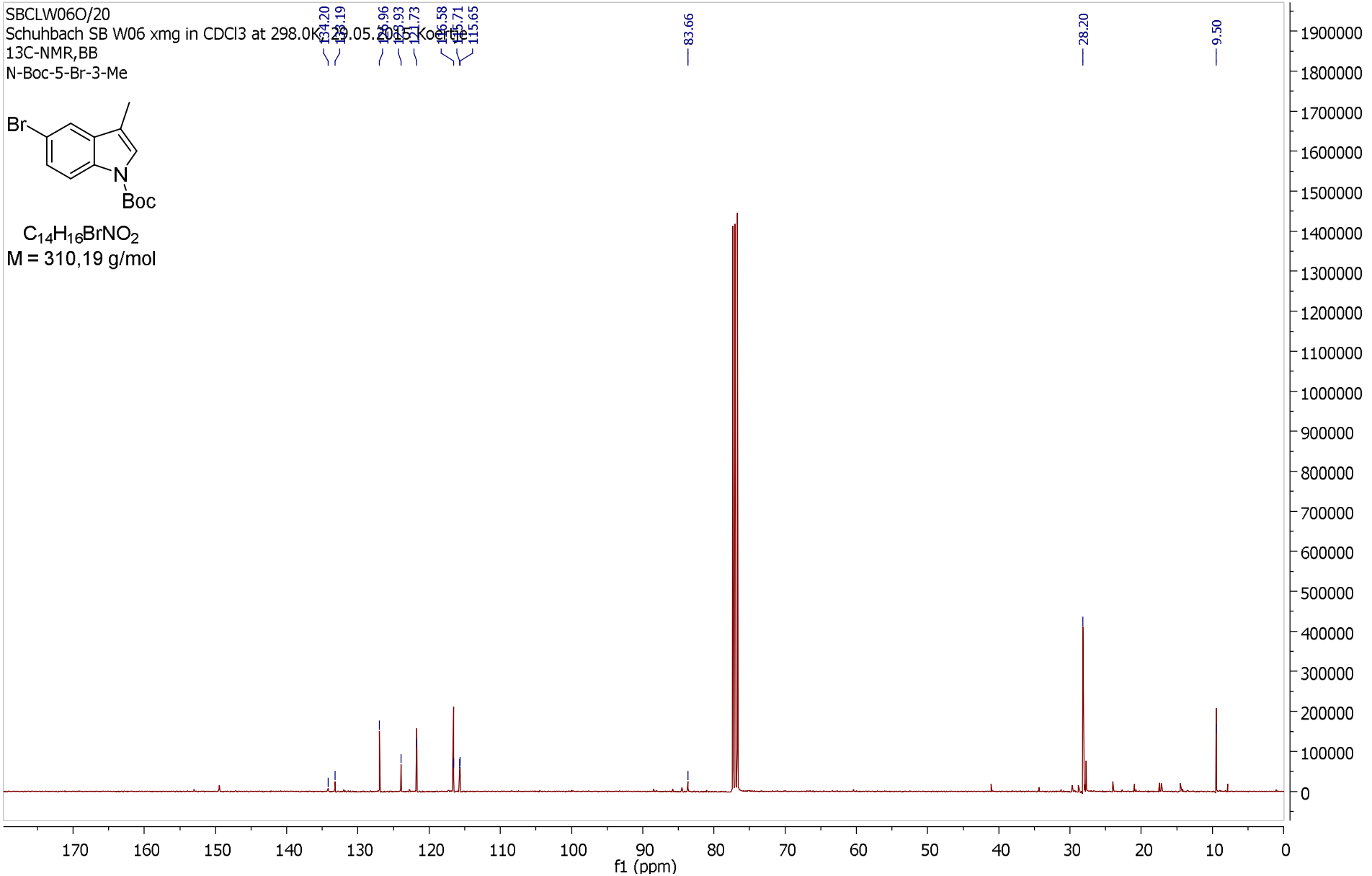

SBHAW01J/10
SW01
7.89
7.52
7.52
7.25
7.24
7.24
7.23
7.13
7.12
7.10
7.10
6.98
6.98
6.97
6.97
6.97
2.28
2.27
Cl
N
H
C9H8ClN
M = 165,62 g/mol
1.05
1.00
2.64
1.20
1.08
3.18
28000
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

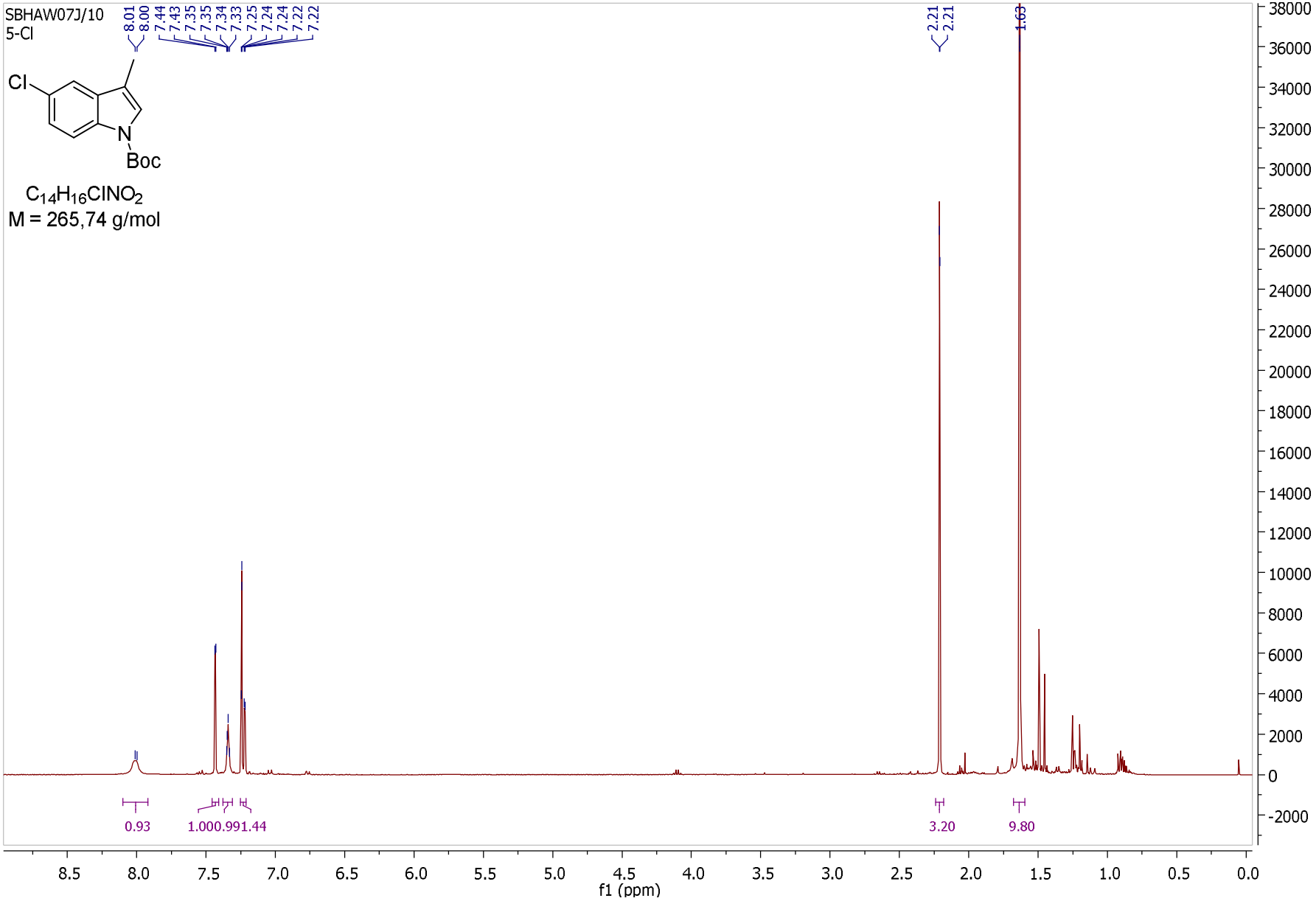

SBCLW01J/10
SW01
Cl
N
H
C9H8ClN
M = 165,62 g/mol
134.56
129.43
124.89
122.95
122.12
118.41
111.89
111.58
77.32
9.54
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
.80
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

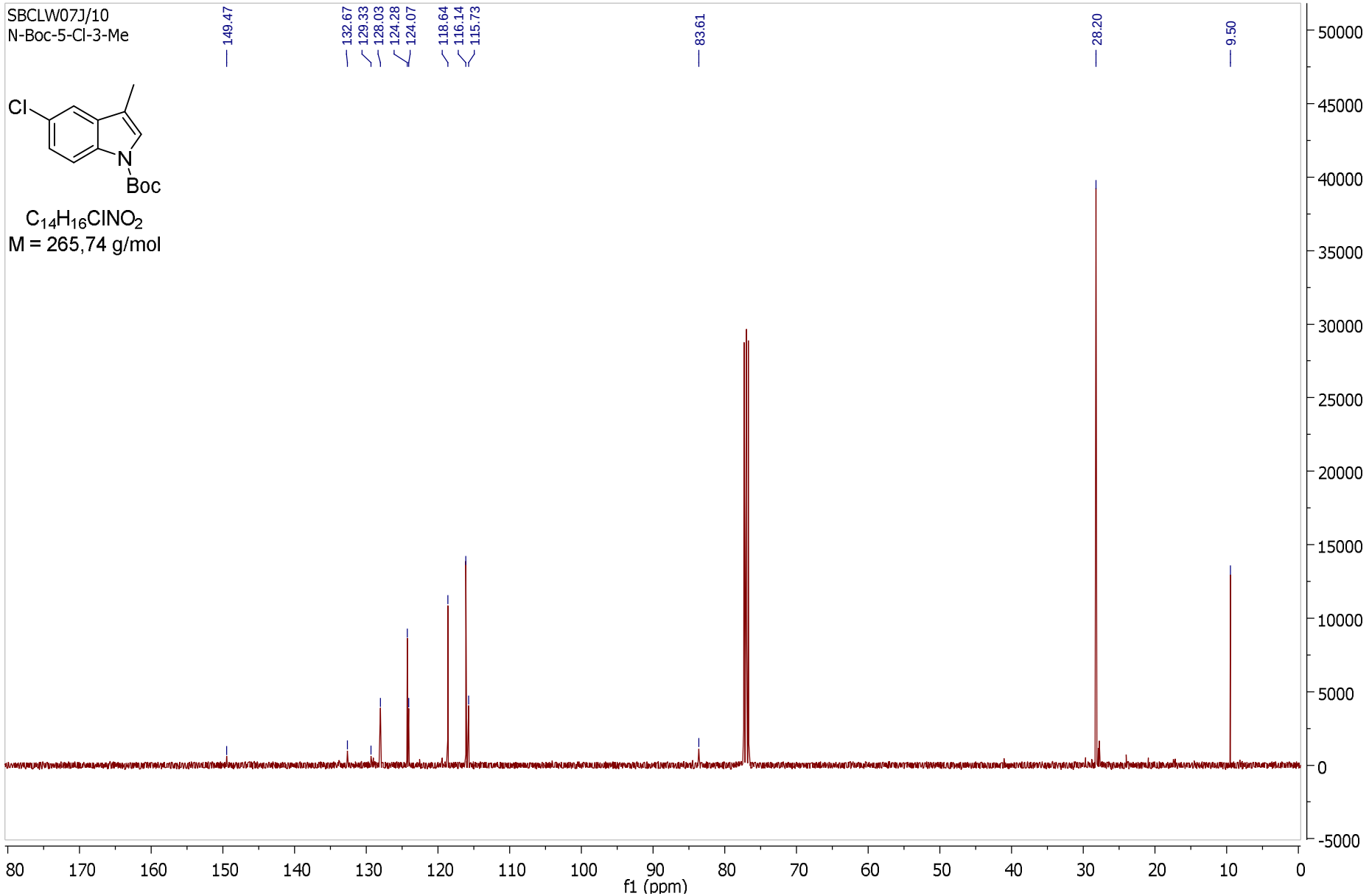

SBHA202J/10
5-Fluor-3-methyl-bocindol
8.03
8.01
7.36
7.24
7.13
7.12
7.10
7.10
7.03
7.02
7.00
7.00
6.98
6.97
2.21
2.21
2.20
2.20
1.64
F
N
Boc
C14H16FNO2
M = 249,29 g/mol
100000
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
0.99
1.00
1.08
1.09
3.34
9.87
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

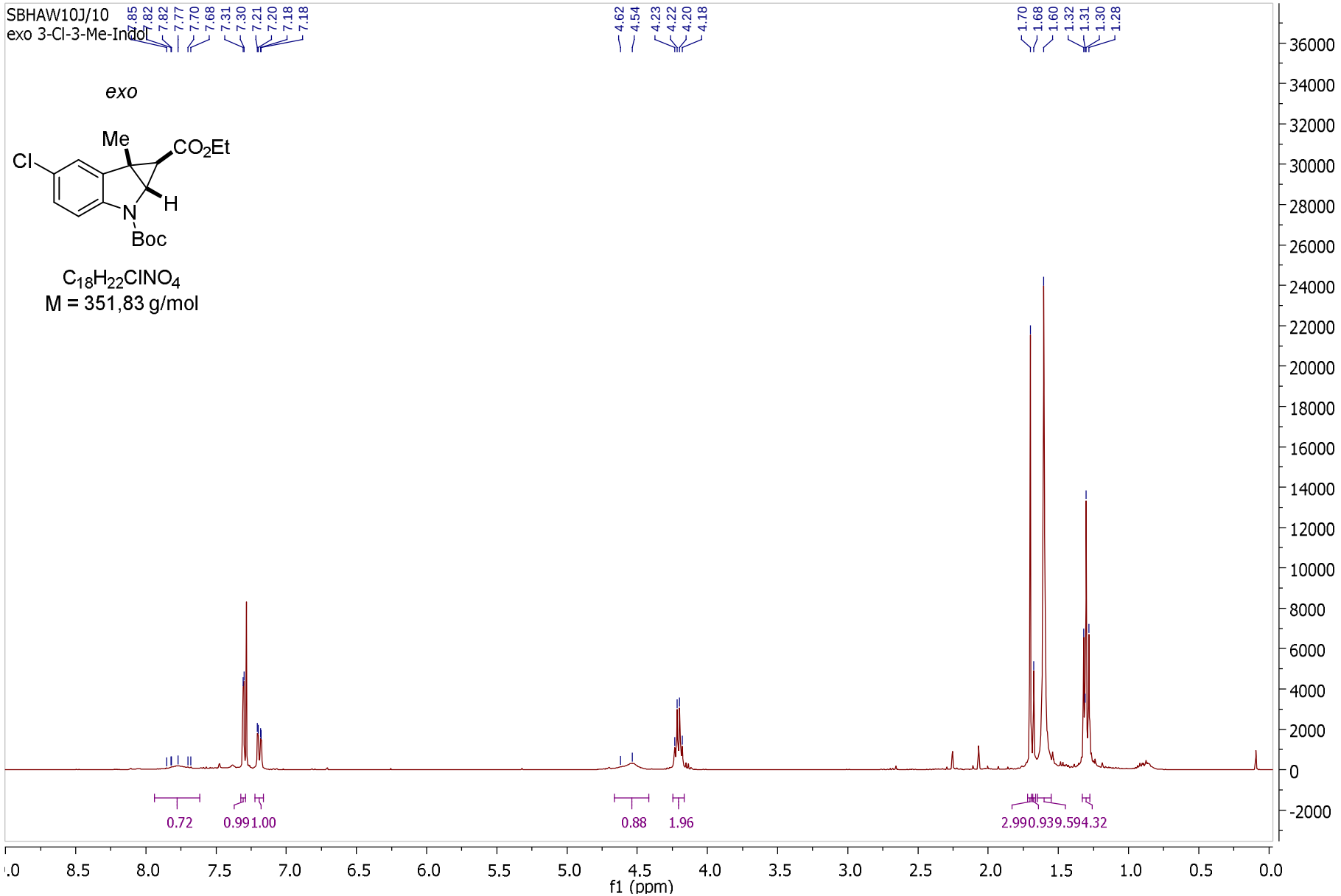

SBCL202J/10
5-Fluor-3-methyl-bocindol
160.32
158.06
132.44
132.35
131.80
124.35
116.07
116.04
115.98
111.93
111.68
104.64
104.40
83.42
77.33 CDCl3
77.02 CDCl3
76.70 CDCl3
28.21
9.57
F
N
Boc
C14H16FNO2
M = 249,29 g/mol
80000
70000
60000
50000
40000
30000
20000
10000
0
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

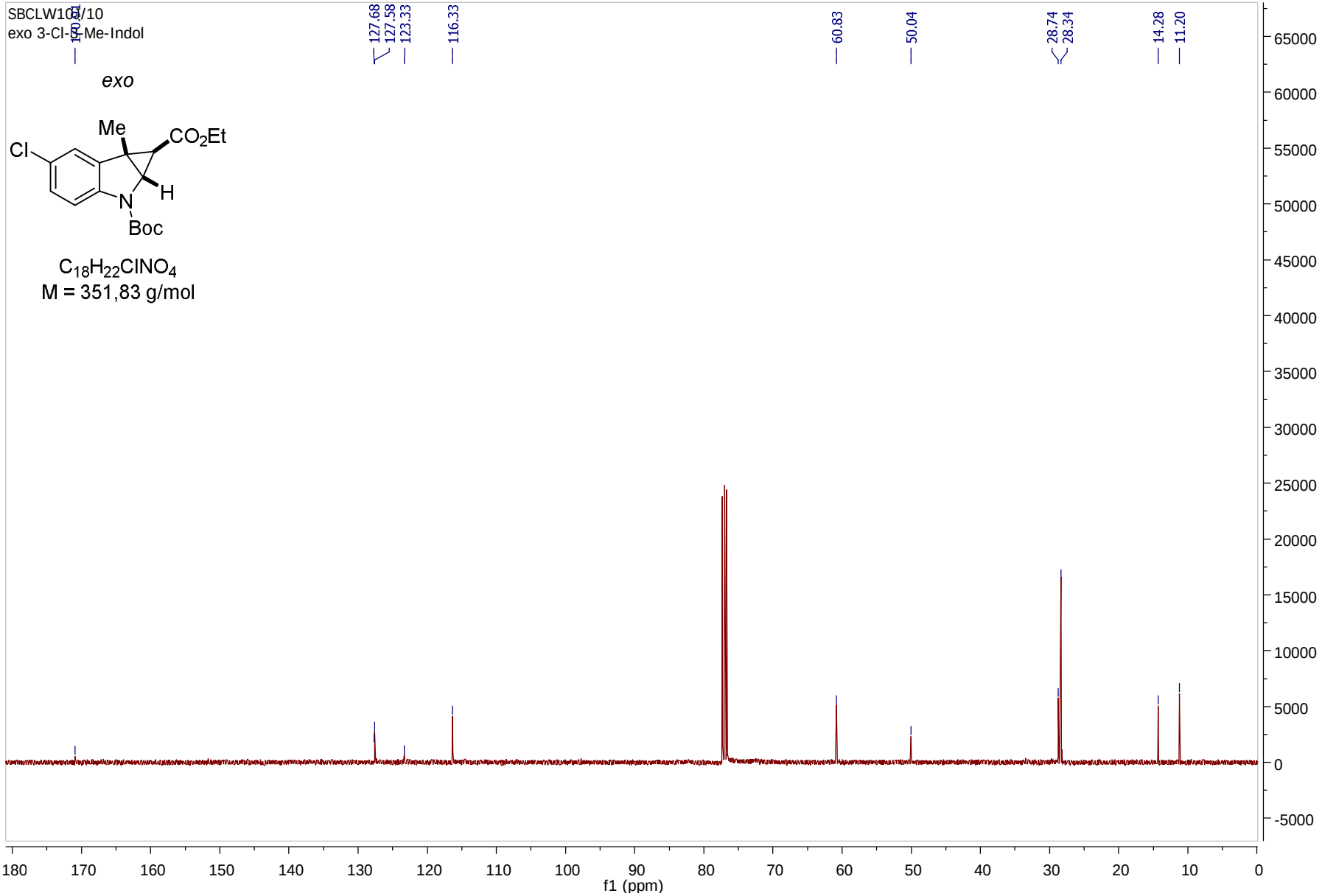

SBHAW06J/10
5-Br
8.01
7.64
7.63
7.43
7.42
7.40
7.40
7.37
7.36
2.25
2.25
1.68
Br
N
Boc
C14H16BrNO2
M = 310,19 g/mol
1.02
1.00
1.10
0.93
3.11
9.26
f1 (ppm)

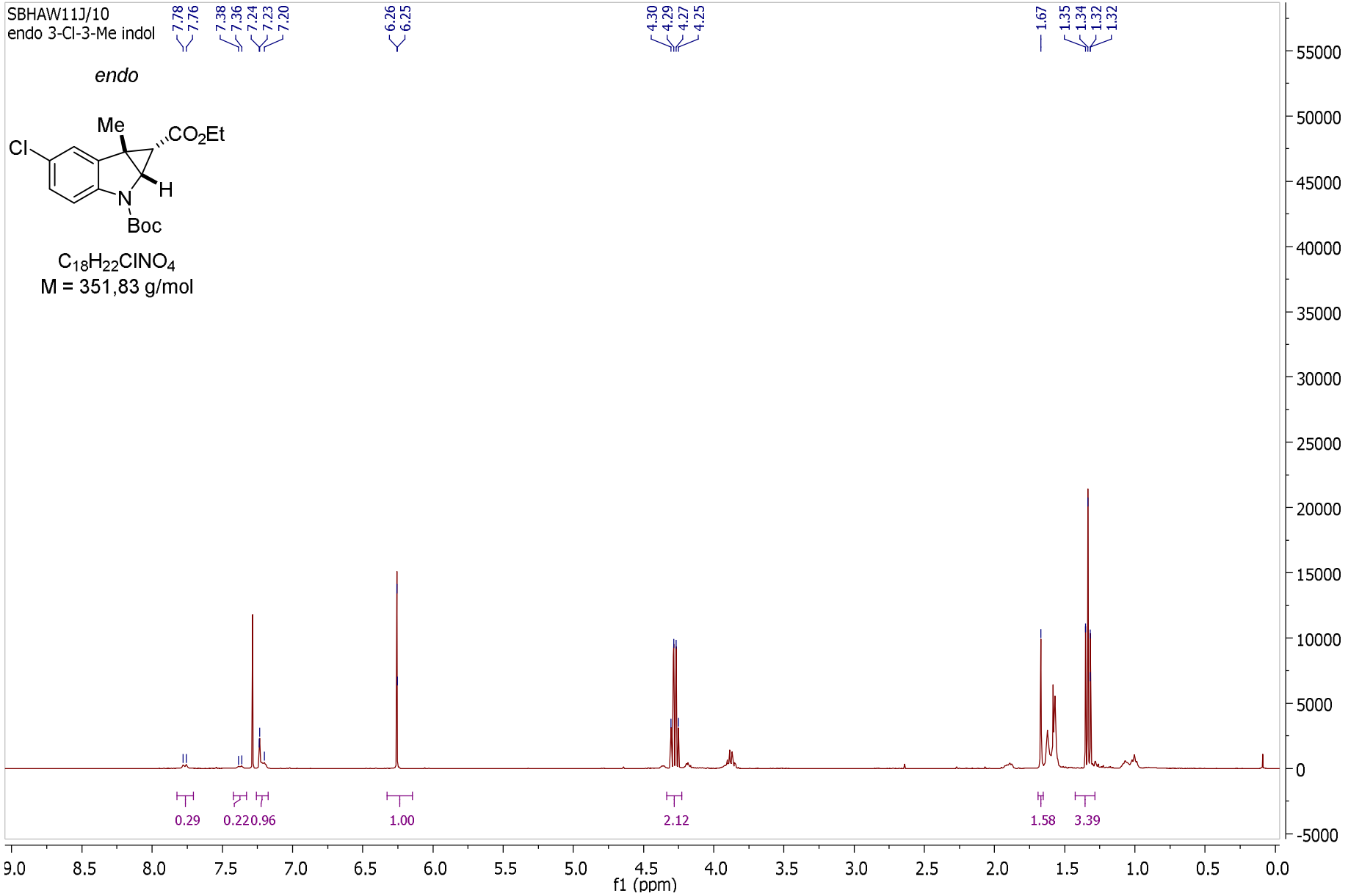

SBCLW06O/20
Schuhbach SB W06 xmg in CDCl3 at 298.0K 29.05.2015 Koertje
13C-NMR,BB
N-Boc-5-Br-3-Me
Br
N
Boc
C14H16BrNO2
M = 310,19 g/mol
134.20
128.19
126.96
123.93
121.73
116.58
115.71
115.65
83.66
28.20
9.50
f1 (ppm)

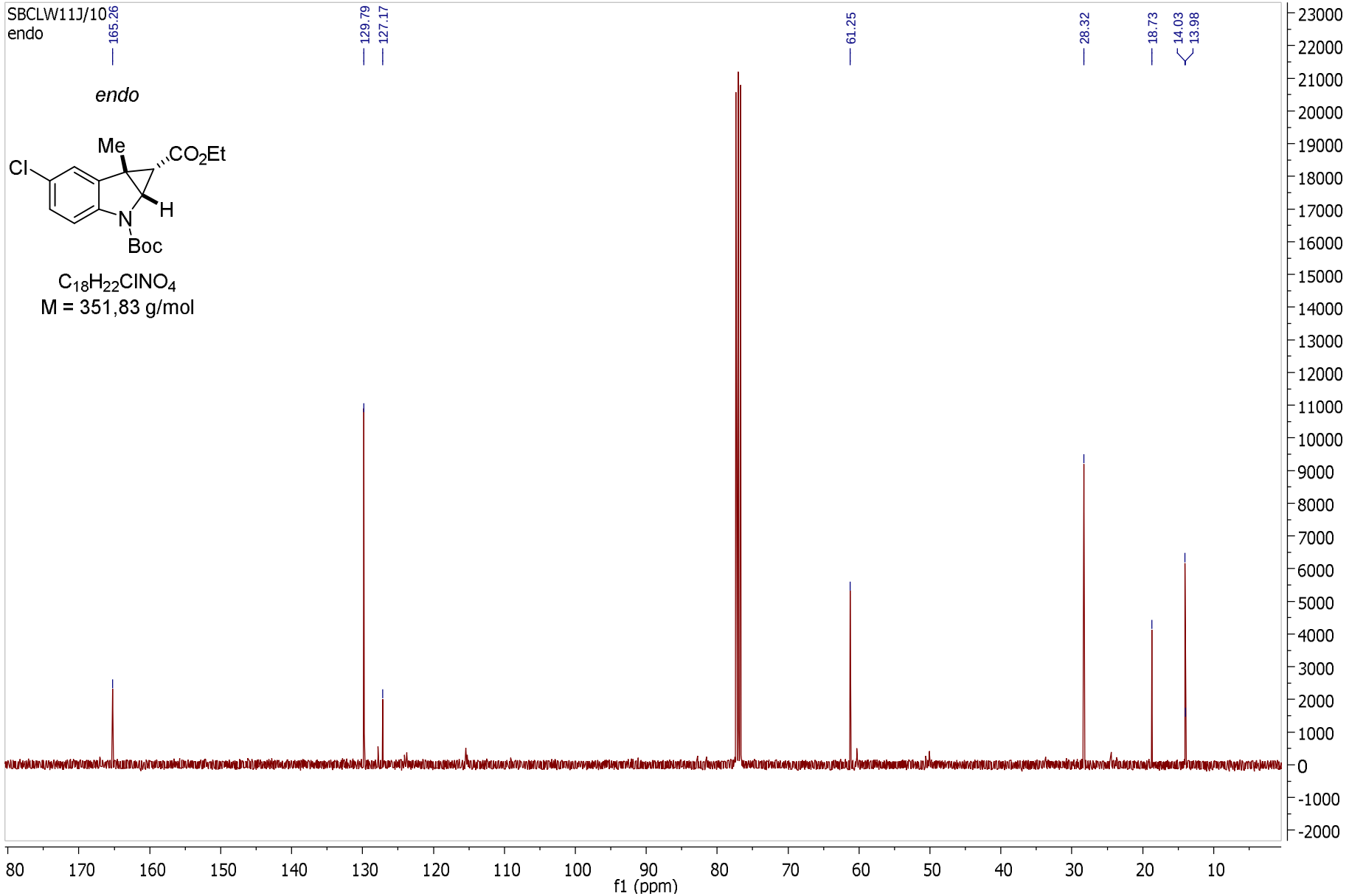

SBHAW07J/10
5-Cl
Cl
N
Boc
C14H16ClNO2
M = 265,74 g/mol
8.01
8.00
7.44
7.43
7.35
7.35
7.34
7.33
7.25
7.24
7.24
7.22
7.22
2.21
2.21
1.63
0.93
1.000.991.44
3.20
9.80
f1 (ppm)


SBCLW07J/10
N-Boc-5-Cl-3-Me
149.47
132.67
129.33
128.03
124.28
124.07
118.64
116.14
115.73
83.61
28.20
9.50
Cl
N
Boc
C14H16ClNO2
M = 265,74 g/mol
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
80
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


SBHAW10J/10
exo 3-Cl-3-Me-Indol
7.85
7.82
7.82
7.77
7.70
7.68
7.31
7.30
7.21
7.20
7.18
7.18
4.62
4.54
4.23
4.22
4.20
4.18
1.70
1.68
1.60
1.32
1.31
1.30
1.28
exo
Me
CO2Et
Cl
H
N
Boc
C18H22ClNO4
M = 351,83 g/mol
0.72
0.99
1.00
0.88
1.96
2.99
0.93
9.59
4.32
f1 (ppm)


SBCLW10/10
exo 3-Cl-5-Me-Indol
170.01
127.68
127.58
123.33
116.33
60.83
50.04
28.74
28.34
14.28
11.20
exo
Me
CO2Et
Cl
H
N
Boc
C18H22ClNO4
M = 351,83 g/mol
65000
60000
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


SBHAW11J/10
endo 3-Cl-3-Me indol
7.78
7.76
7.38
7.36
7.24
7.23
7.20
6.26
6.25
4.30
4.29
4.27
4.25
1.67
1.35
1.34
1.32
1.32
endo
Me
CO2Et
Cl
H
N
Boc
C18H22ClNO4
M = 351,83 g/mol
0.29
0.22
0.96
1.00
2.12
1.58
3.39
f1 (ppm)


SBCLW11J/10
endo
165.26
129.79
127.17
61.25
28.32
18.73
14.03
13.98
endo
Me
CO2Et
Cl
H
N
Boc
C18H22ClNO4
M = 351,83 g/mol
23000
22000
21000
20000
19000
18000
17000
16000
15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
-2000
80
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)