Ruthenium Olefin Metathesis Catalysts Containing Six Membered Sulfone and Sulfoamide Chelating Rings

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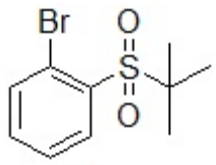
^{1}H and ^{13}C NMR SPECTRA
(LIGANDS and INITIATORS Xa, XIa, XIIa-c, XIIIa)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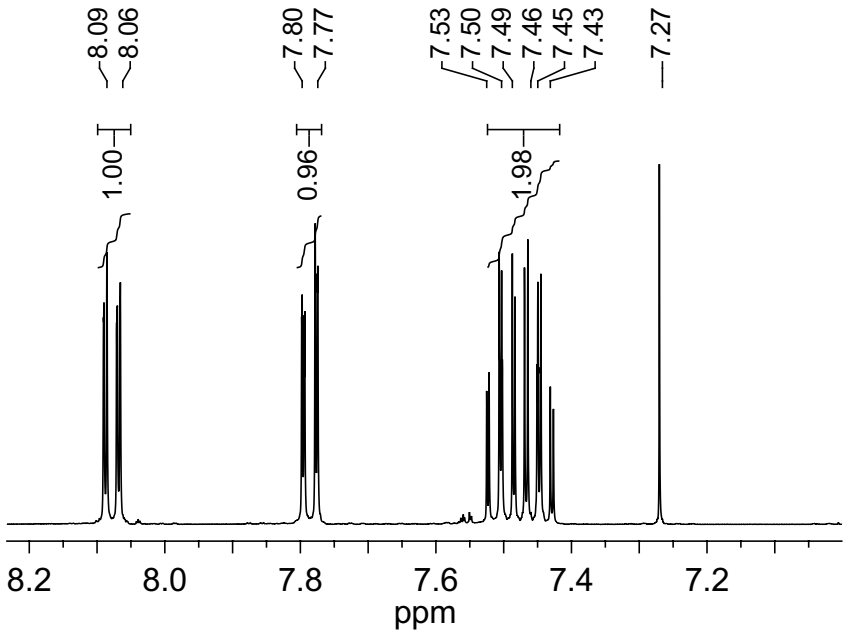
S
O
O

3a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7.45
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0.96
1.98
8.2
8.0
7.8
7.6
7.4
7.2
ppm

9.00
1.42
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7.5
7.0
6.5
6.0
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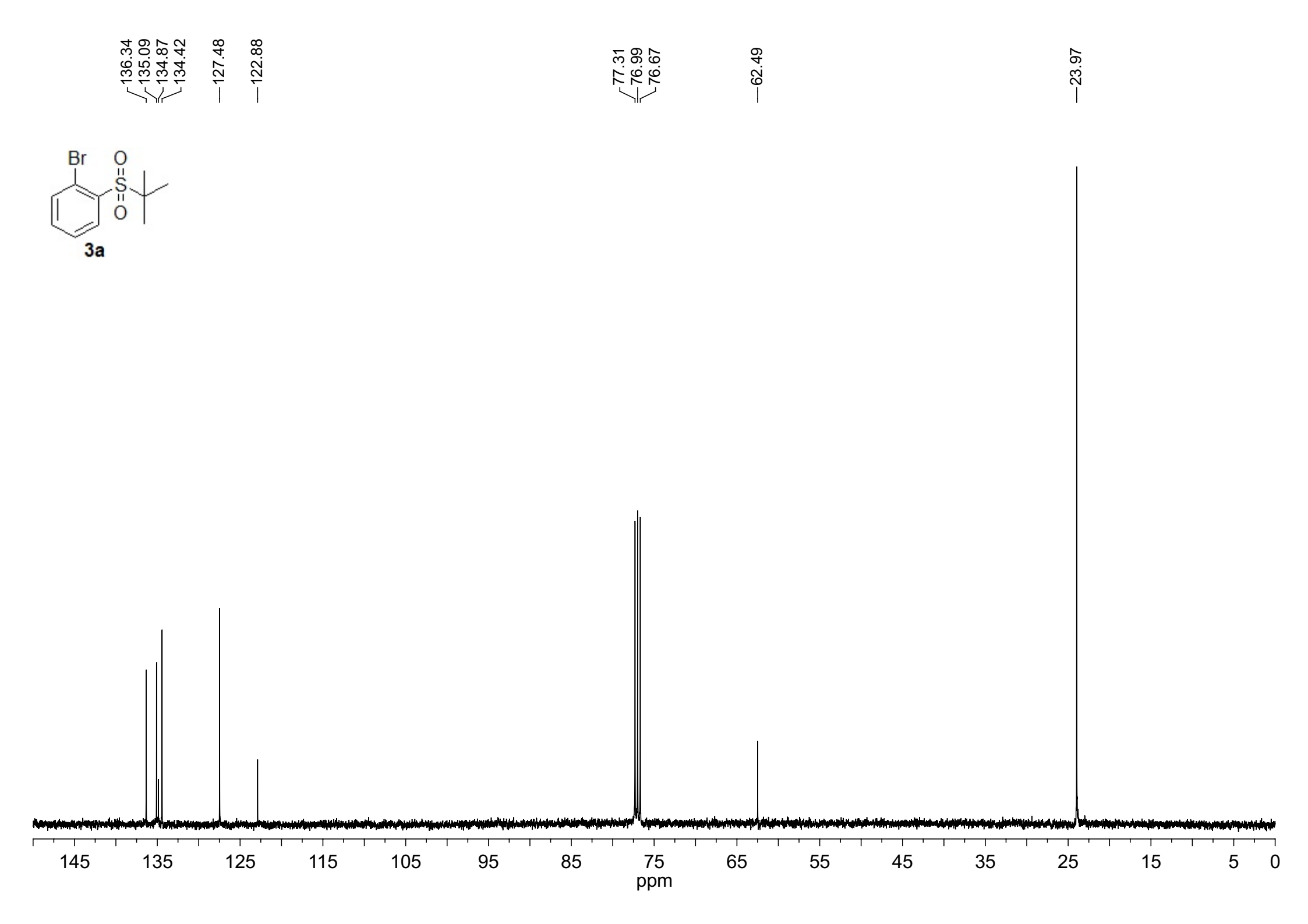
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76.99
76.67
62.49
23.97
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O
S
O
3a
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125
115
105
95
85
75
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55
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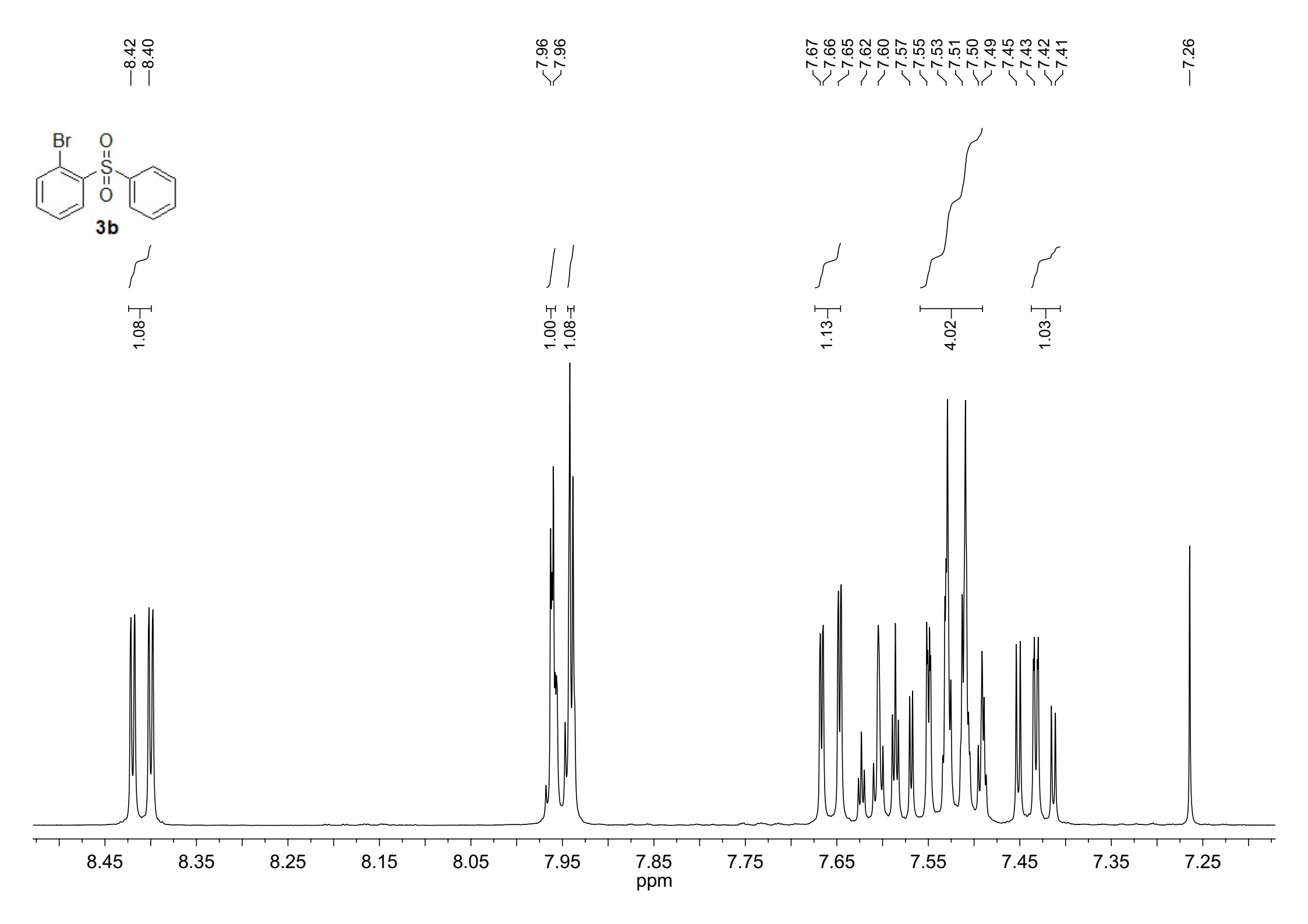
25
15
5
0
ppm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7.65
7.62
7.60
7.57
7.55
7.53
7.51
7.50
7.49
7.45
7.43
7.42
7.41
7.26
Br
O
S
O
3b
1.08
1.00
1.08
1.13
4.02
1.03
8.45
8.35
8.25
8.15
8.05
7.95
7.85
7.75
7.65
7.55
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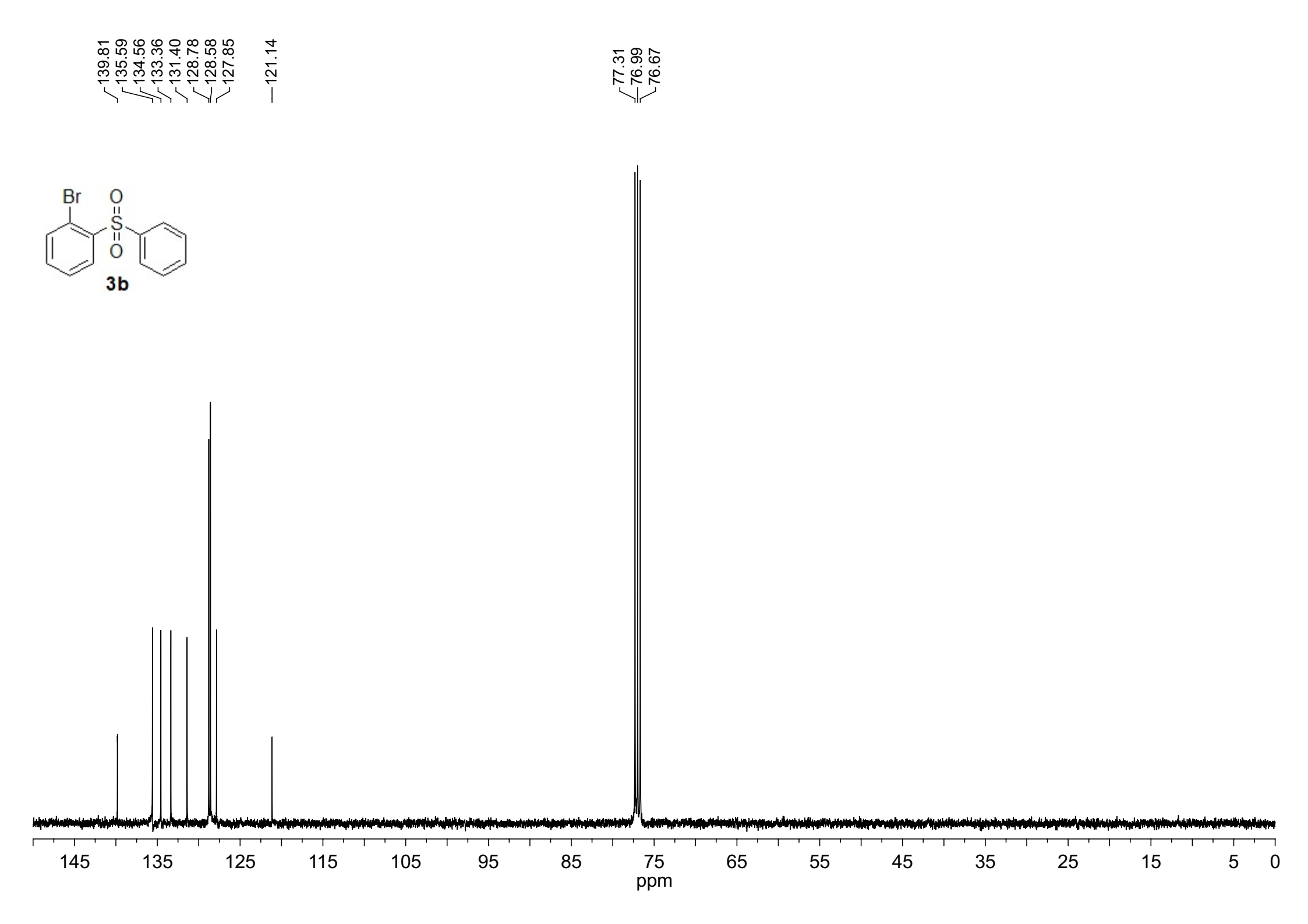
7.35
7.25
ppm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128.78
128.58
127.85
121.14
77.31
76.99
76.67
Br
O
S
O
O
3b
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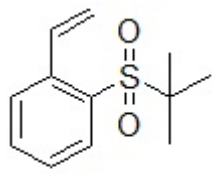
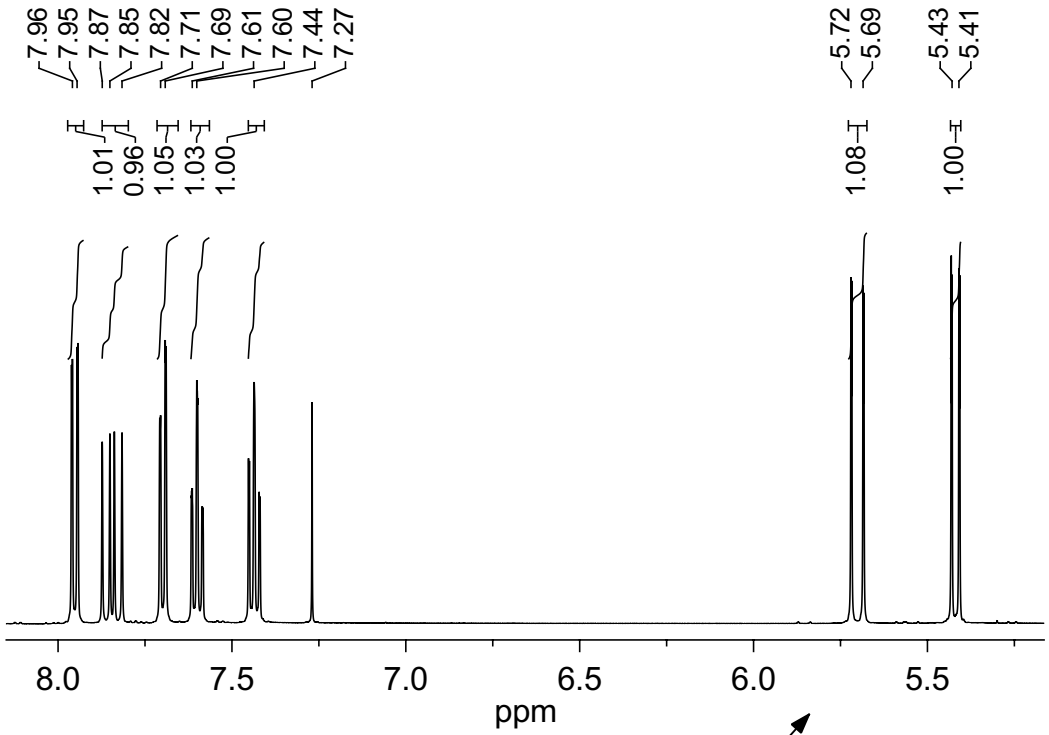
135
125
115
105
95
85
75
65
55
45
35
25
15
5
0
ppm


O
S
O

4a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7.71
7.69
7.61
7.60
7.44
7.27
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5.69
5.43
5.41
1.01
0.96
1.05
1.03
1.00
1.08
1.00
8.0
7.5
7.0
6.5
6.0
5.5
ppm

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7.0
6.5
6.0
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4.0
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3.0
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1.5
1.0
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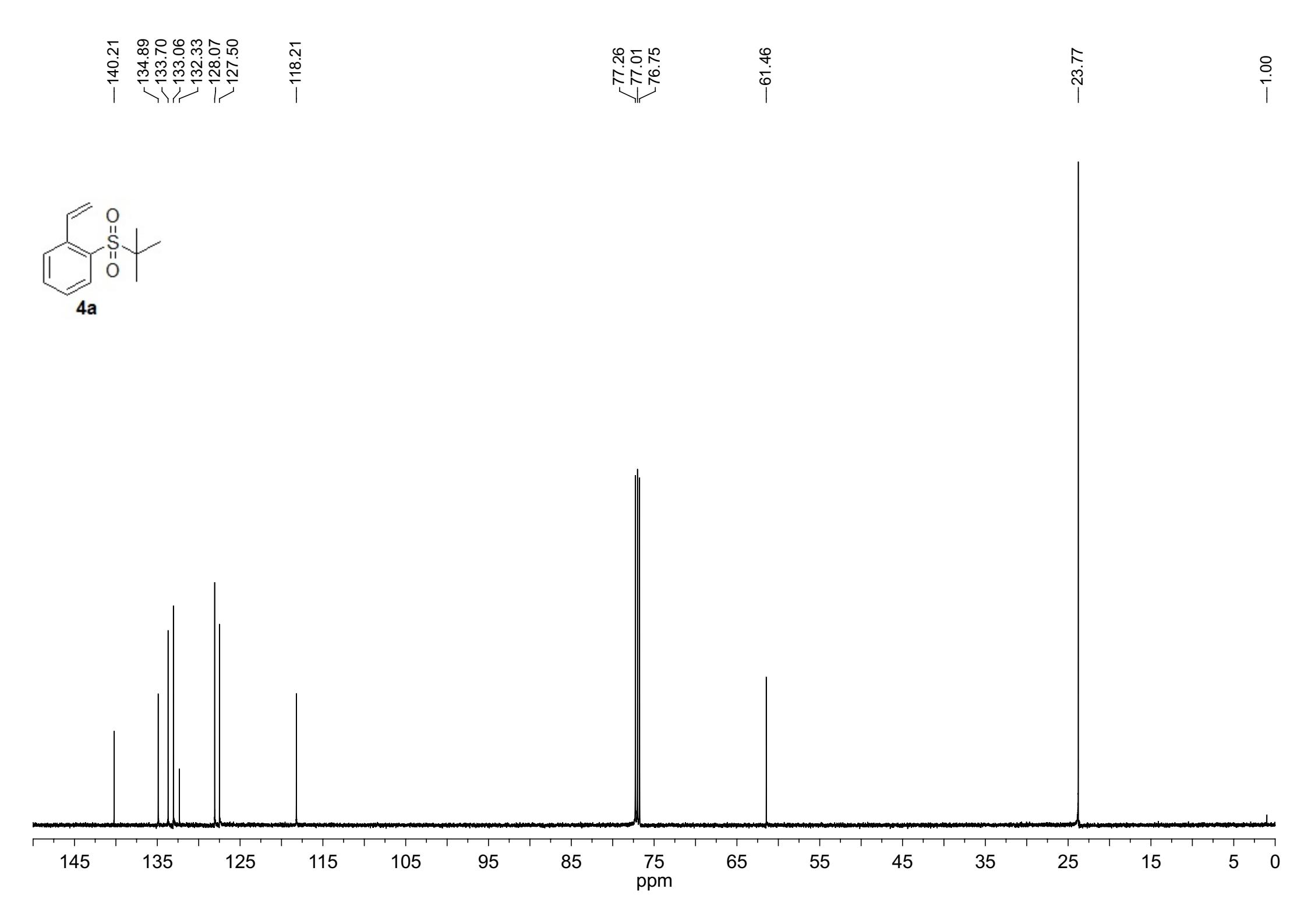
0.0
ppm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118.21
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77.01
76.75
61.46
23.77
1.00
4a
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135
125
115
105
95
85
75
65
55
45
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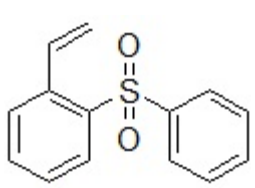
25
15
5
0
ppm



4b

8.21
8.20
7.86
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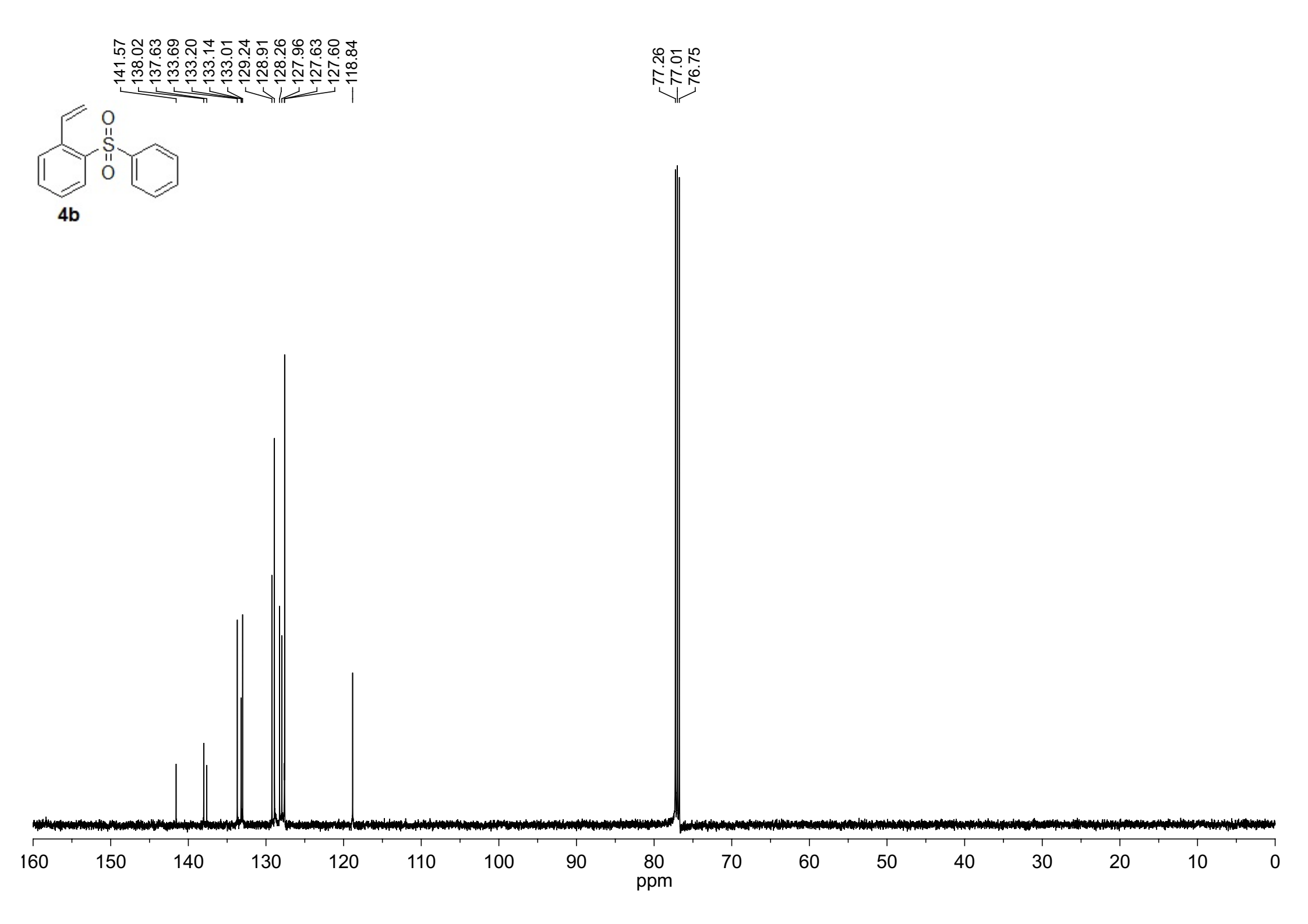
7.56
7.55
7.53
7.51
7.50
7.48
7.46
7.45
5.55
5.51
5.33
5.31
1.09
0.94
8.21
1.13
1.14
9.4 9.2 9.0 8.8 8.6 8.4 8.2 8.0 7.8 7.6 7.4 7.2 7.0 6.8 6.6 6.4 6.2 6.0 5.8 5.6 5.4 5.2 5.0 4.8 4.6
ppm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128.26
127.96
127.63
127.60
118.84
77.26
77.01
76.75
O
S
O
4b
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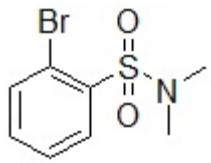
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


Br
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S
O
N

6

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8.08
7.76
7.74
7.48
7.47
7.45
7.43
7.41
7.39
7.37
7.27
2.90
1.04
1.03
1.92
6.00
8.4
8.2
8.0
7.8
7.6
7.4
7.2
ppm
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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4.0
3.5
3.0
2.5
2.0
1.5
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0.5
0.0
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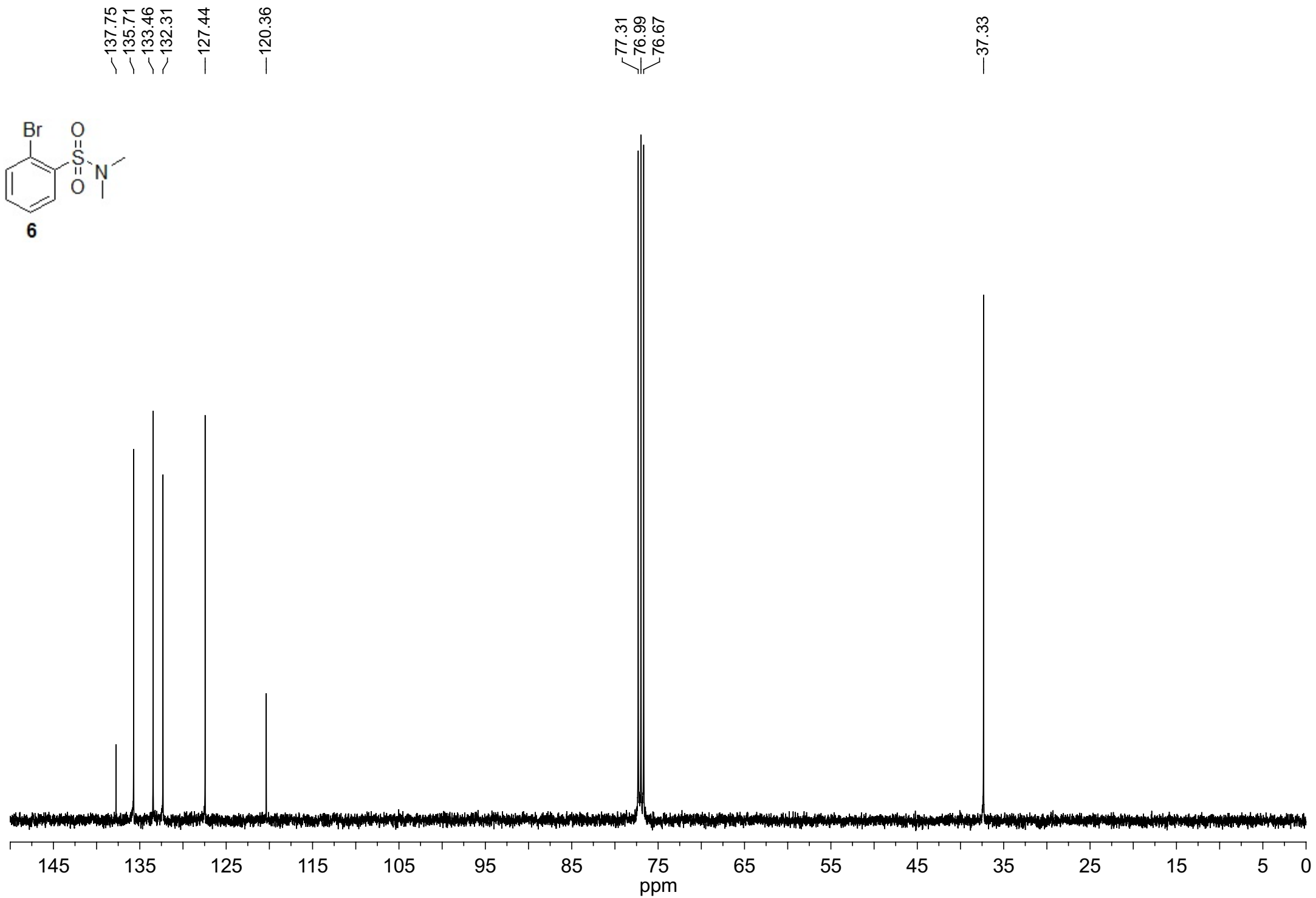
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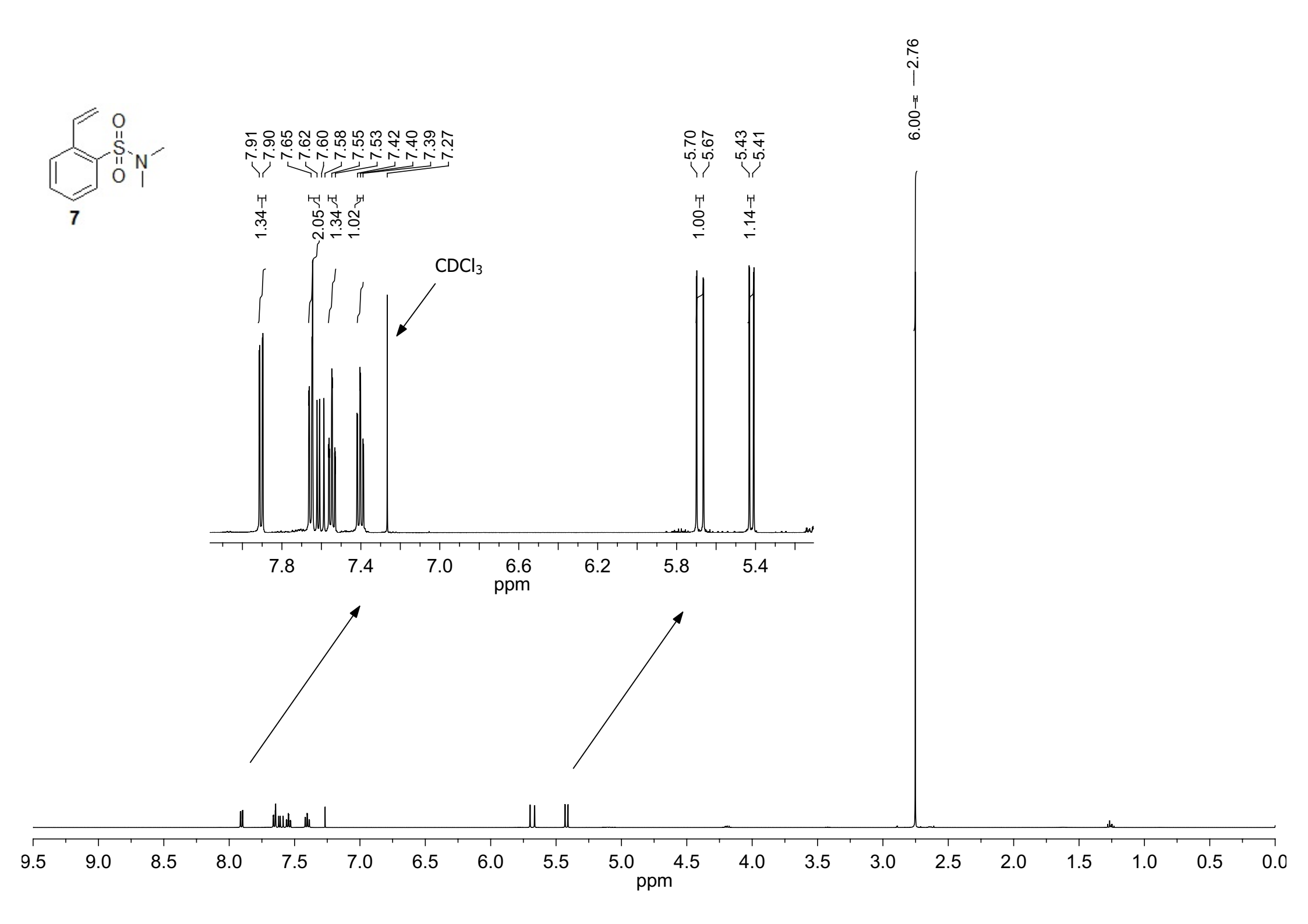
132.31
127.44
120.36
77.31
76.99
76.67
37.33
Br
O
S
N
O
6
145
135
125
115
105
95
85
75
65
55
45
35
25
15
5
0
ppm


7
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7.90
7.65
7.62
7.60
7.58
7.55
7.53
7.42
7.40
7.39
7.27
5.70
5.67
5.43
5.41
6.00
2.76
1.34
2.05
1.34
1.02
1.00
1.14
CDCl3
7.8
7.4
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5.8
5.4
ppm
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8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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4.0
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3.0
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1.5
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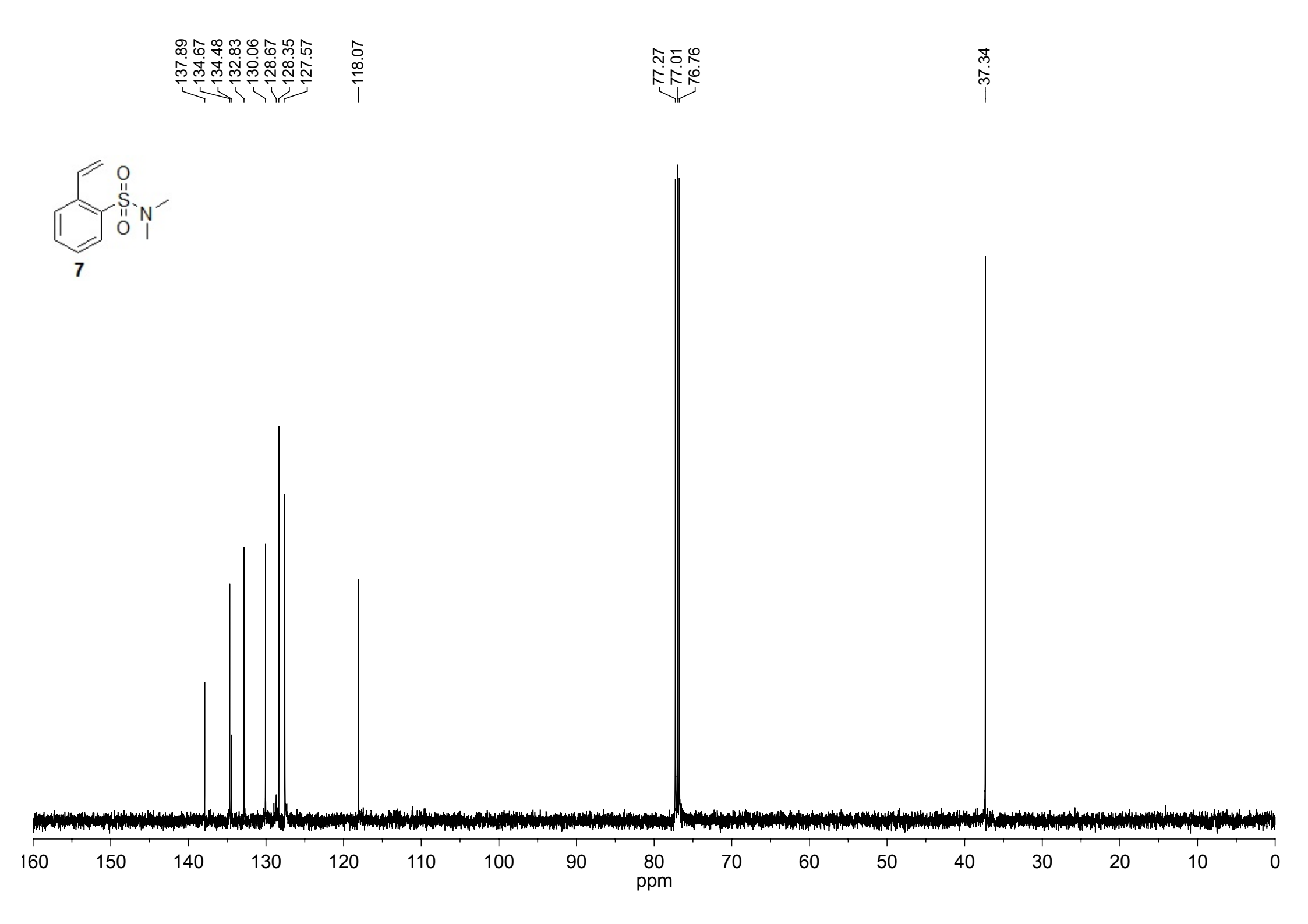
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134.67
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132.83
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128.35
127.57
118.07
77.27
77.01
76.76
37.34
O
S
O
N
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140
130
120
110
100
90
80
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30
20
10
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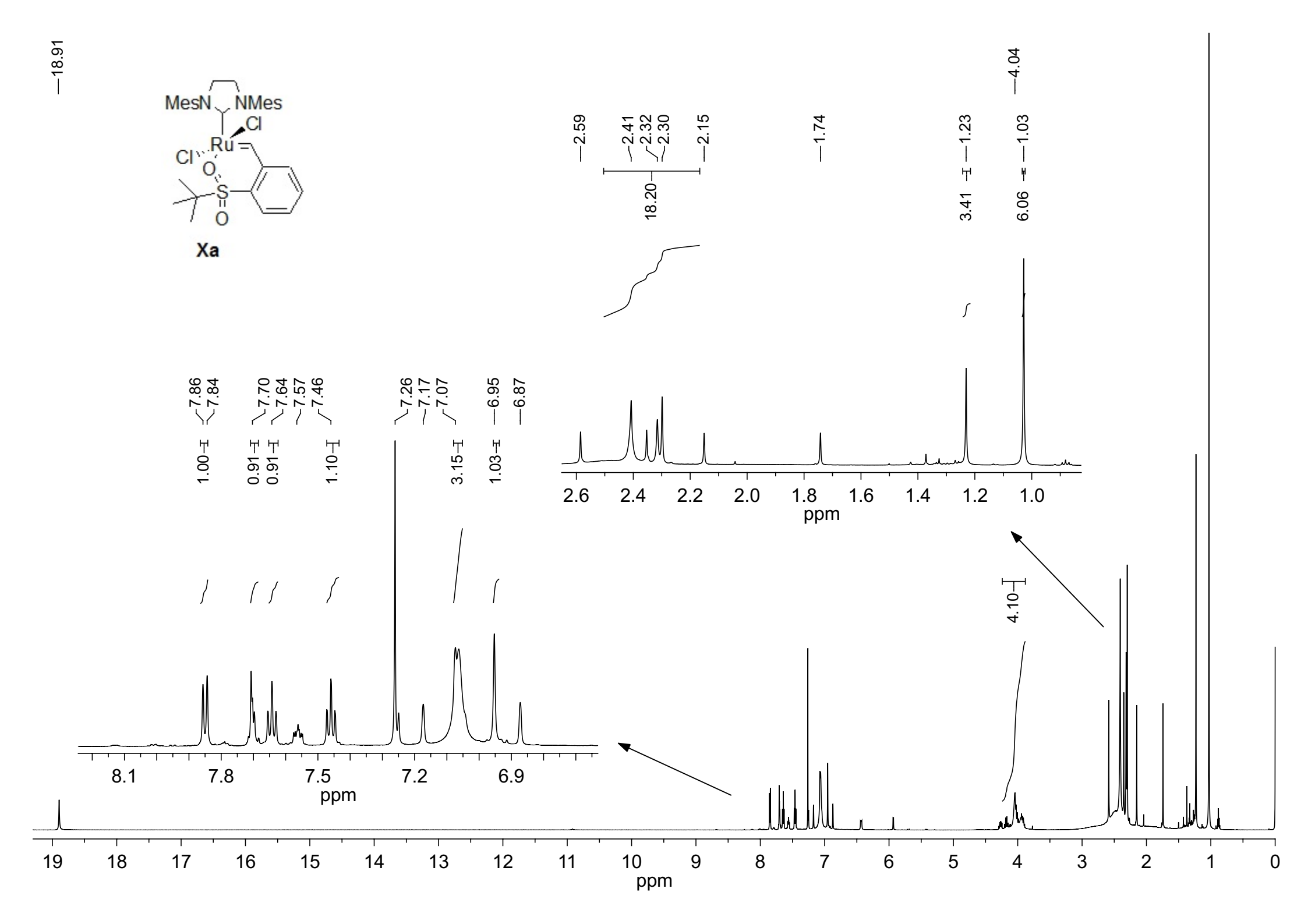
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MesN
NMes
Cl
Ru
Cl
O
S
O
Xa
2.59
2.41
2.32
2.30
2.15
18.20
1.74
3.41
1.23
4.04
6.06
1.03
7.86
7.84
7.70
7.64
7.57
7.46
7.26
7.17
7.07
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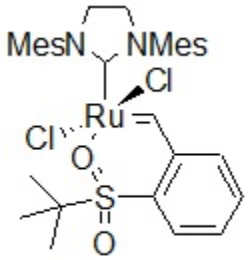
6.87
1.00
0.91
0.91
1.10
3.15
1.03
4.10
ppm
ppm
ppm


MesN
NMes
Cl
Ru
Cl
O
S
O

Xa

271.08
209.00
153.75
147.33
141.41
139.47
138.71
137.65
135.76
135.37
133.89
132.34
129.41
127.49
124.85
120.74
120.00
77.23
76.54
76.11
64.52
62.97
22.95
21.16
20.26
18.97
17.88
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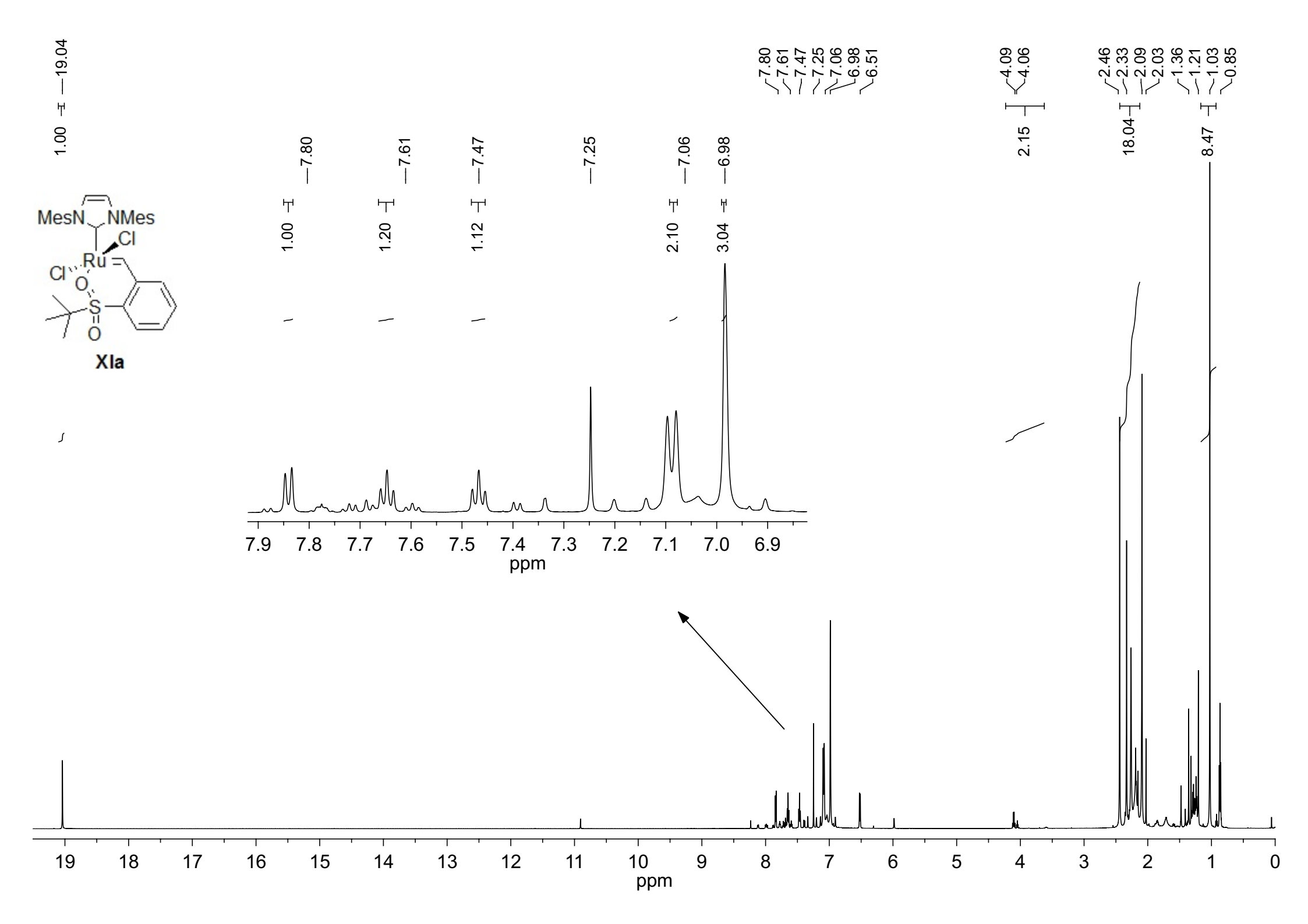
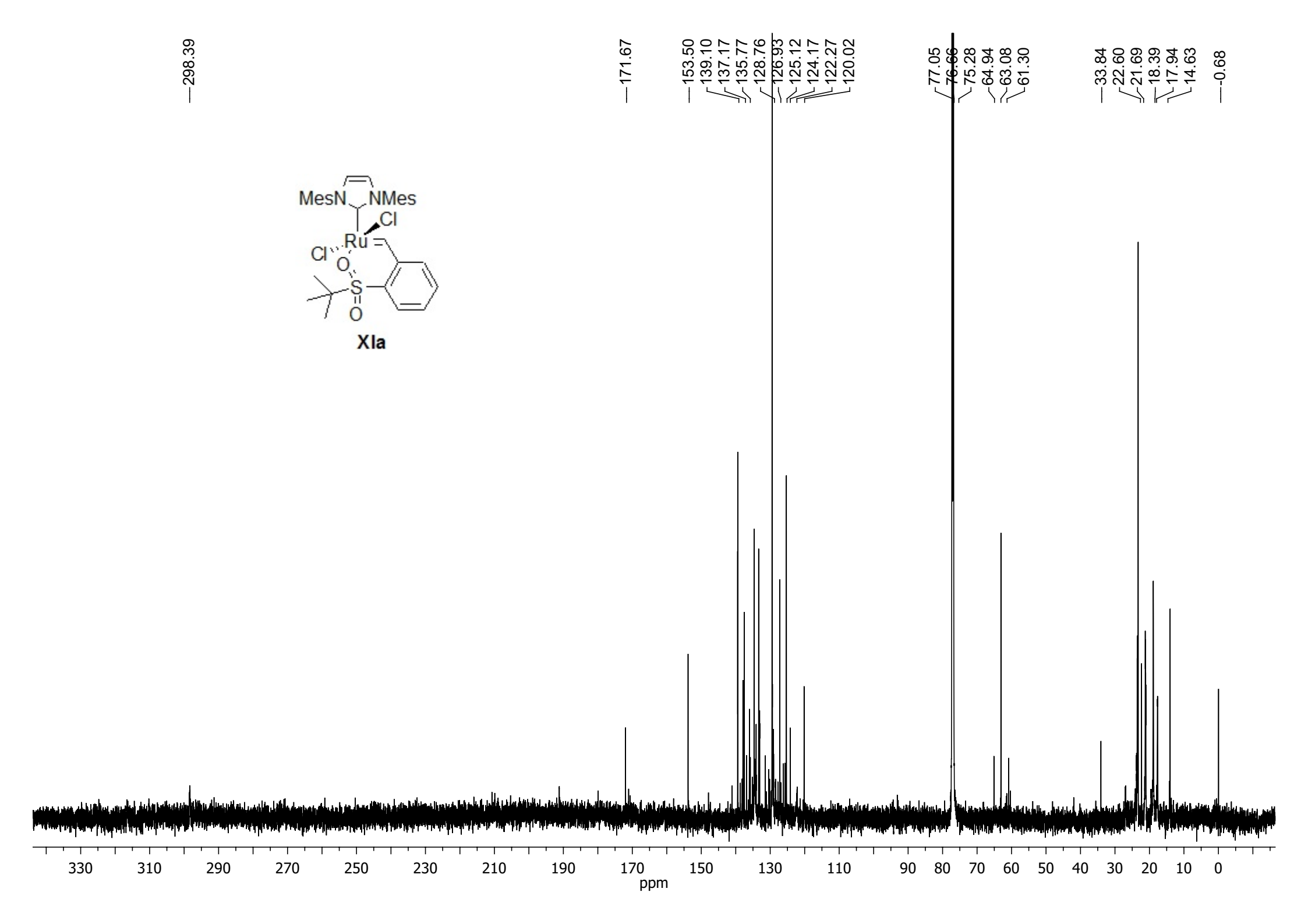
ppm


MesN
NMes
Cl
Ru
Cl
O
S
O
XIa
1.00
19.04
7.80
7.61
7.47
7.25
7.06
6.98
6.51
4.09
4.06
2.46
2.33
2.09
2.03
1.36
1.21
1.03
0.85
2.15
18.04
8.47
ppm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137.17
135.77
128.76
126.93
125.12
124.17
122.27
120.02
77.05
76.66
75.28
64.94
63.08
61.30
33.84
22.60
21.69
18.39
17.94
14.63
-0.68
MesN
NMes
Cl
Ru
Cl
O
S
O
330
310
290
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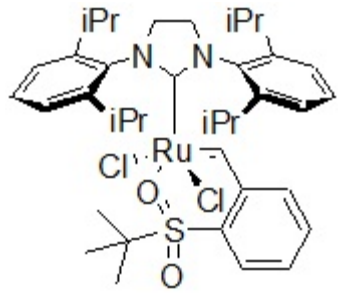
ppm

XIa


iPr
iPr
N
N
iPr
iPr
Ru
Cl
Cl
O
S
O

XIIa

1.00
18.66
7.84
7.62
7.37
7.23
1.12
6.43
4.16
4.10
1.62
13.82
9.62
1.70
1.31
1.00
1.72
3.59
2.09
2.10
7.84
7.62
7.37
7.26
7.23
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
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14
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12
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9
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7
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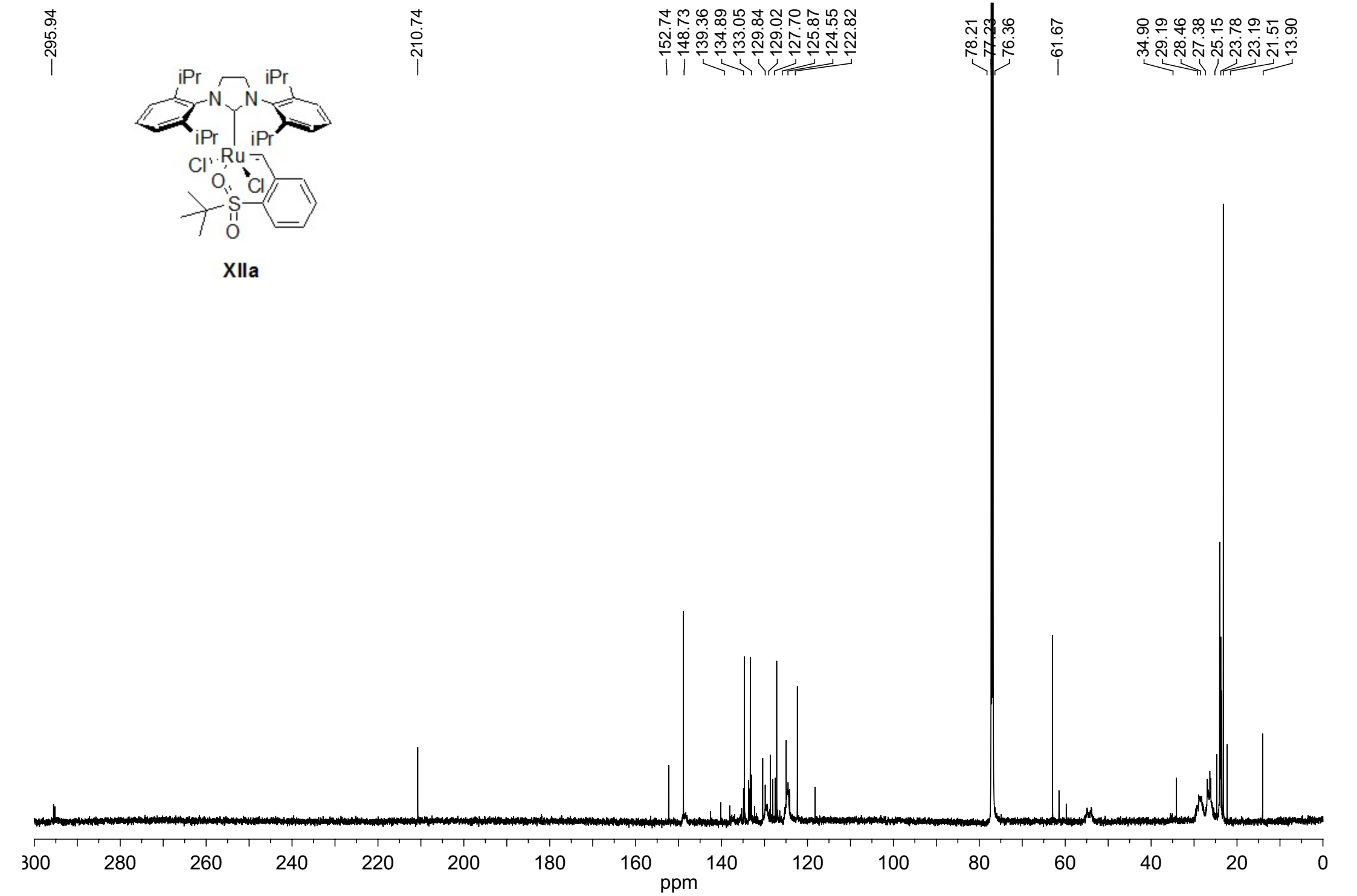
4
3
2
1
ppm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129.84
129.02
127.70
125.87
124.55
122.82
78.21
77.23
76.36
61.67
34.90
29.19
28.46
27.38
25.15
23.78
23.19
21.51
13.90
iPr
iPr
iPr
iPr
N
N
Ru
Cl
Cl
O
S
O
300
280
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240
220
200
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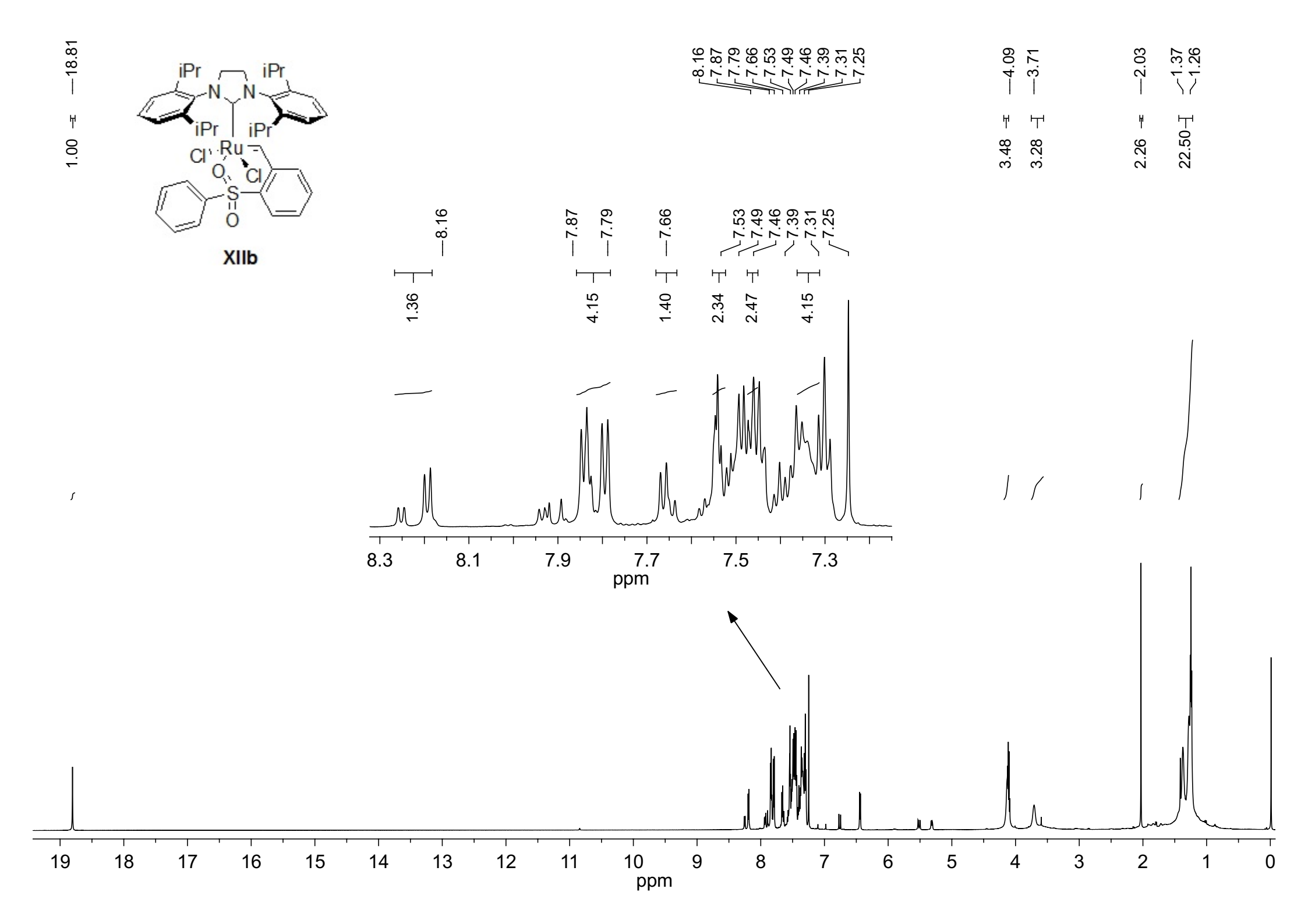
160
140
120
100
80
60
40
20
0
ppm

XIIa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iPr
iPr
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N
Ru
Cl
Cl
O
S
O
XIIb
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7.87
7.79
7.66
7.53
7.49
7.46
7.39
7.31
7.25
4.09
3.71
2.03
1.37
1.26
3.48
3.28
2.26
22.50
1.36
4.15
1.40
2.34
2.47
4.15
8.3
8.1
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ppm
19
18
17
16
15
14
13
12
11
10
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6
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2
1
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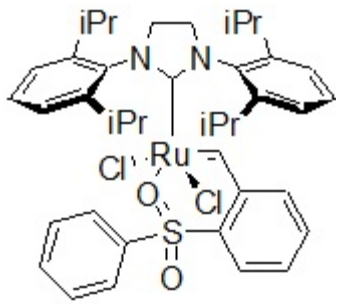
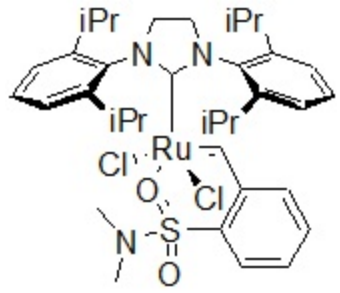


XIIb

297.97
210.33
170.63
148.54
141.87
139.95
137.76
136.57
133.92
133.19
127.97
124.61
118.96
77.40
77.01
76.31
60.17
28.77
26.88
25.73
24.29
21.26
14.52

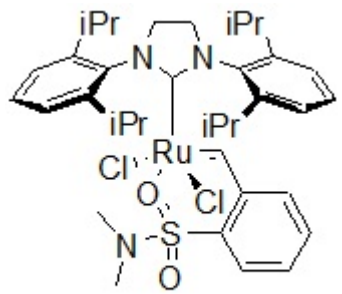
300 280 260 240 220 200 180 160 140 120 100 80 60 40 20

ppm


iPr
iPr
iPr
iPr
N
N
Ru
Cl
Cl
O
O
S
N
O

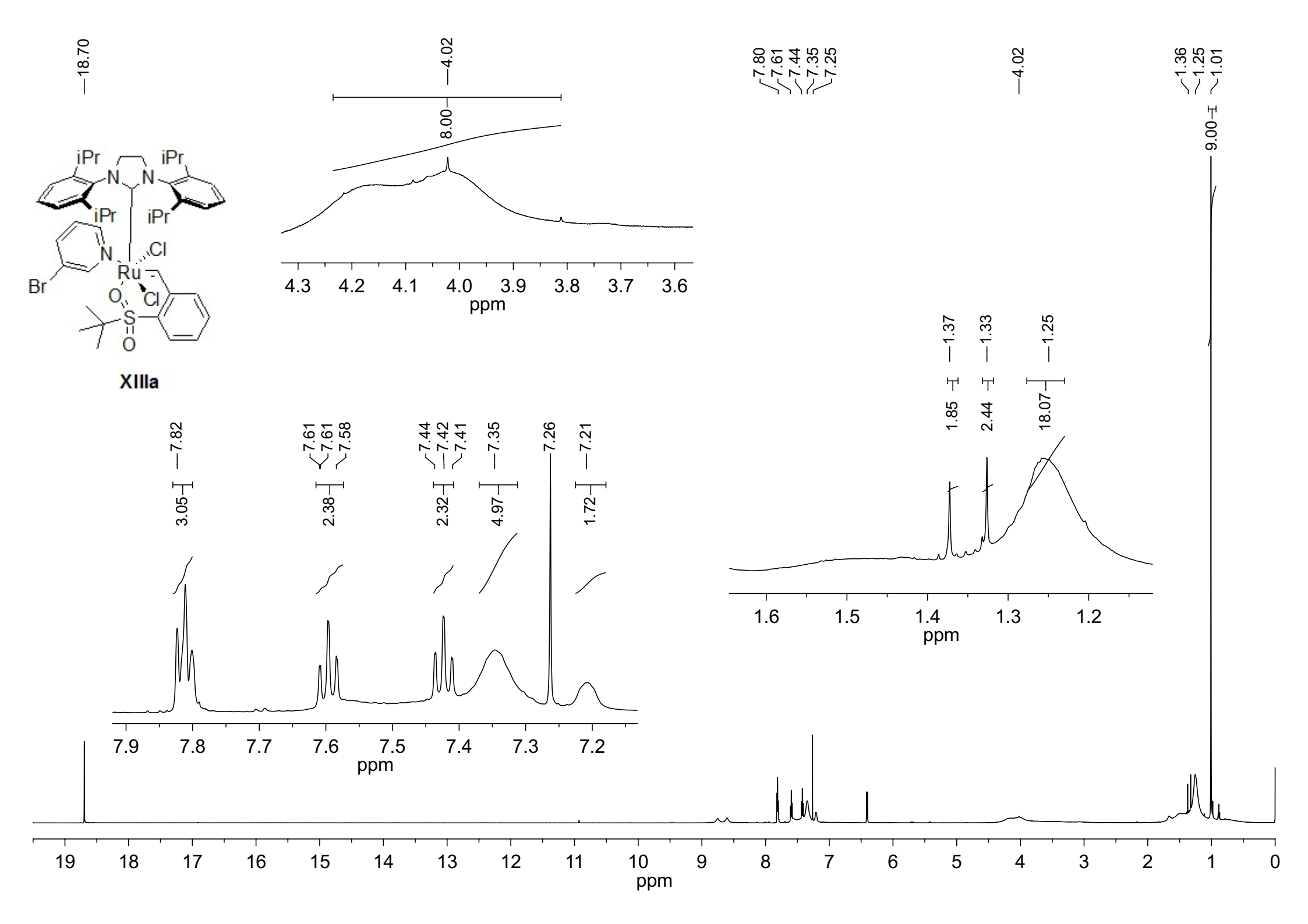
XIIc

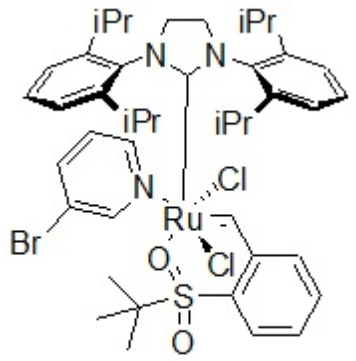
1.12
18.64
7.63
7.49
7.36
7.25
6.48
3.13
4.11
1.54
3.85
0.97
2.77
6.29
2.43
21.08
1.34
1.24
1.82
0.88
7.63
7.49
7.36
7.26
2.82
1.84
6.10
7.60
7.50
7.40
7.30
7.20
ppm
19
18
17
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
ppm


iPr
iPr
N
N
iPr
iPr
Cl
Ru
O
Cl
N
S
O

XIIc

295.69
210.66
150.40
150.30
149.16
148.80
133.50
132.83
130.04
130.04
129.63
128.33
128.21
127.84
127.56
124.68
124.27
77.24
77.13
77.02
76.81
76.31
37.66
37.59
31.55
28.76
28.61
26.45
26.18
23.97
23.70
22.62
14.09
300
280
260
240
220
200
180
160
140
120
100
80
60
40
20
0
ppm


18.70
4.02
8.00
7.80
7.61
7.44
7.35
7.25
4.02
1.36
1.25
1.01
9.00
iPr
iPr
iPr
iPr
N
N
N
Cl
Ru
Cl
Br
O
S
O
O
XIIIa
4.3 4.2 4.1 4.0 3.9 3.8 3.7 3.6
ppm
1.37
1.33
1.25
1.85
2.44
18.07
1.6 1.5 1.4 1.3 1.2
ppm
7.82
7.61
7.61
7.58
7.44
7.42
7.41
7.35
7.26
7.21
3.05
2.38
2.32
4.97
1.72
7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2
ppm
19 18 17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0
ppm



XIIIa

296.31
210.65
152.57
151.32
149.17
148.34
138.57
134.79
133.05
129.22
127.13
124.55
122.11
77.94
77.03
76.29
63.07
28.76
28.35
26.17
25.77
23.70
23.21
14.39

320 290 260 230 200 170 140 110 80 60 40 20 0
ppm