Supplementary Materials (SM)

O,S-Acetals in a new modification of the *oxo*-Friedel-Crafts-Bradsher cyclization – synthesis of fluorescent (hetero)acenes and mechanistic considerations.

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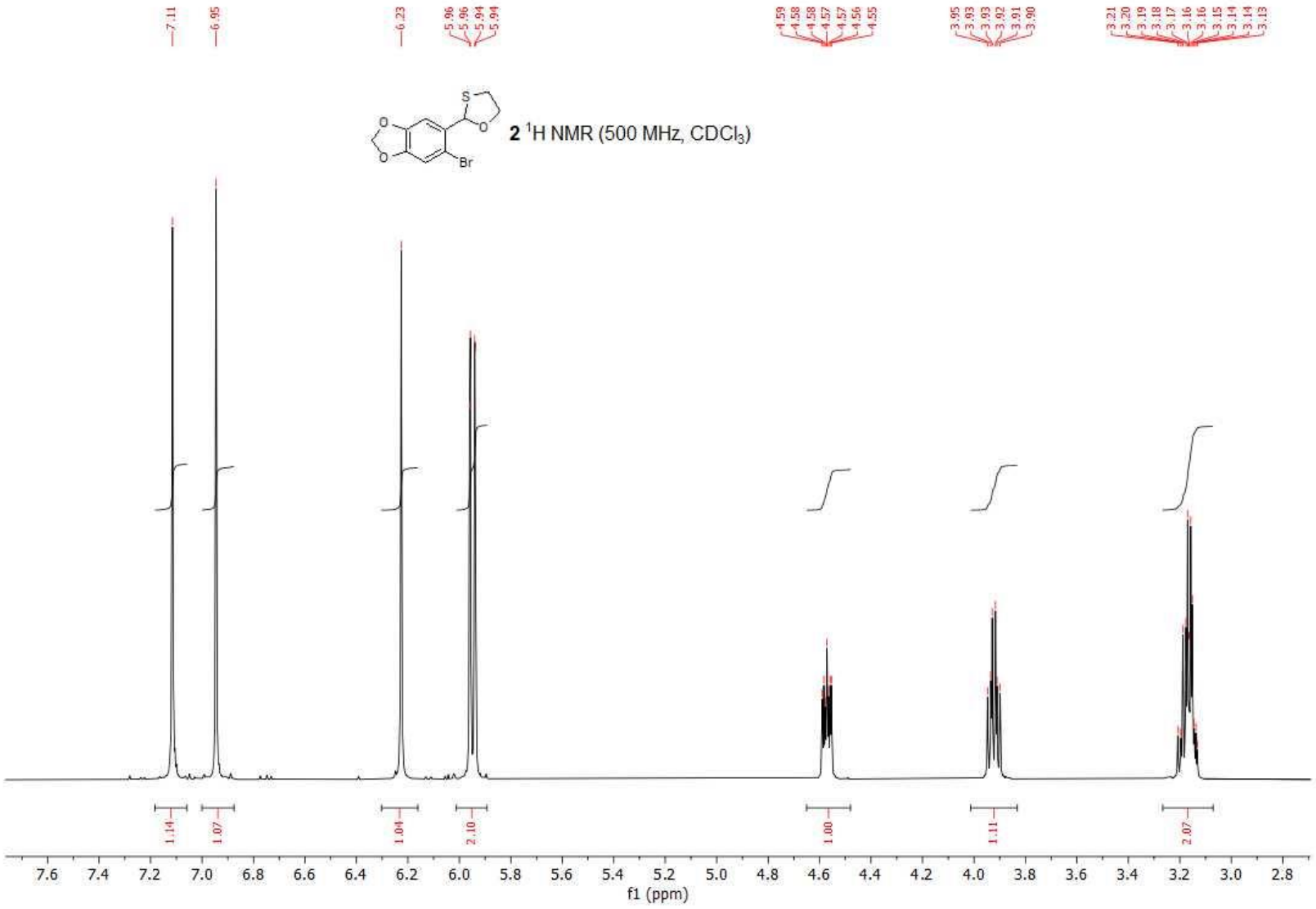
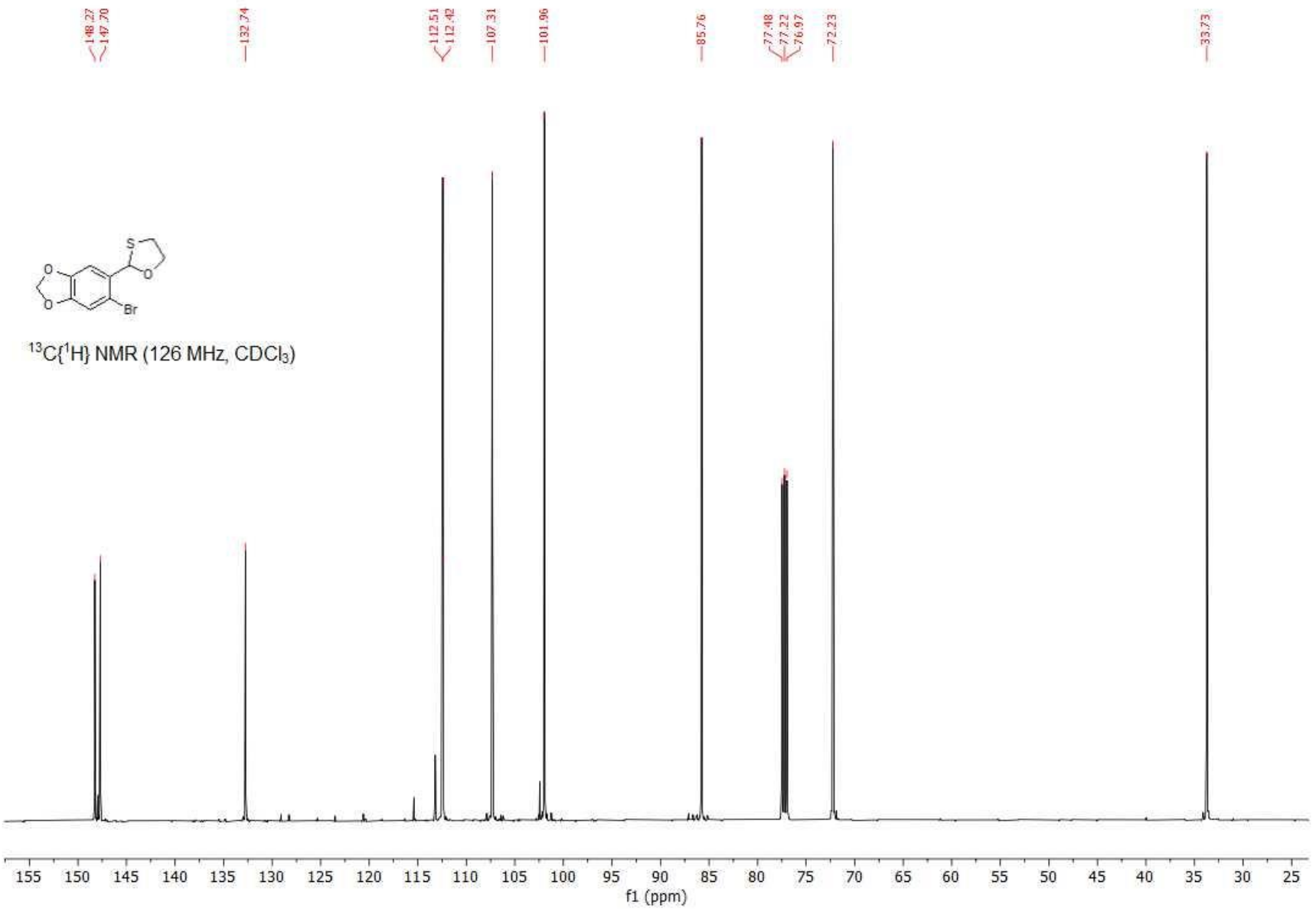
^{1}H and ^{13}C NMR spectra

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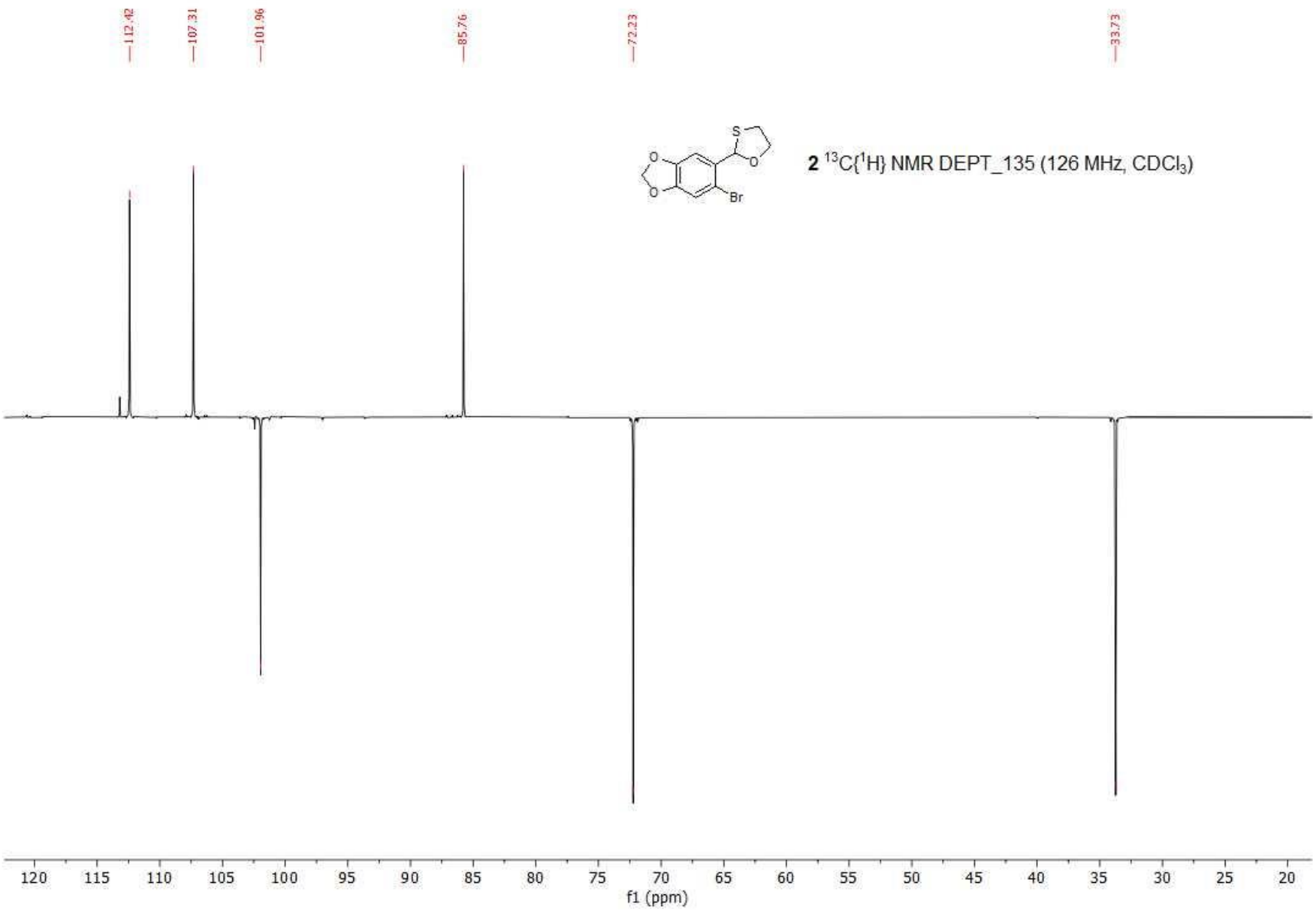
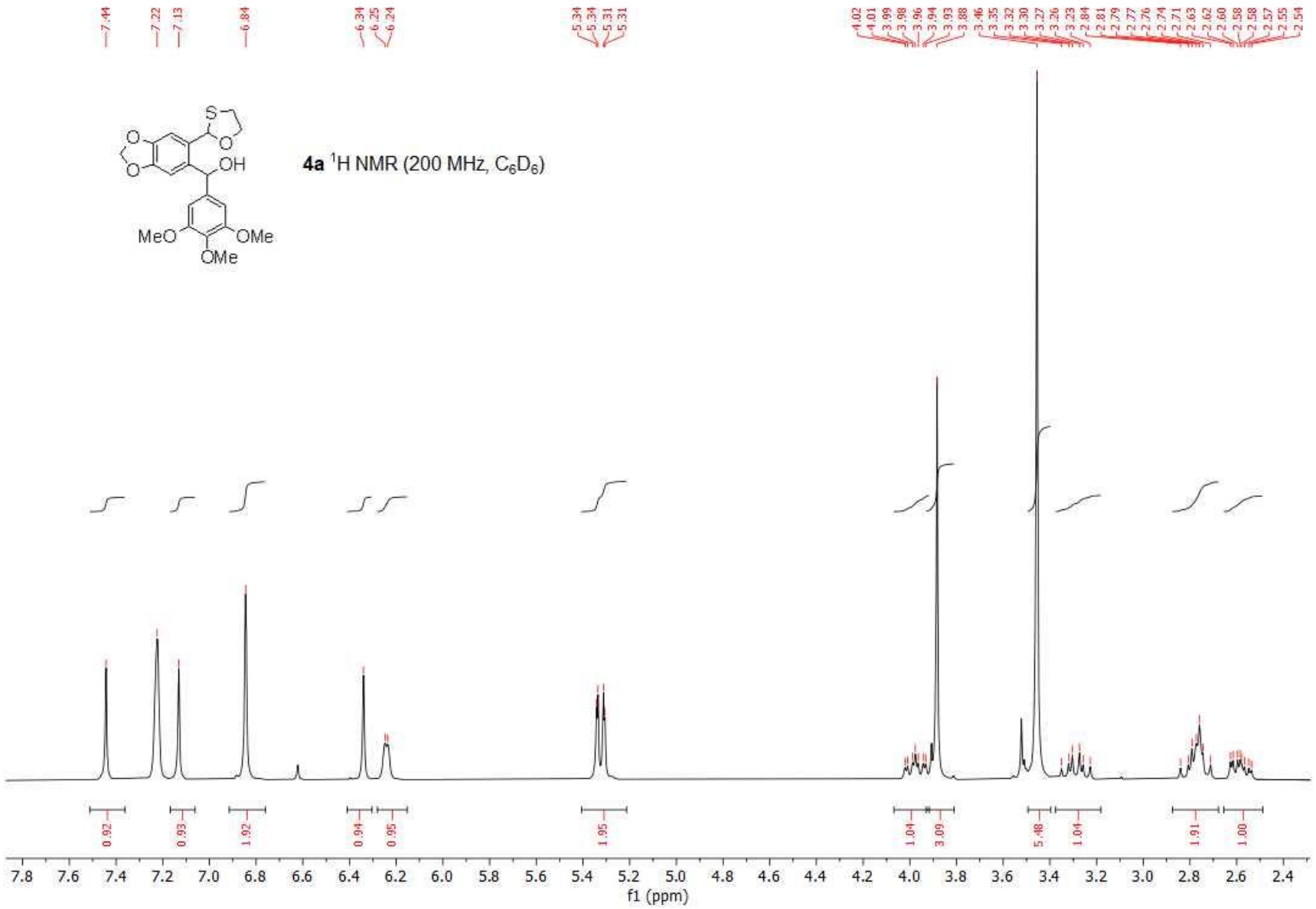
77.22
76.97
72.23
33.73
S
O
O
O
Br
$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$)
155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25
f1 (ppm)


112.42
107.31
101.96
85.76
72.23
33.73
S
O
O
O
Br
2 $^{13}C\{^{1}H\}$ NMR DEPT_135 (126 MHz, $CDCl_3$)
120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20
f1 (ppm)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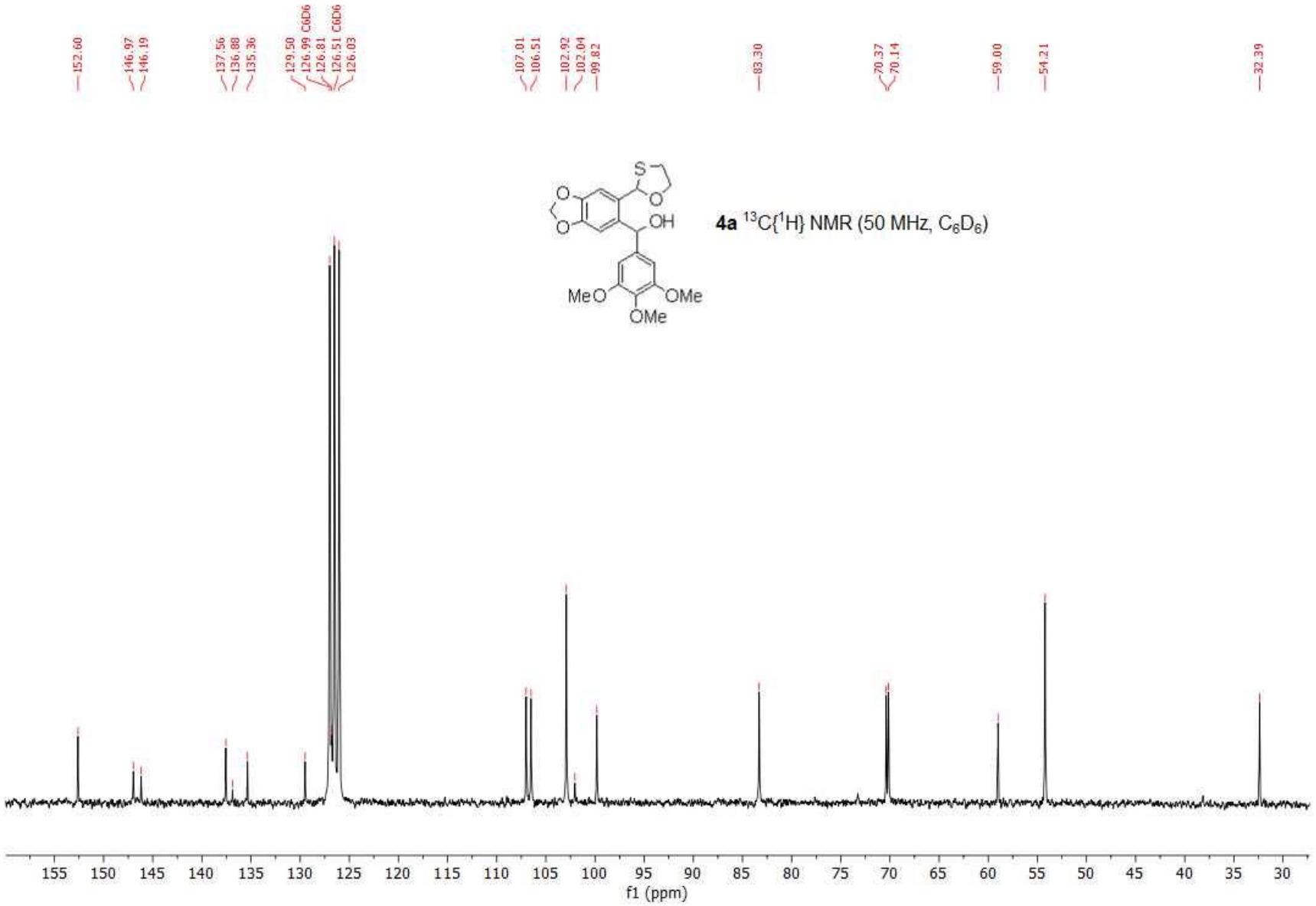
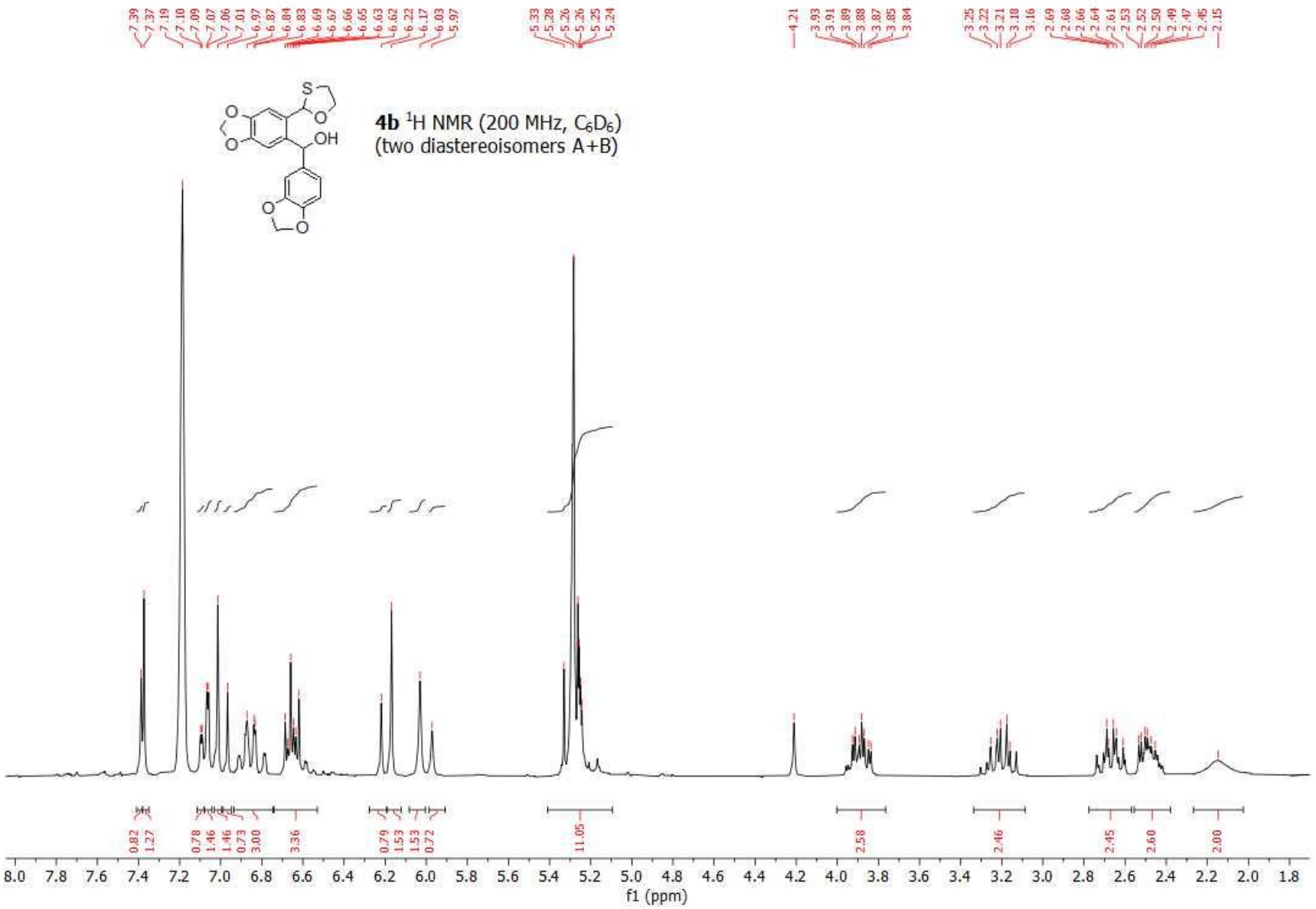
5.31
5.31
4.02
4.01
3.99
3.98
3.96
3.94
3.93
3.88
3.46
3.35
3.32
3.30
3.27
3.26
3.23
2.84
2.81
2.79
2.77
2.76
2.74
2.71
2.63
2.62
2.60
2.58
2.58
2.57
2.55
2.54
S
O
O
O
OH
MeO
OMe
OMe
4a ¹H NMR (200 MHz, C6D6)
0.92
0.93
1.92
0.94
0.95
1.95
1.04
3.09
5.48
1.04
1.91
1.00
7.8
7.6
7.4
7.2
7.0
6.8
6.6
6.4
6.2
6.0
5.8
5.6
5.4
5.2
5.0
4.8
4.6
4.4
4.2
4.0
3.8
3.6
3.4
3.2
3.0
2.8
2.6
2.4
f1 (ppm)



4a $^{13}C\{^{1}H\}$ NMR (50 MHz, C_6D_6)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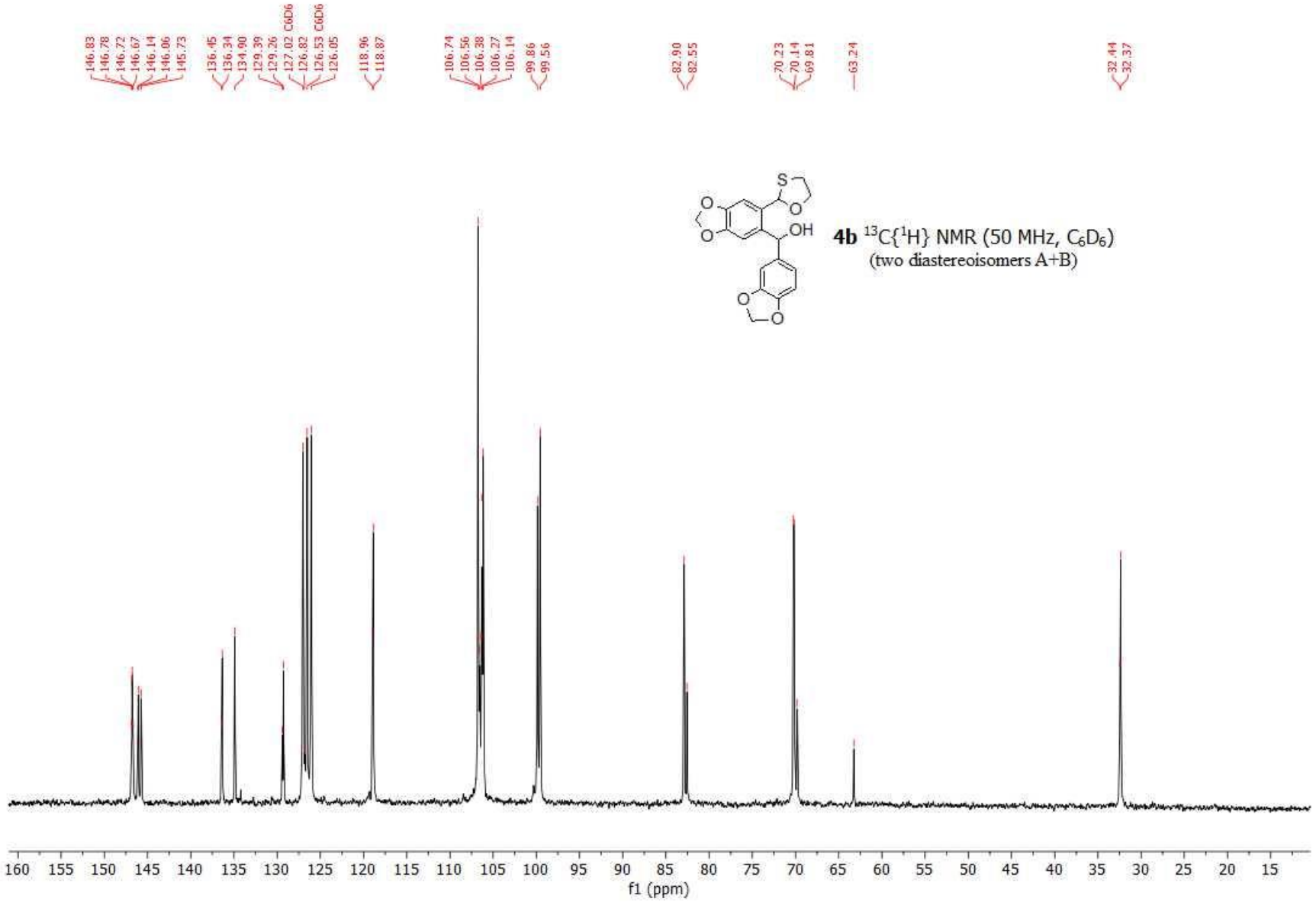
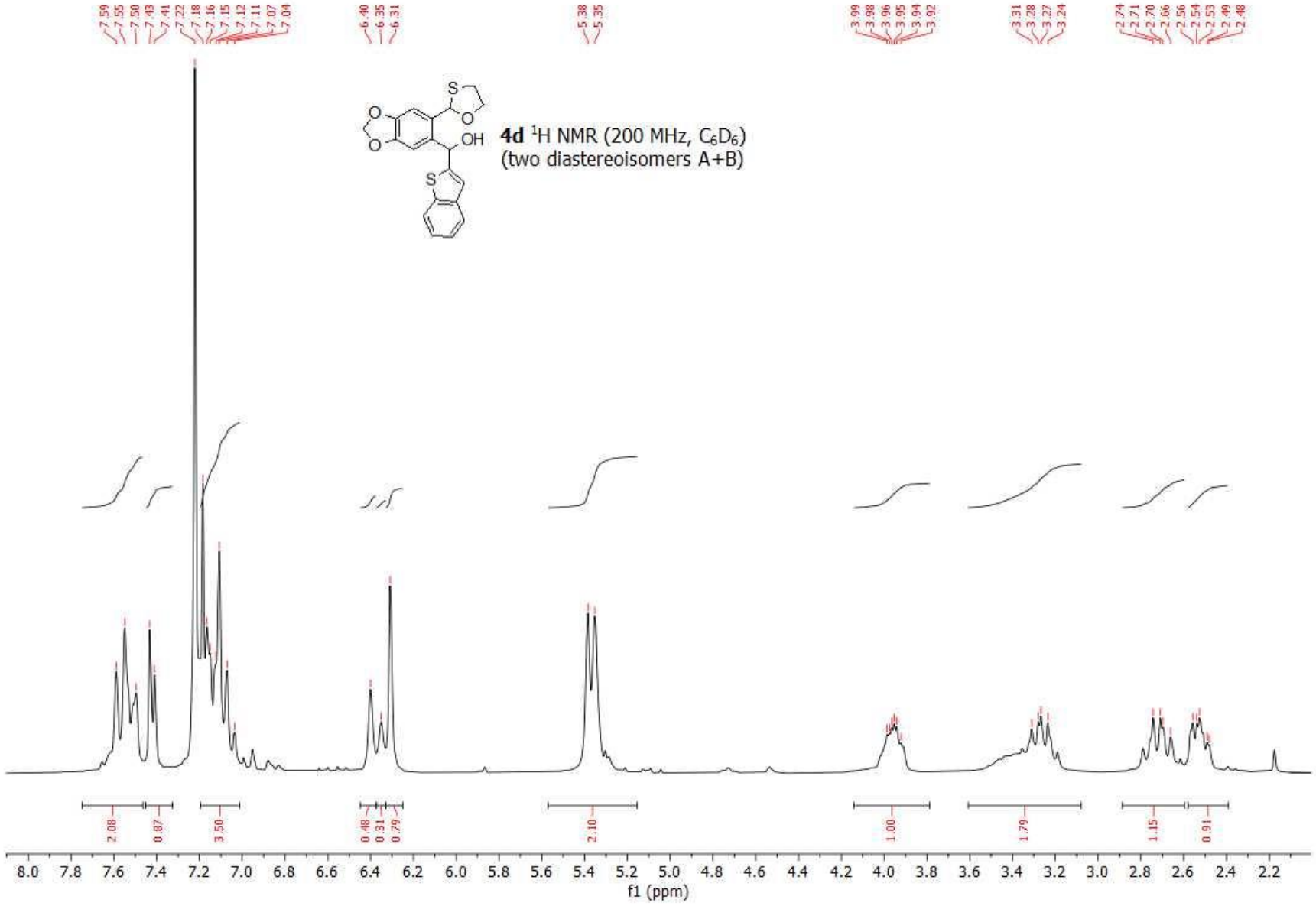
7.19
7.10
7.09
7.07
7.06
7.01
6.97
6.87
6.84
6.83
6.69
6.67
6.66
6.65
6.63
6.62
6.22
6.17
6.03
5.97
5.33
5.28
5.26
5.25
5.24
4.21
3.93
3.91
3.89
3.88
3.87
3.85
3.84
3.25
3.22
3.21
3.18
3.16
2.69
2.68
2.66
2.64
2.61
2.53
2.52
2.50
2.49
2.47
2.45
2.15
S
O
O
O
OH
O
O
4b ¹H NMR (200 MHz, C6D6)
(two diastereoisomers A+B)
0.82
1.27
0.78
1.46
1.46
0.73
3.00
3.36
0.79
1.53
1.53
0.72
11.05
2.58
2.46
2.45
2.60
2.00
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
4.4
4.2
4.0
3.8
3.6
3.4
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
f1 (ppm)



4b $^{13}C\{^{1}H\}$ NMR (50 MHz, C_6D_6)
(two diastereoisomers A+B)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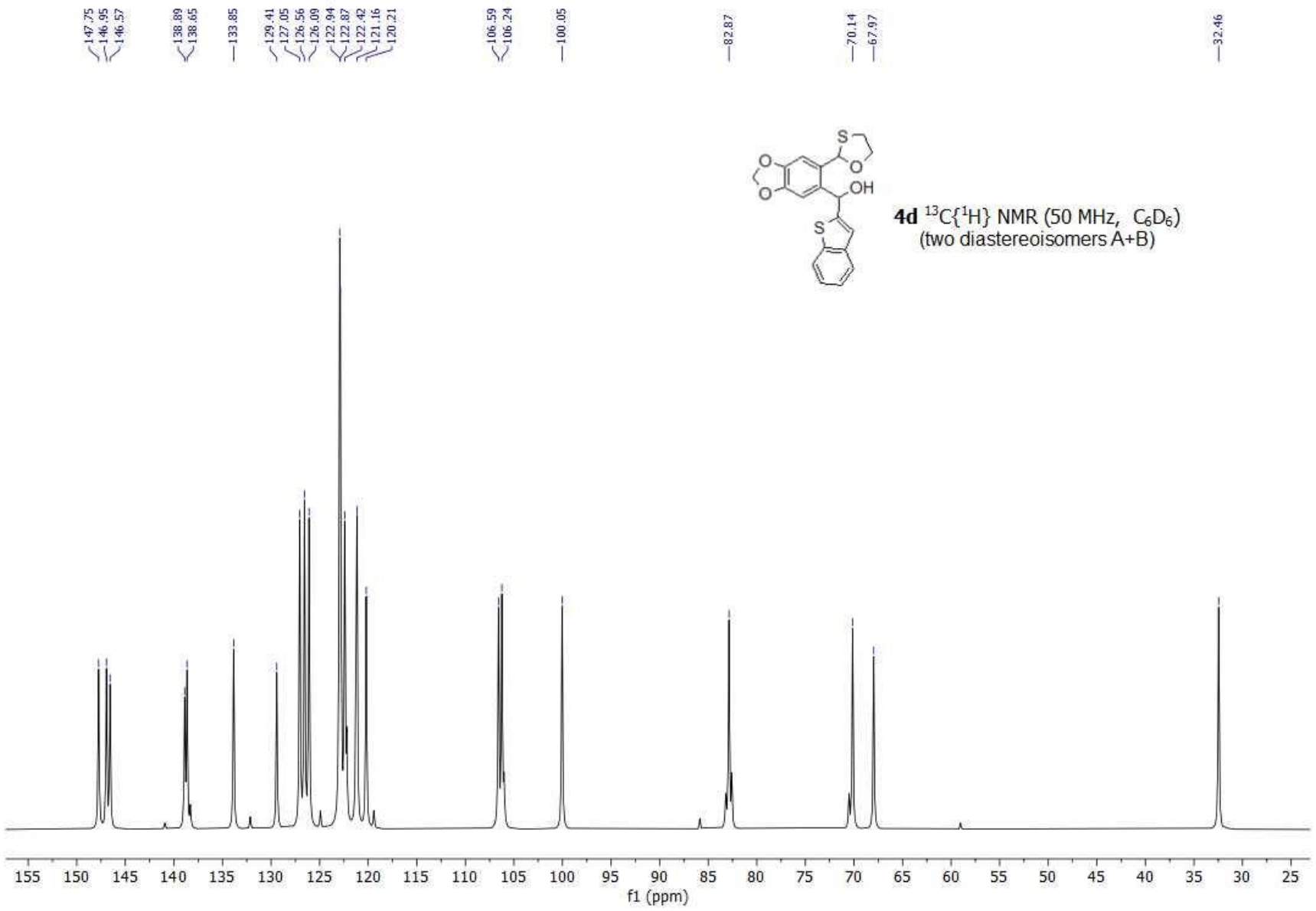
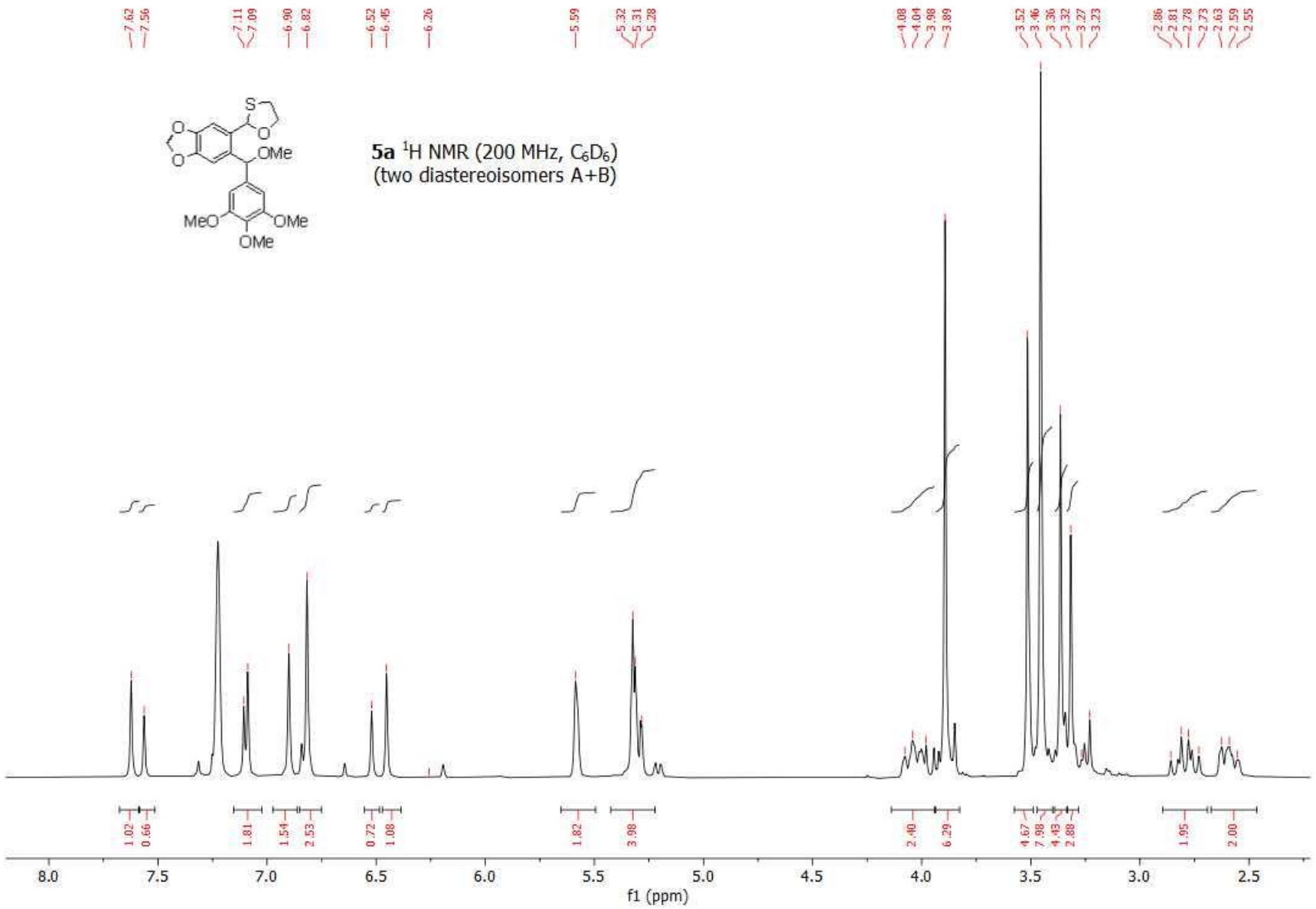
7.55
7.50
7.43
7.41
7.22
7.18
7.16
7.15
7.12
7.11
7.07
7.04
6.40
6.35
6.31
5.38
5.35
3.99
3.98
3.96
3.95
3.94
3.92
3.31
3.28
3.27
3.24
2.74
2.71
2.70
2.66
2.56
2.54
2.53
2.49
2.48
S
O
O
O
OH
S
4d 1H NMR (200 MHz, C6D6)
(two diastereoisomers A+B)
2.08
0.87
3.50
0.48
0.31
0.79
2.10
1.00
1.79
1.15
0.91
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 4.4 4.2 4.0 3.8 3.6 3.4 3.2 3.0 2.8 2.6 2.4 2.2
f1 (ppm)



4d $^{13}C\{^{1}H\}$ NMR (50 MHz, C_6D_6)
(two diastereoisomers A+B)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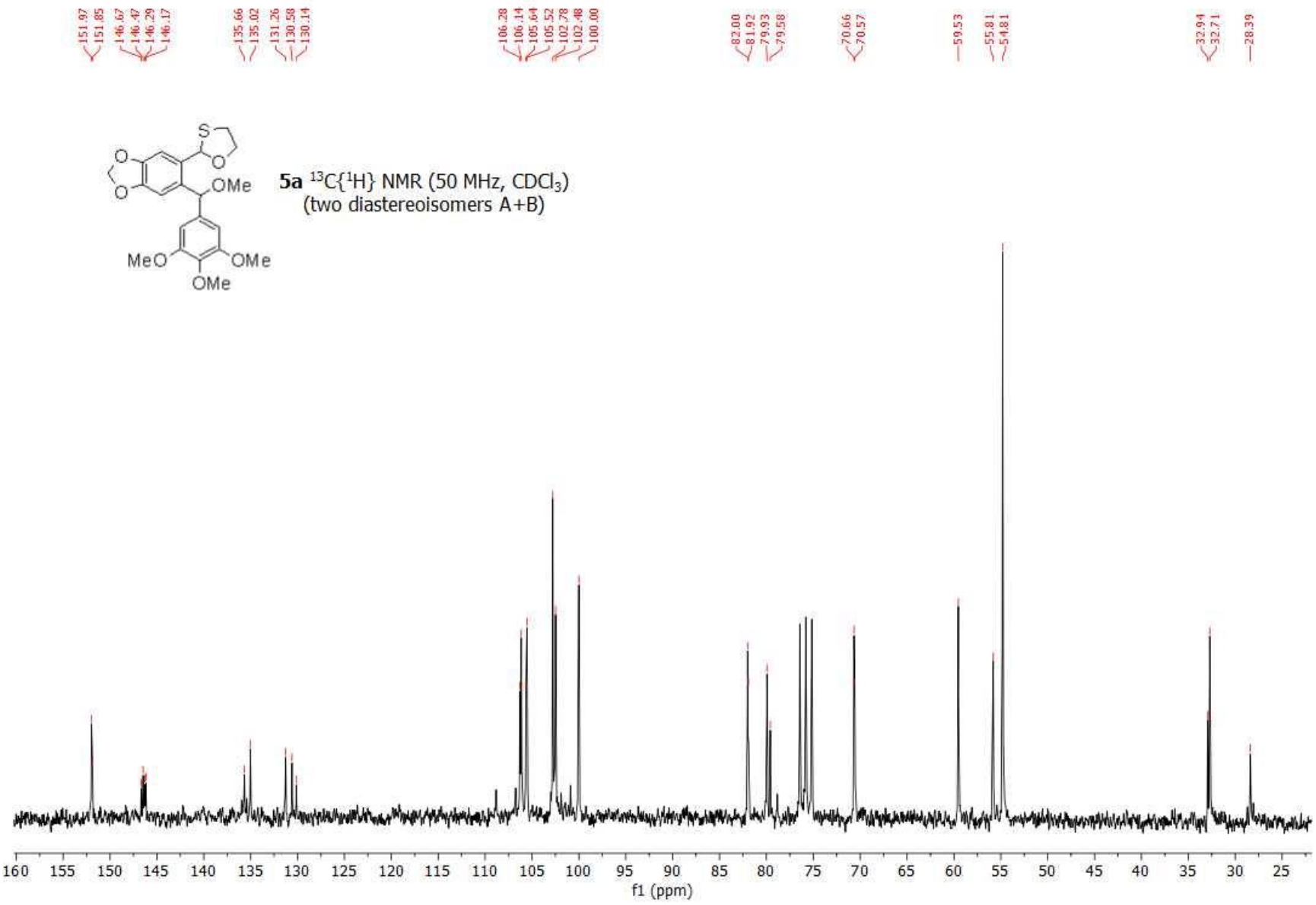
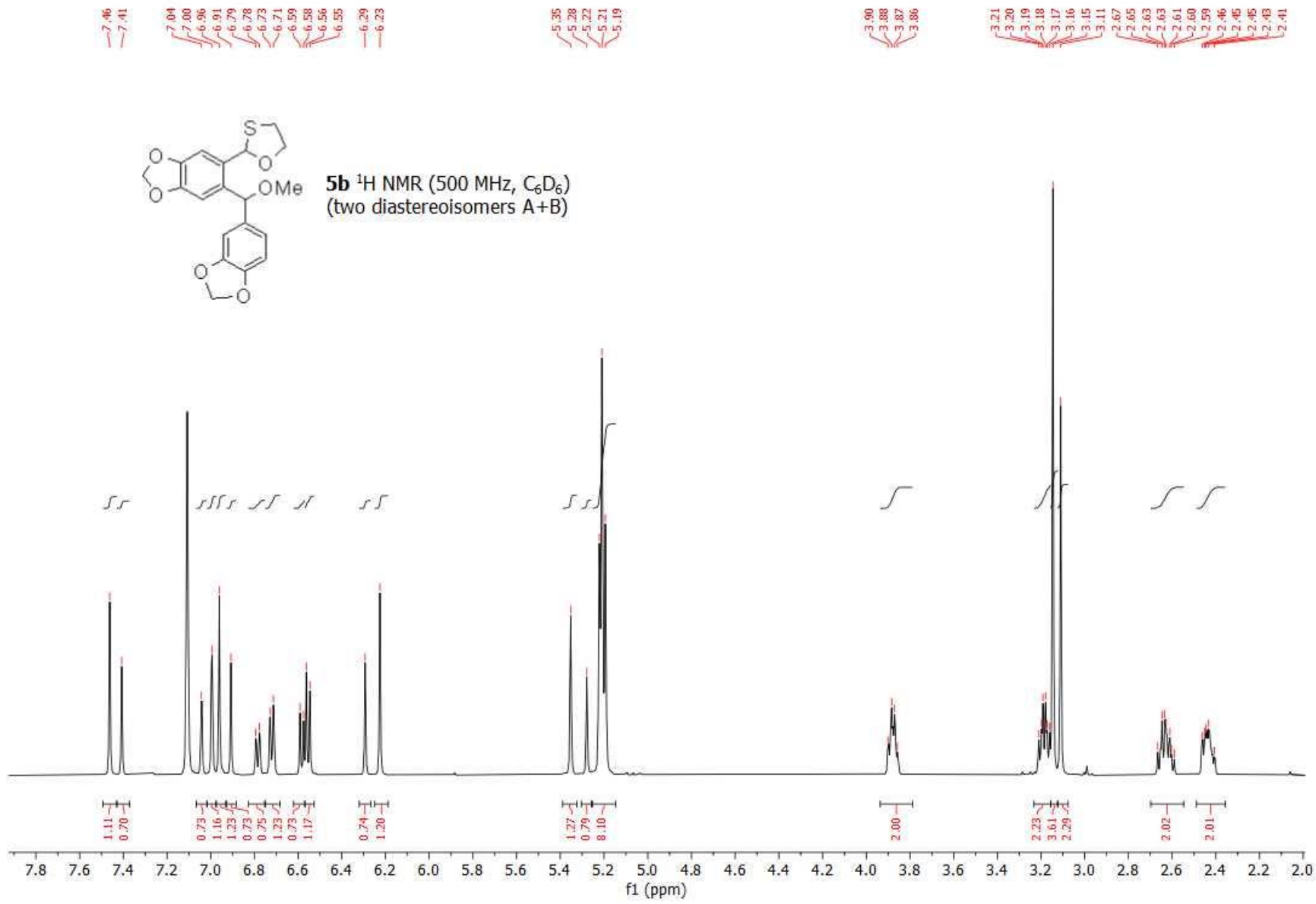
7.56
7.11
7.09
6.90
6.82
6.52
6.45
6.26
5.59
5.32
5.31
5.28
4.08
4.04
3.98
3.89
3.52
3.46
3.36
3.32
3.27
3.23
2.86
2.81
2.78
2.73
2.63
2.59
2.55
S
O
O
O
OMe
MeO
OMe
OMe
5a ¹H NMR (200 MHz, C6D6)
(two diastereoisomers A+B)
1.02
0.66
1.81
1.54
2.53
0.72
1.08
1.82
3.98
2.40
6.29
4.67
7.98
4.43
2.88
1.95
2.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
f1 (ppm)


151.97
151.85
146.67
146.47
146.29
146.17
135.66
135.02
131.26
130.58
130.14
106.28
106.14
105.64
105.52
102.78
102.48
100.00
82.00
81.92
79.93
79.58
70.66
70.57
59.53
55.81
54.81
32.94
32.71
28.39
S
O
O
O
OMe
MeO
OMe
OMe
5a $^{13}C\{^{1}H\}$ NMR (50 MHz, $CDCl_3$)
(two diastereoisomers A+B)
160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25
f1 (ppm)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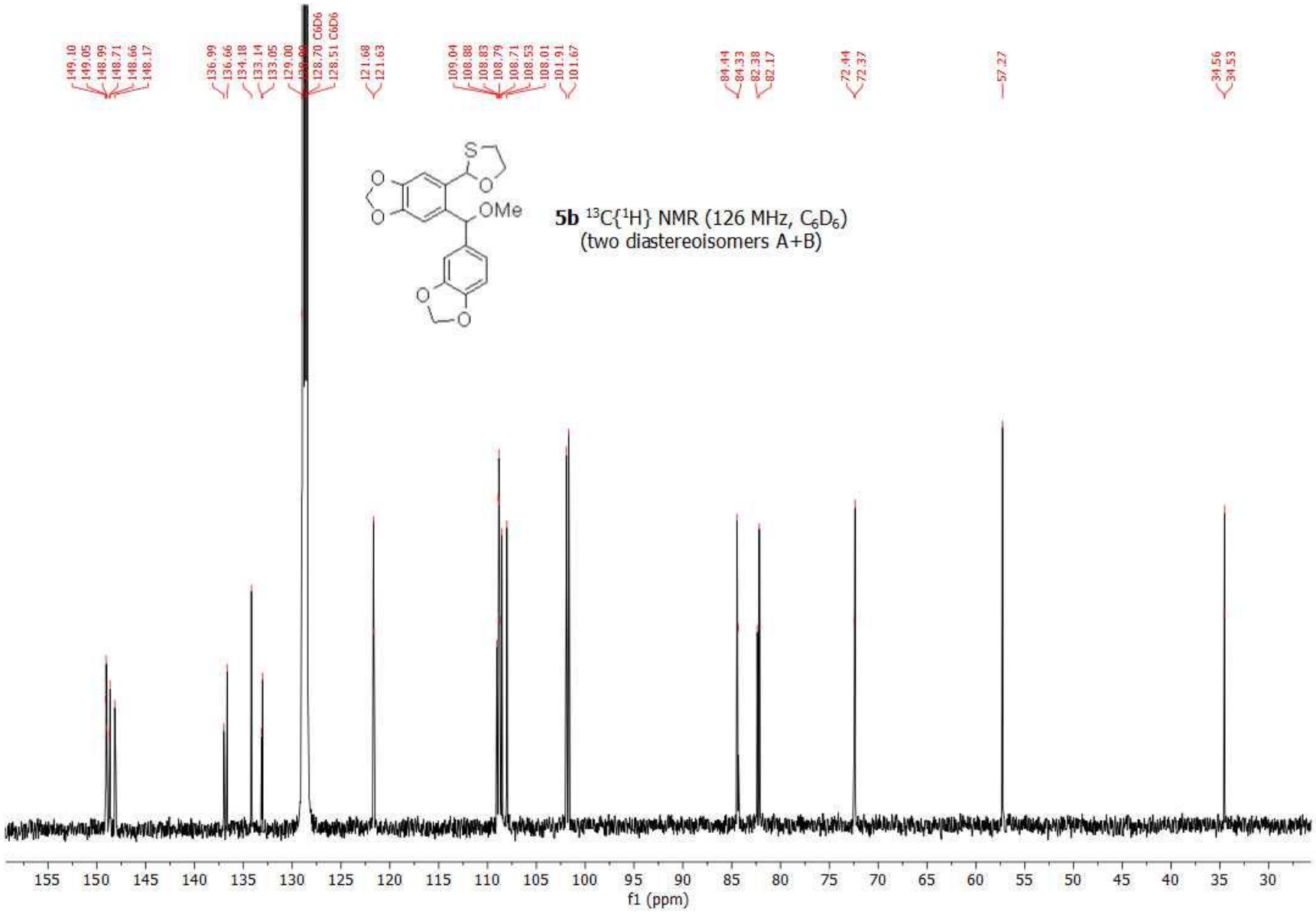
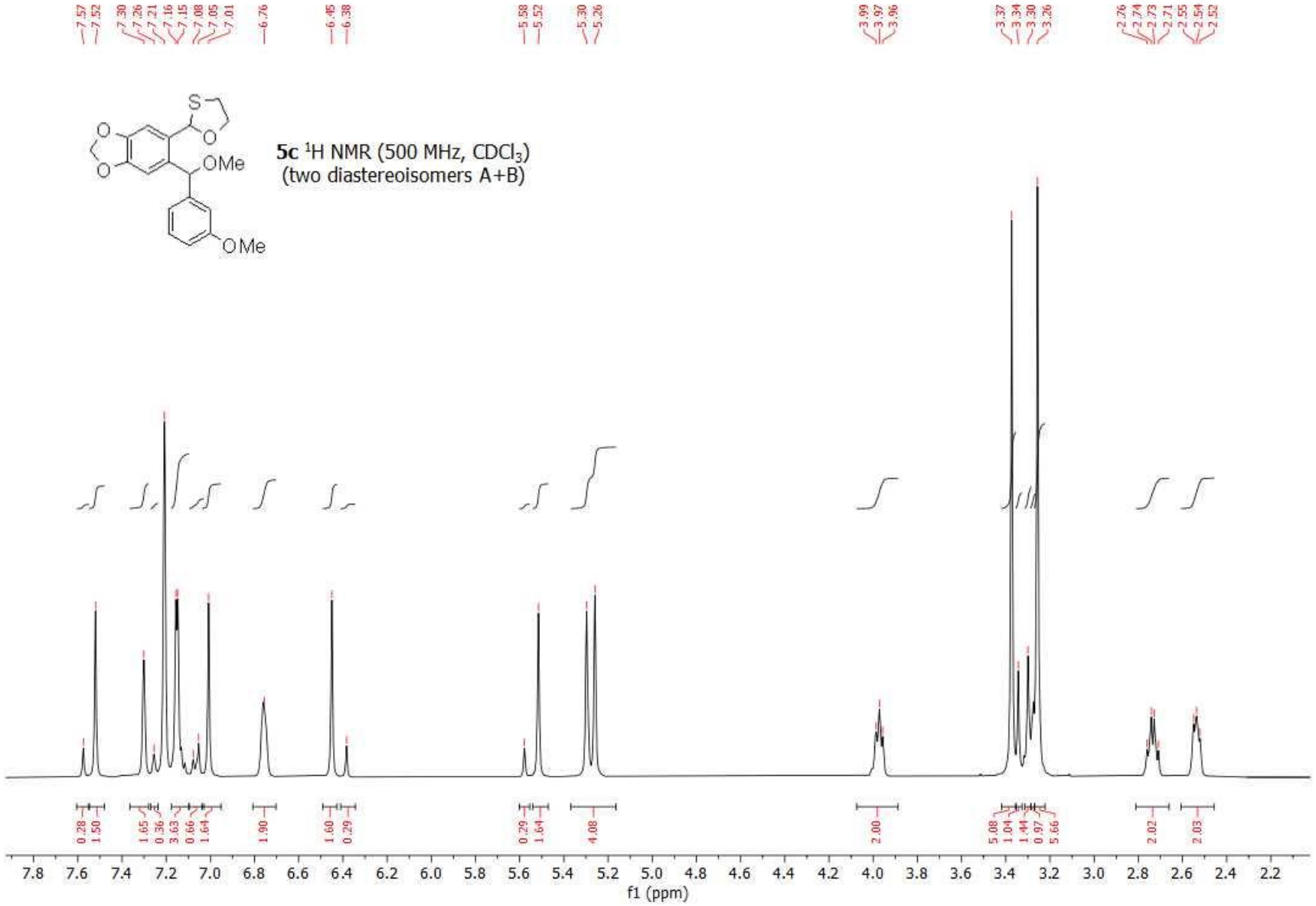
7.04
7.00
6.96
6.91
6.79
6.78
6.73
6.71
6.59
6.58
6.56
6.55
6.29
6.23
5.35
5.28
5.22
5.21
5.19
3.90
3.88
3.87
3.86
3.21
3.20
3.19
3.18
3.17
3.16
3.15
3.11
2.67
2.65
2.63
2.63
2.61
2.60
2.59
2.46
2.45
2.45
2.43
2.41
S
O
O
O
O
OMe
5b ¹H NMR (500 MHz, C6D6)
(two diastereoisomers A+B)
1.11
0.70
0.73
1.16
1.23
0.73
0.75
1.23
0.73
1.17
0.74
1.20
1.27
0.79
8.10
2.00
2.23
3.61
2.29
2.02
2.01
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 4.4 4.2 4.0 3.8 3.6 3.4 3.2 3.0 2.8 2.6 2.4 2.2 2.0
f1 (ppm)



5b $^{13}C\{^{1}H\}$ NMR (126 MHz, C_6D_6)
(two diastereoisomers A+B)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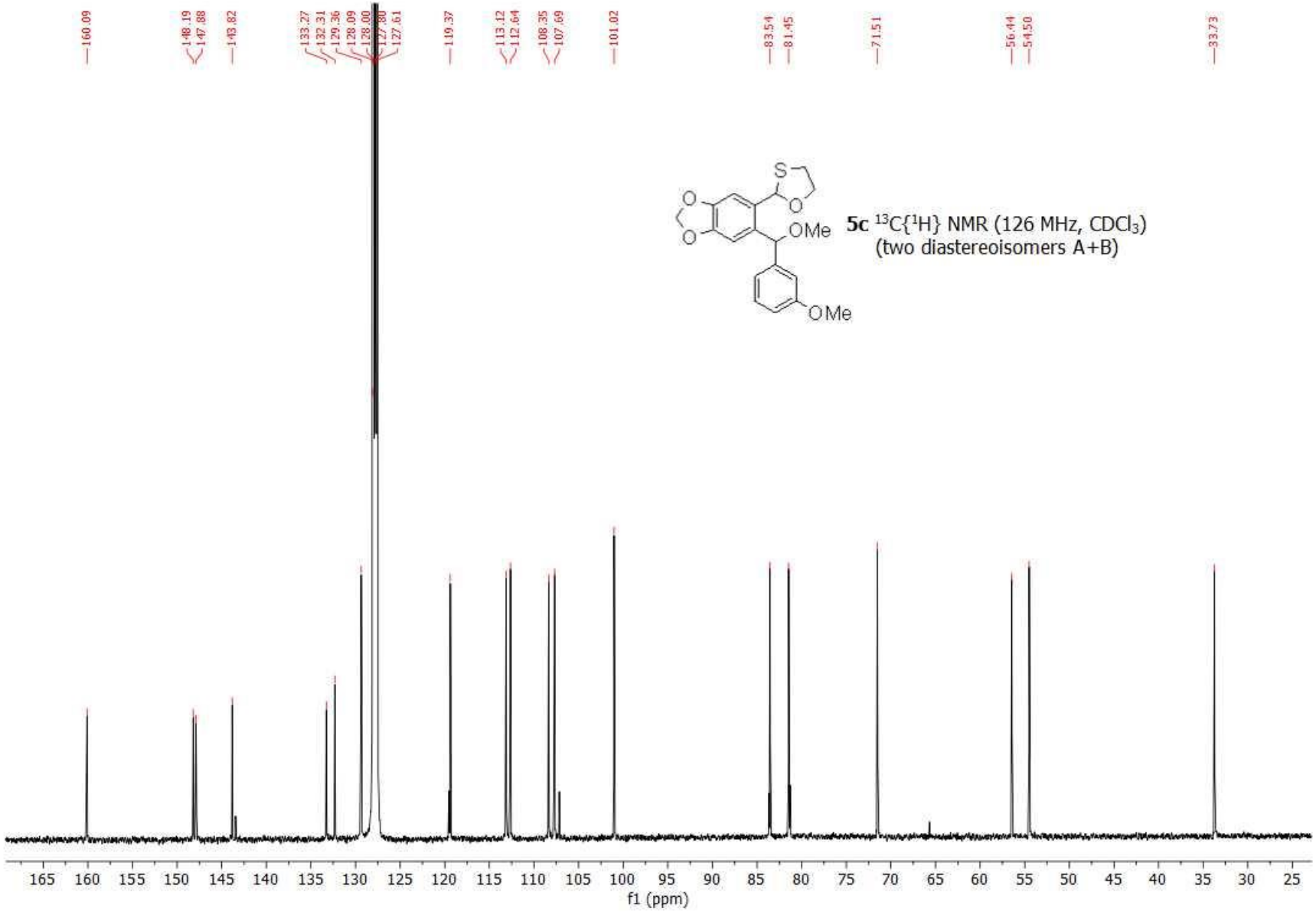
7.52
7.30
7.26
7.21
7.16
7.15
7.08
7.05
7.01
6.76
6.45
6.38
5.58
5.52
5.30
5.26
3.99
3.97
3.96
3.37
3.34
3.30
3.26
2.76
2.74
2.73
2.71
2.55
2.54
2.52
S
O
O
O
OMe
OMe
5c ¹H NMR (500 MHz, CDCl3)
(two diastereoisomers A+B)
0.28
1.50
1.65
0.36
3.63
0.66
1.64
1.90
1.60
0.29
0.29
1.64
4.08
2.00
5.08
1.04
1.44
0.97
5.66
2.02
2.03
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 4.4 4.2 4.0 3.8 3.6 3.4 3.2 3.0 2.8 2.6 2.4 2.2
f1 (ppm)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148.19
147.88
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133.27
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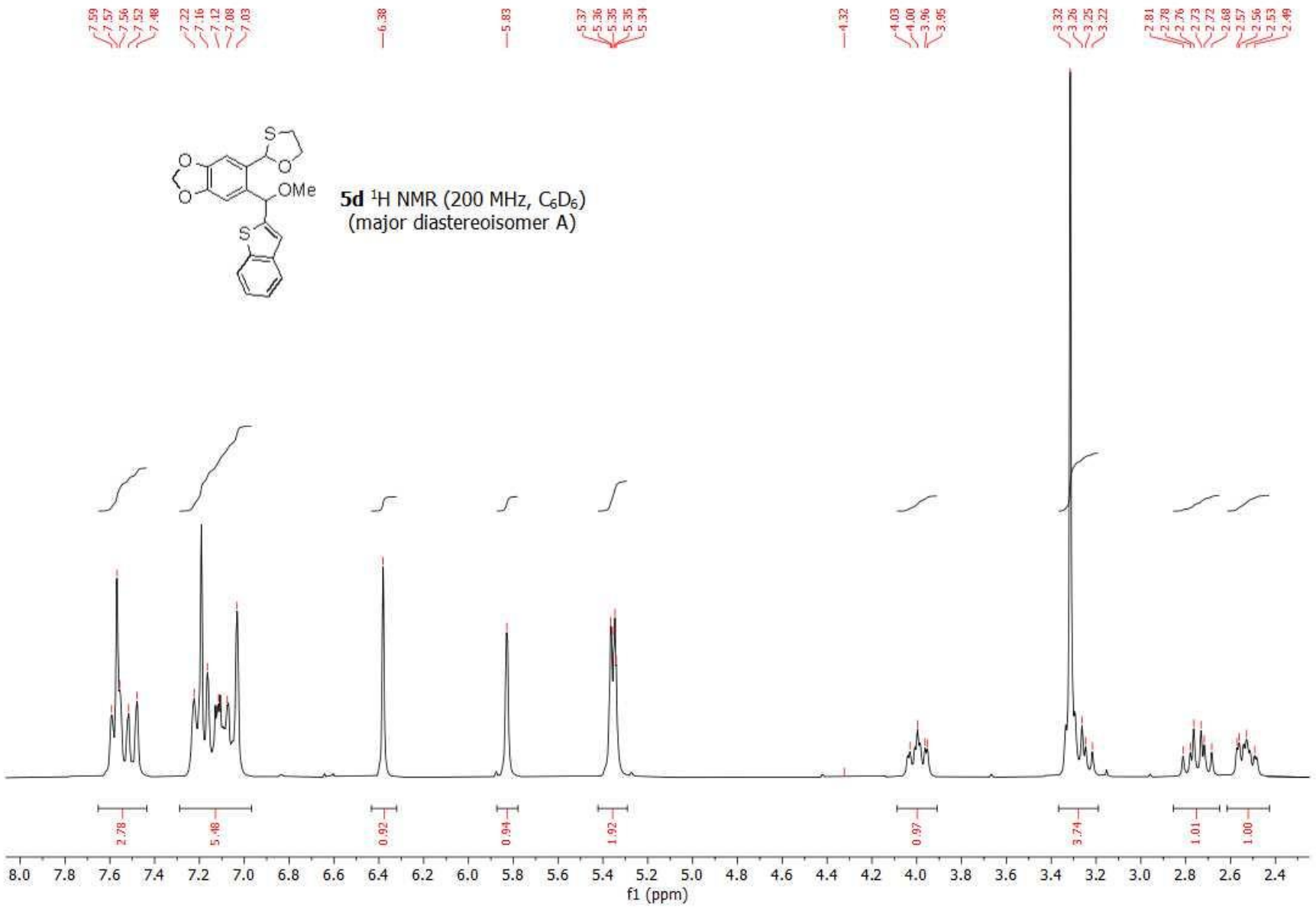
129.36
128.09
128.00
127.80
127.61
119.37
113.12
112.64
108.35
107.69
101.02
83.54
81.45
71.51
56.44
54.50
33.73
S
O
O
O
OMe
OMe
5c $^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$)
(two diastereoisomers A+B)
165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25
f1 (ppm)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7.52
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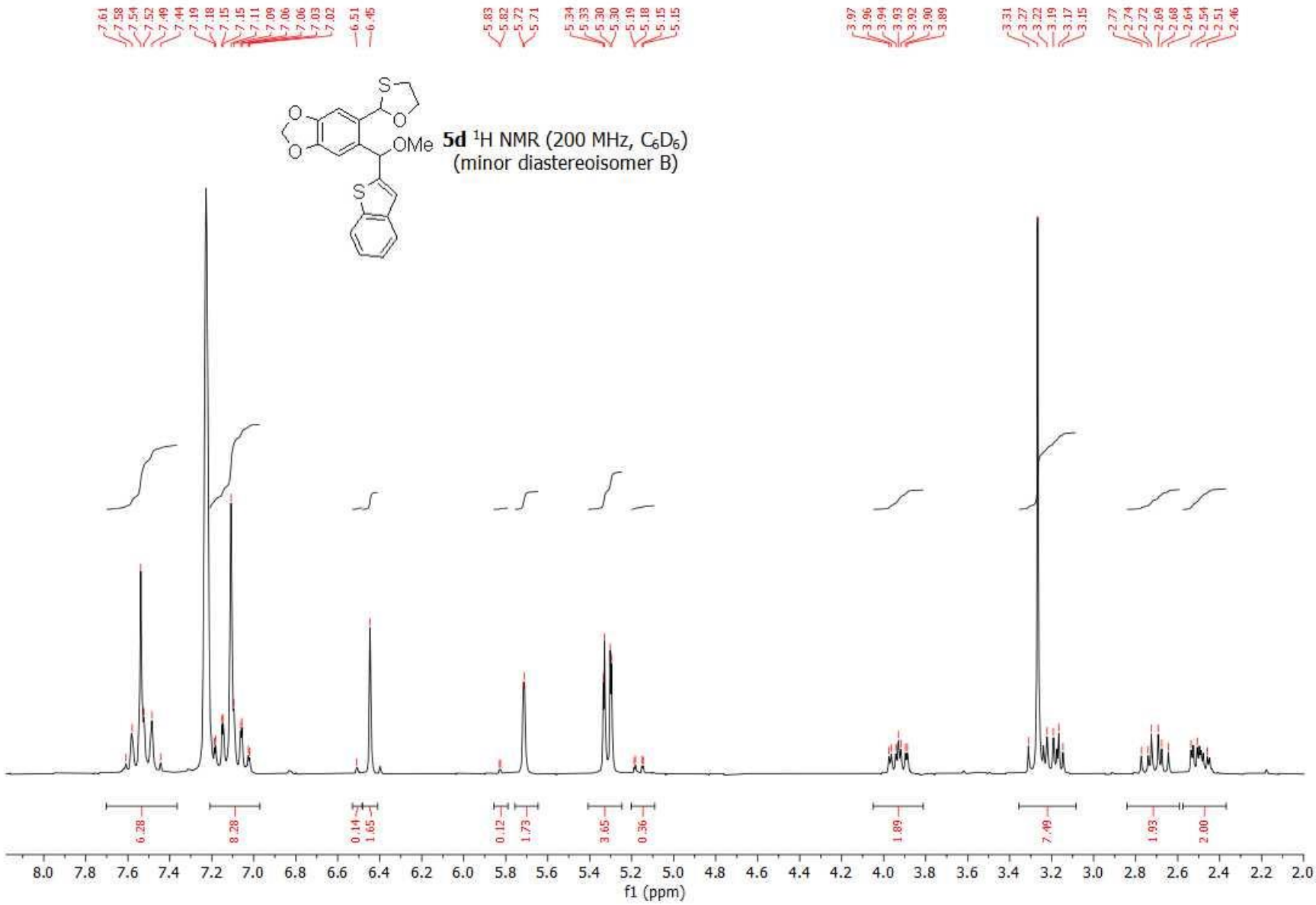
7.22
7.16
7.12
7.08
7.03
6.38
5.83
5.37
5.36
5.35
5.35
5.34
4.32
4.03
4.00
3.96
3.95
3.32
3.26
3.25
3.22
2.81
2.78
2.76
2.73
2.72
2.68
2.57
2.56
2.53
2.49
S
O
O
O
OMe
S
5d 1H NMR (200 MHz, C6D6)
(major diastereoisomer A)
2.78
5.48
0.92
0.94
1.92
0.97
3.74
1.01
1.00
8.0 7.8 7.6 7.4 7.2 7.0 6.8 6.6 6.4 6.2 6.0 5.8 5.6 5.4 5.2 5.0 4.8 4.6 4.4 4.2 4.0 3.8 3.6 3.4 3.2 3.0 2.8 2.6 2.4
f1 (ppm)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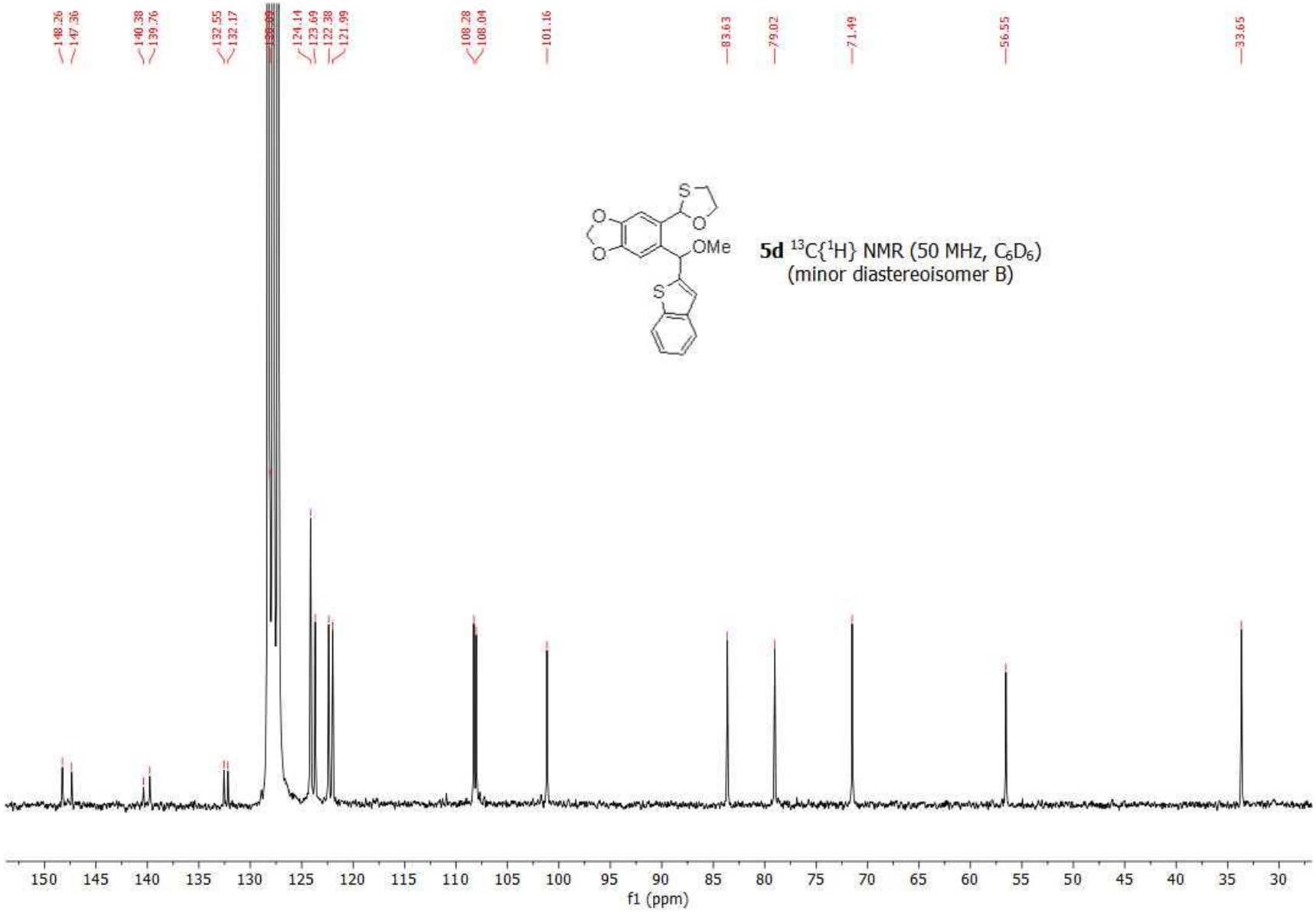
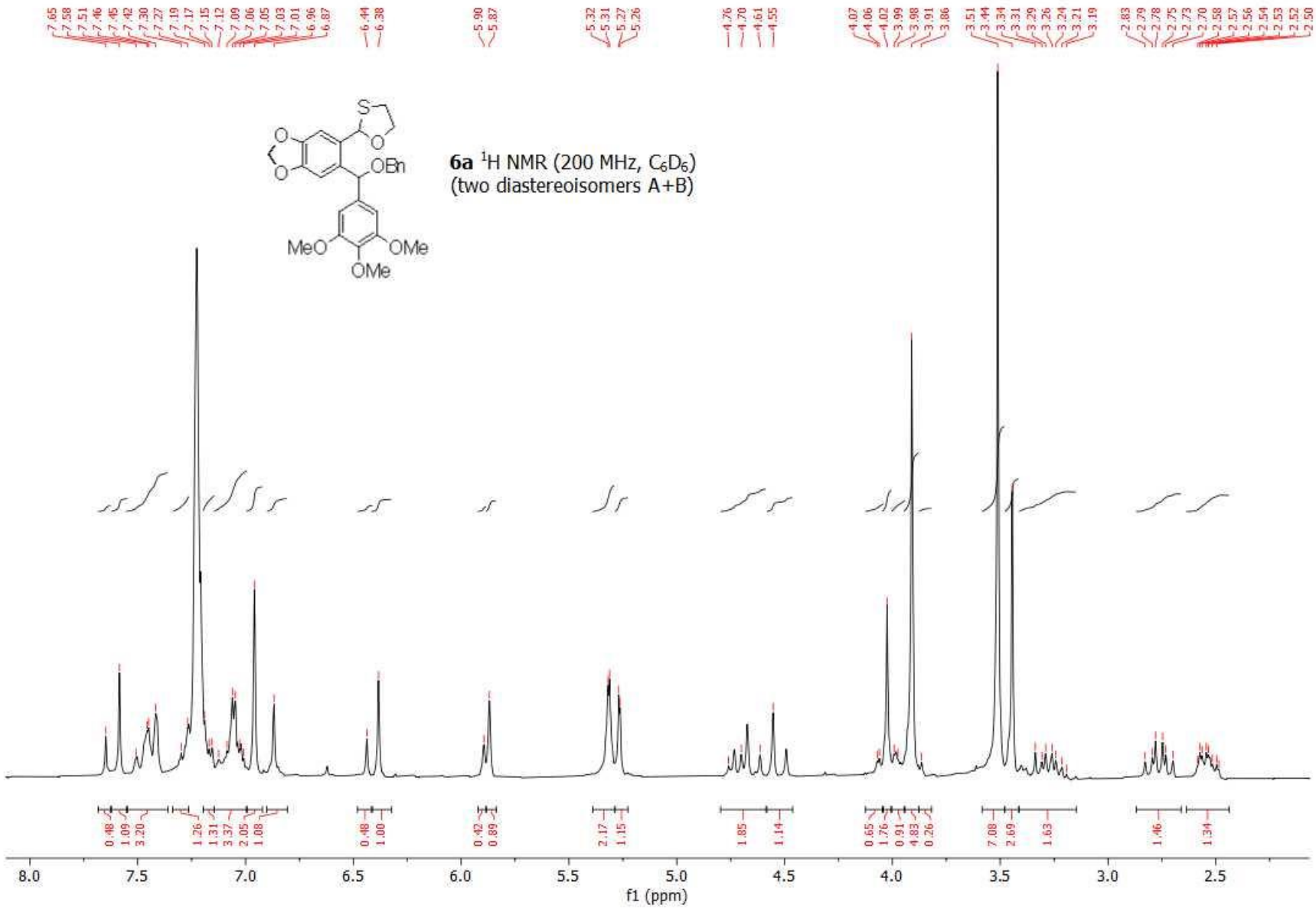
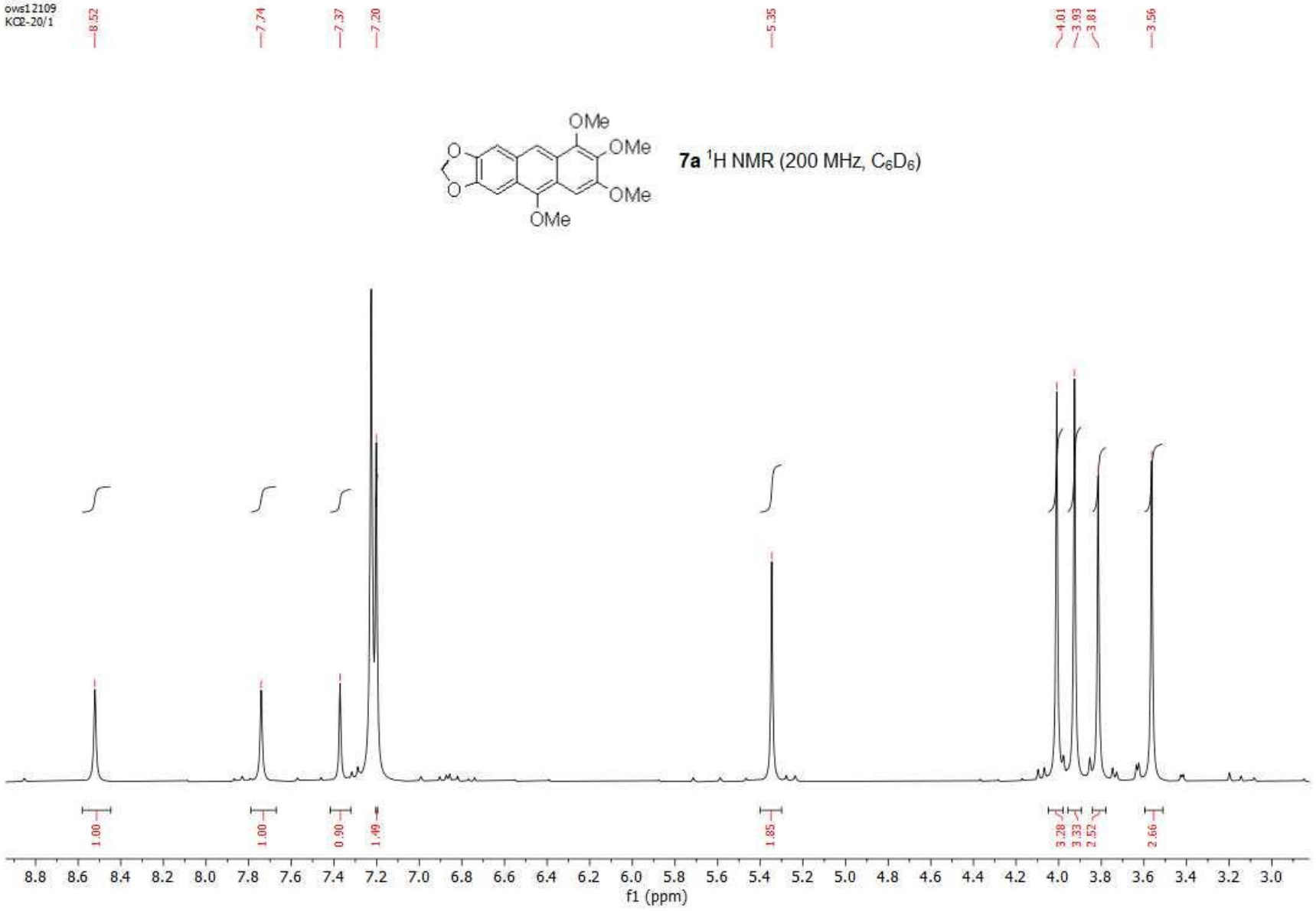
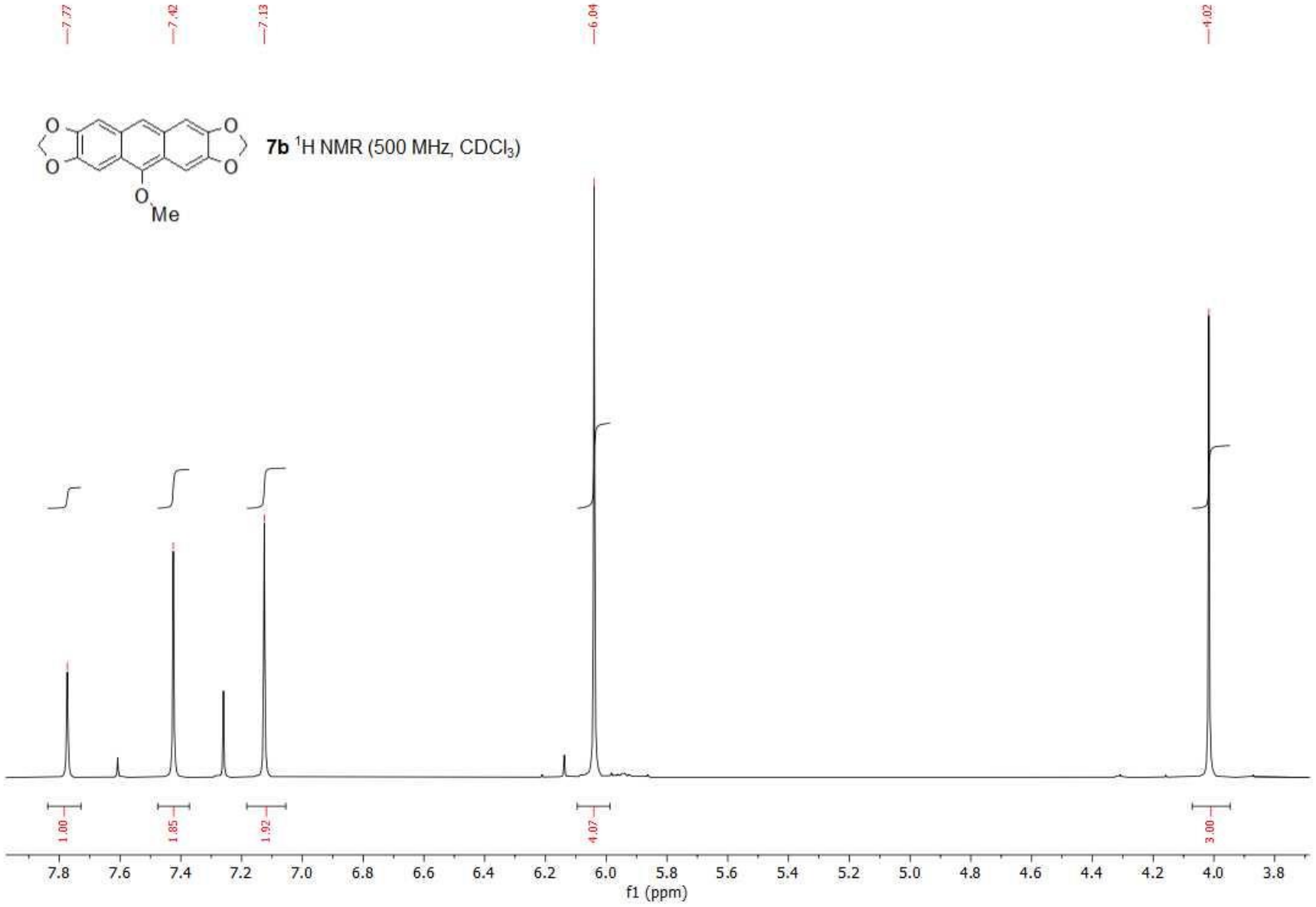
7.52
7.49
7.44
7.19
7.18
7.15
7.15
7.11
7.09
7.06
7.06
7.03
7.02
6.51
6.45
5.83
5.82
5.72
5.71
5.34
5.33
5.30
5.30
5.19
5.18
5.15
5.15
3.97
3.96
3.94
3.93
3.92
3.90
3.89
3.31
3.27
3.22
3.19
3.17
3.15
2.77
2.74
2.72
2.69
2.68
2.64
2.54
2.51
2.46
S
O
O
O
OMe
S
5d 1H NMR (200 MHz, C6D6)
(minor diastereoisomer B)
6.28
8.28
0.14
1.65
0.12
1.73
3.65
0.36
1.89
7.49
1.93
2.00
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 4.4 4.2 4.0 3.8 3.6 3.4 3.2 3.0 2.8 2.6 2.4 2.2 2.0
f1 (ppm)

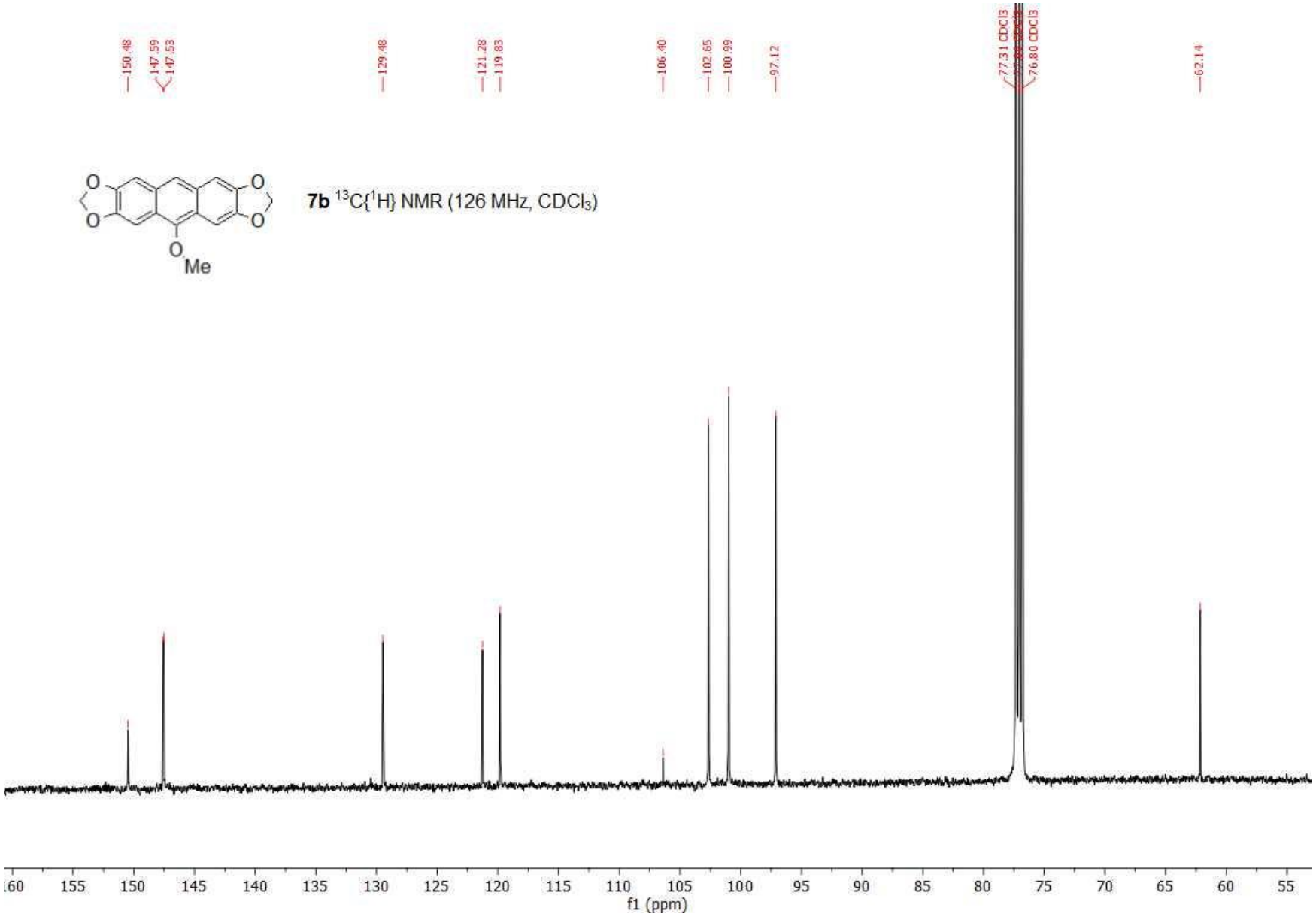


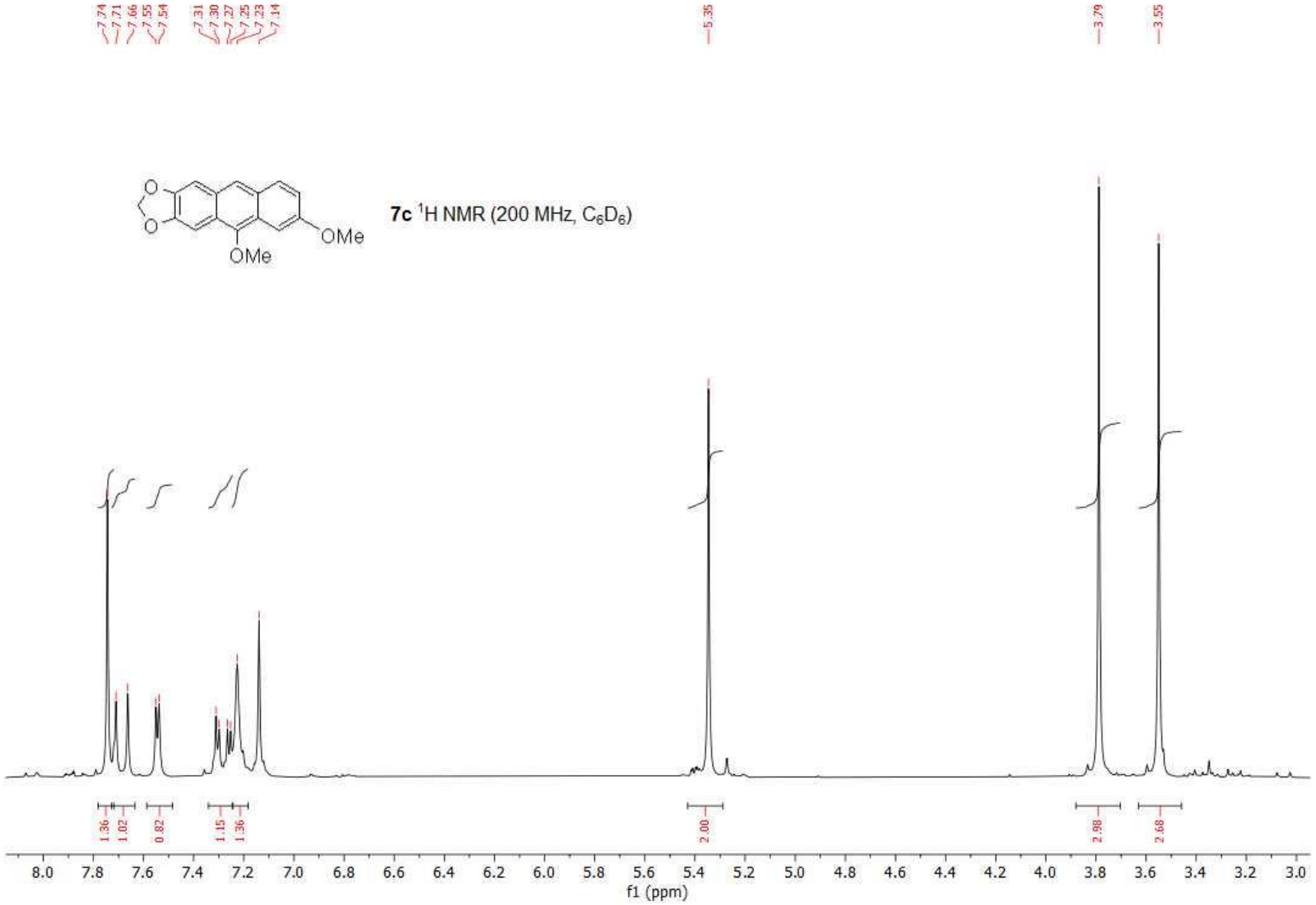
5d $^{13}C\{^{1}H\}$ NMR (50 MHz, C_6D_6)
(minor diastereoisomer B)

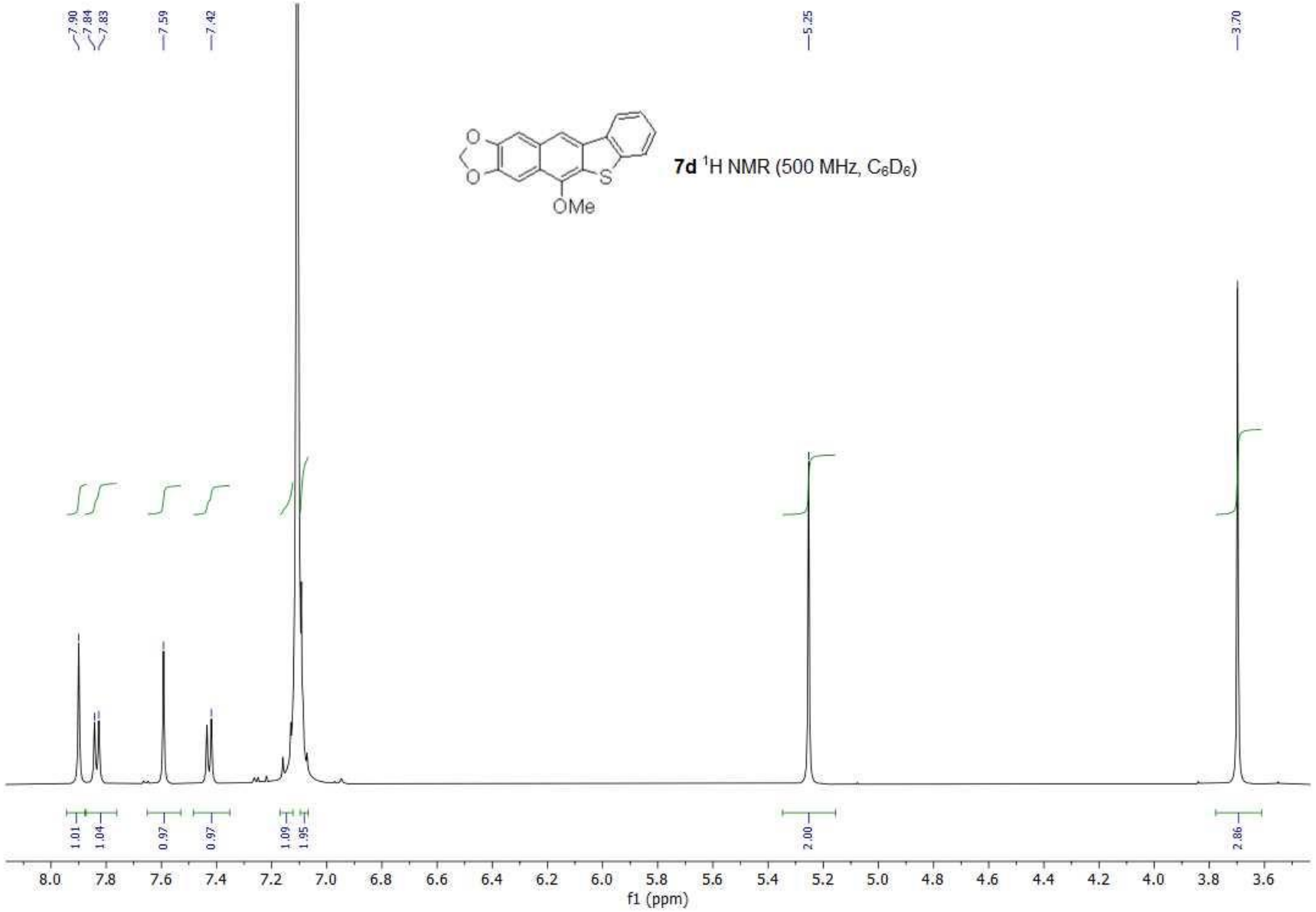

7.65
7.58
7.51
7.46
7.45
7.42
7.30
7.27
7.19
7.17
7.15
7.12
7.09
7.06
7.05
7.03
7.01
6.96
6.87
6.44
6.38
5.90
5.87
5.32
5.31
5.27
5.26
4.76
4.70
4.61
4.55
4.07
4.06
4.02
3.99
3.98
3.91
3.86
3.51
3.44
3.34
3.31
3.29
3.26
3.24
3.21
3.19
2.83
2.79
2.78
2.75
2.73
2.70
2.58
2.57
2.56
2.54
2.53
2.52
2.50
S
O
O
O
OBn
MeO
OMe
OMe
6a ¹H NMR (200 MHz, C6D6)
(two diastereoisomers A+B)
0.48
1.09
3.20
1.26
1.31
3.37
2.05
1.08
0.48
1.00
0.42
0.89
2.17
1.15
1.85
1.14
0.65
1.76
0.91
4.83
0.26
7.08
2.69
1.63
1.46
1.34
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
f1 (ppm)

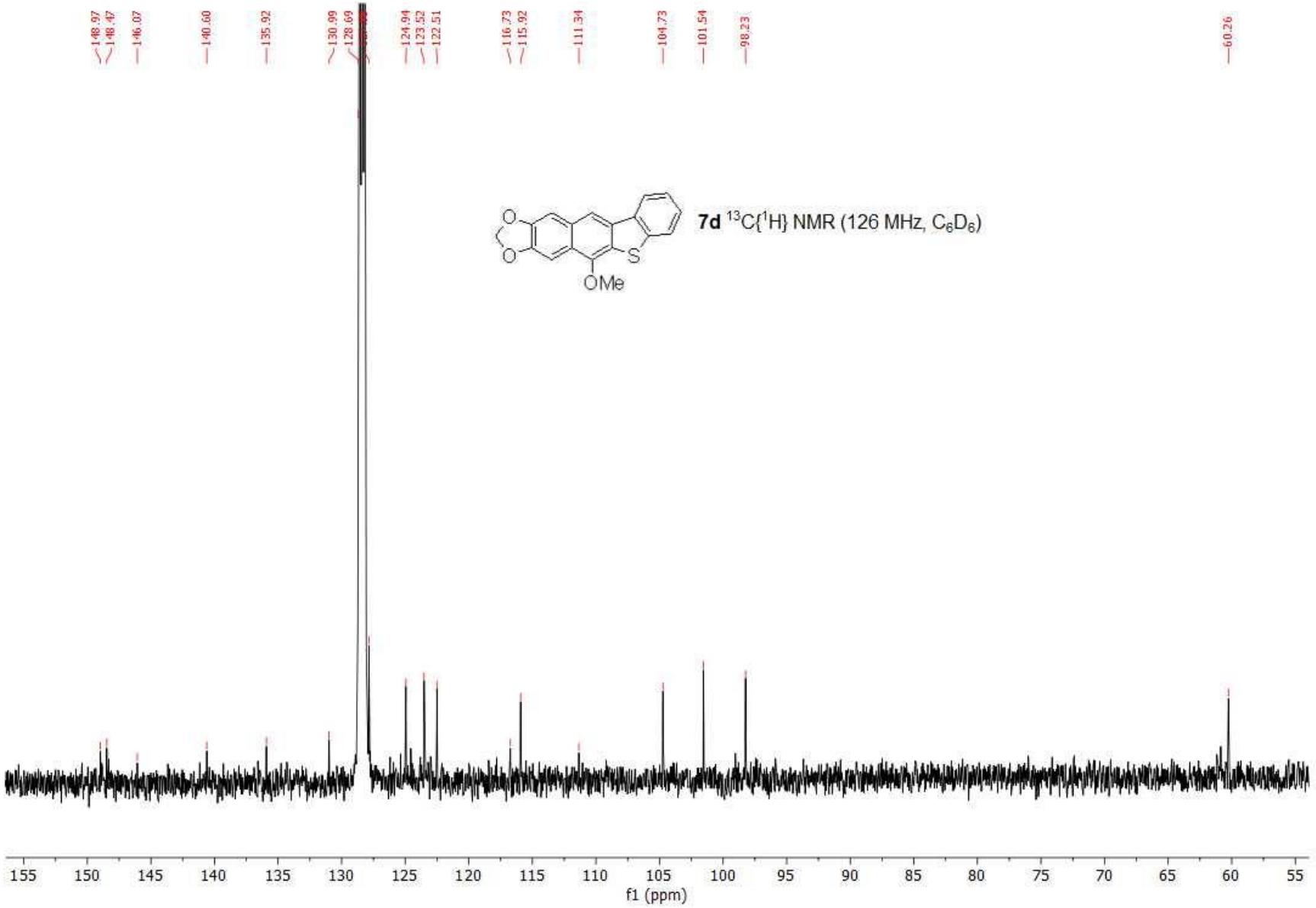

ows12109
KC2-20/1
8.52
7.74
7.37
7.20
5.35
4.01
3.93
3.81
3.56
OMe
OMe
OMe
OMe
O
O
7a ^{1}H NMR (200 MHz, C_6D_6)
1.00
1.00
0.90
1.49
1.85
3.28
3.33
2.52
2.66
8.8 8.6 8.4 8.2 8.0 7.8 7.6 7.4 7.2 7.0 6.8 6.6 6.4 6.2 6.0 5.8 5.6 5.4 5.2 5.0 4.8 4.6 4.4 4.2 4.0 3.8 3.6 3.4 3.2 3.0
f1 (ppm)


7.77
7.42
7.13
6.04
4.02
O
O
O
O
O
Me
7b ^{1}H NMR (500 MHz, $CDCl_3$)
1.00
1.85
1.92
4.07
3.00
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
4.4
4.2
4.0
3.8
f1 (ppm)

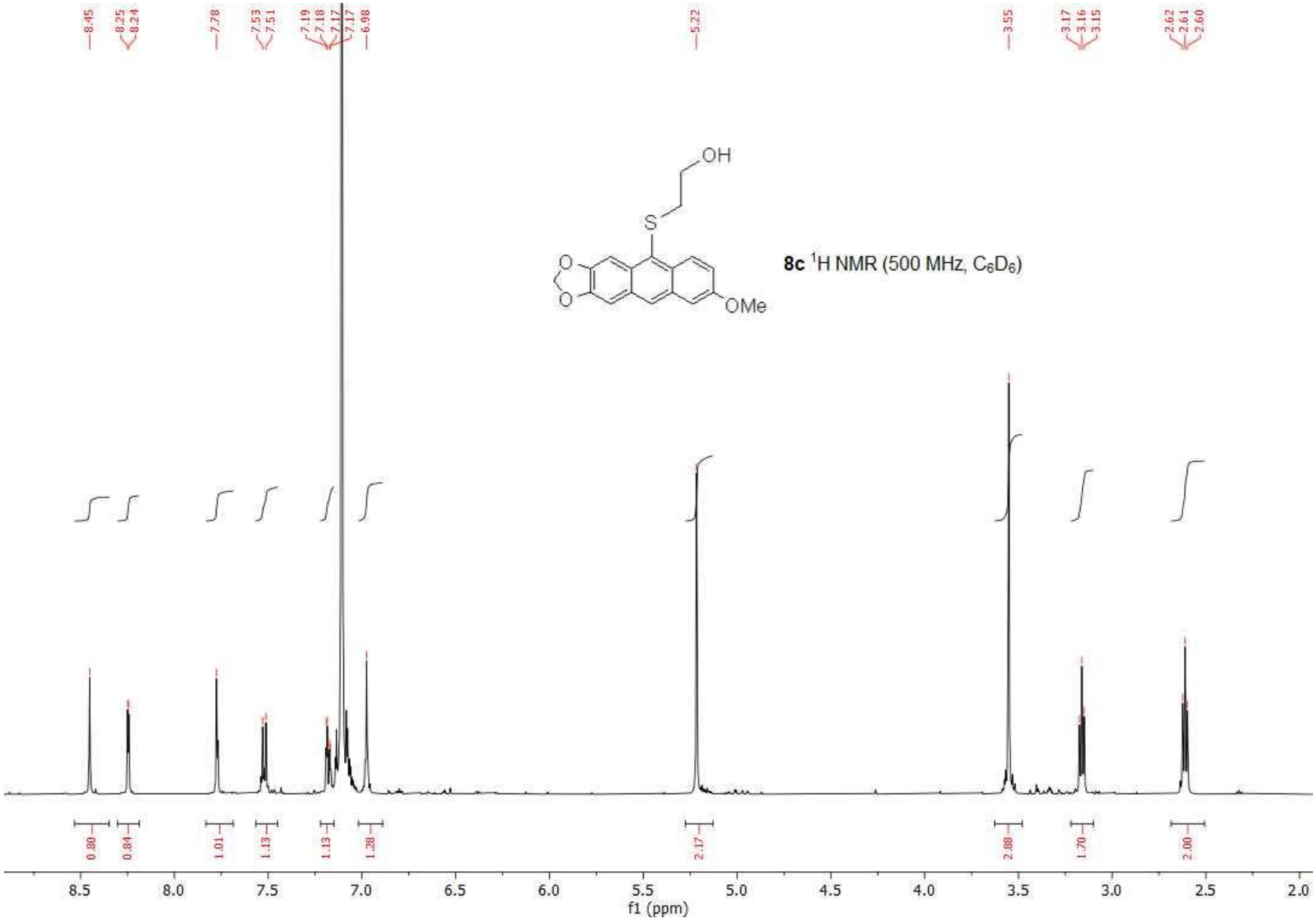

150.48
147.59
147.53
129.48
121.28
119.83
106.40
102.65
100.99
97.12
77.31 CDCl3
76.80 CDCl3
62.14
O
O
O
O
O
Me
7b $^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$)
160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55
f1 (ppm)


7.74
7.71
7.66
7.55
7.54
7.31
7.30
7.27
7.25
7.23
7.14
5.35
3.79
3.55
OMe
OMe
7c ¹H NMR (200 MHz, C6D6)
1.36
1.02
0.82
1.15
1.36
2.00
2.98
2.68
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 4.4 4.2 4.0 3.8 3.6 3.4 3.2 3.0
f1 (ppm)

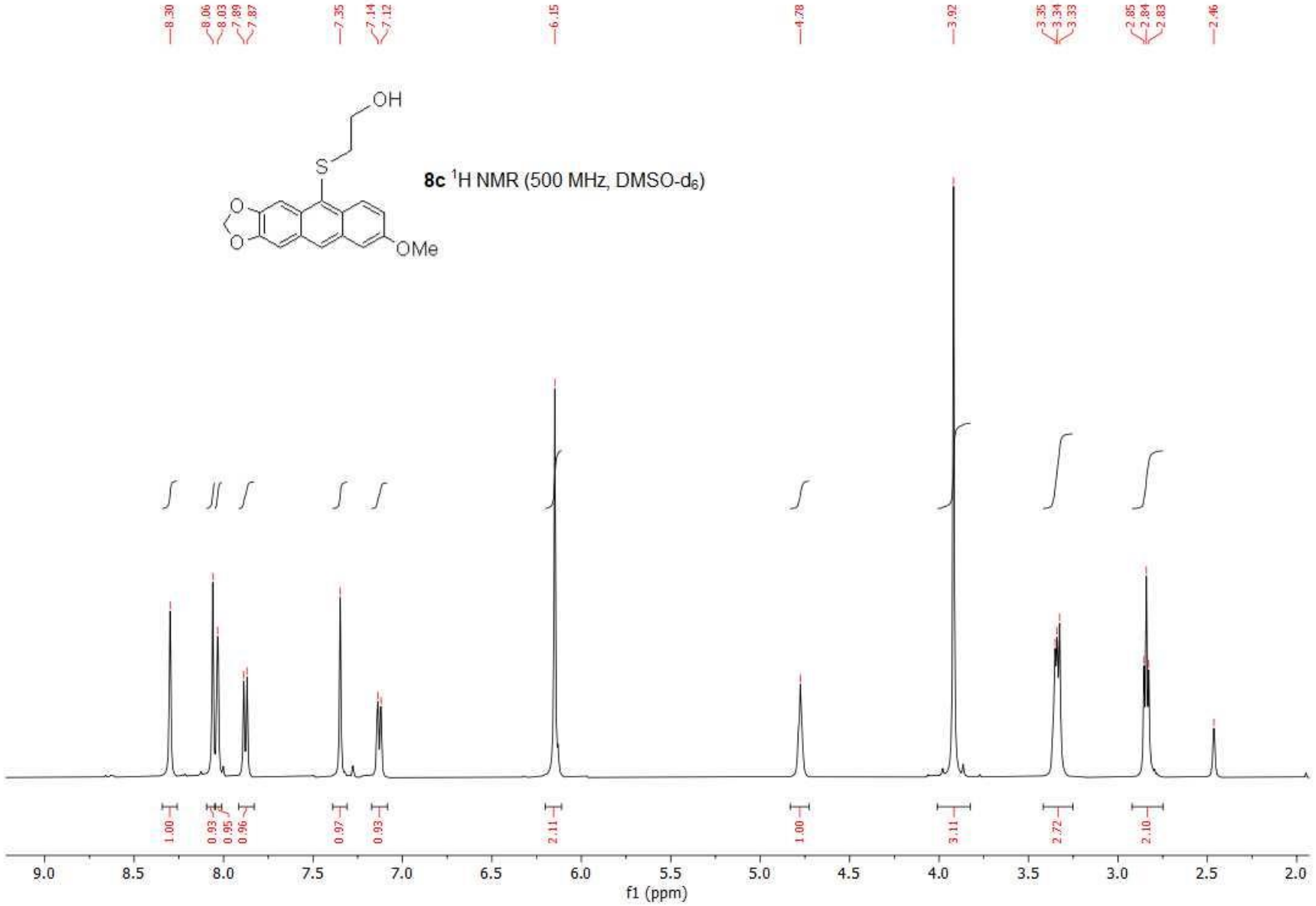

7.90
7.84
7.83
7.59
7.42
5.25
3.70
OMe
7d ^{1}H NMR (500 MHz, C_6D_6)
1.01
1.04
0.97
0.97
1.09
1.95
2.00
2.86
8.0
7.8
7.6
7.4
7.2
7.0
6.8
6.6
6.4
6.2
6.0
5.8
5.6
5.4
5.2
5.0
4.8
4.6
4.4
4.2
4.0
3.8
3.6
f1 (ppm)

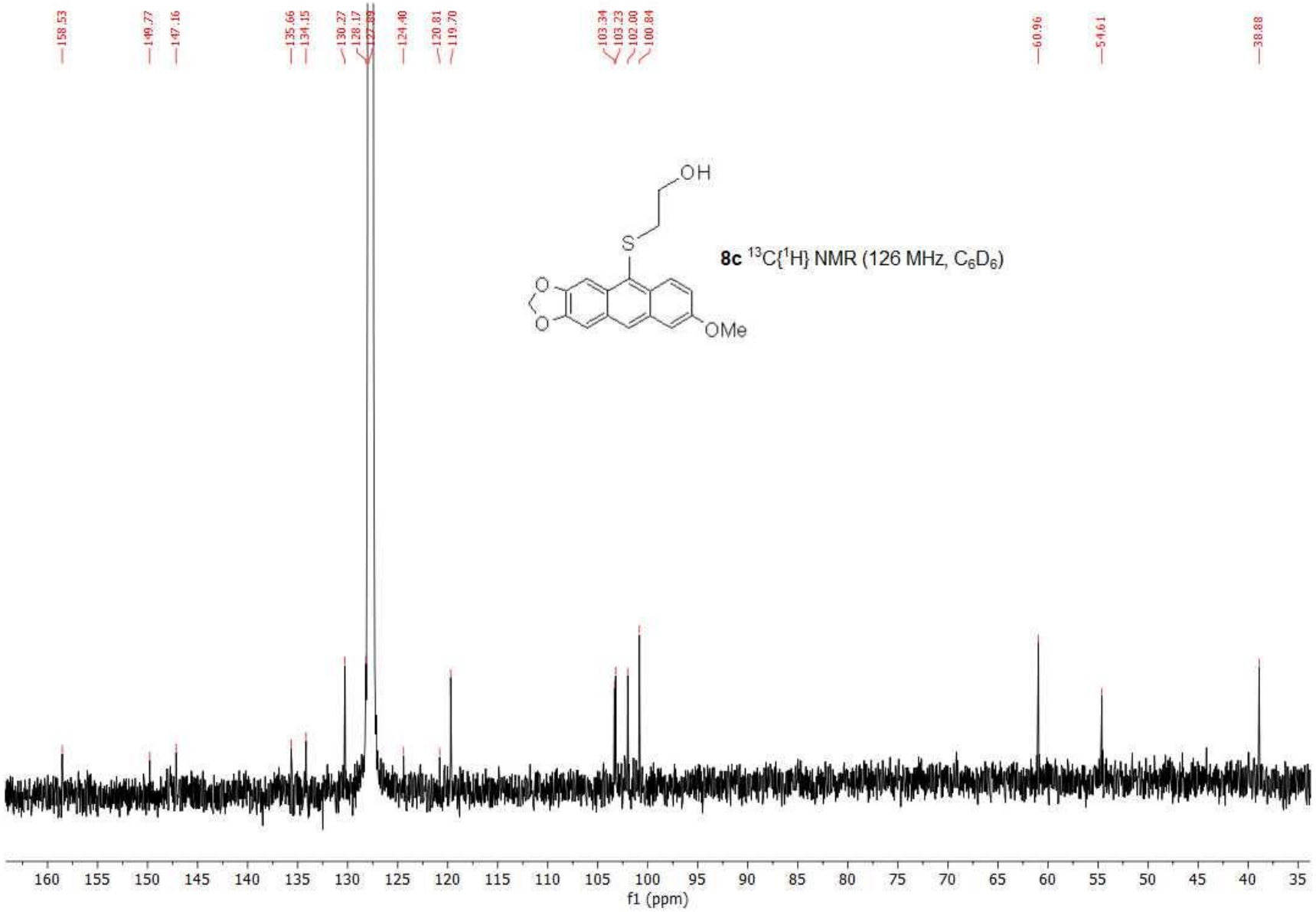


7d $^{13}C\{^{1}H\}$ NMR (126 MHz, C_6D_6)

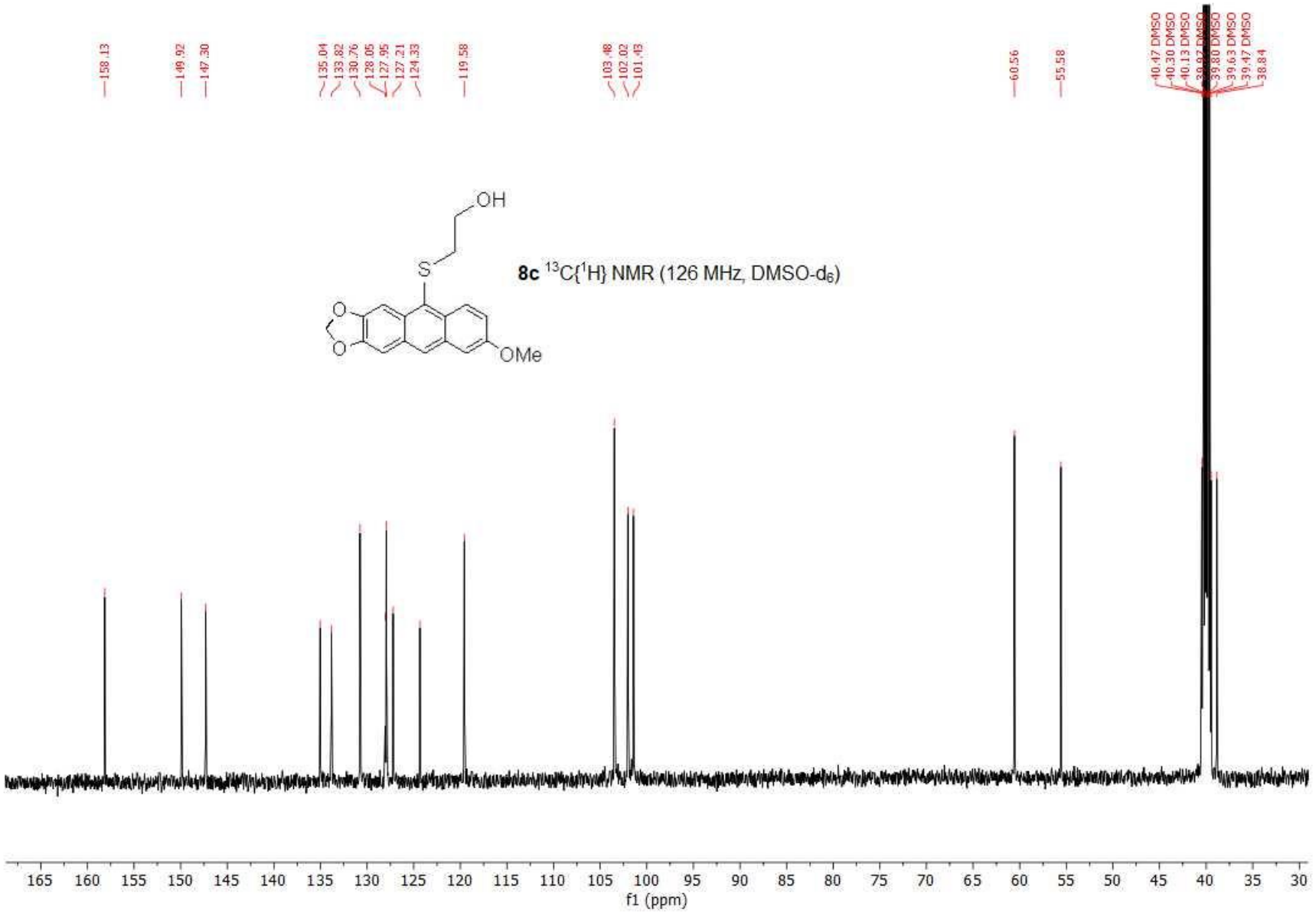


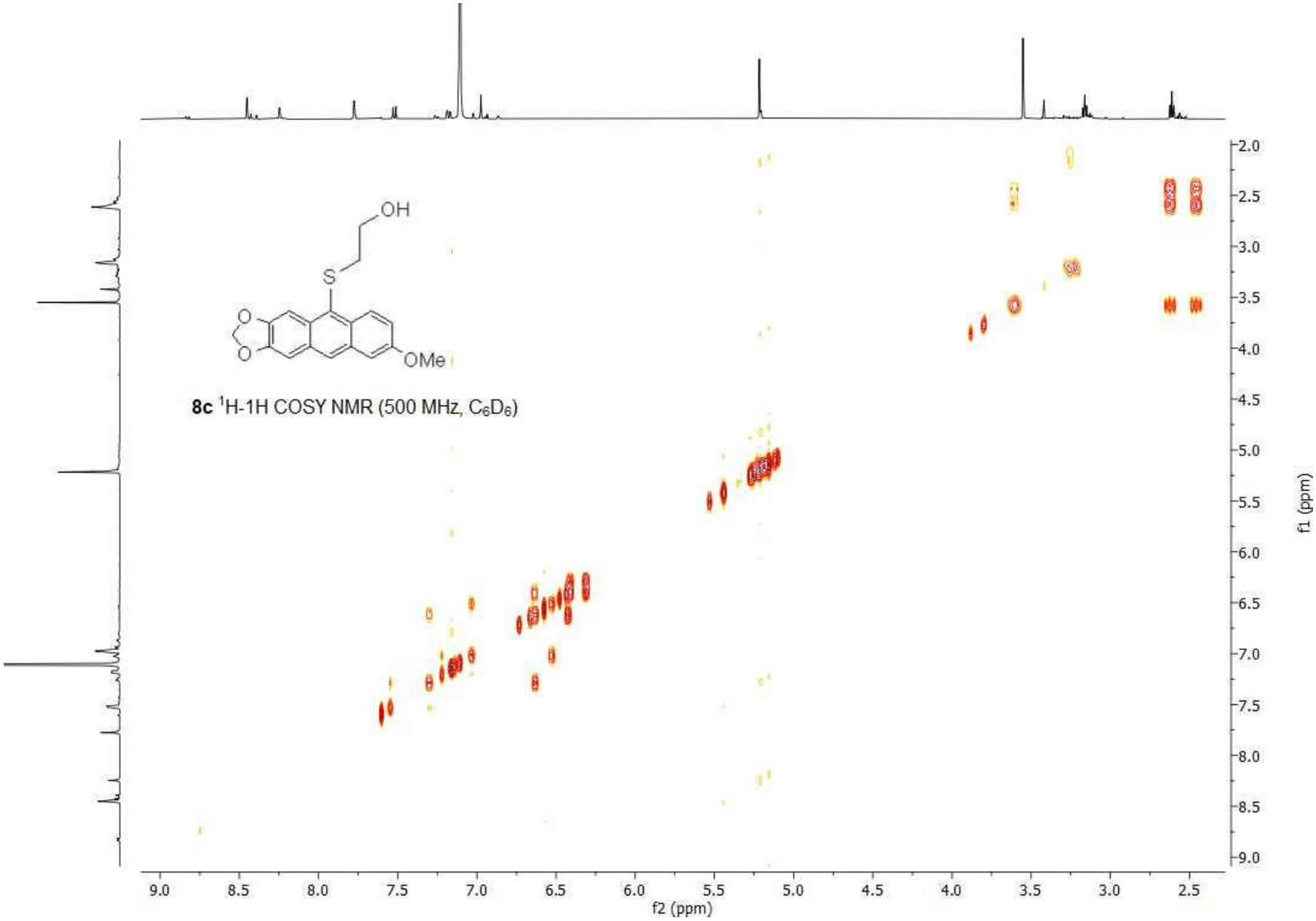
8c ^{1}H NMR (500 MHz, C_6D_6)

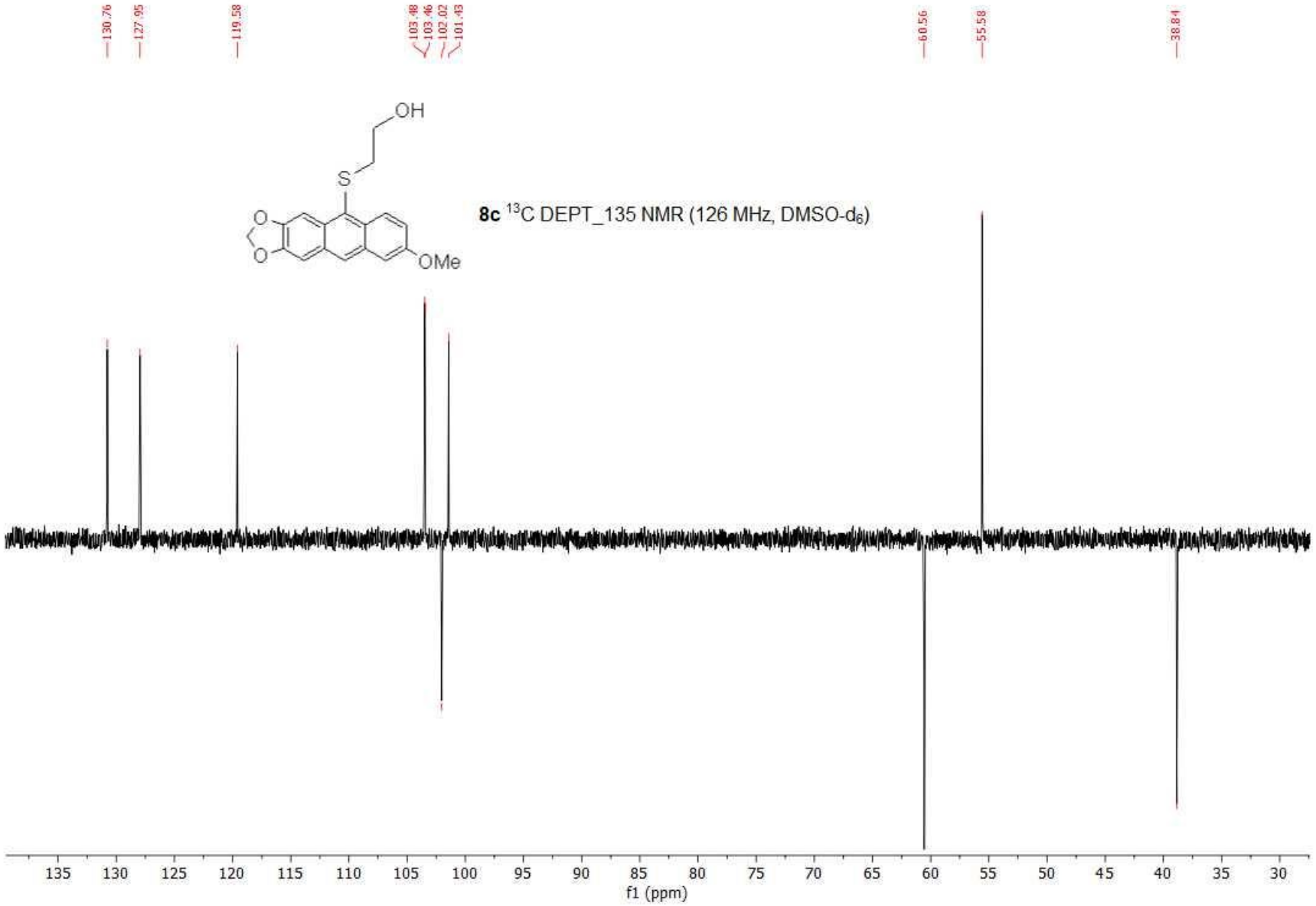

8.30
8.06
8.03
7.89
7.87
7.35
7.14
7.12
6.15
4.78
3.92
3.35
3.34
3.33
2.85
2.84
2.83
2.46
OH
S
O
O
OMe
8c ^{1}H NMR (500 MHz, DMSO-d$_6$)
1.00
0.93
0.95
0.96
0.97
0.93
2.11
1.00
3.11
2.72
2.10
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
f1 (ppm)

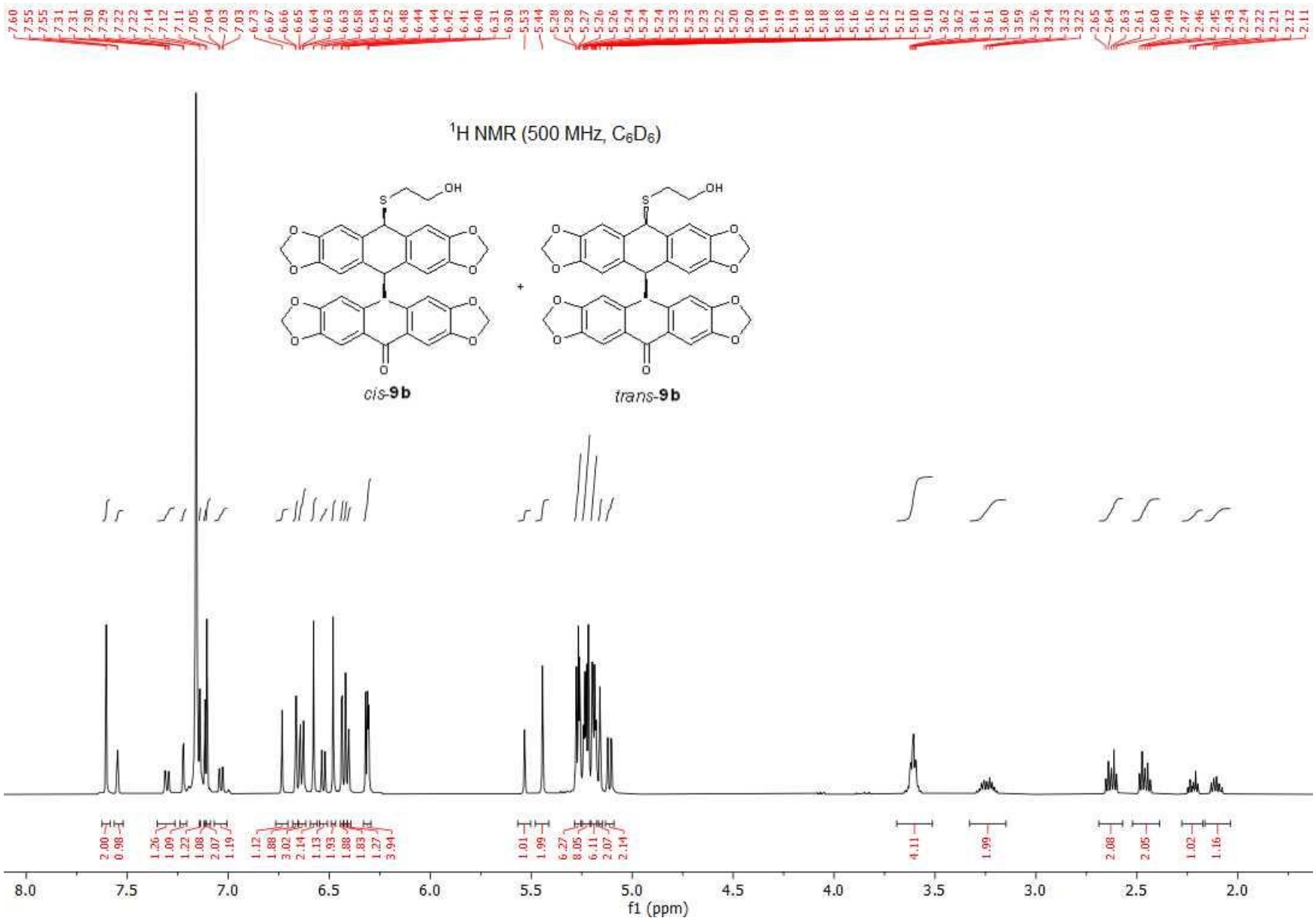


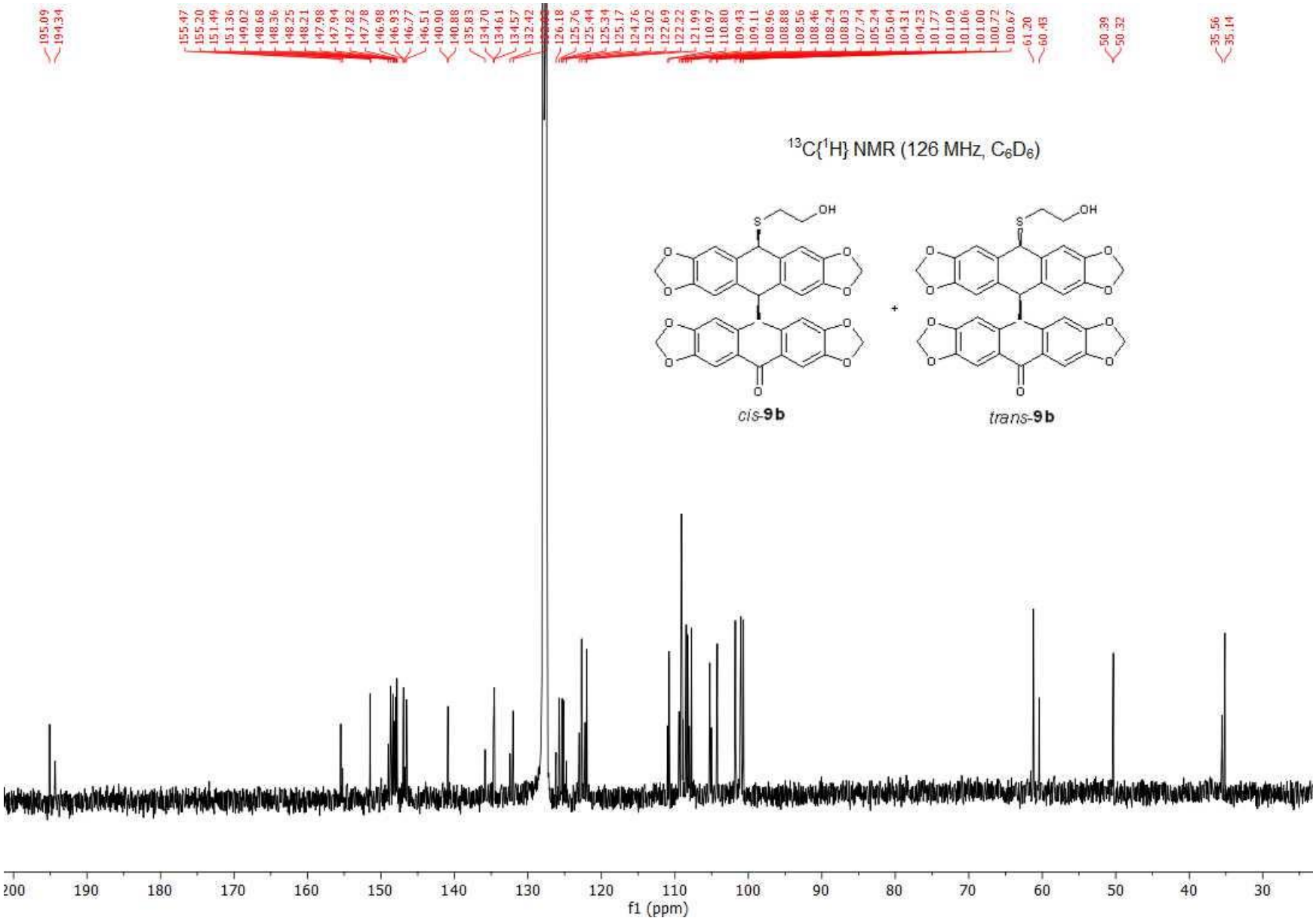
8c $^{13}C\{^{1}H\}$ NMR (126 MHz, C_6D_6)

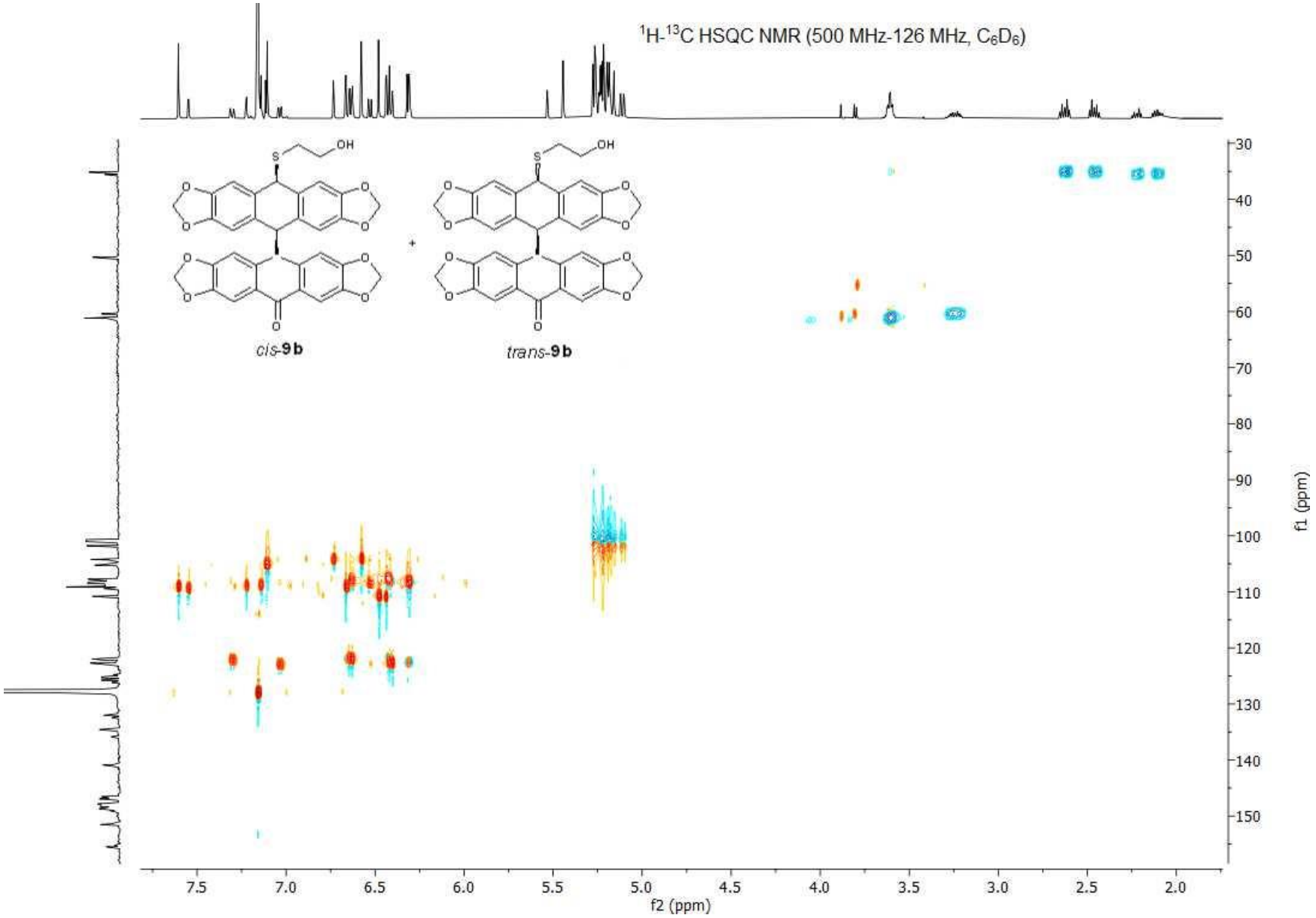

158.13
149.92
147.30
135.04
133.82
130.76
128.05
127.95
127.21
124.33
119.58
103.48
102.02
101.43
60.56
55.58
40.47 DMSO
40.30 DMSO
40.13 DMSO
39.97 DMSO
39.80 DMSO
39.63 DMSO
39.47 DMSO
38.84
OH
S
O
O
OMe
8c $^{13}C\{^{1}H\}$ NMR (126 MHz, DMSO-d_6)
165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30
f1 (ppm)

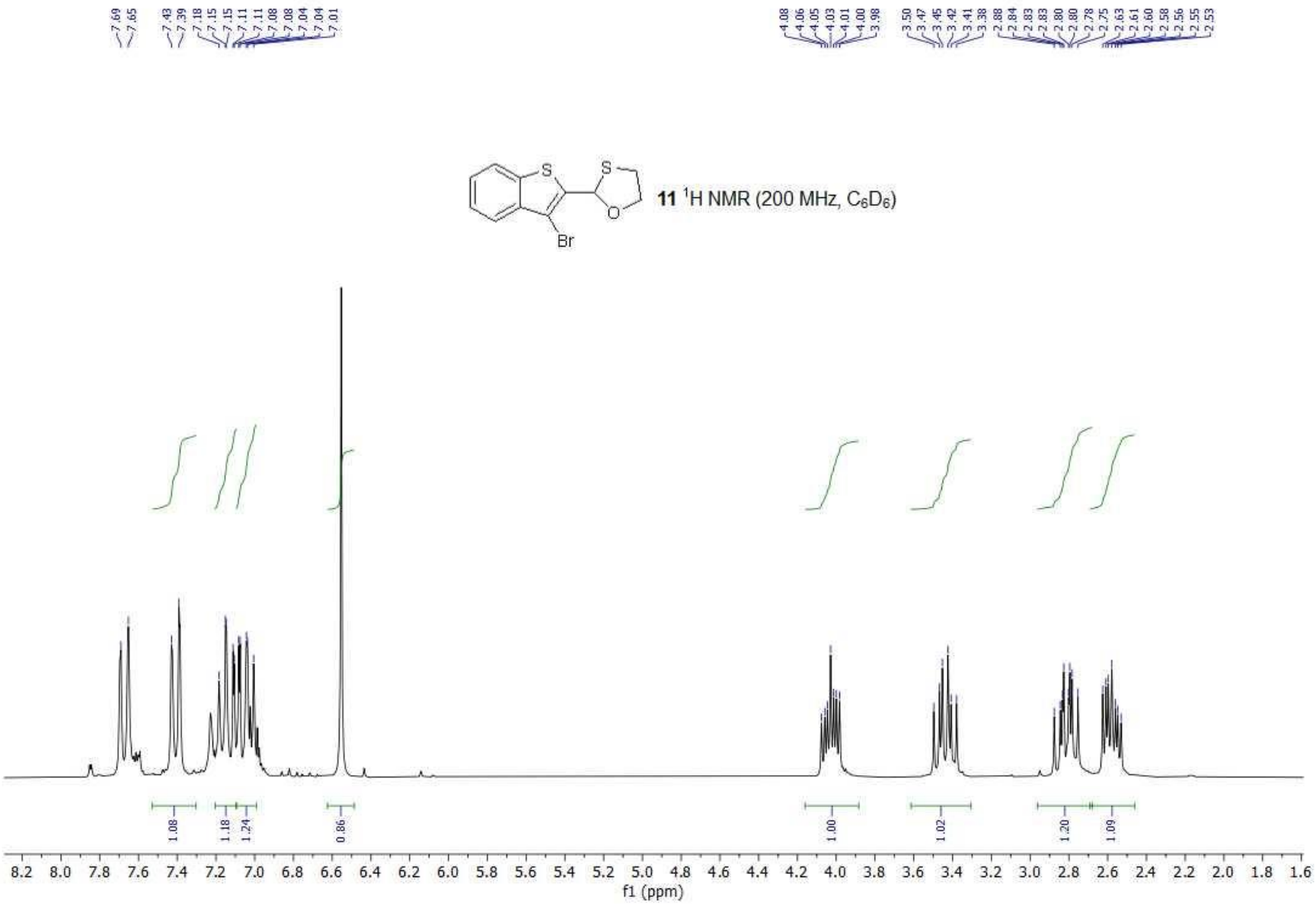

OH
S
O
O
OMe
8c ^{1}H-1H COSY NMR (500 MHz, C_6D_6)
f2 (ppm)
f1 (ppm)

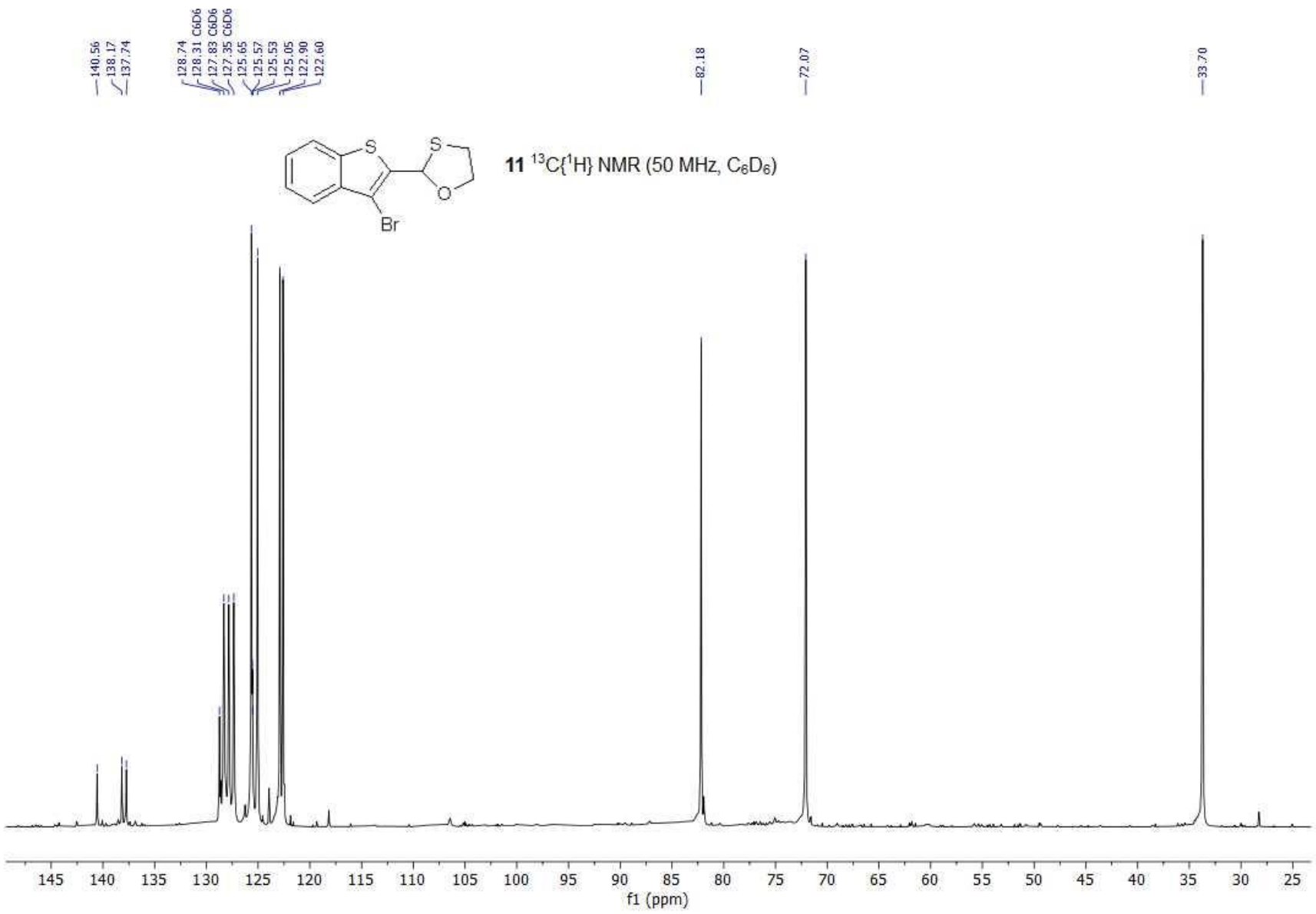

130.76
127.95
119.58
103.48
103.46
102.02
101.43
60.56
55.58
38.84
OH
S
O
O
OMe
8c ^{13}C DEPT_135 NMR (126 MHz, DMSO-d$_6$)
135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30
f1 (ppm)

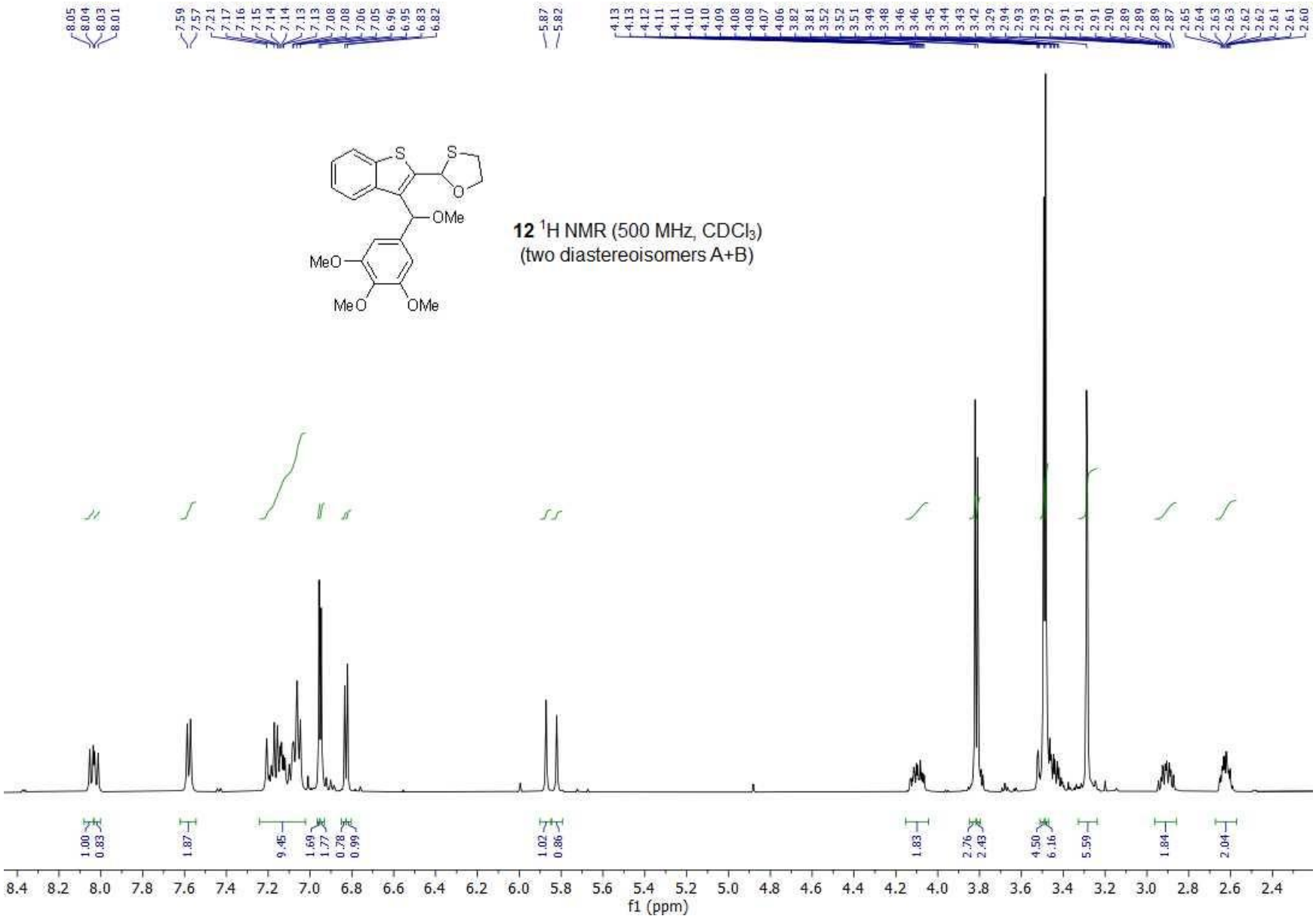

^{1}H NMR (500 MHz, C_6D_6)
cis-9b
trans-9b
f1 (ppm)

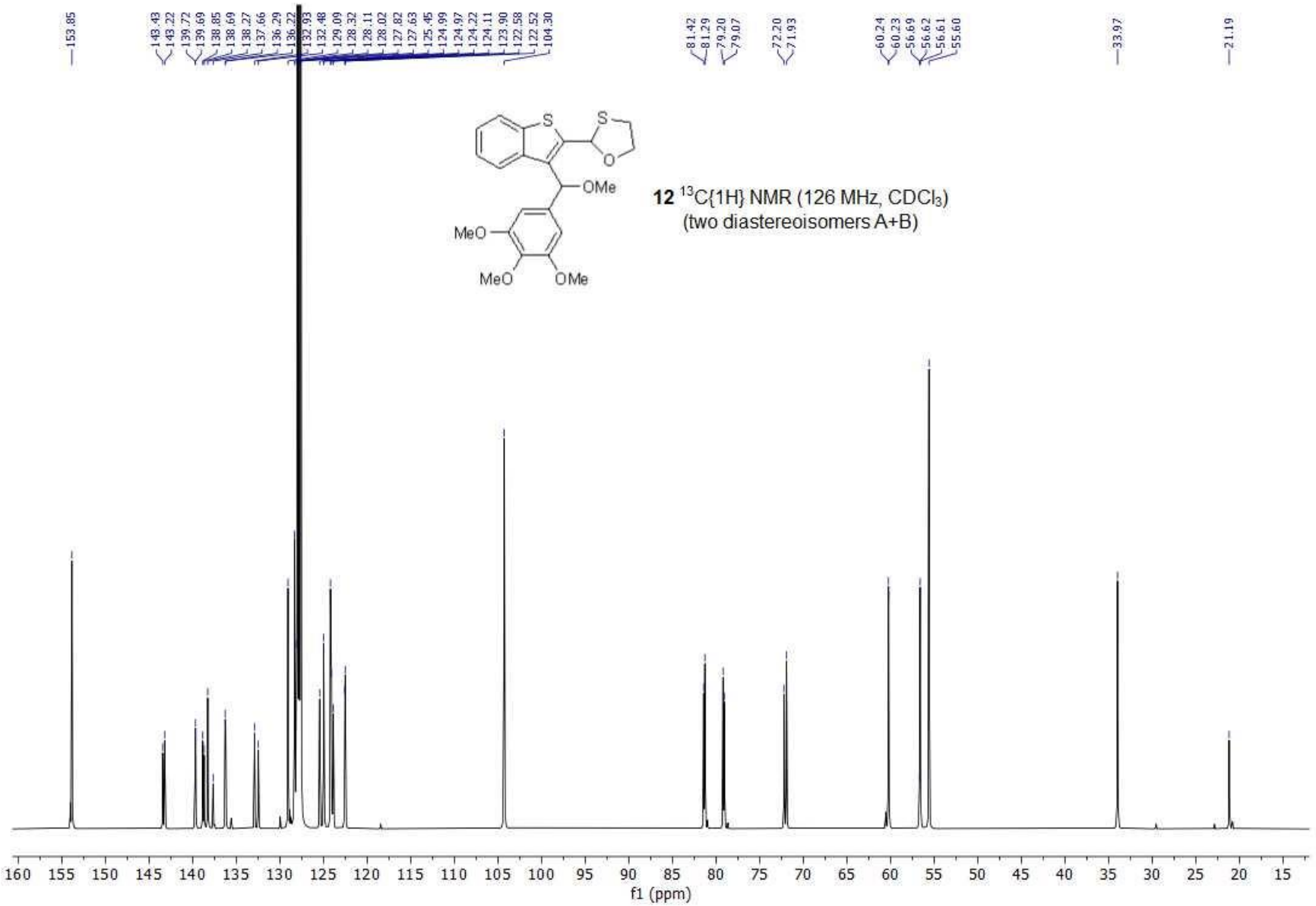

195.09
194.34
155.47
155.20
151.49
151.36
149.02
148.68
148.36
148.25
148.21
147.98
147.94
147.82
147.78
146.98
146.93
146.77
146.51
140.90
140.88
135.83
134.70
134.61
134.57
132.42
126.18
125.76
125.44
125.34
125.17
124.76
123.02
122.69
122.22
121.99
110.97
110.80
109.43
109.11
108.96
108.88
108.56
108.46
108.24
108.03
107.74
105.24
105.04
104.31
104.23
101.77
101.09
101.06
101.00
100.72
100.67
61.20
60.43
50.39
50.32
35.56
35.14
13C{1H} NMR (126 MHz, C6D6)
OH
S
O
cis-9b
+
trans-9b
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
f1 (ppm)


^{1}H-^{13}C HSQC NMR (500 MHz-126 MHz, C_6D_6)
OH
S
O
cis-9b
+
trans-9b
30
40
50
60
70
80
90
100
110
120
130
140
150
f1 (ppm)
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
f2 (ppm)

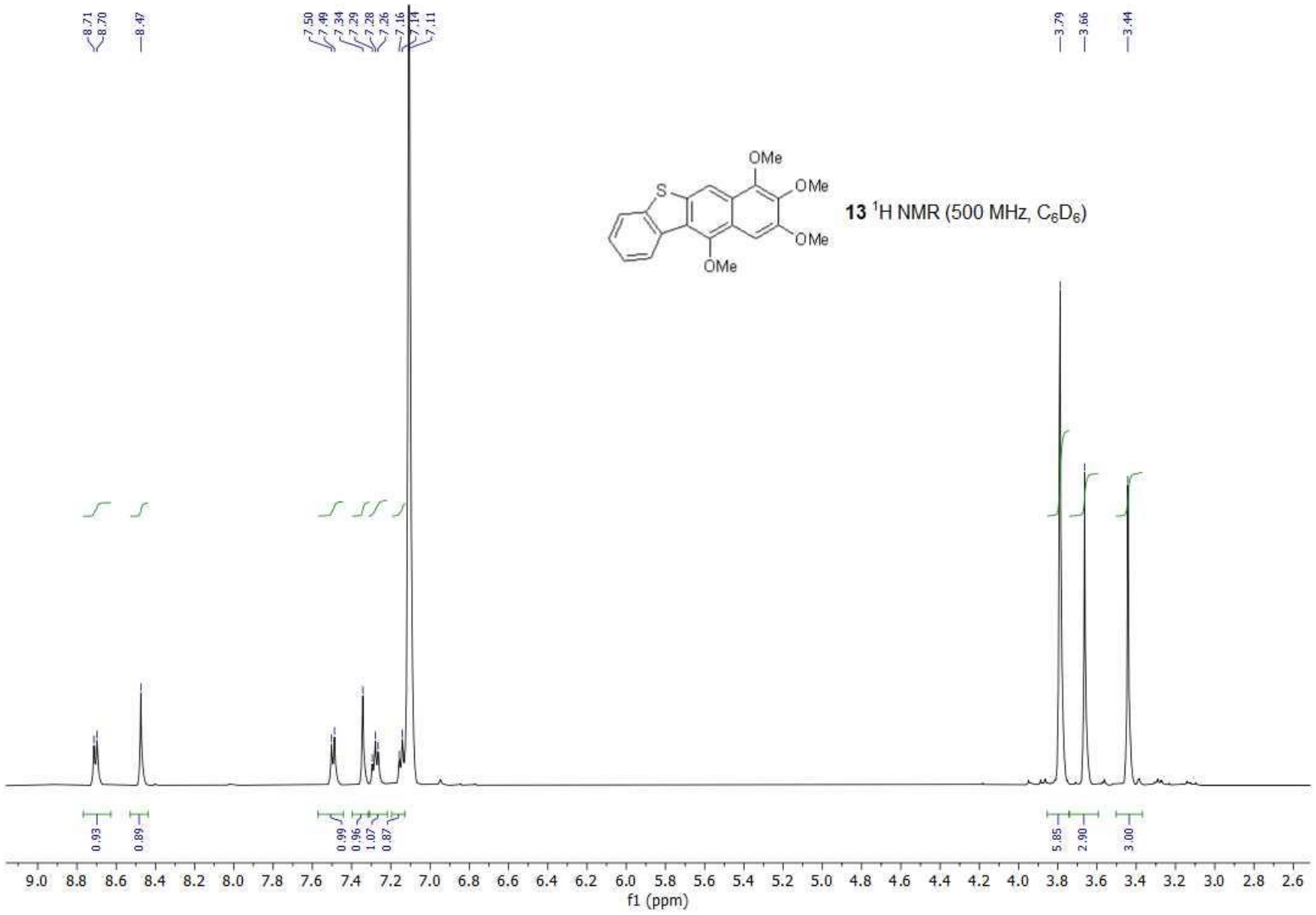

7.69
7.65
7.43
7.39
7.18
7.15
7.15
7.11
7.11
7.08
7.08
7.04
7.04
7.01
4.08
4.06
4.05
4.03
4.01
4.00
3.98
3.50
3.47
3.45
3.42
3.41
3.38
2.88
2.84
2.83
2.83
2.80
2.80
2.78
2.75
2.63
2.61
2.60
2.58
2.56
2.55
2.53
S
S
O
Br
11 1H NMR (200 MHz, C6D6)
1.08
1.18
1.24
0.86
1.00
1.02
1.20
1.09
8.2 8.0 7.8 7.6 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 4.4 4.2 4.0 3.8 3.6 3.4 3.2 3.0 2.8 2.6 2.4 2.2 2.0 1.8 1.6
f1 (ppm)

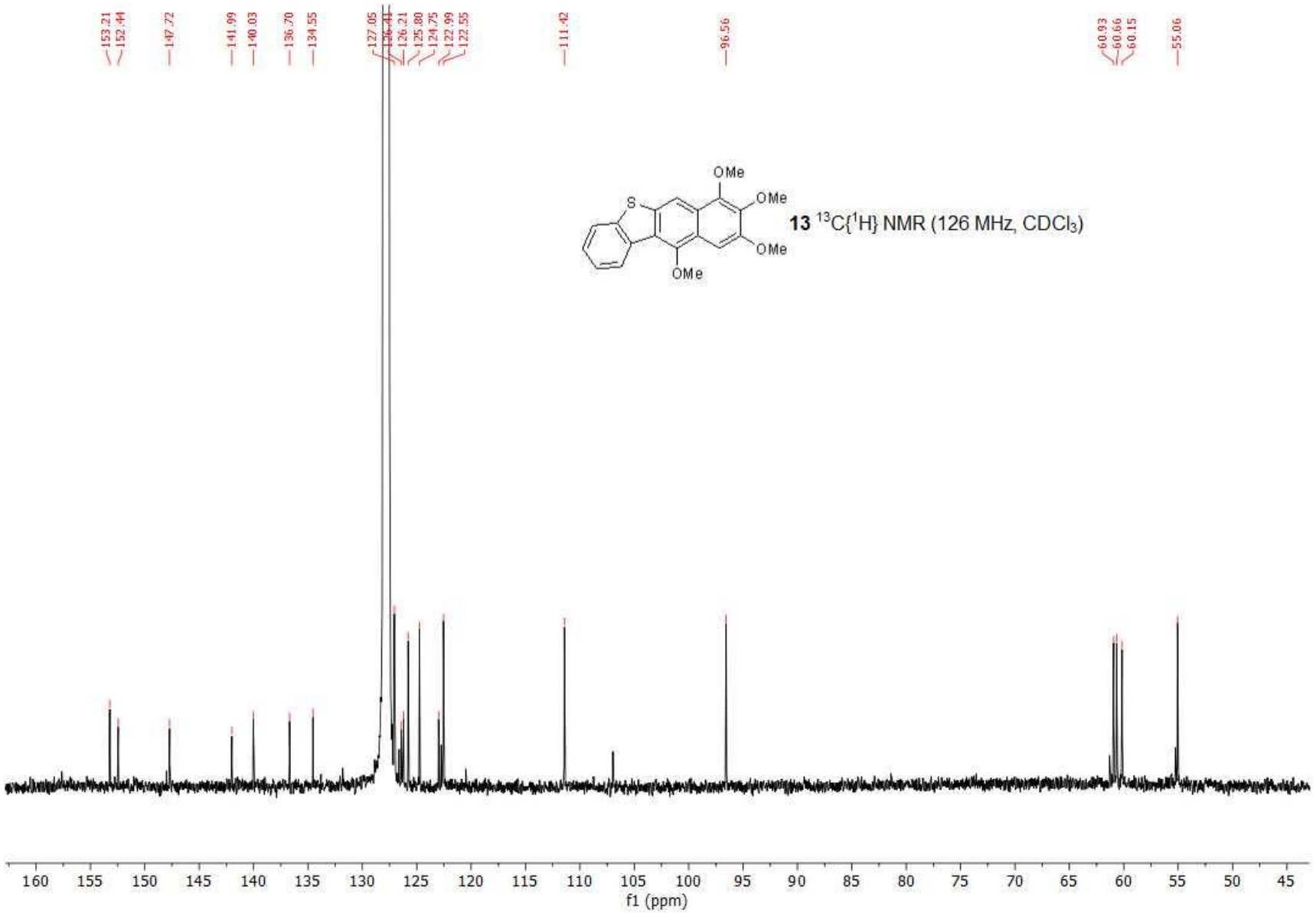

140.56
138.17
137.74
128.74
128.31 C6D6
127.83 C6D6
127.35 C6D6
125.65
125.57
125.53
125.05
122.90
122.60
82.18
72.07
33.70
S
S
O
Br
11 $^{13}C\{^{1}H\}$ NMR (50 MHz, C_6D_6)
145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25
f1 (ppm)


12 ^{1}H NMR (500 MHz, $CDCl_3$)
(two diastereoisomers A+B)
S
S
O
OMe
MeO
MeO
OMe
f1 (ppm)



12 $^{13}C\{1H\}$ NMR (126 MHz, $CDCl_3$)
(two diastereoisomers A+B)


8.71
8.70
8.47
7.50
7.49
7.34
7.29
7.28
7.26
7.16
7.14
7.11
3.79
3.66
3.44
OMe
OMe
OMe
OMe
S
13 ¹H NMR (500 MHz, C6D6)
0.93
0.89
0.99
0.96
1.07
0.87
5.85
2.90
3.00
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 4.4 4.2 4.0 3.8 3.6 3.4 3.2 3.0 2.8 2.6
f1 (ppm)


153.21
152.44
147.72
141.99
140.03
136.70
134.55
127.05
126.41
126.21
125.80
124.75
122.99
122.55
111.42
96.56
60.93
60.66
60.15
55.06
OMe
OMe
OMe
OMe
S
13 $^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$)
160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45
f1 (ppm)

Crystal structure determination

X-ray diffraction data for **13** were collected using an Oxford Diffraction Xcalibur Saphire 3 diffractometer with CuKα radiation. The structures were solved by direct methods and refined by full-matrix least-squares on F^2 with SHELXL-2014 [1]. The carbon, oxygen and sulphur atoms were refined anisotropically. All aromatic H atoms and H atoms of methyl groups were positioned geometrically and constrained to ride on their parent atoms, with C–H distances of 0.93 and 0.96 Å, respectively, and with $U_{iso}(H_{aromatic})$ and $U_{iso}(H_{methyl})$ values of 1.2 $U_{eq}(C_{aromatic})$ and 1.5 $U_{eq}(C_{methyl})$. Details of data collections and structure refinements have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication number CCDC 1475147.

Calculations

The molecular and electronic structures of *cis*-**9b**, *trans*-**9b, 5b, 16a** and **16b** were calculated by DFT method using the gradient corrected three-parameter hybrid functional (B3LYP) with the 6-31++G(d,p) (for *cis*-**9b** and *trans*-**9b**) and 6-311++G(d,p) basis sets (for **5b, 16a** and **16b**). Full geometry optimizations of compounds in the gas phase were performed using its starting geometries prepared manually. The above computations were performed using GAUSSIAN09 quantum chemistry package. In order to check the structural optimizations, the calculated vibrational frequencies of the compounds were used (no imaginary frequencies). GAUSSIAN09 was also used for the TD-DFT (B3LYP 6-311++G(d,p) calculations performed for **7b**.

The calculations in the framework of the noncovalent interactions (NCI) method [2] were performed with the Multiwfn (A Multifunctional Wavefunction Analyzer) software [3]. This method is based on the relationship between the electron density (ρ) and the reduced density gradient ($RDG = \frac{1}{2(3\pi^2)^{1/3}\rho^{4/3}}|\nabla\rho|$), and is a very useful tool for the analysis and visualization of different types of non-covalent interactions. Chemcraft program [4] was employed to visualize the chemical structures and molecular orbitals of investigated compounds, and VMD (Visual Molecular Dynamics) [5] and Multiwfn software[3] were used for visualization of their RDG isosurfaces. The latter software was also used to perform the quantitative analysis of molecular surfaces of **5b**, **16a** and **16b**.

Cartesian coordinates and total energies for the geometries of *cis*-9b and *trans*-9b optimized using Gaussian 09

Table S1. Atom coordinates (Å), total energy (Hartree) and the number of imaginary vibrational frequencies for the geometry of *cis*-**9b** optimized at the B3LYP/6-31++(d,p) level in the gas phase using Gaussian 09.

H	0.515590	-3.776210	0.065460
C	0.343632	-2.702158	0.172555
C	1.458119	-1.952754	-0.513957
C	2.711596	-2.584562	-0.683454
C	3.686621	-1.897029	-1.375815
O	4.954823	-2.311444	-1.717134
C	5.592135	-1.143211	-2.255601
O	4.557124	-0.216292	-2.613136
C	3.446196	-0.636884	-1.915718
C	2.226327	-0.007548	-1.779079
C	1.218969	-0.674027	-1.049490
C	-0.145246	-0.026123	-0.886016
H	-0.293606	0.669623	-1.719168
C	-0.248703	0.890152	0.442795
H	-0.098402	0.217177	1.290334
C	0.844824	1.937684	0.441758
C	2.106780	1.638274	0.993633
C	3.088880	2.603513	0.895589
O	4.387451	2.537380	1.333082
C	4.917479	3.863254	1.156089
O	4.036859	4.562899	0.271000
C	2.870259	3.827772	0.258983
C	1.650537	4.151811	-0.284017
C	0.620561	3.187009	-0.167841
C	-0.745145	3.571878	-0.614353
O	-0.941872	4.568084	-1.312177
C	-1.868956	2.765541	-0.067085
C	-3.163975	3.337923	-0.088908
C	-4.163140	2.639547	0.544603
O	-5.501377	2.952089	0.658712
C	-6.030364	2.015544	1.602807

O	-5.083910	0.938238	1.718412
C	-3.917295	1.420193	1.180685
C	-2.668721	0.831148	1.188482
C	-1.622367	1.519953	0.542032
C	-1.232575	-1.086015	-0.956317
C	-2.459991	-0.789507	-1.589722
C	-3.422166	-1.776138	-1.618430
O	-4.667379	-1.745273	-2.206182
C	-5.324375	-2.935360	-1.748122
O	-4.308809	-3.829289	-1.268973
C	-3.206361	-3.031845	-1.054174
C	-2.009735	-3.357962	-0.454105
C	-1.007661	-2.362685	-0.415305
H	2.894765	-3.587067	-0.311227
H	6.157921	-1.417541	-3.147251
H	6.233885	-0.692429	-1.485274
H	2.047379	0.966745	-2.220707
H	2.301949	0.683485	1.468216
H	5.910126	3.797603	0.707052
H	4.943104	4.372132	2.129634
H	1.449728	5.101447	-0.765779
H	-3.324082	4.294306	-0.572550
H	-6.980078	1.623137	1.234916
H	-6.141844	2.501703	2.581949
H	-2.503630	-0.128019	1.666001
H	-2.641416	0.182532	-2.035123
H	-5.853837	-3.401120	-2.580754
H	-6.003149	-2.680665	-0.921771
H	-1.837565	-4.344662	-0.037183
S	0.229749	-2.404550	2.039398
C	1.838711	-3.014481	2.667770
H	1.963566	-2.548650	3.650130
H	2.650103	-2.653476	2.029498
C	1.900535	-4.530868	2.809400
H	1.718896	-5.014925	1.838528
H	1.122433	-4.868928	3.506735
O	3.206512	-4.852774	3.295439
H	3.264511	-5.804579	3.447583
Total energy		-2460.004177	
Number of imaginary vibrational frequencies		0	

Table S2. Atom coordinates (Å), total energy (Hartree) and the number of imaginary vibrational frequencies for the geometry of *trans*-**9b** optimized at the B3LYP/6-31++(d,p) level in the gas phase using Gaussian 09.

Atom	X	Y	z
O	-4.912202	1.585518	1.488486
C	-3.669161	1.935627	1.027387
C	-2.506630	1.192307	1.065503
C	-1.348807	1.765122	0.500745
C	-1.235952	-0.860491	-1.013824
C	-2.360346	-0.466105	-1.767963
C	-3.430894	-1.334156	-1.821816
O	-4.613102	-1.205602	-2.517457
C	-5.439667	-2.277734	-2.040875
O	-4.579070	-3.238989	-1.413818
C	-3.409092	-2.555675	-1.158781
C	-2.315876	-2.975082	-0.427552
C	-1.203111	-2.109713	-0.364602
H	2.534566	-3.777185	-0.069751
H	6.010289	-2.269314	-3.076157
H	6.191110	-1.424986	-1.480130
H	2.235703	0.684545	-2.331496
H	2.427564	0.372689	1.468983
H	6.431798	2.968457	0.826042
H	5.565748	3.625461	2.277419
H	2.214663	4.944332	-0.598153
H	-2.627630	4.774882	-0.564861
H	-6.677076	2.512083	0.916791
H	-5.839417	3.227924	2.356914
H	-2.494049	0.198912	1.499580
H	-2.384059	0.489197	-2.281215
H	-5.951339	-2.744048	-2.884378
H	-6.149319	-1.885943	-1.297878
H	-2.311932	-3.938039	0.066906
S	0.130985	-4.240127	0.933142
C	0.932765	-4.070302	2.575122
H	1.405111	-5.035133	2.781030
H	1.728302	-3.321076	2.524805
C	-0.052272	-3.729222	3.687147

H	-0.590270	-2.800331	3.447968
H	-0.793870	-4.533789	3.782469
O	0.707958	-3.580372	4.888691
H	0.107642	-3.422282	5.628365
H	0.072027	-1.911156	1.341034
Total energy		-2459.996890	
Number of imaginary vibrational frequencies		0	

Table S3. Atom coordinates (Å), total energy (Hartree) and the number of imaginary vibrational frequencies for the geometry of **5b** optimized at the B3LYP/6-311++(d,p) level in the gas phase using Gaussian 09.

Atom	X	Y	Z
O	4.003551	-2.887588	-0.068798
C	5.127414	-2.263804	-0.706813
H	5.532462	-2.934285	-1.463405
H	5.875831	-2.005209	0.052782
O	4.652318	-1.066696	-1.332568
C	2.672433	0.331054	-0.808993
H	2.975369	1.182700	-1.402091
C	1.445439	0.345175	-0.114939
C	1.043898	-0.763506	0.649892
C	1.873879	-1.901510	0.732739
H	1.578800	-2.762824	1.319850
C	3.062110	-1.892791	0.040291
C	3.451237	-0.795764	-0.717793
C	0.600219	1.586782	-0.229141
H	-0.406597	1.429895	0.151837
O	0.562767	2.027703	-1.567803
C	0.094205	3.368642	-1.607538
H	-0.958877	3.411159	-1.300240
H	0.178892	3.703620	-2.642345
C	0.962915	4.192843	-0.649270
H	1.902274	4.490270	-1.116726
H	0.436677	5.079701	-0.294632
S	1.299917	3.056795	0.757260
C	-0.275931	-0.810897	1.418706
H	-0.253360	-1.730777	2.024343
O	-0.430789	0.290345	2.314258
C	0.443556	0.260736	3.432332
H	0.199582	1.131307	4.040564
H	0.292769	-0.651628	4.025762
H	1.495547	0.318601	3.130571
C	-1.525518	-0.881328	0.540590
C	-1.487787	-1.498469	-0.711344
C	-2.745479	-0.388345	1.048176
C	-2.640297	-1.648613	-1.500370
H	-0.545988	-1.868306	-1.096071

C	-3.864526	-0.543726	0.261968
H	-2.788466	0.107058	2.007582
C	-3.819070	-1.160020	-0.983350
H	-2.600974	-2.116002	-2.475894
O	-5.068580	-1.126733	-1.559908
O	-5.146951	-0.103114	0.506550
C	-5.948761	-0.726500	-0.502630
H	-6.673995	-0.009921	-0.885519
H	-6.436752	-1.615183	-0.081437
Total energy		-1584.317859	
Number of imaginary vibrational frequencies		0	

Table S4. Atom coordinates (Å), total energy (Hartree) and the number of imaginary vibrational frequencies for the geometry of **16a** optimized at the B3LYP/6-311++(d,p) level in the gas phase using Gaussian 09.

Atom	X	Y	Z
C	3.976628	-0.894226	-0.200932
C	2.945527	-1.590379	0.387051
C	1.662135	-1.017971	0.329827
C	1.455522	0.213924	-0.295718
C	2.524757	0.912110	-0.885020
C	3.770572	0.330929	-0.824529
C	0.075109	0.829343	-0.301008
C	0.505287	-1.732794	0.991458
C	-1.013767	-0.224323	-0.349756
C	-0.809819	-1.458362	0.283395
C	-1.796146	-2.459745	0.233845
H	-1.635335	-3.431859	0.684140
C	-2.967432	-2.173515	-0.433692
C	-3.166976	-0.954115	-1.065707
C	-2.205176	0.033057	-1.053162
H	3.116905	-2.538341	0.881829
H	2.376190	1.873248	-1.361627
H	-2.357449	0.962873	-1.587991
H	-0.024191	1.473587	-1.183886
H	0.689707	-2.817199	0.963078
C	-1.091952	2.550765	0.983801

H	-2.019332	2.088928	0.626666
H	-1.214613	2.751930	2.050320
C	-0.815554	3.859980	0.241327
H	0.052929	4.350541	0.680749
H	-0.625422	3.676141	-0.817109
O	0.507737	-1.324241	2.370385
C	-0.342288	-2.075113	3.217959
H	-0.148789	-1.729337	4.233816
H	-1.402660	-1.919886	2.985736
H	-0.120118	-3.151249	3.159449
O	5.312107	-1.218593	-0.255063
O	4.969513	0.816746	-1.291617
C	5.887597	-0.277066	-1.169185
H	6.833401	0.085893	-0.769079
H	6.015753	-0.754303	-2.149080
O	-4.048245	-2.992460	-0.662042
O	-4.378532	-0.965041	-1.715367
C	-5.048892	-2.133089	-1.224553
H	-5.542870	-2.642596	-2.050368
H	-5.758601	-1.841396	-0.440185
O	0.005182	1.652553	0.887332
S	-2.293894	4.958642	0.401606
H	-1.746105	6.036573	-0.193585
Total energy		-1584.320012	
Number of imaginary vibrational frequencies		0	

Table S5. Atom coordinates (Å), total energy (Hartree) and the number of imaginary vibrational frequencies for the geometry of **16b** optimized at the B3LYP/6-311++(d,p) level in the gas phase using Gaussian 09.

Atom	X	Y	Z
C	3.743403	0.332348	-0.843920
C	2.527987	0.974423	-0.822405
C	1.436609	0.281035	-0.262365
C	1.601248	-1.005710	0.258503
C	2.856959	-1.641020	0.230555
C	3.905342	-0.949852	-0.329331
C	0.077881	0.940321	-0.228198

C	0.431888	-1.708818	0.907022
C	-0.884779	-1.336064	0.251651
C	-1.053766	-0.051340	-0.285598
C	-2.255571	0.301531	-0.930945
H	-2.391365	1.275808	-1.383835
C	-3.251286	-0.648513	-0.993307
C	-3.084818	-1.918143	-0.458411
C	-1.912289	-2.292802	0.159424
H	2.416119	1.978304	-1.212882
H	2.992926	-2.632652	0.643955
H	-1.783427	-3.295349	0.549154
H	-0.002310	1.630049	-1.069392
H	0.567753	-2.796895	0.818561
S	0.037539	2.020398	1.321258
C	-1.465994	3.033282	1.074093
H	-2.304450	2.396861	0.784931
H	-1.696324	3.436587	2.063012
C	-1.286541	4.176962	0.086689
H	-0.497761	4.849775	0.442845
H	-0.984011	3.793511	-0.896801
O	-2.541549	4.858064	-0.008778
H	-2.439676	5.621758	-0.584779
O	0.490869	-1.371287	2.305019
C	-0.399753	-2.094342	3.135775
H	-0.165390	-1.808290	4.161419
H	-1.448514	-1.851214	2.929704
H	-0.257756	-3.179989	3.026699
O	4.952302	0.798616	-1.304133
O	5.222175	-1.329035	-0.447146
C	5.819375	-0.342701	-1.297501
H	5.900160	-0.742298	-2.316392
H	6.791113	-0.057856	-0.896355
O	-4.509945	-0.537332	-1.534323
O	-4.236158	-2.649555	-0.639915
C	-5.027199	-1.874613	-1.550002
H	-6.063448	-1.866789	-1.215022
H	-4.928007	-2.289357	-2.561093
Total energy		-1584.330880	
Number of imaginary vibrational frequencies		0	

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