# Supplementary Material

# Ring-closing metathesis in flavonoid synthesis, part 2: neoflav-3-enes

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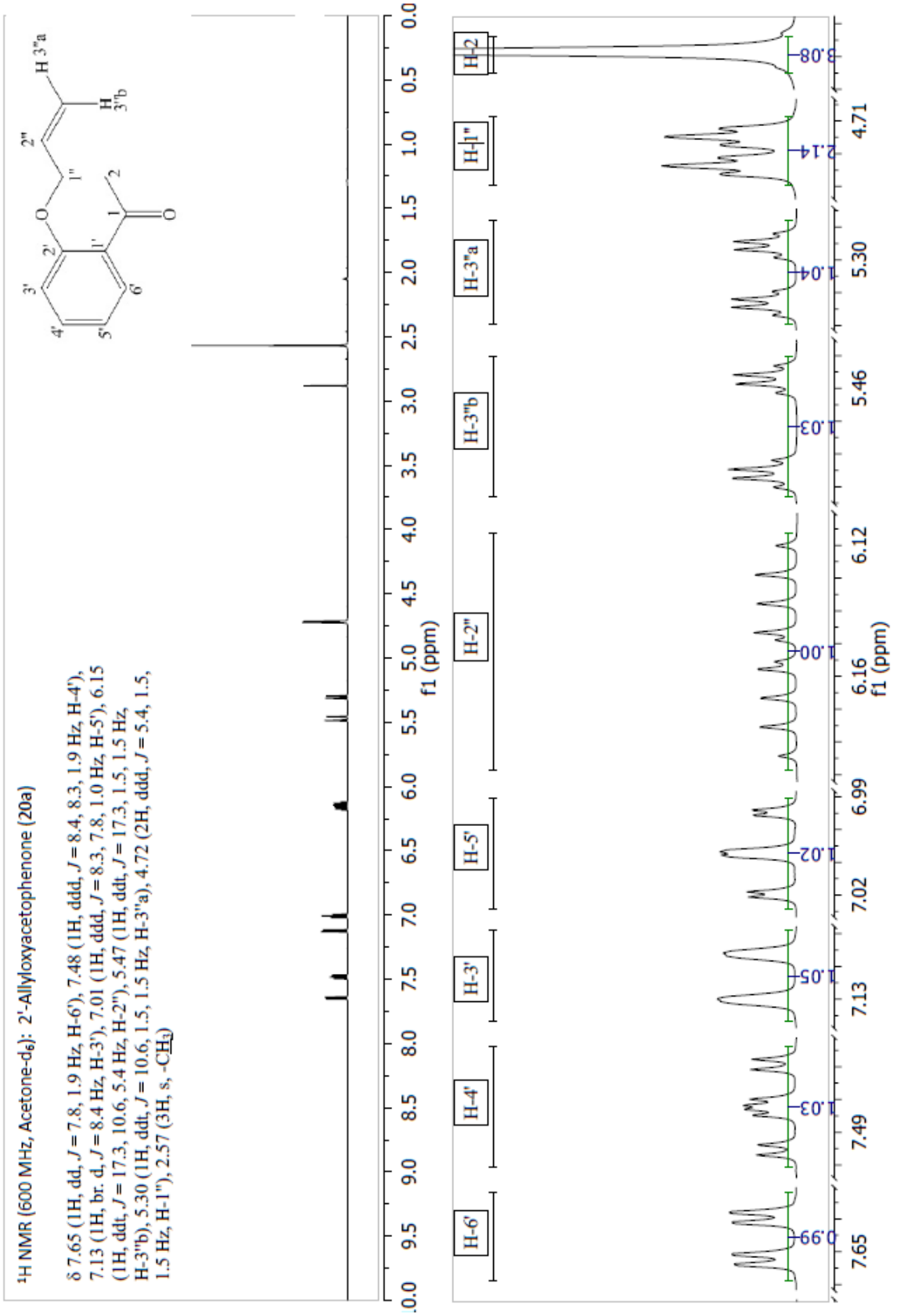
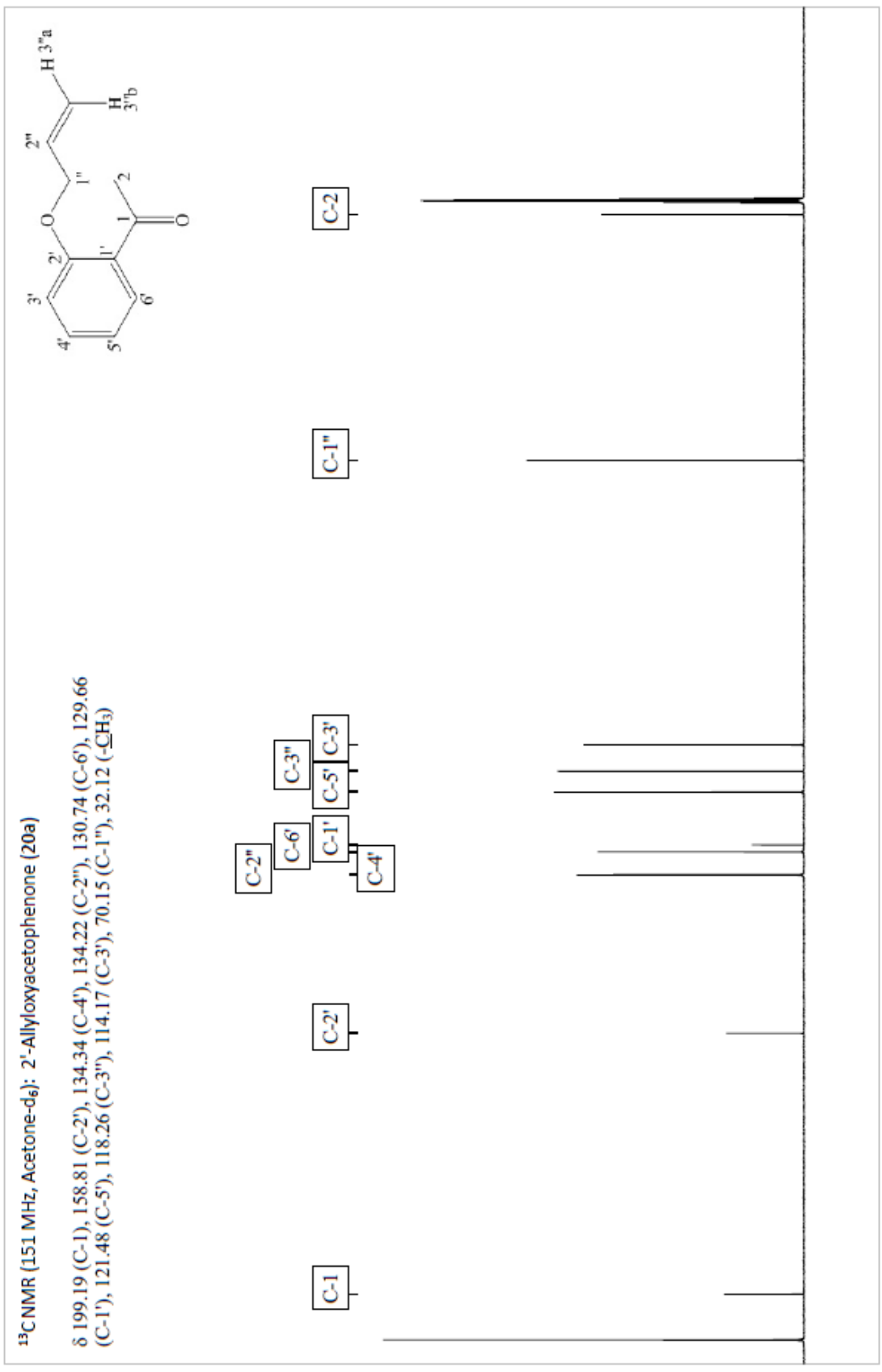
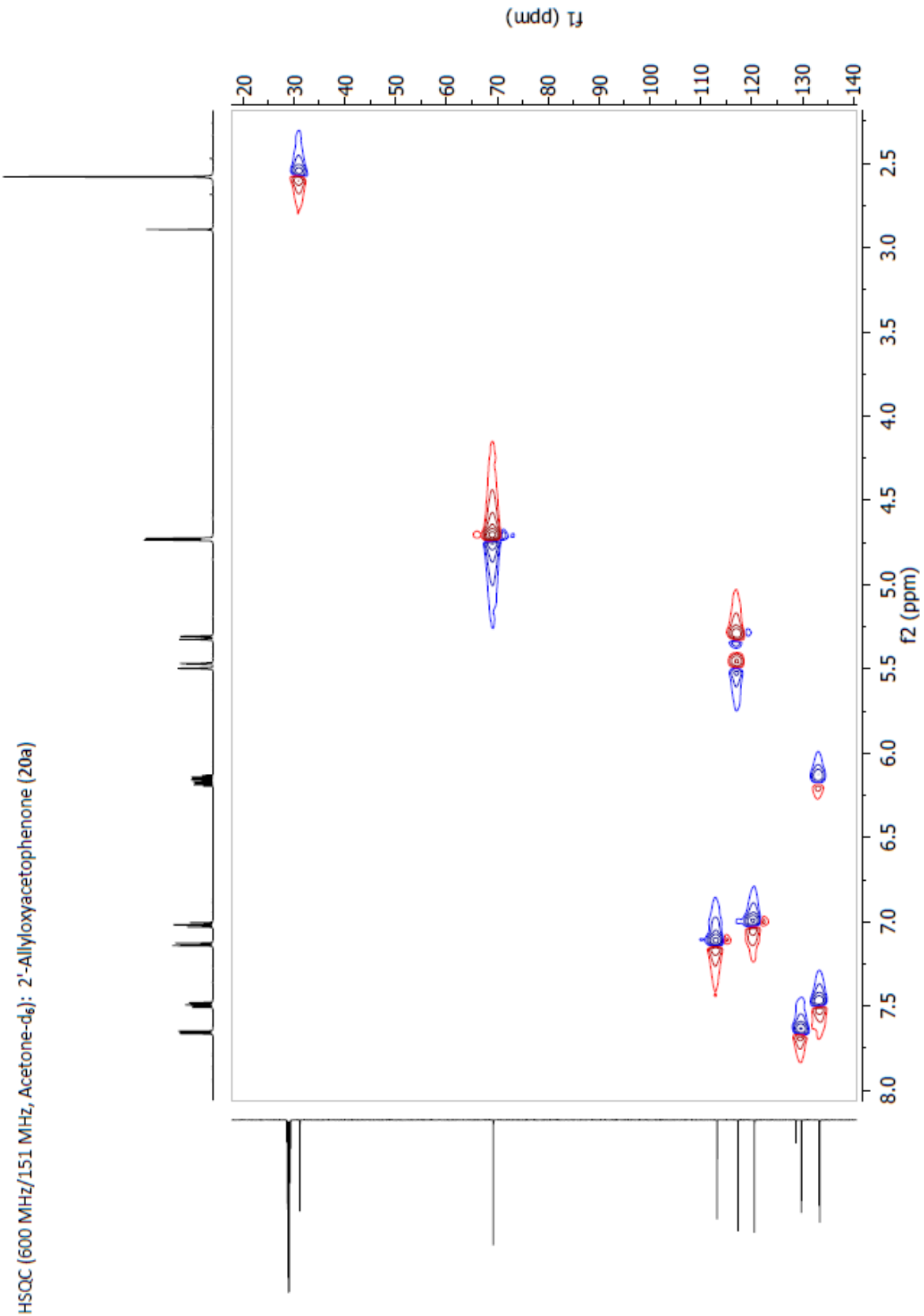
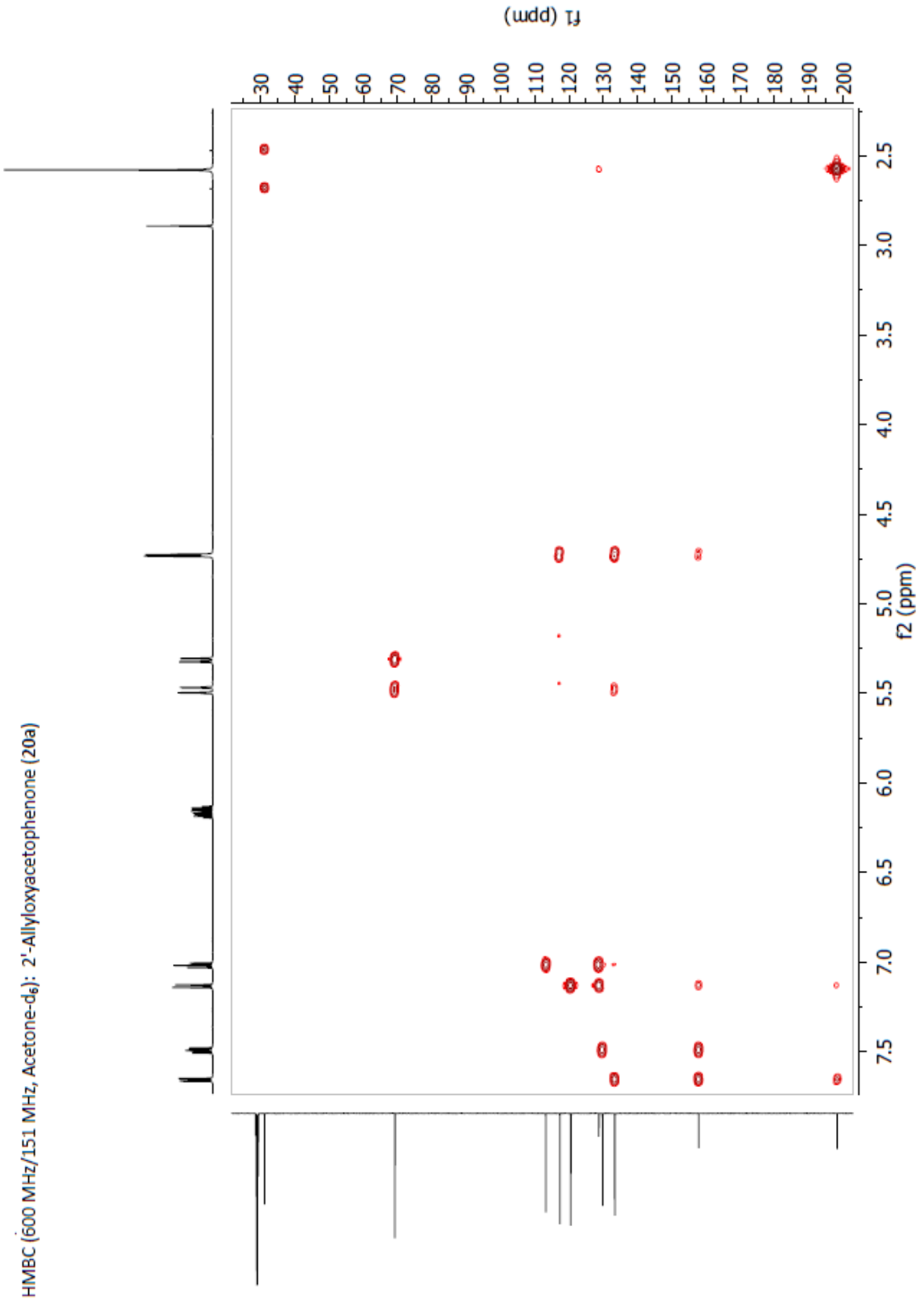

¹H NMR (600 MHz, Acetone-d6): 2'-Allyloxyacetophenone (20a)
δ 7.65 (1H, dd, J = 7.8, 1.9 Hz, H-6'), 7.48 (1H, ddd, J = 8.4, 8.3, 1.9 Hz, H-4'), 7.13 (1H, br. d, J = 8.4 Hz, H-3'), 7.01 (1H, ddd, J = 8.3, 7.8, 1.0 Hz, H-5'), 6.15 (1H, ddt, J = 17.3, 10.6, 5.4 Hz, H-2"), 5.47 (1H, ddt, J = 17.3, 1.5, 1.5 Hz, H-3"b), 5.30 (1H, ddt, J = 10.6, 1.5, 1.5 Hz, H-3"a), 4.72 (2H, ddd, J = 5.4, 1.5, 1.5 Hz, H-1"), 2.57 (3H, s, -CH3)
f1 (ppm)
H-6'
H-4'
H-3'
H-5'
H-2"
H-3"b
H-3"a
H-1"
H-2
3.08
2.14
1.04
1.03
1.00
1.02
1.05
1.03
0.99

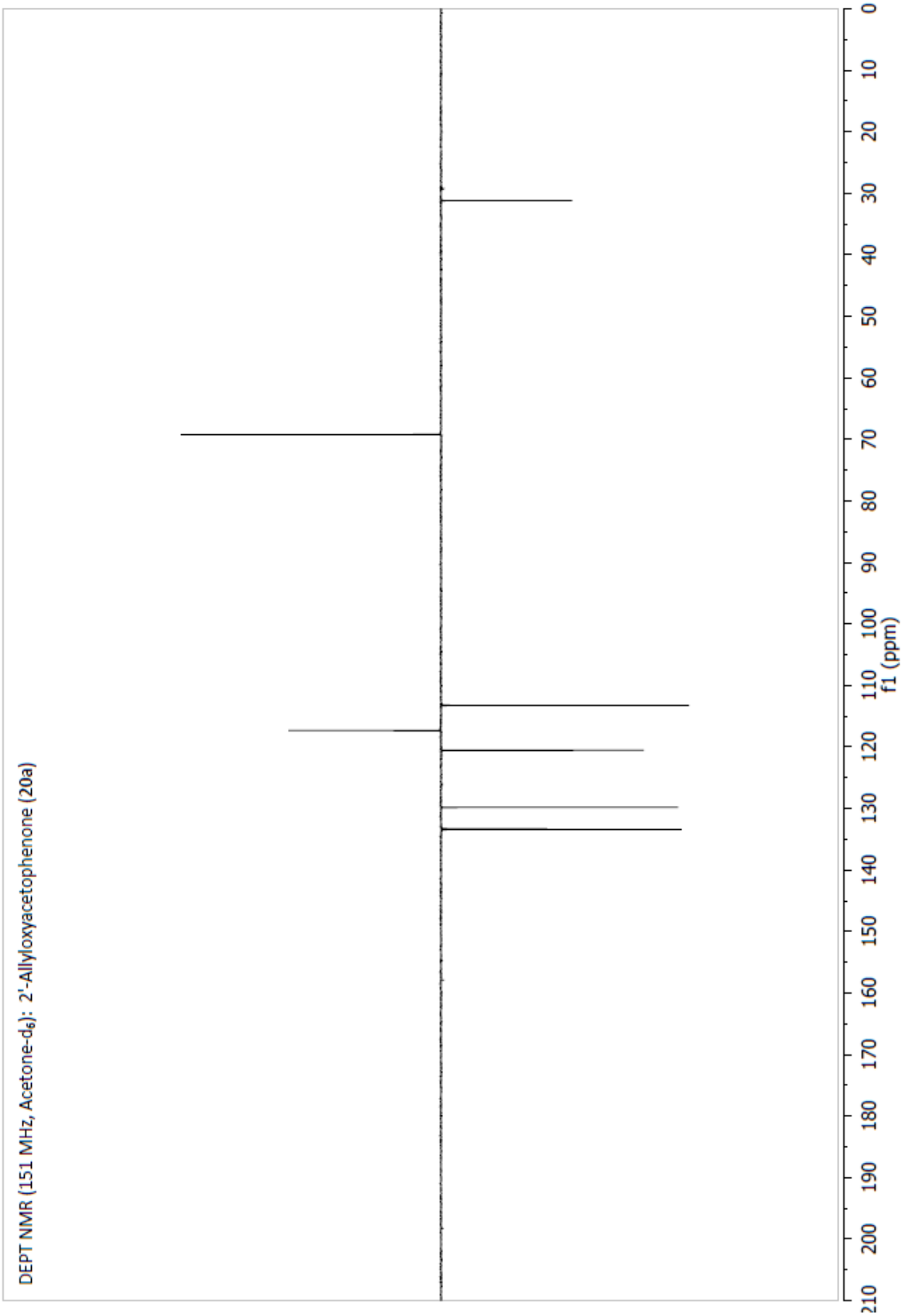

$^{13}$C NMR (151 MHz, Acetone-d$_6$): 2'-Allyloxyacetophenone (20a)
δ 199.19 (C-1), 158.81 (C-2'), 134.34 (C-4'), 134.22 (C-2"), 130.74 (C-6'), 129.66 (C-1'), 121.48 (C-5'), 118.26 (C-3"), 114.17 (C-3'), 70.15 (C-1"), 32.12 (-CH$_3$)
C-1
C-2'
C-2"
C-6'
C-1'
C-4'
C-3"
C-5'
C-3'
C-1"
C-2
f1 (ppm)

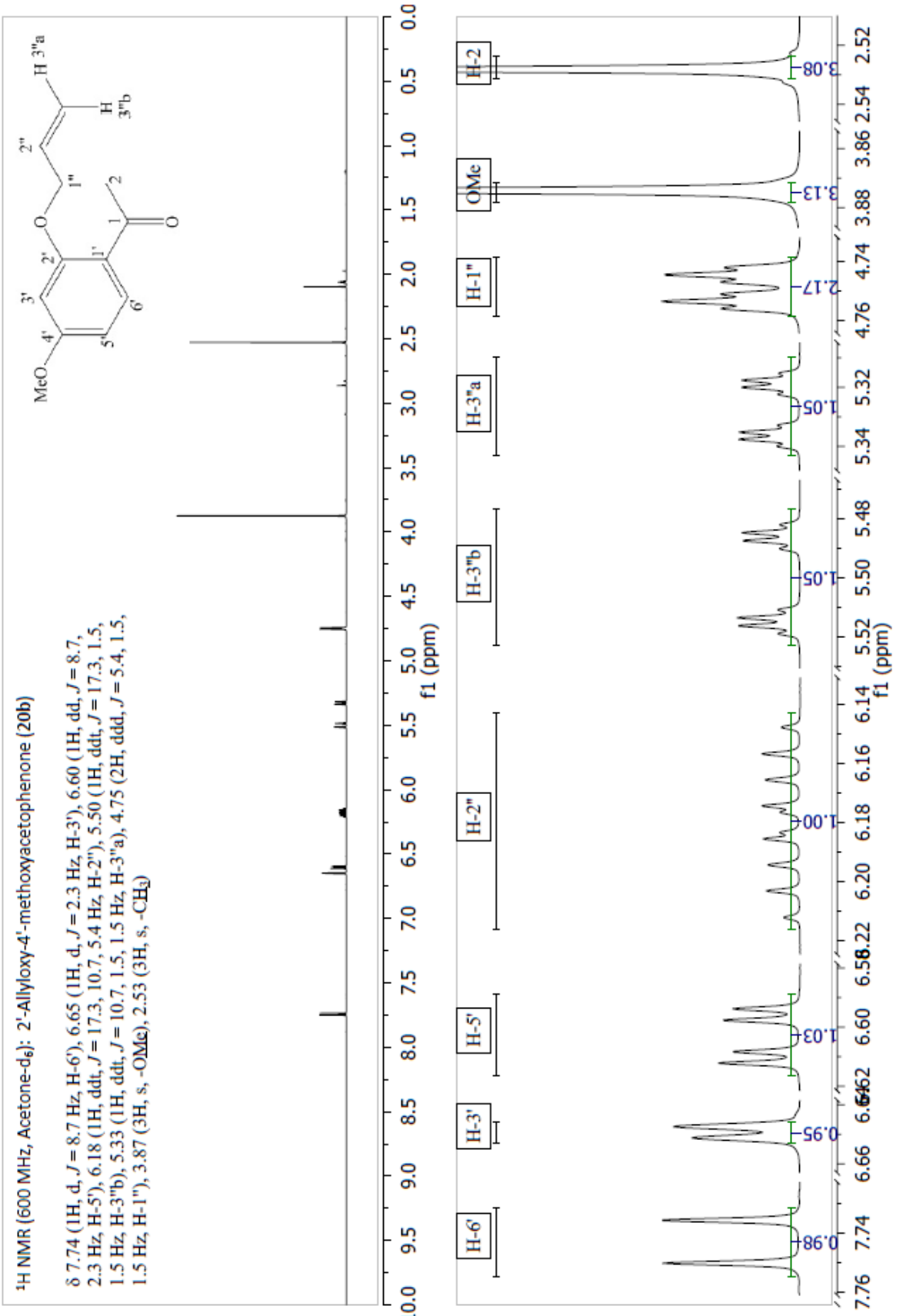



HSQC (600 MHz/151 MHz, Acetone-$d_6$): 2'-Allyloxyacetophenone (20a)



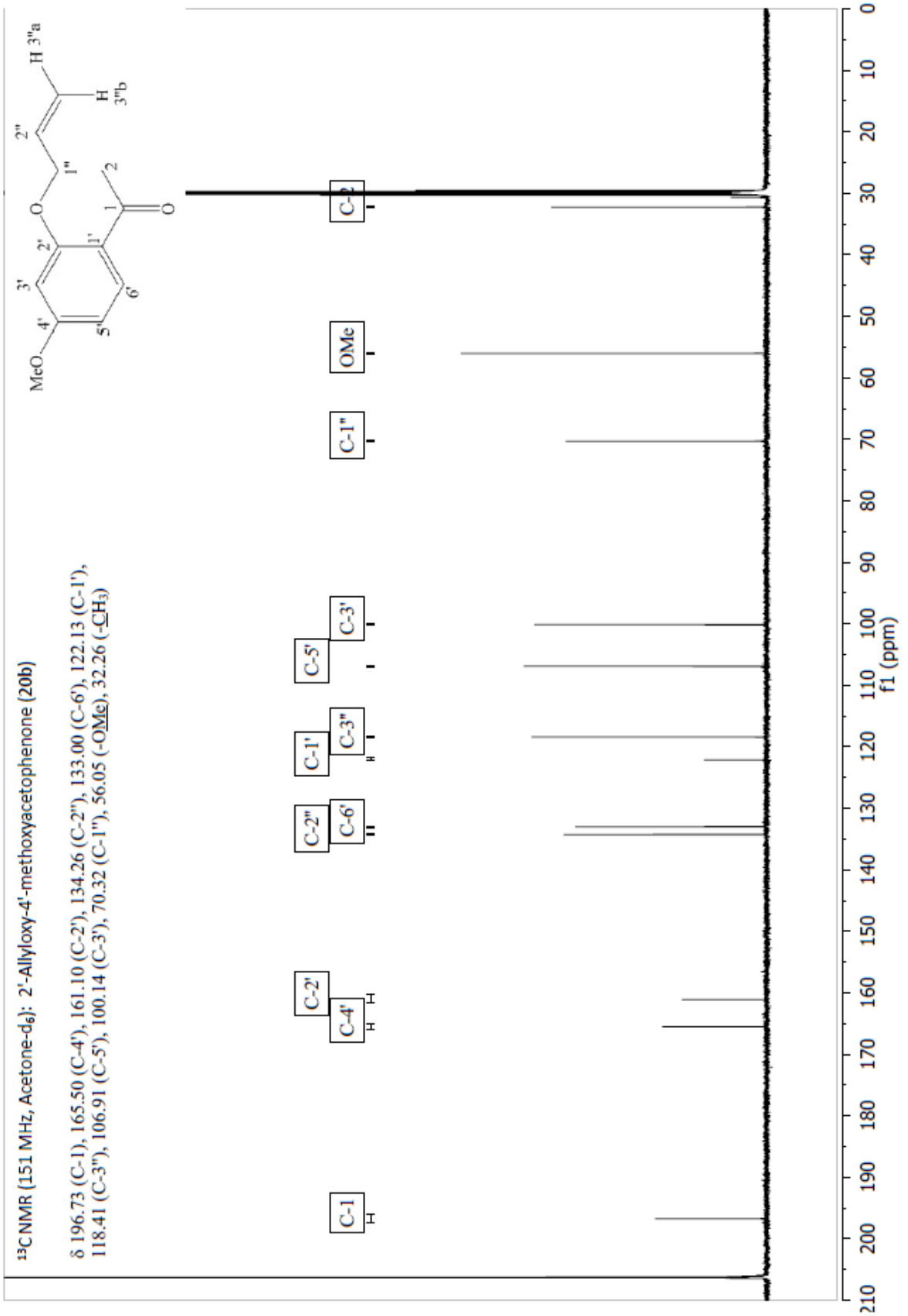

HMBC (600 MHz/151 MHz, Acetone-$d_6$): 2'-Allyloxyacetophenone (20a)

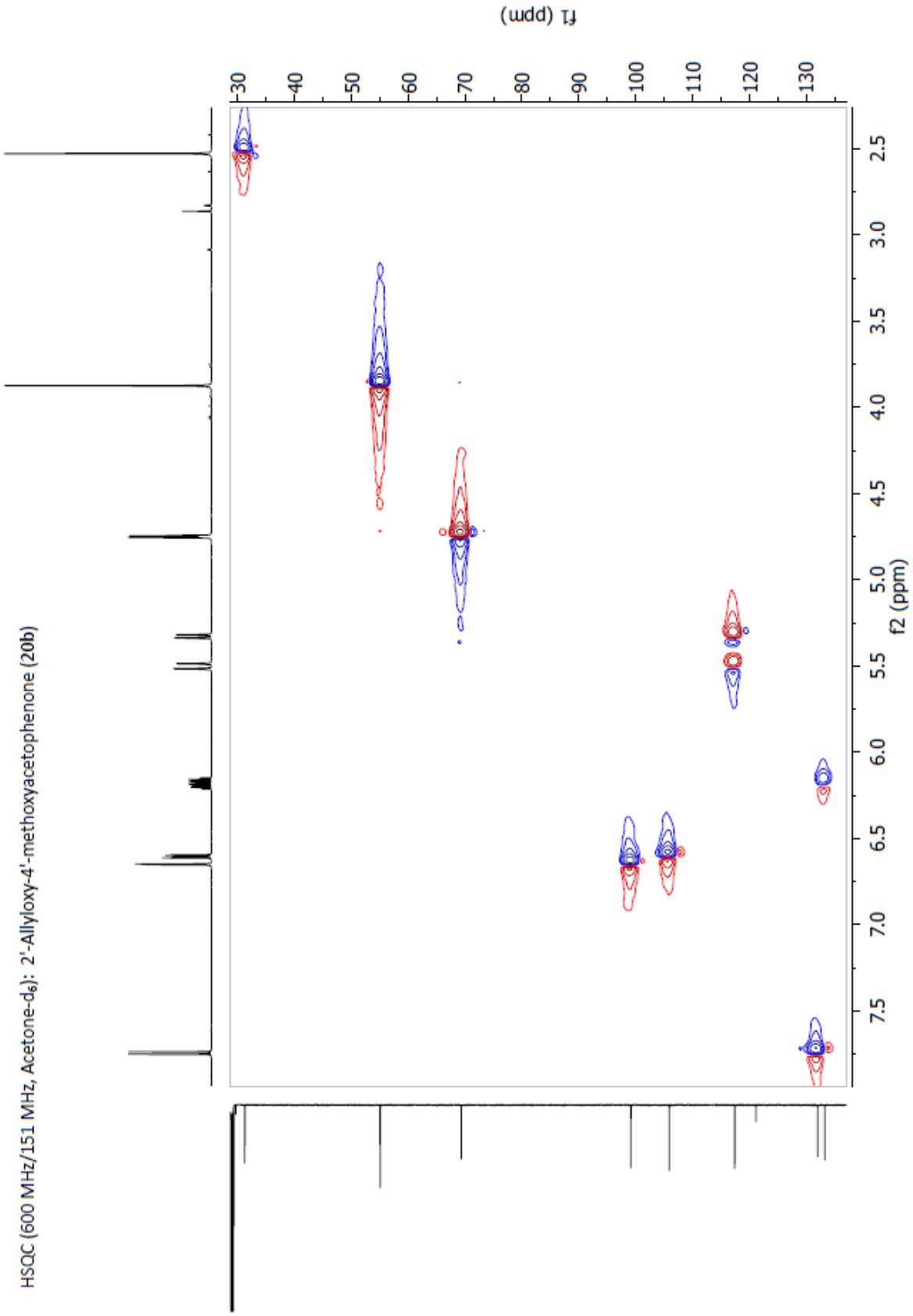

DEPT NMR (151 MHz, Acetone-d6): 2'-Allyloxyacetophenone (20a)
f1 (ppm)
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
210

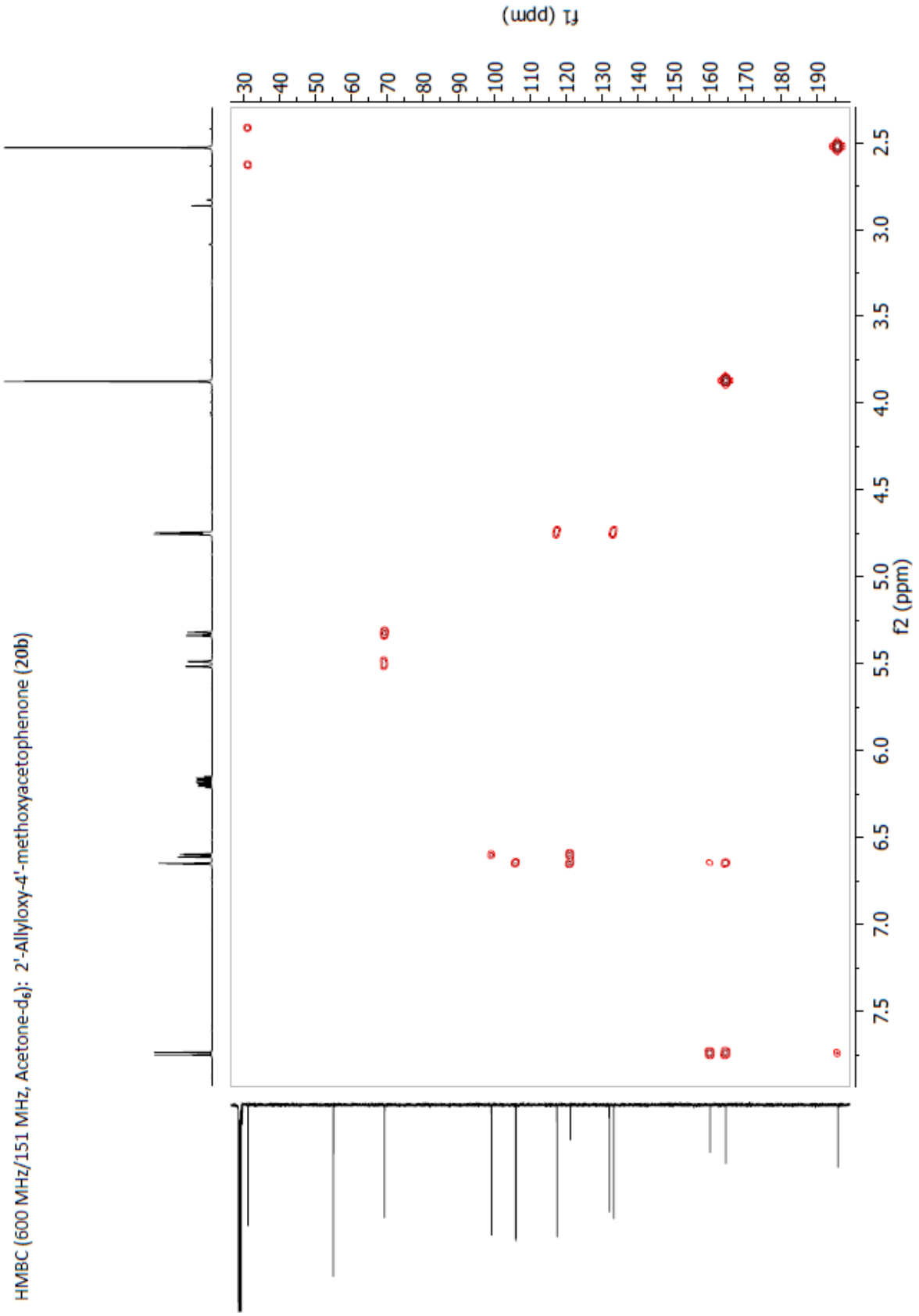


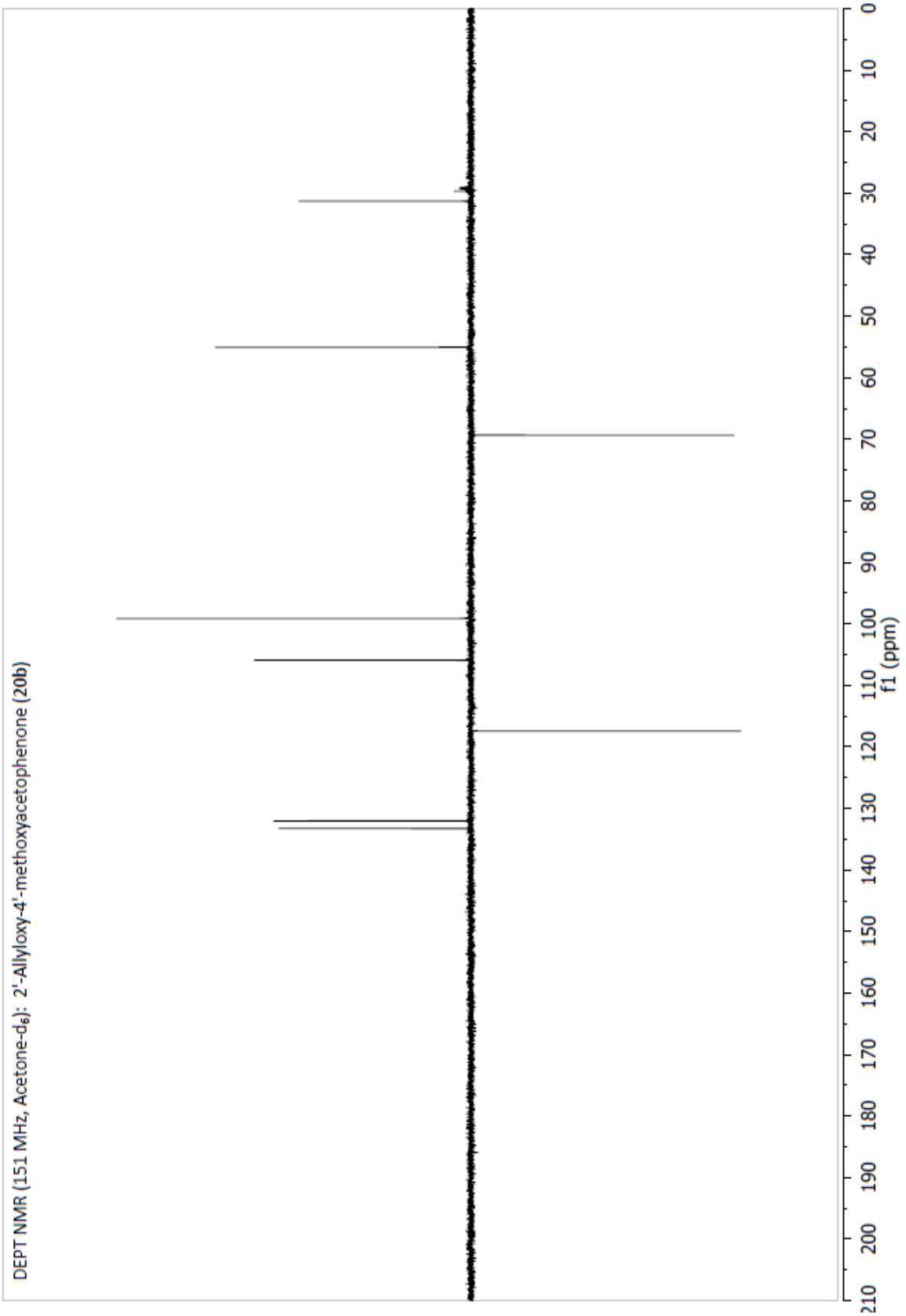

$^1$H NMR (600 MHz, Acetone-$d_6$): 2'-Allyloxy-4'-methoxyacetophenone (**20b**)

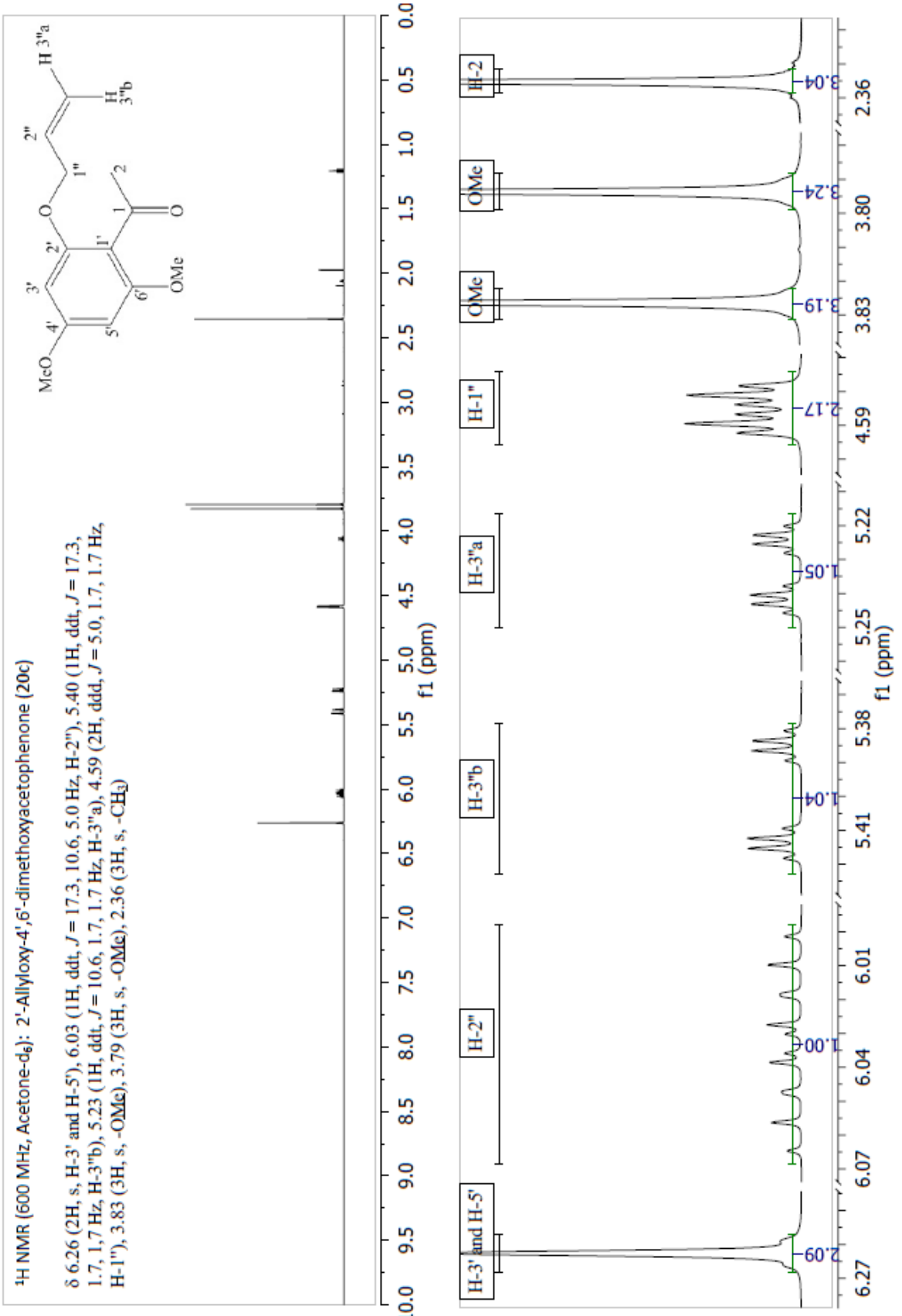
δ 7.74 (1H, d, *J* = 8.7 Hz, H-6'), 6.65 (1H, d, *J* = 2.3 Hz, H-3'), 6.60 (1H, dd, *J* = 8.7, 2.3 Hz, H-5'), 6.18 (1H, ddt, *J* = 17.3, 10.7, 5.4 Hz, H-2"), 5.50 (1H, ddt, *J* = 17.3, 1.5, 1.5 Hz, H-3"b), 5.33 (1H, ddt, *J* = 10.7, 1.5, 1.5 Hz, H-3"a), 4.75 (2H, ddd, *J* = 5.4, 1.5, 1.5 Hz, H-1"), 3.87 (3H, s, -OMe), 2.53 (3H, s, -$CH_3$)

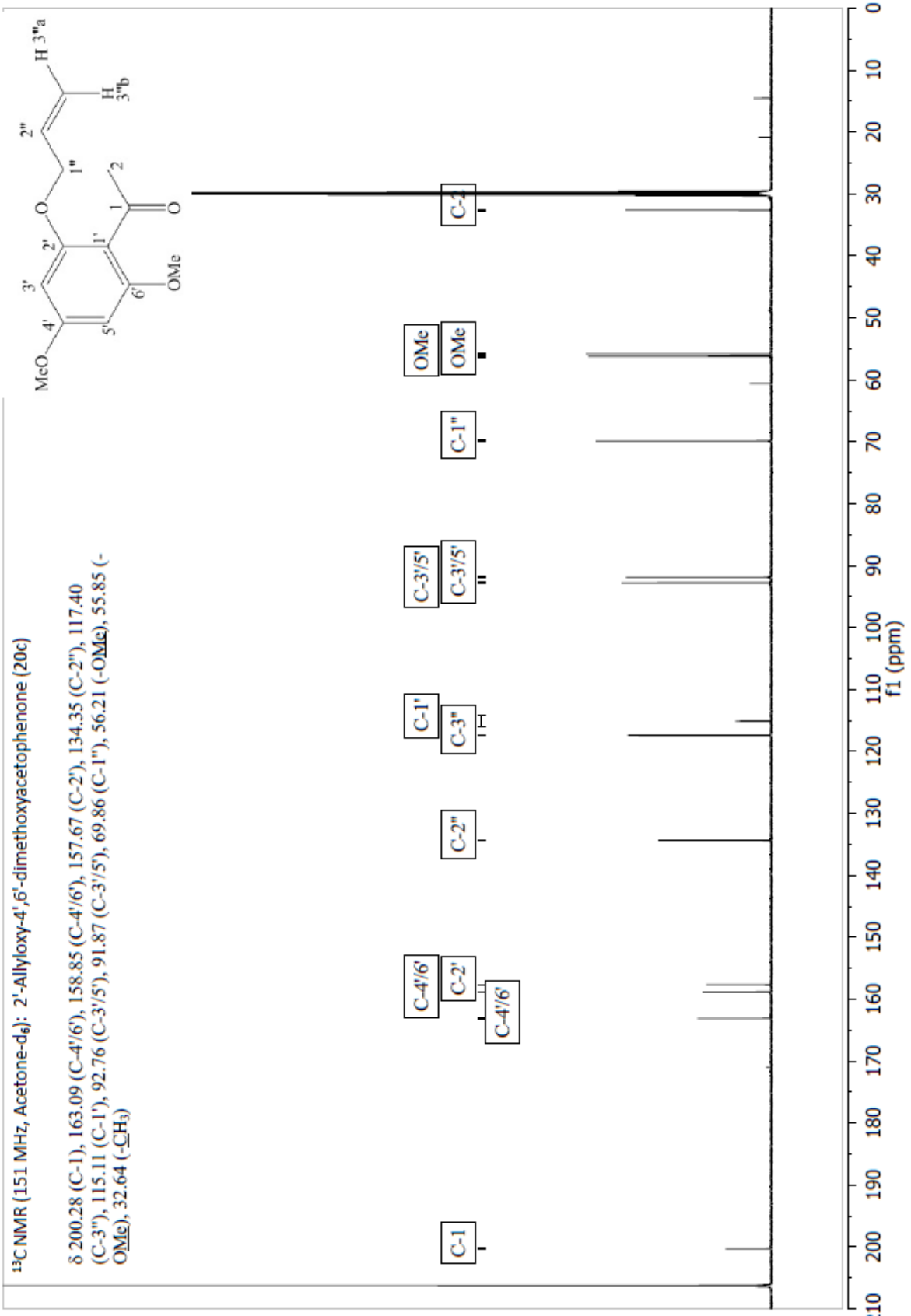

13C NMR (151 MHz, Acetone-d6): 2'-Allyloxy-4'-methoxyacetophenone (20b)
δ 196.73 (C-1), 165.50 (C-4'), 161.10 (C-2'), 134.26 (C-2"), 133.00 (C-6'), 122.13 (C-1'), 118.41 (C-3"), 106.91 (C-5'), 100.14 (C-3'), 70.32 (C-1"), 56.05 (-OMe), 32.26 (-CH3)
C-1
C-2'
C-4'
C-2"
C-6'
C-1'
C-3"
C-5'
C-3'
C-1"
OMe
C-2
MeO
f1 (ppm)

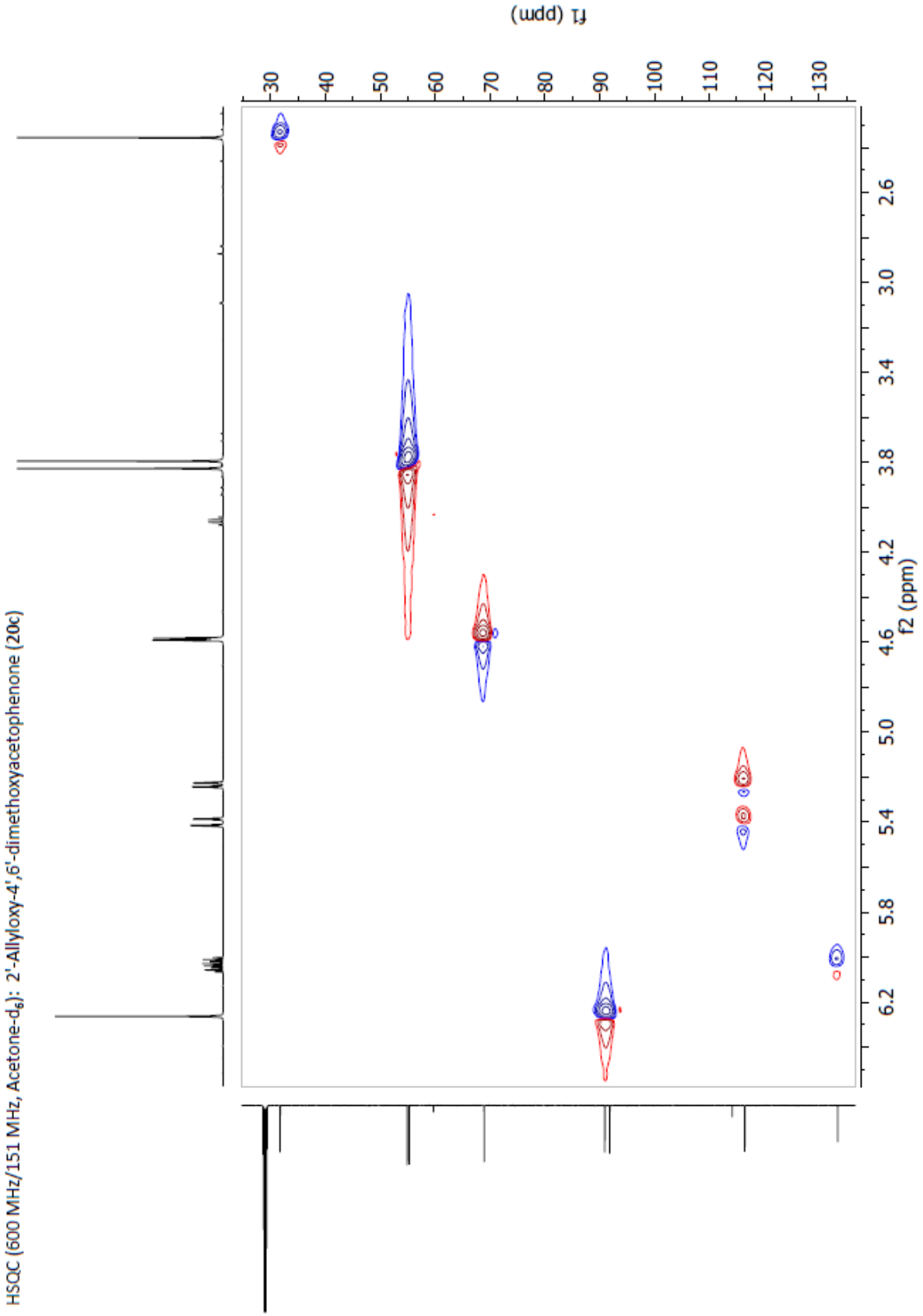

HSQC (600 MHz/151 MHz, Acetone-d6): 2'-Allyloxy-4'-methoxyacetophenone (20b)
f2 (ppm)
f1 (ppm)

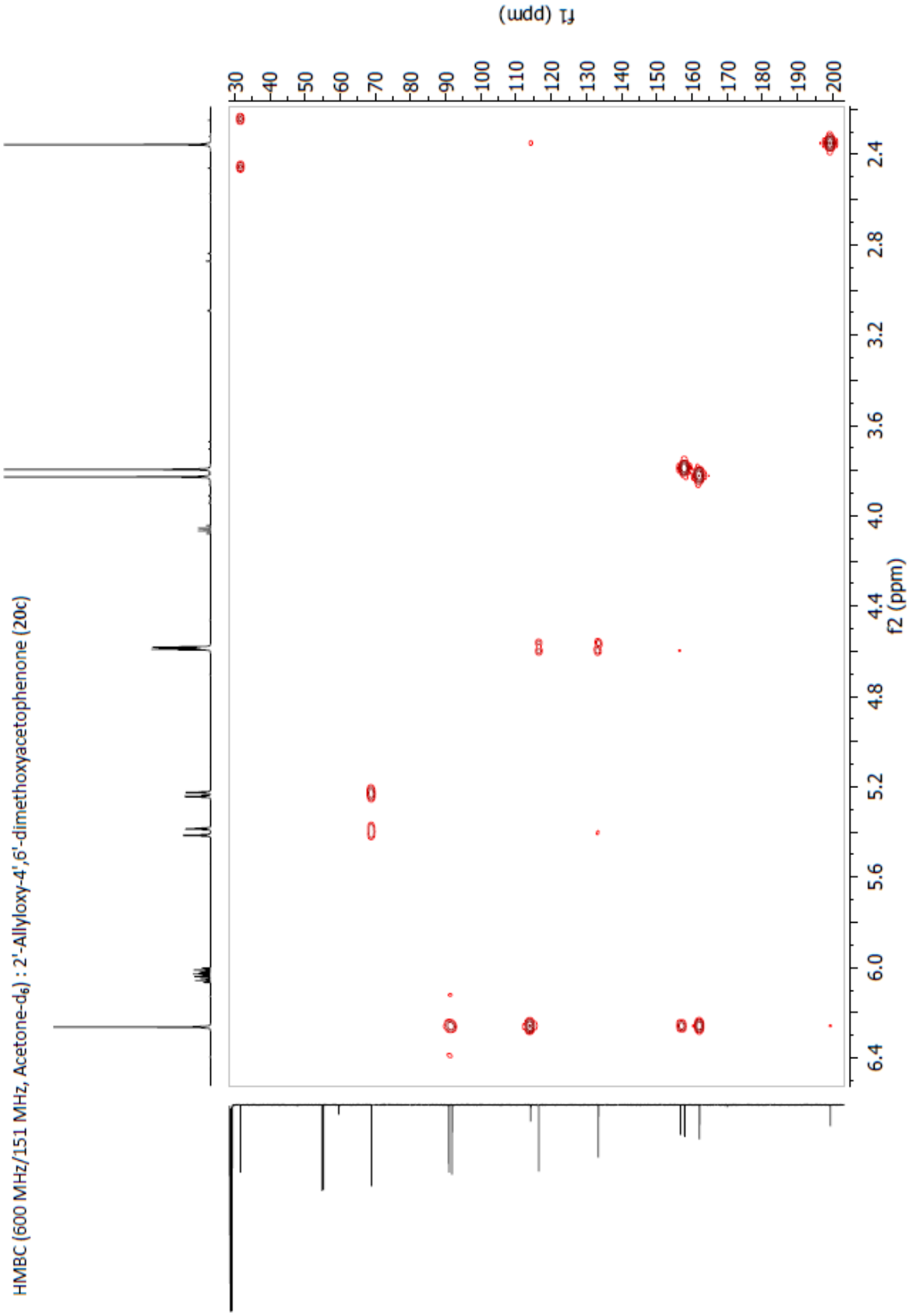

HMBC (600 MHz/151 MHz, Acetone-d6): 2'-Allyloxy-4'-methoxyacetophenone (20b)
f2 (ppm)
f1 (ppm)

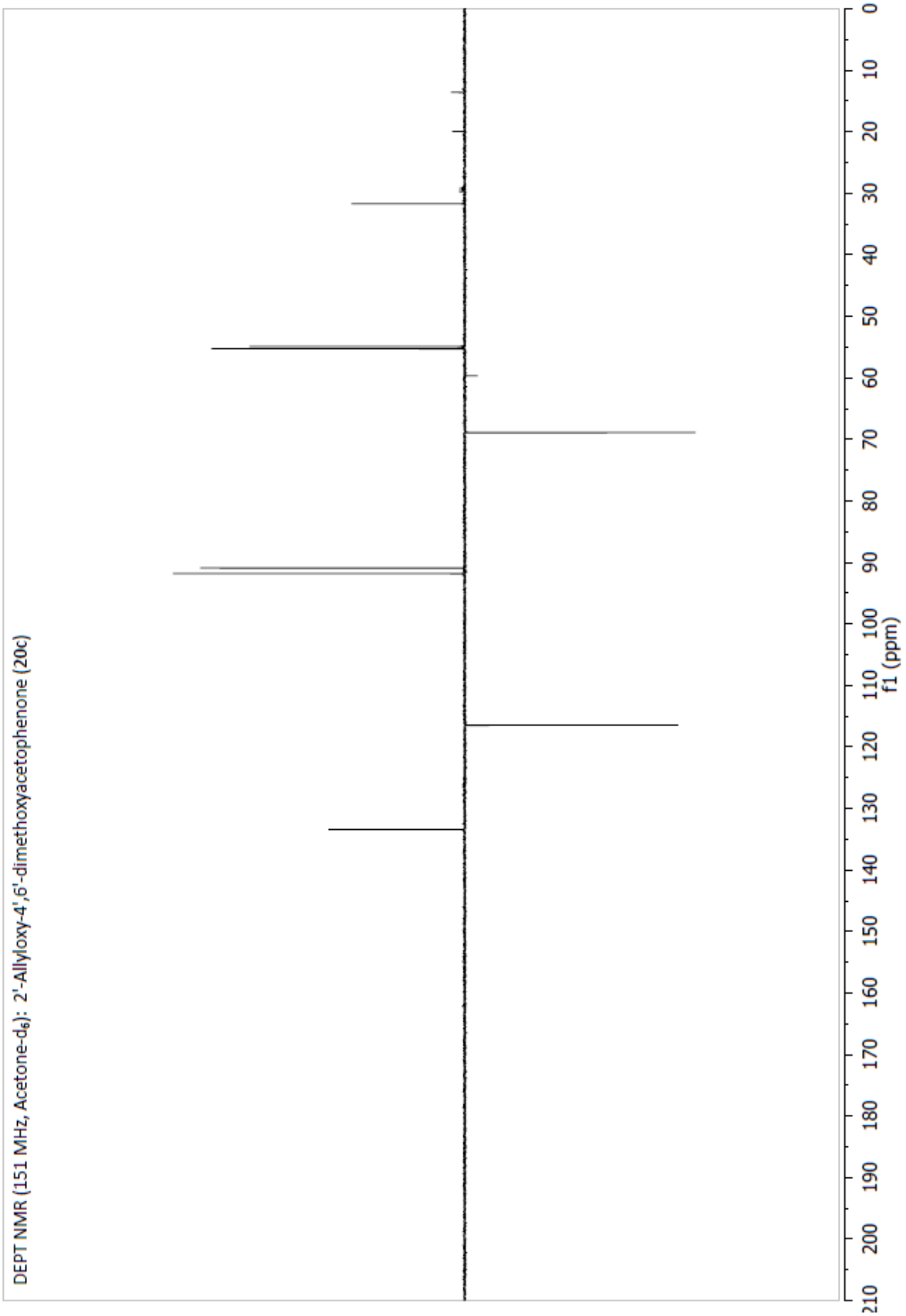

DEPT NMR (151 MHz, Acetone-d6): 2'-Allyloxy-4'-methoxyacetophenone (20b)
f1 (ppm)
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
210

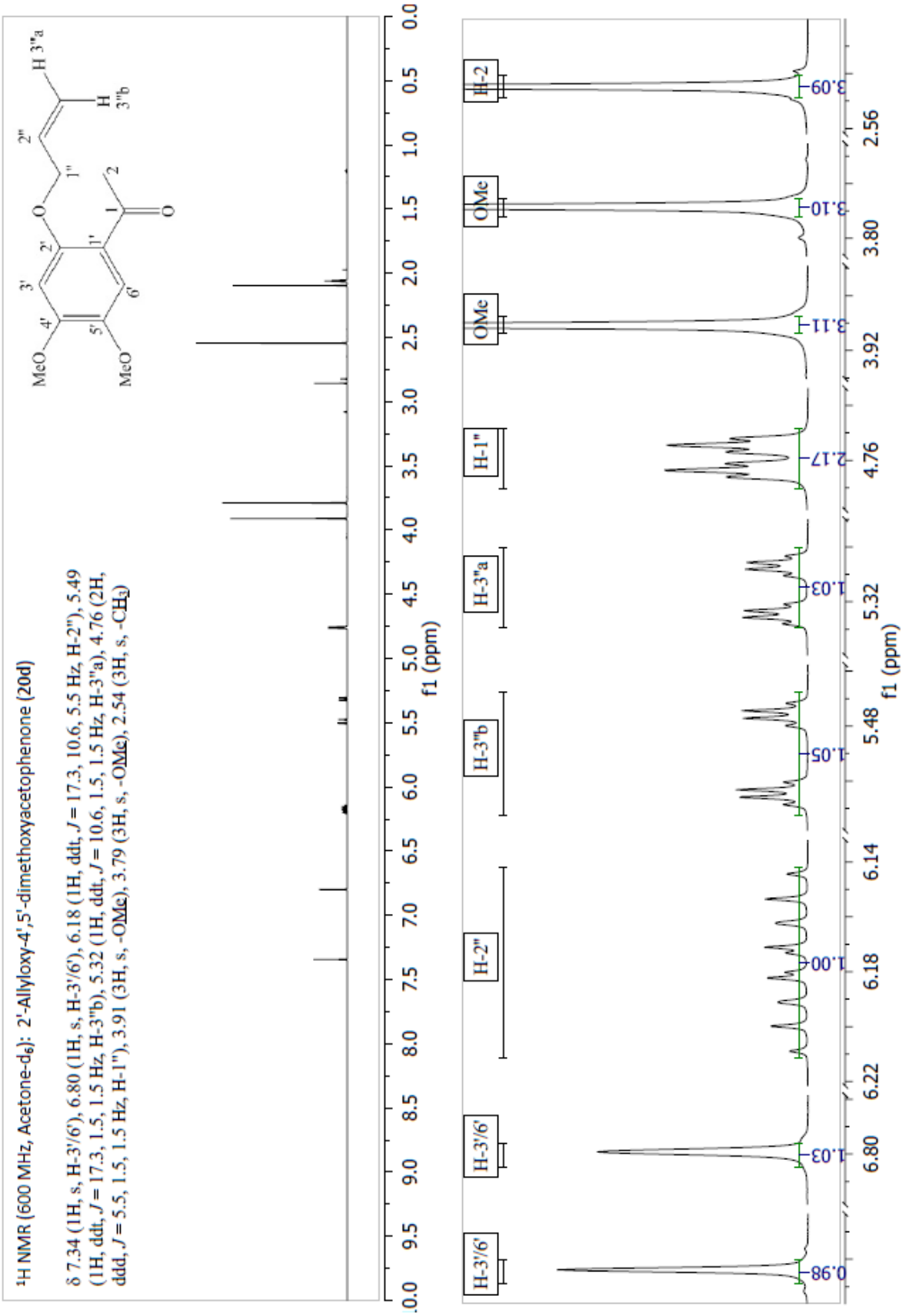

¹H NMR (600 MHz, Acetone-d₆): 2'-Allyloxy-4',6'-dimethoxyacetophenone (20c)
δ 6.26 (2H, s, H-3' and H-5'), 6.03 (1H, ddt, J = 17.3, 10.6, 5.0 Hz, H-2"), 5.40 (1H, ddt, J = 17.3, 1.7, 1,7 Hz, H-3"b), 5.23 (1H, ddt, J = 10.6, 1.7, 1.7 Hz, H-3"a), 4.59 (2H, ddd, J = 5.0, 1.7, 1.7 Hz, H-1"), 3.83 (3H, s, -OMe), 3.79 (3H, s, -OMe), 2.36 (3H, s, -CH3)
f1 (ppm)
H-3' and H-5'
H-2"
H-3"b
H-3"a
H-1"
OMe
OMe
H-2
2.09
1.00
1.04
1.05
2.17
3.19
3.24
3.04


$^{13}$C NMR (151 MHz, Acetone-d$_6$): 2'-Allyloxy-4',6'-dimethoxyacetophenone (20c)
δ 200.28 (C-1), 163.09 (C-4'/6'), 158.85 (C-4'/6'), 157.67 (C-2'), 134.35 (C-2"), 117.40 (C-3"), 115.11 (C-1'), 92.76 (C-3'/5'), 91.87 (C-3'/5'), 69.86 (C-1"), 56.21 (-OMe), 55.85 (-OMe), 32.64 (-CH$_3$)
C-1
C-4'/6'
C-2'
C-4'/6'
C-2"
C-1'
C-3"
C-3'/5'
C-3'/5'
C-1"
OMe
OMe
C-2
f1 (ppm)

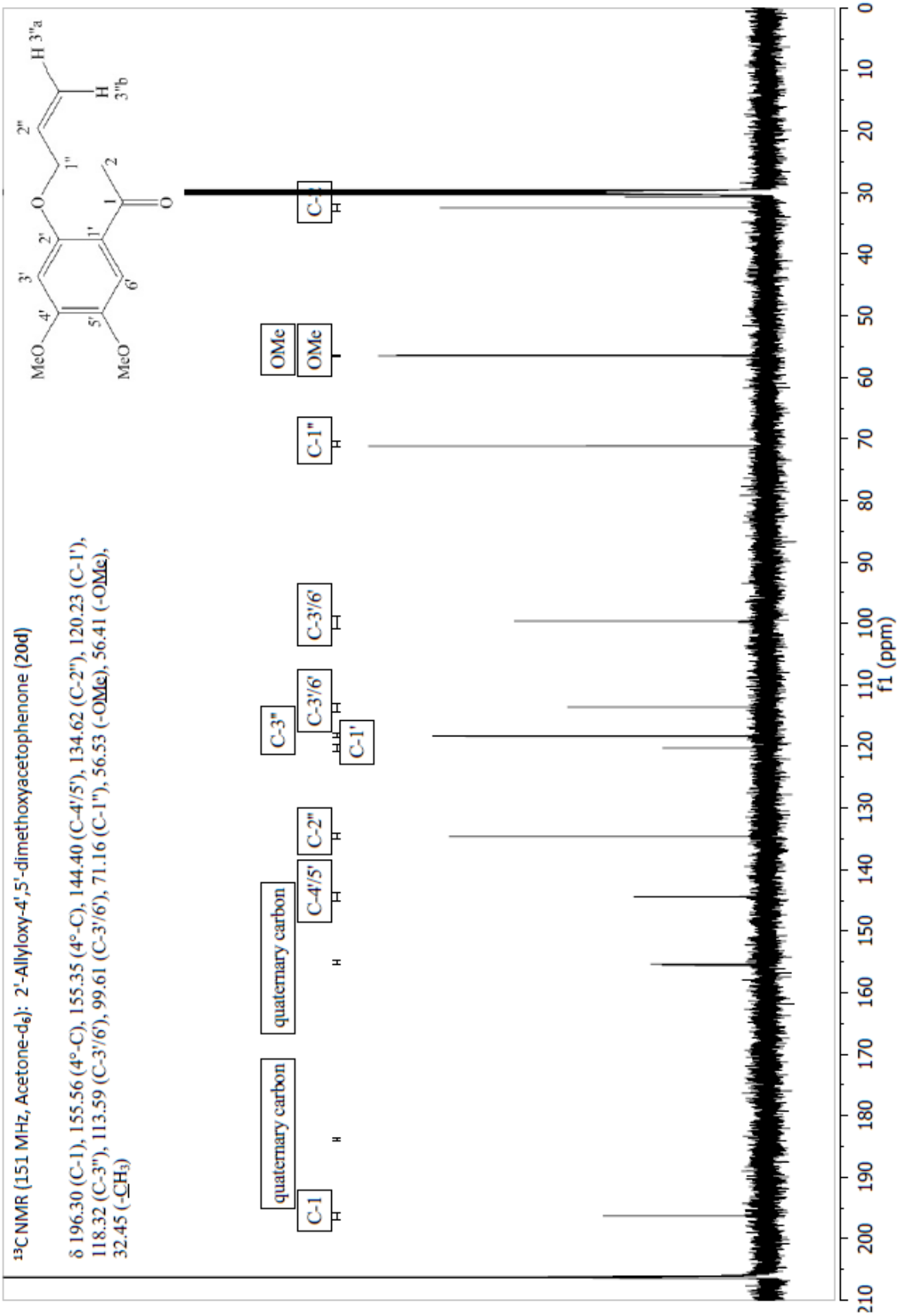

HSQC (600 MHz/151 MHz, Acetone-d6): 2'-Allyloxy-4',6'-dimethoxyacetophenone (20c)
f1 (ppm)
f2 (ppm)
30
40
50
60
70
80
90
100
110
120
130
2.6
3.0
3.4
3.8
4.2
4.6
5.0
5.4
5.8
6.2

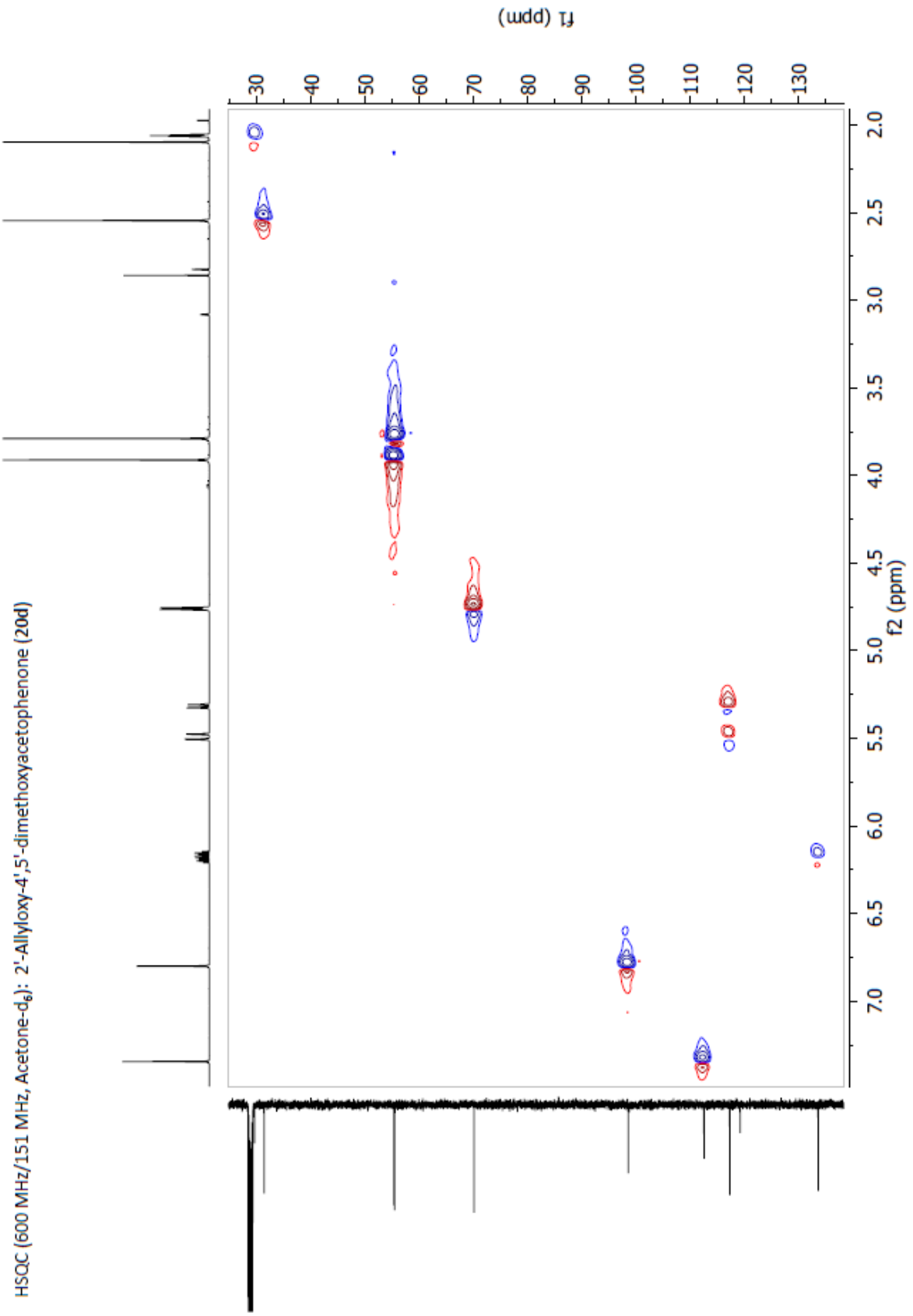

HMBC (600 MHz/151 MHz, Acetone-d6) : 2'-Allyloxy-4',6'-dimethoxyacetophenone (20c)
f1 (ppm)
f2 (ppm)
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
2.4
2.8
3.2
3.6
4.0
4.4
4.8
5.2
5.6
6.0
6.4

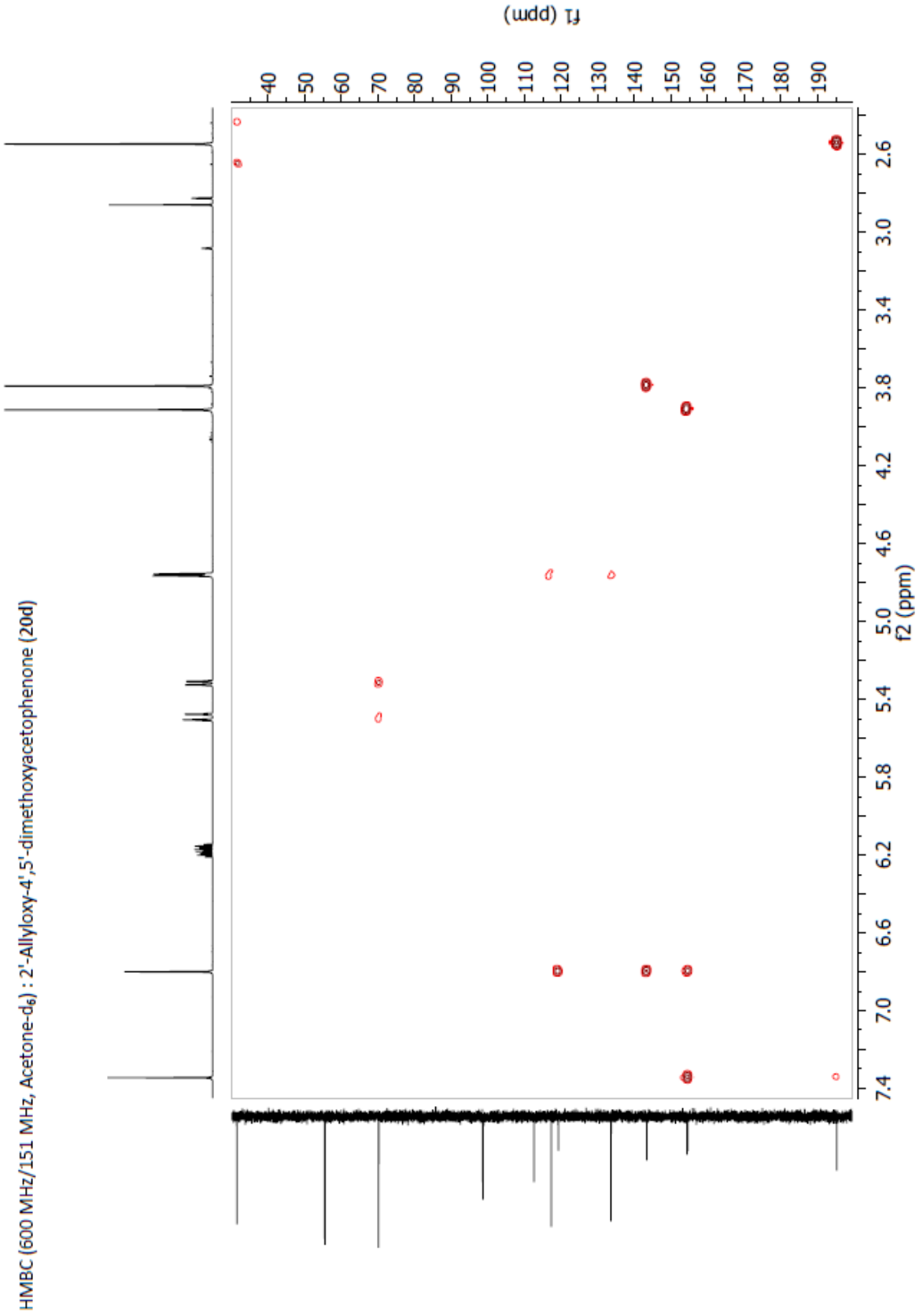

DEPT NMR (151 MHz, Acetone-d6): 2'-Allyloxy-4',6'-dimethoxyacetophenone (20c)
f1 (ppm)
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
210

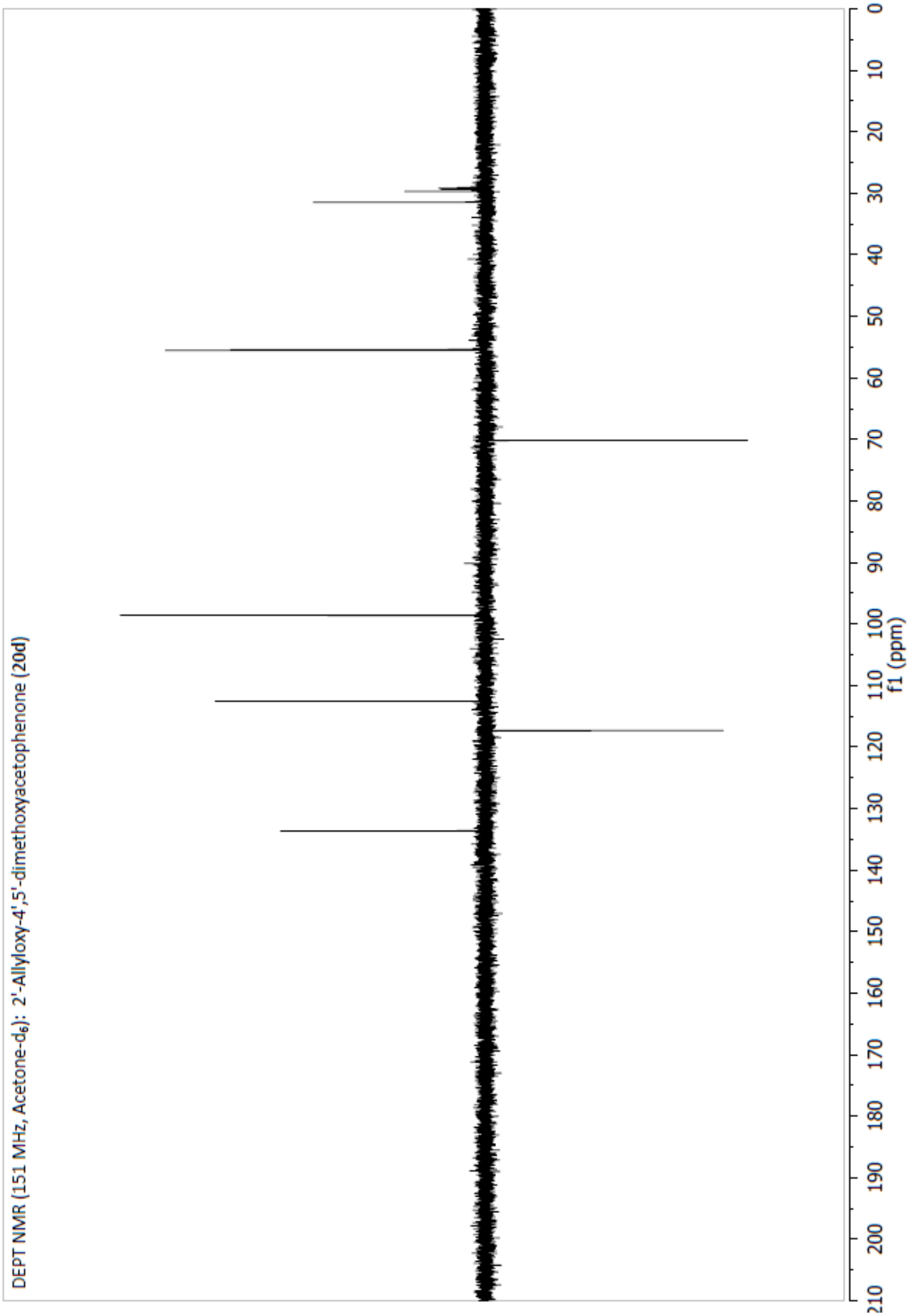

¹H NMR (600 MHz, Acetone-d6): 2'-Allyloxy-4',5'-dimethoxyacetophenone (20d)
δ 7.34 (1H, s, H-3'/6'), 6.80 (1H, s, H-3'/6'), 6.18 (1H, ddt, J = 17.3, 10.6, 5.5 Hz, H-2"), 5.49 (1H, ddt, J = 17.3, 1.5, 1.5 Hz, H-3"b), 5.32 (1H, ddt, J = 10.6, 1.5, 1.5 Hz, H-3"a), 4.76 (2H, ddd, J = 5.5, 1.5, 1.5 Hz, H-1"), 3.91 (3H, s, -OMe), 3.79 (3H, s, -OMe), 2.54 (3H, s, -CH3)
MeO
MeO
f1 (ppm)
H-3'/6'
H-3'/6'
H-2"
H-3"b
H-3"a
H-1"
OMe
OMe
H-2
0.98
1.03
1.00
1.05
1.03
2.17
3.11
3.10
3.09

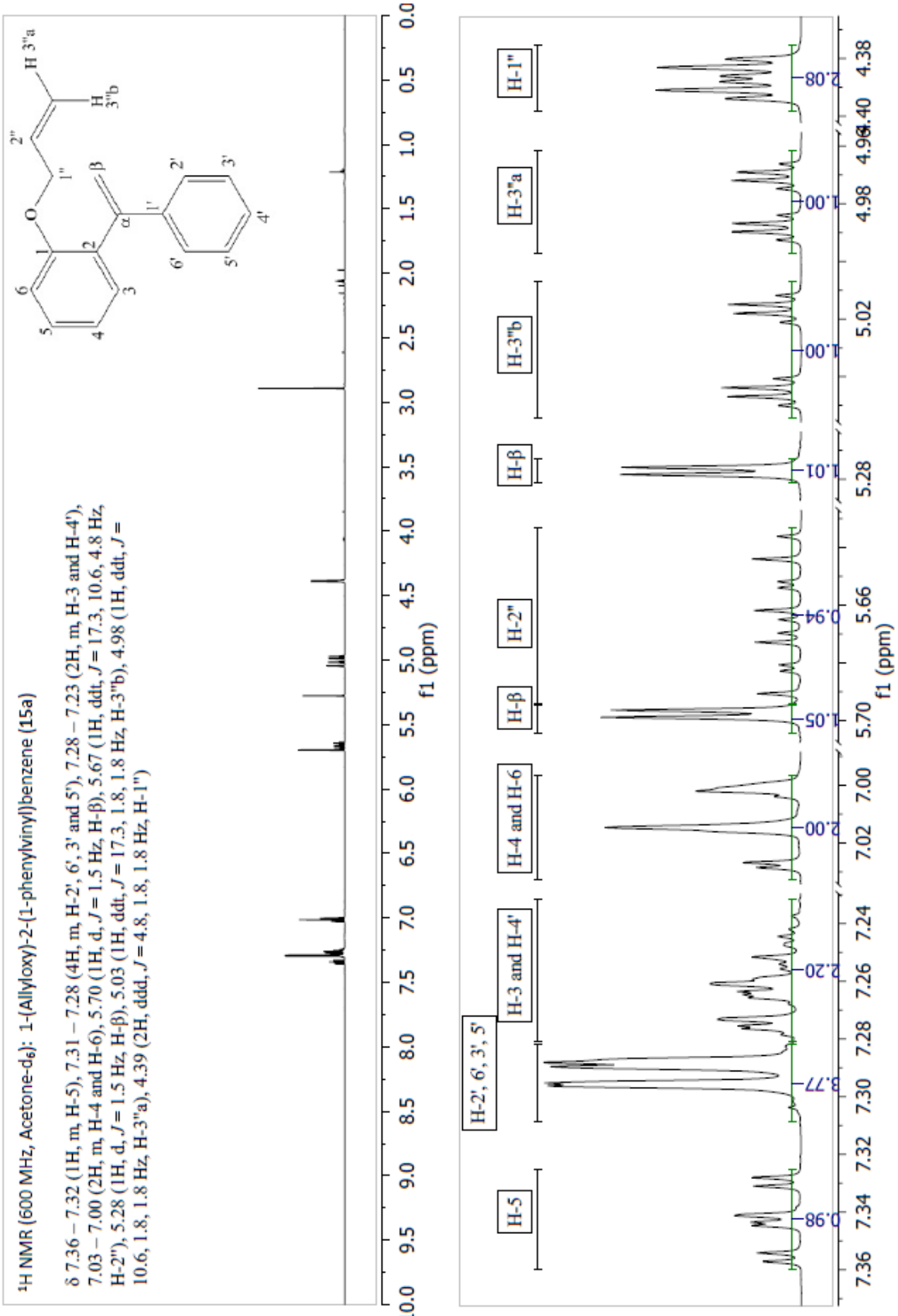
 

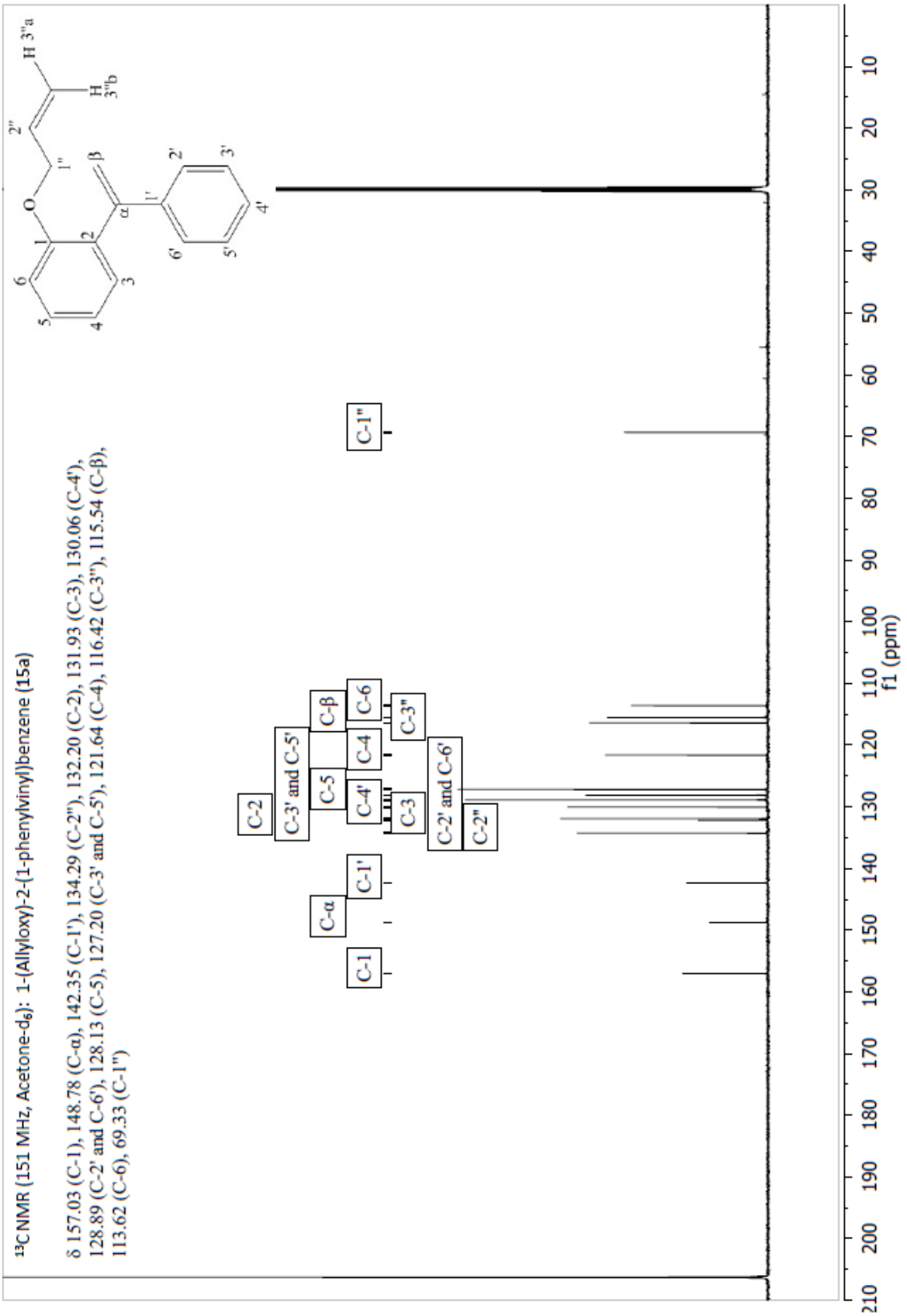

13C NMR (151 MHz, Acetone-d6): 2'-Allyloxy-4',5'-dimethoxyacetophenone (20d)
δ 196.30 (C-1), 155.56 (4'-C), 155.35 (4'-C), 144.40 (C-4'/5'), 134.62 (C-2"), 120.23 (C-1'), 118.32 (C-3"), 113.59 (C-3'/6'), 99.61 (C-3'/6'), 71.16 (C-1"), 56.53 (-OMe), 56.41 (-OMe), 32.45 (-CH3)
quaternary carbon
quaternary carbon
C-1
C-4'/5'
C-2"
C-3"
C-3'/6'
C-3'/6'
C-1'
C-1"
OMe
OMe
C-2
MeO
MeO
H 3"a
H 3"b
f1 (ppm)

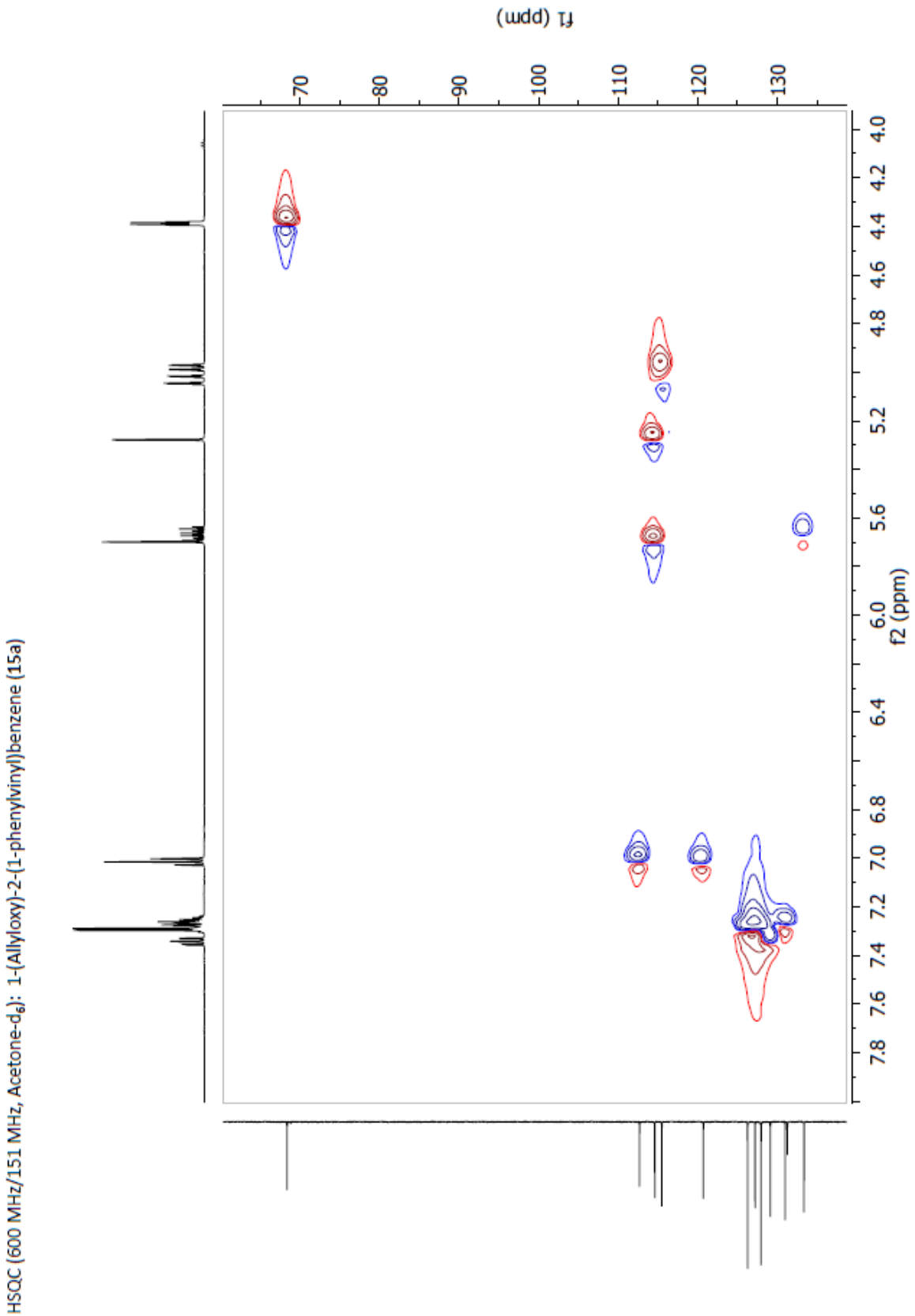

HSQC (600 MHz/151 MHz, Acetone-d6): 2'-Allyloxy-4',5'-dimethoxyacetophenone (20d)
f1 (ppm)
f2 (ppm)
30
40
50
60
70
80
90
100
110
120
130
2.0
2.5
3.0
3.5
4.0
4.5
5.0
5.5
6.0
6.5
7.0


HMBC (600 MHz/151 MHz, Acetone-d6) : 2'-Allyloxy-4',5'-dimethoxyacetophenone (20d)
f1 (ppm)
f2 (ppm)

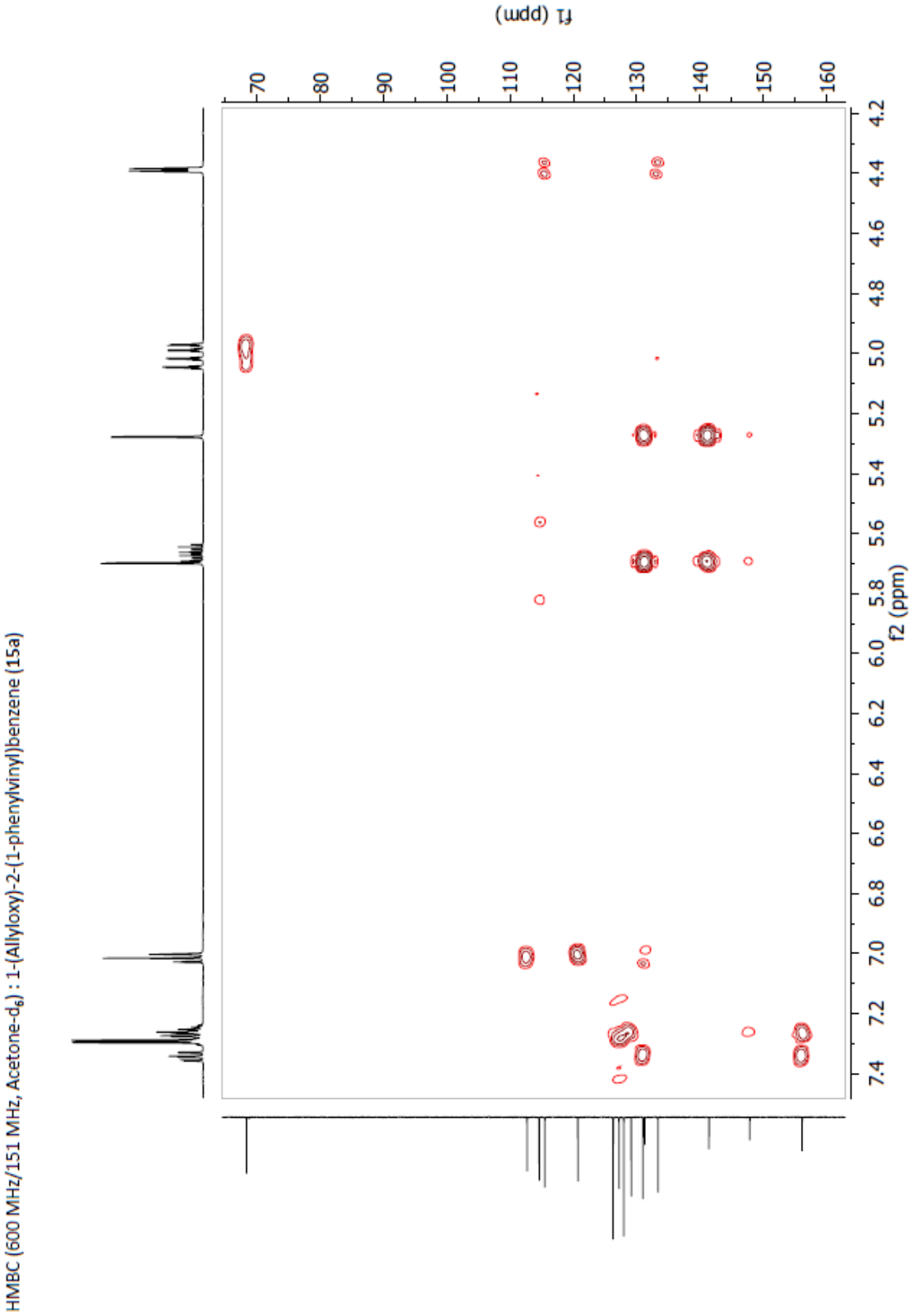

DEPT NMR (151 MHz, Acetone-d6): 2'-Allyloxy-4',5'-dimethoxyacetophenone (20d)
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
210
f1 (ppm)


¹H NMR (600 MHz, Acetone-d6): 1-(Allyloxy)-2-(1-phenylvinyl)benzene (15a)
δ 7.36 – 7.32 (1H, m, H-5), 7.31 – 7.28 (4H, m, H-2', 6', 3' and 5'), 7.28 – 7.23 (2H, m, H-3 and H-4'), 7.03 – 7.00 (2H, m, H-4 and H-6), 5.70 (1H, d, J = 1.5 Hz, H-β), 5.67 (1H, ddt, J = 17.3, 10.6, 4.8 Hz, H-2''), 5.28 (1H, d, J = 1.5 Hz, H-β), 5.03 (1H, ddt, J = 17.3, 1.8, 1.8 Hz, H-3''b), 4.98 (1H, ddt, J = 10.6, 1.8, 1.8 Hz, H-3''a), 4.39 (2H, ddd, J = 4.8, 1.8, 1.8 Hz, H-1'')
f1 (ppm)
H-5
H-2', 6', 3', 5'
H-3 and H-4'
H-4 and H-6
H-β
H-2''
H-β
H-3''b
H-3''a
H-1''

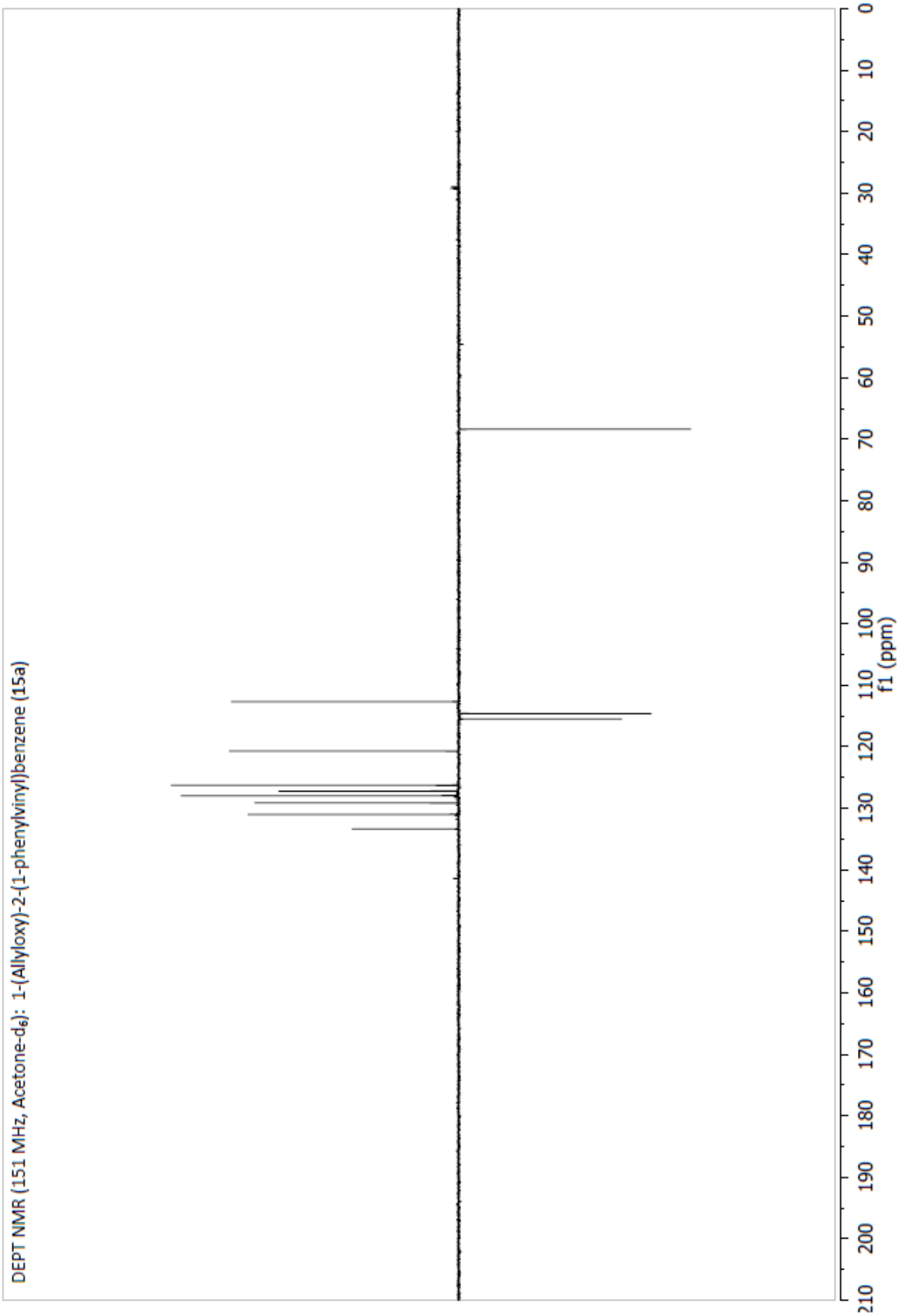

$^{13}$C NMR (151 MHz, Acetone-d$_6$): 1-(Allyloxy)-2-(1-phenylvinyl)benzene (15a)
δ 157.03 (C-1), 148.78 (C-α), 142.35 (C-1'), 134.29 (C-2''), 132.20 (C-2), 131.93 (C-3), 130.06 (C-4'), 128.89 (C-2' and C-6'), 128.13 (C-5), 127.20 (C-3' and C-5'), 121.64 (C-4), 116.42 (C-3''), 115.54 (C-β), 113.62 (C-6), 69.33 (C-1'')
C-1
C-α
C-1'
C-2
C-3' and C-5'
C-5
C-4'
C-3
C-2' and C-6'
C-2''
C-β
C-4
C-6
C-3''
C-1''
f1 (ppm)

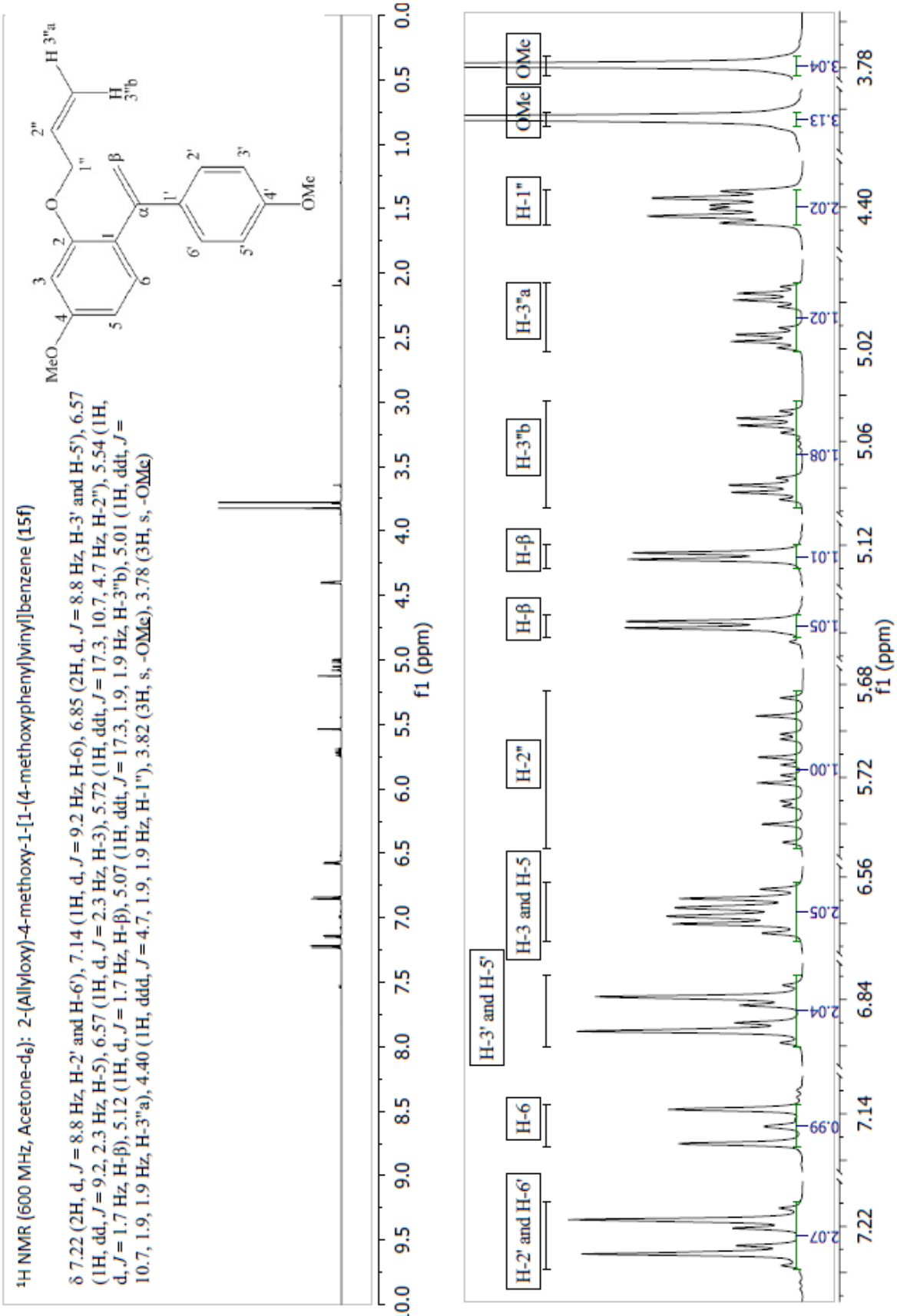



HSQC (600 MHz/151 MHz, Acetone-$d_6$): 1-(Allyloxy)-2-(1-phenylvinyl)benzene (15a)

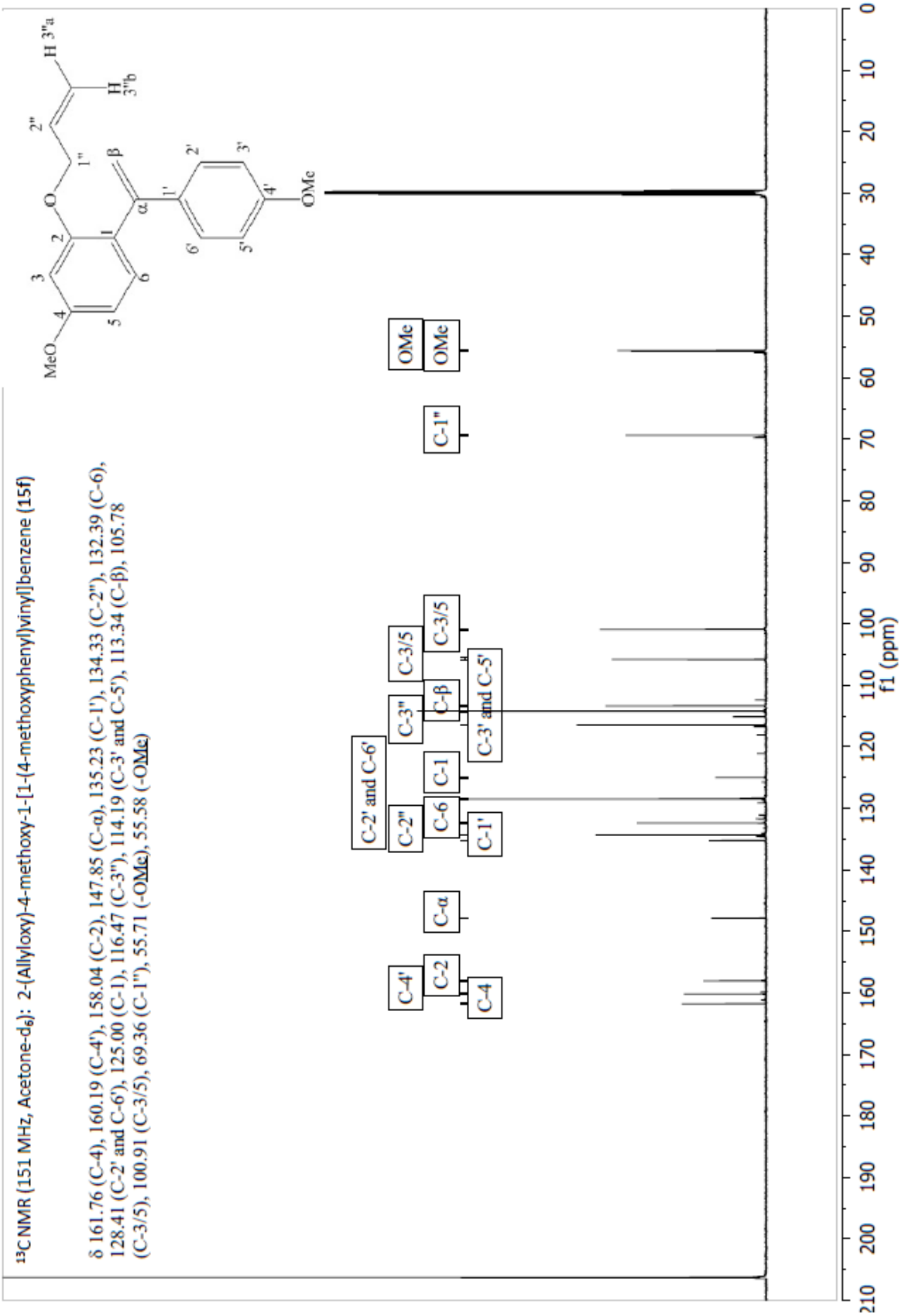


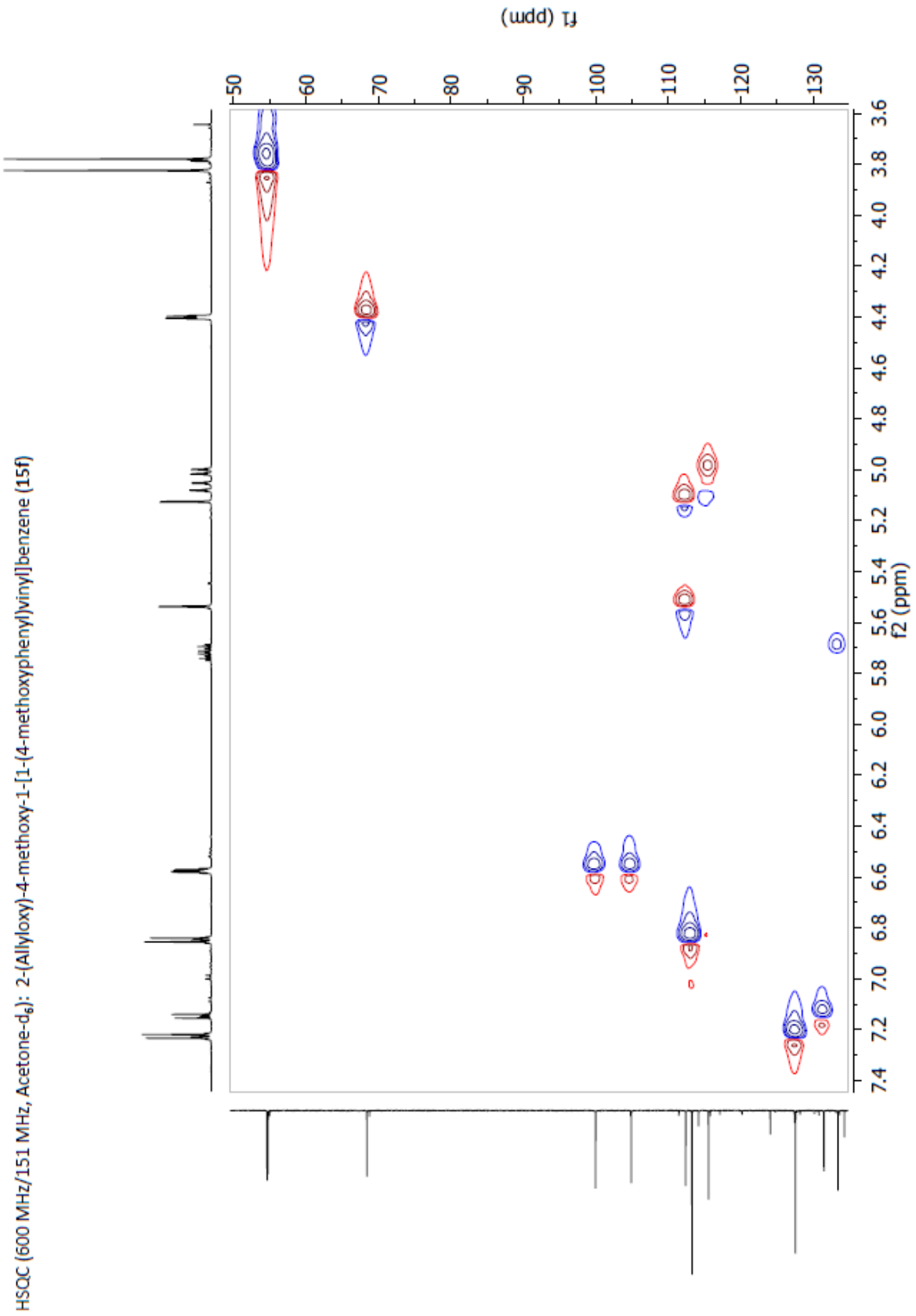

HMBC (600 MHz/151 MHz, Acetone-$d_6$) : 1-(Allyloxy)-2-(1-phenylvinyl)benzene (15a)

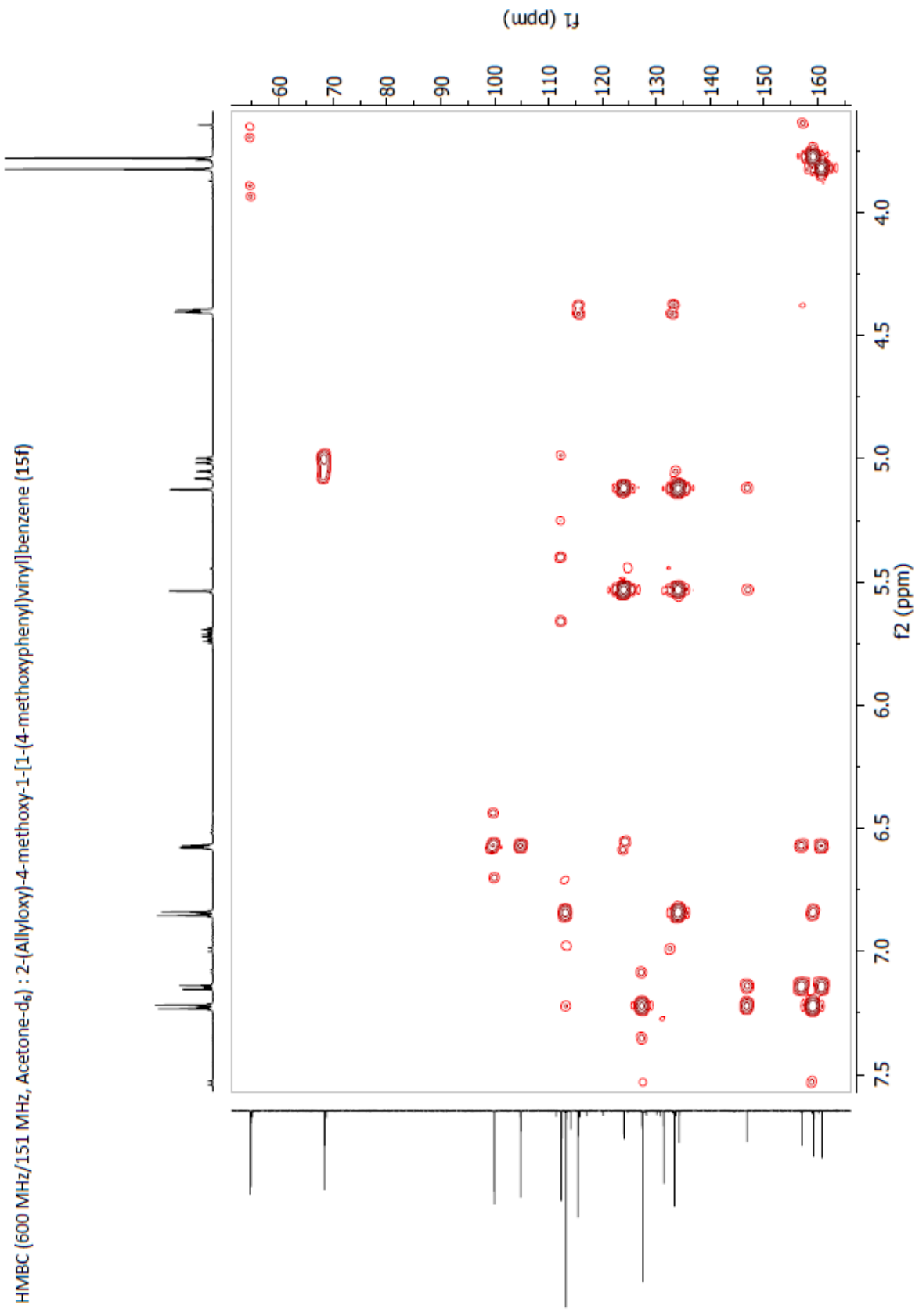

DEPT NMR (151 MHz, Acetone-d6): 1-(Allyloxy)-2-(1-phenylvinyl)benzene (15a)
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
210
f1 (ppm)

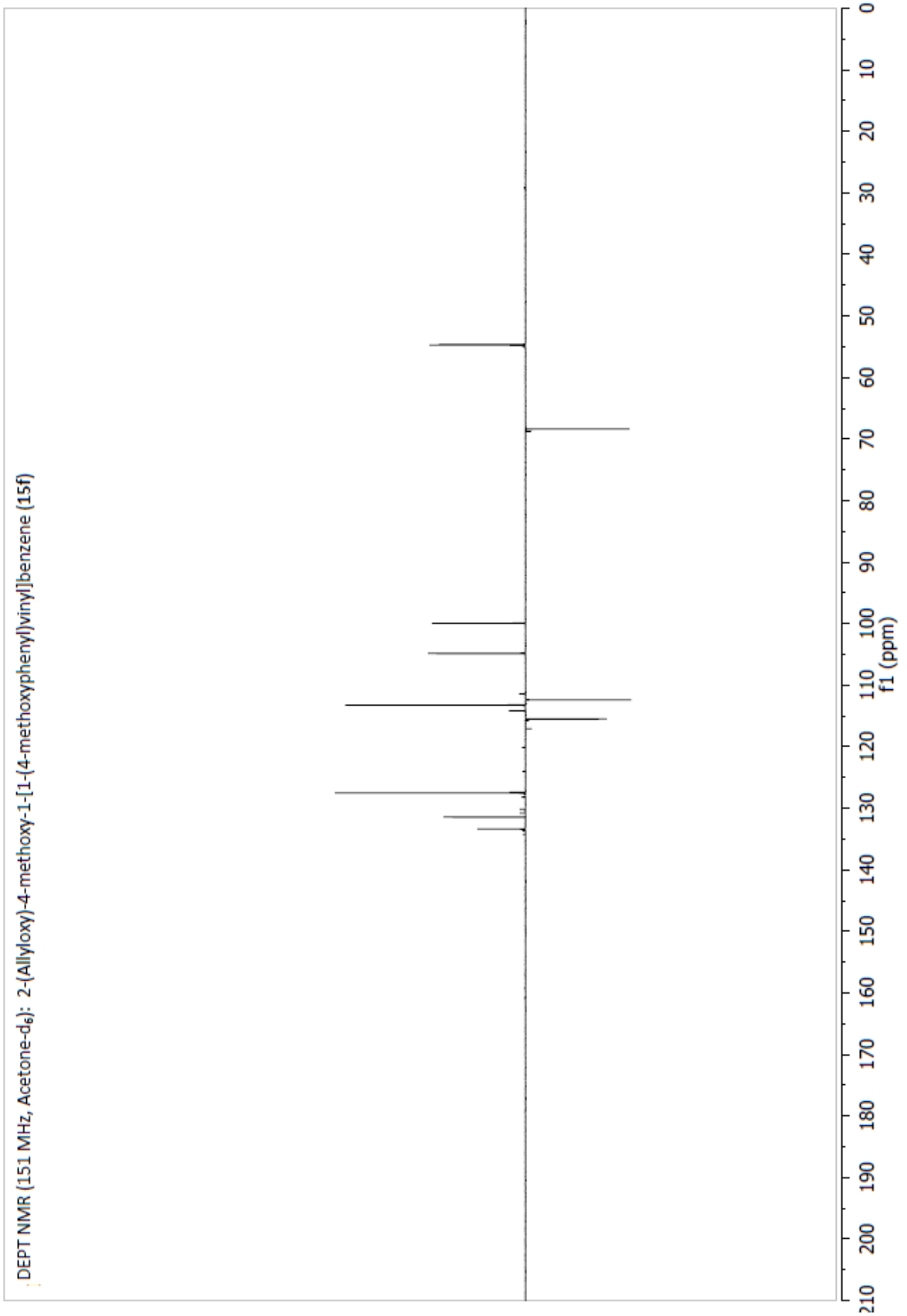

¹H NMR (600 MHz, Acetone-d6): 2-(Allyloxy)-4-methoxy-1-[1-(4-methoxyphenyl)vinyl]benzene (15f)
δ 7.22 (2H, d, J = 8.8 Hz, H-2' and H-6'), 7.14 (1H, d, J = 9.2 Hz, H-6), 6.85 (2H, d, J = 8.8 Hz, H-3' and H-5'), 6.57 (1H, dd, J = 9.2, 2.3 Hz, H-5), 6.57 (1H, d, J = 2.3 Hz, H-3), 5.72 (1H, ddt, J = 17.3, 10.7, 4.7 Hz, H-2"), 5.54 (1H, d, J = 1.7 Hz, H-β), 5.12 (1H, d, J = 1.7 Hz, H-β), 5.07 (1H, ddt, J = 17.3, 1.9, 1.9 Hz, H-3"b), 5.01 (1H, ddt, J = 10.7, 1.9, 1.9 Hz, H-3"a), 4.40 (1H, ddd, J = 4.7, 1.9, 1.9 Hz, H-1"), 3.82 (3H, s, -OMe), 3.78 (3H, s, -OMe)
MeO
OMe
f1 (ppm)
H-2' and H-6'
H-6
H-3' and H-5'
H-3 and H-5
H-2"
H-β
H-β
H-3"b
H-3"a
H-1"
OMe
OMe
2.07
0.99
2.04
2.05
1.00
1.05
1.01
1.08
1.02
2.02
3.13
3.04
7.22
7.14
6.84
6.56
5.72
5.68
5.12
5.06
5.02
4.40
3.78

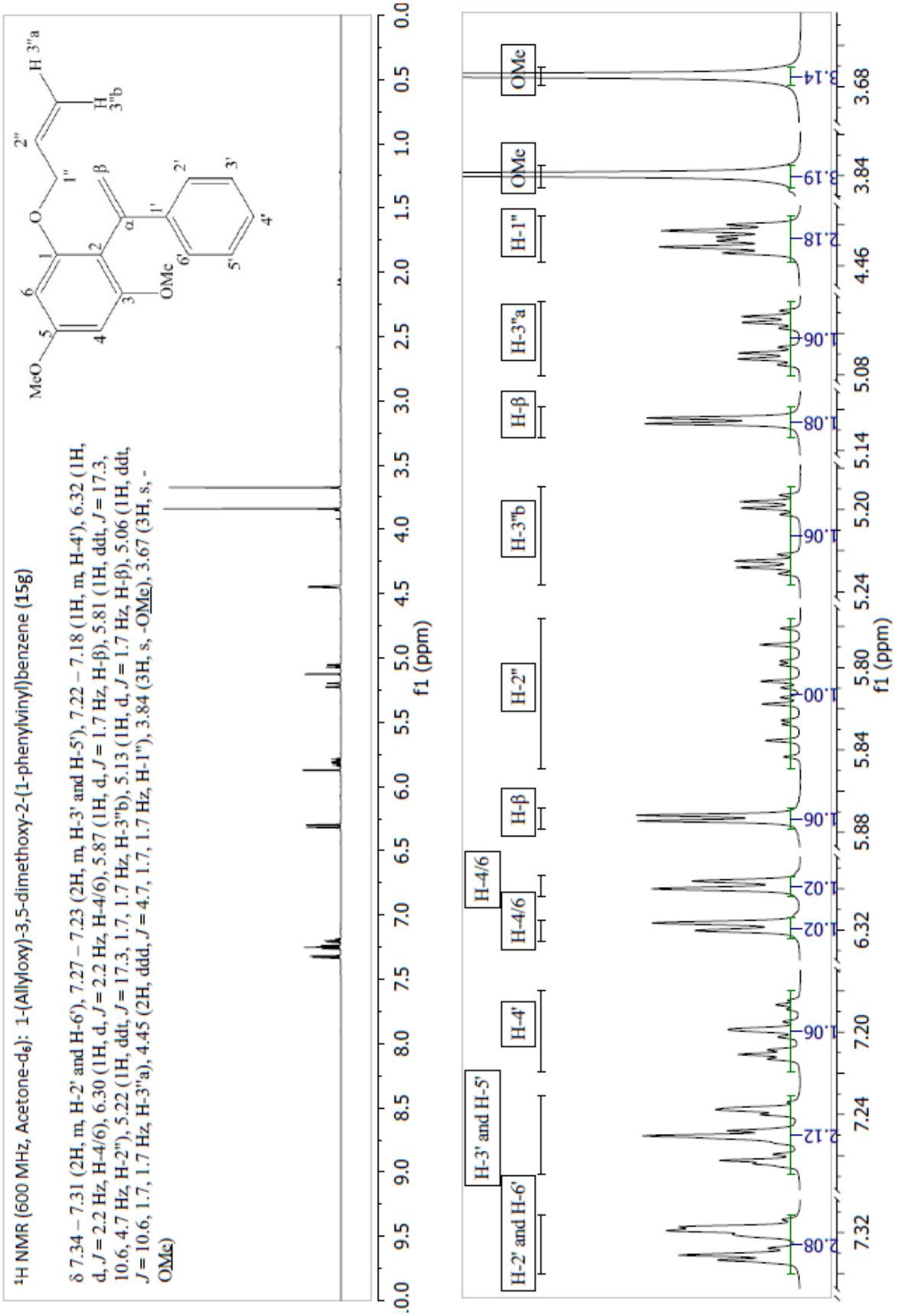
 

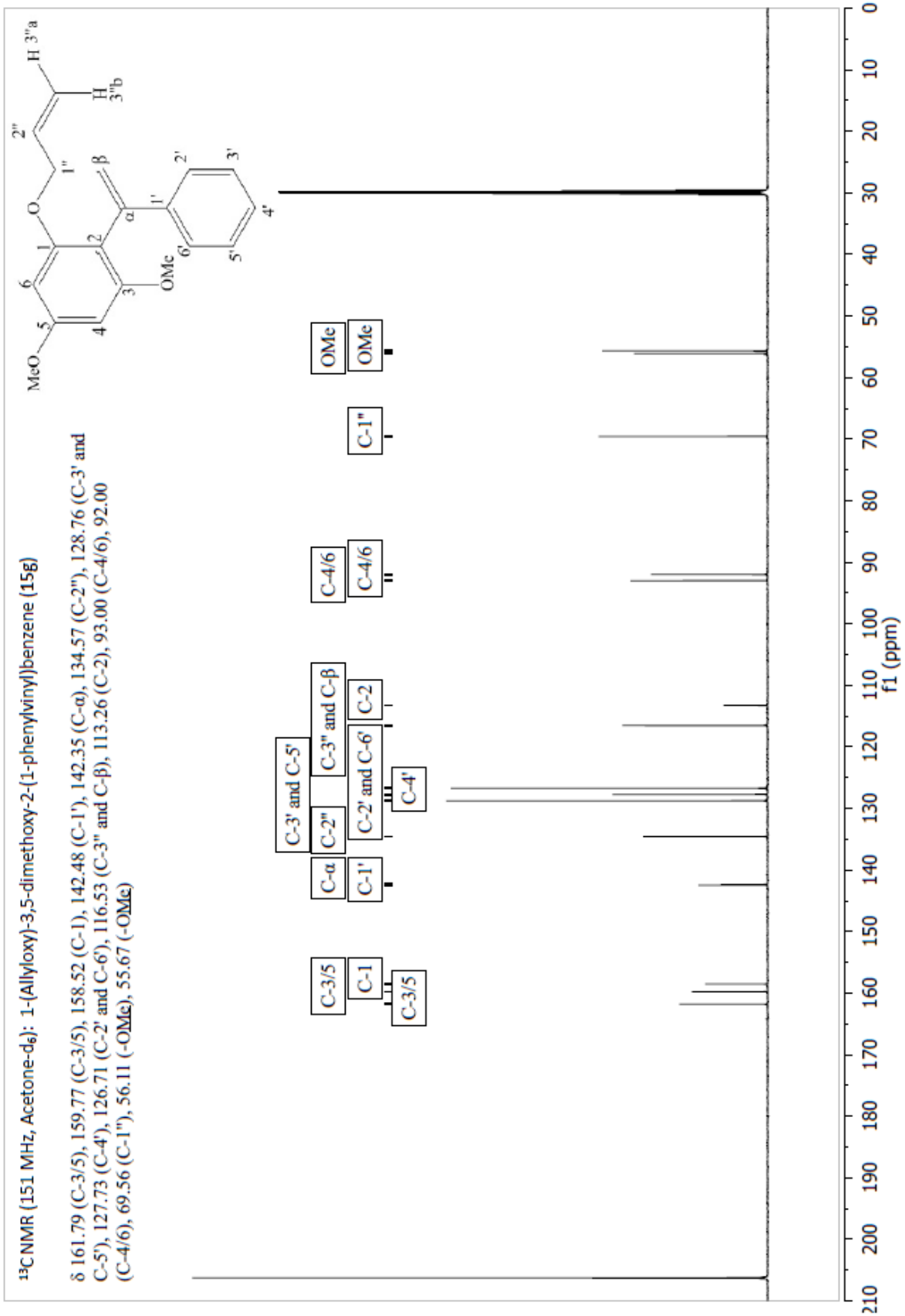

$^{13}$C NMR (151 MHz, Acetone-d$_6$): 2-(Allyloxy)-4-methoxy-1-[1-(4-methoxyphenyl)vinyl]benzene (15f)
δ 161.76 (C-4), 160.19 (C-4'), 158.04 (C-2), 147.85 (C-α), 135.23 (C-1'), 134.33 (C-2"), 132.39 (C-6), 128.41 (C-2' and C-6'), 125.00 (C-1), 116.47 (C-3"), 114.19 (C-3' and C-5'), 113.34 (C-β), 105.78 (C-3/5), 100.91 (C-3/5), 69.36 (C-1"), 55.71 (-OMe), 55.58 (-OMe)
C-4'
C-2
C-4
C-α
C-2' and C-6'
C-2"
C-6
C-1
C-1'
C-3"
C-β
C-3' and C-5'
C-3/5
C-3/5
C-1"
OMe
OMe
MeO
OMe
f1 (ppm)

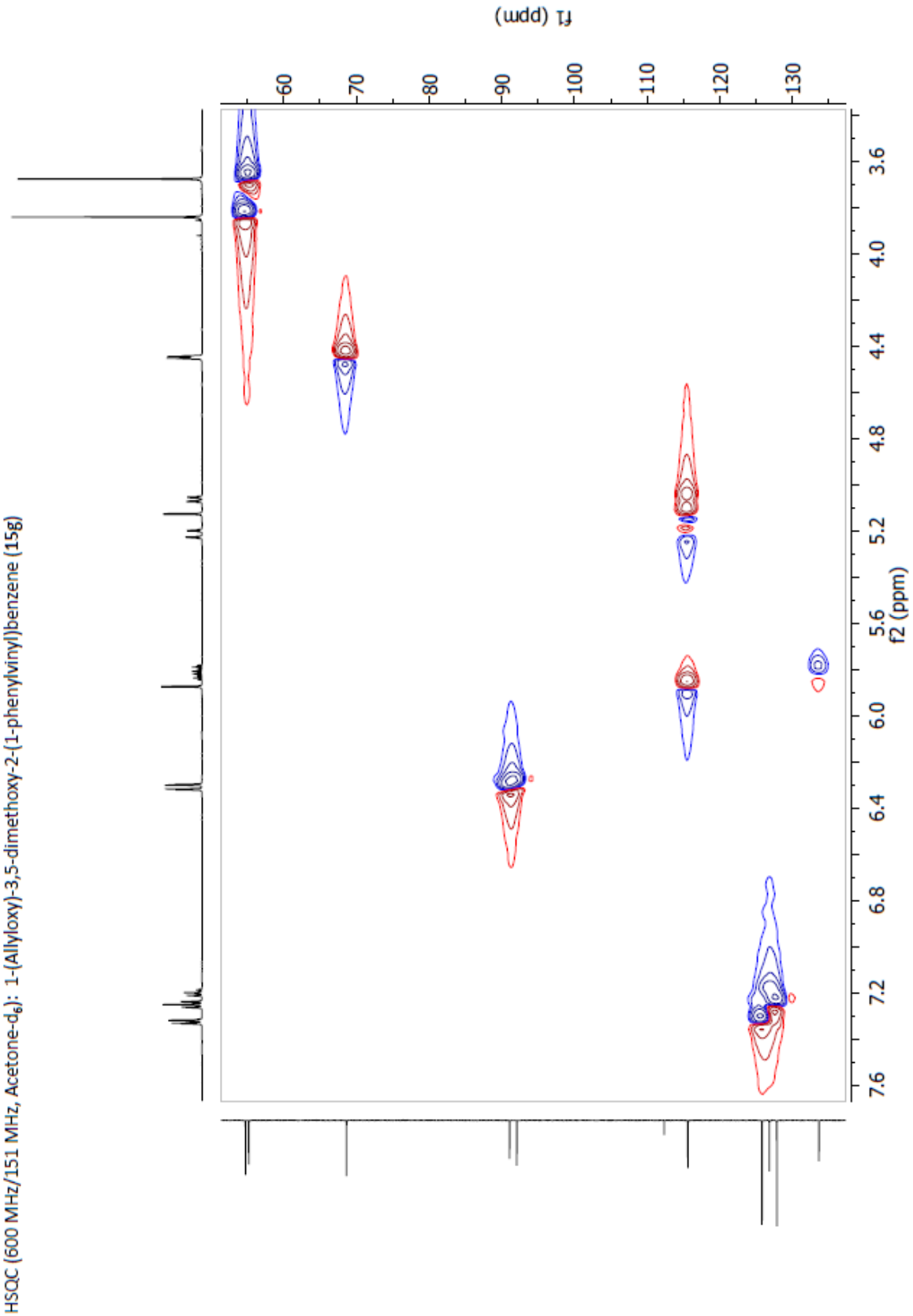

HSQC (600 MHz/151 MHz, Acetone-d6): 2-(Allyloxy)-4-methoxy-1-[1-(4-methoxyphenyl)vinyl]benzene (15f)
f1 (ppm)
f2 (ppm)


HMBC (600 MHz/151 MHz, Acetone-d6) : 2-(Allyloxy)-4-methoxy-1-[1-(4-methoxyphenyl)vinyl]benzene (15f)
f1 (ppm)
f2 (ppm)

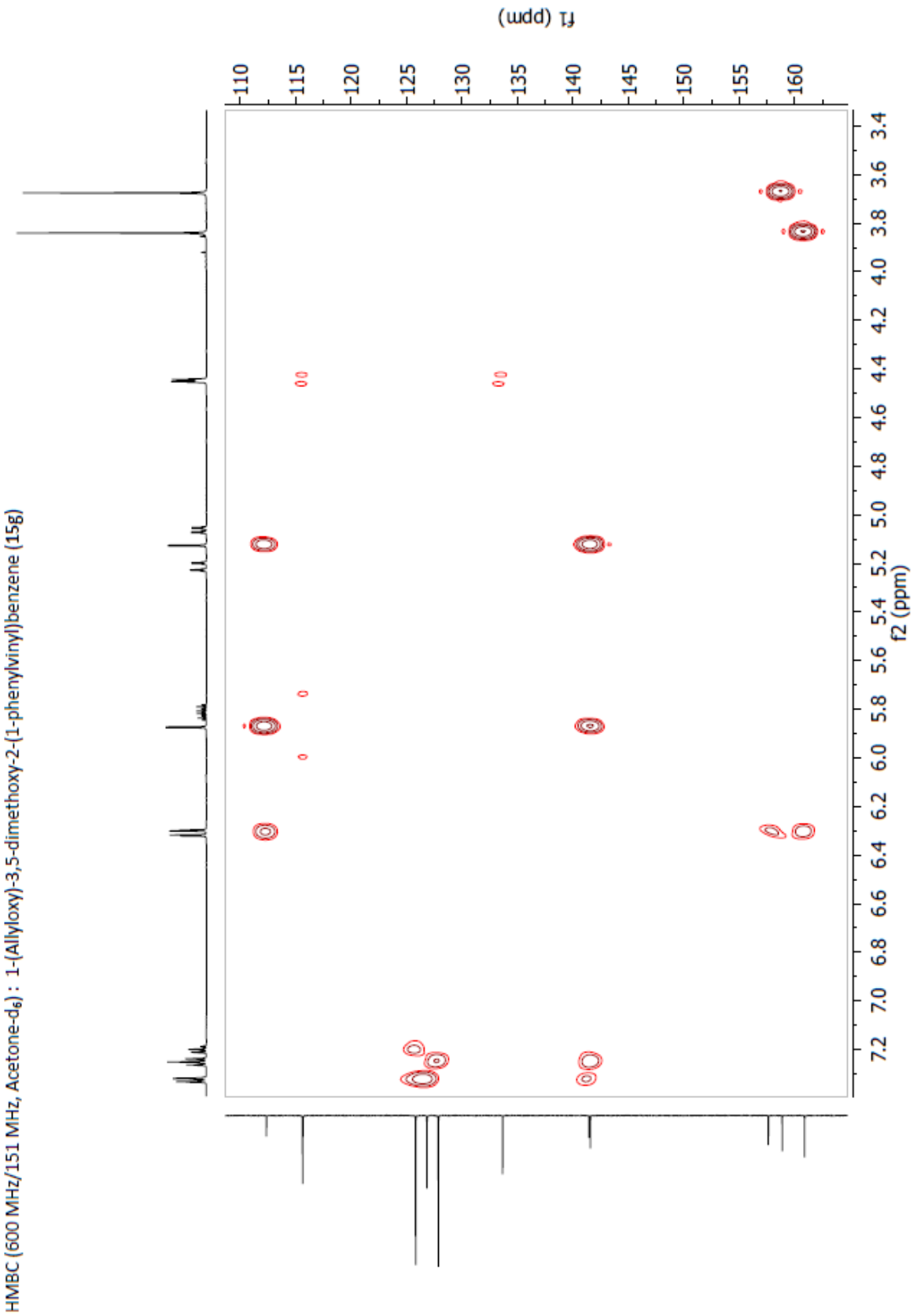

DEPT NMR (151 MHz, Acetone-d6): 2-(Allyloxy)-4-methoxy-1-[1-(4-methoxyphenyl)vinyl]benzene (15f)
f1 (ppm)
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
210

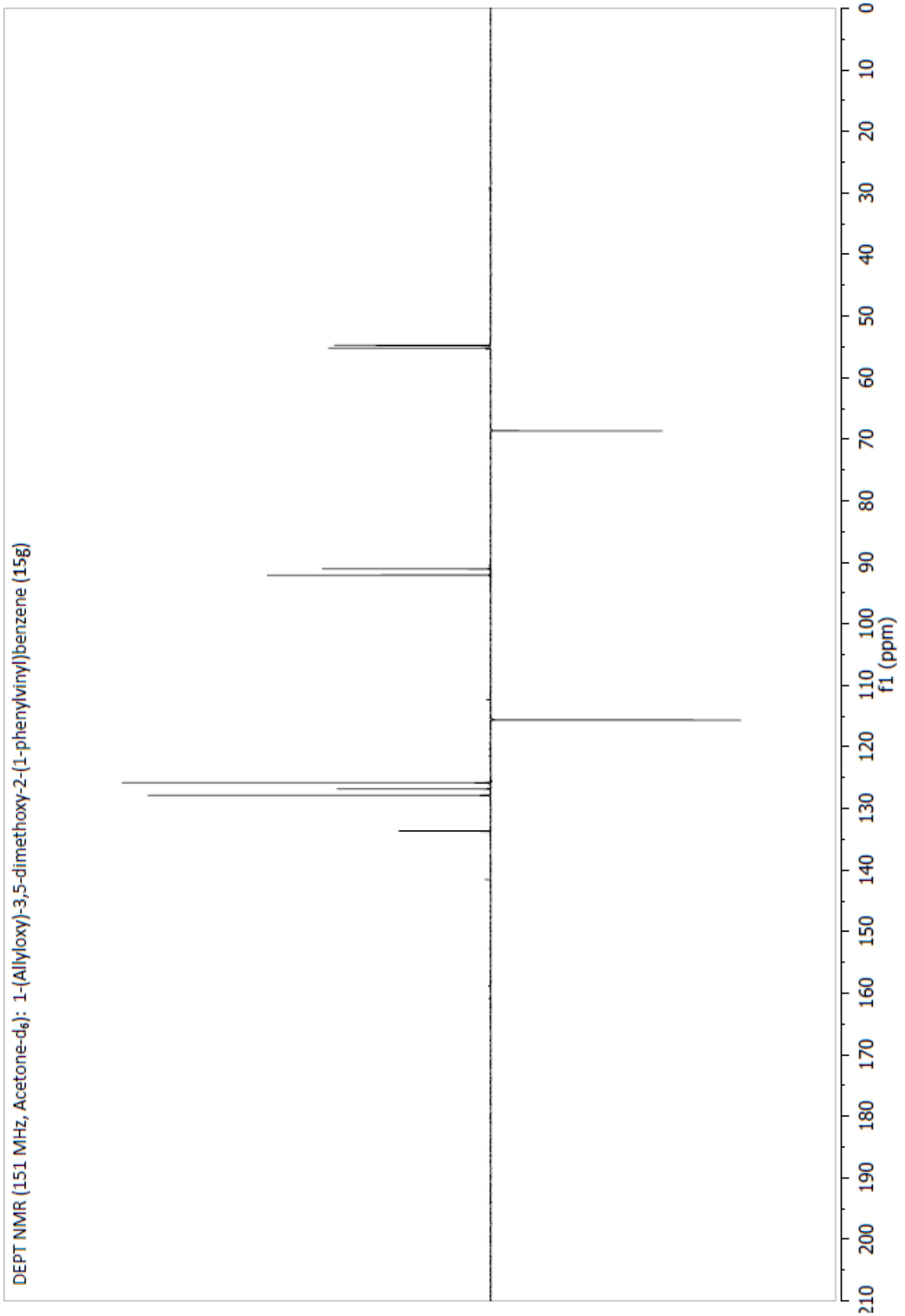

¹H NMR (600 MHz, Acetone-d6): 1-(Allyloxy)-3,5-dimethoxy-2-(1-phenylvinyl)benzene (15g)
δ 7.34 – 7.31 (2H, m, H-2' and H-6'), 7.27 – 7.23 (2H, m, H-3' and H-5'), 7.22 – 7.18 (1H, m, H-4'), 6.32 (1H, d, J = 2.2 Hz, H-4/6), 6.30 (1H, d, J = 2.2 Hz, H-4/6), 5.87 (1H, d, J = 1.7 Hz, H-β), 5.81 (1H, ddt, J = 17.3, 10.6, 4.7 Hz, H-2"), 5.22 (1H, ddt, J = 17.3, 1.7, 1.7 Hz, H-3"b), 5.13 (1H, d, J = 1.7 Hz, H-β), 5.06 (1H, ddt, J = 10.6, 1.7, 1.7 Hz, H-3"a), 4.45 (2H, ddd, J = 4.7, 1.7, 1.7 Hz, H-1"), 3.84 (3H, s, -OMe), 3.67 (3H, s, -OMe)
MeO
OMe
H 3"a
H 3"b
f1 (ppm)
H-2' and H-6'
H-3' and H-5'
H-4'
H-4/6
H-β
H-2"
H-3"b
H-3"a
H-1"
OMe

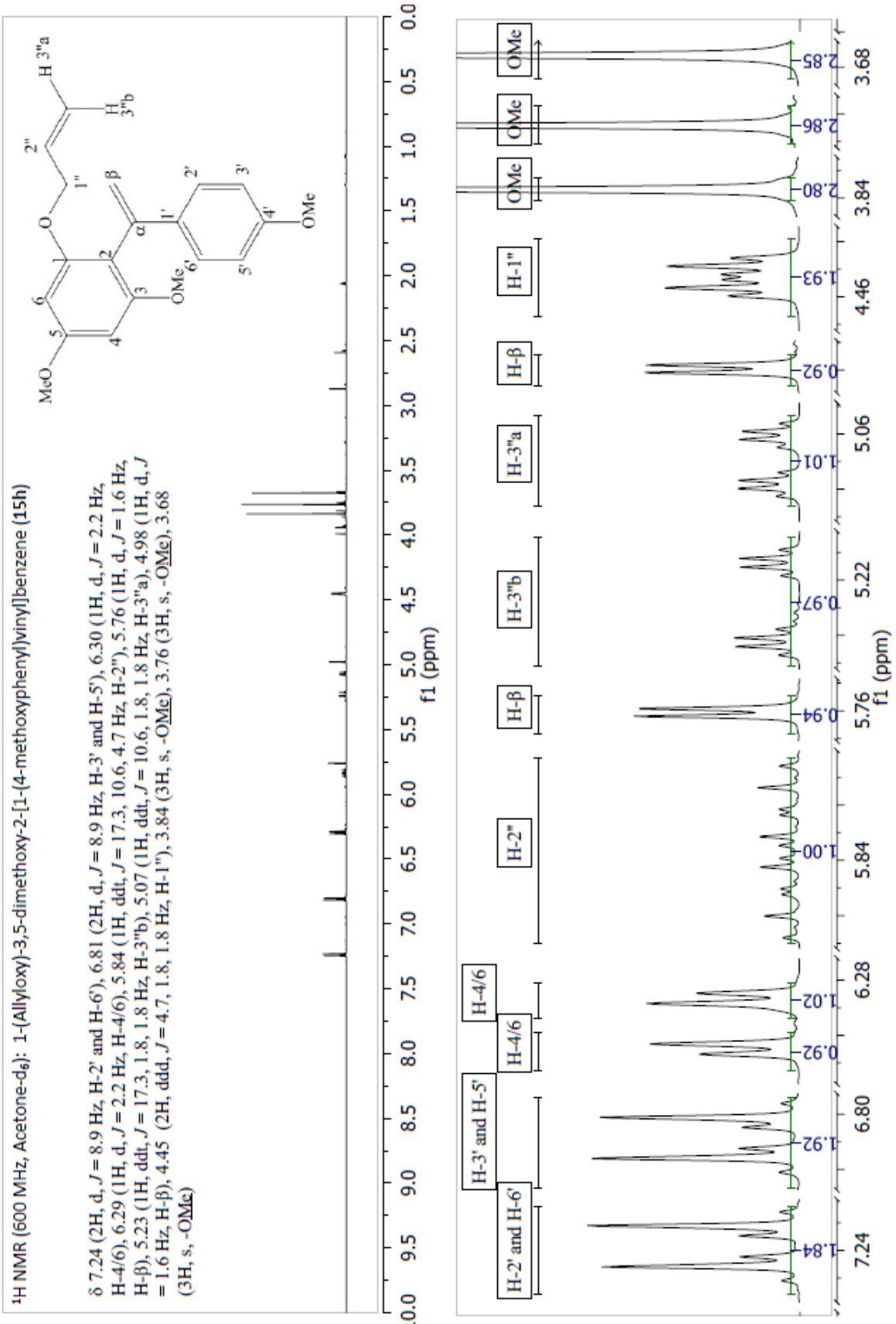

13C NMR (151 MHz, Acetone-d6): 1-(Allyloxy)-3,5-dimethoxy-2-(1-phenylvinyl)benzene (15g)
δ 161.79 (C-3/5), 159.77 (C-3/5), 158.52 (C-1), 142.48 (C-1'), 142.35 (C-α), 134.57 (C-2"), 128.76 (C-3' and C-5'), 127.73 (C-4'), 126.71 (C-2' and C-6'), 116.53 (C-3" and C-β), 113.26 (C-2), 93.00 (C-4/6), 92.00 (C-4/6), 69.56 (C-1"), 56.11 (-OMe), 55.67 (-OMe)
MeO
OMe
H 3"a
H 3"b
C-3/5
C-1
C-3/5
C-α
C-1'
C-3' and C-5'
C-2"
C-2' and C-6'
C-3" and C-β
C-2
C-4'
C-4/6
C-4/6
C-1"
OMe
OMe
f1 (ppm)

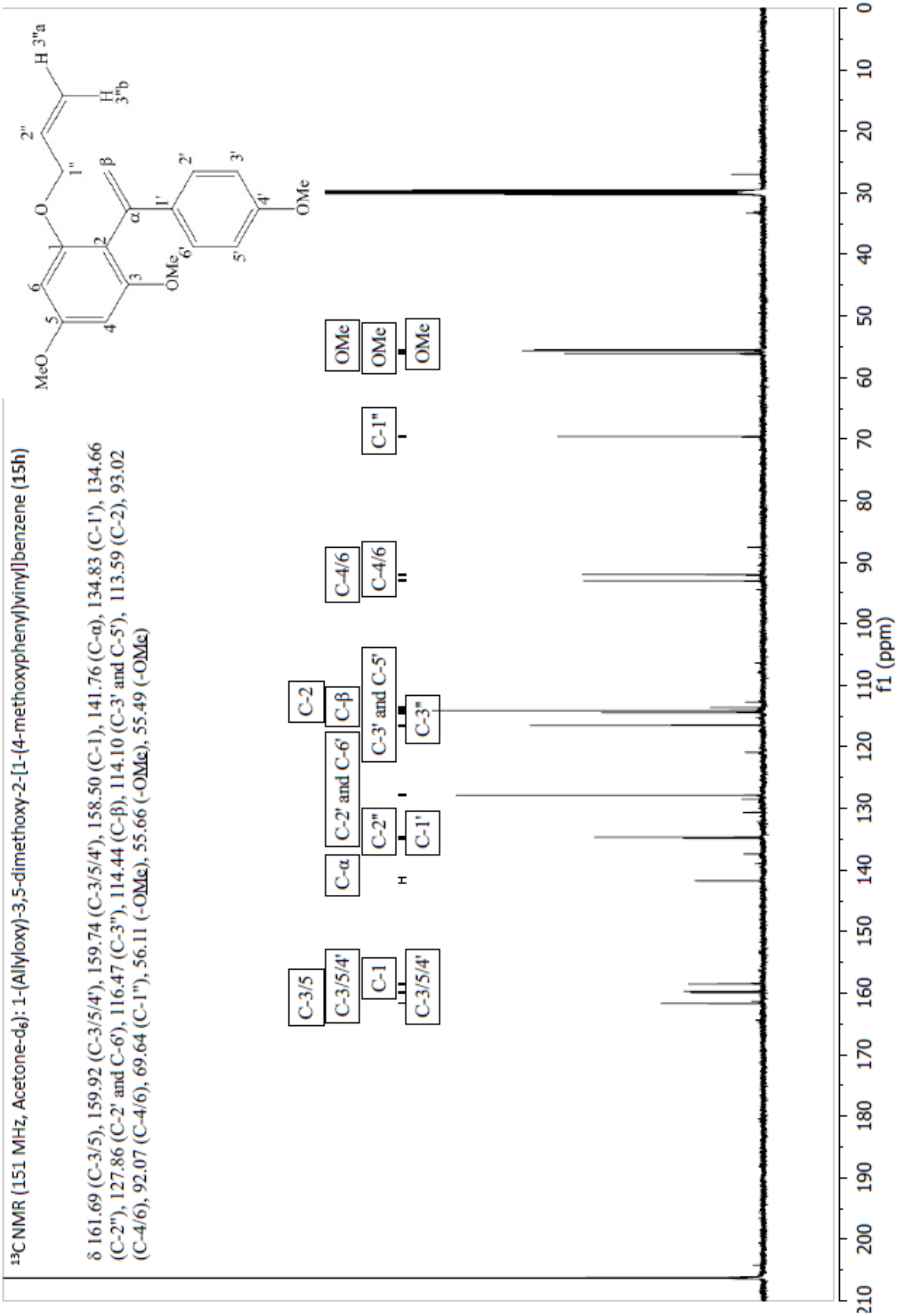


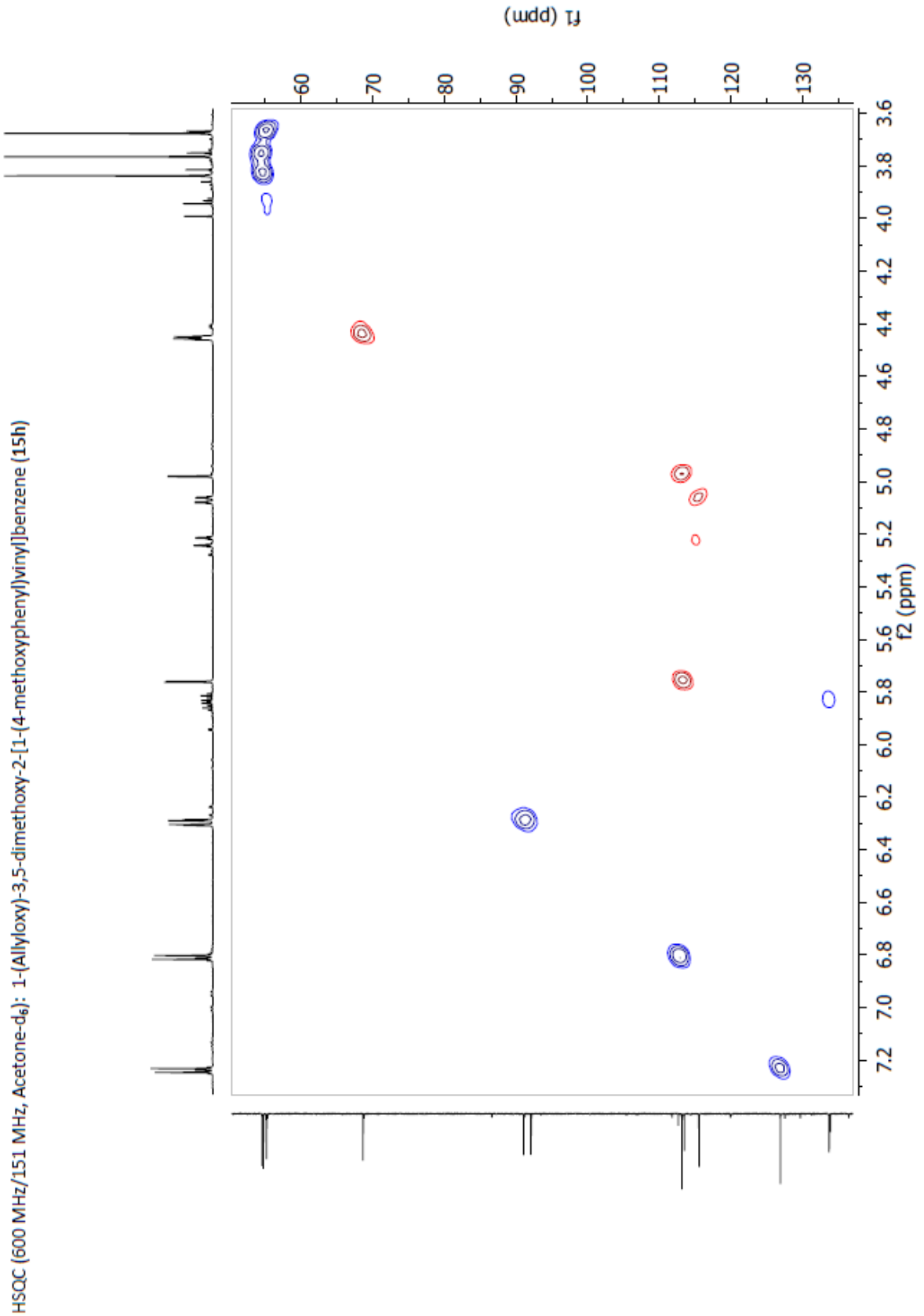

HSQC (600 MHz/151 MHz, Acetone-$d_6$): 1-(Allyloxy)-3,5-dimethoxy-2-(1-phenylvinyl)benzene (15g)


HMBC (600 MHz/151 MHz, Acetone-d6) : 1-(Allyloxy)-3,5-dimethoxy-2-(1-phenylvinyl)benzene (15g)
f1 (ppm)
f2 (ppm)

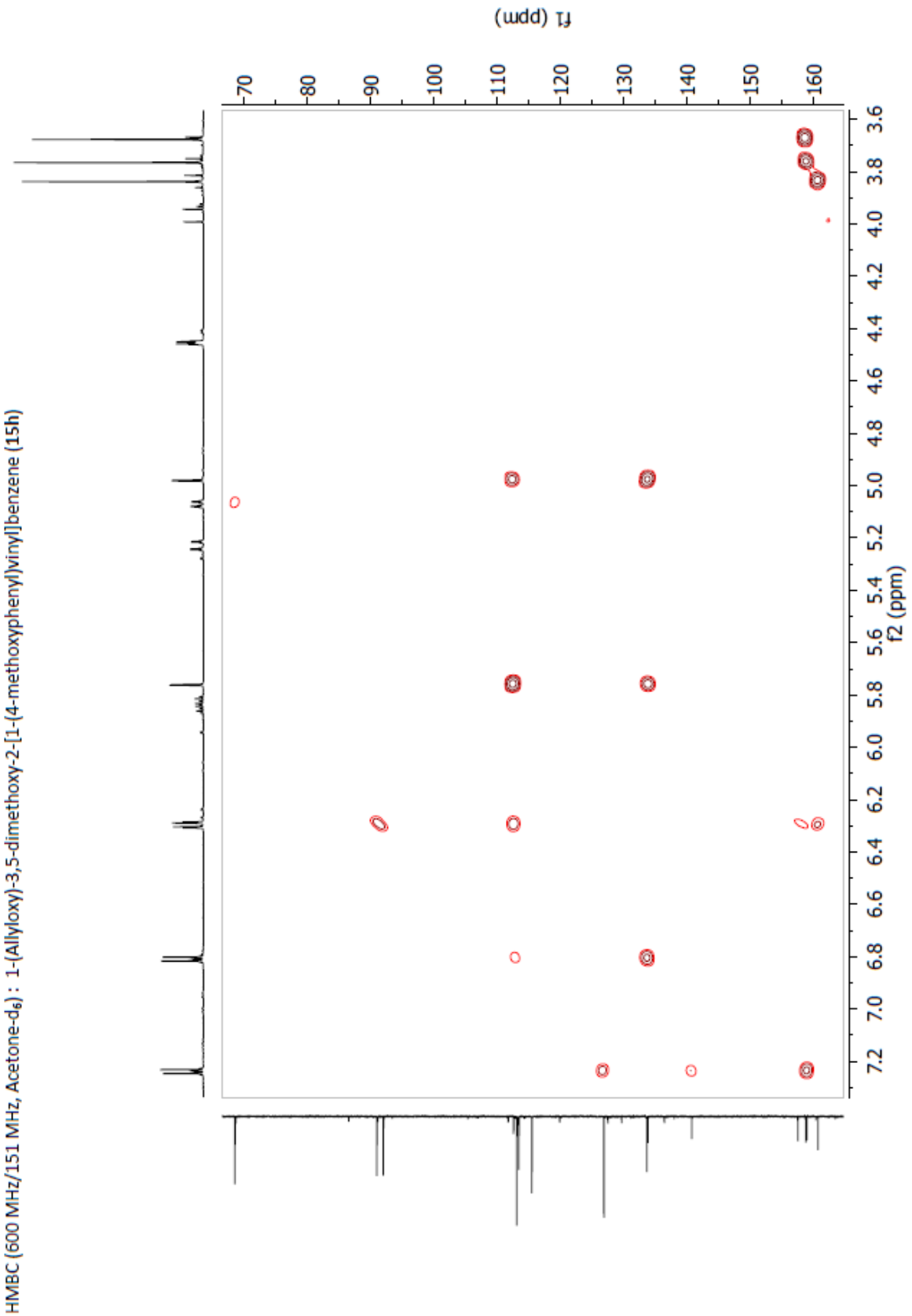

DEPT NMR (151 MHz, Acetone-d6): 1-(Allyloxy)-3,5-dimethoxy-2-(1-phenylvinyl)benzene (15g)
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
210
f1 (ppm)

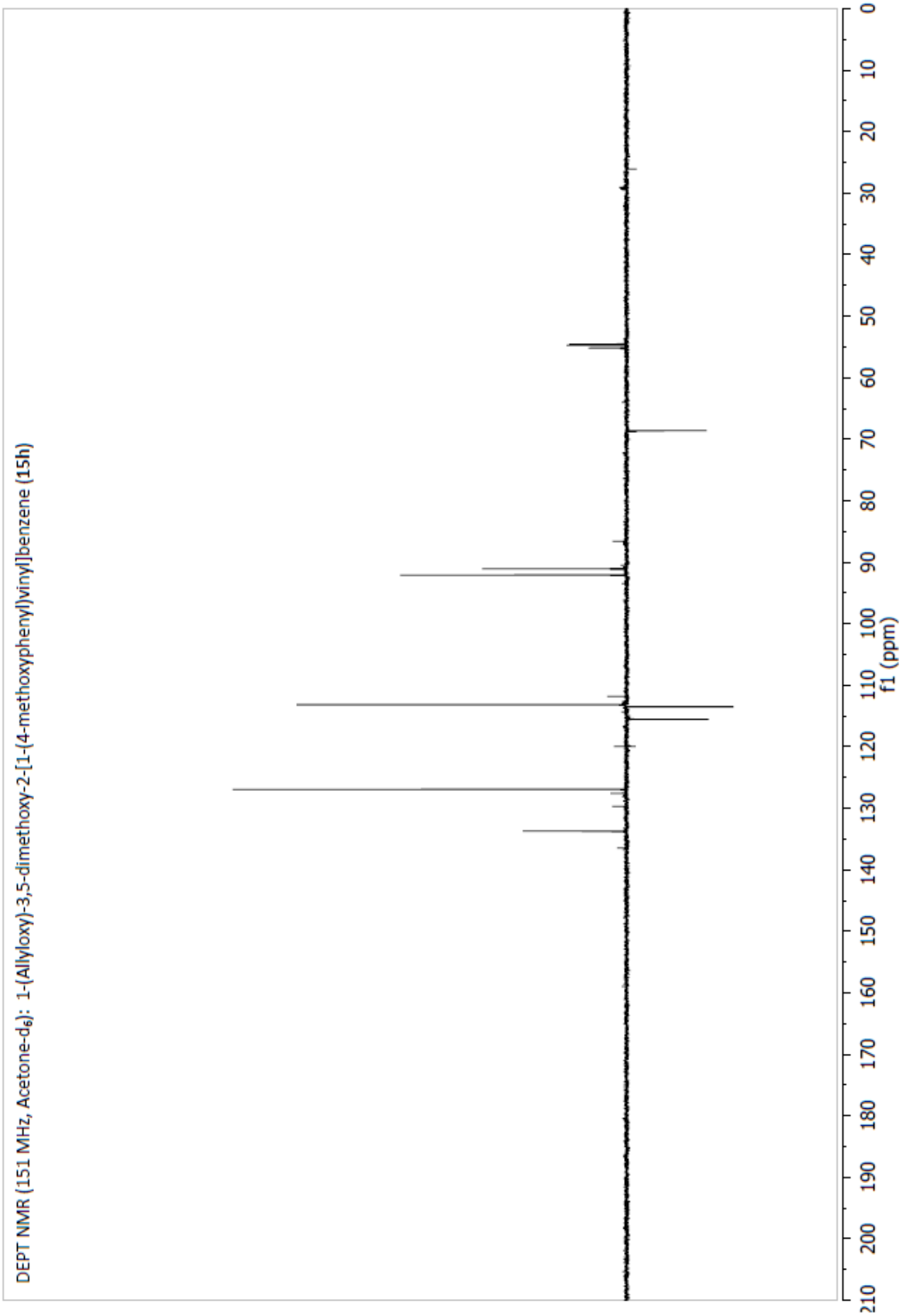

¹H NMR (600 MHz, Acetone-d₆): 1-(Allyloxy)-3,5-dimethoxy-2-[1-(4-methoxyphenyl)vinyl]benzene (15h)
δ 7.24 (2H, d, J = 8.9 Hz, H-2' and H-6'), 6.81 (2H, d, J = 8.9 Hz, H-3' and H-5'), 6.30 (1H, d, J = 2.2 Hz, H-4/6), 6.29 (1H, d, J = 2.2 Hz, H-4/6), 5.84 (1H, ddt, J = 17.3, 10.6, 4.7 Hz, H-2"), 5.76 (1H, d, J = 1.6 Hz, H-β), 5.23 (1H, ddt, J = 17.3, 1.8, 1.8 Hz, H-3"b), 5.07 (1H, ddt, J = 10.6, 1.8, 1.8 Hz, H-3"a), 4.98 (1H, d, J = 1.6 Hz, H-β), 4.45 (2H, ddd, J = 4.7, 1.8, 1.8 Hz, H-1"), 3.84 (3H, s, -OMe), 3.76 (3H, s, -OMe), 3.68 (3H, s, -OMe)
MeO
OMe
OMe
OMe
H 3"a
H 3"b
f1 (ppm)
H-2' and H-6'
H-3' and H-5'
H-4/6
H-4/6
H-2"
H-β
H-3"b
H-3"a
H-β
H-1"
OMe
OMe
OMe
f1 (ppm)

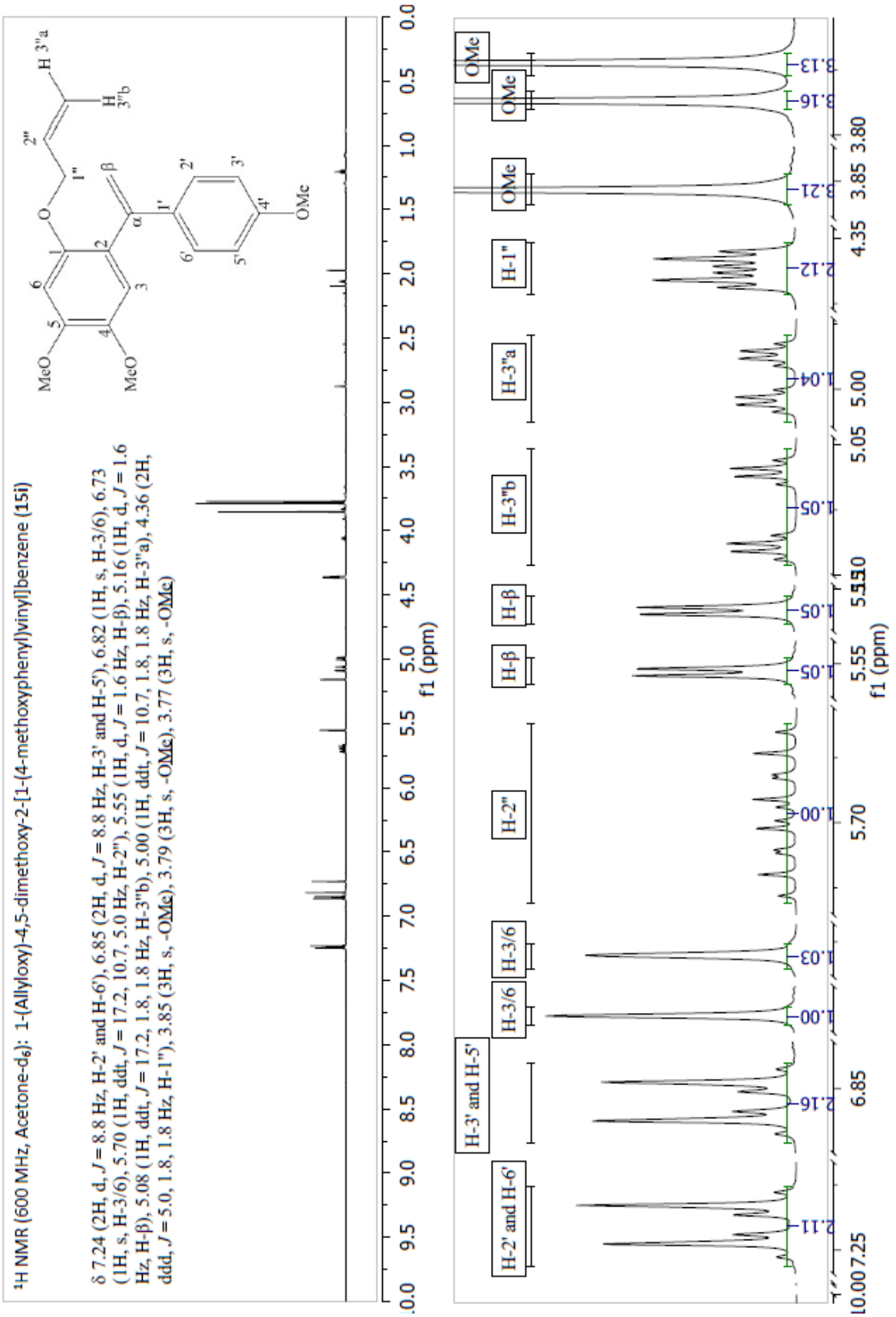

13C NMR (151 MHz, Acetone-d6): 1-(Allyloxy)-3,5-dimethoxy-2-[1-(4-methoxyphenyl)vinyl]benzene (15h)
δ 161.69 (C-3/5), 159.92 (C-3/5/4'), 159.74 (C-3/5/4'), 158.50 (C-1), 141.76 (C-α), 134.83 (C-1'), 134.66 (C-2''), 127.86 (C-2' and C-6'), 116.47 (C-3''), 114.44 (C-β), 114.10 (C-3' and C-5'), 113.59 (C-2), 93.02 (C-4/6), 92.07 (C-4/6), 69.64 (C-1''), 56.11 (-OMe), 55.66 (-OMe), 55.49 (-OMe)
MeO
OMe
OMe
H 3''a
H 3''b
C-3/5
C-3/5/4'
C-1
C-3/5/4'
C-α
C-2
C-2' and C-6'
C-β
C-2''
C-1'
C-3' and C-5'
C-3''
C-4/6
C-4/6
C-1''
OMe
OMe
OMe
f1 (ppm)

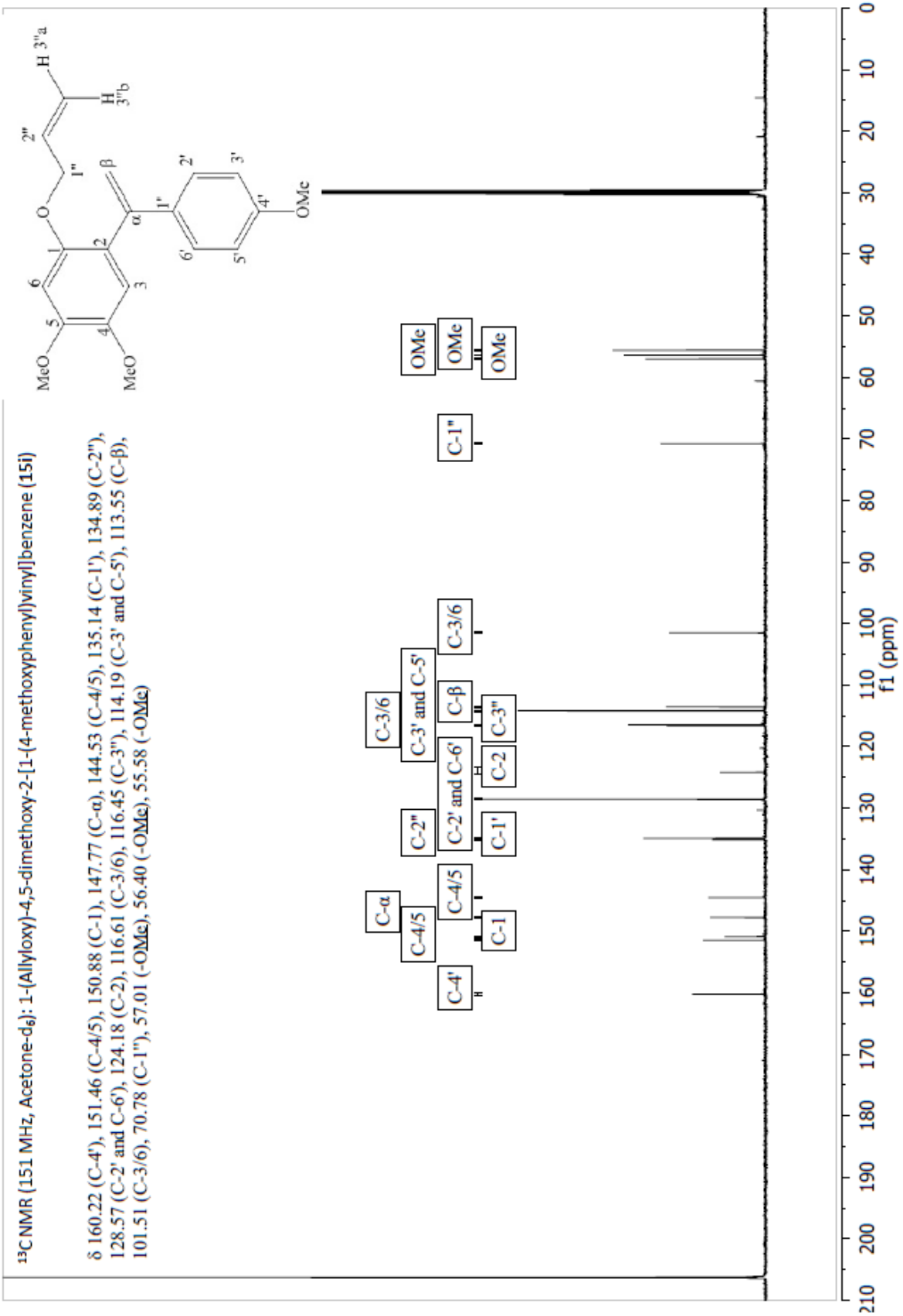


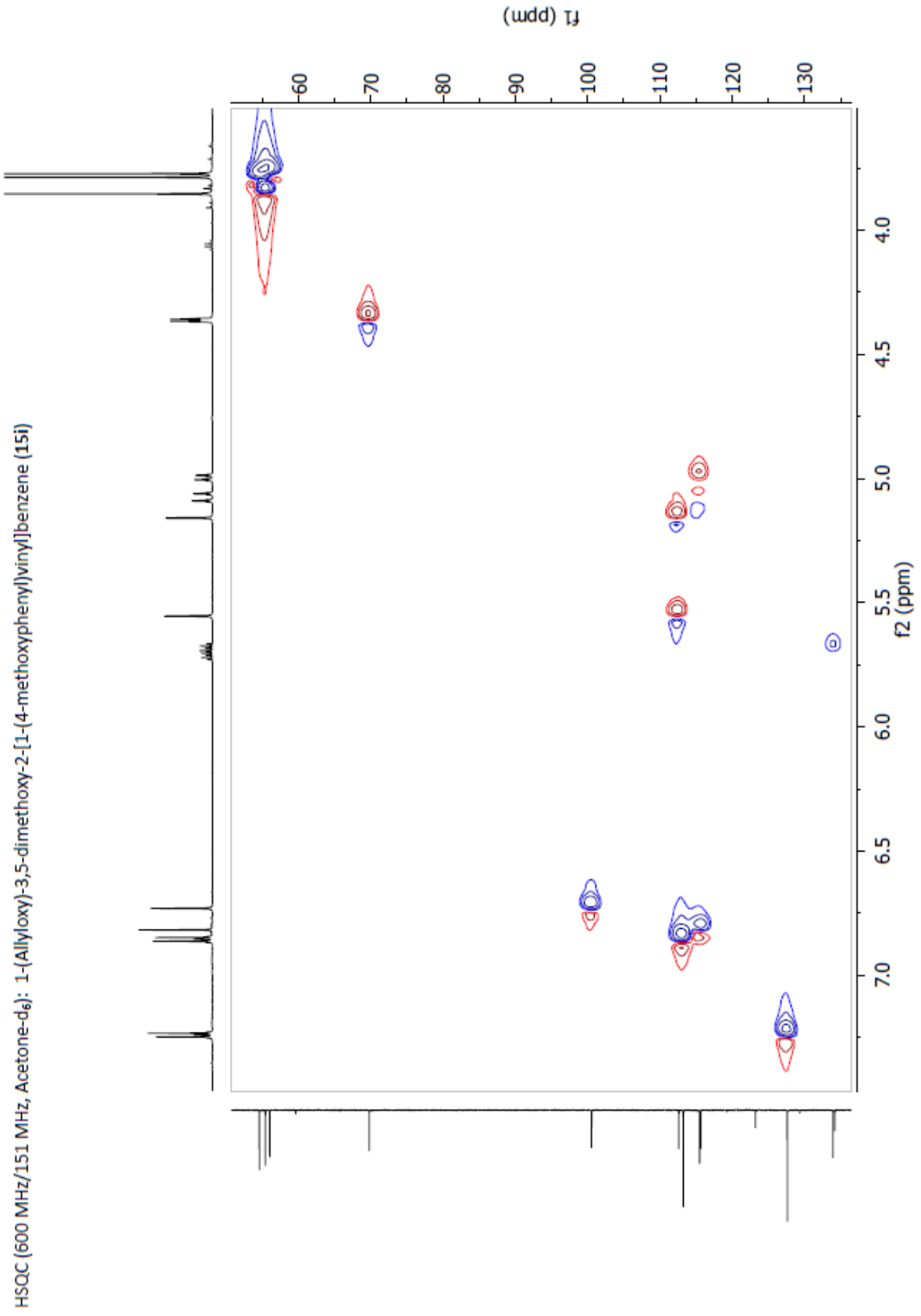

HSQC (600 MHz/151 MHz, Acetone-$d_6$): 1-(Allyloxy)-3,5-dimethoxy-2-[1-(4-methoxyphenyl)vinyl]benzene (**15h**)

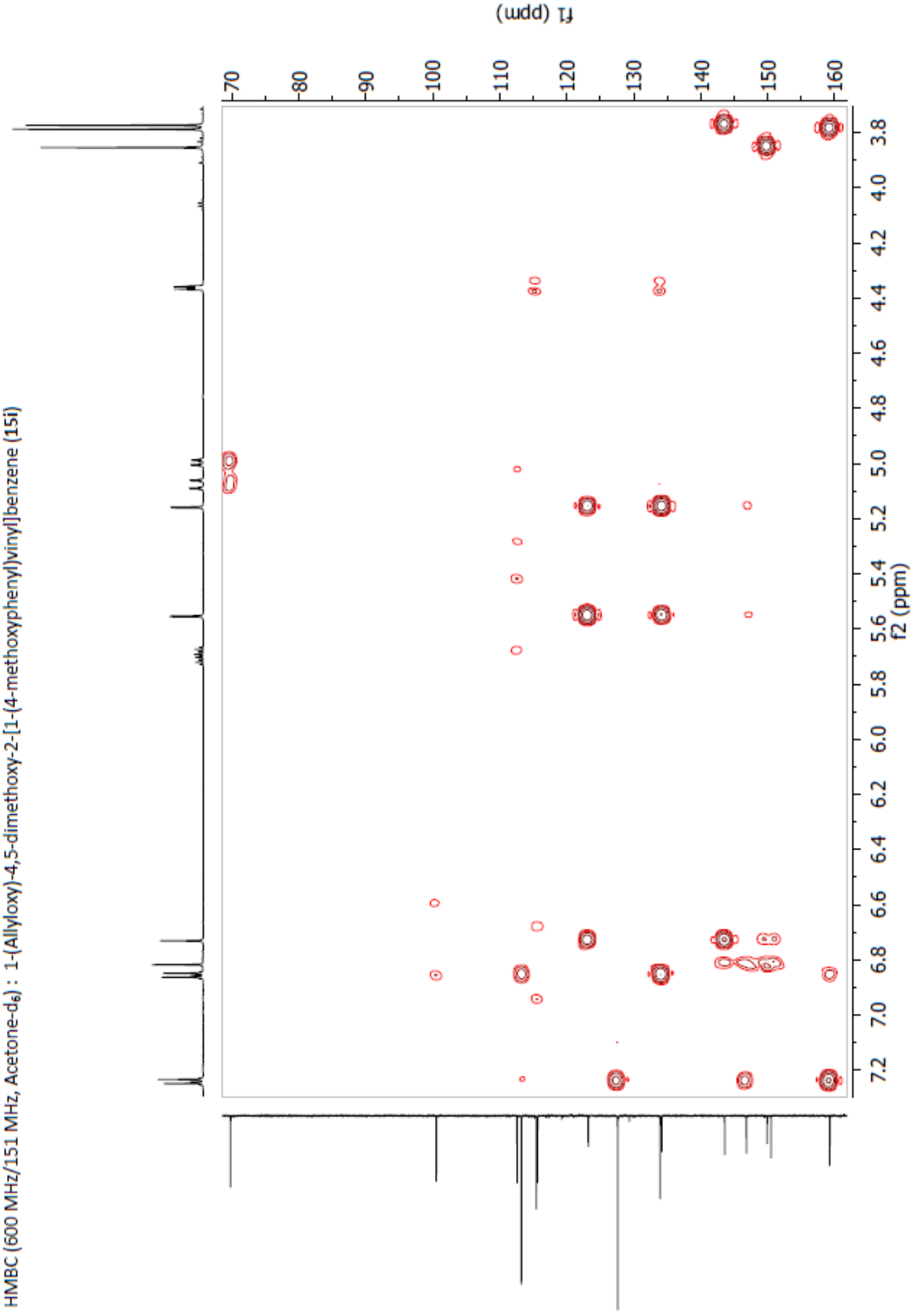

HMBC (600 MHz/151 MHz, Acetone-d6) : 1-(Allyloxy)-3,5-dimethoxy-2-[1-(4-methoxyphenyl)vinyl]benzene (15h)
f1 (ppm)
f2 (ppm)

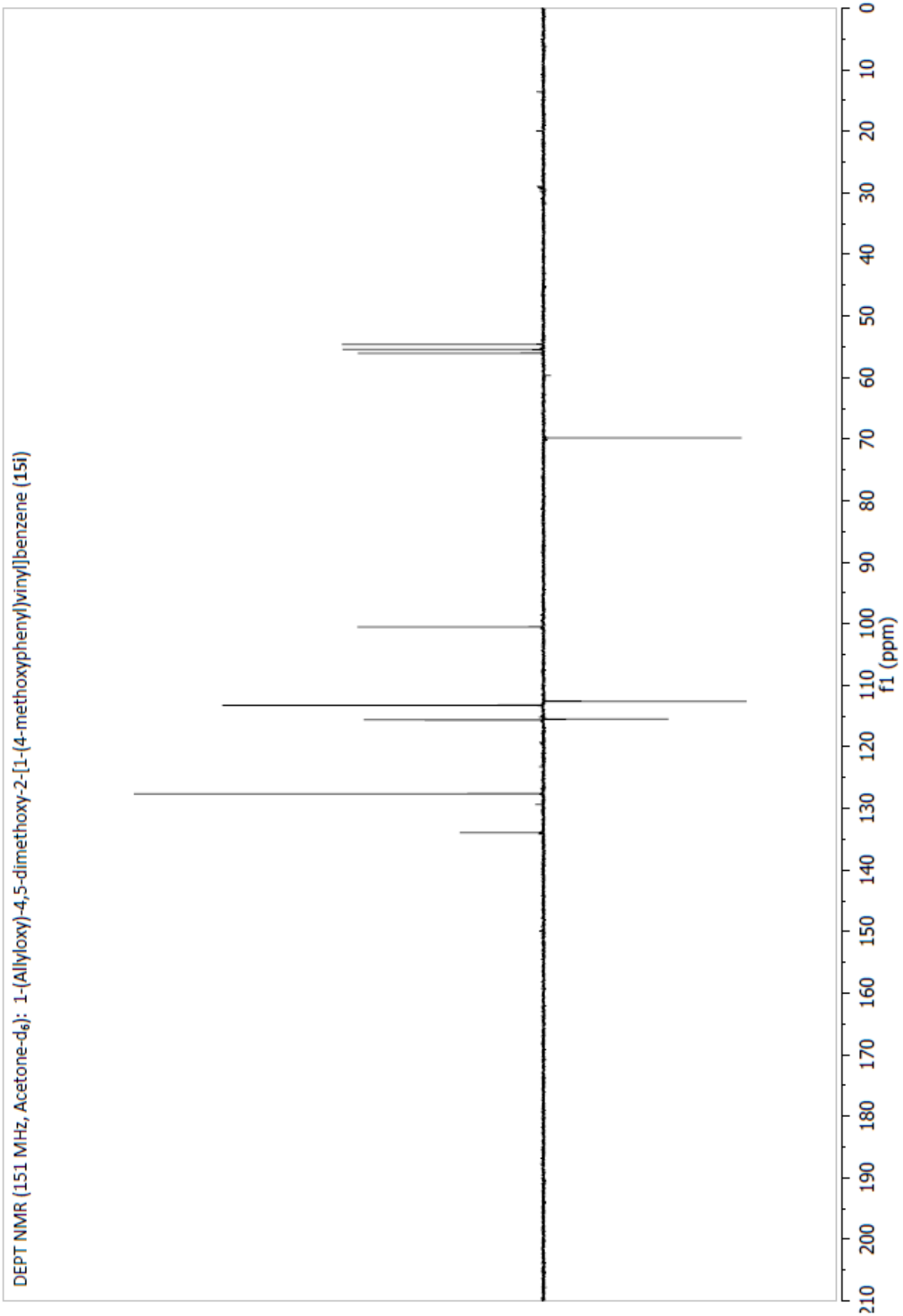

DEPT NMR (151 MHz, Acetone-d6): 1-(Allyloxy)-3,5-dimethoxy-2-[1-(4-methoxyphenyl)vinyl]benzene (15h)
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
210
f1 (ppm)

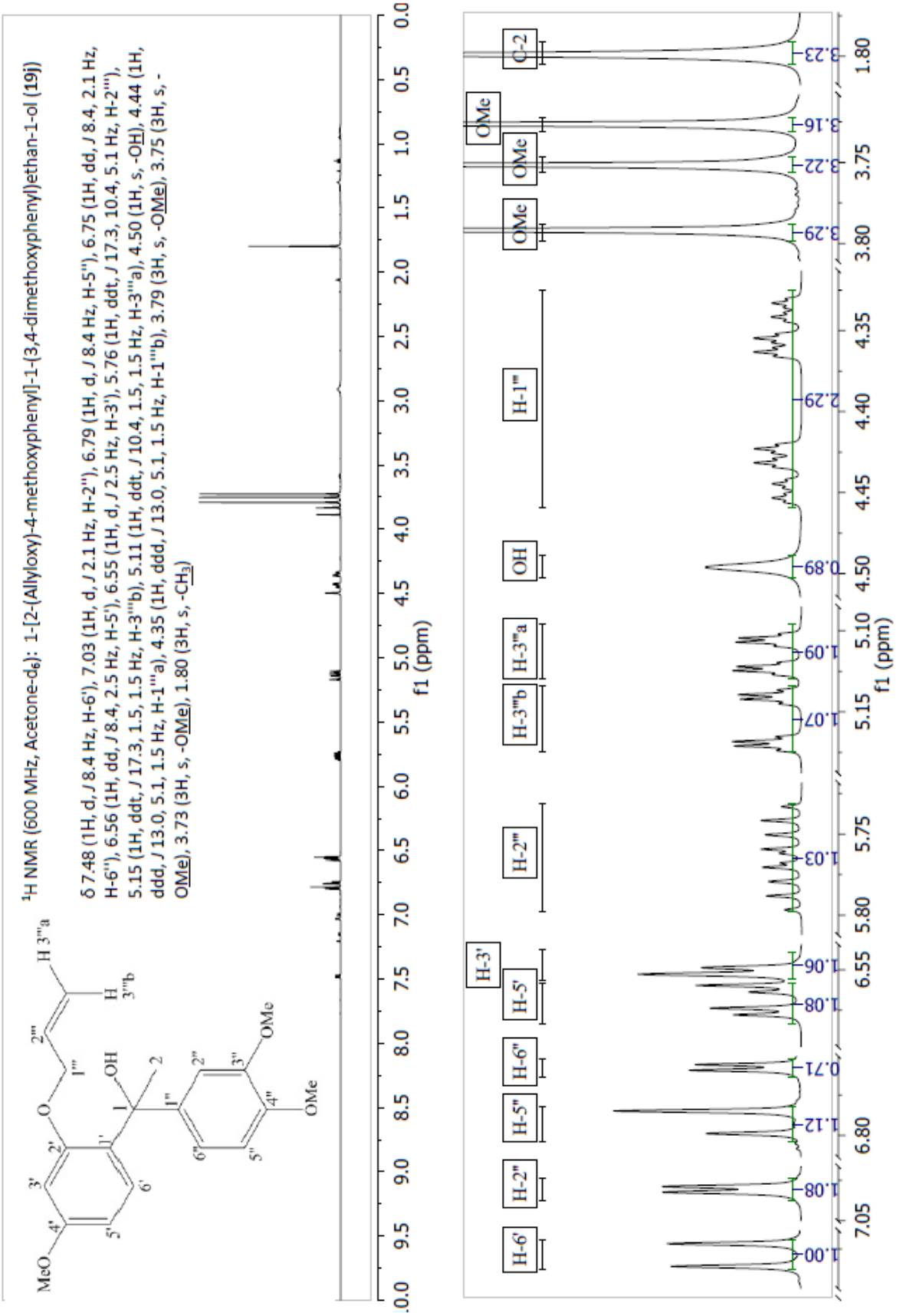

¹H NMR (600 MHz, Acetone-d6): 1-(Allyloxy)-4,5-dimethoxy-2-[1-(4-methoxyphenyl)vinyl]benzene (15i)
δ 7.24 (2H, d, J = 8.8 Hz, H-2' and H-6'), 6.85 (2H, d, J = 8.8 Hz, H-3' and H-5'), 6.82 (1H, s, H-3/6), 6.73 (1H, s, H-3/6), 5.70 (1H, ddt, J = 17.2, 10.7, 5.0 Hz, H-2"), 5.55 (1H, d, J = 1.6 Hz, H-β), 5.16 (1H, d, J = 1.6 Hz, H-β), 5.08 (1H, ddt, J = 17.2, 1.8, 1.8 Hz, H-3"b), 5.00 (1H, ddt, J = 10.7, 1.8, 1.8 Hz, H-3"a), 4.36 (2H, ddd, J = 5.0, 1.8, 1.8 Hz, H-1"), 3.85 (3H, s, -OMe), 3.79 (3H, s, -OMe), 3.77 (3H, s, -OMe)
MeO
MeO
OMe
H 3"a
H 3"b
f1 (ppm)
H-2' and H-6'
H-3' and H-5'
H-3/6
H-3/6
H-2"
H-β
H-β
H-3"b
H-3"a
H-1"
OMe
OMe
OMe
f1 (ppm)

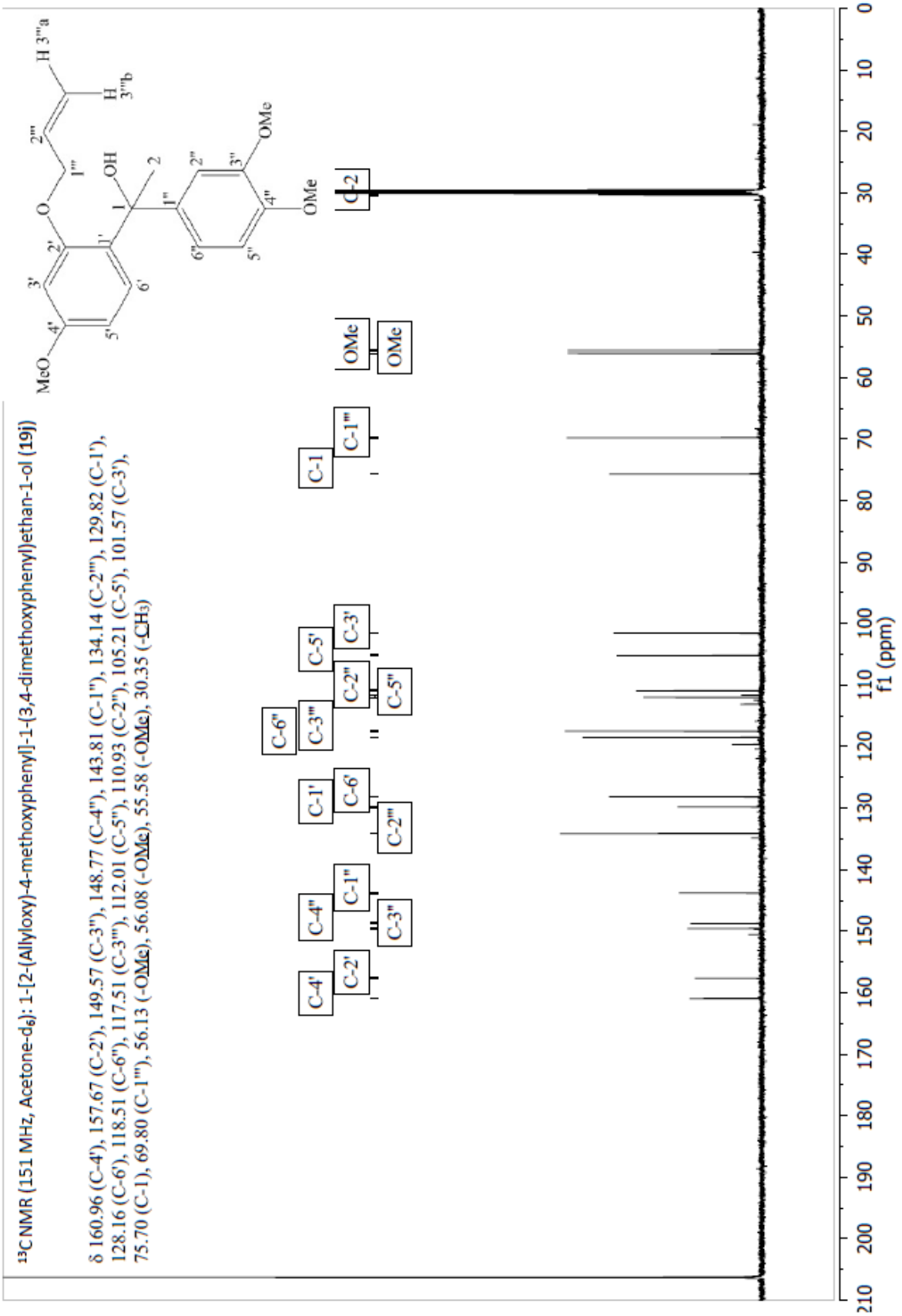

13C NMR (151 MHz, Acetone-d6): 1-(Allyloxy)-4,5-dimethoxy-2-[1-(4-methoxyphenyl)vinyl]benzene (15i)
δ 160.22 (C-4'), 151.46 (C-4/5), 150.88 (C-1), 147.77 (C-α), 144.53 (C-4/5), 135.14 (C-1'), 134.89 (C-2"), 128.57 (C-2' and C-6'), 124.18 (C-2), 116.61 (C-3/6), 116.45 (C-3"), 114.19 (C-3' and C-5'), 113.55 (C-β), 101.51 (C-3/6), 70.78 (C-1"), 57.01 (-OMe), 56.40 (-OMe), 55.58 (-OMe)
MeO
MeO
OMe
C-4'
C-4/5
C-α
C-1
C-4/5
C-2"
C-1'
C-2' and C-6'
C-2
C-3/6
C-3' and C-5'
C-β
C-3"
C-3/6
C-1"
OMe
OMe
OMe
f1 (ppm)

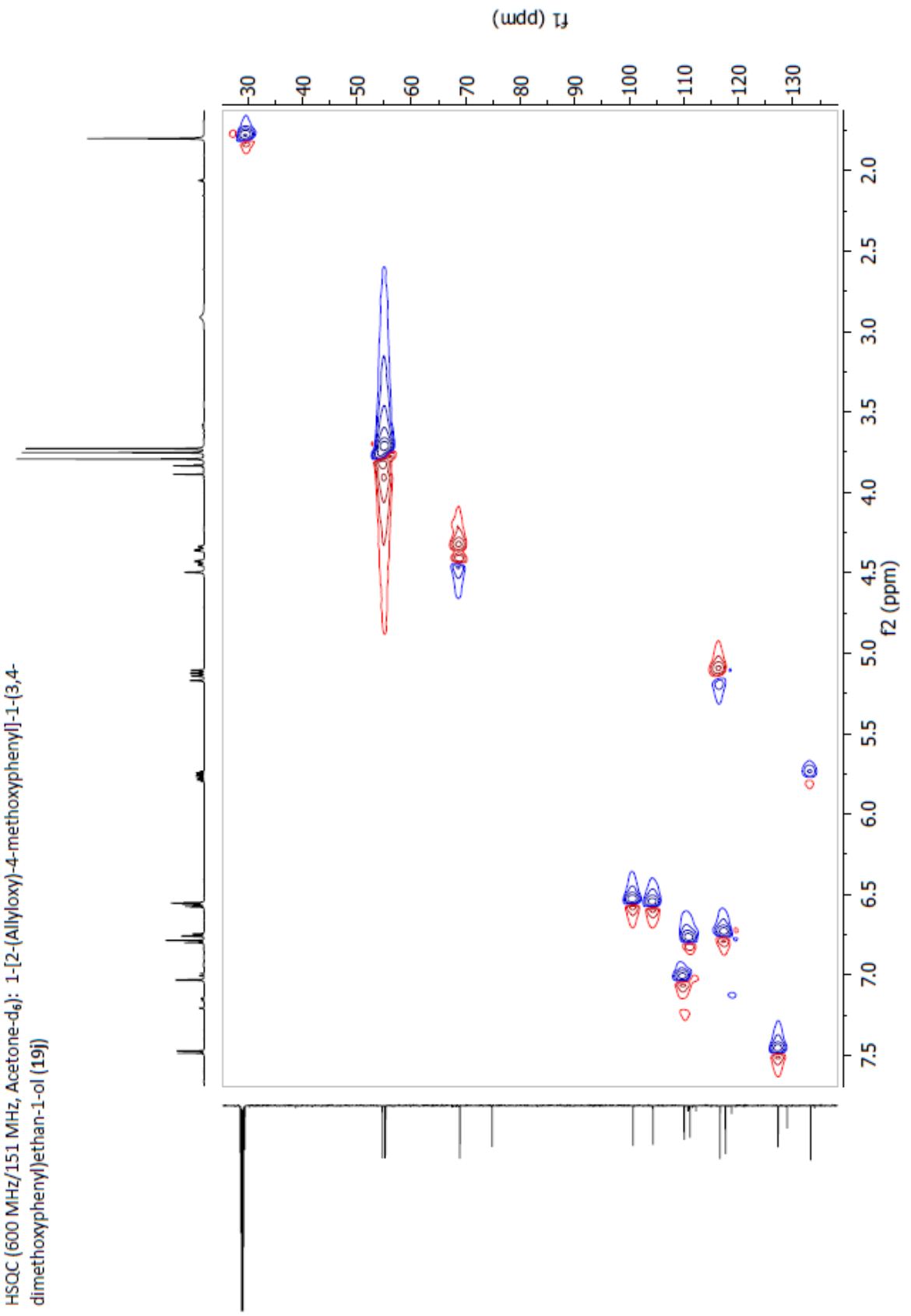

HSQC (600 MHz/151 MHz, Acetone-d6): 1-(Allyloxy)-3,5-dimethoxy-2-[1-(4-methoxyphenyl)vinyl]benzene (15i)
f1 (ppm)
60
70
80
90
100
110
120
130
f2 (ppm)
4.0
4.5
5.0
5.5
6.0
6.5
7.0


HMBC (600 MHz/151 MHz, Acetone-d6) : 1-(Allyloxy)-4,5-dimethoxy-2-[1-(4-methoxyphenyl)vinyl]benzene (15i)
f1 (ppm)
f2 (ppm)

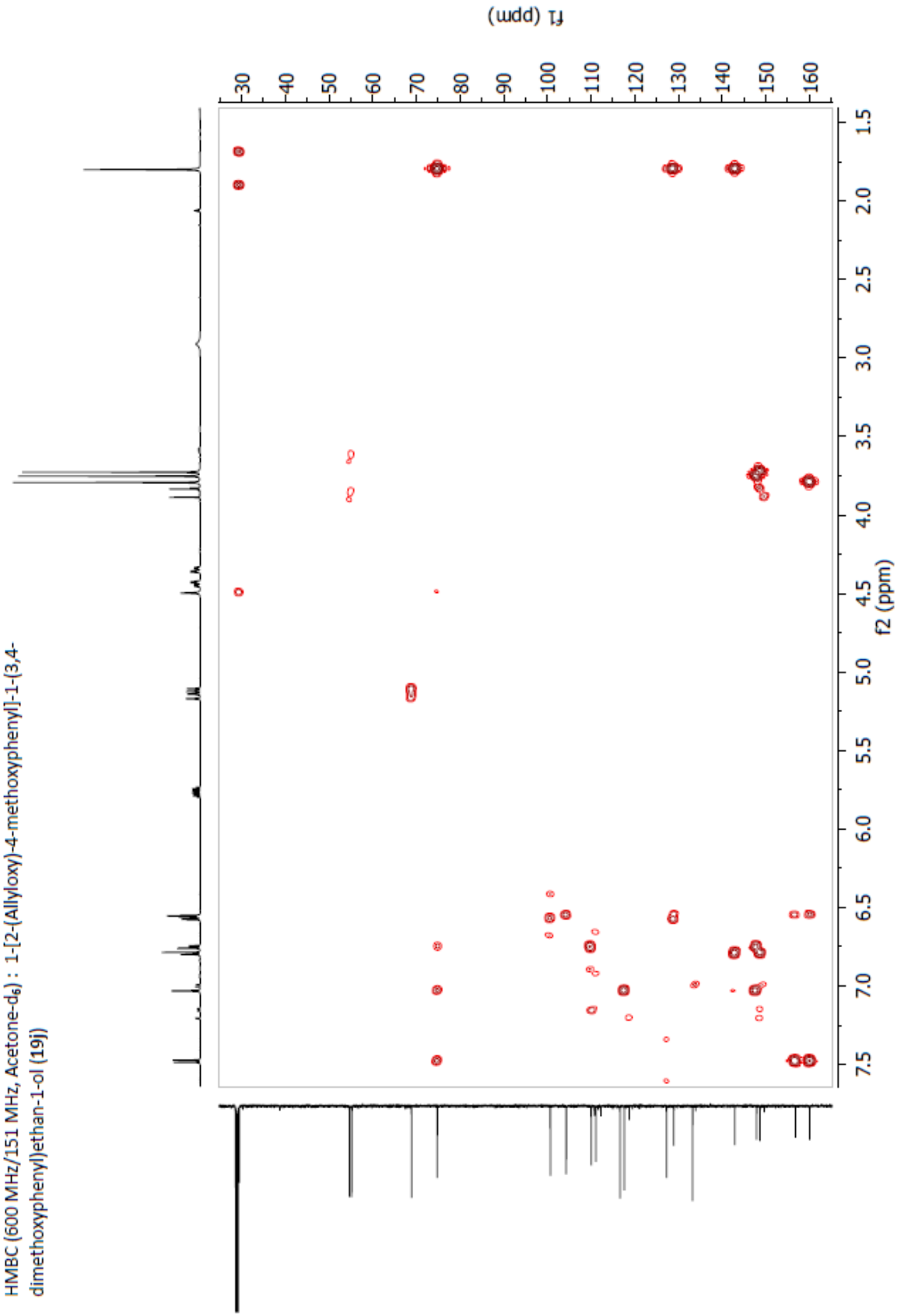

DEPT NMR (151 MHz, Acetone-$d_6$): 1-(Allyloxy)-4,5-dimethoxy-2-[1-(4-methoxyphenyl)vinyl]benzene (15i)
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
210
f1 (ppm)


$^1$H NMR (600 MHz, Acetone-$d_6$): 1-[2-(Allyloxy)-4-methoxyphenyl]-1-(3,4-dimethoxyphenyl)ethan-1-ol (19j)
δ 7.48 (1H, d, J 8.4 Hz, H-6'), 7.03 (1H, d, J 2.1 Hz, H-2''), 6.79 (1H, d, J 8.4 Hz, H-5''), 6.75 (1H, dd, J 8.4, 2.1 Hz, H-6''), 6.56 (1H, dd, J 8.4, 2.5 Hz, H-5'), 6.55 (1H, d, J 2.5 Hz, H-3'), 5.76 (1H, ddt, J 17.3, 10.4, 5.1 Hz, H-2'''), 5.15 (1H, ddt, J 17.3, 1.5, 1.5 Hz, H-3'''b), 5.11 (1H, ddt, J 10.4, 1.5, 1.5 Hz, H-3'''a), 4.50 (1H, s, -OH), 4.44 (1H, ddd, J 13.0, 5.1, 1.5 Hz, H-1'''a), 4.35 (1H, ddd, J 13.0, 5.1, 1.5 Hz, H-1'''b), 3.79 (3H, s, -OMe), 3.75 (3H, s, -OMe), 3.73 (3H, s, -OMe), 1.80 (3H, s, -CH3)
MeO
OMe
OMe
OH
H 3'''a
H 3'''b
f1 (ppm)
H-6'
H-2''
H-5''
H-6''
H-5'
H-3'
H-2'''
H-3'''b
H-3'''a
OH
H-1'''
OMe
OMe
OMe
C-2

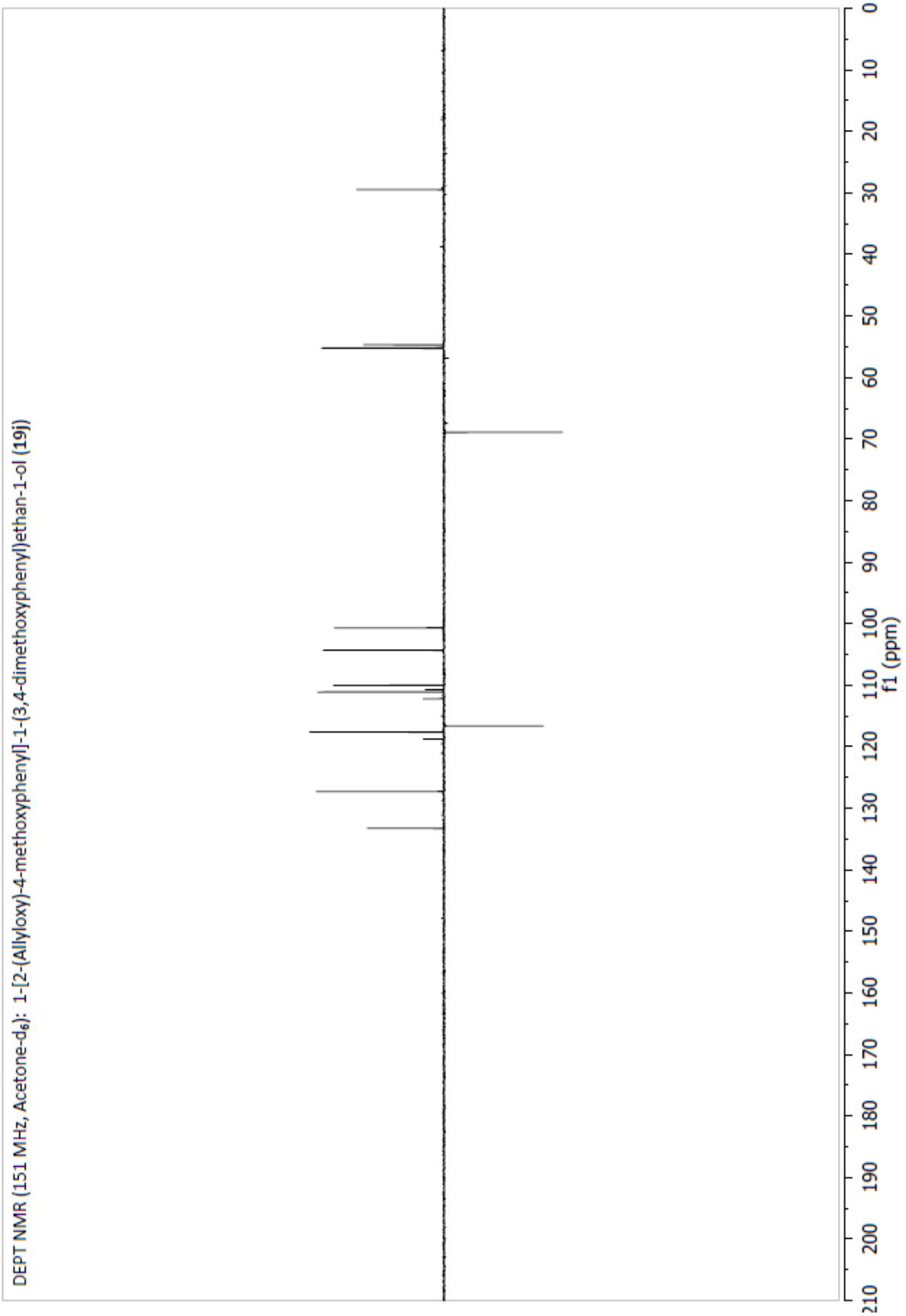

$^{13}$C NMR (151 MHz, Acetone-$d_6$): 1-[2-(Allyloxy)-4-methoxyphenyl]-1-(3,4-dimethoxyphenyl)ethan-1-ol (19j)
δ 160.96 (C-4'), 157.67 (C-2'), 149.57 (C-3"), 148.77 (C-4"), 143.81 (C-1"), 134.14 (C-2'"), 129.82 (C-1'), 128.16 (C-6'), 118.51 (C-6"), 117.51 (C-3'"), 112.01 (C-5"), 110.93 (C-2"), 105.21 (C-5'), 101.57 (C-3'), 75.70 (C-1), 69.80 (C-1'"), 56.13 (-OMe), 56.08 (-OMe), 55.58 (-OMe), 30.35 (-CH3)
C-4'
C-2'
C-4"
C-1"
C-3"
C-1'
C-6'
C-2'"
C-6"
C-3'"
C-5'
C-2"
C-3'
C-5"
C-1
C-1'"
OMe
OMe
C-2
f1 (ppm)

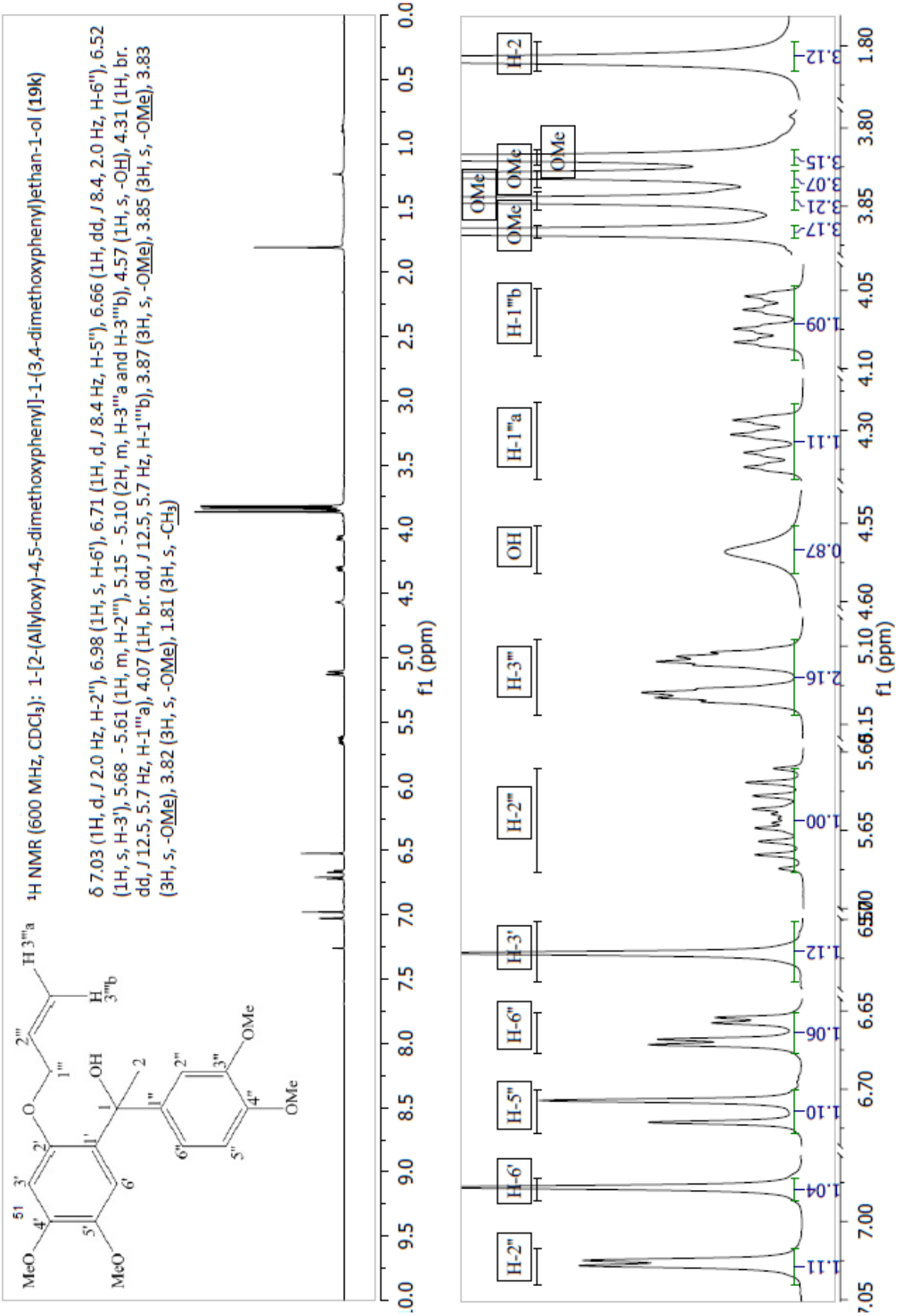


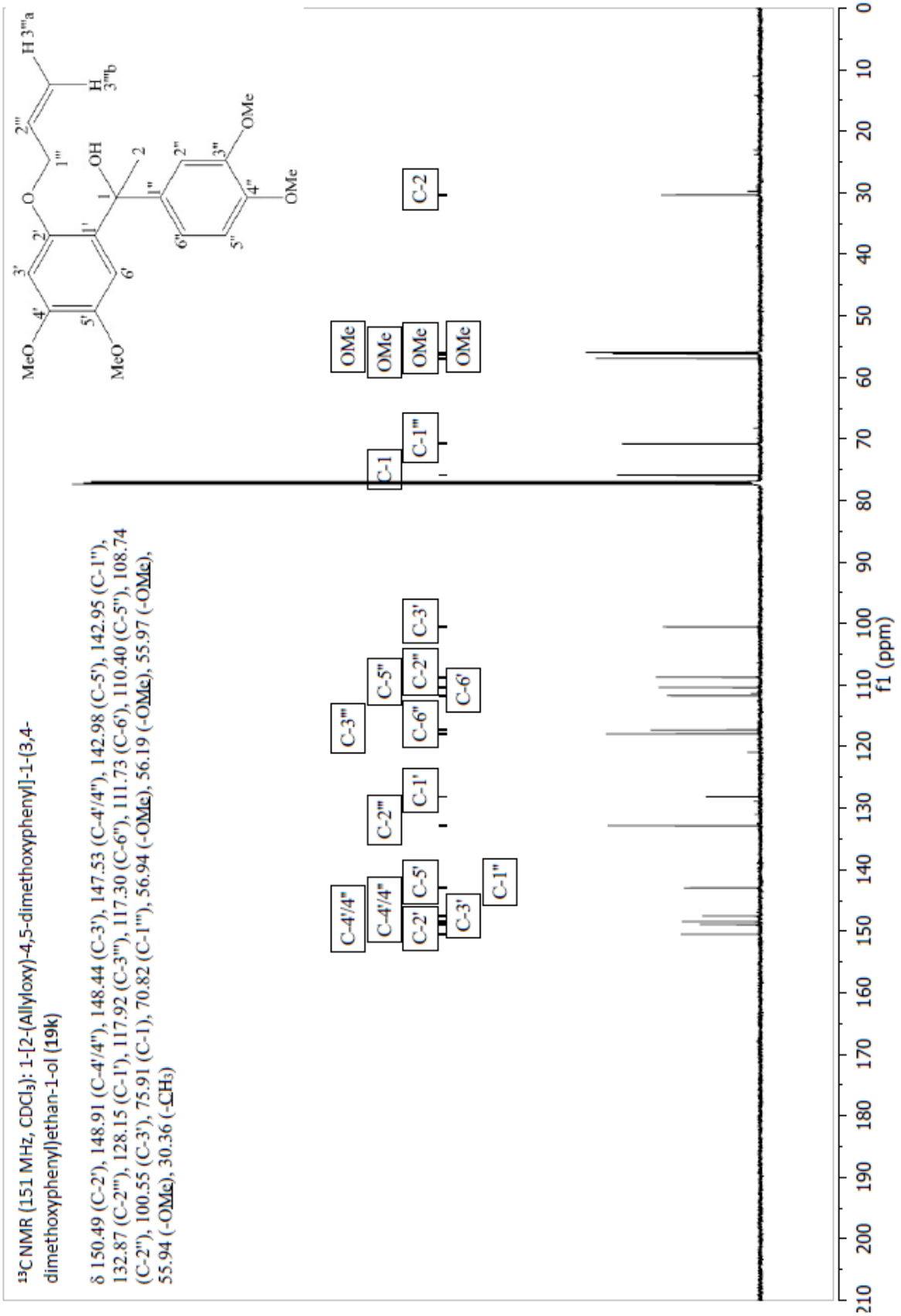

HSQC (600 MHz/151 MHz, Acetone-$d_6$): 1-[2-(Allyloxy)-4-methoxyphenyl]-1-(3,4-dimethoxyphenyl)ethan-1-ol (**19j**)




HMBC (600 MHz/151 MHz, Acetone-$d_6$) : 1-[2-(Allyloxy)-4-methoxyphenyl]-1-(3,4-dimethoxyphenyl)ethan-1-ol (**19j**)

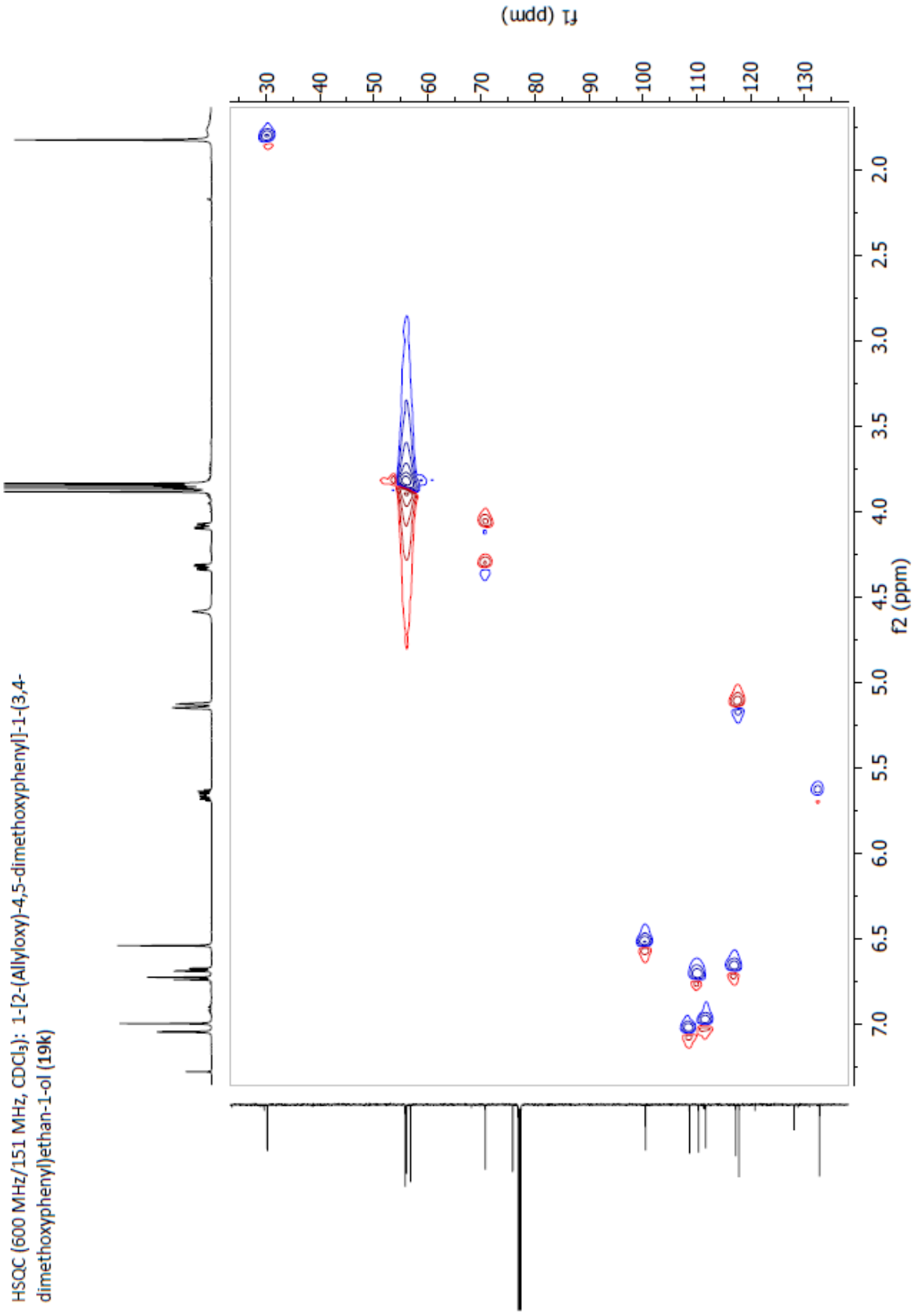

DEPT NMR (151 MHz, Acetone-d6): 1-[2-(Allyloxy)-4-methoxyphenyl]-1-(3,4-dimethoxyphenyl)ethan-1-ol (19j)
f1 (ppm)
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
210


1H NMR (600 MHz, CDCl3): 1-[2-(Allyloxy)-4,5-dimethoxyphenyl]-1-(3,4-dimethoxyphenyl)ethan-1-ol (19k)
δ 7.03 (1H, d, J 2.0 Hz, H-2''), 6.98 (1H, s, H-6'), 6.71 (1H, d, J 8.4 Hz, H-5''), 6.66 (1H, dd, J 8.4, 2.0 Hz, H-6''), 6.52 (1H, s, H-3'), 5.68 - 5.61 (1H, m, H-2'''), 5.15 - 5.10 (2H, m, H-3'''a and H-3'''b), 4.57 (1H, s, -OH), 4.31 (1H, br. dd, J 12.5, 5.7 Hz, H-1'''a), 4.07 (1H, br. dd, J 12.5, 5.7 Hz, H-1'''b), 3.87 (3H, s, -OMe), 3.85 (3H, s, -OMe), 3.83 (3H, s, -OMe), 3.82 (3H, s, -OMe), 1.81 (3H, s, -CH3)
f1 (ppm)
H-2''
H-6'
H-5''
H-6''
H-3'
H-2'''
H-3''
OH
H-1'''a
H-1'''b
OMe
OMe
OMe
OMe
H-2
f1 (ppm)

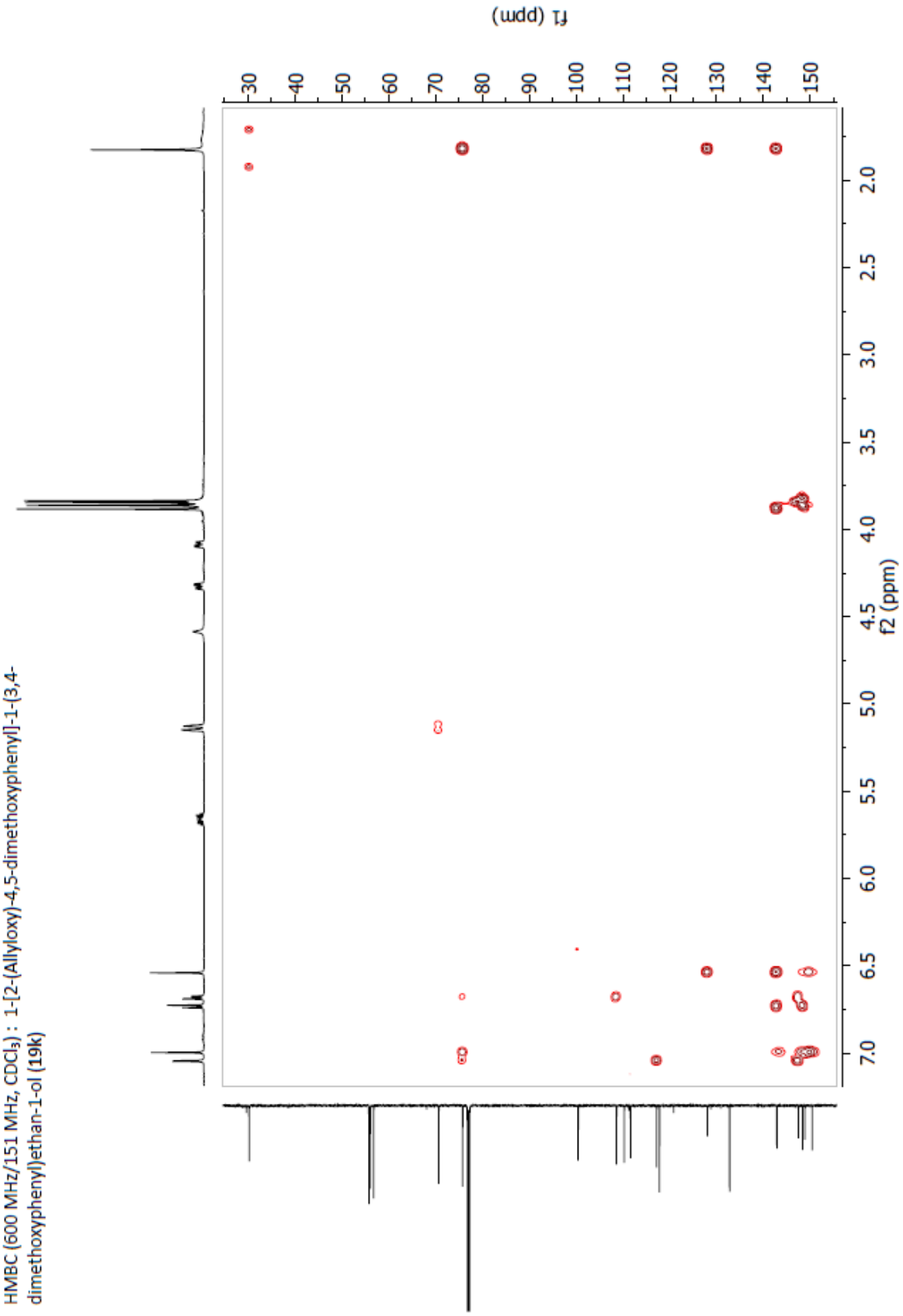



$^{13}$C NMR (151 MHz, $CDCl_3$): 1-[2-(Allyloxy)-4,5-dimethoxyphenyl]-1-(3,4-dimethoxyphenyl)ethan-1-ol (**19k**)

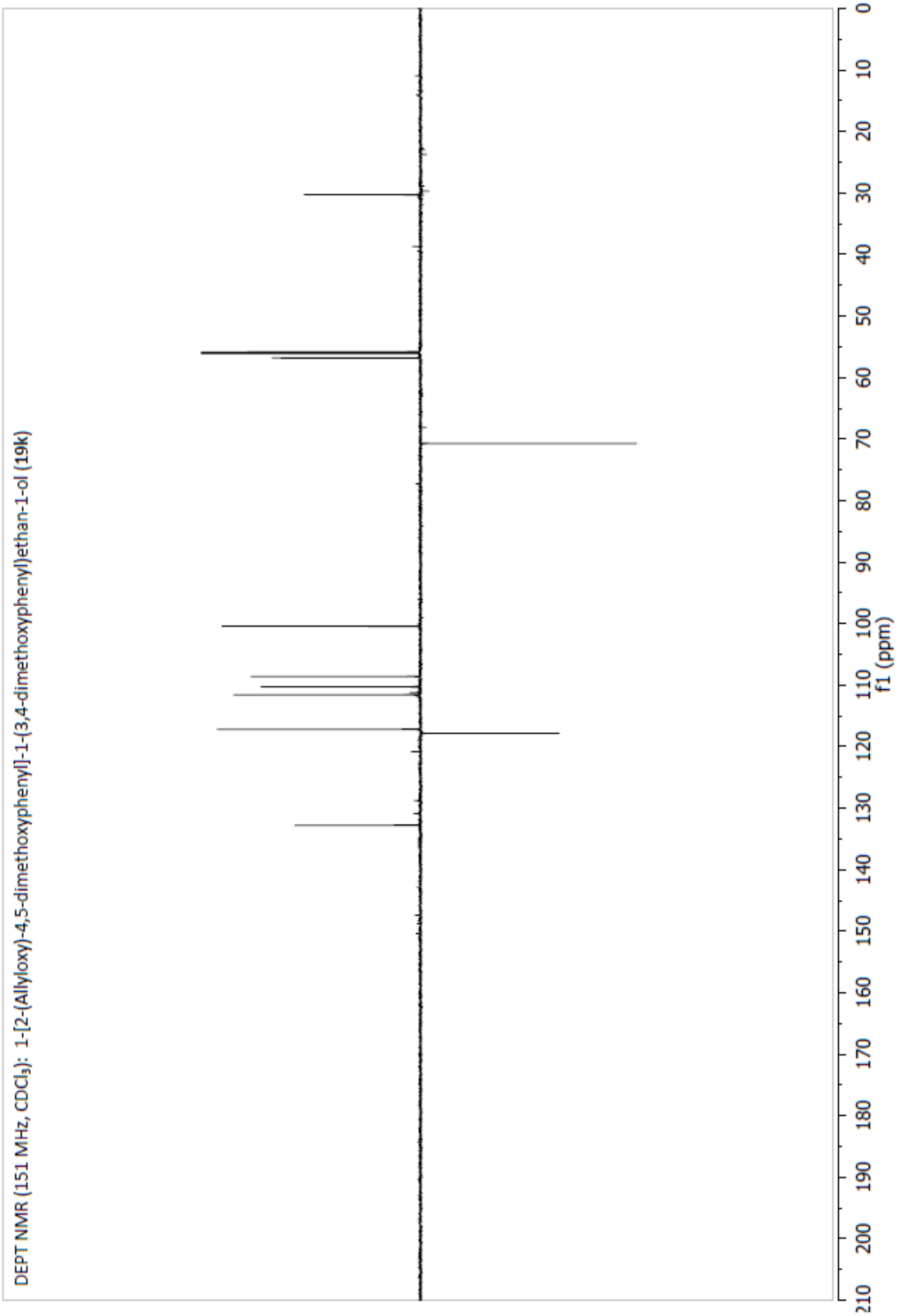
δ 150.49 (C-2'), 148.91 (C-4'/4"), 148.44 (C-3'), 147.53 (C-4'/4"), 142.98 (C-5'), 142.95 (C-1"), 132.87 (C-2'''), 128.15 (C-1'), 117.92 (C-3'''), 117.30 (C-6"), 111.73 (C-6'), 110.40 (C-5"), 108.74 (C-2"), 100.55 (C-3'), 75.91 (C-1), 70.82 (C-1'''), 56.94 (-OMe), 56.19 (-OMe), 55.97 (-OMe), 55.94 (-OMe), 30.36 (-$\underline{C}H_3$)

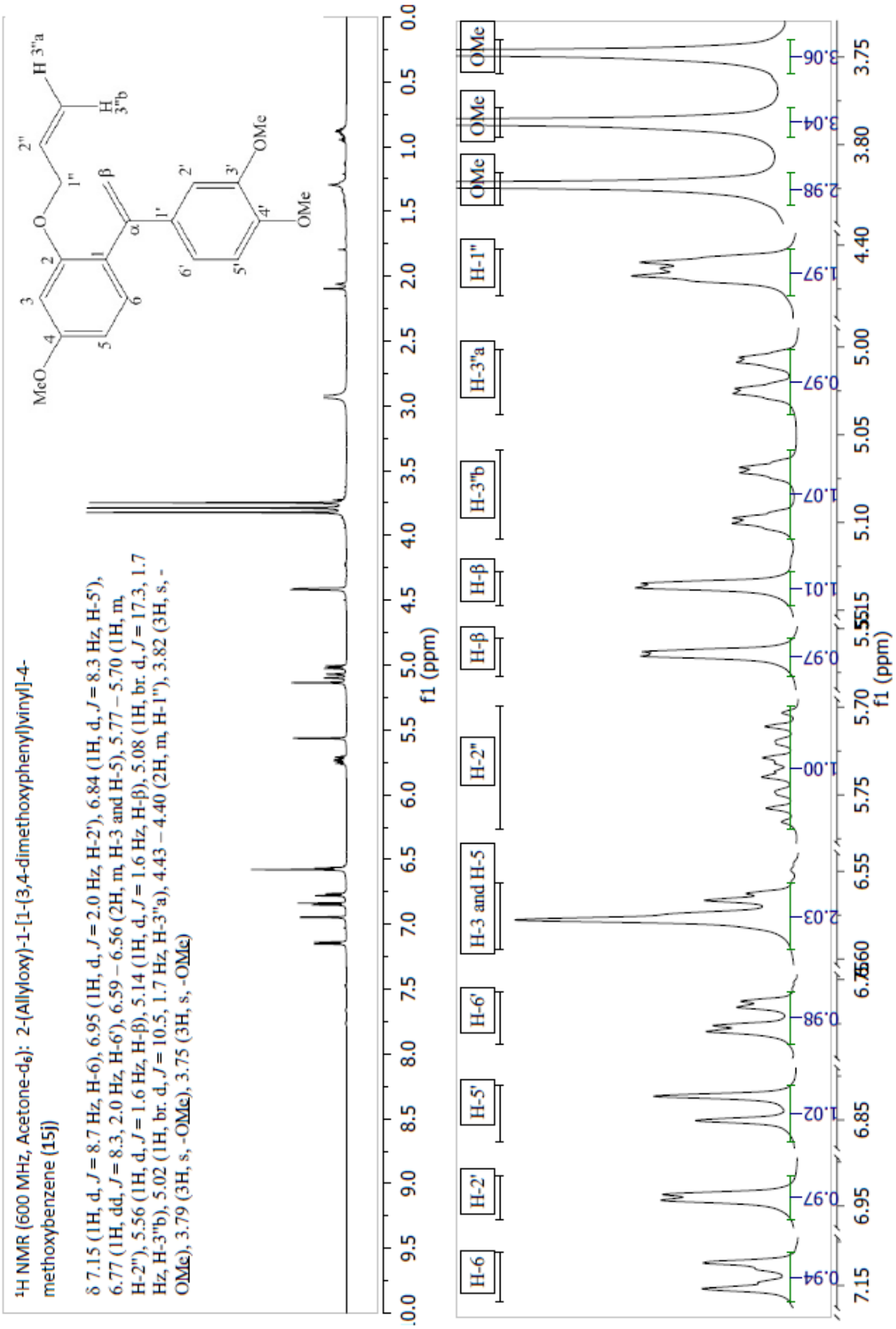


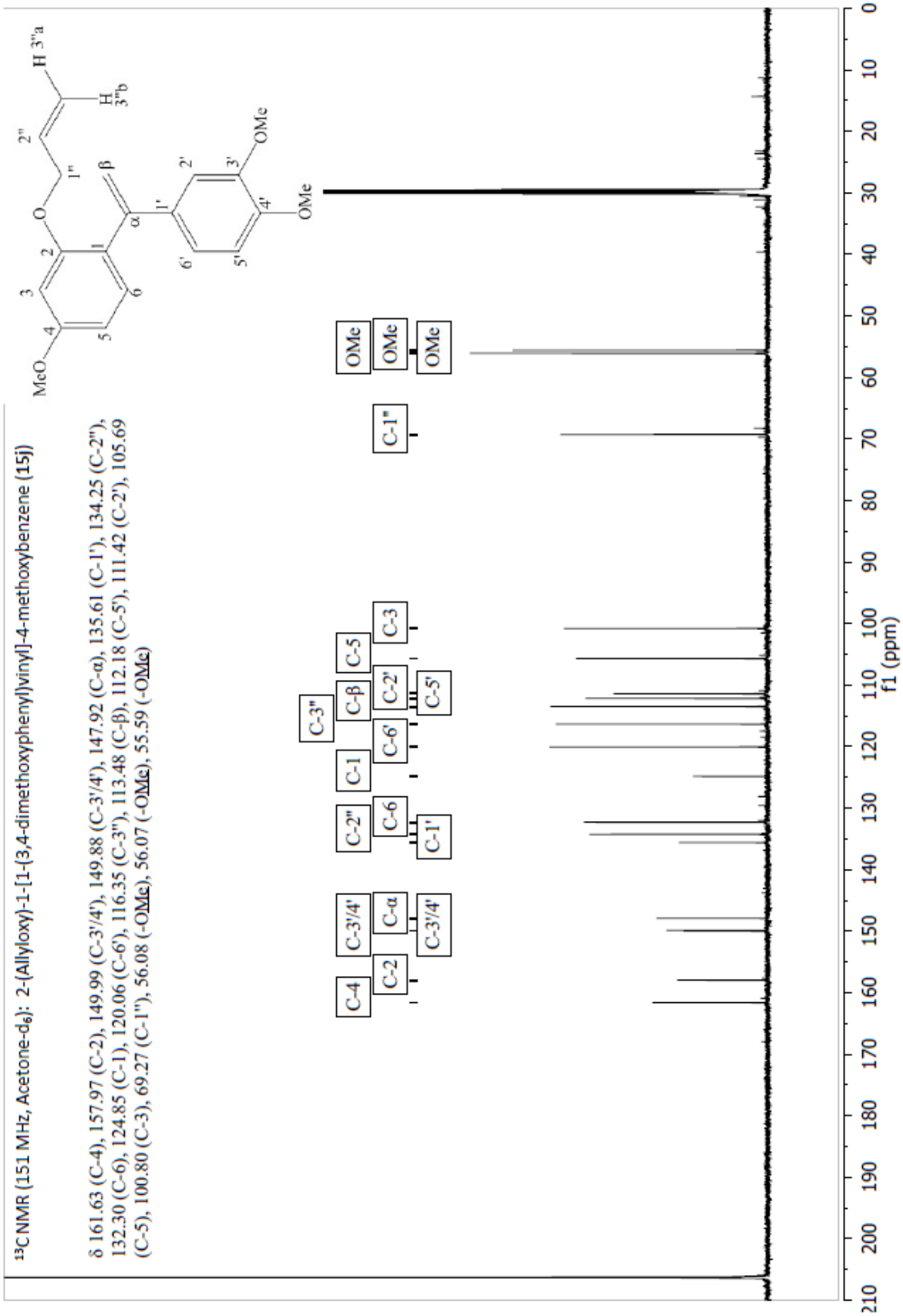

HSQC (600 MHz/151 MHz, $CDCl_3$): 1-[2-(Allyloxy)-4,5-dimethoxyphenyl]-1-(3,4-dimethoxyphenyl)ethan-1-ol (**19k**)

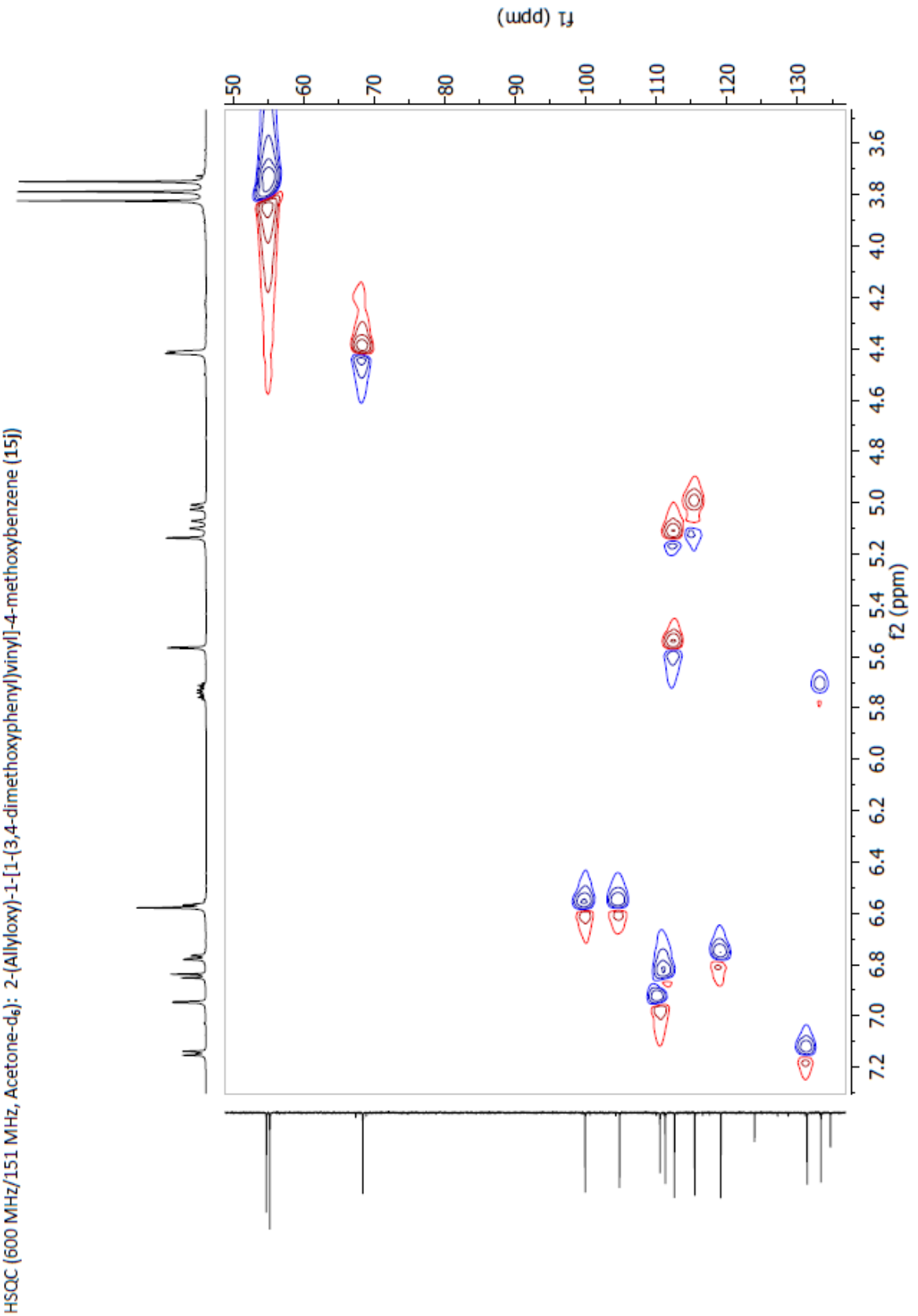


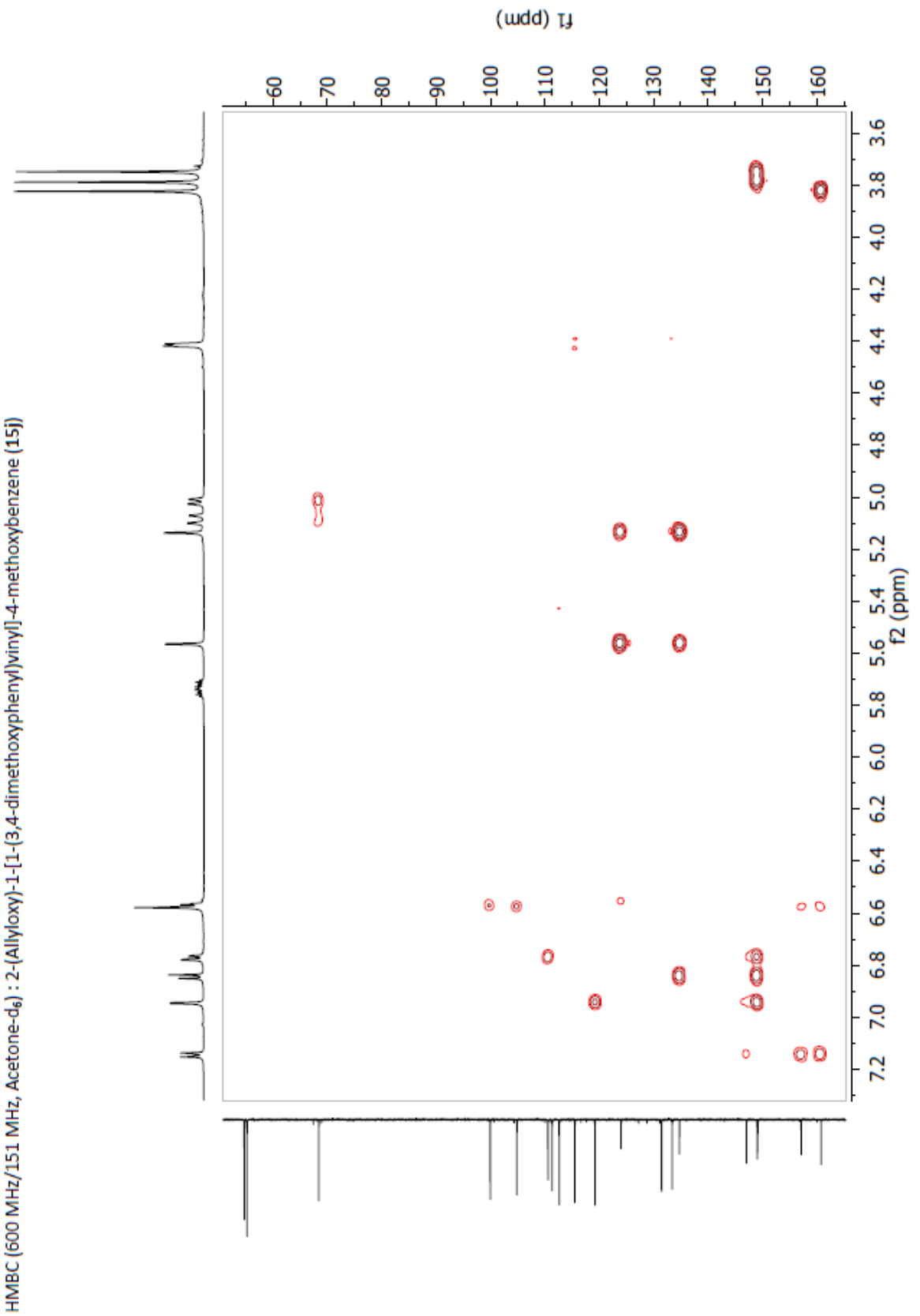

HMBC (600 MHz/151 MHz, $CDCl_3$) : 1-[2-(Allyloxy)-4,5-dimethoxyphenyl]-1-(3,4-dimethoxyphenyl)ethan-1-ol (**19k**)


DEPT NMR (151 MHz, CDCl3): 1-[2-(Allyloxy)-4,5-dimethoxyphenyl]-1-(3,4-dimethoxyphenyl)ethan-1-ol (19k)
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
210
f1 (ppm)

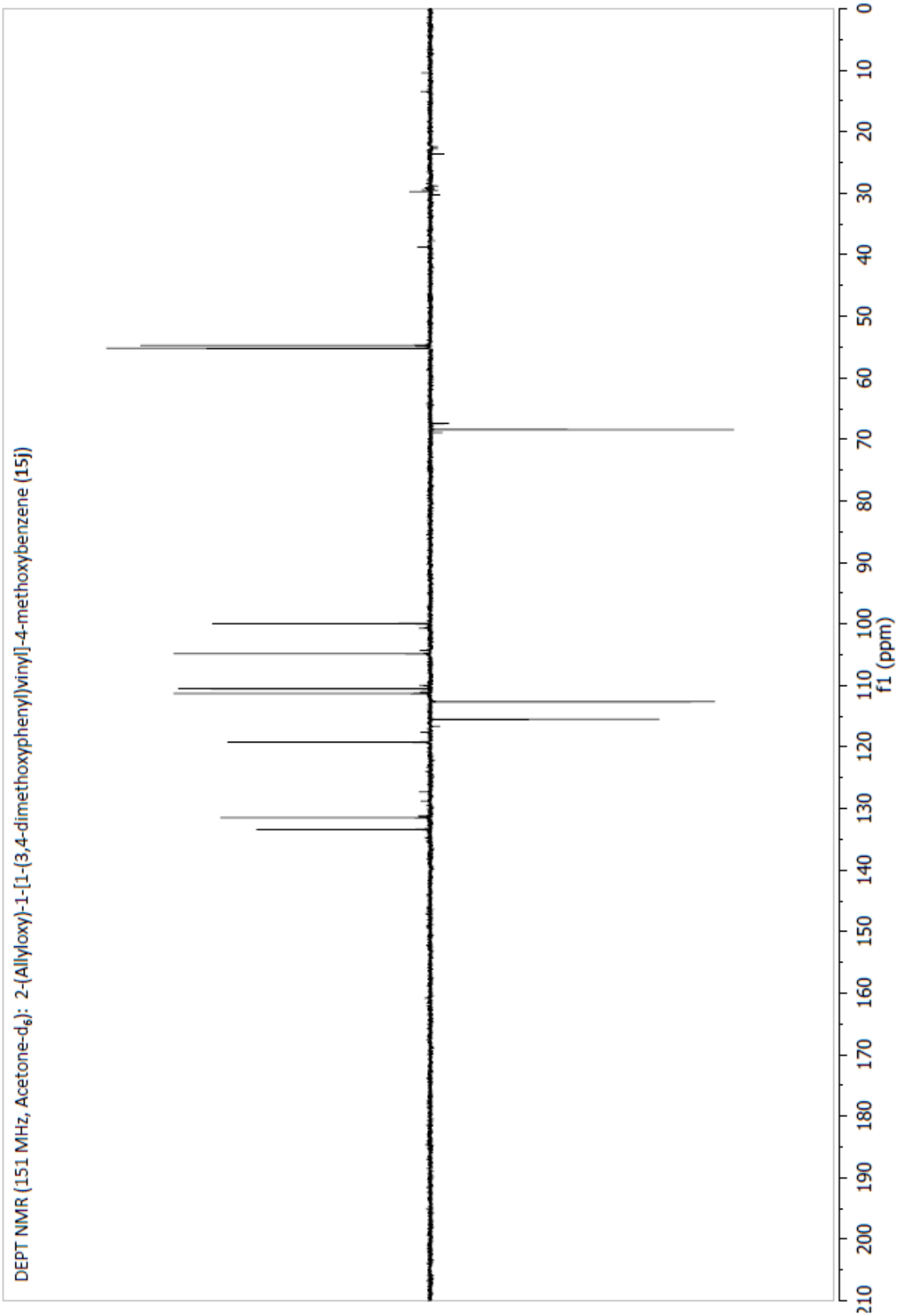

¹H NMR (600 MHz, Acetone-d6): 2-(Allyloxy)-1-[1-(3,4-dimethoxyphenyl)vinyl]-4-methoxybenzene (15j)
δ 7.15 (1H, d, J = 8.7 Hz, H-6), 6.95 (1H, d, J = 2.0 Hz, H-2'), 6.84 (1H, d, J = 8.3 Hz, H-5'), 6.77 (1H, dd, J = 8.3, 2.0 Hz, H-6'), 6.59 – 6.56 (2H, m, H-3 and H-5), 5.77 – 5.70 (1H, m, H-2"), 5.56 (1H, d, J = 1.6 Hz, H-β), 5.14 (1H, d, J = 1.6 Hz, H-β), 5.08 (1H, br. d, J = 17.3, 1.7 Hz, H-3"b), 5.02 (1H, br. d, J = 10.5, 1.7 Hz, H-3"a), 4.43 – 4.40 (2H, m, H-1"), 3.82 (3H, s, -OMe), 3.79 (3H, s, -OMe), 3.75 (3H, s, -OMe)
MeO
OMe
OMe
f1 (ppm)
H-6
H-2'
H-5'
H-6'
H-3 and H-5
H-2"
H-β
H-β
H-3"b
H-3"a
H-1"
OMe
OMe
OMe
f1 (ppm)

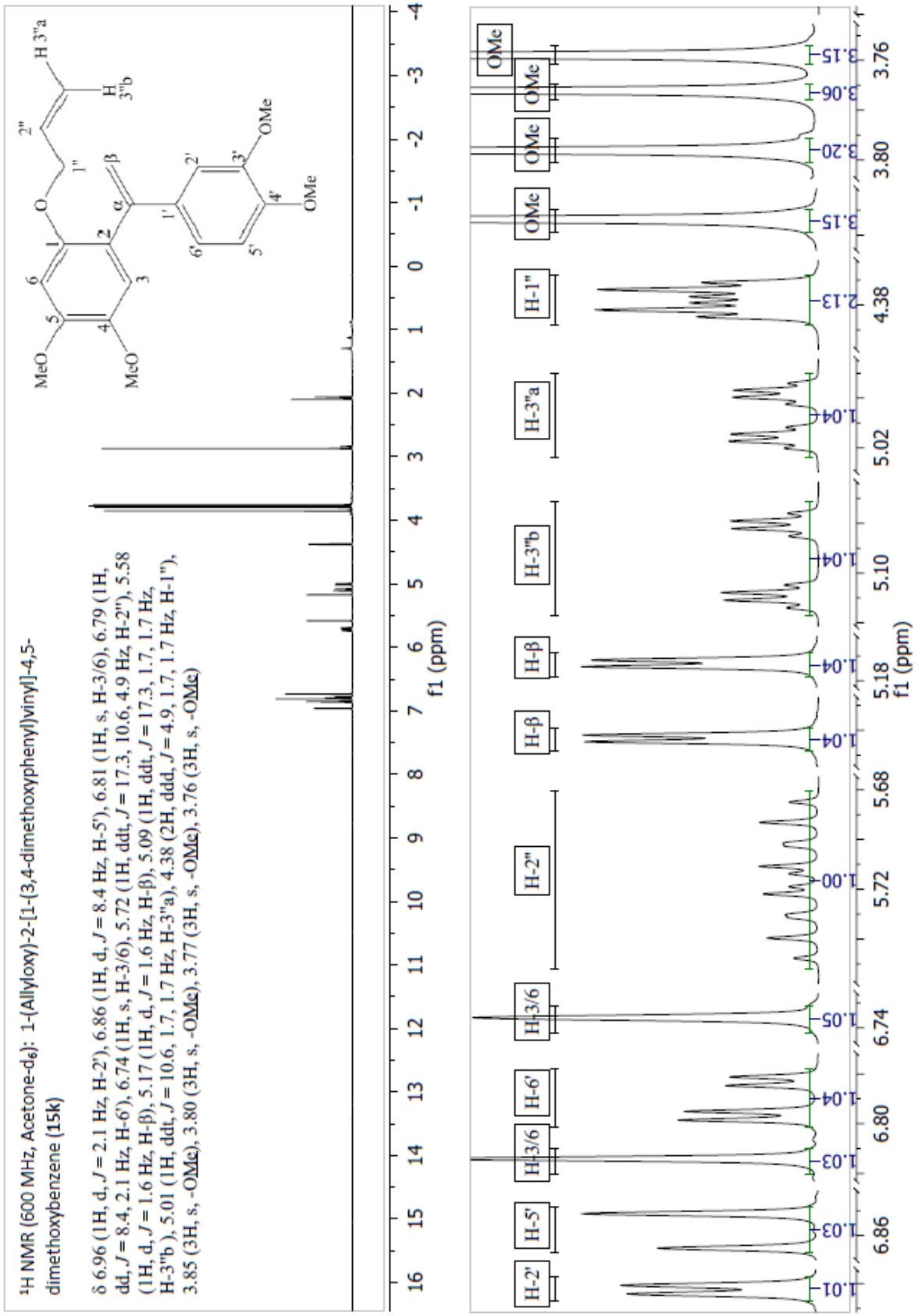

$^{13}$C NMR (151 MHz, Acetone-d$_6$): 2-(Allyloxy)-1-[1-(3,4-dimethoxyphenyl)vinyl]-4-methoxybenzene (15j)
δ 161.63 (C-4), 157.97 (C-2), 149.99 (C-3'/4'), 149.88 (C-3'/4'), 147.92 (C-α), 135.61 (C-1'), 134.25 (C-2''), 132.30 (C-6), 124.85 (C-1), 120.06 (C-6'), 116.35 (C-3''), 113.48 (C-β), 112.18 (C-5'), 111.42 (C-2'), 105.69 (C-5), 100.80 (C-3), 69.27 (C-1''), 56.08 (-OMe), 56.07 (-OMe), 55.59 (-OMe)
MeO
OMe
OMe
OMe
OMe
C-4
C-2
C-3'/4'
C-α
C-3'/4'
C-2''
C-6
C-1'
C-1
C-3''
C-β
C-6'
C-5
C-2'
C-5'
C-3
C-1''
f1 (ppm)


HSQC (600 MHz/151 MHz, Acetone-d6): 2-(Allyloxy)-1-[1-(3,4-dimethoxyphenyl)vinyl]-4-methoxybenzene (15j)
f1 (ppm)
f2 (ppm)

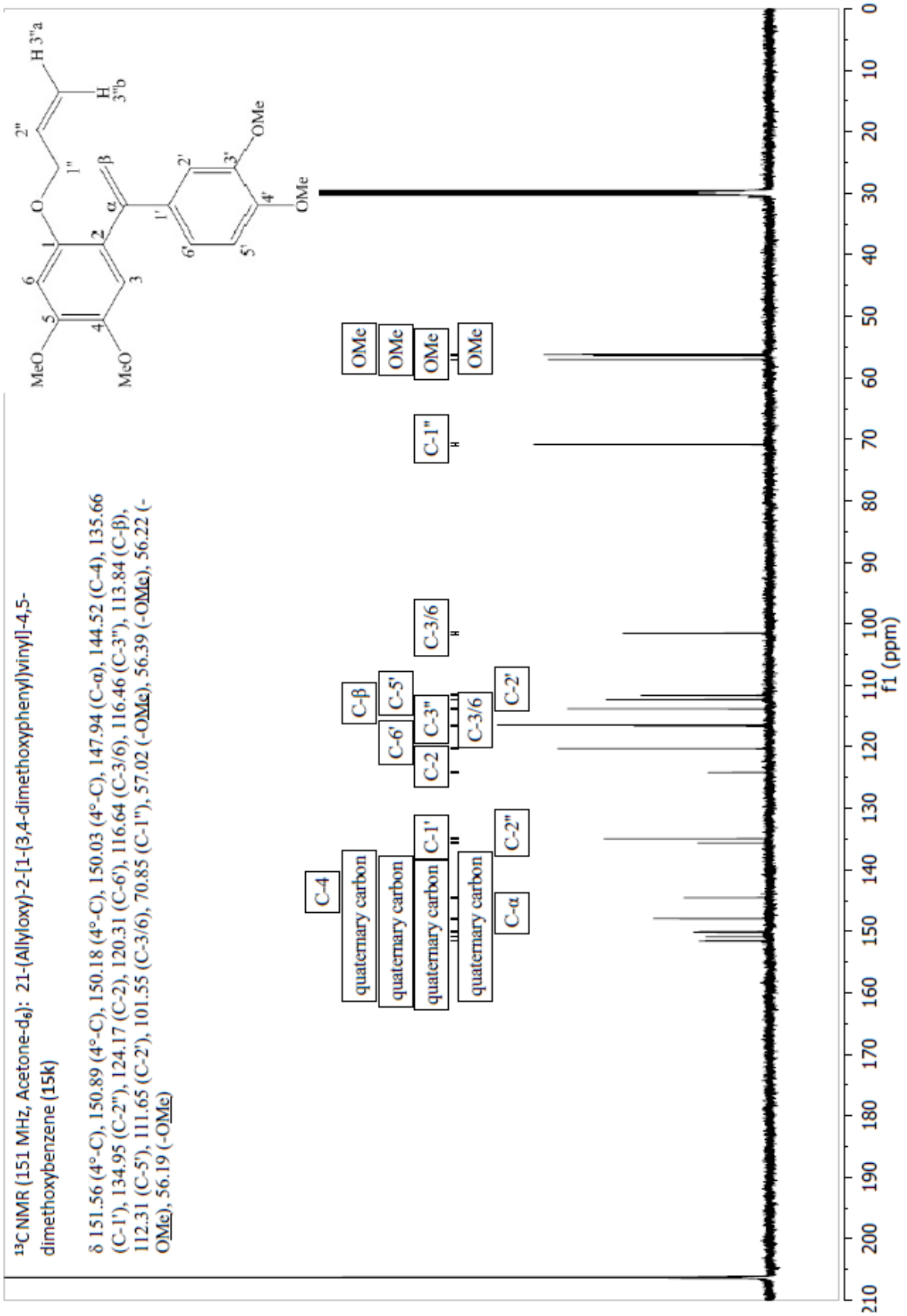


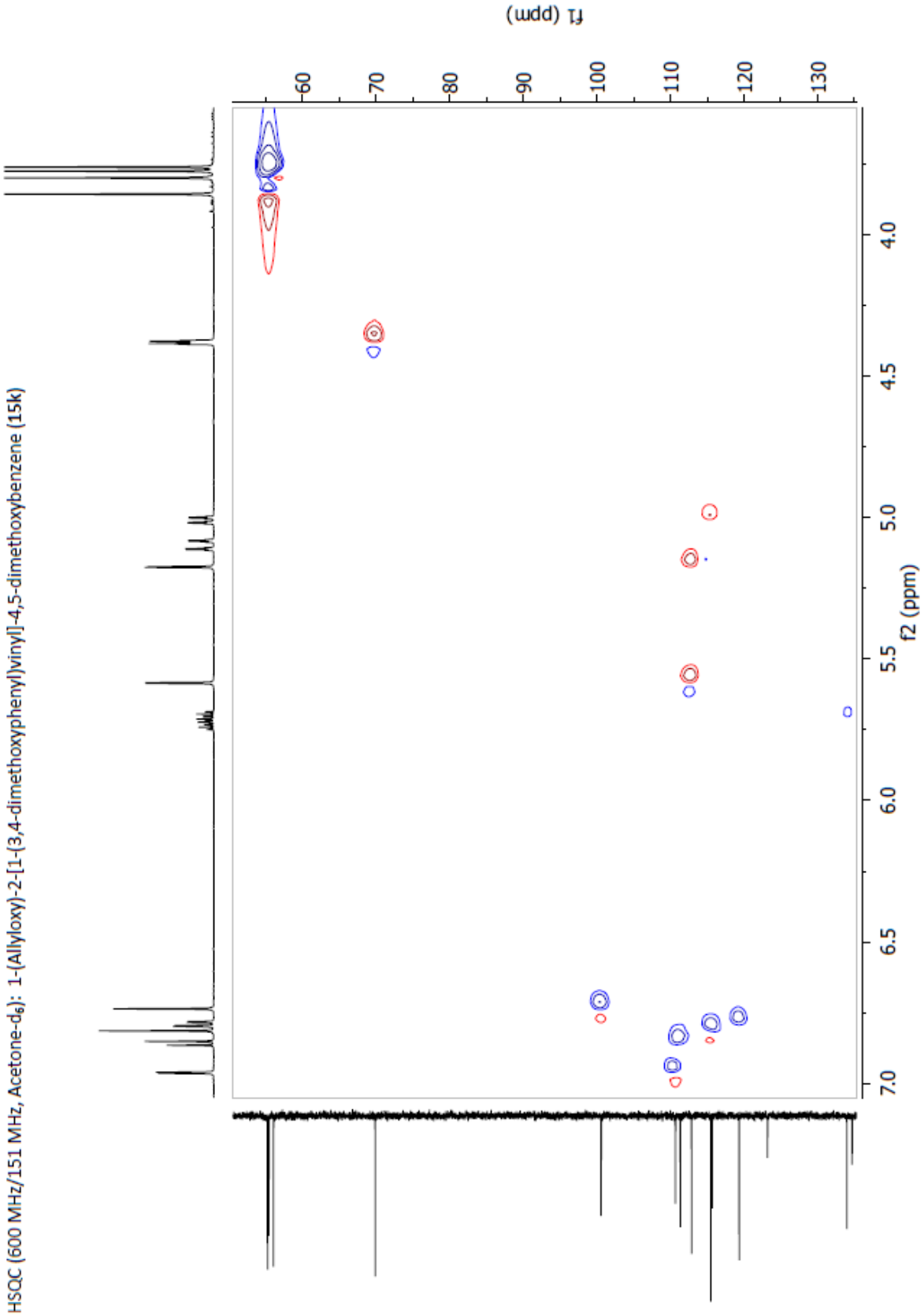

HMBC (600 MHz/151 MHz, Acetone-$d_6$) : 2-(Allyloxy)-1-[1-(3,4-dimethoxyphenyl)vinyl]-4-methoxybenzene (15j)

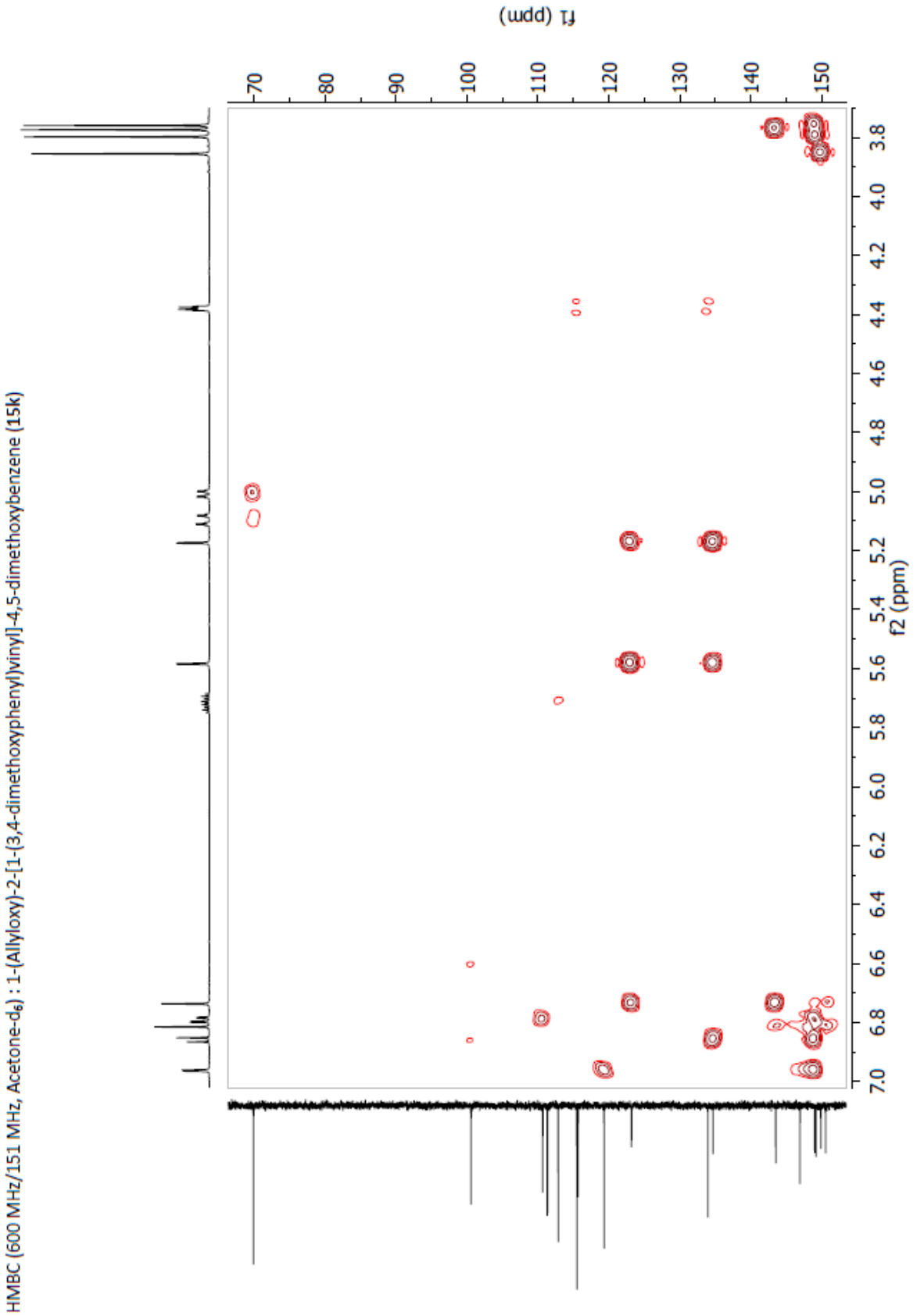

DEPT NMR (151 MHz, Acetone-d6): 2-(Allyloxy)-1-[1-(3,4-dimethoxyphenyl)vinyl]-4-methoxybenzene (15j)
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
210
f1 (ppm)


¹H NMR (600 MHz, Acetone-d₆): 1-(Allyloxy)-2-[1-(3,4-dimethoxyphenyl)vinyl]-4,5-dimethoxybenzene (15k)
δ 6.96 (1H, d, J = 2.1 Hz, H-2'), 6.86 (1H, d, J = 8.4 Hz, H-5'), 6.81 (1H, s, H-3/6), 6.79 (1H, dd, J = 8.4, 2.1 Hz, H-6'), 6.74 (1H, s, H-3/6), 5.72 (1H, ddt, J = 17.3, 10.6, 4.9 Hz, H-2"), 5.58 (1H, d, J = 1.6 Hz, H-β), 5.17 (1H, d, J = 1.6 Hz, H-β), 5.09 (1H, ddt, J = 17.3, 1.7, 1.7 Hz, H-3"b ), 5.01 (1H, ddt, J = 10.6, 1.7, 1.7 Hz, H-3"a), 4.38 (2H, ddd, J = 4.9, 1.7, 1.7 Hz, H-1"), 3.85 (3H, s, -OMe), 3.80 (3H, s, -OMe), 3.77 (3H, s, -OMe), 3.76 (3H, s, -OMe)
MeO
MeO
OMe
OMe
H 3"a
H 3"b
f1 (ppm)
H-2'
H-5'
H-3/6
H-3/6
H-6'
H-3/6
H-2"
H-β
H-β
H-3"b
H-3"a
H-1"
OMe
OMe
OMe
OMe
f1 (ppm)

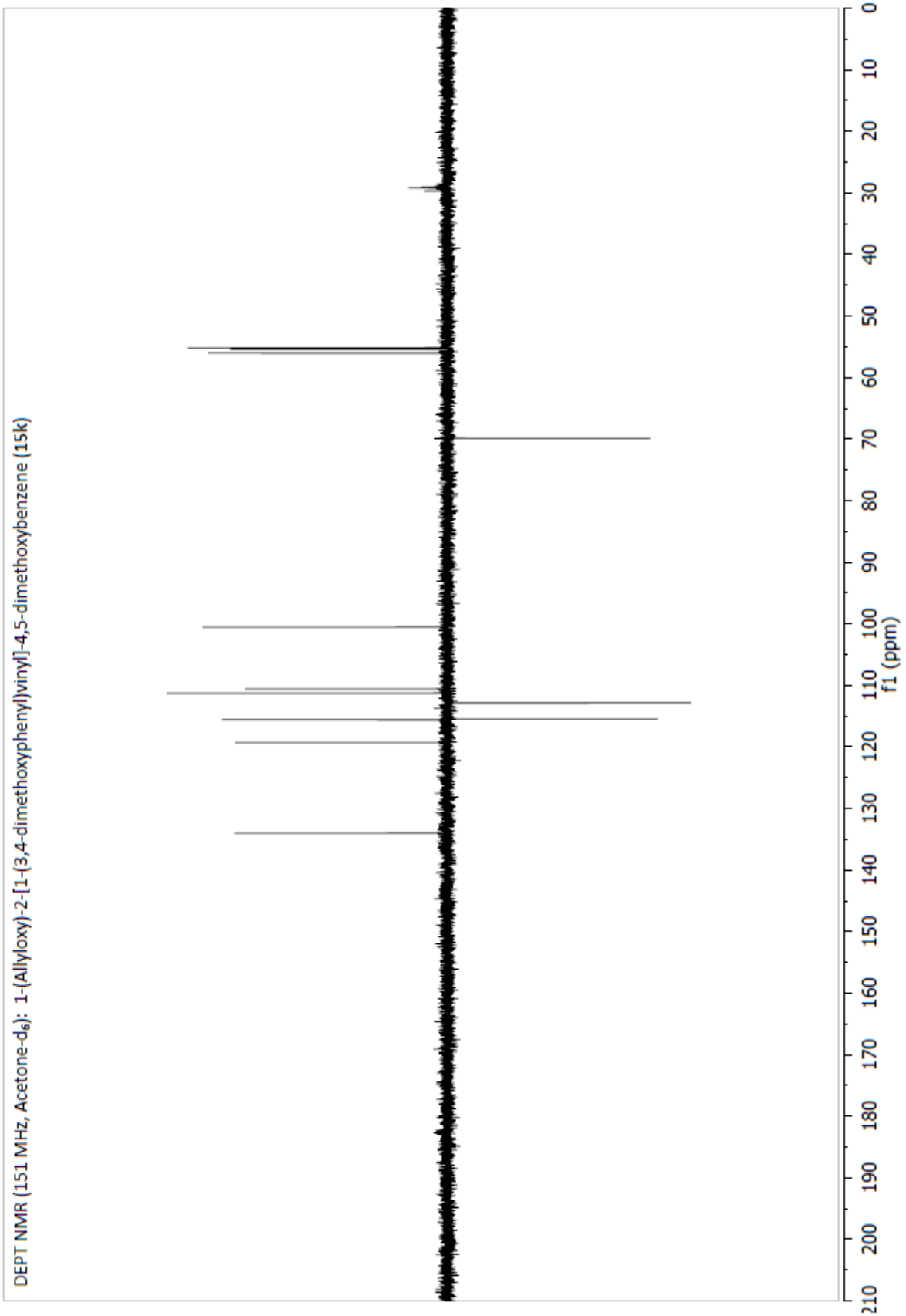
 

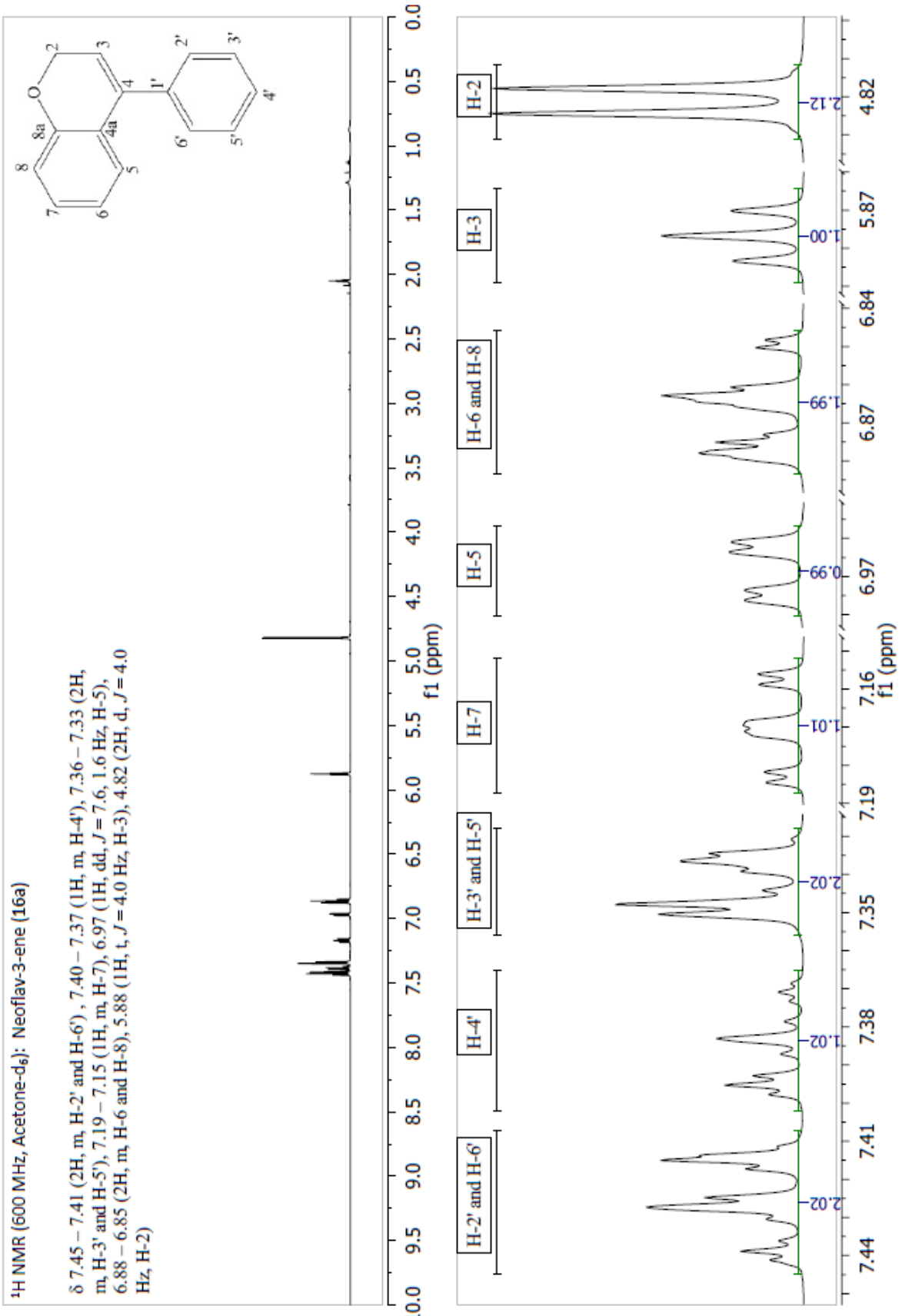

13C NMR (151 MHz, Acetone-d6): 21-(Allyloxy)-2-[1-(3,4-dimethoxyphenyl)vinyl]-4,5-dimethoxybenzene (15k)
δ 151.56 (4°-C), 150.89 (4°-C), 150.18 (4°-C), 150.03 (4°-C), 147.94 (C-α), 144.52 (C-4), 135.66 (C-1'), 134.95 (C-2"), 124.17 (C-2), 120.31 (C-6'), 116.64 (C-3/6), 116.46 (C-3"), 113.84 (C-β), 112.31 (C-5'), 111.65 (C-2'), 101.55 (C-3/6), 70.85 (C-1"), 57.02 (-OMe), 56.39 (-OMe), 56.22 (-OMe), 56.19 (-OMe)
C-4
quaternary carbon
quaternary carbon
quaternary carbon
quaternary carbon
C-1'
C-α
C-2"
C-β
C-6'
C-5'
C-2
C-3"
C-3/6
C-3/6
C-2'
C-1"
OMe
OMe
OMe
OMe
MeO
MeO
OMe
OMe
f1 (ppm)

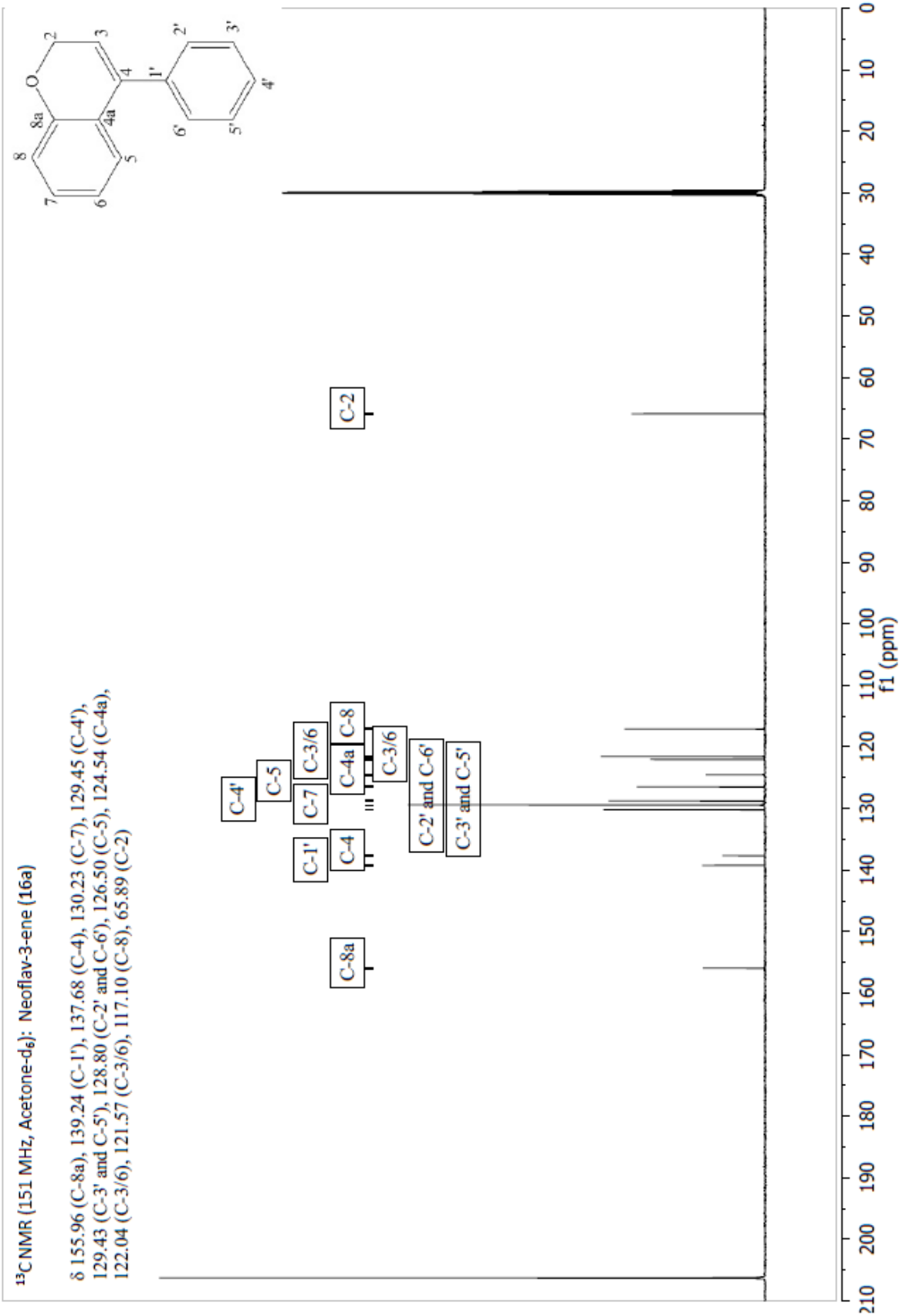

HSQC (600 MHz/151 MHz, Acetone-d6): 1-(Allyloxy)-2-[1-(3,4-dimethoxyphenyl)vinyl]-4,5-dimethoxybenzene (15k)
f1 (ppm)
60
70
80
90
100
110
120
130
f2 (ppm)
4.0
4.5
5.0
5.5
6.0
6.5
7.0

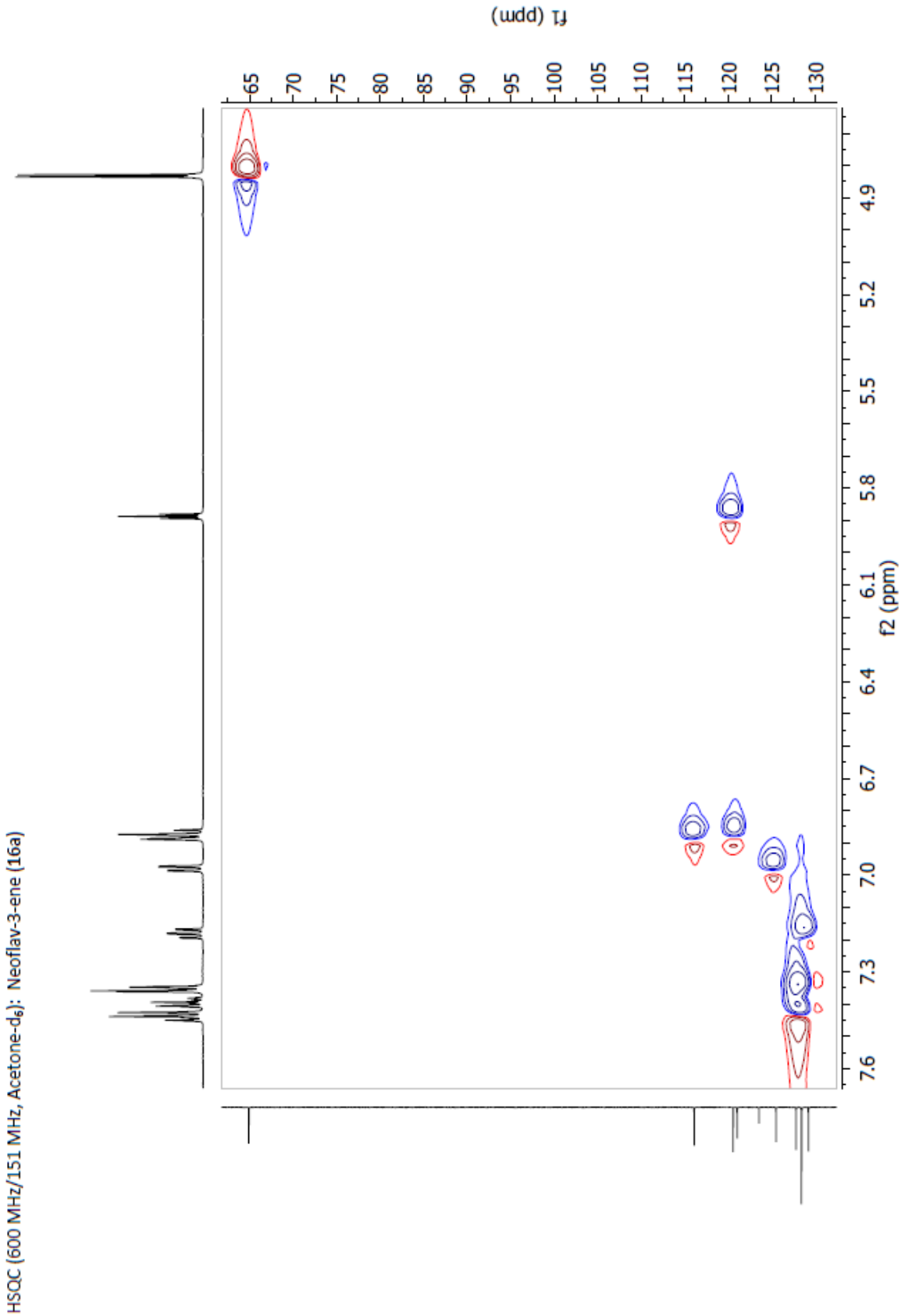



HMBC (600 MHz/151 MHz, Acetone-$d_6$) : 1-(Allyloxy)-2-[1-(3,4-dimethoxyphenyl)vinyl]-4,5-dimethoxybenzene (**15k**)

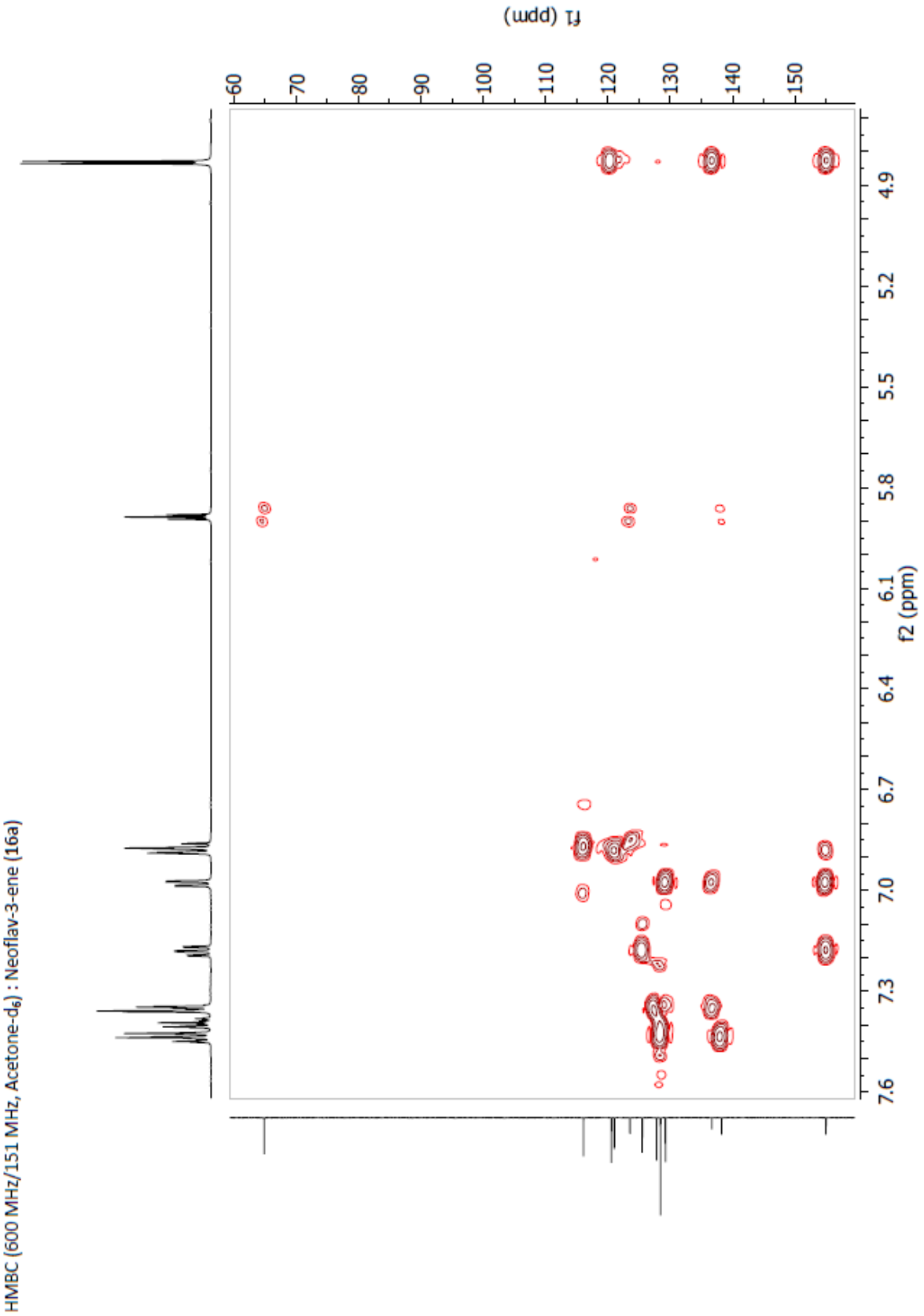

DEPT NMR (151 MHz, Acetone-d6): 1-(Allyloxy)-2-[1-(3,4-dimethoxyphenyl)vinyl]-4,5-dimethoxybenzene (15k)
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
210
f1 (ppm)

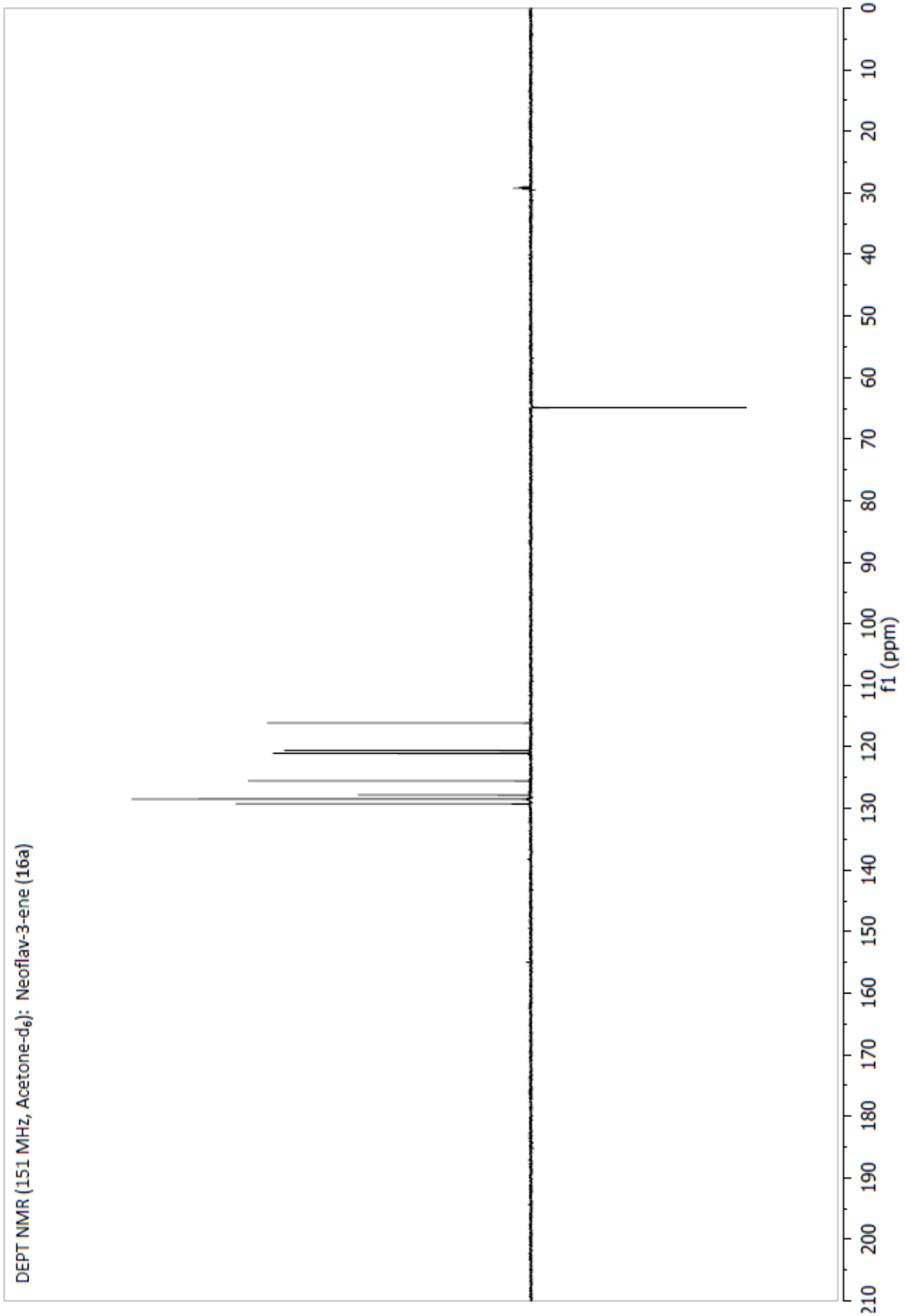

¹H NMR (600 MHz, Acetone-d₆): Neoflav-3-ene (16a)
δ 7.45 – 7.41 (2H, m, H-2' and H-6') , 7.40 – 7.37 (1H, m, H-4'), 7.36 – 7.33 (2H, m, H-3' and H-5'), 7.19 – 7.15 (1H, m, H-7), 6.97 (1H, dd, J = 7.6, 1.6 Hz, H-5), 6.88 – 6.85 (2H, m, H-6 and H-8), 5.88 (1H, t, J = 4.0 Hz, H-3), 4.82 (2H, d, J = 4.0 Hz, H-2)
f1 (ppm)
H-2' and H-6'
H-4'
H-3' and H-5'
H-7
H-5
H-6 and H-8
H-3
H-2
2.12
1.00
1.99
0.99
1.01
2.02
1.02
2.02

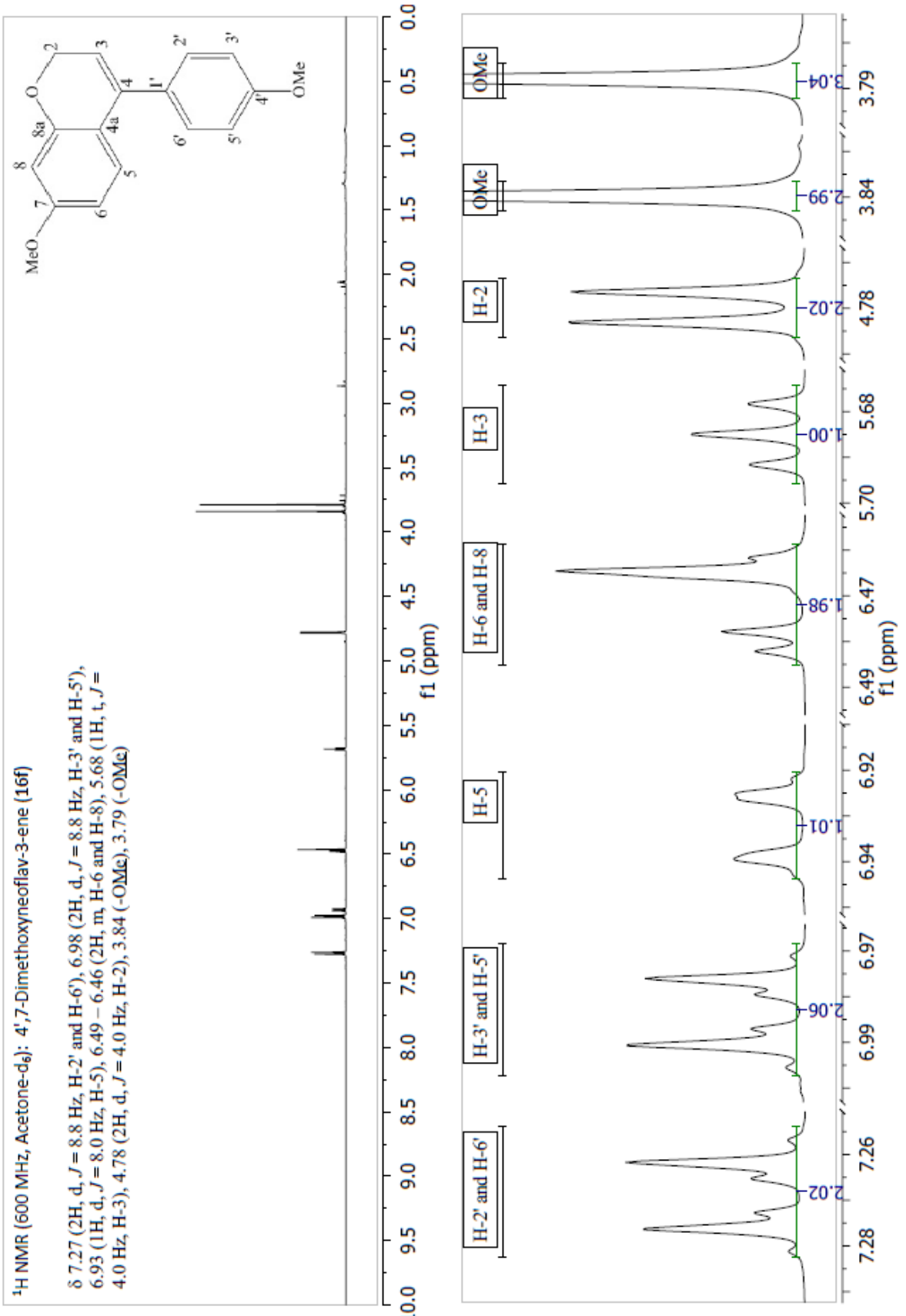

$^{13}$C NMR (151 MHz, Acetone-$d_6$): Neoflav-3-ene (16a)
δ 155.96 (C-8a), 139.24 (C-1'), 137.68 (C-4), 130.23 (C-7), 129.45 (C-4'), 129.43 (C-3' and C-5'), 128.80 (C-2' and C-6'), 126.50 (C-5), 124.54 (C-4a), 122.04 (C-3/6), 121.57 (C-3/6), 117.10 (C-8), 65.89 (C-2)
C-8a
C-4
C-1'
C-7
C-5
C-4'
C-4a
C-3/6
C-8
C-3/6
C-2' and C-6'
C-3' and C-5'
C-2
f1 (ppm)

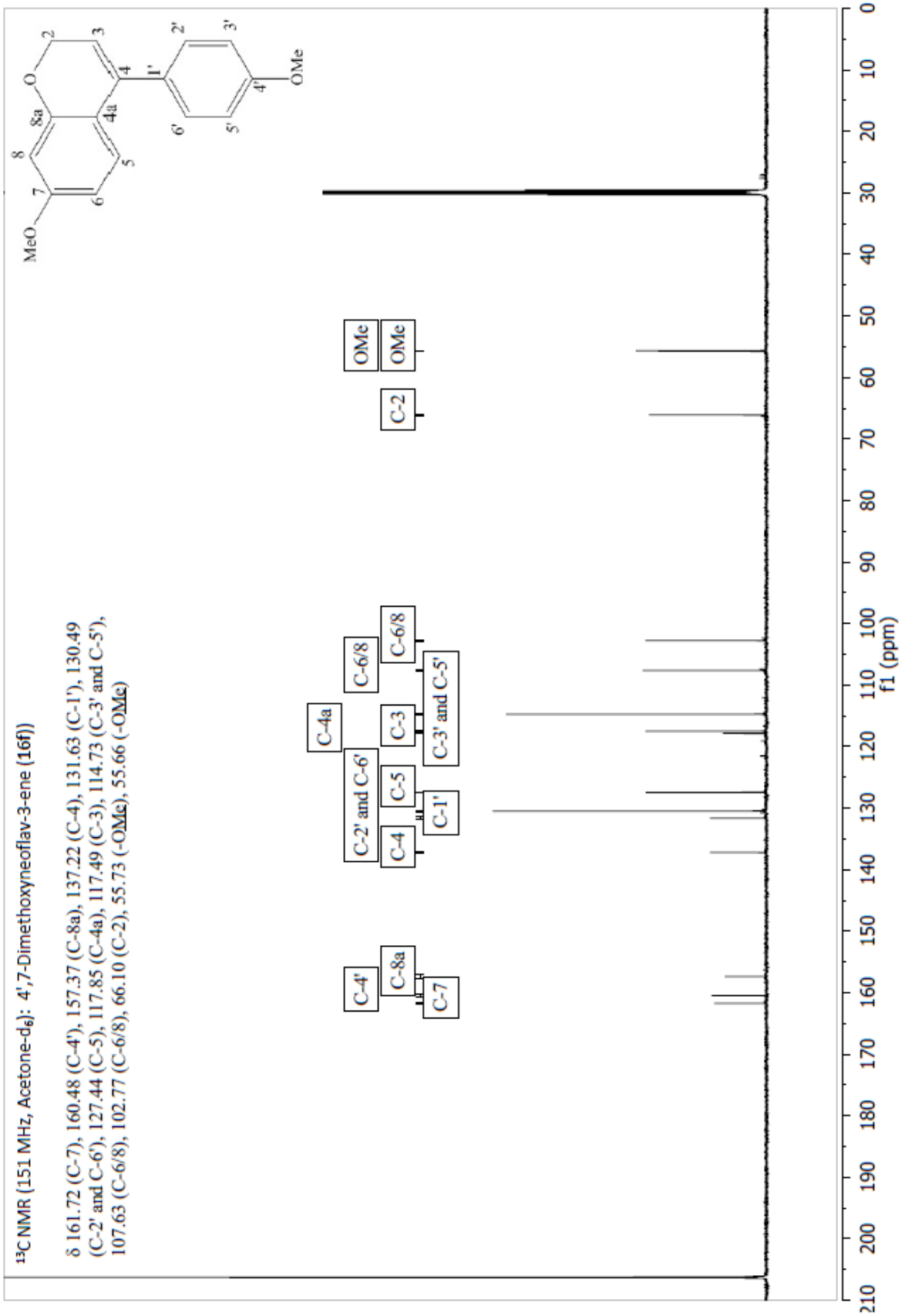


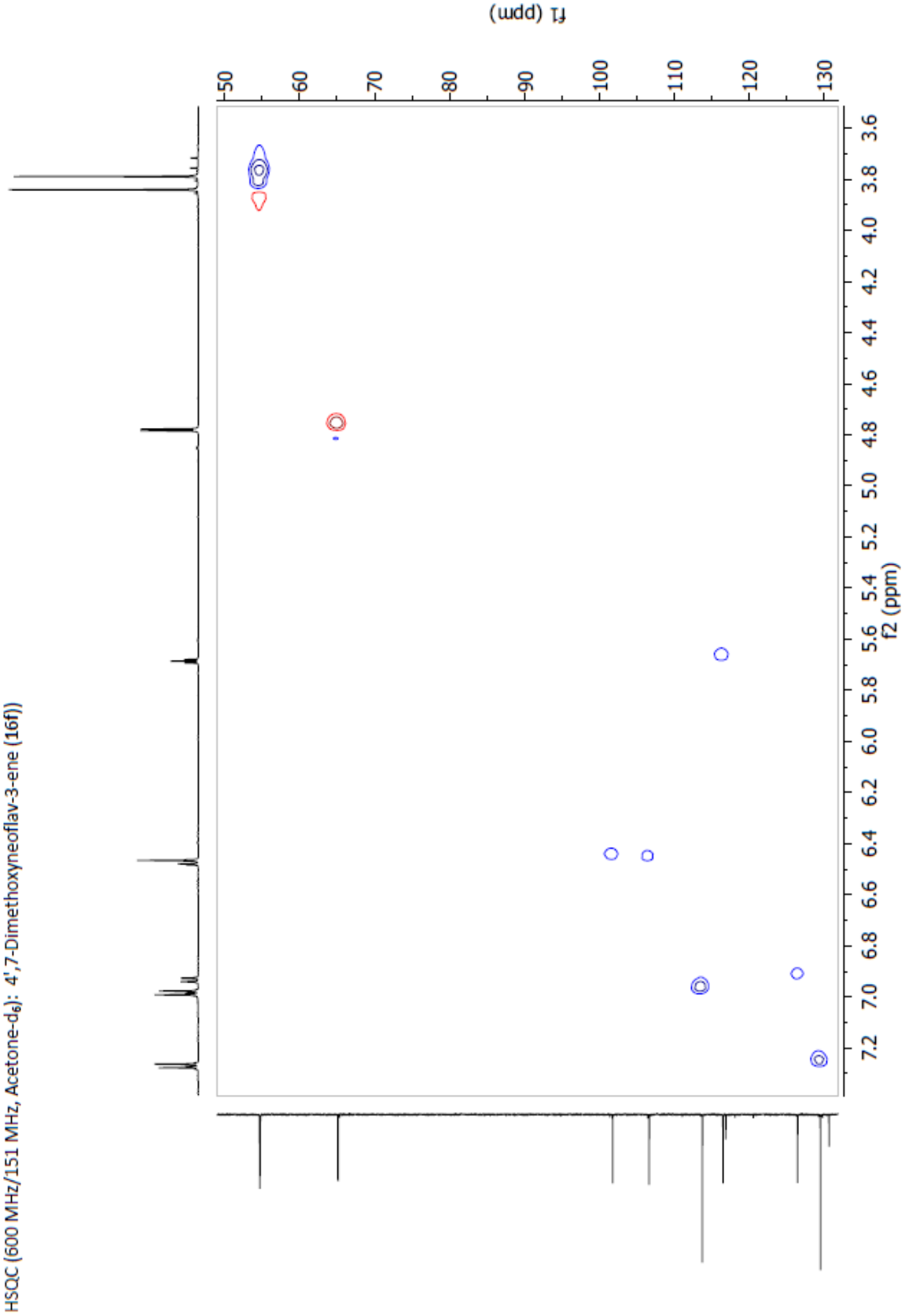

HSQC (600 MHz/151 MHz, Acetone-$d_6$): Neoflav-3-ene (16a)


HMBC (600 MHz/151 MHz, Acetone-d6) : Neoflav-3-ene (16a)
f1 (ppm)
60
70
80
90
100
110
120
130
140
150
f2 (ppm)
4.9
5.2
5.5
5.8
6.1
6.4
6.7
7.0
7.3
7.6

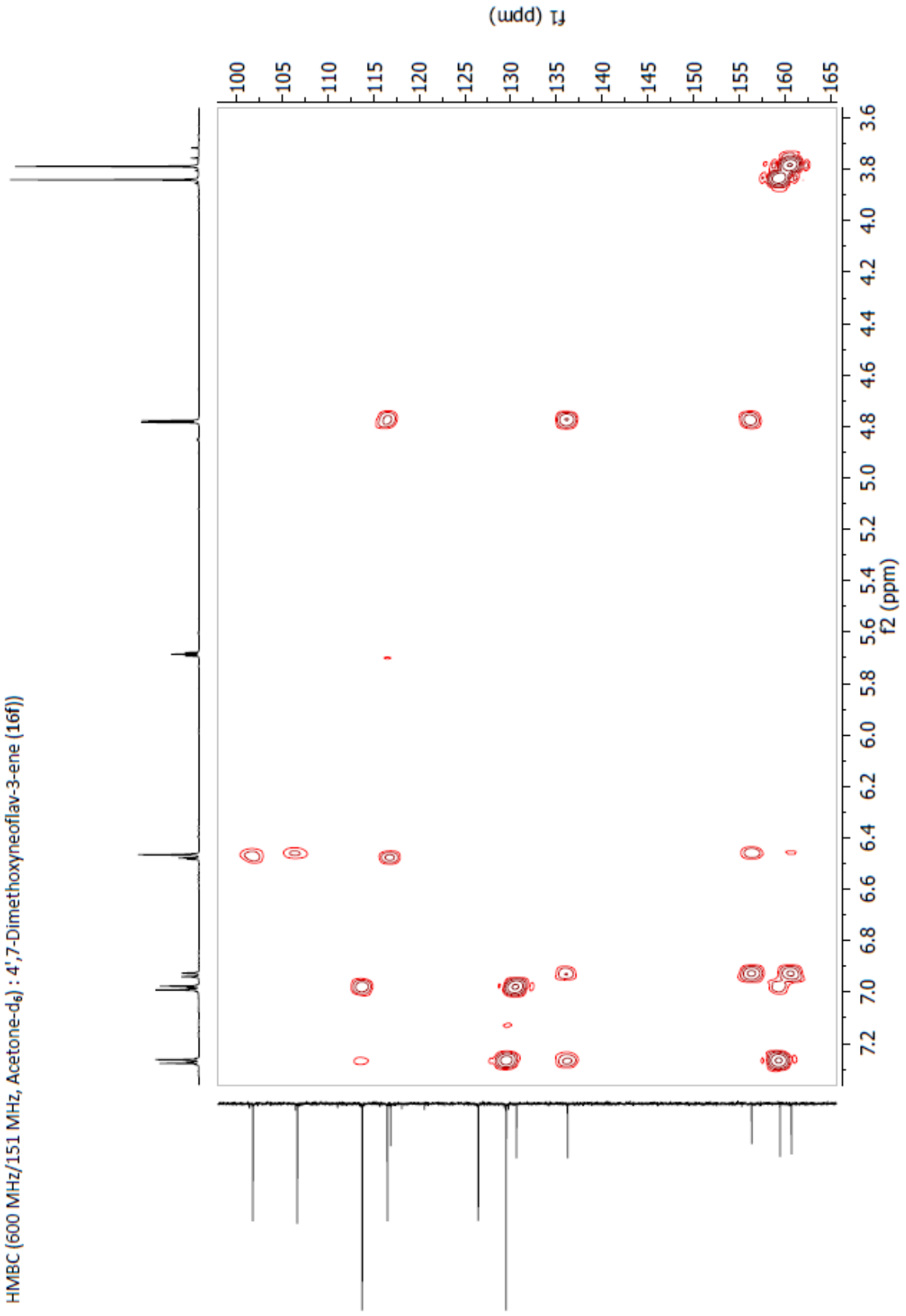

DEPT NMR (151 MHz, Acetone-d6): Neoflav-3-ene (16a)
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
210
f1 (ppm)

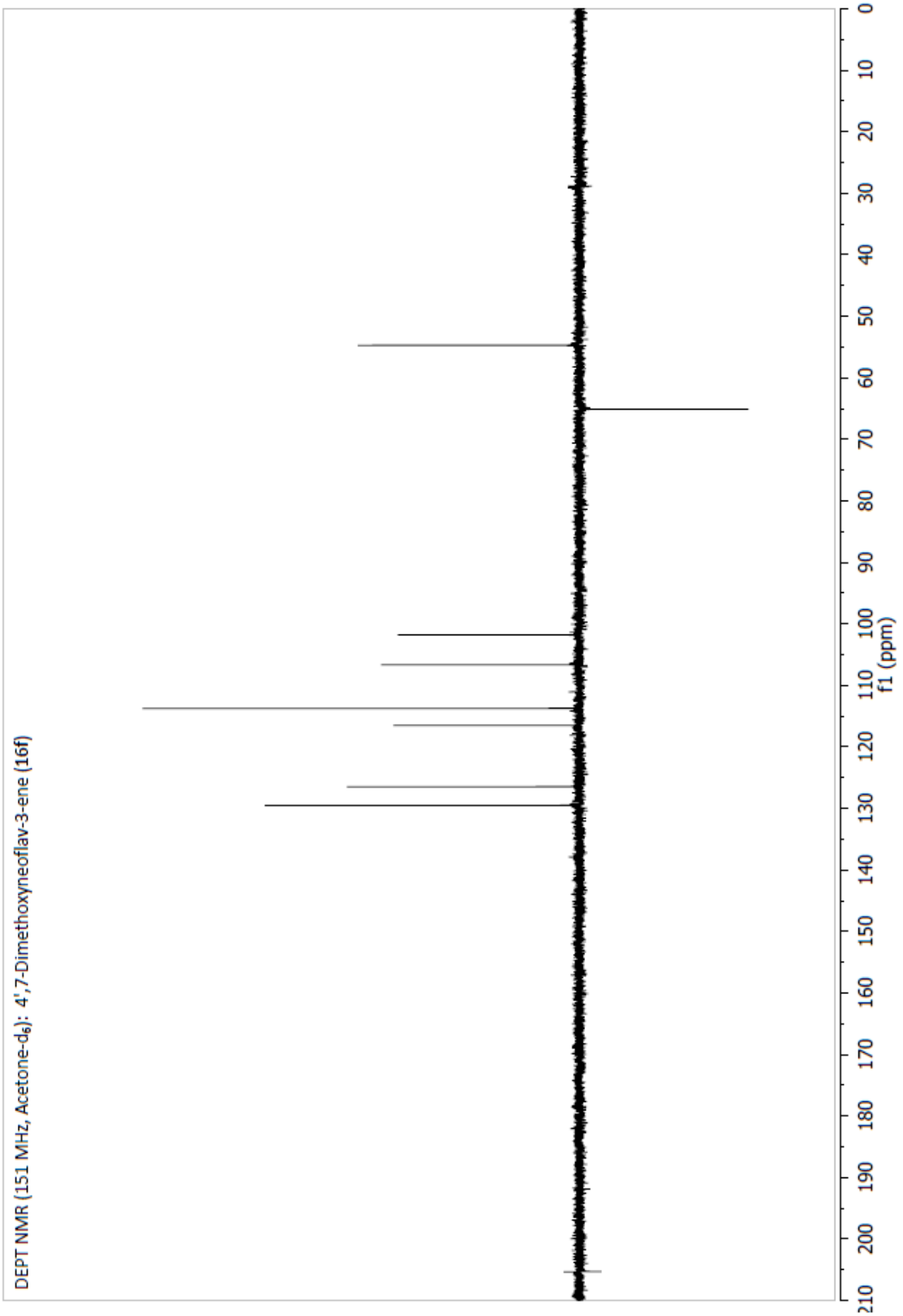

¹H NMR (600 MHz, Acetone-d₆): 4',7-Dimethoxyneoflav-3-ene (16f)
δ 7.27 (2H, d, J = 8.8 Hz, H-2' and H-6'), 6.98 (2H, d, J = 8.8 Hz, H-3' and H-5'), 6.93 (1H, d, J = 8.0 Hz, H-5), 6.49 – 6.46 (2H, m, H-6 and H-8), 5.68 (1H, t, J = 4.0 Hz, H-3), 4.78 (2H, d, J = 4.0 Hz, H-2), 3.84 (-OMe), 3.79 (-OMe)
MeO
OMe
f1 (ppm)
H-2' and H-6'
H-3' and H-5'
H-5
H-6 and H-8
H-3
H-2
OMe
OMe
2.02
2.06
1.01
1.98
1.00
2.02
2.99
3.04


MeO
OMe
δ 161.72 (C-7), 160.48 (C-4'), 157.37 (C-8a), 137.22 (C-4), 131.63 (C-1'), 130.49 (C-2' and C-6'), 127.44 (C-5), 117.85 (C-4a), 117.49 (C-3), 114.73 (C-3' and C-5'), 107.63 (C-6/8), 102.77 (C-6/8), 66.10 (C-2), 55.73 (-OMe), 55.66 (-OMe)
C-4'
C-8a
C-7
C-4
C-2' and C-6'
C-4a
C-1'
C-5
C-3
C-3' and C-5'
C-6/8
C-6/8
C-2
OMe
OMe
f1 (ppm)

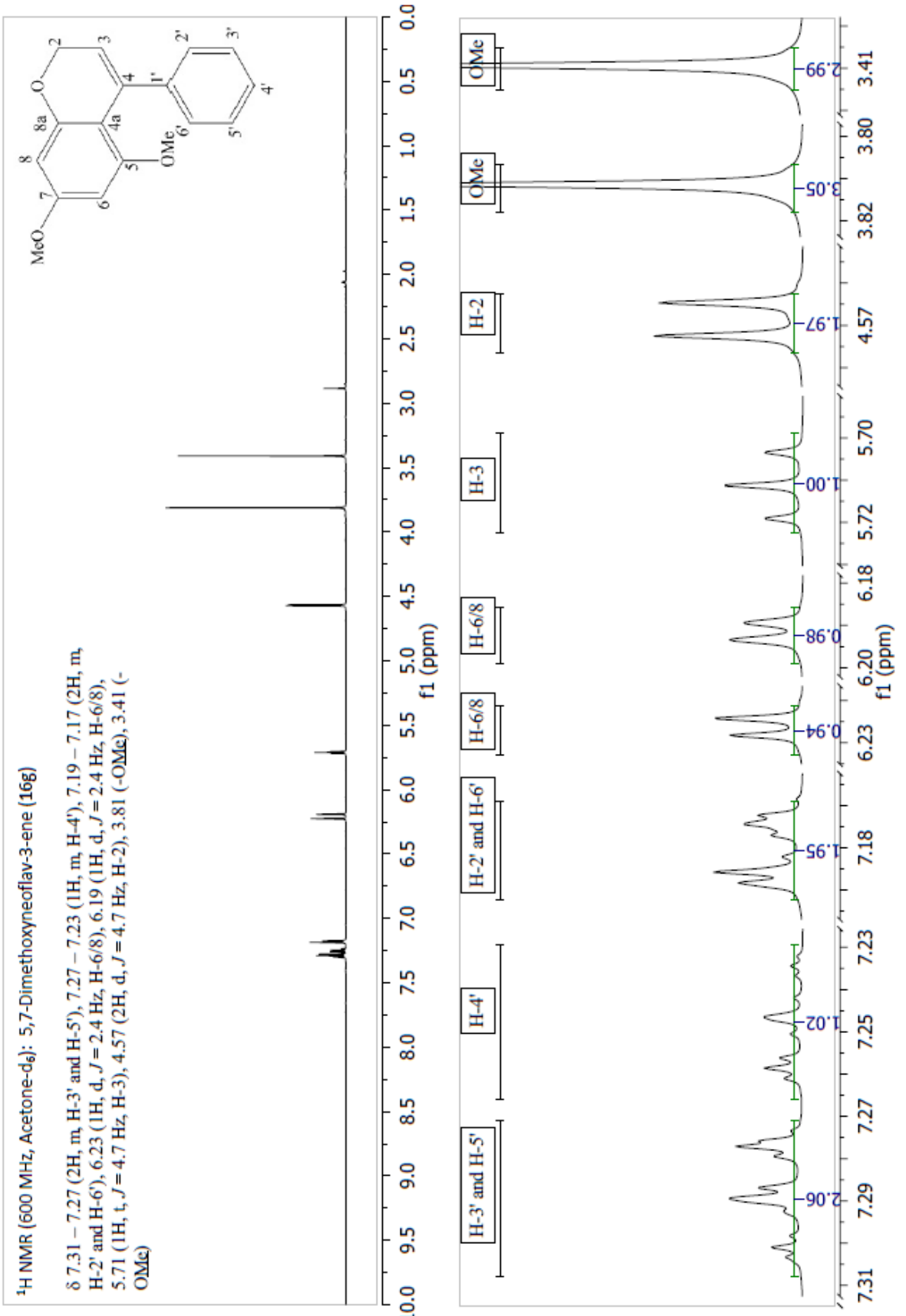



HSQC (600 MHz/151 MHz, Acetone-$d_6$): 4',7-Dimethoxyneoflav-3-ene (**16f**))


HMBC (600 MHz/151 MHz, Acetone-d6) : 4',7-Dimethoxyneoflav-3-ene (16f))
f1 (ppm)
f2 (ppm)

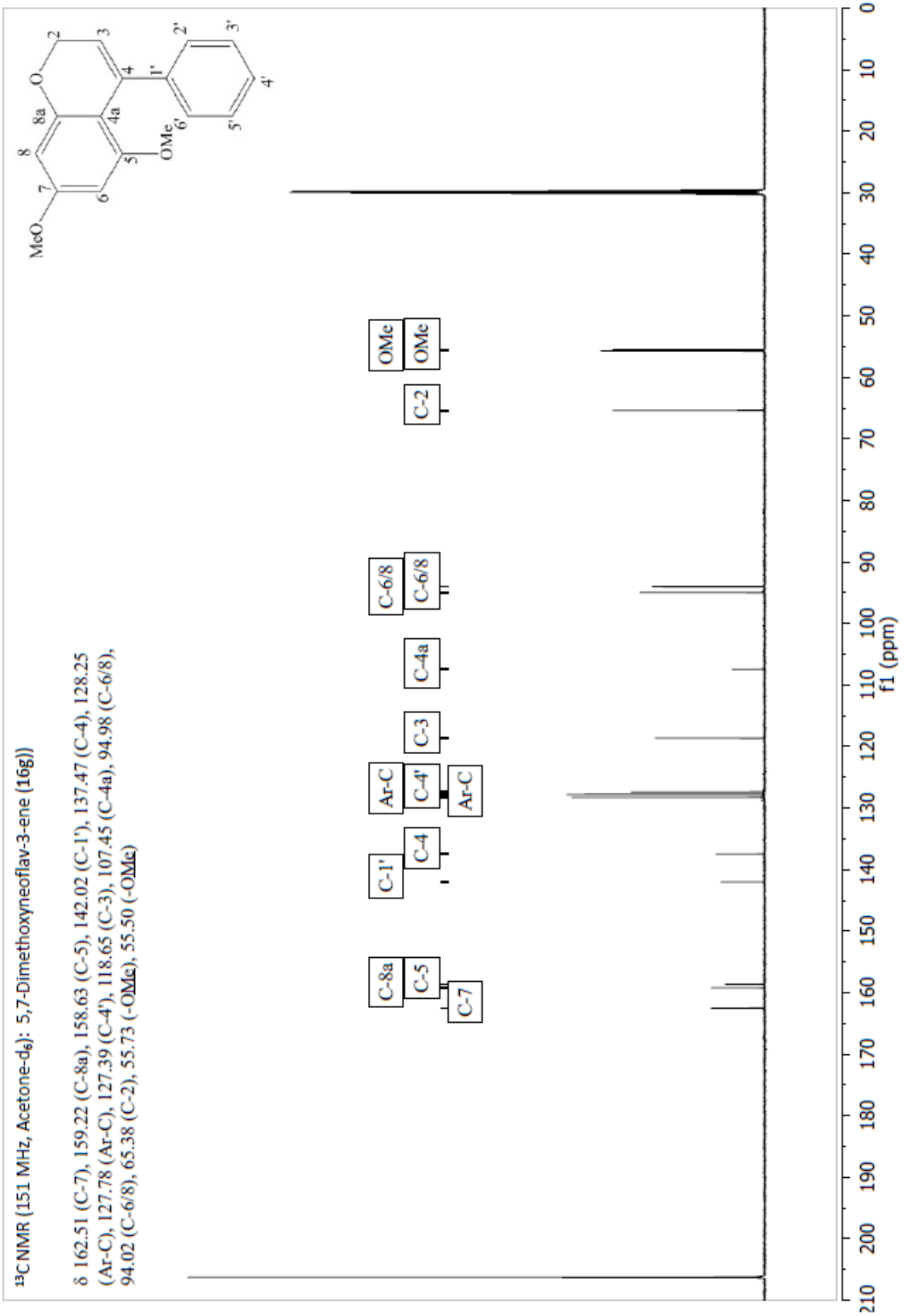

DEPT NMR (151 MHz, Acetone-d6): 4',7-Dimethoxyneoflav-3-ene (16f)
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
210
f1 (ppm)



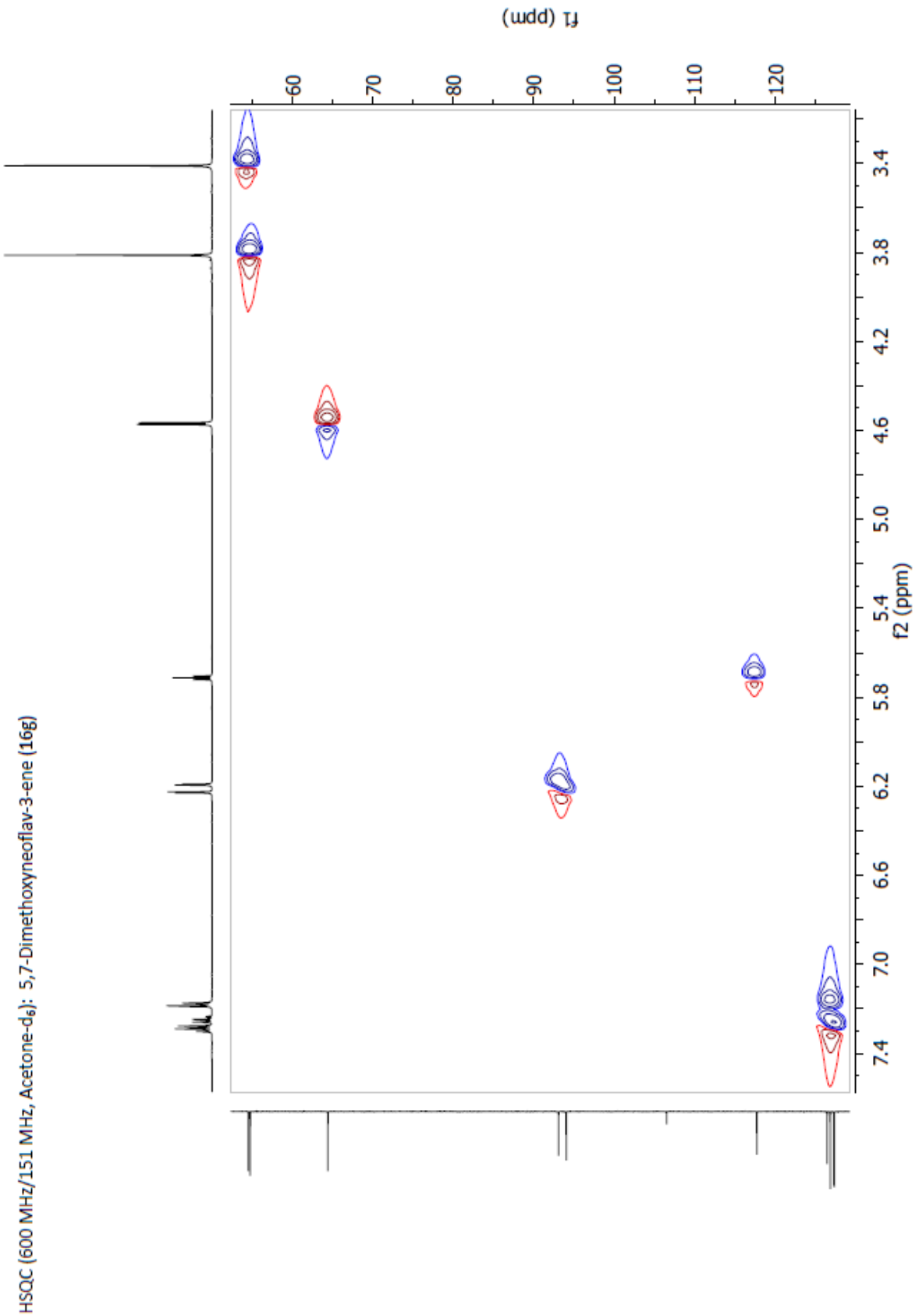

$^1$H NMR (600 MHz, Acetone-$d_6$): 5,7-Dimethoxyneoflav-3-ene (16g)

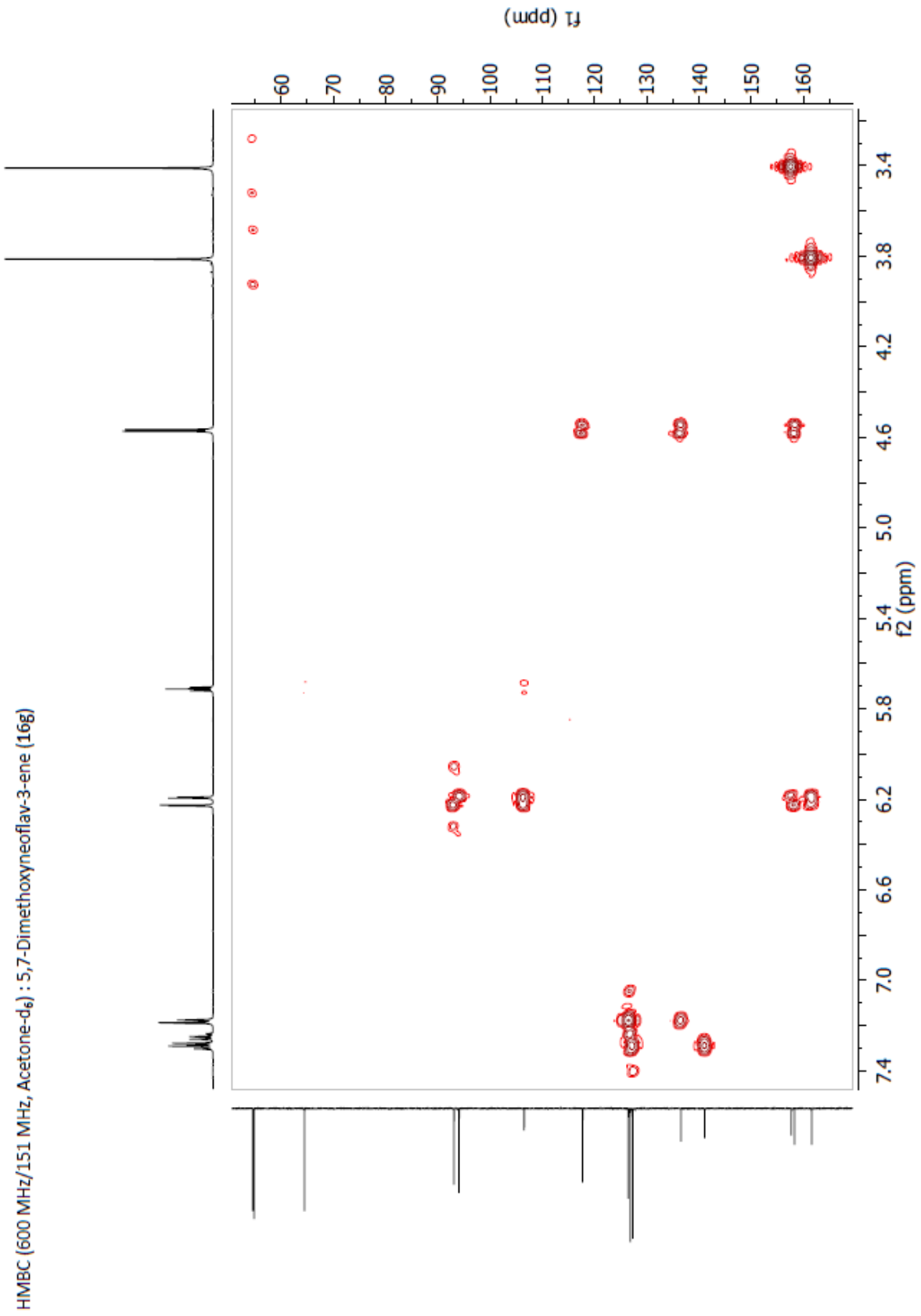
δ 7.31 – 7.27 (2H, m, H-3' and H-5'), 7.27 – 7.23 (1H, m, H-4'), 7.19 – 7.17 (2H, m, H-2' and H-6'), 6.23 (1H, d, *J* = 2.4 Hz, H-6/8), 6.19 (1H, d, *J* = 2.4 Hz, H-6/8), 5.71 (1H, t, *J* = 4.7 Hz, H-3), 4.57 (2H, d, *J* = 4.7 Hz, H-2), 3.81 (-OMe), 3.41 (-OMe)



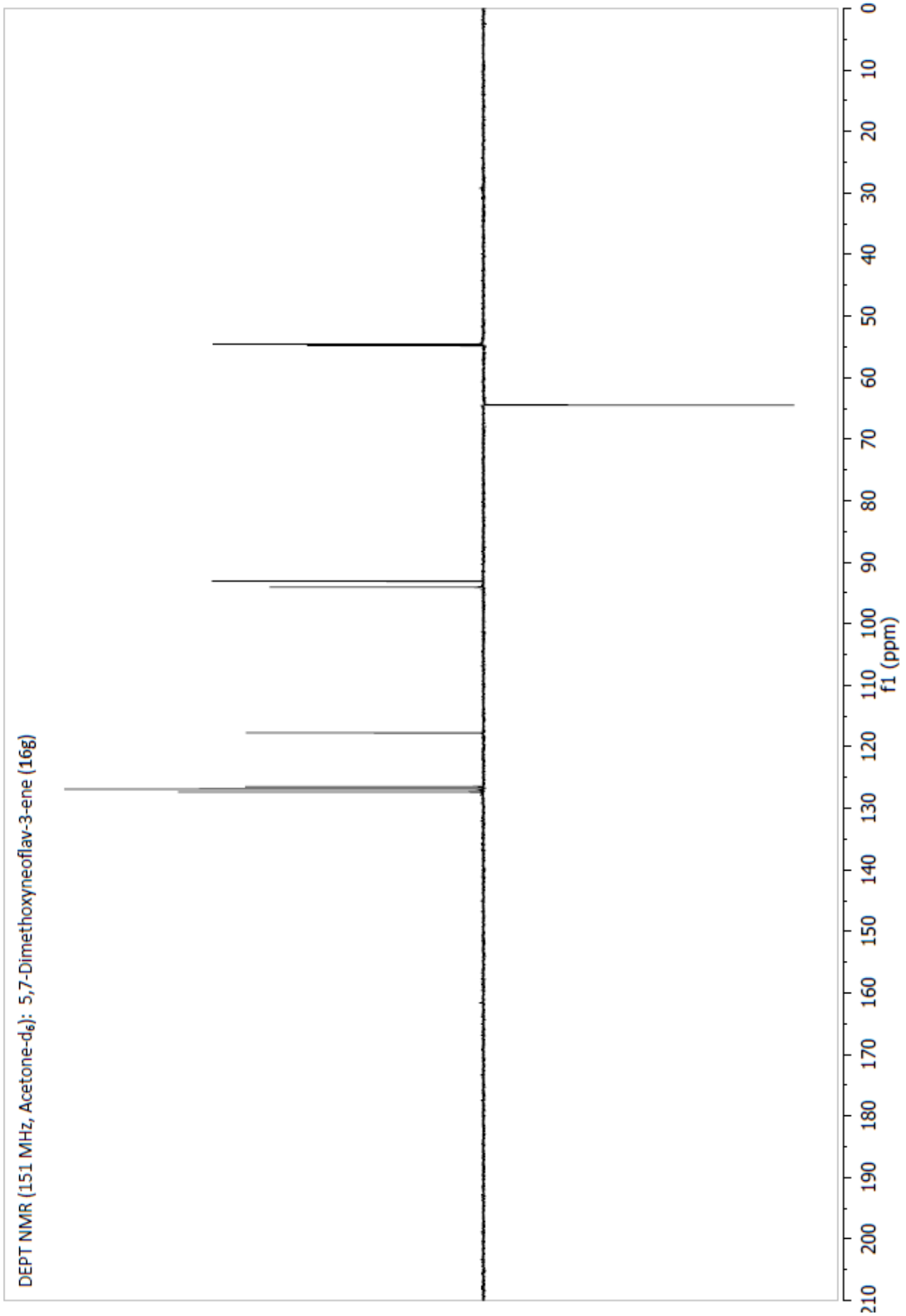

$^{13}$C NMR (151 MHz, Acetone-$d_6$): 5,7-Dimethoxyneoflav-3-ene (16g))

δ 162.51 (C-7), 159.22 (C-8a), 158.63 (C-5), 142.02 (C-1'), 137.47 (C-4), 128.25 (Ar-C), 127.78 (Ar-C), 127.39 (C-4'), 118.65 (C-3), 107.45 (C-4a), 94.98 (C-6/8), 94.02 (C-6/8), 65.38 (C-2), 55.73 (-OMe), 55.50 (-OMe)


HSQC (600 MHz/151 MHz, Acetone-d6): 5,7-Dimethoxyneoflav-3-ene (16g)
f1 (ppm)
60
70
80
90
100
110
120
f2 (ppm)
3.4
3.8
4.2
4.6
5.0
5.4
5.8
6.2
6.6
7.0
7.4



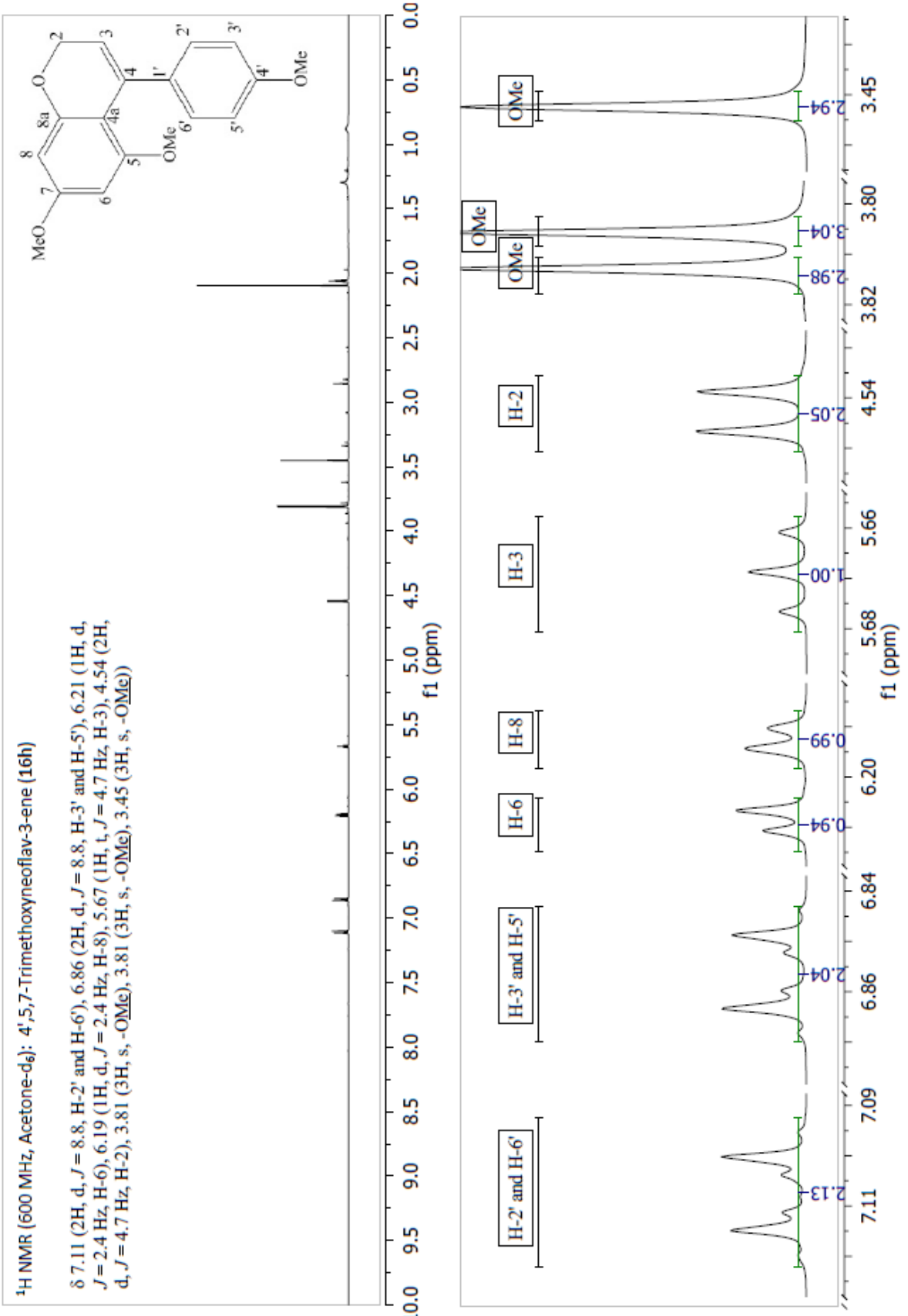

HMBC (600 MHz/151 MHz, Acetone-$d_6$) : 5,7-Dimethoxyneoflav-3-ene (**16g**)

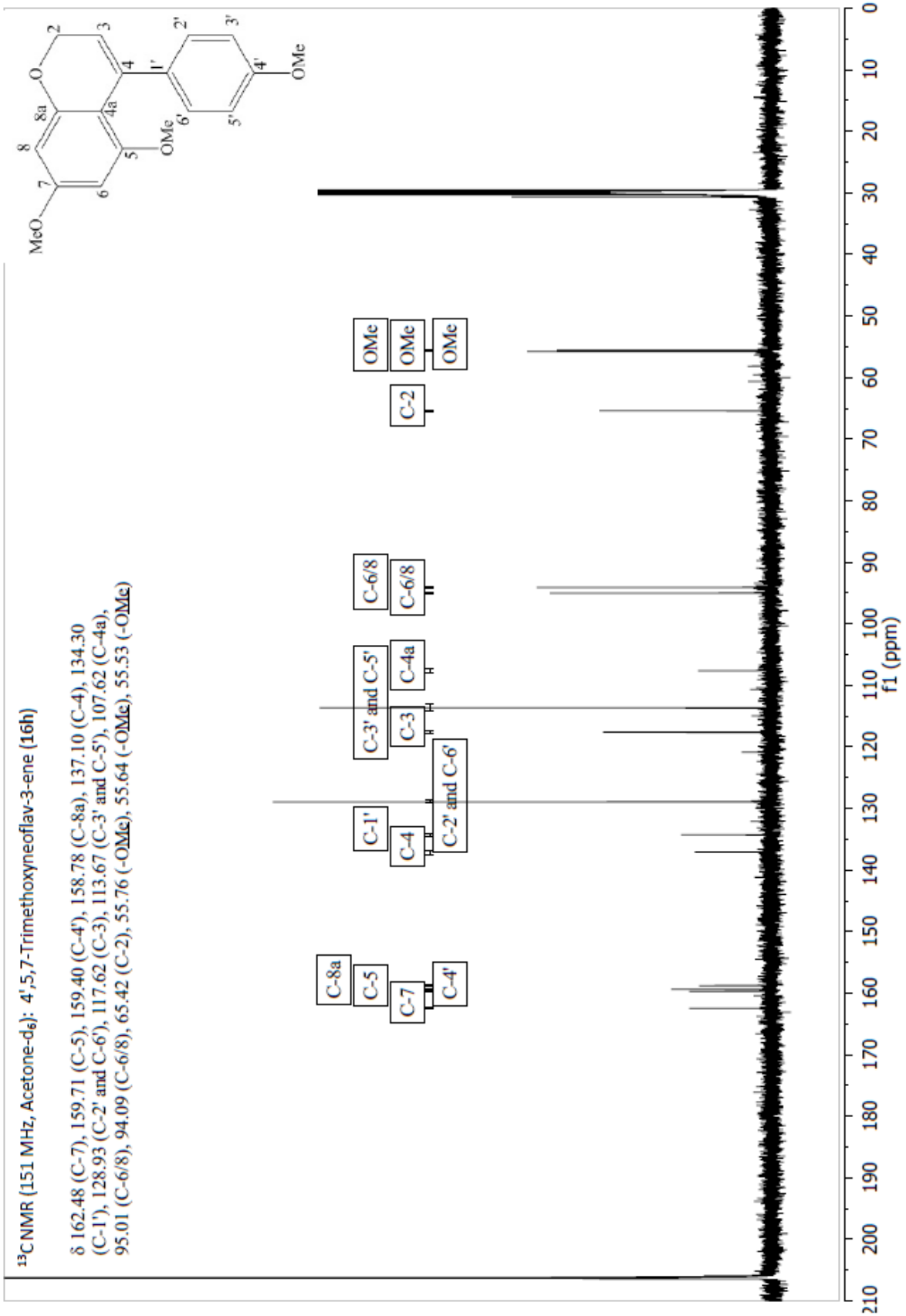

DEPT NMR (151 MHz, Acetone-d6): 5,7-Dimethoxyneoflav-3-ene (16g)
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
210
f1 (ppm)

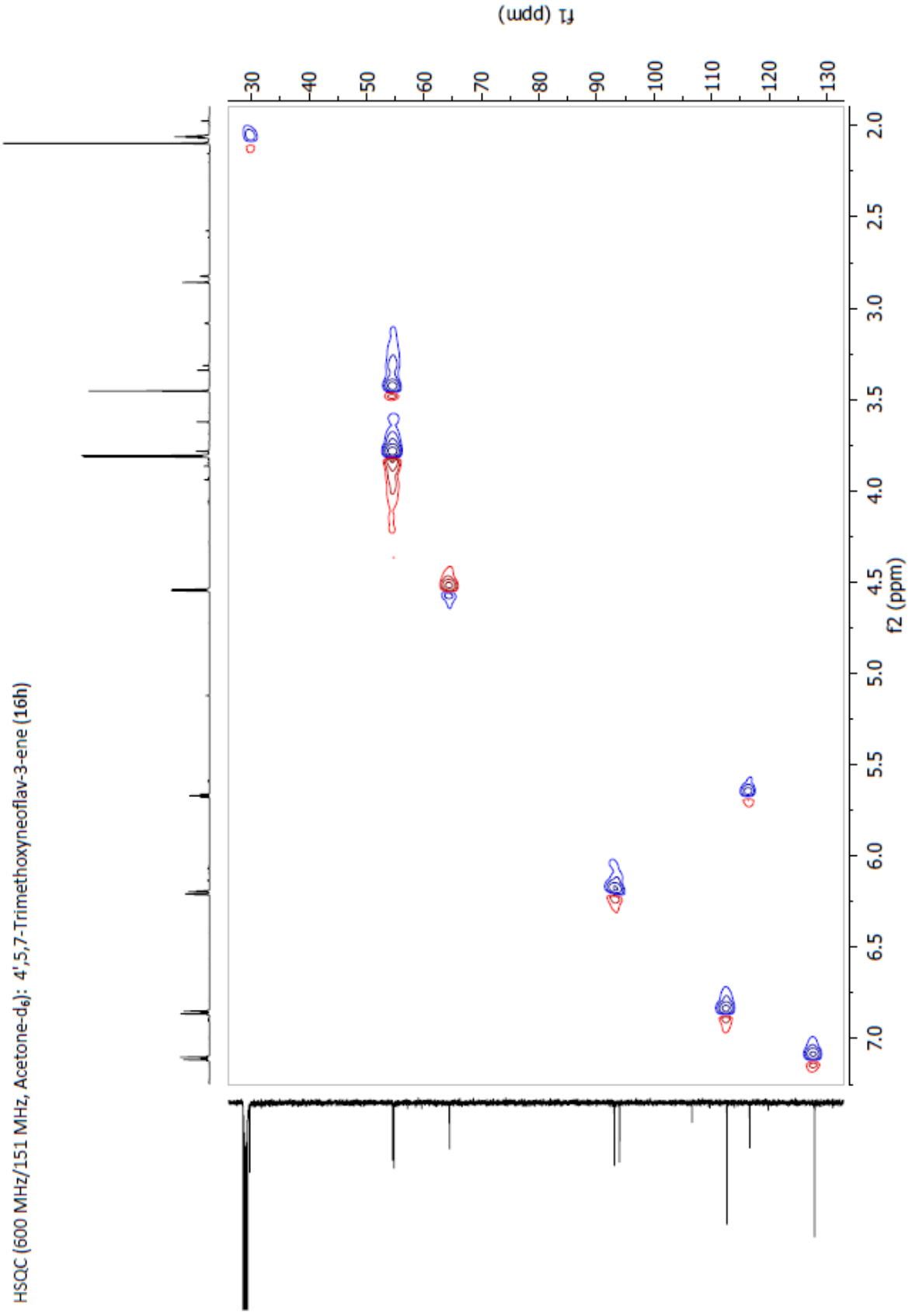
 

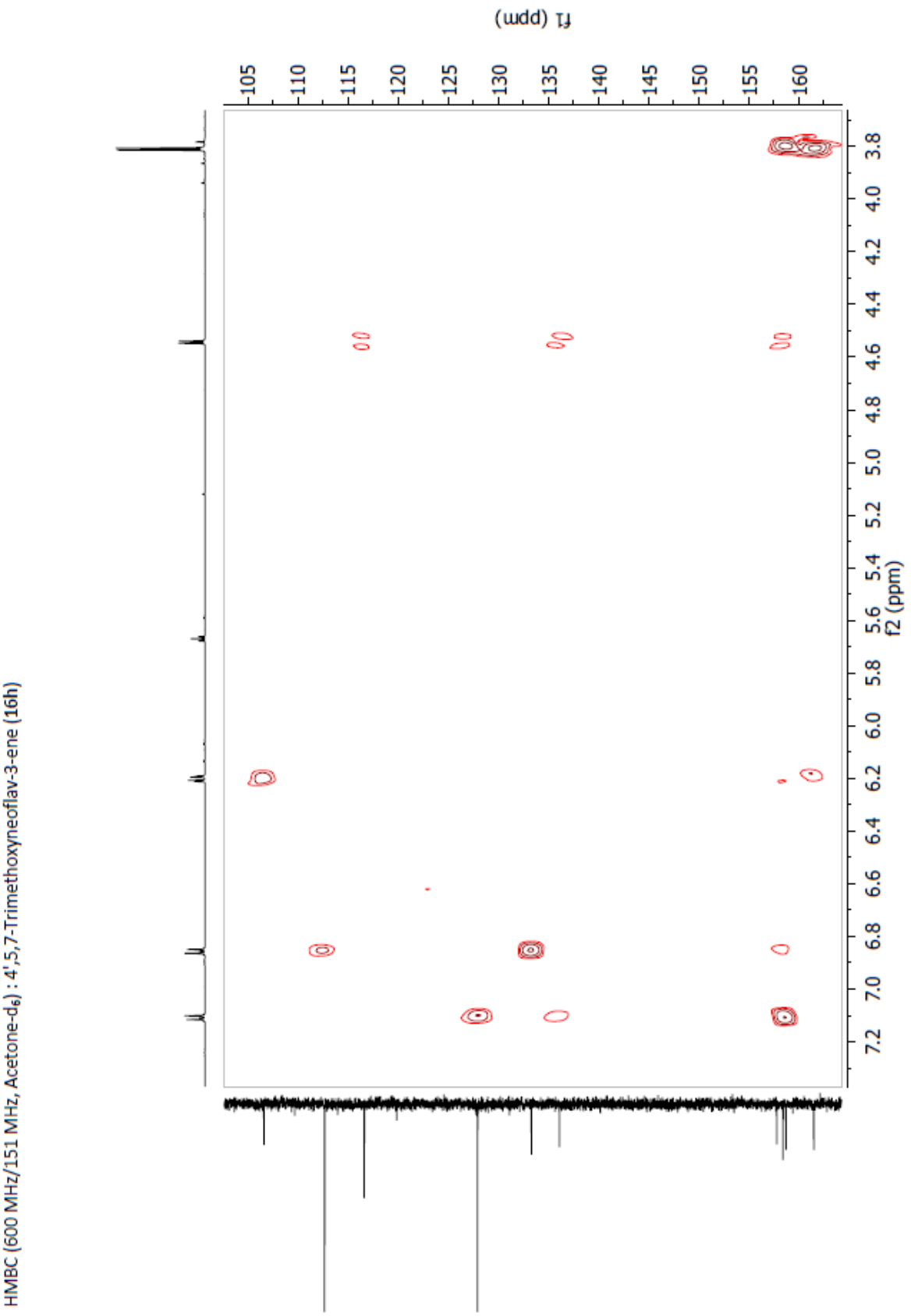
$^1$H NMR (600 MHz, Acetone-$d_6$): 4',5,7-Trimethoxyneoflav-3-ene (**16h**)

δ 7.11 (2H, d, *J* = 8.8, H-2' and H-6'), 6.86 (2H, d, *J* = 8.8, H-3' and H-5'), 6.21 (1H, d, *J* = 2.4 Hz, H-6), 6.19 (1H, d, *J* = 2.4 Hz, H-8), 5.67 (1H, t, *J* = 4.7 Hz, H-3), 4.54 (2H, d, *J* = 4.7 Hz, H-2), 3.81 (3H, s, -OMe), 3.45 (3H, s, -OMe))

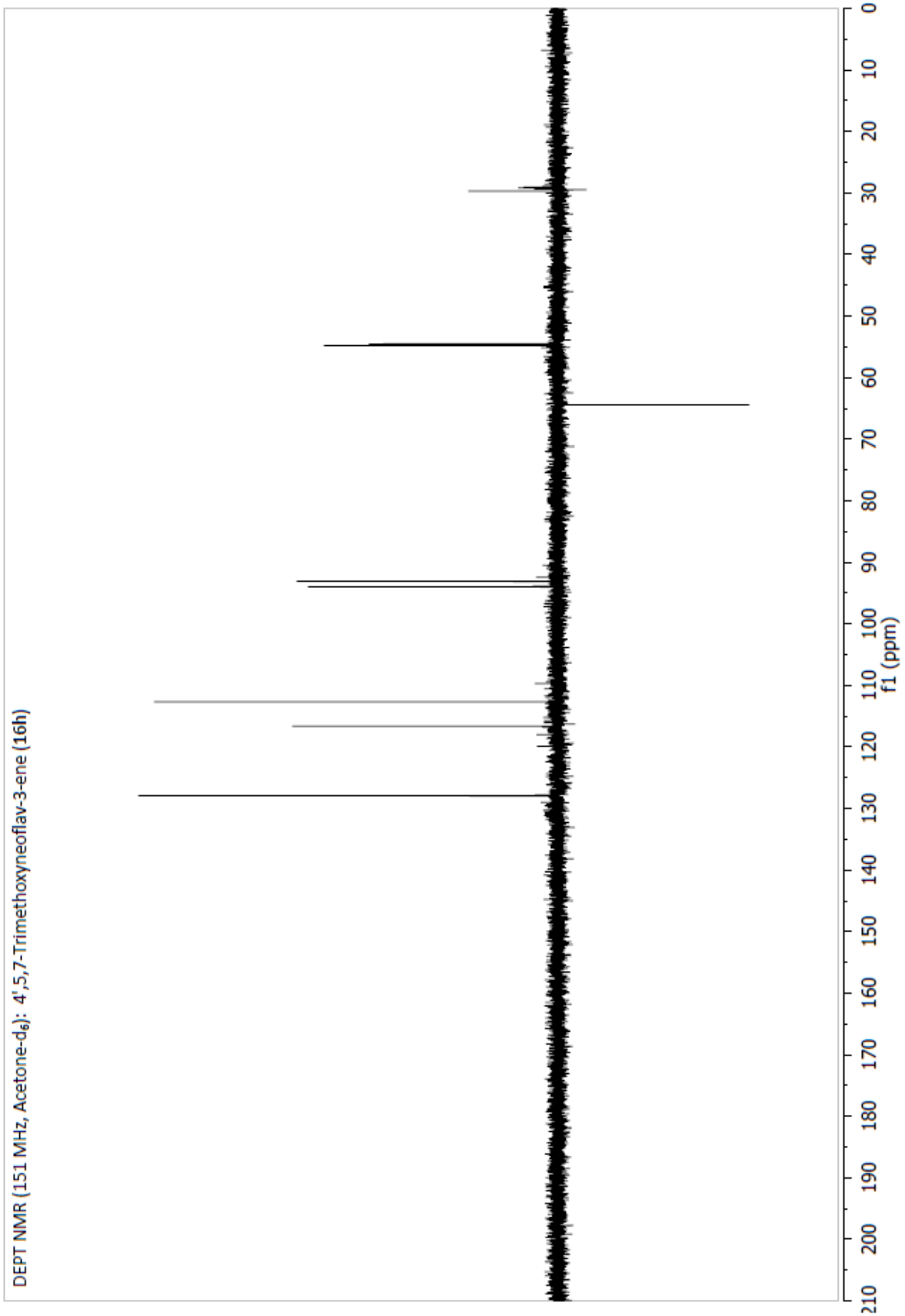


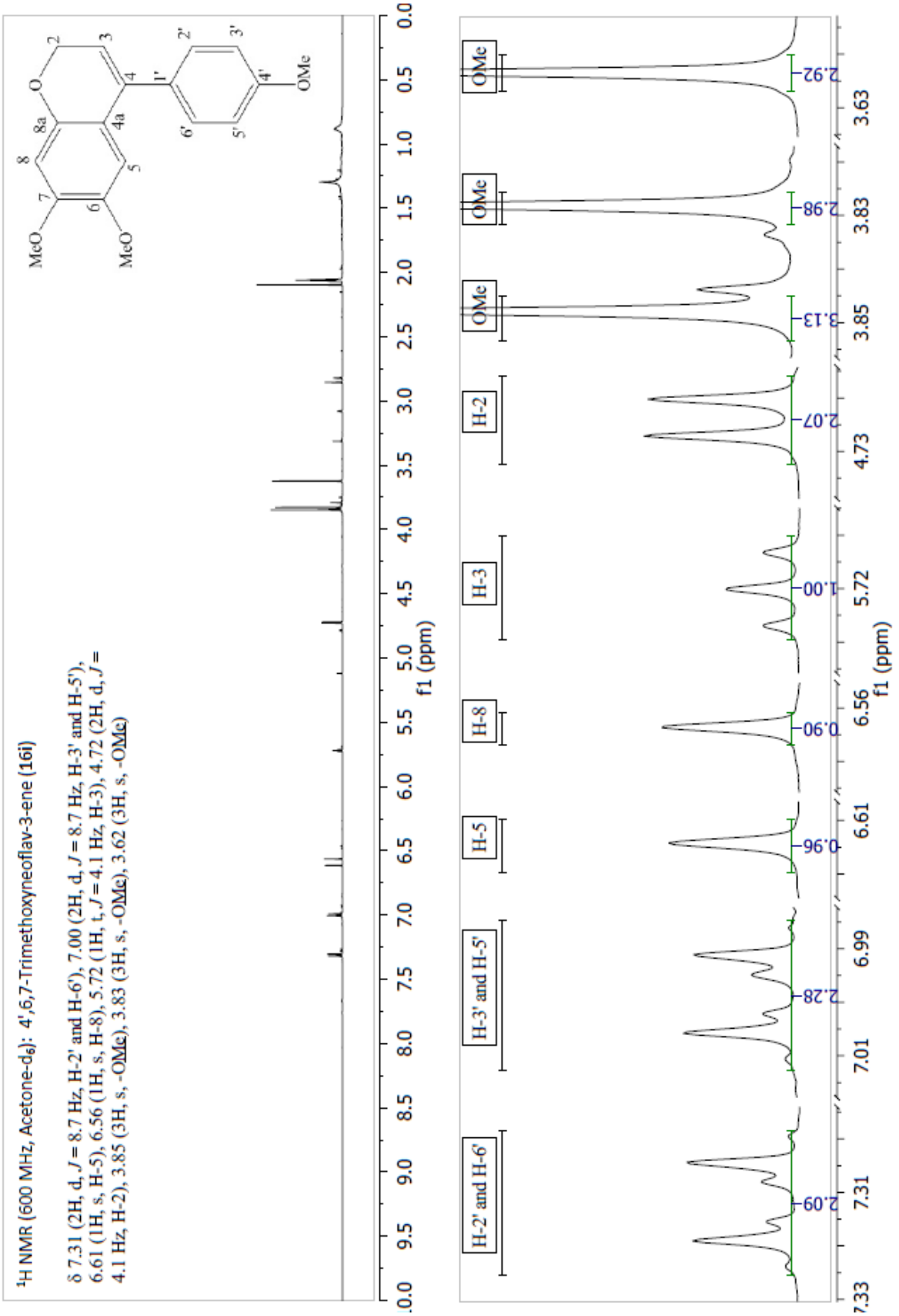

13C NMR (151 MHz, Acetone-d6): 4',5,7-Trimethoxyneoflav-3-ene (16h)
δ 162.48 (C-7), 159.71 (C-5), 159.40 (C-4'), 158.78 (C-8a), 137.10 (C-4), 134.30 (C-1'), 128.93 (C-2' and C-6'), 117.62 (C-3), 113.67 (C-3' and C-5'), 107.62 (C-4a), 95.01 (C-6/8), 94.09 (C-6/8), 65.42 (C-2), 55.76 (-OMe), 55.64 (-OMe), 55.53 (-OMe)
C-8a
C-5
C-7
C-4'
C-1'
C-4
C-2' and C-6'
C-3' and C-5'
C-3
C-4a
C-6/8
C-6/8
C-2
OMe
OMe
OMe
MeO
OMe
OMe
f1 (ppm)

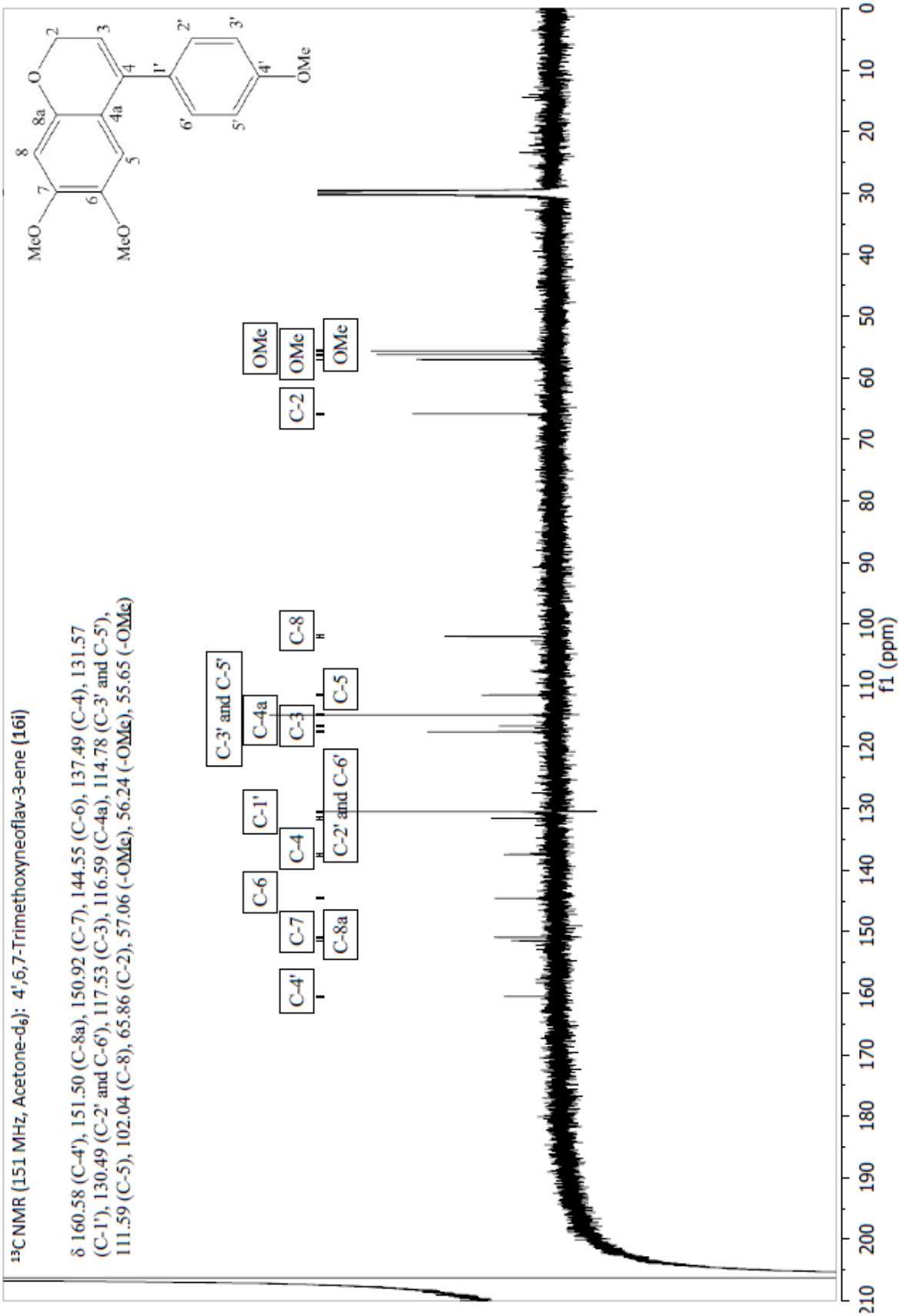

HSQC (600 MHz/151 MHz, Acetone-d6): 4',5,7-Trimethoxyneoflav-3-ene (16h)
f1 (ppm)
f2 (ppm)

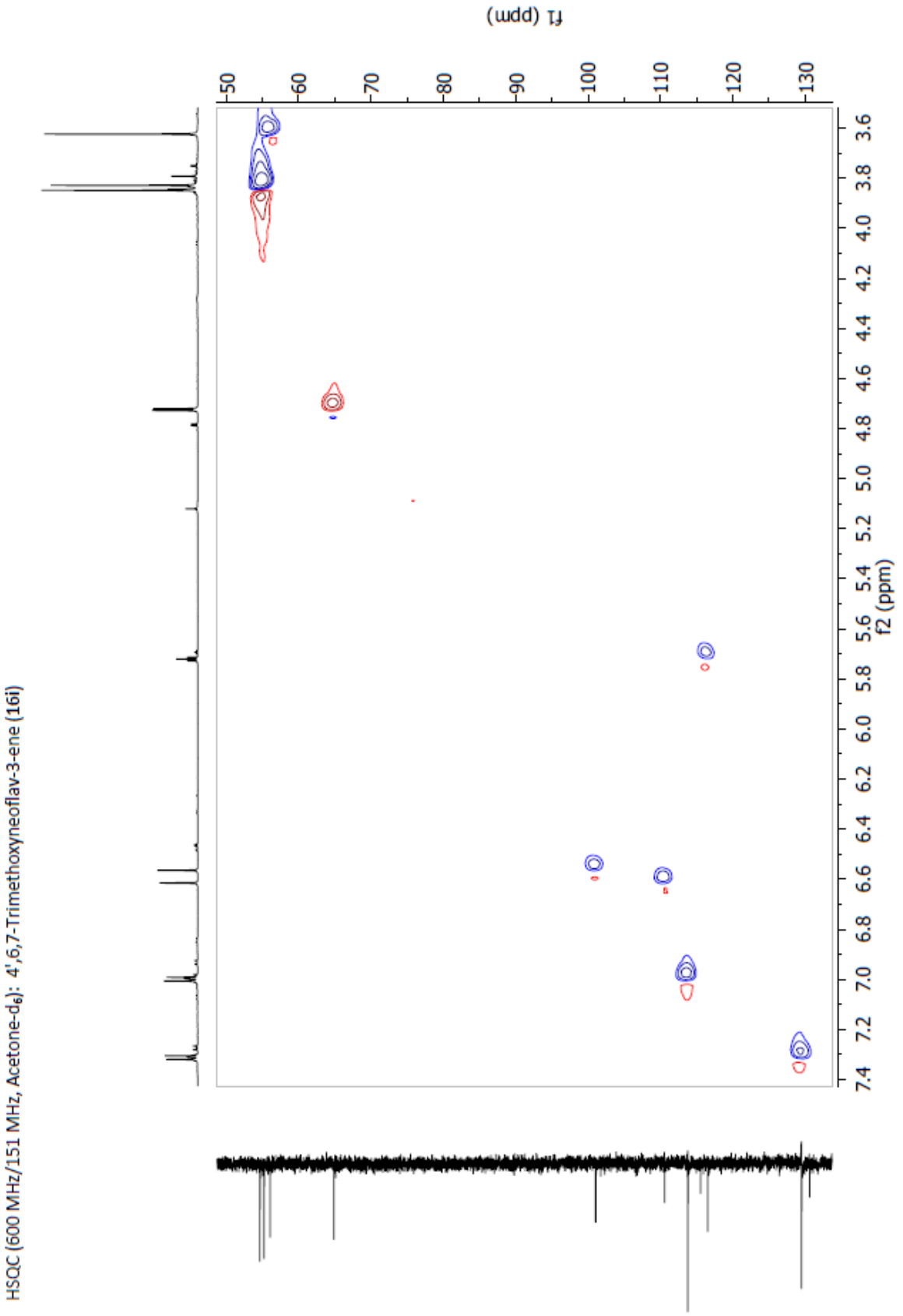



HMBC (600 MHz/151 MHz, Acetone-$d_6$) : 4',5,7-Trimethoxyneoflav-3-ene (**16h**)

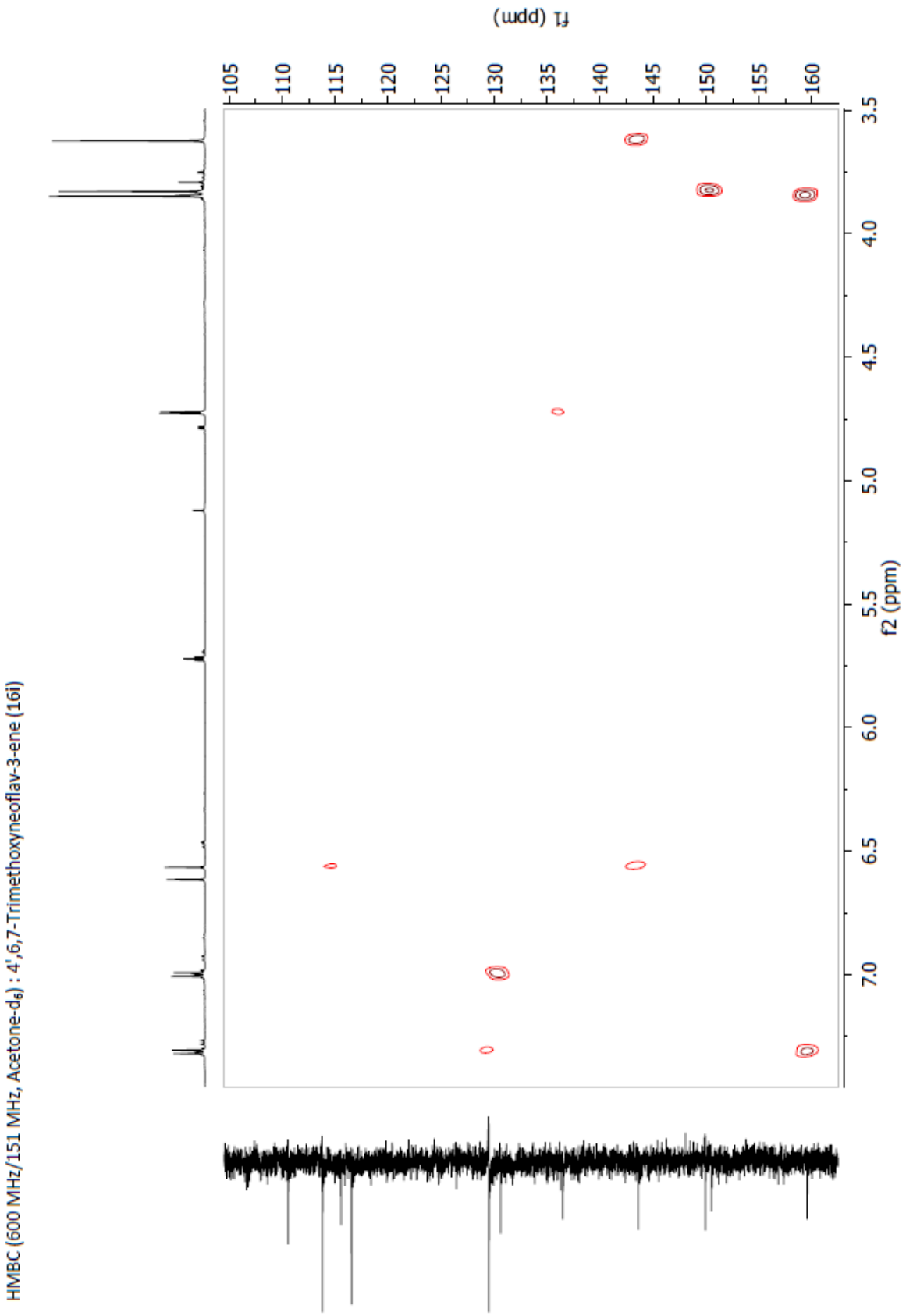

DEPT NMR (151 MHz, Acetone-d6): 4',5,7-Trimethoxyneoflav-3-ene (16h)
f1 (ppm)
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
210


$^1$H NMR (600 MHz, Acetone-$d_6$): 4',6,7-Trimethoxyneoflav-3-ene (16i)
δ 7.31 (2H, d, J = 8.7 Hz, H-2' and H-6'), 7.00 (2H, d, J = 8.7 Hz, H-3' and H-5'), 6.61 (1H, s, H-5), 6.56 (1H, s, H-8), 5.72 (1H, t, J = 4.1 Hz, H-3), 4.72 (2H, d, J = 4.1 Hz, H-2), 3.85 (3H, s, -OMe), 3.83 (3H, s, -OMe), 3.62 (3H, s, -OMe)
MeO
MeO
OMe
f1 (ppm)
H-2' and H-6'
H-3' and H-5'
H-5
H-8
H-3
H-2
OMe
OMe
OMe
2.09
2.28
0.96
0.90
1.00
2.07
3.13
2.98
2.92
f1 (ppm)

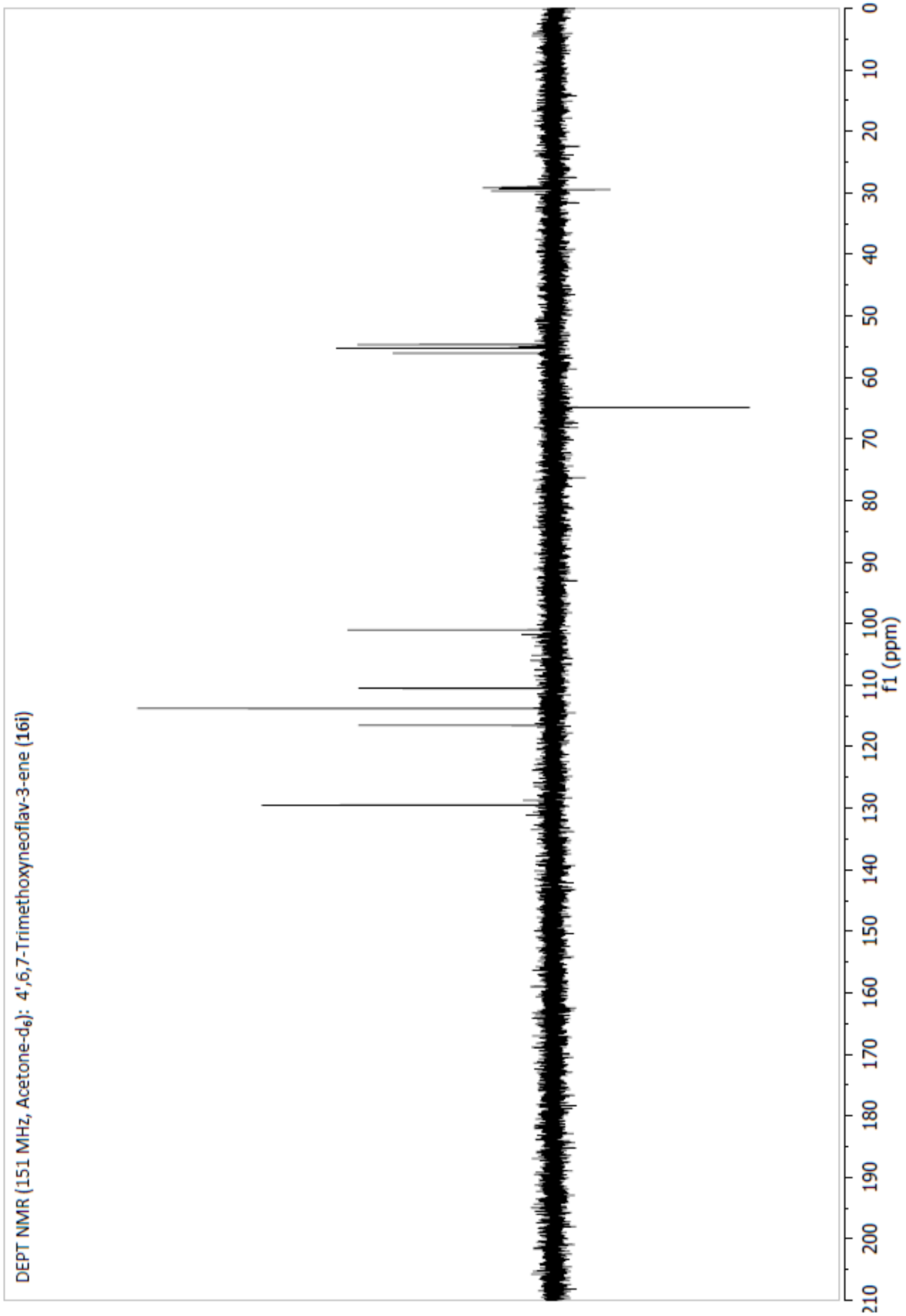

$^{13}$CNMR (151 MHz, Acetone-d$_6$): 4',6,7-Trimethoxyneoflav-3-ene (16i)
δ 160.58 (C-4'), 151.50 (C-8a), 150.92 (C-7), 144.55 (C-6), 137.49 (C-4), 131.57 (C-1'), 130.49 (C-2' and C-6'), 117.53 (C-3), 116.59 (C-4a), 114.78 (C-3' and C-5'), 111.59 (C-5), 102.04 (C-8), 65.86 (C-2), 57.06 (-OMe), 56.24 (-OMe), 55.65 (-OMe)
C-4'
C-7
C-8a
C-6
C-1'
C-4
C-2' and C-6'
C-3' and C-5'
C-4a
C-3
C-5
C-8
C-2
OMe
OMe
OMe
MeO
MeO
OMe
f1 (ppm)

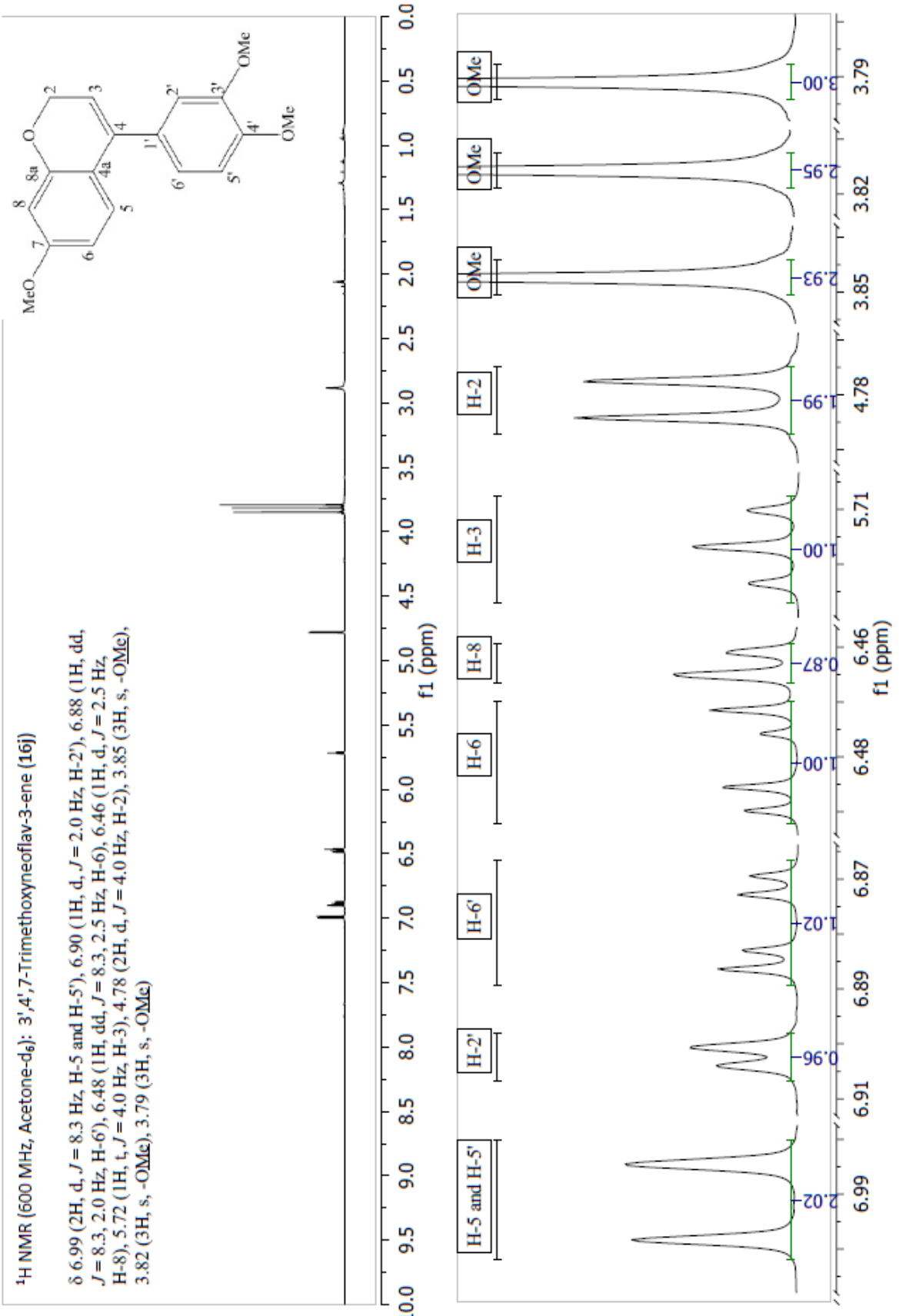



HSQC (600 MHz/151 MHz, Acetone-$d_6$): 4',6,7-Trimethoxyneoflav-3-ene (16i)



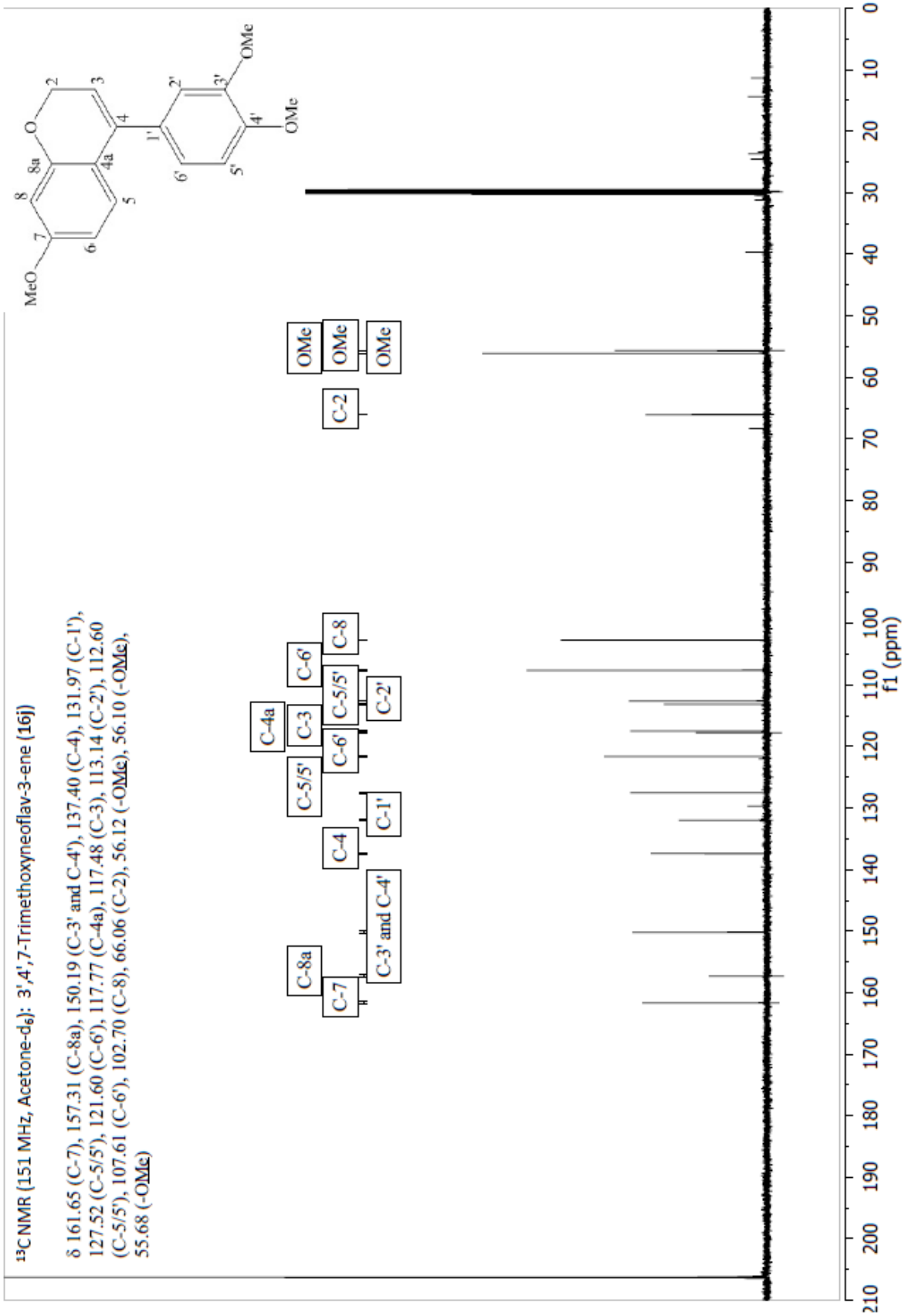

HMBC (600 MHz/151 MHz, Acetone-$d_6$) : 4',6,7-Trimethoxyneoflav-3-ene (16i)

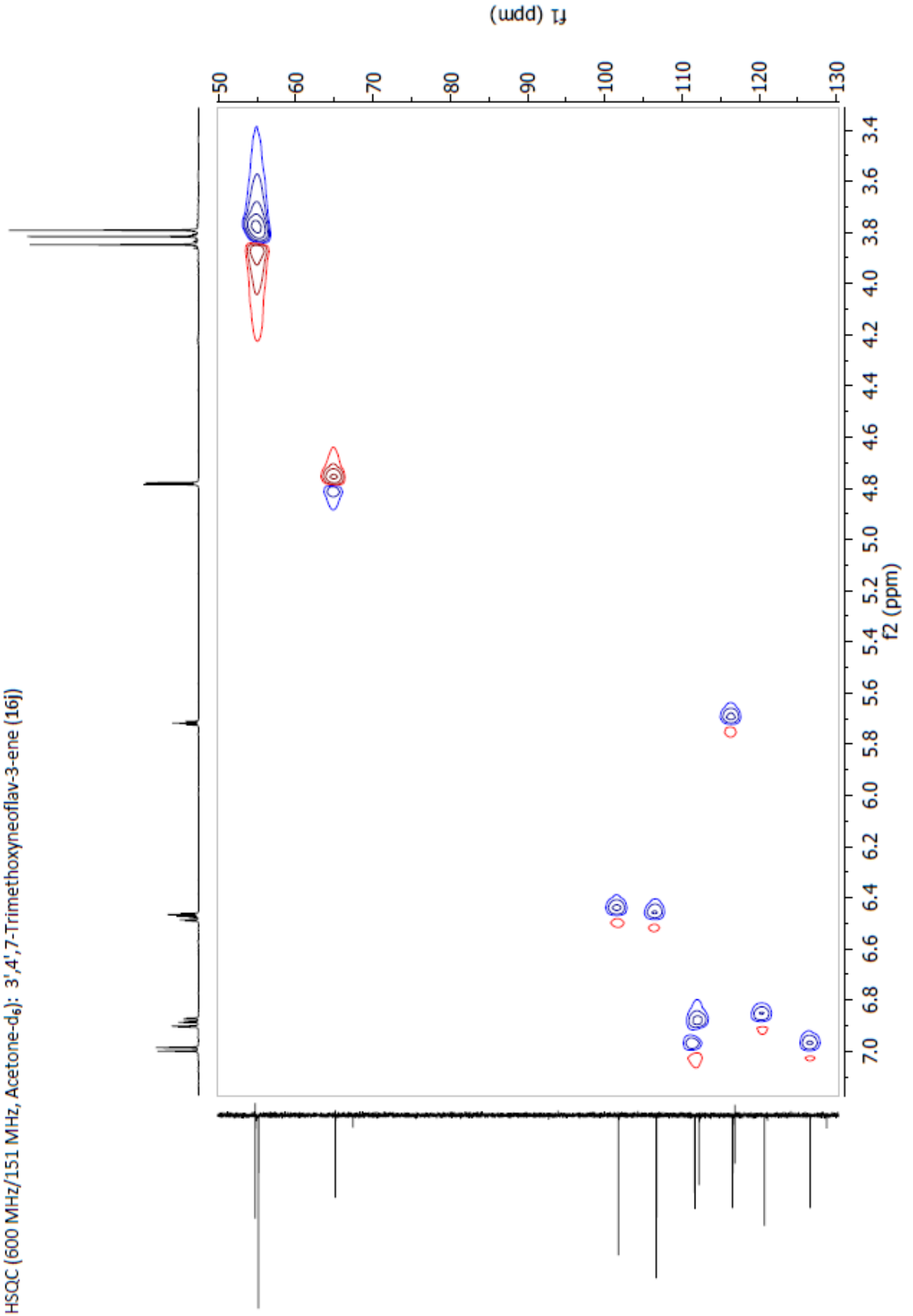

DEPT NMR (151 MHz, Acetone-d6): 4',6,7-Trimethoxyneoflav-3-ene (16i)
f1 (ppm)
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
210



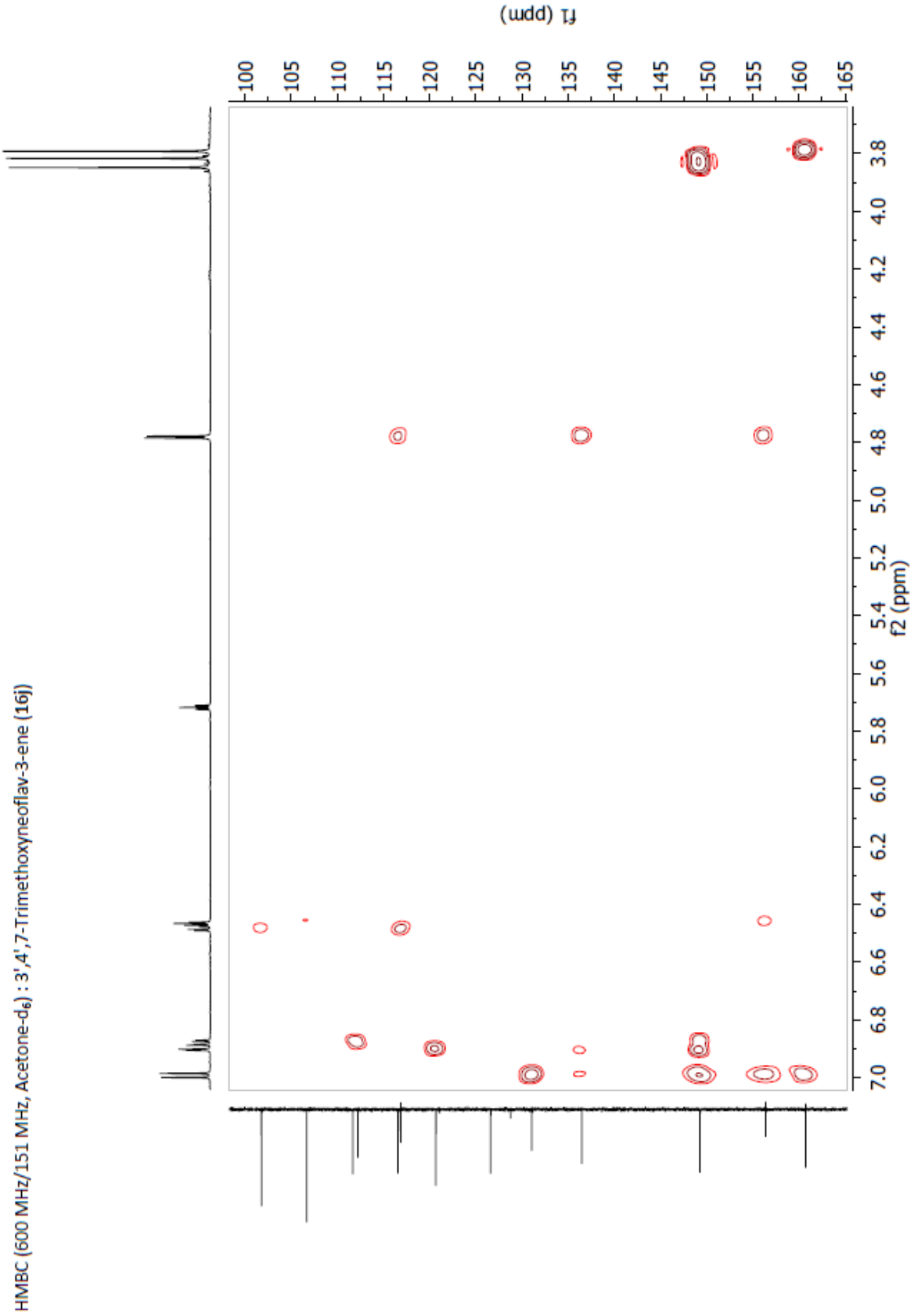

$^1$H NMR (600 MHz, Acetone-$d_6$): 3',4',7-Trimethoxyneoflav-3-ene (**16j**)

δ 6.99 (2H, d, *J* = 8.3 Hz, H-5 and H-5'), 6.90 (1H, d, *J* = 2.0 Hz, H-2'), 6.88 (1H, dd, *J* = 8.3, 2.0 Hz, H-6'), 6.48 (1H, dd, *J* = 8.3, 2.5 Hz, H-6), 6.46 (1H, d, *J* = 2.5 Hz, H-8), 5.72 (1H, t, *J* = 4.0 Hz, H-3), 4.78 (2H, d, *J* = 4.0 Hz, H-2), 3.85 (3H, s, -OMe), 3.82 (3H, s, -OMe), 3.79 (3H, s, -OMe)

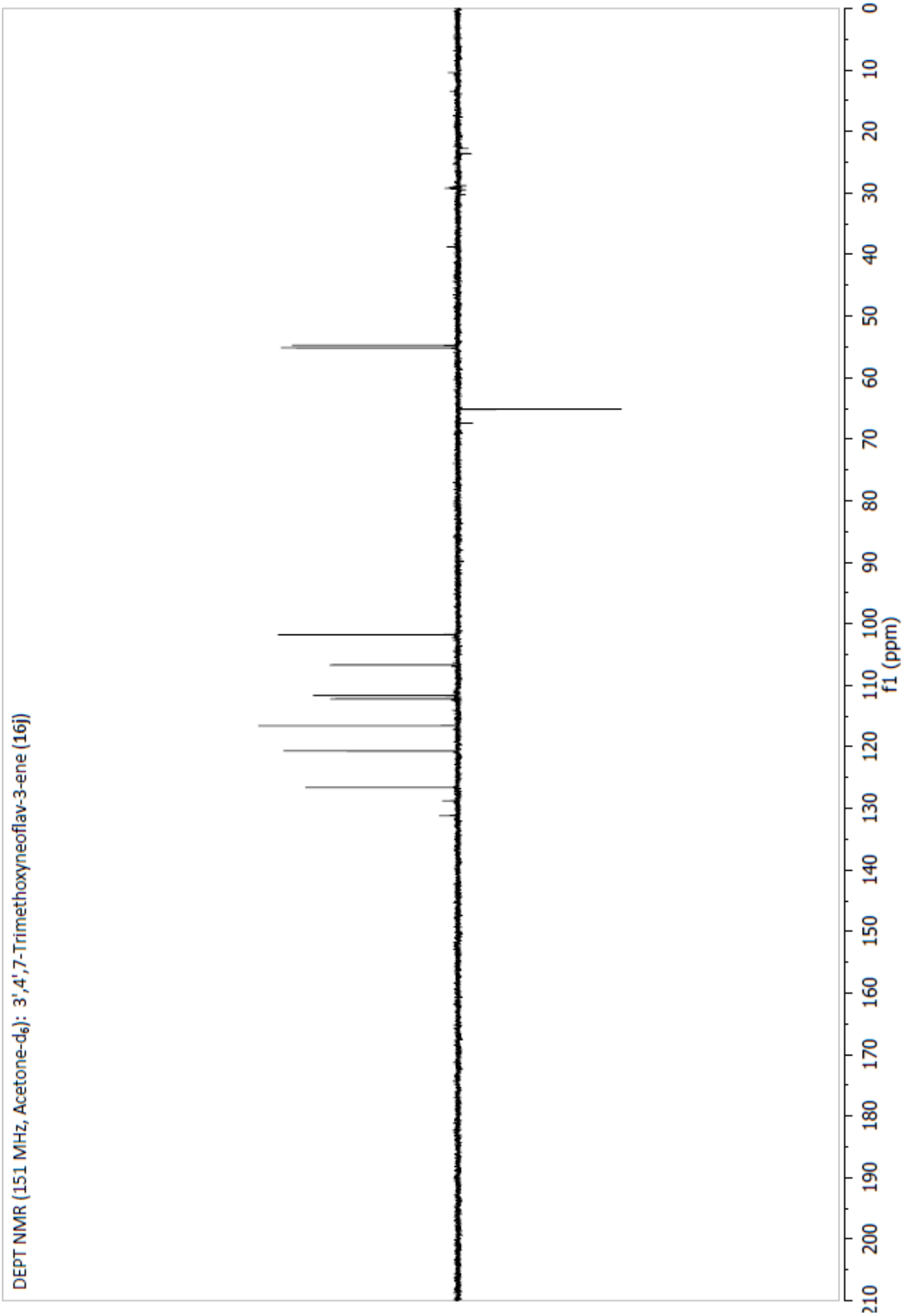

$^{13}$C NMR (151 MHz, Acetone-d$_6$): 3',4',7-Trimethoxyneoflav-3-ene (16j)
δ 161.65 (C-7), 157.31 (C-8a), 150.19 (C-3' and C-4'), 137.40 (C-4), 131.97 (C-1'), 127.52 (C-5/5'), 121.60 (C-6'), 117.77 (C-4a), 117.48 (C-3), 113.14 (C-2'), 112.60 (C-5/5'), 107.61 (C-6'), 102.70 (C-8), 66.06 (C-2), 56.12 (-OMe), 56.10 (-OMe), 55.68 (-OMe)
MeO
OMe
OMe
C-8a
C-7
C-3' and C-4'
C-4
C-1'
C-4a
C-5/5'
C-3
C-6'
C-5/5'
C-6'
C-2'
C-8
C-2
OMe
OMe
OMe
f1 (ppm)

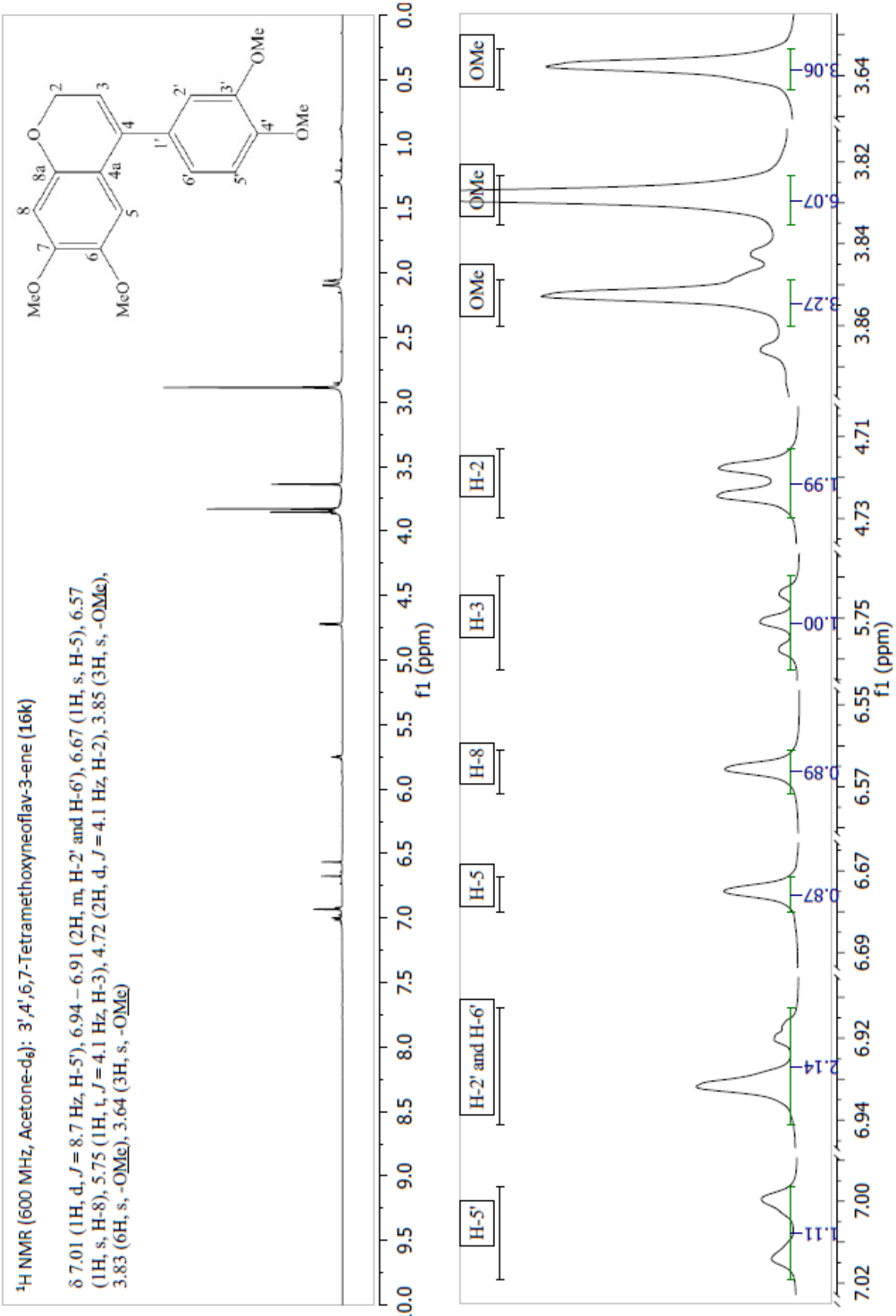


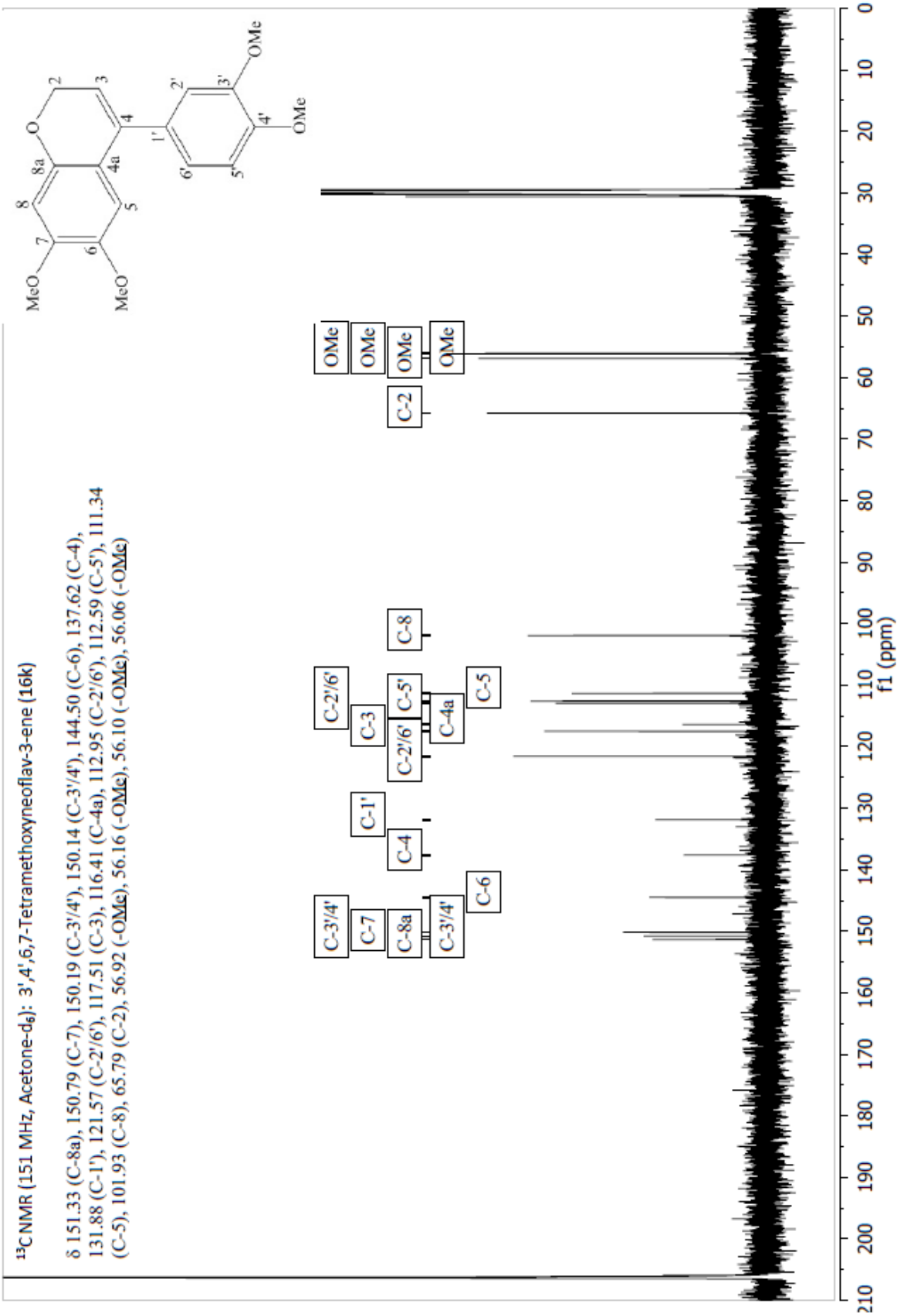

HSQC (600 MHz/151 MHz, Acetone-$d_6$): 3',4',7-Trimethoxyneoflav-3-ene (**16j**)

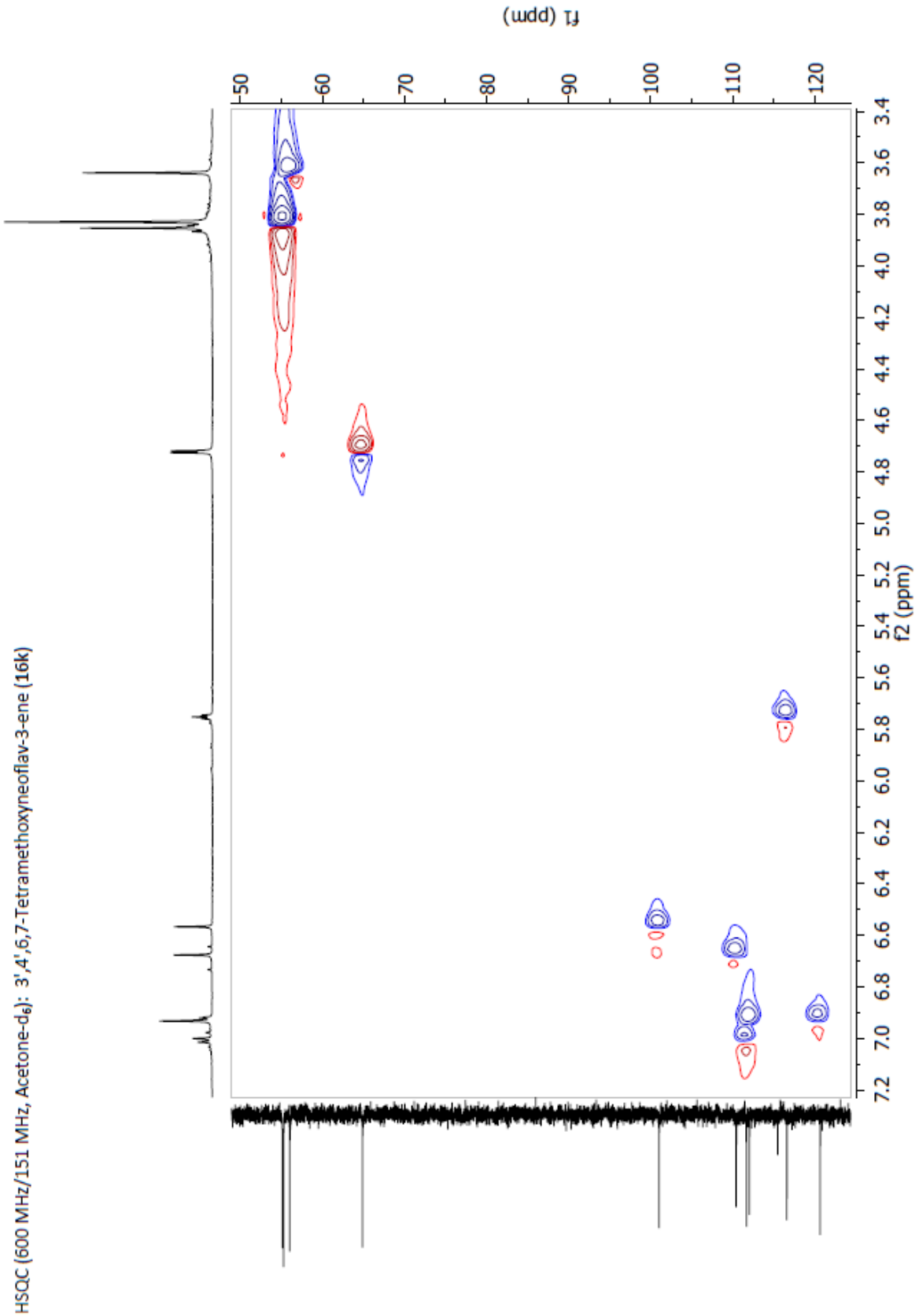


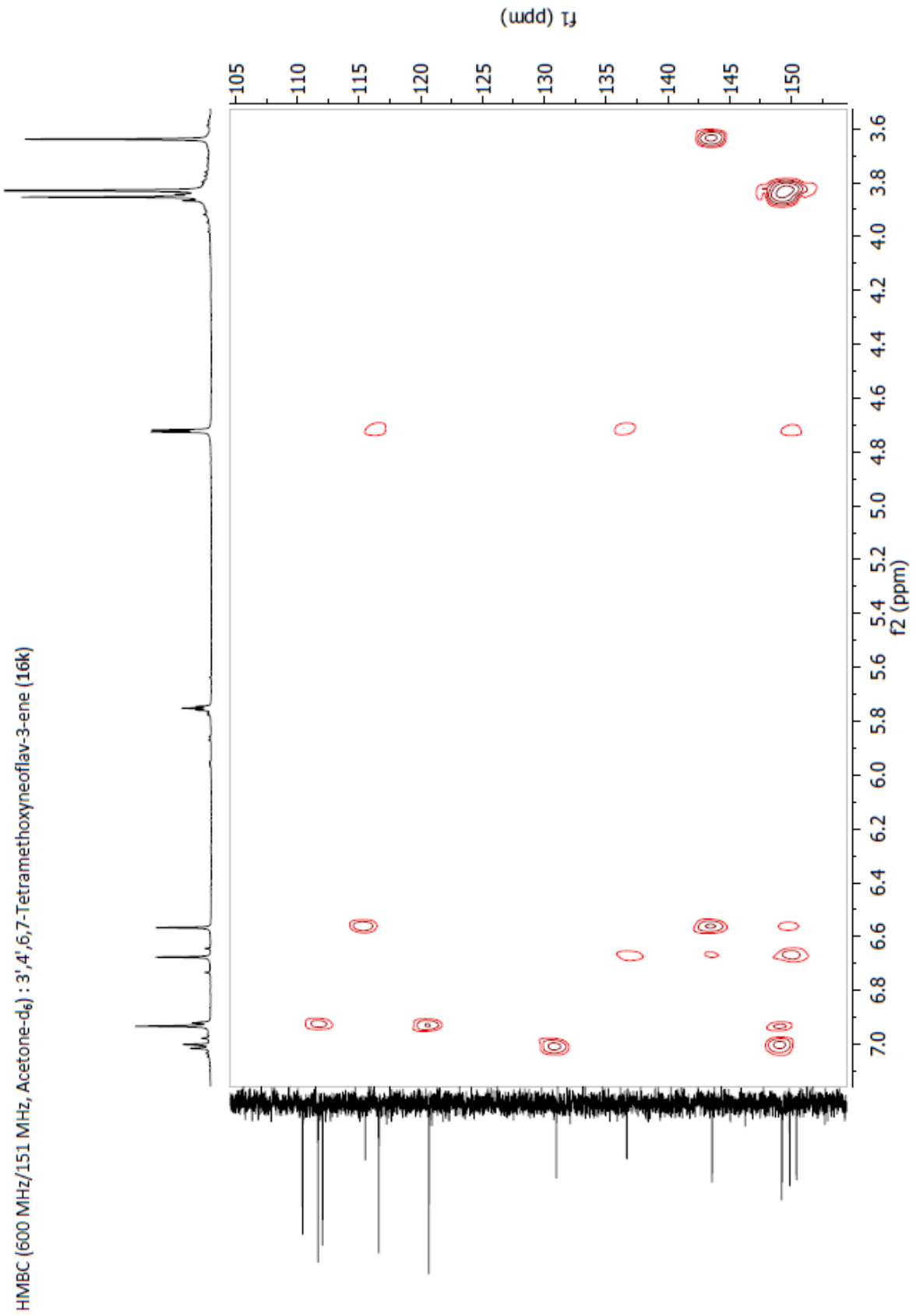

HMBC (600 MHz/151 MHz, Acetone-$d_6$) : 3',4',7-Trimethoxyneoflav-3-ene (**16j**)

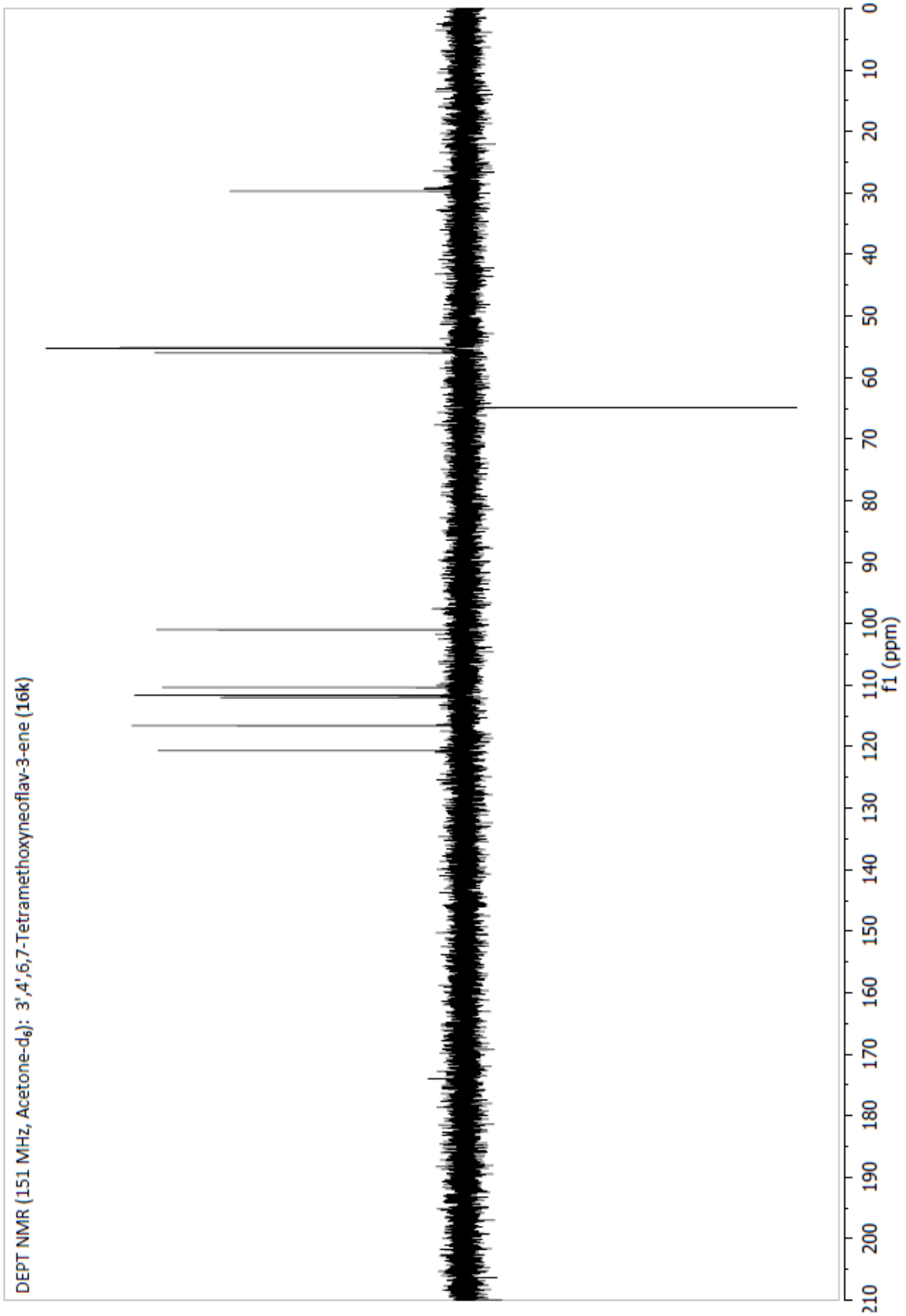

DEPT NMR (151 MHz, Acetone-d6): 3',4',7-Trimethoxyneoflav-3-ene (16j)
f1 (ppm)
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
210


$^1$H NMR (600 MHz, Acetone-$d_6$): 3',4',6,7-Tetramethoxyneoflav-3-ene (16k)
δ 7.01 (1H, d, J = 8.7 Hz, H-5'), 6.94 – 6.91 (2H, m, H-2' and H-6'), 6.67 (1H, s, H-5), 6.57 (1H, s, H-8), 5.75 (1H, t, J = 4.1 Hz, H-3), 4.72 (2H, d, J = 4.1 Hz, H-2), 3.85 (3H, s, -OMe), 3.83 (6H, s, -OMe), 3.64 (3H, s, -OMe)
MeO
MeO
OMe
OMe
f1 (ppm)
H-5'
H-2' and H-6'
H-5
H-8
H-3
H-2
OMe
OMe
OMe
1.11
2.14
0.87
0.89
1.00
1.99
6.07
3.27
3.06
f1 (ppm)


13C NMR (151 MHz, Acetone-d6): 3',4',6,7-Tetramethoxyneoflav-3-ene (16k)
δ 151.33 (C-8a), 150.79 (C-7), 150.19 (C-3'/4'), 150.14 (C-3'/4'), 144.50 (C-6), 137.62 (C-4), 131.88 (C-1'), 121.57 (C-2'/6'), 117.51 (C-3), 116.41 (C-4a), 112.95 (C-2'/6'), 112.59 (C-5'), 111.34 (C-5), 101.93 (C-8), 65.79 (C-2), 56.92 (-OMe), 56.16 (-OMe), 56.10 (-OMe), 56.06 (-OMe)
MeO
MeO
OMe
OMe
C-3'/4'
C-7
C-8a
C-3'/4'
C-6
C-4
C-1'
C-2'/6'
C-3
C-2'/6'
C-5'
C-4a
C-5
C-8
C-2
OMe
OMe
OMe
OMe
f1 (ppm)


HSQC (600 MHz/151 MHz, Acetone-d6): 3',4',6,7-Tetramethoxyneoflav-3-ene (16k)
f1 (ppm)
50
60
70
80
90
100
110
120
f2 (ppm)
3.4
3.6
3.8
4.0
4.2
4.4
4.6
4.8
5.0
5.2
5.4
5.6
5.8
6.0
6.2
6.4
6.6
6.8
7.0
7.2


HMBC (600 MHz/151 MHz, Acetone-d6) : 3',4',6,7-Tetramethoxyneoflav-3-ene (16k)
f1 (ppm)
105
110
115
120
125
130
135
140
145
150
f2 (ppm)
3.6
3.8
4.0
4.2
4.4
4.6
4.8
5.0
5.2
5.4
5.6
5.8
6.0
6.2
6.4
6.6
6.8
7.0


DEPT NMR (151 MHz, Acetone-d6): 3',4',6,7-Tetramethoxyneoflav-3-ene (16k)
f1 (ppm)
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
210