Supplementary Material

Inhibitory effects of a novel chrysin-derivative, CPD 6, on acute and chronic skin inflammation

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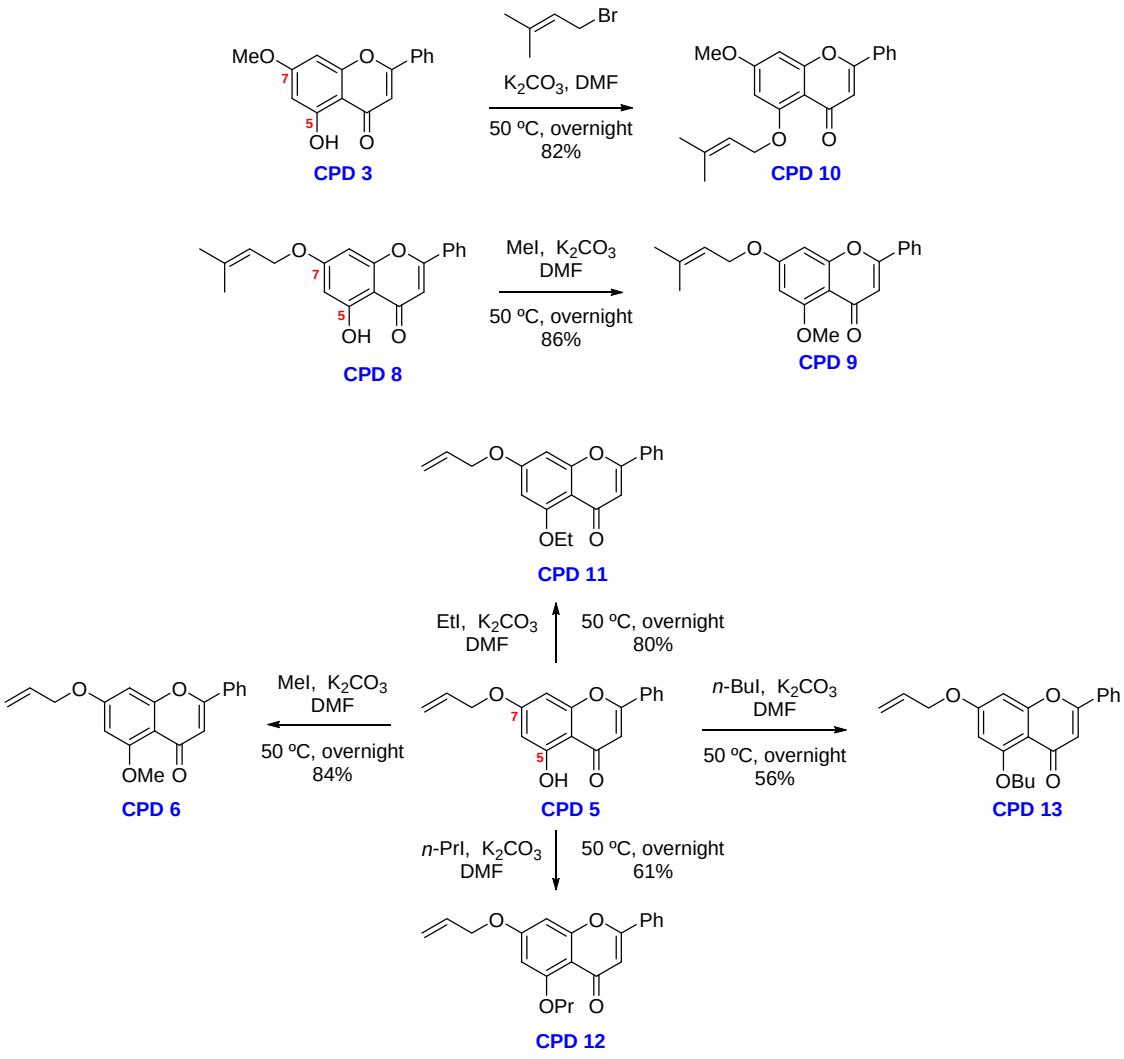
Synthesis of CPD 1-14

CPD 1 (chrysin) was purchased from Sigma-Aldrich (MO, USA). **CPDs 2-8** and **CPD14** were synthesized by according to the literature procedure [1–7]. **CPD 9** and **CPD 10** were prepared from **CPD 8** and **CPD 3** by methylation and prenylation, respectively (Scheme 1). **CPDs 6** and **11–13** were prepared from **CPD 5** by alkylation (methylation, ethylation, *n*-propylation, and *n*-butylation).

Scheme 1. Preparation of **CPDs 6**, **9–13**



CPD-6: m.p 128.1 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.89-7.85 (m, 2 H), 7.52-7.48 (m, 3 H), 6.69 (d, *J* = 0.6 Hz, 1 H), 6.58 (d, *J* = 2.4 Hz, 1 H), 6.43 (d, *J* = 2.4 Hz, 1 H), 6.09 (dddd, *J* = 17.4, 10.8, 5.4, 5.4 Hz, 1 H), 5.48 (dddd, *J* = 17.4, 1.8, 1.8, 1.8 Hz, 1 H), 5.37 (dddd, *J* = 10.8, 1.2, 1.2, 1.2 Hz, 1 H), 4.65 (ddd, *J* = 13.2, 7.8, 4.8 Hz, 2 H), 3.97 (s, 3 H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 177.6, 163.0, 161.0, 160.7, 159.8, 132.1, 131.2, 128.9, 126.0, 118.6, 109.4, 109.1, 96.6, 93.7, 69.3, 56.5.

CPD-9: m.p 121.2 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.90-7.85 (m, 2 H), 7.54-7.46 (m, 3 H), 6.68 (s, 1 H), 6.59 (d, *J* = 2.4 Hz, 1 H), 6.40 (d, *J* = 2.4 Hz, 1 H), 5.53 (dddd, *J* = 7.2, 7.2, 1.2, 1.2 Hz, 1 H), 4.61 (d, *J* = 7.2 Hz, 2 H), 3.95 (s, 3 H), 1.84 (s, 3 H), 1.80 (s, 3 H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 177.6, 163.3, 160.9, 160.6, 159.9, 139.6, 131.6, 131.1, 128.9, 126.0, 118.5, 109.3, 109.1, 96.7, 93.5, 65.3, 56.4, 25.8, 18.3.

CPD-10: m.p 138.3 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.91-7.85 (m, 2 H), 7.54-7.45 (m, 3 H), 6.65 (s, 1 H), 6.56 (dd, *J* = 2.4, 0.6 Hz, 1 H), 6.38 (d, *J* = 2.4 Hz, 1 H), 5.58 (dddd, *J* = 6.6, 6.6, 1.2, 1.2 Hz, 2 H), 4.69 (d, *J* = 6.6 Hz, 2 H), 3.90 (s, 3 H), 1.79 (s, 3 H), 1.76 (s, 3 H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 177.4, 163.8, 160.5, 160.2, 159.9, 137.4, 131.7, 131.1, 128.9, 125.9, 119.5, 109.7, 109.1, 97.6, 92.9, 66.6, 55.7, 25.8, 18.4.

CPD-11: m.p 146.3 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.89-7.86 (m, 2 H), 7.52-7.47 (m, 3 H), 6.65 (s, 1 H), 6.56 (d, *J* = 2.4 Hz, 1 H), 6.41 (d, *J* = 2.4 Hz, 1 H), 6.08 (dddd, *J* = 17.4, 10.8, 5.4, 5.4 Hz, 1 H), 5.47 (dddd, *J* = 17.4, 1.8, 1.8, 1.8 Hz, 1 H), 5.37 (dddd, *J* = 10.8, 1.2, 1.2, 1.2 Hz, 1 H), 4.63 (ddd, *J* = 5.4, 1.8, 1.8 Hz, 2 H), 4.16 (ddd, *J* = 7.2, 7.2, 7.2 Hz, 2 H), 1.56 (dd, *J* = 7.2, 7.2 Hz, 3 H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 177.5, 162.9, 160.5, 160.3, 159.8, 132.2, 131.7, 131.1, 128.9, 126.0, 118.5, 109.6, 109.1, 97.5, 93.6, 69.2, 65.0, 14.5.

CPD-12: mp 112.6 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.89-7.85 (m, 2 H), 7.53-7.46 (m, 3 H), 6.63 (s, 1 H), 6.55 (d, *J* = 2.4 Hz, 1 H), 6.40 (d, *J* = 2.4 Hz, 1 H), 6.08 (dddd, *J* = 17.4, 10.8, 5.4, 5.4 Hz, 1 H), 5.47 (dddd, *J* = 17.4, 1.8, 1.8, 1.8 Hz, 1 H), 5.36 (dddd, *J* = 10.8, 1.2, 1.2, 1.2 Hz, 1 H), 4.63 (ddd, *J* = 5.4, 1.8, 1.8 Hz, 2 H), 4.03 (dd, *J* = 6.6, 6.6 Hz, 2 H), 1.96 (ddddd, *J* = 7.2, 7.2, 7.2, 7.2, 7.2 Hz, 2 H), 1.13 (dd, *J* = 7.2, 7.2 Hz, 3 H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 177.4, 162.9, 160.5, 160.5, 159.8, 132.2, 131.7, 131.1, 128.9, 126.0, 118.5, 109.7, 109.2, 97.4, 93.5, 70.9, 69.2, 22.3, 10.5.

CPD-13: mp 117.9 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.91-7.84 (m, 2 H), 7.54-7.46 (m, 3 H), 6.62 (s, 1 H), 6.55 (d, *J* = 2.4 Hz, 1 H), 6.40 (d, *J* = 2.4 Hz, 1 H), 6.08 (dddd, *J* = 17.4, 10.2, 6.0, 6.0 Hz, 1 H), 5.47 (dddd, *J* = 17.4, 1.8, 1.8, 1.8 Hz, 1 H), 5.36 (dddd, *J* = 10.8, 1.2, 1.2, 1.2 Hz, 1 H), 4.63 (ddd, *J* = 5.4, 1.8, 1.8 Hz, 2 H), 4.07 (dd, *J* = 6.6, 6.6 Hz, 2 H), 1.97-1.87 (m, 2 H), 1.64-1.56 (m, 2 H), 1.00 (dd, *J* = 7.2, 7.2 Hz, 3 H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 177.4, 162.9, 160.6, 160.5, 159.8, 132.2, 131.7, 131.1, 128.9, 126.0, 118.5, 109.7, 109.2, 97.4, 93.5, 69.2, 30.9, 19.2, 13.8.

References

1. For **CPD 2**: Daskiewicz, J.B.; Depeint, F.; Viornery, L.; Bayet, C.; Comte-Sarrazin, G.; Comte, G.; Gee, J.M.; Johnson, I.T.; Ndjoko, K.; Hostettmann, K.; Barron, D. Effects of Flavonoids on Cell Proliferation and Caspase Activation in a Human Colonic Cell Line HT29: An SAR Study. *J. Med. Chem.* **2005**, *48*, 2790–2804.

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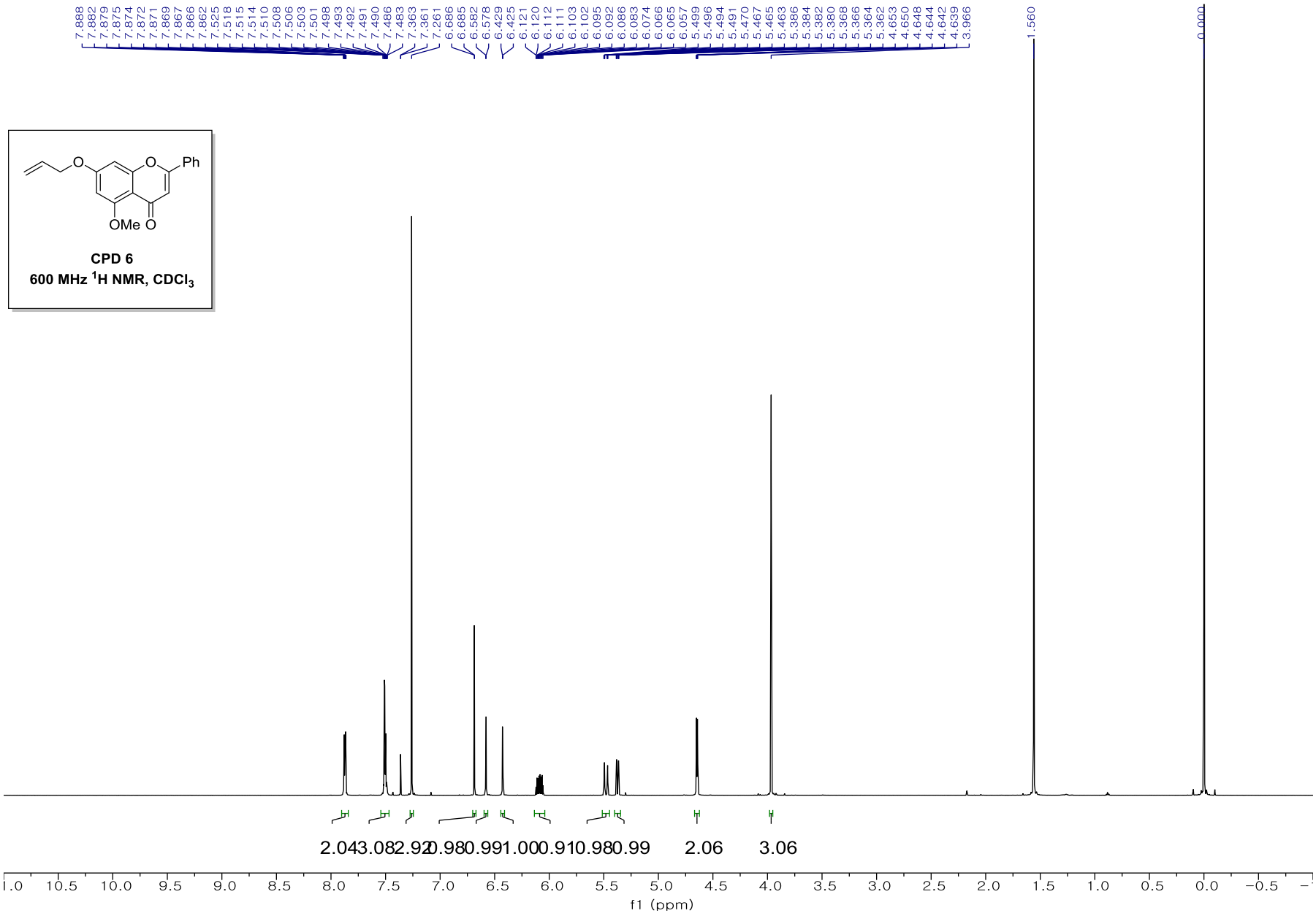
6. For **CPD 7**: Khanna, R. N.; Seshadri, T. R. Synthesis of isomers of kanjone. *Indian. J. Chem.*, **1963**, *1*, 385–387.

7. For **CPD 8**: a) Hwang, S. H.; Kim, H. Y.; Zuo, G.; Wang, Z.; Lee, J.-Y.; Lim, S. S. Anti-glycation, Carbonyl Trapping and Anti-inflammatory Activities of Chrysin Derivatives. *Molecules* **2018**, *23*, 1752. b) Wang, S.H.; Chen, C.H.; Lo, C.Y.; Feng, J.Z.; Lin, H.J.; Chang, P.Y.; Yang, L. L.; Chen, L.G.; Liu, Y. W.; Kuo, C. D.; Wu, J.Y. Synthesis and biological evaluation of novel 7-O-lipophilic substituted baicalein derivatives as potential anticancer agents. *Med. Chem. Comm.* **2015**, *6*, 1864–1873.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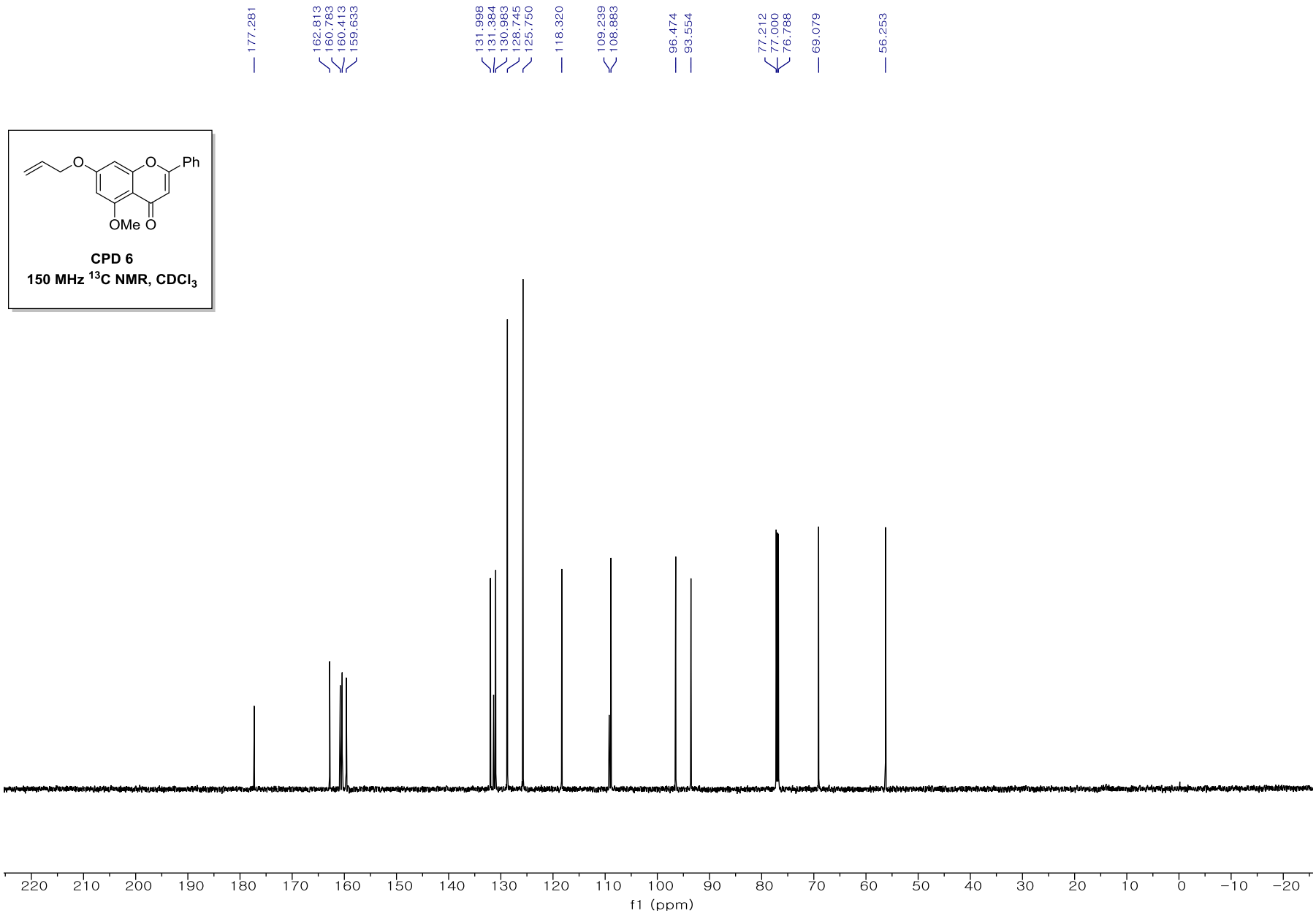
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77.000
76.788
69.079
56.253
O
O
Ph
OMe O
CPD 6
150 MHz 13C NMR, CDCl3
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10 −20
f1 (ppm)

State Parameter Editor

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Entrance Potential (EP):		10.0
Q1 Resolution:	Unit	
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CEM (CEM):	2500.0	

Mass Spectrometer Method Properties

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Scans in Period:	594
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Experiments in Period:	1

Period 1 Experiment 1:

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Parameter Table(Period 1 Experiment 1):

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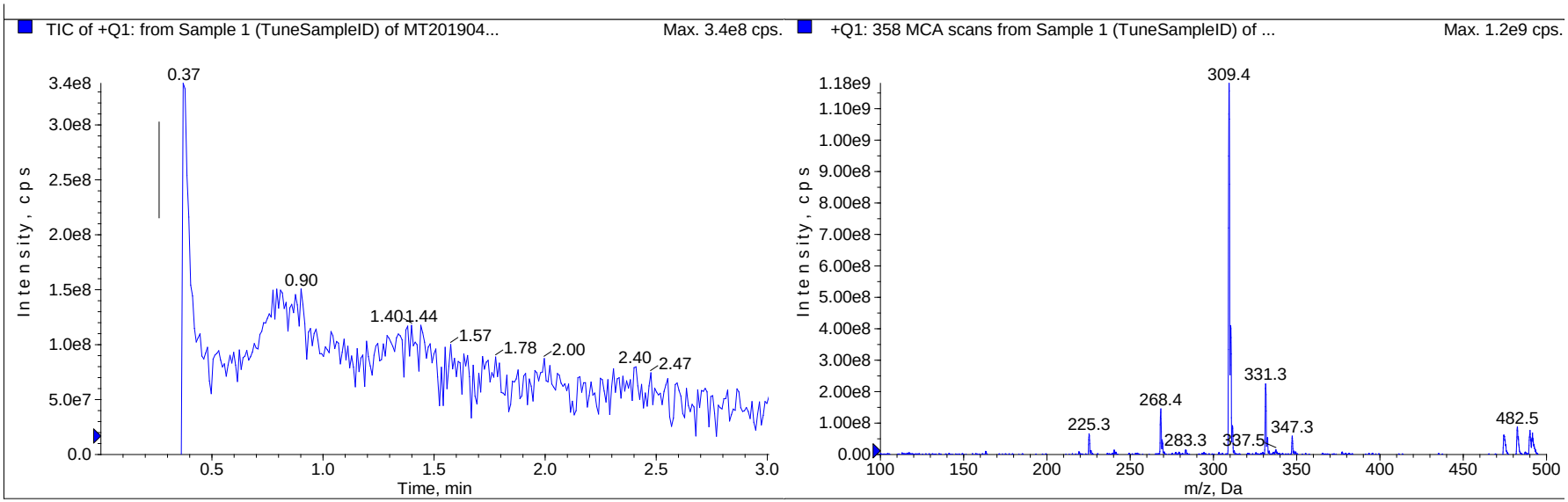
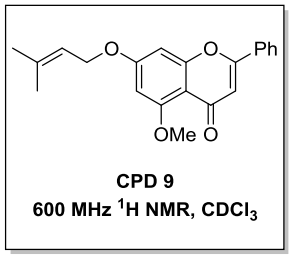
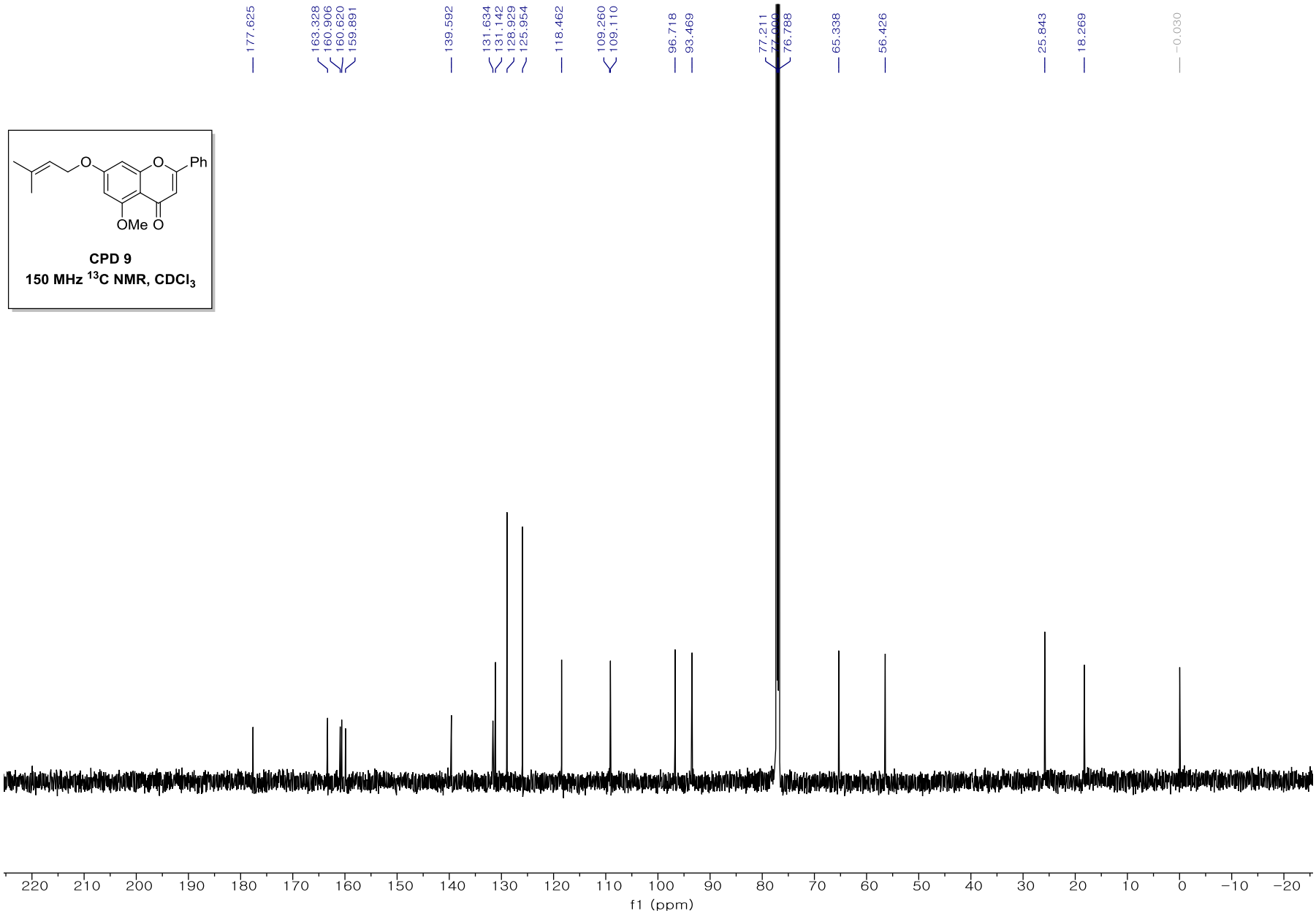




CPD 9
600 MHz ^{1}H NMR, $CDCl_3$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Ph
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150 MHz 13C NMR, CDCl3
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State Parameter Editor

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Interface Heater (ihe):	On	
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Entrance Potential (EP):		10.0
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Mass Spectrometer Method Properties

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Scans in Period:	356
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Experiments in Period:	1

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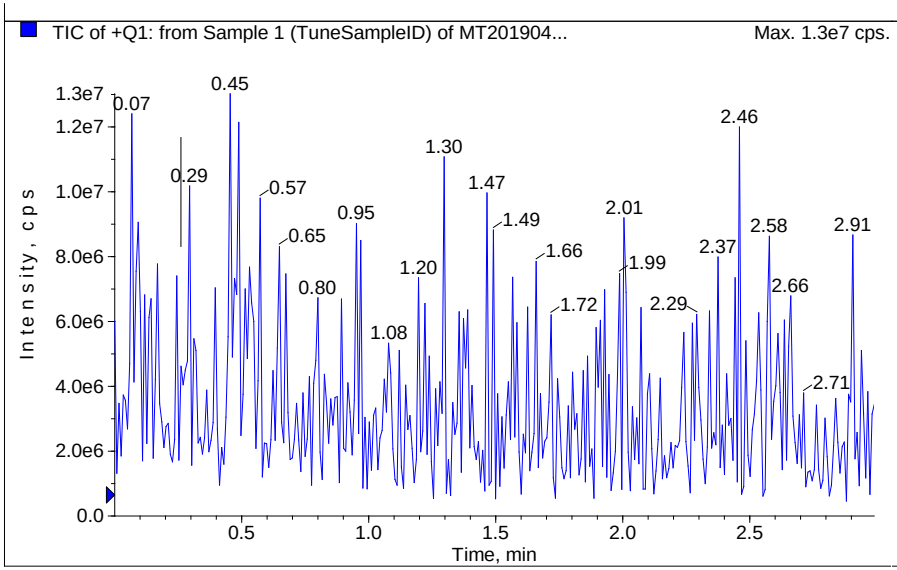

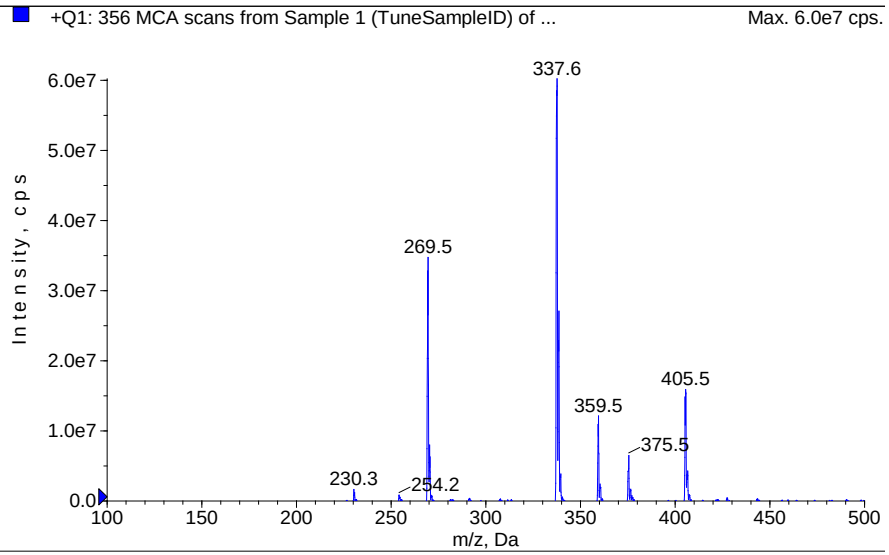

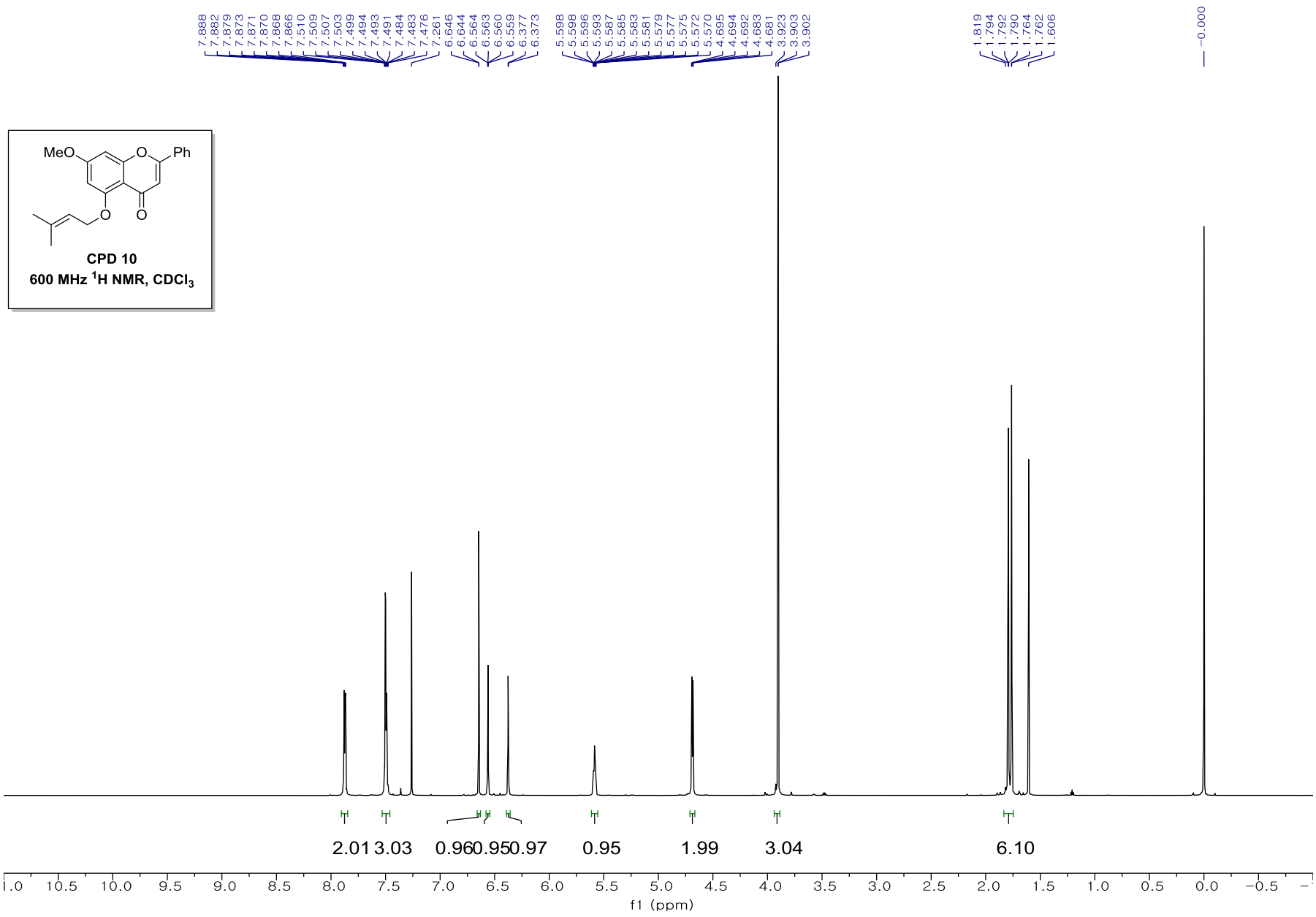
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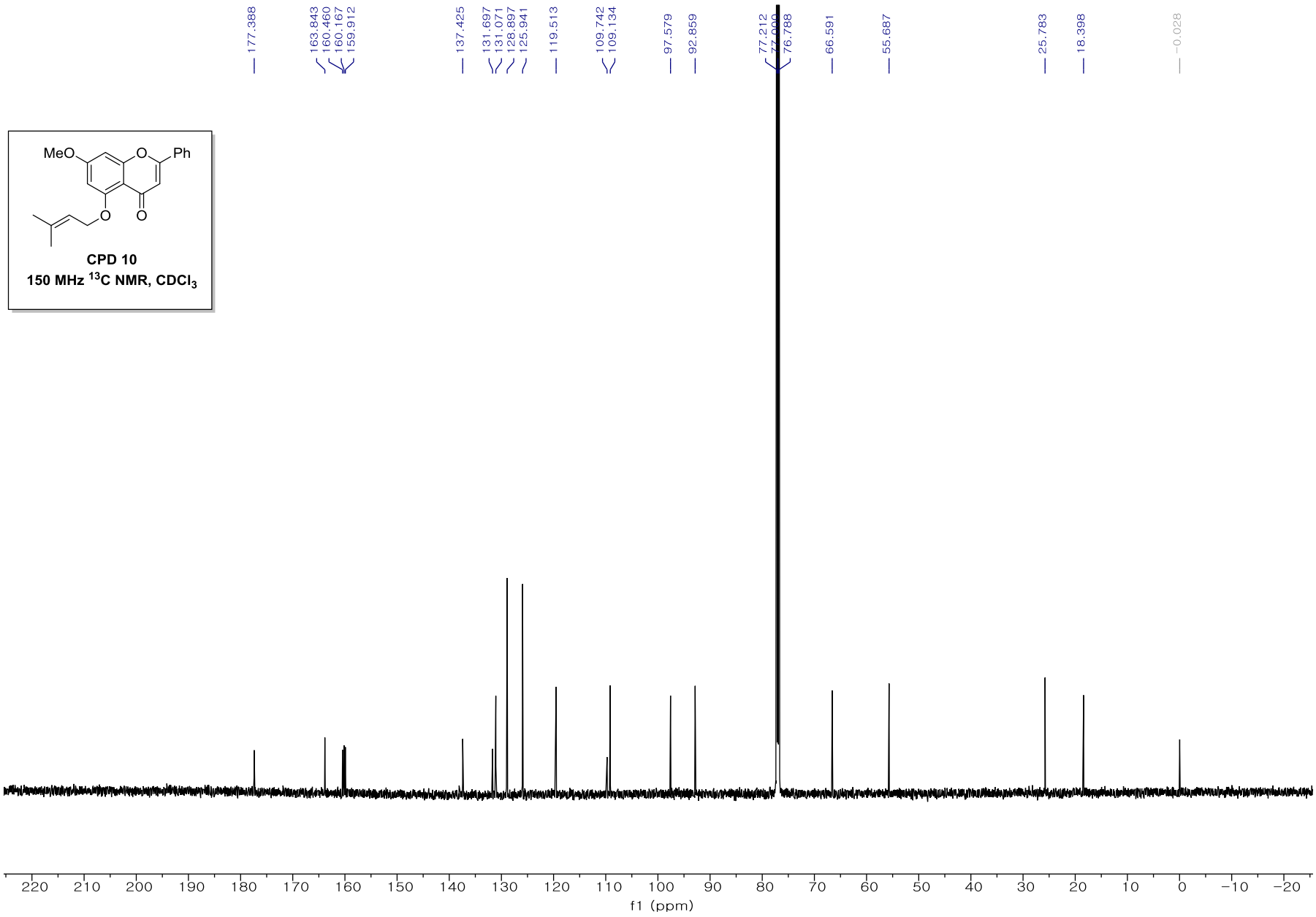
f1 (ppm)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CPD 10
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f1 (ppm)

State Parameter Editor

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Interface Heater (ihe):	On	
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Entrance Potential (EP):		10.0
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Mass Spectrometer Method Properties

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Experiments in Period:    1

Period 1  Experiment   1:
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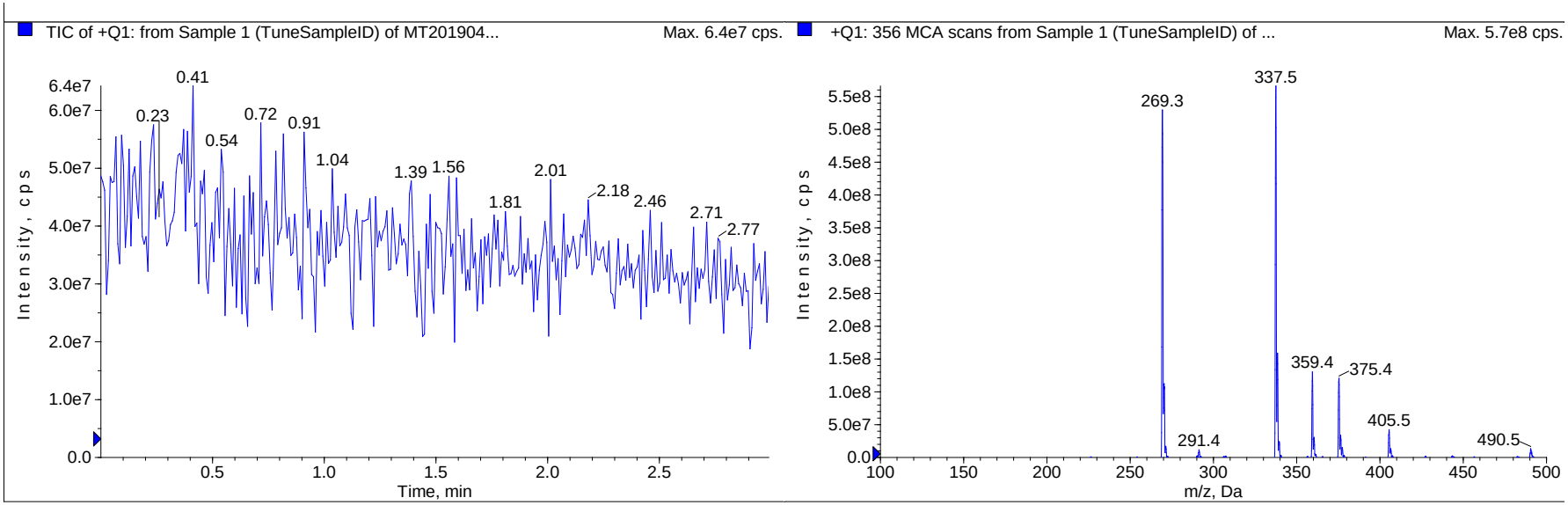

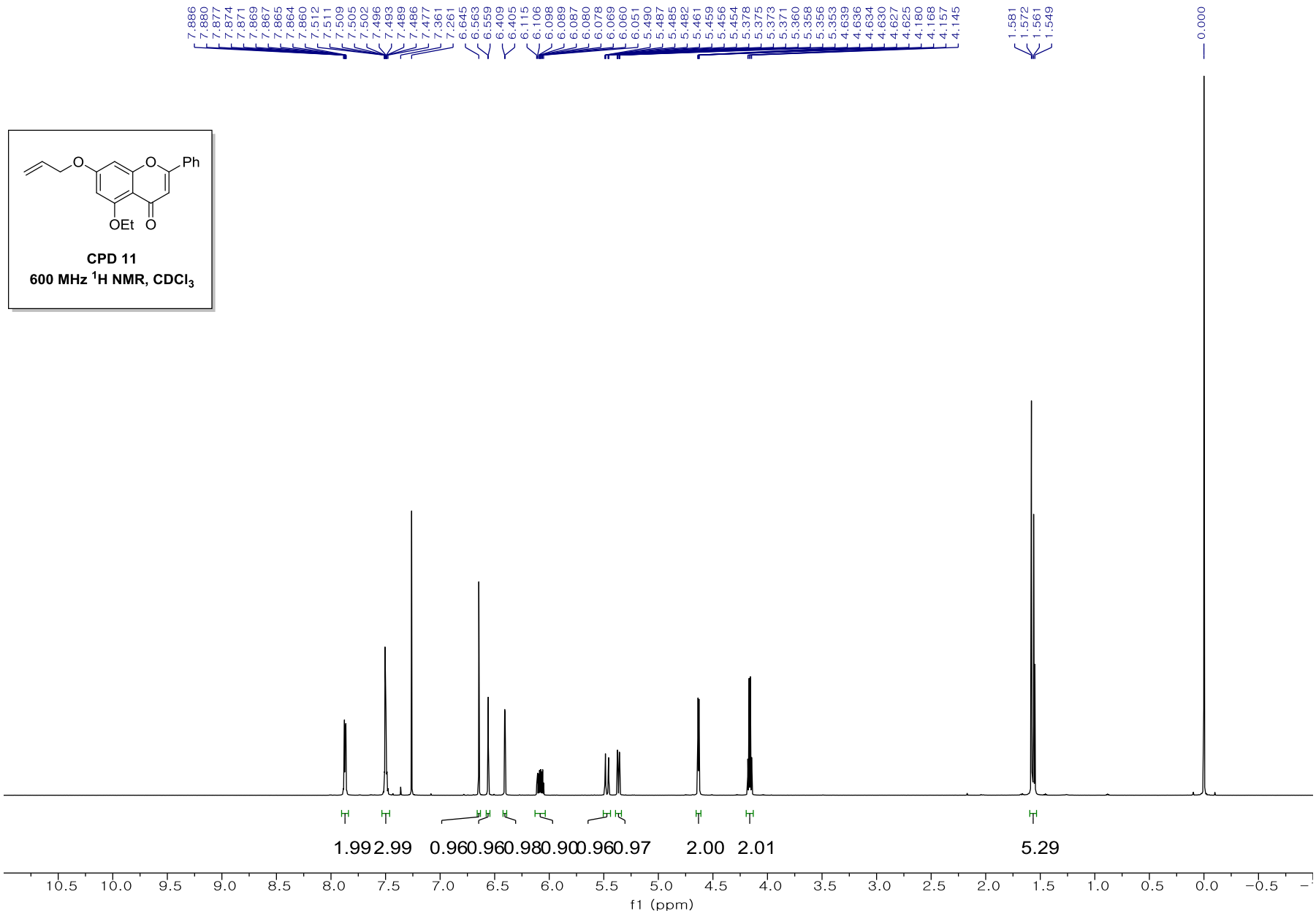
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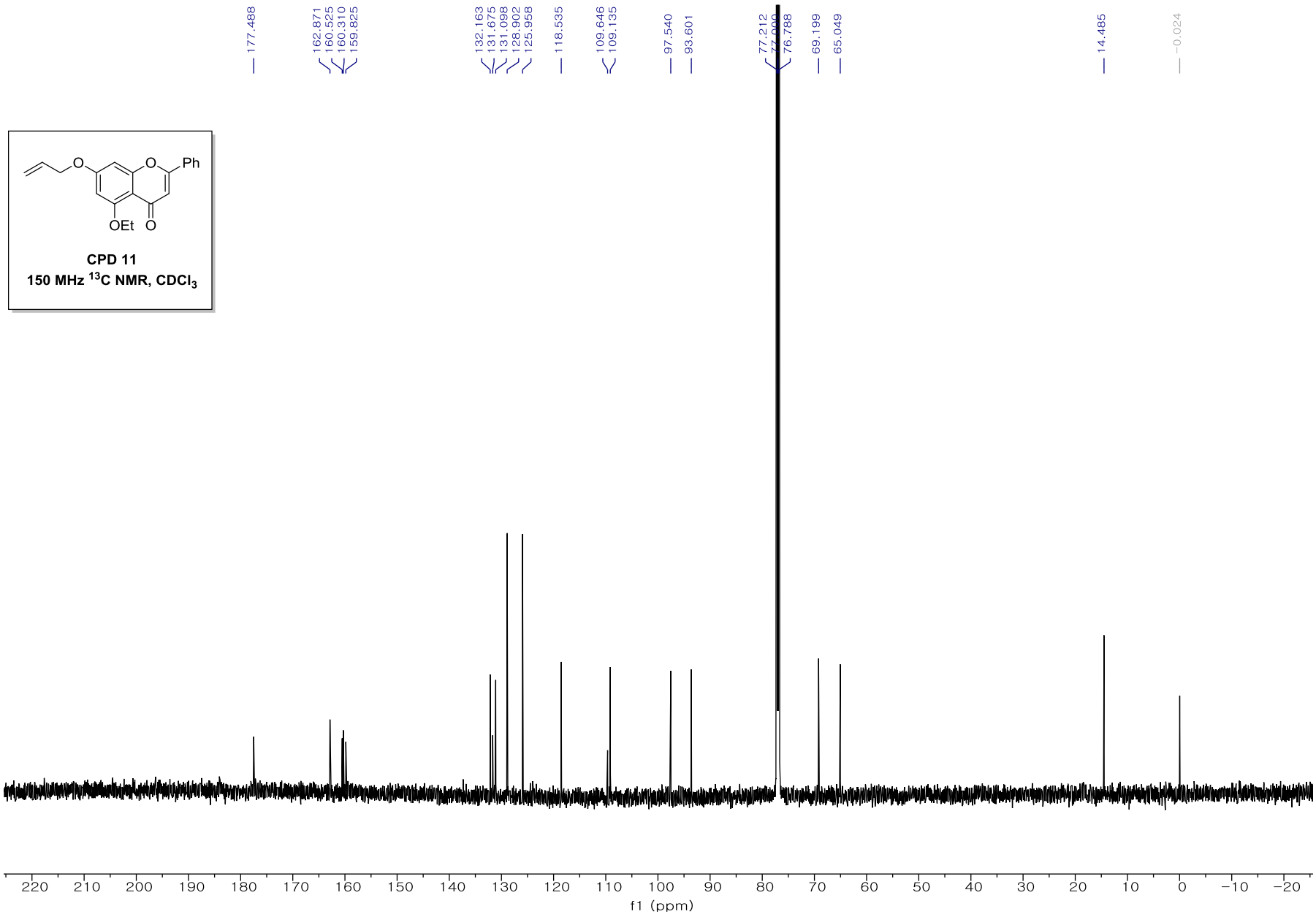
f1 (ppm)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118.535
109.646
109.135
97.540
93.601
77.212
77.000
76.788
69.199
65.049
14.485
-0.024
O
O
Ph
OEt
O
CPD 11
150 MHz 13C NMR, CDCl3
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
f1 (ppm)

State Parameter Editor

Ion Source:	Turbo Spray	
Ion Source Temperature Reached		
Curtain Gas (CUR):	10.0	
IonSpray Voltage (IS):	5500.0	
Temperature (TEM):	0.0	
Ion Source Gas 1 (GS1):	12.0	
Ion Source Gas 2 (GS2):	0.0	
Interface Heater (ihe):	On	
Declustering Potential (DP):		70.0
Entrance Potential (EP):		10.0
Q1 Resolution:	Unit	
Ion Energy 1 (IE1):	1.0	
Deflector (DF):	-200.0	
CEM (CEM):	2500.0	

Mass Spectrometer Method Properties

Period 1:

Scans in Period:	356
Relative Start Time:	0.00 msec
Experiments in Period:	1

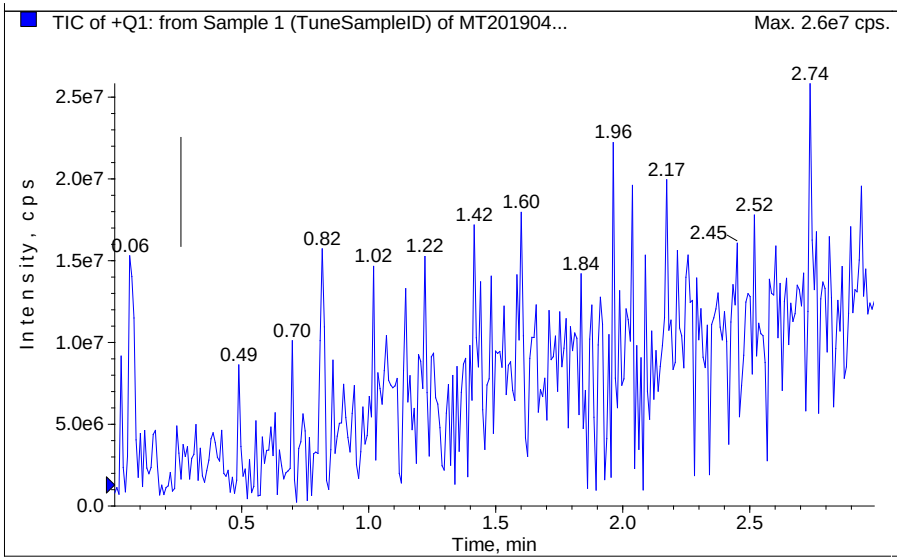
Period 1 Experiment 1:

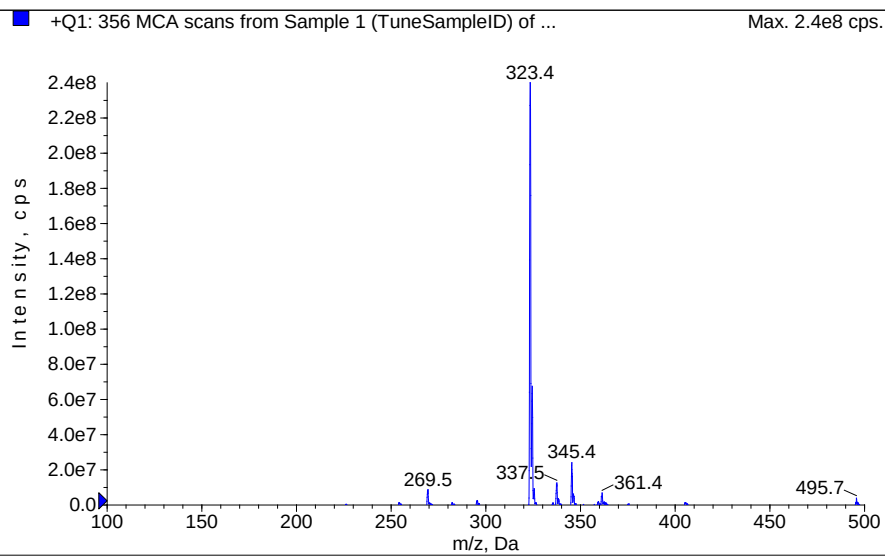
Scan Type:	Q1 MS (Q1)
Polarity:	Positive
Scan Mode:	Profile
Ion Source:	Turbo Spray
Resolution Q1:	Unit
Intensity Thres.:	0.00 cps
Settling Time:	0.0000 msec
MR Pause:	5.0070 msec
MCA:	Yes
Center/Width:	No
Step Size:	0.10 Da

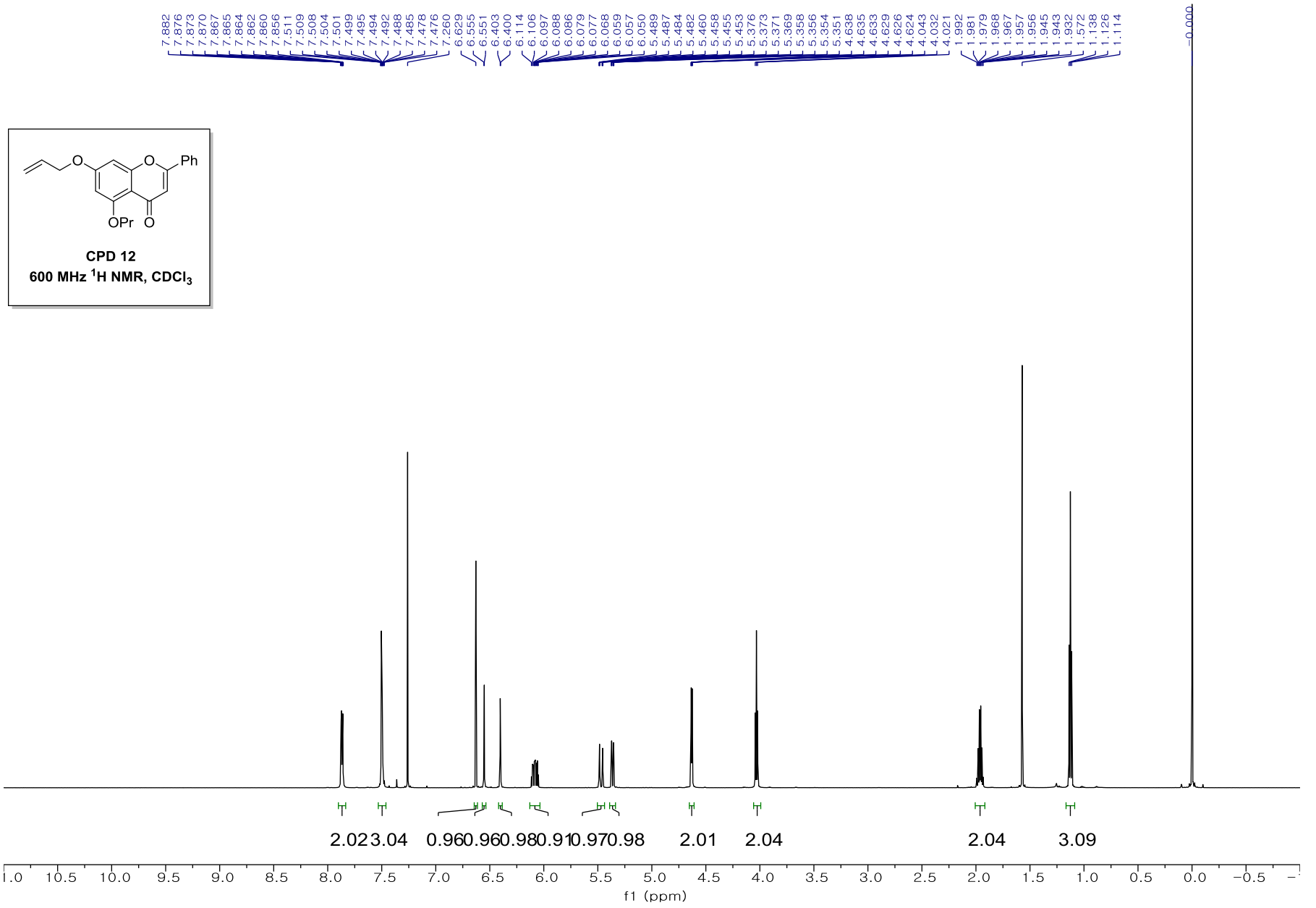
Start (Da)	Stop (Da)	Time (sec)	Param	Start	Stop
100.00	500.00	0.50	CEP	7.84	19.33

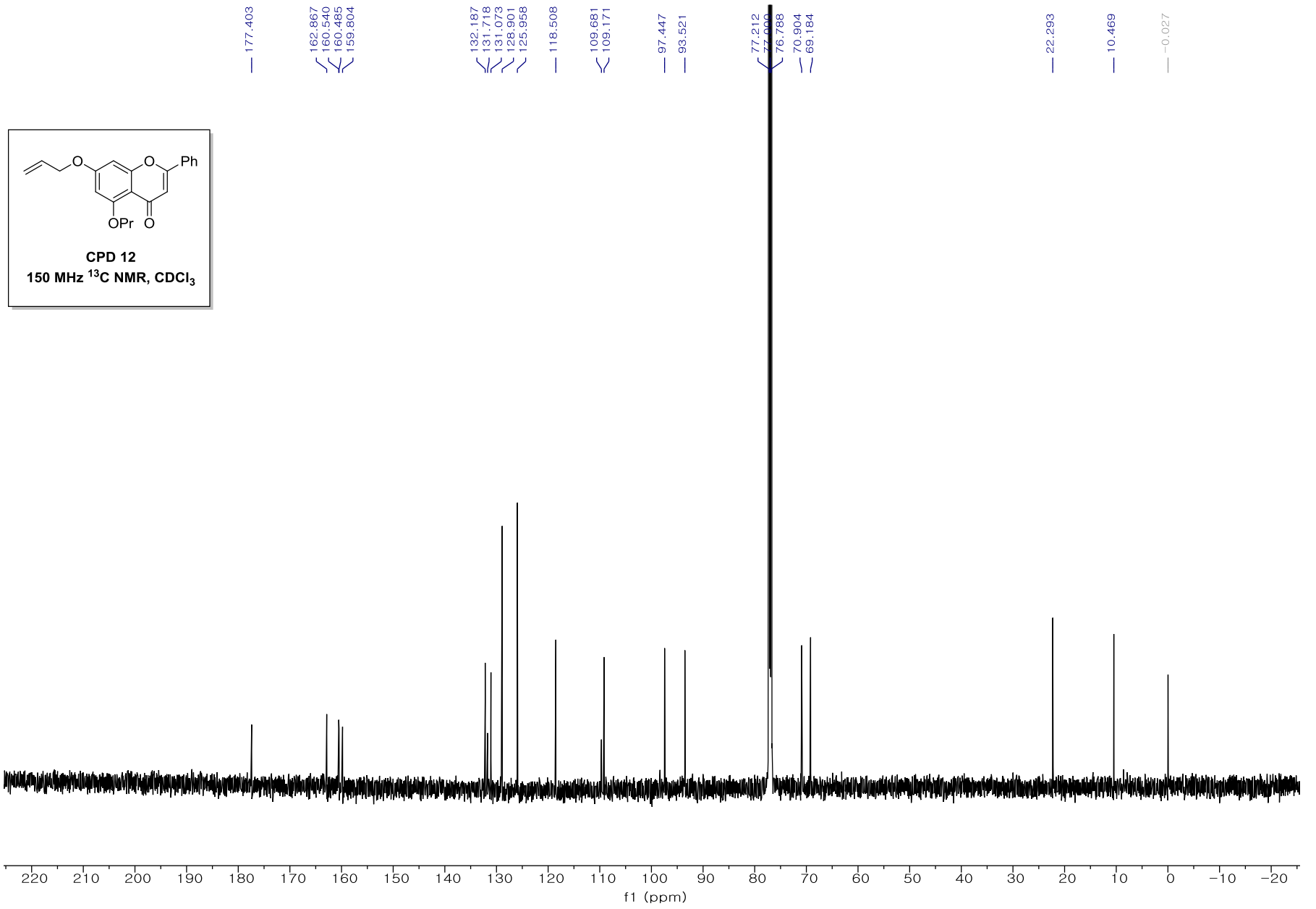
Parameter Table(Period 1 Experiment 1):

CUR:	10.00
TEM:	0.00
GS1:	12.00
GS2:	0.00
ihe:	ON
IS:	5500.00
DP	70.00
EP	10.00






7.882 7.876 7.873 7.870 7.867 7.865 7.864 7.862 7.860 7.856 7.511 7.509 7.508 7.504 7.501 7.499 7.495 7.494 7.492 7.488 7.485 7.478 7.476 7.260 6.629 6.555 6.551 6.403 6.400 6.114 6.106 6.097 6.088 6.086 6.079 6.077 6.068 6.059 6.057 6.050 5.489 5.487 5.484 5.482 5.460 5.458 5.455 5.453 5.376 5.373 5.371 5.369 5.358 5.356 5.354 5.351 4.638 4.635 4.633 4.629 4.626 4.624 4.043 4.032 4.021 1.992 1.981 1.979 1.968 1.967 1.957 1.956 1.945 1.943 1.932 1.572 1.138 1.126 1.114 0.000
O
O
Ph
OPr
O
CPD 12
600 MHz 1H NMR, CDCl3
2.02 3.04 0.96 0.96 0.98 0.91 0.97 0.98 2.01 2.04 2.04 3.09
f1 (ppm)


177.403
162.867
160.540
160.485
159.804
132.187
131.718
131.073
128.901
125.958
118.508
109.681
109.171
97.447
93.521
77.212
76.788
70.904
69.184
22.293
10.469
-0.027
O
O
Ph
OPr
O
CPD 12
150 MHz 13C NMR, CDCl3
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
−20
f1 (ppm)

State Parameter Editor

Ion Source:	Turbo Spray	
Ion Source Temperature Reached		
Curtain Gas (CUR):	10.0	
IonSpray Voltage (IS):	5500.0	
Temperature (TEM):	0.0	
Ion Source Gas 1 (GS1):	12.0	
Ion Source Gas 2 (GS2):	0.0	
Interface Heater (ihe):	On	
Declustering Potential (DP):		70.0
Entrance Potential (EP):		10.0
Q1 Resolution:	Unit	
Ion Energy 1 (IE1):	1.0	
Deflector (DF):	-200.0	
CEM (CEM):	2500.0	

Mass Spectrometer Method Properties

Period 1:

Scans in Period:	356
Relative Start Time:	0.00 msec
Experiments in Period:	1

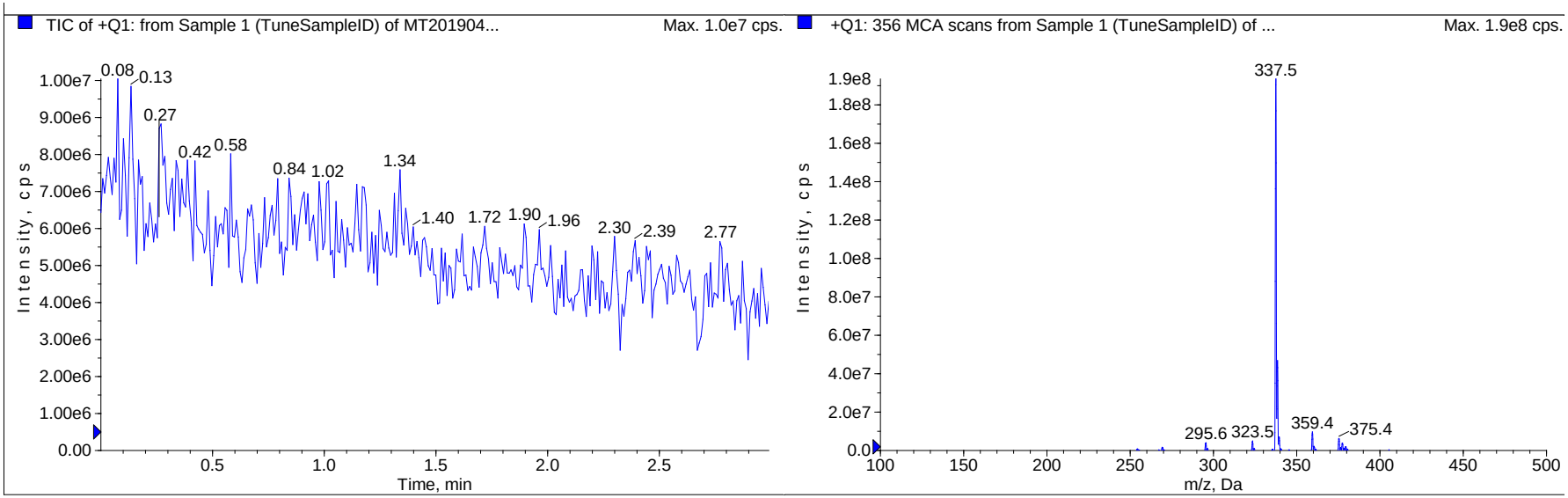
Period 1 Experiment 1:

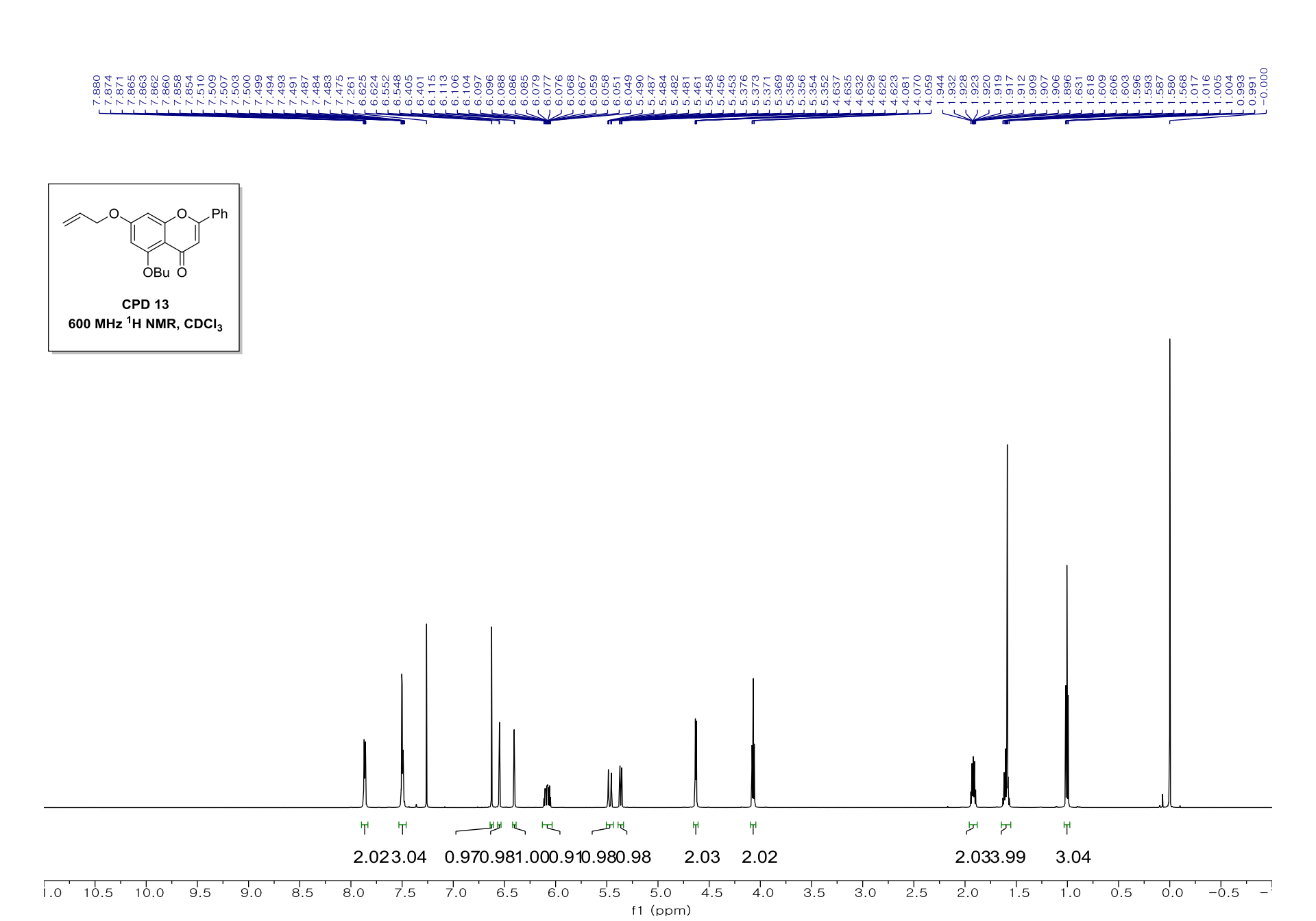
Scan Type:	Q1 MS (Q1)
Polarity:	Positive
Scan Mode:	Profile
Ion Source:	Turbo Spray
Resolution Q1:	Unit
Intensity Thres.:	0.00 cps
Settling Time:	0.0000 msec
MR Pause:	5.0070 msec
MCA:	Yes
Center/Width:	No
Step Size:	0.10 Da

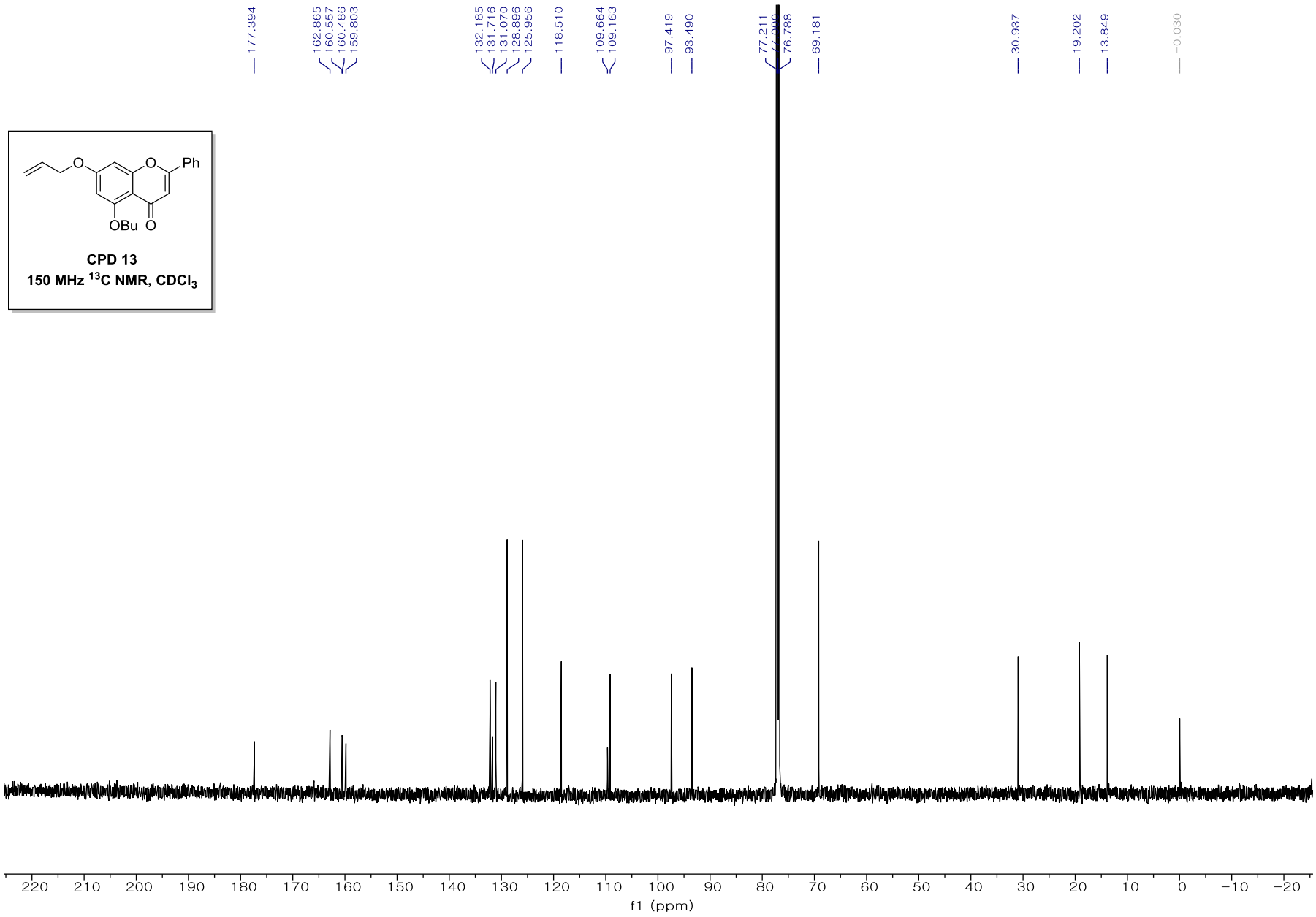
Start (Da)	Stop (Da)	Time (sec)	Param	Start	Stop
100.00	500.00	0.50	CEP	7.84	19.33

Parameter Table(Period 1 Experiment 1):

CUR:	10.00
TEM:	0.00
GS1:	12.00
GS2:	0.00
ihe:	ON
IS:	5500.00
DP	70.00
EP	10.00




7.880 7.874 7.871 7.865 7.863 7.862 7.860 7.858 7.854 7.510 7.509 7.507 7.503 7.500 7.499 7.494 7.493 7.491 7.487 7.484 7.483 7.475 7.261 6.625 6.624 6.552 6.548 6.405 6.401 6.115 6.113 6.106 6.104 6.097 6.096 6.088 6.086 6.085 6.079 6.077 6.076 6.068 6.067 6.059 6.058 6.051 6.049 5.490 5.487 5.484 5.482 5.481 5.461 5.458 5.456 5.453 5.376 5.373 5.371 5.369 5.358 5.356 5.354 5.352 4.637 4.635 4.632 4.629 4.626 4.623 4.081 4.070 4.059 1.944 1.932 1.928 1.923 1.920 1.919 1.917 1.912 1.909 1.907 1.906 1.896 1.631 1.618 1.609 1.606 1.603 1.596 1.593 1.587 1.580 1.568 1.017 1.016 1.005 1.004 0.993 0.991 0.000
O
O
Ph
OBu
O
CPD 13
600 MHz ^{1}H NMR, $CDCl_3$
2.02 3.04 0.97 0.98 1.00 0.91 0.98 0.98 2.03 2.02 2.03 3.99 3.04
f1 (ppm)


177.394
162.865
160.557
160.486
159.803
132.185
131.716
131.070
128.896
125.956
118.510
109.664
109.163
97.419
93.490
77.211
76.788
69.181
30.937
19.202
13.849
-0.030
O
O
Ph
OBu
O
CPD 13
150 MHz 13C NMR, CDCl3
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)

State Parameter Editor

Ion Source:	Turbo Spray	
Ion Source Temperature Reached		
Curtain Gas (CUR):	10.0	
IonSpray Voltage (IS):	5500.0	
Temperature (TEM):	0.0	
Ion Source Gas 1 (GS1):	12.0	
Ion Source Gas 2 (GS2):	0.0	
Interface Heater (ihe):	On	
Declustering Potential (DP):		70.0
Entrance Potential (EP):		10.0
Q1 Resolution:	Unit	
Ion Energy 1 (IE1):	1.0	
Deflector (DF):	-200.0	
CEM (CEM):	2500.0	

Mass Spectrometer Method Properties

Period 1:

Scans in Period:	356
Relative Start Time:	0.00 msec
Experiments in Period:	1

Period 1 Experiment 1:

Scan Type:	Q1 MS (Q1)
Polarity:	Positive
Scan Mode:	Profile
Ion Source:	Turbo Spray
Resolution Q1:	Unit
Intensity Thres.:	0.00 cps
Settling Time:	0.0000 msec
MR Pause:	5.0070 msec
MCA:	Yes
Center/Width:	No
Step Size:	0.10 Da

Start (Da)	Stop (Da)	Time (sec)	Param	Start	Stop
100.00	500.00	0.50	CEP	7.84	19.33

Parameter Table(Period 1 Experiment 1):

CUR:	10.00
TEM:	0.00
GS1:	12.00
GS2:	0.00
ihe:	ON
IS:	5500.00
DP	70.00
EP	10.00