Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.
This journal is © The Royal Society of Chemistry 2017

Supporting Information

Palladium-catalyzed C-H olefination of uracils and caffeines using molecular oxygen as the sole oxidant

Xinyu Zhang, Lv Su, Lin Qiu, Zhenwei fan, Xiaofeng Zhang, Shen Lin and Qiufeng Huang*

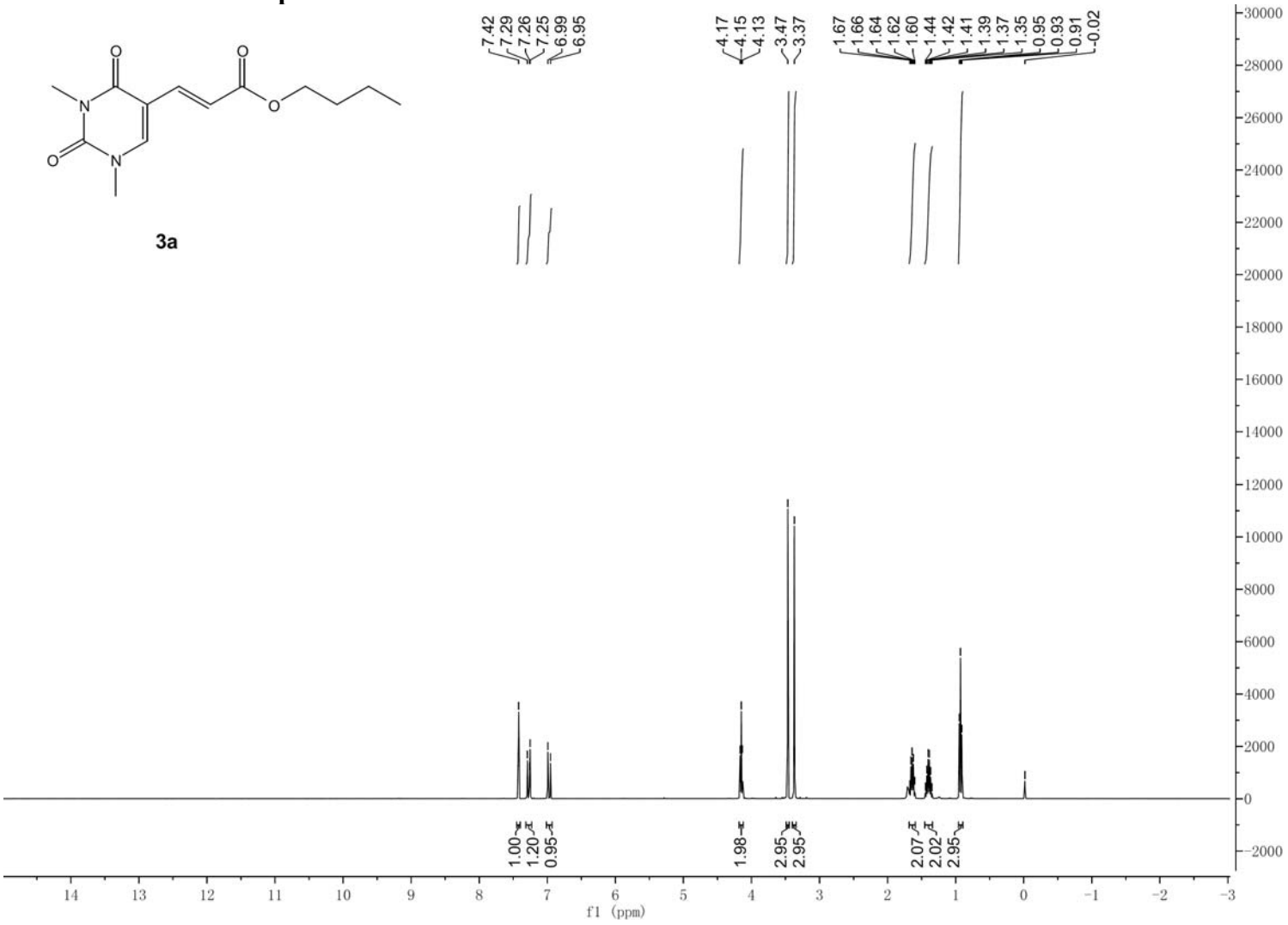
College of Chemistry & Chemical Engineering, Fujian Normal University, Fuzhou 350007, P. R. China and Fujian Key Laboratory of Polymer Materials, Fuzhou 350007, P. R. China.

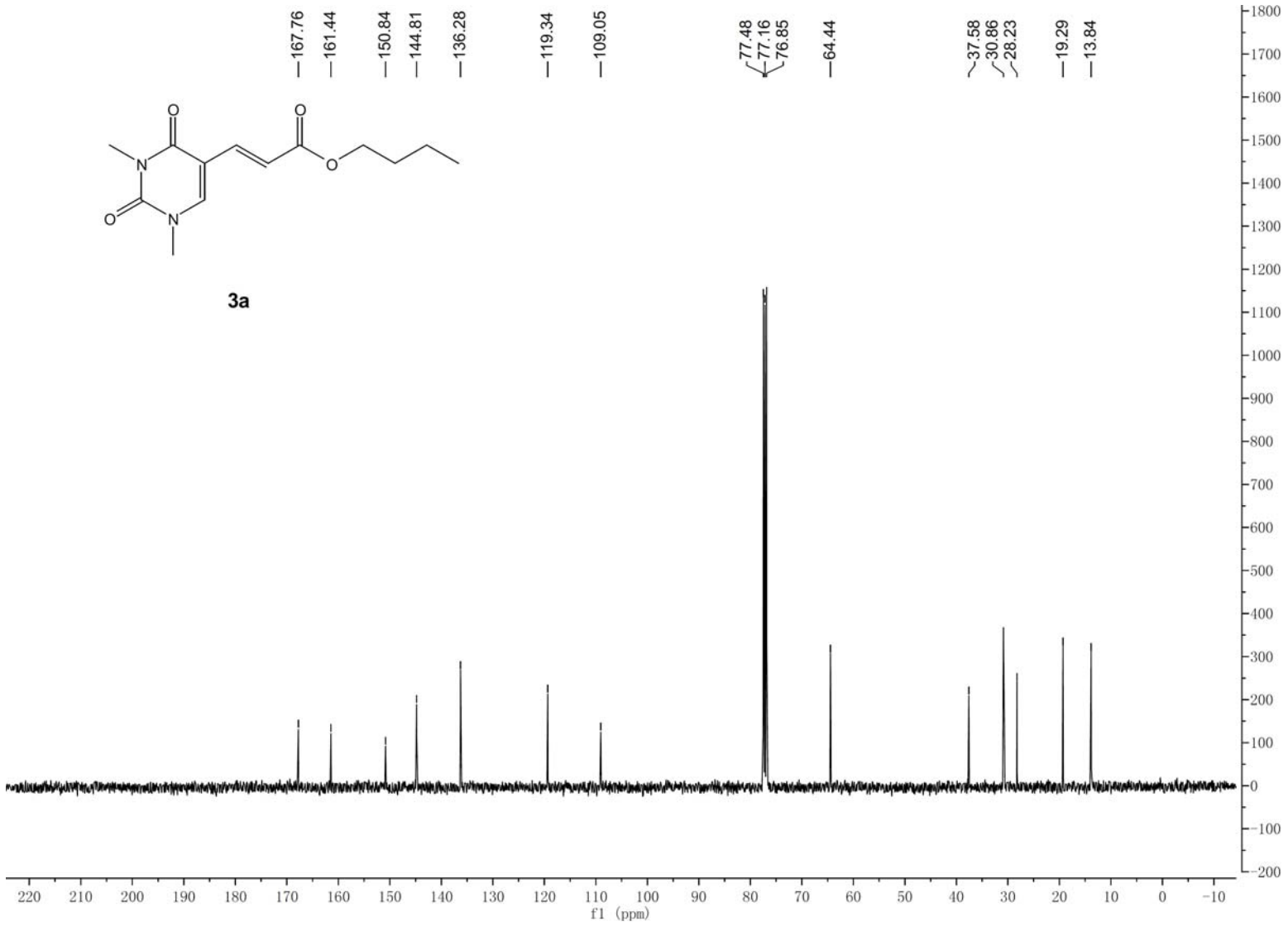
qiufenghuang@fjnu.edu.cn

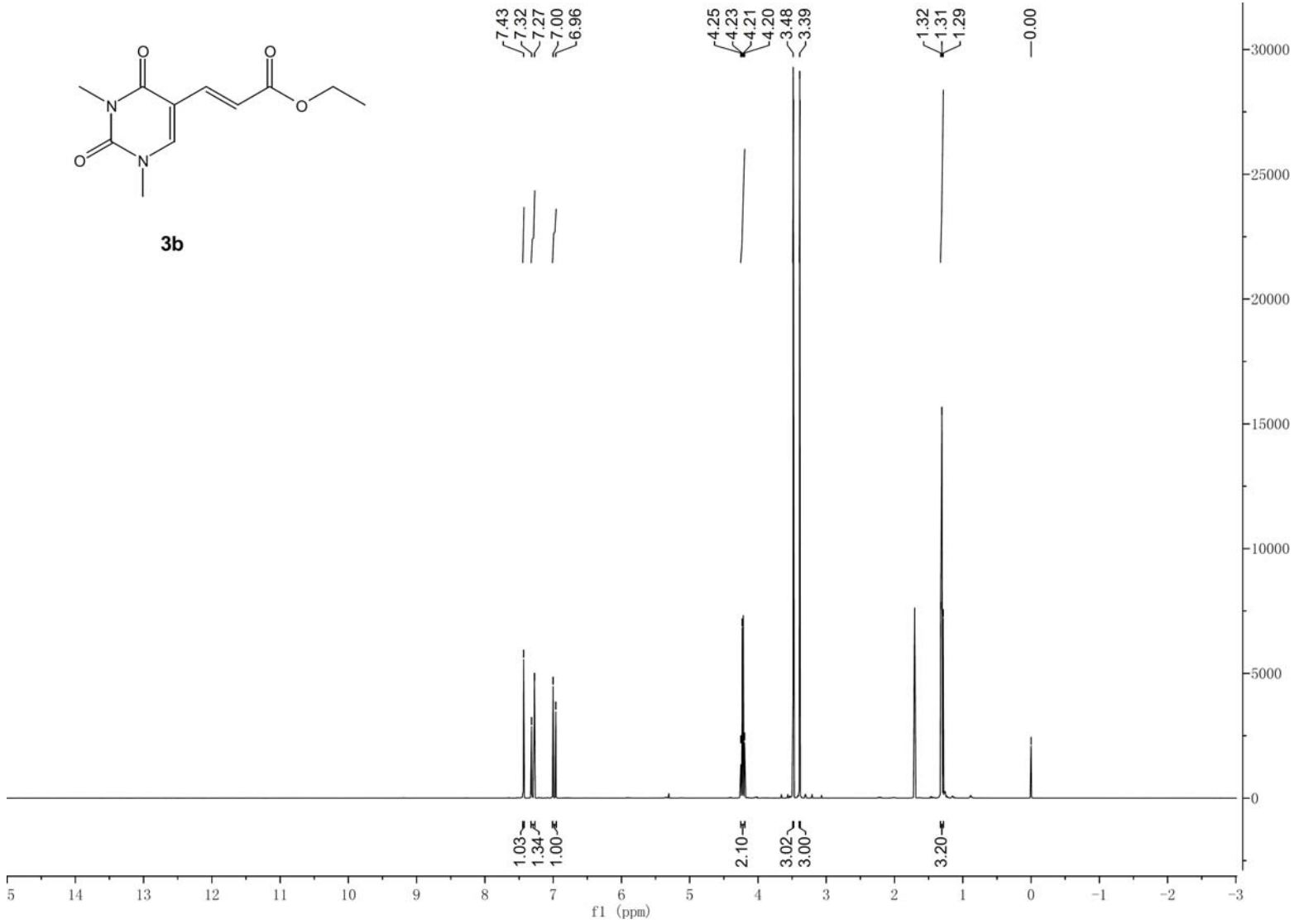
Contents:

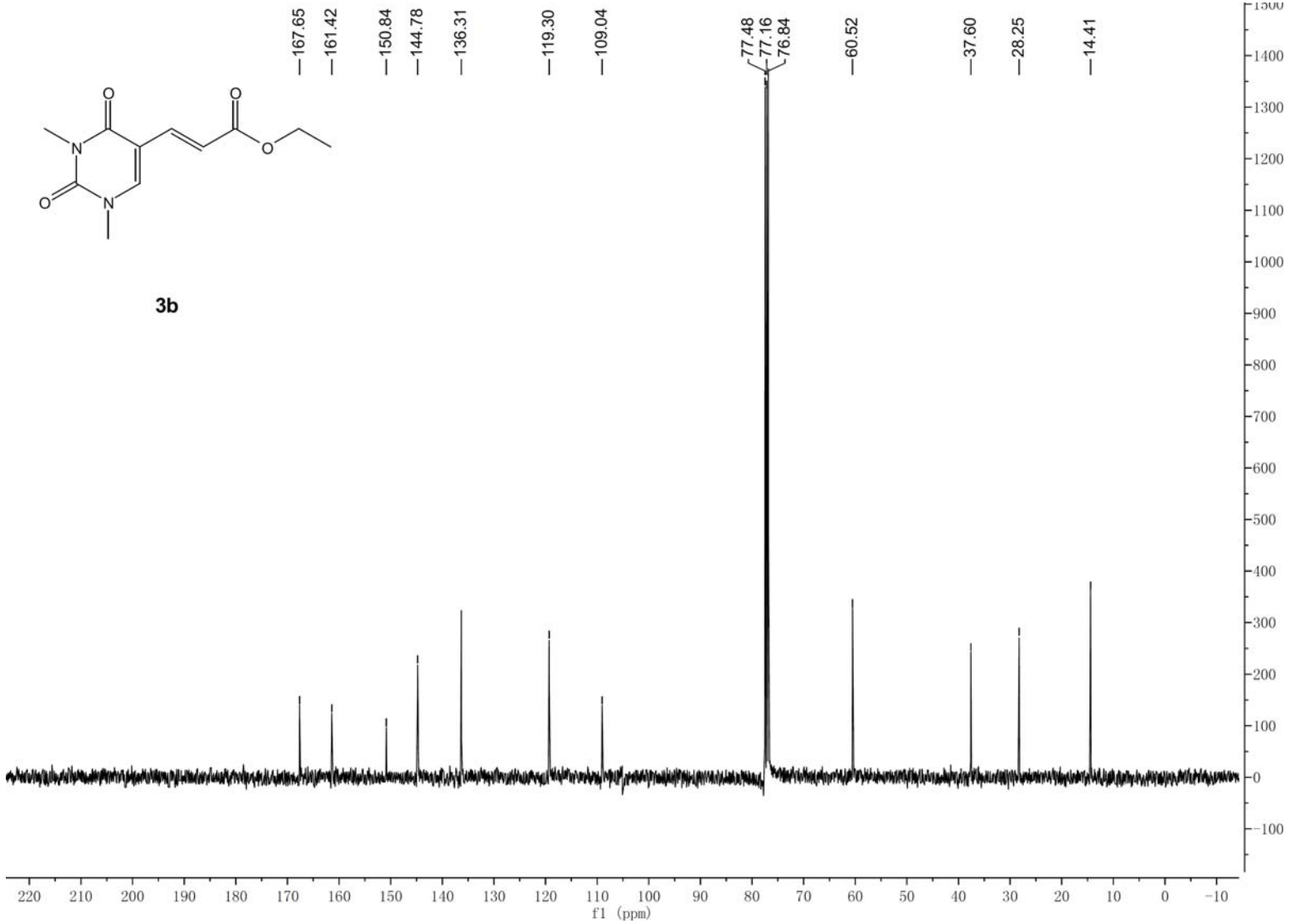
Copies of ^{1}H NMR and ^{13}C NMR charts for compounds **3a~3t**, **4a~4p S**2 to S72

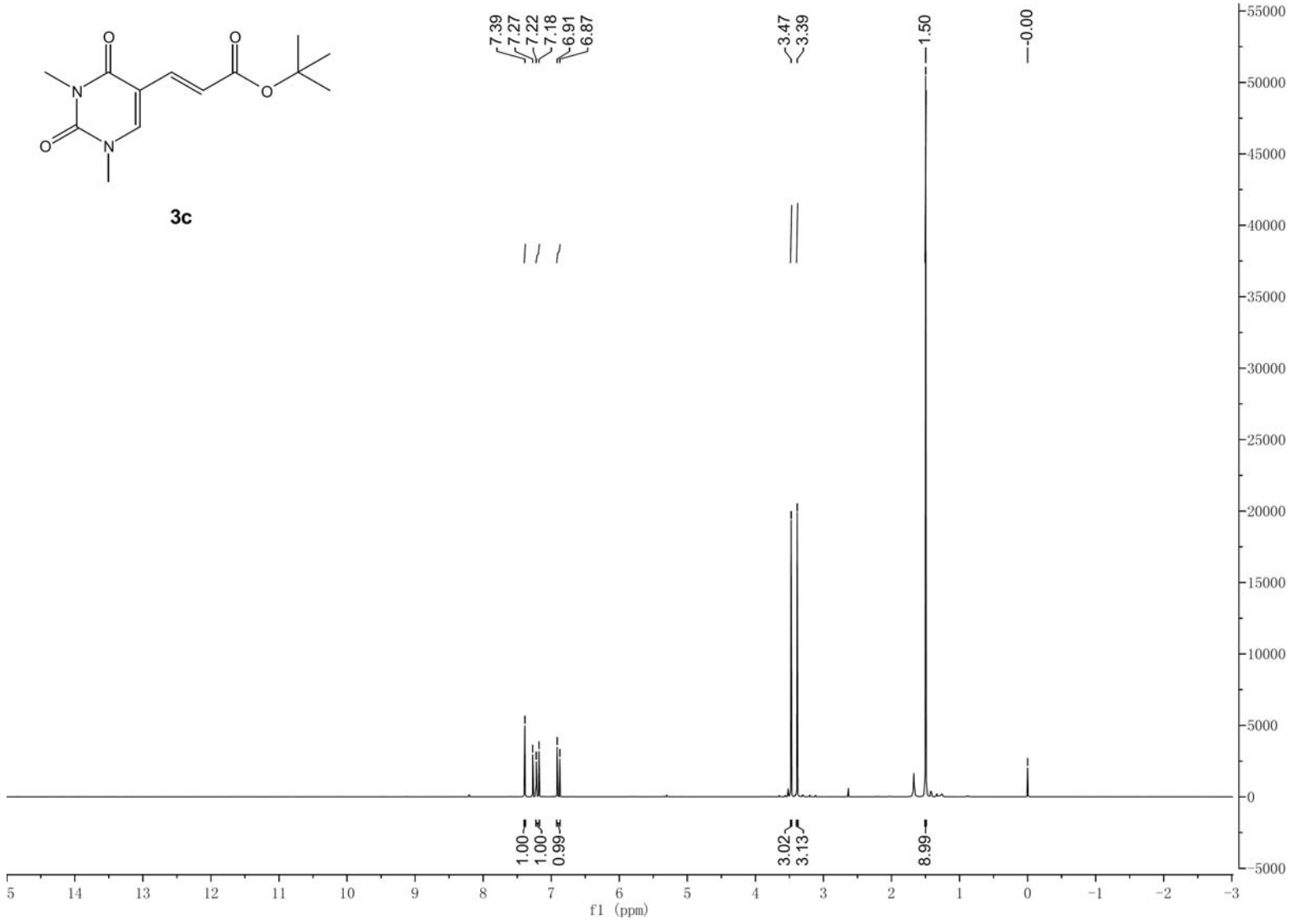
Copies of ^{1}H and ^{13}C-NMR charts of products

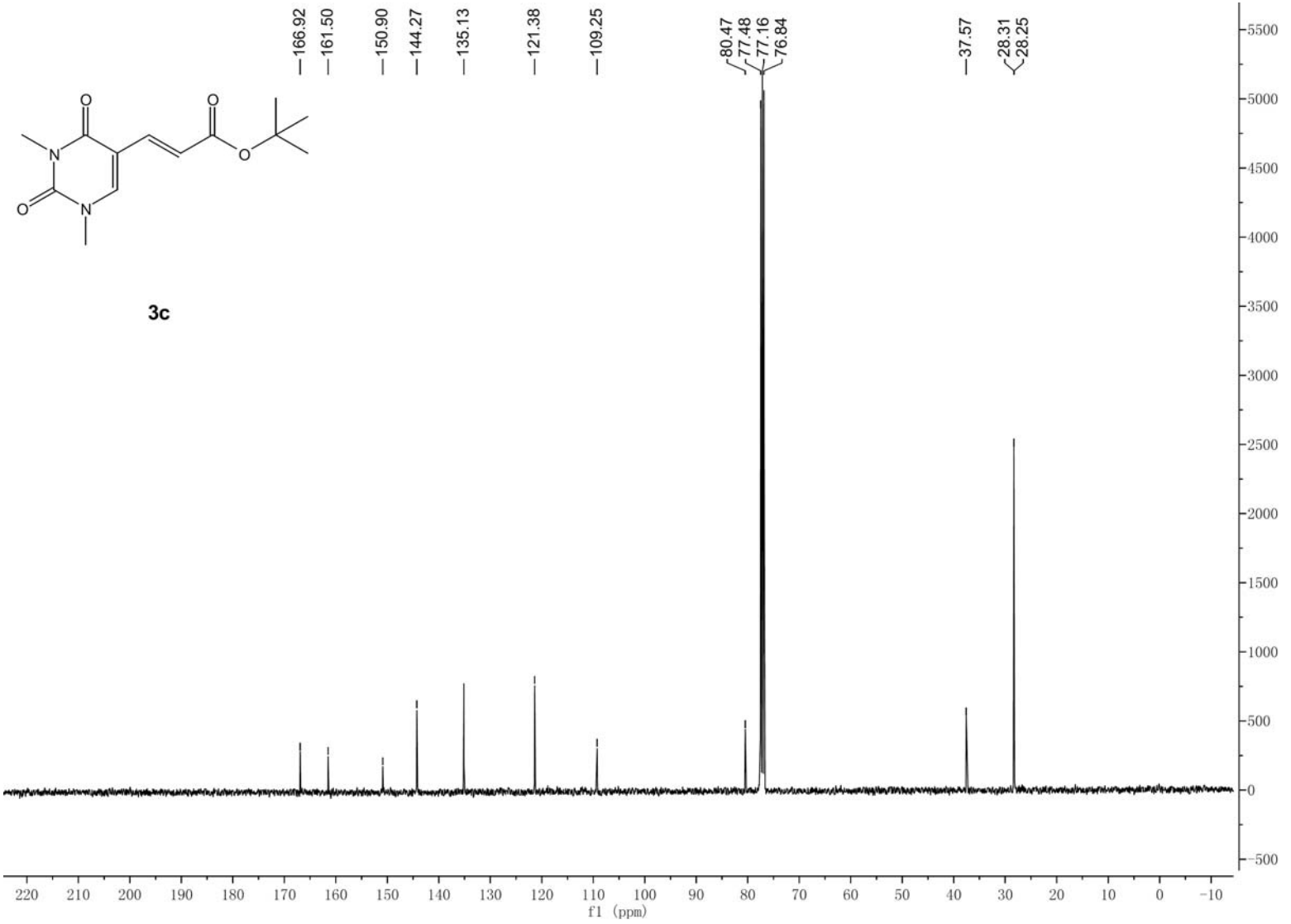


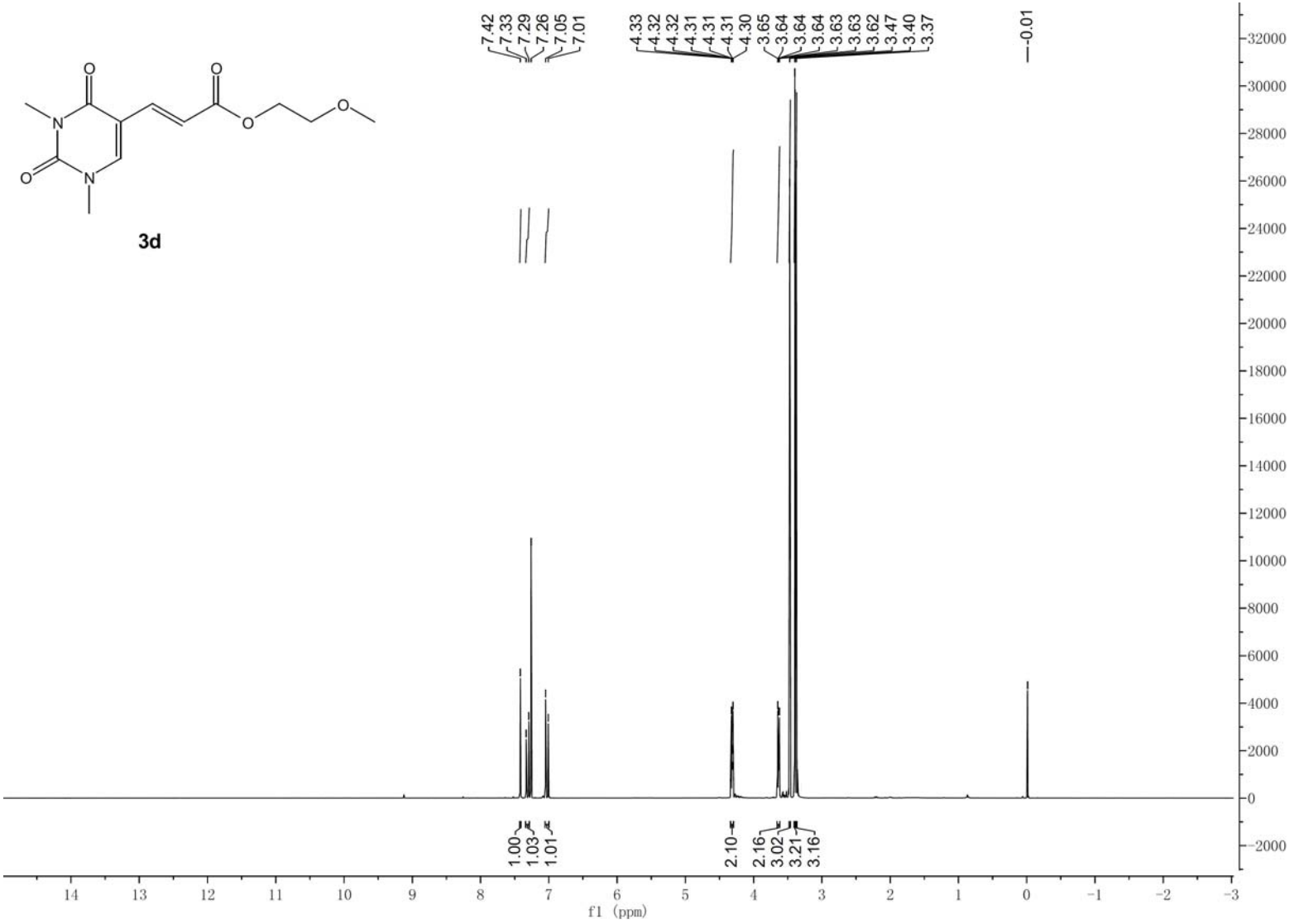

167.76
161.44
150.84
144.81
136.28
119.34
109.05
77.48
77.16
76.85
64.44
37.58
30.86
28.23
19.29
13.84
3a
f1 (ppm)

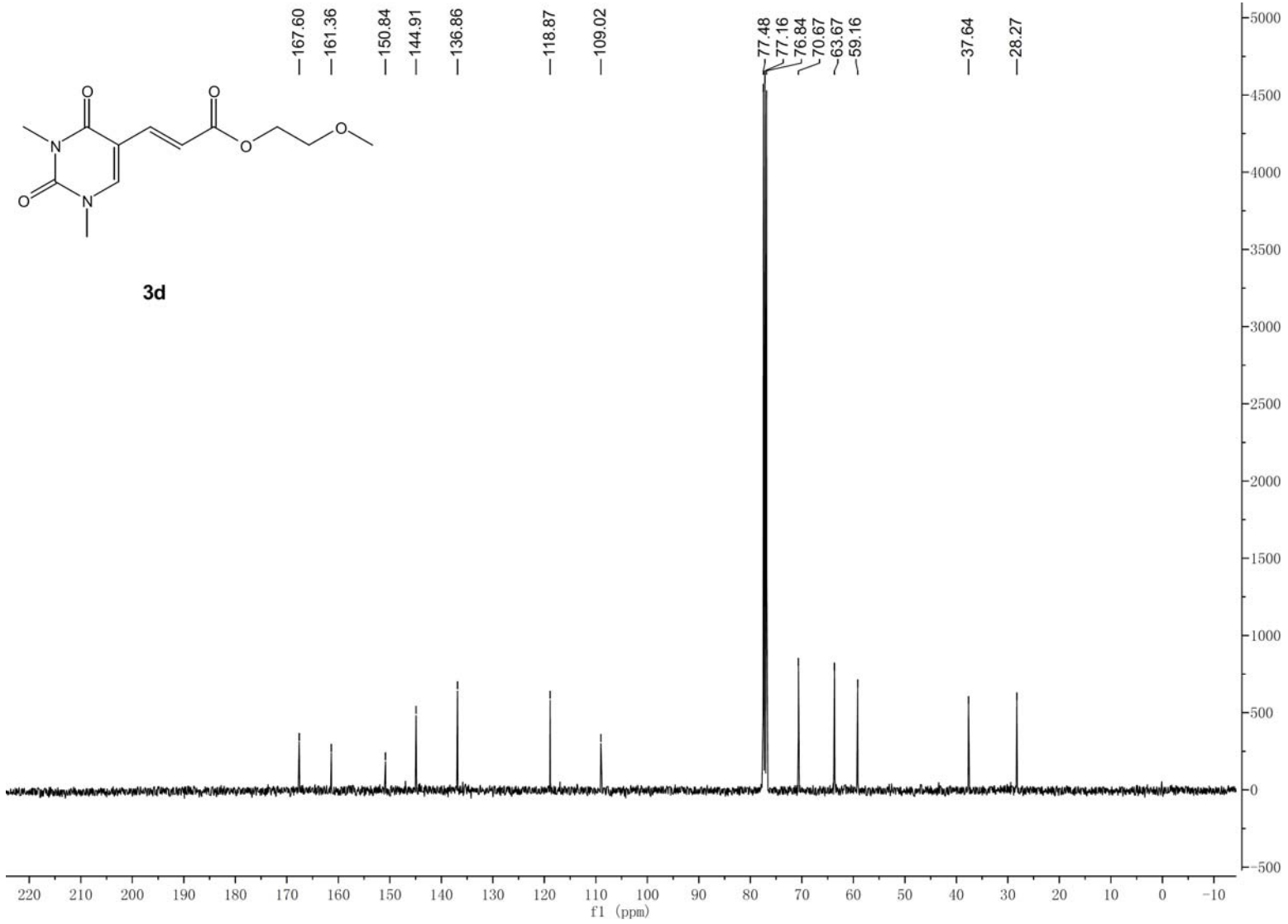

3b
7.43
7.32
7.27
7.00
6.96
4.25
4.23
4.21
4.20
3.48
3.39
1.32
1.31
1.29
0.00
1.03
1.34
1.00
2.10
3.02
3.00
3.20
f1 (ppm)

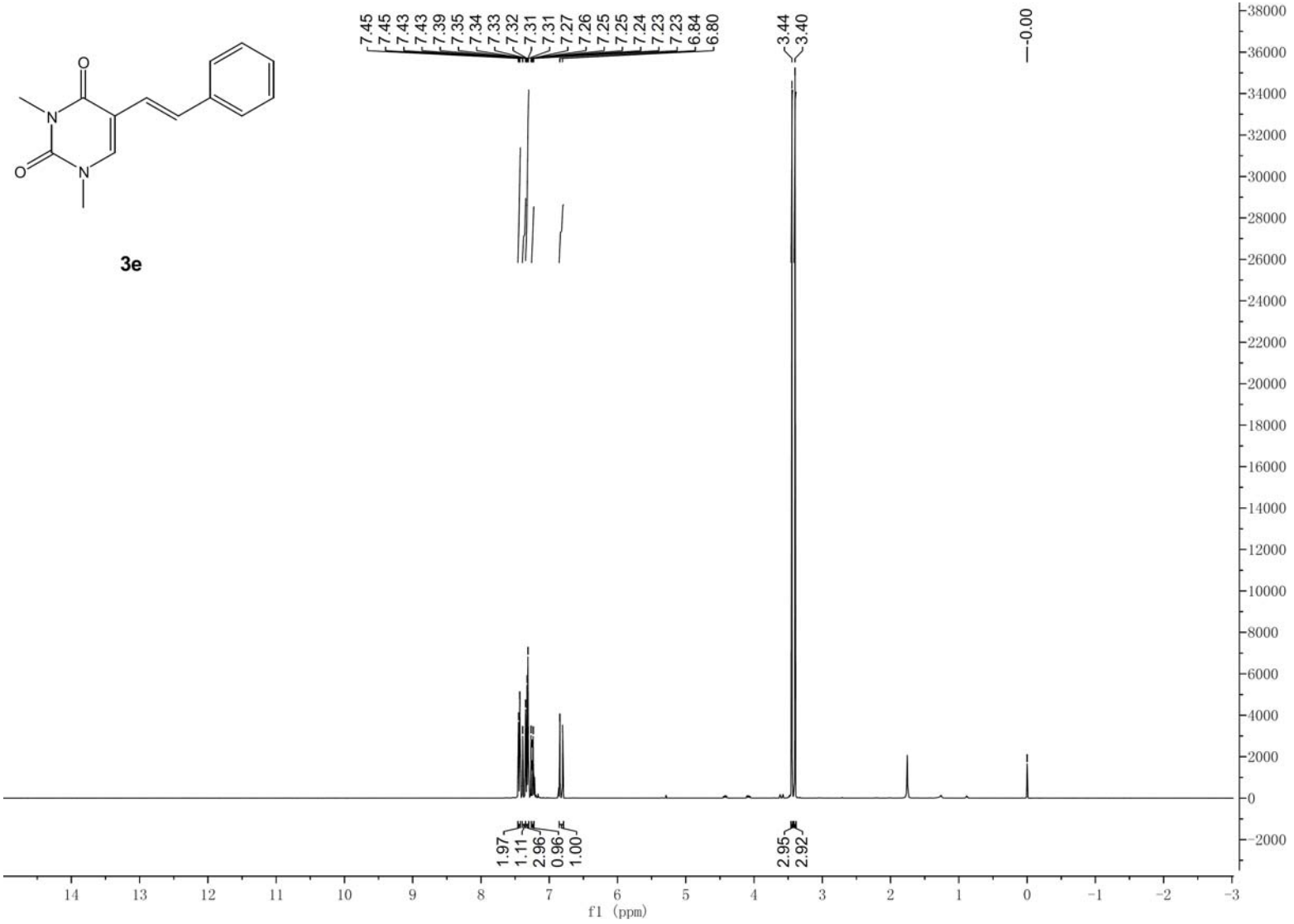

167.65
161.42
150.84
144.78
136.31
119.30
109.04
77.48
77.16
76.84
60.52
37.60
28.25
14.41
3b
f1 (ppm)

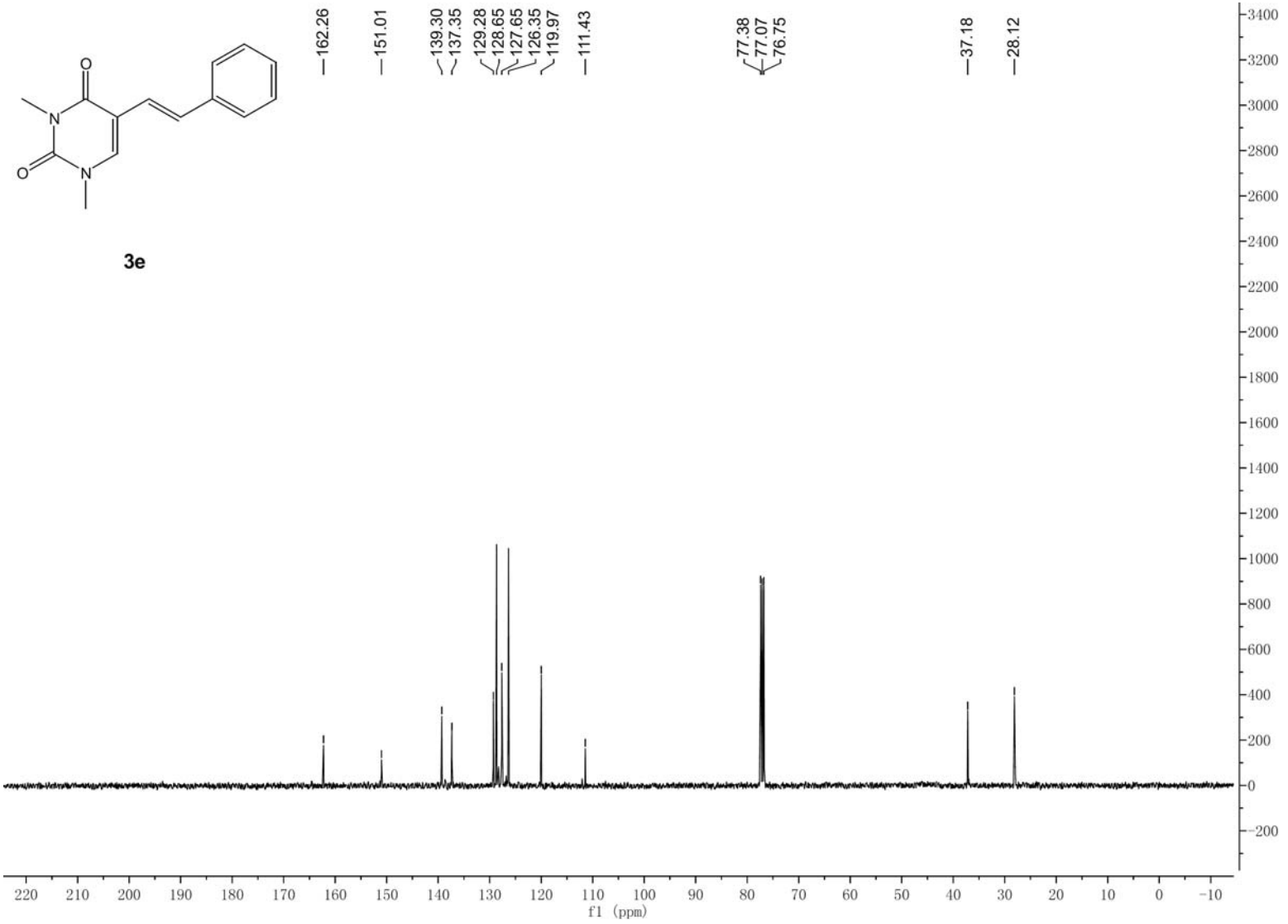

3c
7.39
7.27
7.22
7.18
6.91
6.87
3.47
3.39
1.50
0.00
1.00
1.00
0.99
3.02
3.13
8.99
f1 (ppm)

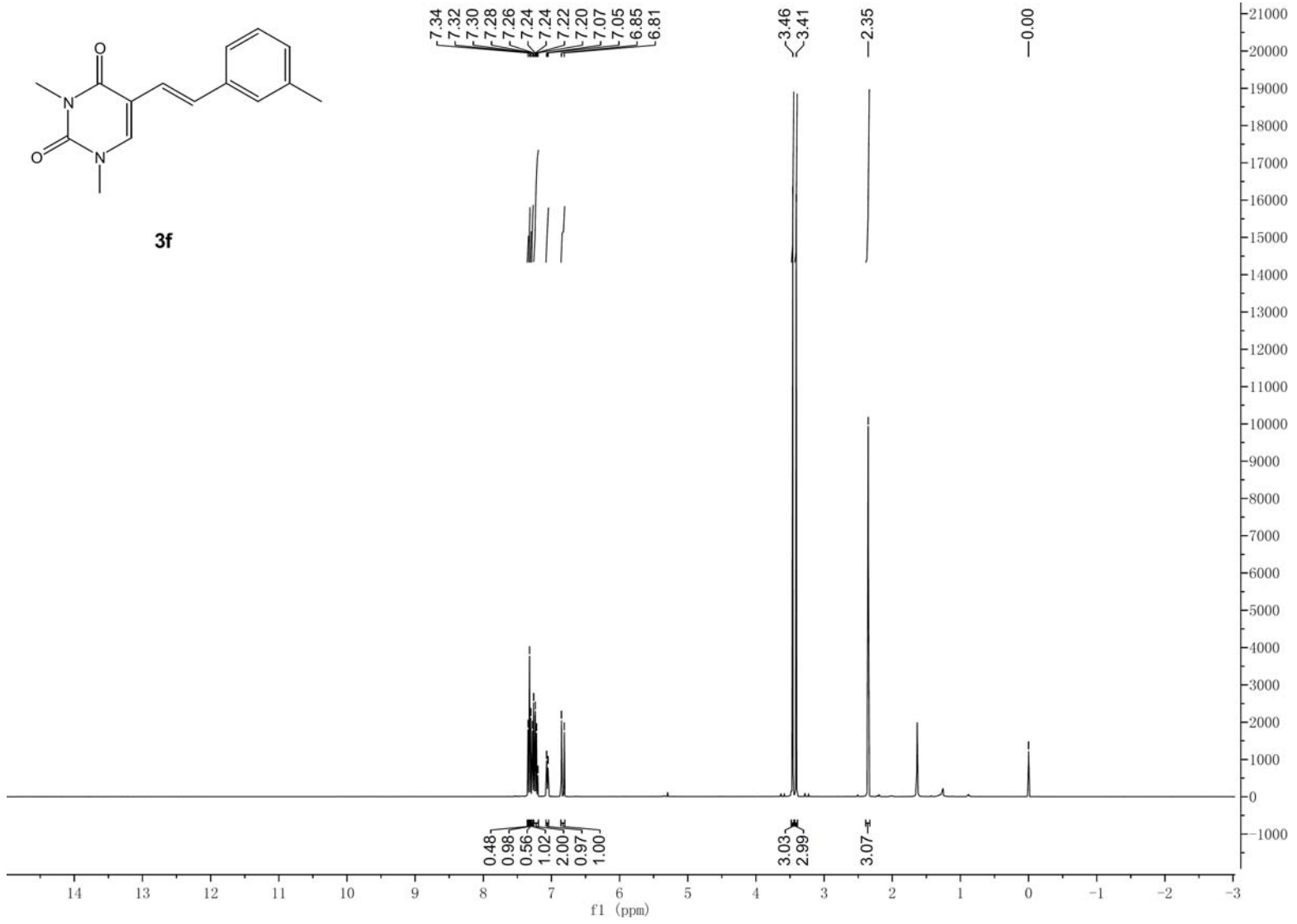

166.92
161.50
150.90
144.27
135.13
121.38
109.25
80.47
77.48
77.16
76.84
37.57
28.31
28.25
3c
f1 (ppm)

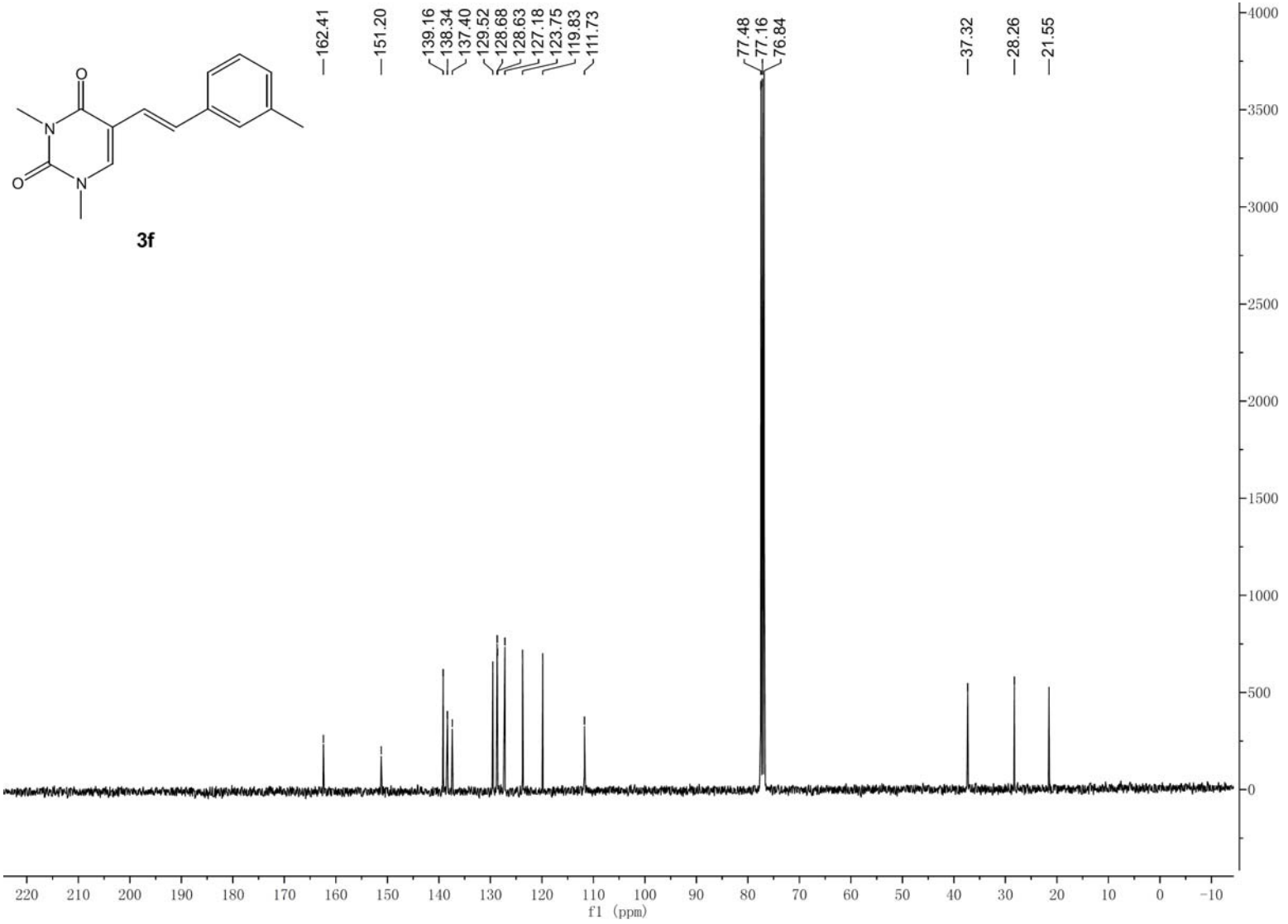

3d
7.42
7.33
7.29
7.26
7.05
7.01
4.33
4.32
4.32
4.31
4.31
4.31
4.30
3.65
3.64
3.64
3.64
3.63
3.63
3.62
3.47
3.40
3.37
0.01
1.00
1.03
1.01
2.10
2.16
3.02
3.21
3.16
f1 (ppm)

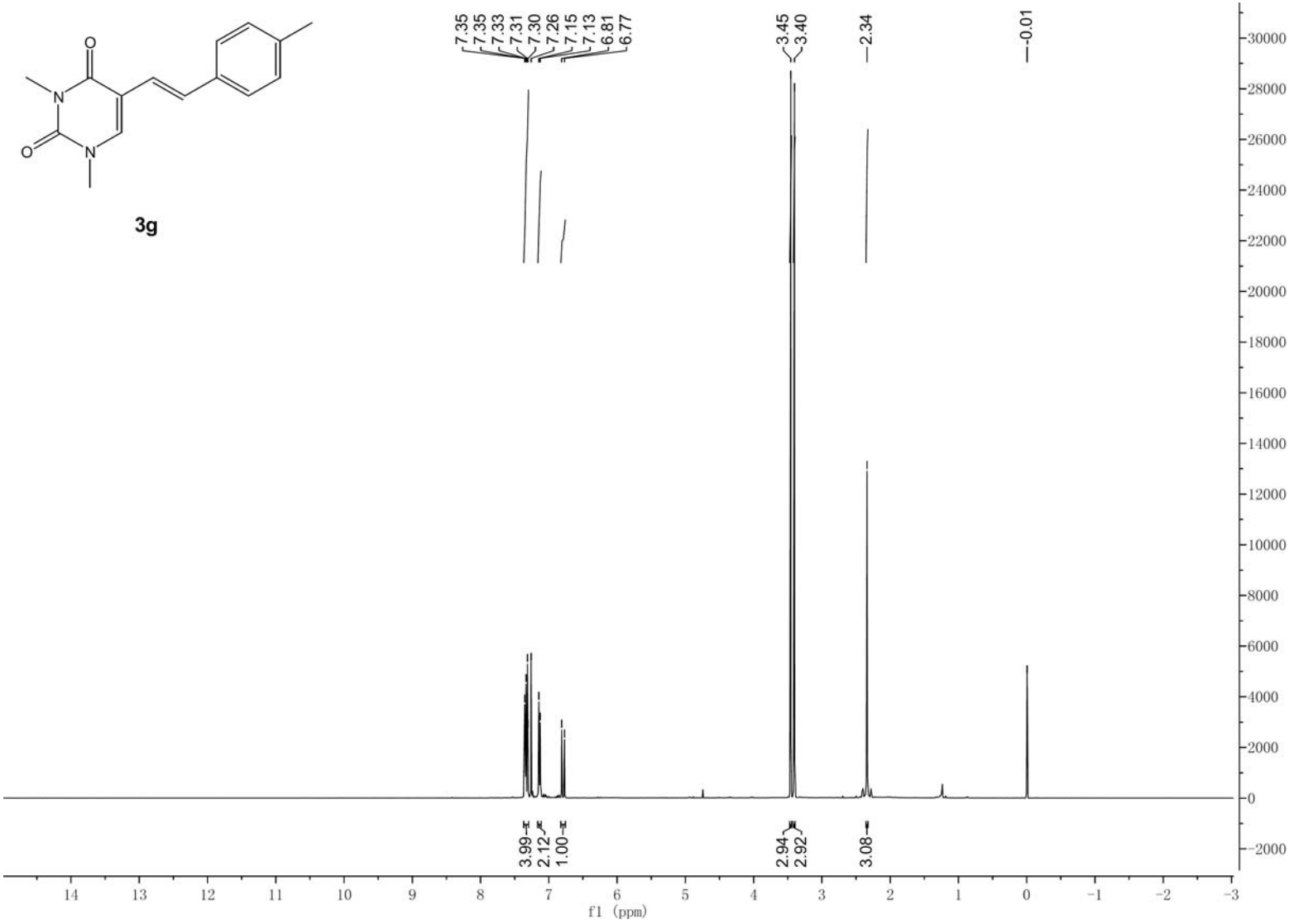

167.60
161.36
150.84
144.91
136.86
118.87
109.02
77.48
77.16
76.84
70.67
63.67
59.16
37.64
28.27
3d
f1 (ppm)

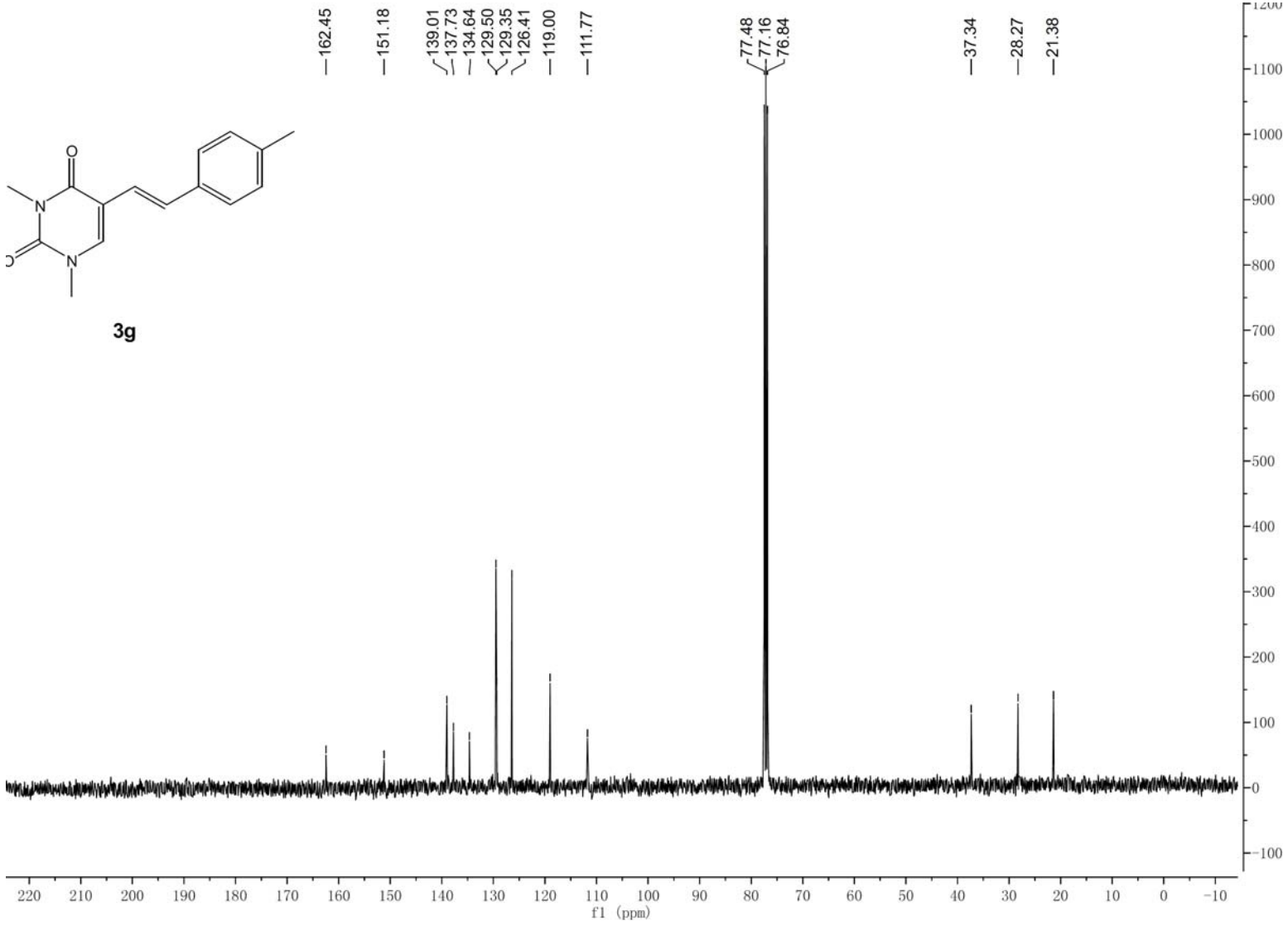

3e
7.45
7.45
7.43
7.43
7.39
7.35
7.34
7.33
7.32
7.31
7.31
7.27
7.26
7.25
7.25
7.24
7.23
7.23
6.84
6.80
3.44
3.40
0.00
1.97
1.11
2.96
0.96
1.00
2.95
2.92
f1 (ppm)

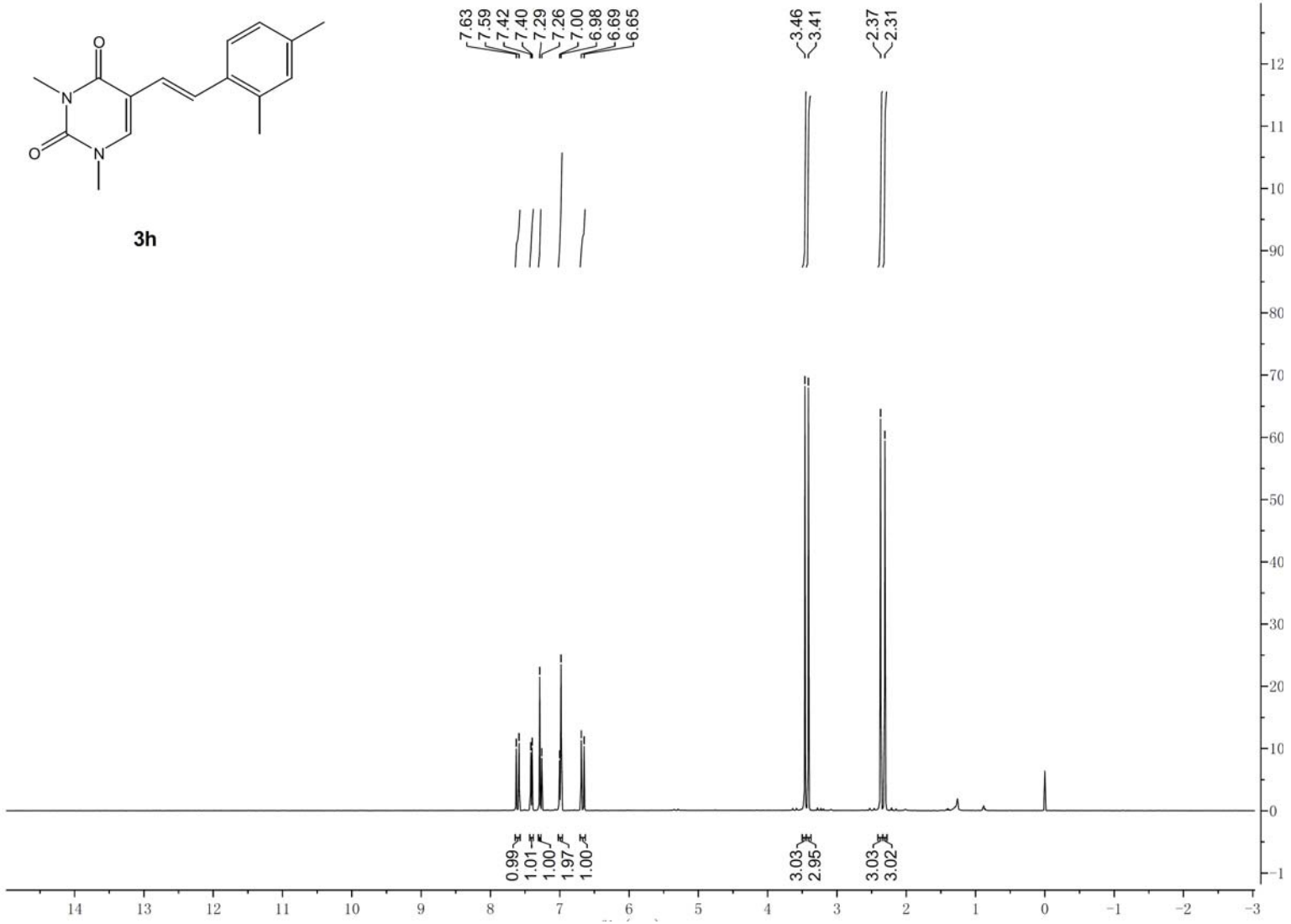

162.26
151.01
139.30
137.35
129.28
128.65
127.65
126.35
119.97
111.43
77.38
77.07
76.75
37.18
28.12
3e
f1 (ppm)

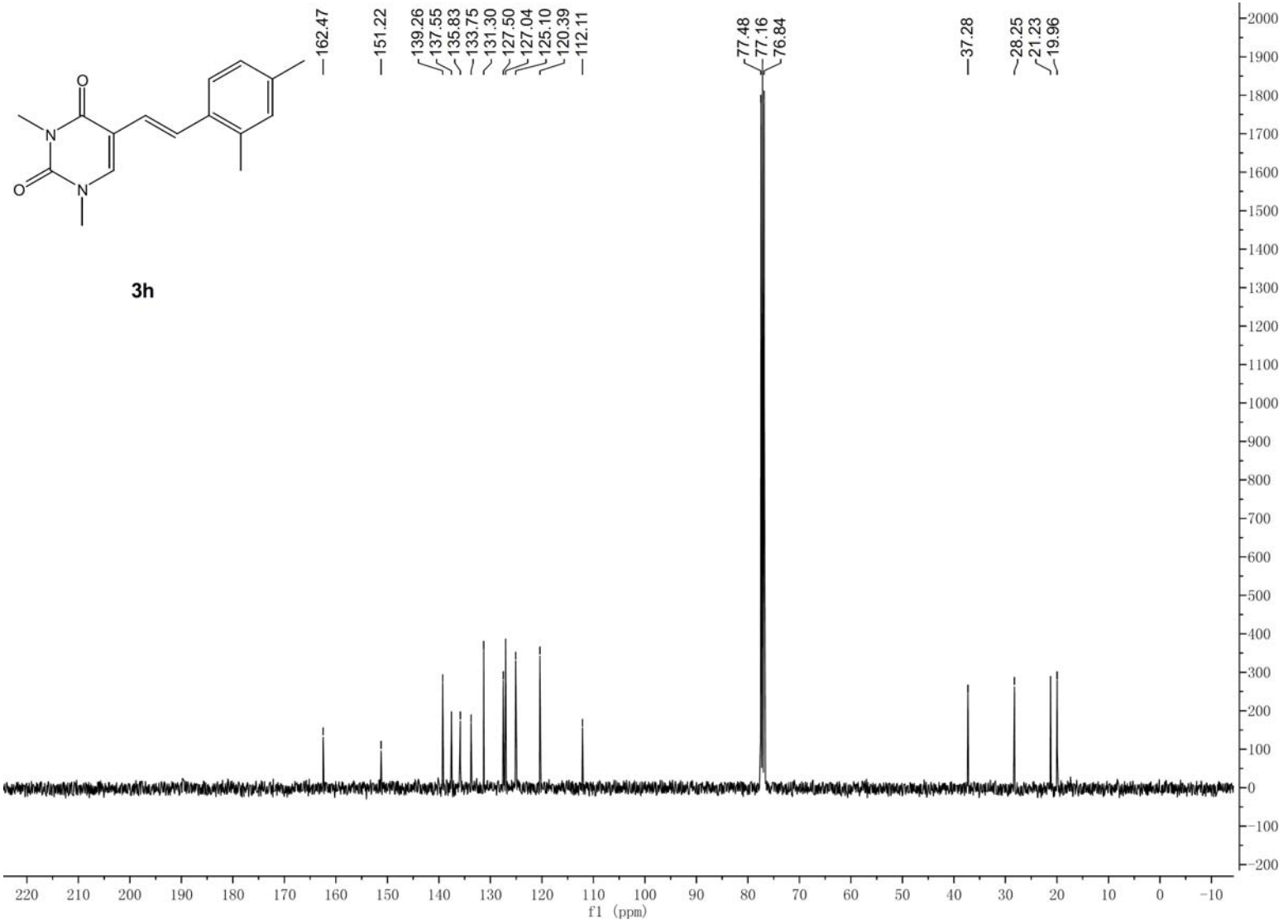

3f
7.34
7.32
7.30
7.28
7.26
7.24
7.24
7.22
7.20
7.07
7.05
6.85
6.81
3.46
3.41
2.35
0.00
0.48
0.98
0.56
1.02
2.00
0.97
1.00
3.03
2.99
3.07
f1 (ppm)

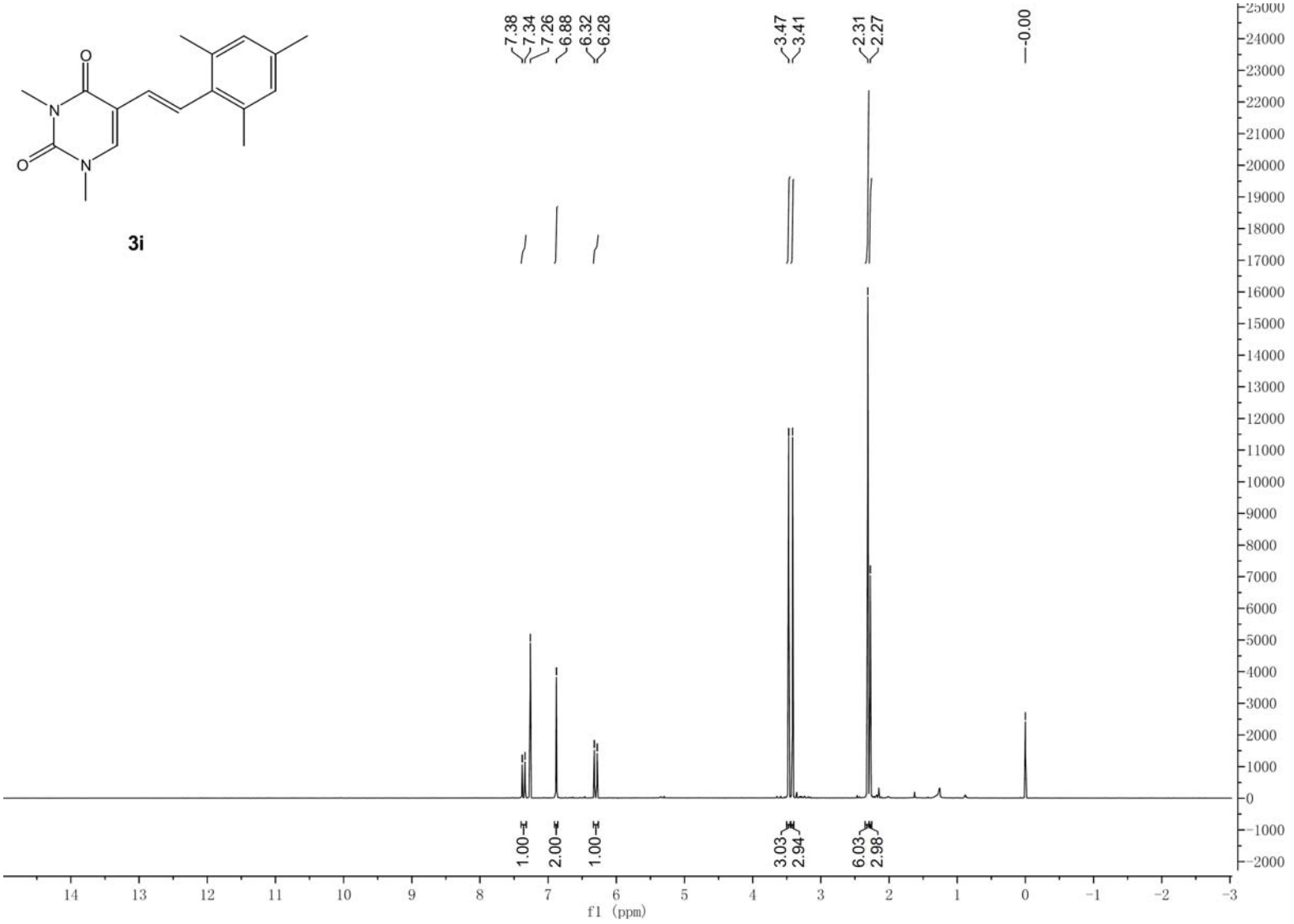

3f
162.41
151.20
139.16
138.34
137.40
129.52
128.68
128.63
127.18
123.75
119.83
111.73
77.48
77.16
76.84
37.32
28.26
21.55
f1 (ppm)

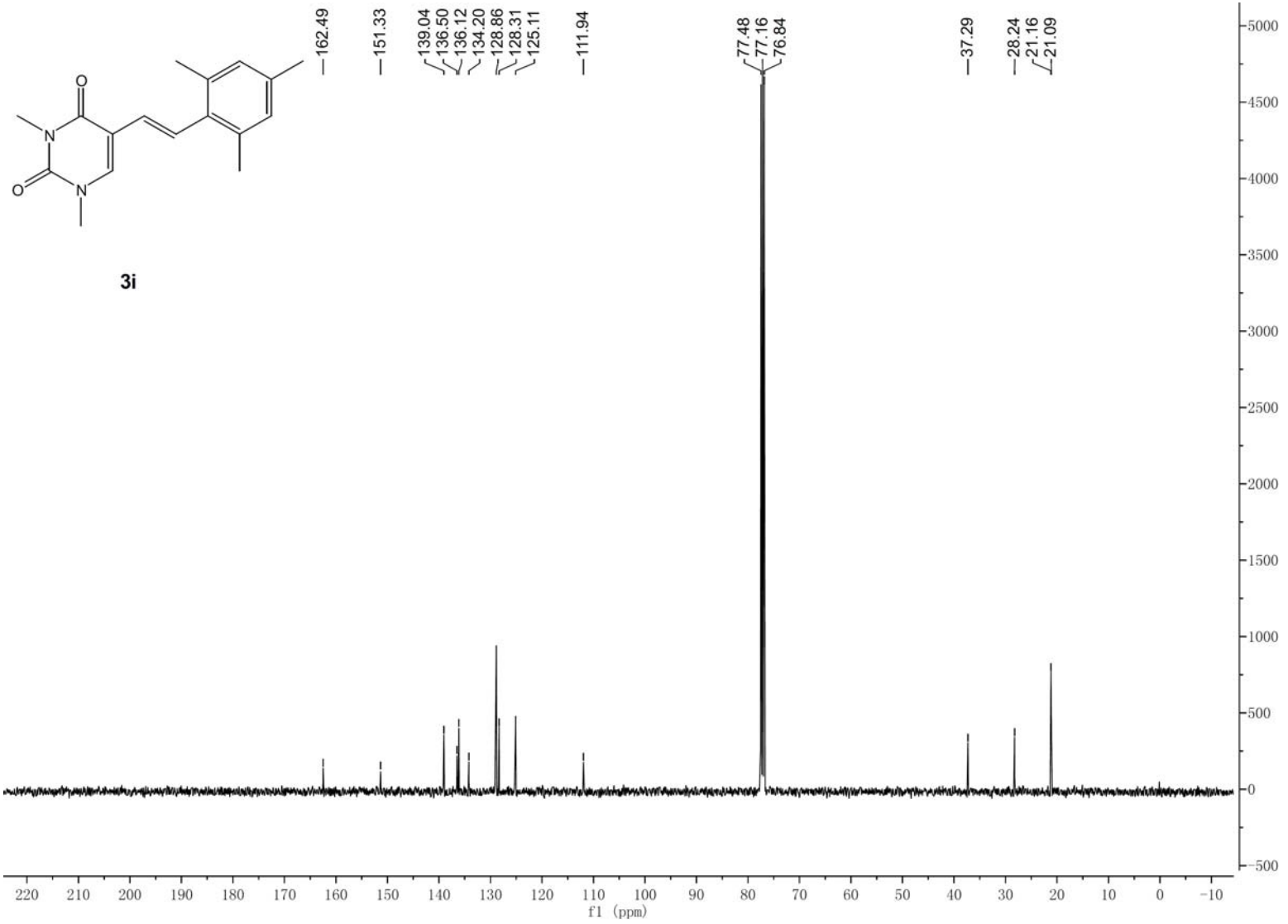

3g
7.35
7.35
7.33
7.31
7.30
7.26
7.15
7.13
6.81
6.77
3.45
3.40
2.34
0.01
3.99
2.12
1.00
2.94
2.92
3.08
f1 (ppm)

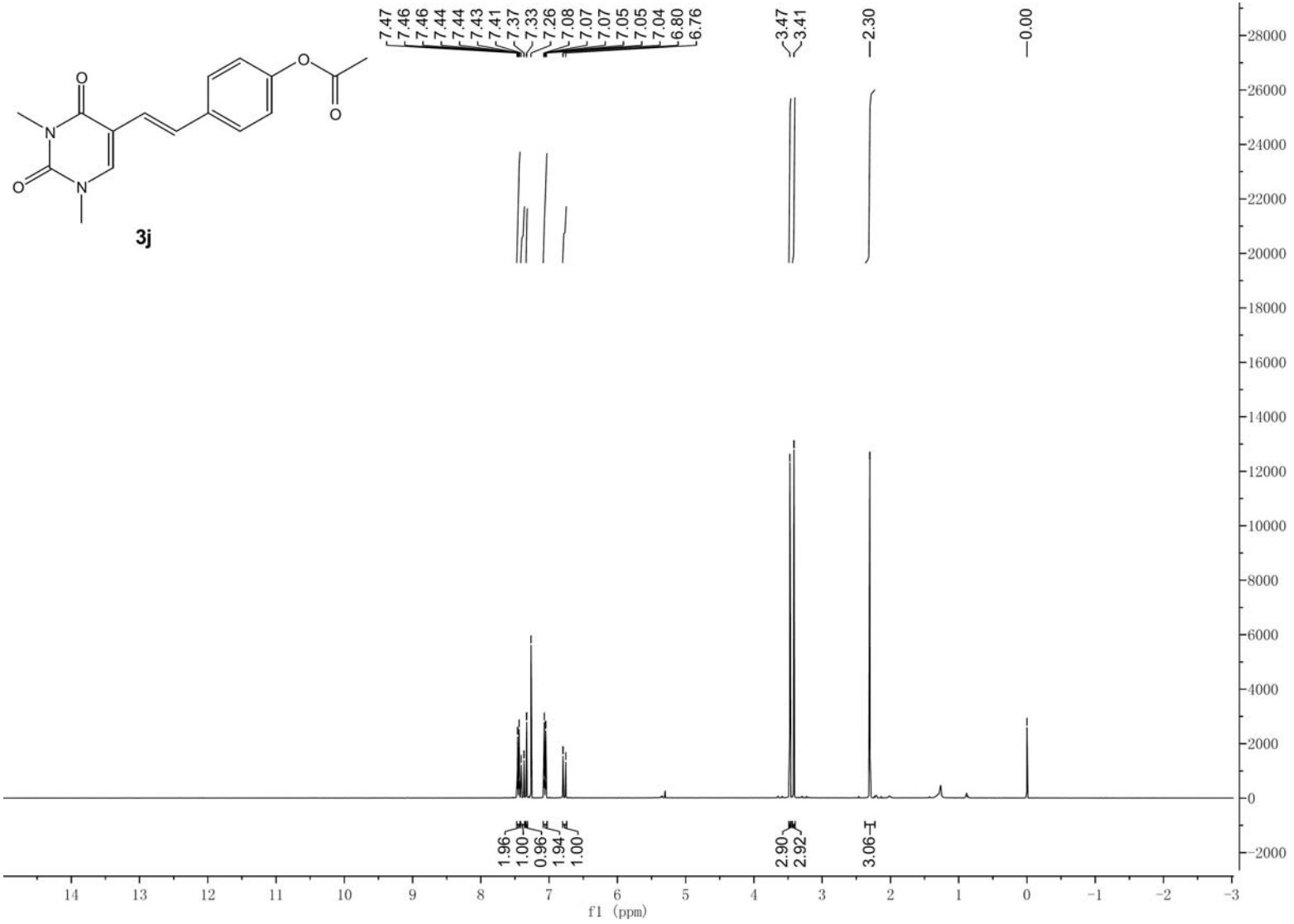

162.45
151.18
139.01
137.73
134.64
129.50
129.35
126.41
119.00
111.77
77.48
77.16
76.84
37.34
28.27
21.38
3g
f1 (ppm)

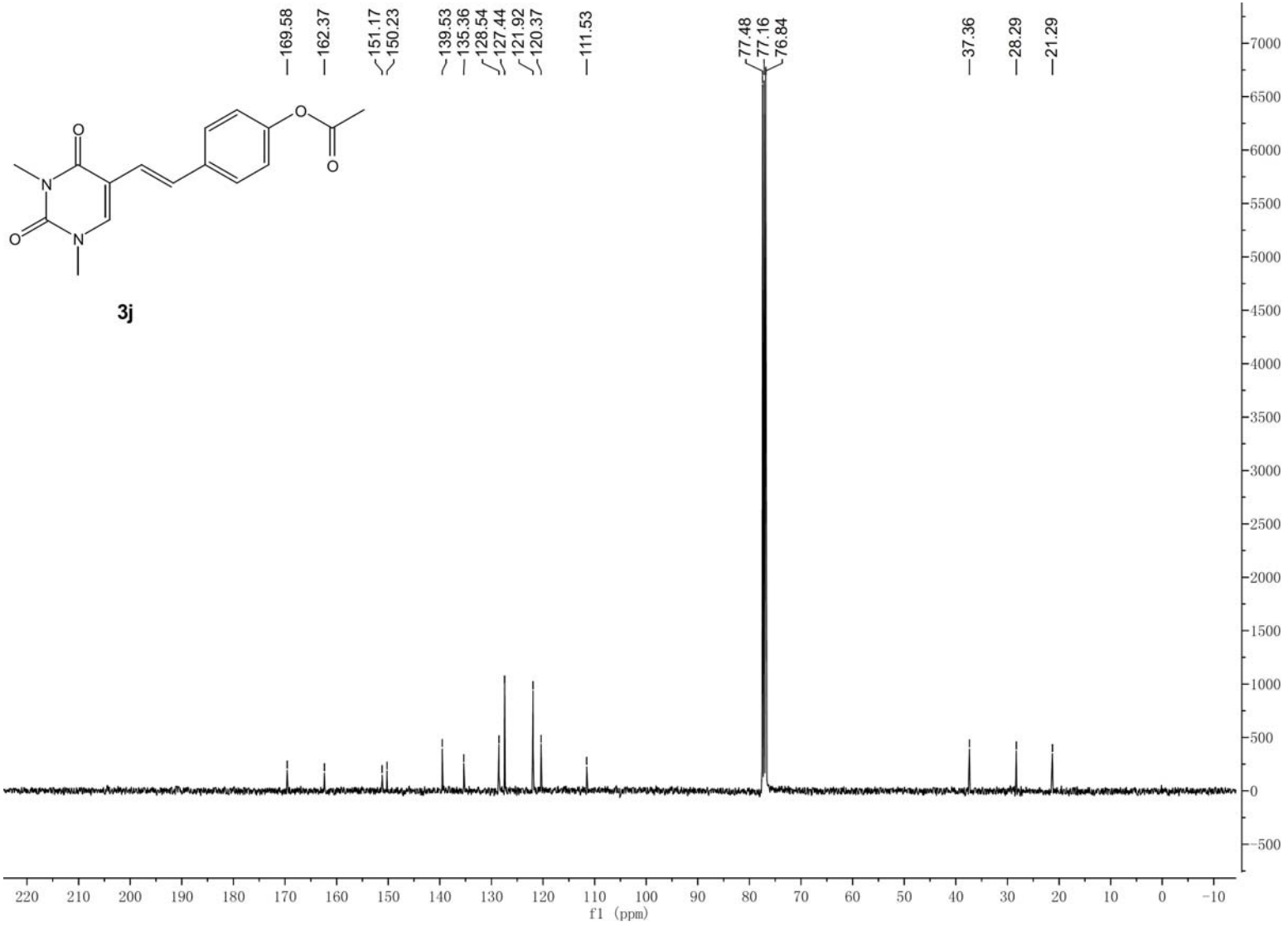

3h
7.63
7.59
7.42
7.40
7.29
7.26
7.00
6.98
6.69
6.65
3.46
3.41
2.37
2.31
0.99
1.01
1.00
1.97
1.00
3.03
2.95
3.03
3.02

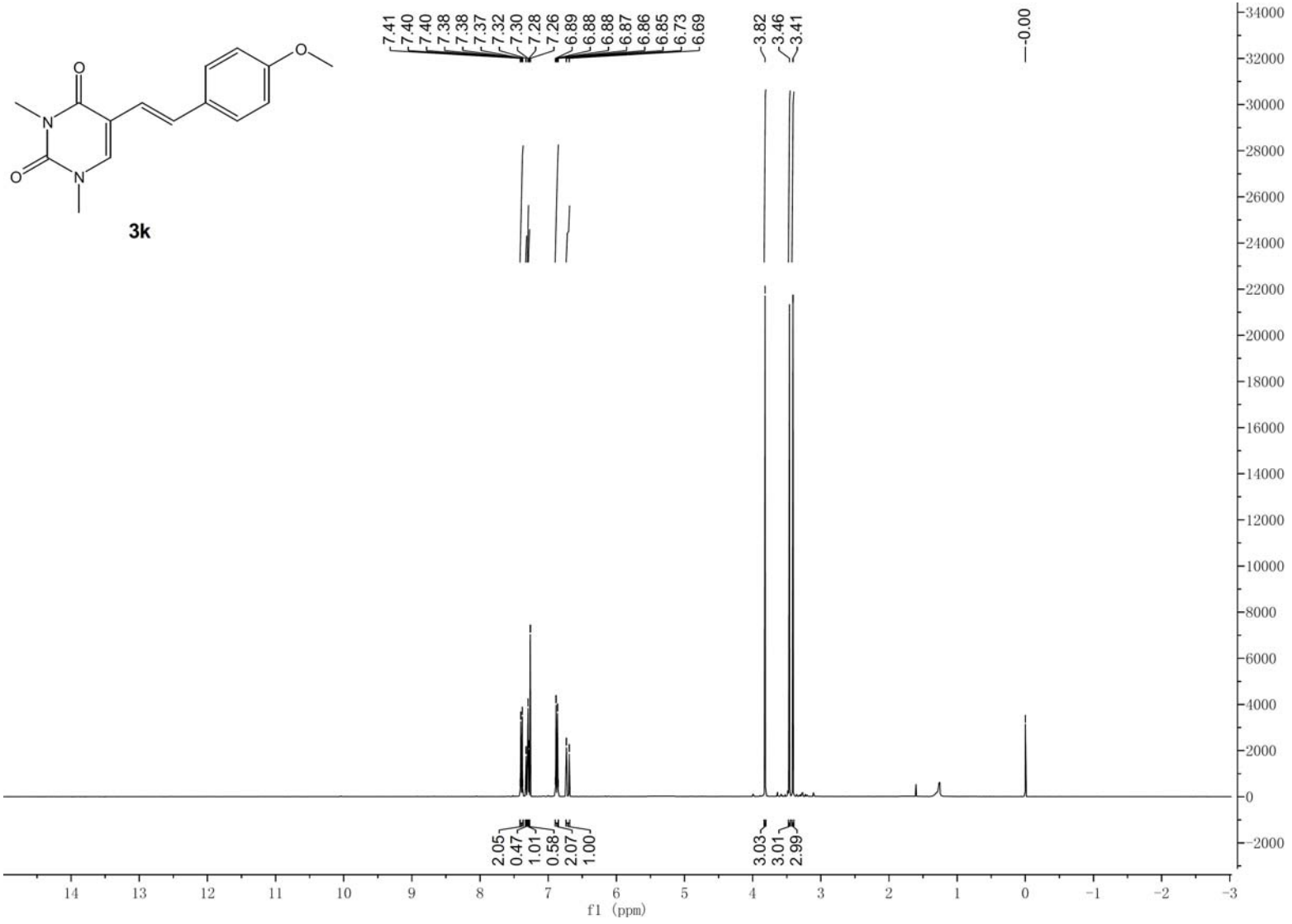

162.47
151.22
139.26
137.55
135.83
133.75
131.30
127.50
127.04
125.10
120.39
112.11
77.48
77.16
76.84
37.28
28.25
21.23
19.96
3h
f1 (ppm)

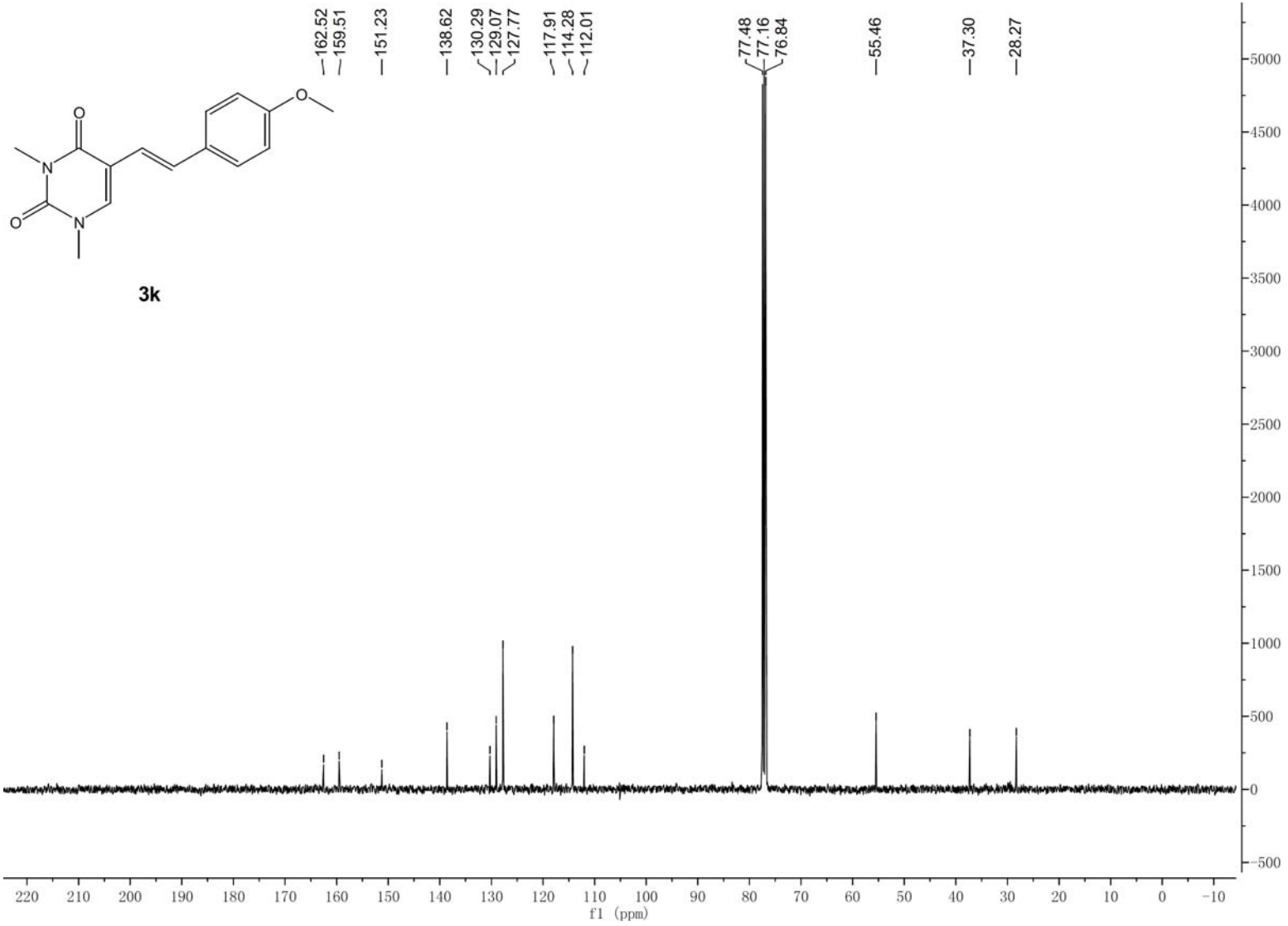

3i
7.38
7.34
7.26
6.88
6.32
6.28
3.47
3.41
2.31
2.27
0.00
1.00
2.00
1.00
3.03
2.94
6.03
2.98
f1 (ppm)

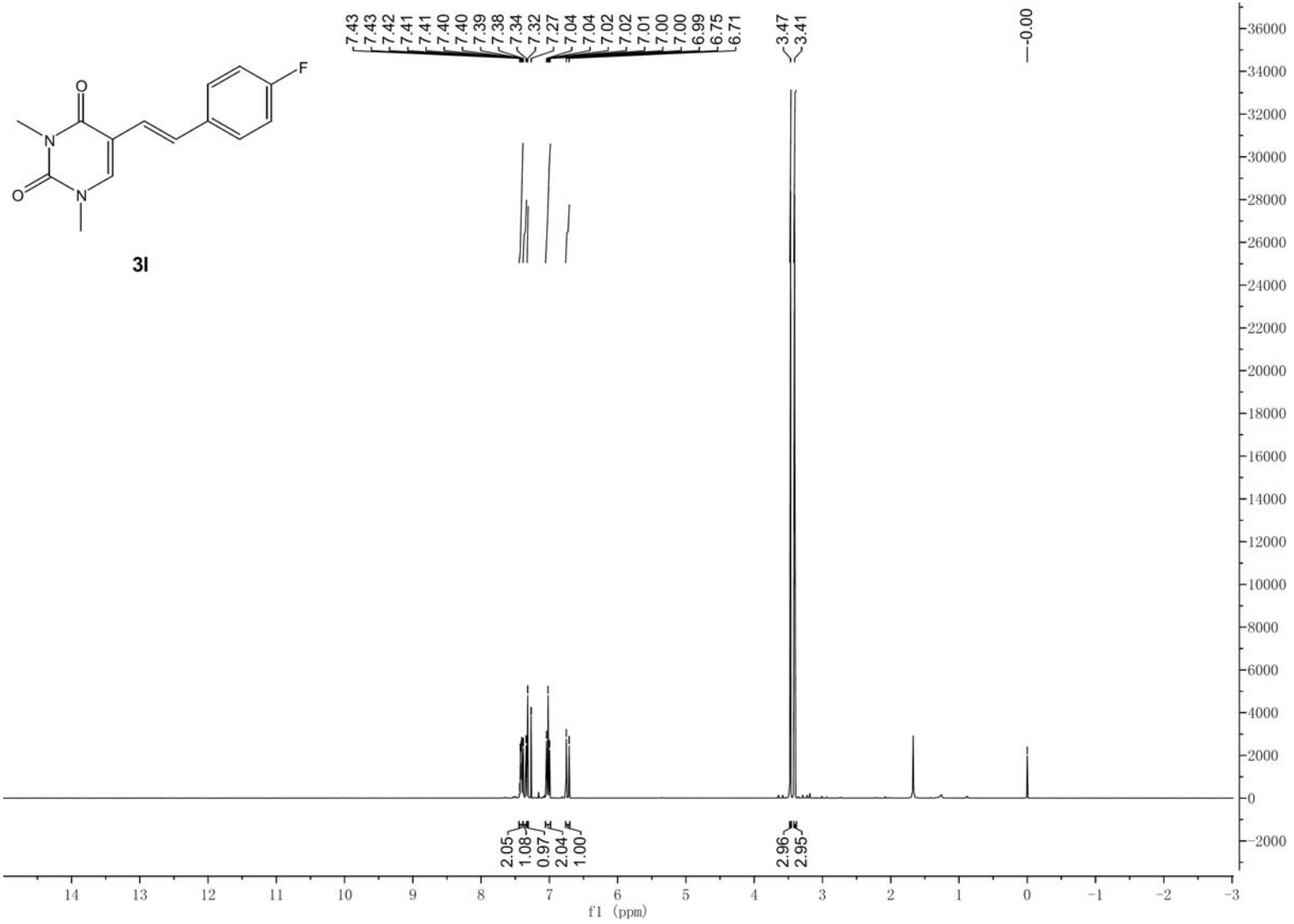

162.49
151.33
139.04
136.50
136.12
134.20
128.86
128.31
125.11
111.94
77.48
77.16
76.84
37.29
28.24
21.16
21.09
3i
f1 (ppm)

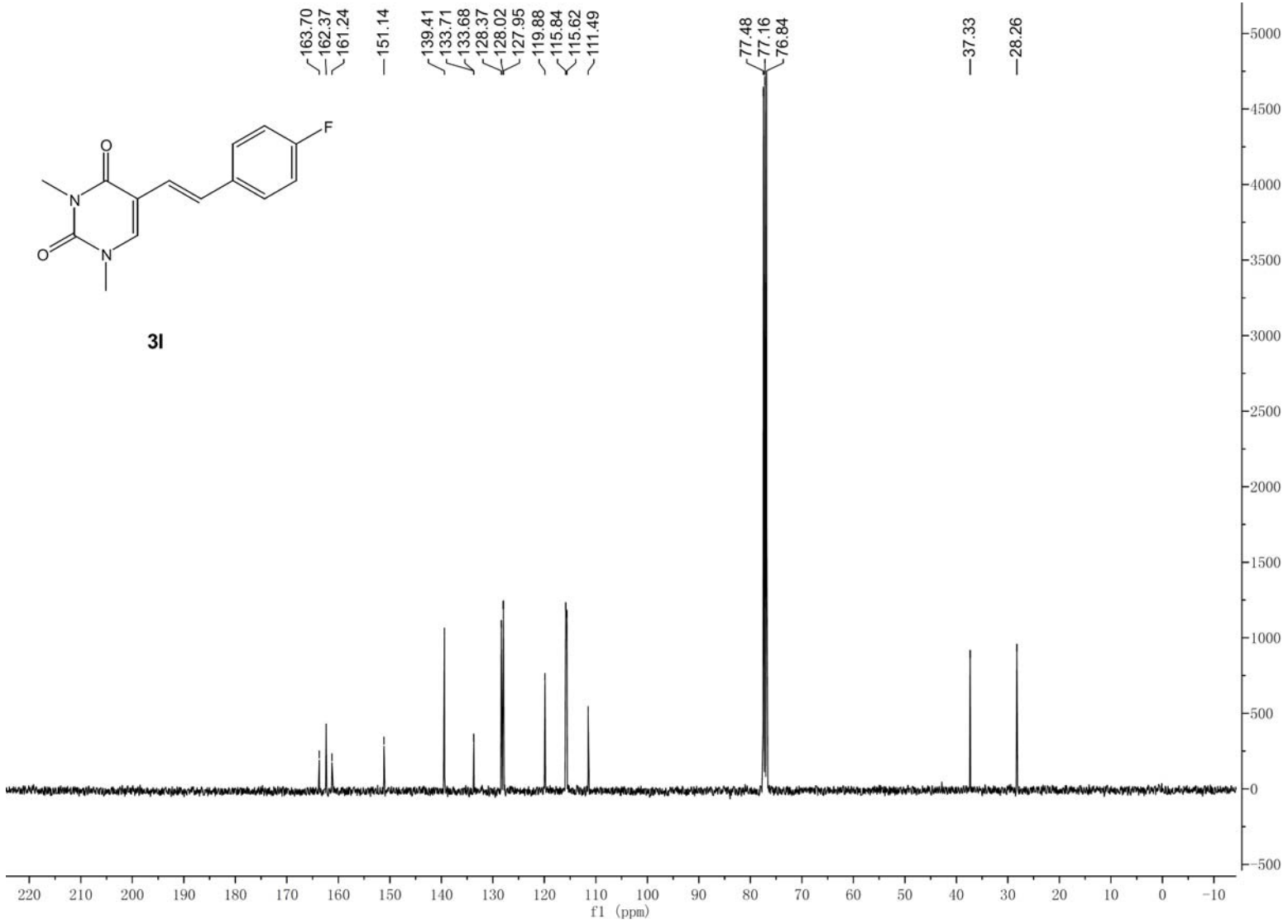

3j
7.47
7.46
7.46
7.44
7.44
7.43
7.41
7.37
7.33
7.26
7.08
7.07
7.07
7.05
7.05
7.04
6.80
6.76
3.47
3.41
2.30
0.00
1.96
1.00
0.96
1.94
1.00
2.90
2.92
3.06
f1 (ppm)

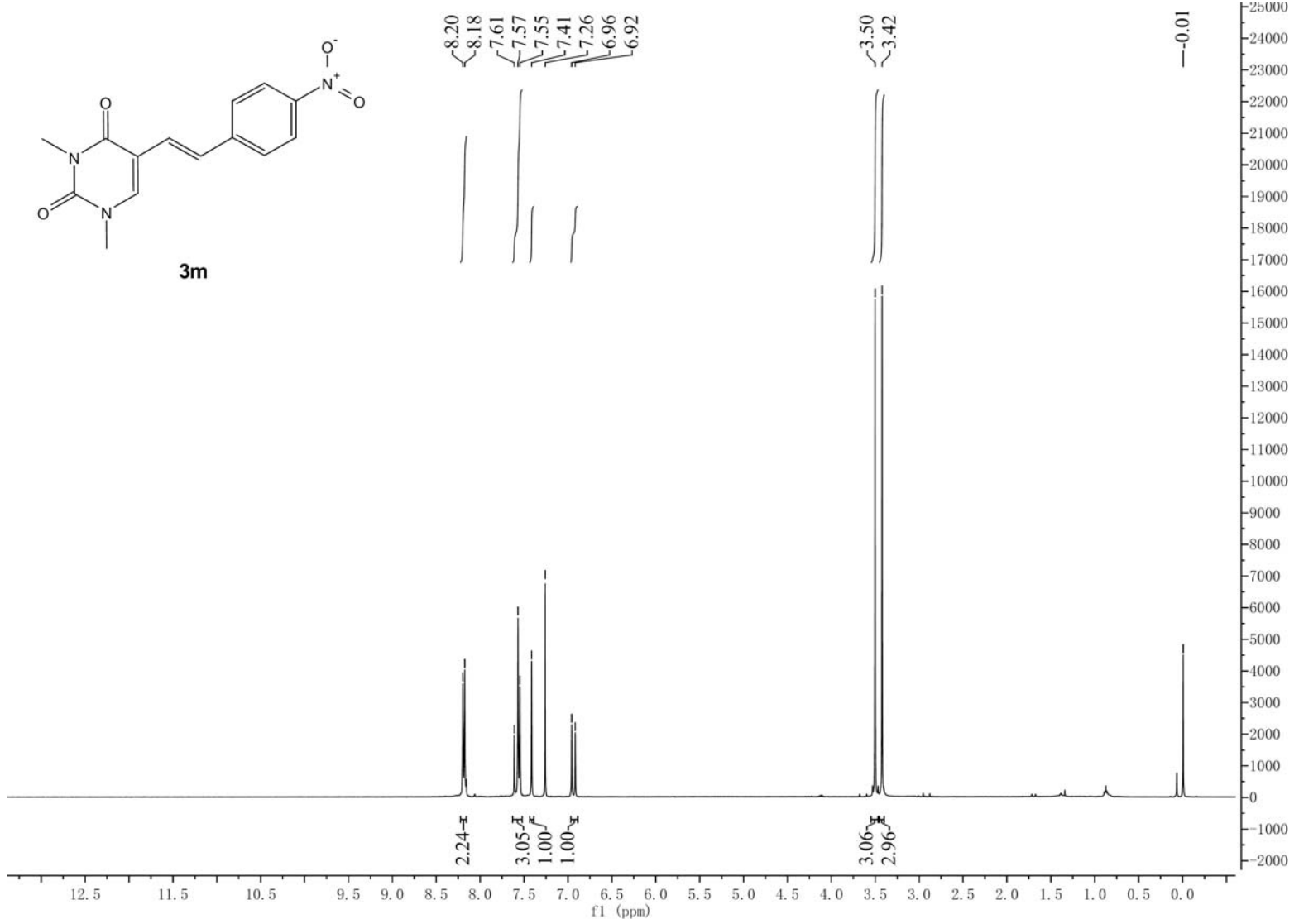

169.58
162.37
151.17
150.23
139.53
135.36
128.54
127.44
121.92
120.37
111.53
77.48
77.16
76.84
37.36
28.29
21.29
O
N
O
N
O
O
3j
7000
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
−500
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)

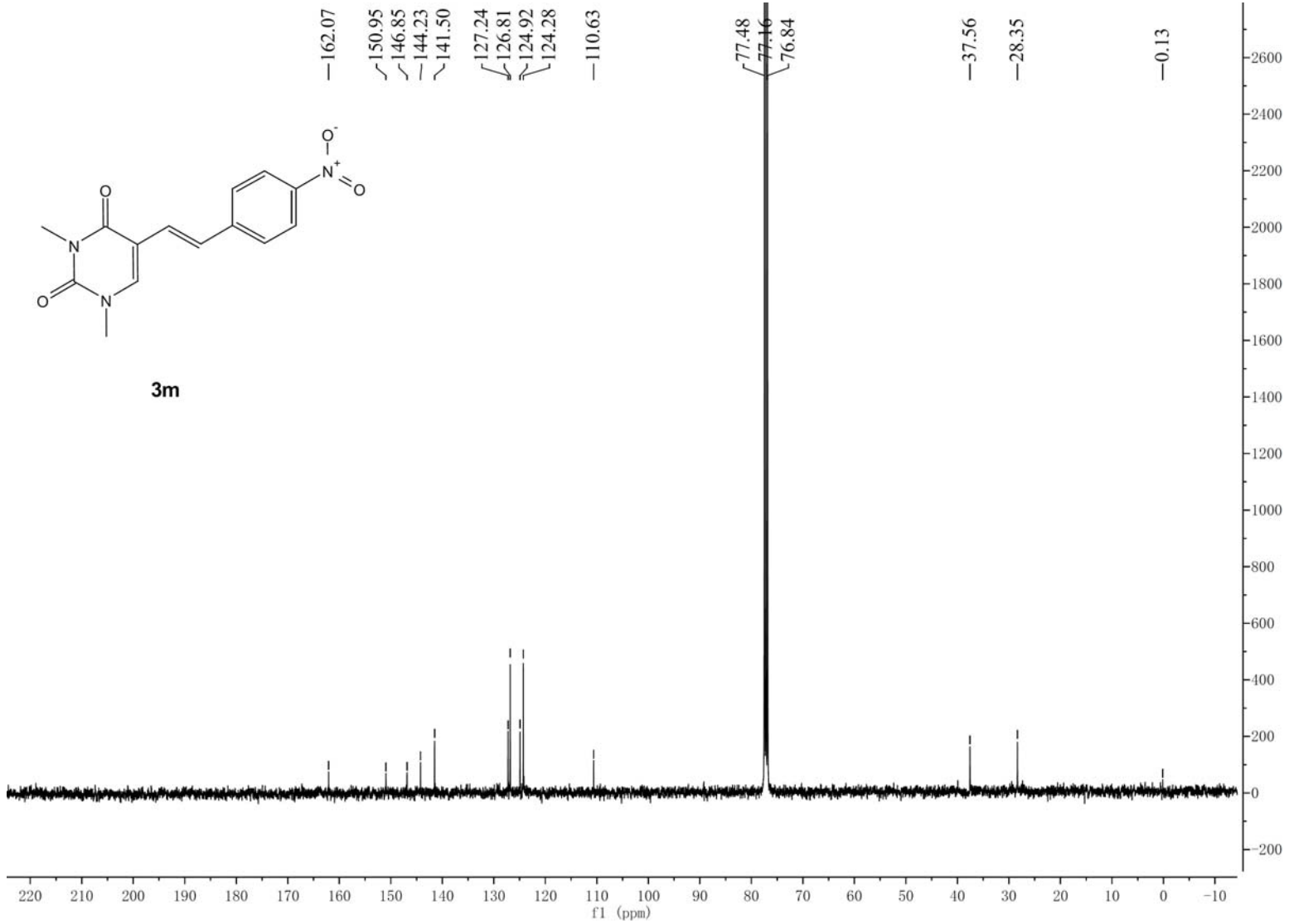

3k
7.41
7.40
7.40
7.38
7.38
7.37
7.32
7.30
7.28
7.26
6.89
6.88
6.88
6.87
6.86
6.85
6.73
6.69
3.82
3.46
3.41
0.00
2.05
0.47
1.01
0.58
2.07
1.00
3.03
3.01
2.99
f1 (ppm)

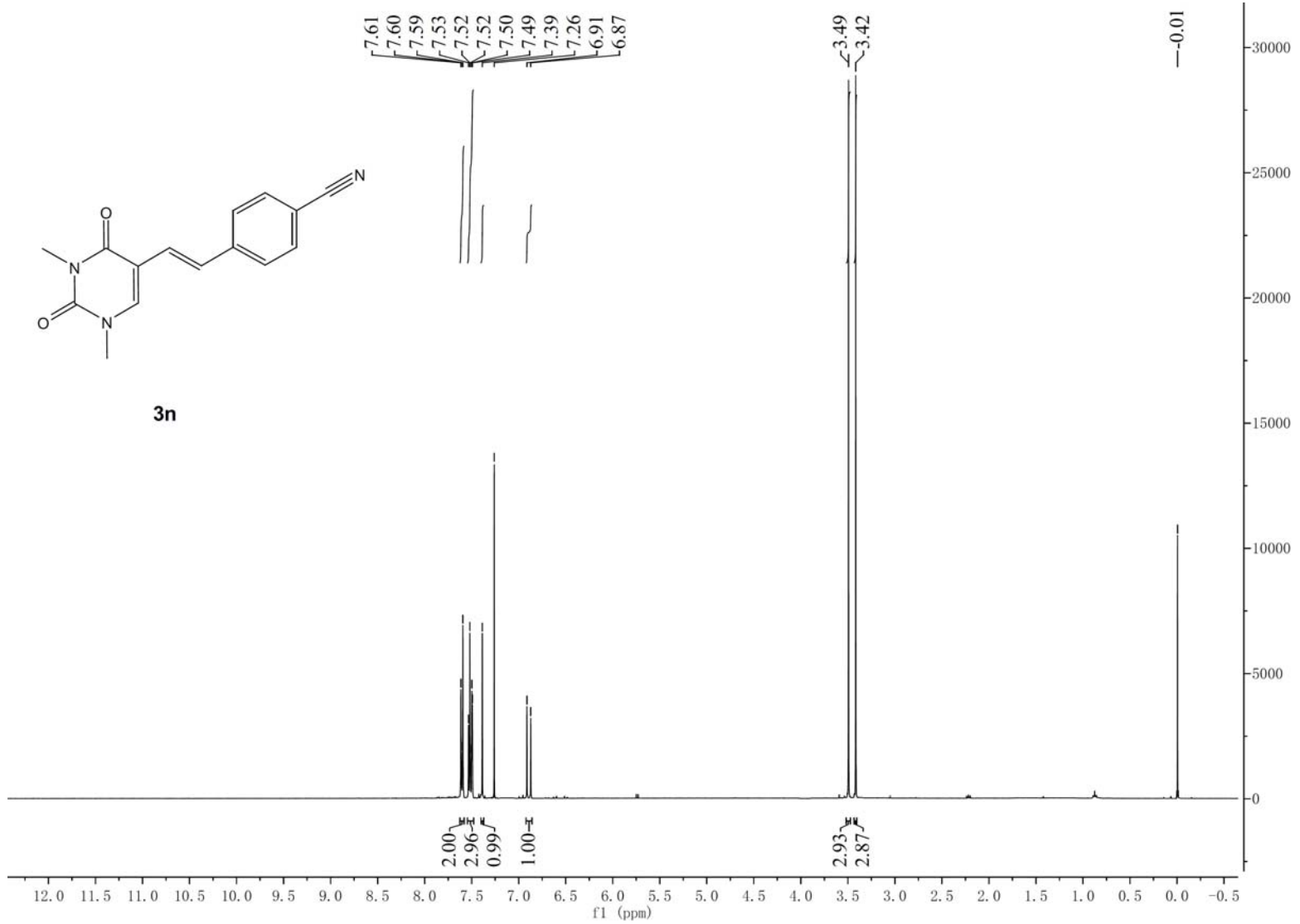

162.52
159.51
151.23
138.62
130.29
129.07
127.77
117.91
114.28
112.01
77.48
77.16
76.84
55.46
37.30
28.27
O
N
O
N
O
3k
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

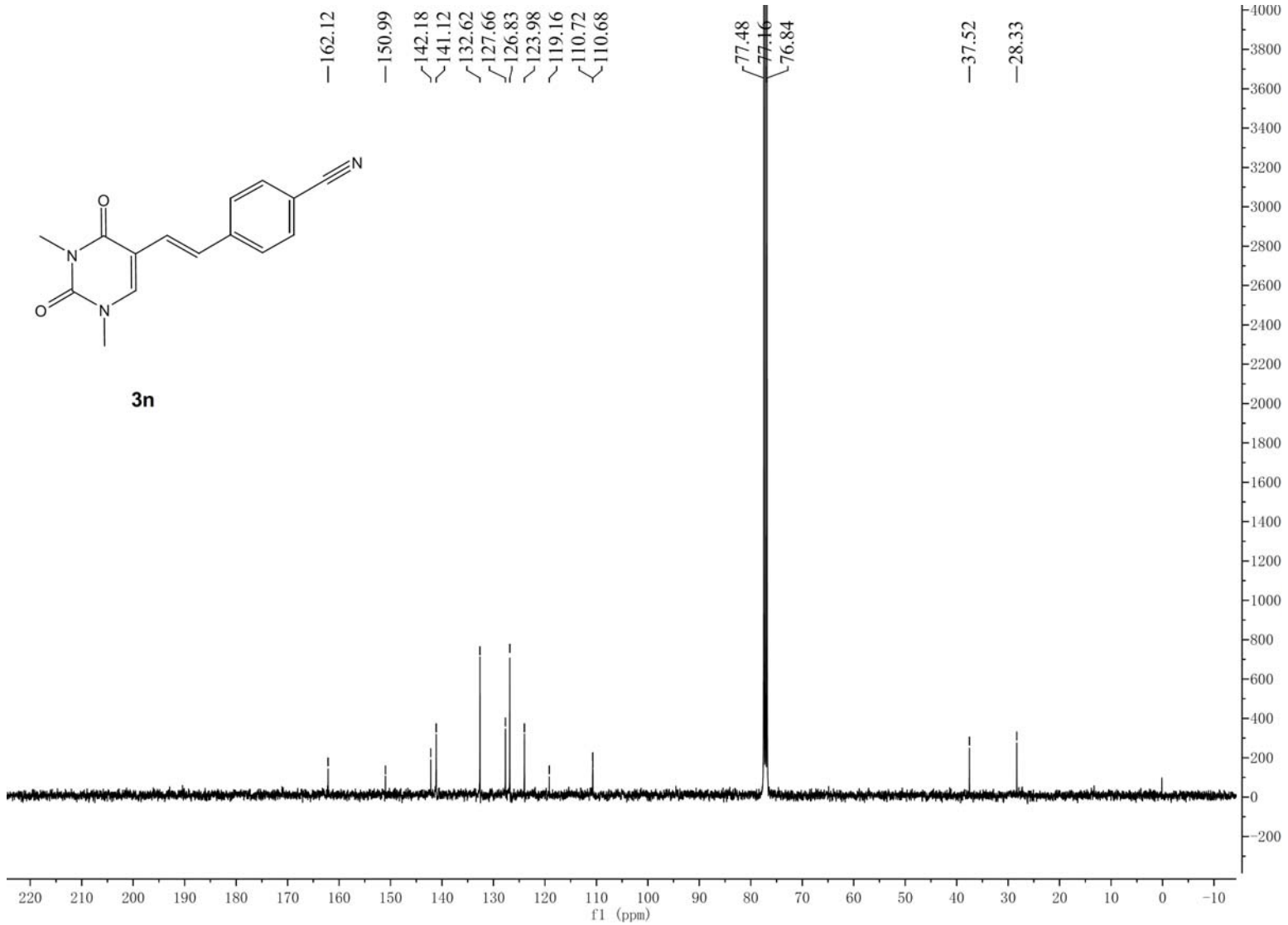

3l
7.43
7.43
7.42
7.41
7.41
7.40
7.40
7.39
7.38
7.34
7.32
7.27
7.04
7.04
7.02
7.02
7.01
7.00
7.00
6.99
6.75
6.71
3.47
3.41
0.00
2.05
1.08
0.97
2.04
1.00
2.96
2.95
f1 (ppm)

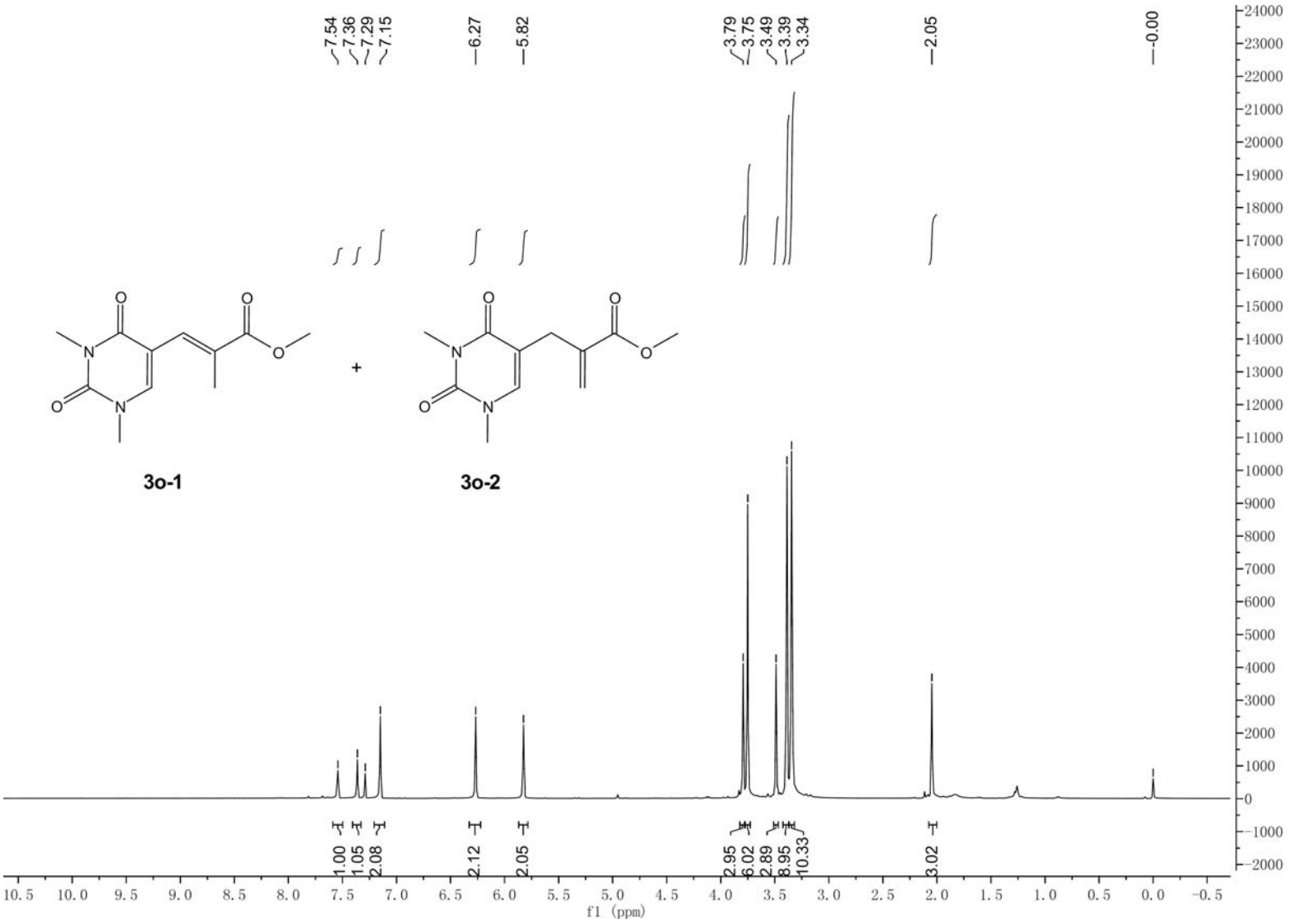

163.70
162.37
161.24
151.14
139.41
133.71
133.68
128.37
128.02
127.95
119.88
115.84
115.62
111.49
77.48
77.16
76.84
37.33
28.26
O
N
O
N
F
3l
f1 (ppm)

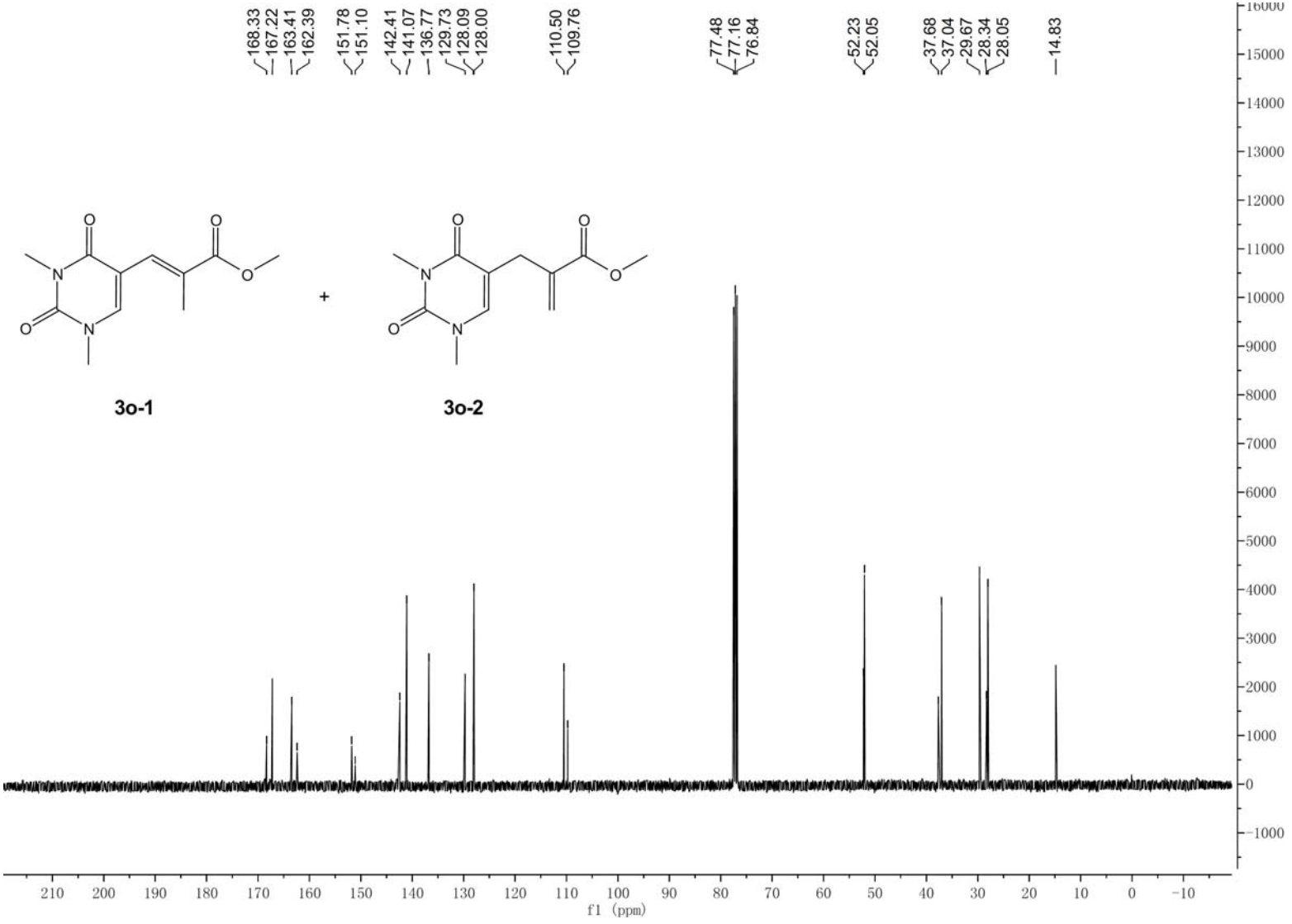

3m
8.20
8.18
7.61
7.57
7.55
7.41
7.26
6.96
6.92
3.50
3.42
-0.01
2.24
3.05
1.00
1.00
3.06
2.96
f1 (ppm)

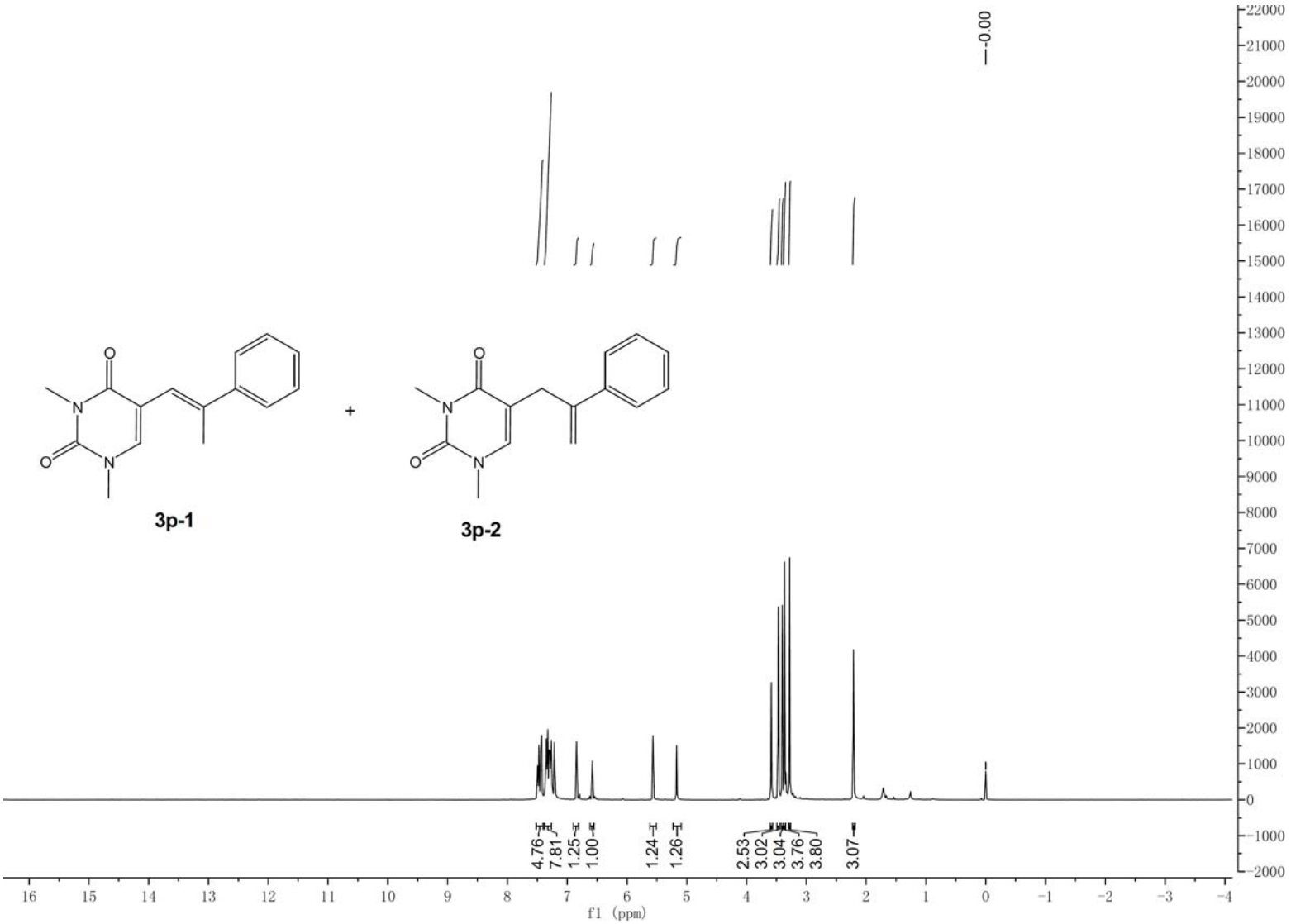

162.07
150.95
146.85
144.23
141.50
127.24
126.81
124.92
124.28
110.63
77.48
77.16
76.84
37.56
28.35
0.13
3m
f1 (ppm)

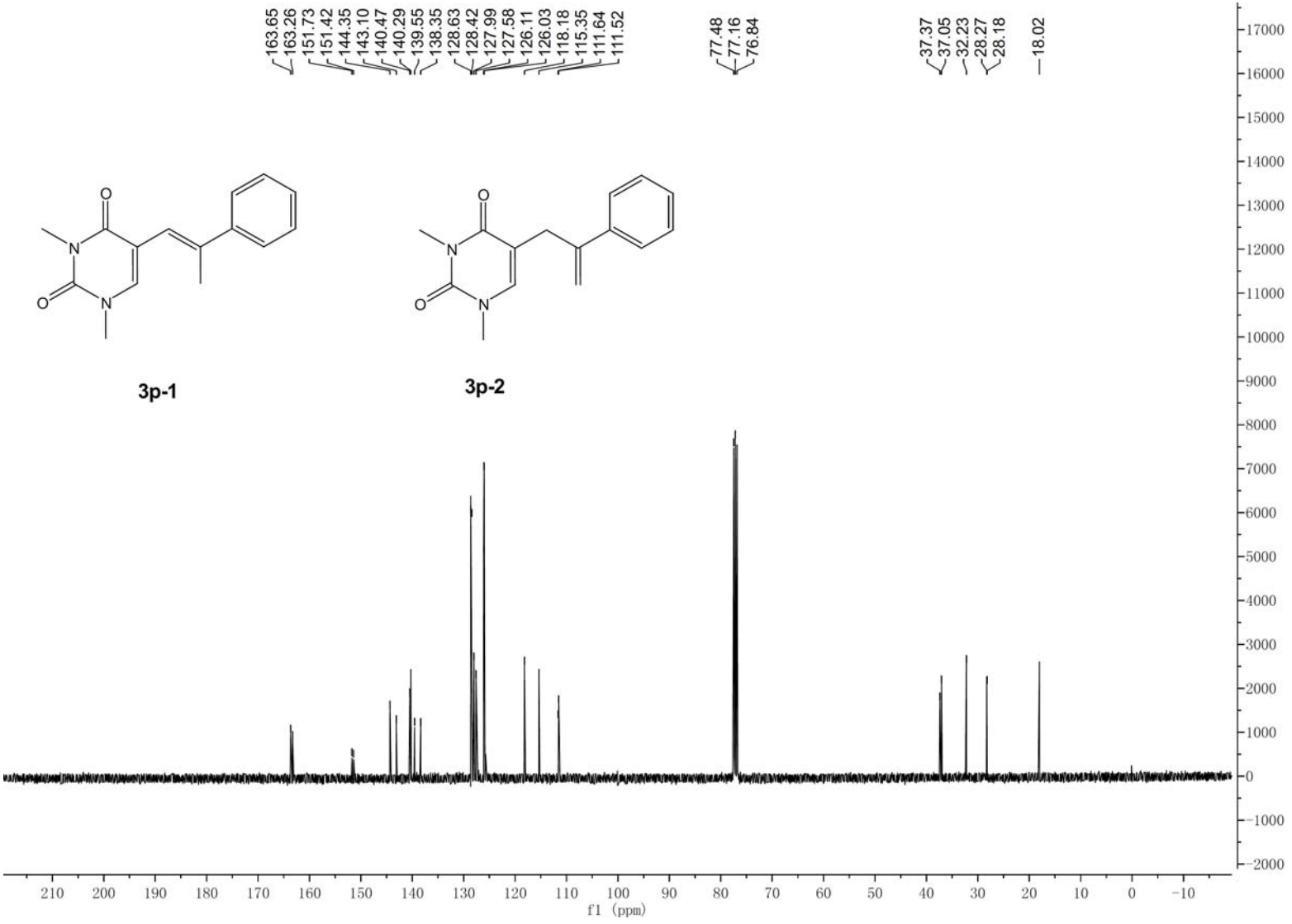

7.61
7.60
7.59
7.53
7.52
7.52
7.50
7.49
7.39
7.26
6.91
6.87
3.49
3.42
-0.01
O
N
O
N
N
3n
2.00
2.96
0.99
1.00
2.93
2.87
f1 (ppm)

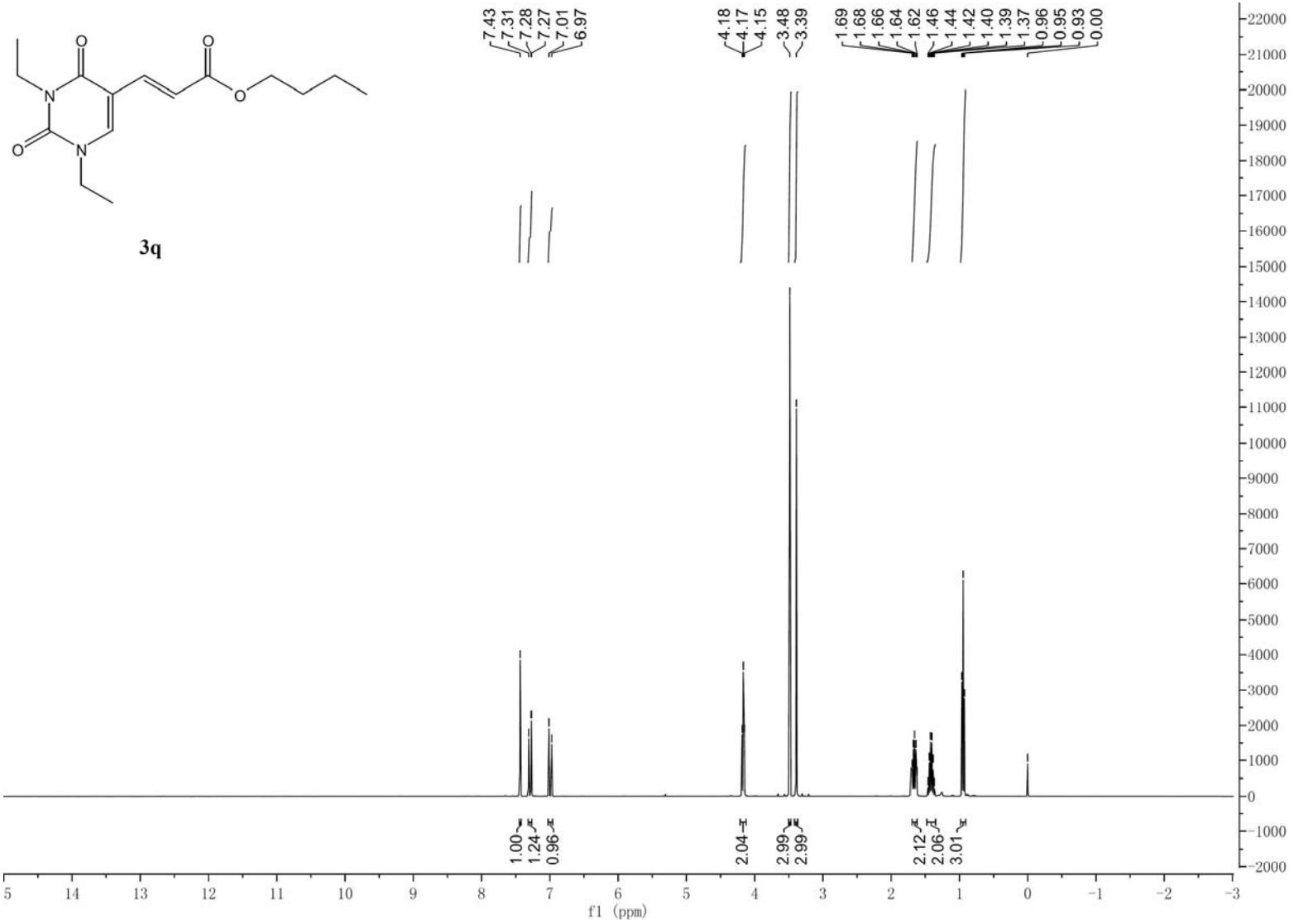

162.12
150.99
142.18
141.12
132.62
127.66
126.83
123.98
119.16
110.72
110.68
77.48
77.16
76.84
37.52
28.33
O
N
O
N
N
3n
f1 (ppm)

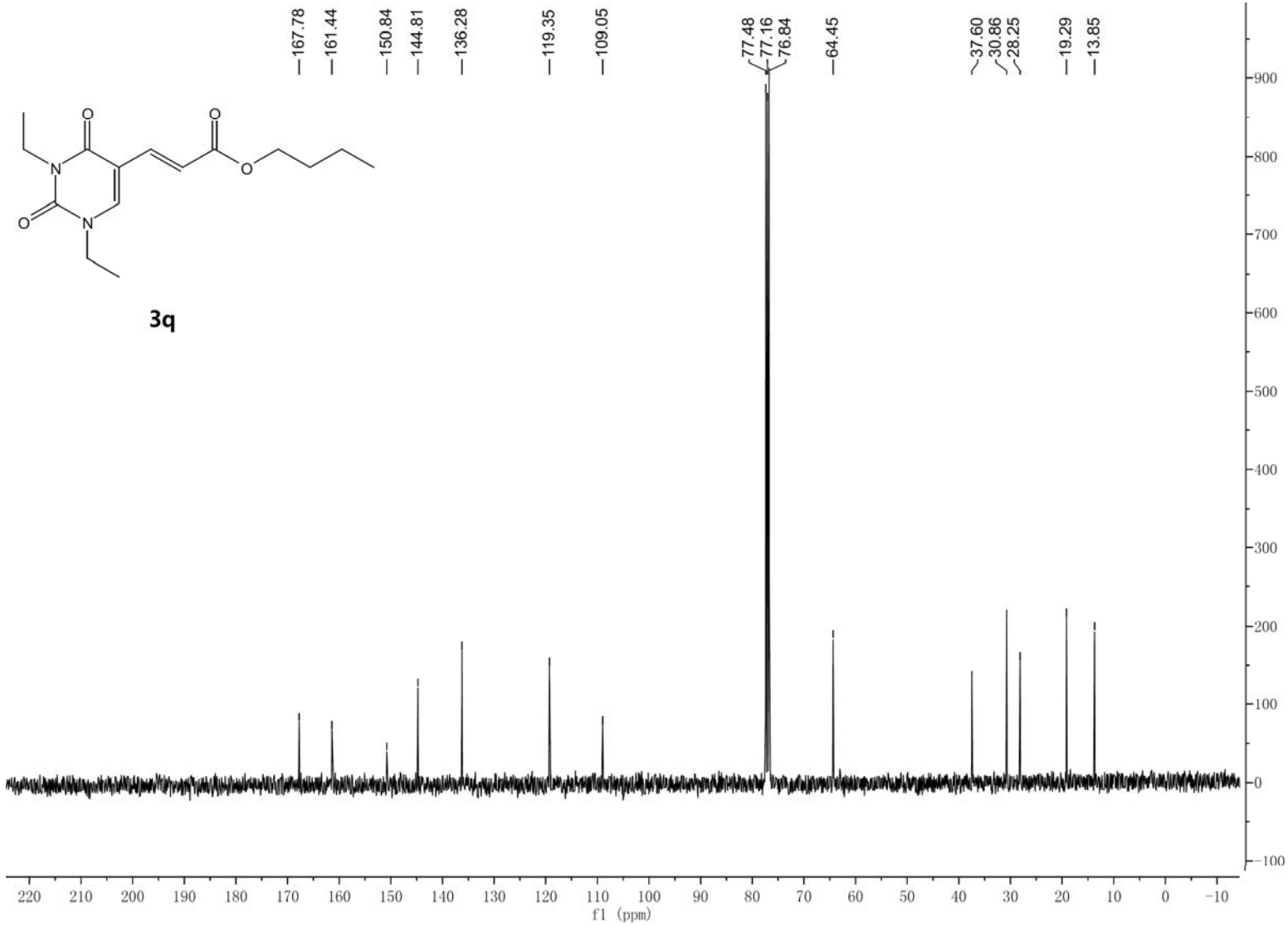

7.54
7.36
7.29
7.15
6.27
5.82
3.79
3.75
3.49
3.39
3.34
2.05
0.00
3o-1
3o-2
1.00
1.05
2.08
2.12
2.05
2.95
6.02
2.89
8.95
10.33
3.02
f1 (ppm)

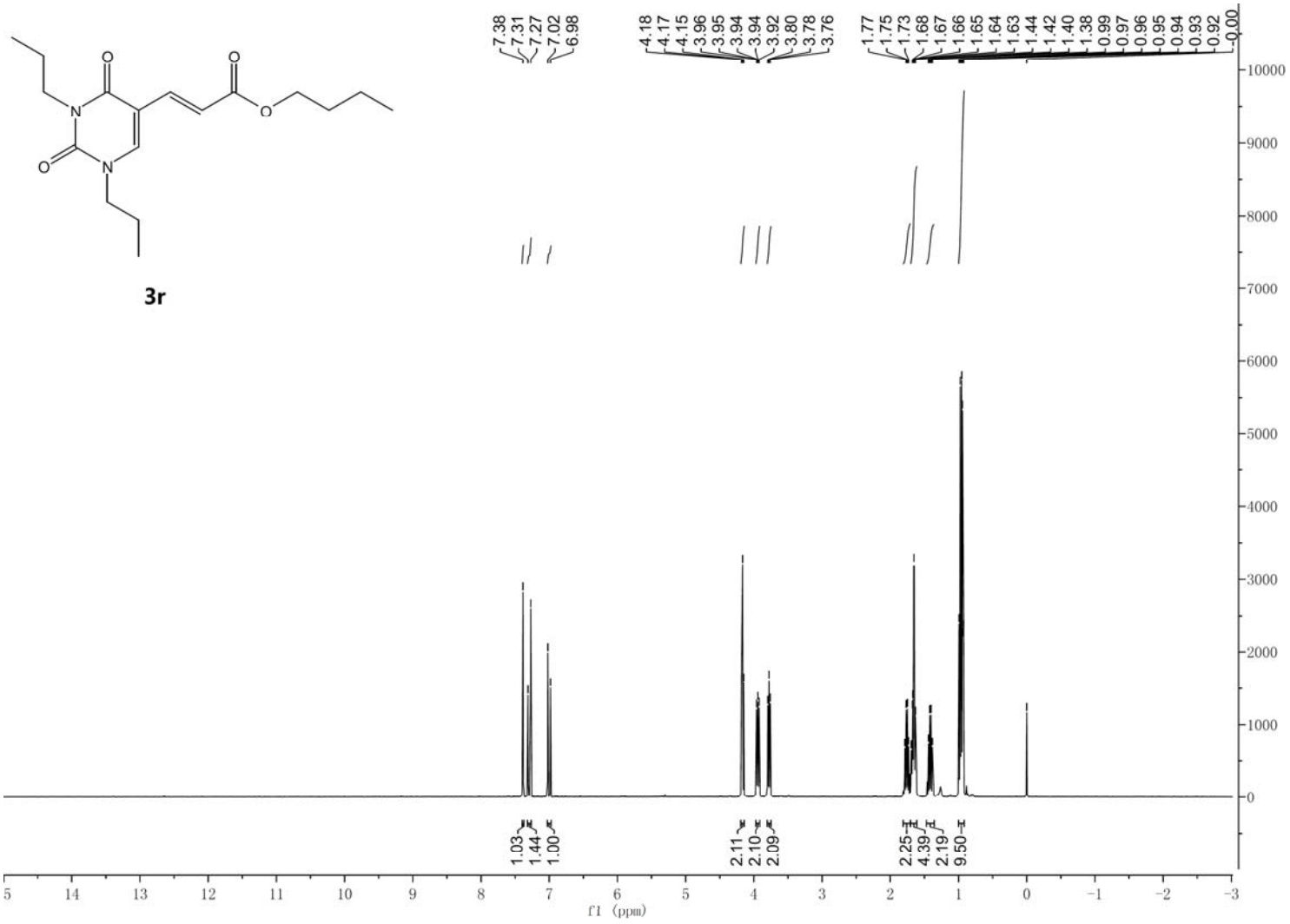

168.33
167.22
163.41
162.39
151.78
151.10
142.41
141.07
136.77
129.73
128.09
128.00
110.50
109.76
77.48
77.16
76.84
52.23
52.05
37.68
37.04
29.67
28.34
28.05
14.83
3o-1
+
3o-2
f1 (ppm)

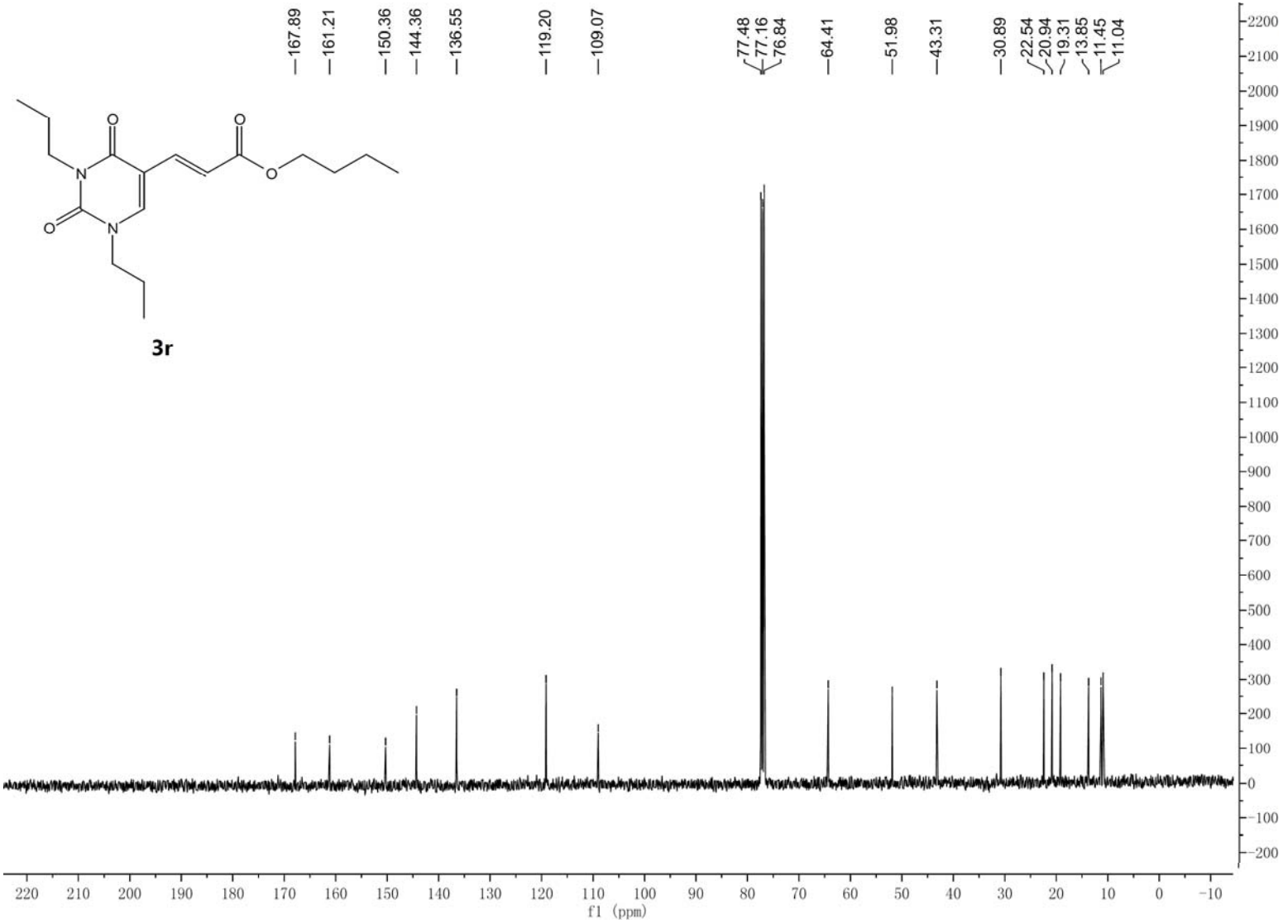

3p-1
+
3p-2
—0.00
4.76
7.81
1.25
1.00
1.24
1.26
2.53
3.02
3.04
3.76
3.80
3.07
f1 (ppm)

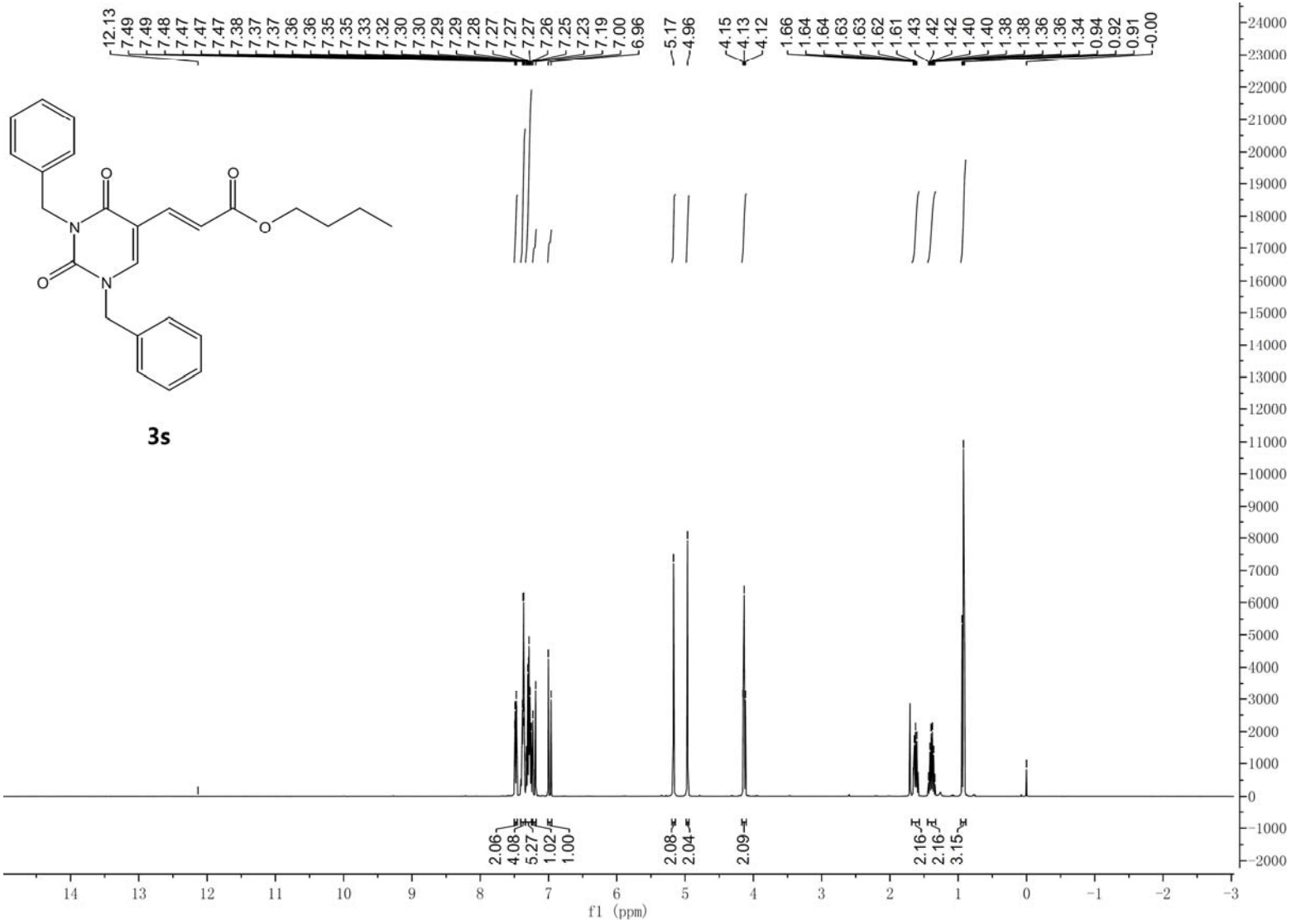

163.65
163.26
151.73
151.42
144.35
143.10
140.47
140.29
139.55
138.35
128.63
128.42
127.99
127.58
126.11
126.03
118.18
115.35
111.64
111.52
77.48
77.16
76.84
37.37
37.05
32.23
28.27
28.18
18.02
3p-1
3p-2
f1 (ppm)

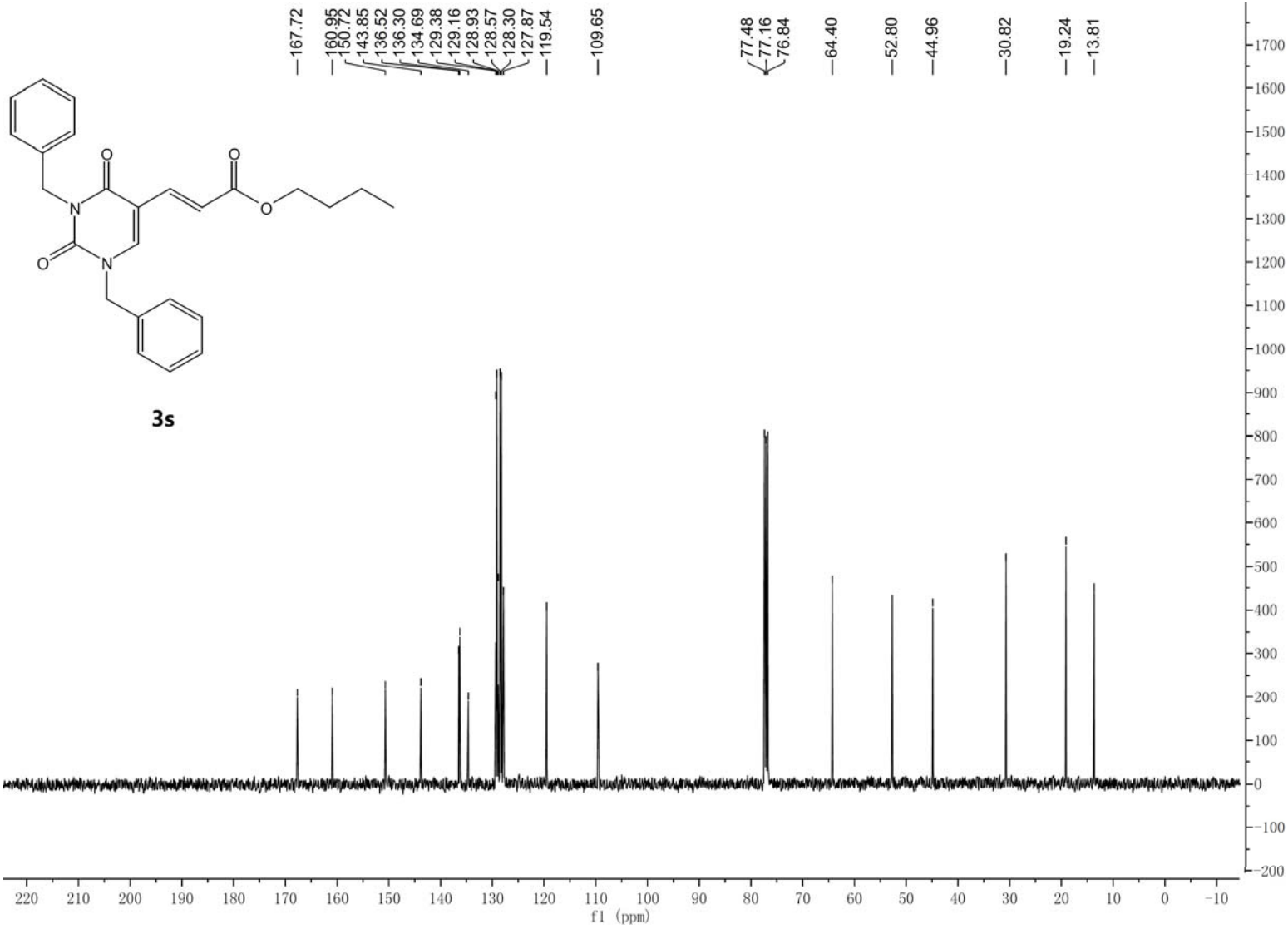

3q
7.43
7.31
7.28
7.27
7.01
6.97
4.18
4.17
4.15
3.48
3.39
1.69
1.68
1.66
1.64
1.62
1.46
1.44
1.42
1.40
1.39
1.37
0.96
0.95
0.93
0.00
1.00
1.24
0.96
2.04
2.99
2.99
2.12
2.06
3.01
f1 (ppm)

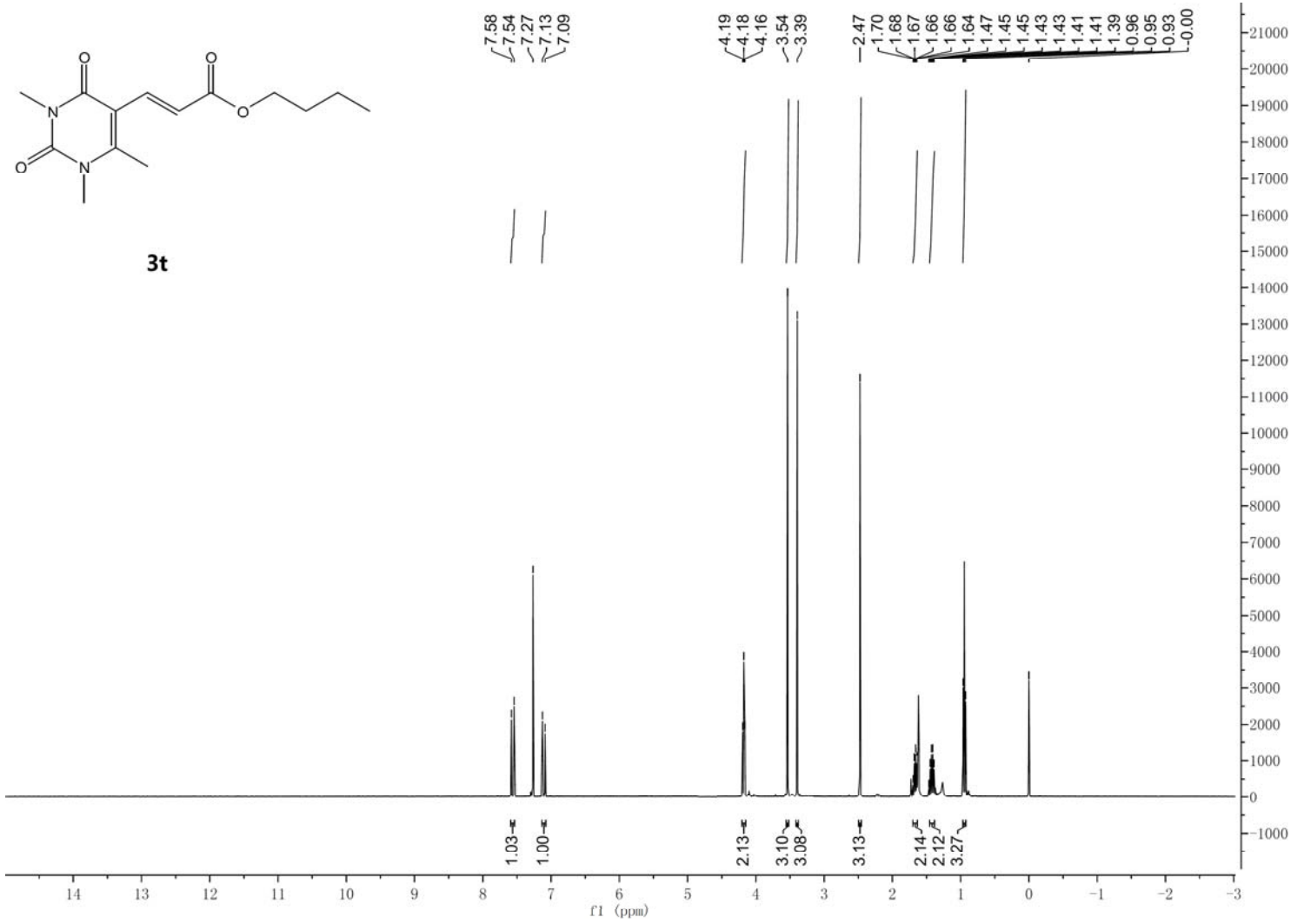

167.78
161.44
150.84
144.81
136.28
119.35
109.05
77.48
77.16
76.84
64.45
37.60
30.86
28.25
19.29
13.85
3q
f1 (ppm)

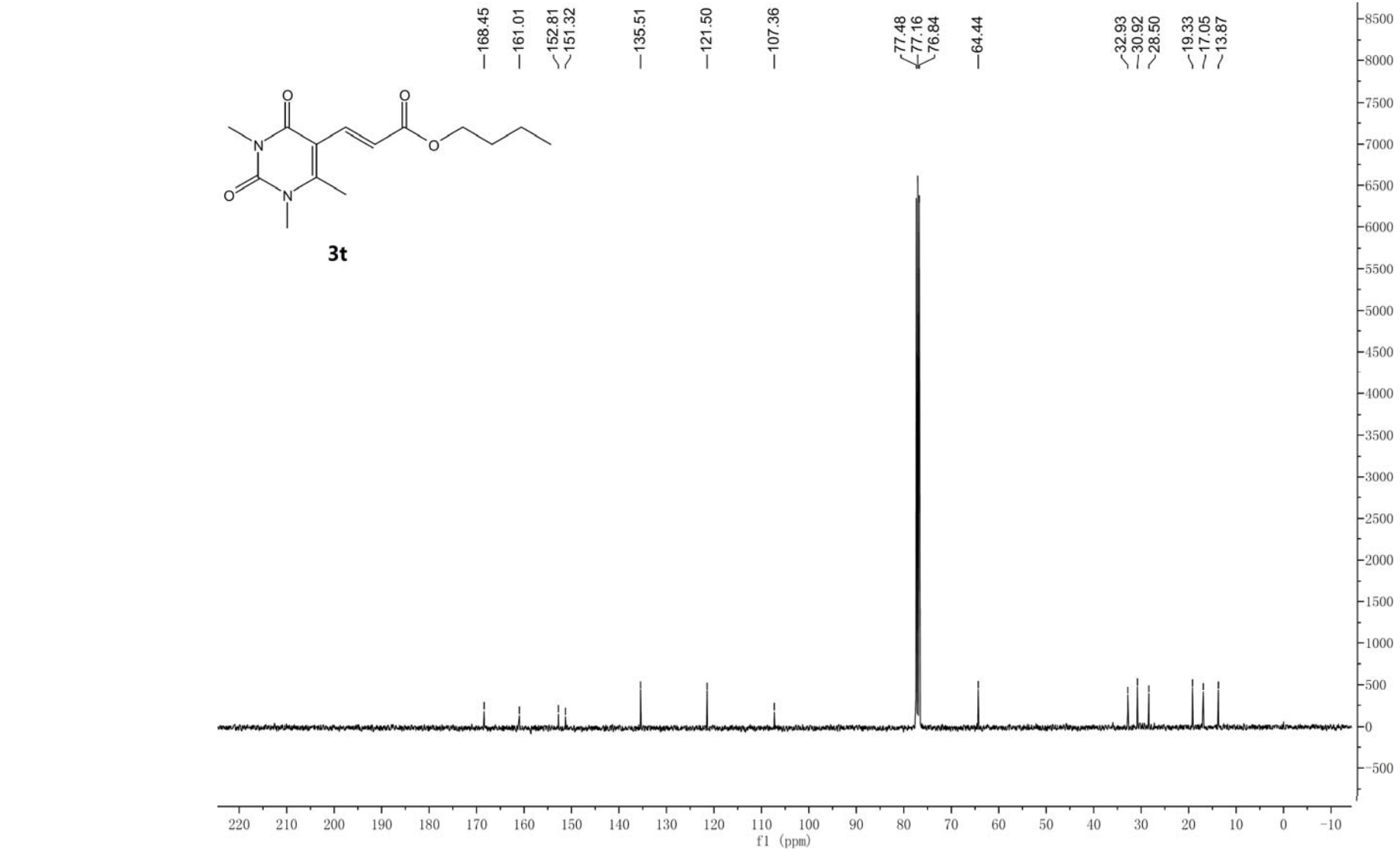

3r
7.38
7.31
7.27
7.02
6.98
4.18
4.17
4.15
3.96
3.95
3.94
3.94
3.92
3.80
3.78
3.76
1.77
1.75
1.73
1.68
1.67
1.66
1.65
1.64
1.63
1.44
1.42
1.40
1.38
0.99
0.97
0.96
0.95
0.94
0.93
0.92
0.00
1.03
1.44
1.00
2.11
2.10
2.09
2.25
4.39
2.19
9.50
f1 (ppm)

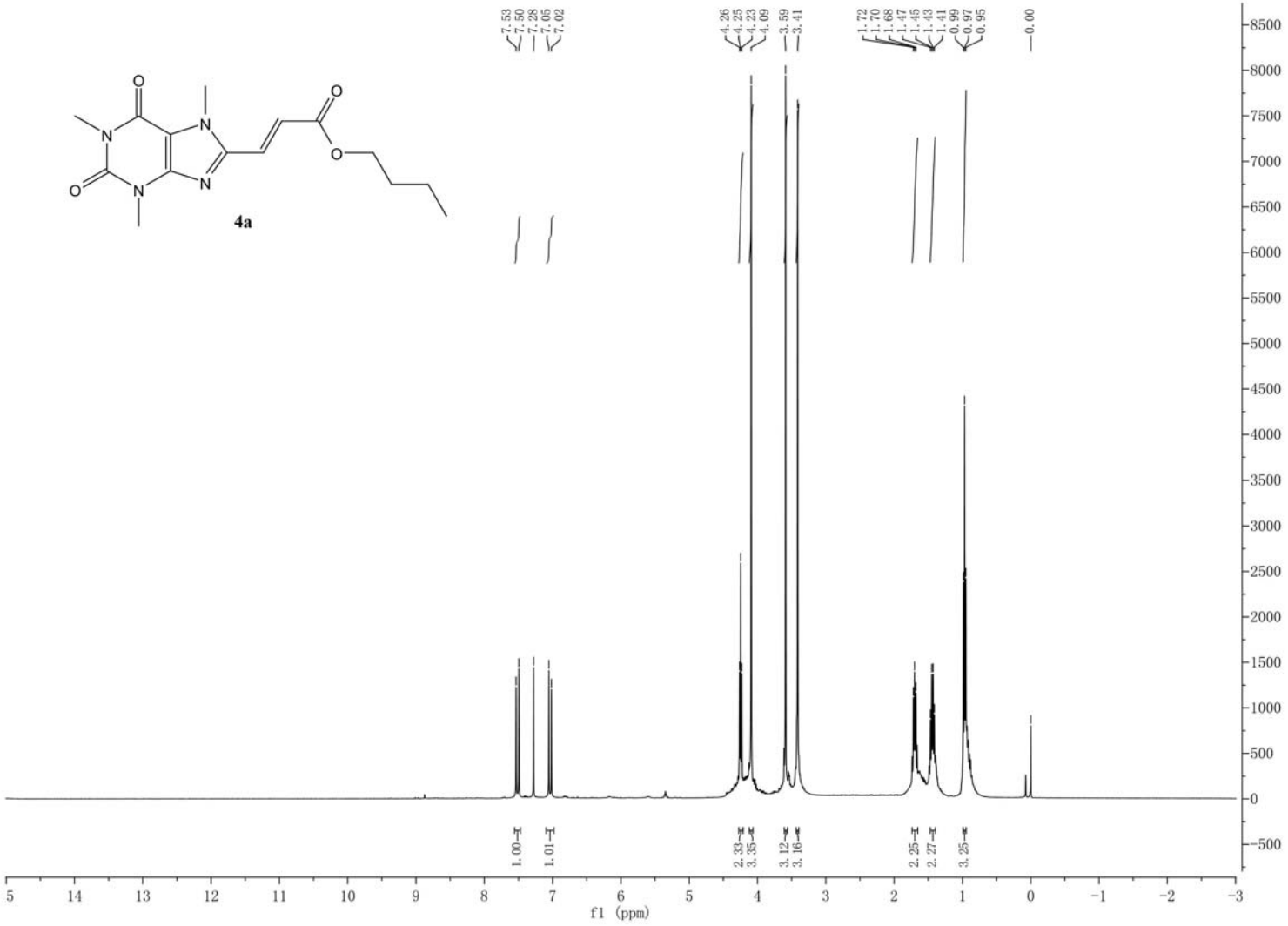

167.89
161.21
150.36
144.36
136.55
119.20
109.07
77.48
77.16
76.84
64.41
51.98
43.31
30.89
22.54
20.94
19.31
13.85
11.45
11.04
3r
f1 (ppm)

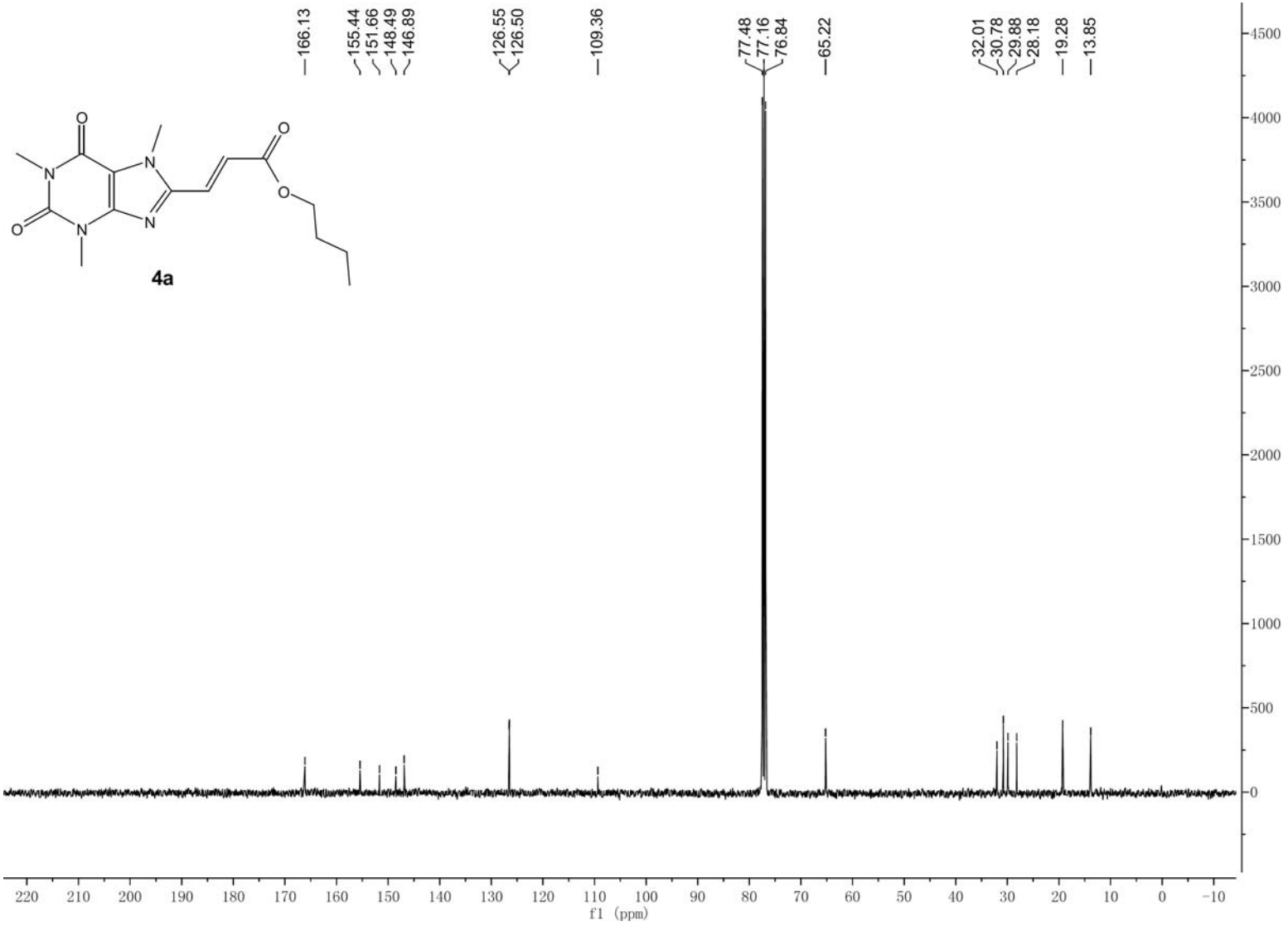

12.13
7.49
7.49
7.48
7.47
7.47
7.47
7.38
7.37
7.37
7.36
7.36
7.35
7.35
7.33
7.32
7.30
7.30
7.29
7.29
7.28
7.27
7.27
7.27
7.26
7.25
7.23
7.19
7.00
6.96
5.17
4.96
4.15
4.13
4.12
1.66
1.64
1.64
1.63
1.63
1.62
1.61
1.43
1.42
1.42
1.40
1.40
1.38
1.38
1.36
1.36
1.34
0.94
0.92
0.91
0.00
O
O
N
O
O
N
3s
2.06
4.08
5.27
1.02
1.00
2.08
2.04
2.09
2.16
2.16
3.15
f1 (ppm)

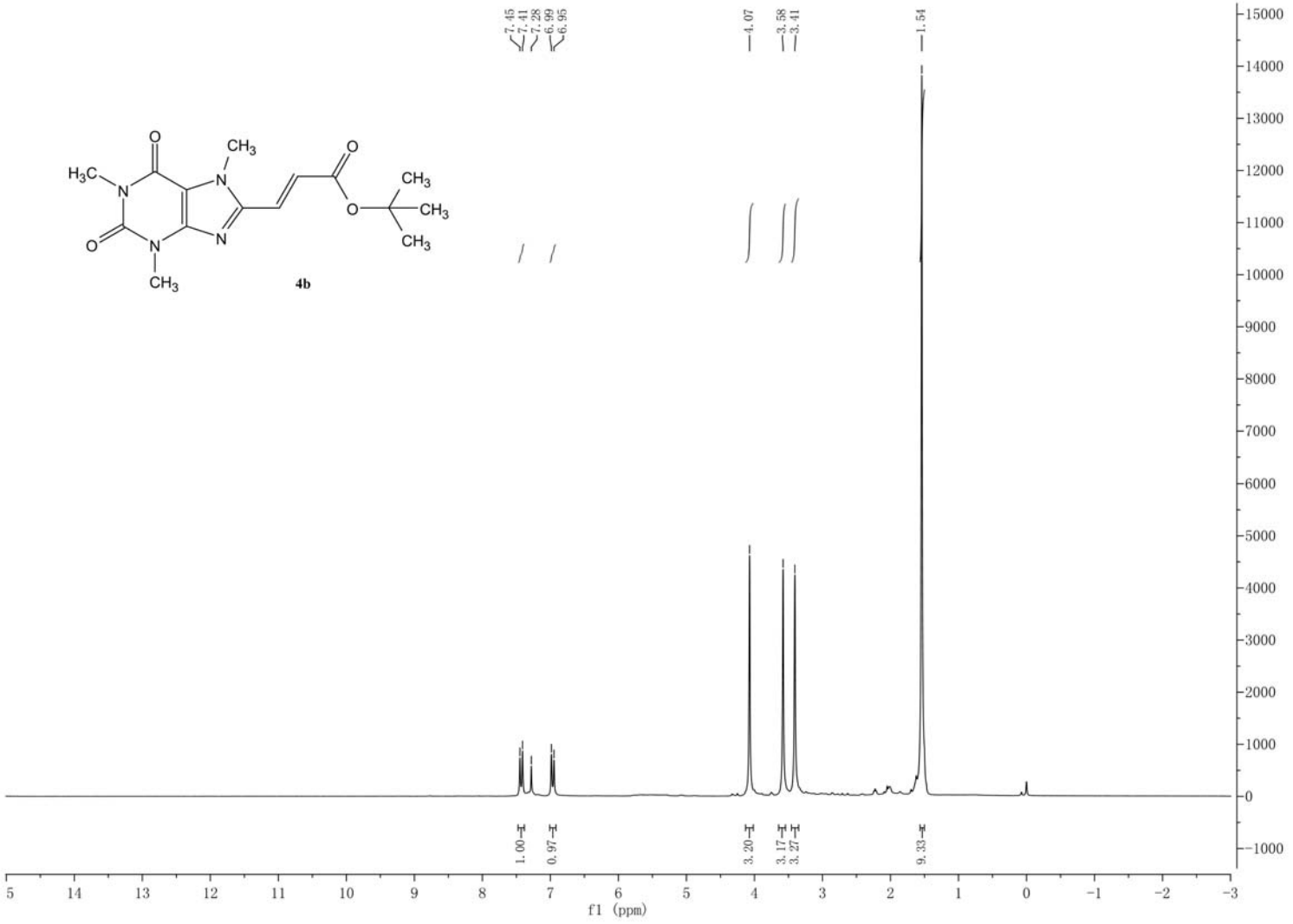

167.72
160.95
150.72
143.85
136.52
136.30
134.69
129.38
129.16
128.93
128.57
128.30
127.87
119.54
109.65
77.48
77.16
76.84
64.40
52.80
44.96
30.82
19.24
13.81
3s
f1 (ppm)

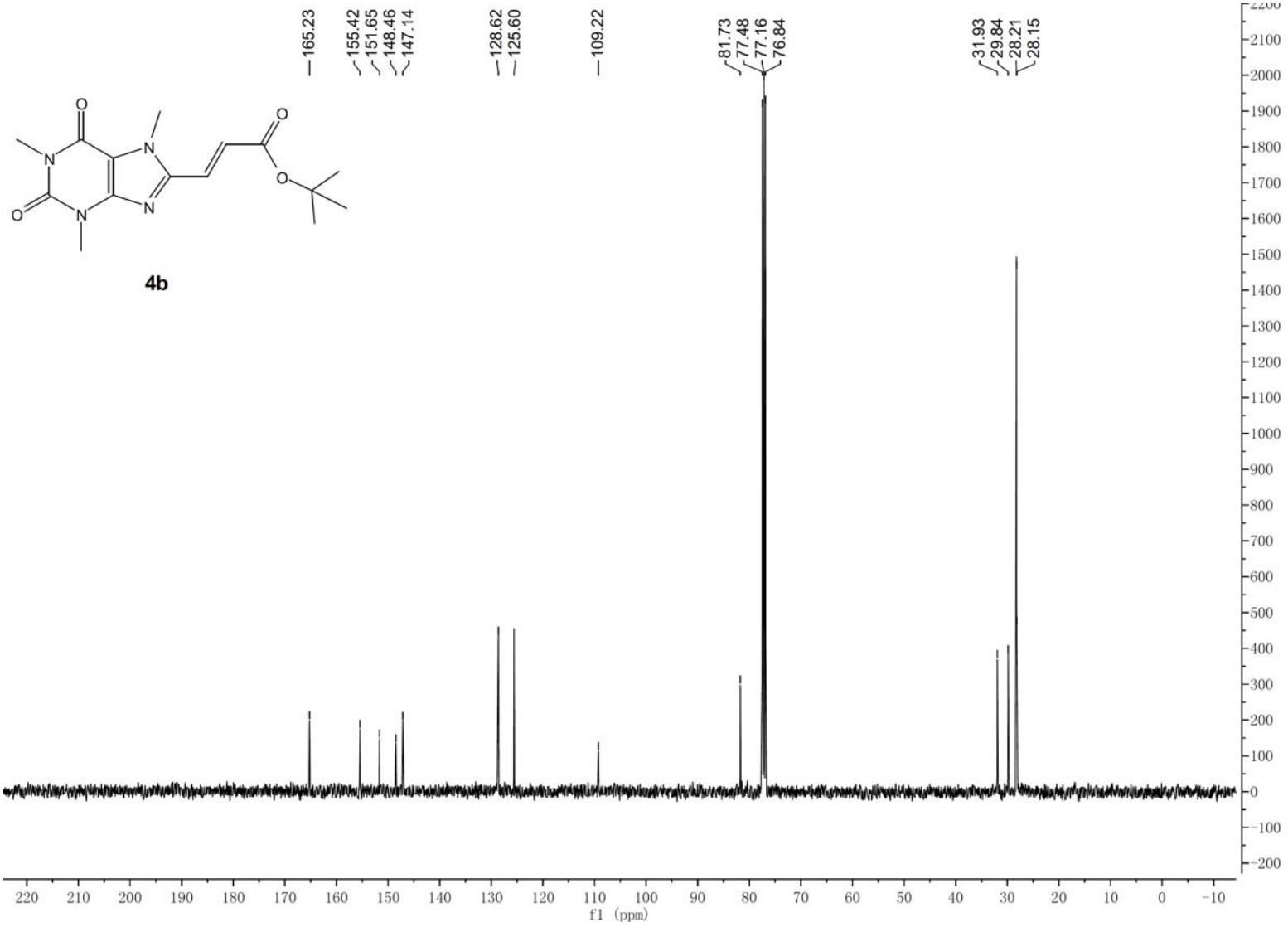

3t
7.58
7.54
7.27
7.13
7.09
4.19
4.18
4.16
3.54
3.39
2.47
1.70
1.68
1.67
1.66
1.66
1.64
1.47
1.45
1.45
1.43
1.43
1.41
1.41
1.39
0.96
0.95
0.93
0.00
1.03
1.00
2.13
3.10
3.08
3.13
2.14
2.12
3.27
f1 (ppm)

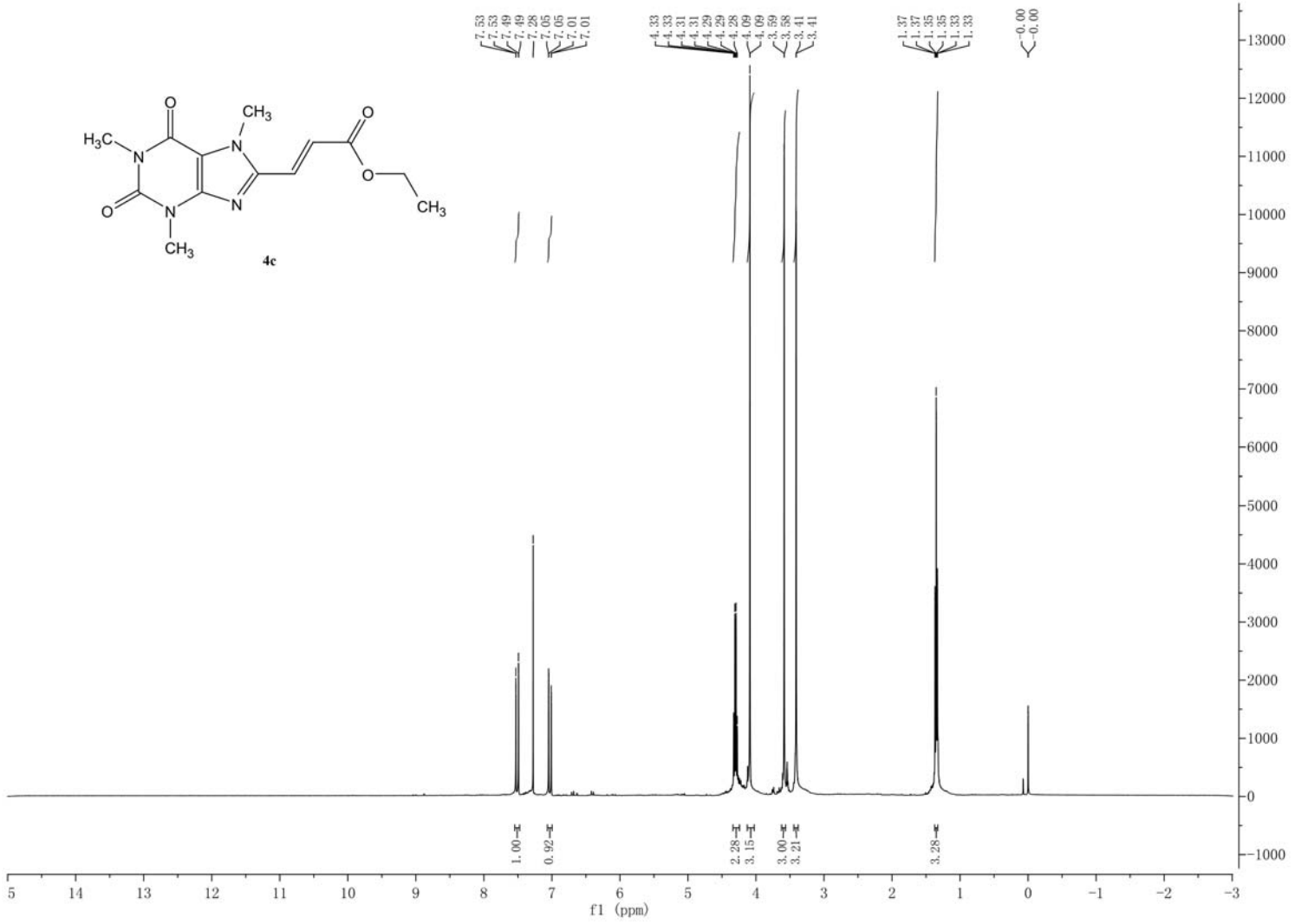

168.45
161.01
152.81
151.32
135.51
121.50
107.36
77.48
77.16
76.84
64.44
32.93
30.92
28.50
19.33
17.05
13.87
3t
f1 (ppm)

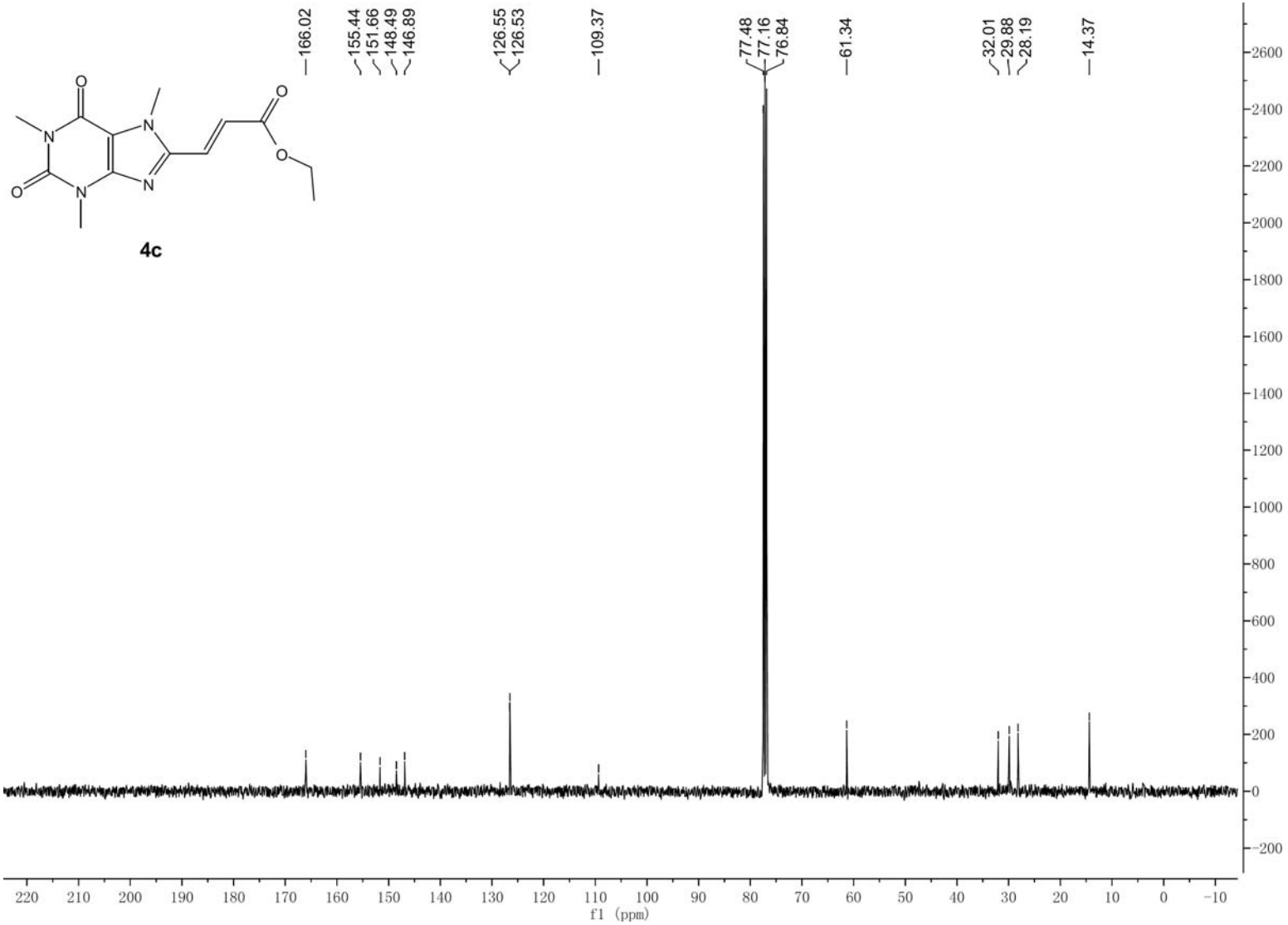

4a
7.53
7.50
7.28
7.05
7.02
4.26
4.25
4.23
4.09
3.59
3.41
1.72
1.70
1.68
1.47
1.45
1.43
1.41
0.99
0.97
0.95
0.00
1.00
1.01
2.33
3.35
3.12
3.16
2.25
2.27
3.25
f1 (ppm)

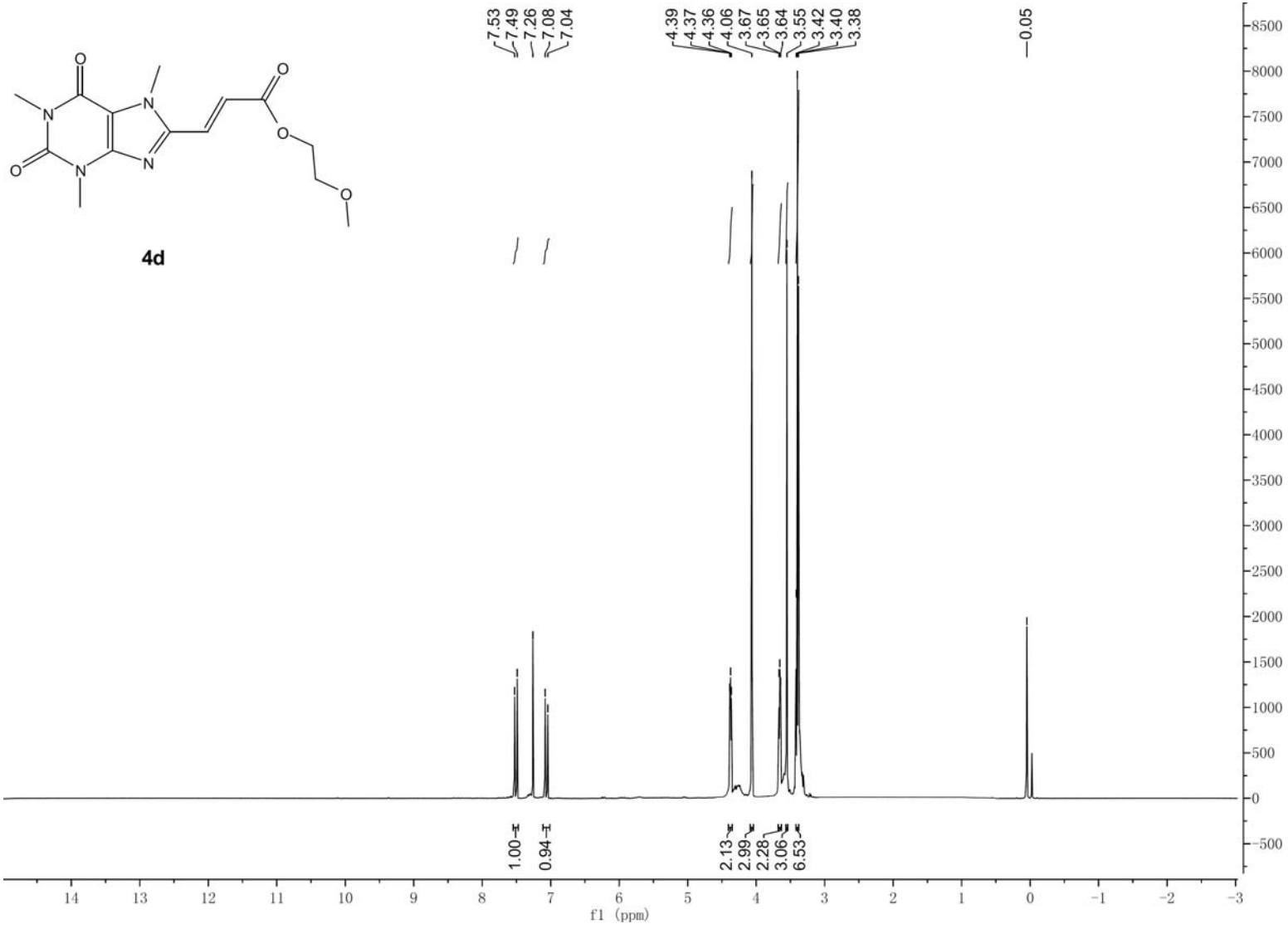

166.13
155.44
151.66
148.49
146.89
126.55
126.50
109.36
77.48
77.16
76.84
65.22
32.01
30.78
29.88
28.18
19.28
13.85
4a
f1 (ppm)

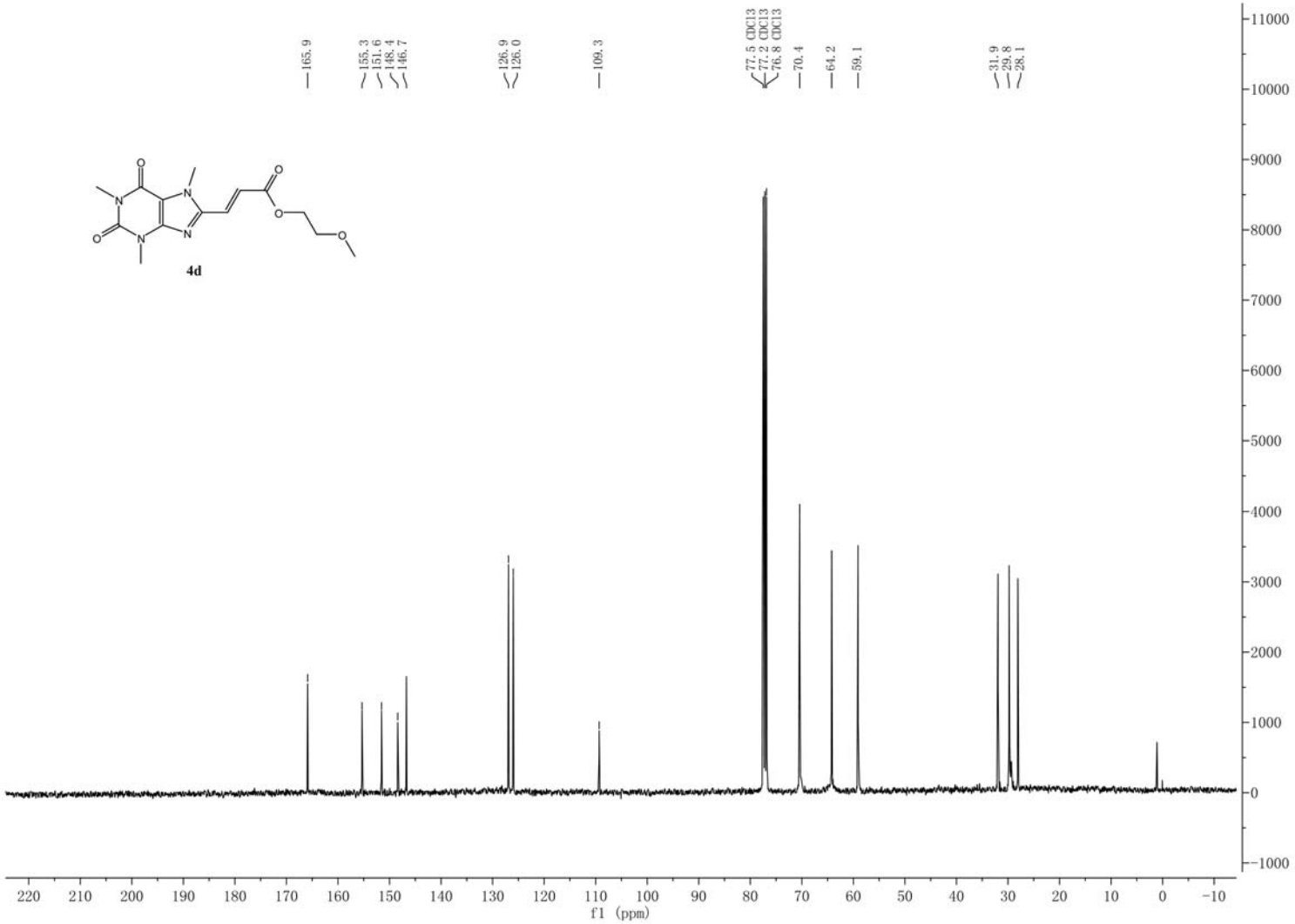

7.45
7.41
7.28
6.99
6.95
4.07
3.58
3.41
1.54
4b
1.00
0.97
3.20
3.17
3.27
9.33
f1 (ppm)

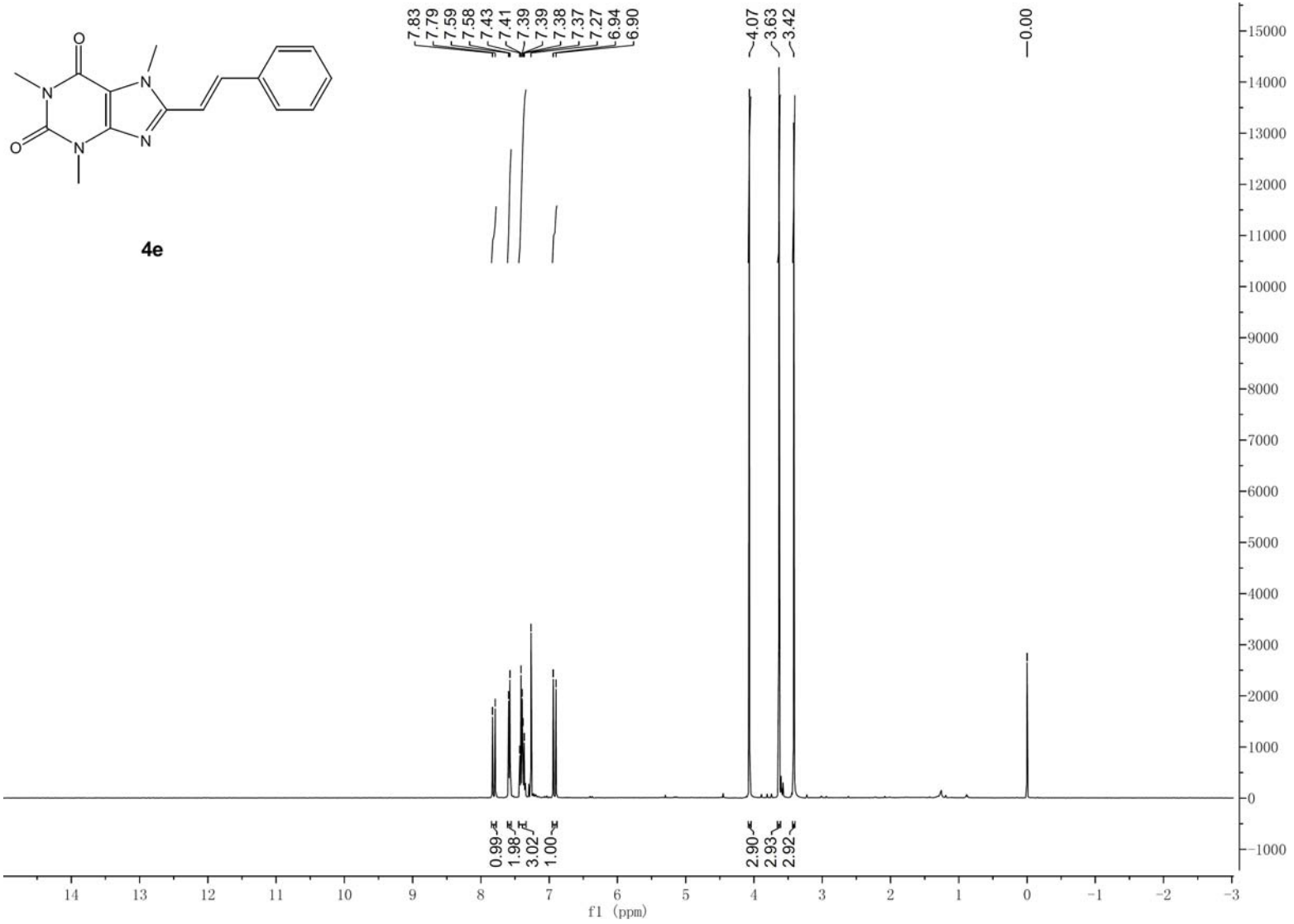

165.23
155.42
151.65
148.46
147.14
128.62
125.60
109.22
81.73
77.48
77.16
76.84
31.93
29.84
28.21
28.15
4b
f1 (ppm)

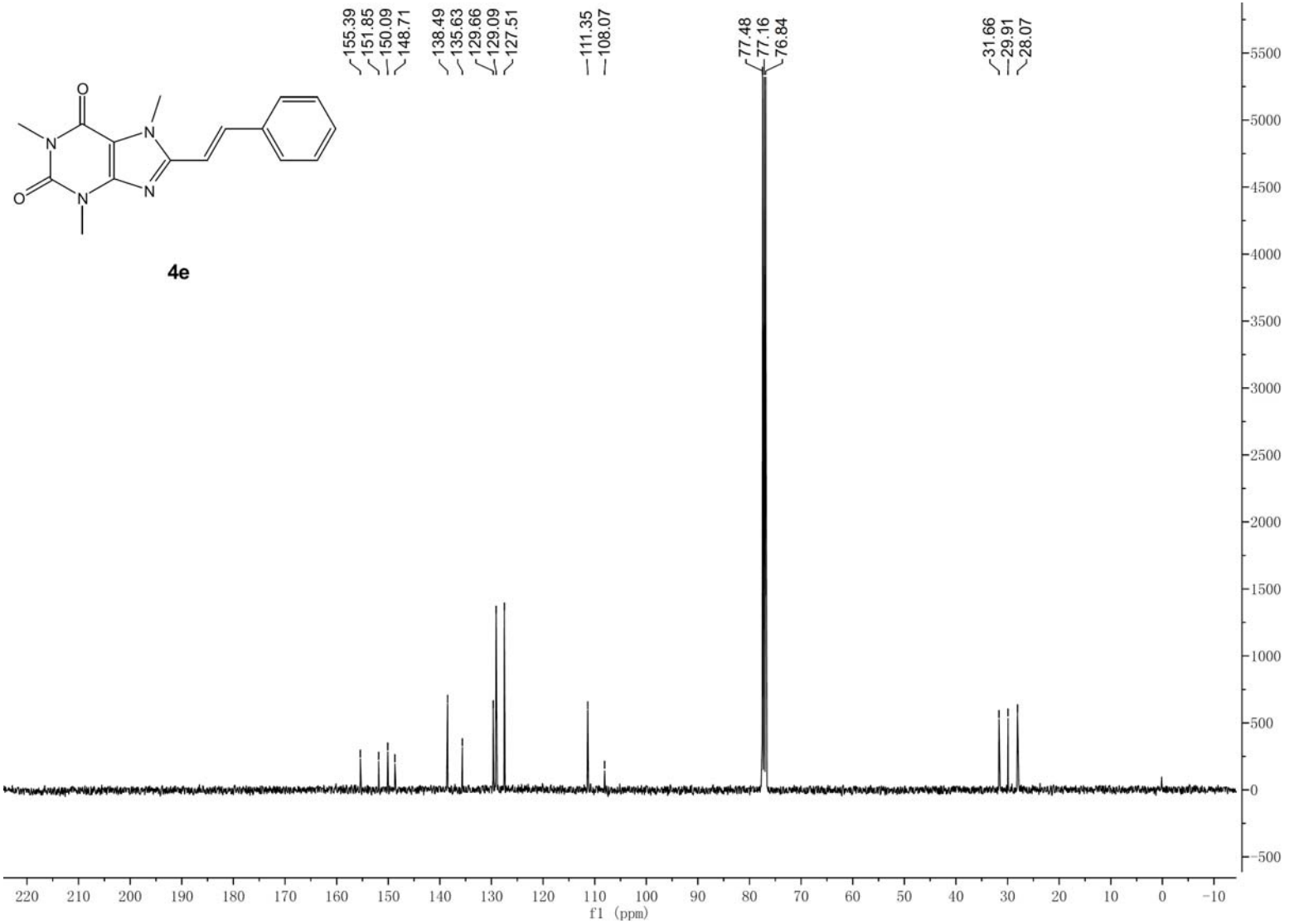

4c
7.53
7.53
7.49
7.49
7.28
7.05
7.05
7.01
7.01
4.33
4.33
4.31
4.31
4.29
4.29
4.28
4.09
4.09
3.59
3.58
3.41
3.41
1.37
1.37
1.35
1.35
1.33
1.33
-0.00
-0.00
1.00
0.92
2.28
3.15
3.00
3.21
3.28
f1 (ppm)

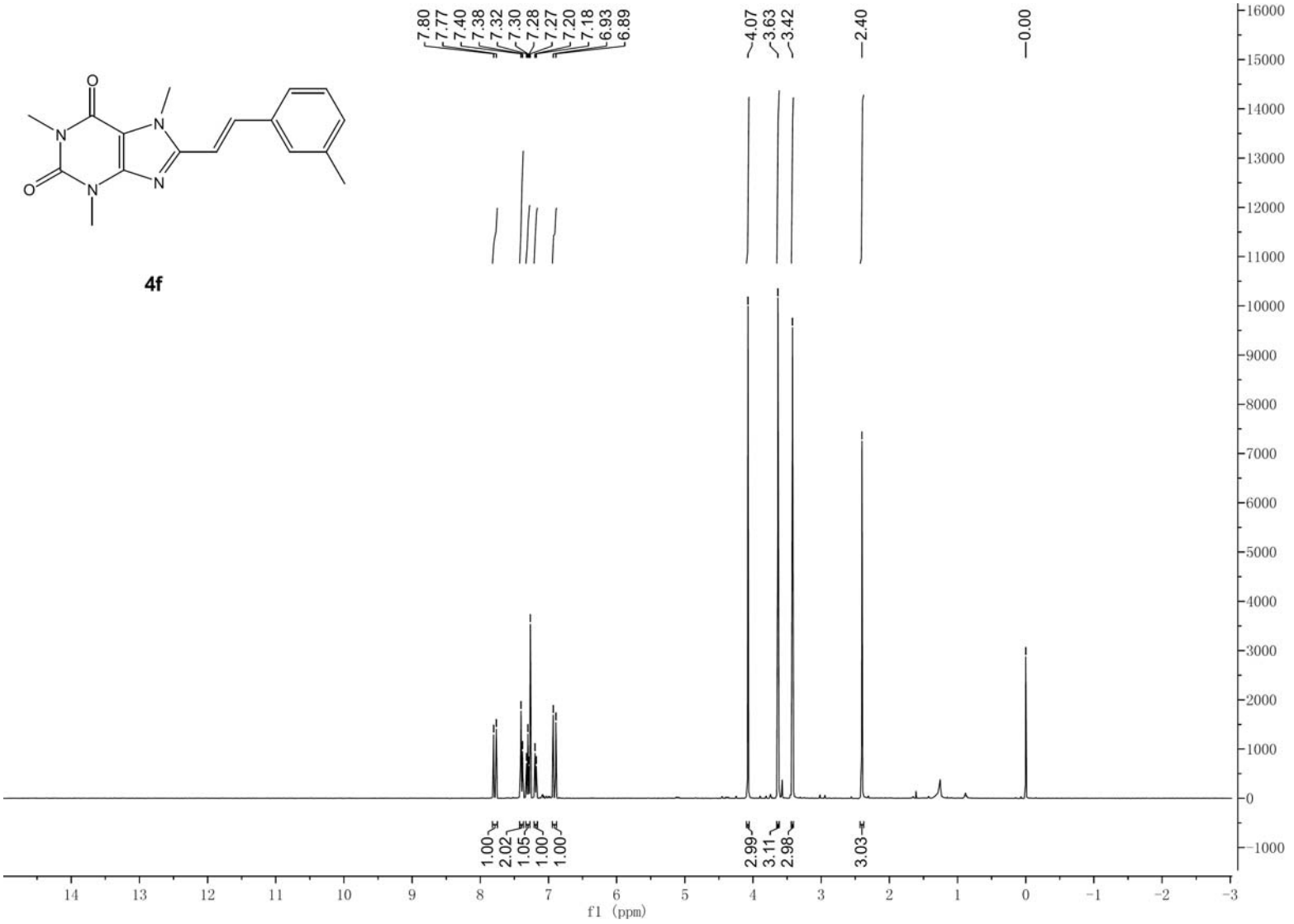

166.02
155.44
151.66
148.49
146.89
126.55
126.53
109.37
77.48
77.16
76.84
61.34
32.01
29.88
28.19
14.37
4c
f1 (ppm)

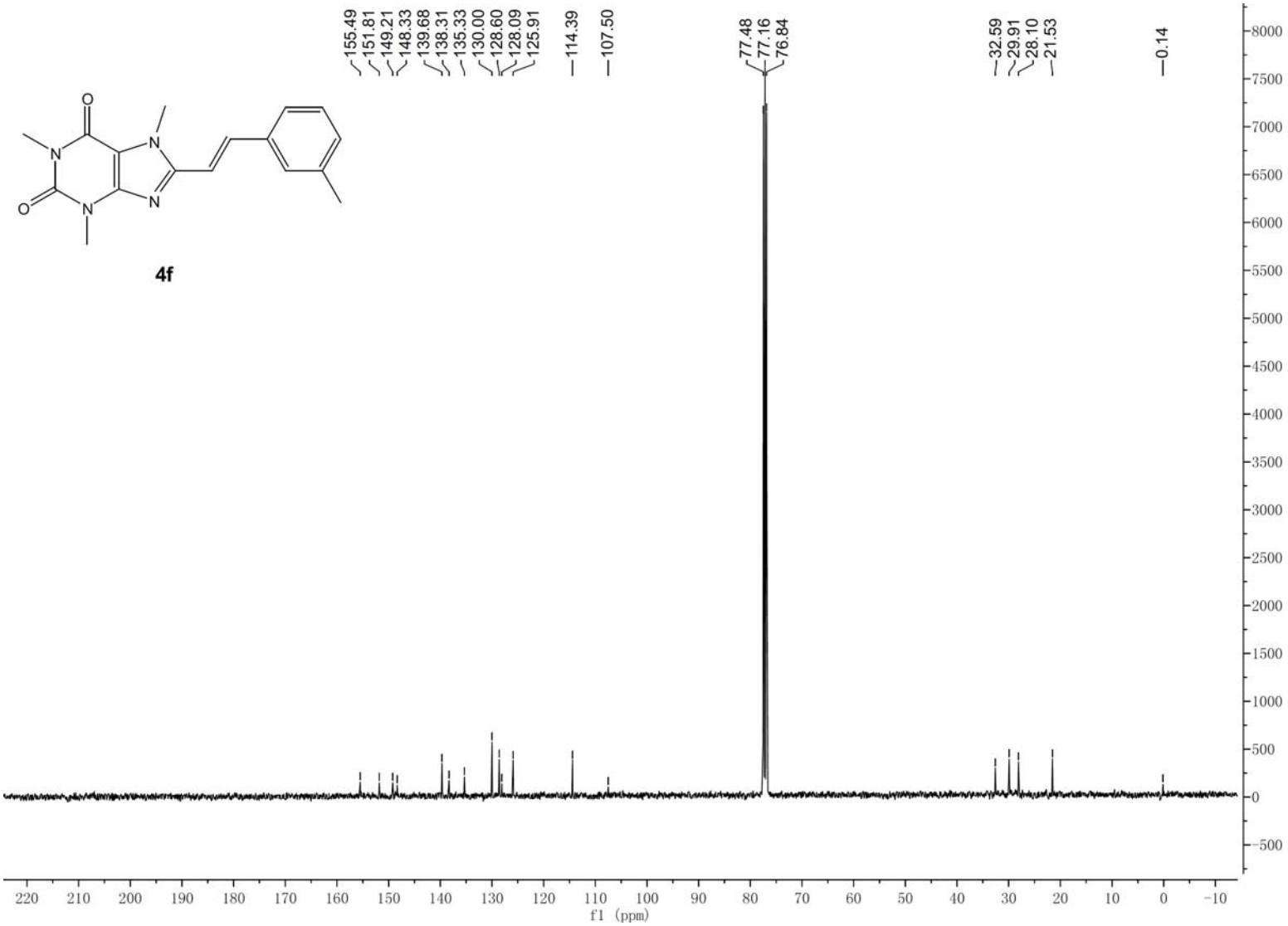

4d
7.53
7.49
7.26
7.08
7.04
4.39
4.37
4.36
4.06
3.67
3.65
3.64
3.55
3.42
3.40
3.38
0.05
1.00
0.94
2.13
2.99
2.28
3.06
6.53
f1 (ppm)

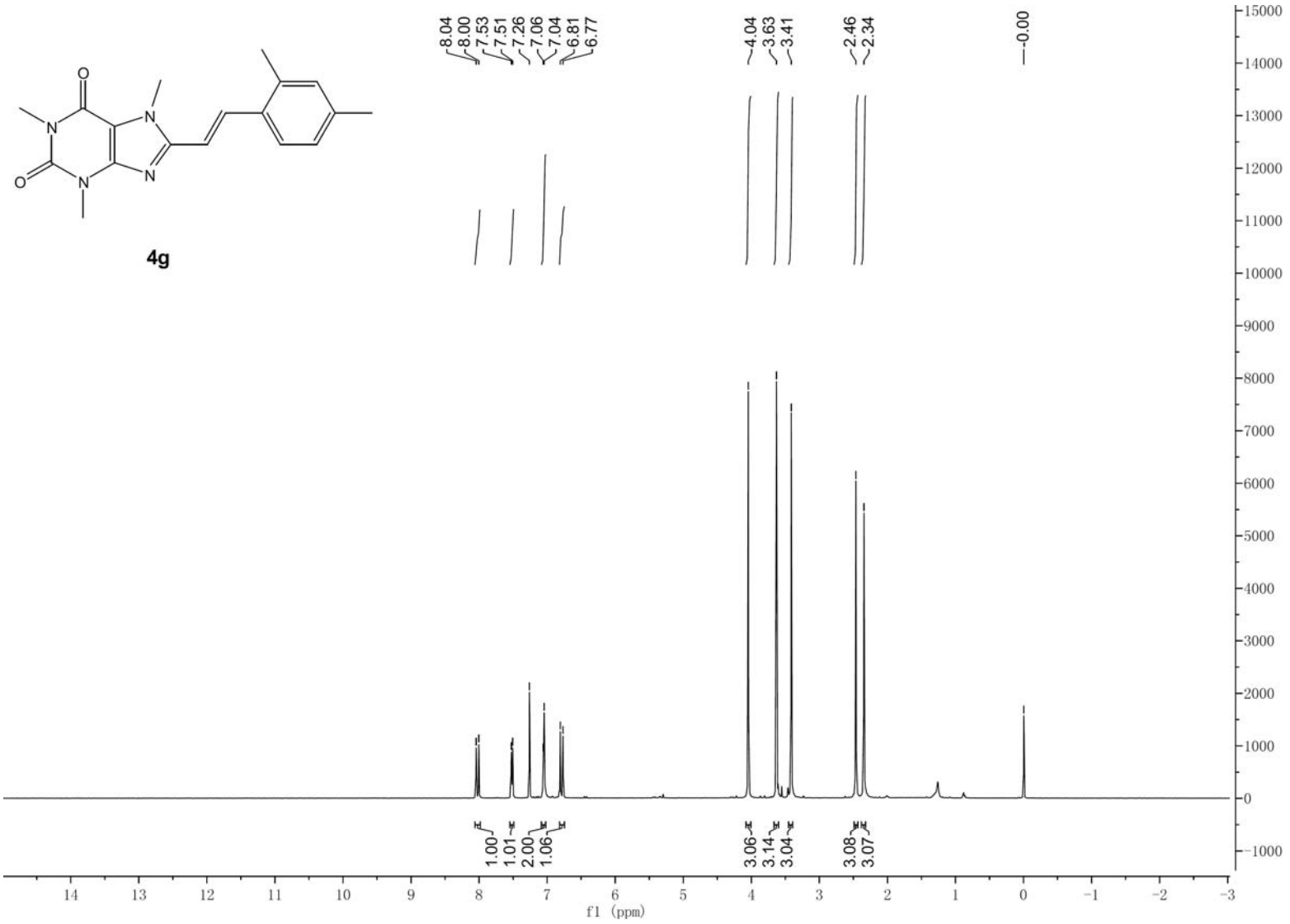

165.9
155.3
151.6
148.4
146.7
126.9
126.0
109.3
77.5 CDCl3
77.2 CDCl3
76.8 CDCl3
70.4
64.2
59.1
31.9
29.8
28.1
4d
f1 (ppm)

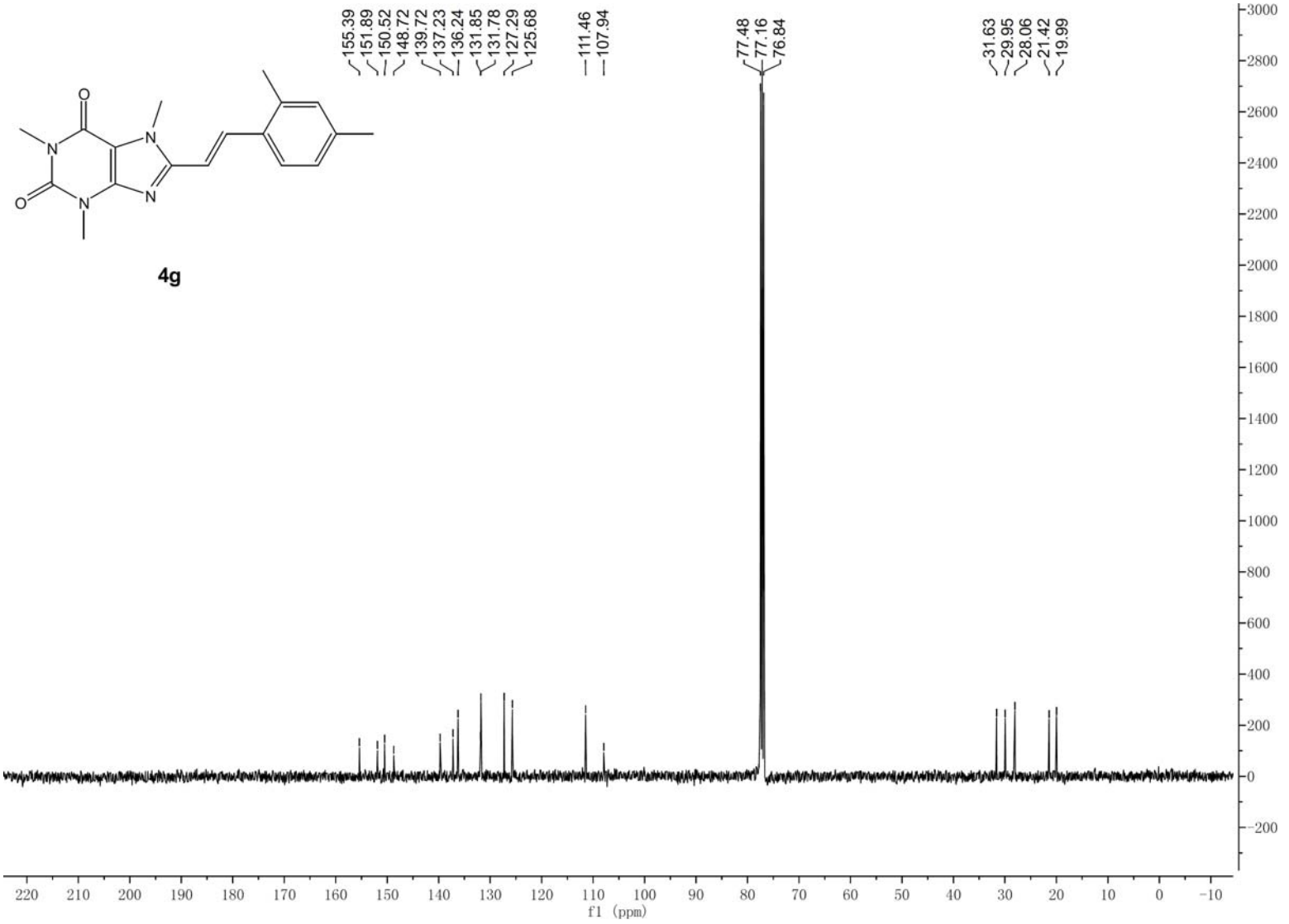

4e
7.83
7.79
7.59
7.58
7.43
7.41
7.39
7.39
7.38
7.37
7.27
6.94
6.90
4.07
3.63
3.42
0.00
0.99
1.98
3.02
1.00
2.90
2.93
2.92
f1 (ppm)

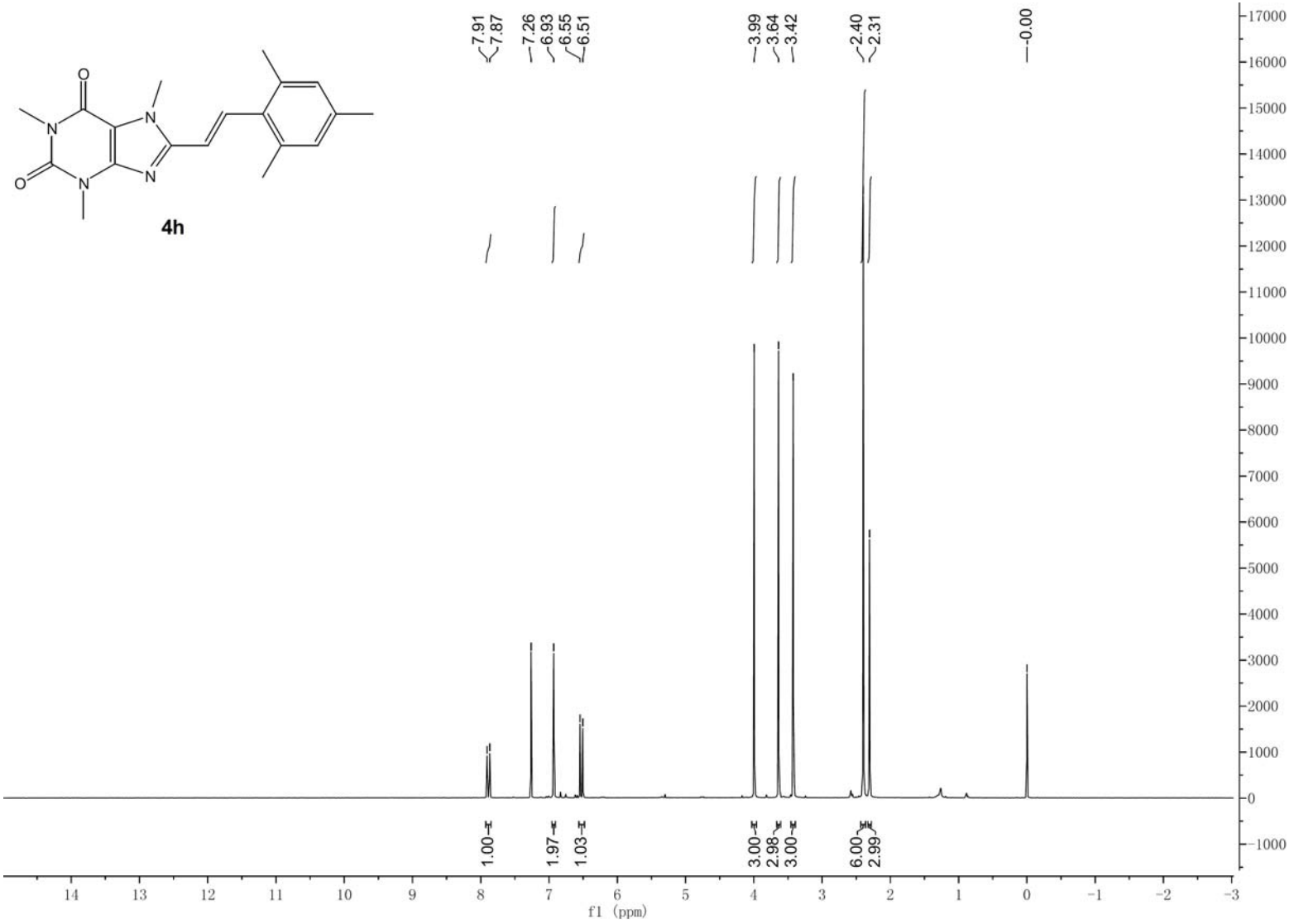

155.39
151.85
150.09
148.71
138.49
135.63
129.66
129.09
127.51
111.35
108.07
77.48
77.16
76.84
31.66
29.91
28.07
4e
f1 (ppm)

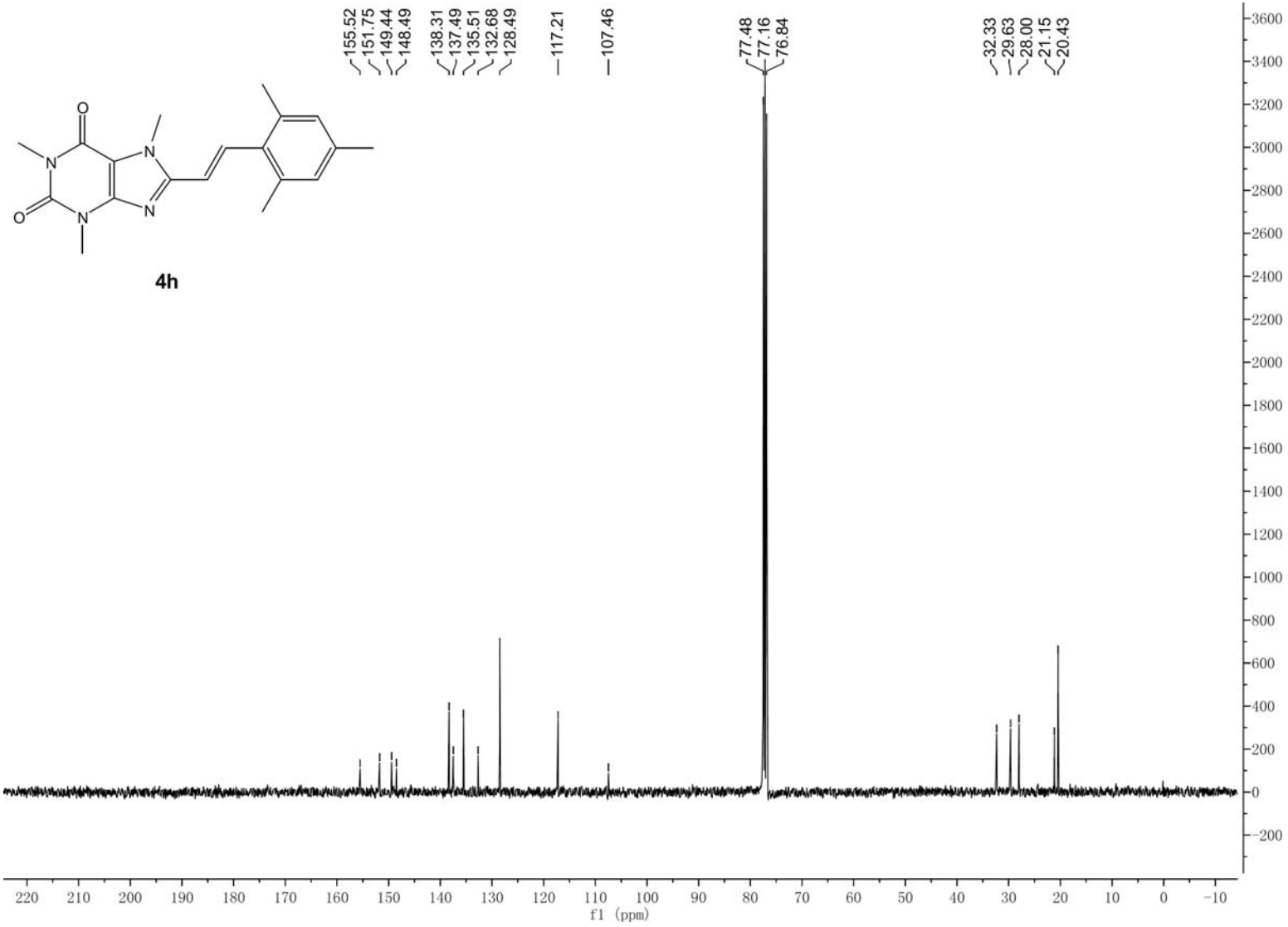

4f
7.80
7.77
7.40
7.38
7.32
7.30
7.28
7.27
7.20
7.18
6.93
6.89
4.07
3.63
3.42
2.40
0.00
1.00
2.02
1.05
1.00
1.00
2.99
3.11
2.98
3.03
f1 (ppm)

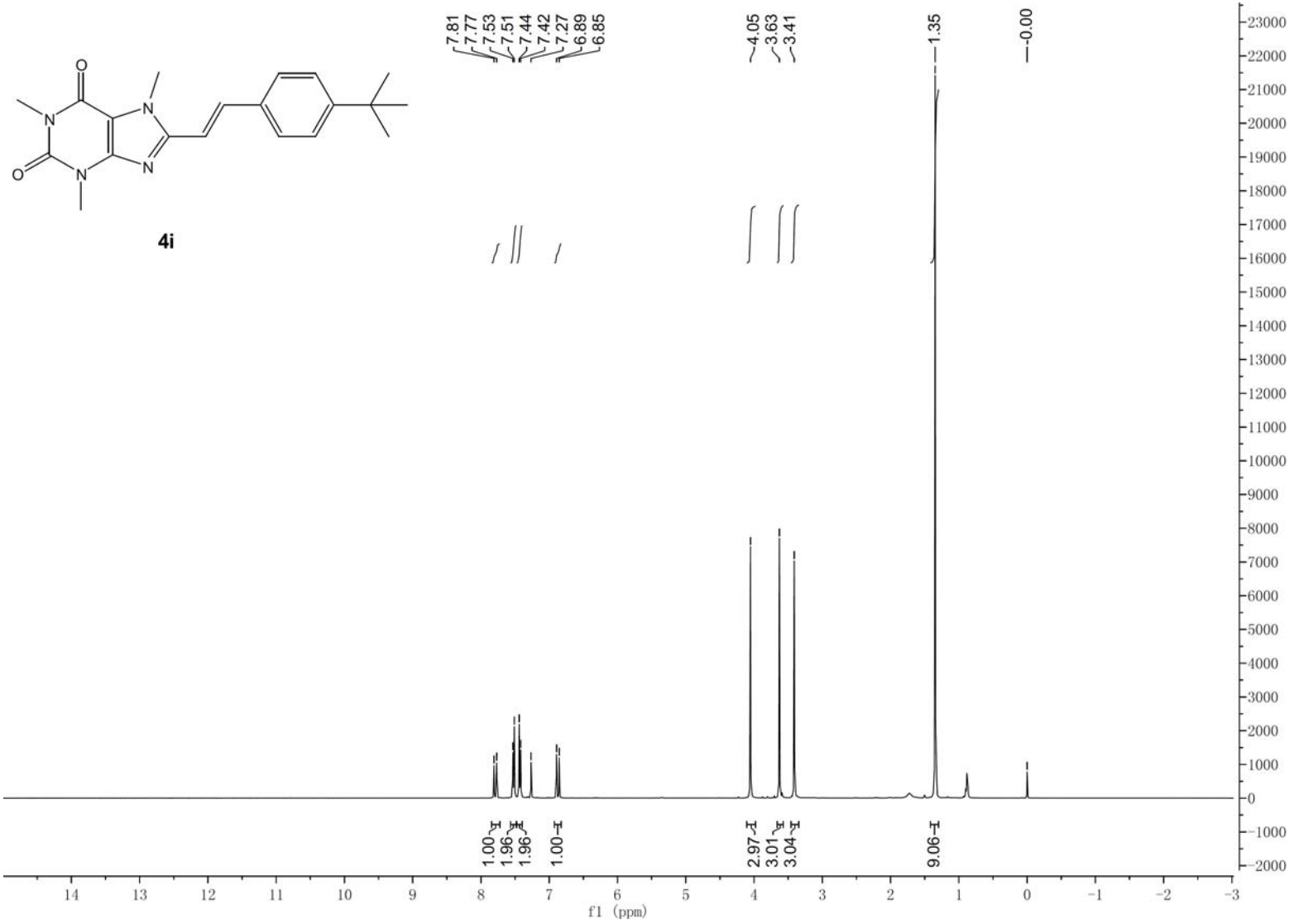

155.49
151.81
149.21
148.33
139.68
138.31
135.33
130.00
128.60
128.09
125.91
114.39
107.50
77.48
77.16
76.84
32.59
29.91
28.10
21.53
0.14
4f
f1 (ppm)

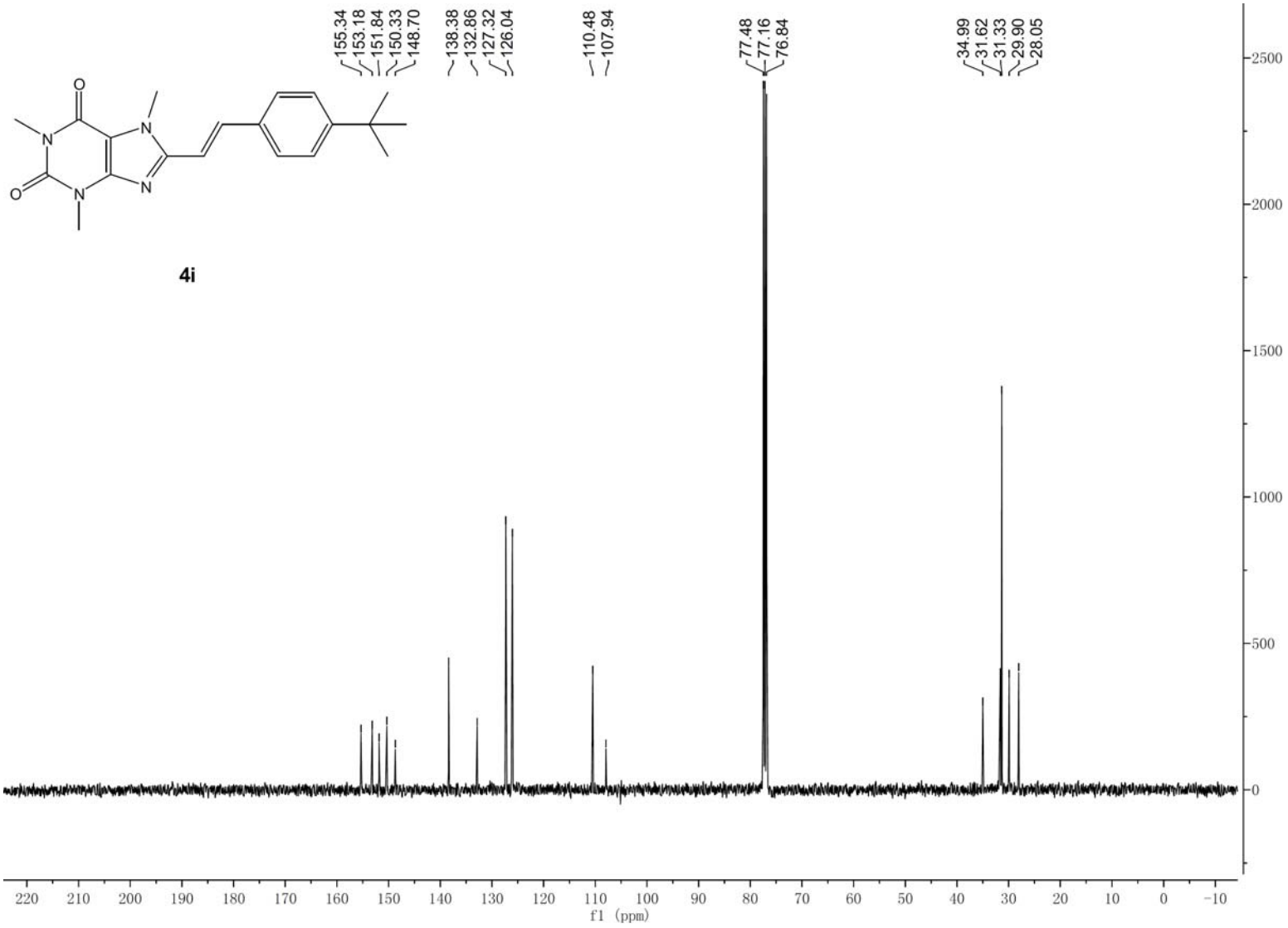

4g
8.04
8.00
7.53
7.51
7.26
7.06
7.04
6.81
6.77
4.04
3.63
3.41
2.46
2.34
0.00
1.00
1.01
2.00
1.06
3.06
3.14
3.04
3.08
3.07
f1 (ppm)

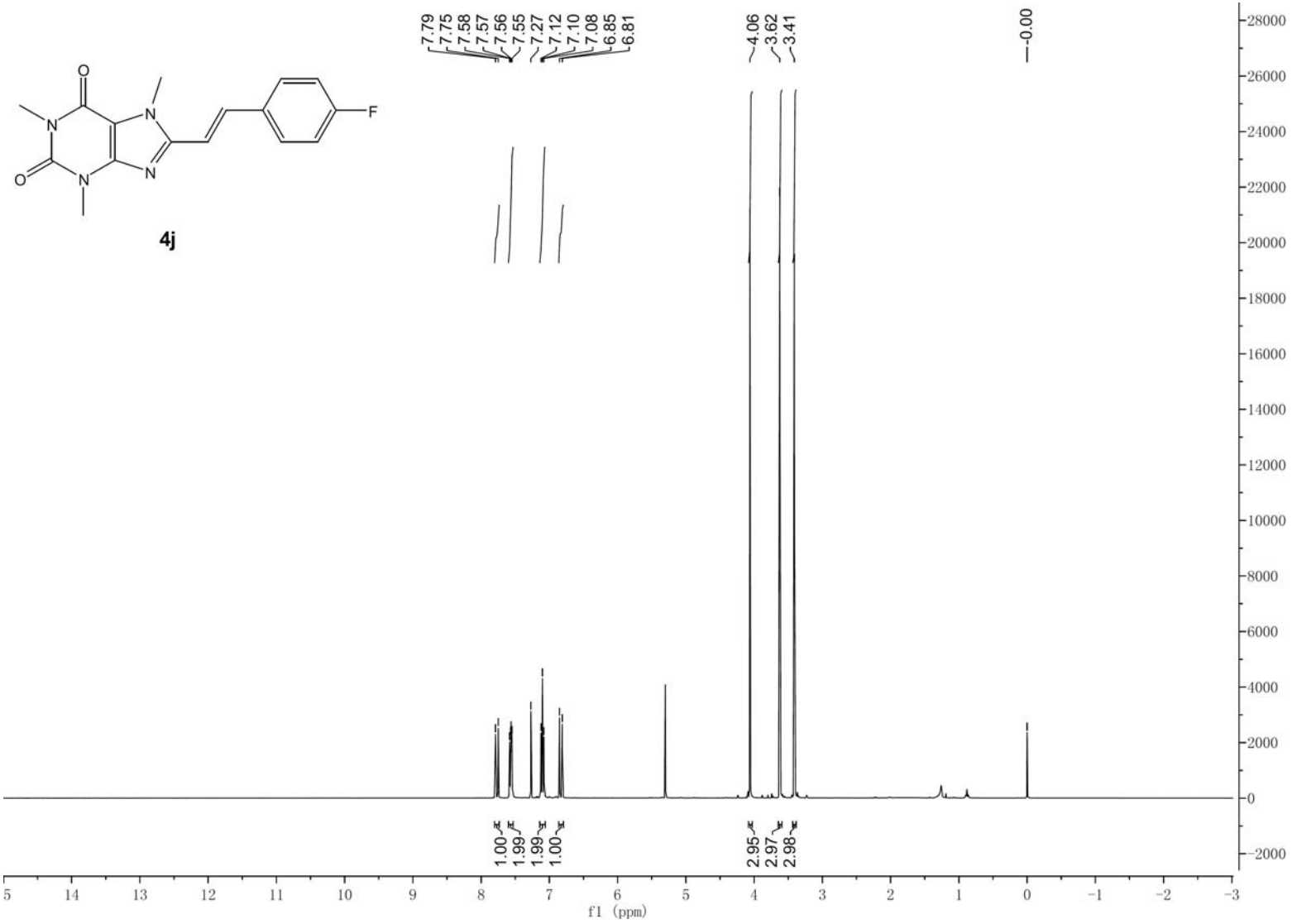

155.39
151.89
150.52
148.72
139.72
137.23
136.24
131.85
131.78
127.29
125.68
111.46
107.94
77.48
77.16
76.84
31.63
29.95
28.06
21.42
19.99
4g
f1 (ppm)

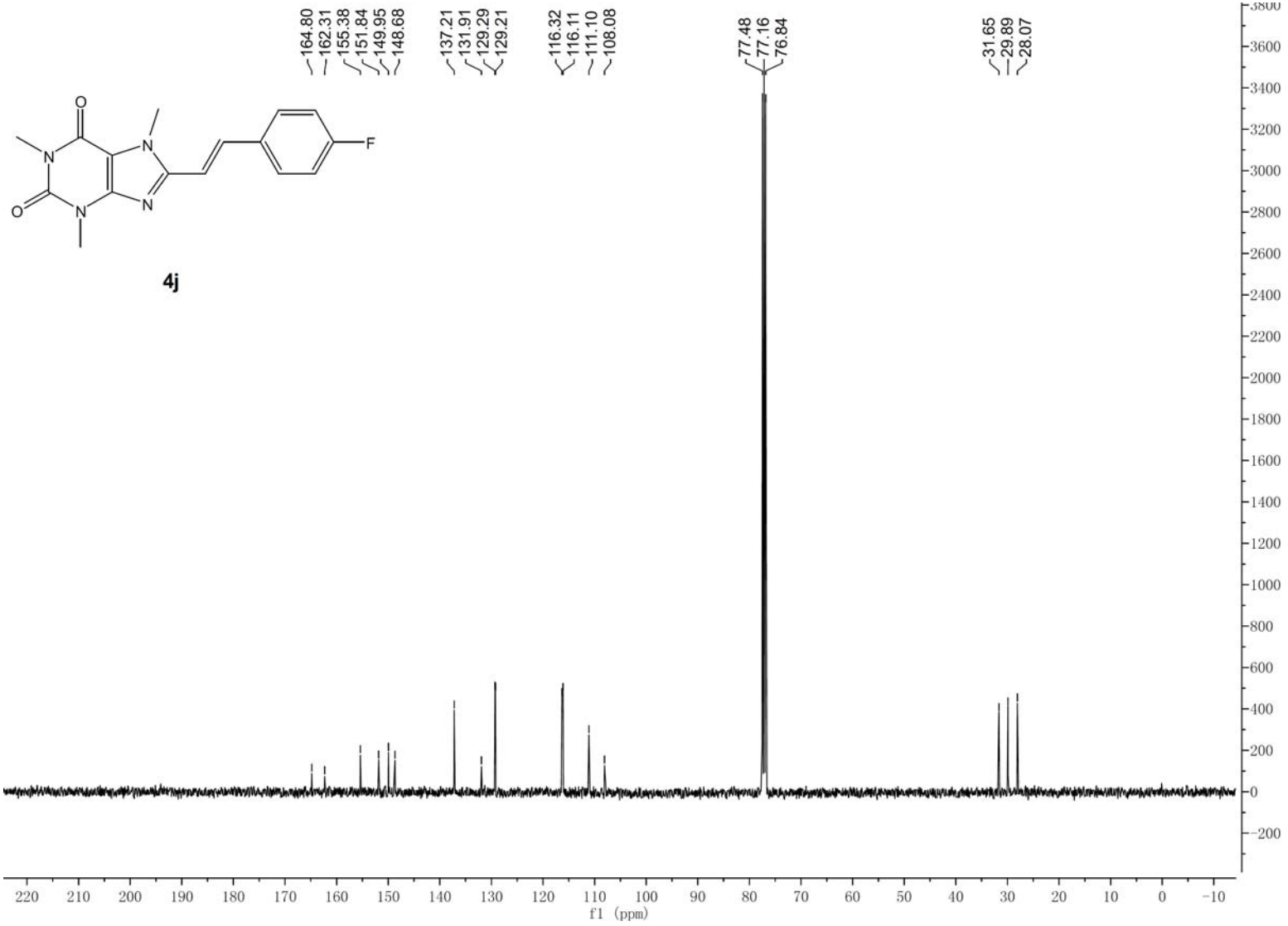

4h
7.91
7.87
7.26
6.93
6.55
6.51
3.99
3.64
3.42
2.40
2.31
0.00
1.00
1.97
1.03
3.00
2.98
3.00
6.00
2.99
f1 (ppm)

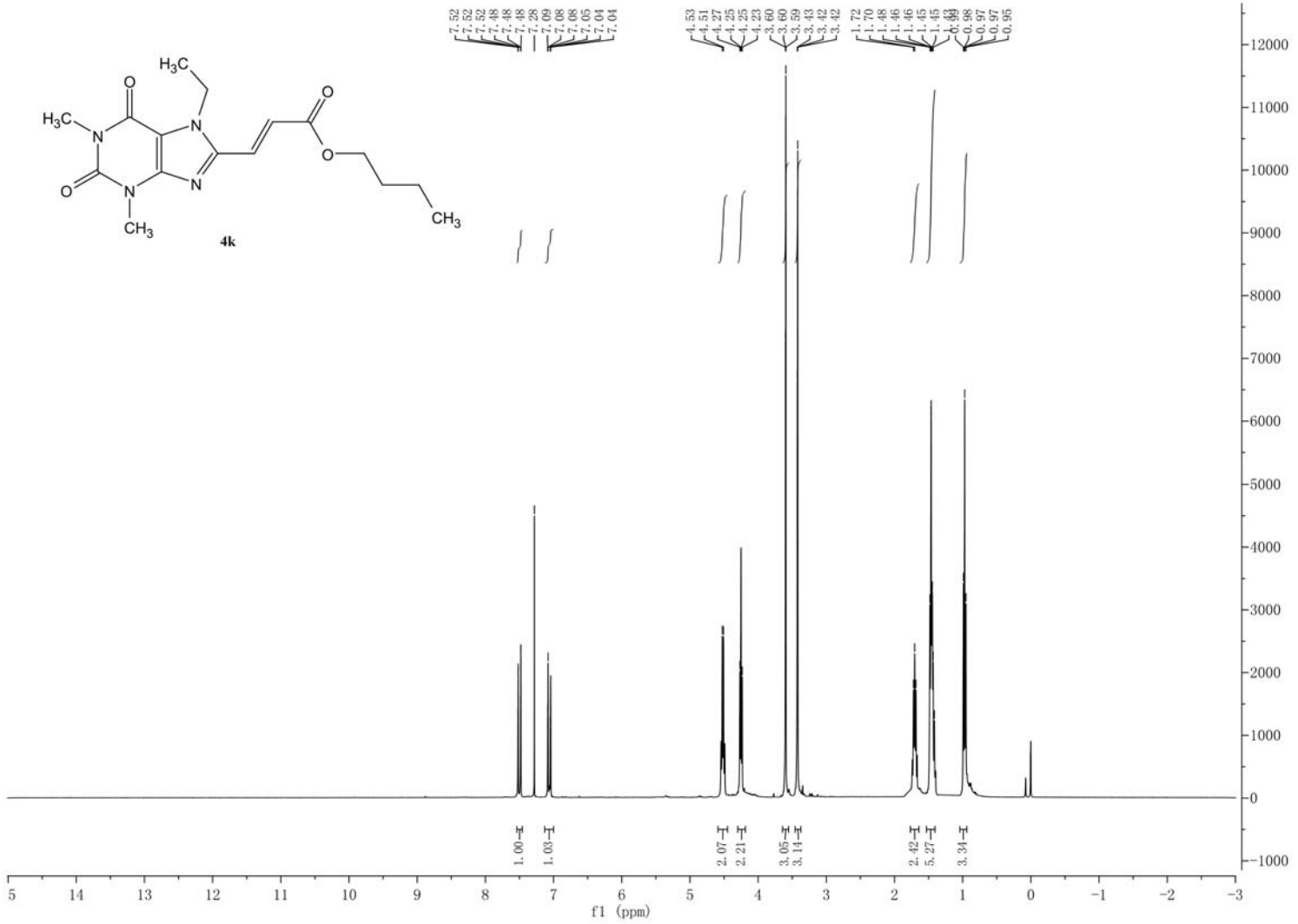

155.52
151.75
149.44
148.49
138.31
137.49
135.51
132.68
128.49
117.21
107.46
77.48
77.16
76.84
32.33
29.63
28.00
21.15
20.43
4h
f1 (ppm)

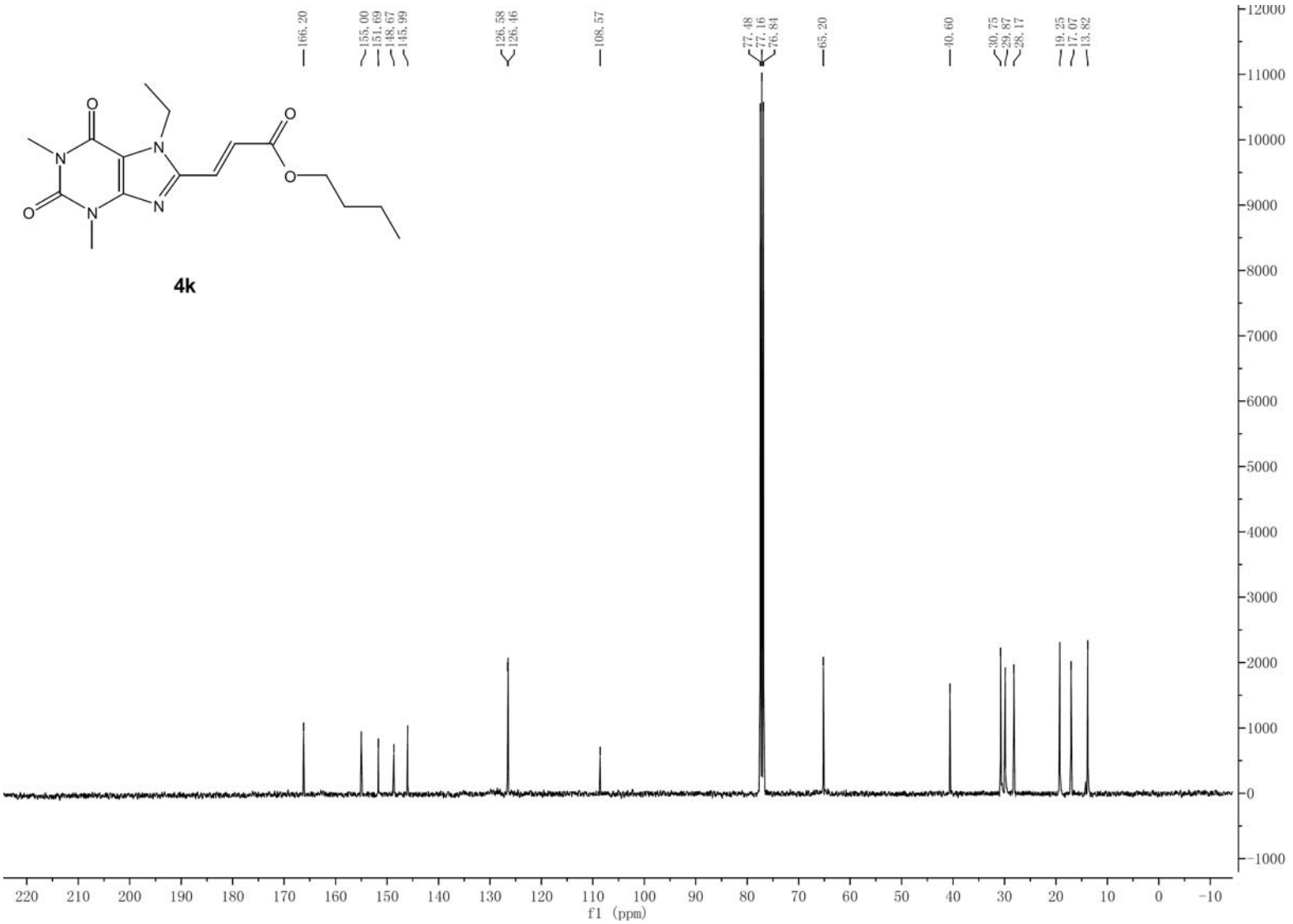

4i
7.81
7.77
7.53
7.51
7.44
7.42
7.27
6.89
6.85
4.05
3.63
3.41
1.35
0.00
1.00
1.96
1.96
1.00
2.97
3.01
3.04
9.06
f1 (ppm)

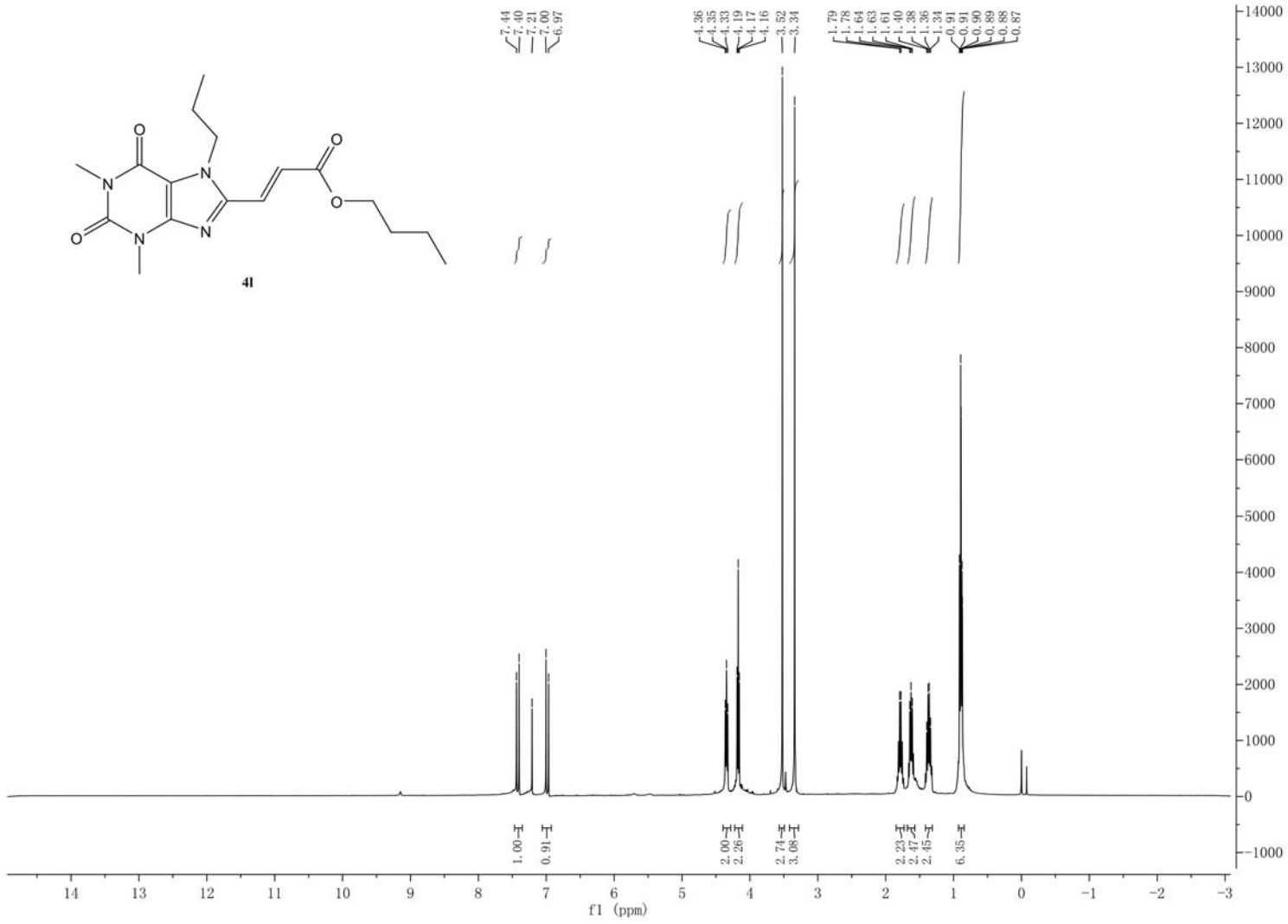

155.34
153.18
151.84
150.33
148.70
138.38
132.86
127.32
126.04
110.48
107.94
77.48
77.16
76.84
34.99
31.62
31.33
29.90
28.05
4i
2500
2000
1500
1000
500
0
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


4j
7.79
7.75
7.58
7.57
7.56
7.55
7.27
7.12
7.10
7.08
6.85
6.81
4.06
3.62
3.41
0.00
1.00
1.99
1.99
1.00
2.95
2.97
2.98
f1 (ppm)

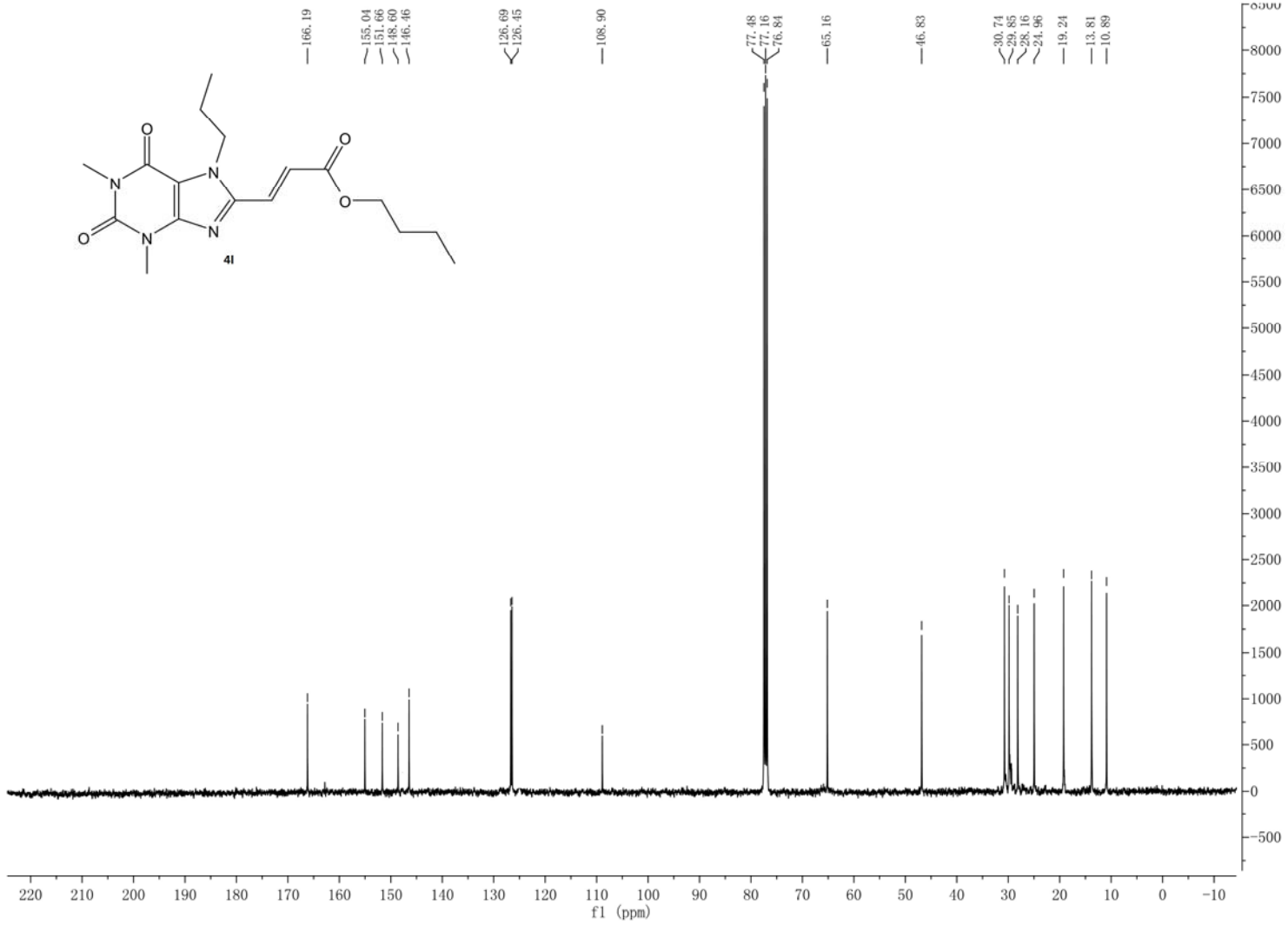

164.80
162.31
155.38
151.84
149.95
148.68
137.21
131.91
129.29
129.21
116.32
116.11
111.10
108.08
77.48
77.16
76.84
31.65
29.89
28.07
O
N
N
O
N
N
F
4j
f1 (ppm)

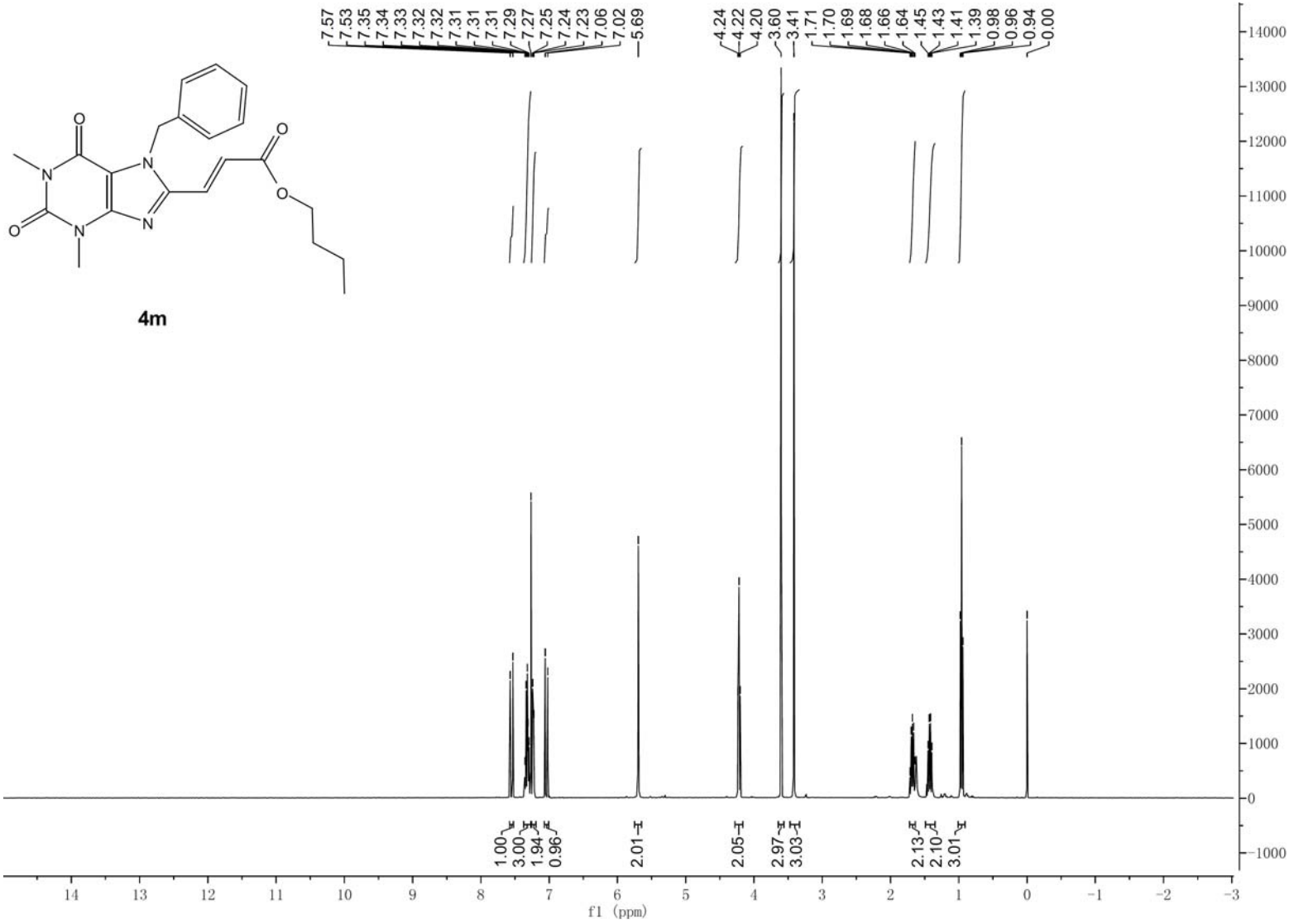

4k
7.52
7.52
7.52
7.48
7.48
7.48
7.28
7.09
7.08
7.08
7.05
7.04
7.04
4.53
4.51
4.27
4.25
4.25
4.23
3.60
3.60
3.59
3.43
3.42
3.42
1.72
1.70
1.48
1.46
1.46
1.45
1.45
0.98
0.97
0.97
0.95
1.00
1.03
2.07
2.21
3.05
3.14
2.42
5.27
3.34
f1 (ppm)

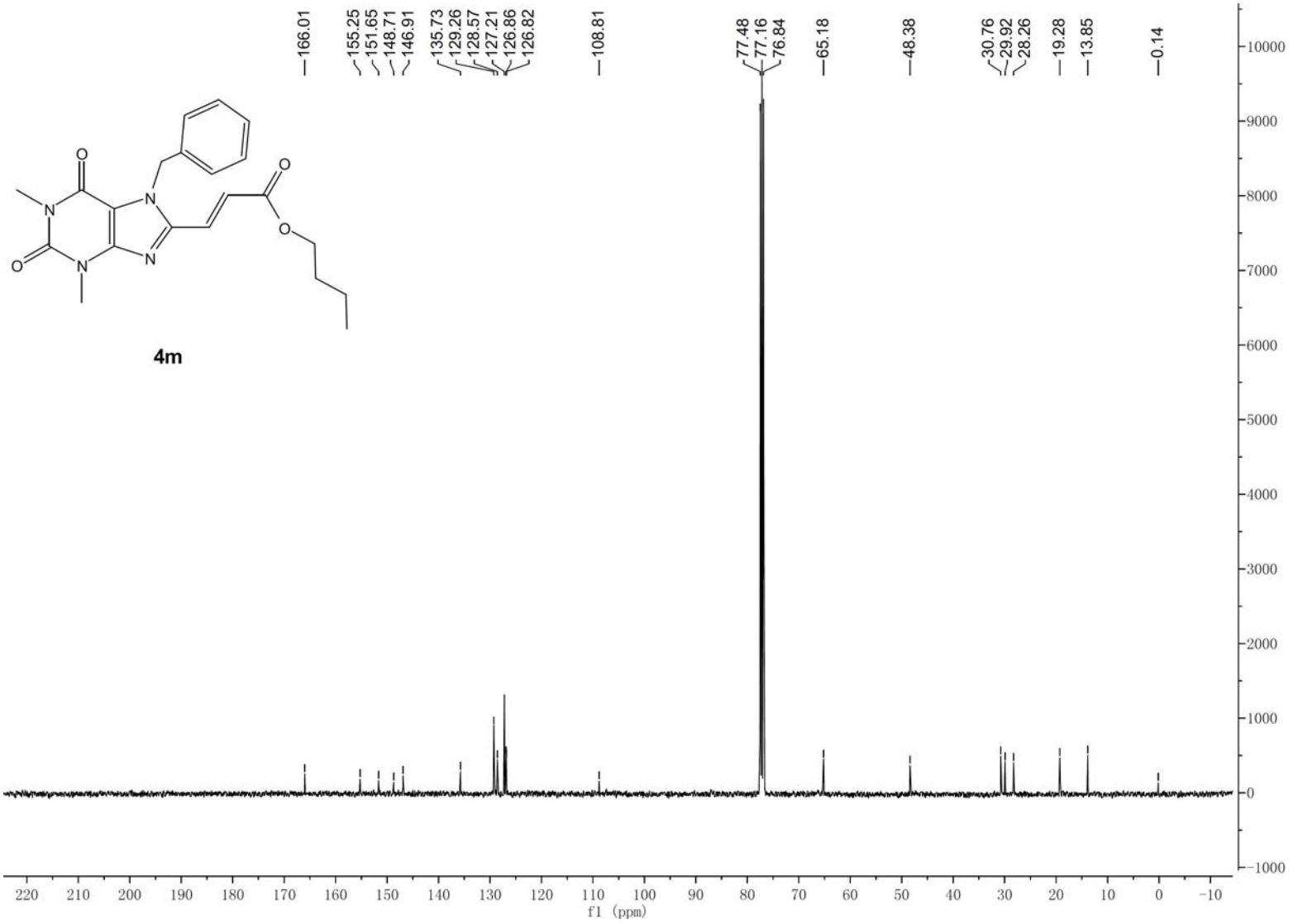

166.20
155.00
151.69
148.67
145.99
126.58
126.46
108.57
77.48
77.16
76.84
65.20
40.60
30.75
29.87
28.17
19.25
17.07
13.82
4k
f1 (ppm)

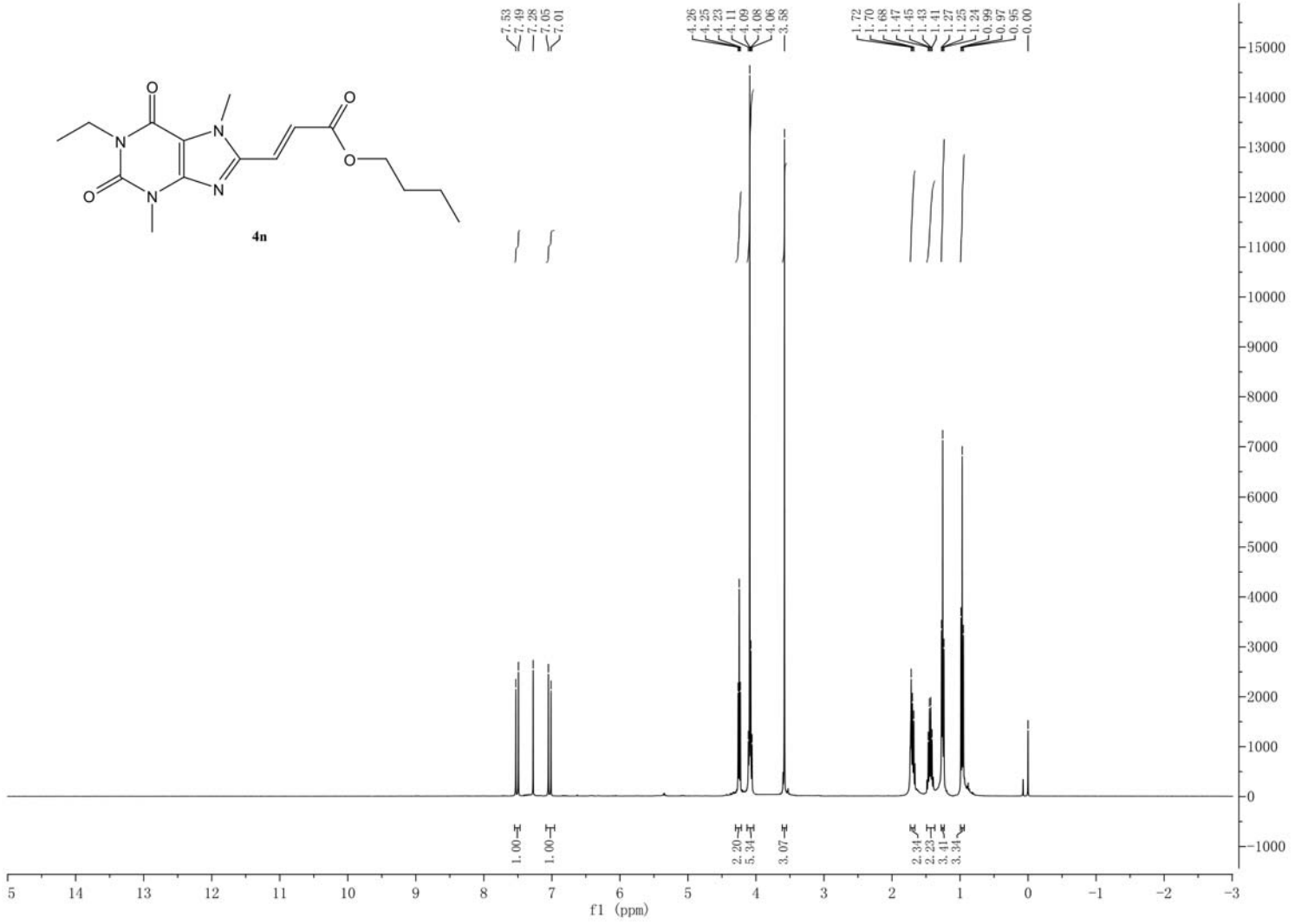

7.44
7.40
7.21
7.00
6.97
4.36
4.35
4.33
4.19
4.17
4.16
3.52
3.34
1.79
1.78
1.64
1.63
1.61
1.40
1.38
1.36
1.34
0.91
0.91
0.90
0.89
0.88
0.87
1.00
0.91
2.00
2.26
2.74
3.08
2.23
2.47
2.45
6.35
f1 (ppm)

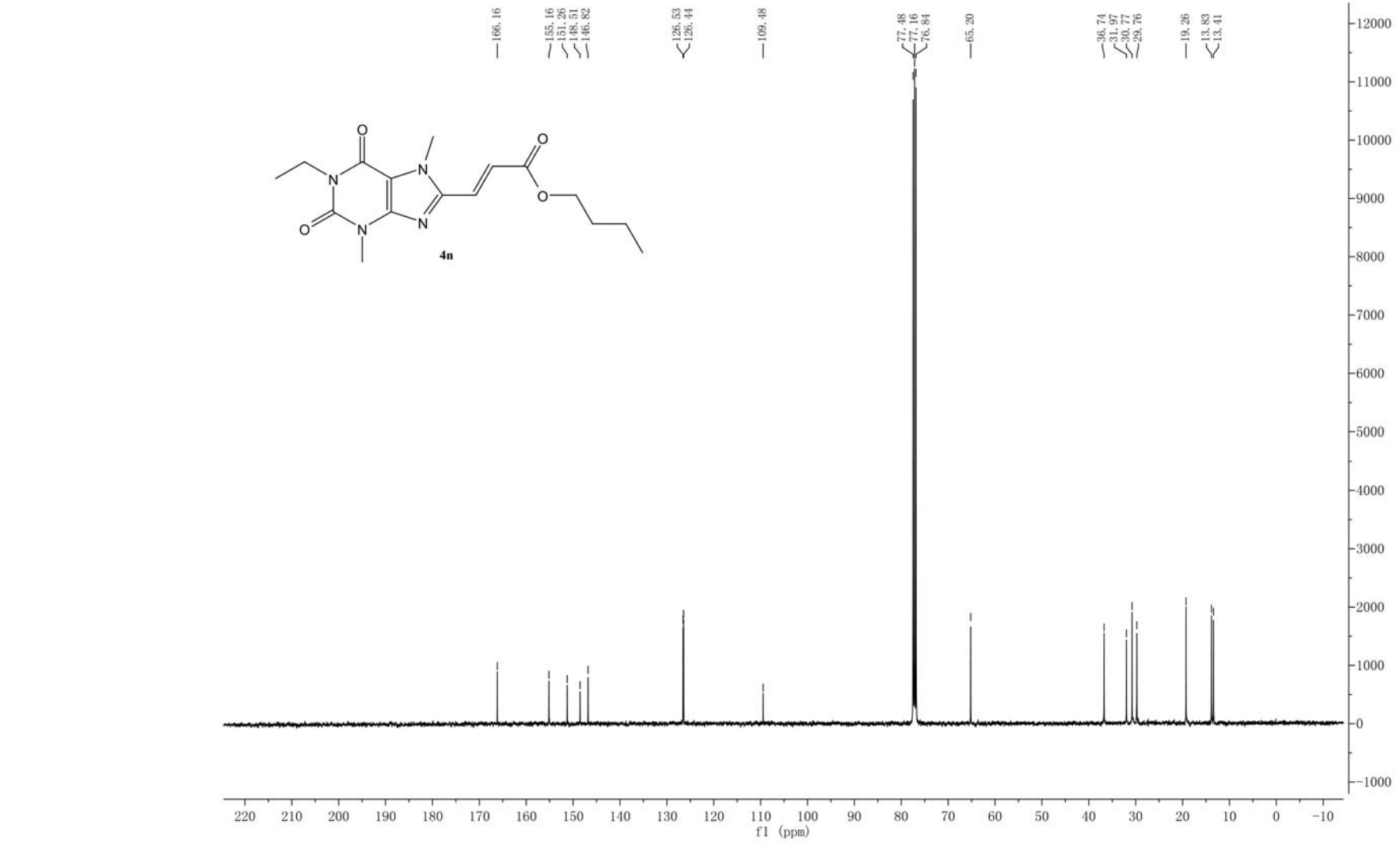
4l

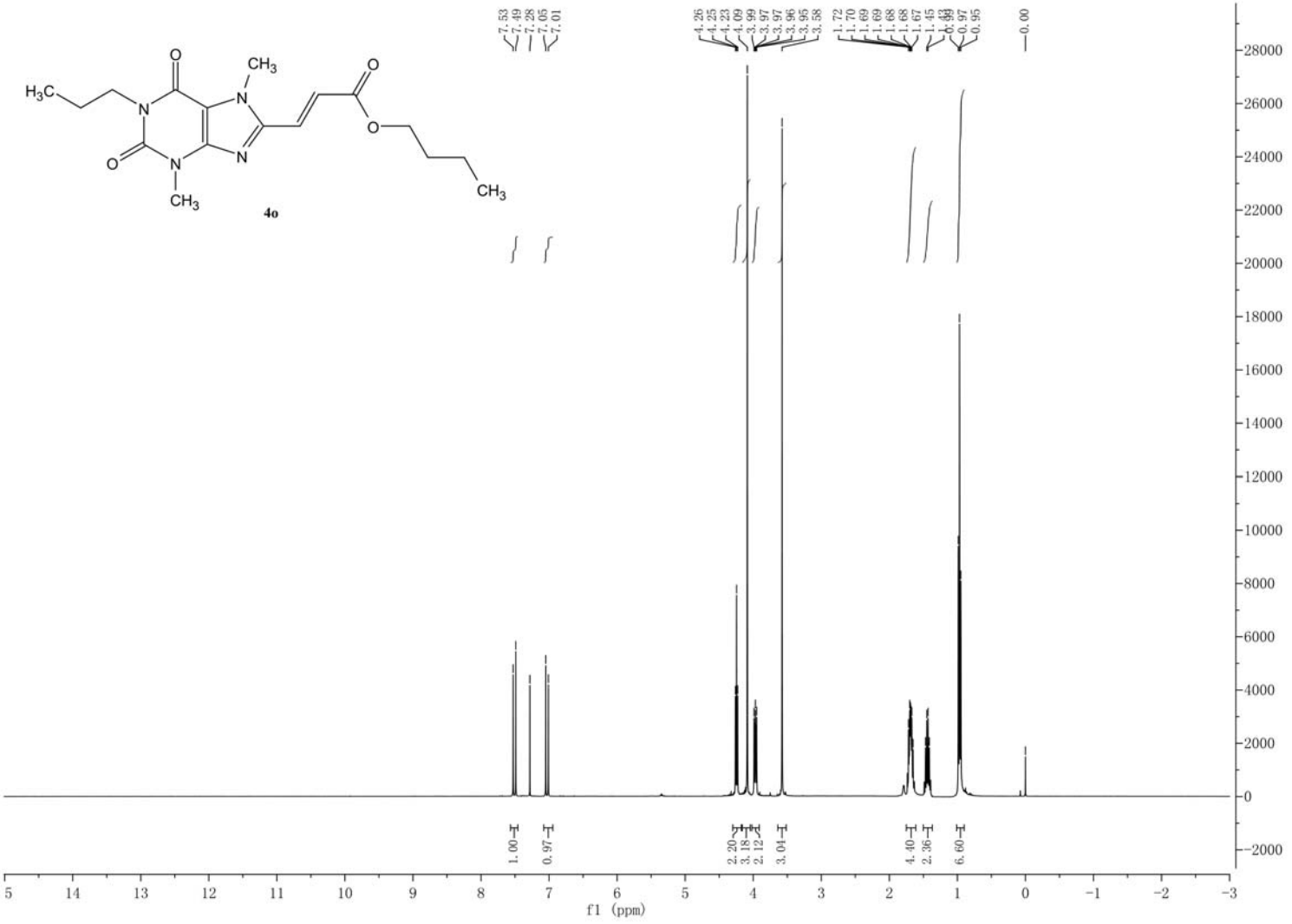

166.19
155.04
151.66
148.60
146.46
126.69
126.45
108.90
77.48
77.16
76.84
65.16
46.83
30.74
29.85
28.16
24.96
19.24
13.81
10.89
4l
f1 (ppm)

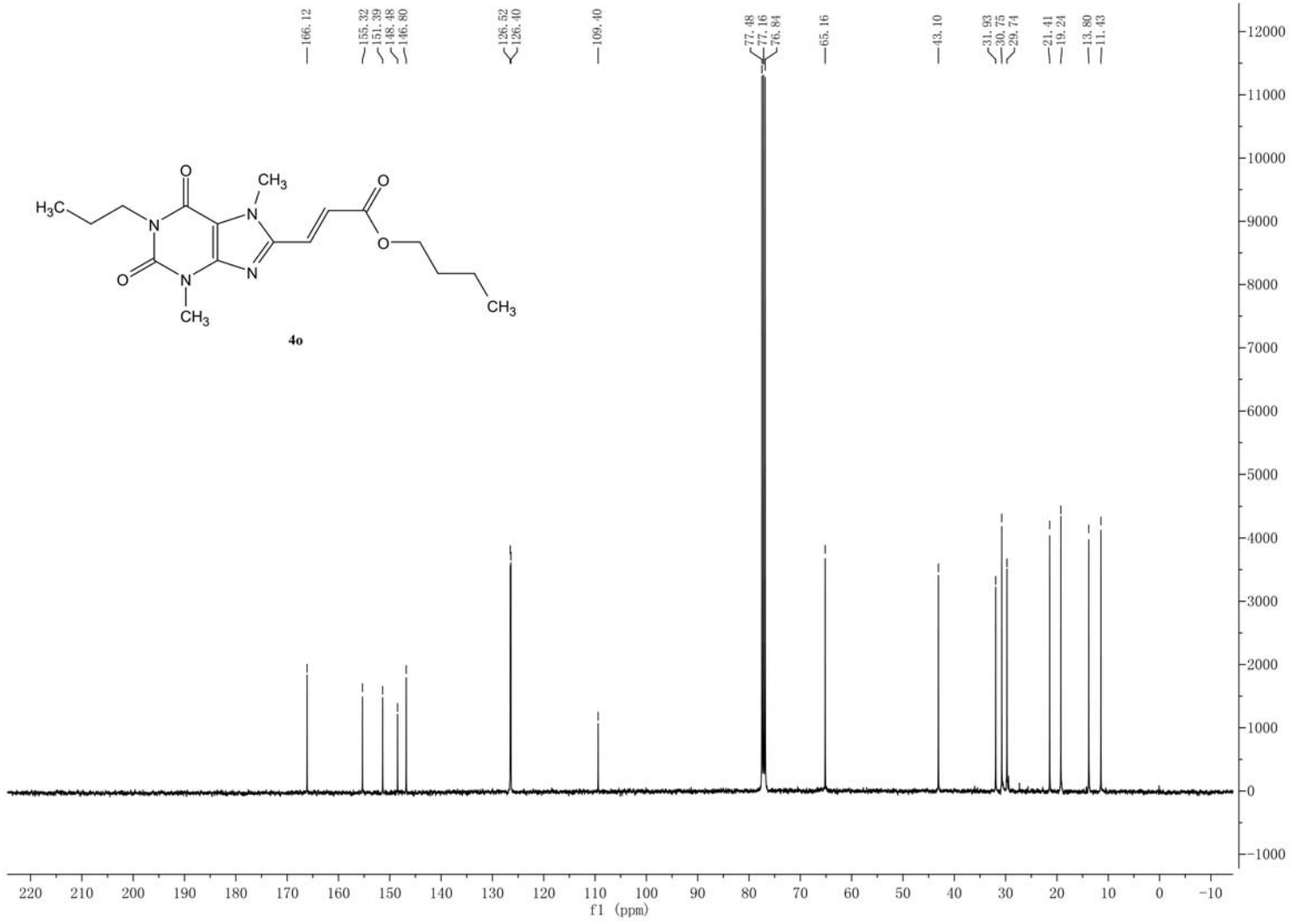

4m
7.57
7.53
7.35
7.34
7.33
7.32
7.32
7.31
7.31
7.31
7.29
7.27
7.25
7.24
7.23
7.06
7.02
5.69
4.24
4.22
4.20
3.60
3.41
1.71
1.70
1.69
1.68
1.66
1.64
1.45
1.43
1.41
1.39
0.98
0.96
0.94
0.00
1.00
3.00
1.94
0.96
2.01
2.05
2.97
3.03
2.13
2.10
3.01
f1 (ppm)

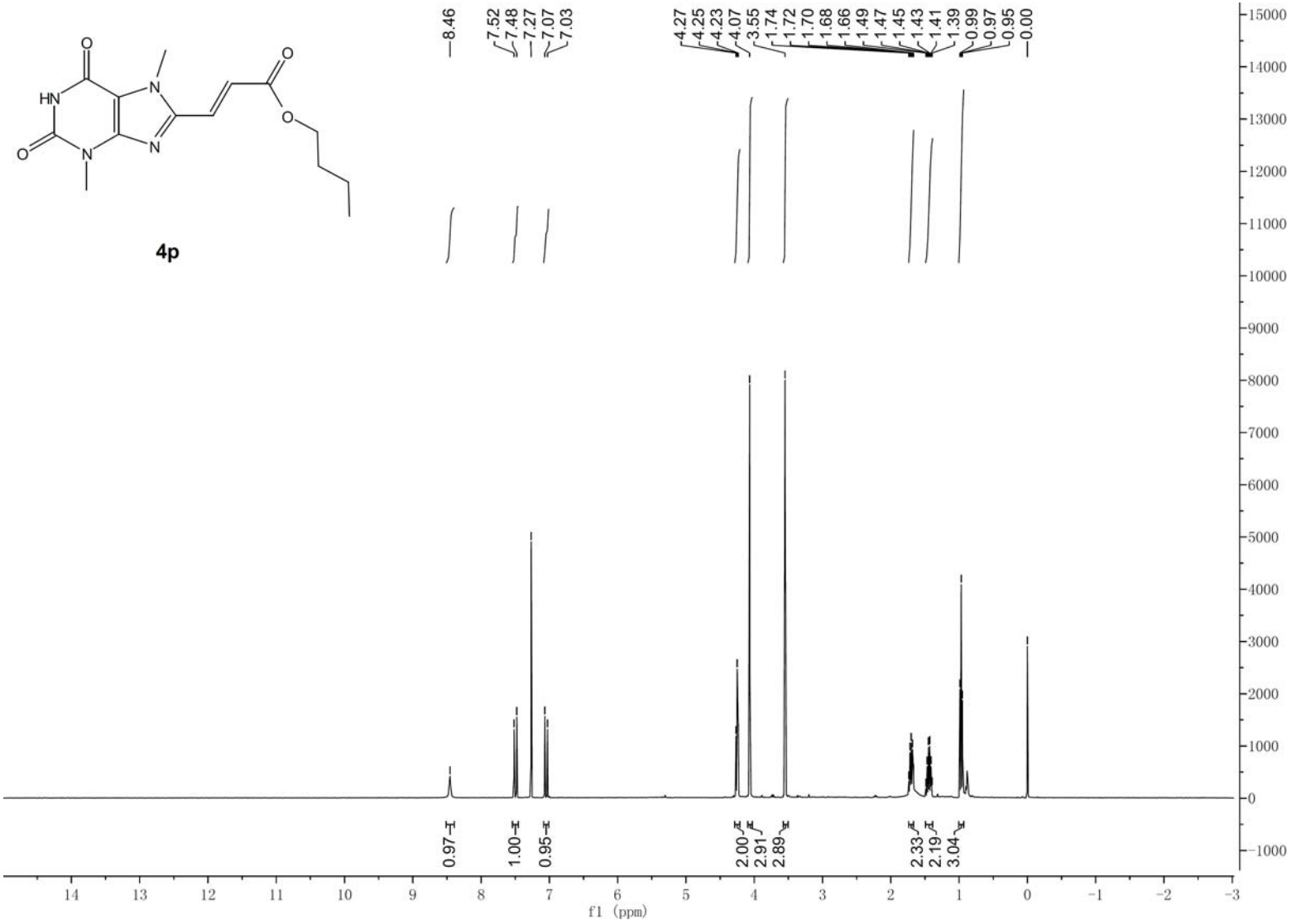

166.01
155.25
151.65
148.71
146.91
135.73
129.26
128.57
127.21
126.86
126.82
108.81
77.48
77.16
76.84
65.18
48.38
30.76
29.92
28.26
19.28
13.85
0.14
4m
f1 (ppm)


4n
7.53
7.49
7.28
7.05
7.01
4.26
4.25
4.23
4.11
4.09
4.08
4.06
3.58
1.72
1.70
1.68
1.47
1.45
1.43
1.41
1.27
1.25
1.24
0.99
0.97
0.95
0.00
1.00
1.00
2.20
5.34
3.07
2.34
2.23
3.41
3.34
f1 (ppm)


166.16
155.16
151.26
148.51
146.82
126.53
126.44
109.48
77.48
77.16
76.84
65.20
36.74
31.97
30.77
29.76
19.26
13.83
13.41
4n
f1 (ppm)


4o
f1 (ppm)


166.12
155.32
151.39
148.48
146.80
126.52
126.40
109.40
77.48
77.16
76.84
65.16
43.10
31.93
30.75
29.74
21.41
19.24
13.80
11.43
4o
f1 (ppm)


4p
8.46
7.52
7.48
7.27
7.07
7.03
4.27
4.25
4.23
4.07
3.55
1.74
1.72
1.70
1.68
1.66
1.49
1.47
1.45
1.43
1.41
1.39
0.99
0.97
0.95
0.00
0.97
1.00
0.95
2.00
2.91
2.89
2.33
2.19
3.04
f1 (ppm)