Supporting Information for

Original article

Novel PF74-like small molecules targeting the HIV-1 capsid protein: balance of potency and metabolic stability

Lei Wang[a,d], Mary C. Casey[b], Sanjeev Kumar V. Vernekar[a], Rajkumar Lalji Sahani[a], Karen A. Kirby[c], Haijuan Du[c], Huanchun Zhang[c], Philip R. Tedbury[c], Jiashu Xie[a], Stefan G. Sarafianos[c], Zhengqiang Wang[a,*]

[a]*Center for Drug Design, College of Pharmacy, University of Minnesota, Minneapolis, MN 55455, USA*

[b]*Department of Molecular Microbiology and Immunology, University of Missouri School of Medicine, Christopher S. Bond Life Sciences Center, Columbia, MO 65211, USA*

[c]*Laboratory of Biochemical Pharmacology, Department of Pediatrics, Emory University School of Medicine, Atlanta, GA 30322, USA*

[d]*Department of Pharmaceutical Sciences, School of Chemical Engineering, Dalian University of Technology, Dalian 116024, China*

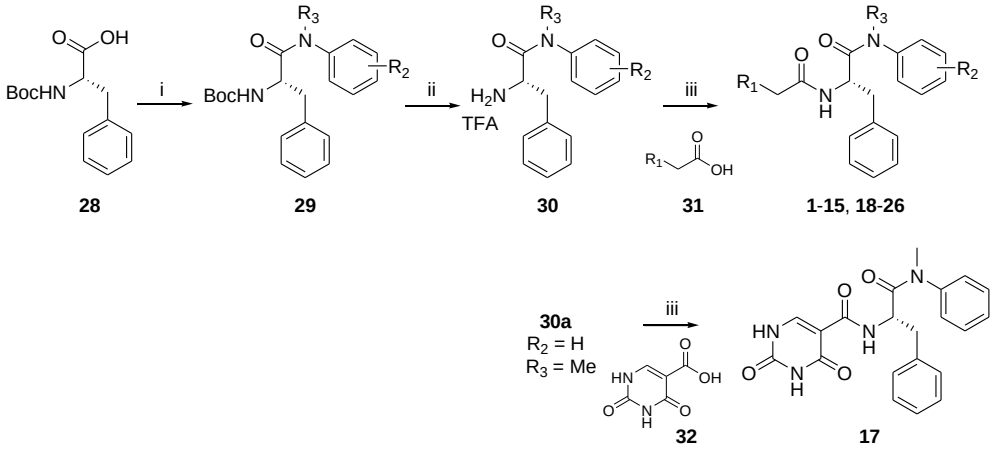
[*]Corresponding author. Tel.: +1 612 6267025.

E-mail address: wangx472@umn.edu (Zhengqiang Wang).

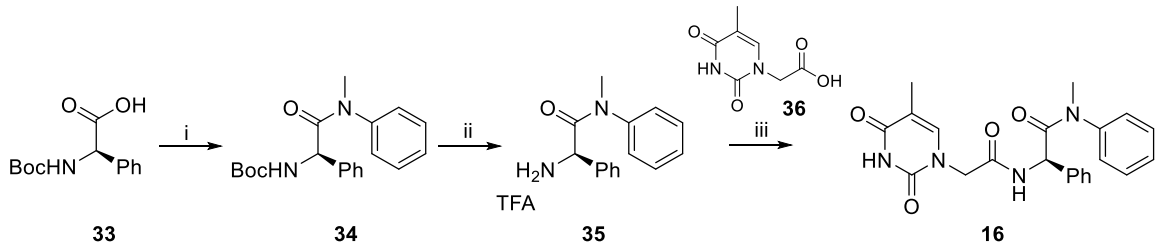
Received 17 June 2020; received in revised form 8 July 2020; accepted 20 July 2020

Table of contents

1. Synthesis of intermediates



Reagents and conditions: (i) amine, T_3P, DIPEA, DMF, rt, 12 h; (ii) TFA; DCM, rt, 4−6 h; (iii) HATU, DIPEA, DMF, rt, 12 h.



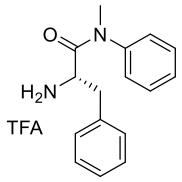
Reagents and conditions: (i) *N*-methylaniline, T_3P, DIPEA, DMF, rt, 12 h; (i) TFA; DCM, rt, 6 h; (iii) HATU, DIPEA, DMF, rt, 12 h.

*1.1. Synthesis of **29***

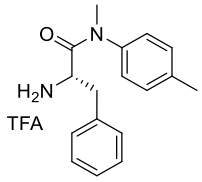
To a solution of (*tert*-butoxycarbonyl)-L-phenylalanine (1.0 g, 1 equiv.) in DMF (5 mL), T_3P (2 equiv.) and DIPEA (3 equiv.) were add and the mixture was stirred at room temperature for 20 min before amine (1.5 equiv.) was added. The mixture was further stirred at room temperature overnight. Upon completion, H_2O was added and the reaction mixture was extracted with EtOAc (3×50 mL). The organic phases were combined and washed with brine, dried over anhydrous $MgSO_4$, filtered and concentrated. The product was purified by Combi-flash on silica gel using EtOAc/hexane.

*1.2. Synthesis of **30***

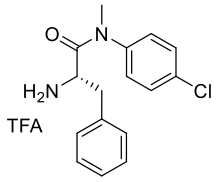
TFA (5 equiv.) was added dropwise to a solution of **29** (1 equiv.) in DCM (5 mL) and the mixture was stirred at room temperature for 4−6 h. The solvent was evaporated to give the product as a TFA salt.



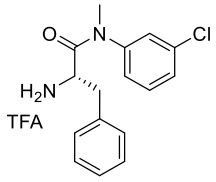
^{1}H NMR (600 MHz, DMSO-d_6) δ 7.36–7.31 (m, 3H), 7.20–7.14 (m, 3H), 6.96–6.90 (m, 2H), 6.83 (d, J = 8.2 Hz, 2H), 3.30 (t, J = 6.8 Hz, 1H), 3.06 (s, 3H), 2.71 (dd, J = 12.7, 6.8 Hz, 1H), 2.43 (dd, J = 13.2, 7.8 Hz, 1H).



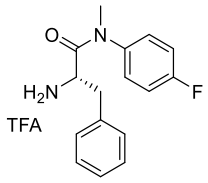
^{1}H NMR (600 MHz, DMSO-d_6) δ 7.20–7.12 (m, 5H), 6.86–6.80 (m, 4H), 3.33–3.30 (m, 1H), 3.02 (s, 3H), 2.71 (dd, J = 13.1, 7.3 Hz, 1H), 2.44 (dd, J = 12.8, 6.8 Hz, 1H), 2.28 (s, 3H).



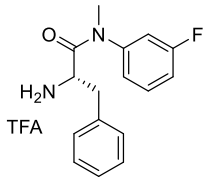
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.37–7.20 (m, 6H), 6.98–6.97 (m, 3H), 4.12–4.10 (m, 1H), 3.10 (s, 3H), 3.08–3.02 (m, 2H).



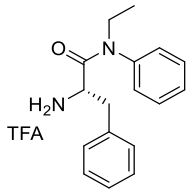
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.37–7.21 (m, 7H), 6.98–6.97 (m, 2H), 4.15–4.12 (m, 1H), 3.12 (s, 3H), 3.10–3.03 (m, 2H).



^{1}H NMR (600 MHz, $CDCl_3$) δ 7.32–7.27 (m, 4H), 6.98–6.93 (m, 5H), 4.09–4.06 (m, 1H), 3.12 (s, 3H), 3.05–3.04 (m, 2H).



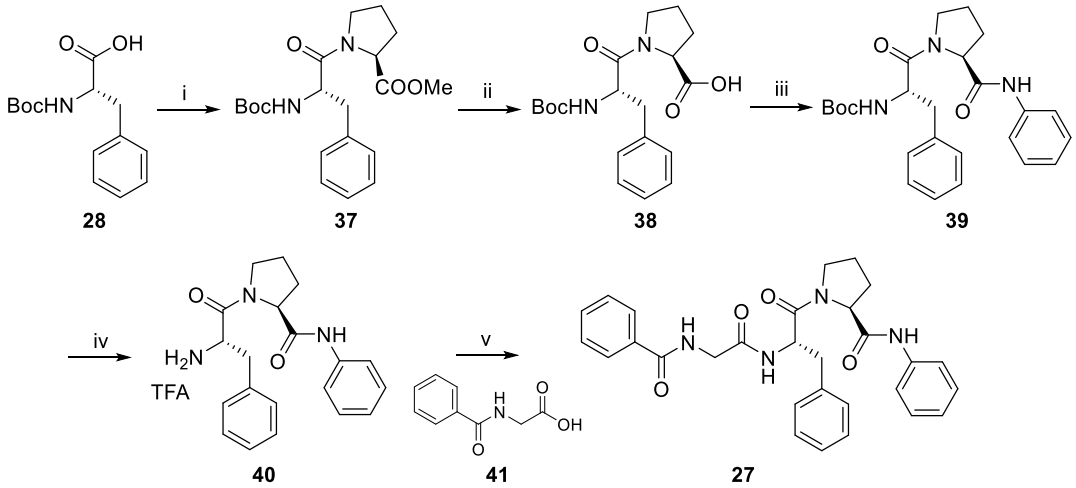
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.32–7.22 (m, 5H), 7.00–6.97 (m, 4H), 4.17–4.14 (m, 1H), 3.11 (s, 3H), 3.10–3.03 (m, 2H).



^{1}H NMR (600 MHz, $CDCl_3$) δ 7.31–7.23 (m, 8H), 6.97–6.96 (m, 2H), 4.03–4.00 (m, 1H), 3.76–3.72 (m, 1H), 3.48–3.43 (m, 1H), 3.08–3.01 (m, 2H), 1.00 (t, J = 7.2 Hz, 3H).

*1.3. Synthesis of **35***

Synthesis of **35** is similar to the synthesis of **30** except (*R*)-2-((*tert*-butoxycarbonyl)amino)-2-phenylacetic acid (**33**) was used in the first step. ^{1}H NMR (600 MHz, DMSO-d_6) δ 8.53 (s, 3H), 7.39–7.25 (m, 6H), 6.99–6.95 (m, 2H), 6.89–6.86 (m, 2H), 4.91 (s, 1H), 3.19 (s, 3H).



Reagents and conditions: (i) L-proline methyl ester hydrochloride, T_3P, DIPEA, DMF, rt, 12 h; (ii) LiOH, MeOH/H_2O, rt, overnight; (iii) aniline, HATU, DIPEA, DMF, rt, 12 h; (iv) TFA; DCM, rt, 6 h; (v) HATU, DIPEA, DMF, rt, 12 h.

*1.4. Synthesis of **37***

To a solution of (*tert*-butoxycarbonyl)-L-phenylalanine (0.5 g, 1 equiv.) in DMF (5 mL), T_3P (2 equiv.) and DIPEA (3 equiv.) were add and the mixture was stirred at room temperature for 20 min before L-proline methyl ester hydrochloride (1.5 equiv.) was added. The mixture was further stirred at room temperature overnight. Upon completion, H_2O was added and the reaction mixture was extracted with EtOAc (3×50 mL). The organic phases were combined and washed with brine, dried over anhydrous $MgSO_4$, filtered and concentrated. The product was purified by Combi-flash on silica gel using EtOAc/hexane.

*1.5. Synthesis of **38***

Compound **37** (1 equiv.) and LiOH (3 equiv.) were dissolved in 10 mL mixture of H_2O/MeOH (2:8). The reaction mixture was stirred for overnight. Solvent was removed under vacuum and the solution was acidified to pH 2 by HCl 2N. The crude mixture was filtered to give desired product.

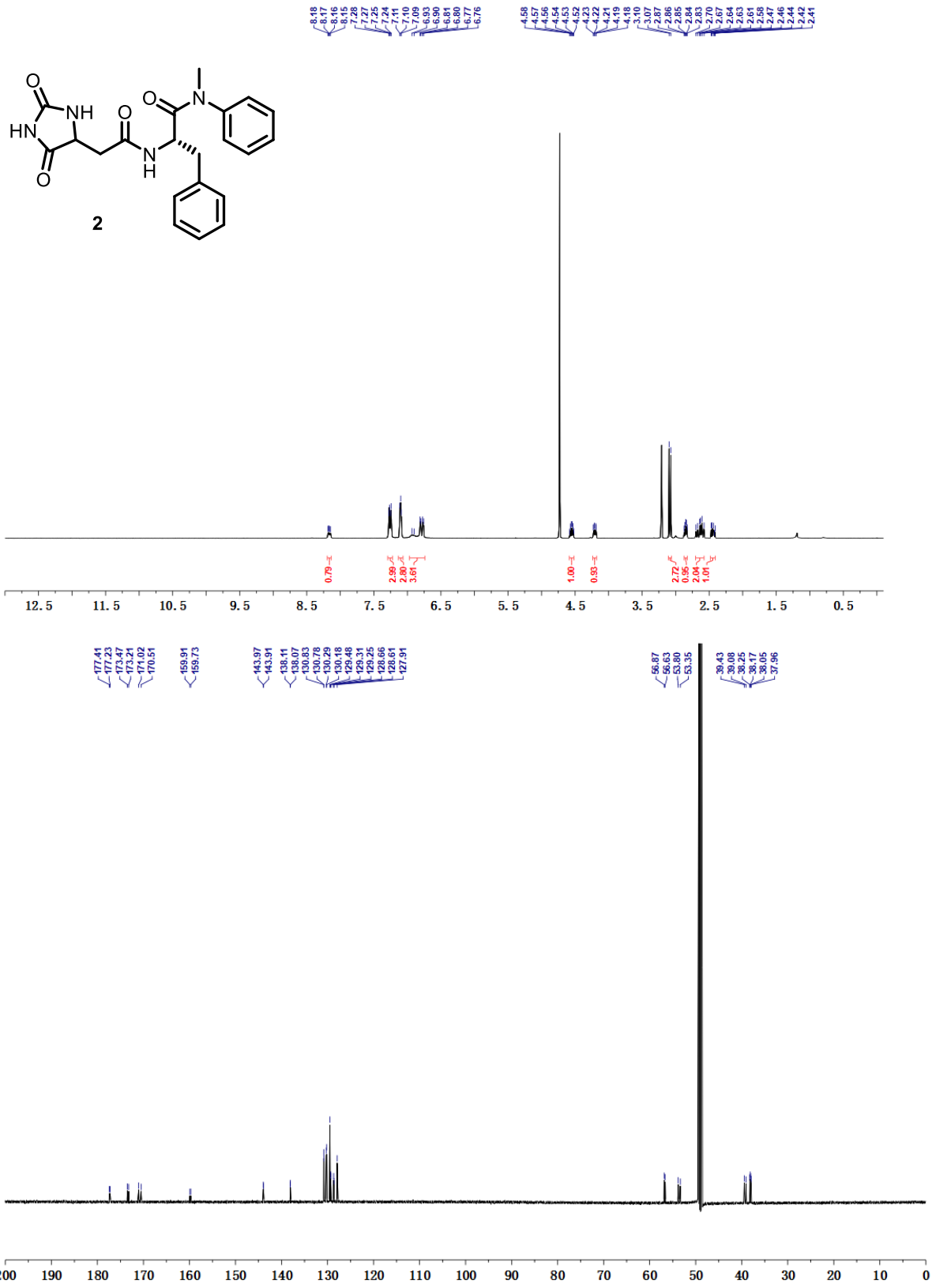
*1.6. Synthesis of **39***

To a solution of **38** (1 equiv.) in DMF, HATU (2 equiv.) and DIPEA (3 equiv.) were add and the mixture was stirred at room temperature for 20 min before aniline (1.5 equiv.) was added. The mixture was further stirred at RT overnight. Upon completion, H_2O was added and the reaction mixture was extracted with EtOAc (3×50 mL). The organic phases were combined and washed with brine, dried over anhydrous $MgSO_4$, filtered and concentrated. The product was purified by Combi-flash on silica gel using EtOAc/hexane.

*1.7. Synthesis of **40***

TFA (5 equiv.) was added dropwise to a solution of **39** (1 equiv.) in DCM (5 mL) and the mixture was stirred at room temperature for 6 h. The solvent was evaporated to give the product **40** as a TFA salt. ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.25 (s, 1H), 7.61 (d, J = 7.8 Hz, 2H), 7.31–7.28 (m, 2H), 7.19–7.14 (m, 3H), 7.12–7.06 (m, 3H), 4.50–4.45 (m, 1H), 4.20–4.14 (m, 1H), 3.19 (q, J = 7.2 Hz, 1H), 3.06–2.95 (m, 2H), 2.71–2.63 (m, 1H), 2.07–2.04 (m, 1H), 1.90–1.82 (m, 2H), 1.80–1.71 (m, 1H).

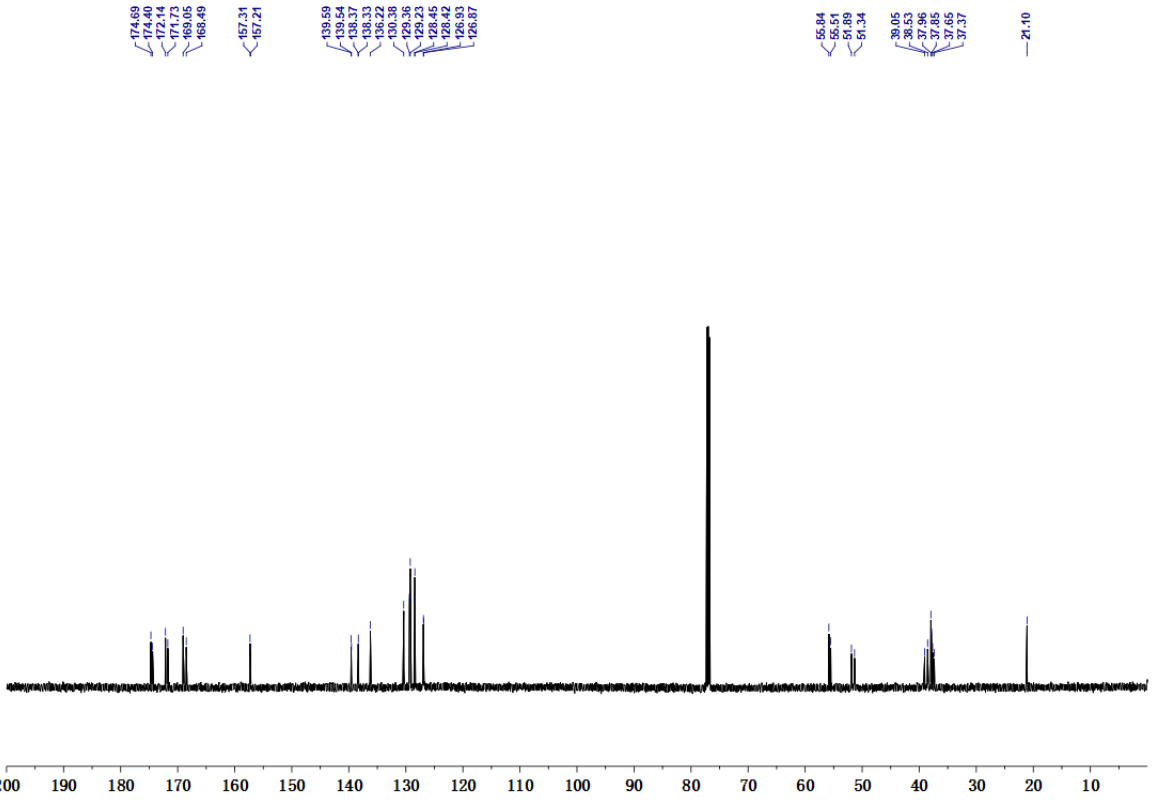
2. NMR spectra

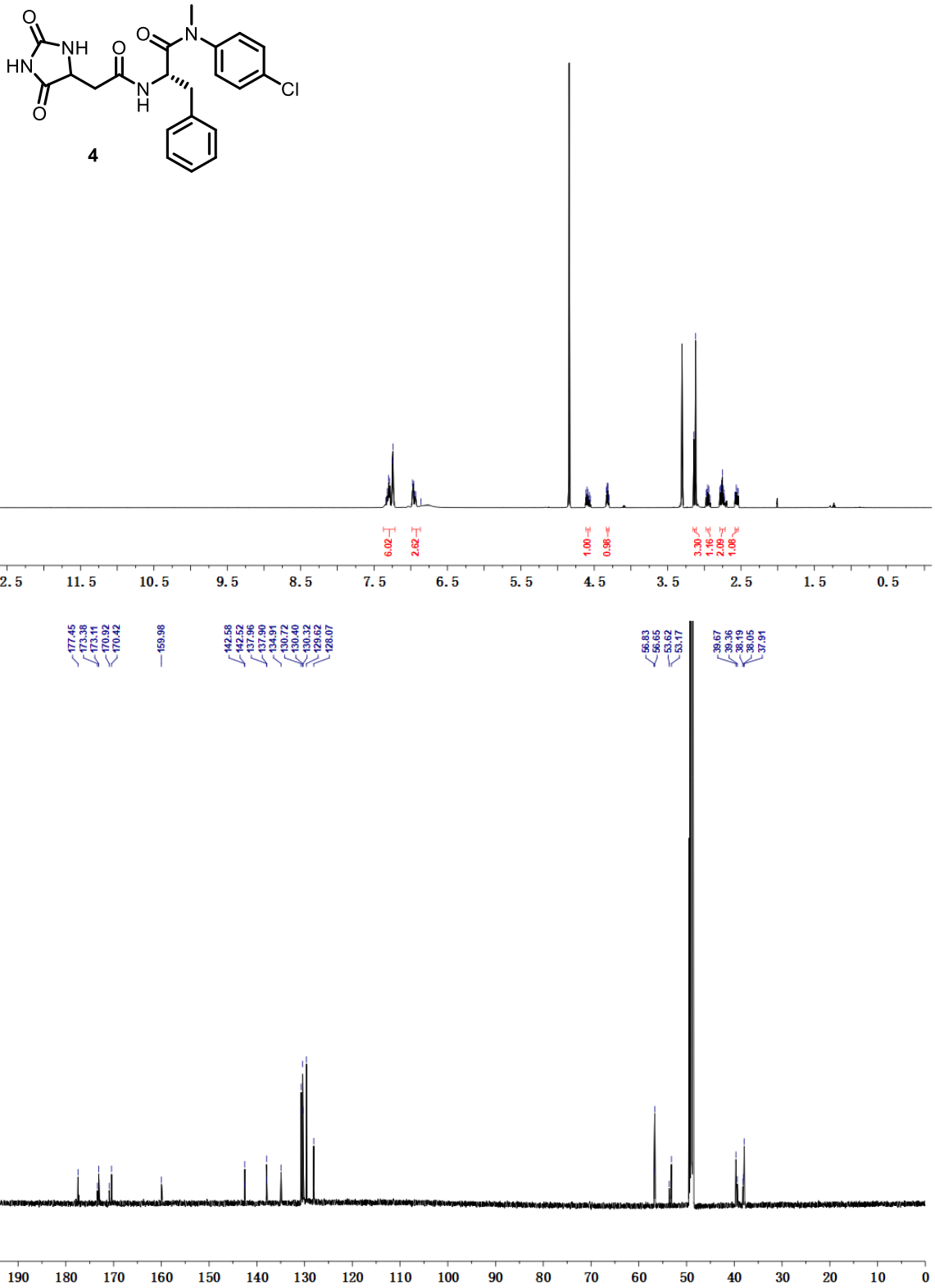


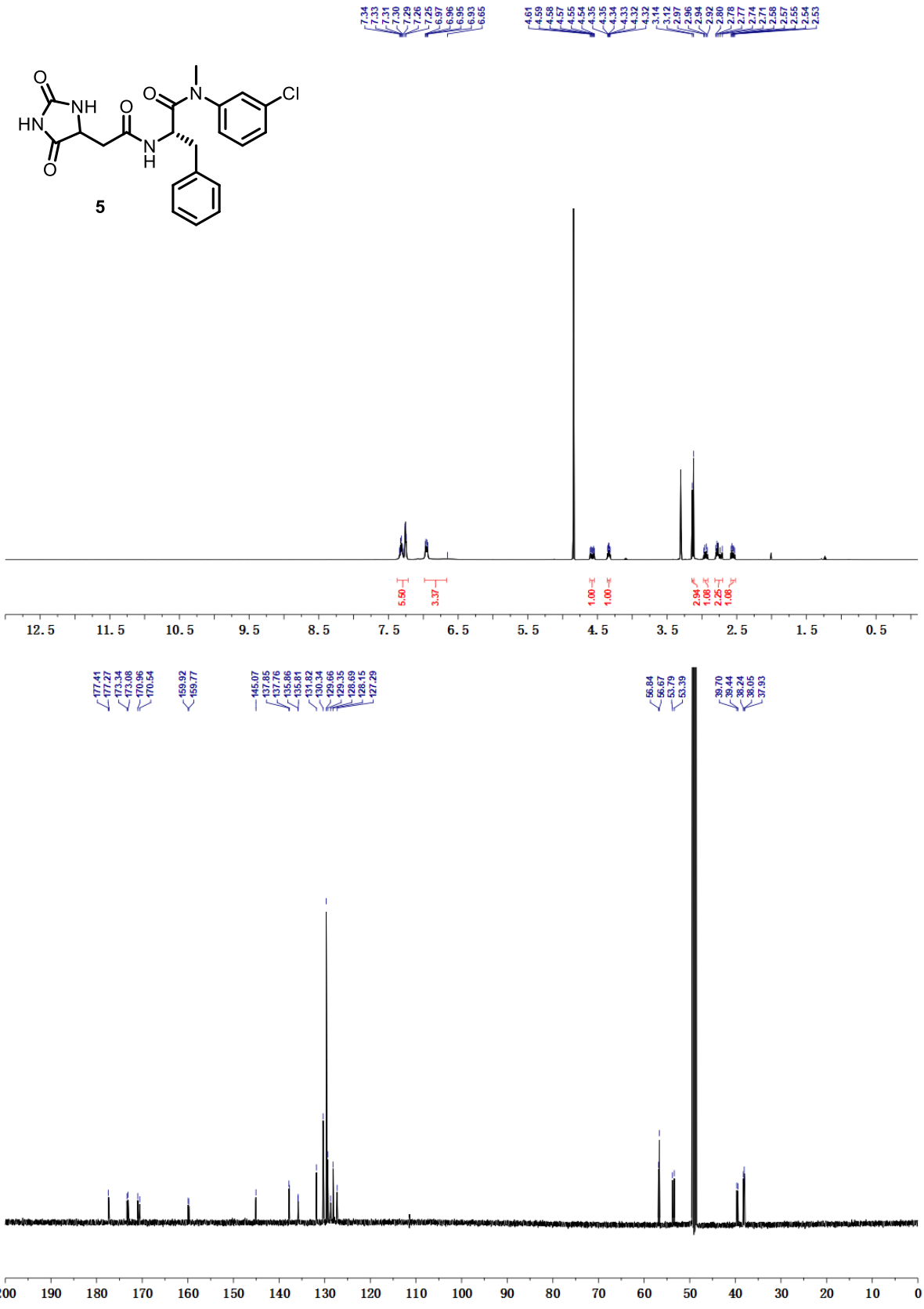
O
NH
HN
O
O
N
O
N
H

3

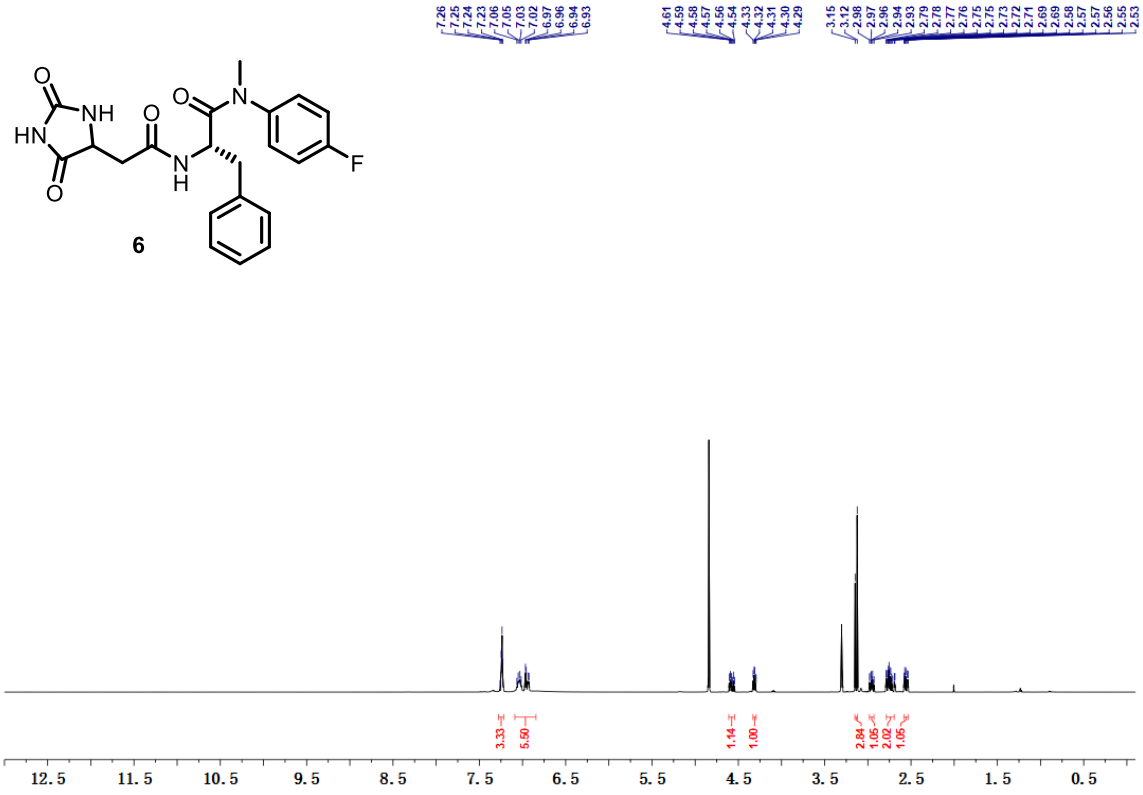

9.52
9.36
7.52
7.50
7.38
7.36
7.22
7.21
7.20
7.19
7.16
7.15
7.14
6.91
6.90
6.89
6.87
6.86
6.78
4.85
4.84
4.82
4.81
4.79
4.78
4.77
4.35
4.34
4.33
4.32
2.92
2.91
2.90
2.89
2.88
2.86
2.84
2.81
2.74
2.73
2.72
2.70
2.51
2.49
2.48
2.46
2.47
2.45
2.37
2.36
1.32
1.13
4.20
3.95
1.00
0.93
1.99
0.96
1.00
2.67
12.5
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5


174.69
174.40
172.14
171.73
169.05
168.49
157.31
157.21
139.59
139.54
138.37
138.33
136.22
130.38
129.36
129.23
128.45
128.42
126.93
126.87
55.84
55.51
54.89
51.34
39.05
38.53
37.96
37.85
37.65
37.37
21.10
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10

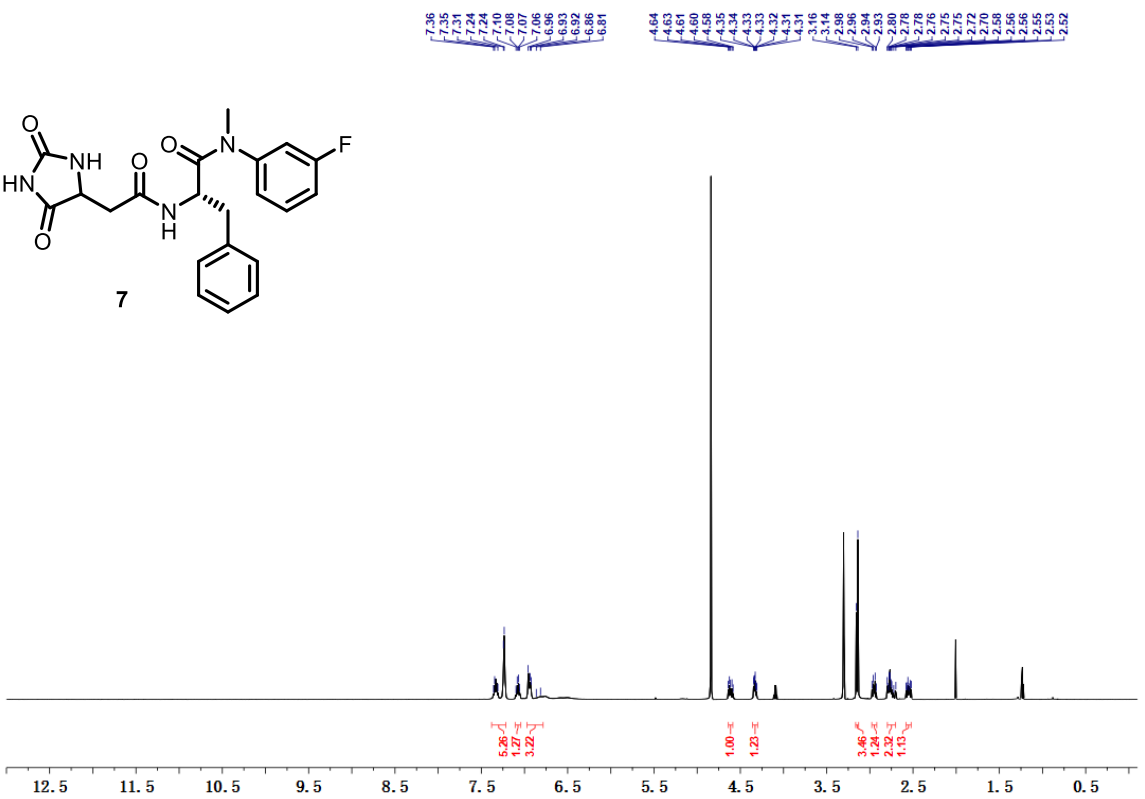

7.34
7.32
7.30
7.29
7.25
7.24
6.98
6.96
6.95
6.93
6.86
4.61
4.60
4.59
4.58
4.56
4.55
4.33
4.32
4.31
4.30
3.14
3.12
2.98
2.96
2.95
2.94
2.92
2.79
2.78
2.76
2.75
2.74
2.73
2.72
2.58
2.56
2.55
2.54
O
NH
HN
O
O
N
N
H
Cl
4
6.02
2.62
1.00
0.98
3.30
1.16
2.09
1.08
12.5
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
177.45
173.38
173.11
170.92
170.42
159.98
142.58
142.52
137.96
137.90
134.91
130.72
130.40
130.32
129.62
128.07
56.83
56.65
53.62
53.17
39.67
39.36
39.19
38.05
37.91
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0


7.34
7.33
7.31
7.30
7.29
7.26
7.25
6.97
6.96
6.95
6.93
6.65
4.61
4.59
4.58
4.57
4.55
4.54
4.35
4.34
4.33
4.32
3.14
3.12
2.97
2.96
2.94
2.92
2.80
2.78
2.77
2.74
2.71
2.68
2.57
2.55
2.54
2.53
O
NH
HN
O
O
N
O
N
H
Cl
5
5.50
3.37
1.00
1.00
2.94
1.08
2.25
1.08
12.5
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
177.41
177.27
173.34
173.08
170.96
170.54
159.92
159.77
145.07
137.85
137.76
135.86
135.81
131.82
130.34
129.66
129.35
128.69
128.15
127.29
56.84
56.67
53.79
53.39
39.70
39.44
38.24
38.05
37.93
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

6

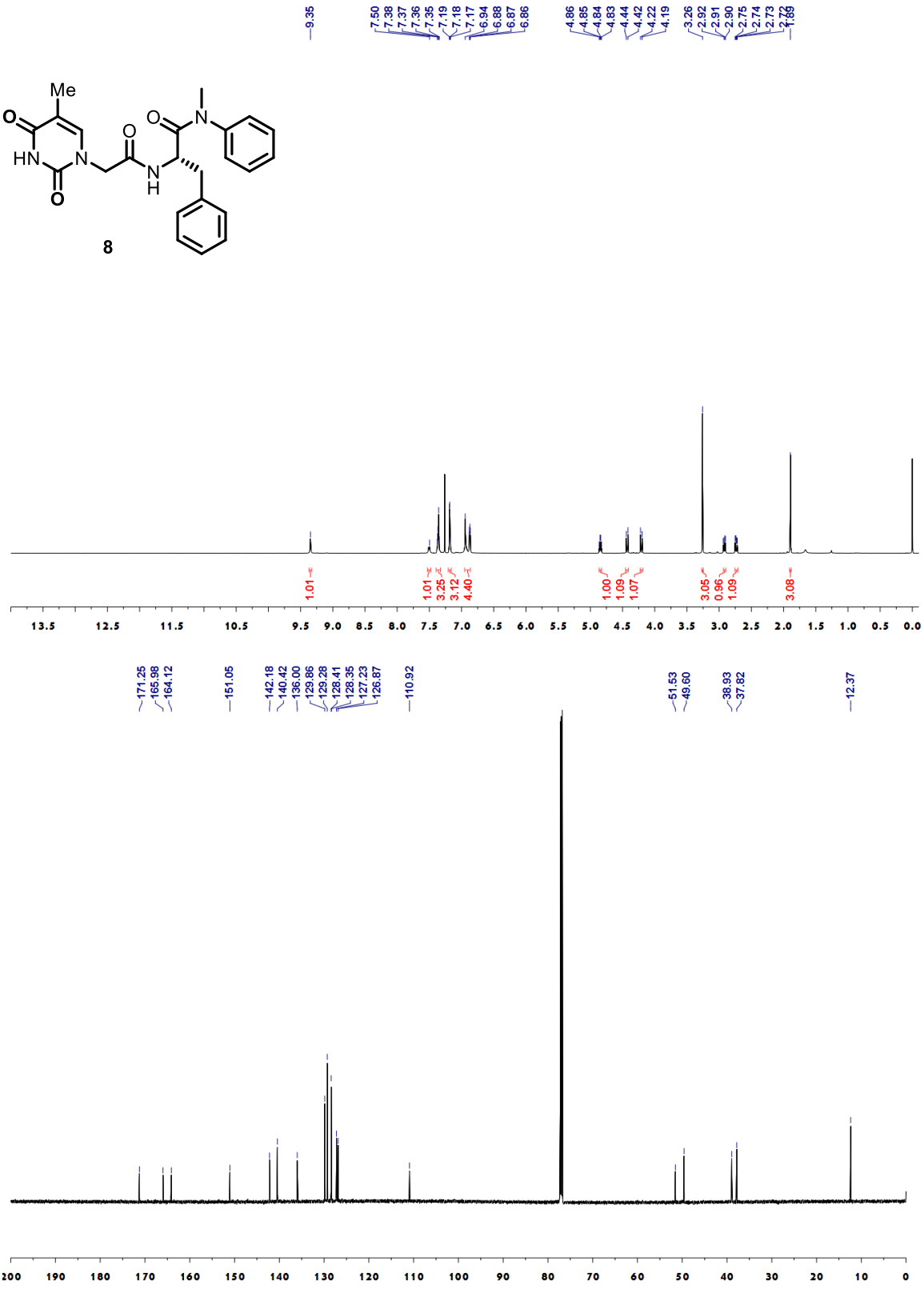


7



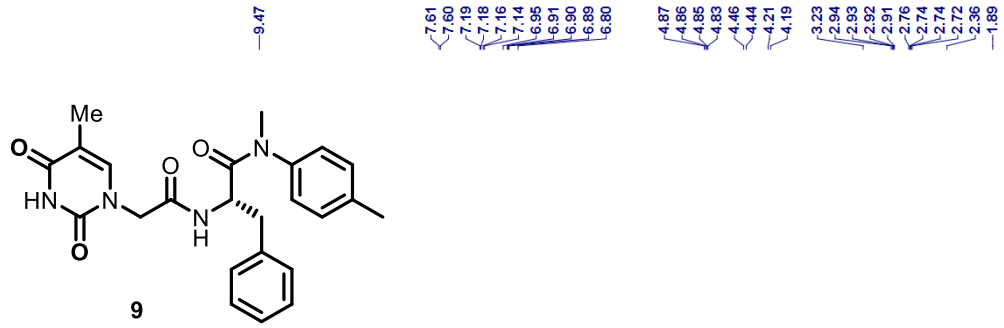
Me
O
HN
N
O
O
N
N
H

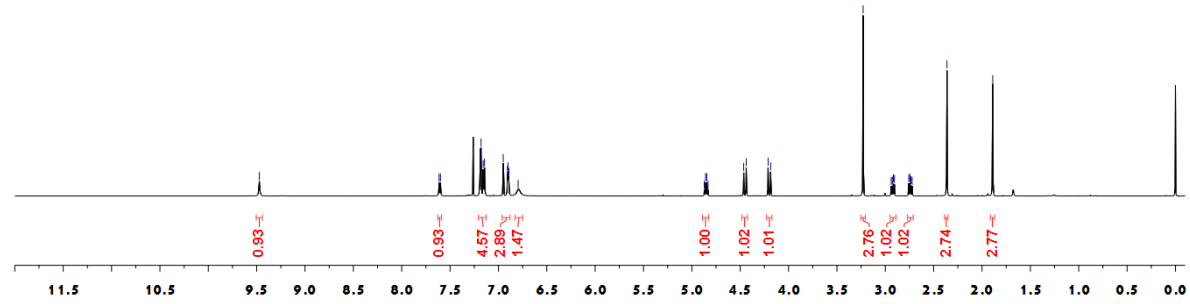
8

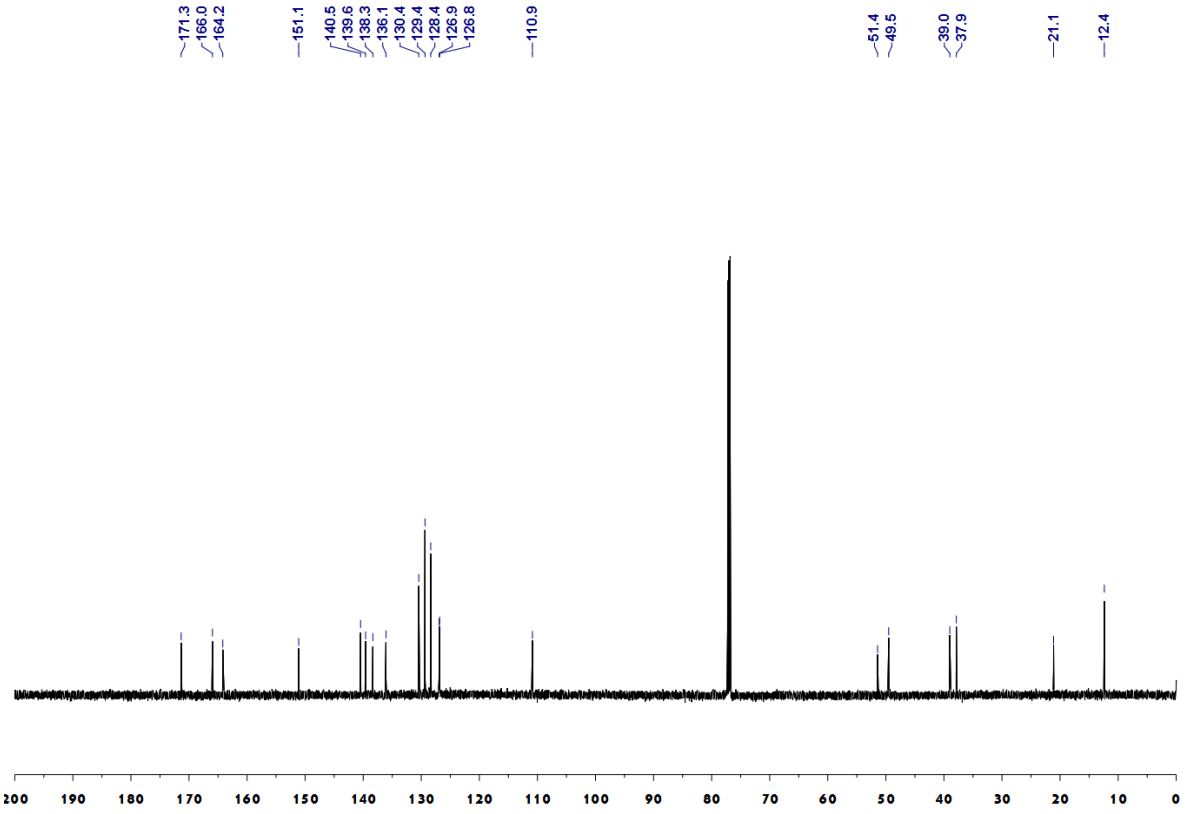

9.35
7.50
7.38
7.37
7.36
7.35
7.19
7.18
7.17
6.94
6.88
6.87
6.86
4.86
4.85
4.84
4.83
4.44
4.42
4.22
4.19
3.26
2.92
2.91
2.90
2.75
2.74
2.73
1.88
1.01
1.01
3.25
3.12
4.40
1.00
1.09
1.07
3.05
0.96
1.09
3.08
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
171.25
165.98
164.12
151.05
142.18
140.42
136.00
129.86
129.28
128.41
128.35
127.23
126.87
110.92
51.53
49.60
38.93
37.82
12.37
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

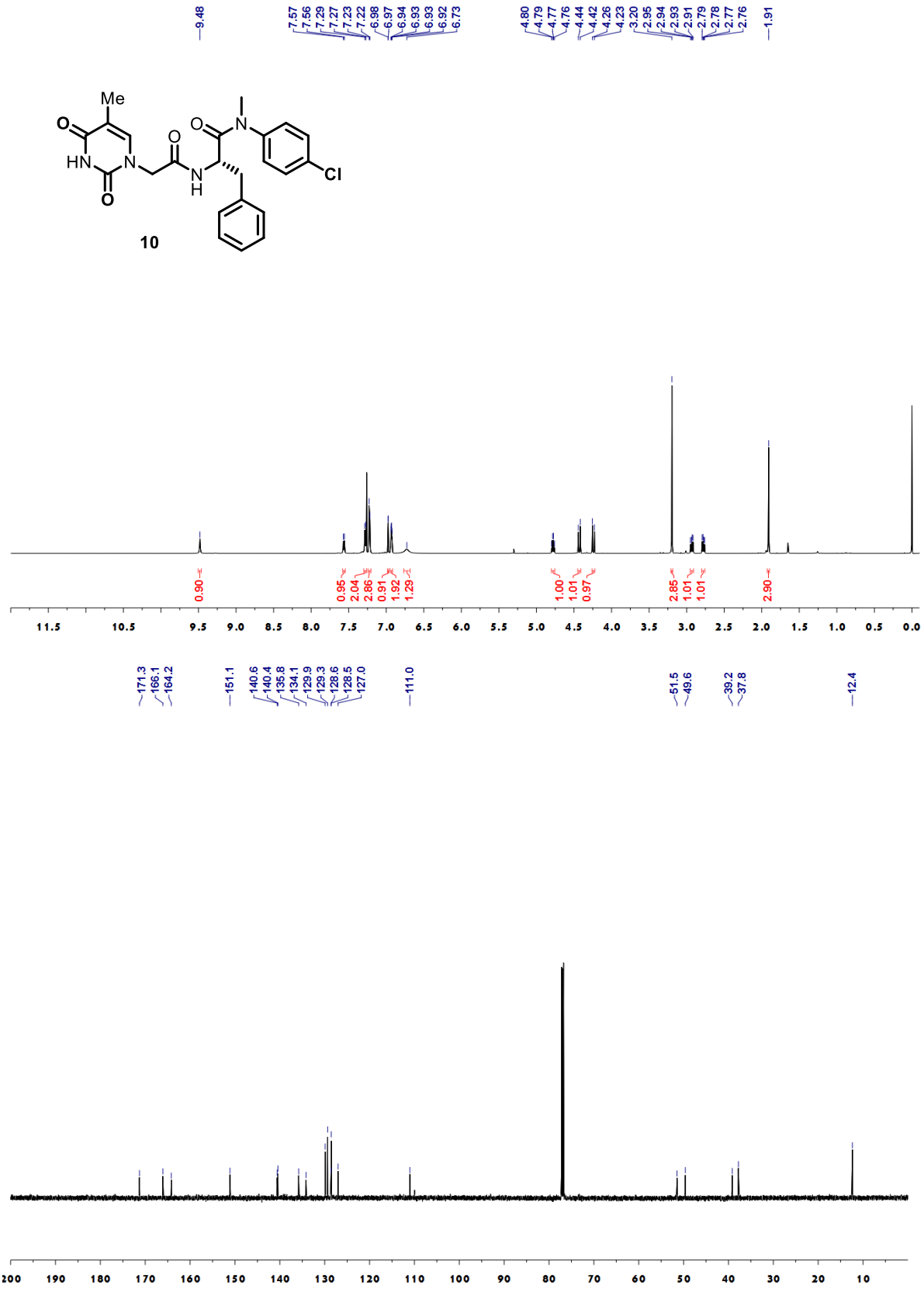
Me
O
HN
N
O
O
N
H
O
N

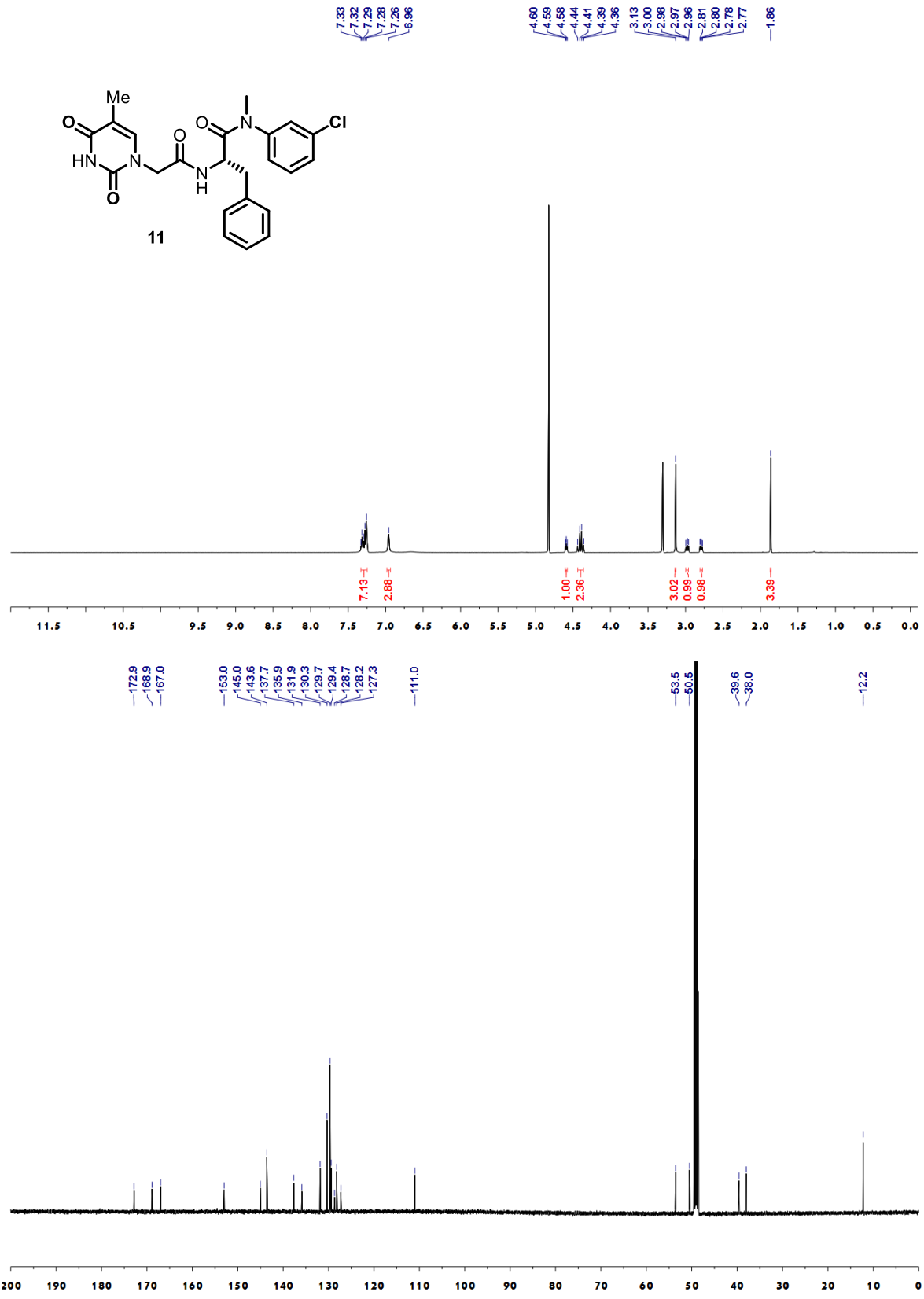
9


9.47
7.61
7.60
7.19
7.18
7.16
7.14
6.95
6.91
6.90
6.89
6.80
4.87
4.86
4.85
4.83
4.46
4.44
4.21
4.19
3.23
2.94
2.93
2.92
2.91
2.76
2.74
2.74
2.72
2.36
1.89


0.93
0.93
4.57
2.89
1.47
1.00
1.02
1.01
2.76
1.02
1.02
2.74
2.77
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

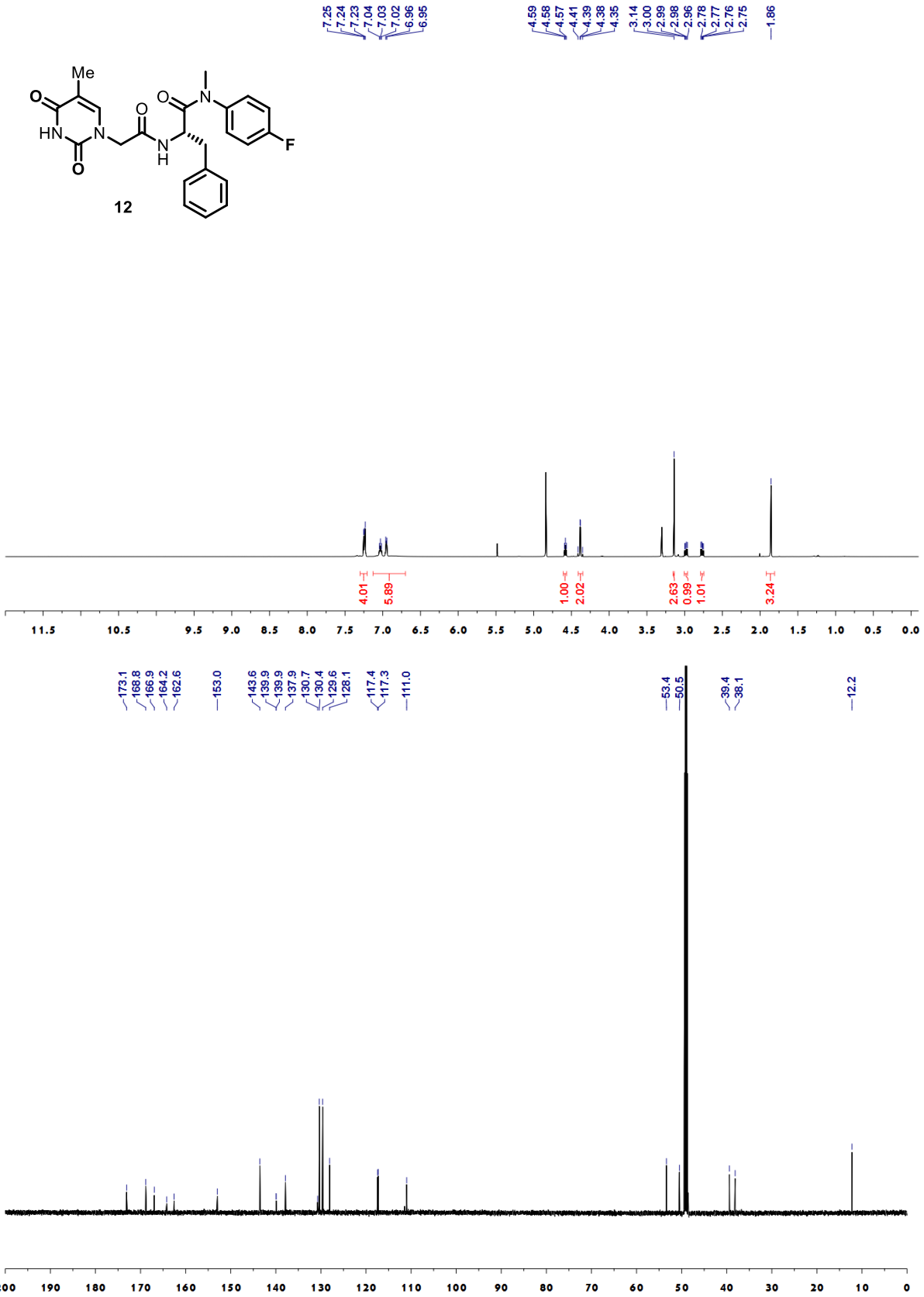

171.3
166.0
164.2
151.1
140.5
139.6
138.3
136.1
130.4
129.4
128.4
126.9
126.8
110.9
51.4
49.5
39.0
37.9
21.1
12.4
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0


9.48
7.57
7.56
7.29
7.27
7.23
7.22
6.98
6.97
6.94
6.93
6.93
6.92
6.73
4.80
4.79
4.77
4.76
4.44
4.42
4.26
4.23
3.20
2.95
2.94
2.93
2.91
2.79
2.78
2.77
2.76
1.91
Me
O
HN
N
O
O
N
H
O
N
Cl
10
0.90
0.95
2.04
2.86
0.91
1.92
1.29
1.00
1.01
0.97
2.85
1.01
1.01
2.90
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
171.3
166.1
164.2
151.1
140.6
140.4
135.8
134.1
129.9
129.3
128.6
128.5
127.0
111.0
51.5
49.6
39.2
37.8
12.4
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10


7.33
7.32
7.29
7.28
7.26
6.96
4.60
4.59
4.58
4.44
4.41
4.39
4.36
3.13
3.00
2.98
2.97
2.96
2.81
2.80
2.78
2.77
1.86
Me
O
HN
N
O
O
N
H
O
N
Cl
11
7.13
2.88
1.00
2.36
3.02
0.99
0.98
3.39
172.9
168.9
167.0
153.0
145.0
143.6
137.7
135.9
131.9
130.3
129.7
129.4
128.7
128.2
127.3
111.0
53.5
50.5
39.6
38.0
12.2

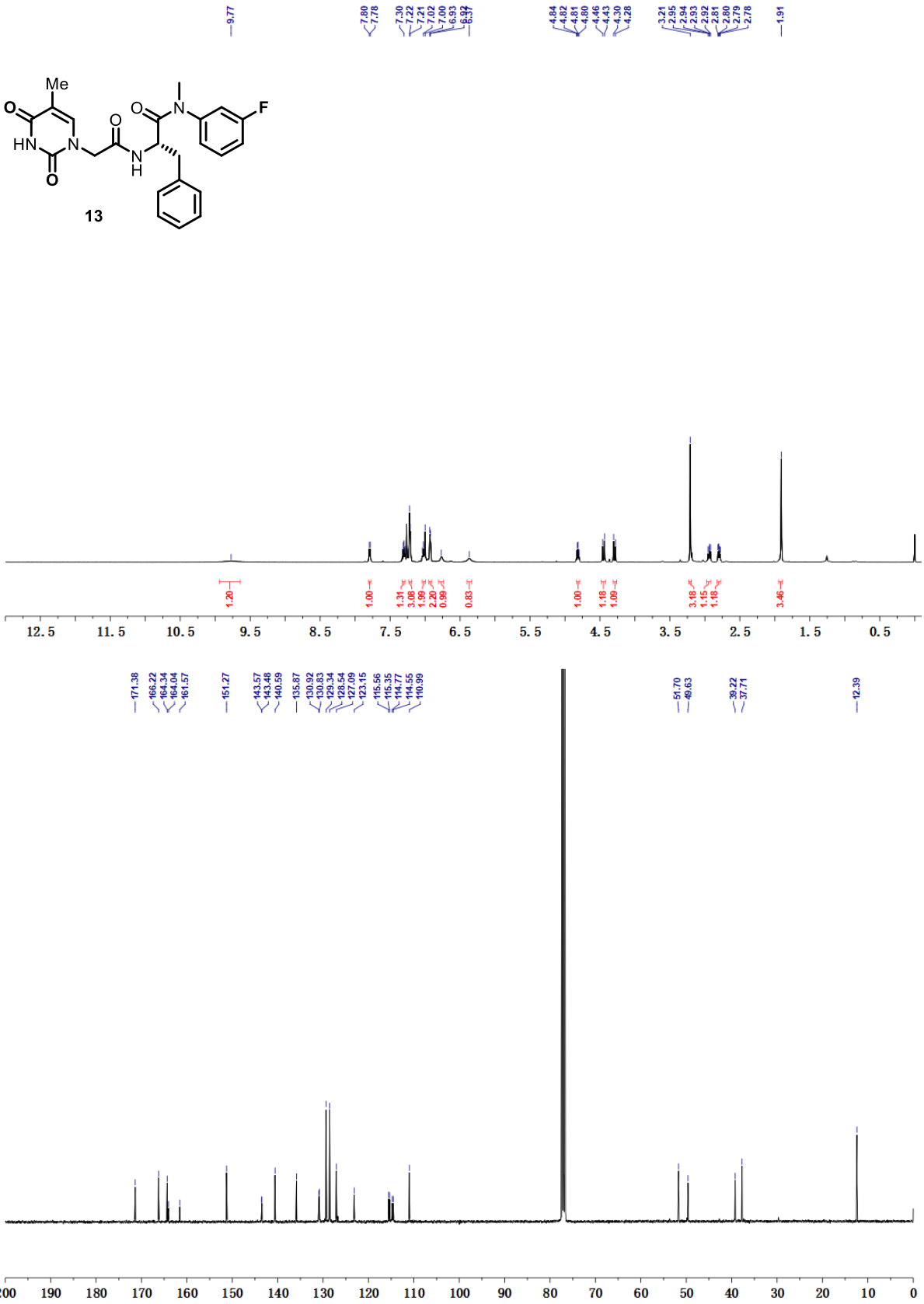
Me
O
HN
N
O
O
N
H
O
N
F

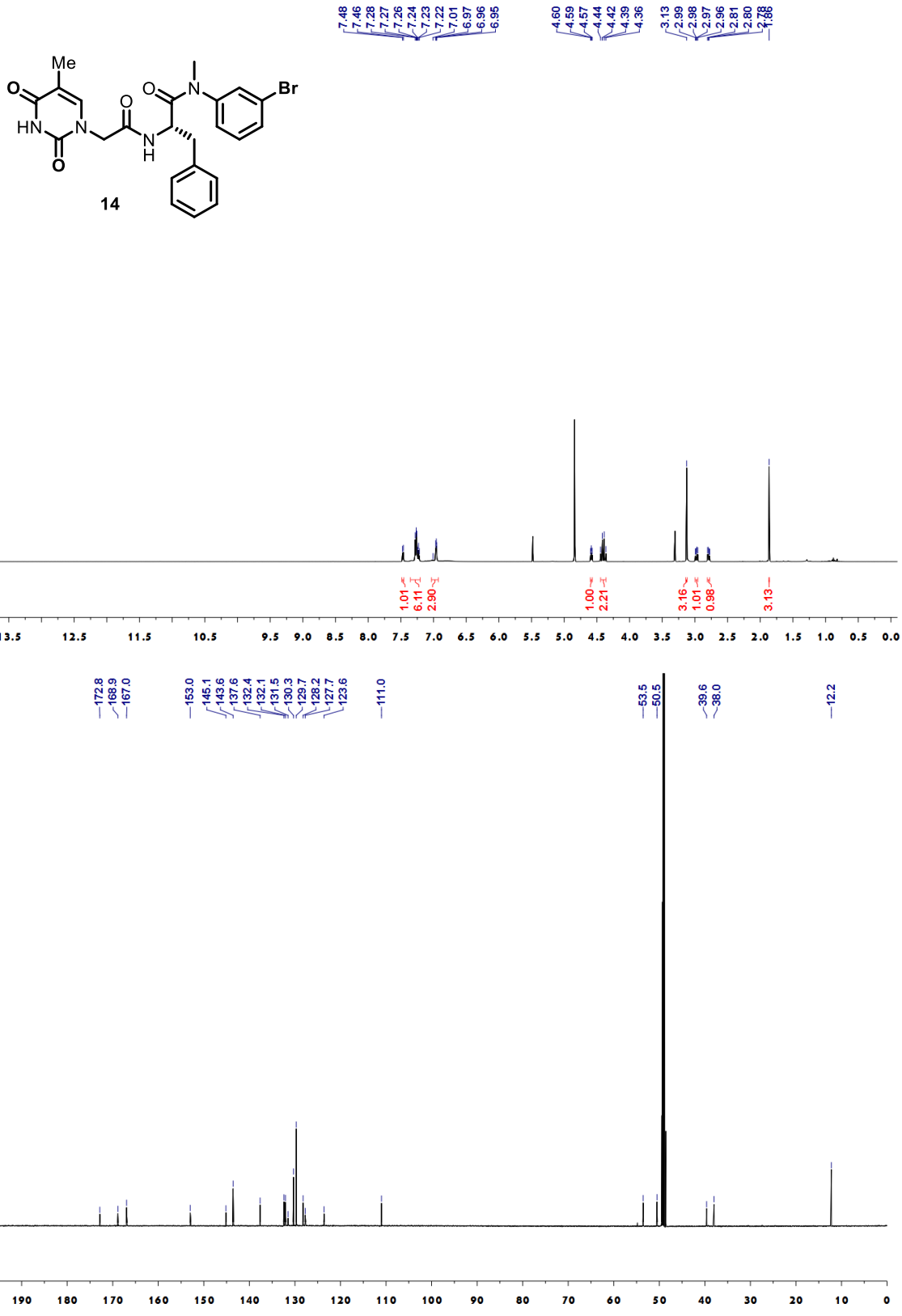
12


7.25
7.24
7.23
7.04
7.03
7.02
6.96
6.95
4.59
4.58
4.57
4.41
4.39
4.38
4.35
3.14
3.00
2.99
2.98
2.96
2.78
2.77
2.76
2.75
1.86
4.01
5.89
1.00
2.02
2.63
0.99
1.01
3.24
173.1
168.8
166.9
164.2
162.6
153.0
143.6
139.9
139.9
137.9
130.7
130.4
129.6
128.1
117.4
117.3
111.0
53.4
50.5
39.4
38.1
12.2

Me
O
HN
N
O
O
N
H
O
N
F

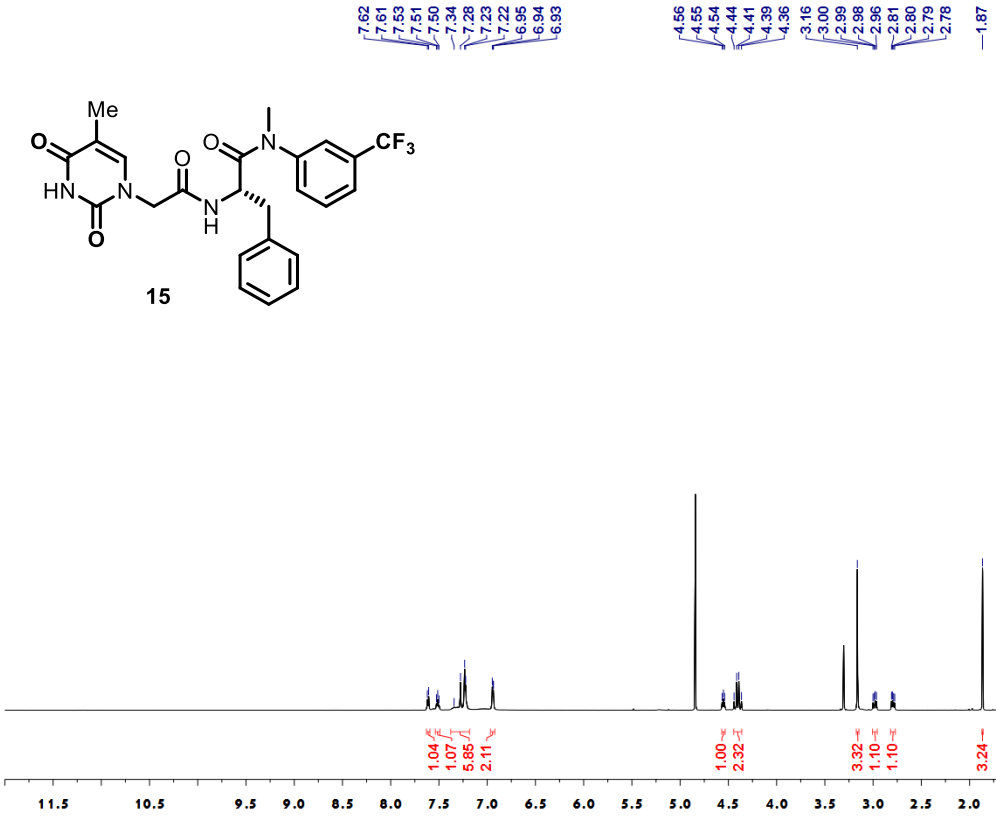
13

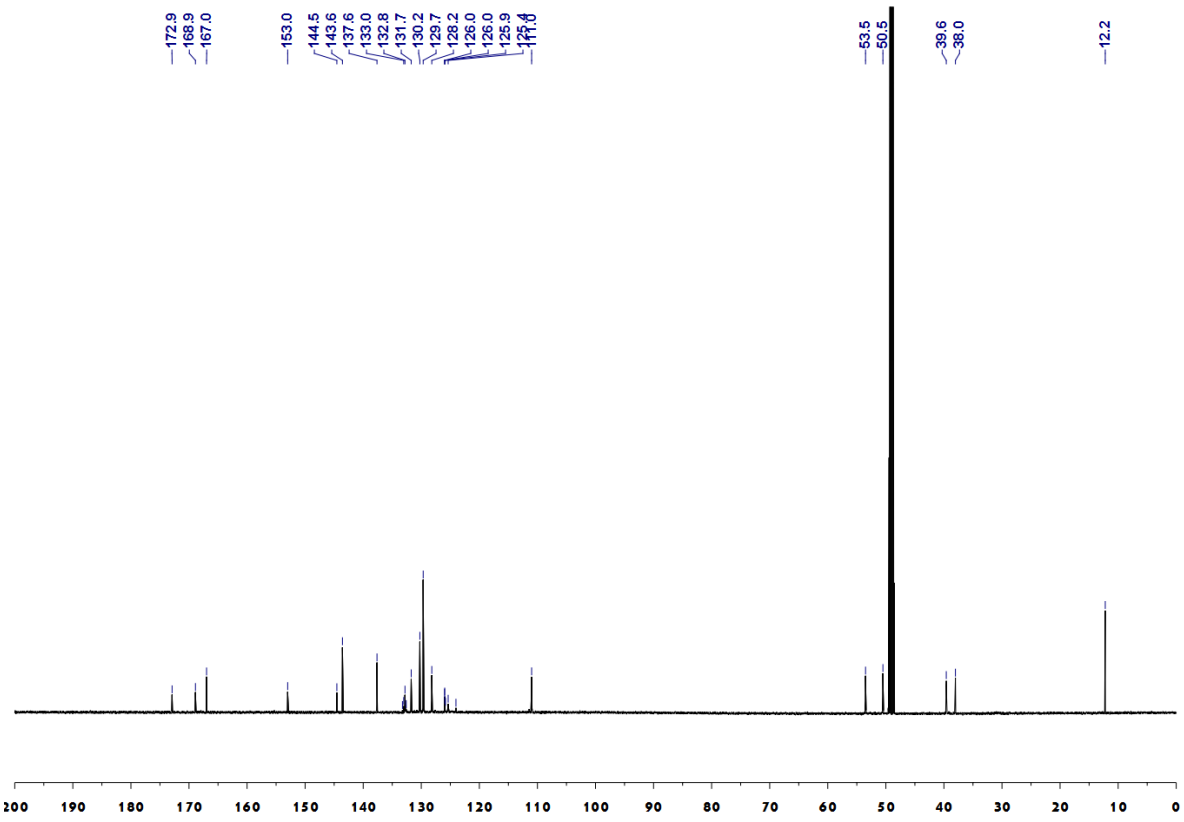

9.77
7.80
7.78
7.30
7.22
7.21
7.02
7.00
6.93
6.37
4.84
4.82
4.81
4.80
4.46
4.43
4.30
4.28
3.21
2.95
2.94
2.93
2.92
2.81
2.80
2.79
2.78
1.91
1.20
1.00
1.31
3.08
1.99
2.20
0.99
0.83
1.00
1.18
1.09
3.18
1.15
1.18
3.46
12.5
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
171.38
166.22
164.34
164.04
161.57
151.27
143.57
143.48
140.59
135.87
130.92
130.83
129.34
128.54
127.09
123.15
115.56
115.35
114.77
114.55
110.99
51.70
49.63
39.22
37.71
12.39
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0


Me
O
HN
N
O
O
N
H
O
N
Br
14
7.48
7.46
7.28
7.27
7.26
7.24
7.23
7.22
7.01
6.97
6.96
6.95
4.60
4.59
4.57
4.44
4.42
4.39
4.36
3.13
2.99
2.98
2.97
2.96
2.81
2.80
1.01
6.11
2.90
1.00
2.21
3.16
1.01
0.98
3.13
172.8
168.9
167.0
153.0
145.1
143.6
137.6
132.4
132.1
131.5
130.3
129.7
128.2
127.7
123.6
111.0
53.5
50.5
39.6
38.0
12.2

Me
O
HN
N
O
O
N
H
O
N
CF3

15

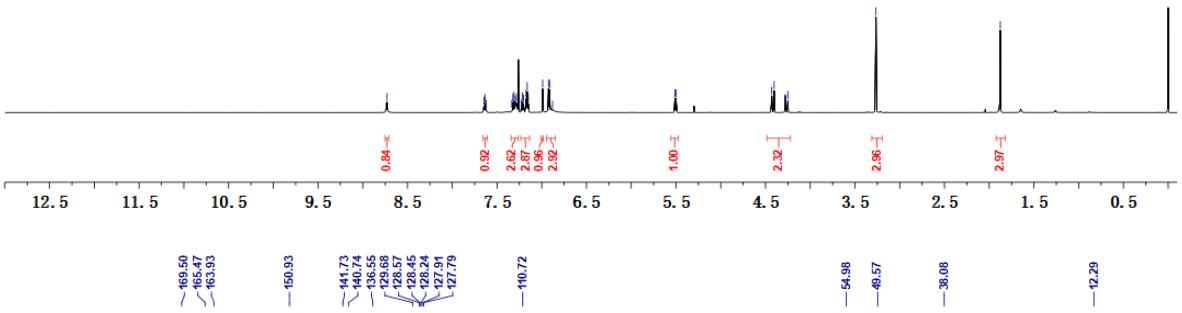

7.62
7.61
7.53
7.51
7.50
7.34
7.28
7.23
7.22
6.95
6.94
6.93
4.56
4.55
4.54
4.44
4.41
4.39
4.36
3.16
3.00
2.99
2.98
2.96
2.81
2.80
2.79
2.78
1.87
1.04
1.07
5.85
2.11
1.00
2.32
3.32
1.10
1.10
3.24
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0


172.9
168.9
167.0
153.0
144.5
143.6
137.6
133.0
132.8
131.7
130.2
129.7
128.2
126.0
126.0
125.9
53.5
50.5
39.6
38.0
12.2
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

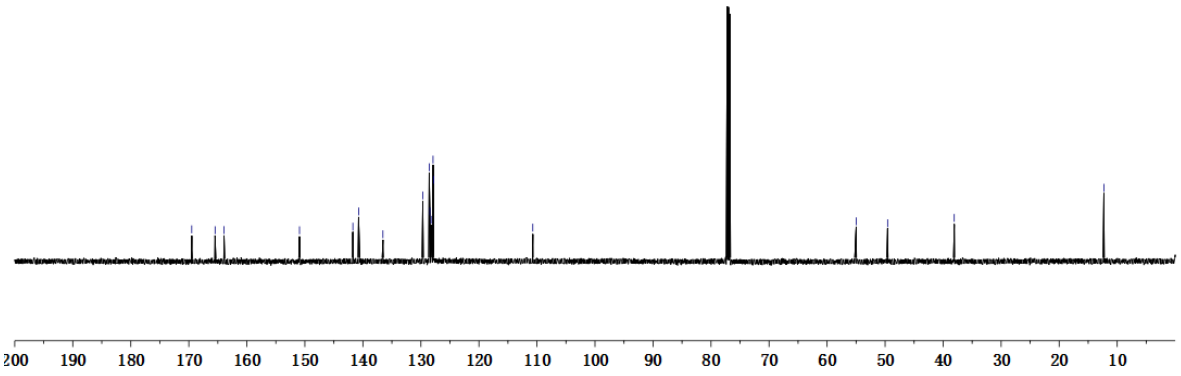

8.73
7.65
7.63
7.62
7.33
7.32
7.31
7.30
7.28
7.23
7.22
7.20
7.16
7.15
6.99
6.92
6.91
6.88
5.51
5.50
4.43
4.40
4.28
4.25
3.27
1.88

Me
O
HN
N
O
O
N
H
O
N

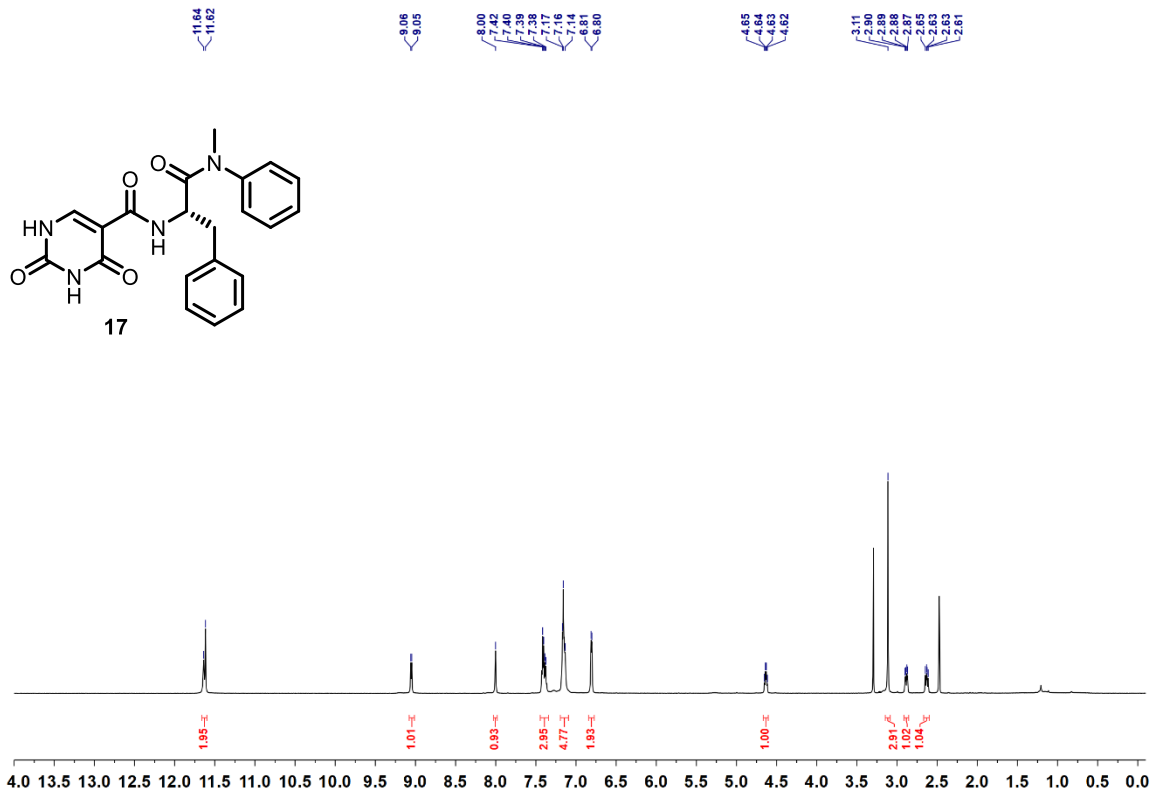
16

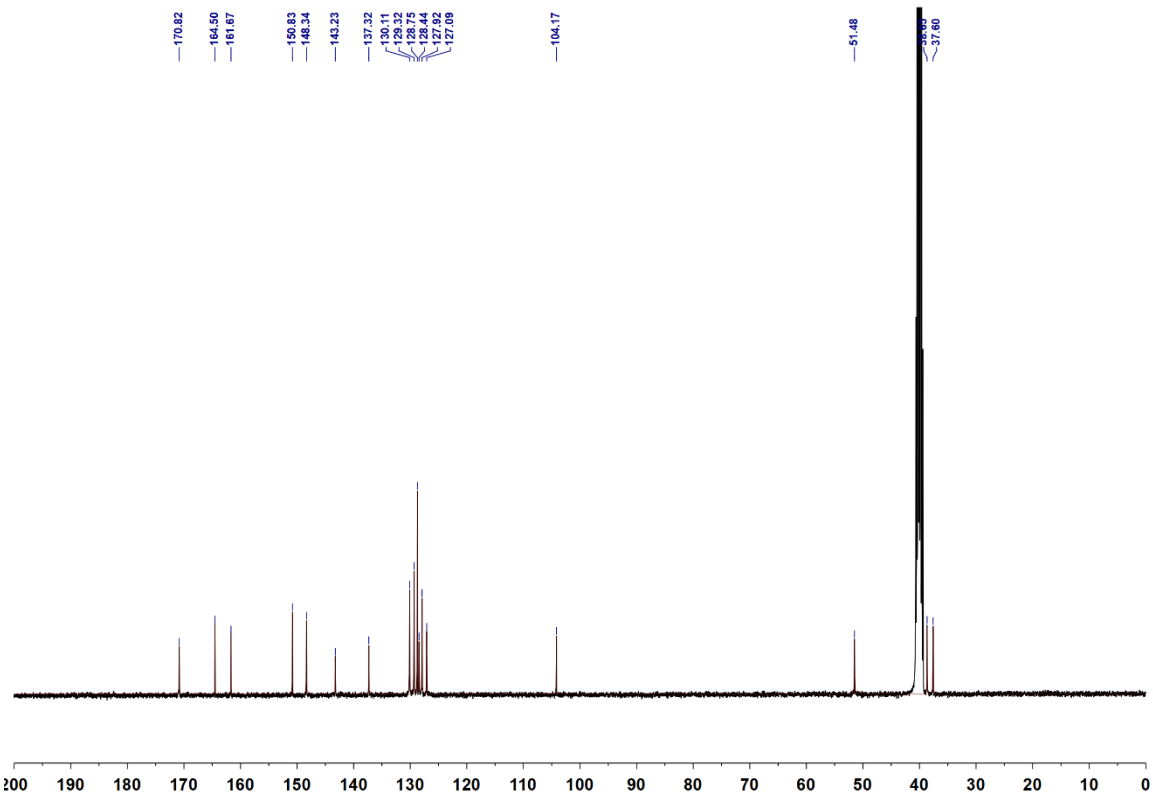

0.84
0.92
2.62
2.67
0.96
2.92
1.00
2.32
2.96
2.97
12.5
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5

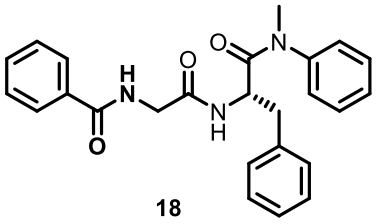
169.50
165.47
163.93
150.93
141.73
140.74
136.55
129.68
129.57
128.45
128.24
127.91
127.79
110.72
54.98
49.57
38.08
12.29


200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10

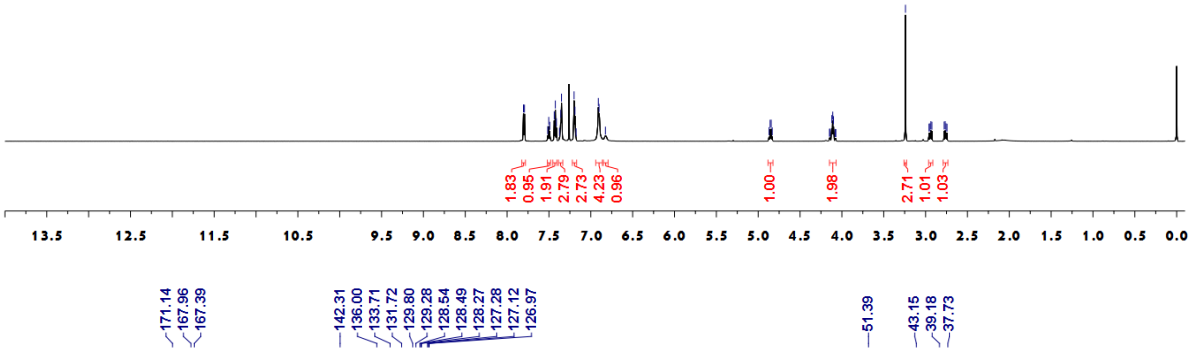
17

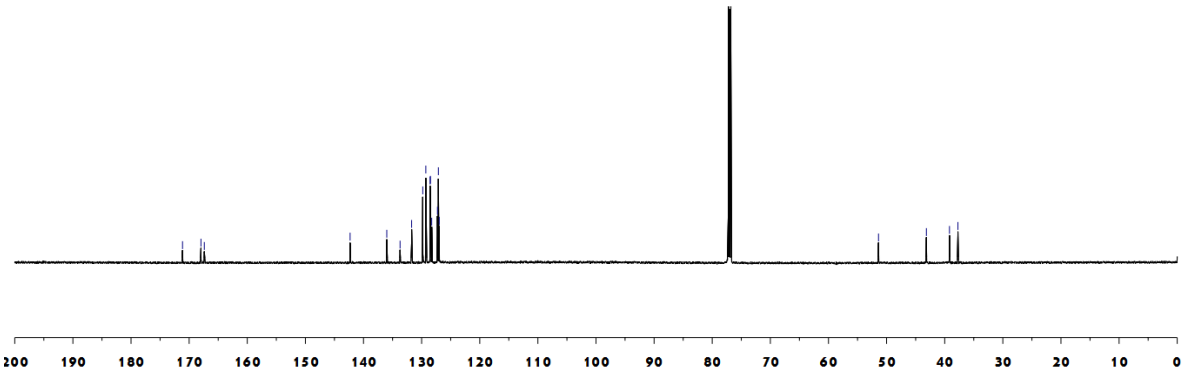


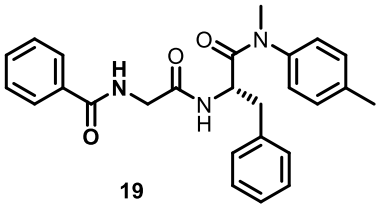




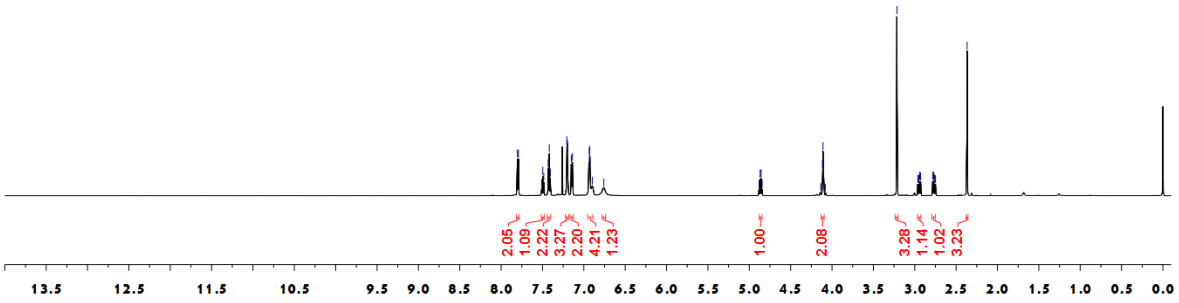
18

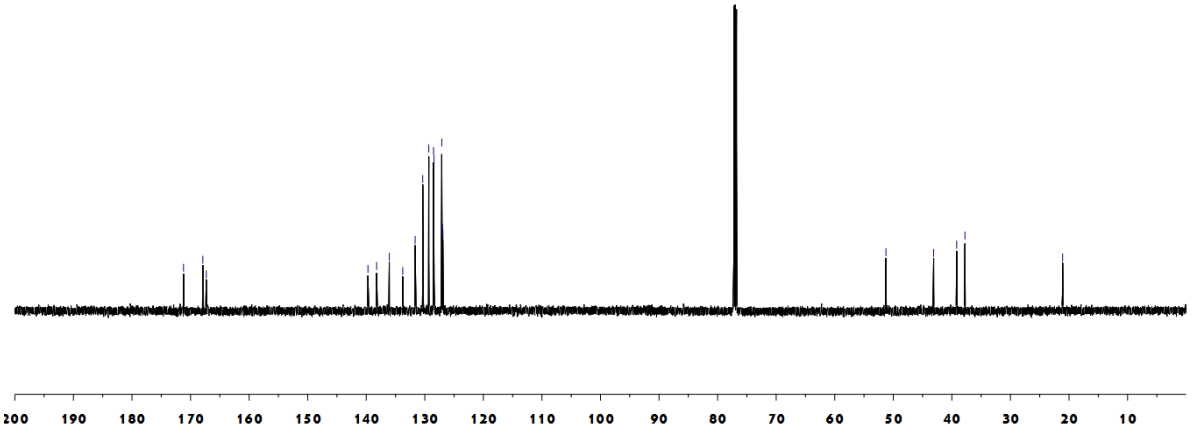


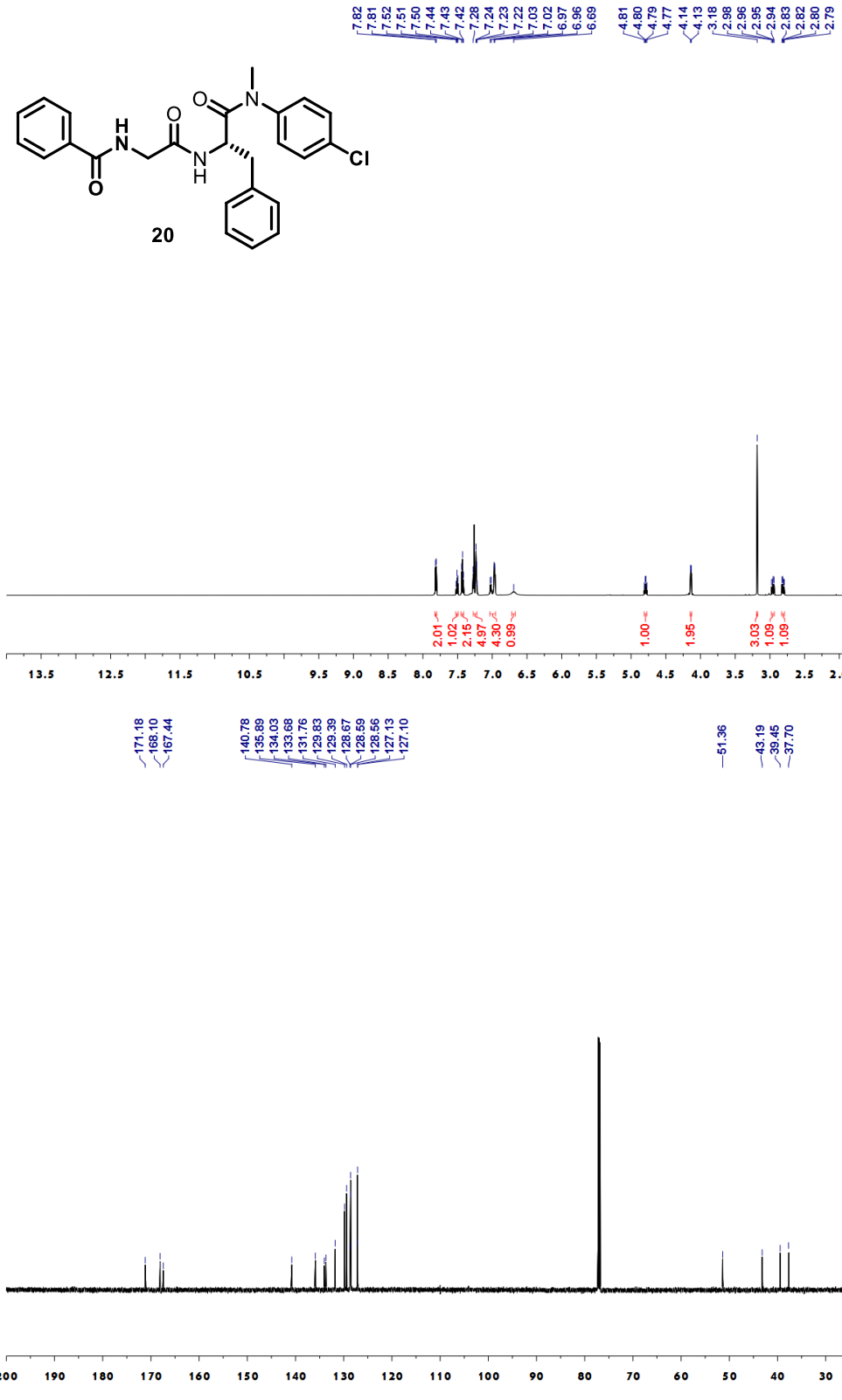


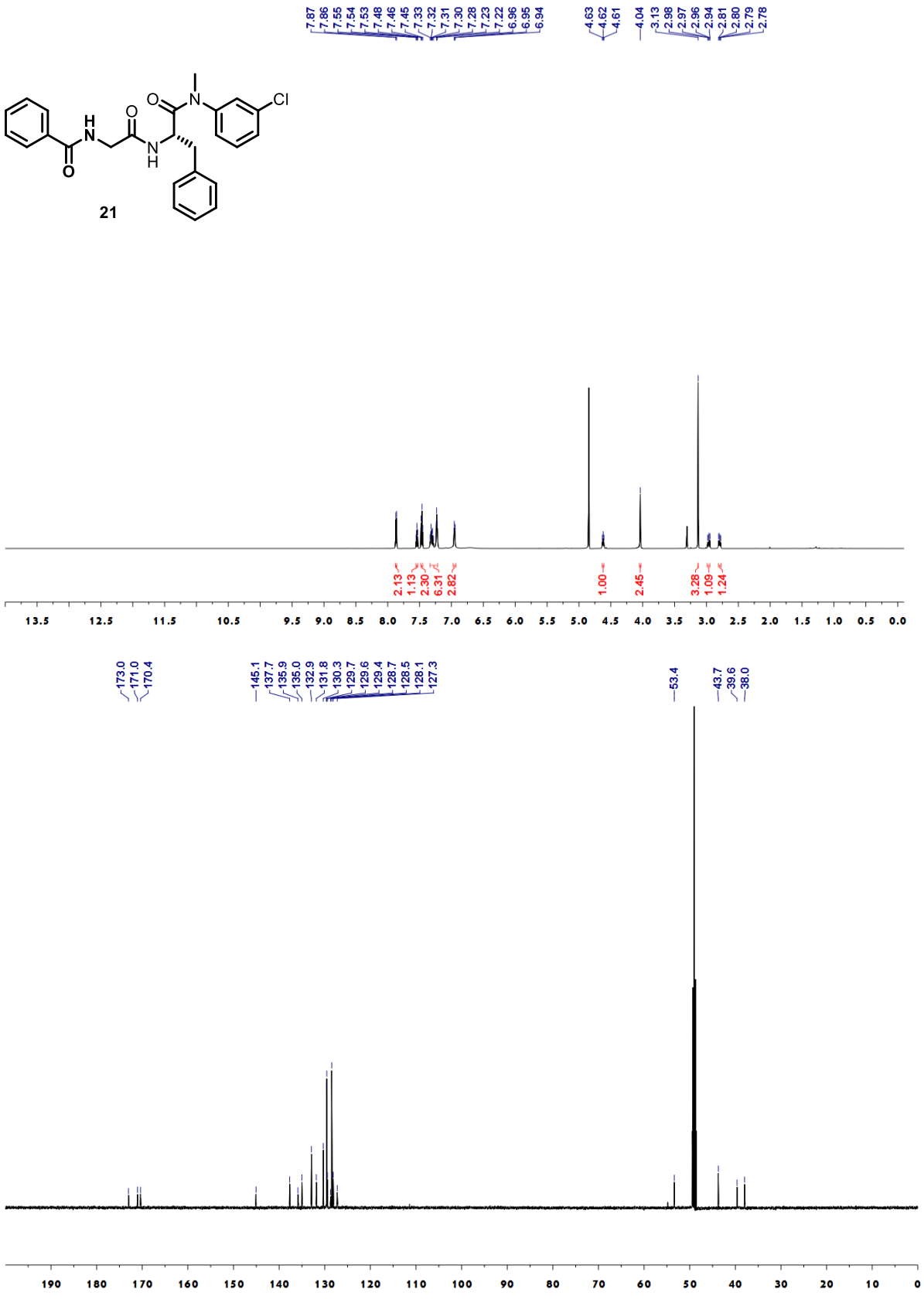


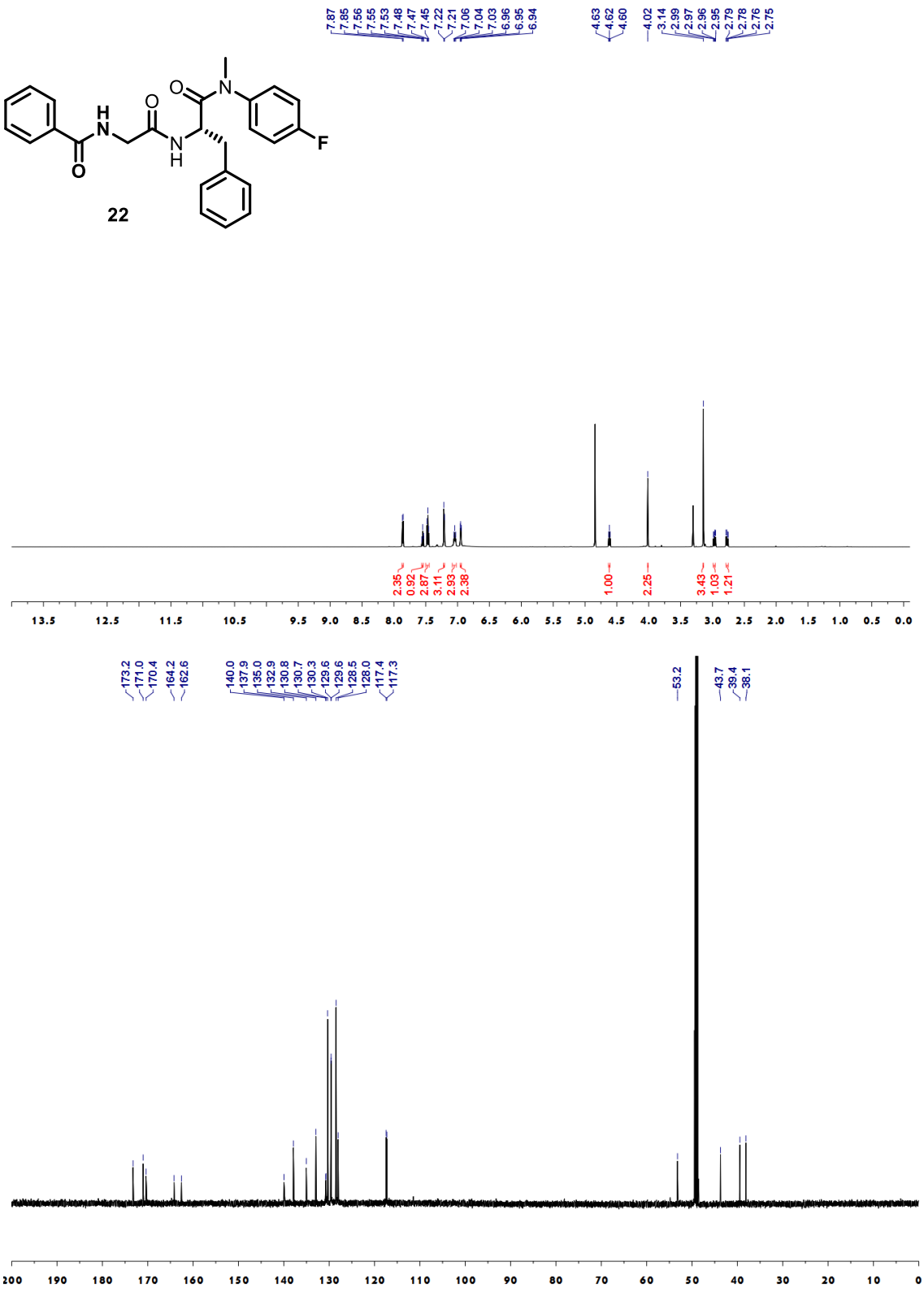
19



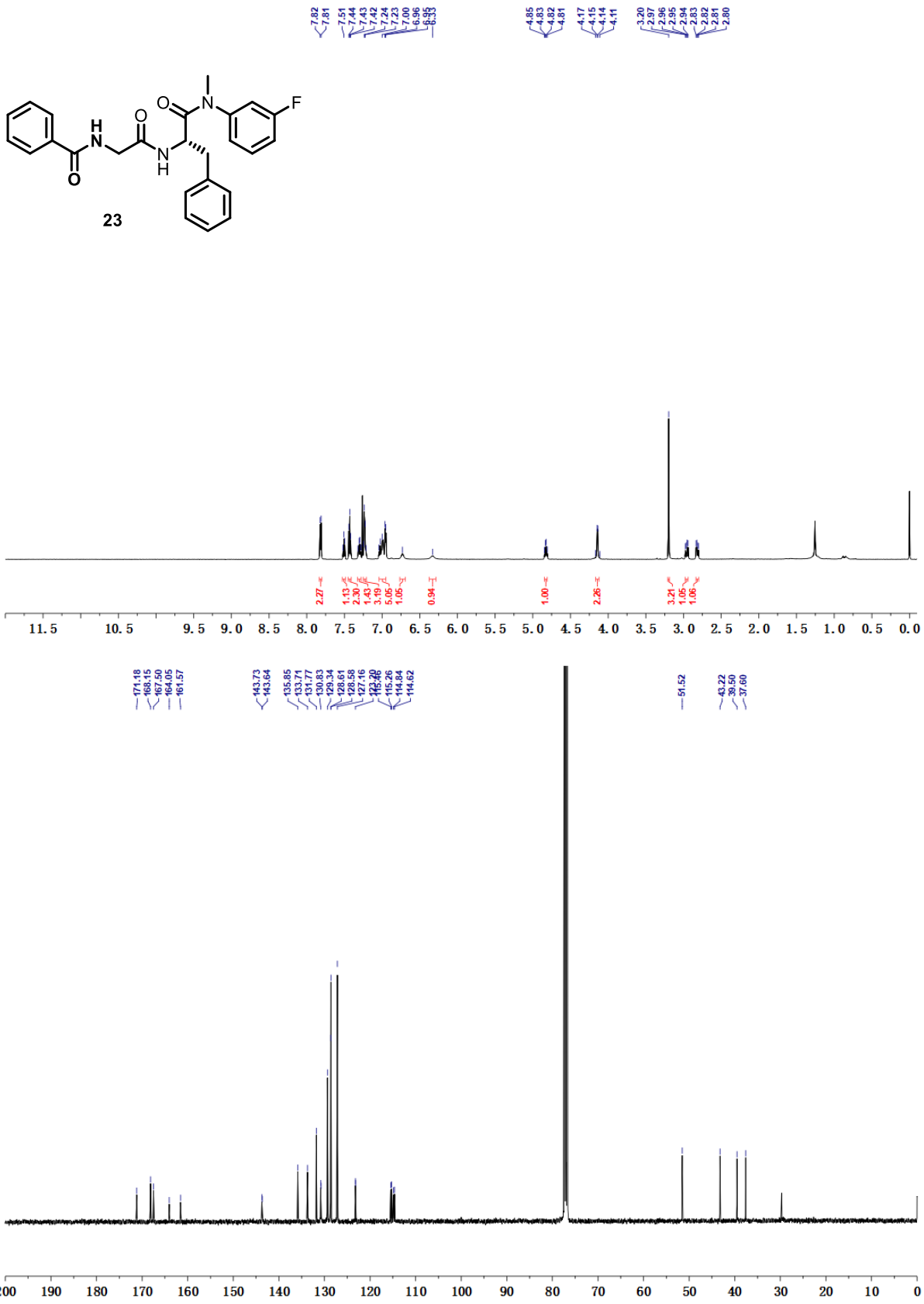



7.82
7.81
7.52
7.51
7.50
7.44
7.43
7.42
7.28
7.24
7.23
7.22
7.03
7.02
6.97
6.96
6.69
4.81
4.80
4.79
4.77
4.14
4.13
3.18
2.98
2.96
2.95
2.94
2.83
2.82
2.80
2.79
O
N
H
N
O
O
H
Cl
20
2.01
1.02
2.15
4.97
4.30
0.99
1.00
1.95
3.03
1.09
1.09
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
171.18
168.10
167.44
140.78
135.89
134.03
133.68
131.76
129.83
129.39
128.67
128.59
128.56
127.13
127.10
51.36
43.19
39.45
37.70
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0


7.87
7.86
7.55
7.54
7.53
7.48
7.46
7.45
7.33
7.32
7.31
7.30
7.28
7.23
7.22
6.96
6.95
6.94
4.63
4.62
4.61
4.04
3.13
2.98
2.97
2.96
2.94
2.81
2.80
2.79
2.78
O
N
Cl
H
N
O
N
H
O
21
2.13
1.13
2.30
6.31
2.82
1.00
2.45
3.28
1.09
1.24
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
173.0
171.0
170.4
145.1
137.7
135.9
135.0
132.9
131.8
130.3
129.7
129.6
129.4
128.7
128.5
128.1
127.3
53.4
43.7
39.6
38.0
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

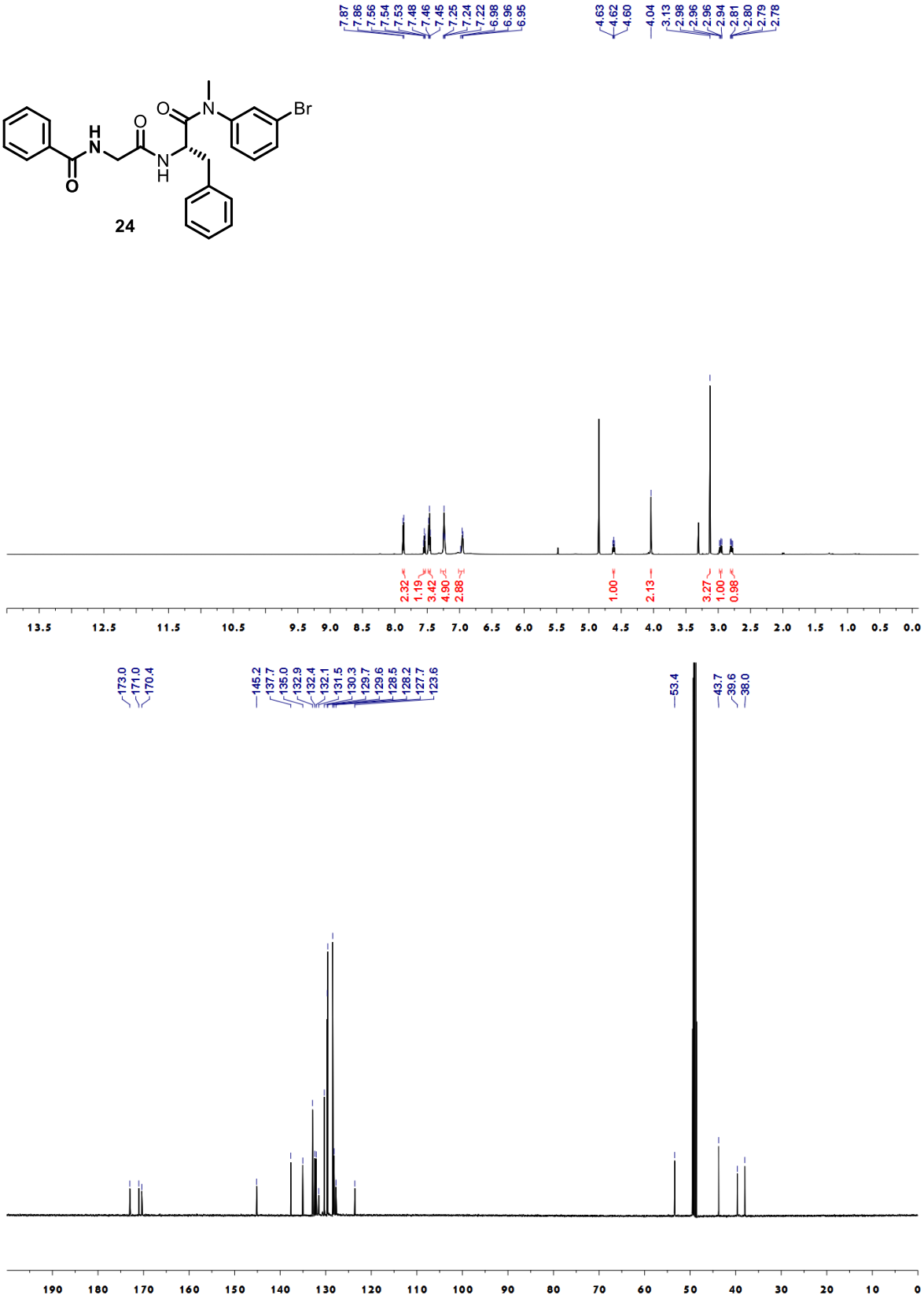

7.87
7.85
7.56
7.55
7.53
7.48
7.47
7.45
7.22
7.21
7.06
7.04
7.03
6.96
6.95
6.94
4.63
4.62
4.60
4.02
3.14
2.99
2.97
2.96
2.95
2.79
2.78
2.76
2.75
O
N
H
N
O
O
H
N
F
22
2.35
0.92
2.87
3.11
2.93
2.38
1.00
2.25
3.43
1.03
1.21
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
173.2
171.0
170.4
164.2
162.6
140.0
137.9
135.0
132.9
130.8
130.7
130.3
129.6
129.6
128.5
128.0
117.4
117.3
53.2
43.7
39.4
38.1
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

23

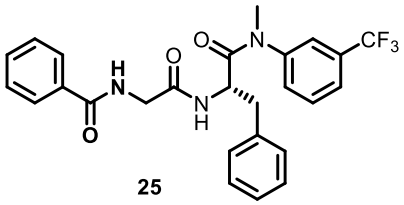


O
N
Br
H
N
O
N
H
O

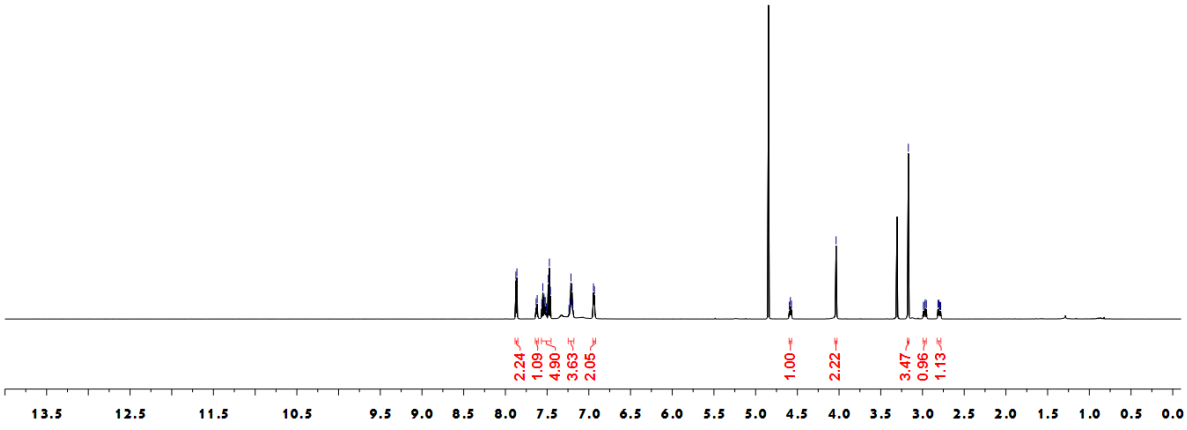
24

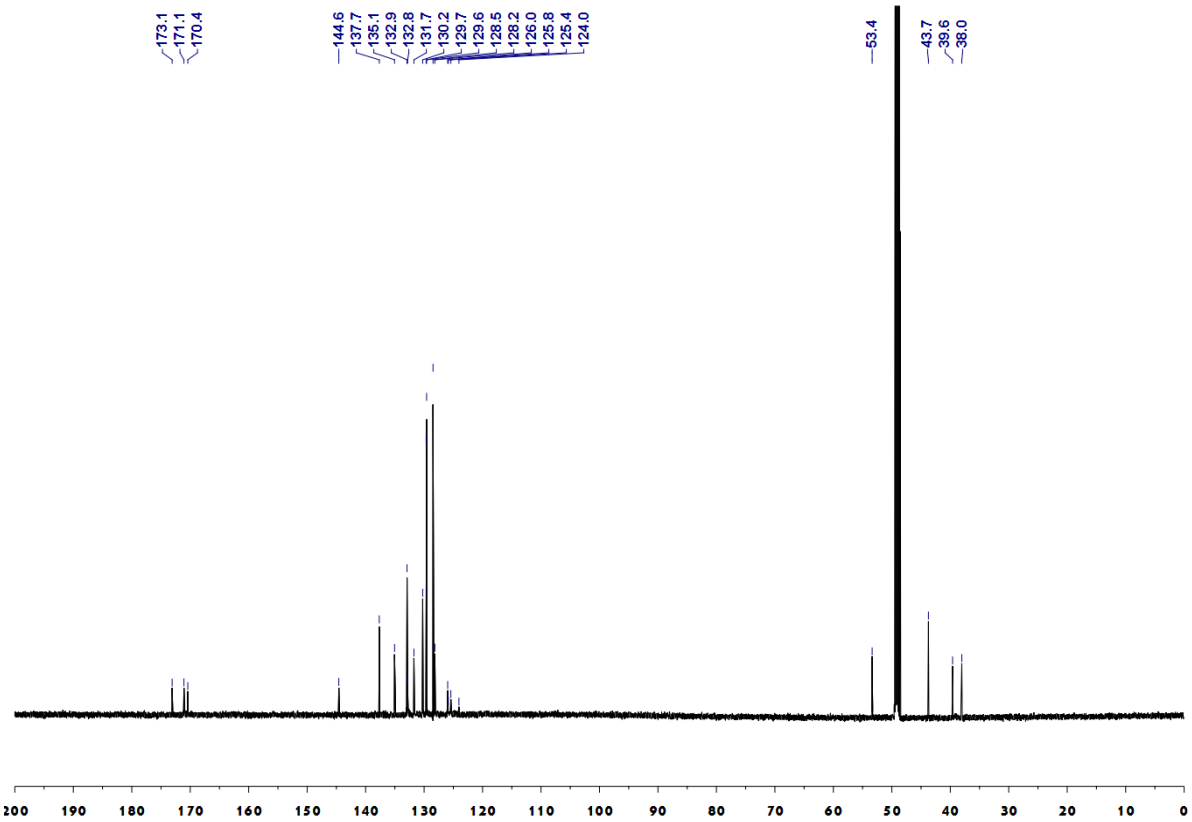

7.87
7.86
7.56
7.54
7.53
7.48
7.46
7.45
7.25
7.24
7.22
6.98
6.96
6.95
4.63
4.62
4.60
4.04
3.13
2.98
2.96
2.96
2.94
2.81
2.80
2.79
2.78
2.32
1.19
3.42
4.90
2.88
1.00
2.13
3.27
1.00
0.98
173.0
171.0
170.4
145.2
137.7
135.0
132.9
132.4
132.1
131.5
130.3
129.7
129.6
128.5
128.2
127.7
123.6
53.4
43.7
39.6
38.0

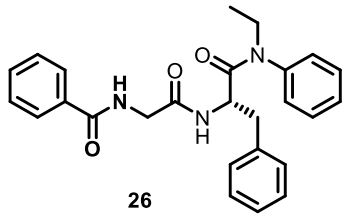

7.87
7.86
7.63
7.62
7.56
7.55
7.54
7.52
7.51
7.49
7.47
7.46
7.24
7.23
7.21
7.20
7.19
6.94
6.93
4.60
4.58
4.57
4.04
3.17
2.99
2.97
2.97
2.95
2.81
2.80
2.79
2.78


O
N
CF3
H
N
O
O
N
H

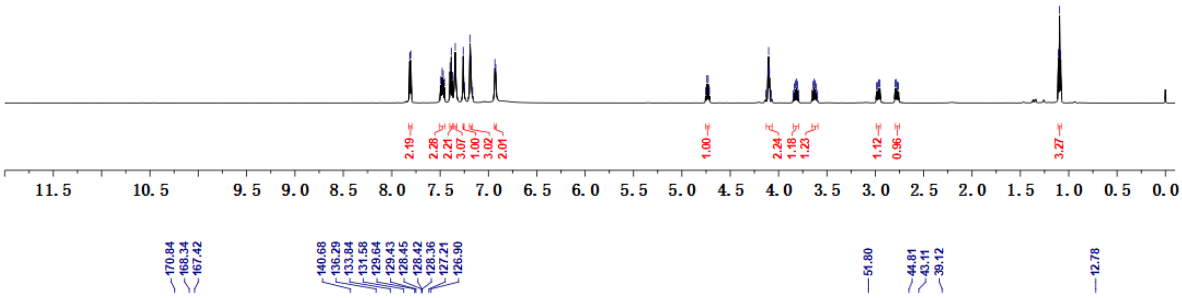
25

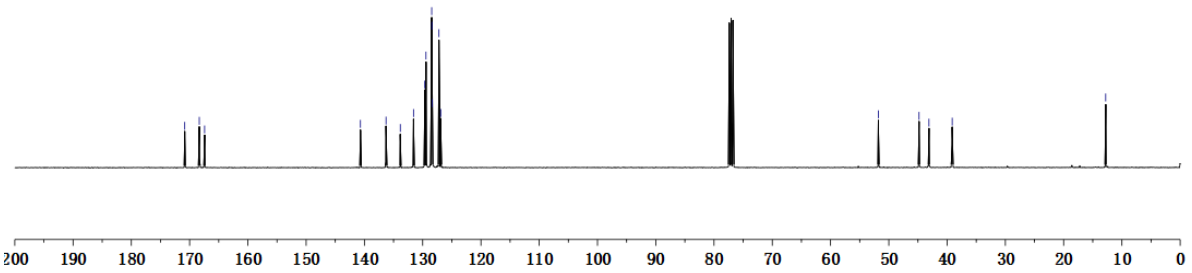

2.24
1.09
4.90
3.63
2.05
1.00
2.22
3.47
0.96
1.13
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0


173.1
171.1
170.4
144.6
137.7
135.1
132.9
132.8
131.7
130.2
129.7
129.6
128.5
128.2
126.0
125.8
125.4
124.0
53.4
43.7
39.6
38.0
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

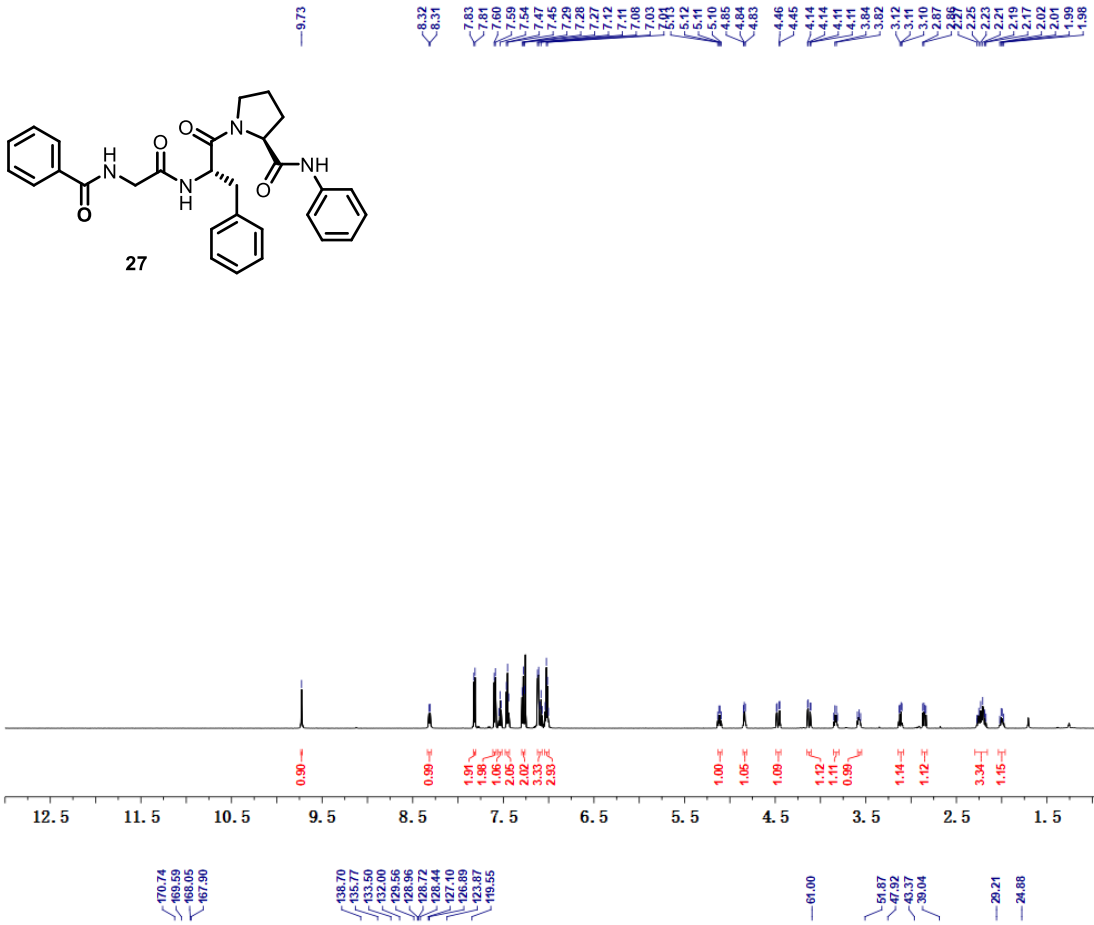


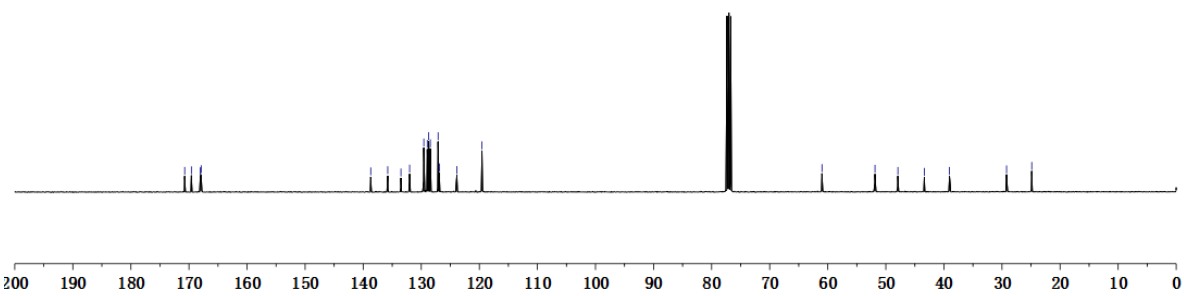
26



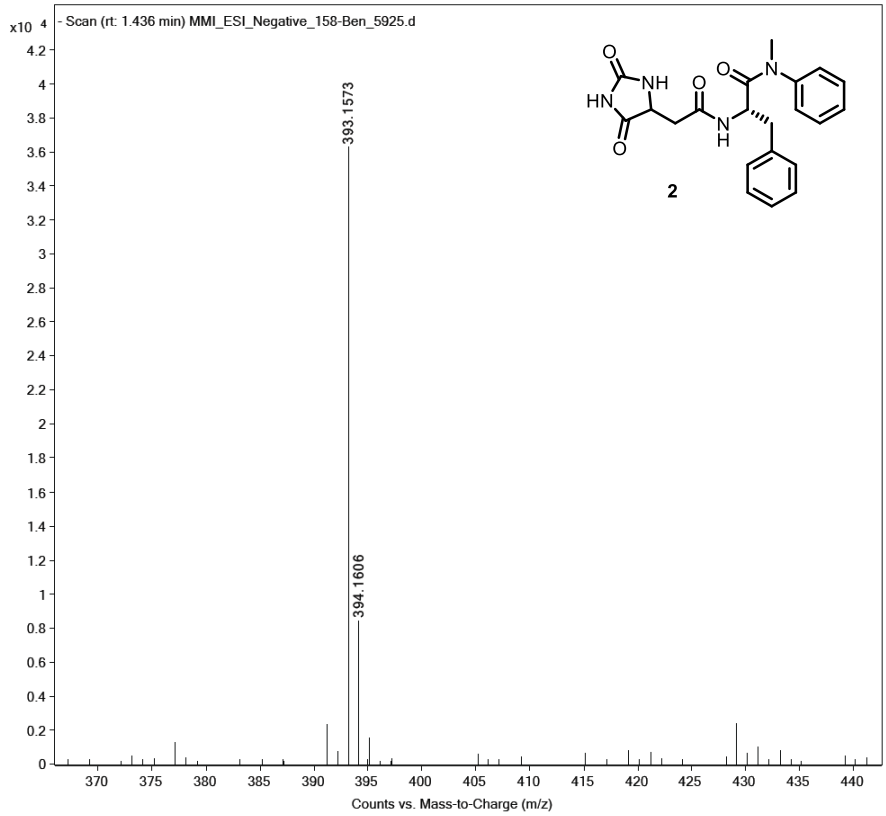


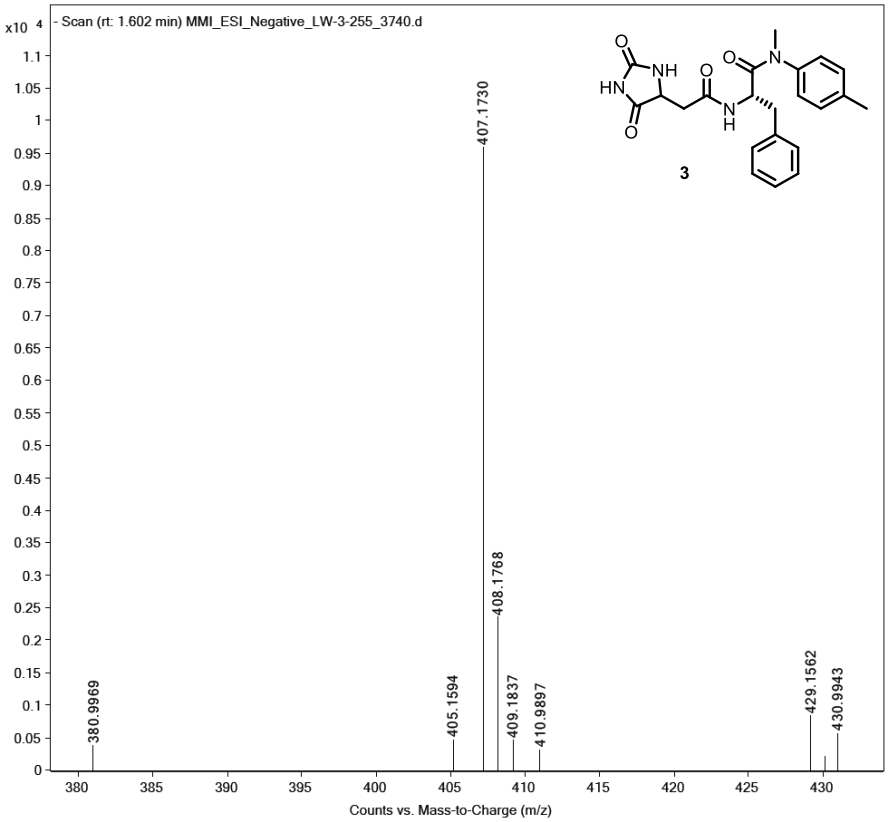
27

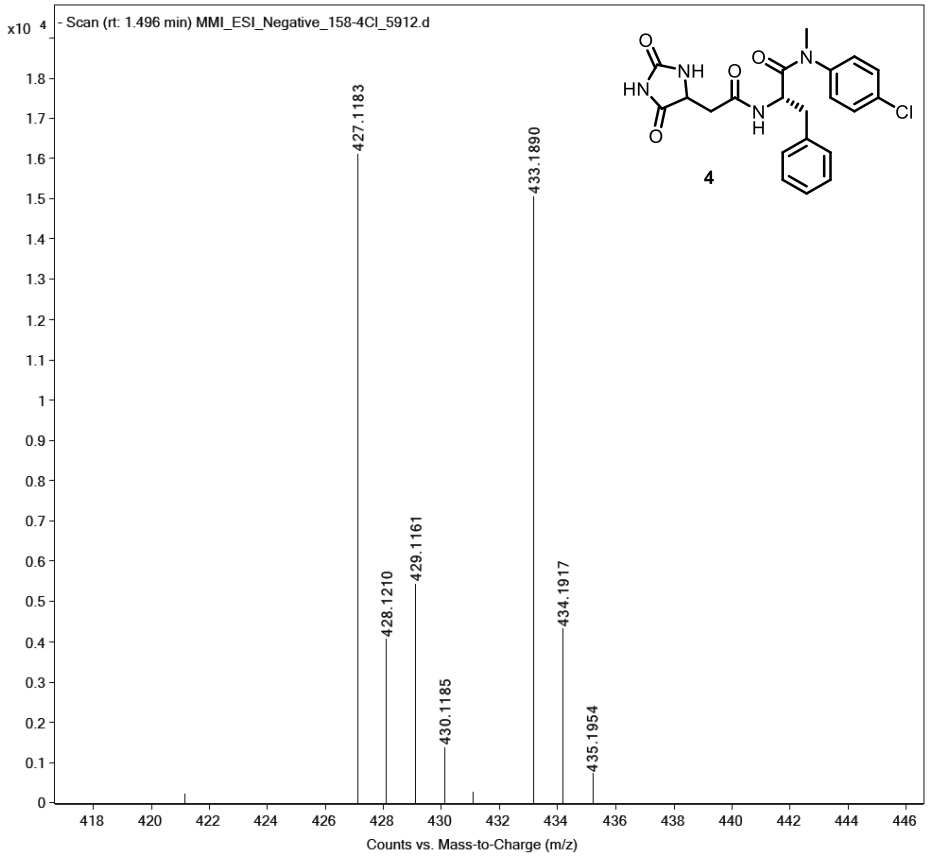


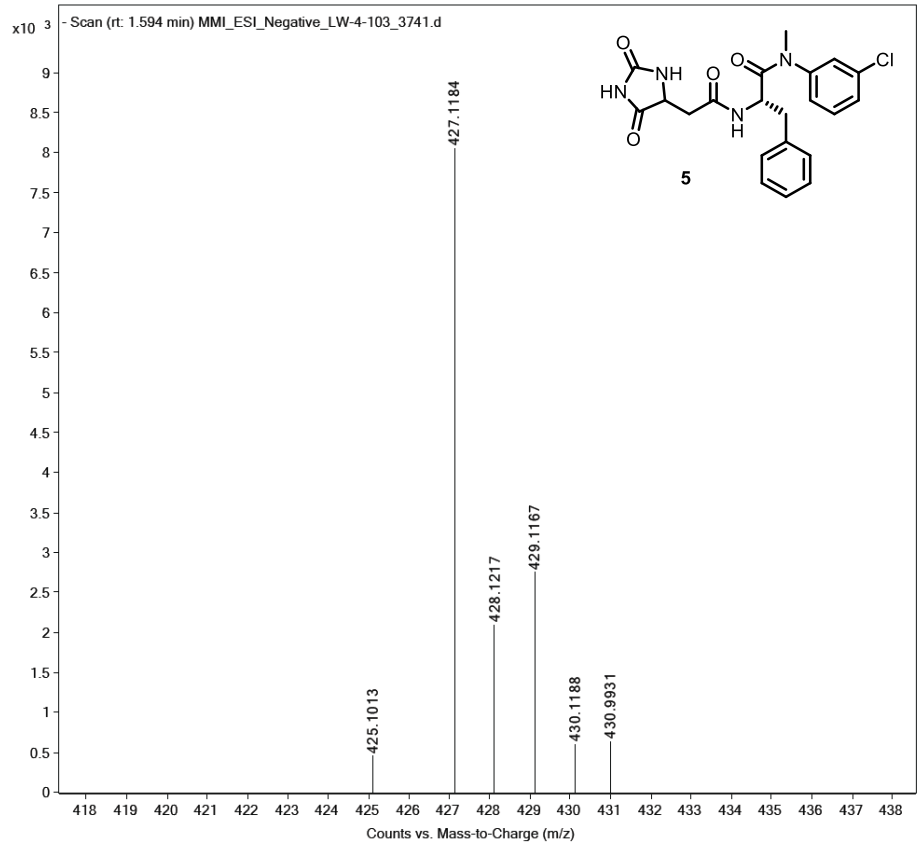


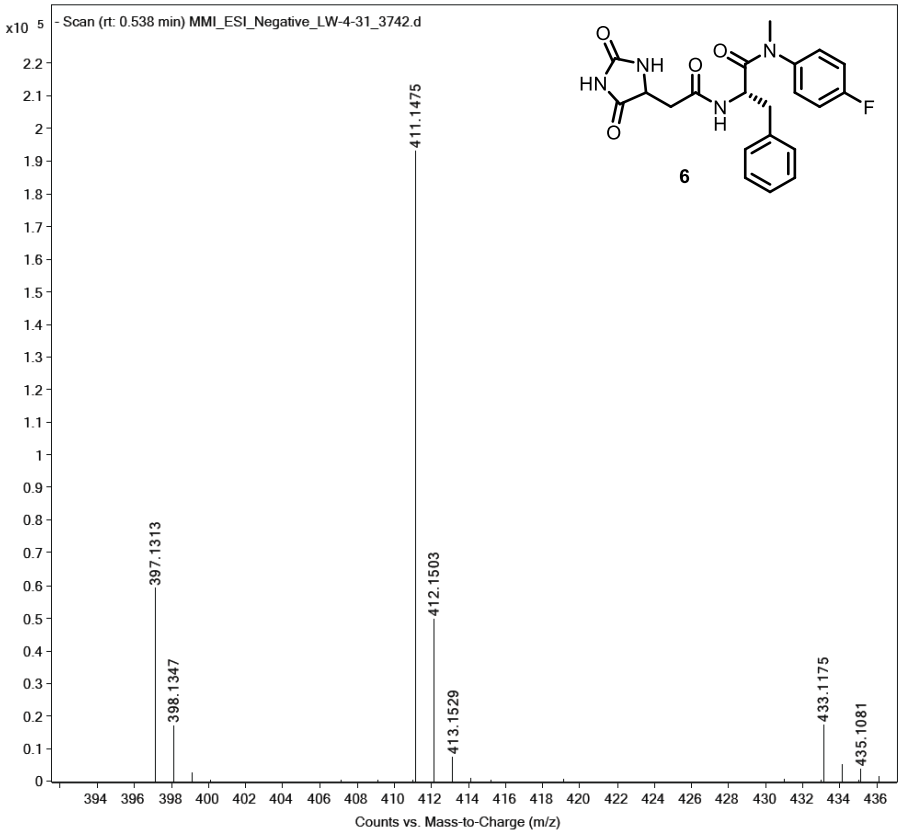
3. HR-MS spectra

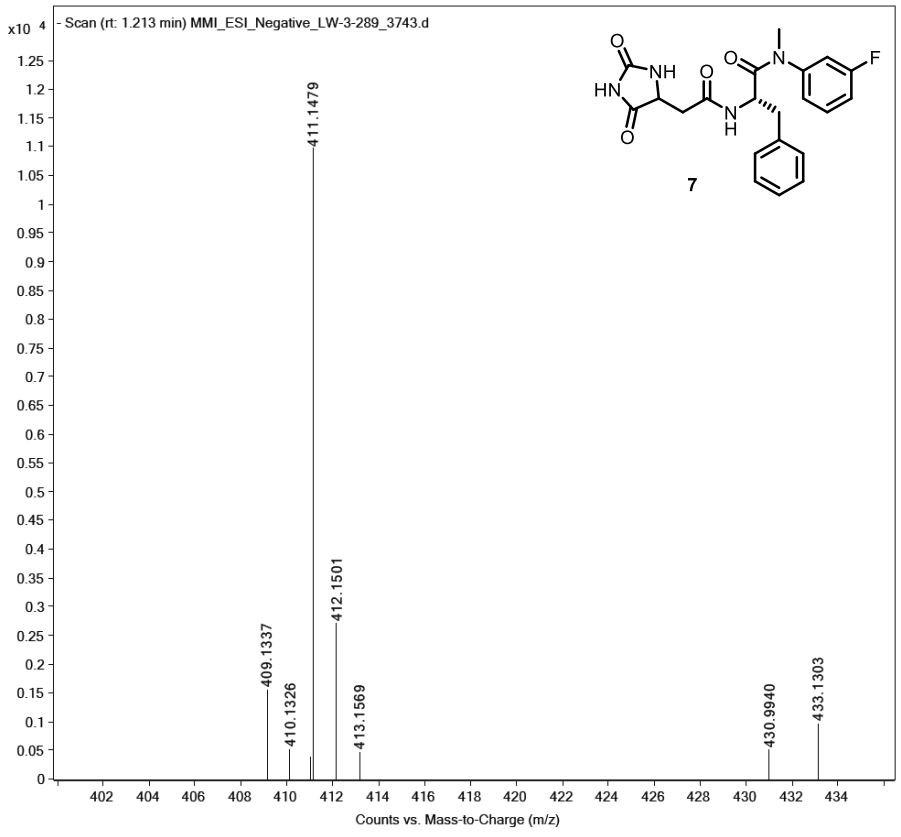


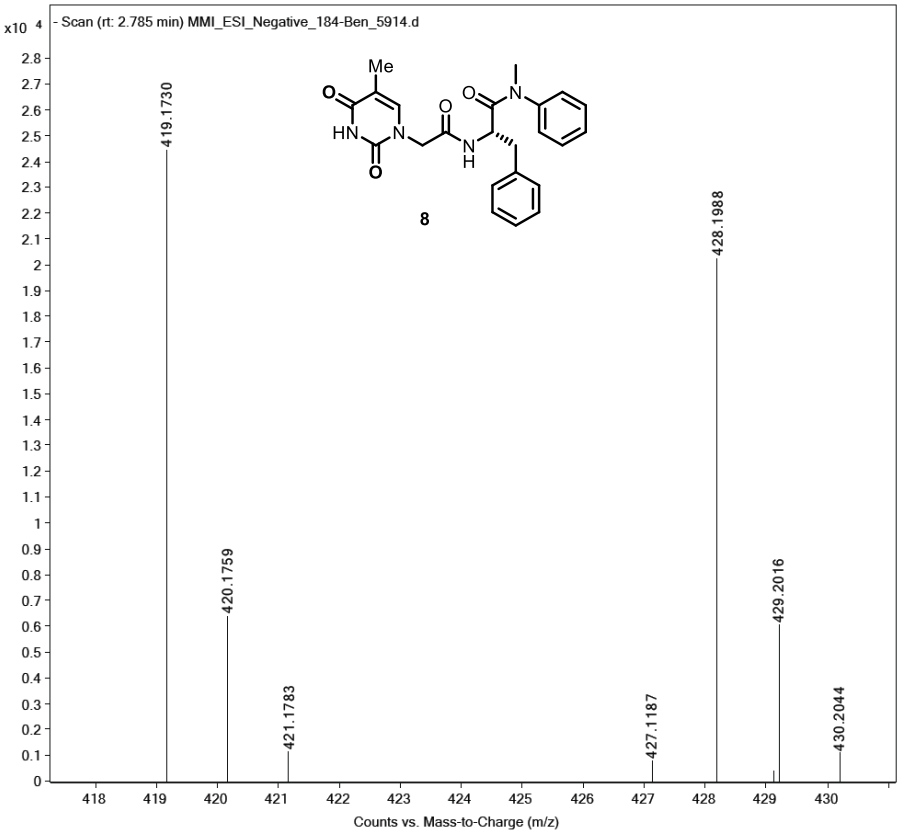


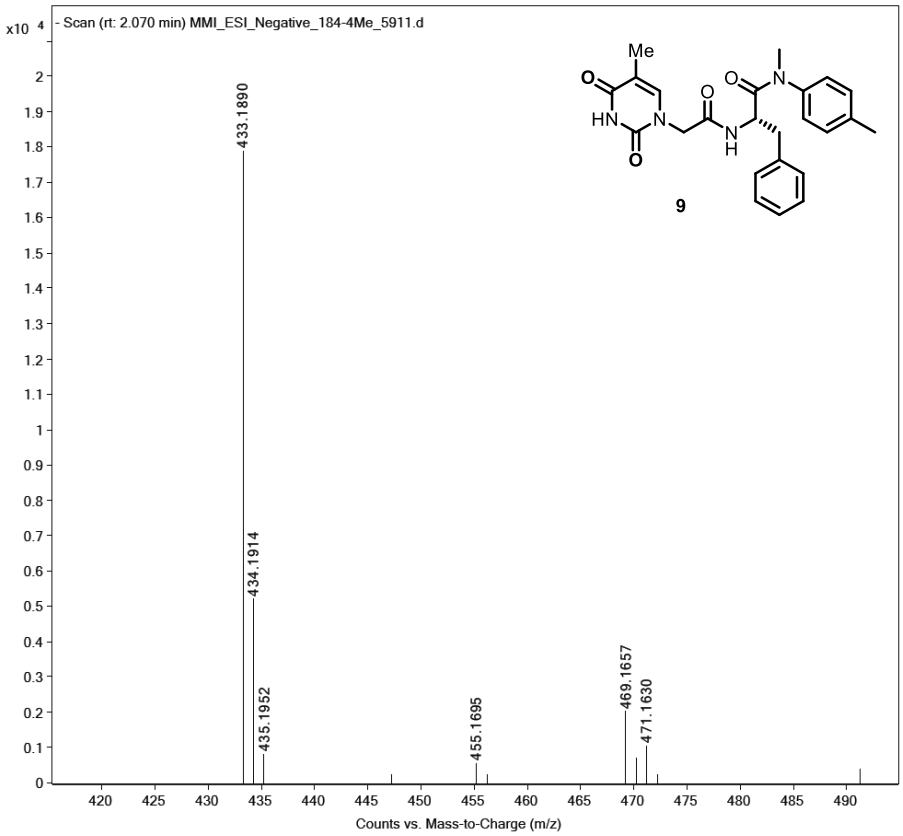

- Scan (rt: 1.496 min) MMI_ESI_Negative_158-4Cl_5912.d
x10 4
427.1183
433.1890
429.1161
428.1210
434.1917
430.1185
435.1954
Counts vs. Mass-to-Charge (m/z)
4

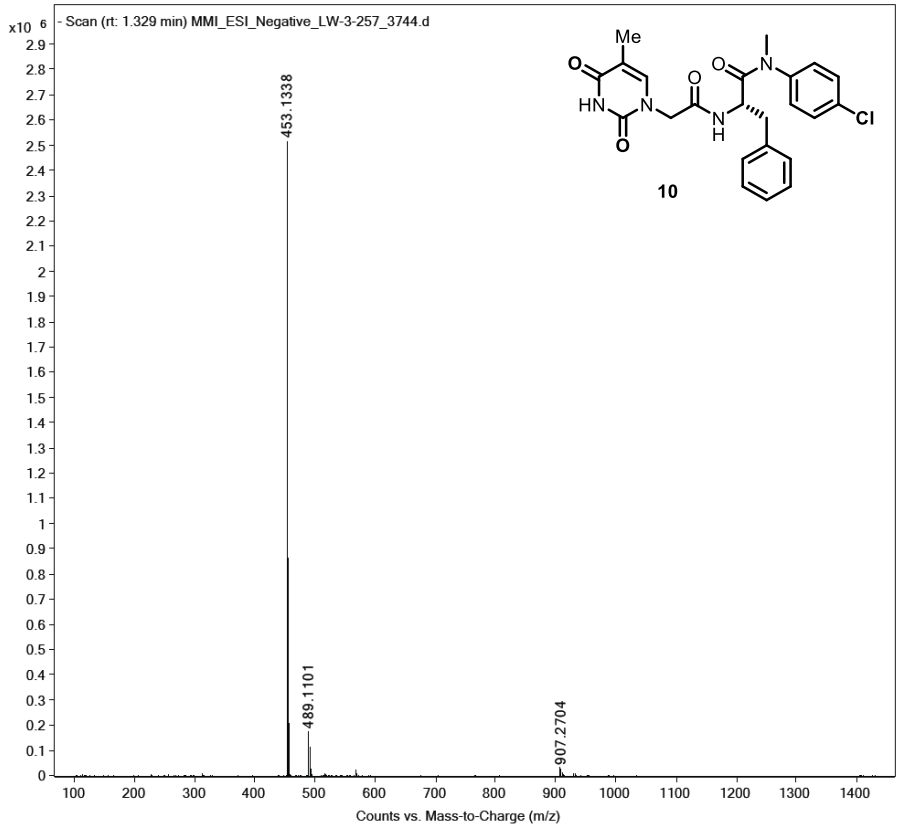

- Scan (rt: 1.594 min) MMI_ESI_Negative_LW-4-103_3741.d
x10 3
427.1184
429.1167
428.1217
425.1013
430.1188
430.9931
Counts vs. Mass-to-Charge (m/z)
5

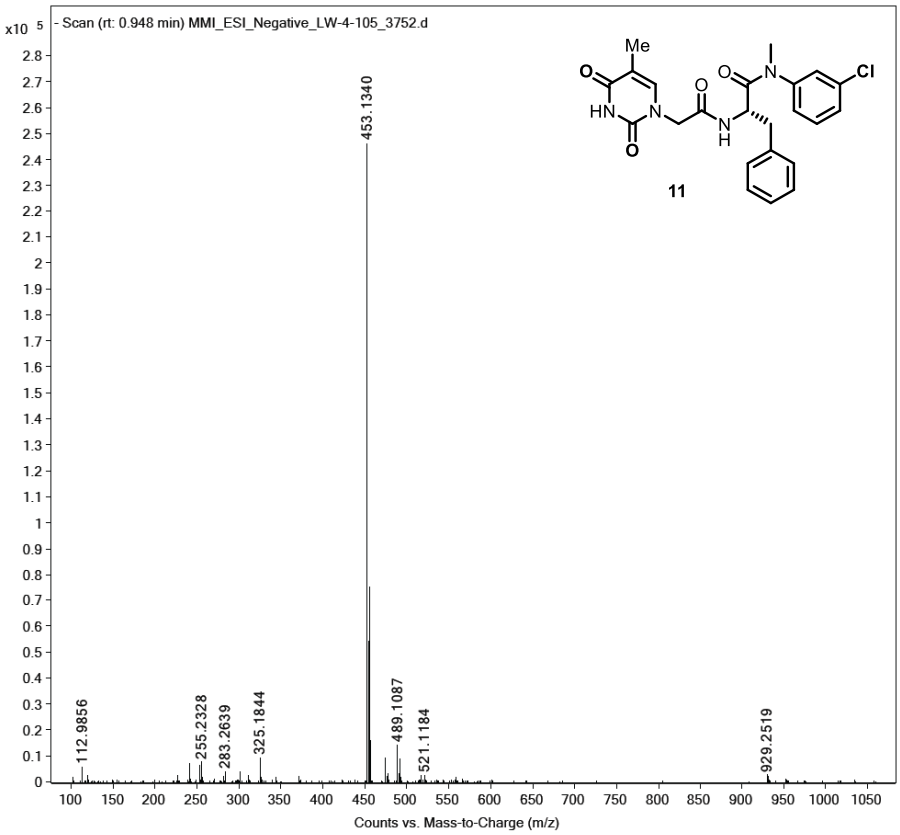

- Scan (rt: 0.538 min) MMI_ESI_Negative_LW-4-31_3742.d
x10 5
411.1475
397.1313
412.1503
398.1347
413.1529
433.1175
435.1081
Counts vs. Mass-to-Charge (m/z)
6

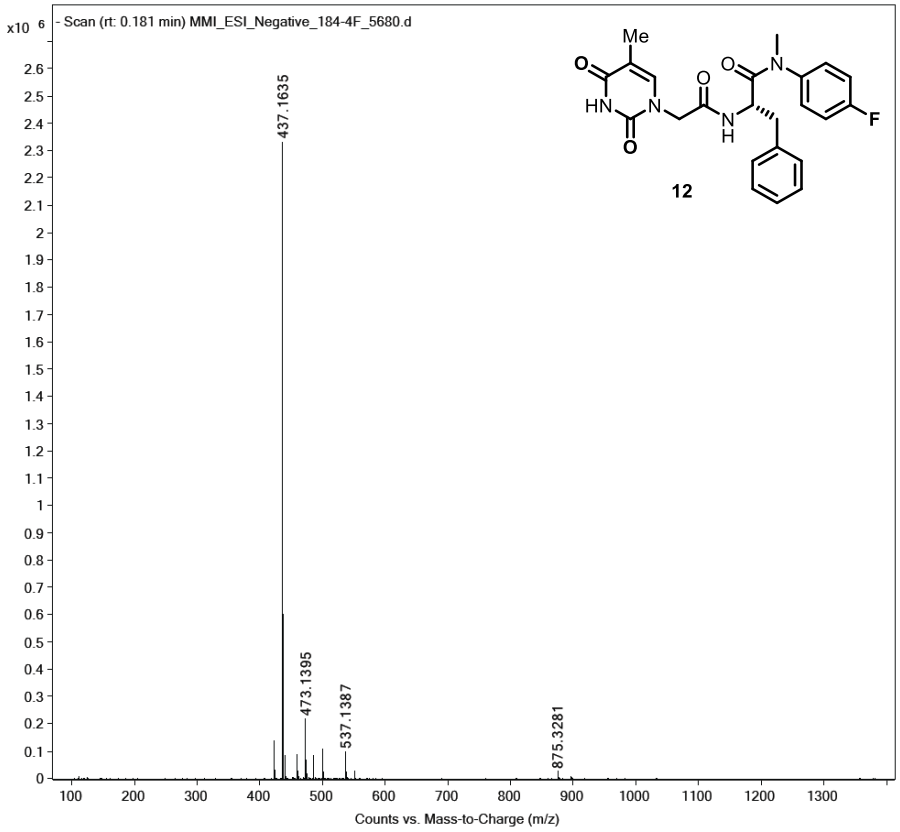

- Scan (rt: 1.213 min) MMI_ESI_Negative_LW-3-289_3743.d
x10 4
411.1479
412.1501
409.1337
410.1326
413.1569
430.9940
433.1303
Counts vs. Mass-to-Charge (m/z)
7

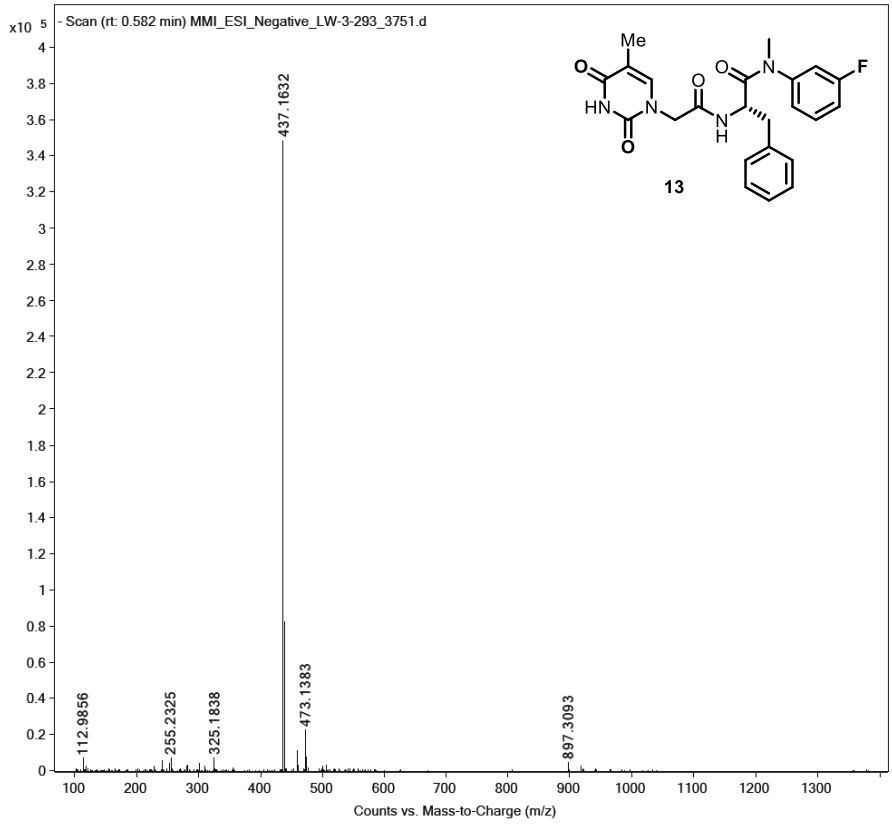

- Scan (rt: 2.785 min) MMI_ESI_Negative_184-Ben_5914.d
x10 4
419.1730
420.1759
421.1783
427.1187
428.1988
429.2016
430.2044
Counts vs. Mass-to-Charge (m/z)
8

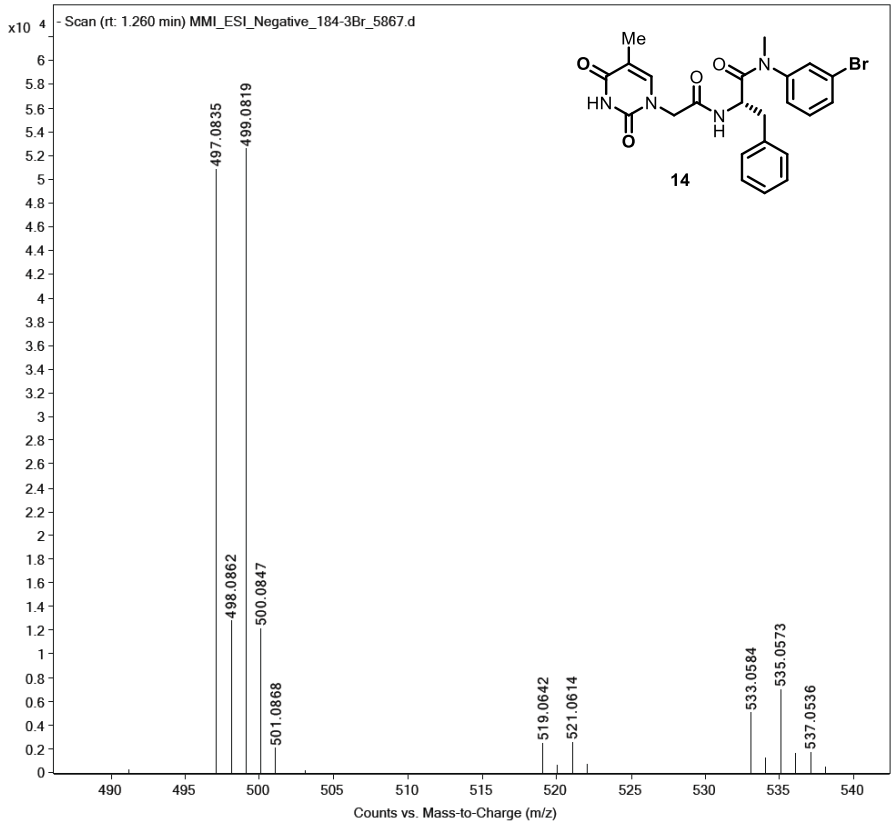

- Scan (rt: 2.070 min) MMI_ESI_Negative_184-4Me_5911.d
x10 4
433.1890
434.1914
435.1952
455.1695
469.1657
471.1630
Counts vs. Mass-to-Charge (m/z)
9

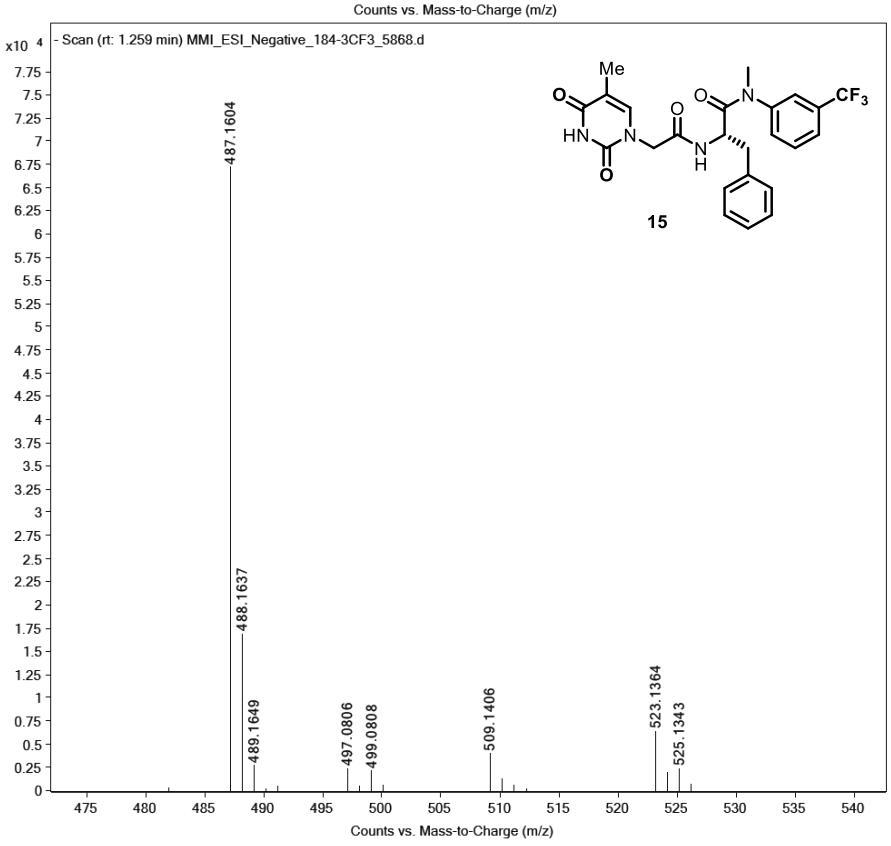

- Scan (rt: 1.329 min) MMI_ESI_Negative_LW-3-257_3744.d
x10 6
453.1338
489.1101
907.2704
Counts vs. Mass-to-Charge (m/z)
10

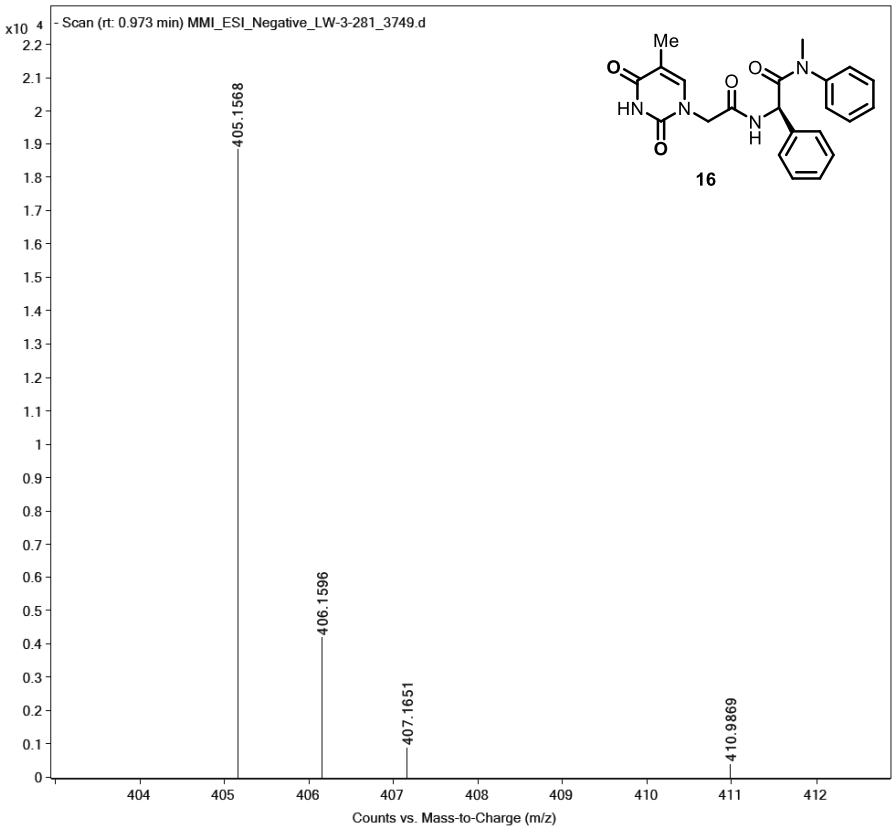

- Scan (rt: 0.948 min) MMI_ESI_Negative_LW-4-105_3752.d
x10 5
453.1340
112.9856
255.2328
283.2639
325.1844
489.1087
521.1184
929.2519
Counts vs. Mass-to-Charge (m/z)
11

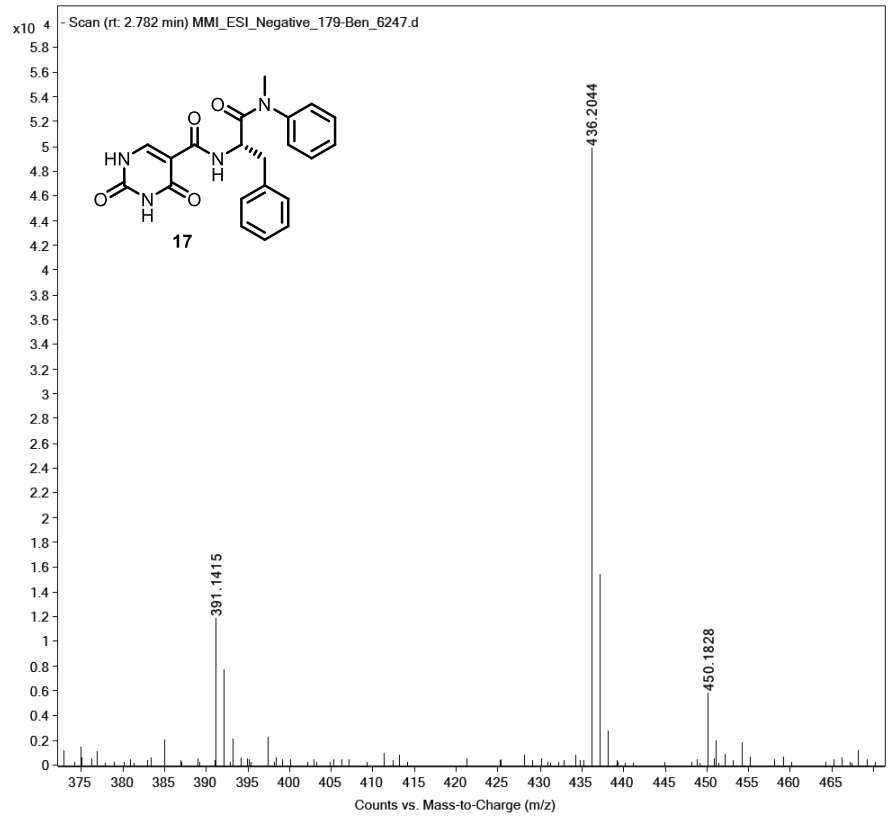

x10 6
- Scan (rt: 0.181 min) MMI_ESI_Negative_184-4F_5680.d
437.1635
473.1395
537.1387
875.3281
Counts vs. Mass-to-Charge (m/z)
12

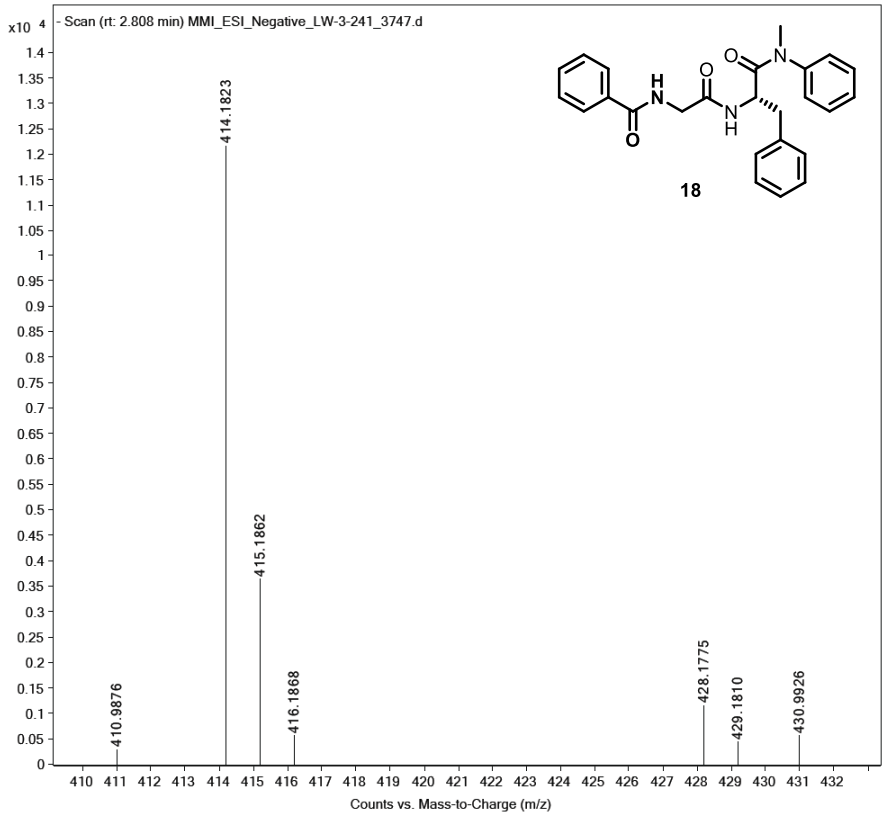

x10 5
- Scan (rt: 0.582 min) MMI_ESI_Negative_LW-3-293_3751.d
437.1632
112.9856
255.2325
325.1838
473.1383
897.3093
Counts vs. Mass-to-Charge (m/z)
13

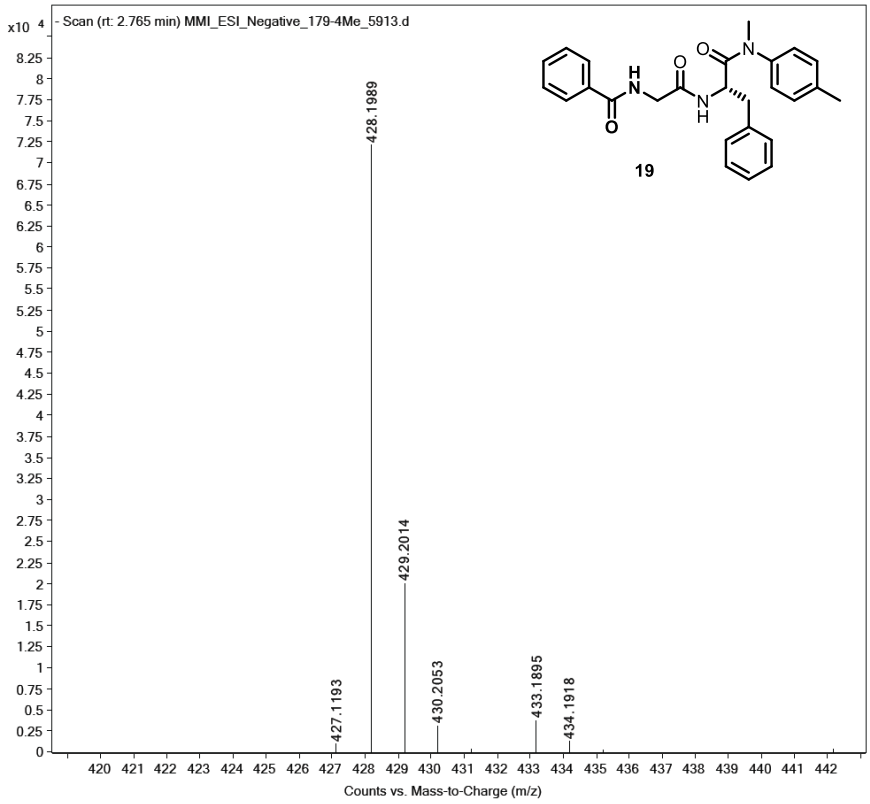

- Scan (rt: 1.260 min) MMI_ESI_Negative_184-3Br_5867.d
x10 4
497.0835
499.0819
498.0862
500.0847
501.0868
519.0642
521.0614
533.0584
535.0573
537.0536
Counts vs. Mass-to-Charge (m/z)
Me
Br
14

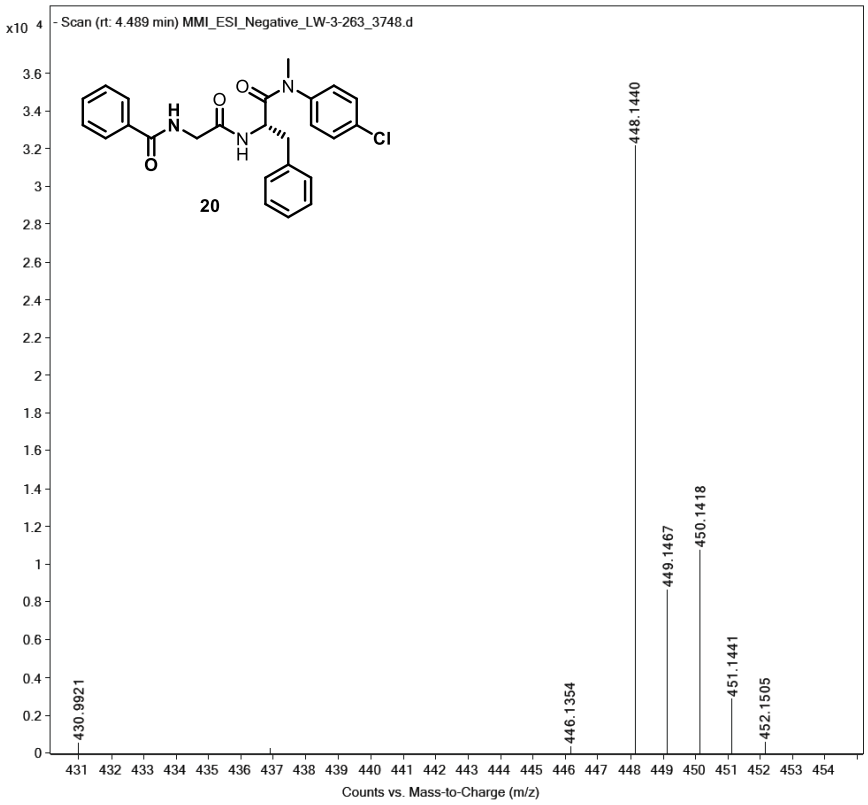

- Scan (rt: 1.259 min) MMI_ESI_Negative_184-3CF3_5868.d
x10 4
487.1604
488.1637
489.1649
497.0806
499.0808
509.1406
523.1364
525.1343
Counts vs. Mass-to-Charge (m/z)
Me
CF3
15

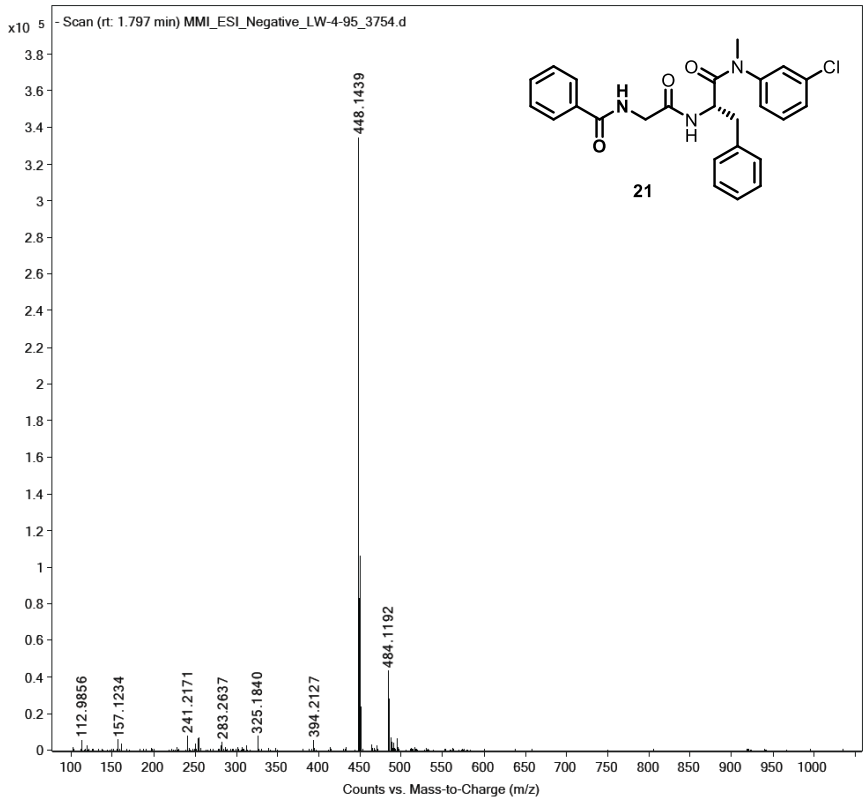

- Scan (rt: 0.973 min) MMI_ESI_Negative_LW-3-281_3749.d
x10 4
405.1568
406.1596
407.1651
410.9869
Counts vs. Mass-to-Charge (m/z)
16

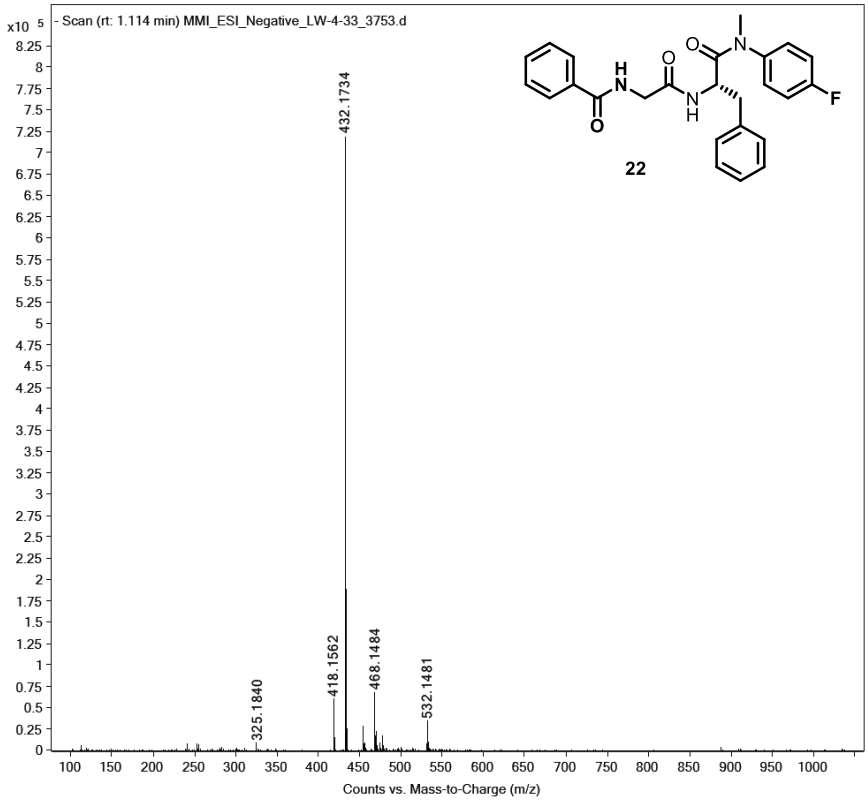

- Scan (rt: 2.782 min) MMI_ESI_Negative_179-Ben_6247.d
x10 4
436.2044
391.1415
450.1828
Counts vs. Mass-to-Charge (m/z)
17

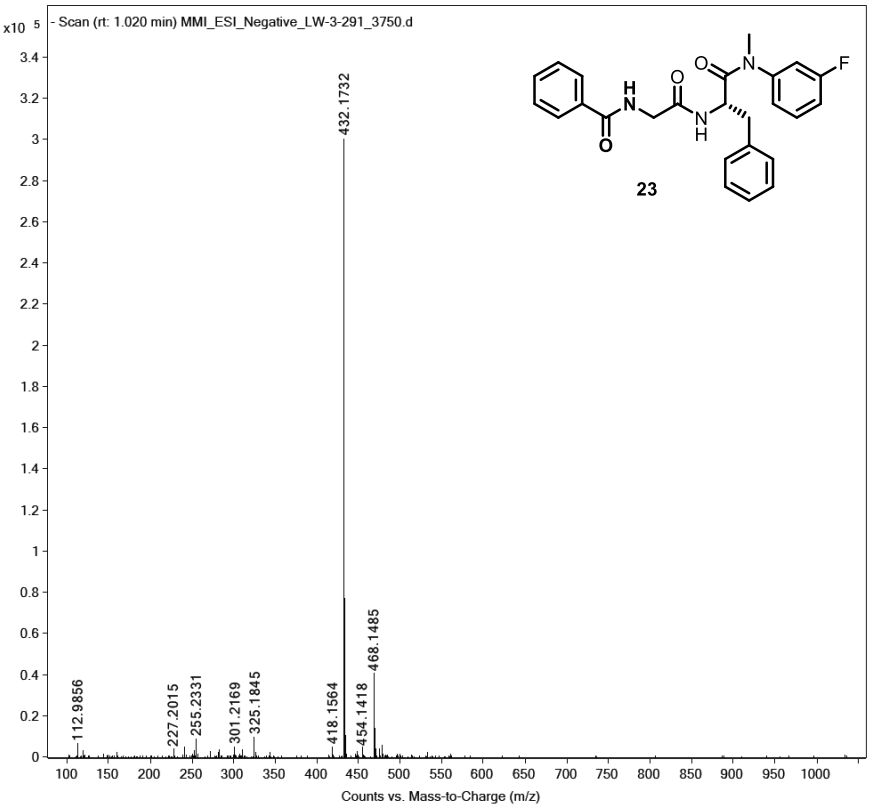

- Scan (rt: 2.808 min) MMI_ESI_Negative_LW-3-241_3747.d
x10 4
414.1823
415.1862
416.1868
410.9876
428.1775
429.1810
430.9926
Counts vs. Mass-to-Charge (m/z)
18

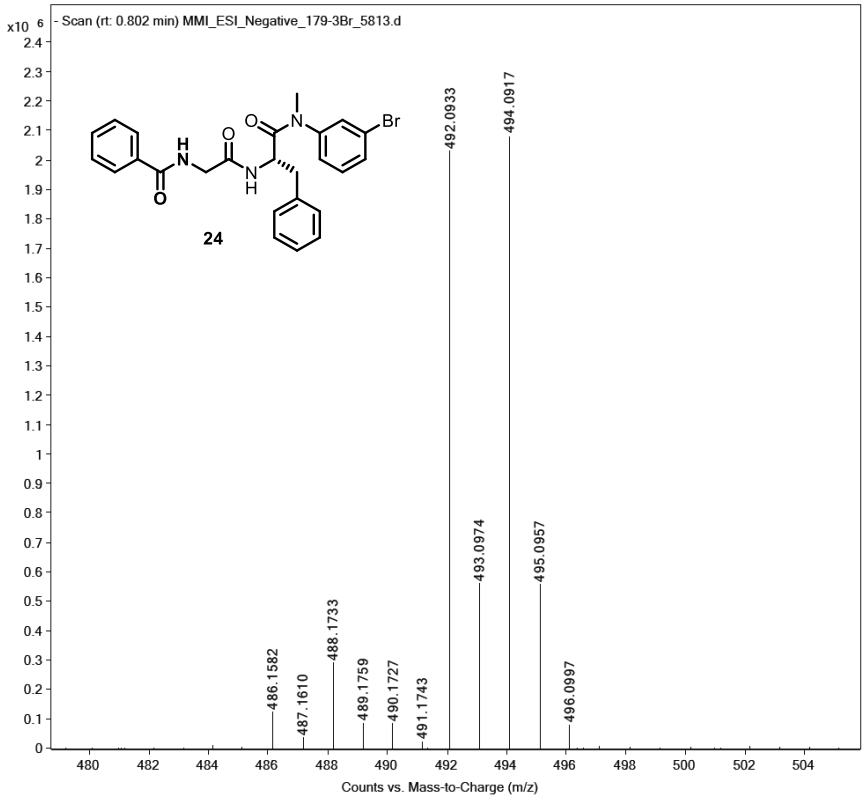

- Scan (rt: 2.765 min) MMI_ESI_Negative_179-4Me_5913.d
x10 4
428.1989
429.2014
427.1193
430.2053
433.1895
434.1918
Counts vs. Mass-to-Charge (m/z)
19

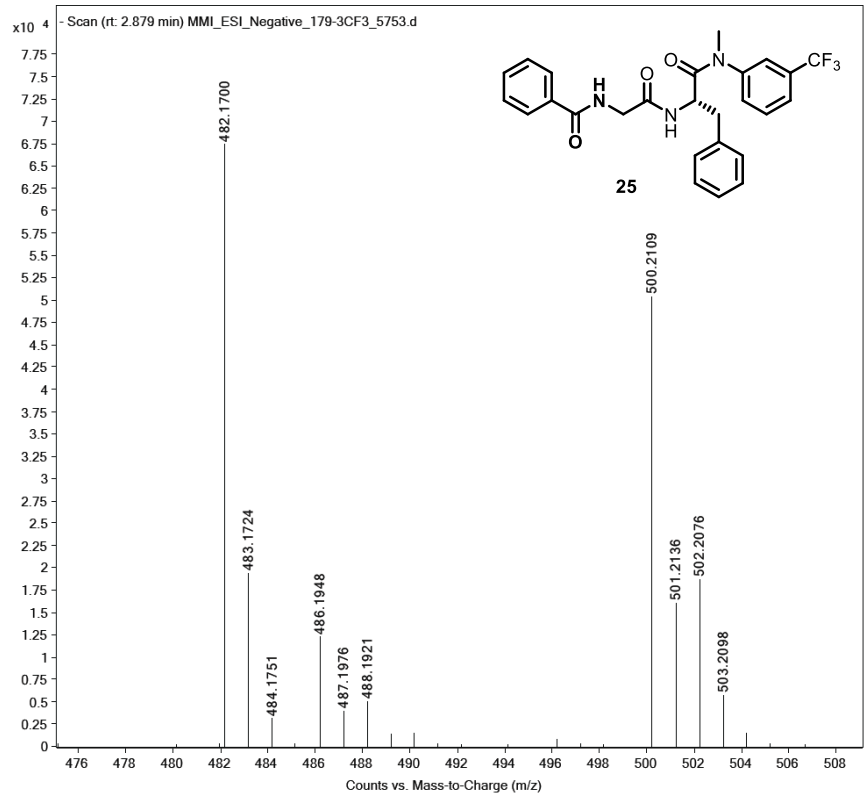

- Scan (rt: 4.489 min) MMI_ESI_Negative_LW-3-263_3748.d
x10 4
20
448.1440
449.1467
450.1418
451.1441
452.1505
430.9921
446.1354
Counts vs. Mass-to-Charge (m/z)

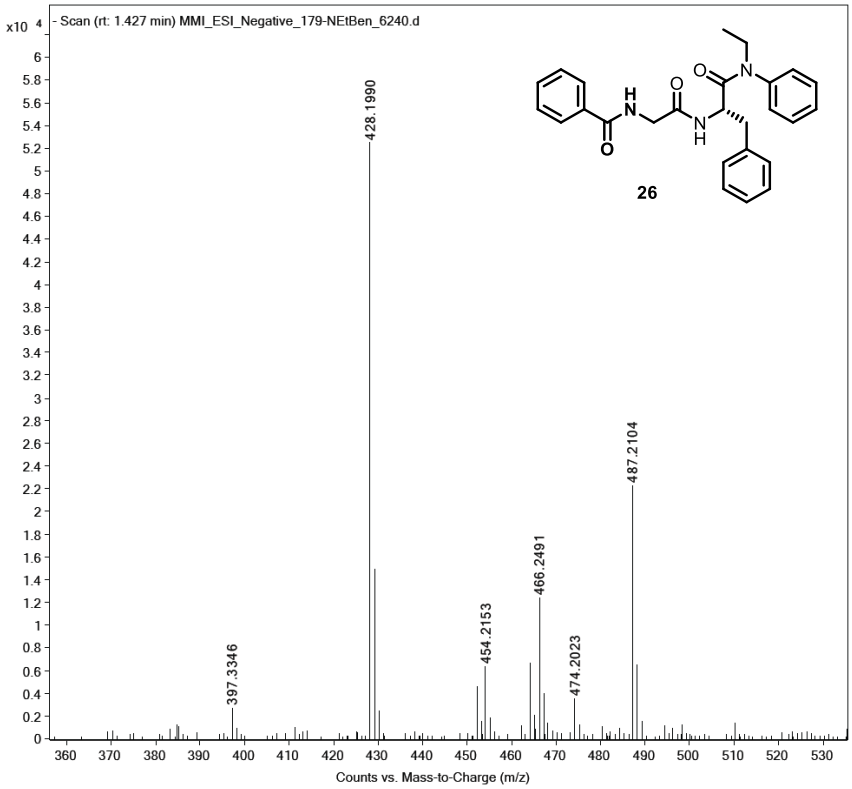

- Scan (rt: 1.797 min) MMI_ESI_Negative_LW-4-95_3754.d
x10 5
21
448.1439
484.1192
112.9856
157.1234
241.2171
283.2637
325.1840
394.2127
Counts vs. Mass-to-Charge (m/z)

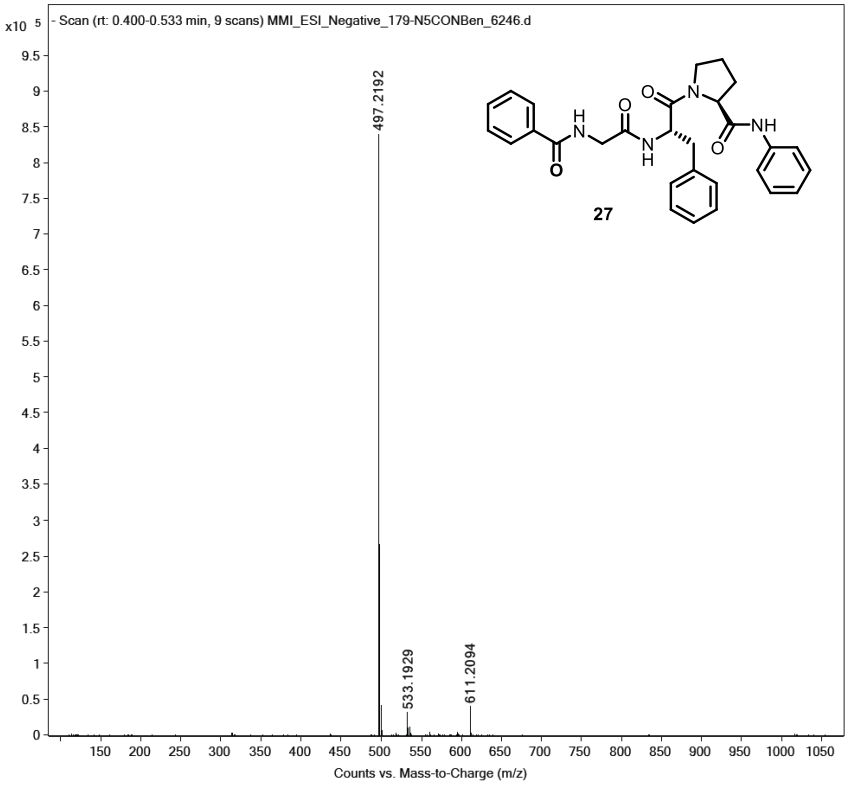

- Scan (rt: 1.114 min) MMI_ESI_Negative_LW-4-33_3753.d
x10 5
8.25
8
7.75
7.5
7.25
7
6.75
6.5
6.25
6
5.75
5.5
5.25
5
4.75
4.5
4.25
4
3.75
3.5
3.25
3
2.75
2.5
2.25
2
1.75
1.5
1.25
1
0.75
0.5
0.25
0
432.1734
418.1562
468.1484
325.1840
532.1481
100 150 200 250 300 350 400 450 500 550 600 650 700 750 800 850 900 950 1000
Counts vs. Mass-to-Charge (m/z)
22


- Scan (rt: 1.020 min) MMI_ESI_Negative_LW-3-291_3750.d
x10 5
3.4
3.2
3
2.8
2.6
2.4
2.2
2
1.8
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
432.1732
468.1485
112.9856
227.2015
255.2331
301.2169
325.1845
418.1564
454.1418
100 150 200 250 300 350 400 450 500 550 600 650 700 750 800 850 900 950 1000
Counts vs. Mass-to-Charge (m/z)
23


- Scan (rt: 0.802 min) MMI_ESI_Negative_179-3Br_5813.d
x10 6
24
492.0933
494.0917
493.0974
495.0957
488.1733
486.1582
487.1610
489.1759
490.1727
491.1743
496.0997
Counts vs. Mass-to-Charge (m/z)


- Scan (rt: 2.879 min) MMI_ESI_Negative_179-3CF3_5753.d
x10 4
25
482.1700
500.2109
483.1724
501.2136
502.2076
486.1948
503.2098
484.1751
487.1976
488.1921
Counts vs. Mass-to-Charge (m/z)


- Scan (rt: 1.427 min) MMI_ESI_Negative_179-NEtBen_6240.d
x10 4
428.1990
487.2104
466.2491
454.2153
474.2023
397.3346
Counts vs. Mass-to-Charge (m/z)
26


- Scan (rt: 0.400-0.533 min, 9 scans) MMI_ESI_Negative_179-N5CONBen_6246.d
x10 5
497.2192
533.1929
611.2094
Counts vs. Mass-to-Charge (m/z)
27