Supporting Information

Sulfur(VI) fluoride exchange as a key reaction for synthesizing biaryl sulfate core derivatives as potent hepatitis C virus NS5A inhibitors and their structure-activity relationship studies

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[e.] Department of Life Sciences, Pohang University of Science and Technology, Pohang 37673, South Korea.

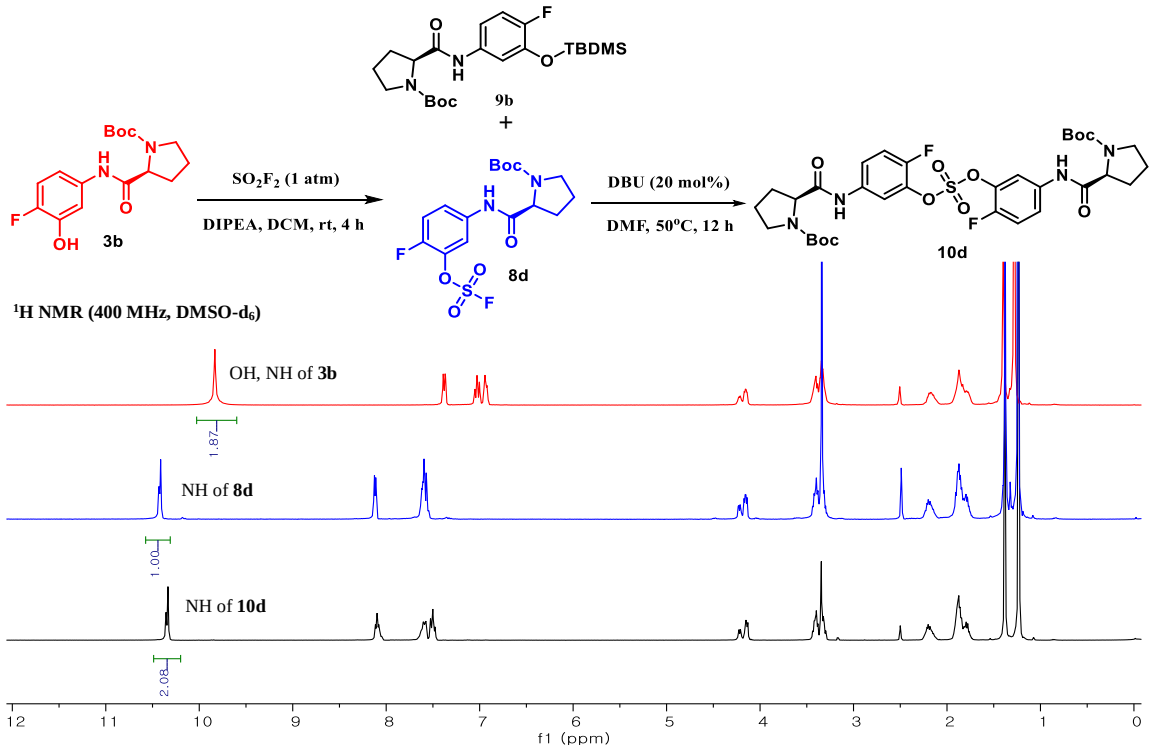


Figure S1. Representative ^{1}H NMR (400 MHz, DMSO-d$_6$) Analysis of Fosylation and SuFEx. Reaction illustrated a Starting Material (red) and fosylated compound (blue) and SuFEx product (black).

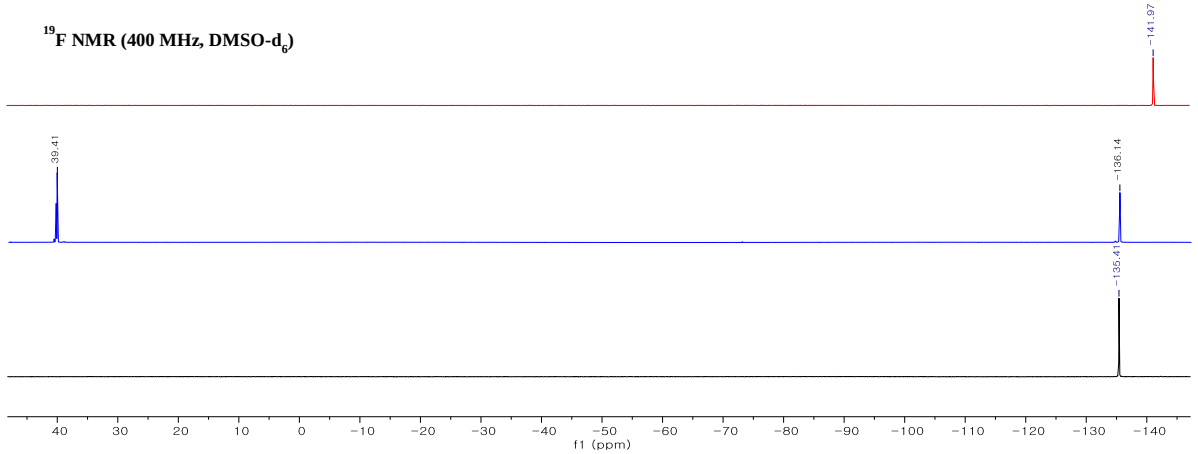


Figure S2. Representative ^{19}F NMR (400 MHz, DMSO-d$_6$) Analysis of Fosylation and SuFEx. Reaction illustrated a Starting Material (red) and fosylated compound (blue) and SuFEx product (black).

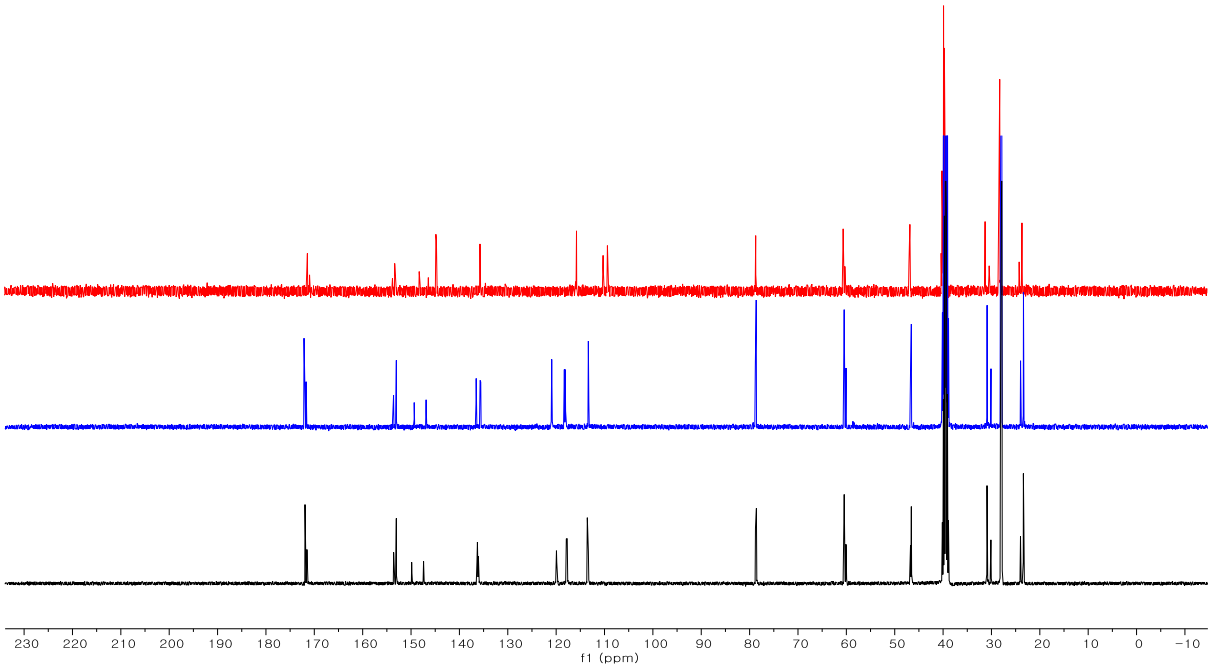
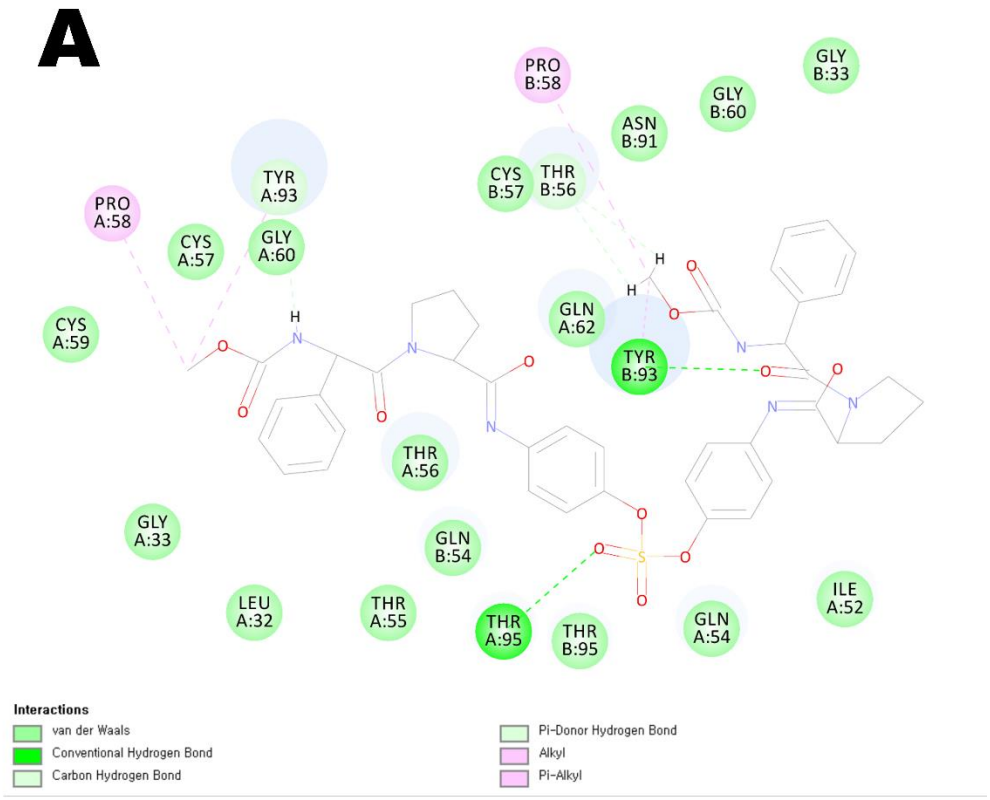
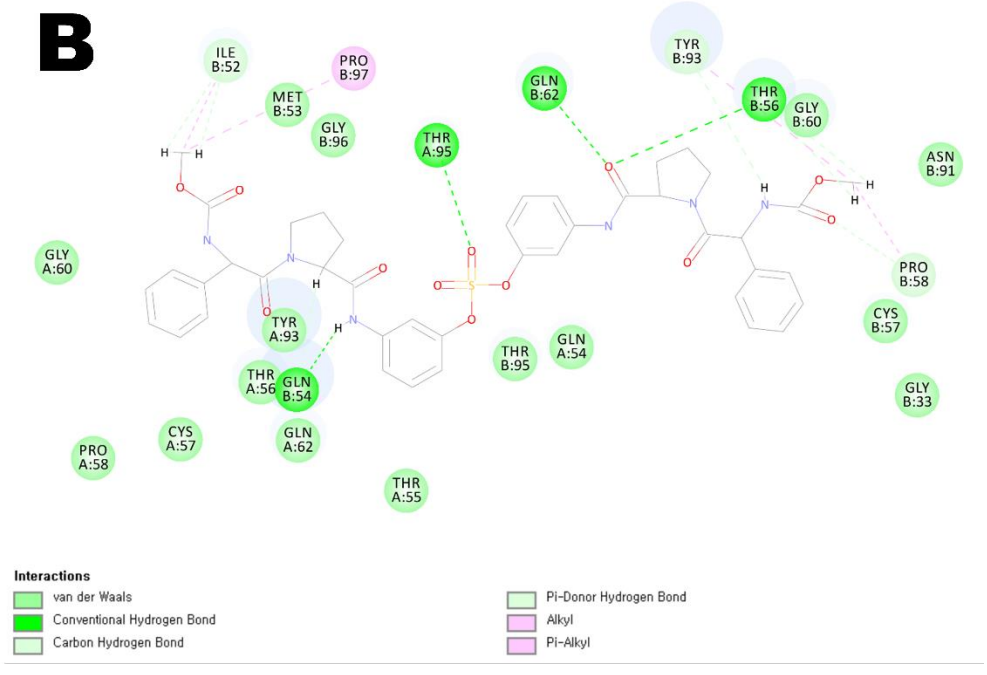


Figure S3. Representative ^{13}C NMR (400 MHz, DMSO-d_6) Analysis of Fosylation and SuFEx. Reaction illustrated a Starting Material (red) and fosylated compound (blue) and SuFEx product (black).

Molecular docking study





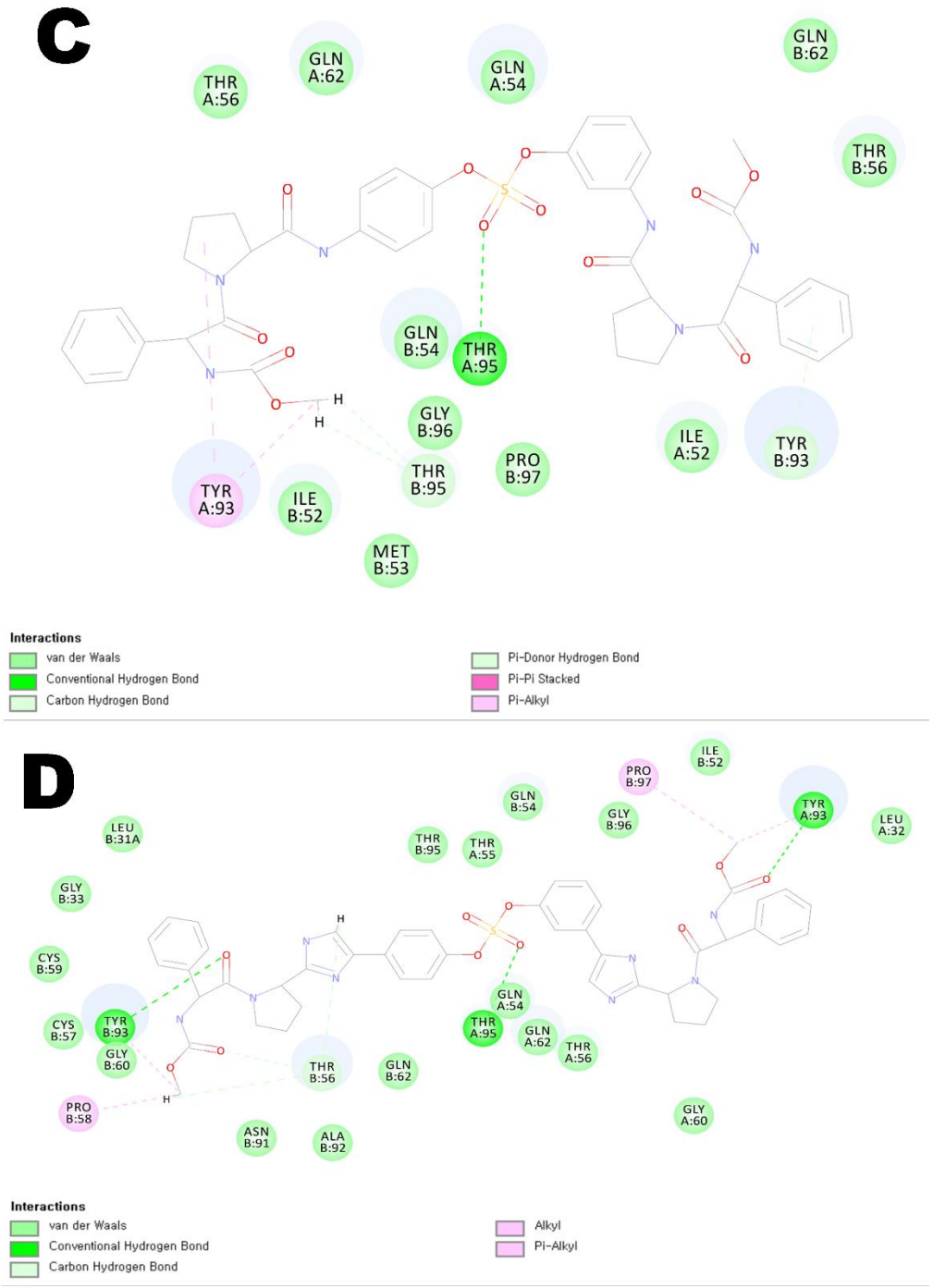


Figure S4. 2D-interaction docking model of (A) **BMK-21007**, (B) **BMK-21014**, (C) compound **11**, and (D) compound **22** inside NS5A dimer model (3FQQ). Various interactions are depicted by different color legends. Inhibitors are shown by line, interacting residues by colored sphere, and interactions by dash lines.

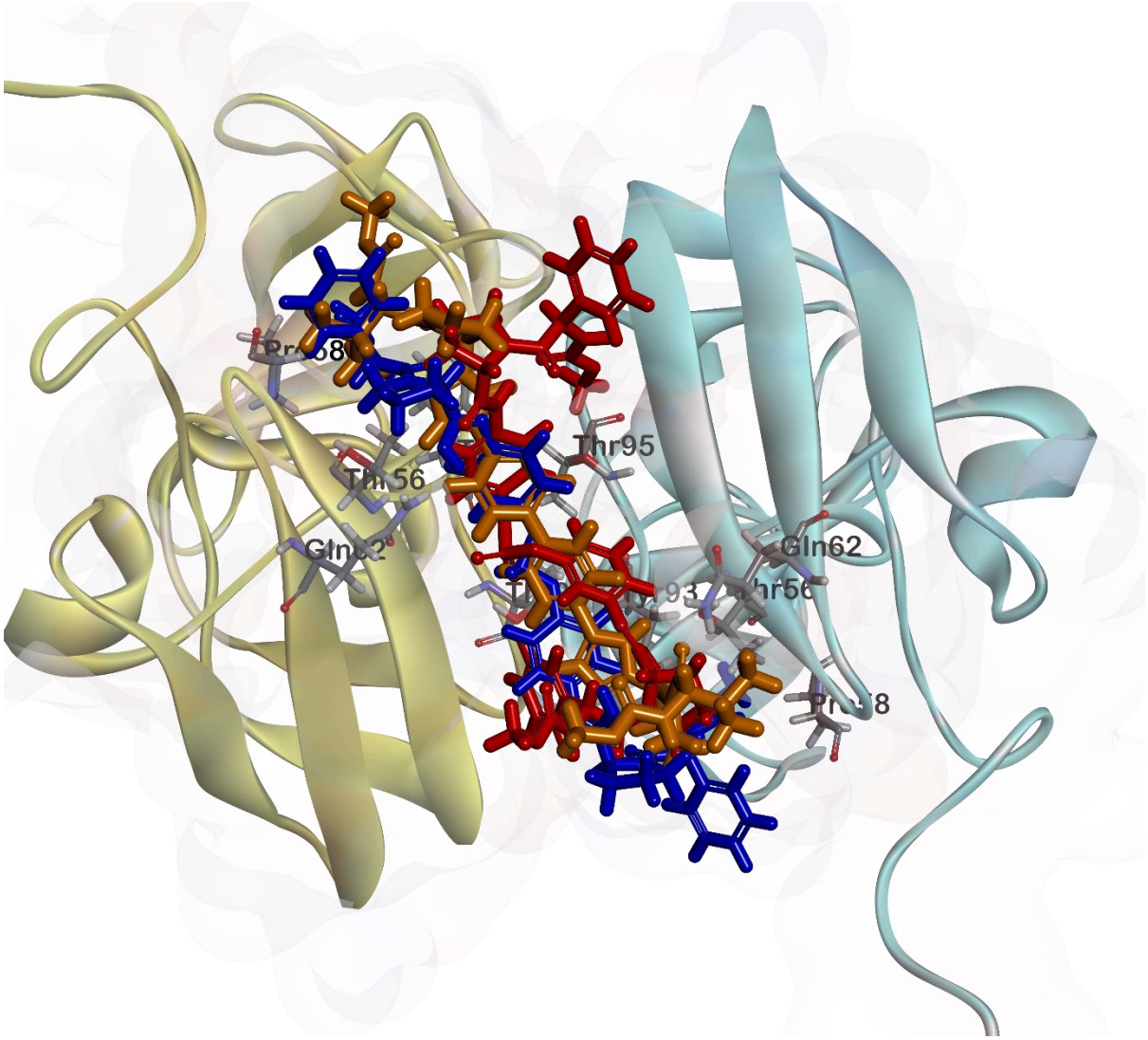


Figure S5. Superposed model of inhibitors inside NS5A dimer model (3FQQ). Daclatasvir, **BMK-21007**, and compound **11** shown by orange, blue, and red, respectively.

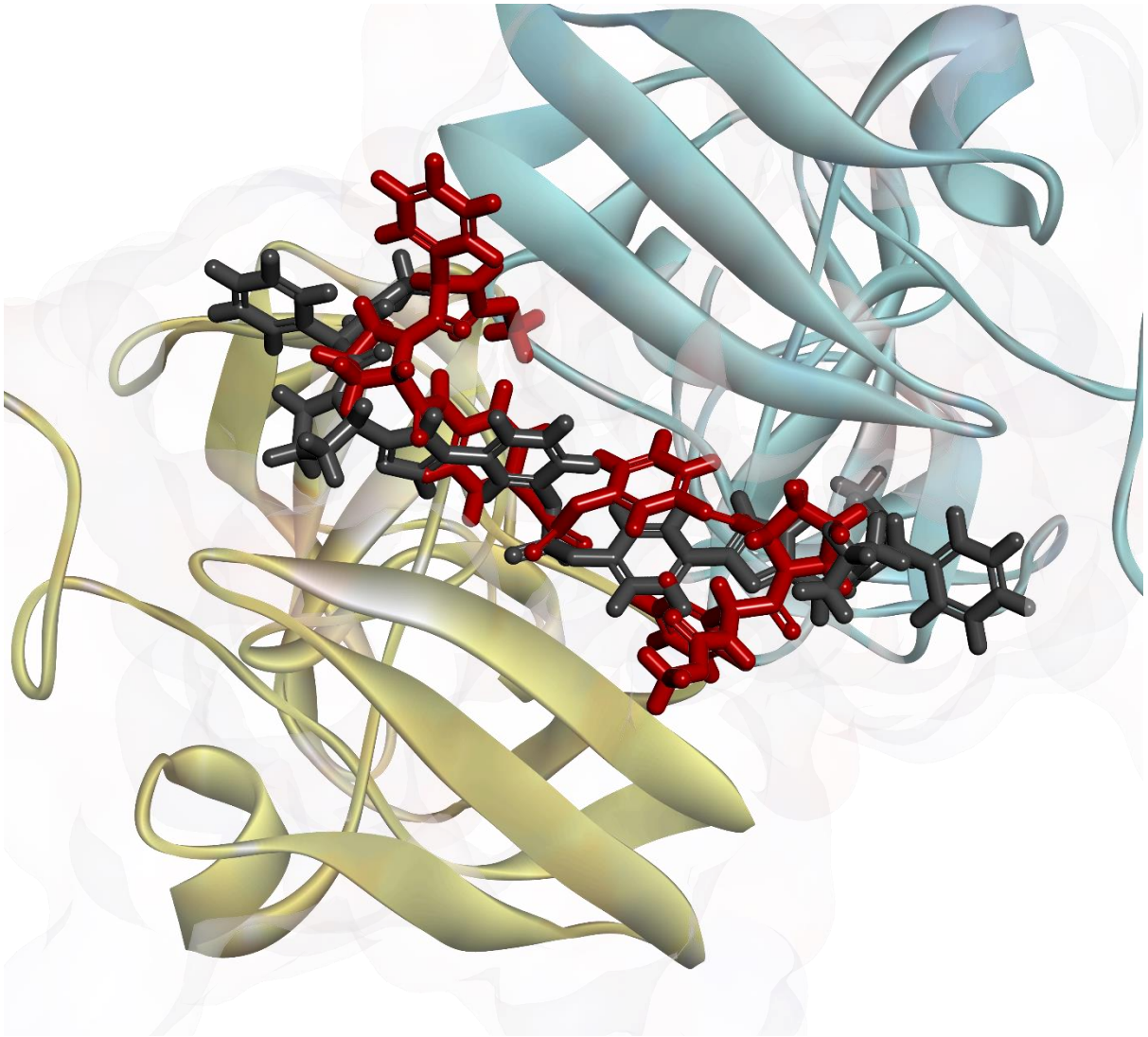
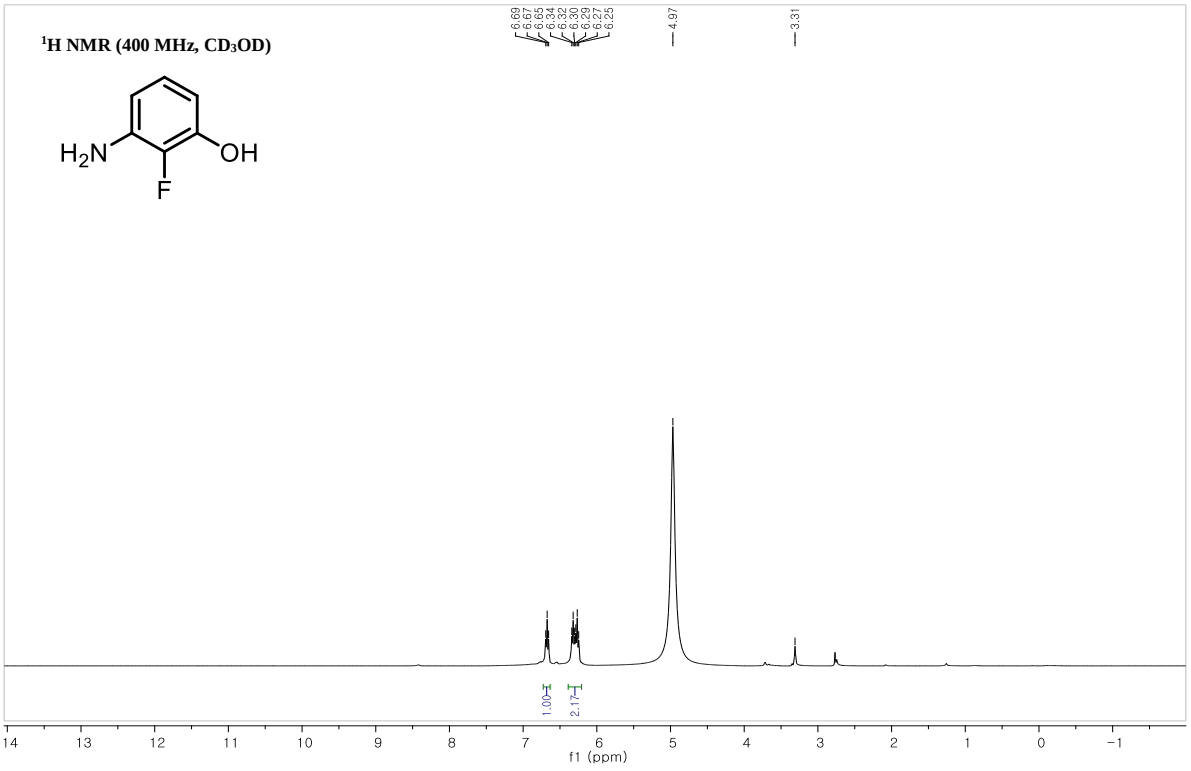
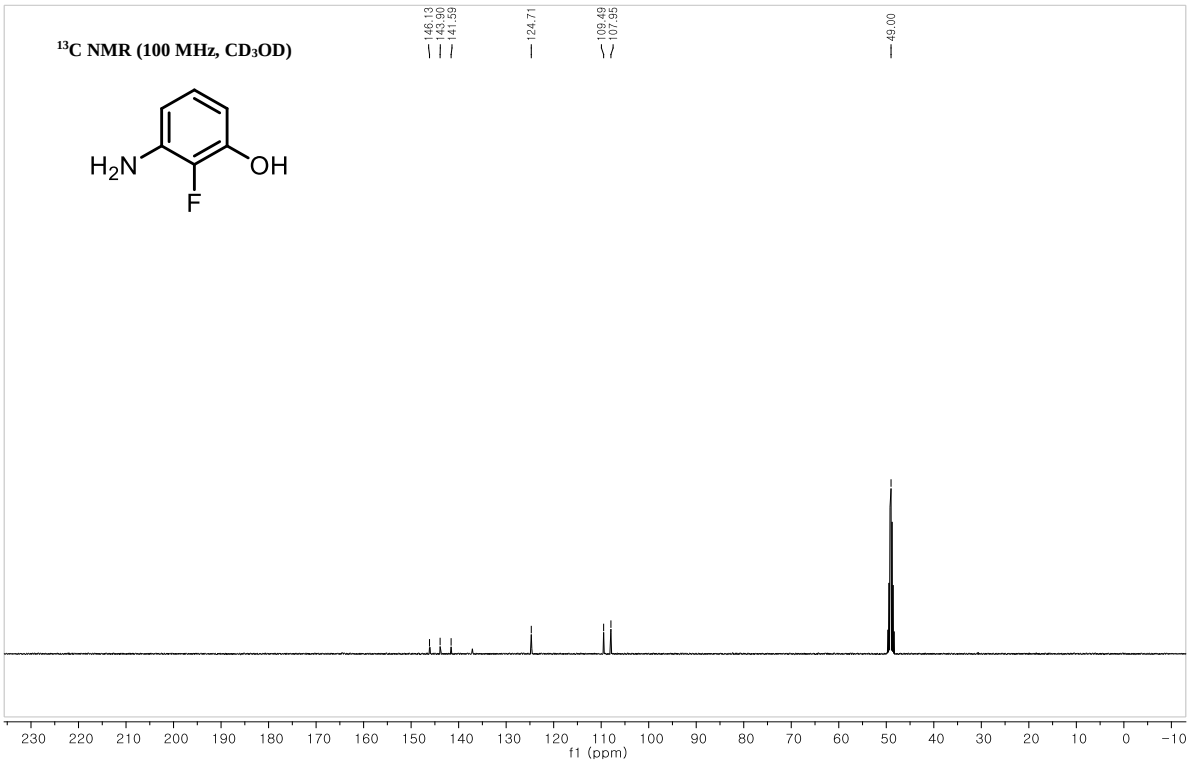


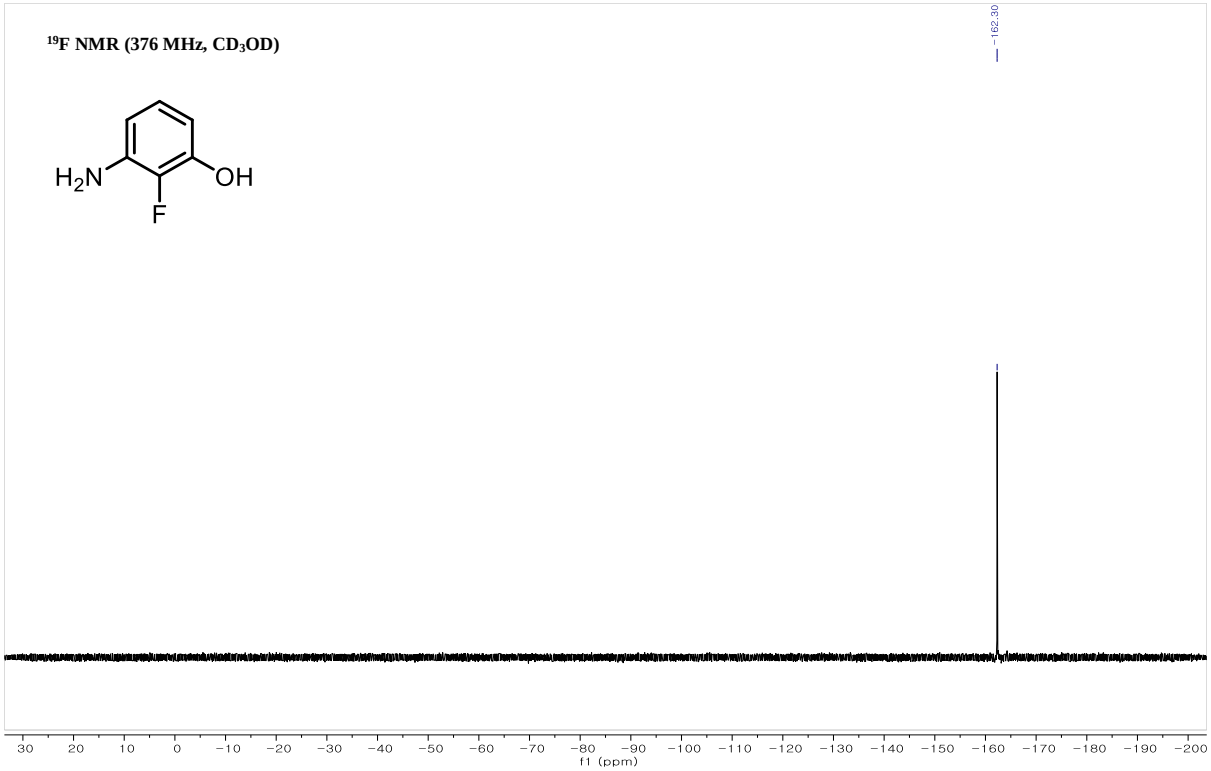
Figure S6. Superposed model of inhibitors inside NS5A dimer model (3FQQ). Compounds **11** a nd **22** shown by red and grey, respectively.

NMR Spectra

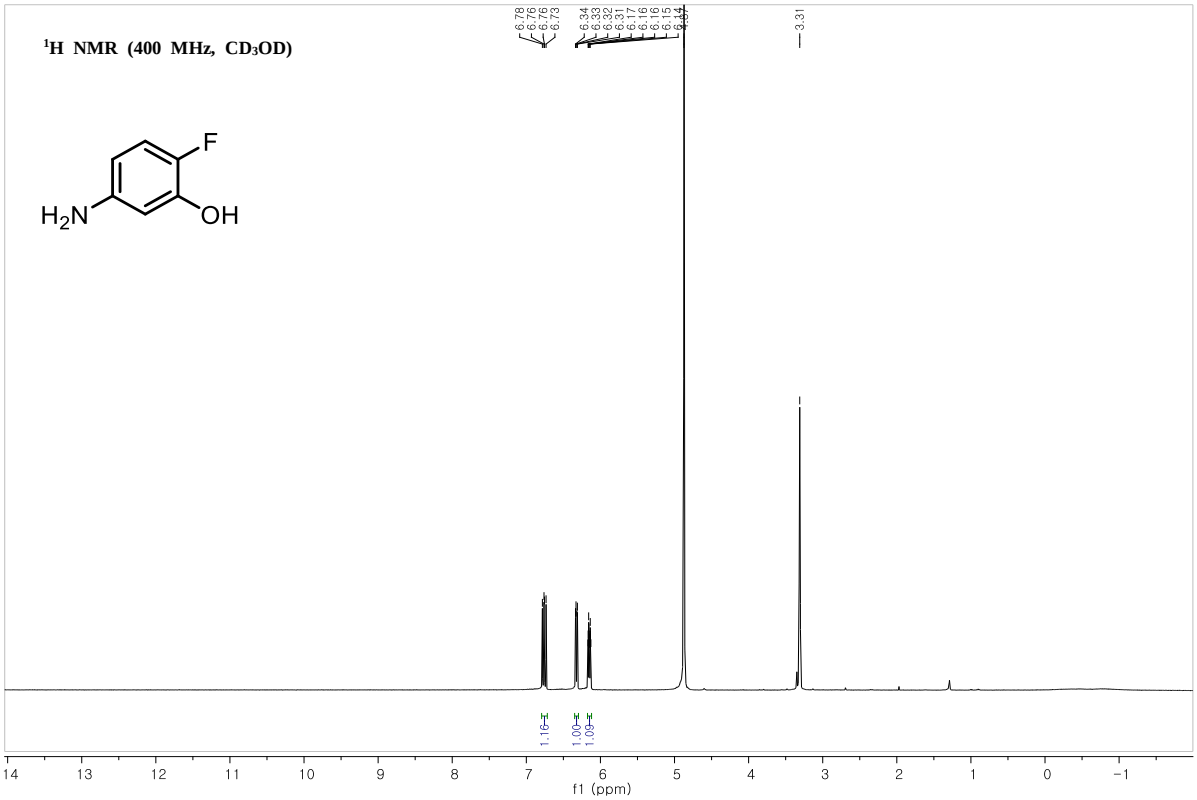
Compound 2a



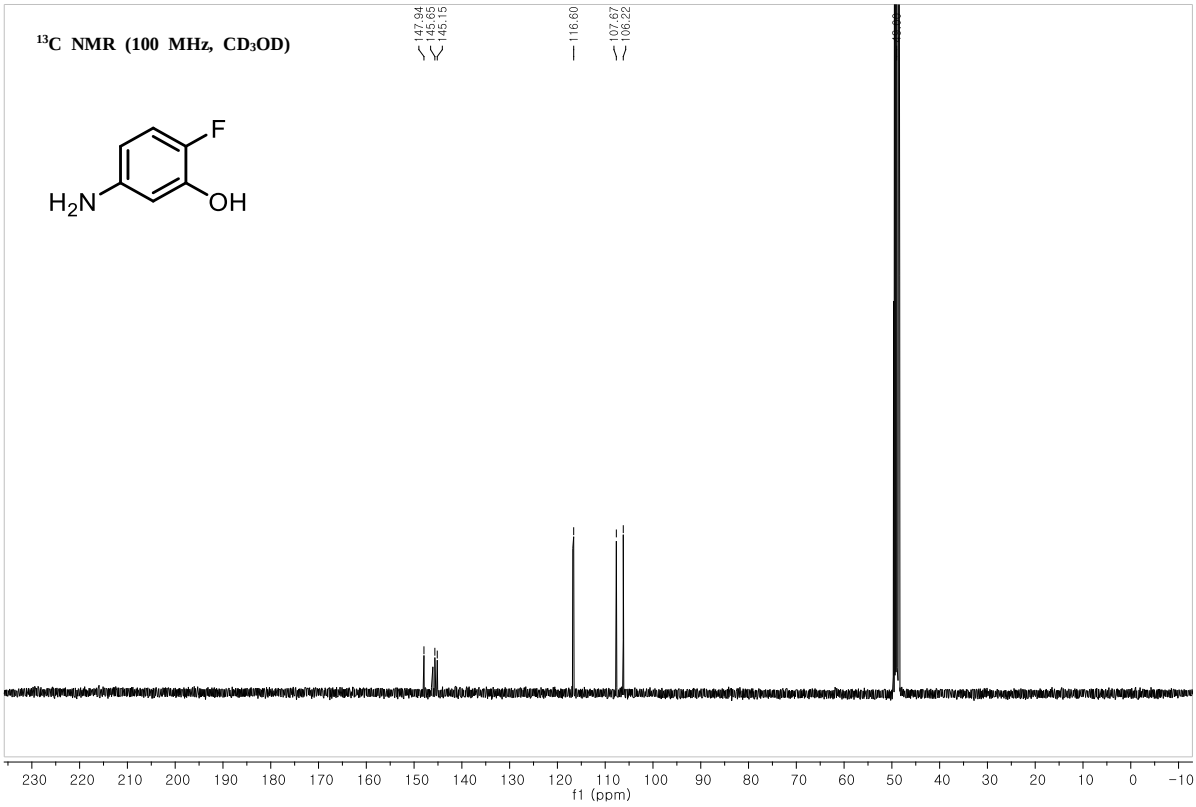



19F NMR (376 MHz, CD3OD)
H2N
OH
F
-162.30
30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

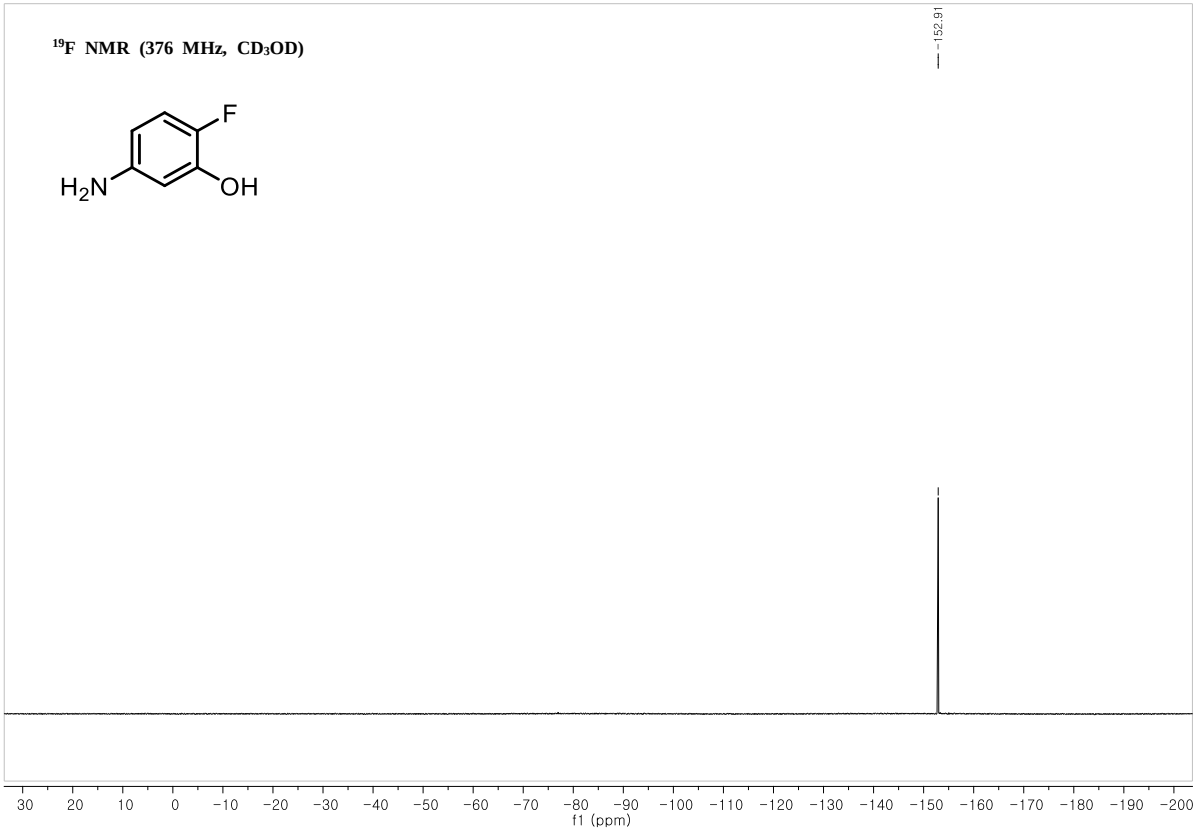
Compound 2b


1H NMR (400 MHz, CD3OD)
F
H2N
OH
6.78
6.76
6.75
6.73
6.34
6.33
6.32
6.31
6.17
6.16
6.16
6.15
6.14
6.13
3.31
1.16
1.00
1.05
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)

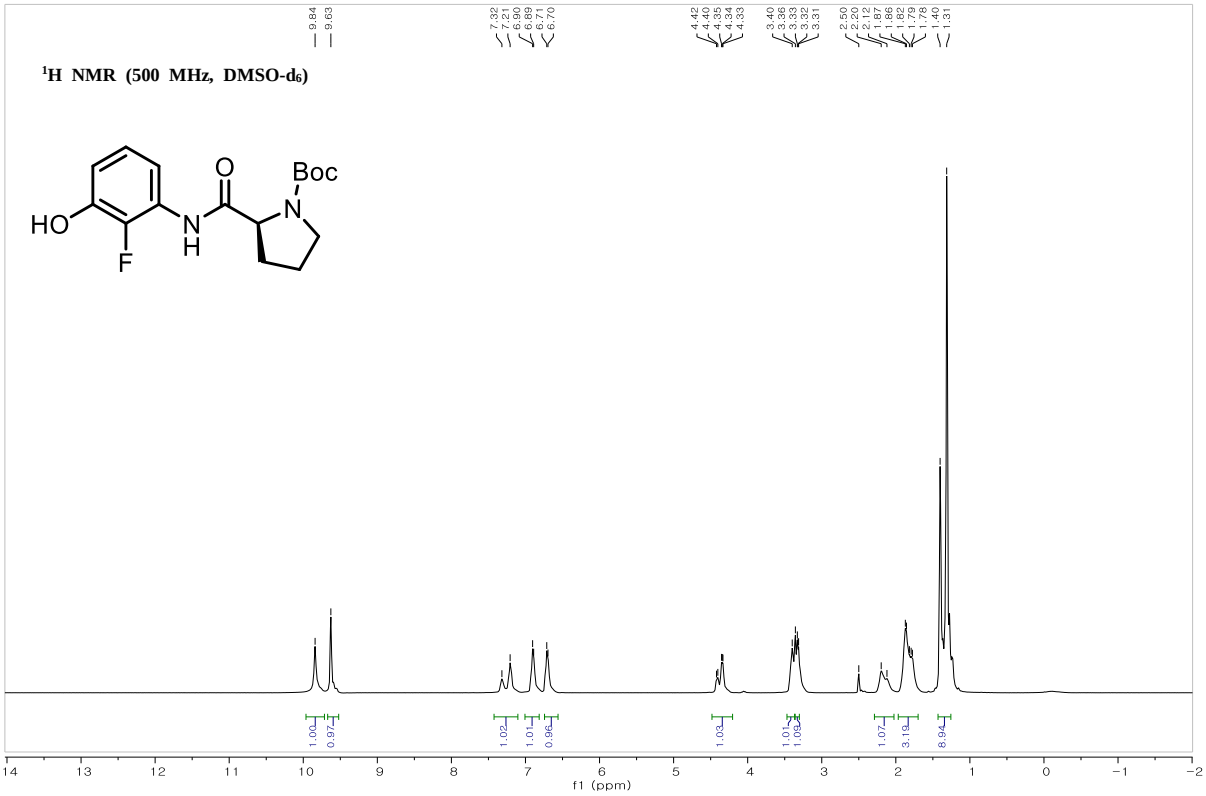
^{13}C NMR (100 MHz, CD_3OD)



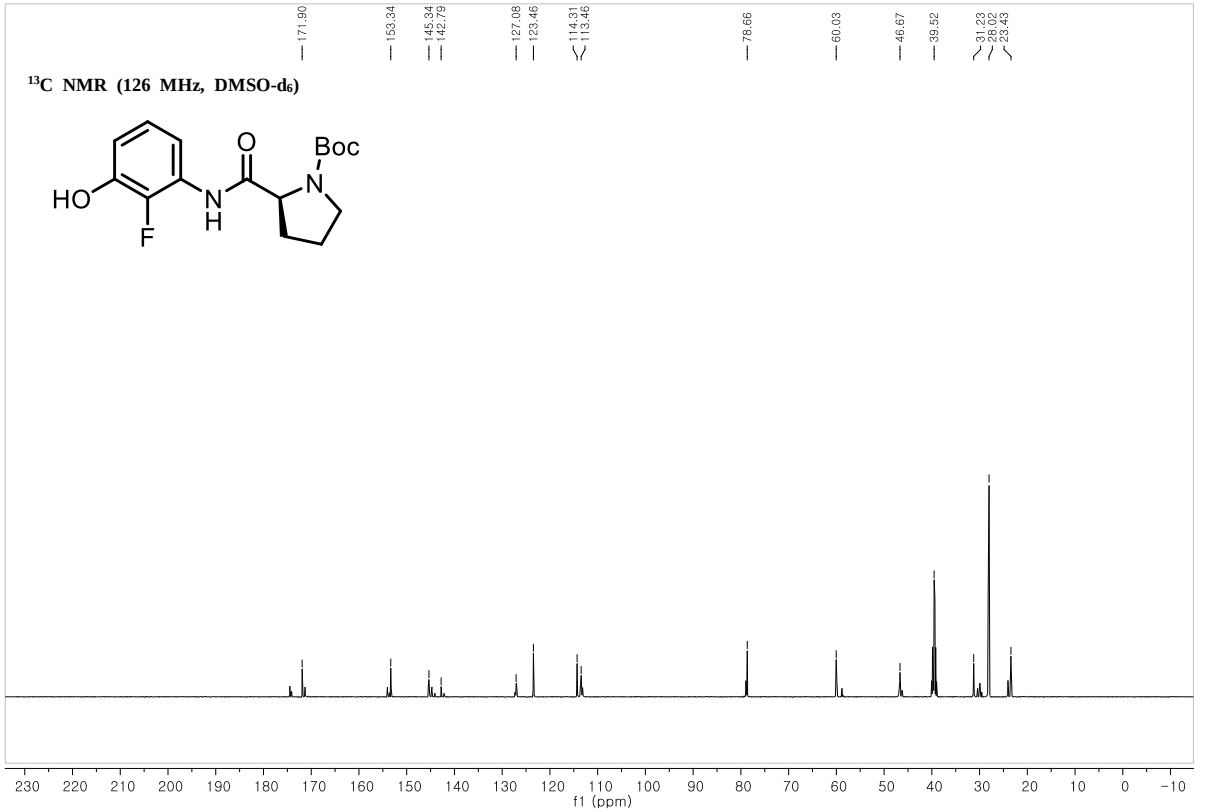
^{19}F NMR (376 MHz, CD_3OD)



Compound 3a

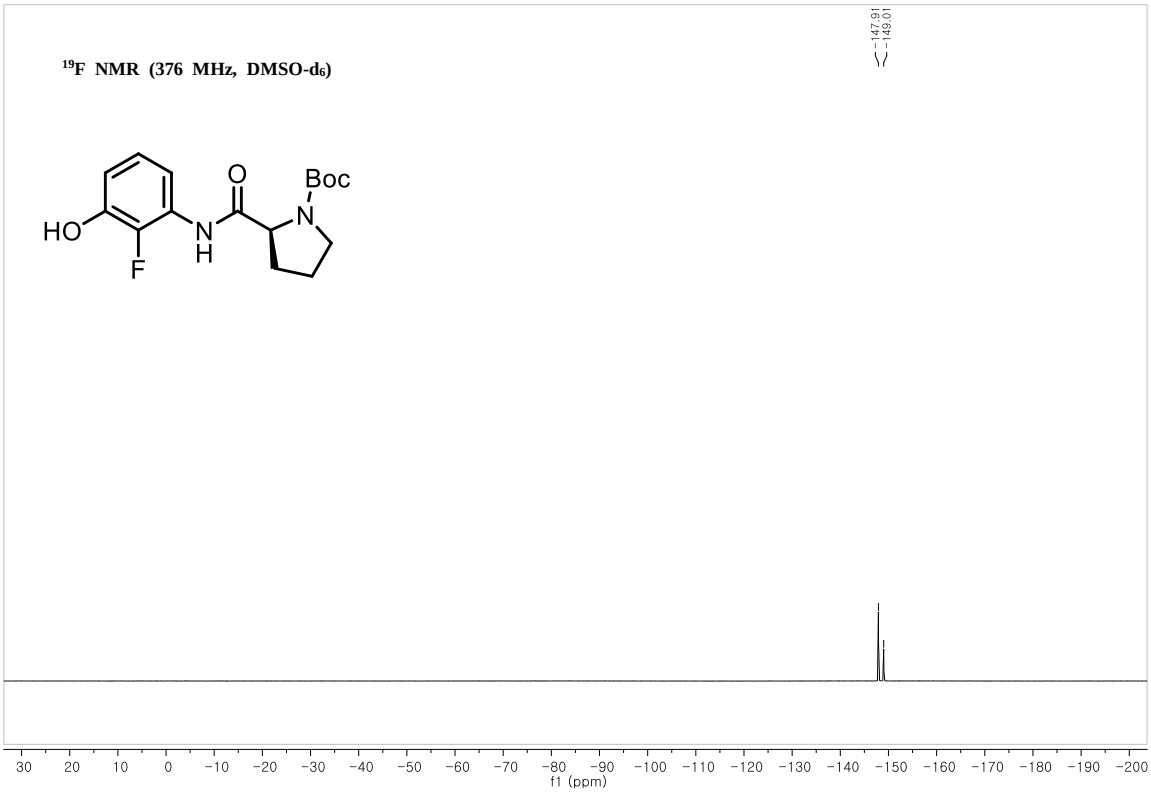


^{1}H NMR (500 MHz, DMSO-d_6)



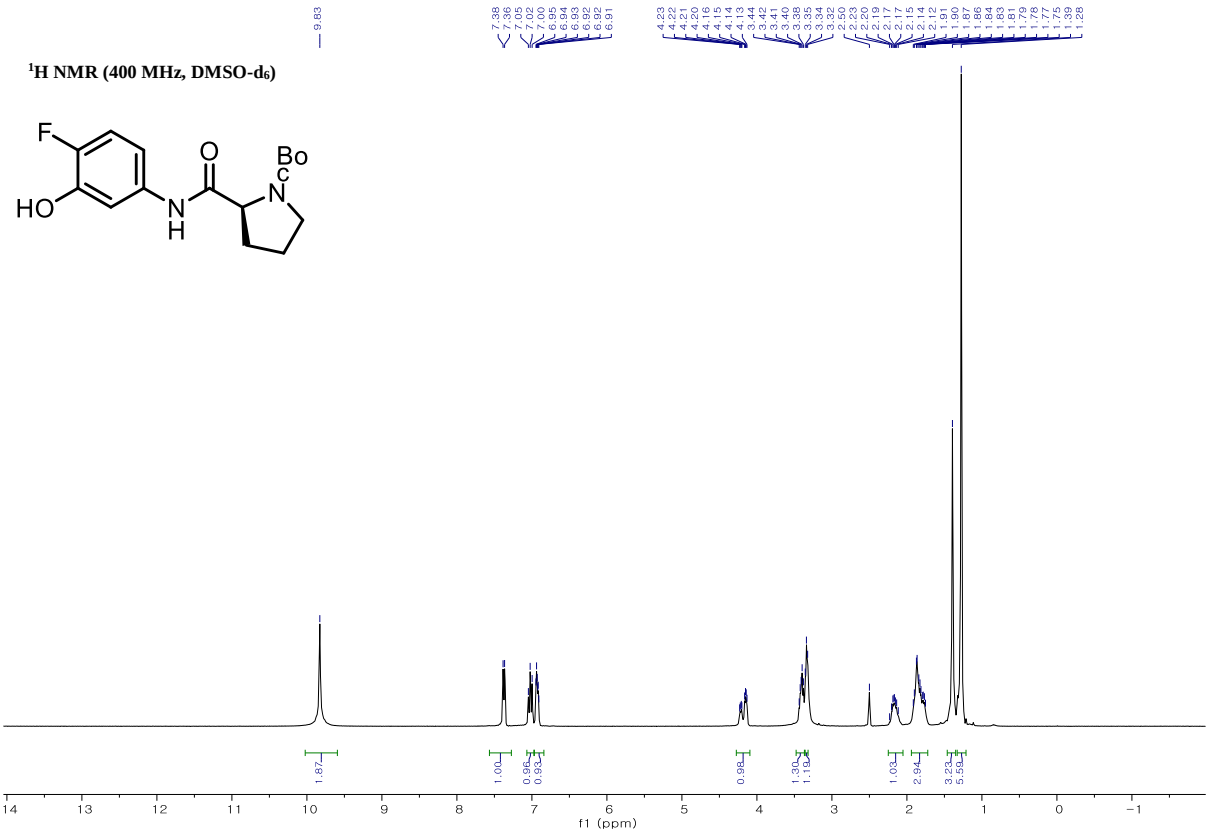
^{13}C NMR (126 MHz, DMSO-d_6)

^{19}F NMR (376 MHz, DMSO-d$_6$)

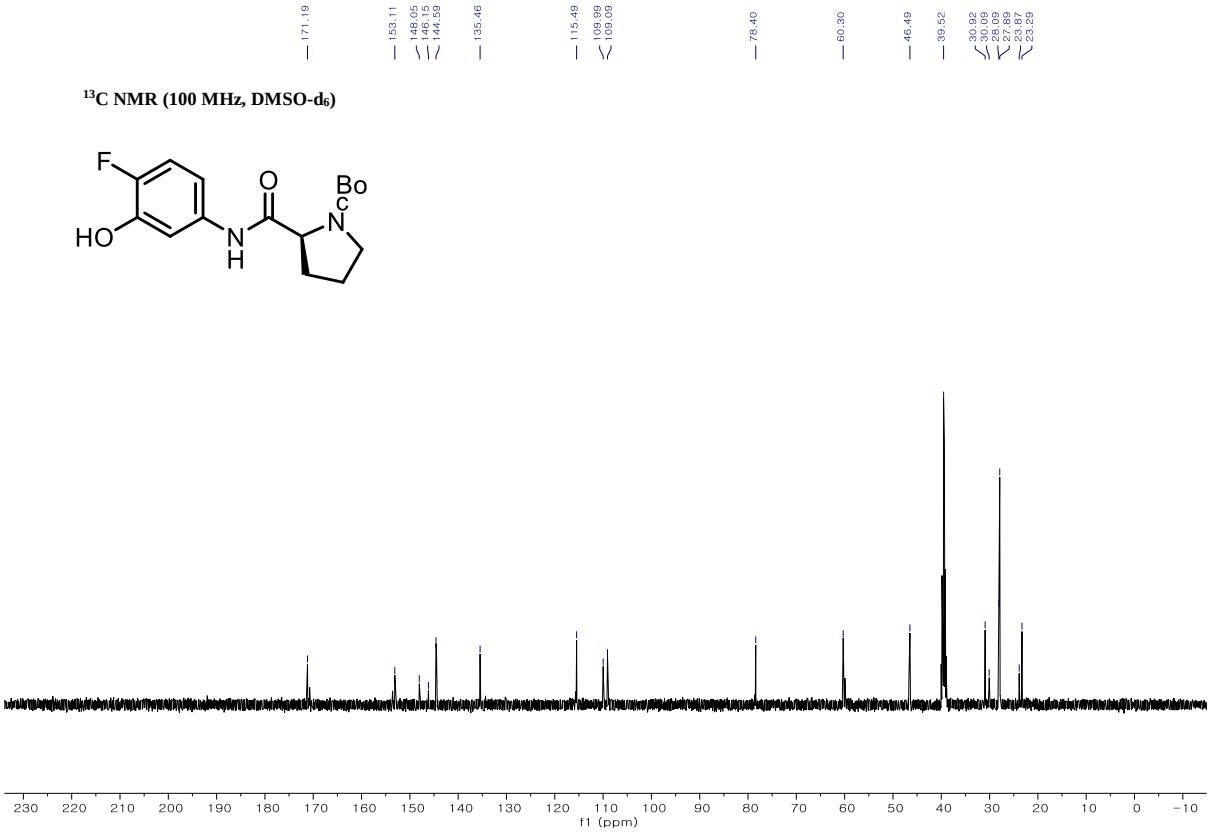


Compound 3b

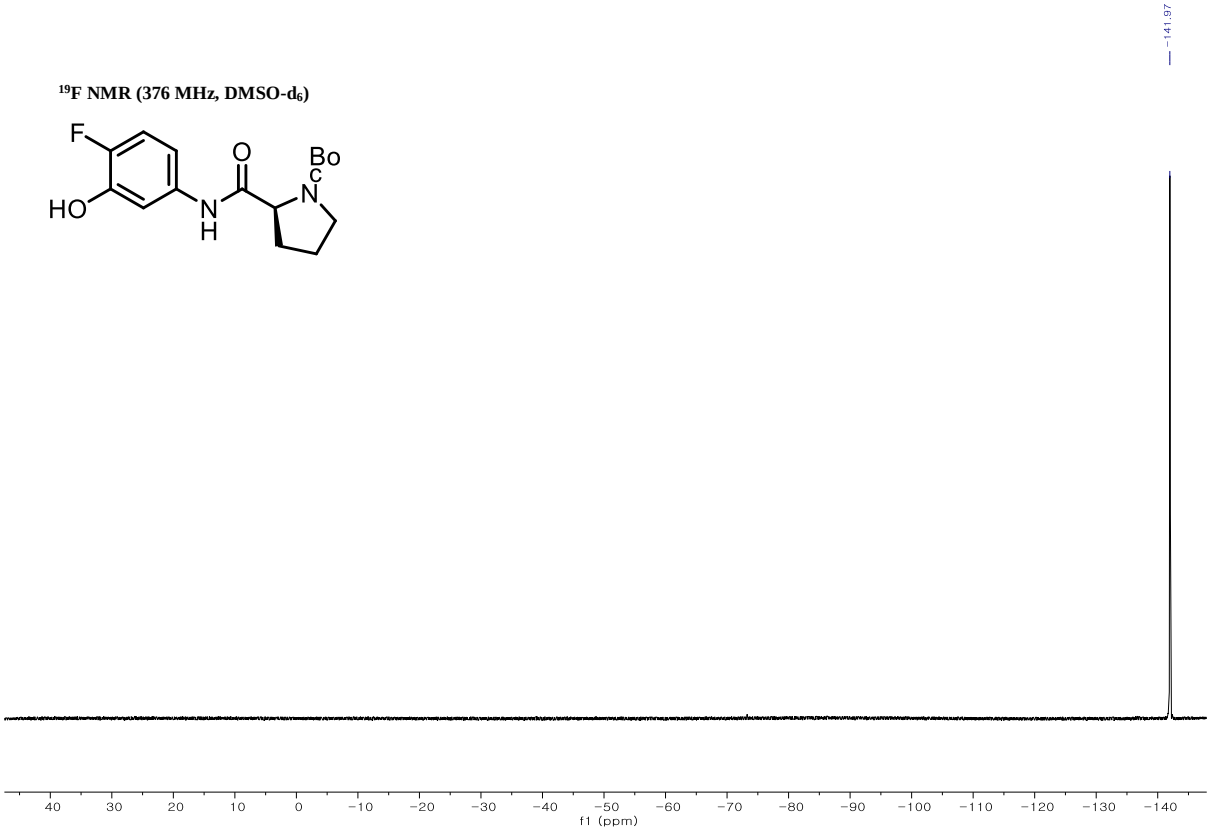
^{1}H NMR (400 MHz, DMSO-d$_6$)



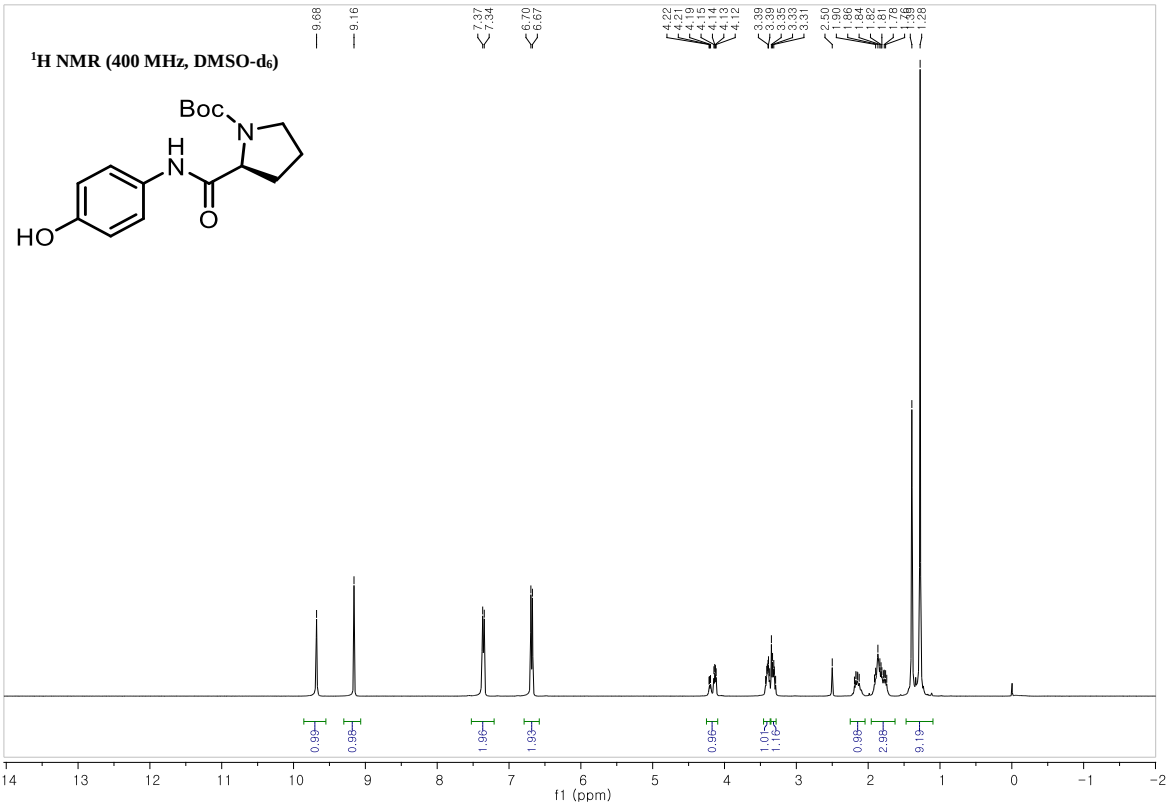
^{13}C NMR (100 MHz, DMSO-d$_6$)

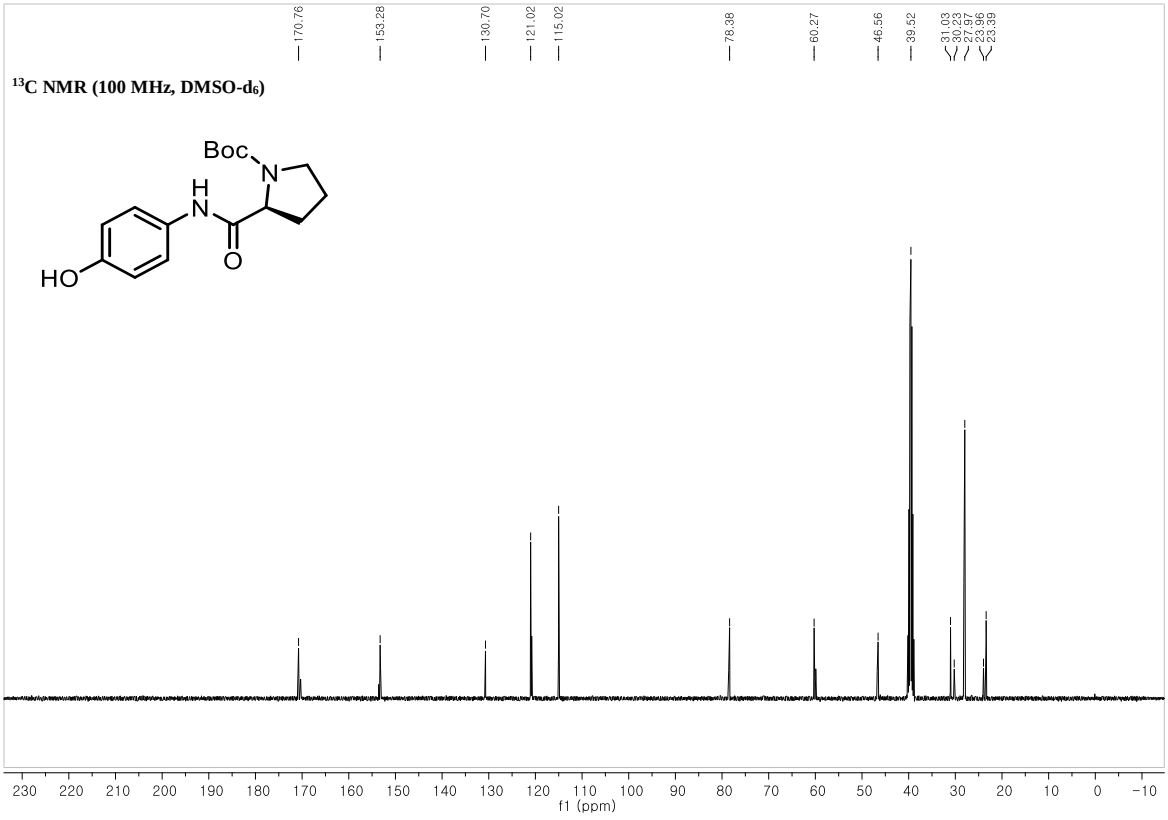


^{19}F NMR (376 MHz, DMSO-d$_6$)

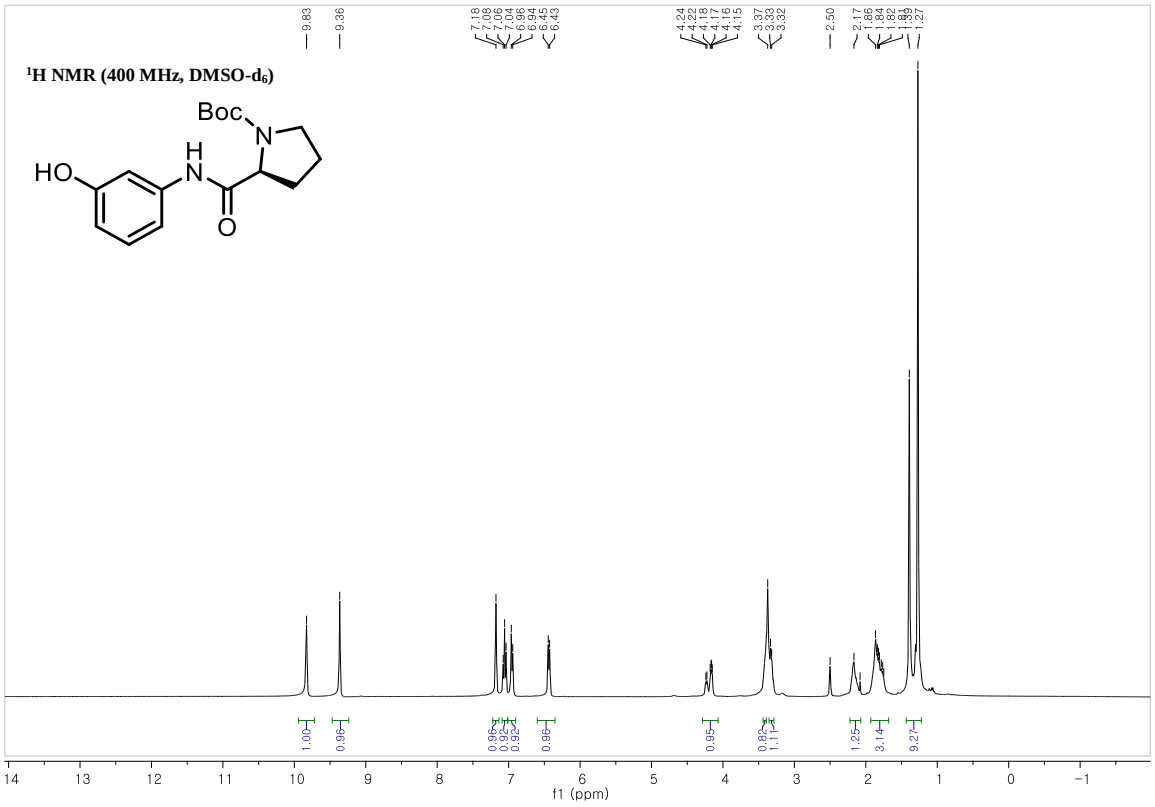


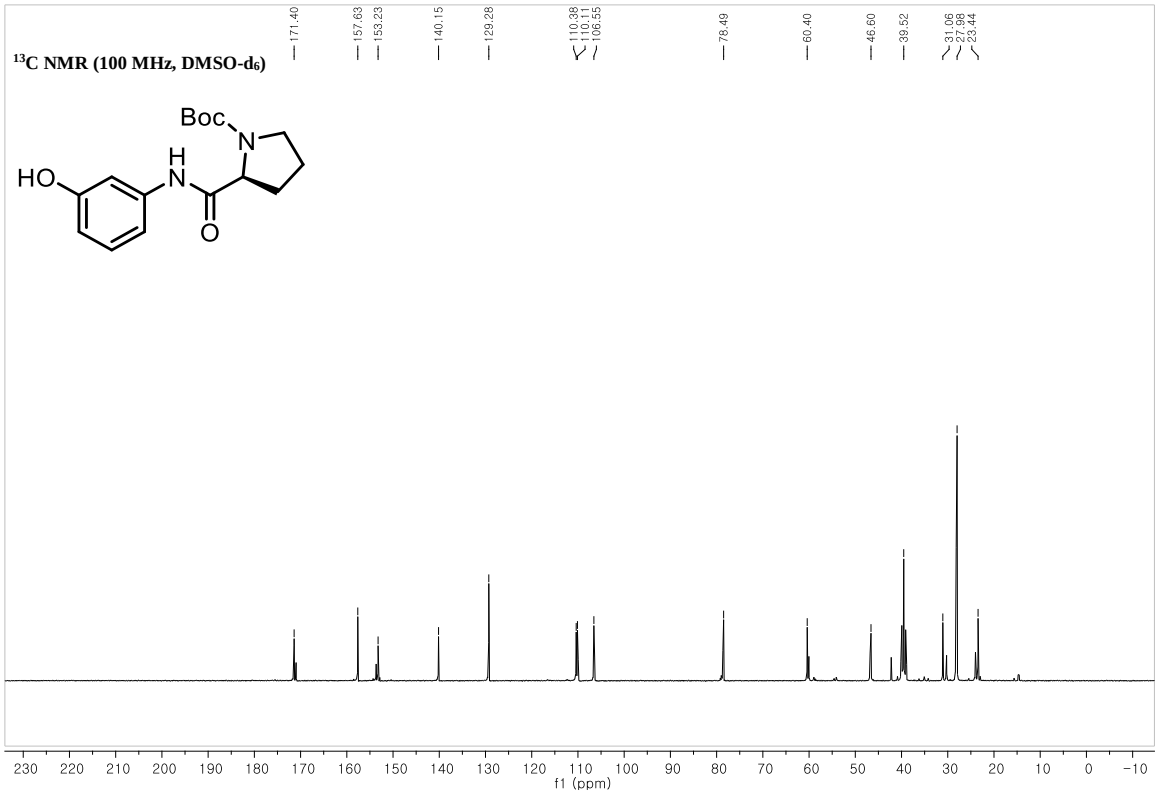
Compound 3c


^{1}H NMR (400 MHz, DMSO-d$_6$)
Boc
N
H
N
O
HO
9.68
9.16
7.37
7.34
6.70
6.67
4.22
4.21
4.19
4.15
4.14
4.13
4.12
3.39
3.39
3.35
3.33
3.31
2.50
1.90
1.86
1.84
1.82
1.81
1.78
1.39
1.28
0.99
0.98
1.96
1.93
0.96
1.01
1.16
0.99
2.99
9.19
f1 (ppm)

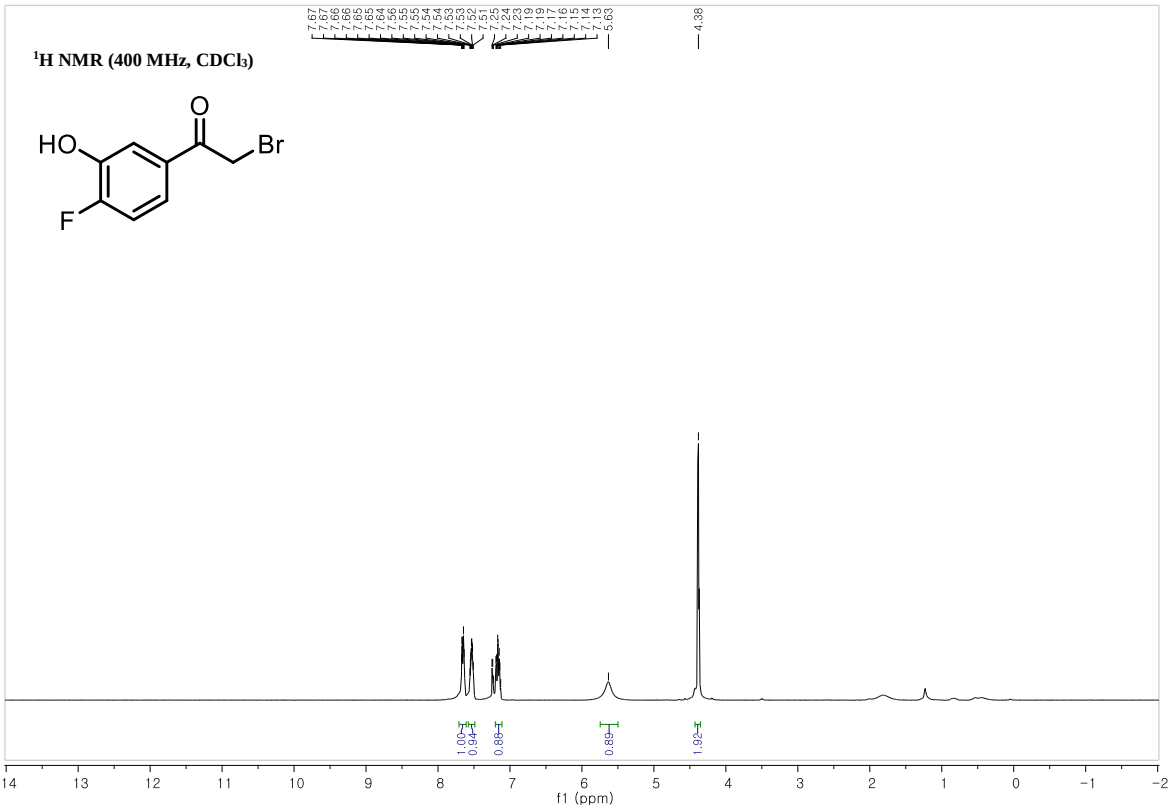

^{13}C NMR (100 MHz, DMSO-d$_6$)
Boc
N
H
N
O
HO
170.76
153.28
130.70
121.02
115.02
78.38
60.27
46.56
39.52
31.03
30.23
27.97
23.96
23.39
f1 (ppm)

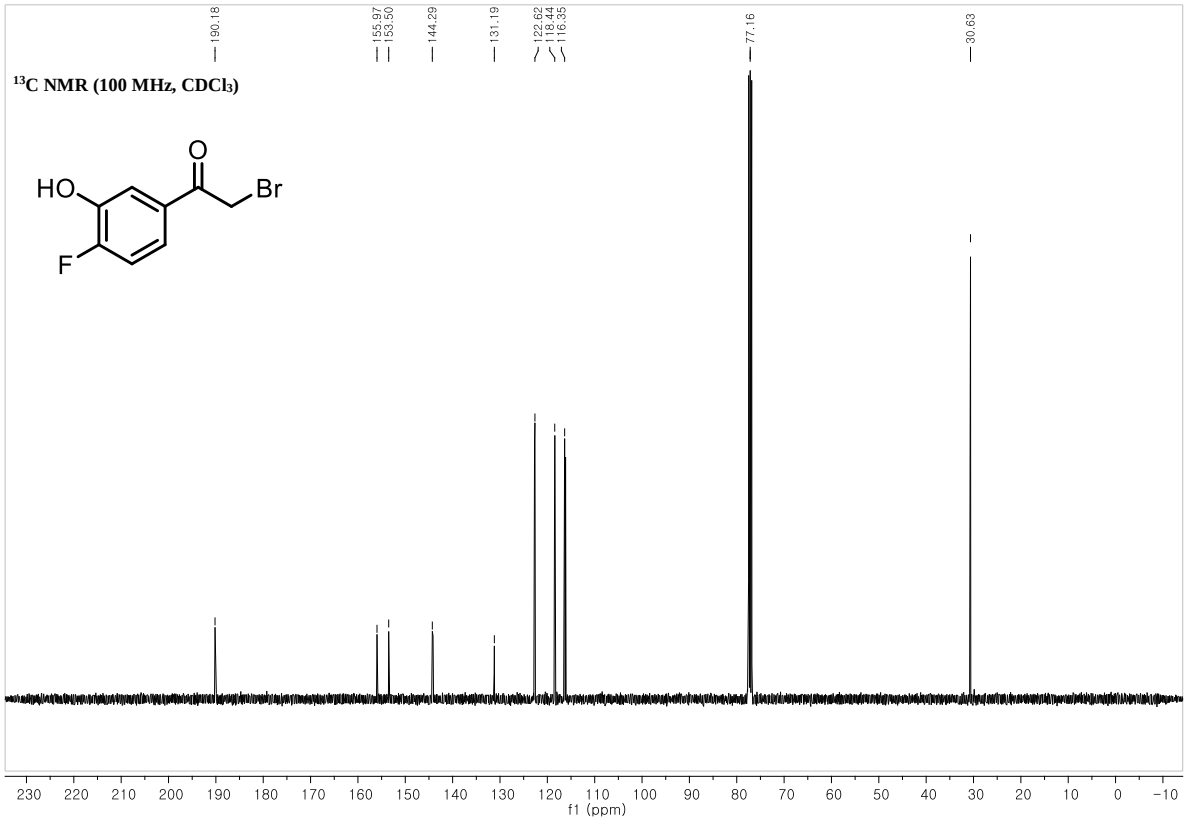
Compound 3d

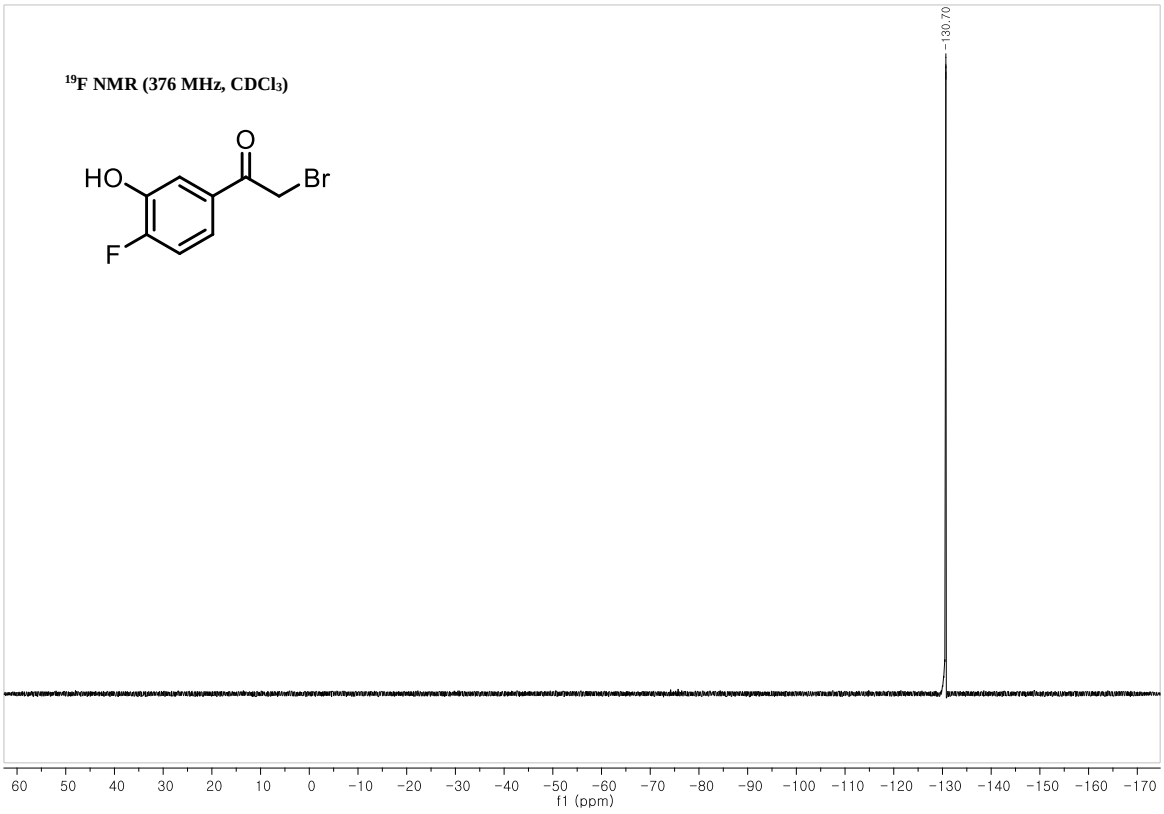

9.83
9.36
7.18
7.08
7.06
7.04
6.96
6.94
6.45
6.43
4.24
4.22
4.18
4.17
4.16
4.15
3.37
3.33
3.32
2.50
2.17
1.86
1.84
1.82
1.81
1.27
1H NMR (400 MHz, DMSO-d6)
Boc
N
H
N
HO
O
1.00
0.96
0.95
0.92
0.92
0.96
0.95
0.82
1.11
1.25
3.14
9.27
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1
f1 (ppm)


171.40
157.63
153.23
140.15
129.28
110.88
110.11
106.55
78.49
60.40
46.60
39.52
31.06
27.98
23.44
13C NMR (100 MHz, DMSO-d6)
Boc
N
H
N
HO
O
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)

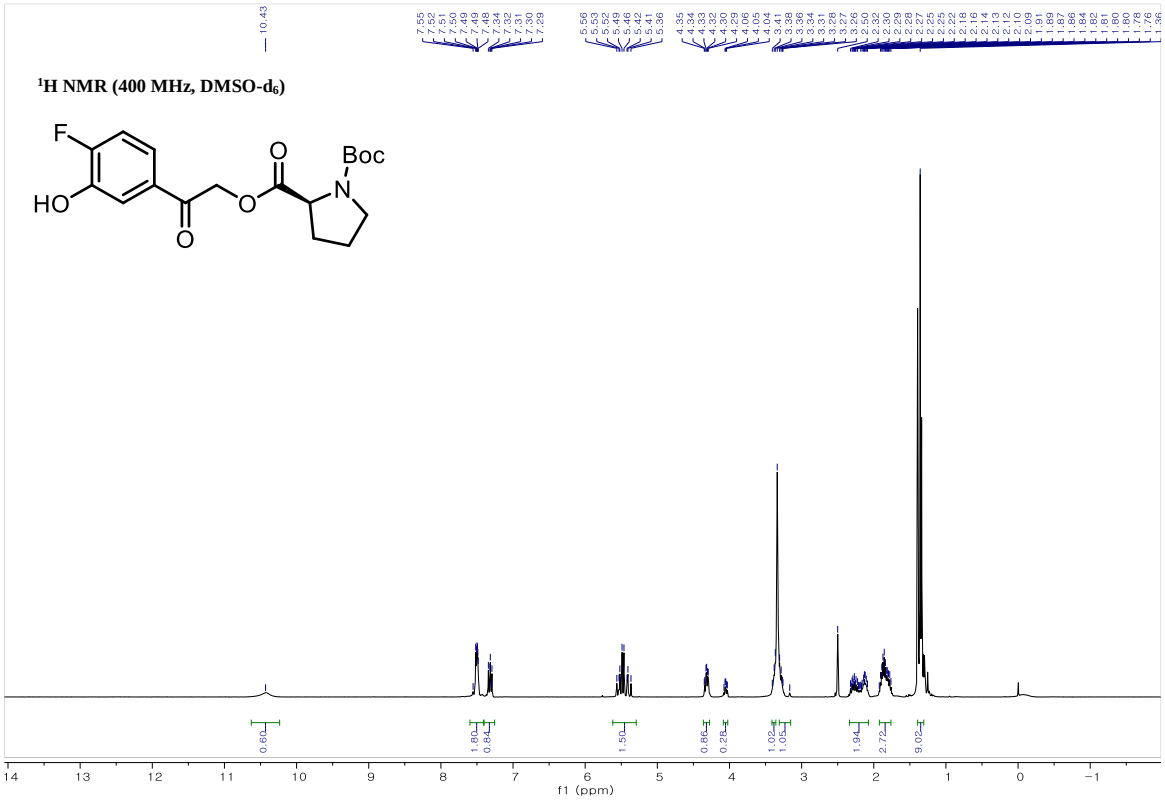
Compound 5a


7.67
7.67
7.66
7.66
7.65
7.65
7.64
7.56
7.55
7.55
7.54
7.54
7.53
7.53
7.52
7.51
7.25
7.24
7.23
7.19
7.19
7.17
7.16
7.15
7.14
7.13
5.63
4.38
1H NMR (400 MHz, CDCl3)
O
HO
Br
F
1.00
0.94
0.88
0.89
1.92
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2
f1 (ppm)

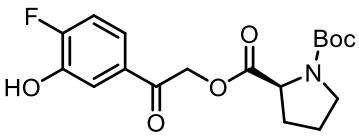

190.18
155.97
153.50
144.29
131.19
122.62
118.44
116.35
77.16
30.63
13C NMR (100 MHz, CDCl3)
O
HO
Br
F
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)


19F NMR (376 MHz, CDCl3)
HO
F
O
Br
-130.70
f1 (ppm)

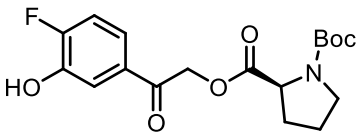
Compound 6a


1H NMR (400 MHz, DMSO-d6)
F
HO
O
O
O
N
Boc
10.43
f1 (ppm)

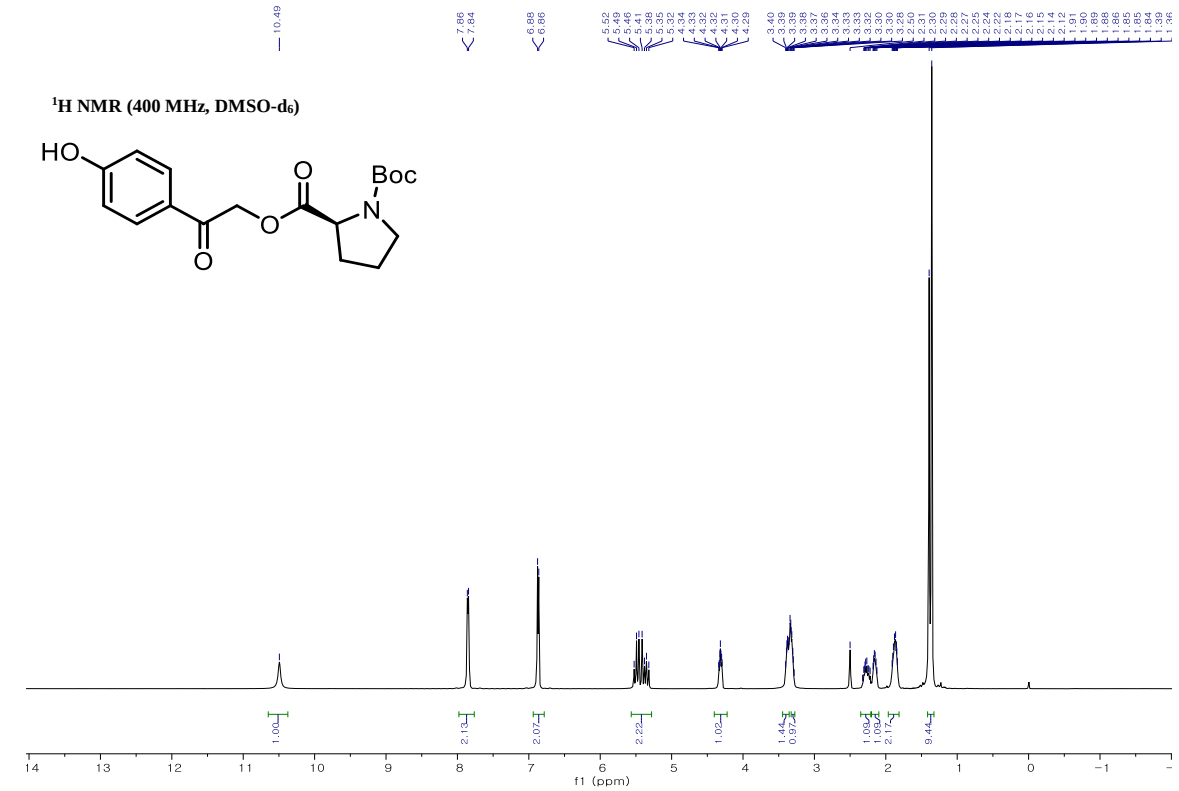
^{13}C NMR (100 MHz, DMSO-d$_6$)

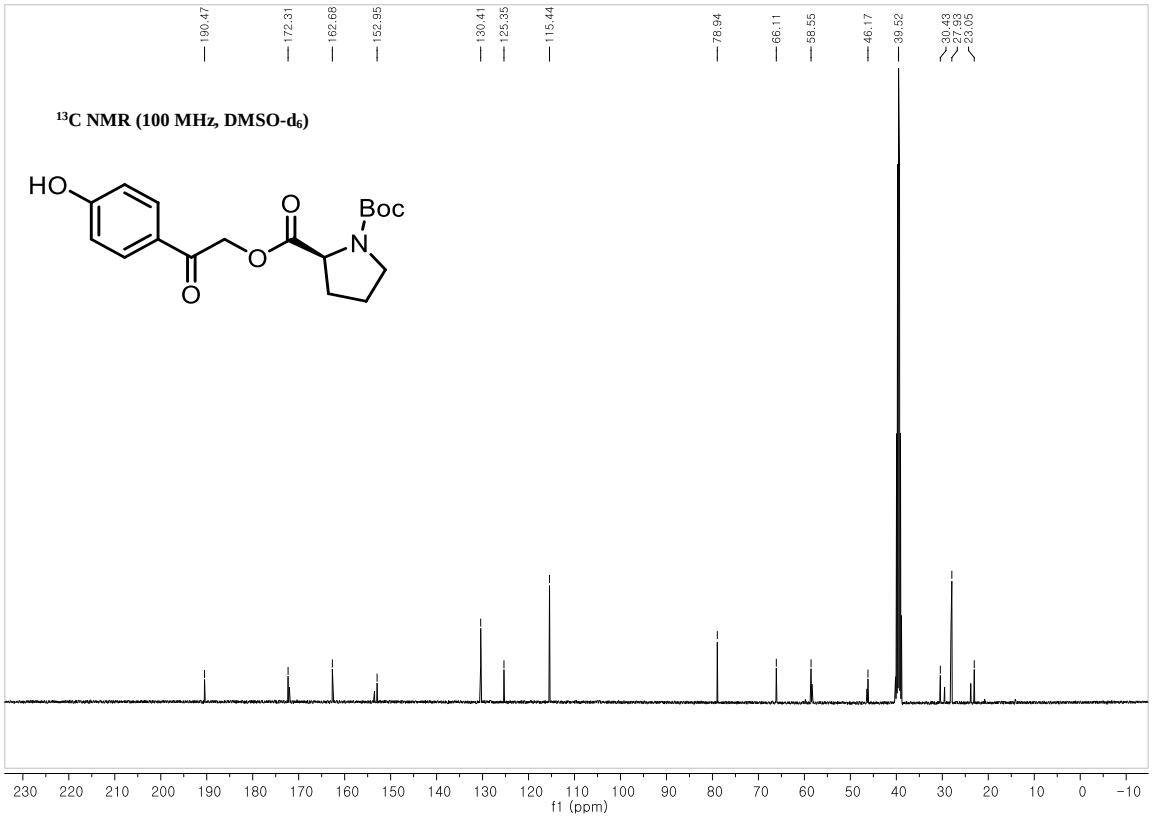


^{19}F NMR (376 MHz, DMSO-d$_6$)

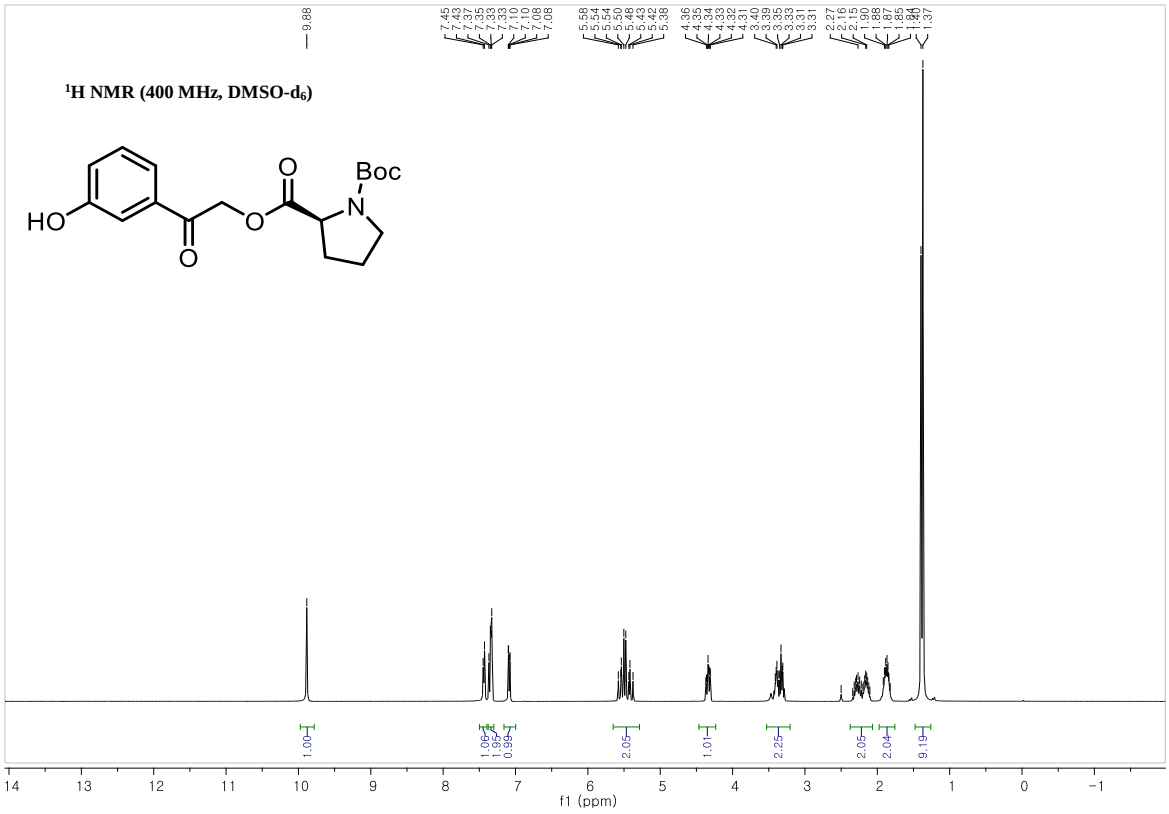


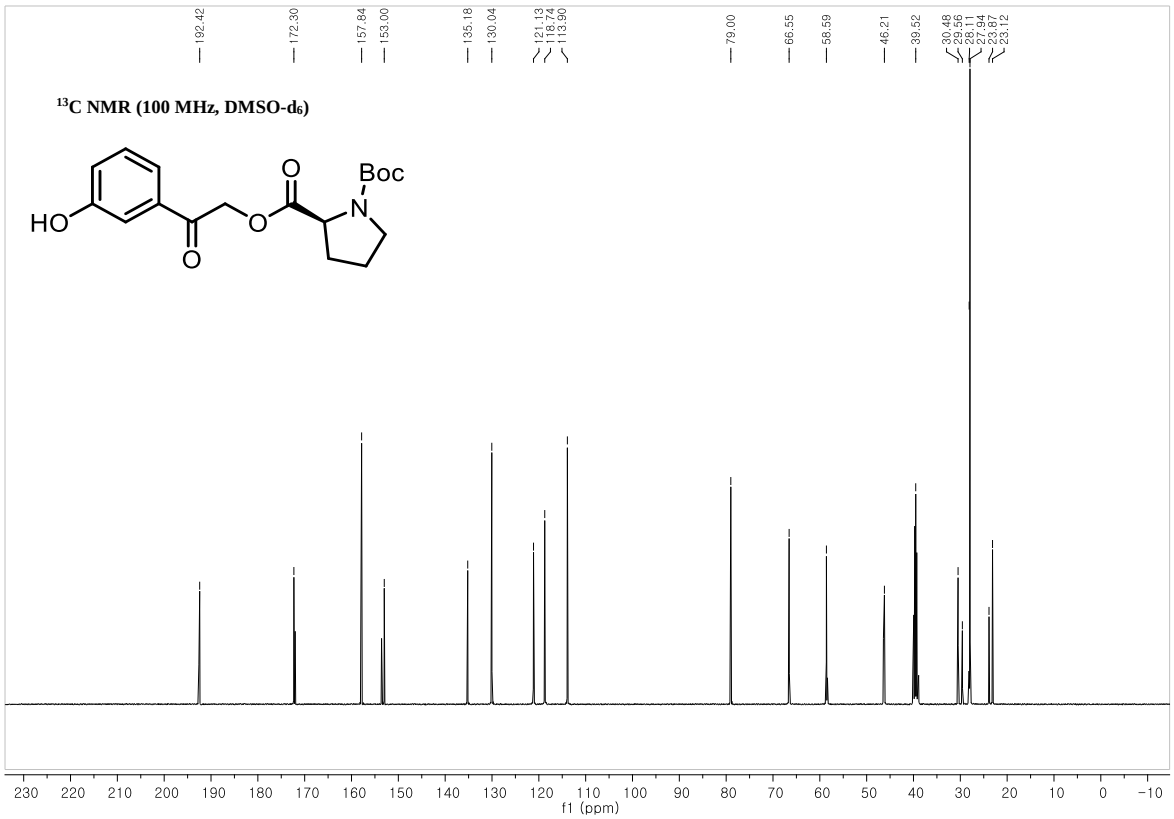
Compound 6b


^{1}H NMR (400 MHz, DMSO-d$_6$)
HO
O
Boc
N
O
O
f1 (ppm)

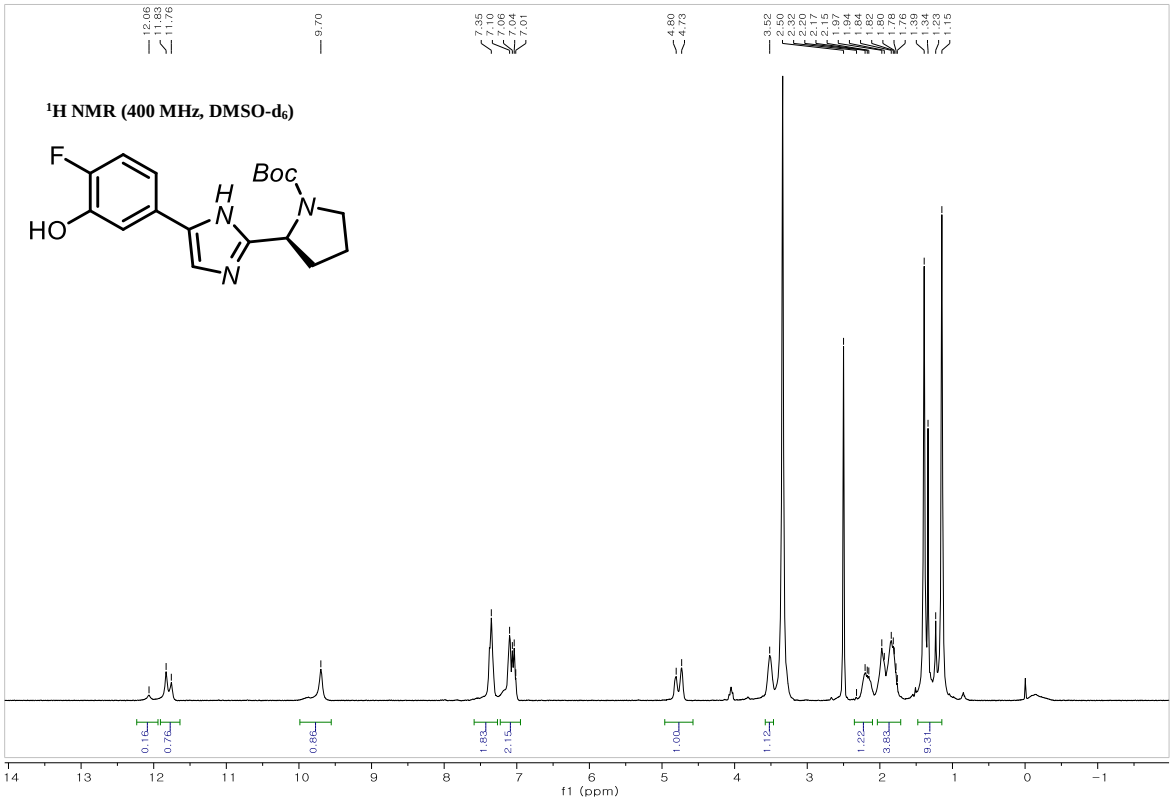

^{13}C NMR (100 MHz, DMSO-d$_6$)
HO
O
Boc
N
O
O
f1 (ppm)

Compound 6c

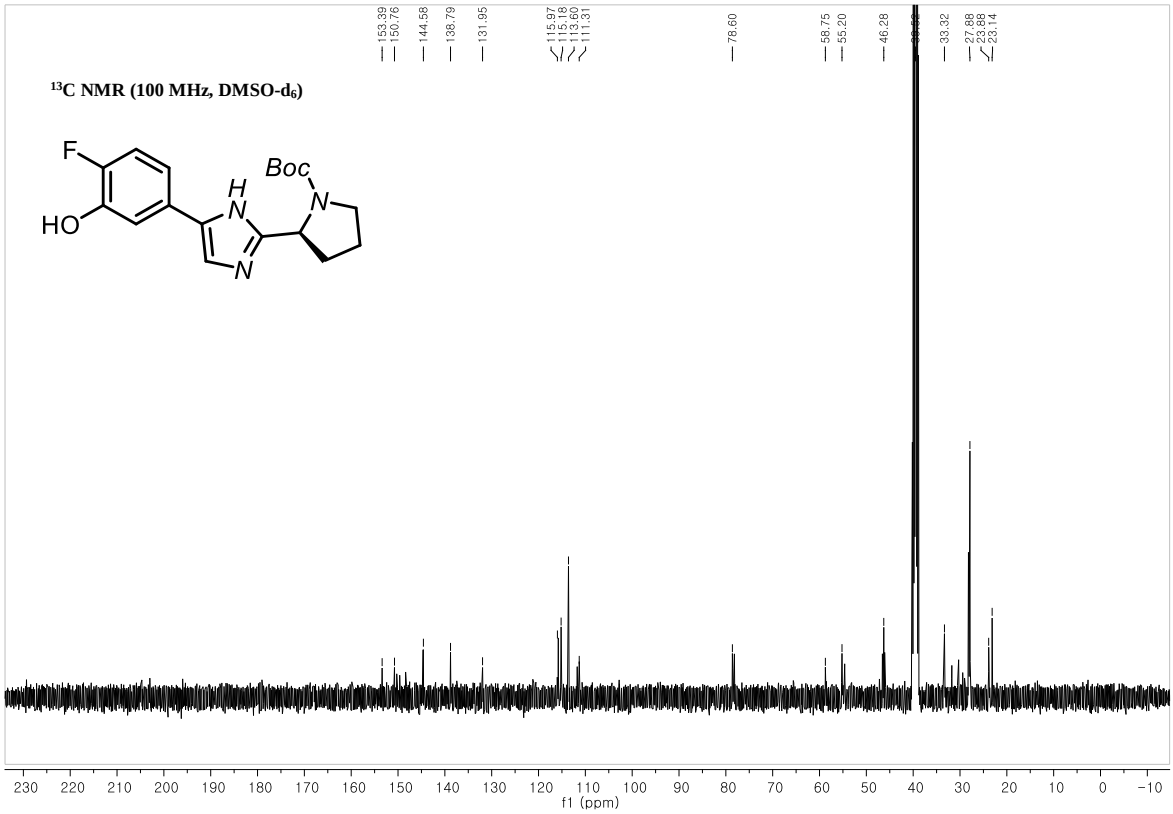

9.88
7.45
7.43
7.37
7.35
7.33
7.13
7.10
7.08
5.58
5.54
5.50
5.48
5.43
5.42
5.38
4.36
4.35
4.34
4.33
4.32
4.31
3.40
3.39
3.35
3.33
3.31
3.31
2.27
2.16
2.15
1.90
1.88
1.87
1.85
1.37
1H NMR (400 MHz, DMSO-d6)
HO
O
O
O
N
Boc
1.00
1.06
1.95
0.99
2.05
1.01
2.25
2.05
2.04
9.19
f1 (ppm)


192.42
172.30
157.84
153.00
135.18
130.04
121.13
118.74
113.90
79.00
66.55
58.59
46.21
39.52
30.48
29.56
28.11
27.94
23.37
23.12
13C NMR (100 MHz, DMSO-d6)
HO
O
O
O
N
Boc
f1 (ppm)

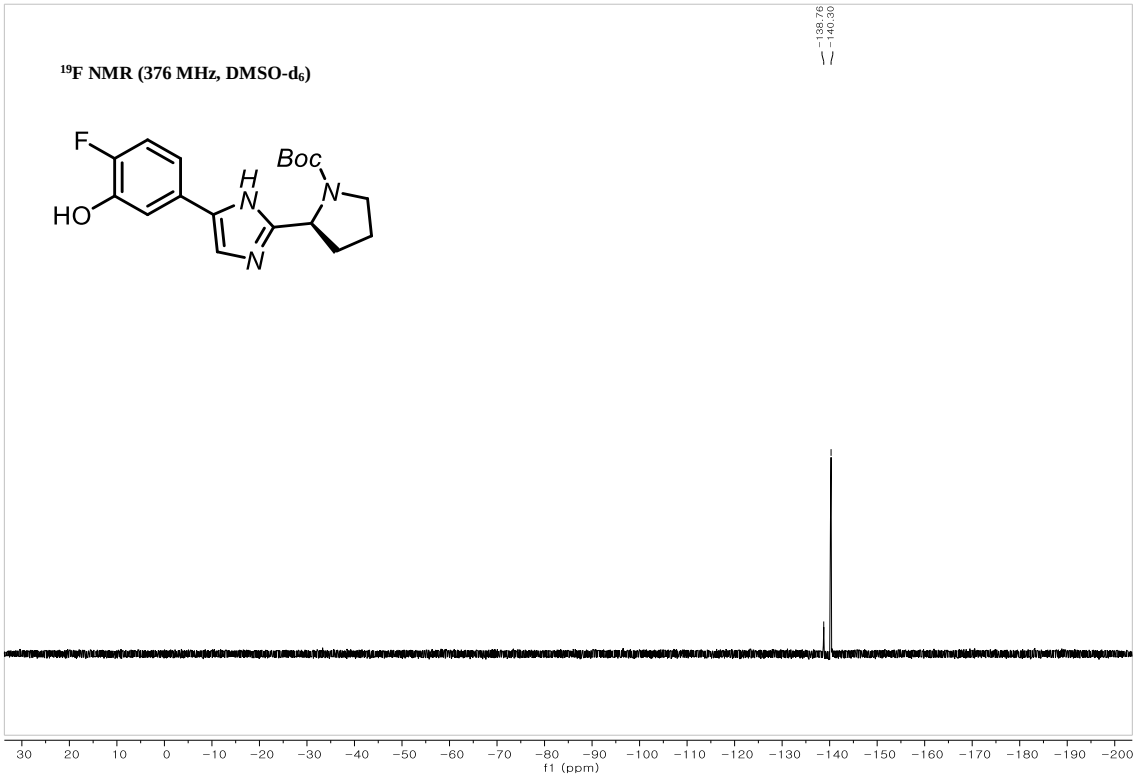
Compound 7a



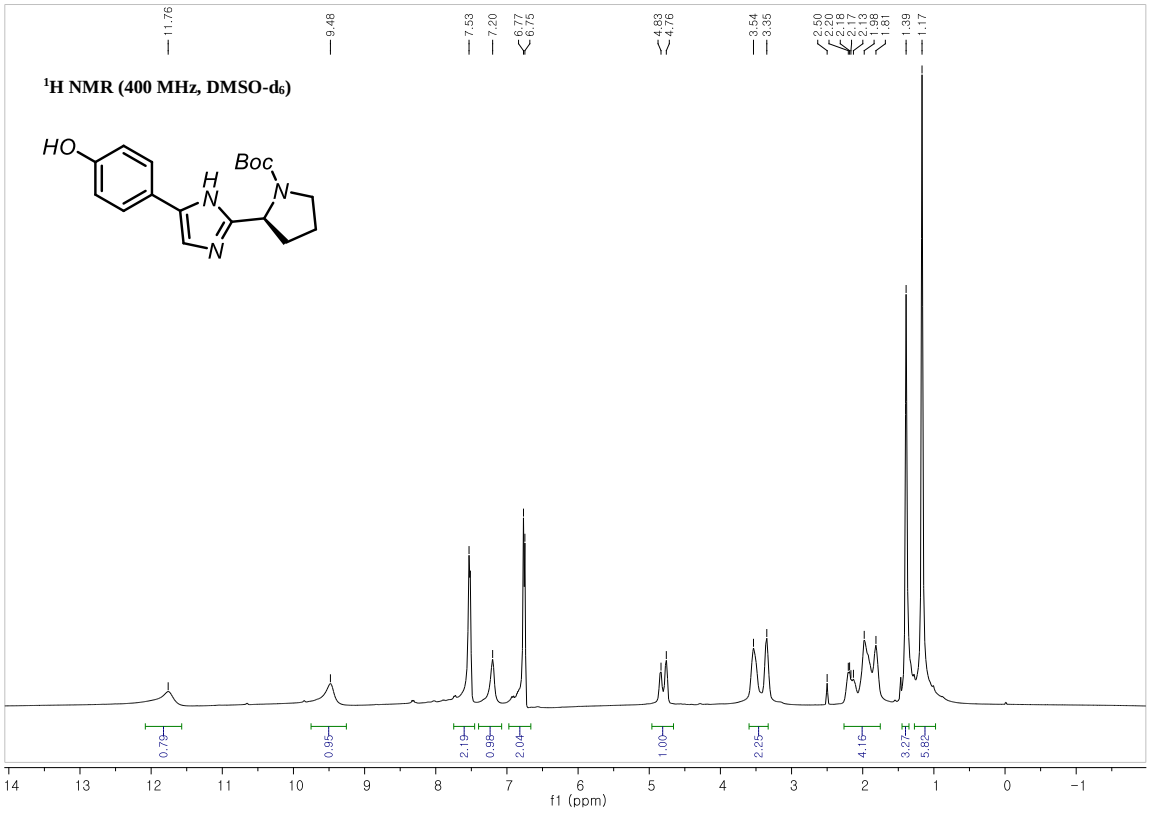
^{1}H NMR (400 MHz, DMSO-d_6)

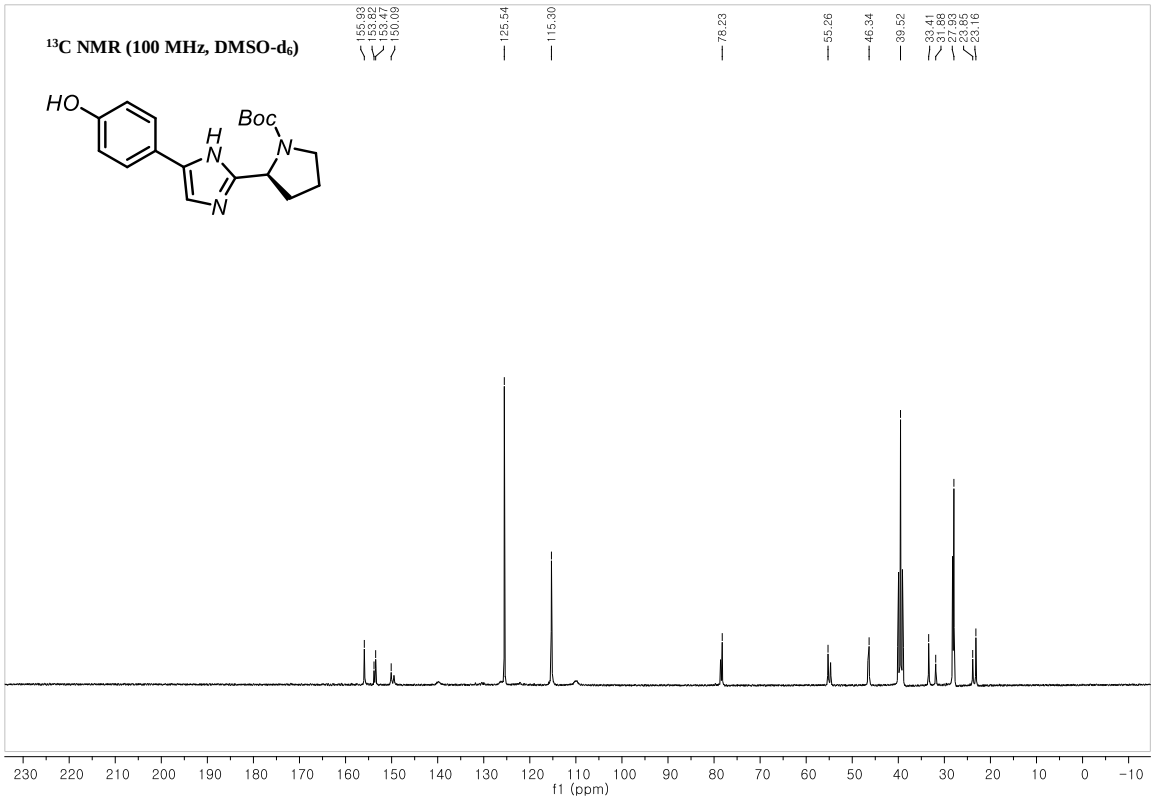


^{13}C NMR (100 MHz, DMSO-d_6)

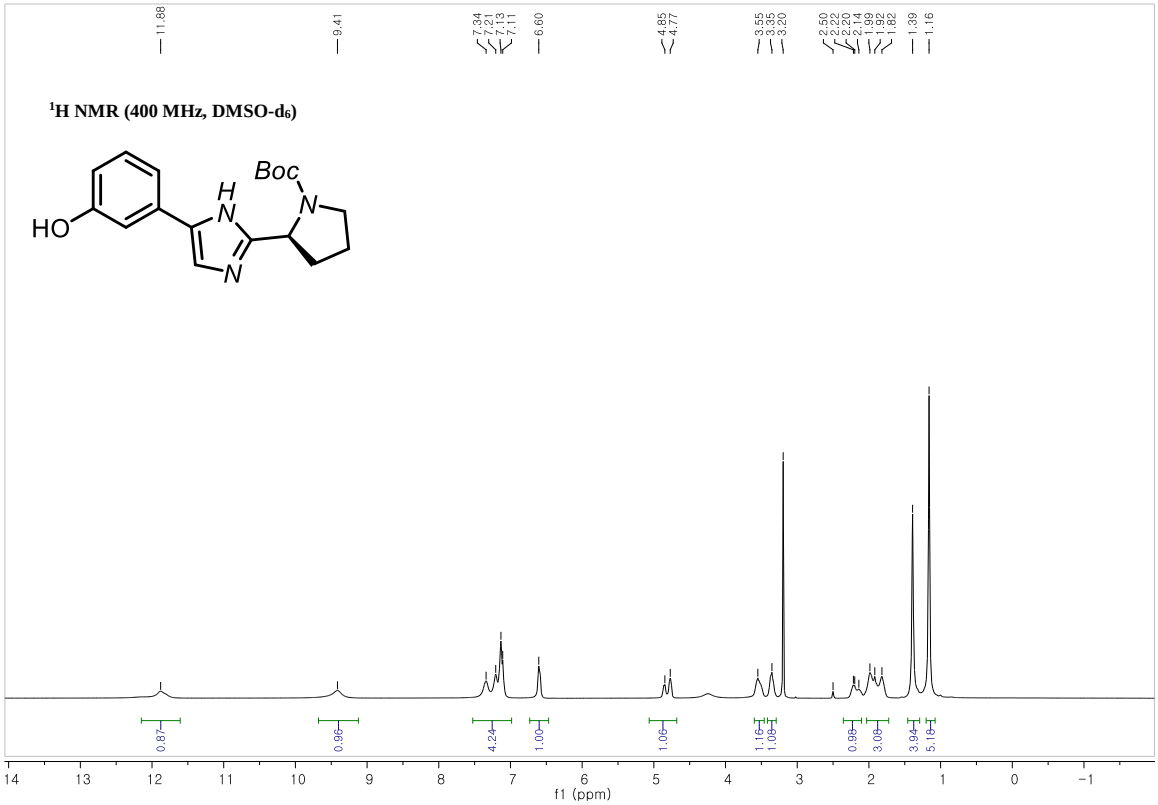

19F NMR (376 MHz, DMSO-d6)
F
HO
H
N
N
Boc
N
-138.76
-140.30
30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

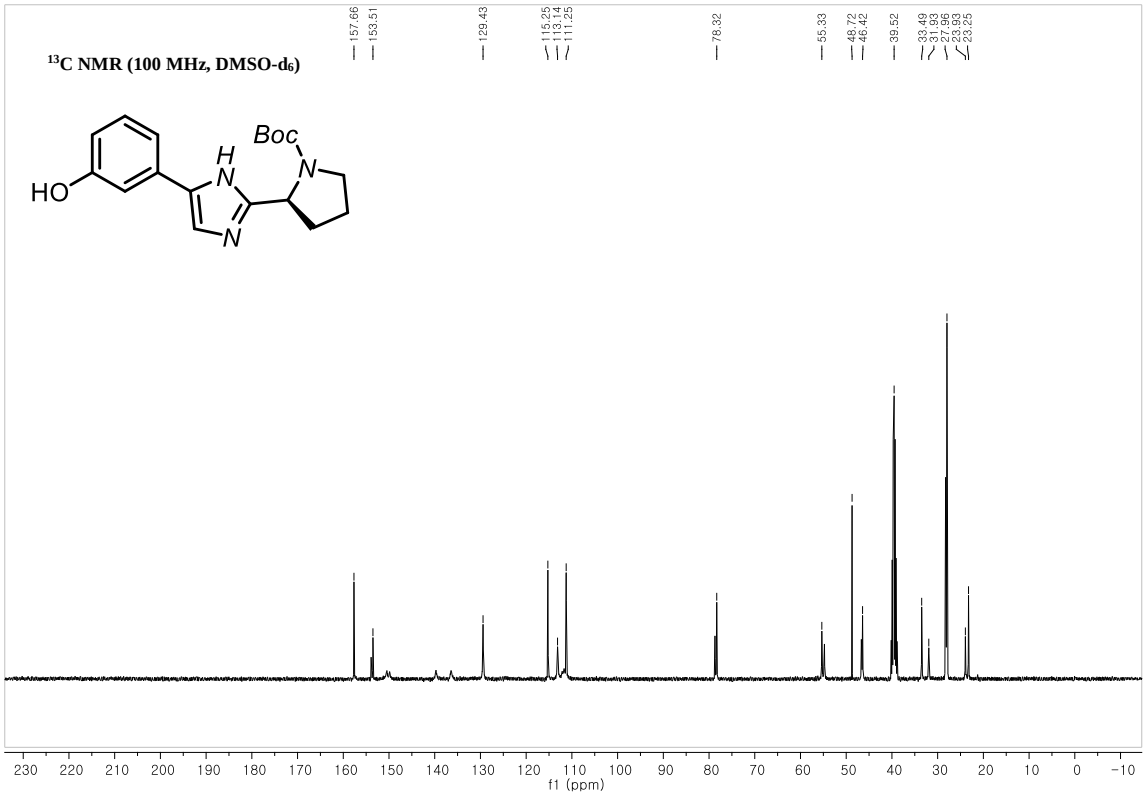
Compound 7b


11.76
9.48
7.53
7.20
6.77
6.75
4.83
4.76
3.54
3.35
2.50
2.20
2.18
2.17
2.13
1.98
1.81
1.39
1.17
1H NMR (400 MHz, DMSO-d6)
HO
H
N
N
Boc
N
0.79
0.95
2.19
0.98
2.04
1.00
2.25
4.16
3.27
5.82
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)

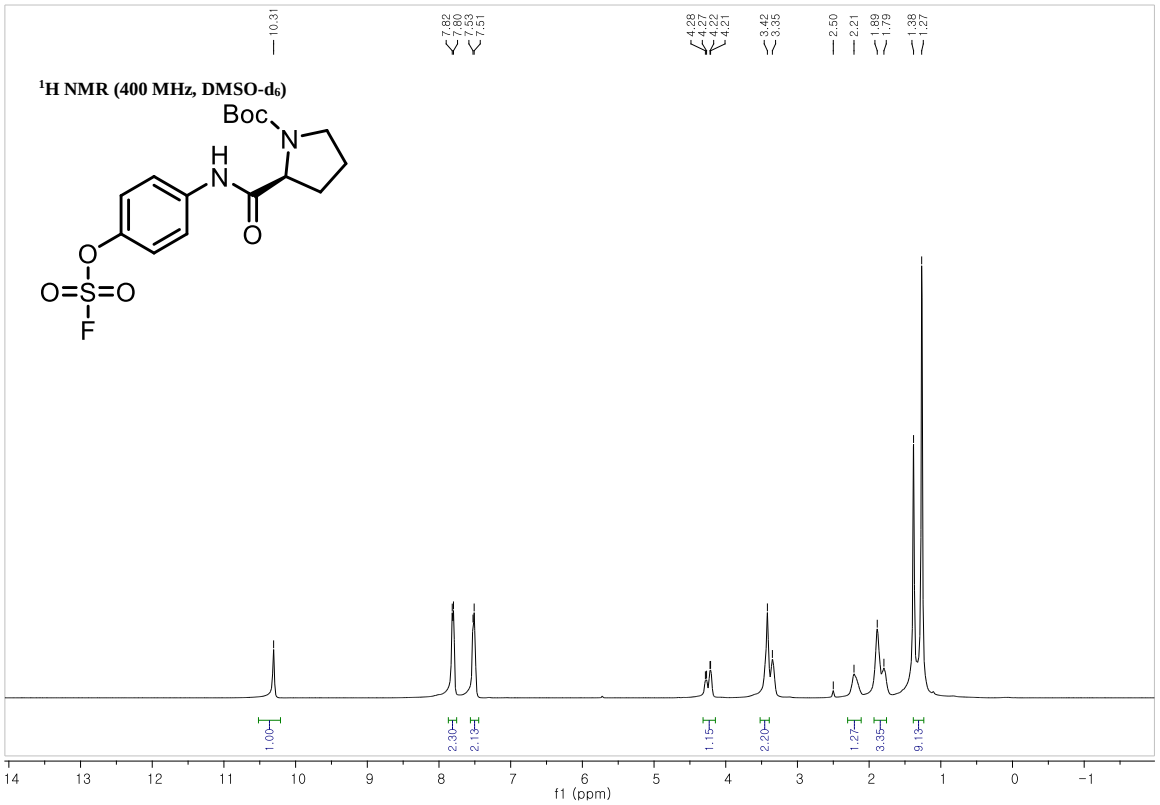

13C NMR (100 MHz, DMSO-d6)
155.93
153.82
153.47
150.09
125.54
115.30
78.23
55.26
46.34
39.52
33.41
31.88
27.93
23.85
23.16
HO
Boc
H
N
N
N
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)

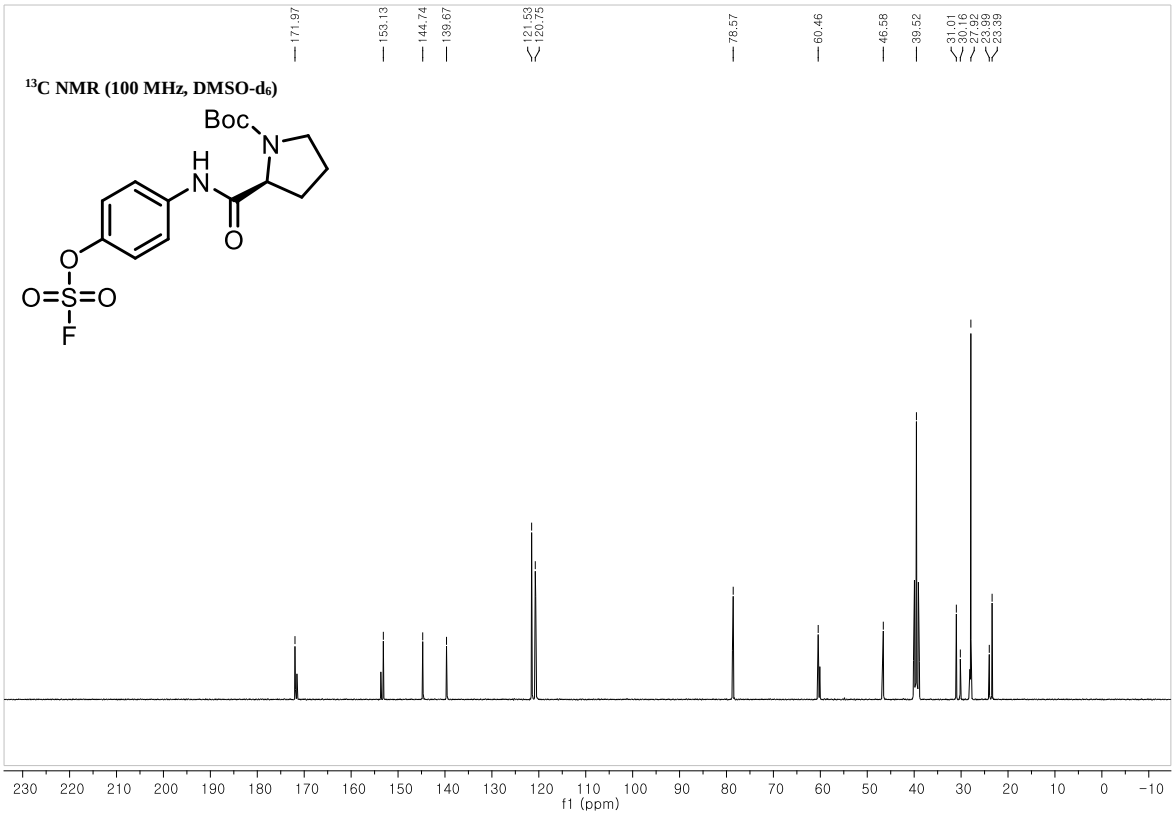
Compound 7c

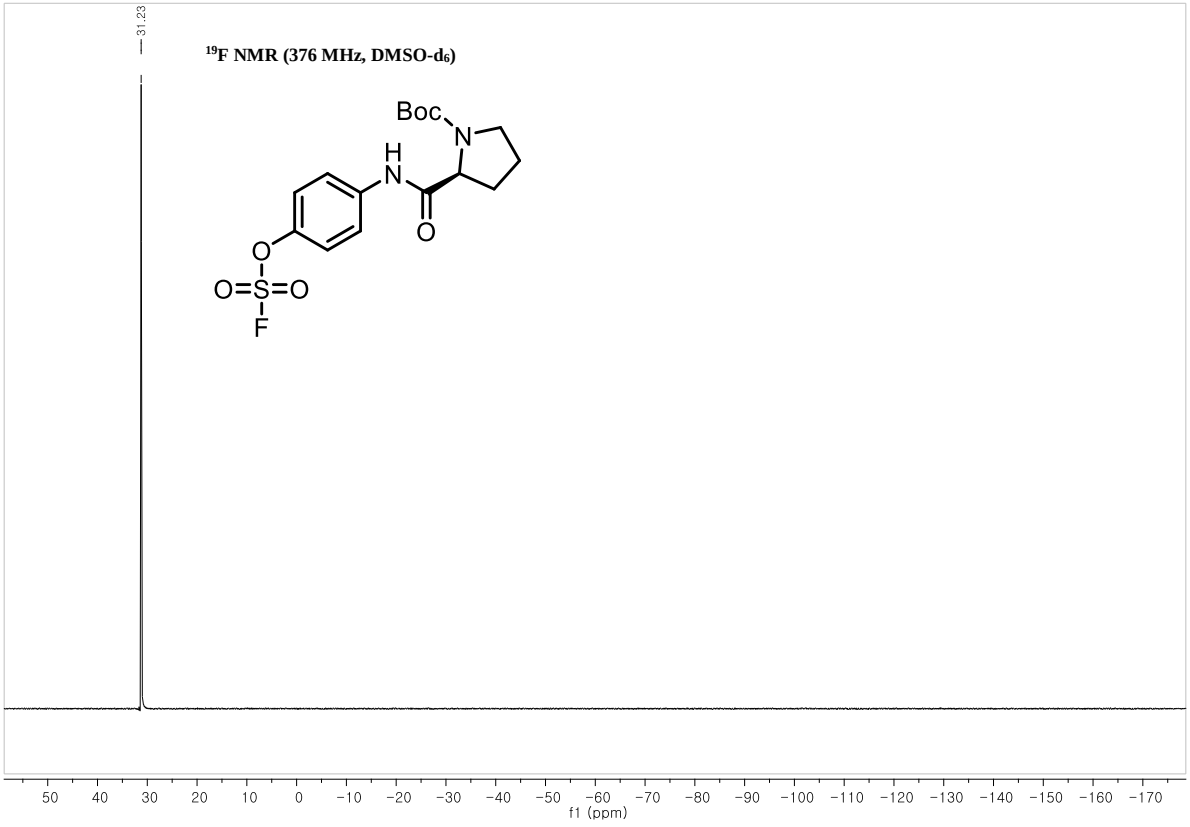

11.88
9.41
7.34
7.21
7.13
7.11
6.60
4.85
4.77
3.55
3.35
3.20
2.50
2.22
2.20
2.14
1.99
1.92
1.82
1.39
1.16
1H NMR (400 MHz, DMSO-d6)
HO
Boc
H
N
N
N
0.87
0.96
4.24
1.00
1.00
1.16
1.05
0.98
3.05
3.94
5.18
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1
f1 (ppm)


157.66
153.51
129.43
115.25
113.44
111.25
78.32
55.33
49.72
46.42
39.52
33.49
31.93
27.96
23.93
23.25
13C NMR (100 MHz, DMSO-d6)
HO
H
N
N
Boc
N
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

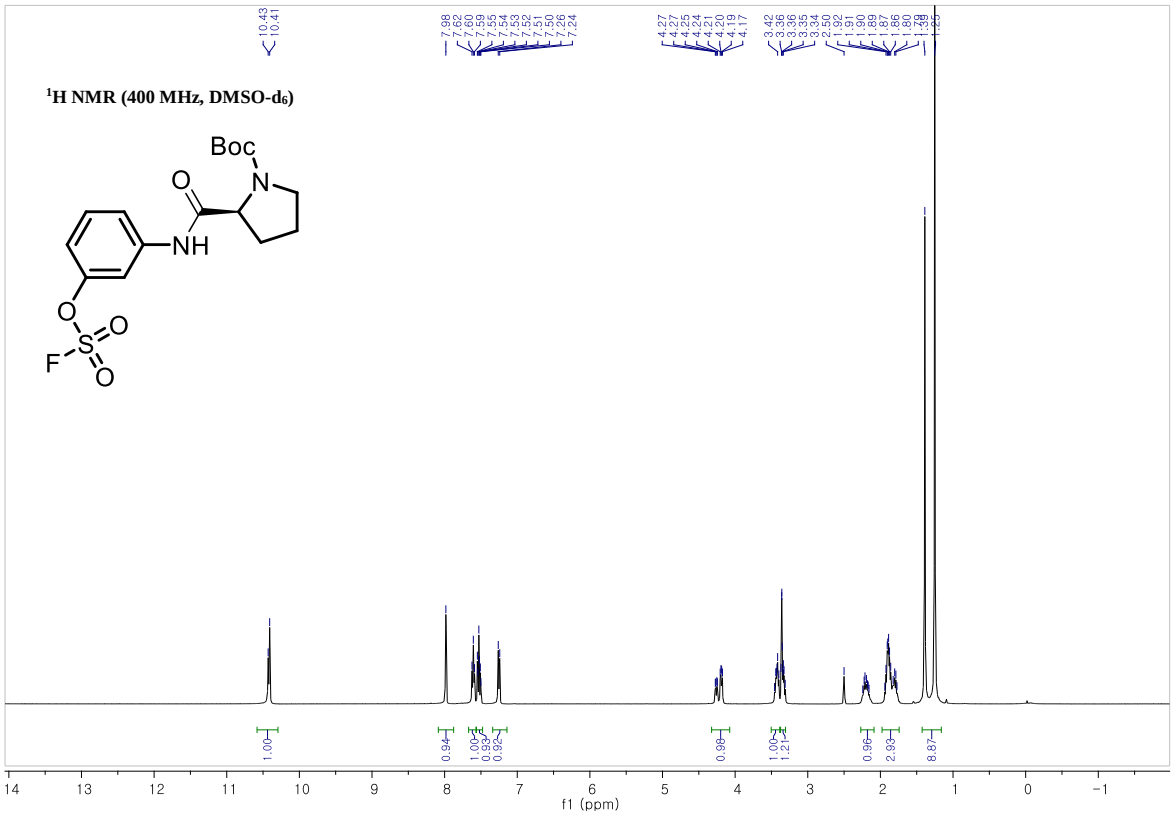
Compound 8a

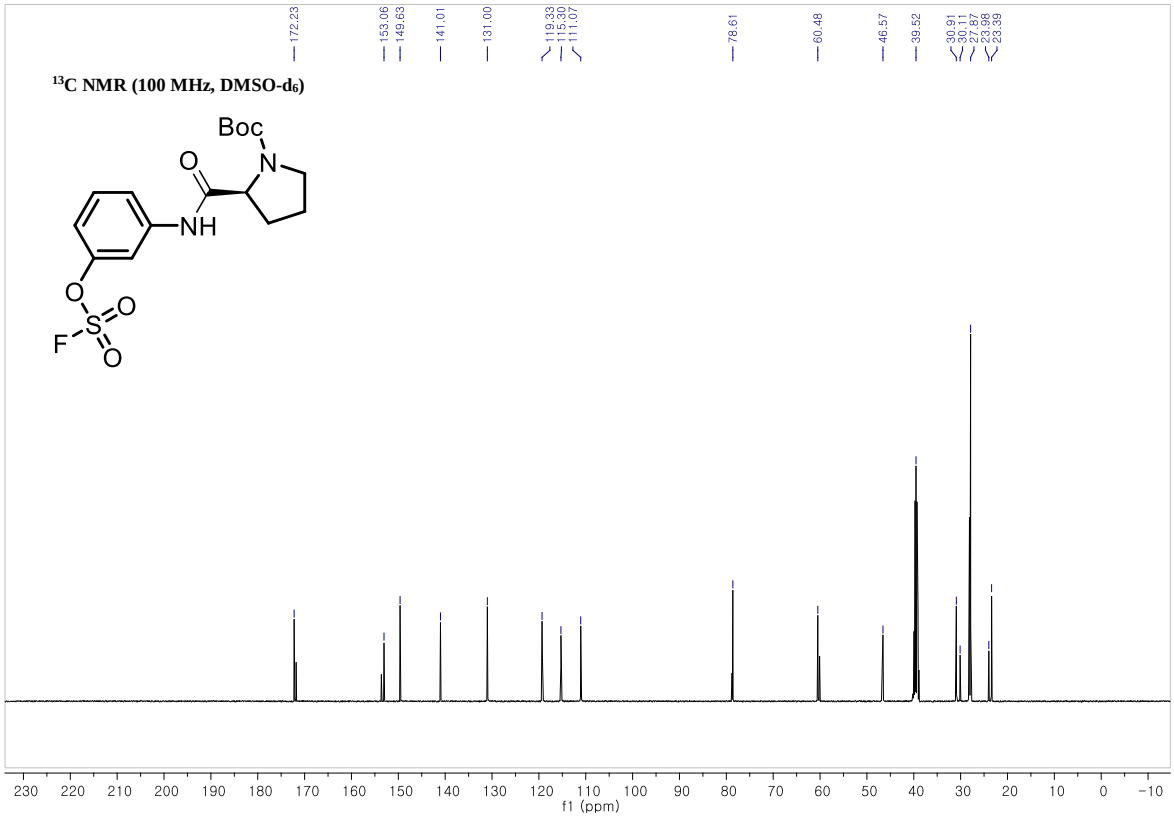

10.31
7.82
7.80
7.53
7.51
4.28
4.27
4.22
4.21
3.42
3.35
2.50
2.21
1.89
1.79
1.38
1.27
1H NMR (400 MHz, DMSO-d6)
Boc
N
H
N
O
O
O=S=O
F
1.00
2.30
2.13
1.15
2.20
1.27
3.35
9.13
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)

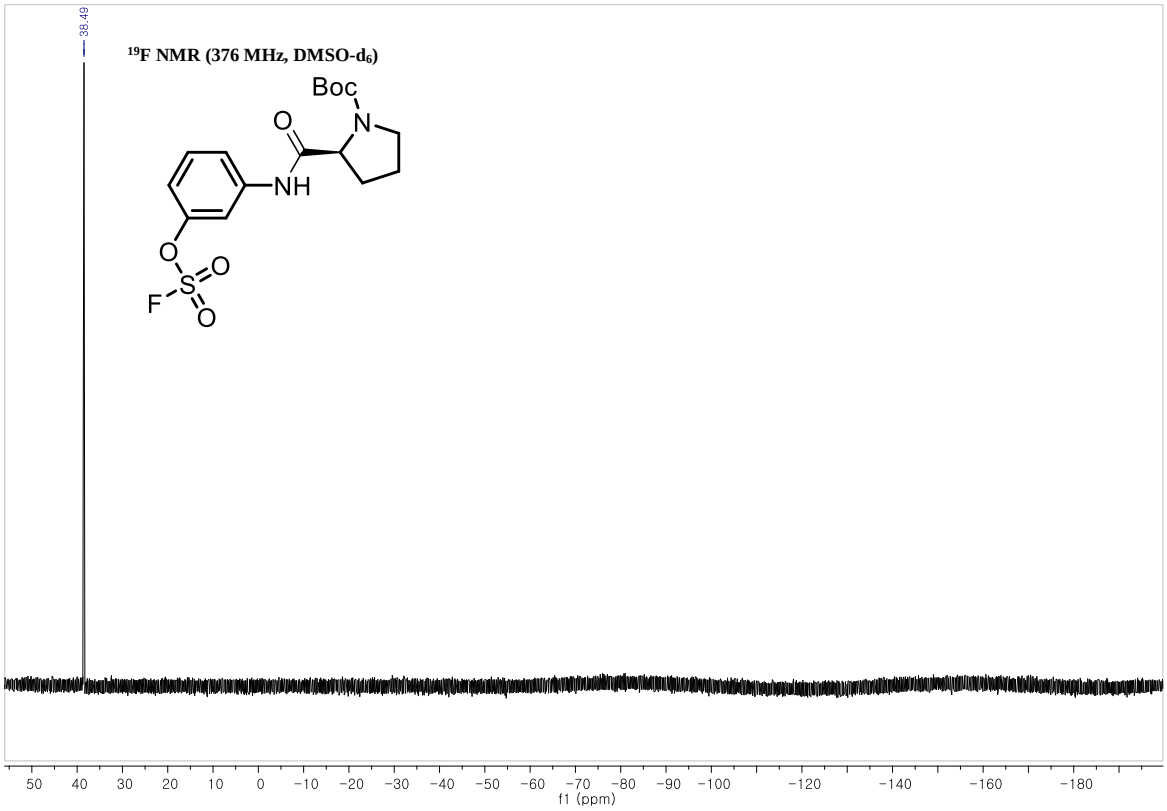

171.97
153.13
144.74
139.67
121.53
120.75
78.57
60.46
46.58
39.52
31.01
30.16
27.92
23.99
23.39
13C NMR (100 MHz, DMSO-d6)
Boc
N
H
N
O
O
O=S=O
F
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


31.23
19F NMR (376 MHz, DMSO-d6)
Boc
N
H
N
O
O
O=S=O
F
50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170
f1 (ppm)

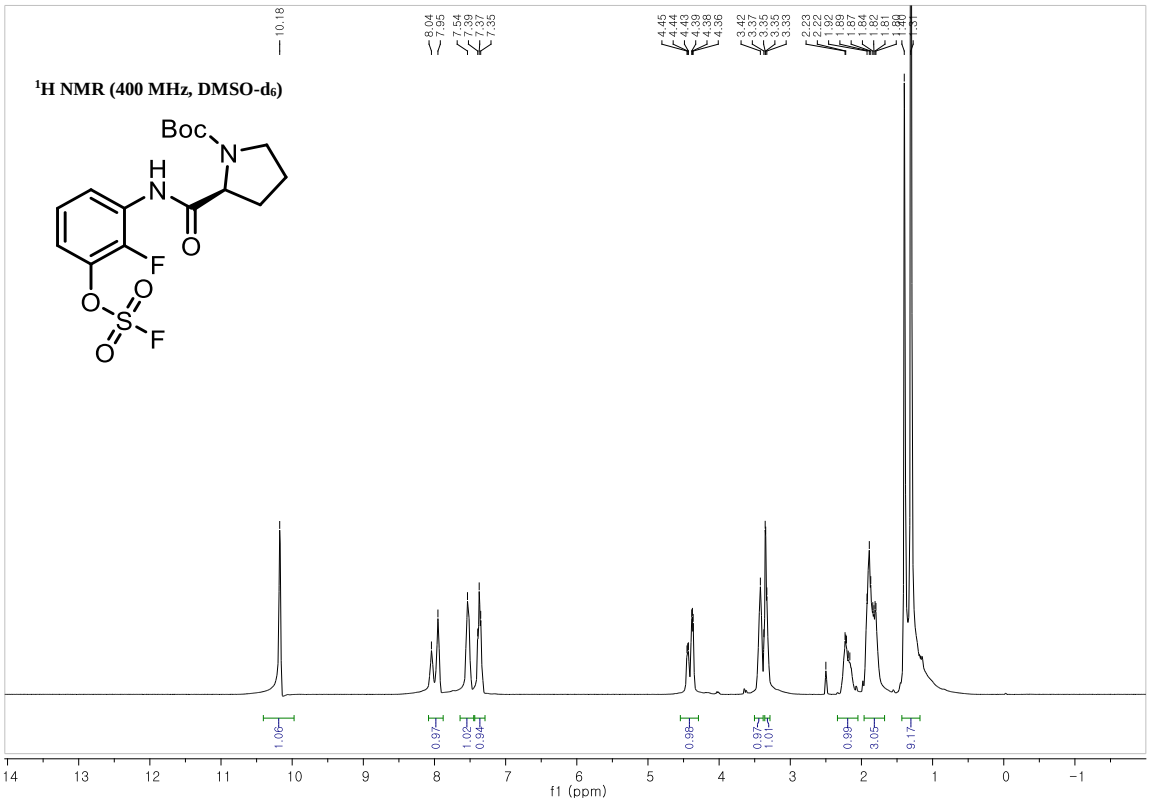
Compound 8b

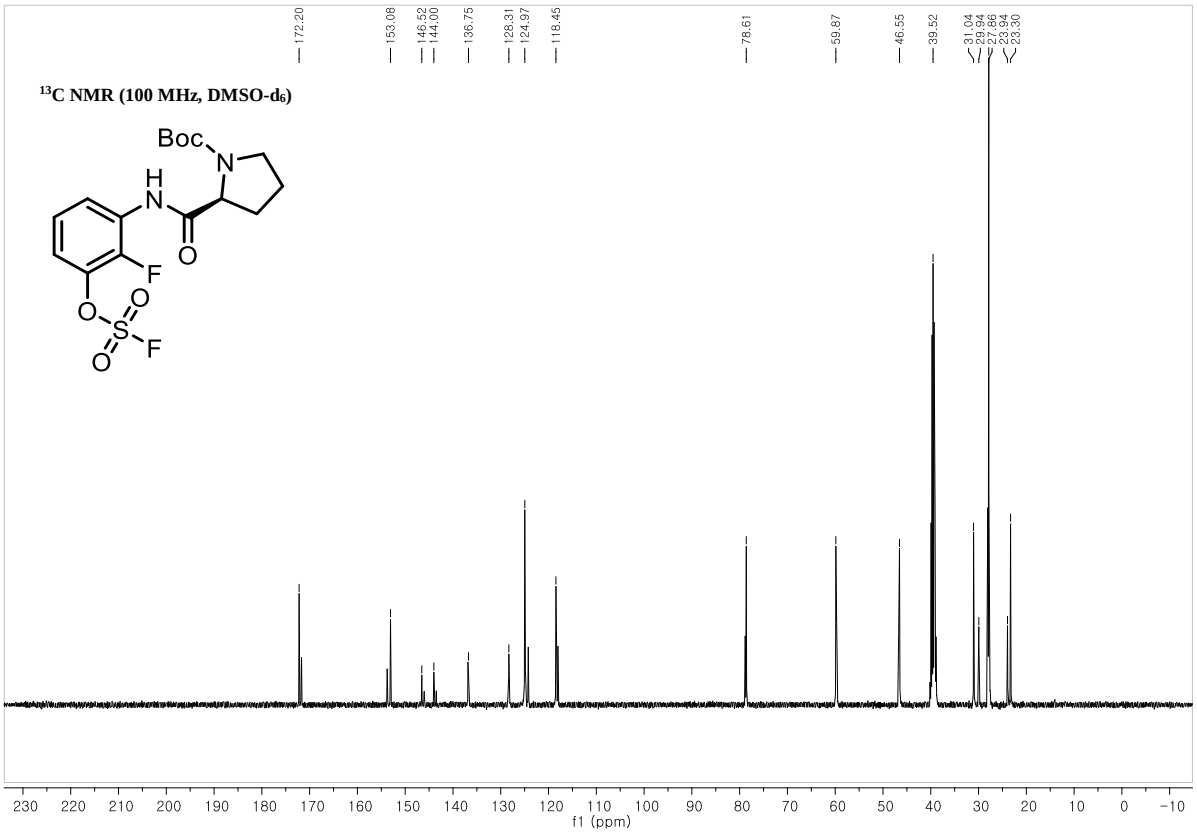

^{1}H NMR (400 MHz, DMSO-d$_6$)
Boc
N
O
NH
O
F
S
O
O
f1 (ppm)

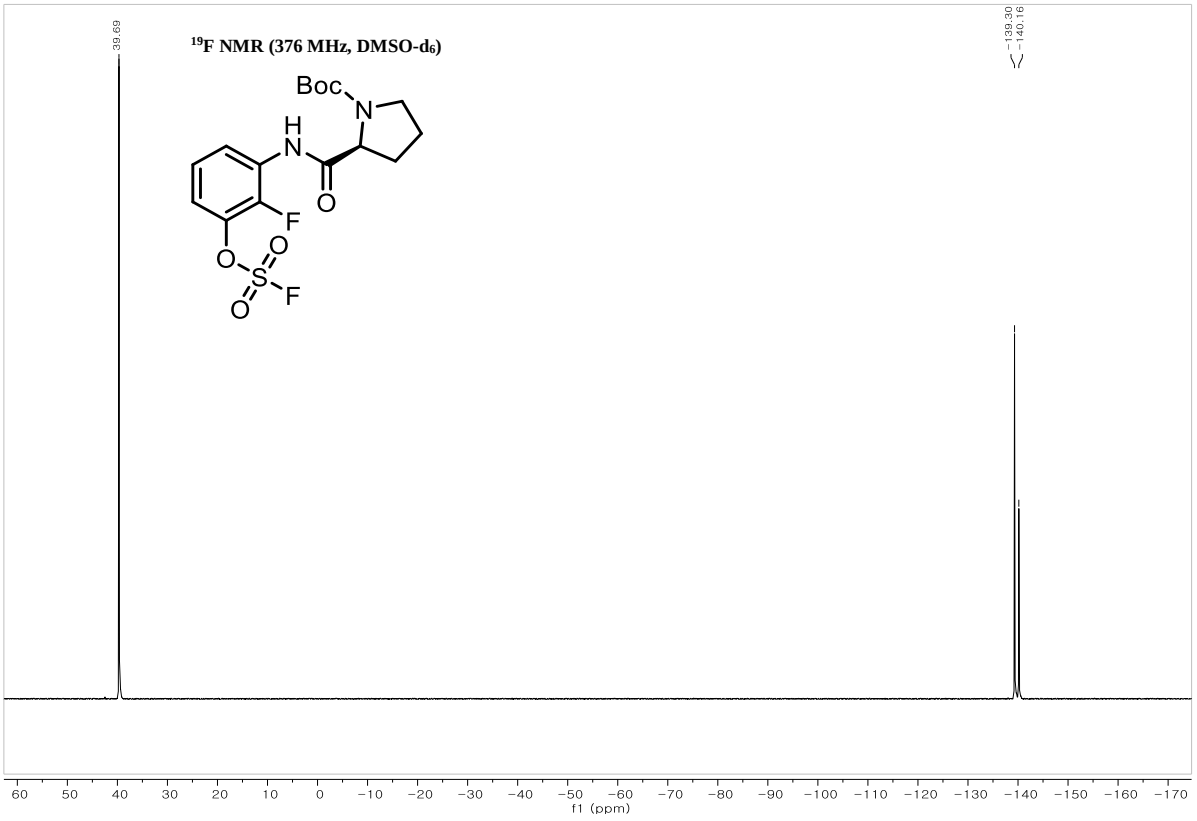

^{13}C NMR (100 MHz, DMSO-d$_6$)
Boc
N
O
NH
O
F
S
O
O
f1 (ppm)


38.49
19F NMR (376 MHz, DMSO-d6)
Boc
N
O
NH
O
S
O
F
O
50 40 30 20 10 0 −10 −20 −30 −40 −50 −60 −70 −80 −90 −100 −120 −140 −160 −180
f1 (ppm)

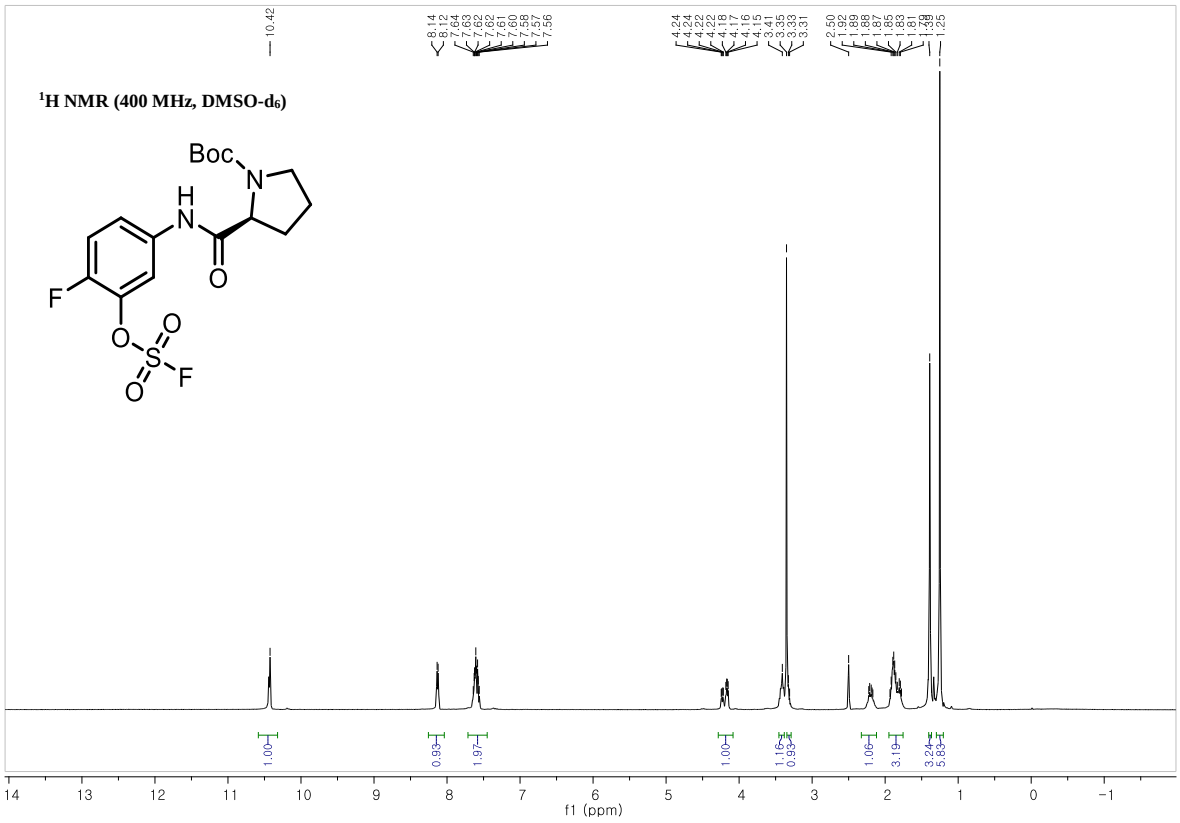
Compound 8c


10.18
8.04
7.95
7.54
7.39
7.37
7.35
4.45
4.44
4.43
4.39
4.38
4.36
3.42
3.37
3.35
3.35
3.33
2.23
2.22
1.92
1.89
1.87
1.84
1.82
1.81
1.31
1H NMR (400 MHz, DMSO-d6)
Boc
N
H
N
O
F
O
O
S
O
F
1.06
0.97
1.02
0.94
0.98
0.97
1.01
0.99
3.05
9.17
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1
f1 (ppm)

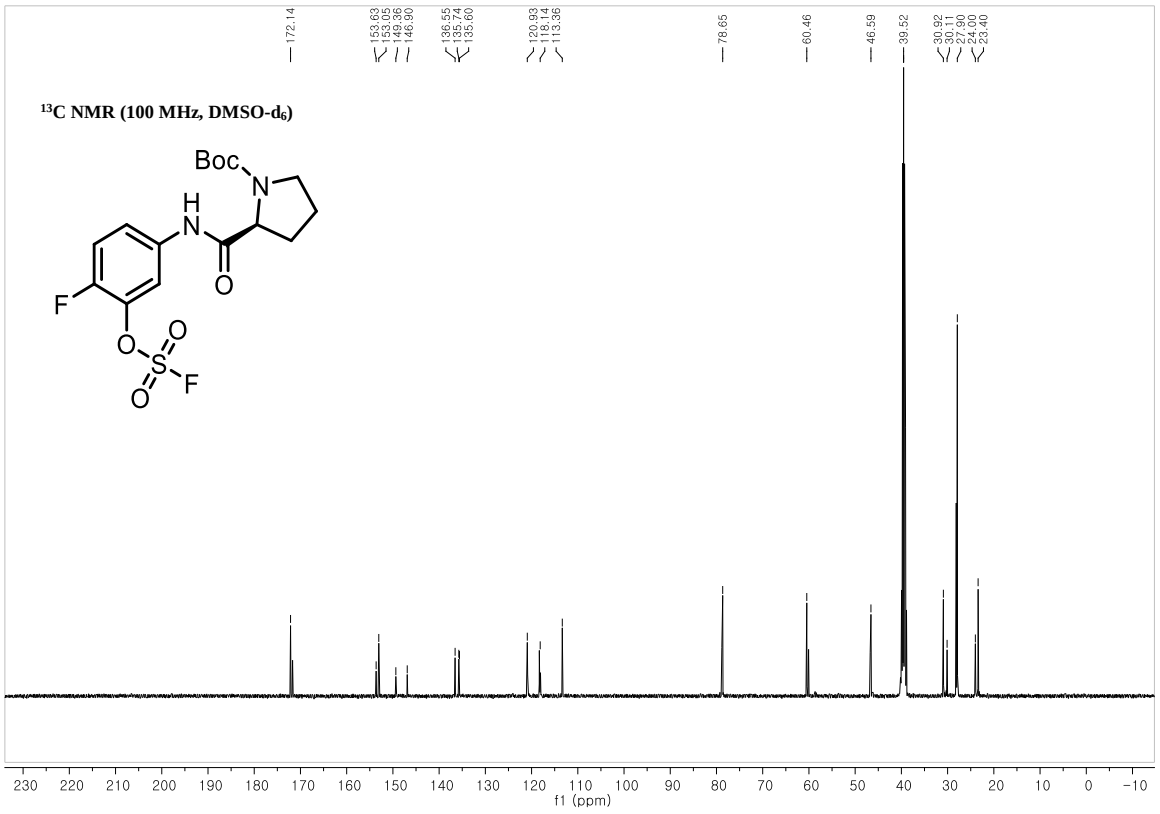

172.20
153.08
146.52
144.00
136.75
128.31
124.97
118.45
78.61
59.87
46.55
39.52
31.04
29.94
27.86
23.84
23.30
13C NMR (100 MHz, DMSO-d6)
Boc
N
H
N
O
F
O
O
S
O
O
F
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)


39.69
−139.30
−140.16
19F NMR (376 MHz, DMSO-d6)
Boc
N
H
N
O
F
O
O
S
O
O
F
60 50 40 30 20 10 0 −10 −20 −30 −40 −50 −60 −70 −80 −90 −100 −110 −120 −130 −140 −150 −160 −170
f1 (ppm)

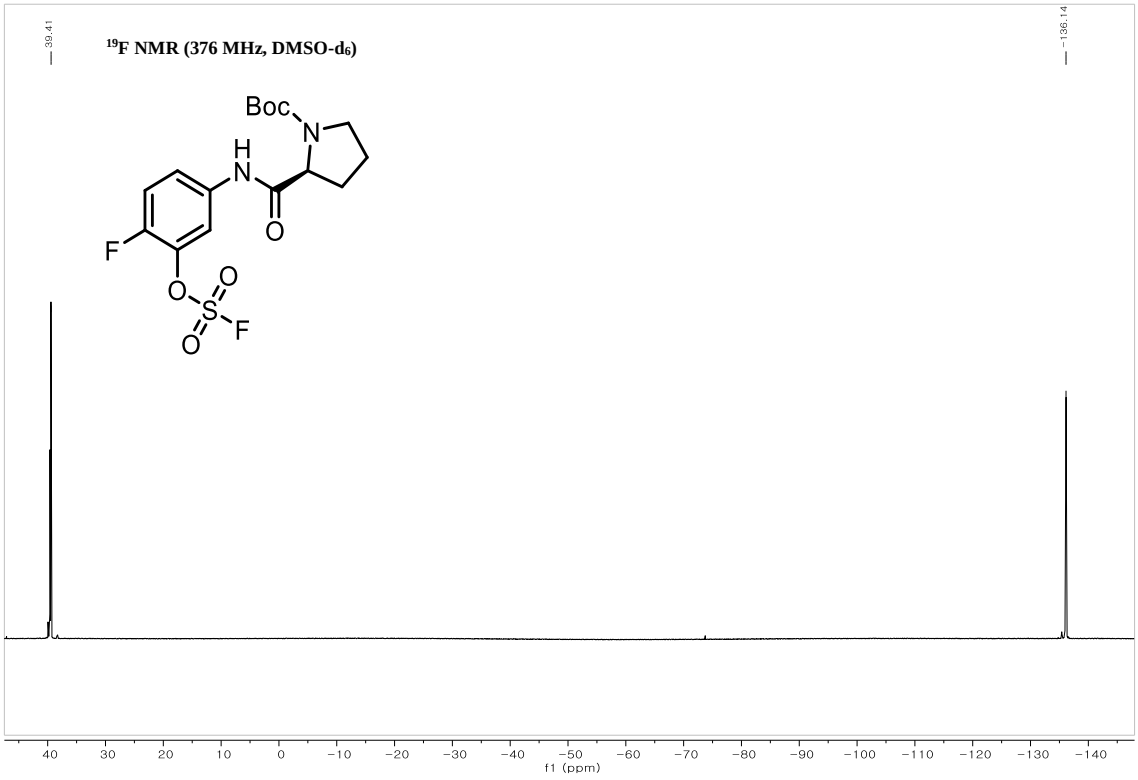
Compound 8d



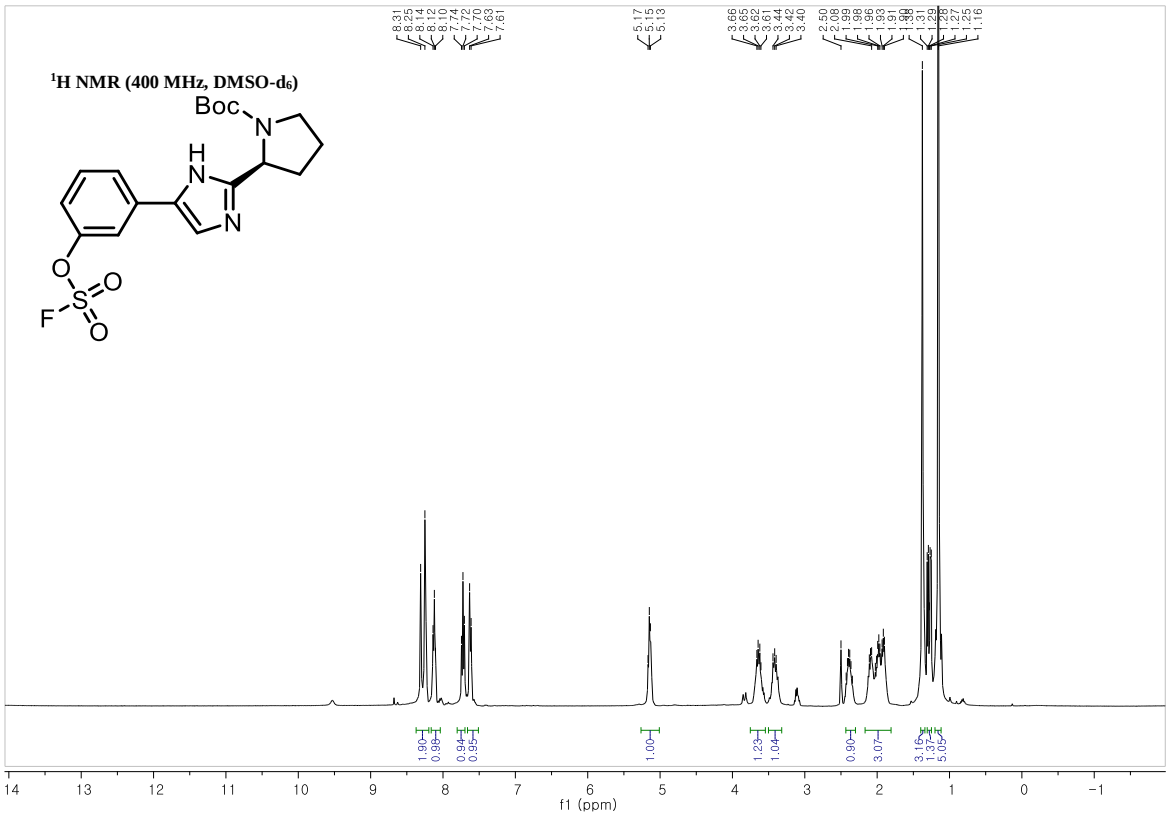
^{1}H NMR (400 MHz, DMSO-d_6)



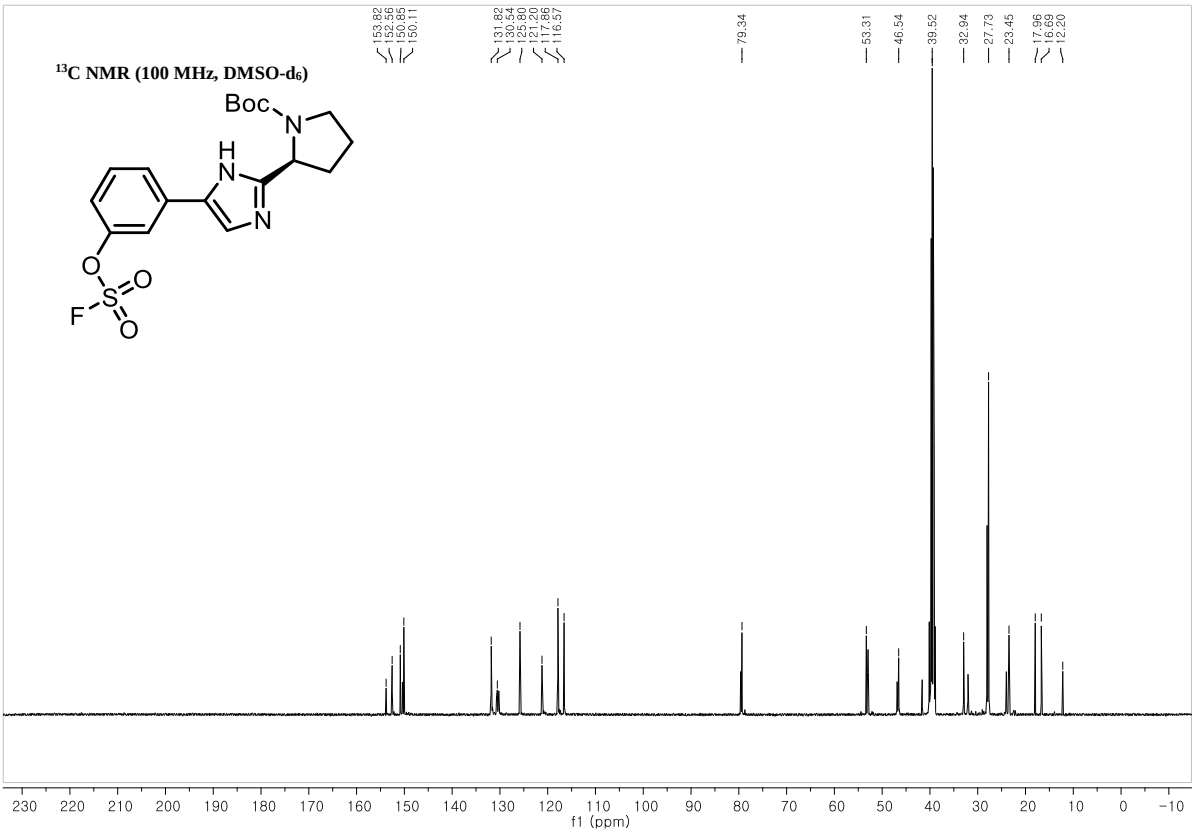
^{13}C NMR (100 MHz, DMSO-d_6)


39.41
-136.14
19F NMR (376 MHz, DMSO-d6)
Boc
N
H
N
O
F
O
S
O
O
F
40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140
f1 (ppm)

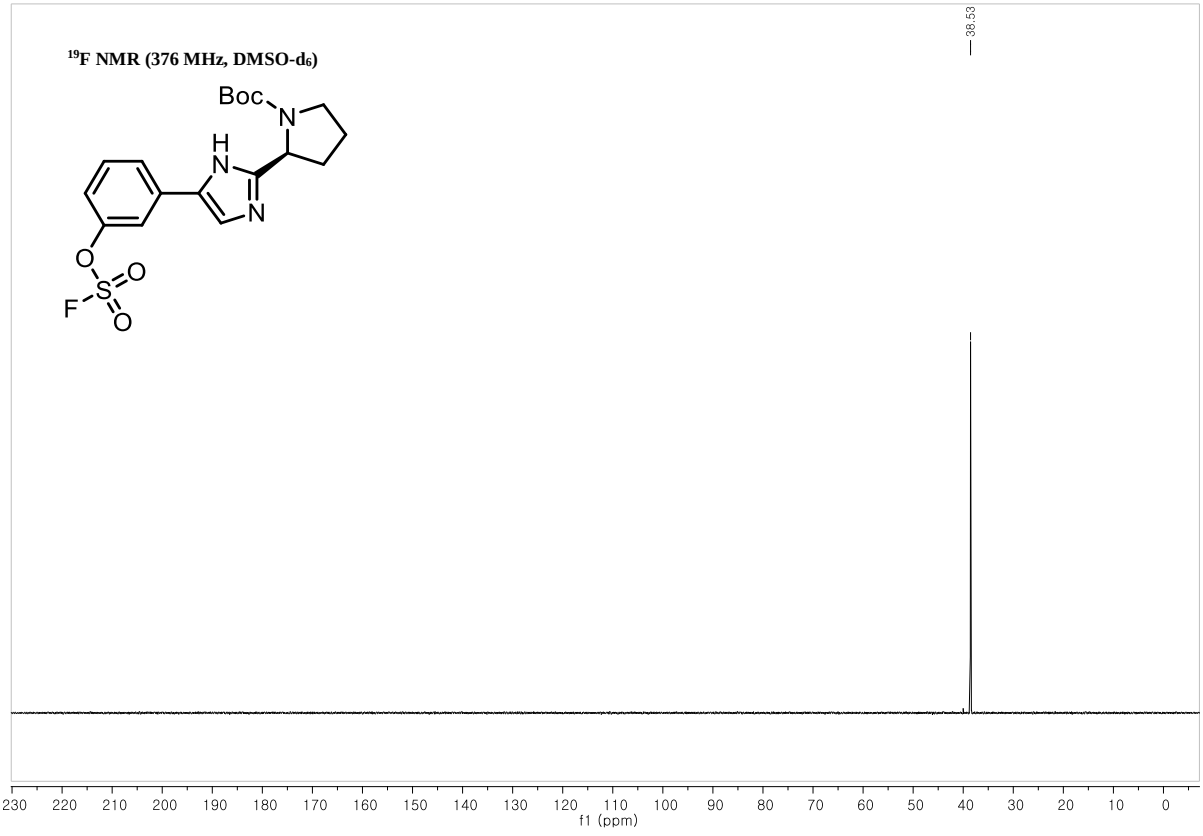
Compound 8e


8.31
8.25
8.14
8.12
8.10
7.74
7.72
7.70
7.63
7.61
5.17
5.15
5.13
3.66
3.65
3.62
3.61
3.44
3.42
3.40
2.50
2.08
1.99
1.98
1.96
1.93
1.91
1.38
1.31
1.29
1.28
1.27
1.25
1.16
1H NMR (400 MHz, DMSO-d6)
Boc
N
H
N
N
O
F
S
O
O
1.90
0.98
0.94
0.95
1.00
1.23
1.04
0.90
3.07
3.16
1.37
5.05
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)

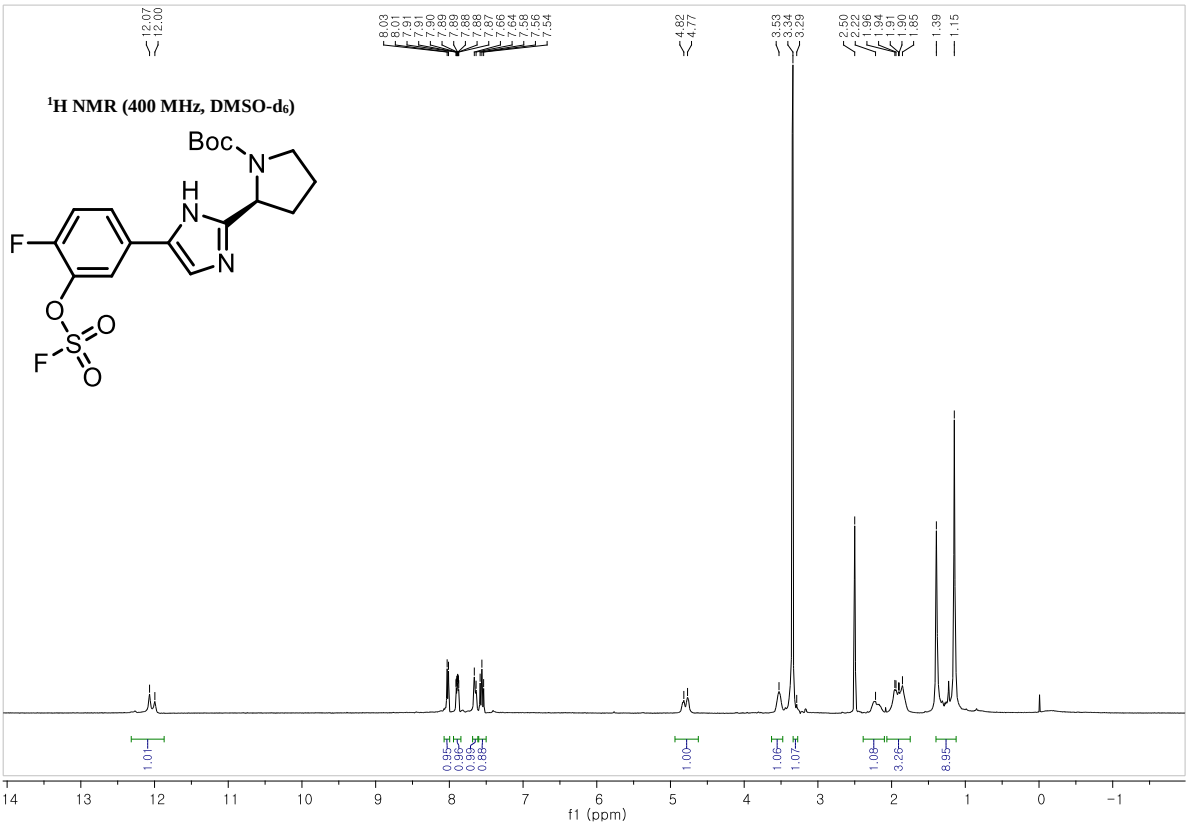
^{13}C NMR (100 MHz, DMSO-d$_6$)

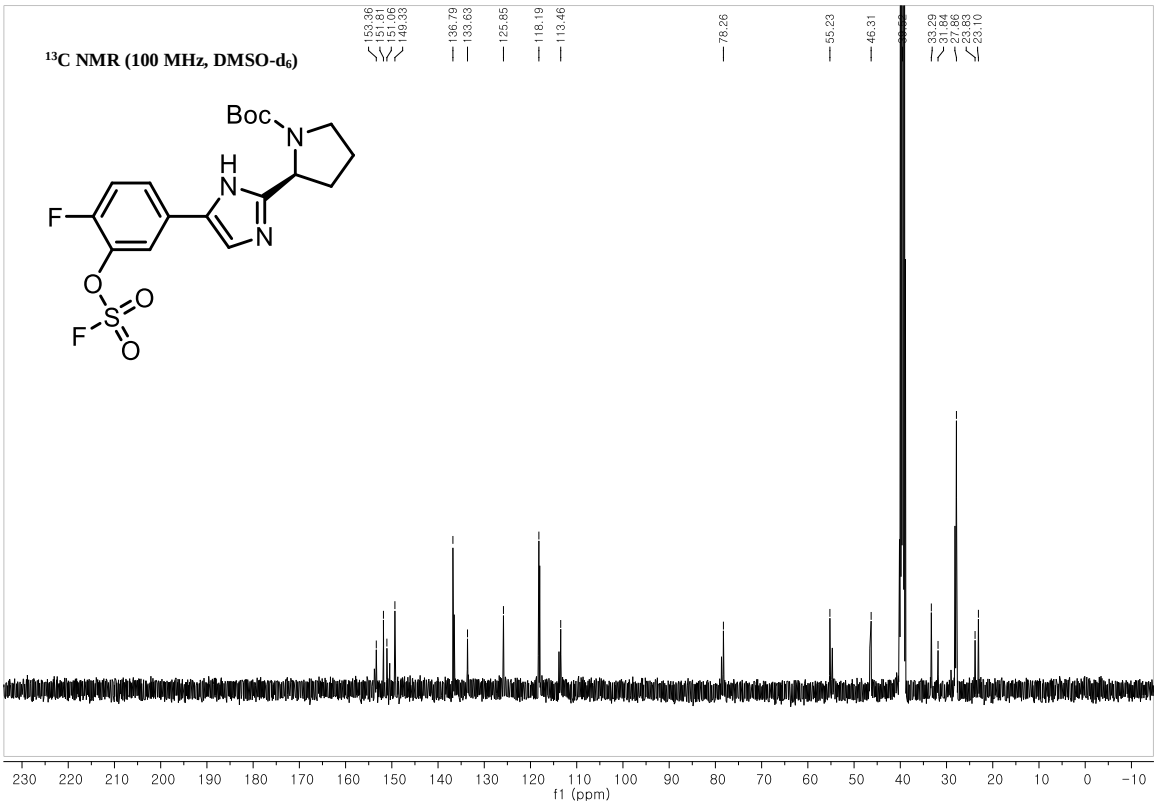


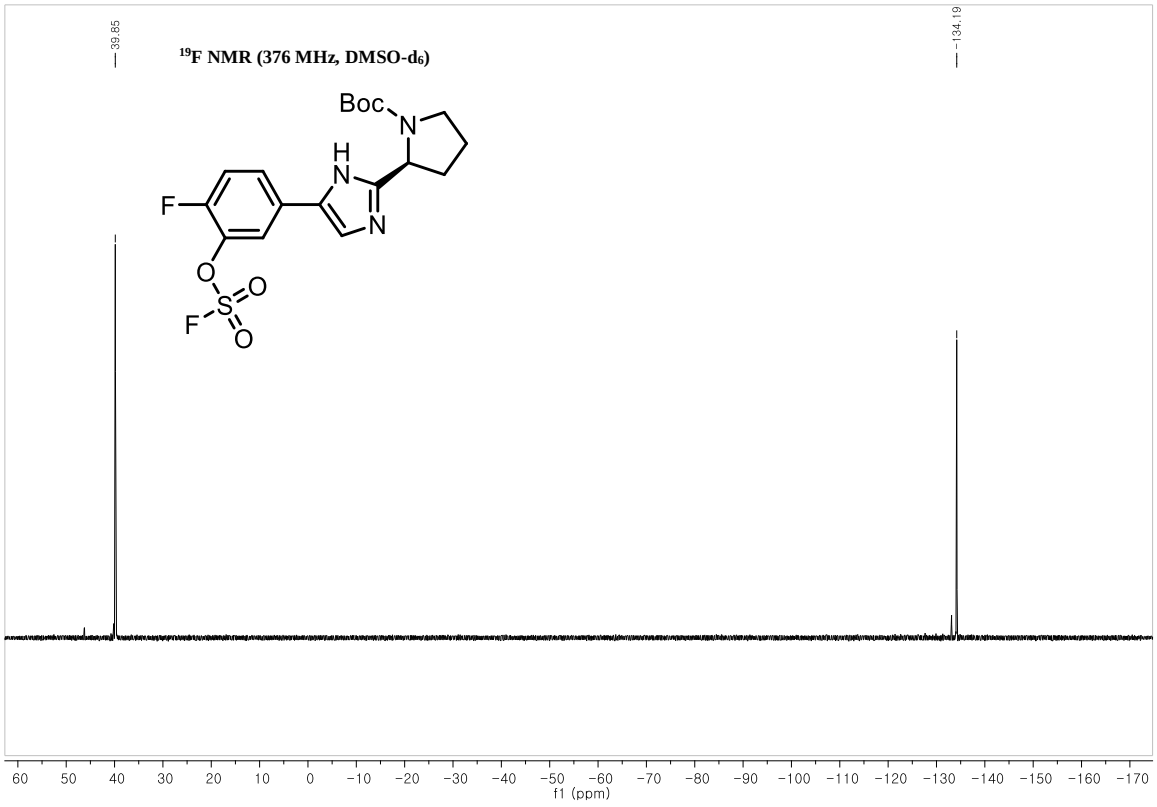
^{19}F NMR (376 MHz, DMSO-d$_6$)



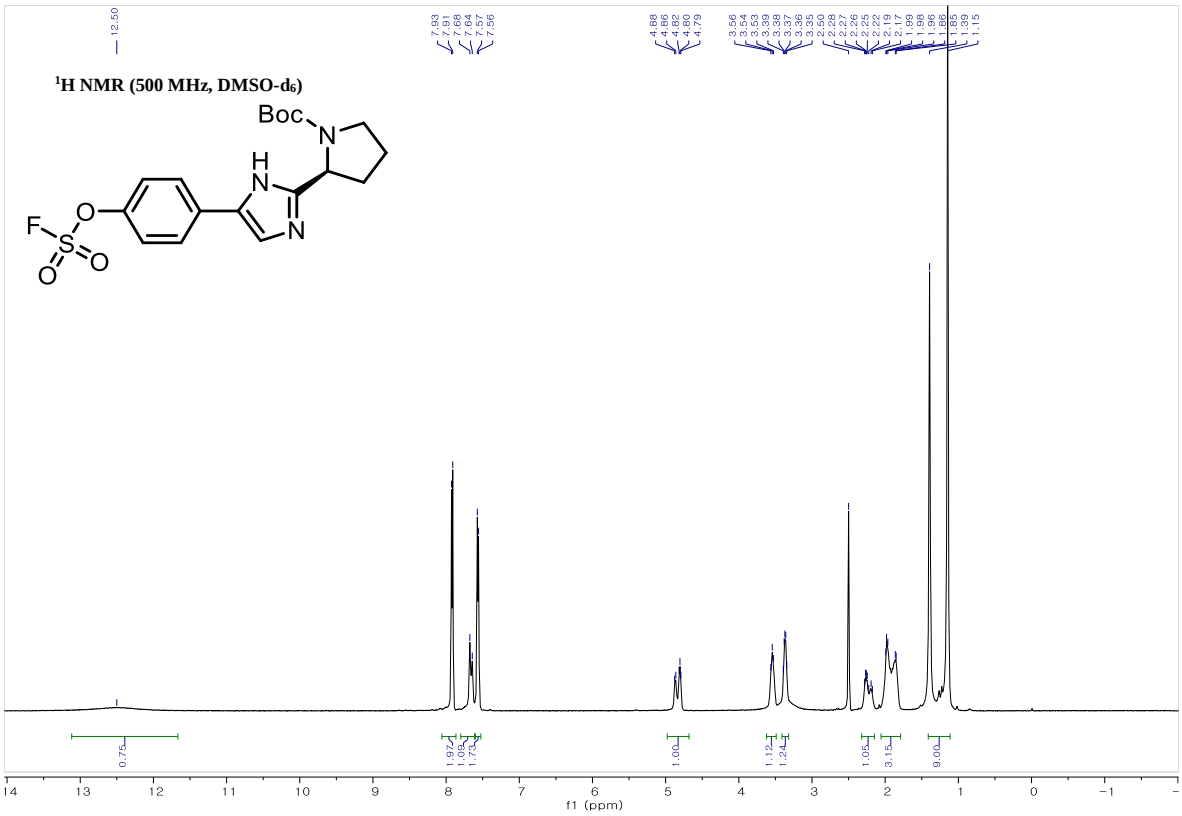
Compound 8f


12.07
12.00
8.03
8.01
7.91
7.90
7.89
7.89
7.88
7.88
7.87
7.66
7.64
7.58
7.56
7.54
4.82
4.77
3.53
3.34
3.29
2.50
2.22
1.96
1.94
1.91
1.90
1.85
1.39
1.15
1H NMR (400 MHz, DMSO-d6)
Boc
N
H
N
N
F
O
S
O
F
O
1.01
0.95
0.96
0.96
0.89
1.00
1.06
1.07
1.08
3.26
8.95
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
−1
f1 (ppm)

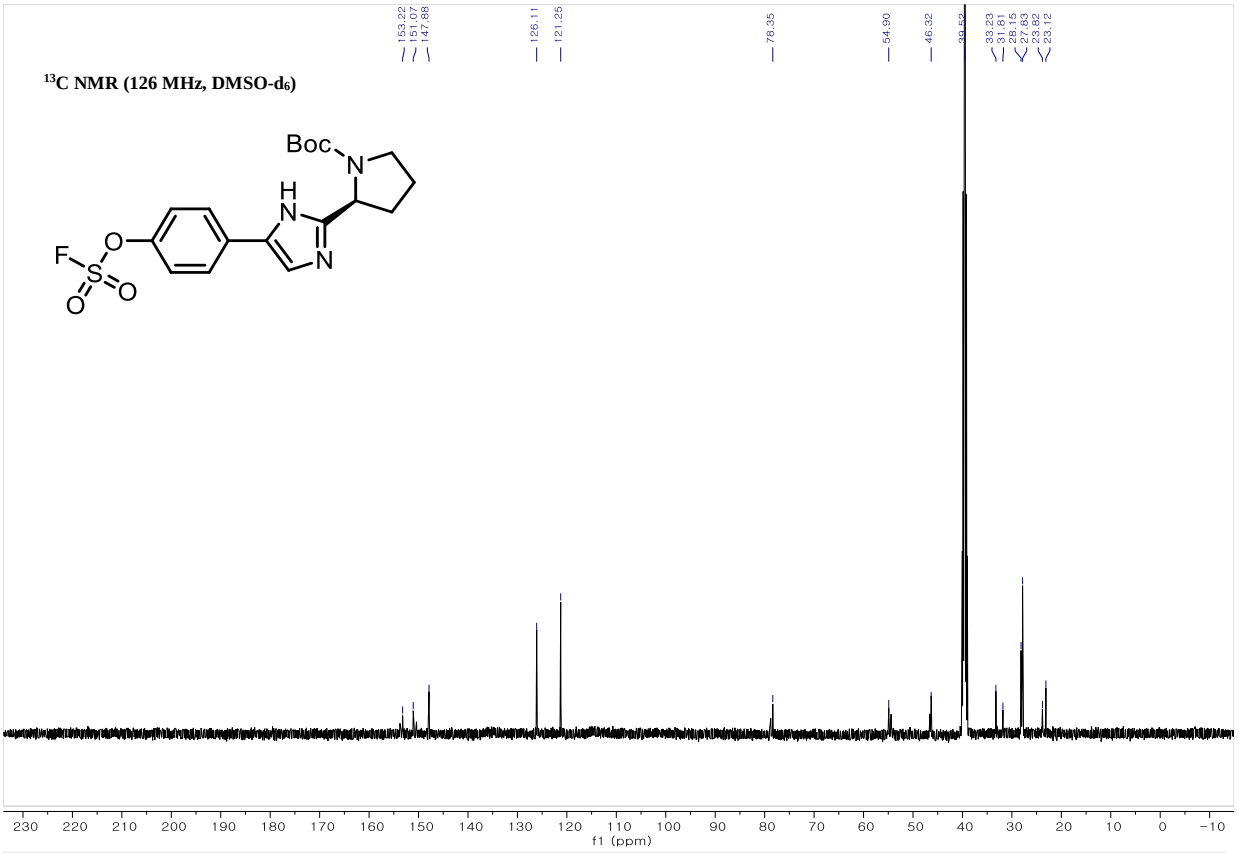

153.36
151.81
151.06
149.33
136.79
133.63
125.85
118.19
113.46
78.26
55.23
46.31
33.29
31.84
27.86
23.83
23.10
13C NMR (100 MHz, DMSO-d6)
Boc
N
H
N
N
F
O
S
O
F
O
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)


39.85
-134.19
19F NMR (376 MHz, DMSO-d6)
Boc
N
H
N
N
F
O
S
O
F
O
60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170
f1 (ppm)

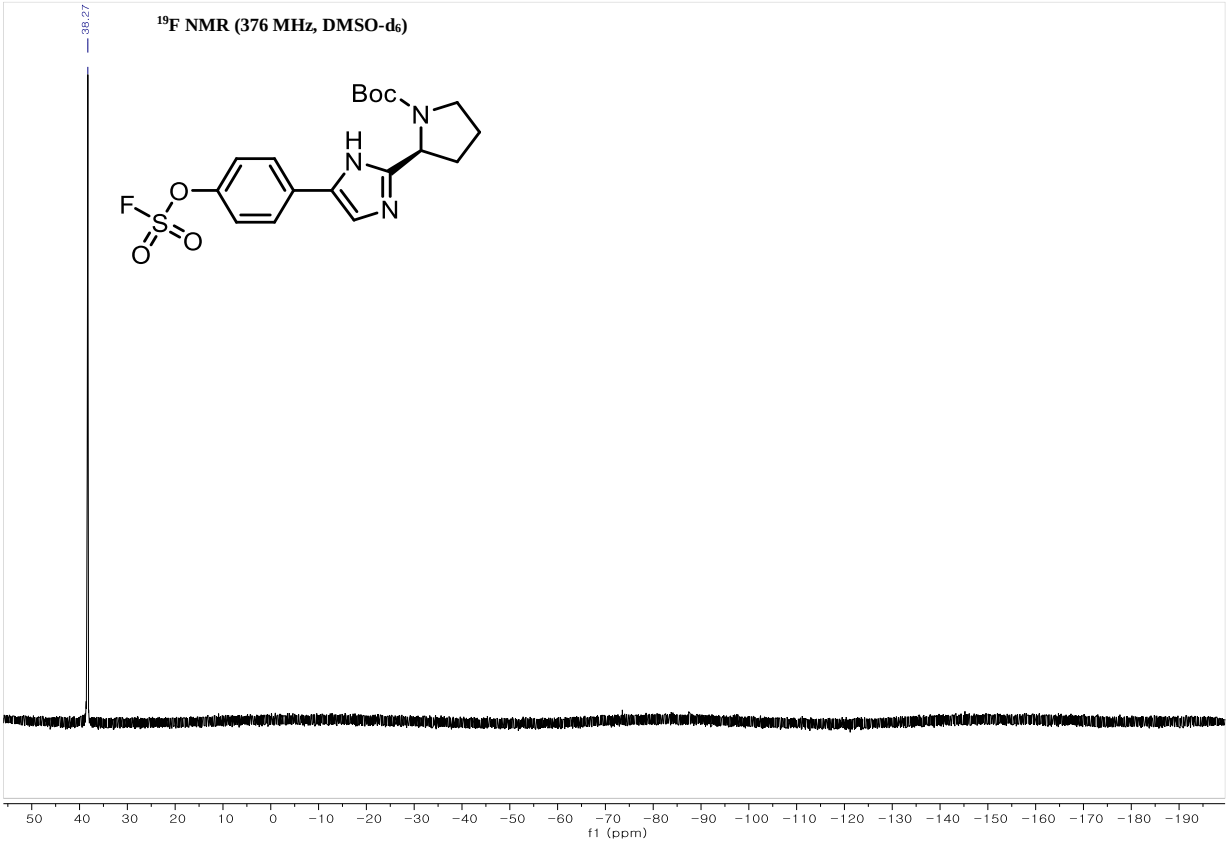
Compound 8g


12.50
7.93
7.91
7.68
7.64
7.57
7.56
4.88
4.86
4.82
4.80
4.79
3.56
3.54
3.53
3.39
3.38
3.37
3.36
3.35
2.50
2.28
2.27
2.26
2.25
2.22
2.19
2.17
1.99
1.98
1.96
1.86
1.85
1.39
1.15
1H NMR (500 MHz, DMSO-d6)
Boc
N
H
N
N
F
O
S
O
O
0.75
1.97
1.09
1.73
1.00
1.12
1.24
1.05
3.15
9.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)

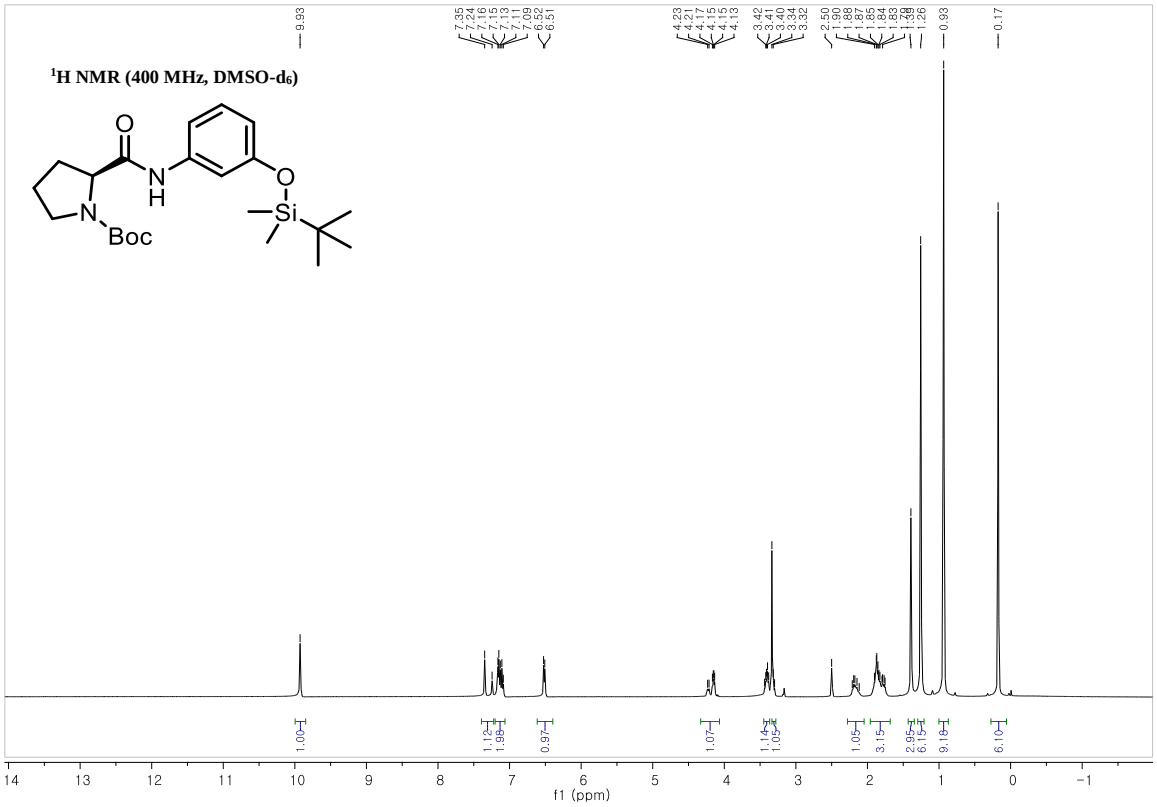
^{13}C NMR (126 MHz, DMSO-d_6)

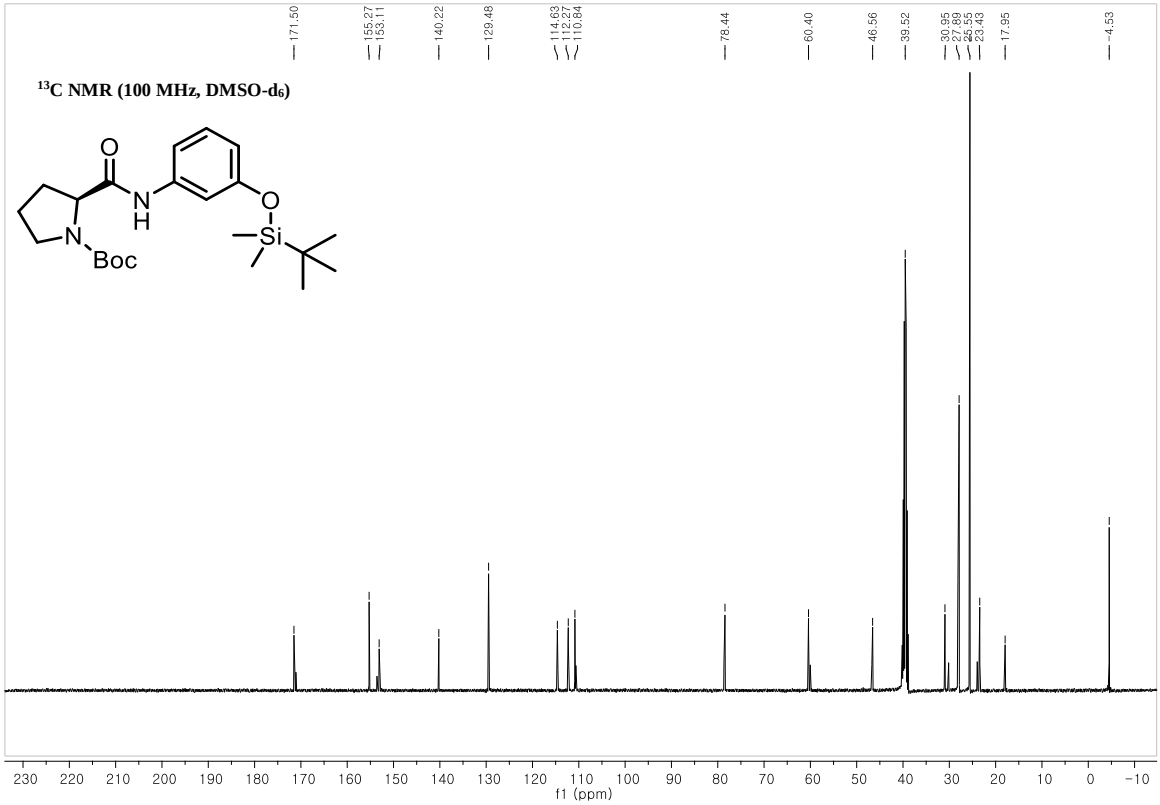


^{19}F NMR (376 MHz, DMSO-d_6)

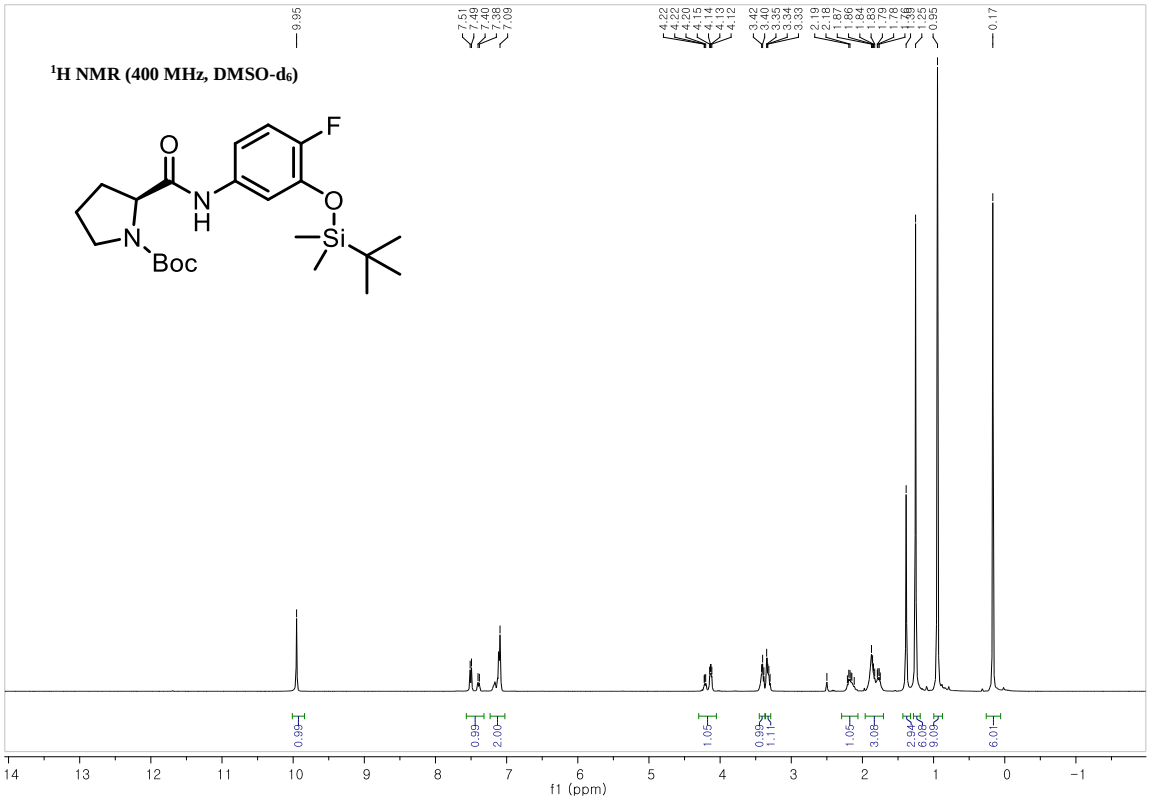


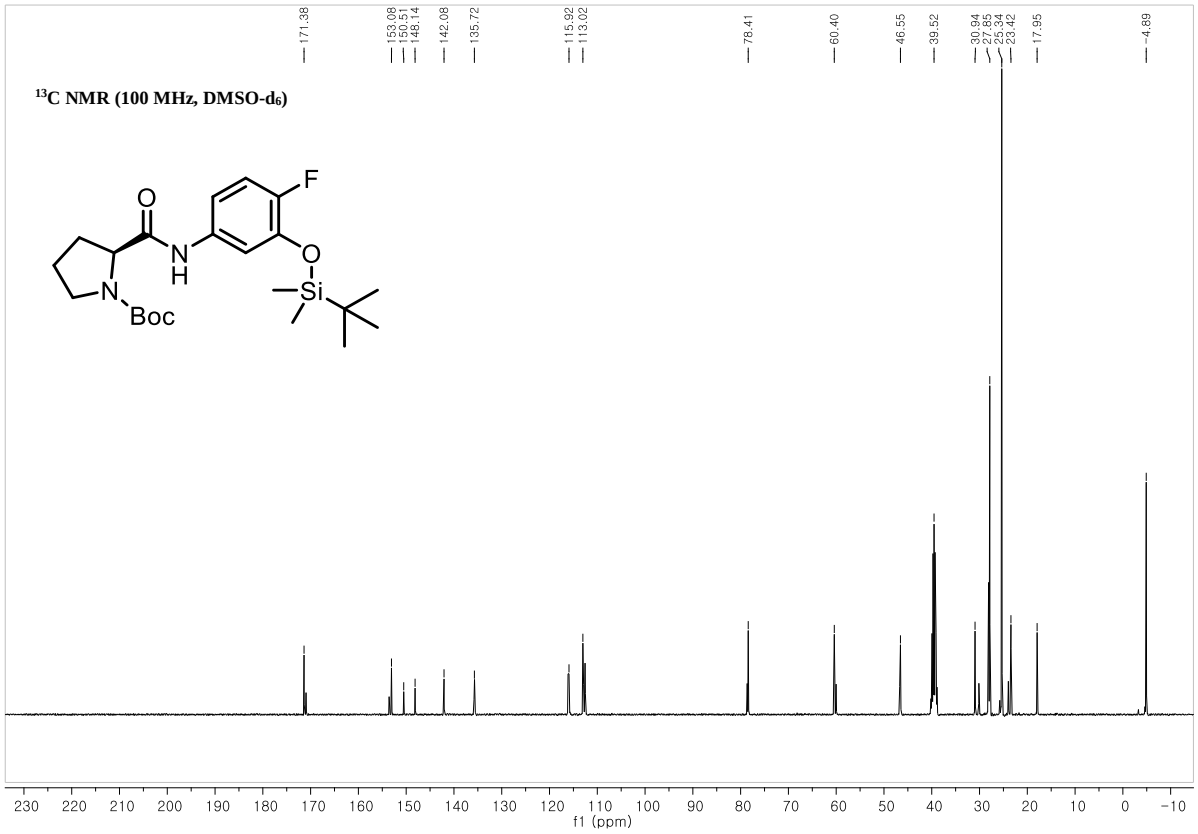
Compound 9a

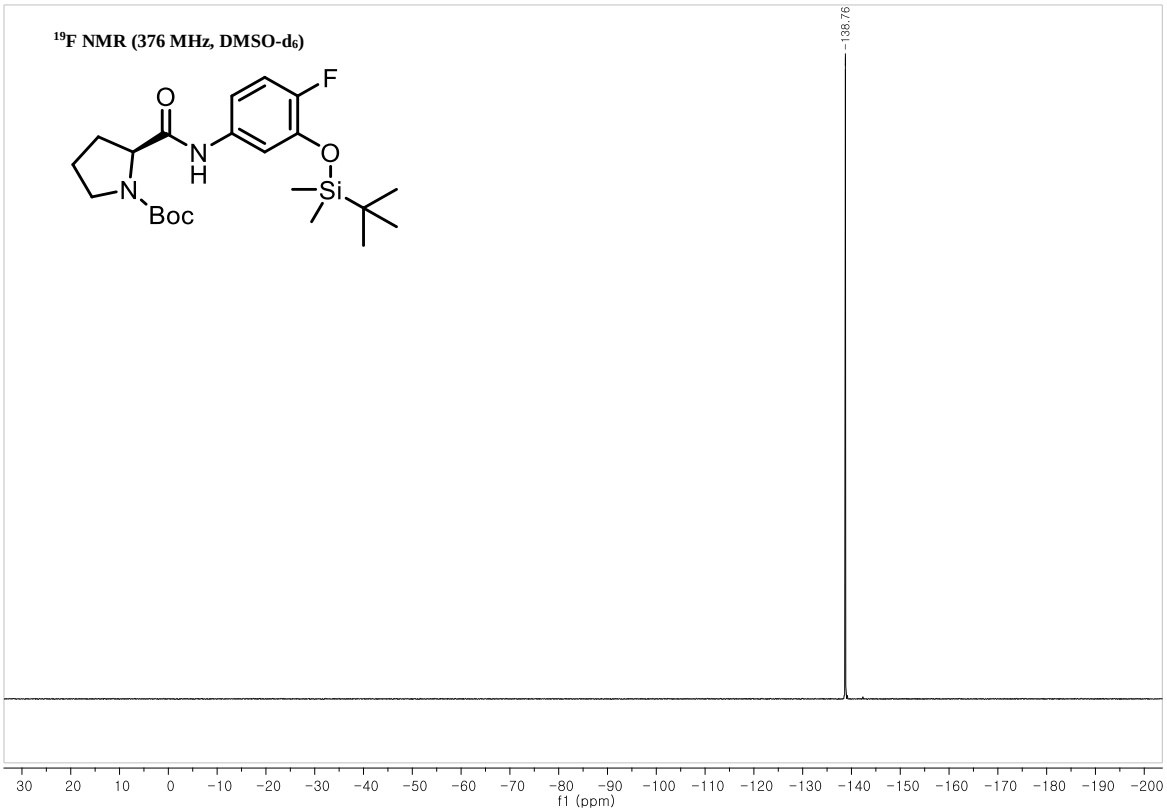

9.93
7.35
7.24
7.16
7.15
7.13
7.11
7.09
6.52
6.51
4.23
4.21
4.17
4.15
4.15
4.13
3.42
3.41
3.40
3.34
3.32
2.50
1.90
1.88
1.87
1.85
1.84
1.83
1.79
1.39
1.26
0.93
0.17
1.00
1.12
1.98
0.97
1.07
1.14
1.05
1.05
3.15
2.95
6.15
9.18
6.10
f1 (ppm)


171.50
155.27
153.11
140.22
129.48
114.63
112.27
110.84
78.44
60.40
46.56
39.52
30.95
27.89
26.55
23.43
17.95
-4.53
f1 (ppm)

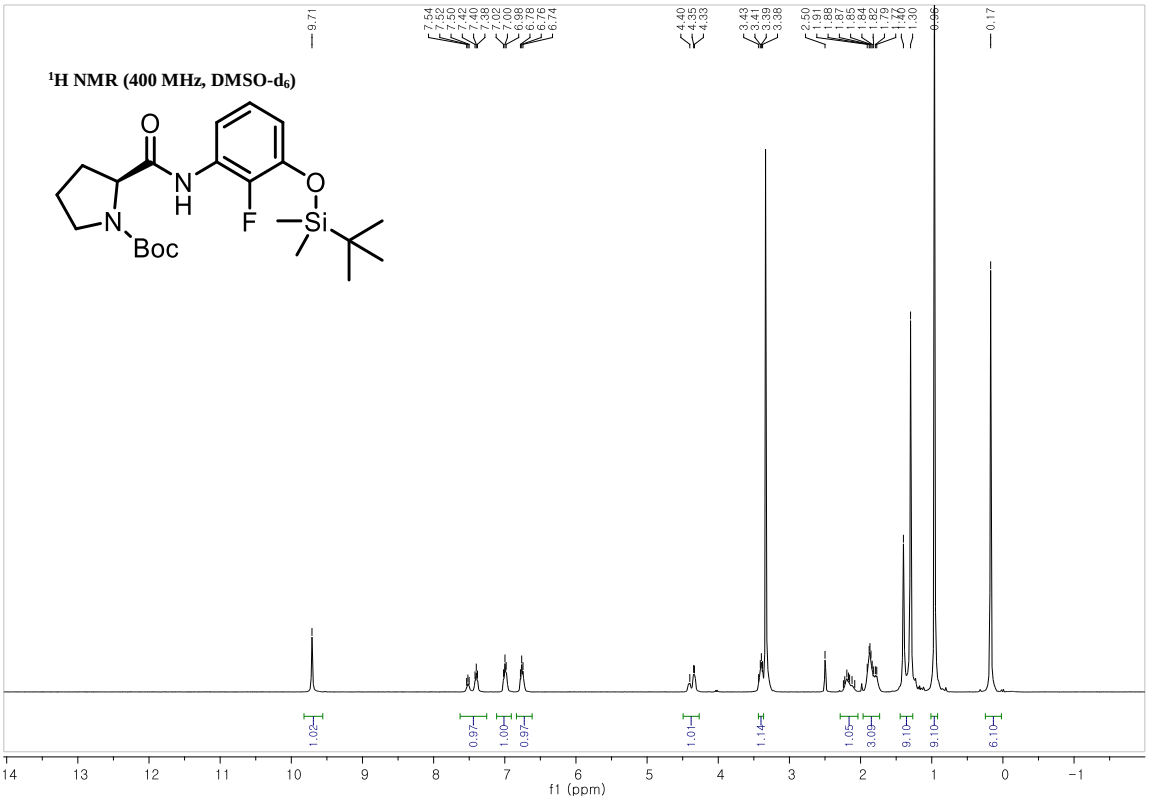
Compound 9b



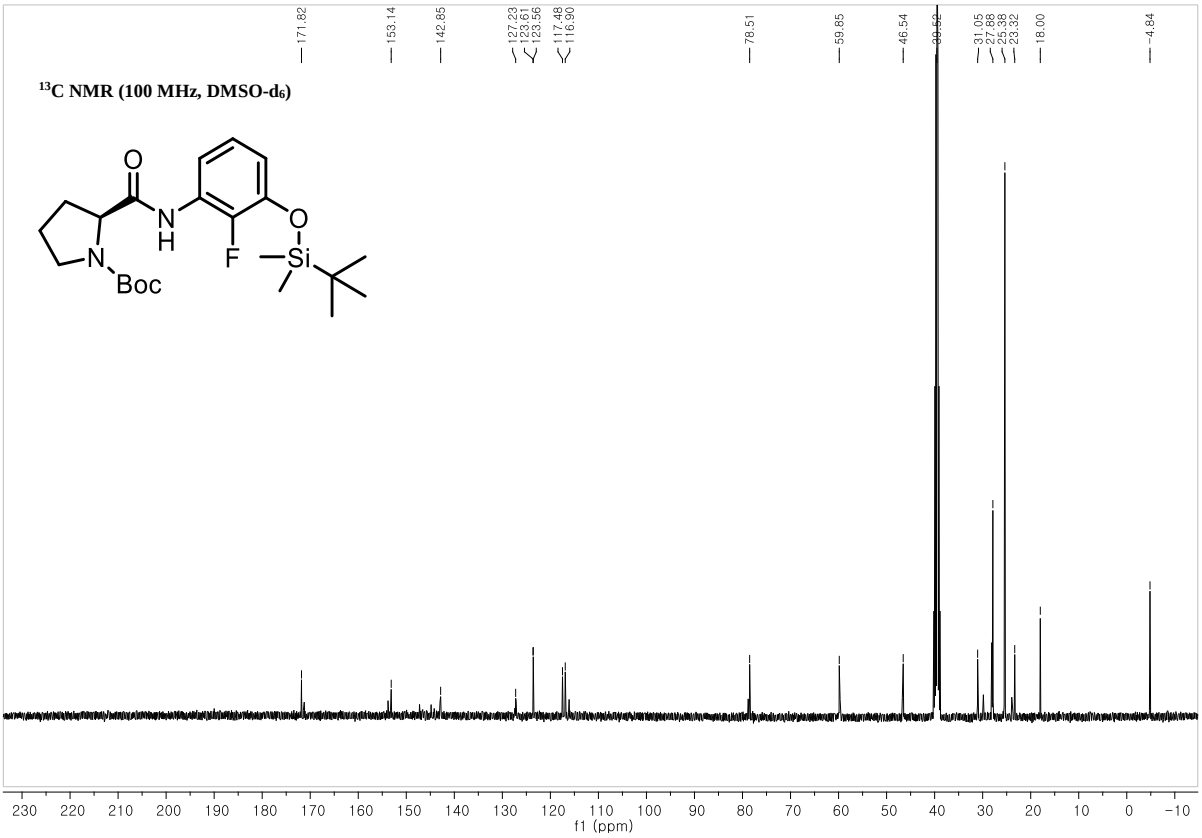



19F NMR (376 MHz, DMSO-d6)
-138.76
f1 (ppm)

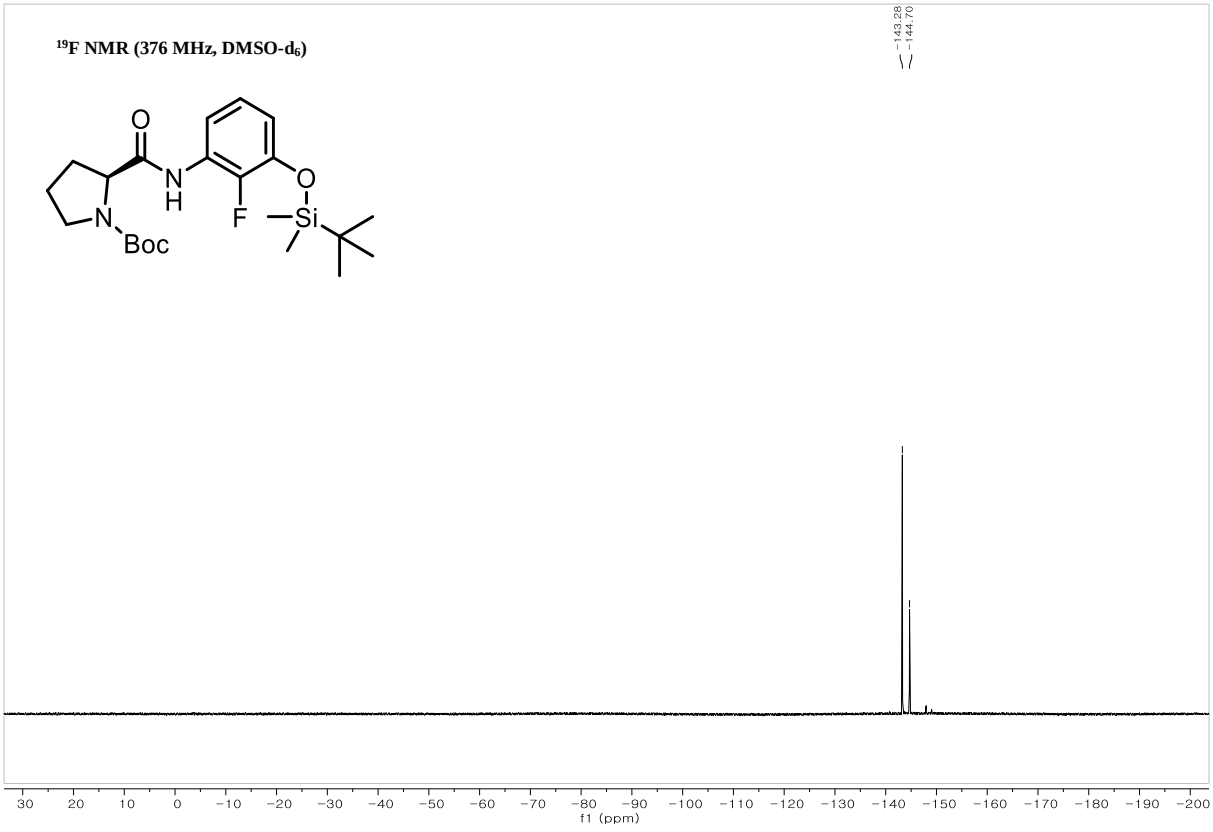
Compound 9c


1H NMR (400 MHz, DMSO-d6)
9.71
7.54
7.52
7.50
7.42
7.40
7.38
7.02
7.00
6.98
6.78
6.76
6.74
4.40
4.35
4.33
3.43
3.41
3.39
3.38
2.50
1.91
1.88
1.87
1.85
1.84
1.82
1.79
1.77
1.47
1.30
0.17
1.02
0.97
1.00
0.97
1.01
1.14
1.05
3.09
9.16
9.16
6.16
f1 (ppm)

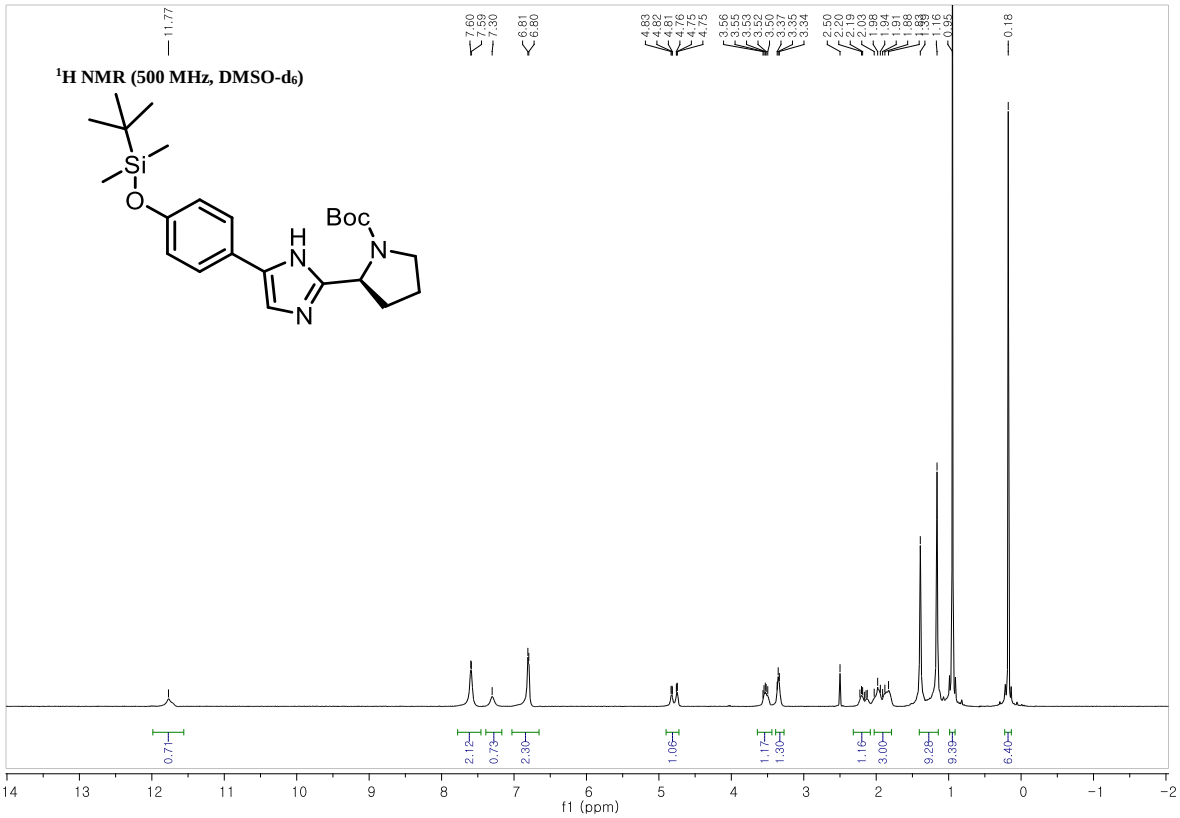
^{13}C NMR (100 MHz, DMSO-d_6)

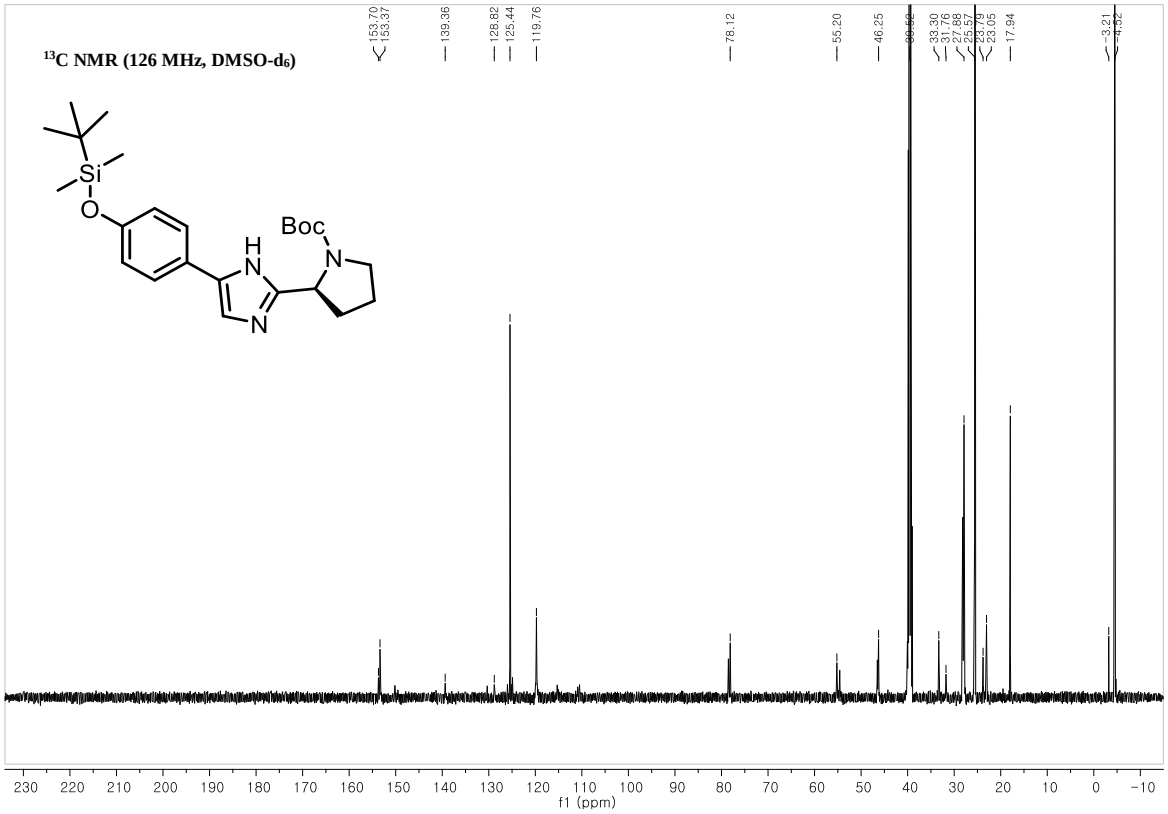


^{19}F NMR (376 MHz, DMSO-d_6)

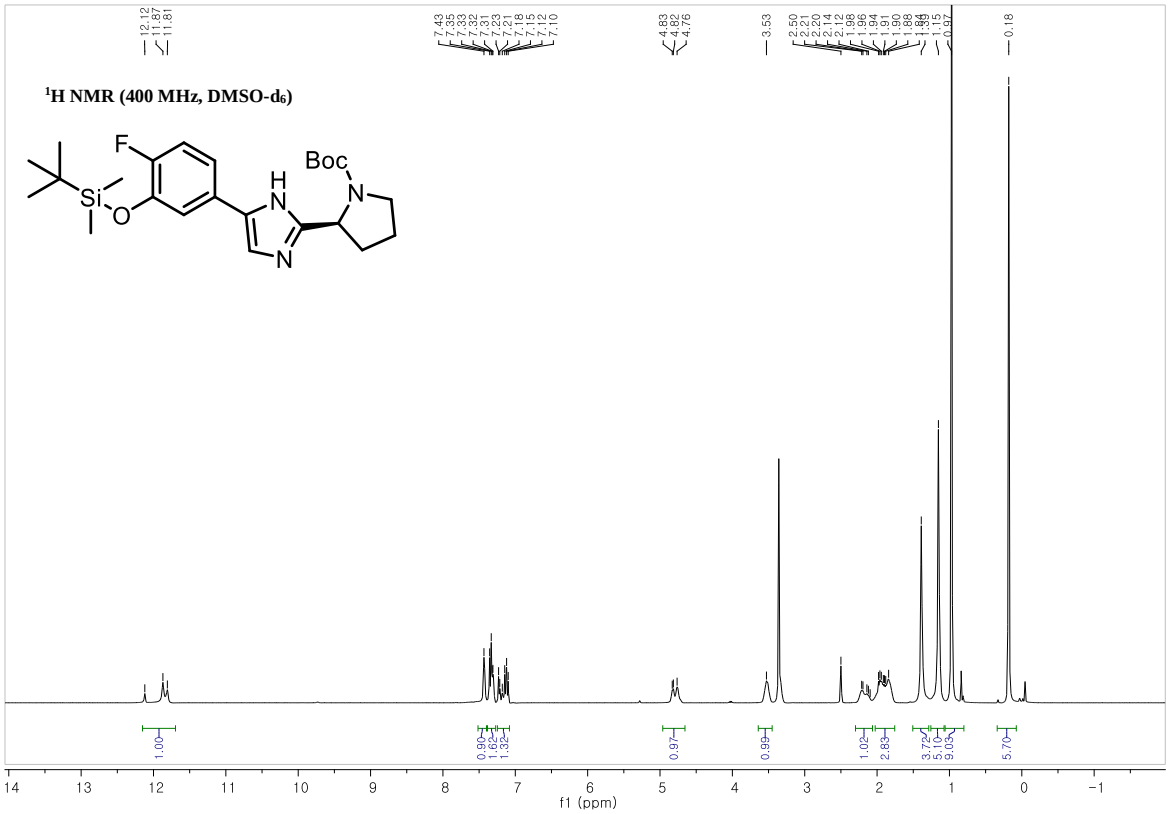


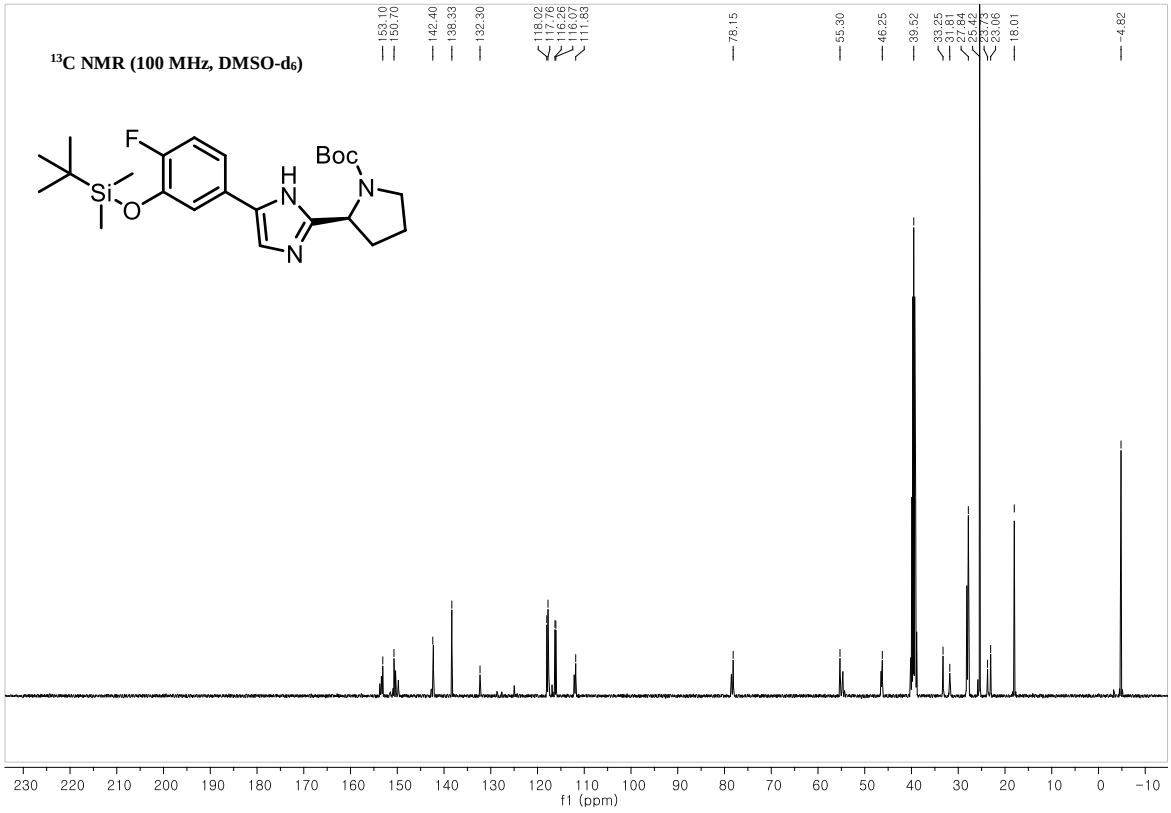
Compound 9d

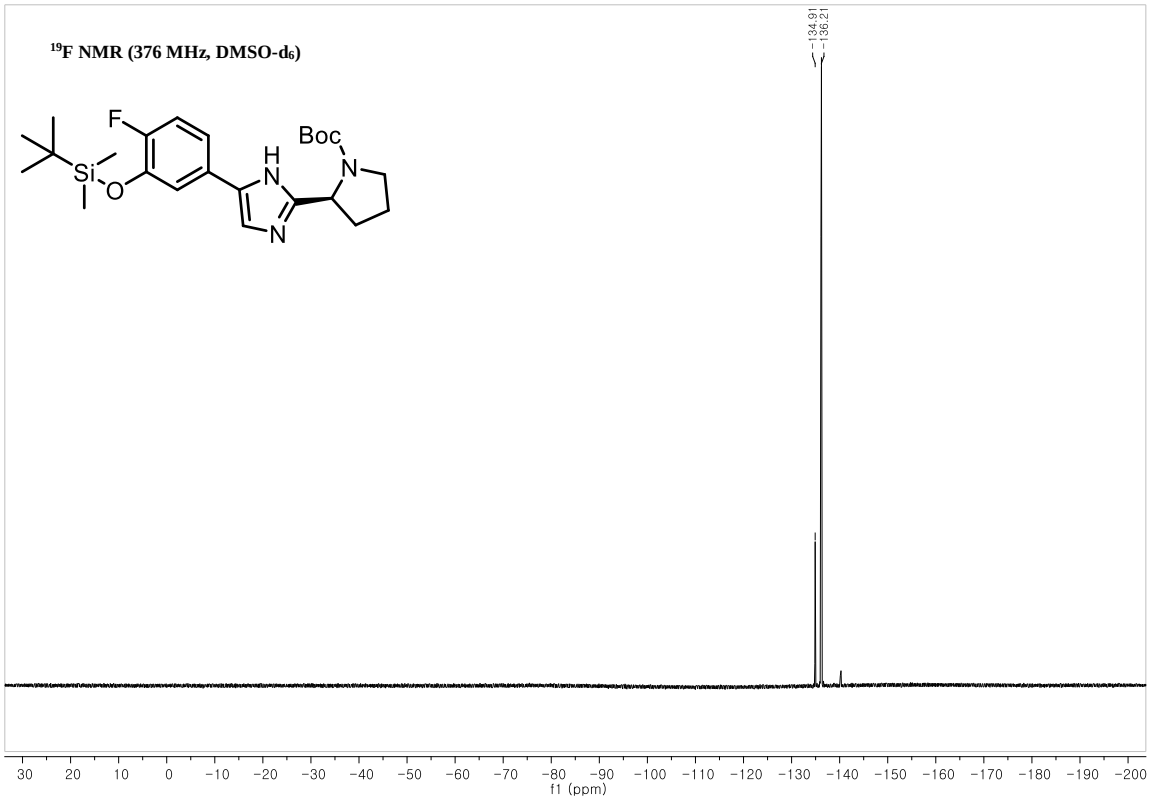

^{1}H NMR (500 MHz, DMSO-d$_6$)
Si
O
H
N
N
Boc
N
f1 (ppm)


^{13}C NMR (126 MHz, DMSO-d$_6$)
Si
O
H
N
N
Boc
N
f1 (ppm)

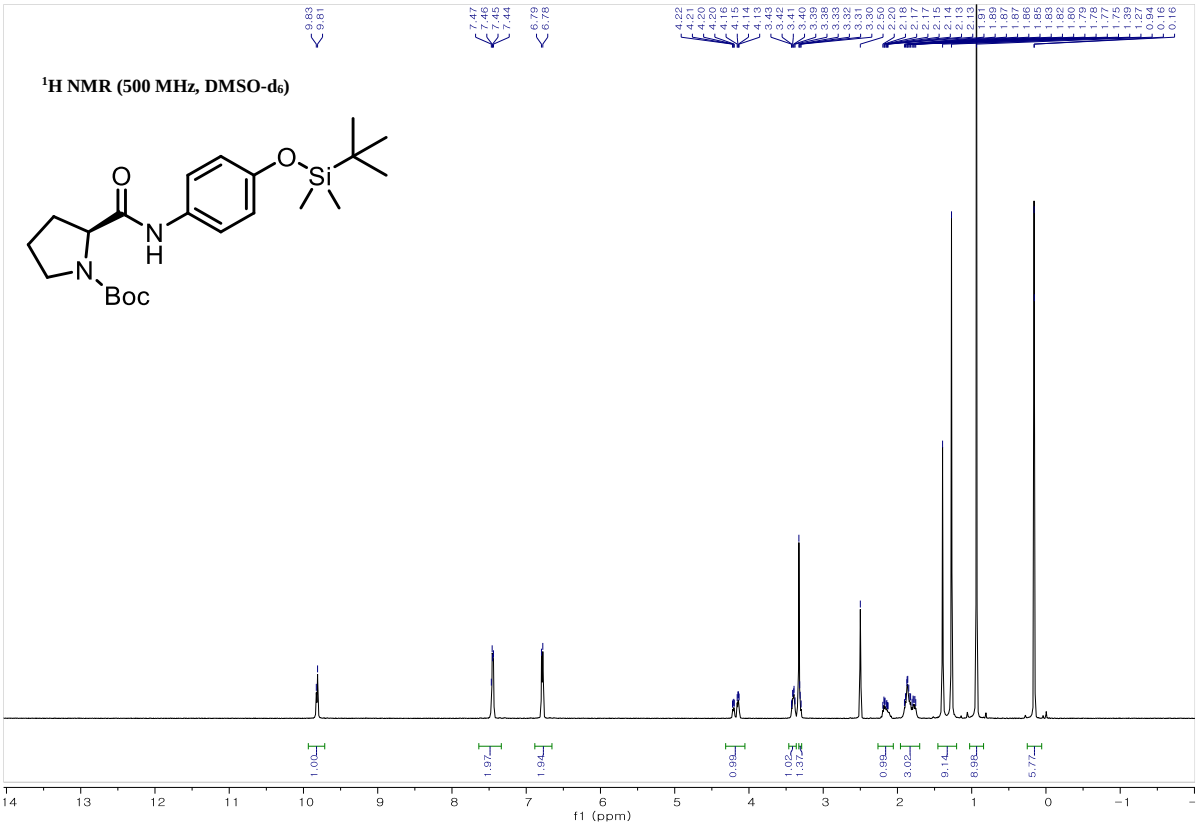
Compound 9e

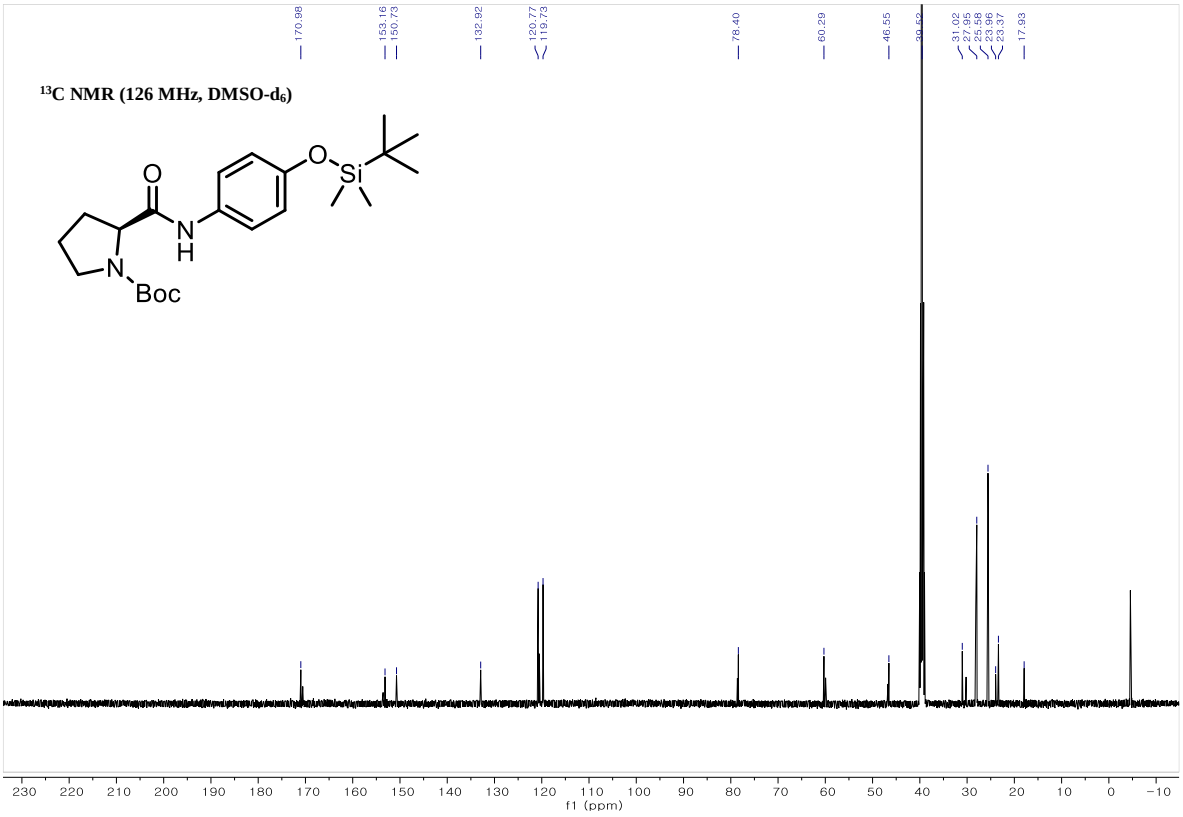

1H NMR (400 MHz, DMSO-d6)
F
Si
O
H
N
N
Boc
N
f1 (ppm)


13C NMR (100 MHz, DMSO-d6)
F
Si
O
H
N
N
Boc
N
f1 (ppm)

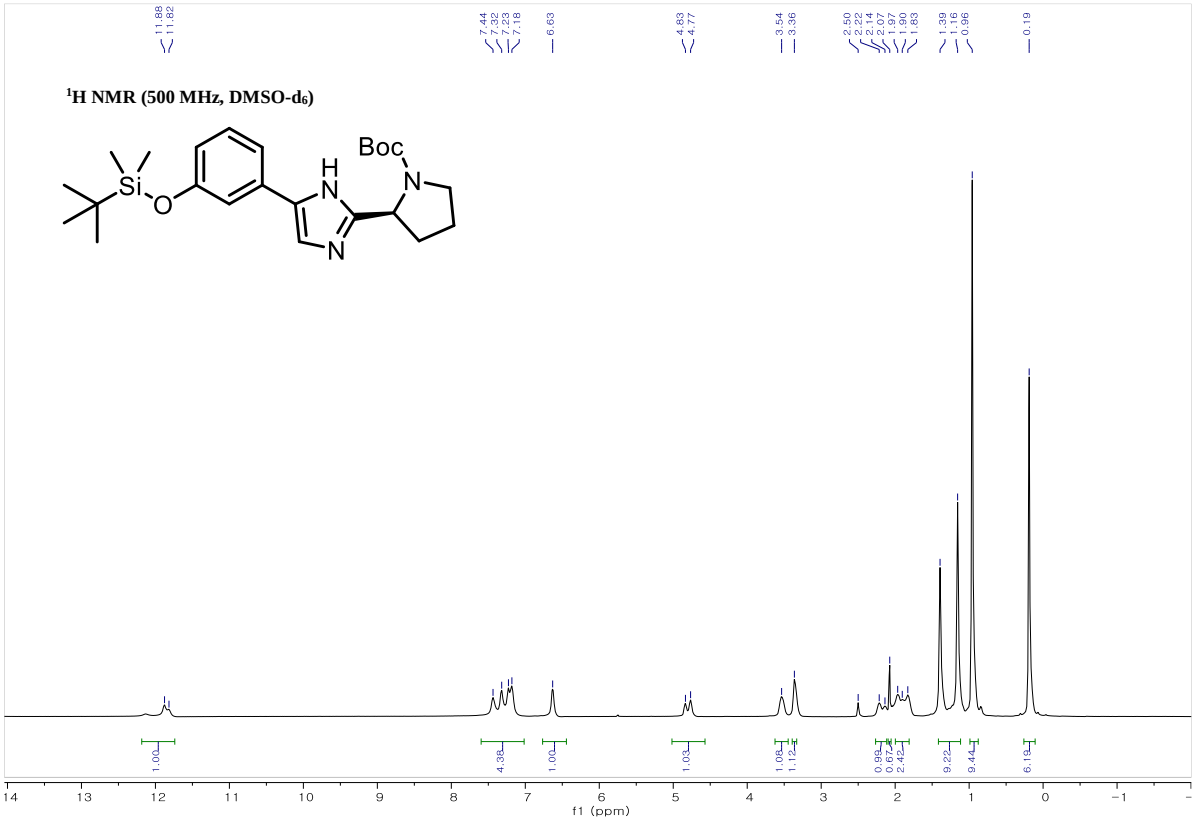

^{19}F NMR (376 MHz, DMSO-d$_6$)
F
Si
O
H
N
N
Boc
N
-134.91
-136.21
f1 (ppm)

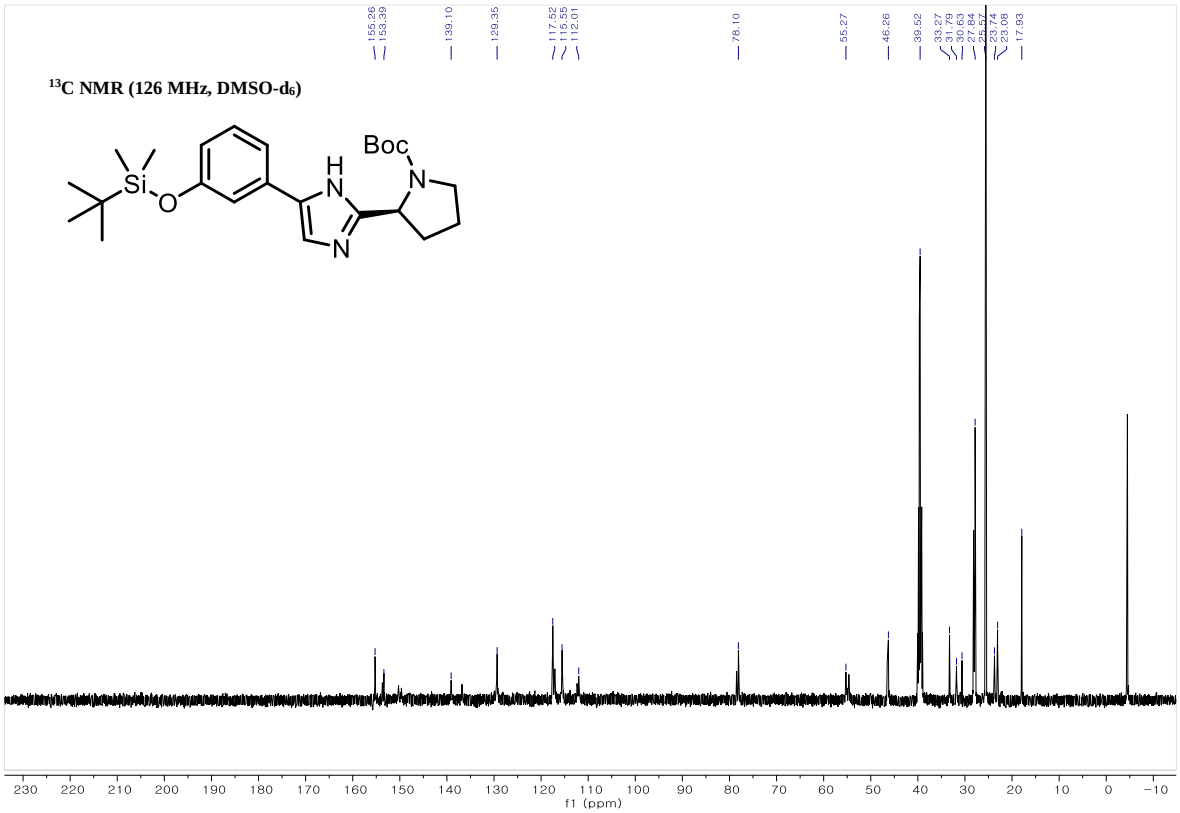
Compound 9f


^{1}H NMR (500 MHz, DMSO-d$_6$)
O
N
H
N
Boc
O
Si
9.83
9.81
7.47
7.46
7.45
7.44
6.79
6.78
1.00
1.97
1.94
0.99
1.02
1.37
0.99
3.02
9.14
8.98
5.77
f1 (ppm)

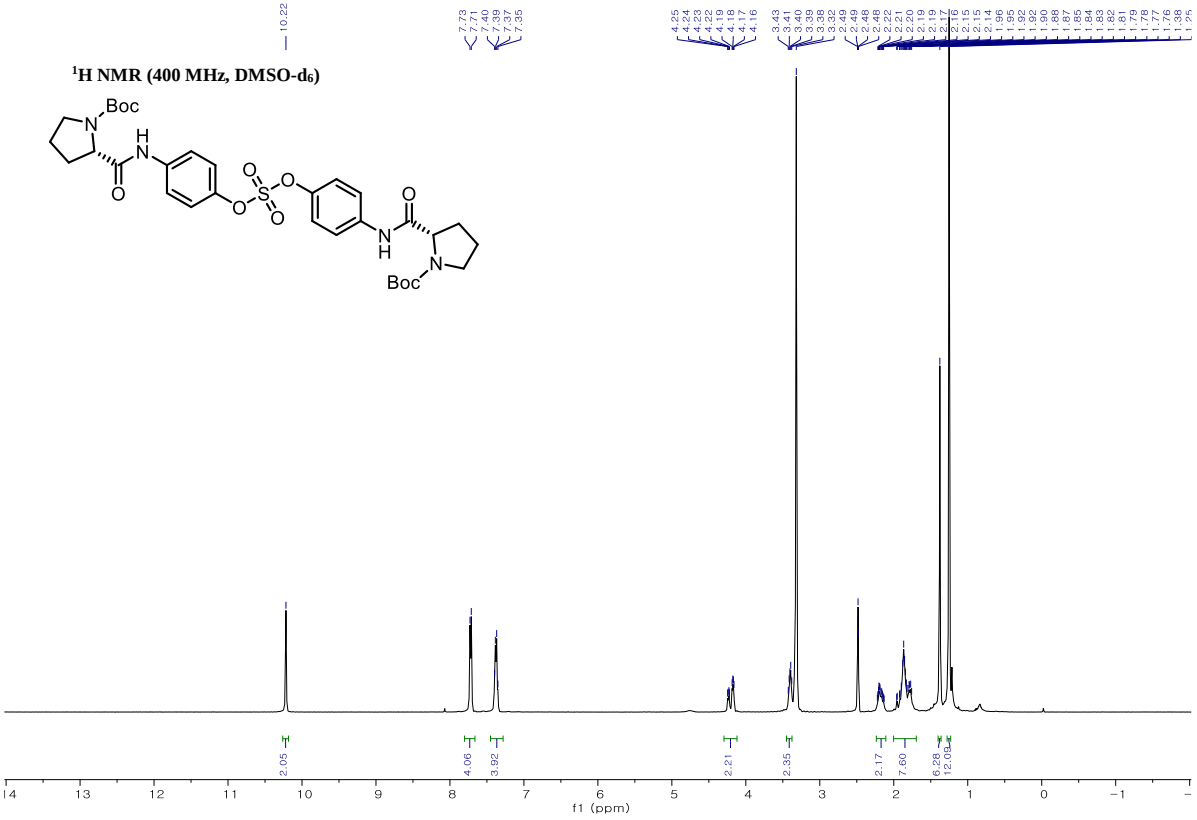

170.98
153.16
150.73
132.92
120.77
119.73
78.40
60.29
46.55
39.62
31.02
27.95
25.58
23.96
23.37
17.93
13C NMR (126 MHz, DMSO-d6)
O
Si
N
H
N
Boc
f1 (ppm)

Compound 9g

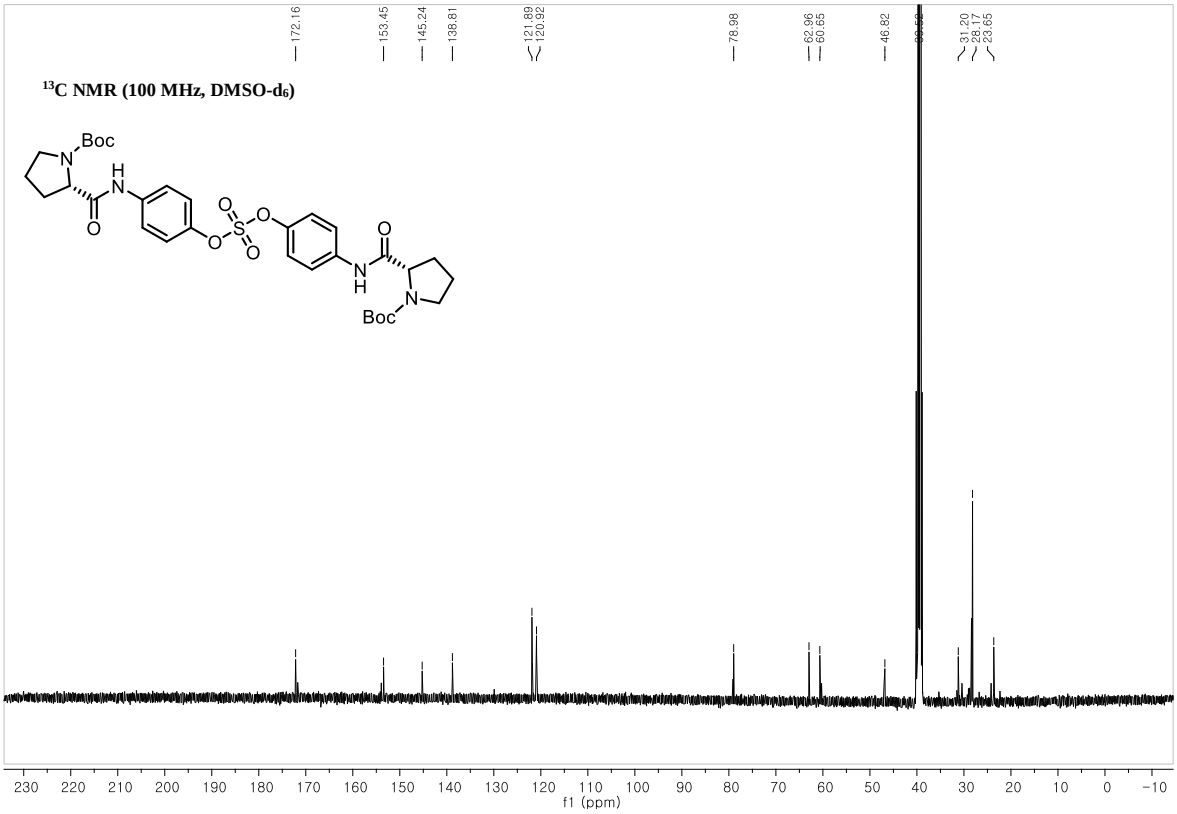

11.88
11.82
7.44
7.32
7.23
7.18
6.63
4.83
4.77
3.54
3.36
2.50
2.22
2.14
2.07
1.97
1.90
1.83
1.39
1.16
0.96
0.19
1H NMR (500 MHz, DMSO-d6)
Si
O
H
N
N
Boc
N
1.00
4.38
1.00
1.03
1.08
1.12
0.93
0.87
2.42
9.22
9.44
6.19
f1 (ppm)



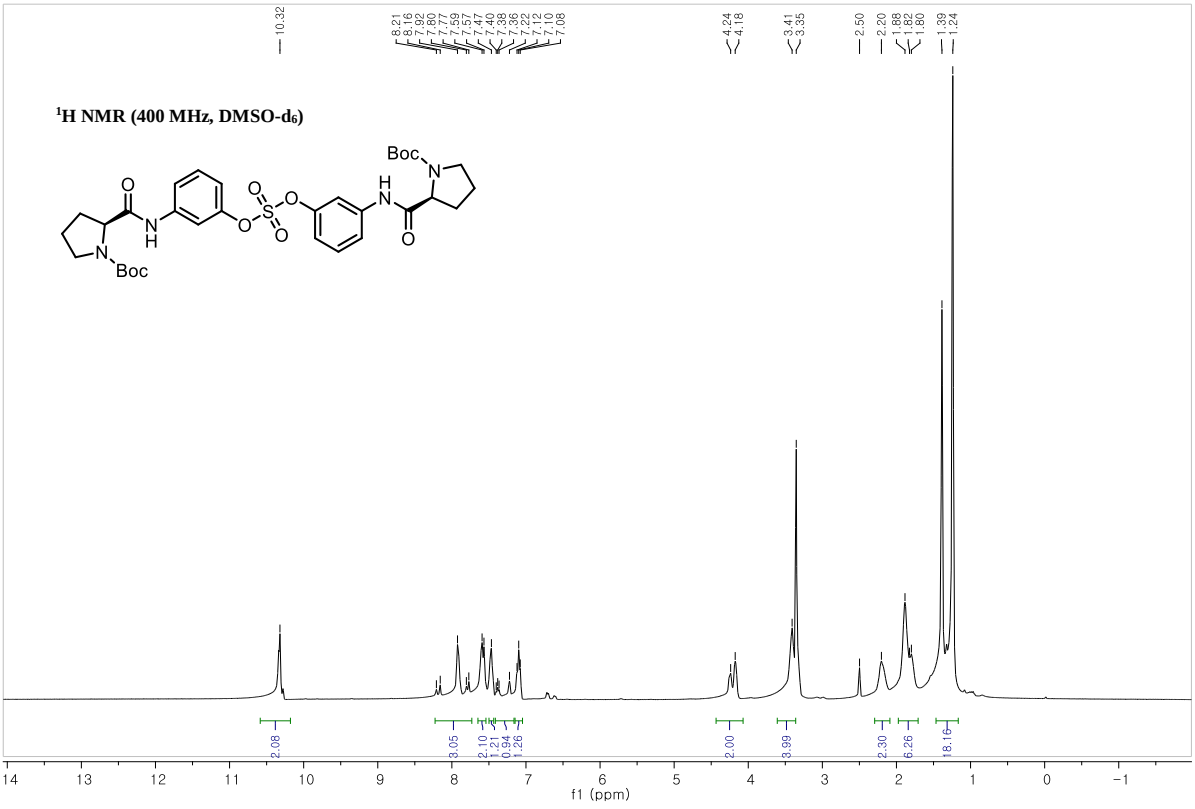
Compound 10a

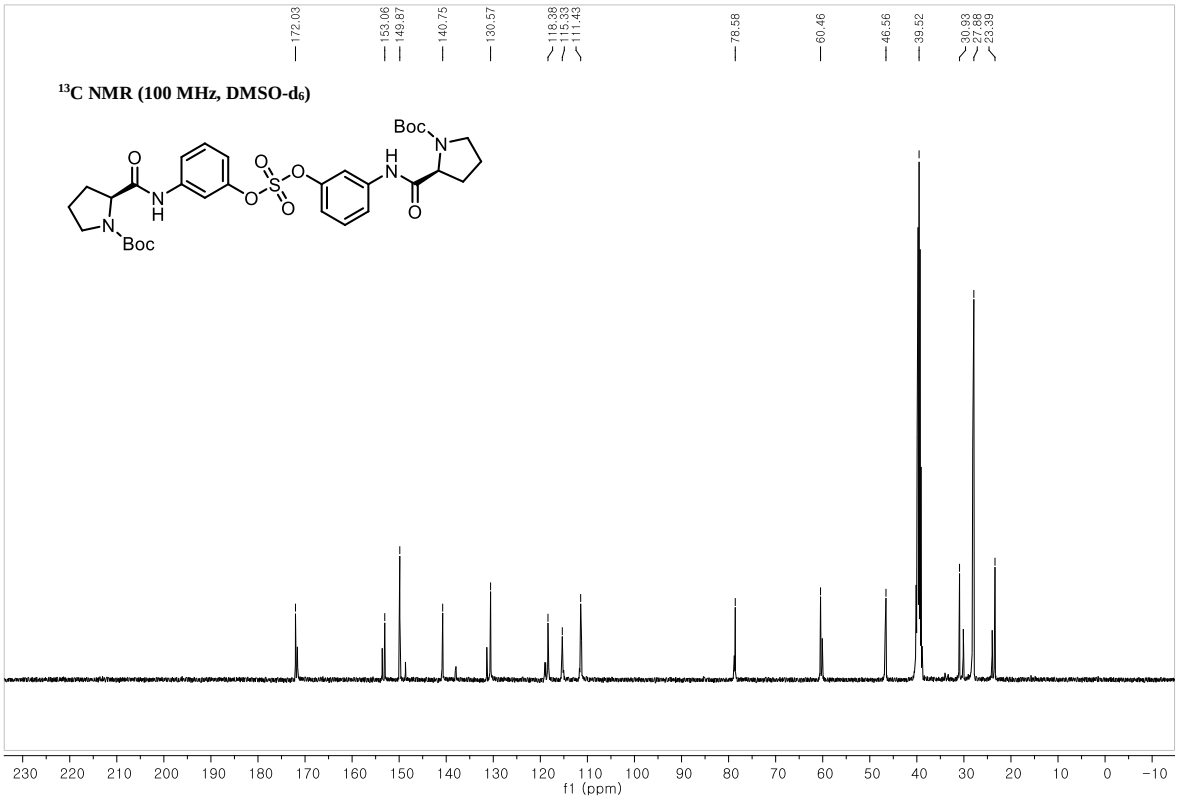


Boc

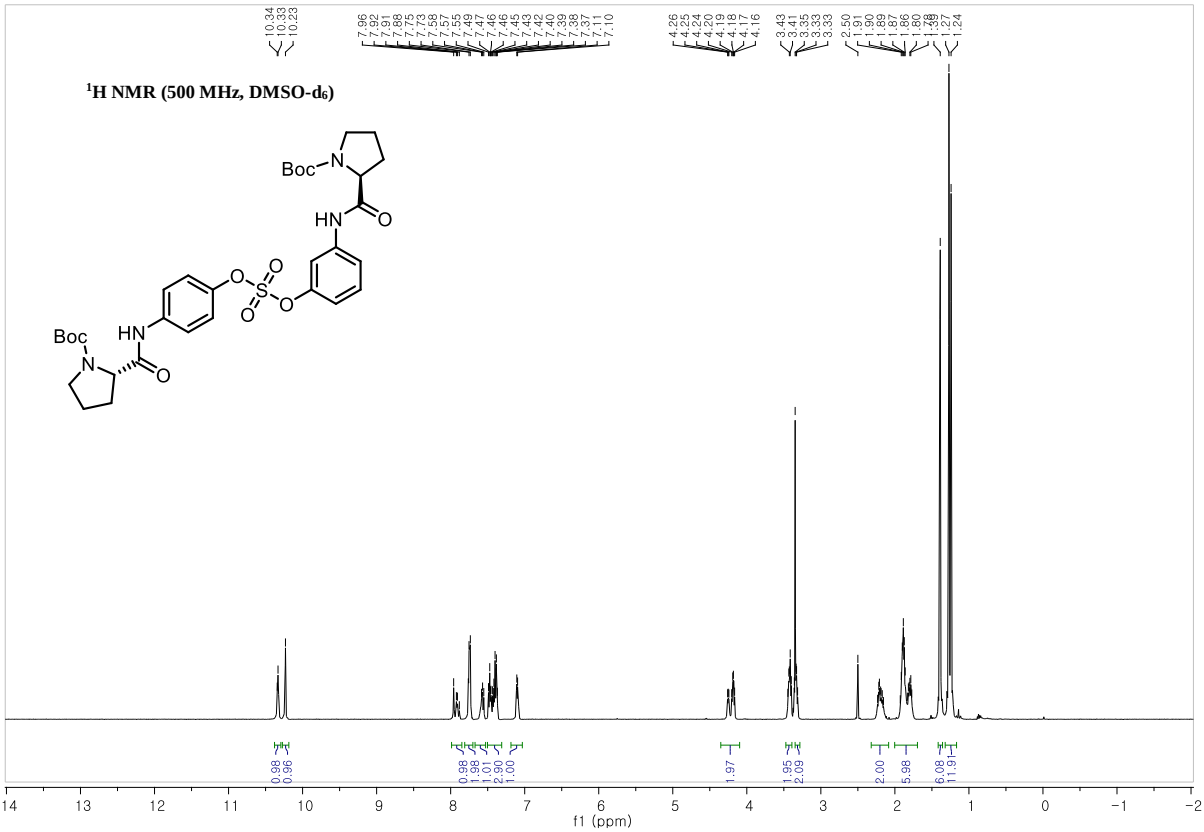


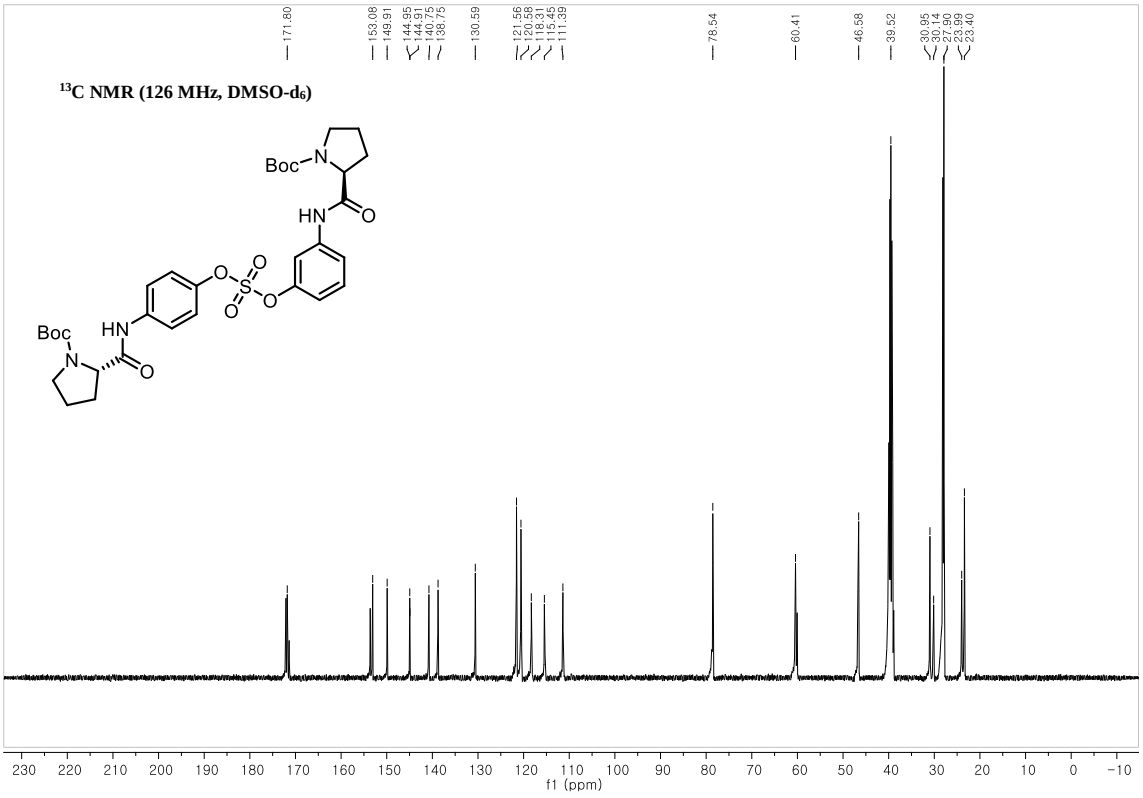
Compound 10b



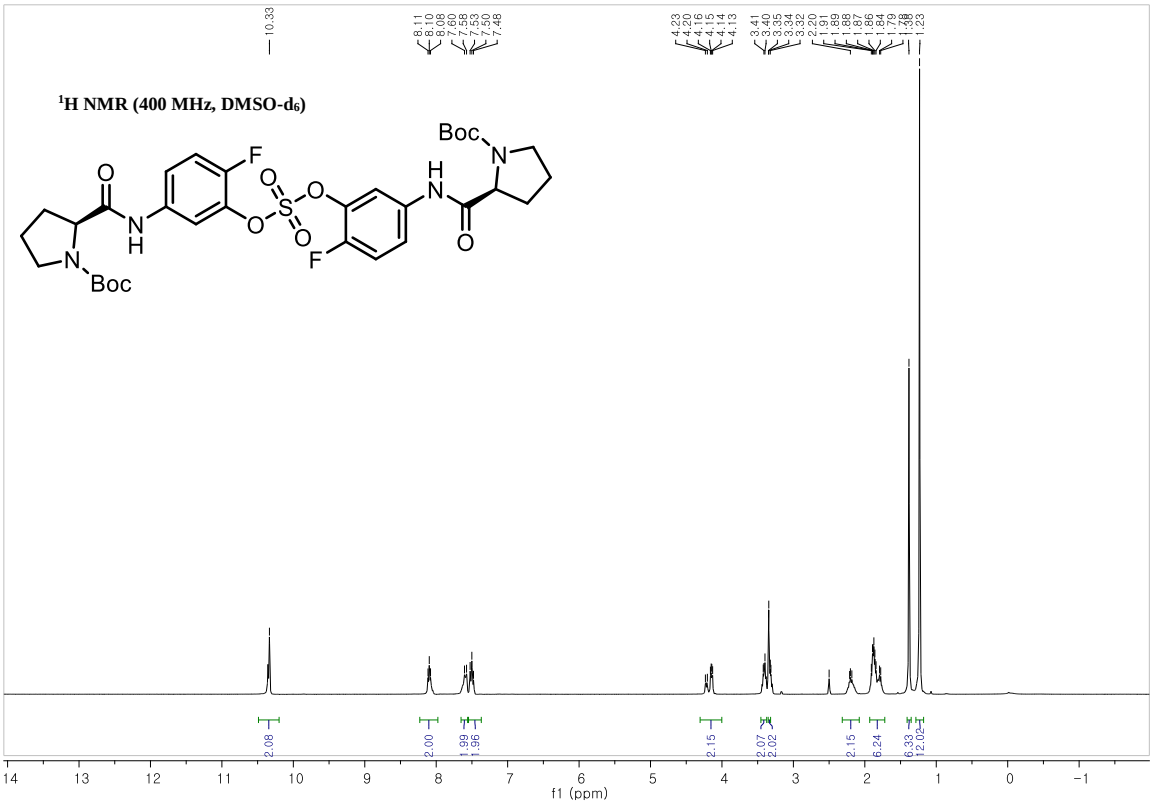


Compound 10c

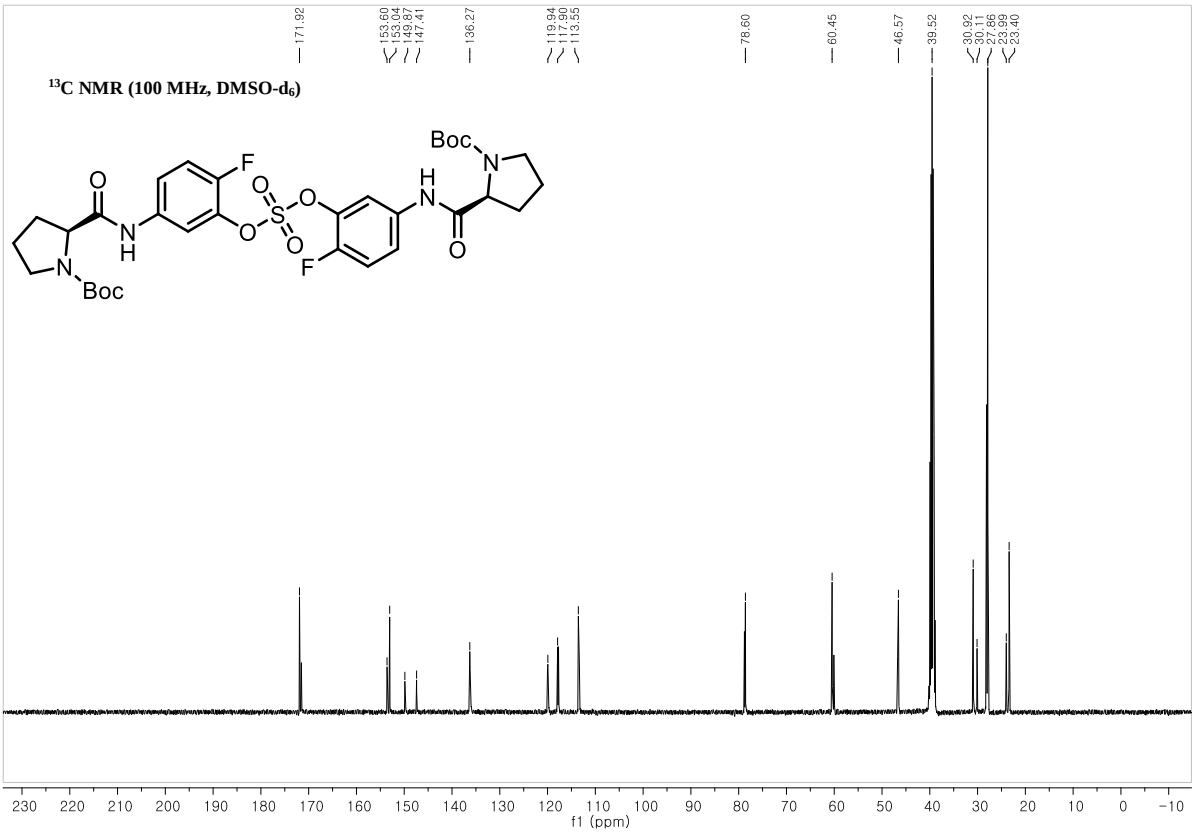




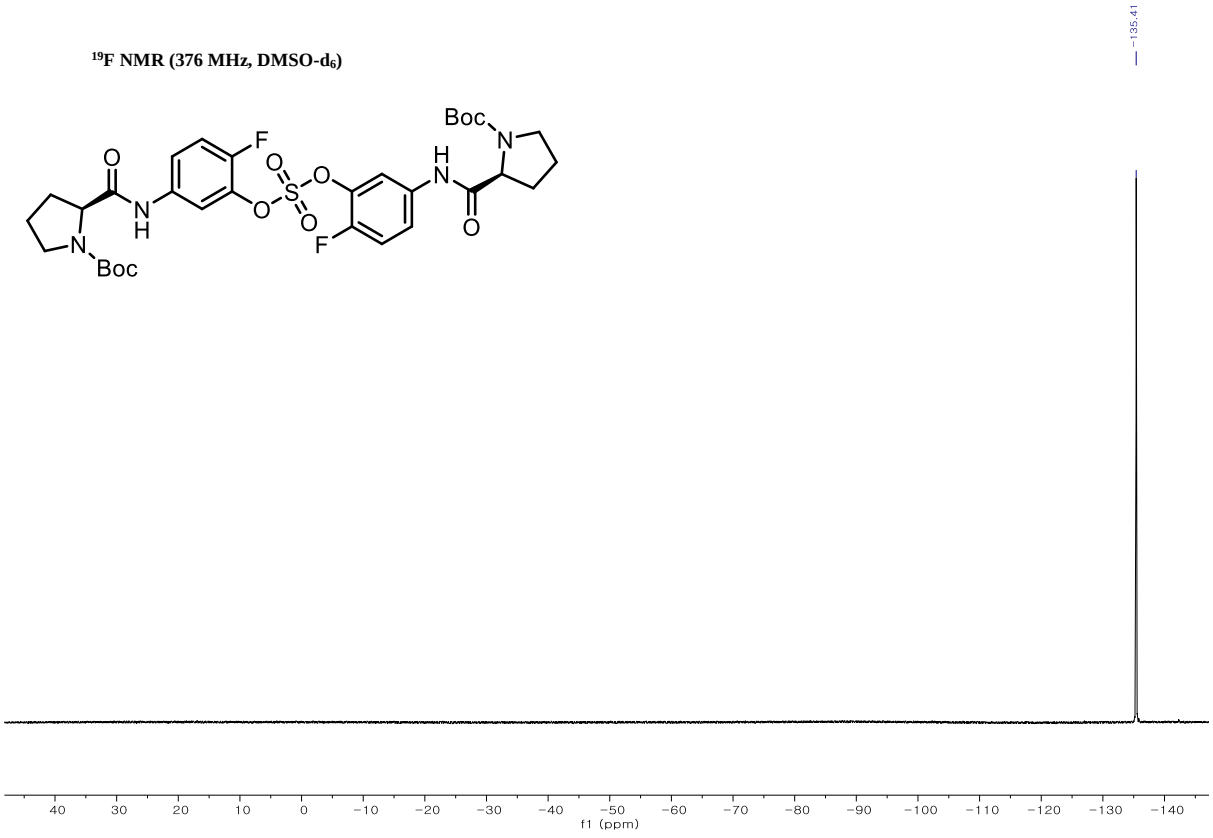
Compound 10d



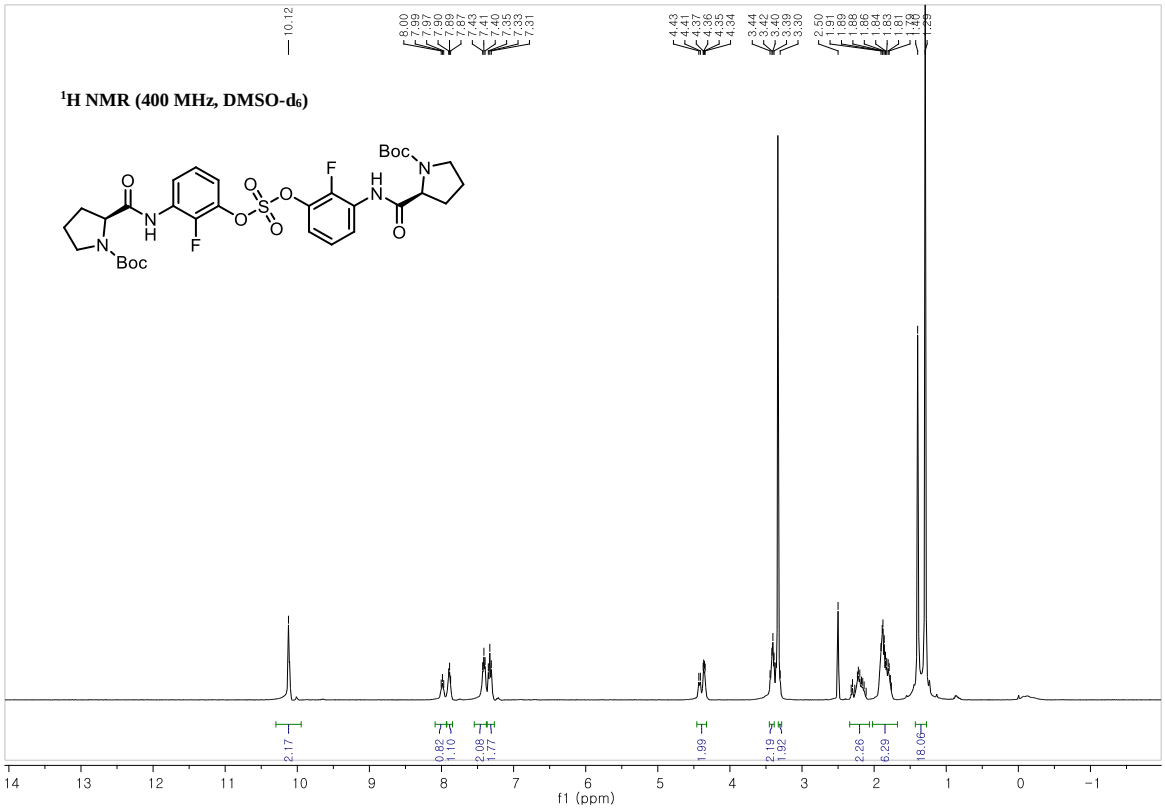
^{13}C NMR (100 MHz, DMSO-d_6)

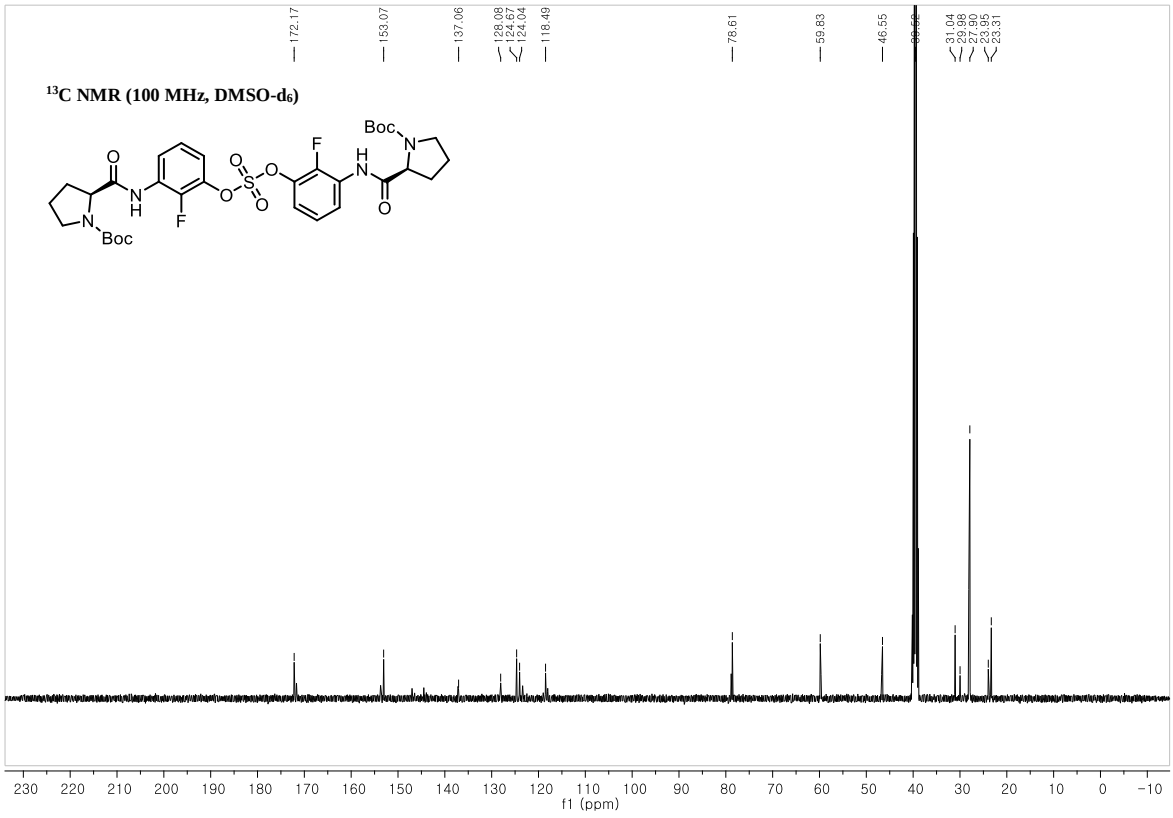


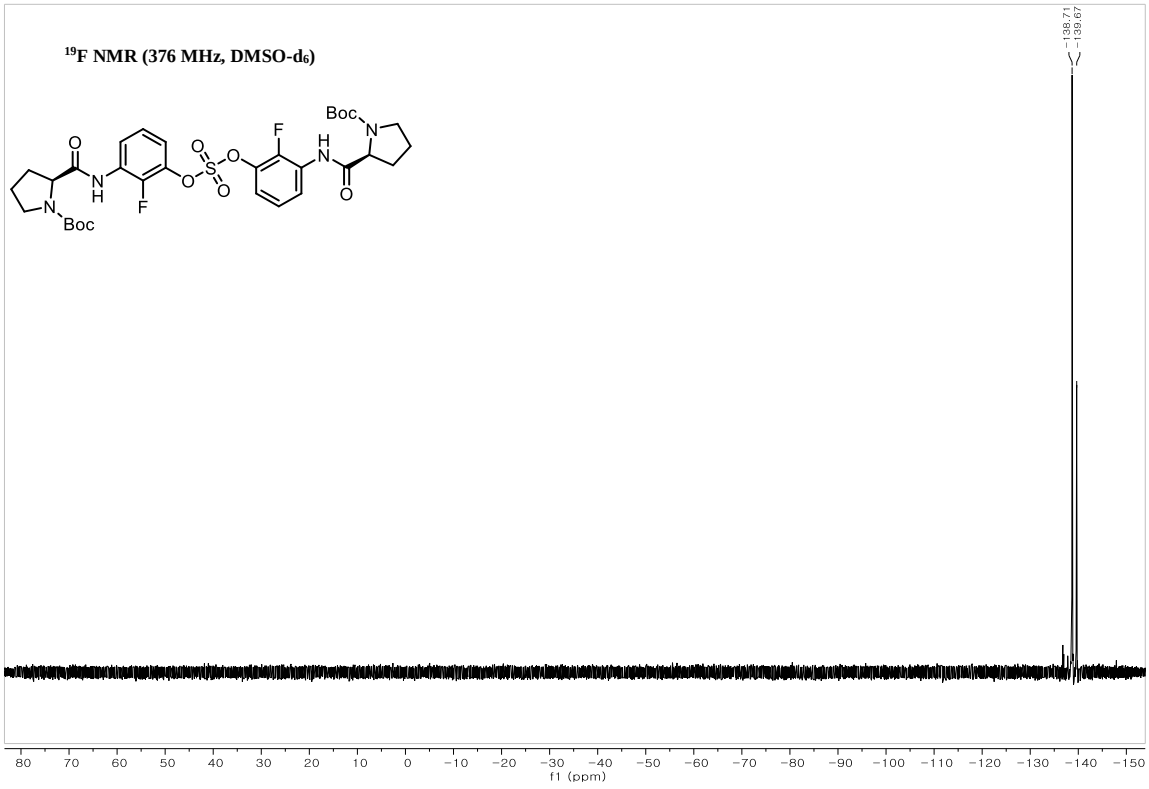
^{19}F NMR (376 MHz, DMSO-d_6)



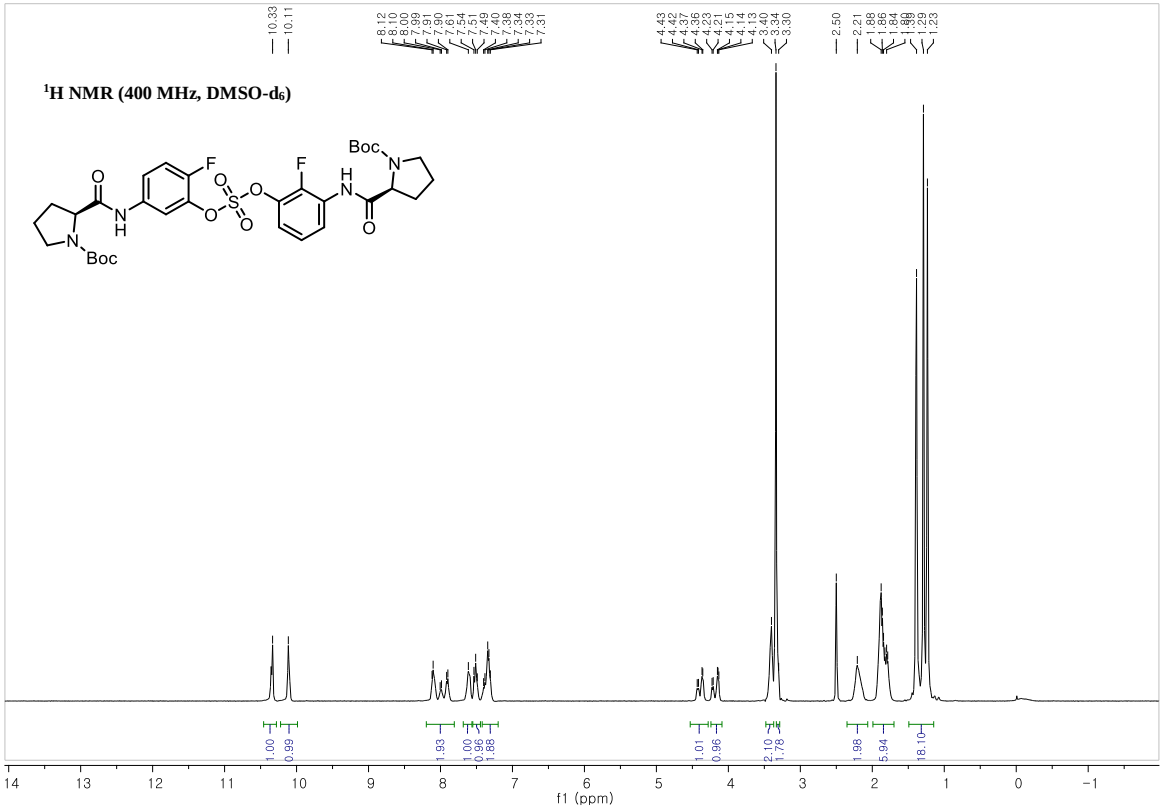
Compound 10e



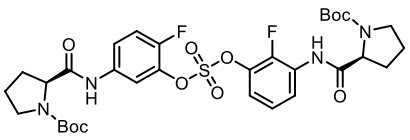




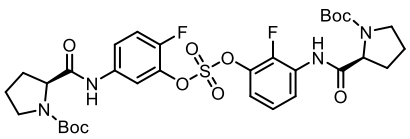
Compound 10f



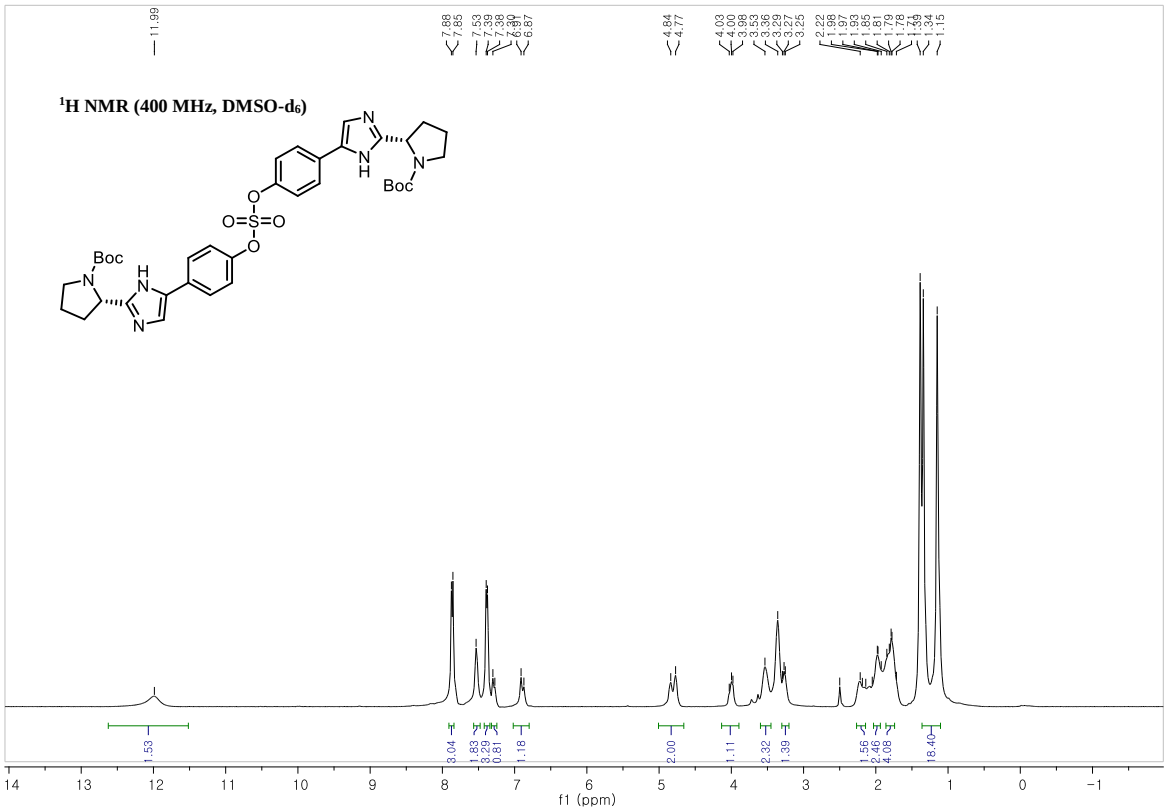
^{13}C NMR (100 MHz, DMSO-d$_6$)

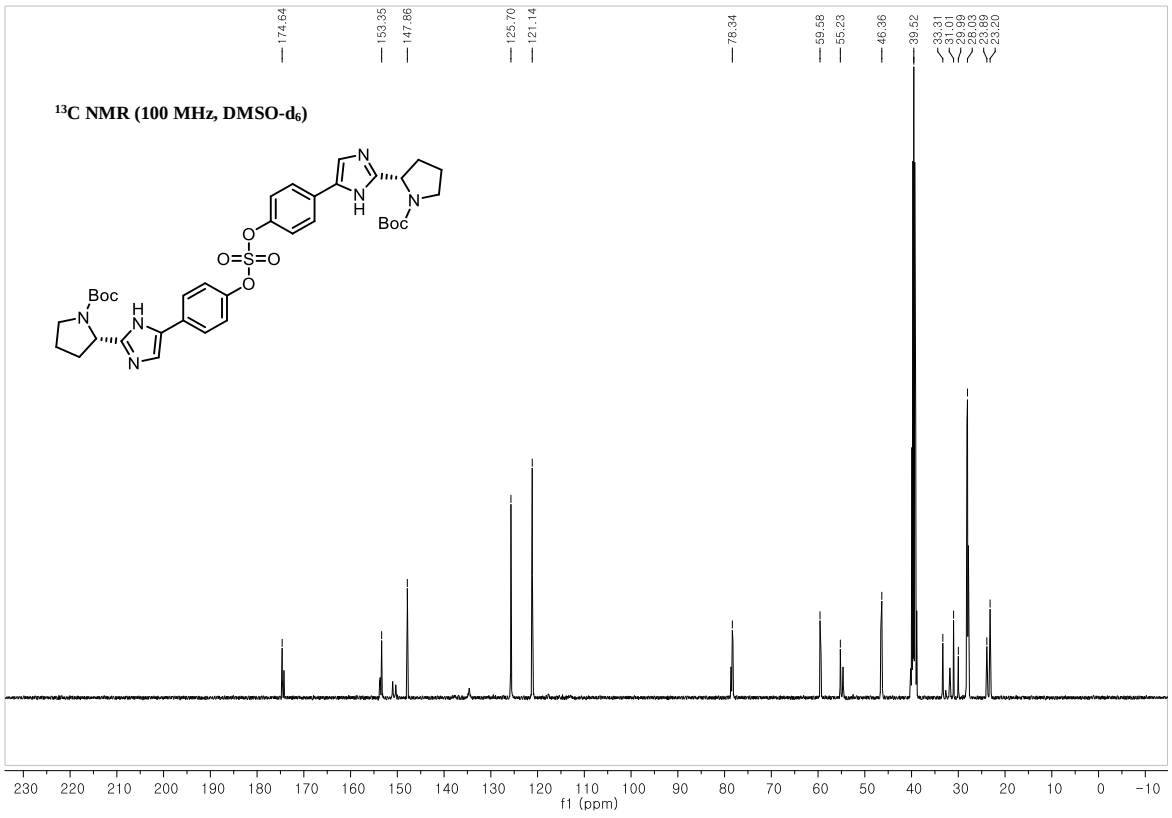


^{19}F NMR (376 MHz, DMSO-d$_6$)

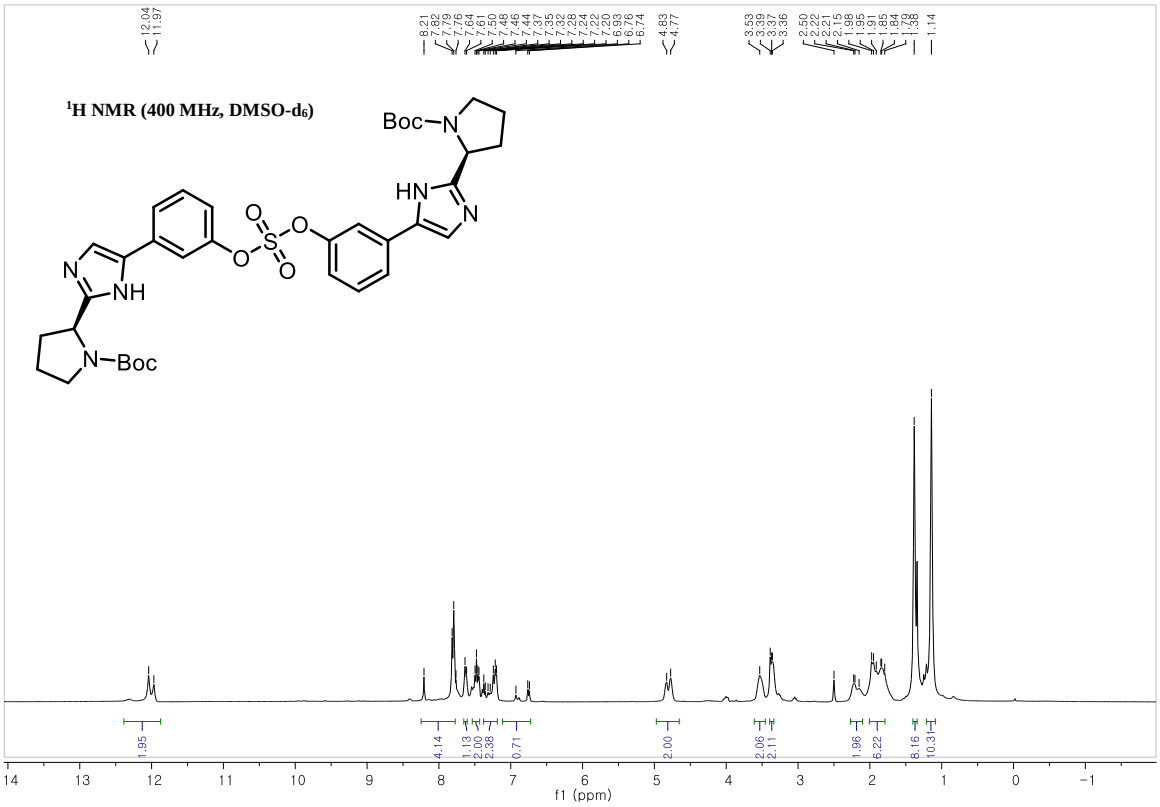


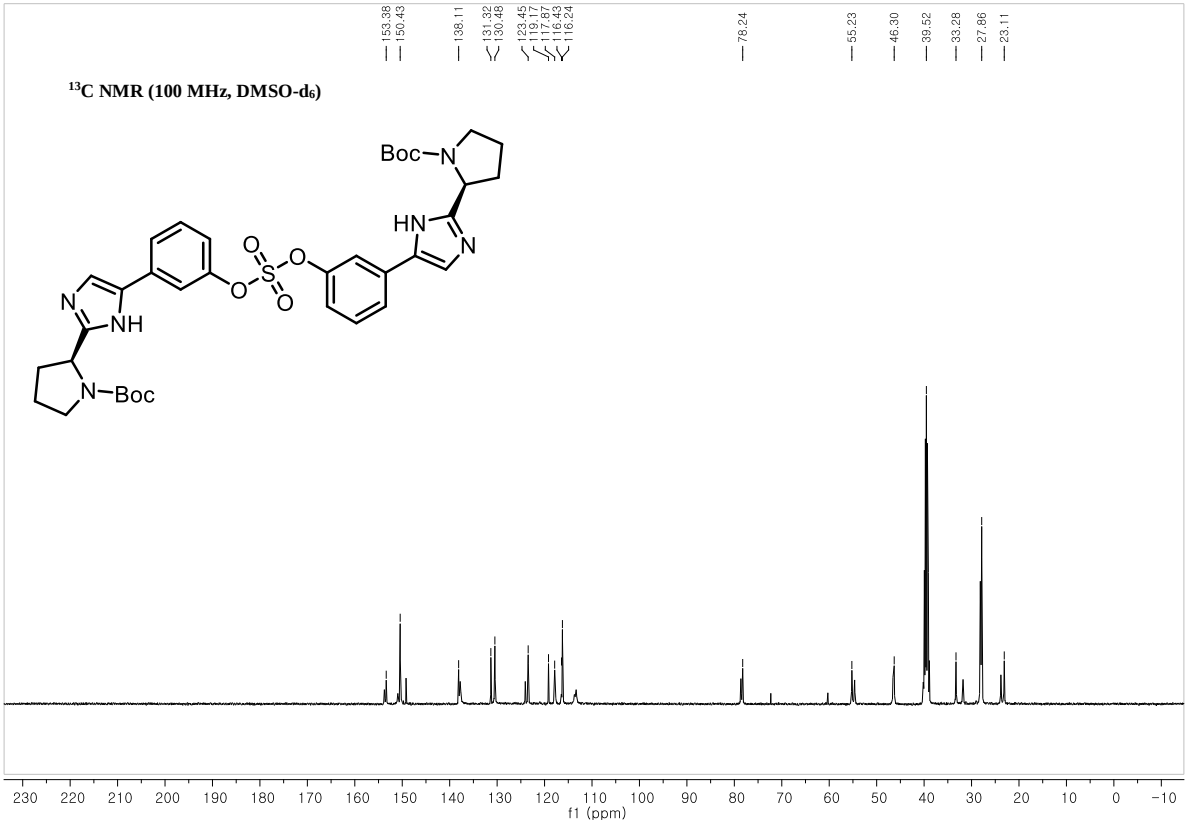
Compound 10g



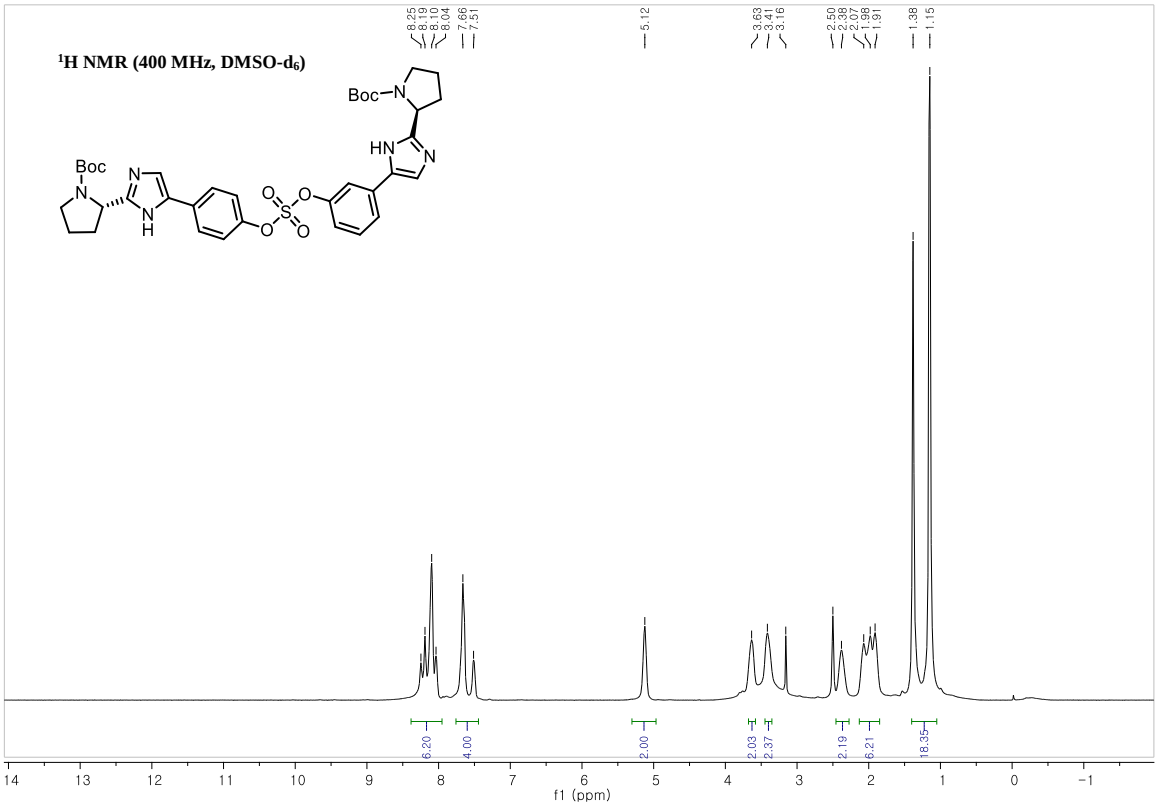


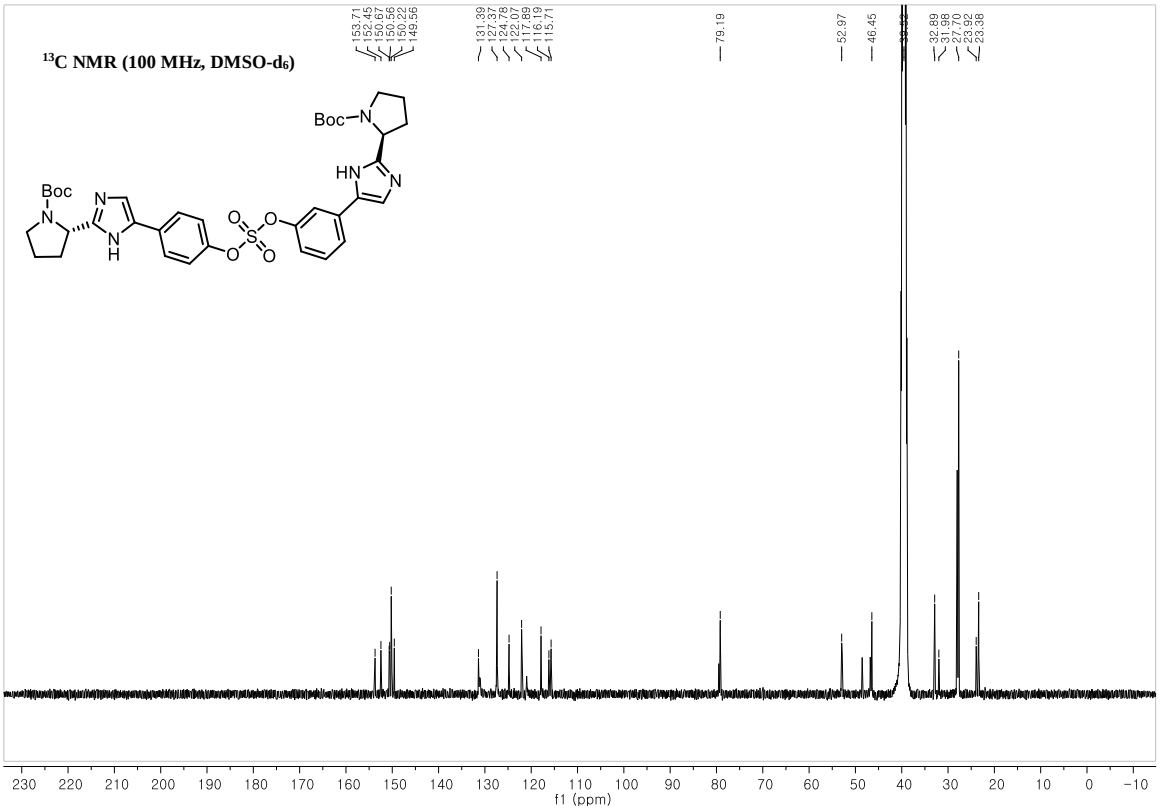
Compound 10h



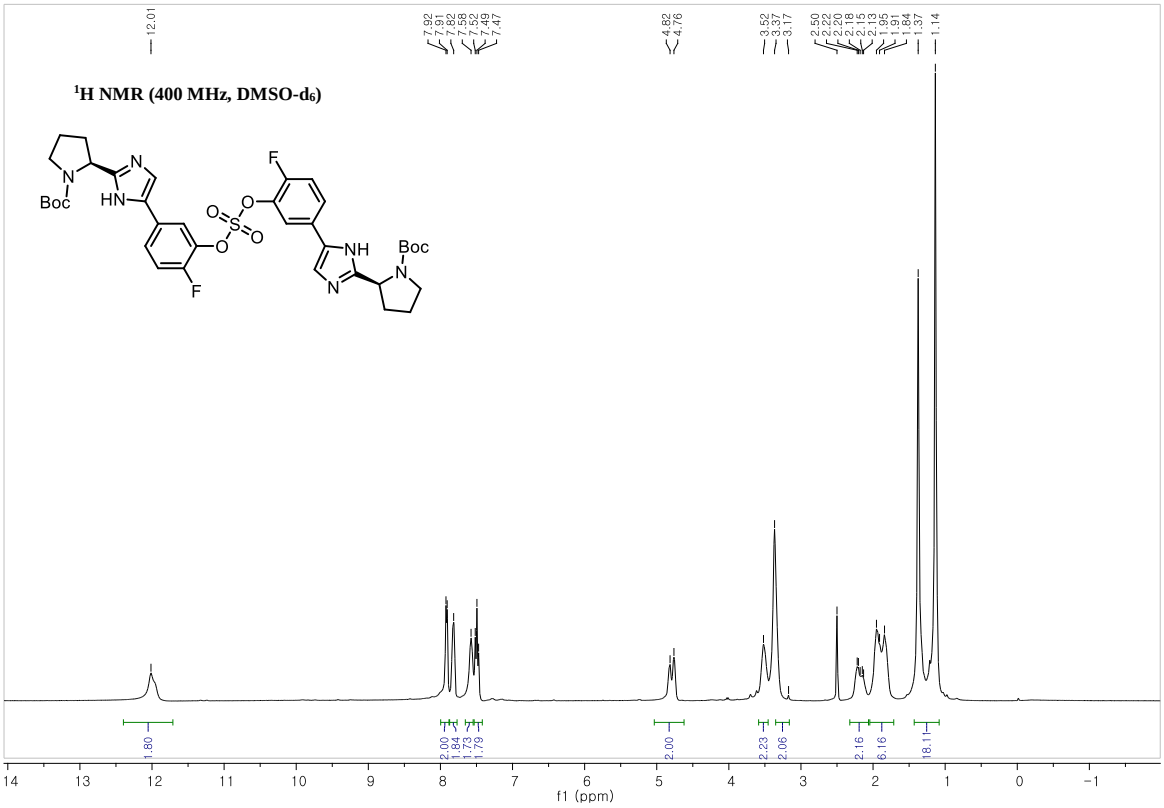


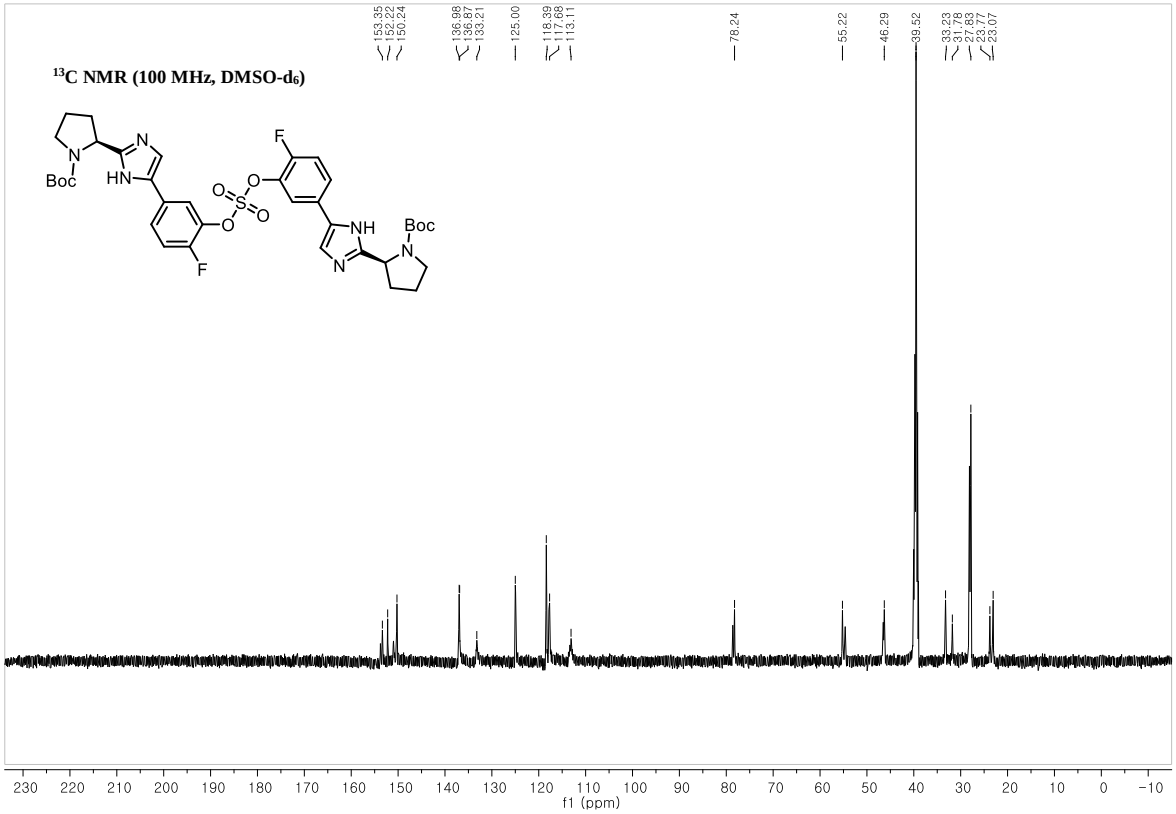
Compound 10i

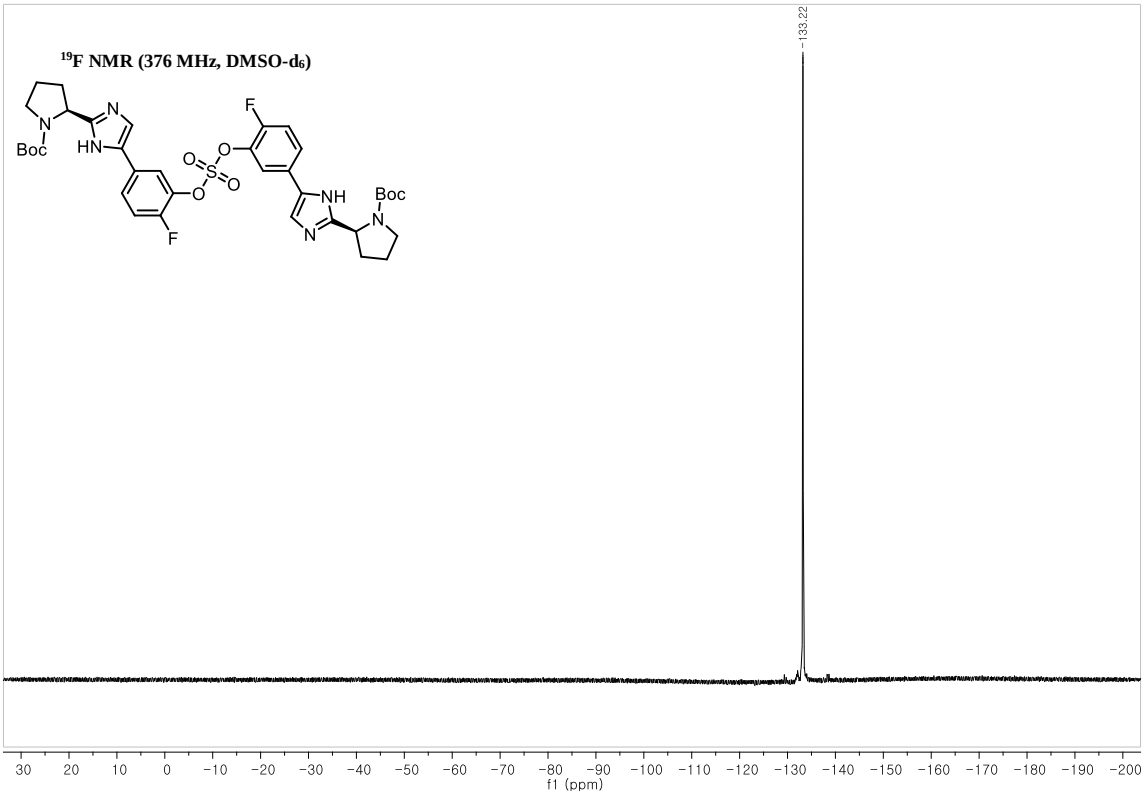




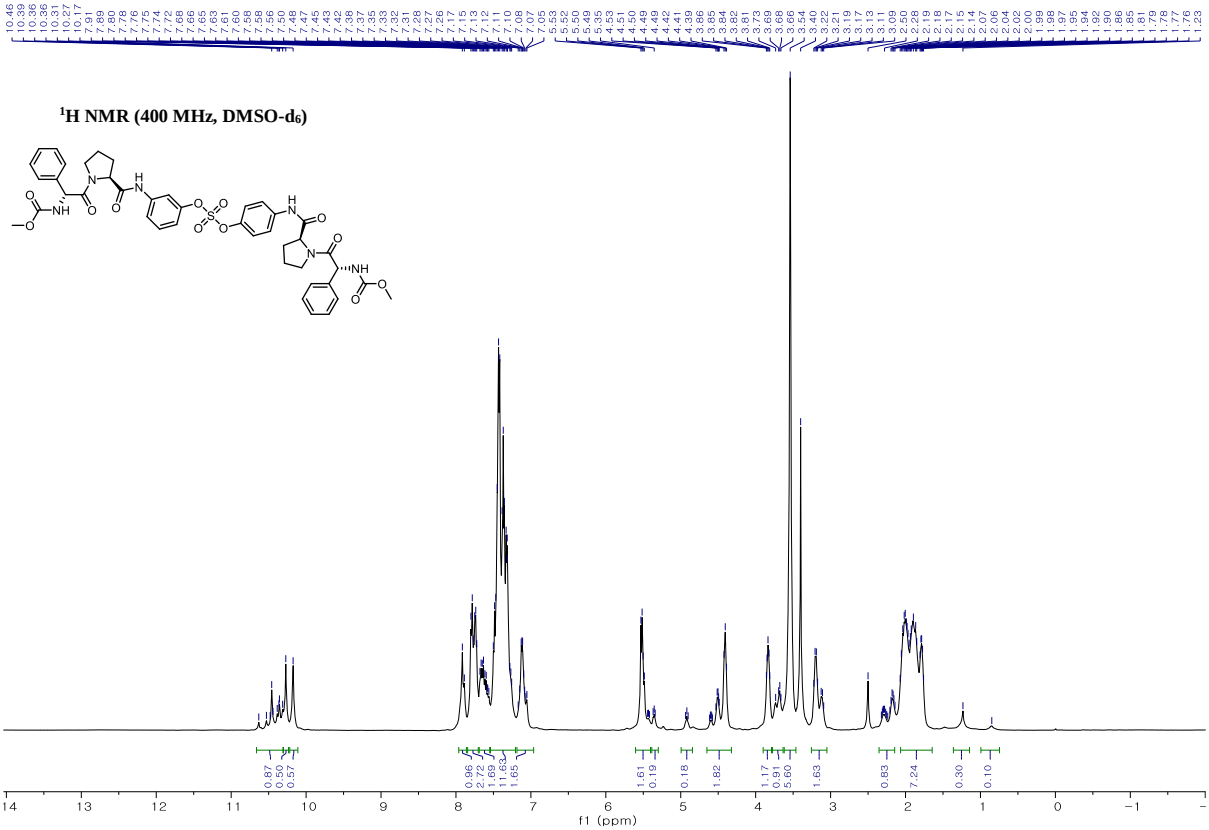
Compound 10j

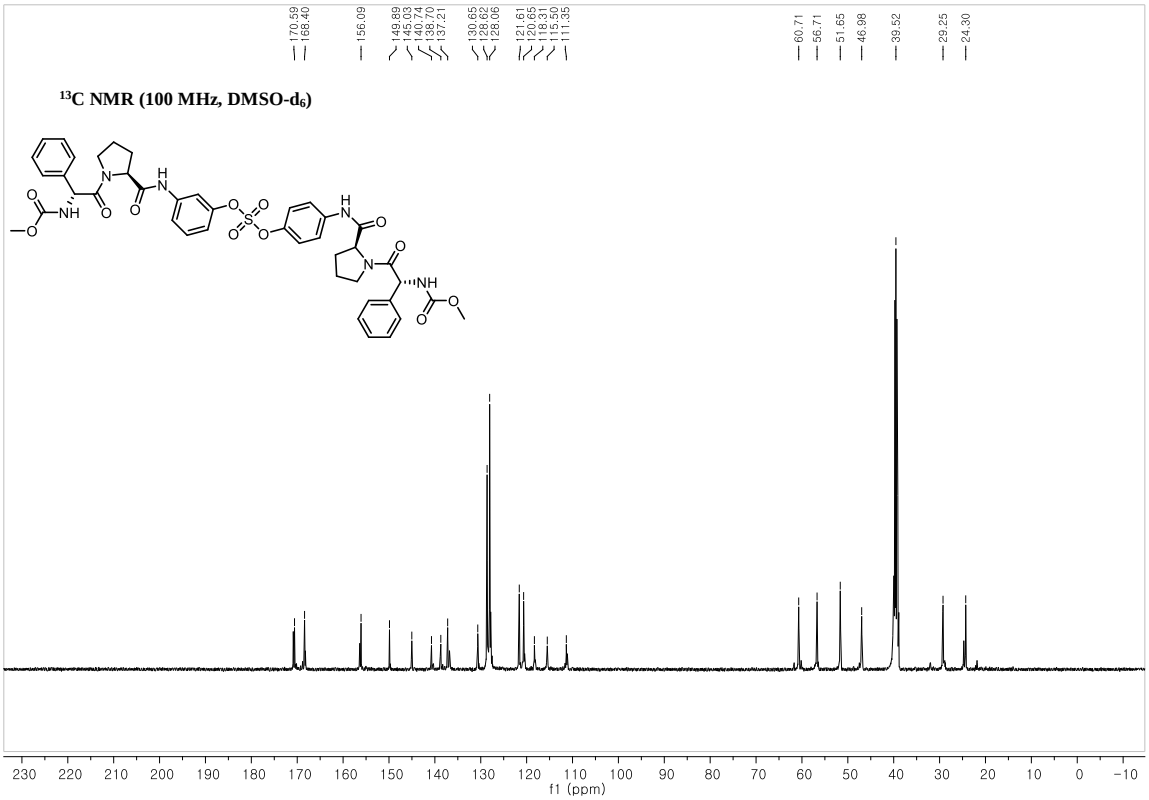




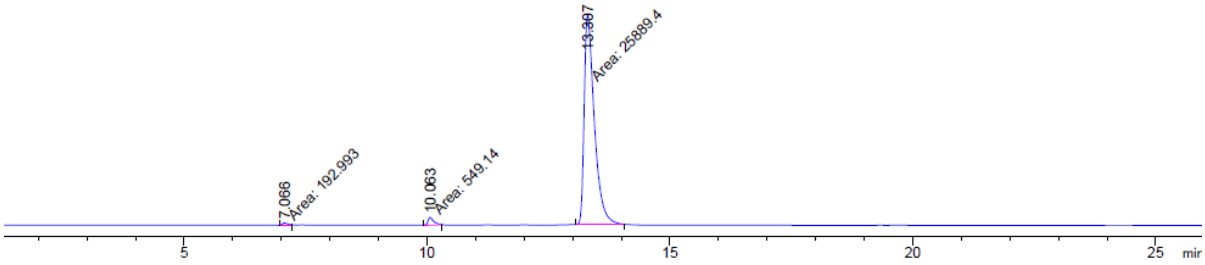

19F NMR (376 MHz, DMSO-d6)
-133.22
f1 (ppm)

Compound 11

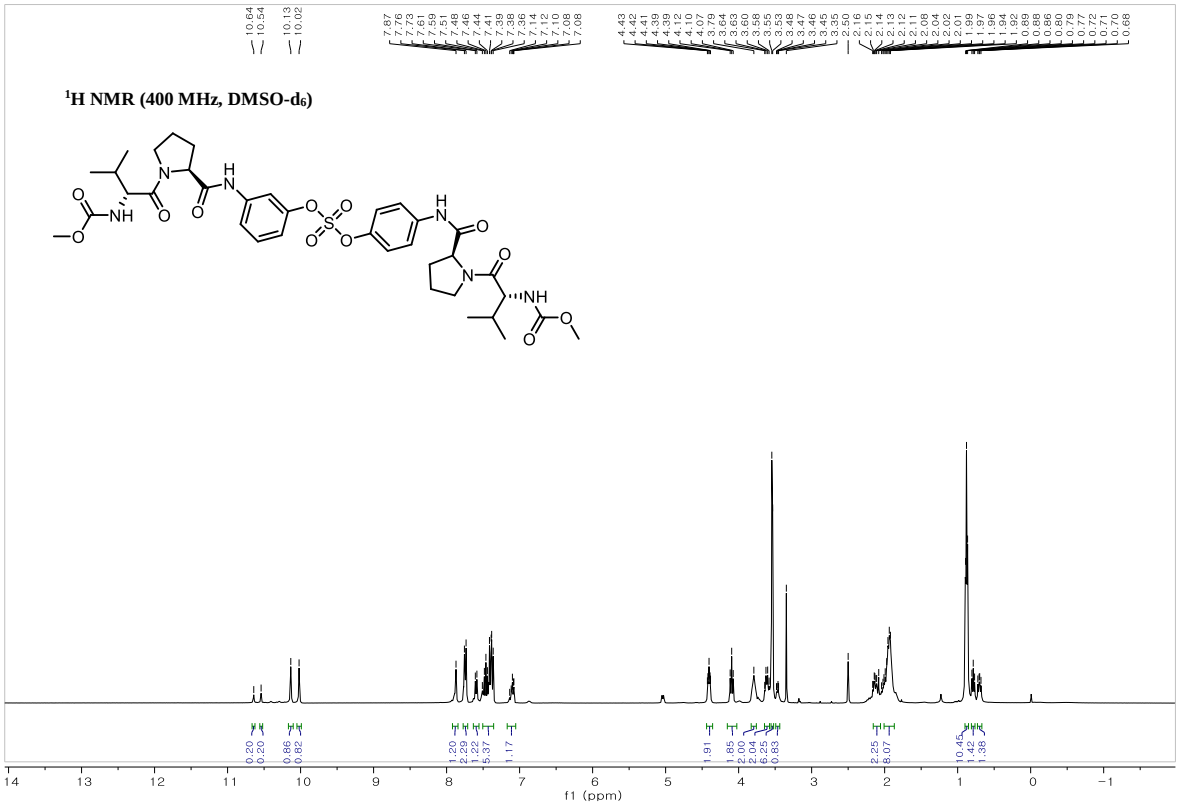

1H NMR (400 MHz, DMSO-d6)
f1 (ppm)

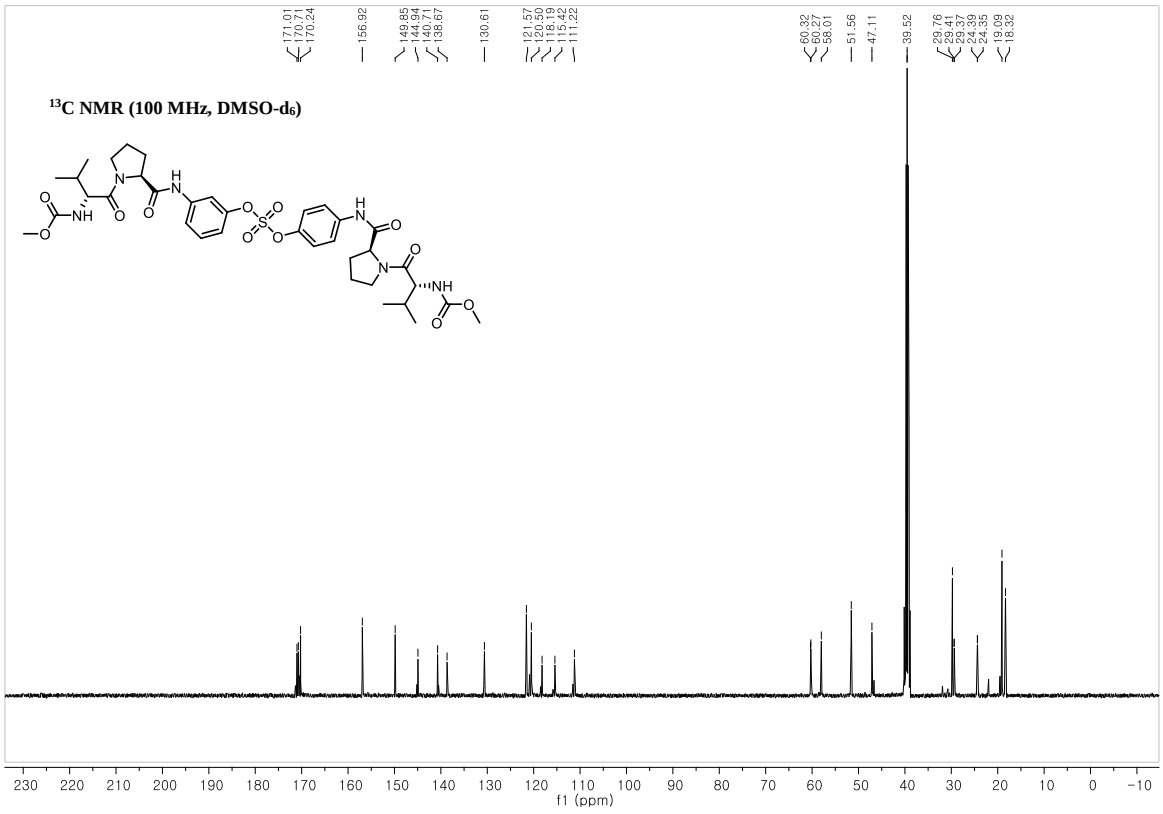


HPLC (compound 11, wavelength = 254 nm)

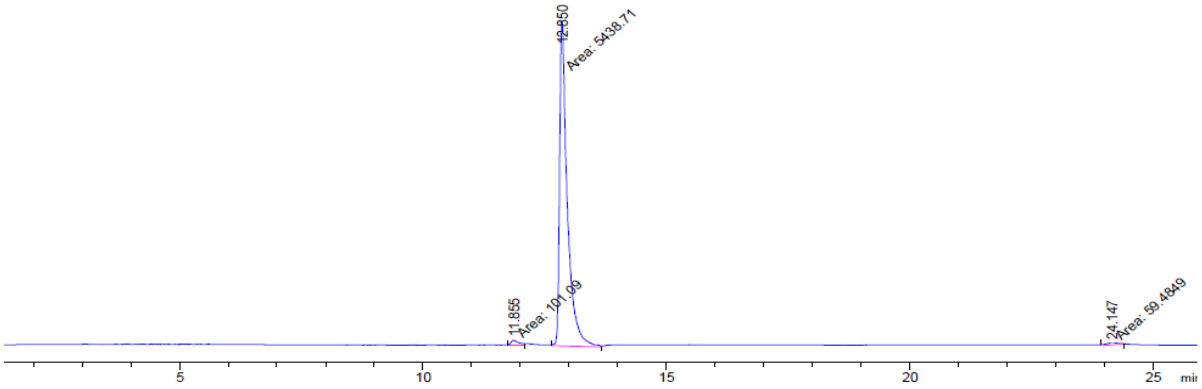


Compound 12

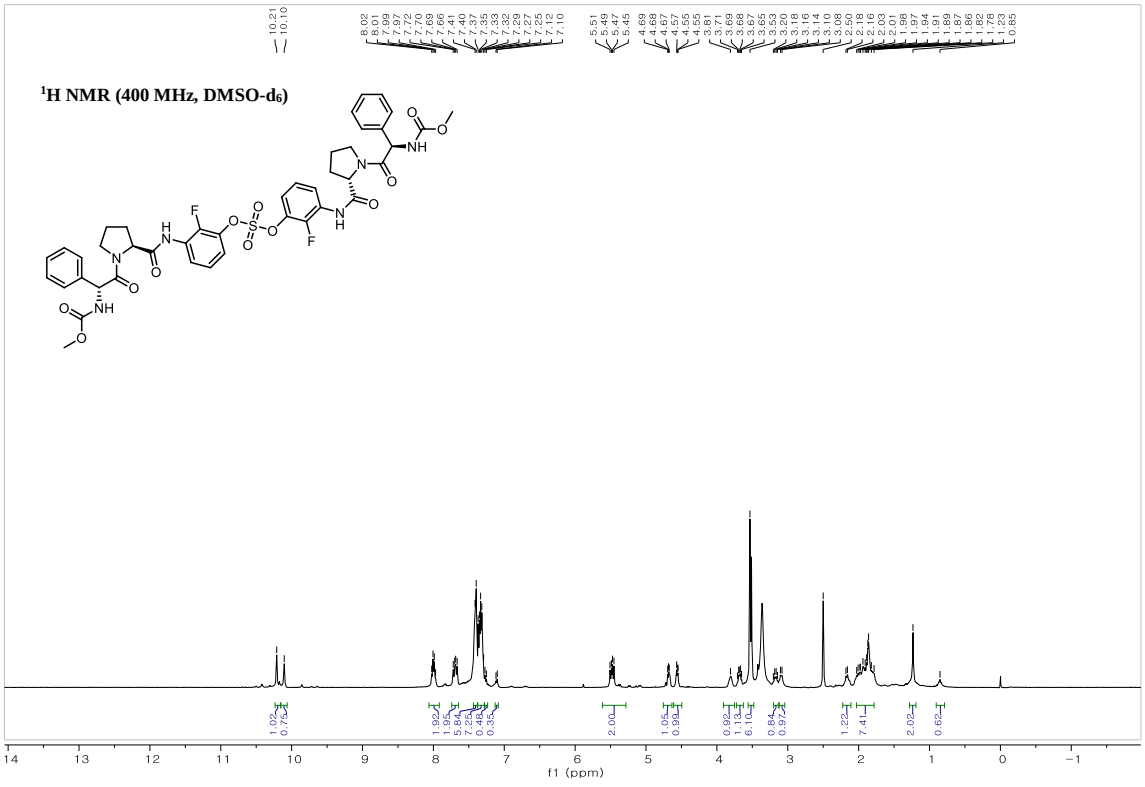




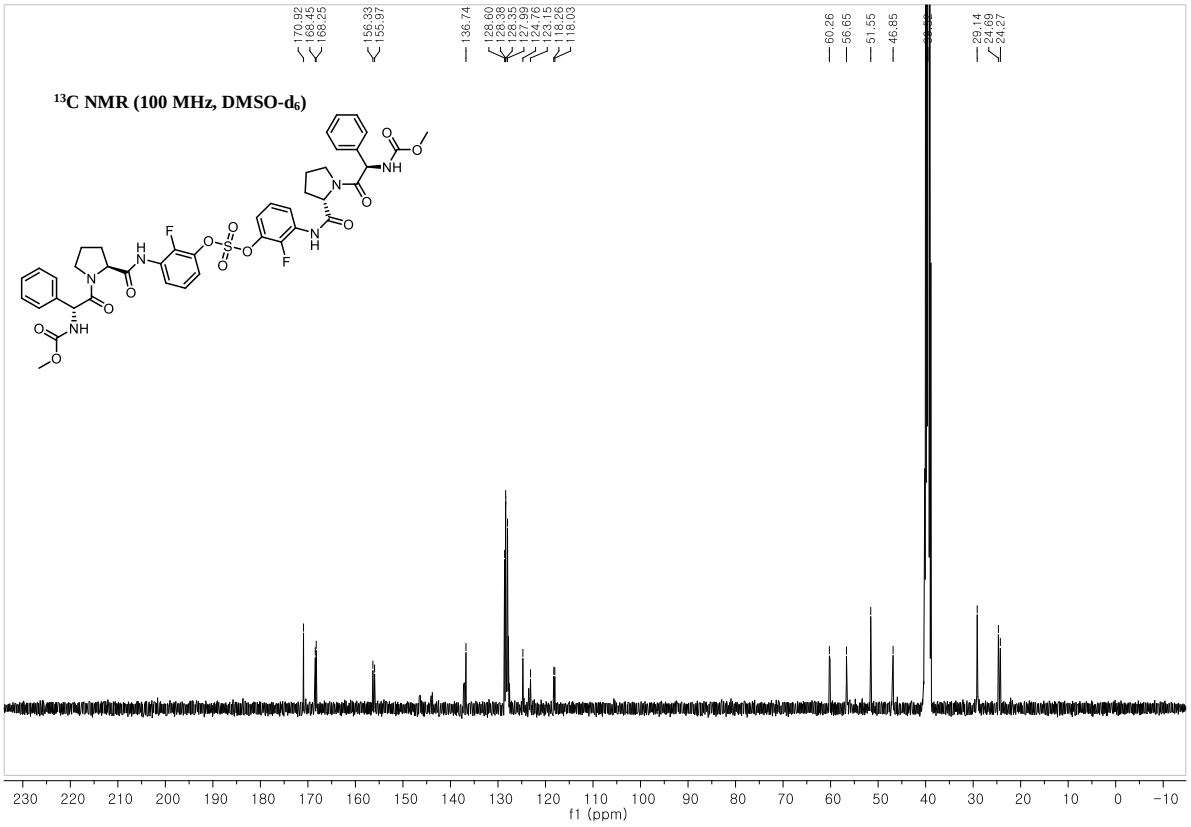
HPLC (compound 12, wavelength = 254 nm)



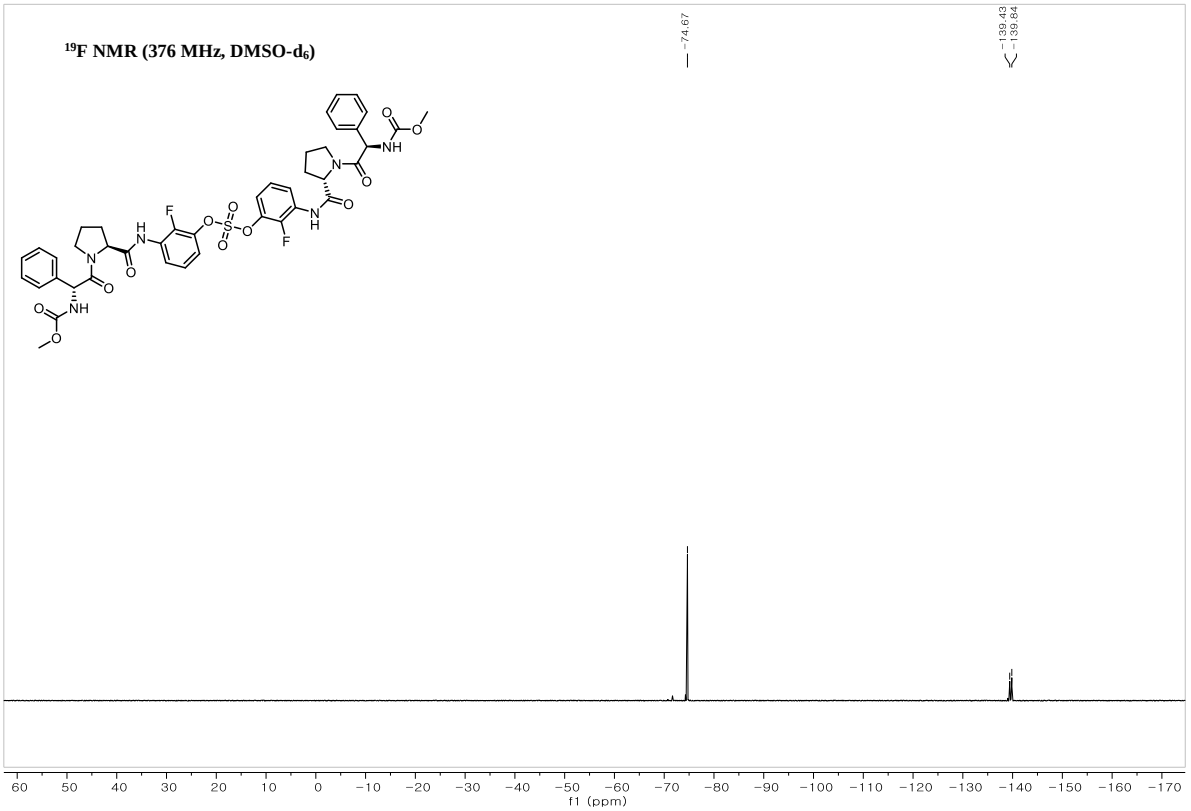
Compound 13



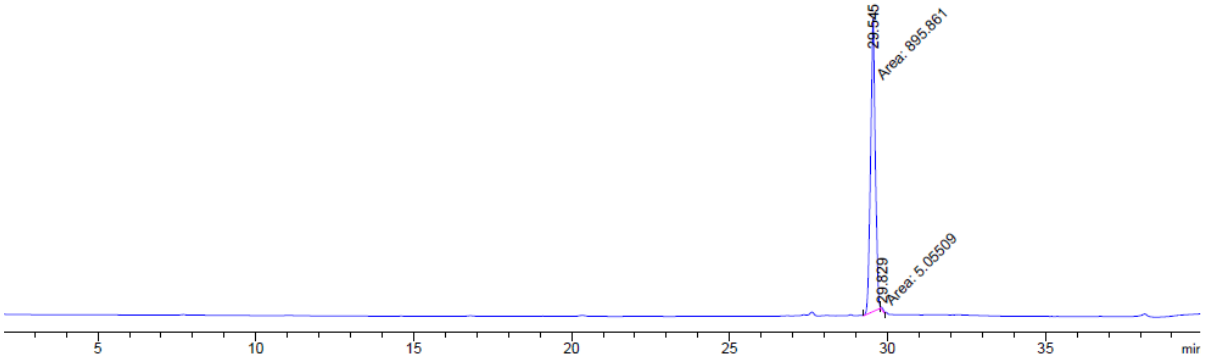
^{13}C NMR (100 MHz, DMSO-d_6)



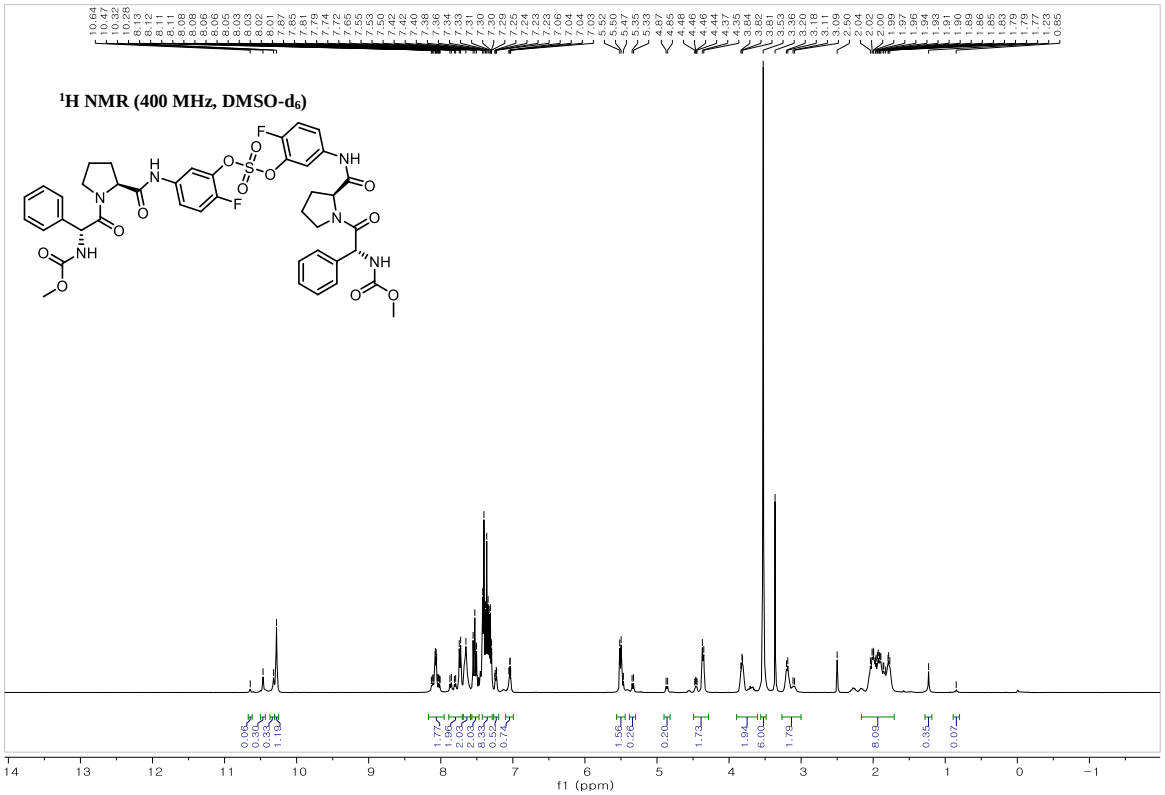
^{19}F NMR (376 MHz, DMSO-d_6)



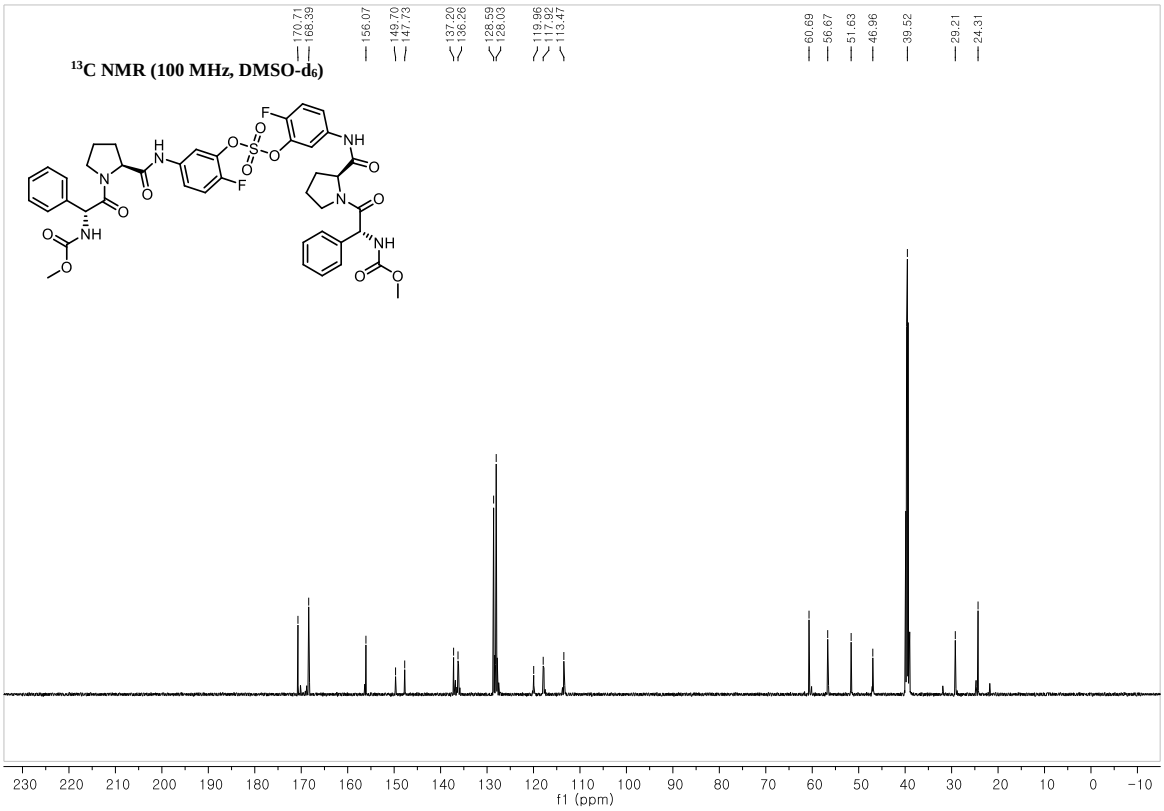
HPLC (compound 13, wavelength = 254 nm)



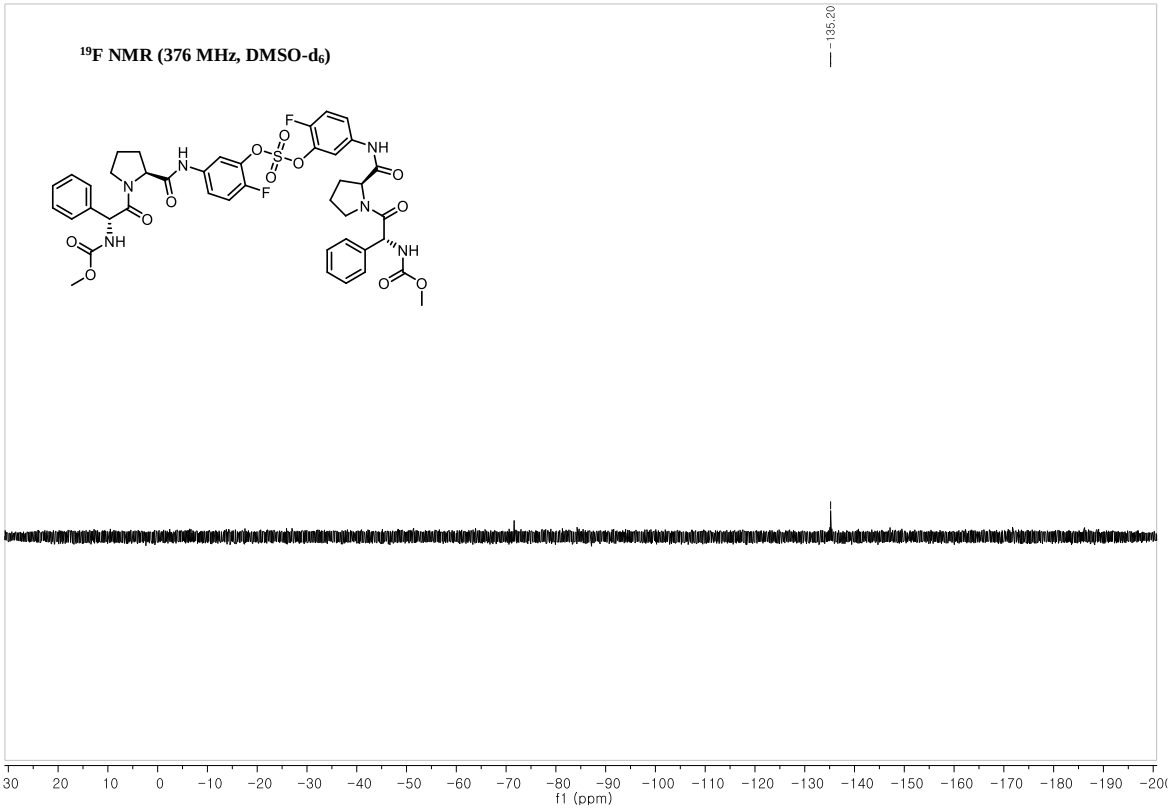
Compound 14



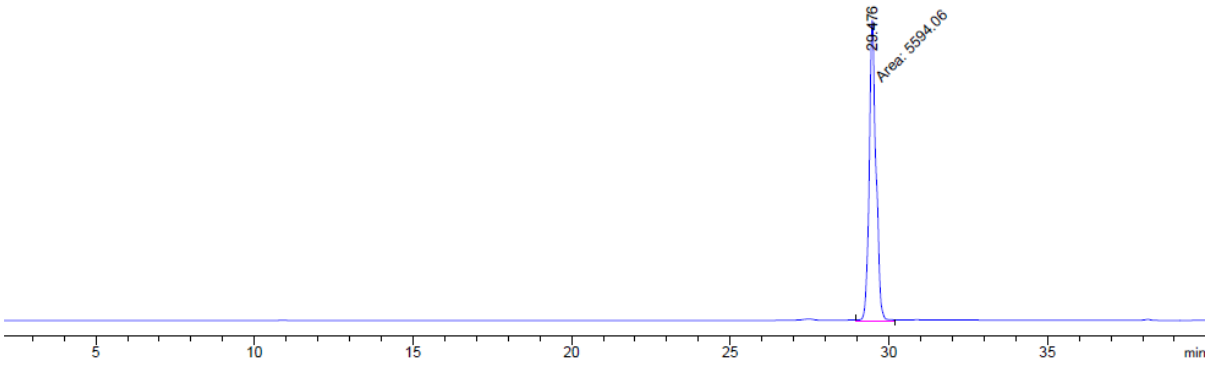
^{13}C NMR (100 MHz, DMSO-d$_6$)



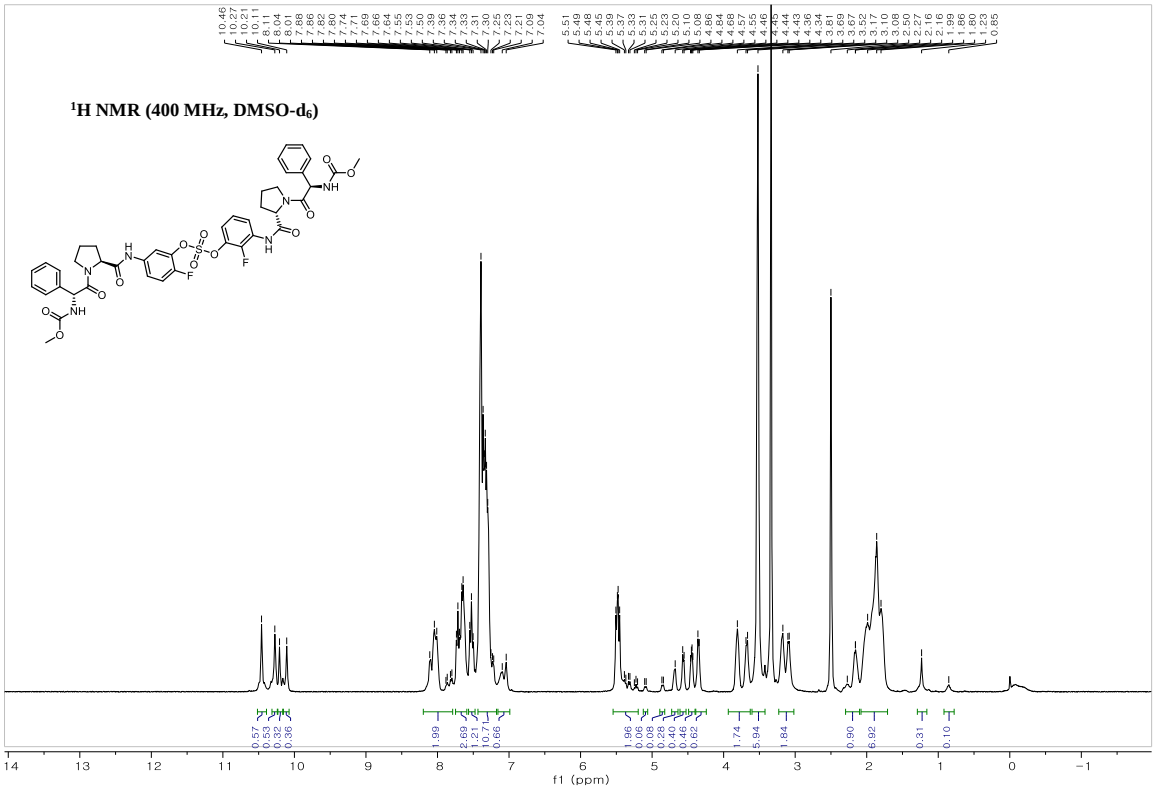
^{19}F NMR (376 MHz, DMSO-d$_6$)



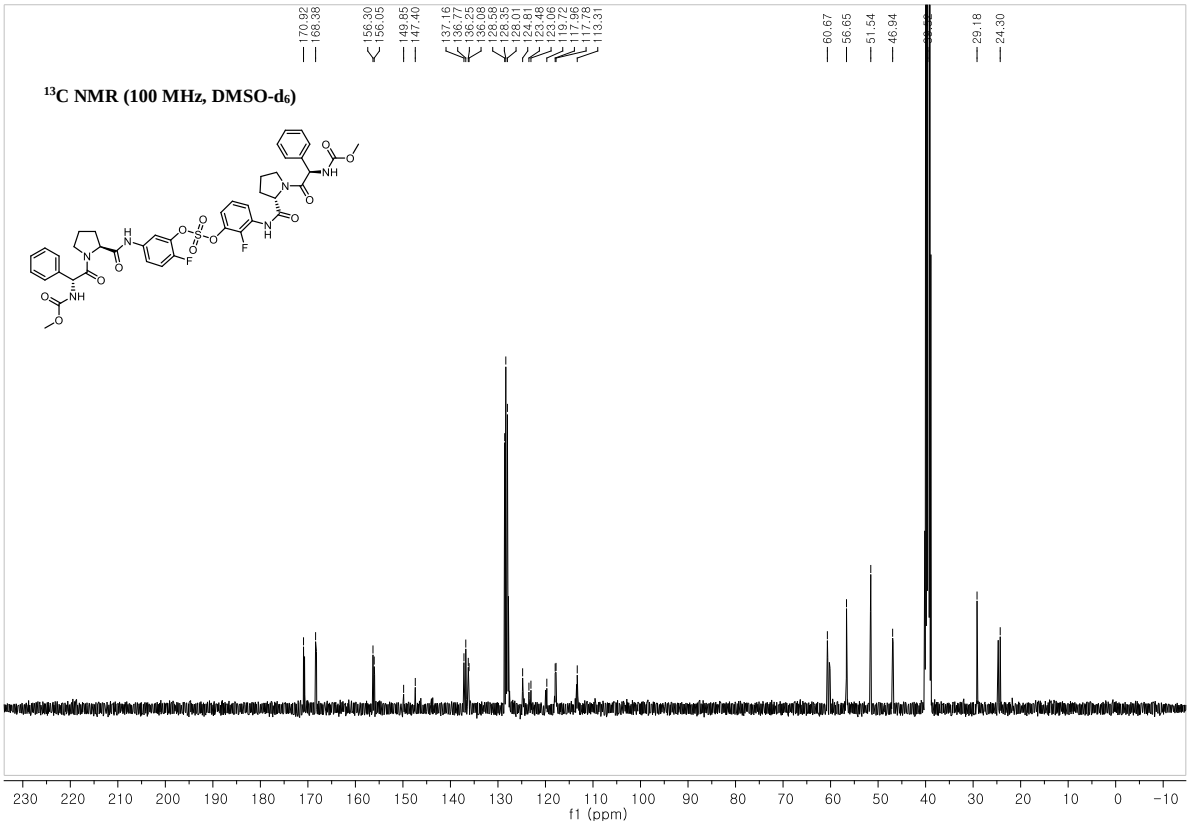
HPLC (compound 14, wavelength = 254 nm)



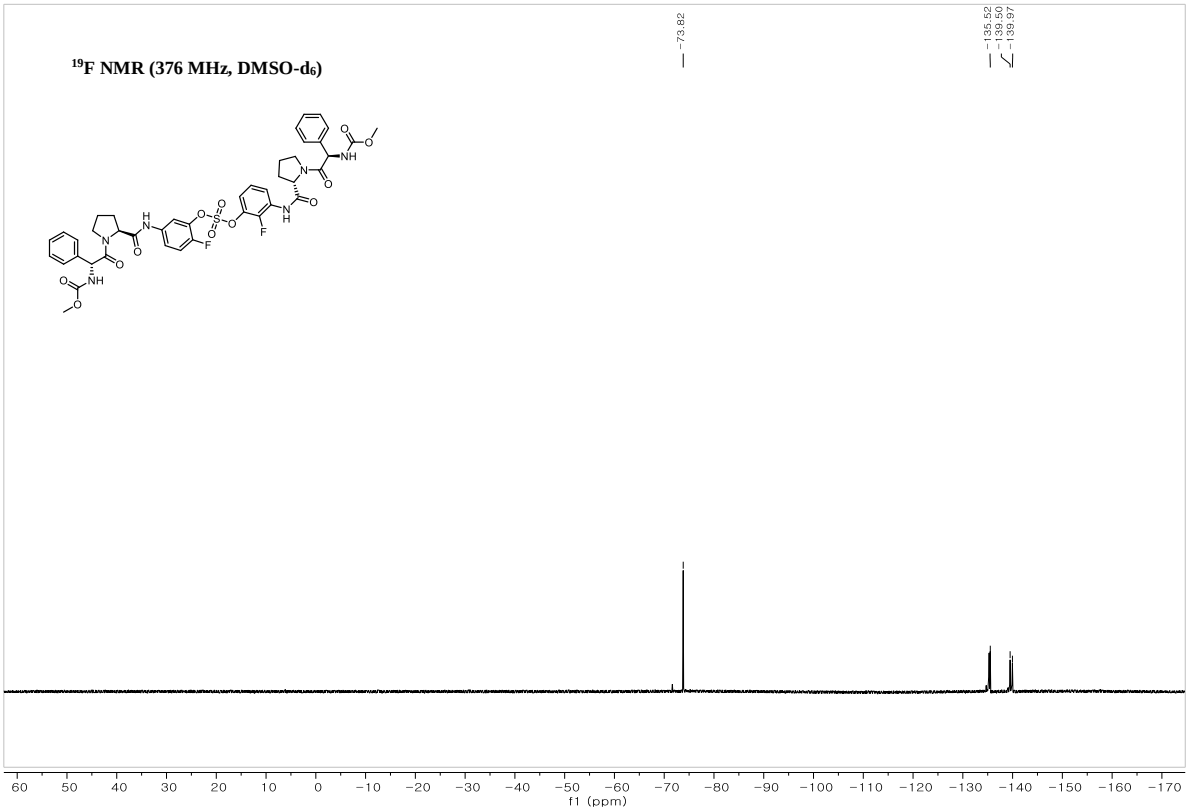
Compound 15



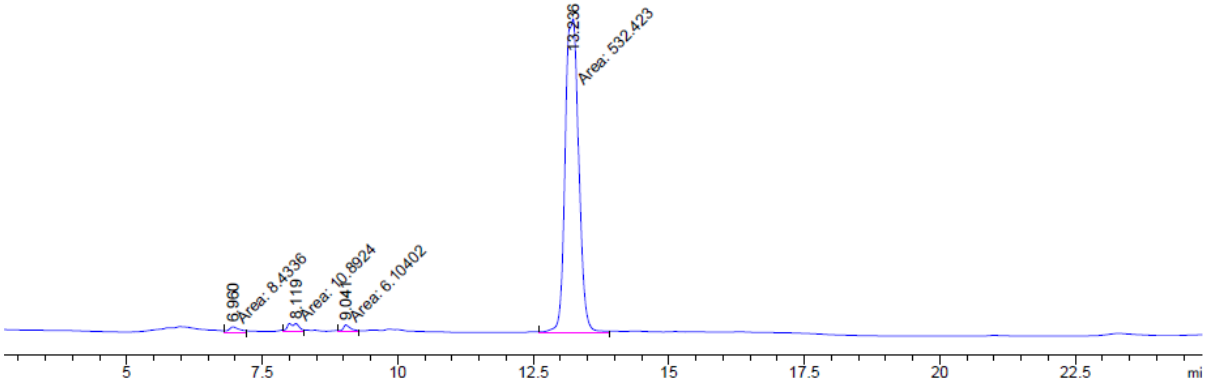
^{13}C NMR (100 MHz, DMSO-d$_6$)



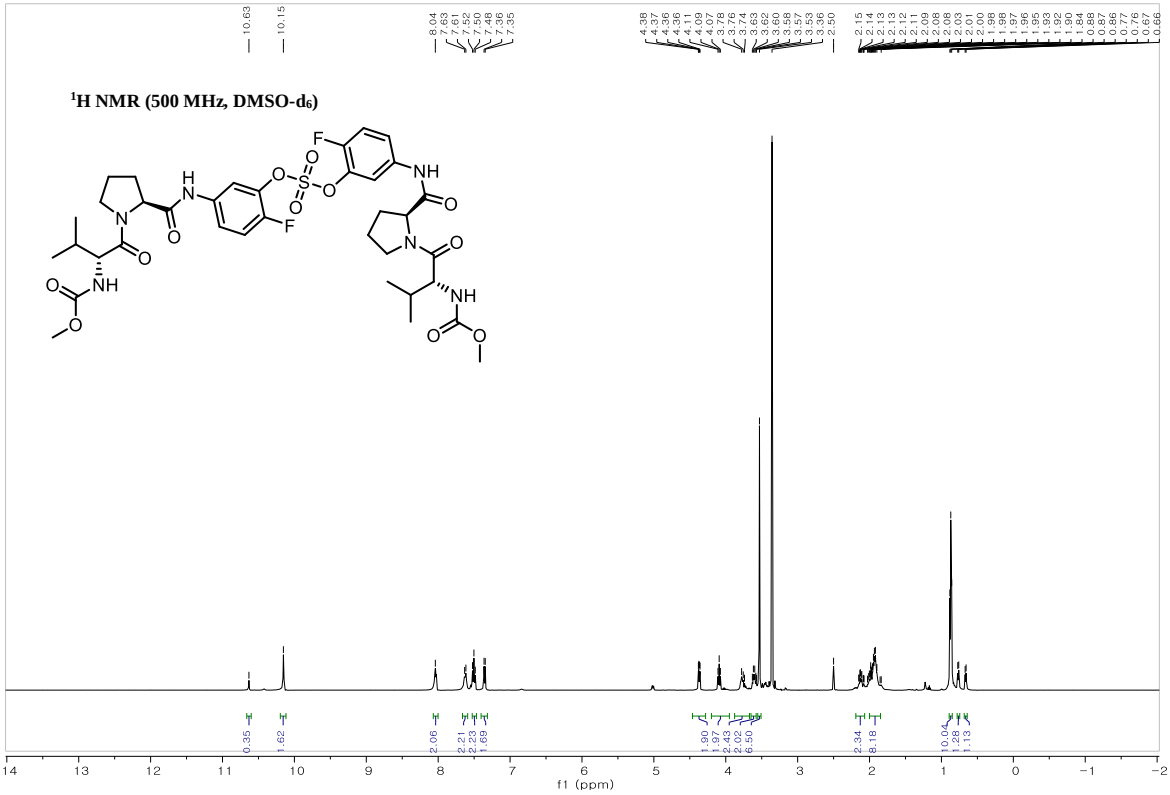
^{19}F NMR (376 MHz, DMSO-d$_6$)

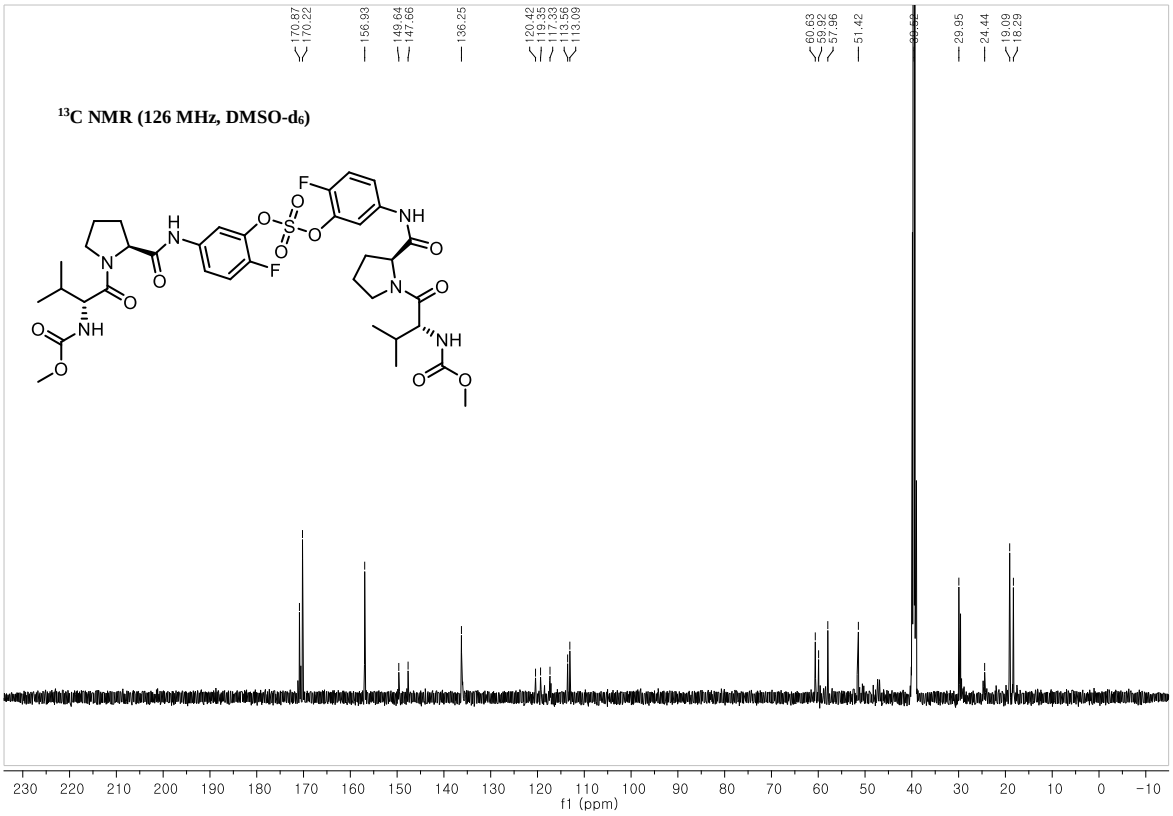


HPLC (compound 15, wavelength = 254 nm)

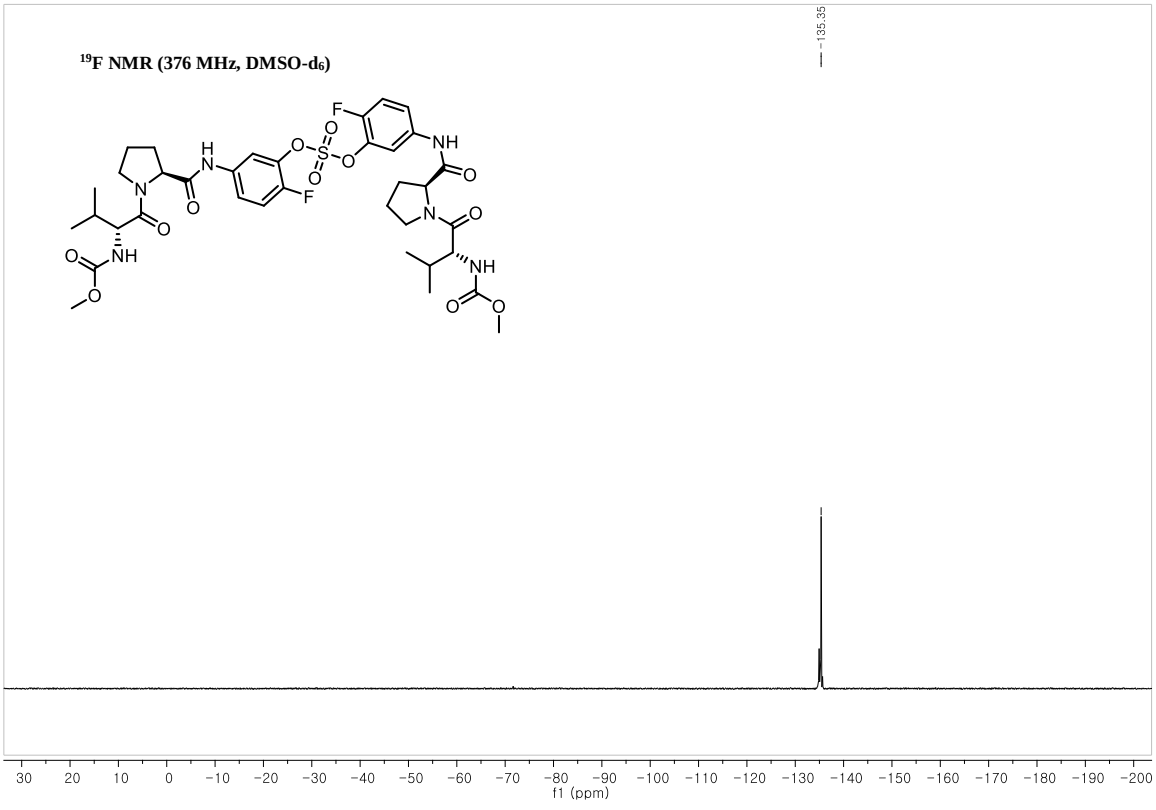


Compound 16



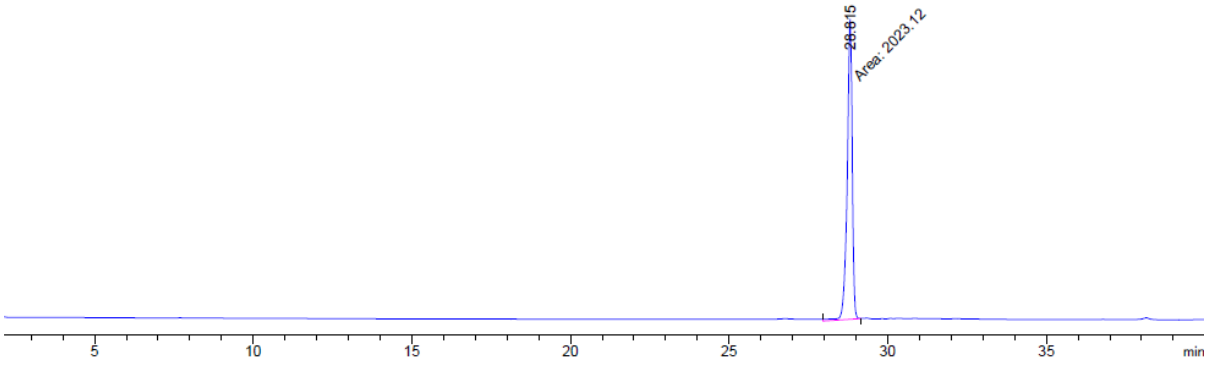


^{13}C NMR (126 MHz, DMSO-d$_6$)

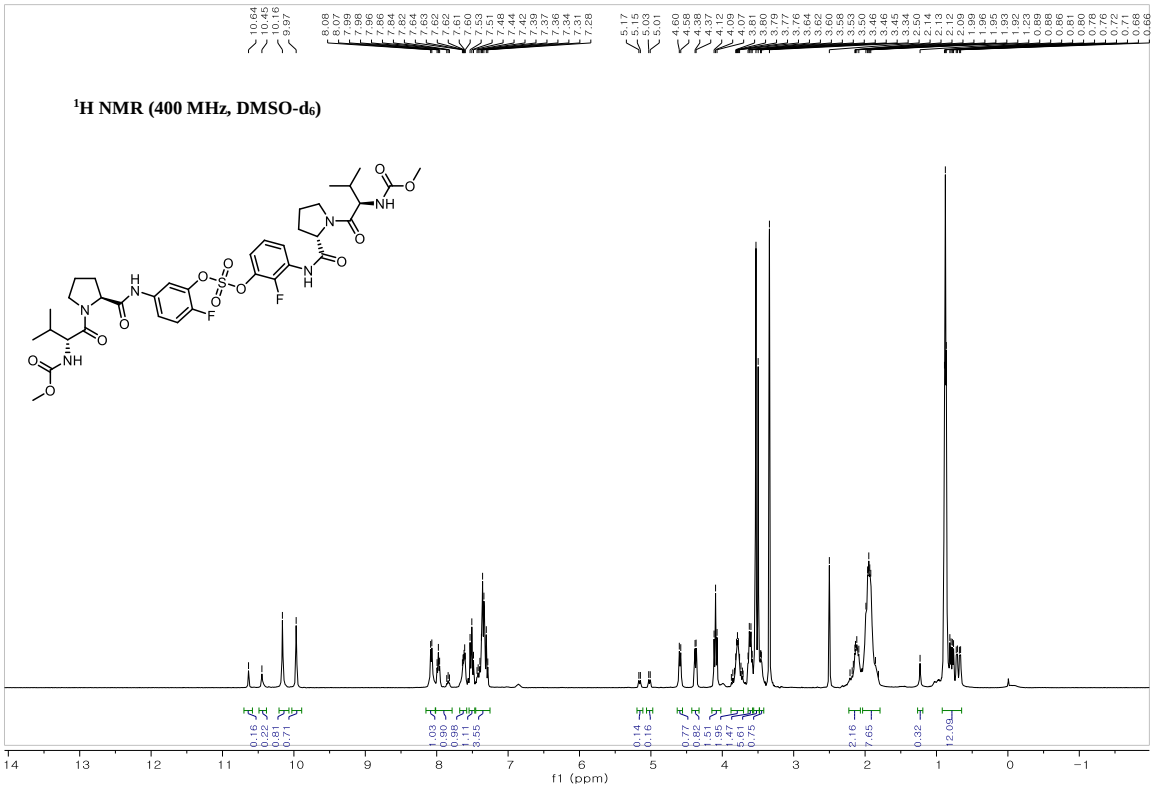


^{19}F NMR (376 MHz, DMSO-d$_6$)

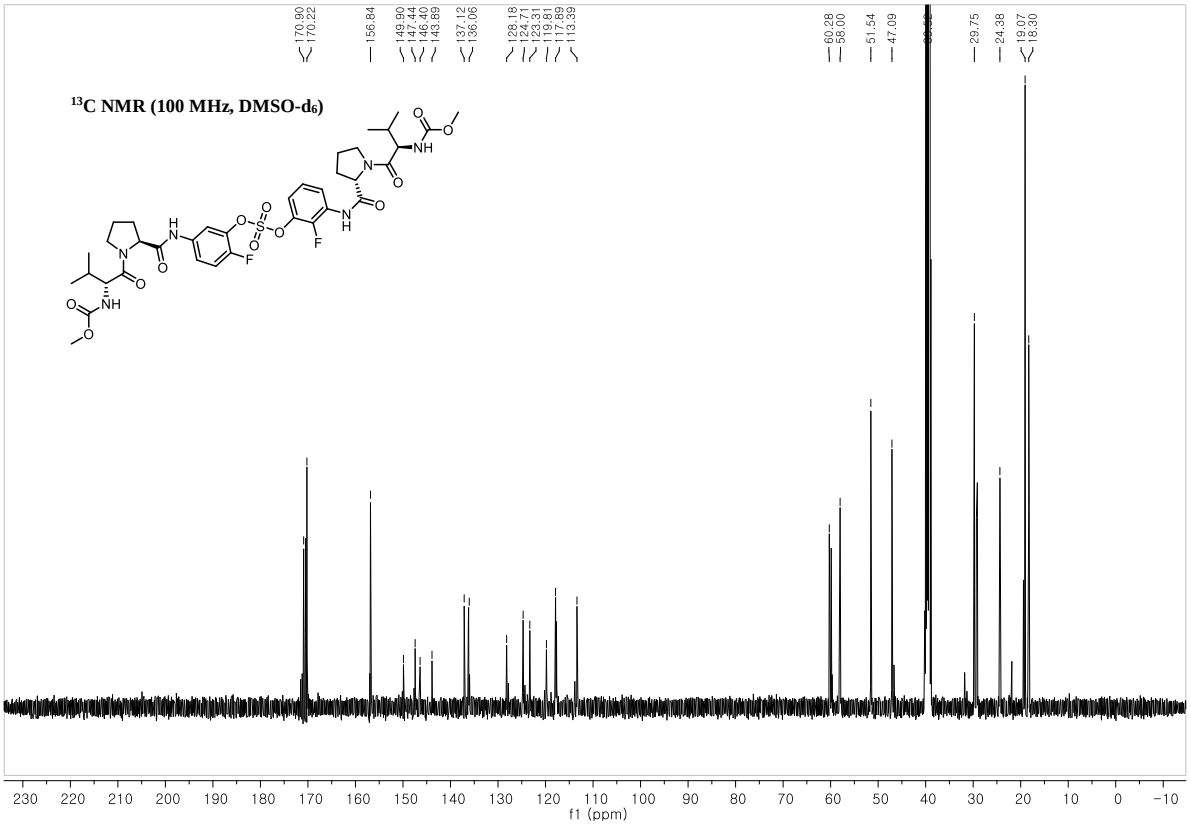
HPLC (compound 16, wavelength = 254 nm)



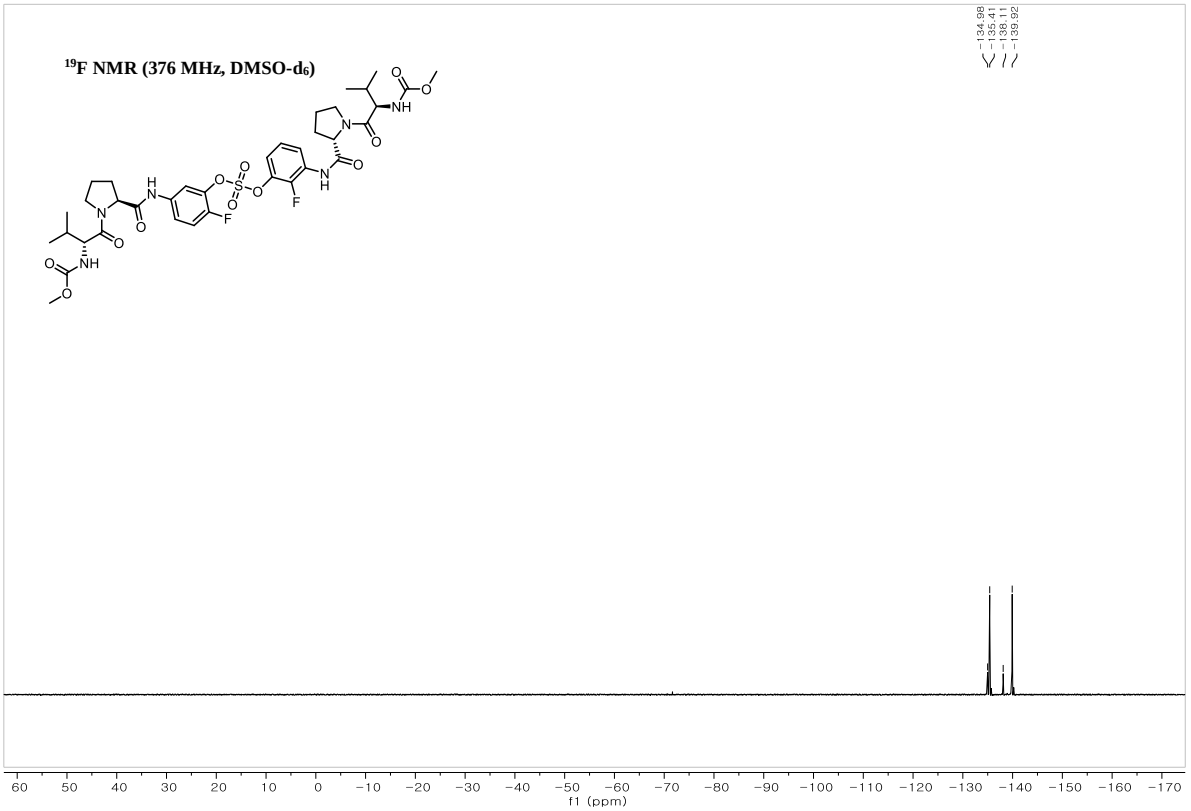
Compound 17



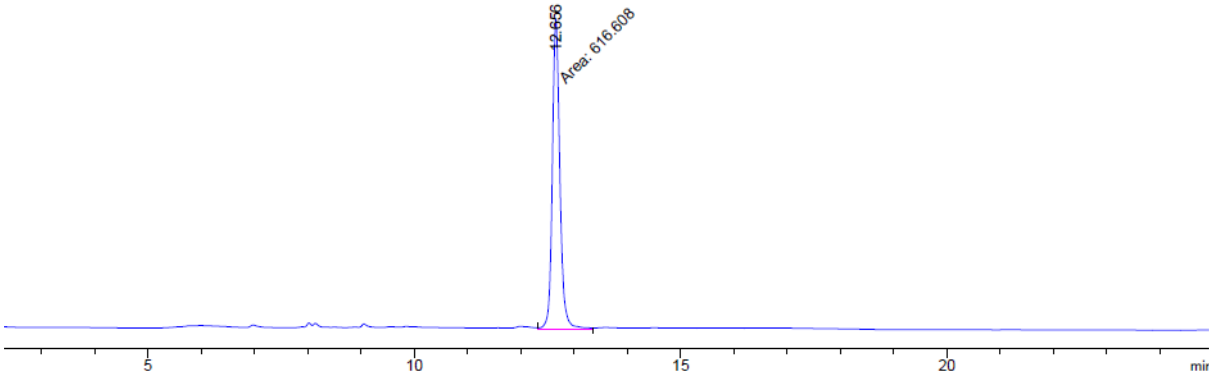
^{13}C NMR (100 MHz, DMSO-d$_6$)



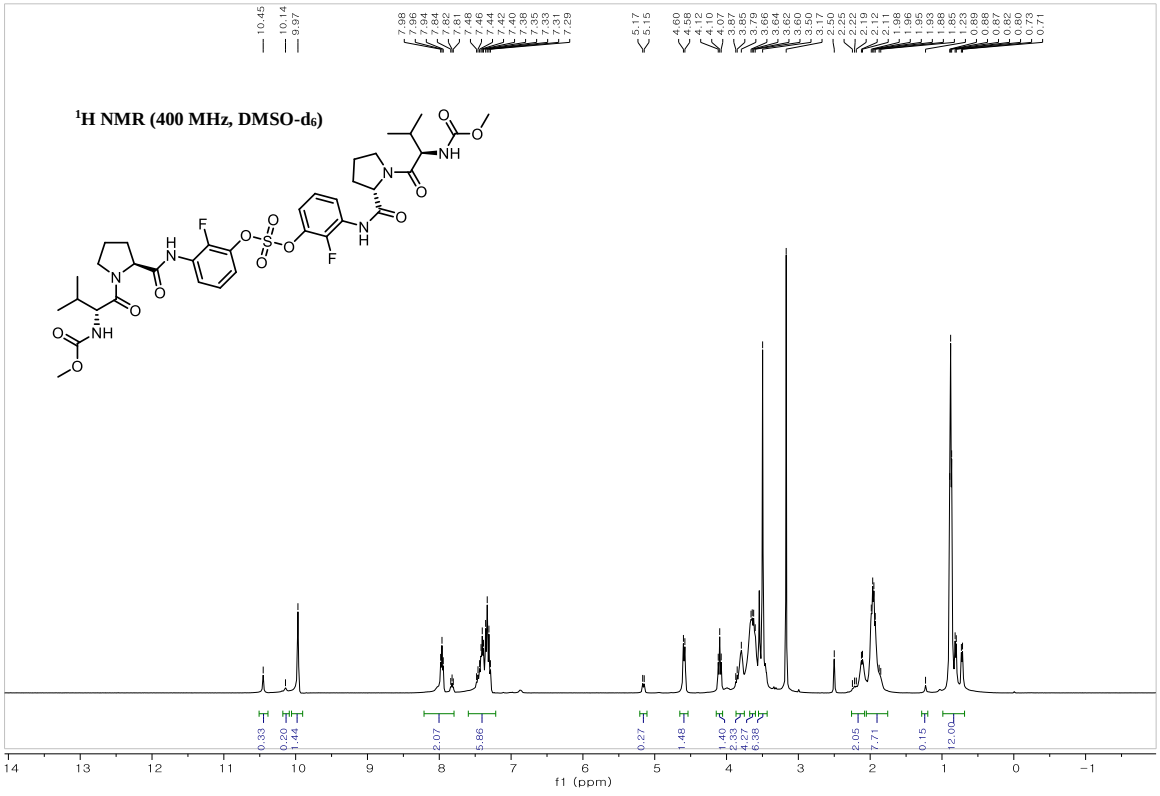
^{19}F NMR (376 MHz, DMSO-d$_6$)

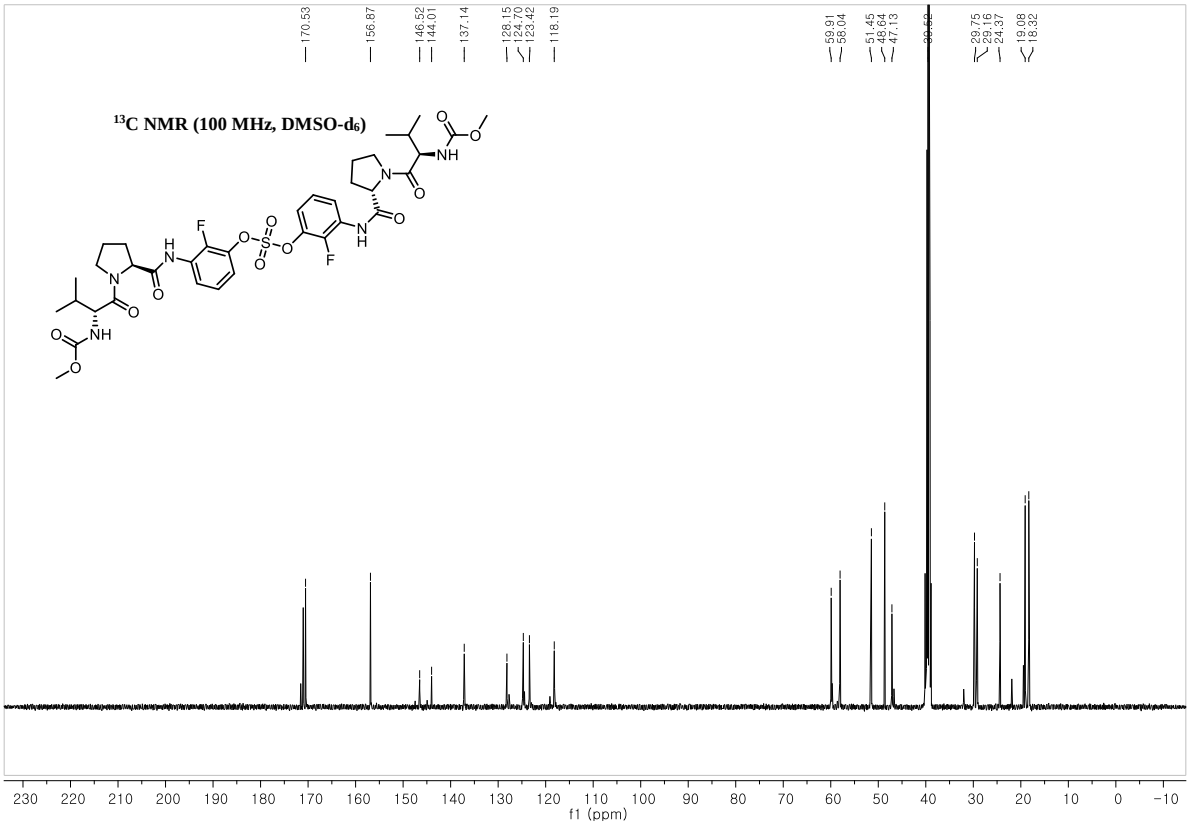


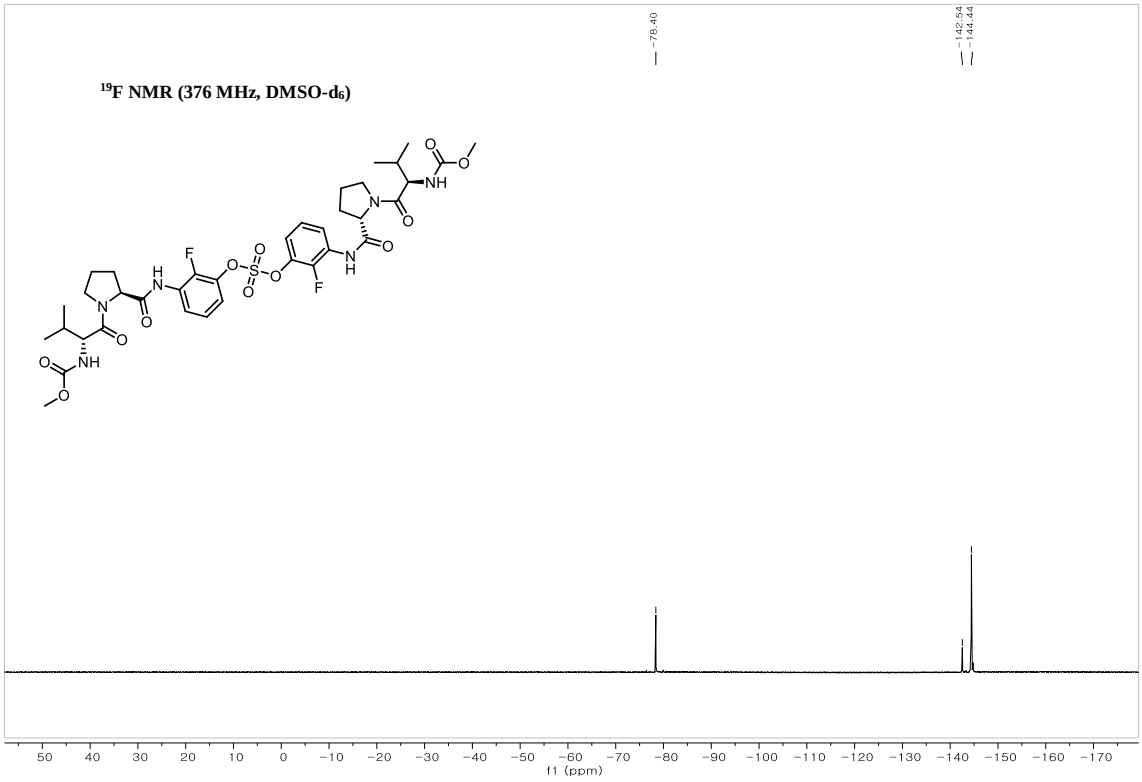
HPLC (compound 17, wavelength = 254 nm)



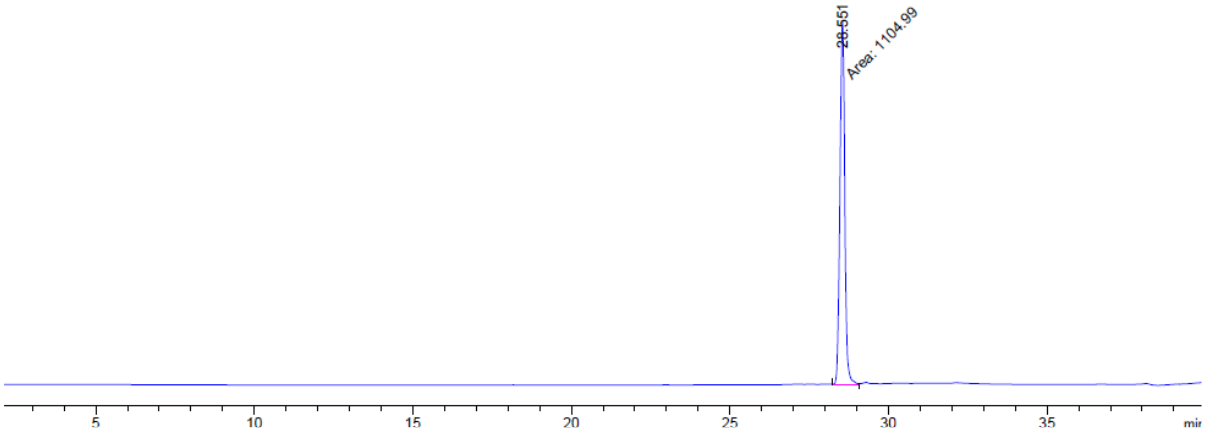
Compound 18



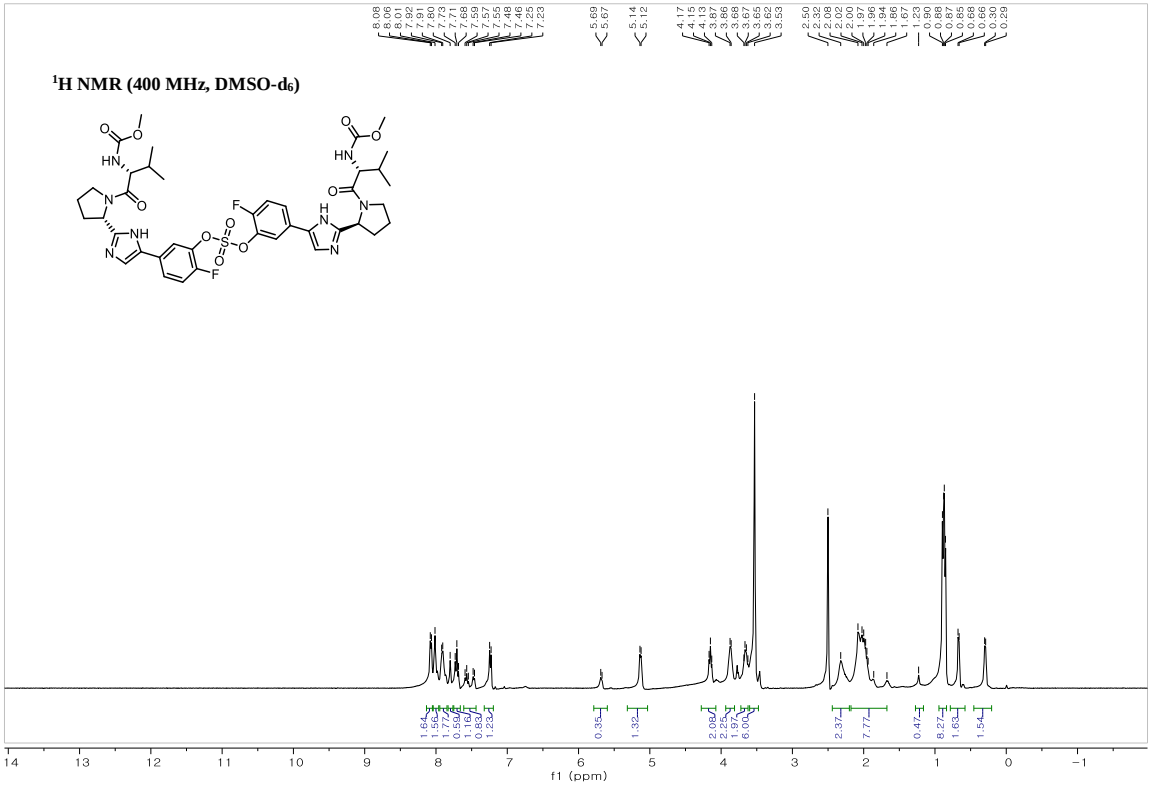

170.53
156.87
146.52
144.01
137.14
128.15
124.70
123.42
118.19
59.91
58.04
51.45
48.64
47.13
39.58
29.75
29.16
24.37
19.08
18.32
13C NMR (100 MHz, DMSO-d6)
f1 (ppm)


-78.40
-142.54
-144.44
19F NMR (376 MHz, DMSO-d6)
f1 (ppm)

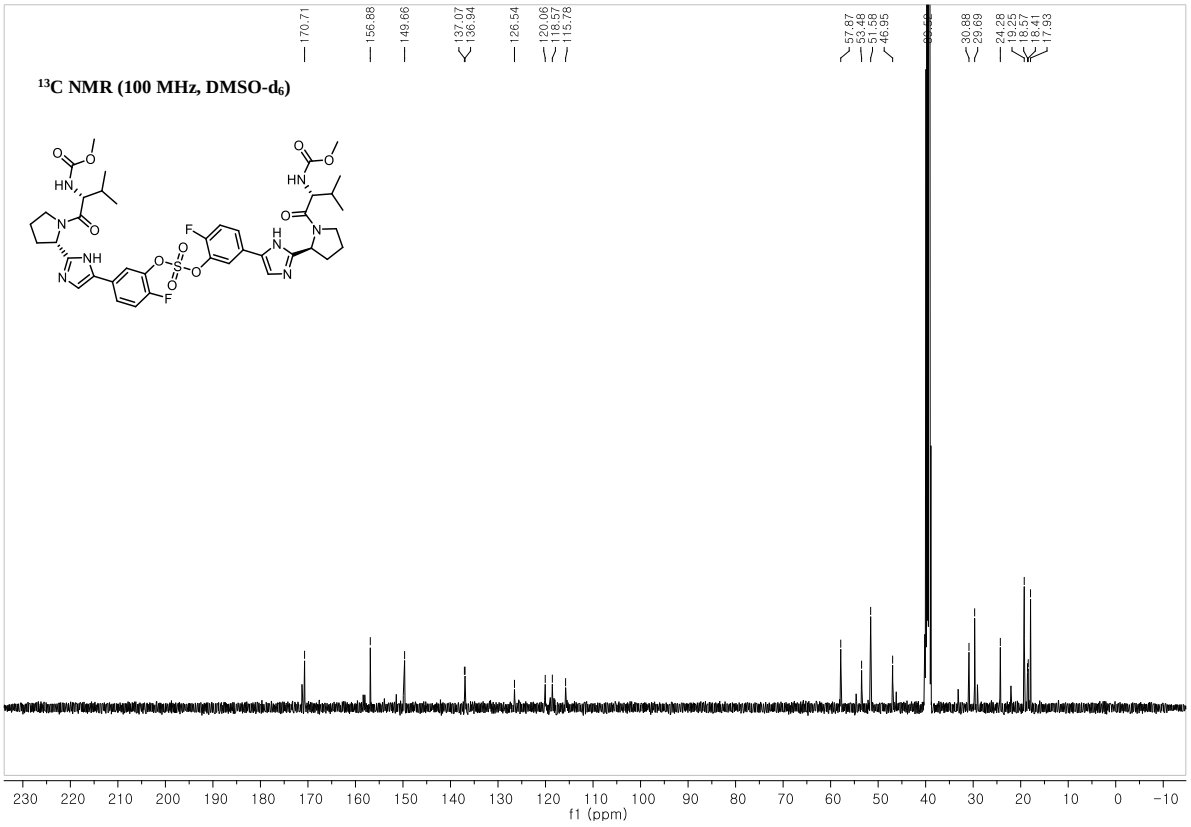
HPLC (compound 18, wavelength = 254 nm)



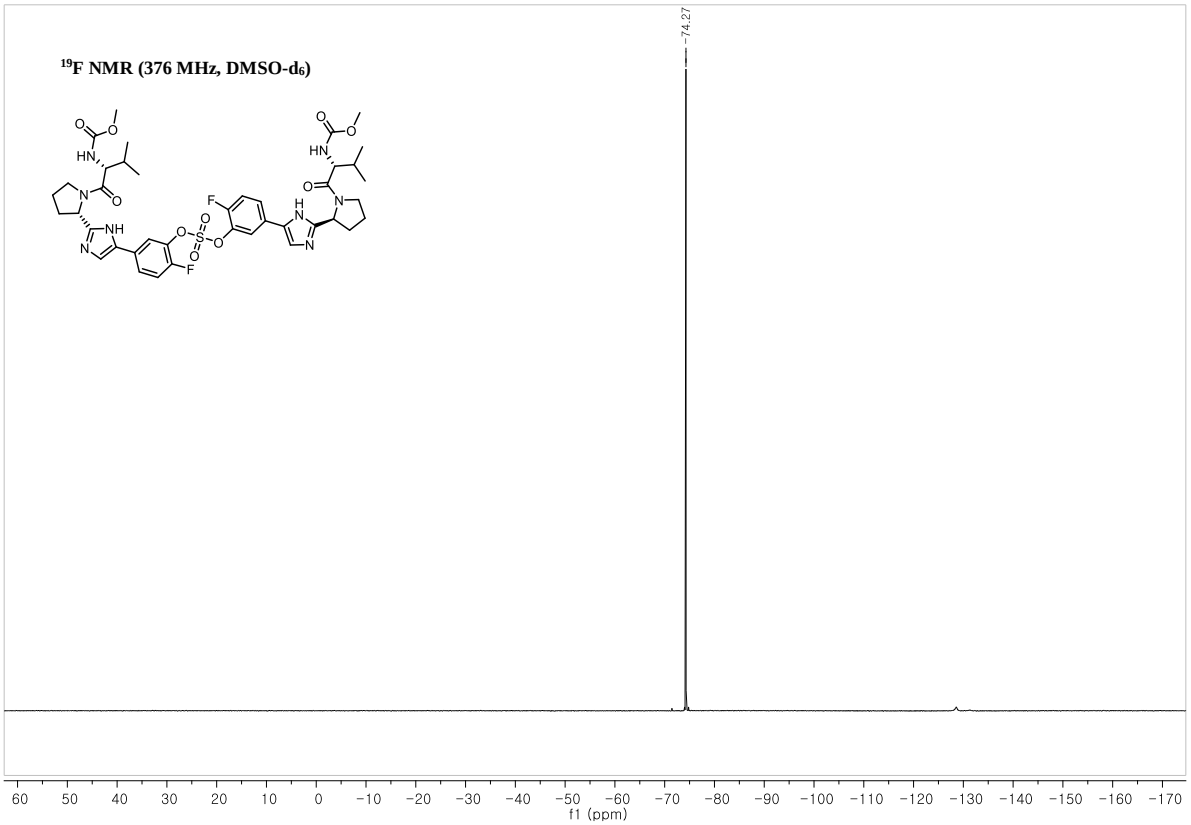
Compound 19



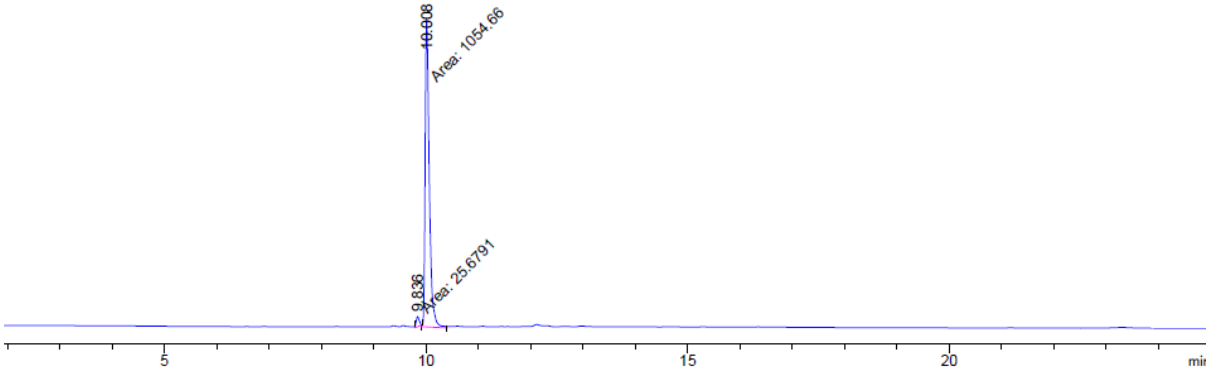
^{13}C NMR (100 MHz, DMSO-d_6)



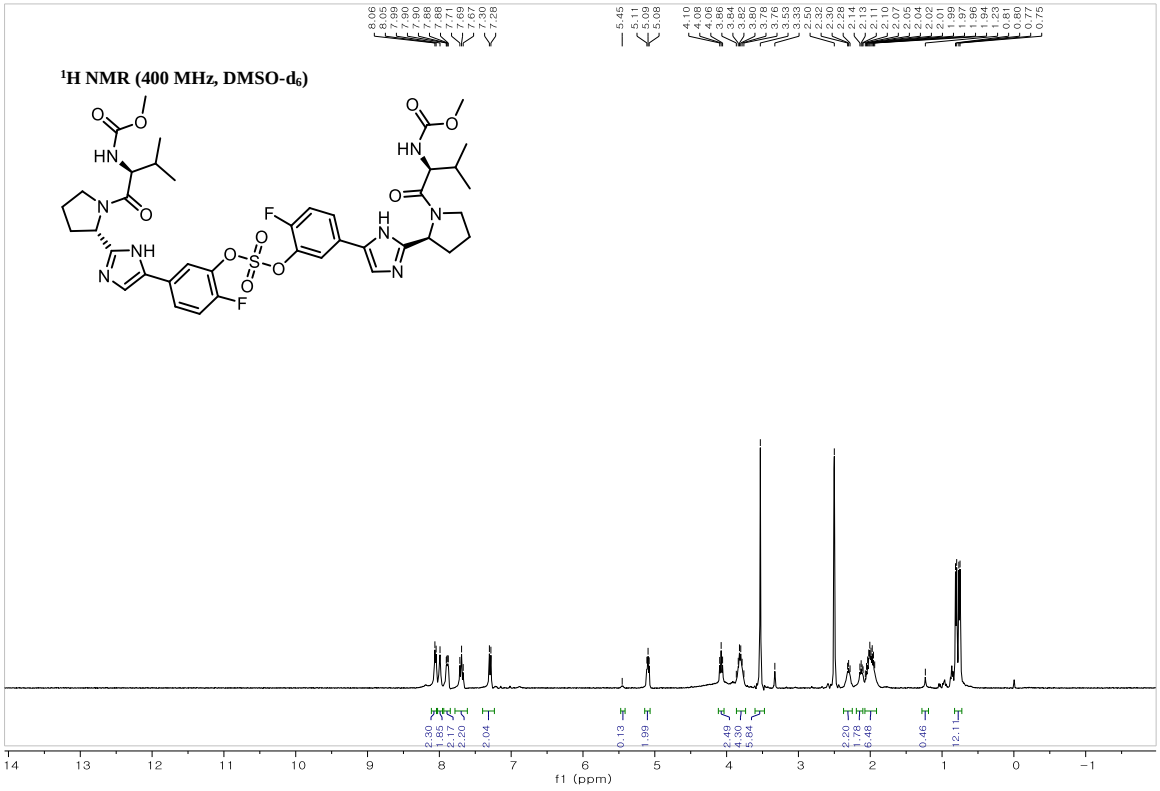
^{19}F NMR (376 MHz, DMSO-d_6)

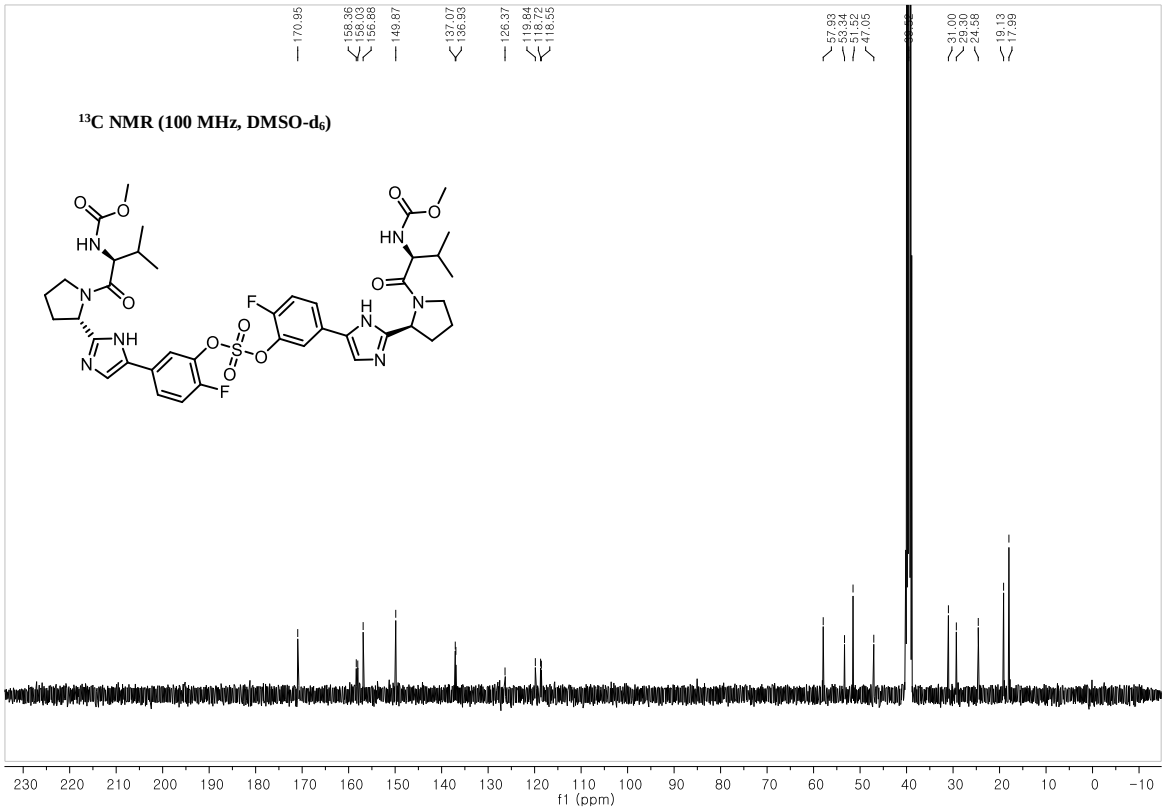


HPLC (compound 19, wavelength = 254 nm)

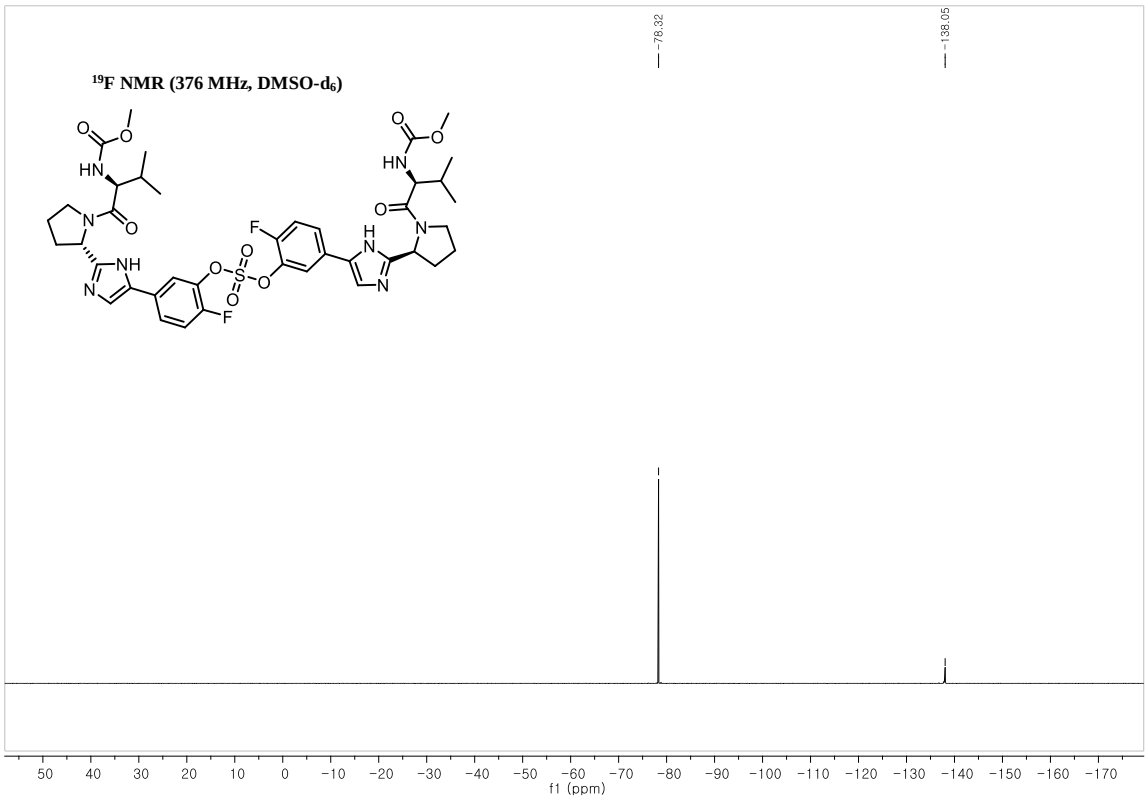


Compound 20



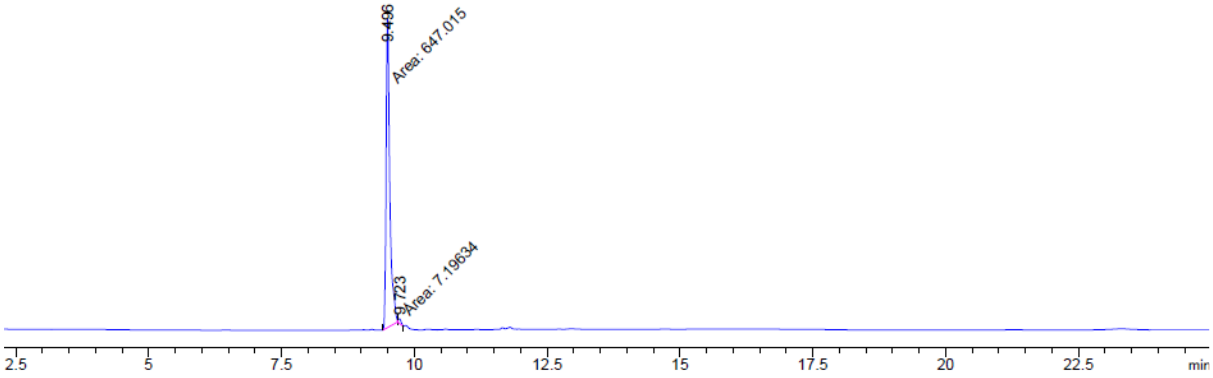


^{13}C NMR (100 MHz, DMSO-d$_6$)

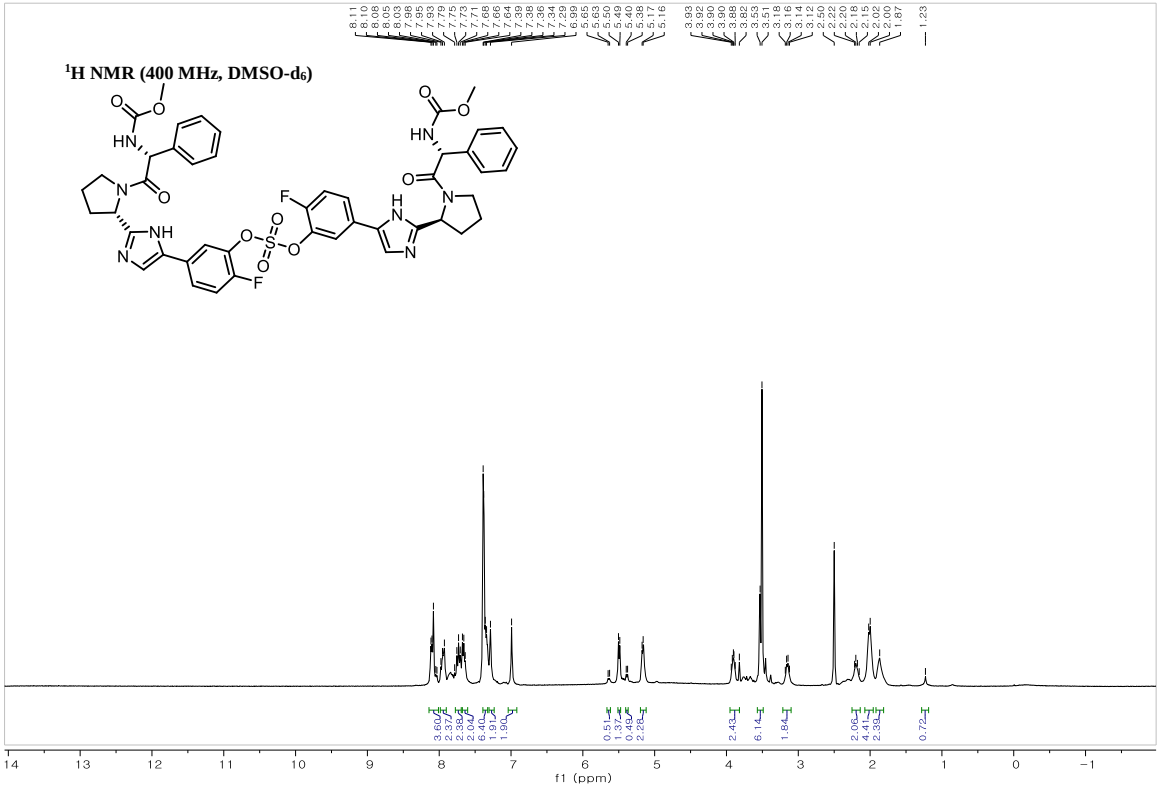


^{19}F NMR (376 MHz, DMSO-d$_6$)

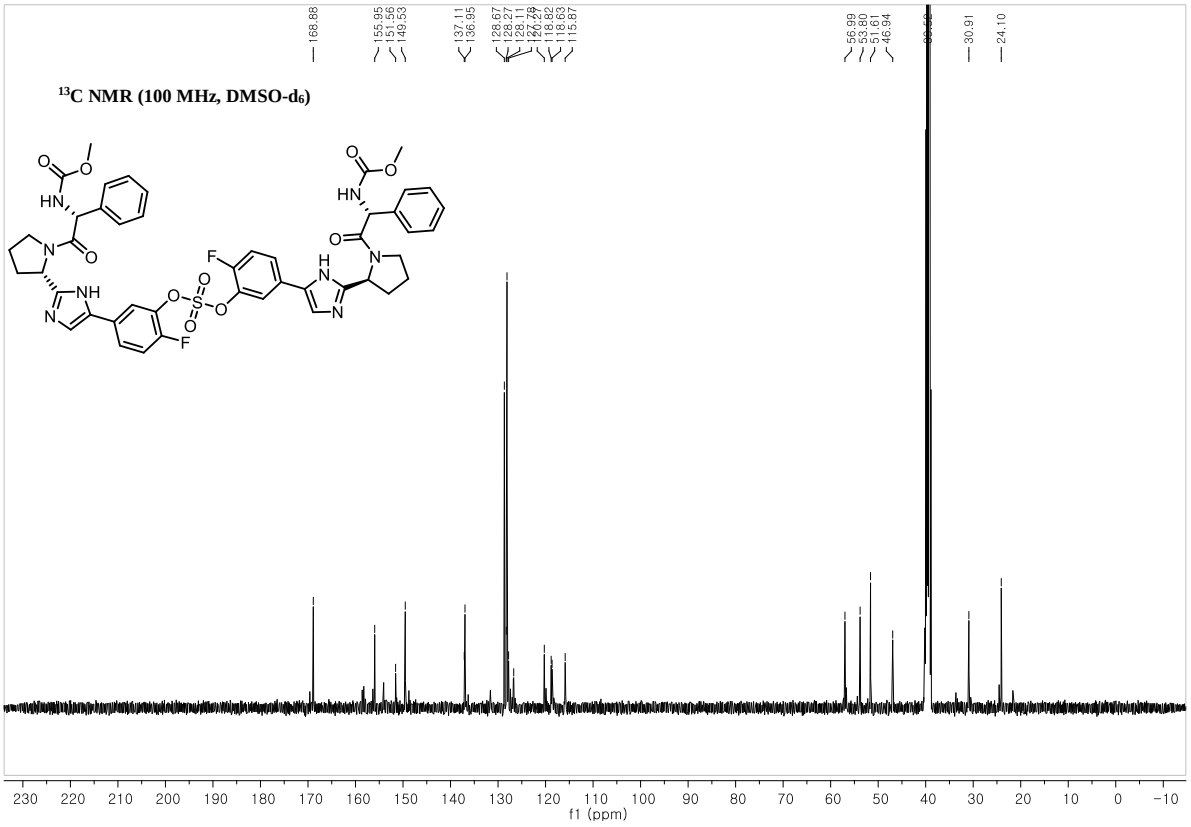
HPLC (compound 20, wavelength = 254 nm)



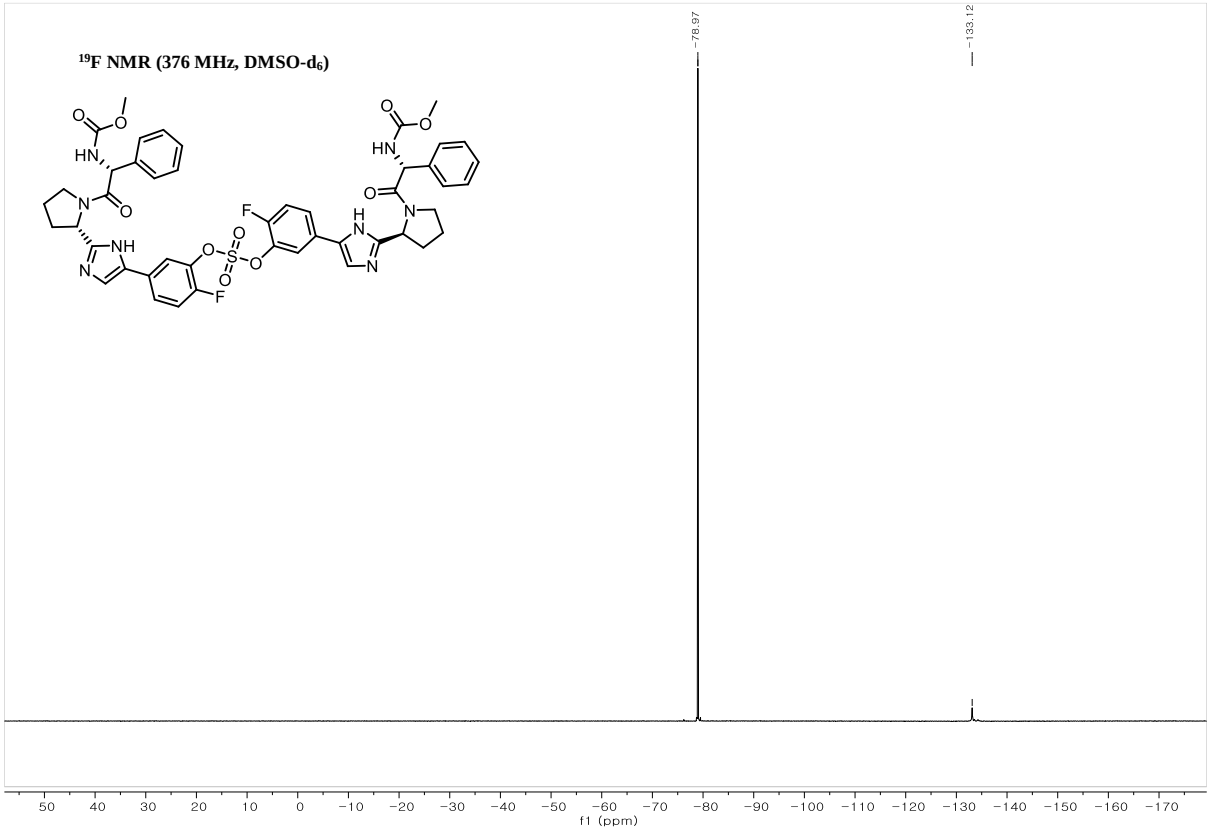
Compound 21



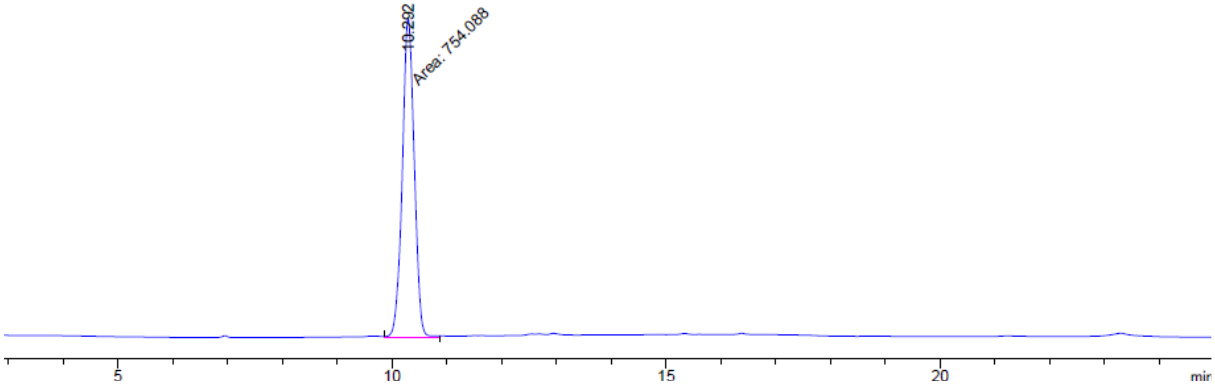
^{13}C NMR (100 MHz, DMSO-d$_6$)



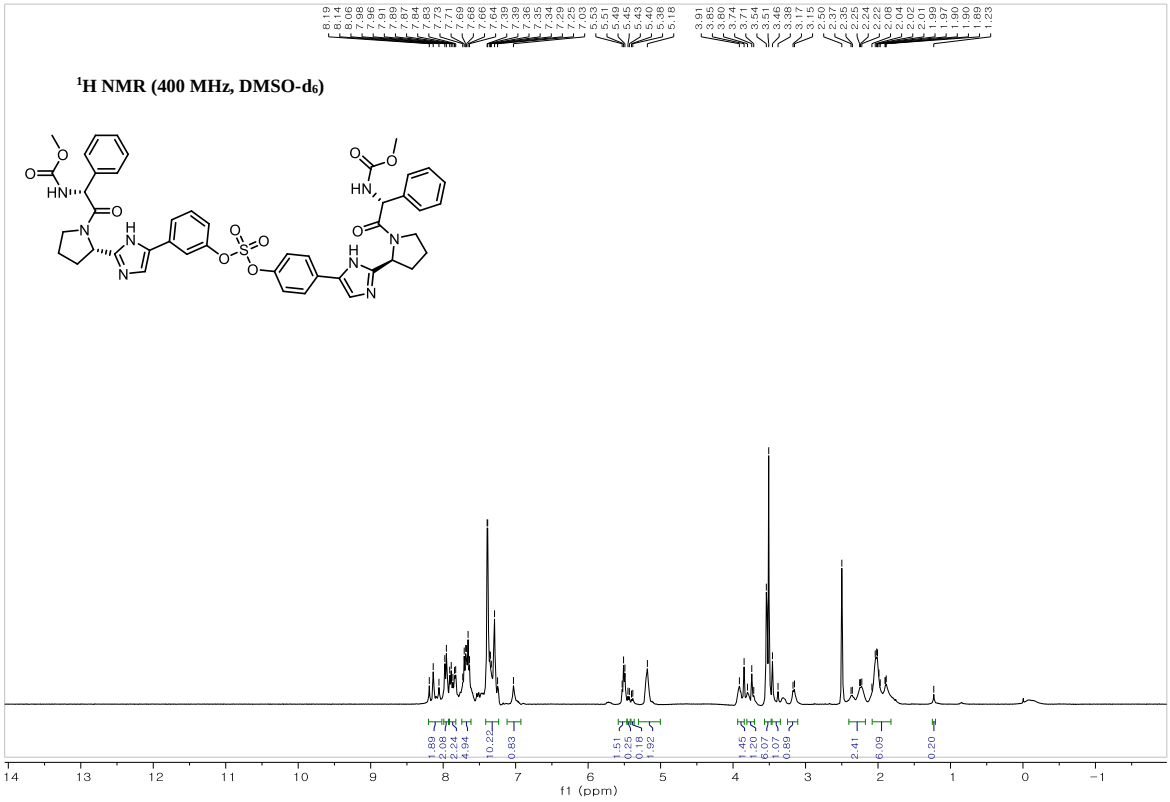
^{19}F NMR (376 MHz, DMSO-d$_6$)

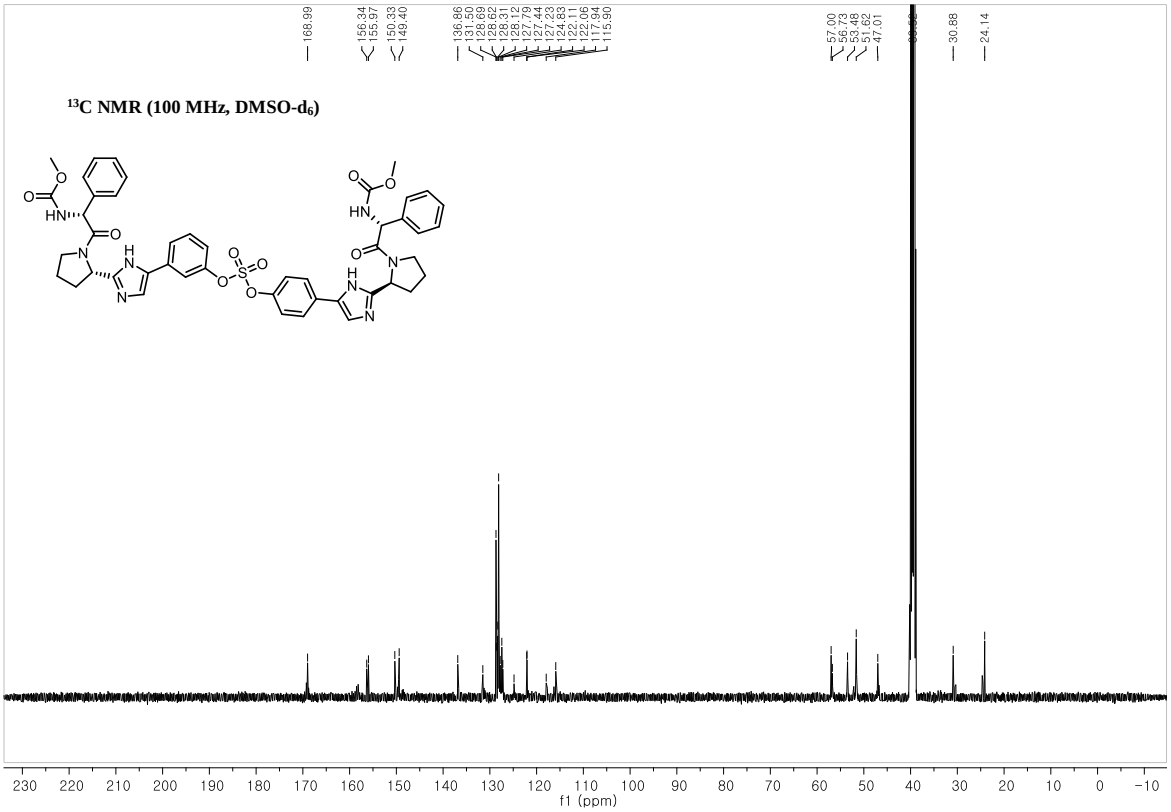


HPLC (compound 21, wavelength = 254 nm)

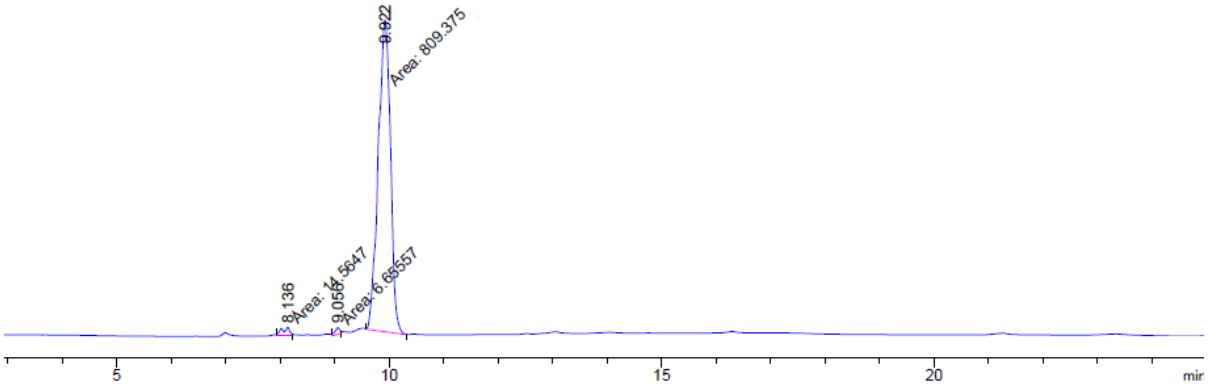


Compound 22

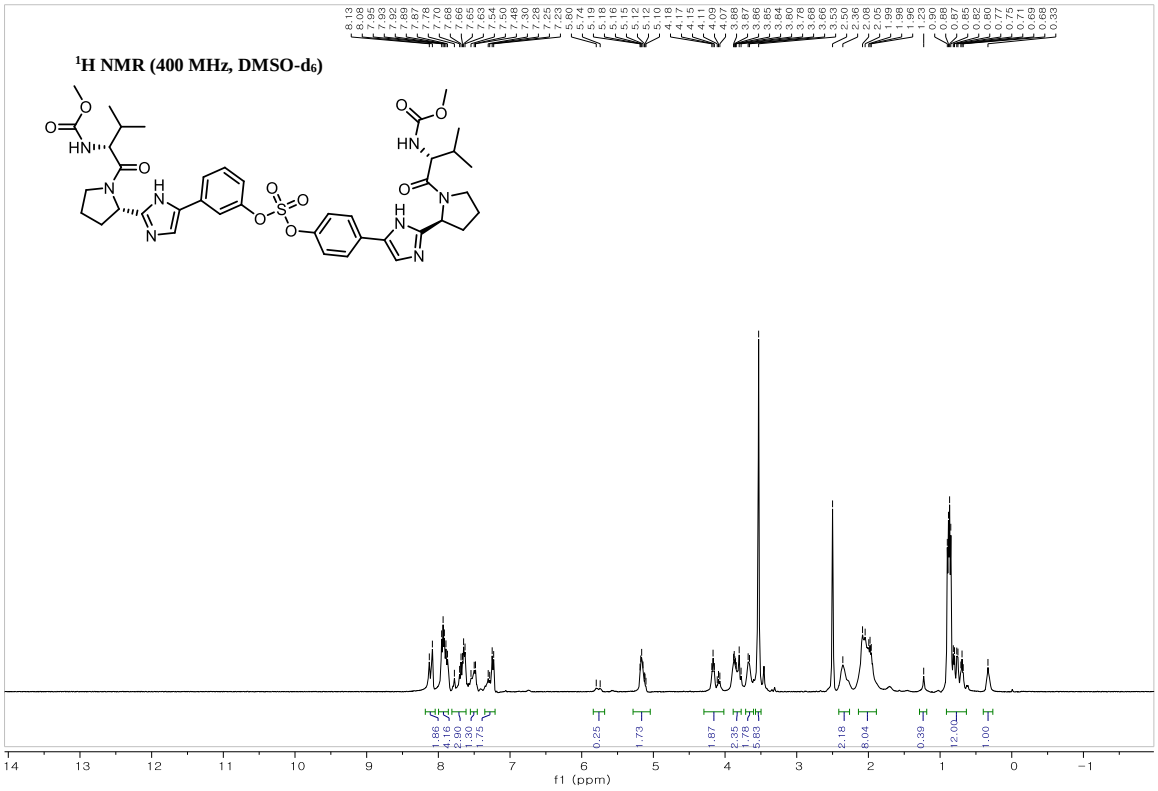


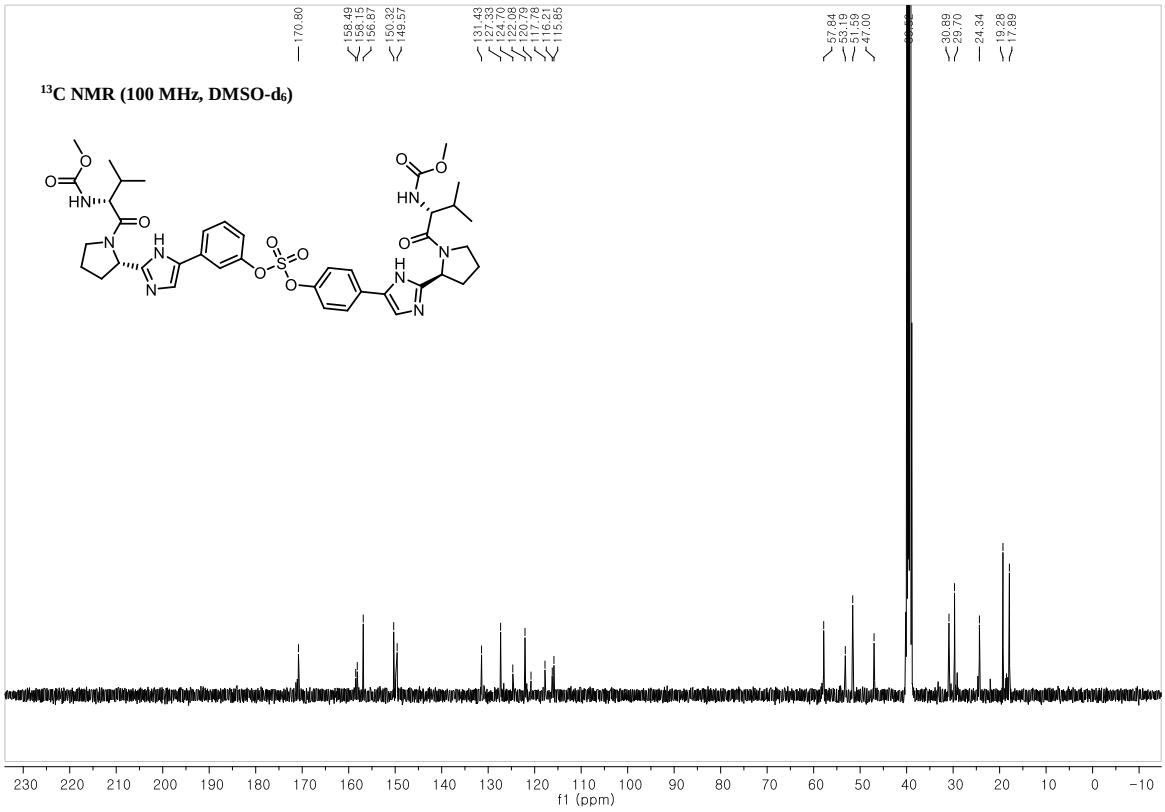


HPLC (compound 22, wavelength = 254 nm)

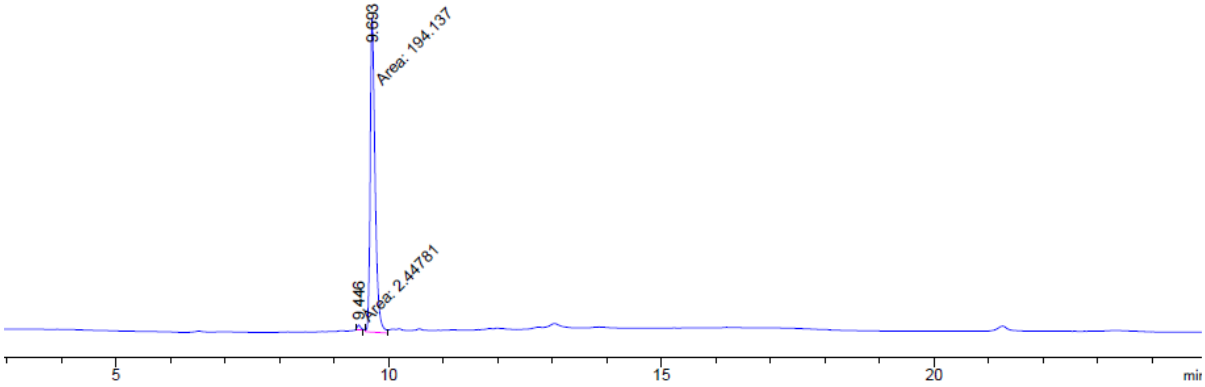


Compound 23

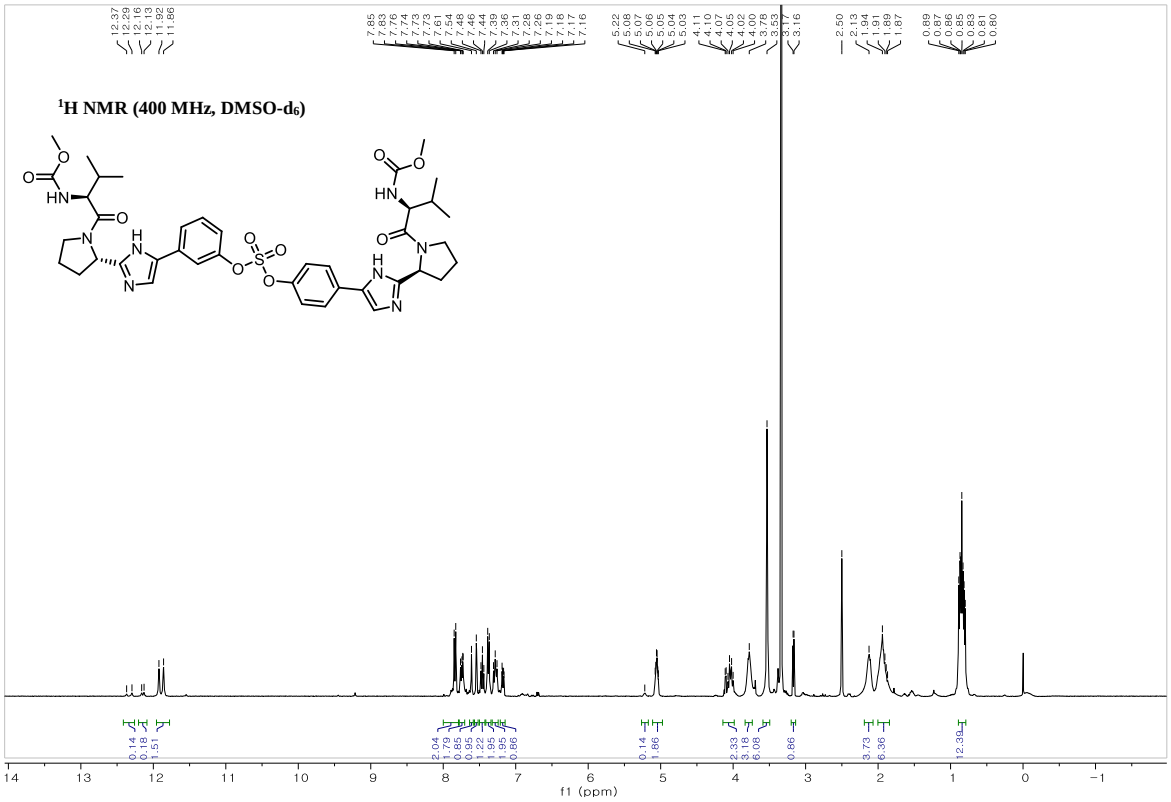


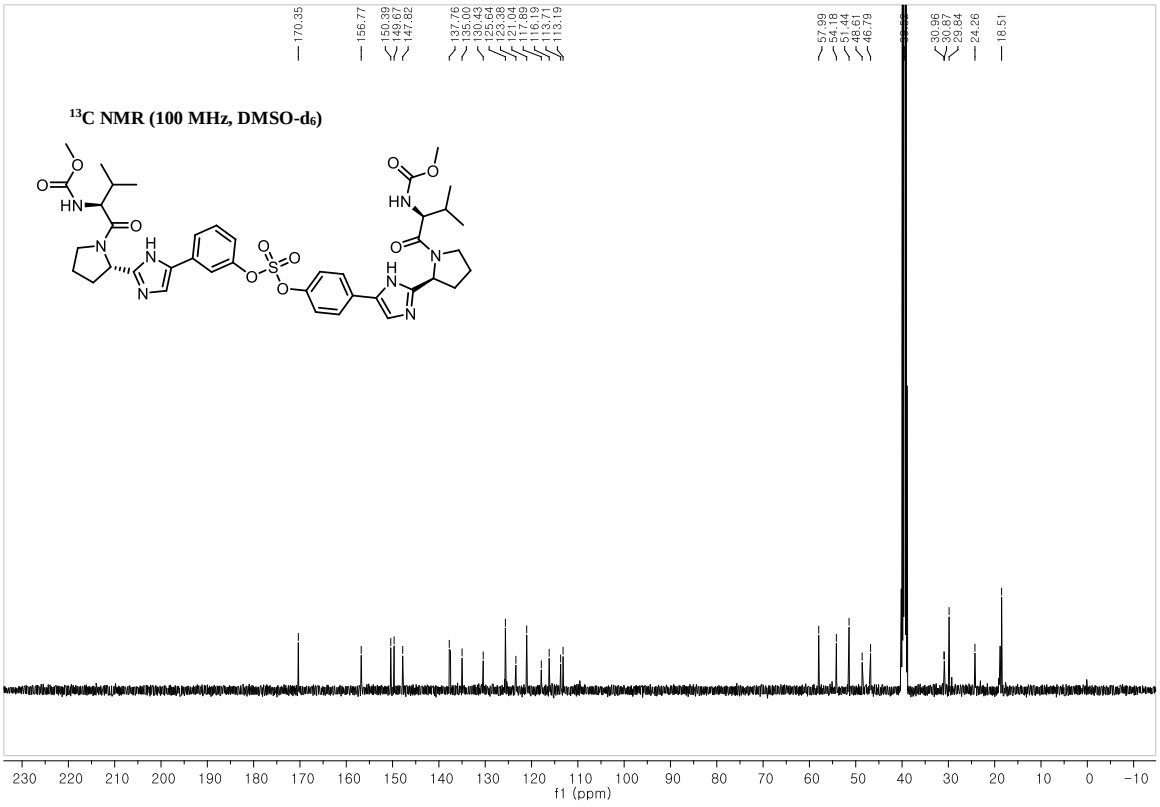


HPLC (compound 23, wavelength = 254 nm)

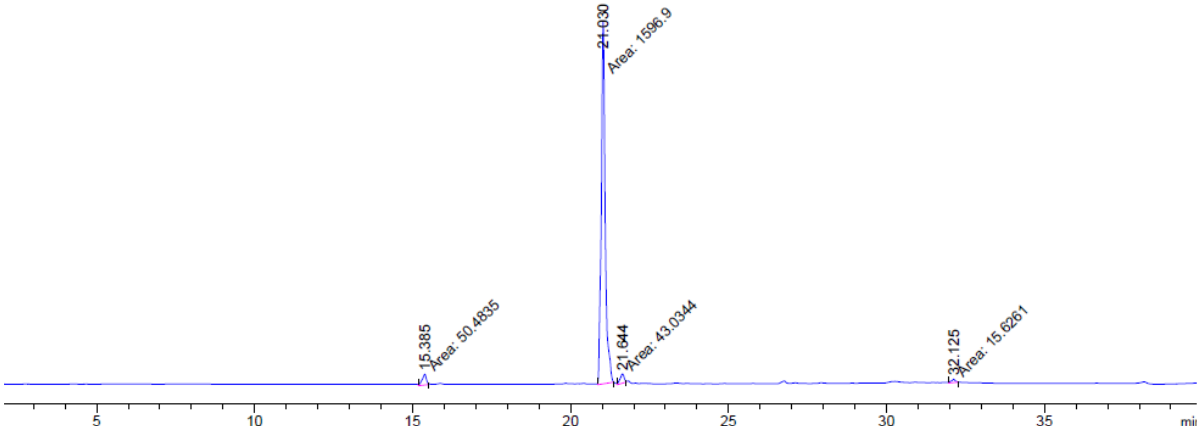


Compound 24

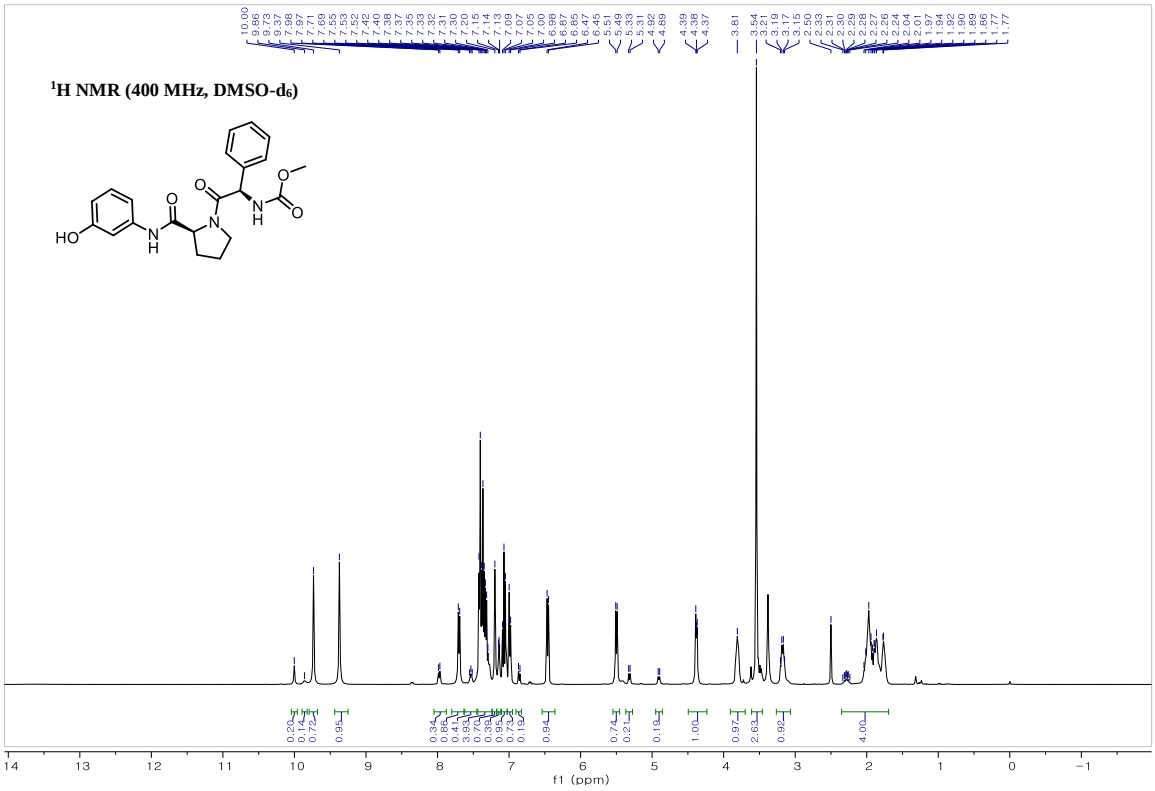


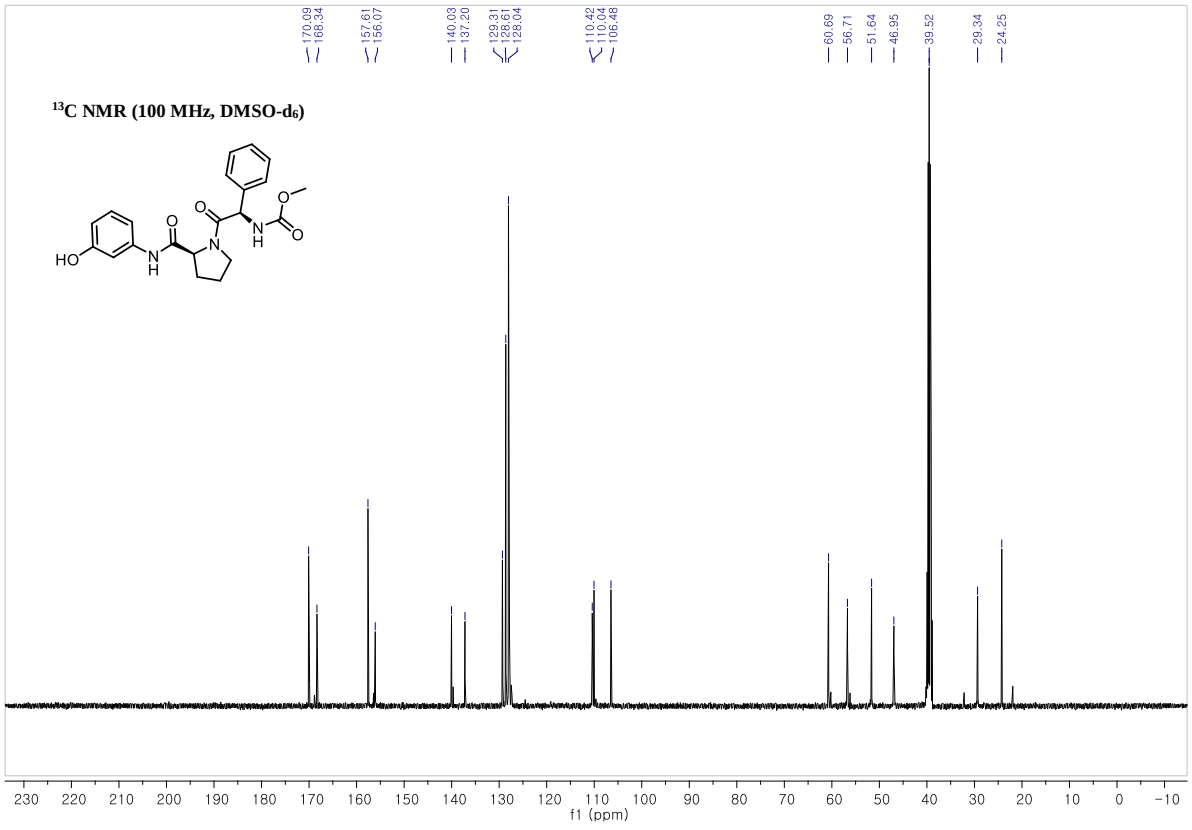


HPLC (compound 24, wavelength = 254 nm)

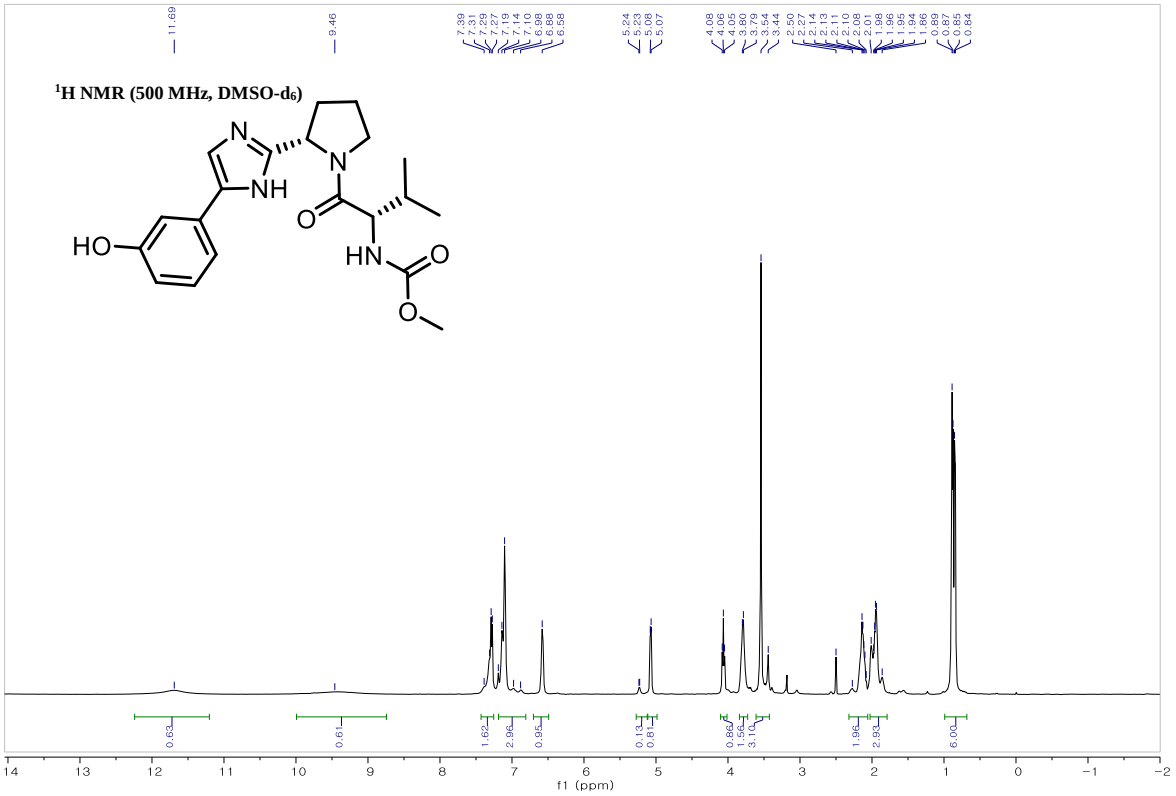


Compound 25

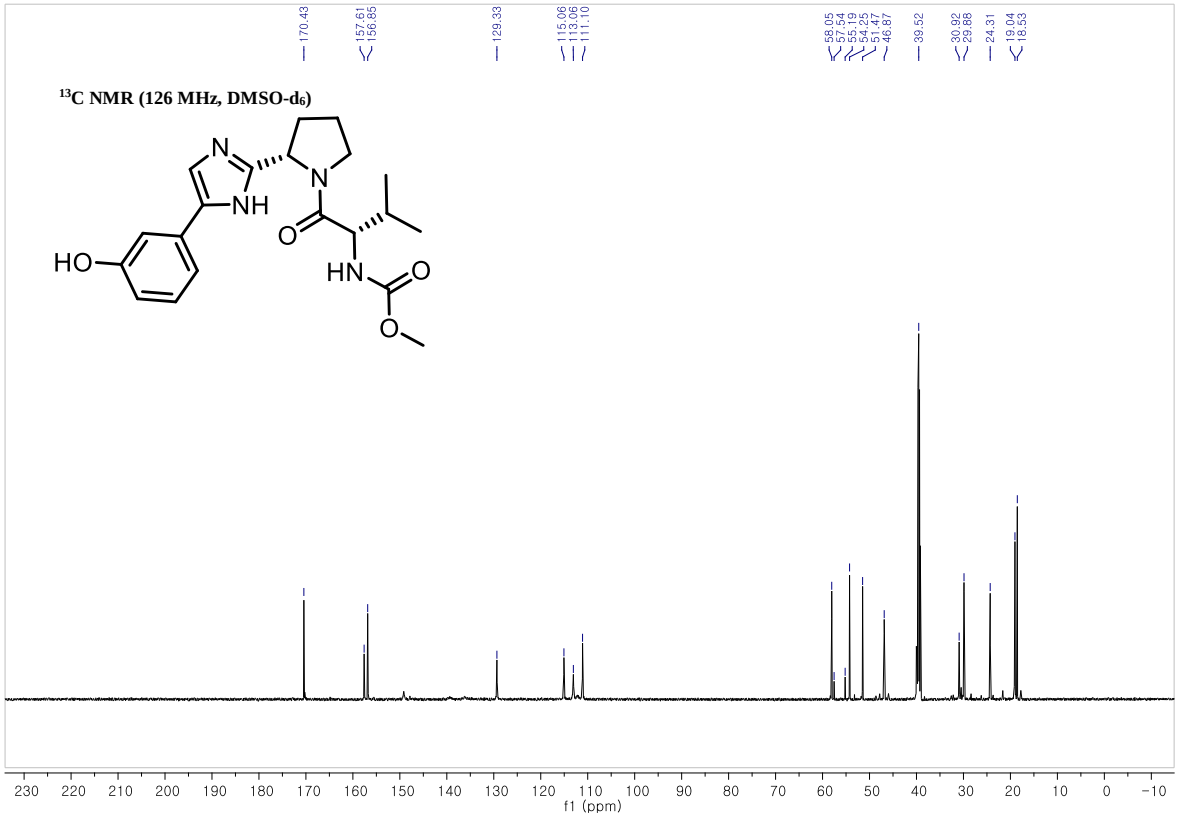




Compound 26

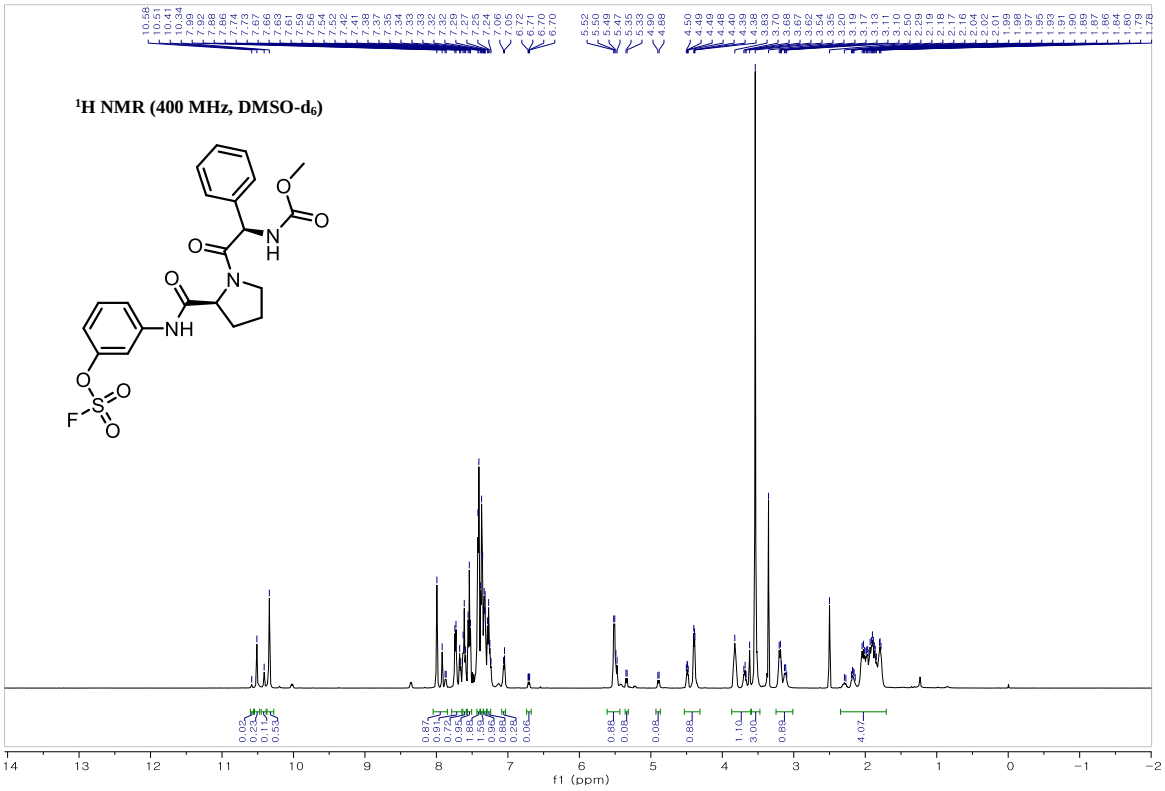


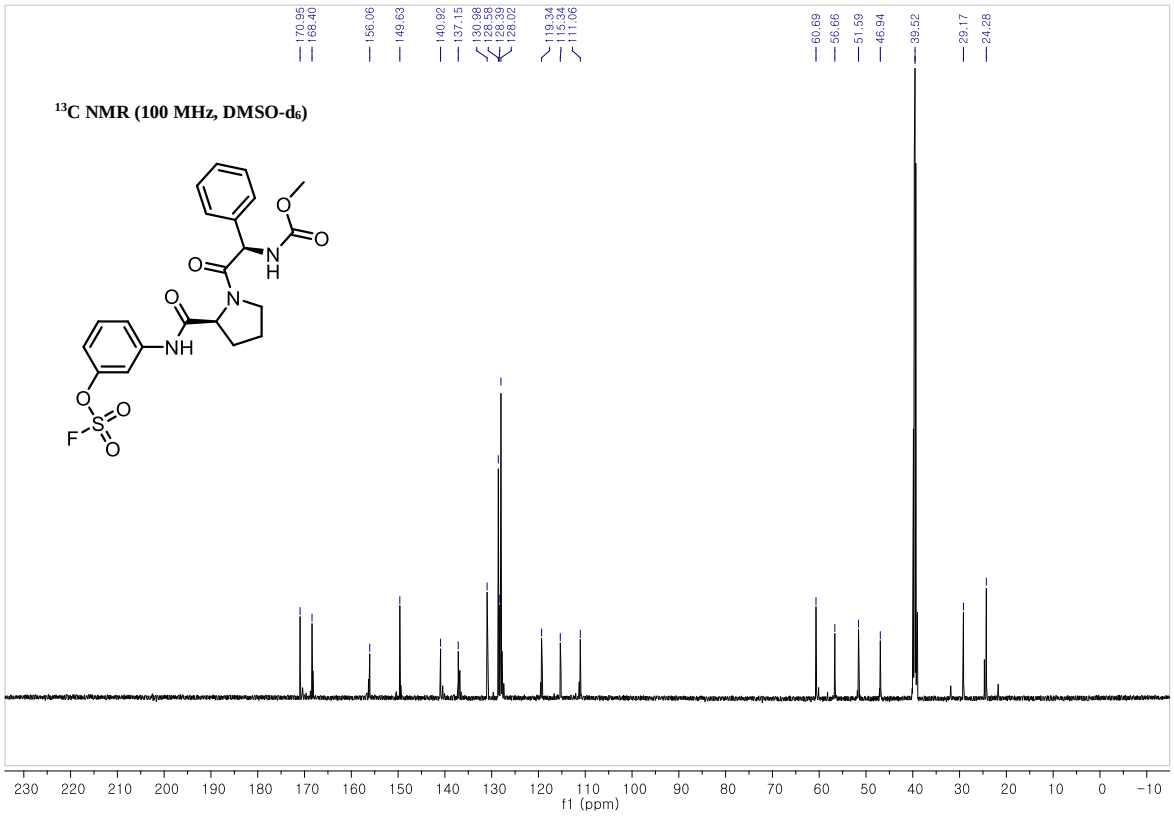
^{1}H NMR (500 MHz, DMSO-d$_6$)

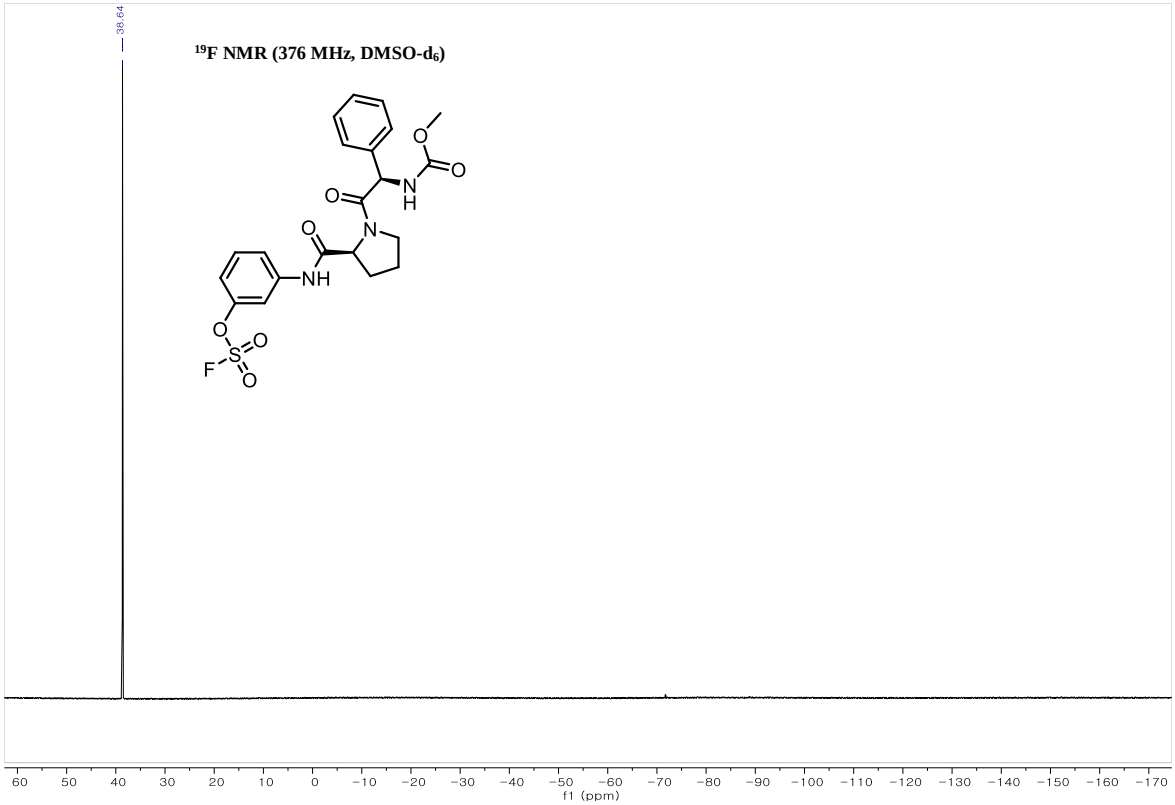


^{13}C NMR (126 MHz, DMSO-d$_6$)

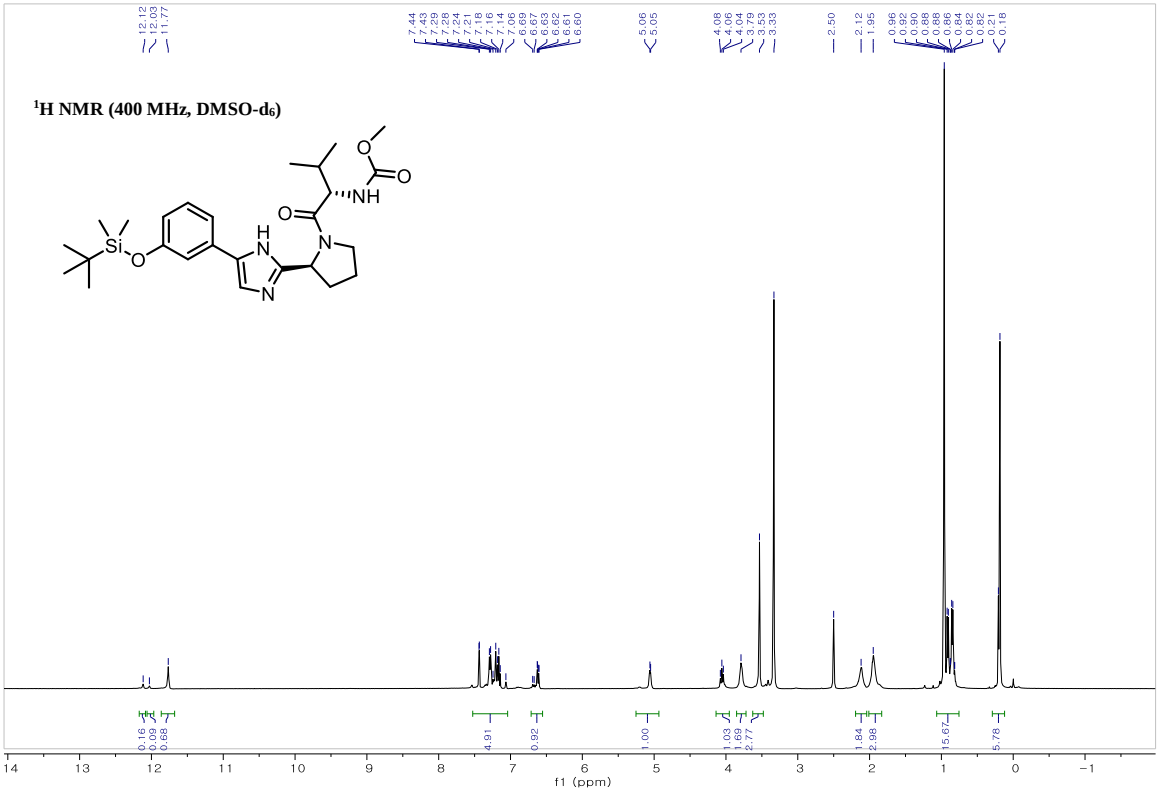
Compound 27

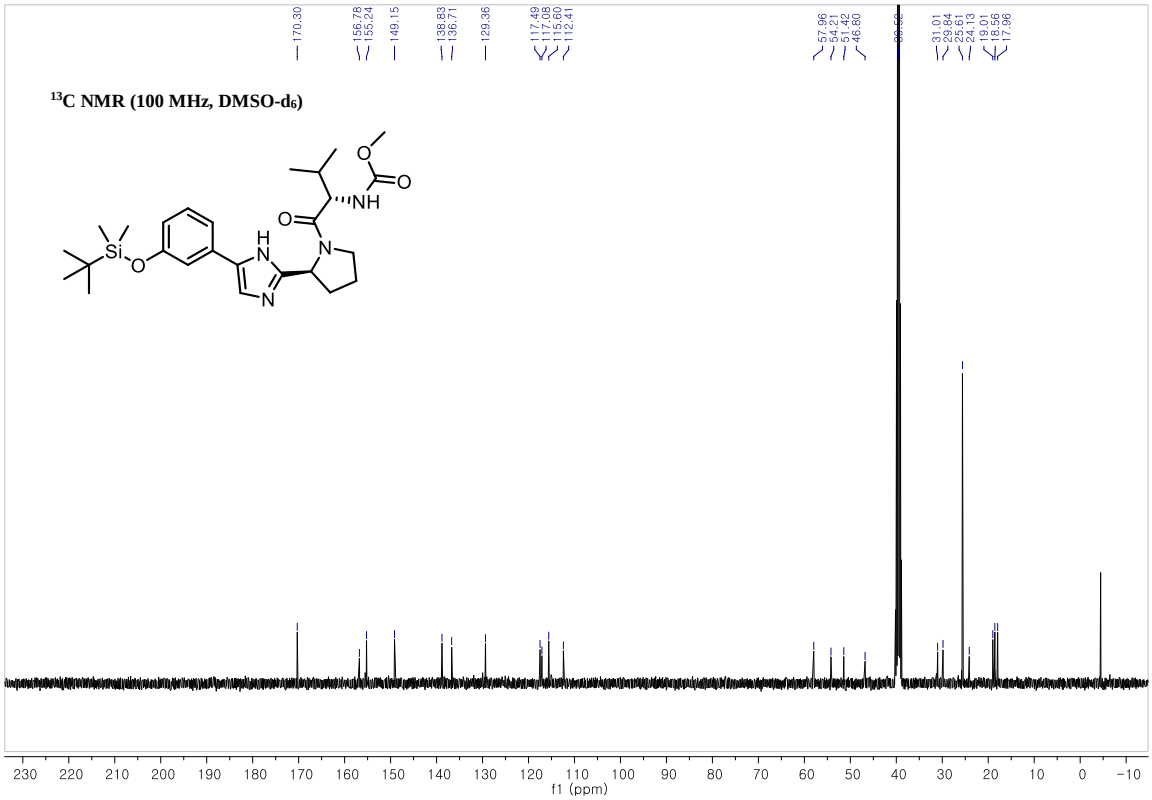




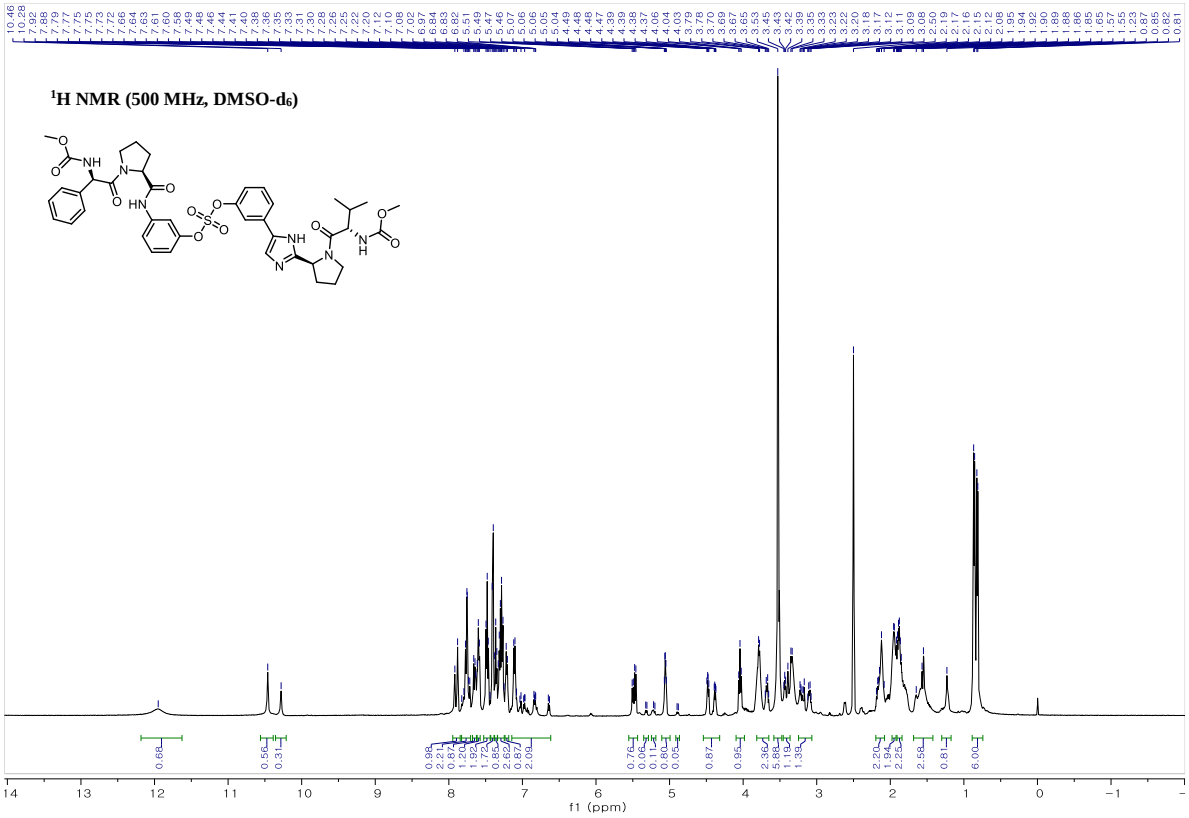


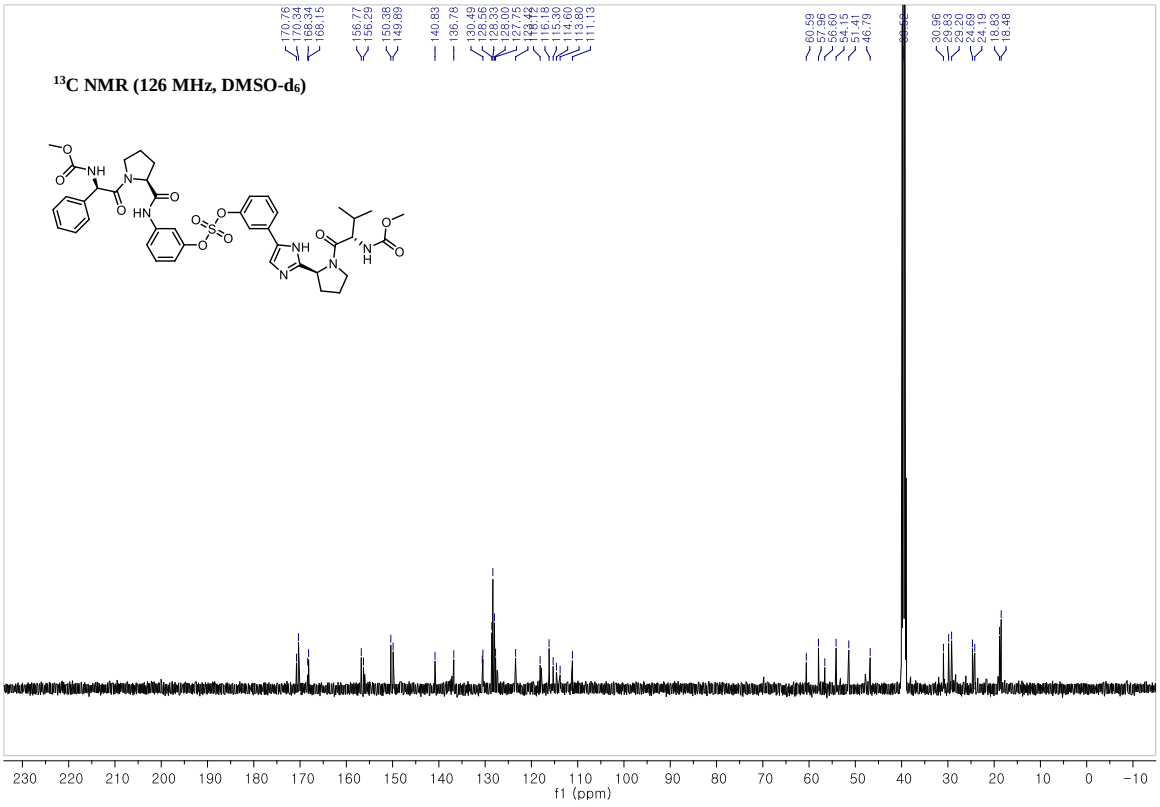
Compound 28



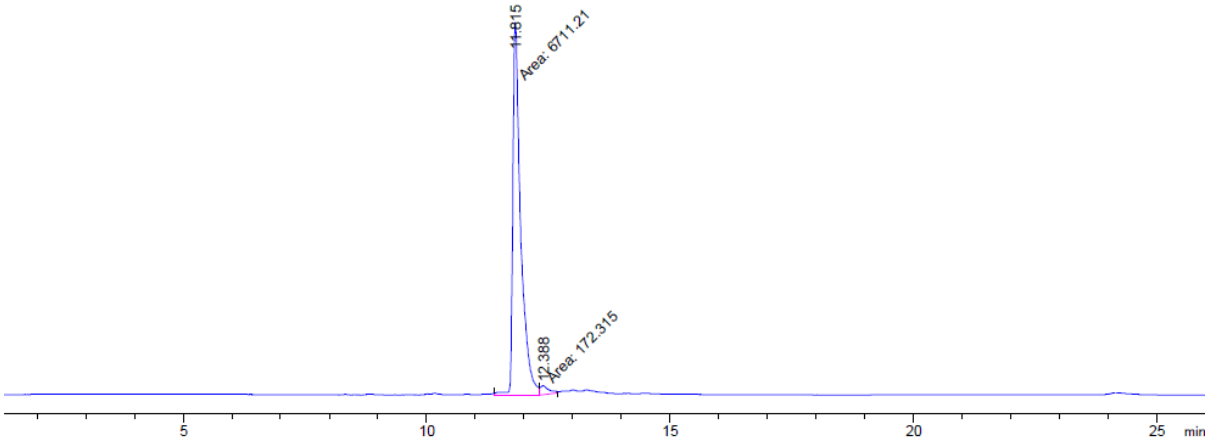

13C NMR (100 MHz, DMSO-d6)
170.30
156.78
155.24
149.15
138.83
136.71
129.36
117.49
117.08
115.60
112.41
57.96
54.21
51.42
46.80
39.56
31.01
29.84
25.61
24.13
19.01
18.56
17.96
f1 (ppm)

Compound 29

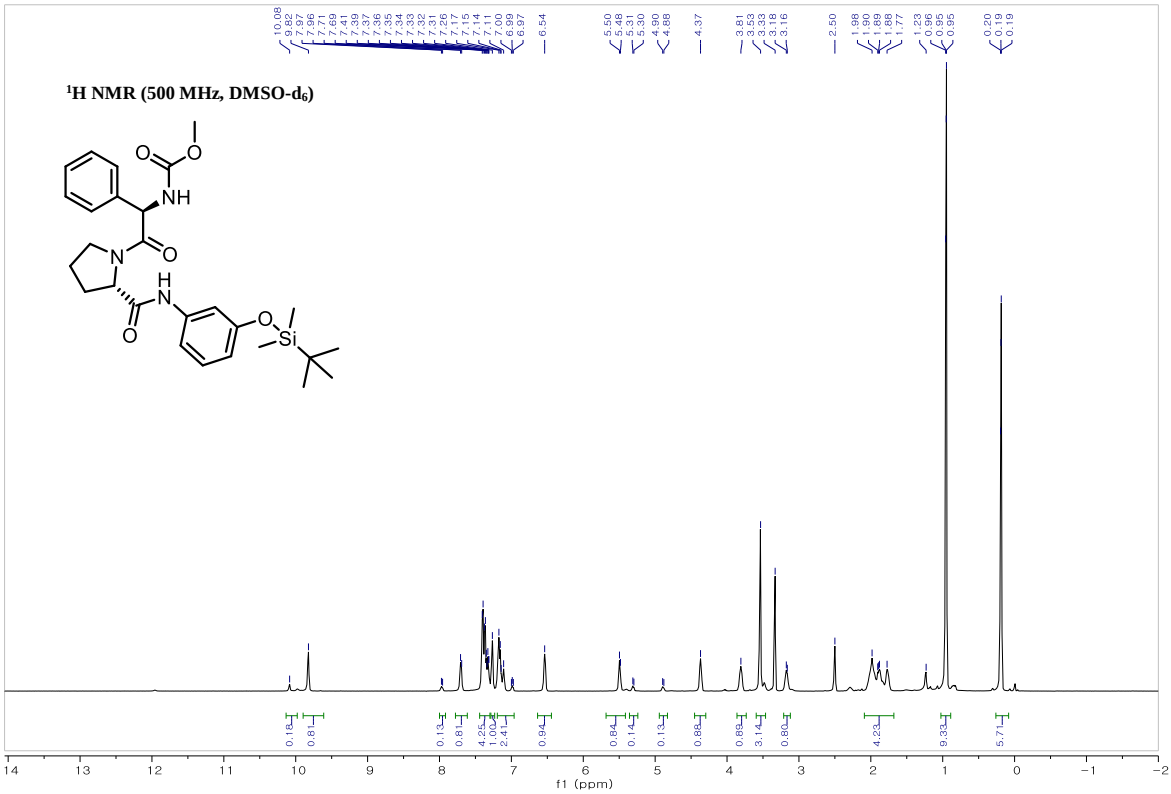

1H NMR (500 MHz, DMSO-d6)
f1 (ppm)

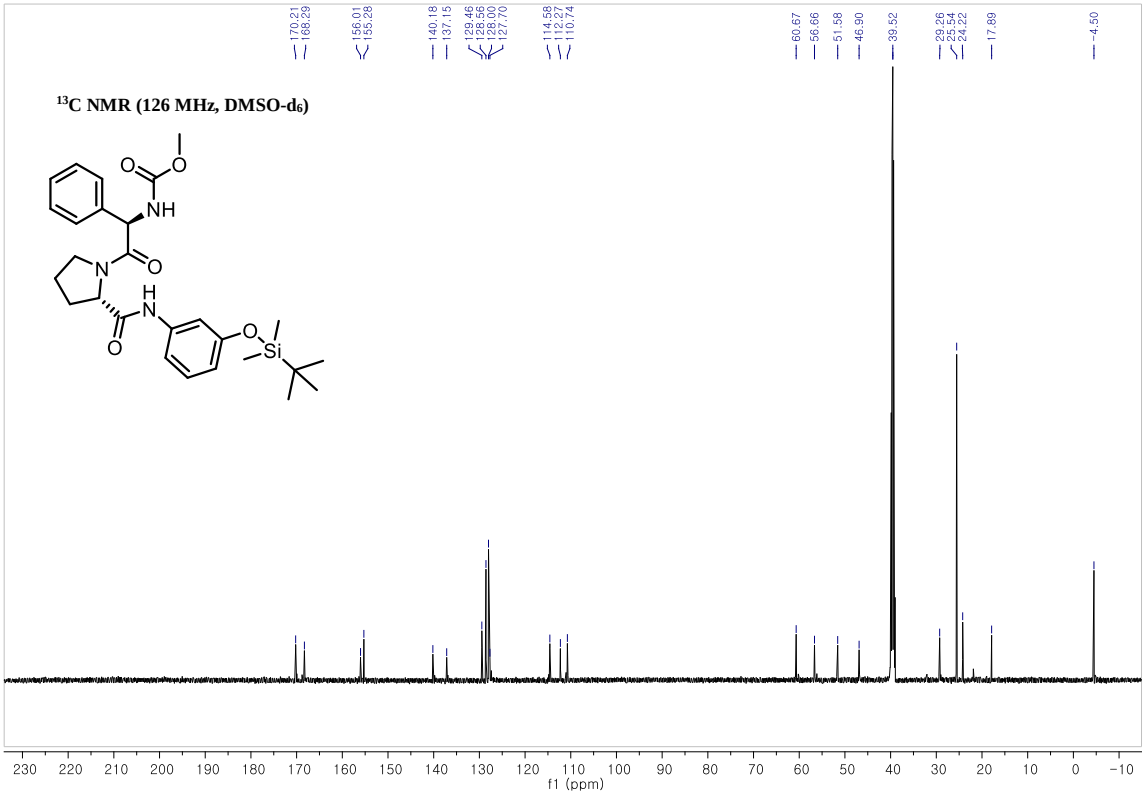


HPLC (compound 29, wavelength = 254 nm)

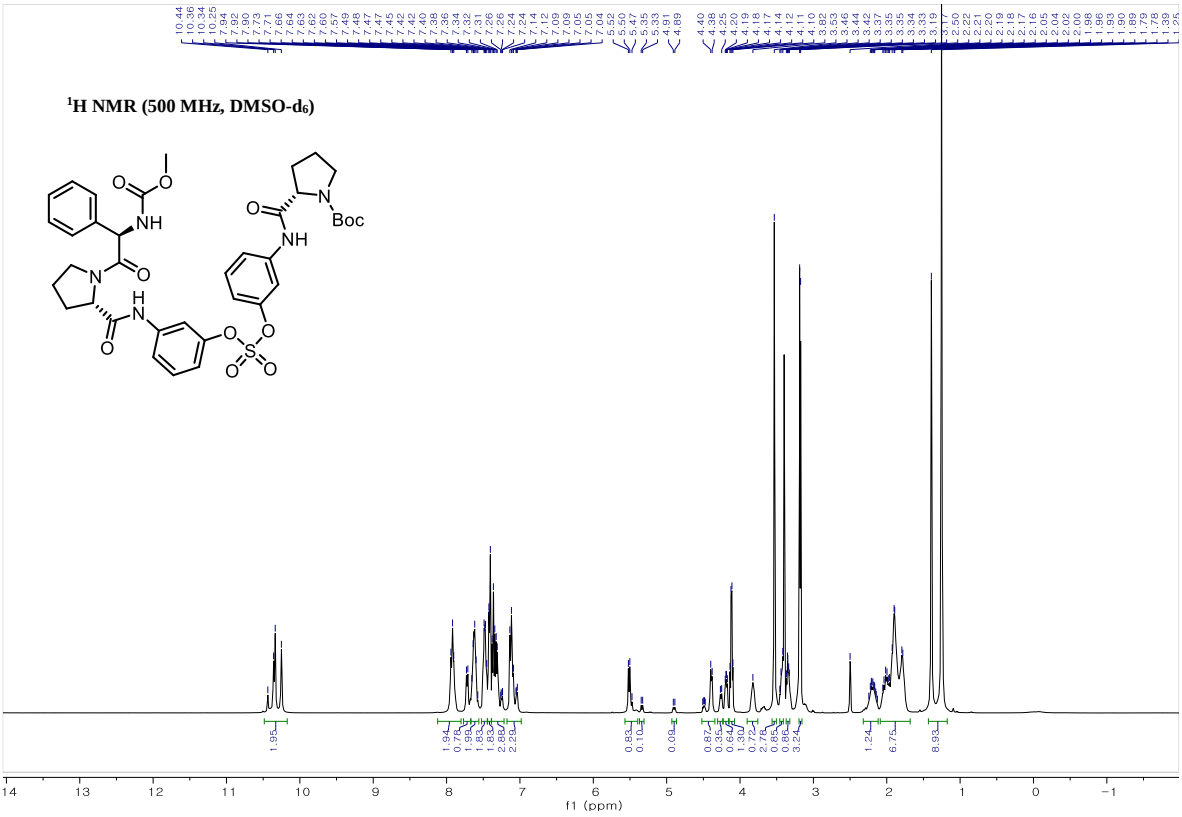


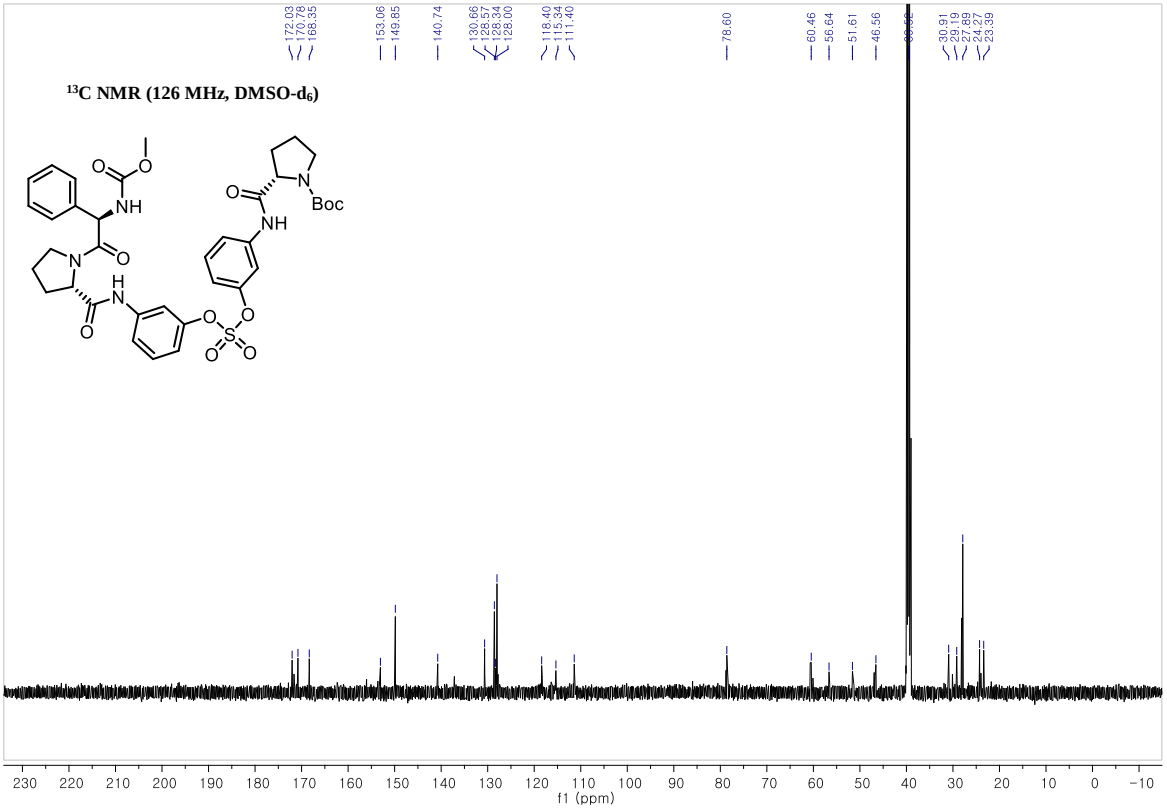
Compound 30



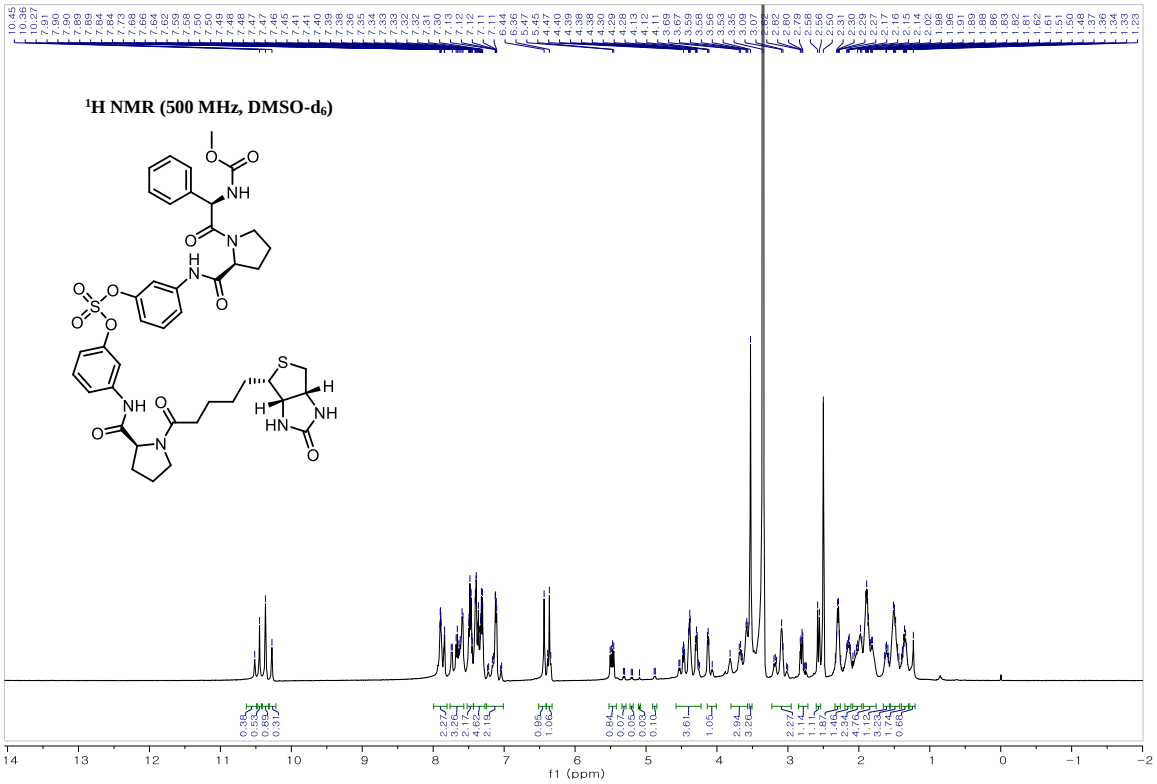


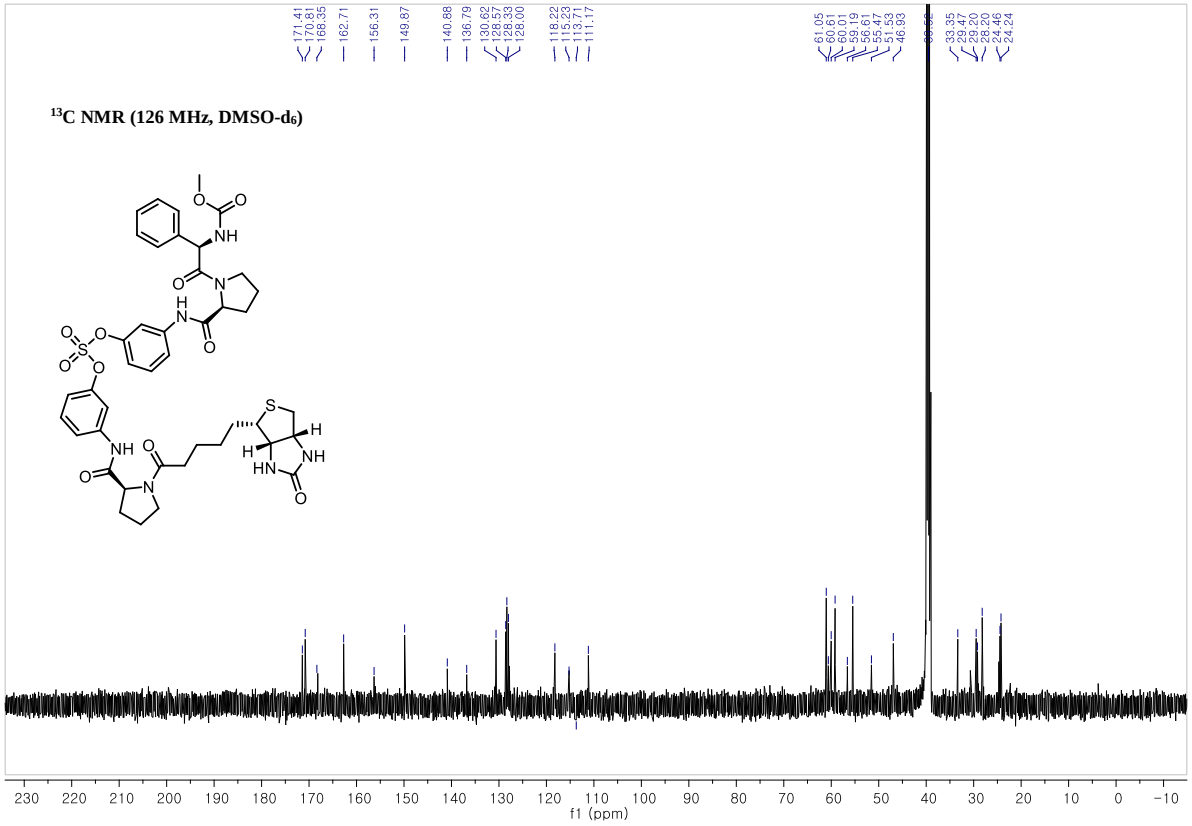
Compound 31





Compound 32





HPLC (compound 32, wavelength = 254 nm)