

Supporting Information for

Original article

Structure–activity relationship of pyrazol-4-yl-pyridine derivatives and identification of a radiofluorinated probe for imaging the muscarinic acetylcholine receptor M₄

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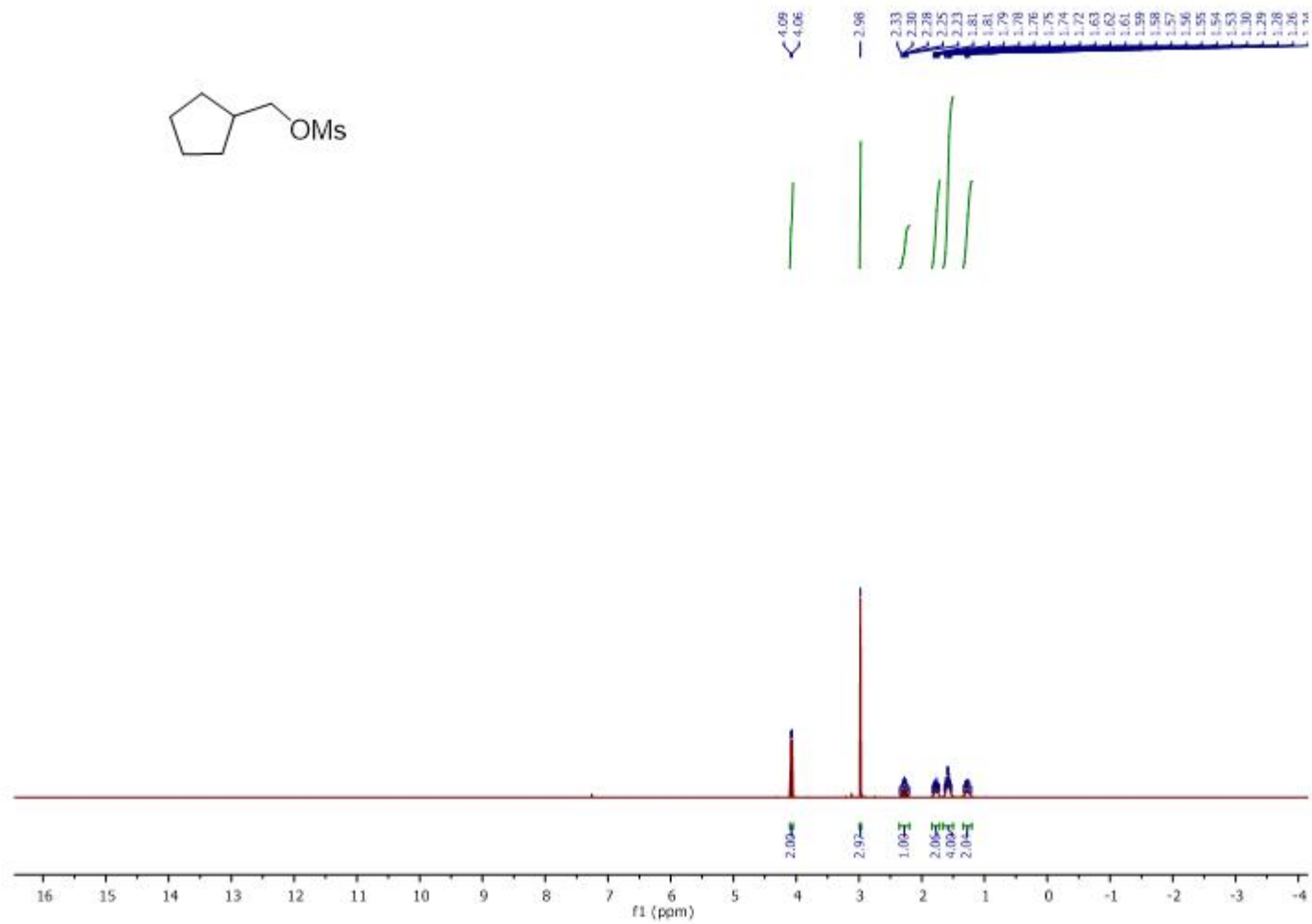
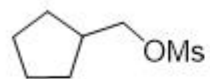
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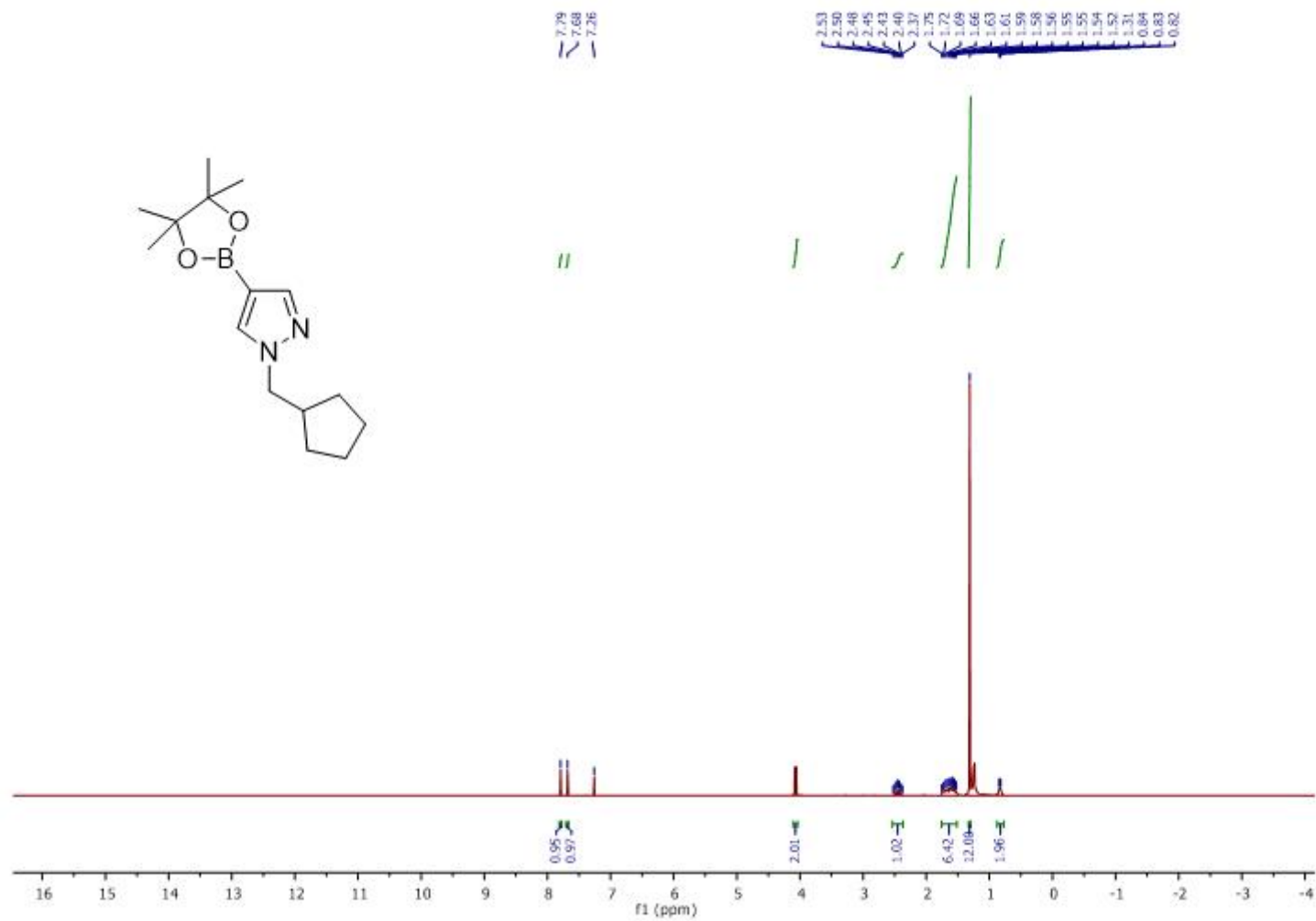
E-mail addresses: liang.steven@mgh.harvard.edu (Steven H. Liang).

Running title: Imaging muscarinic acetylcholine receptor M₄

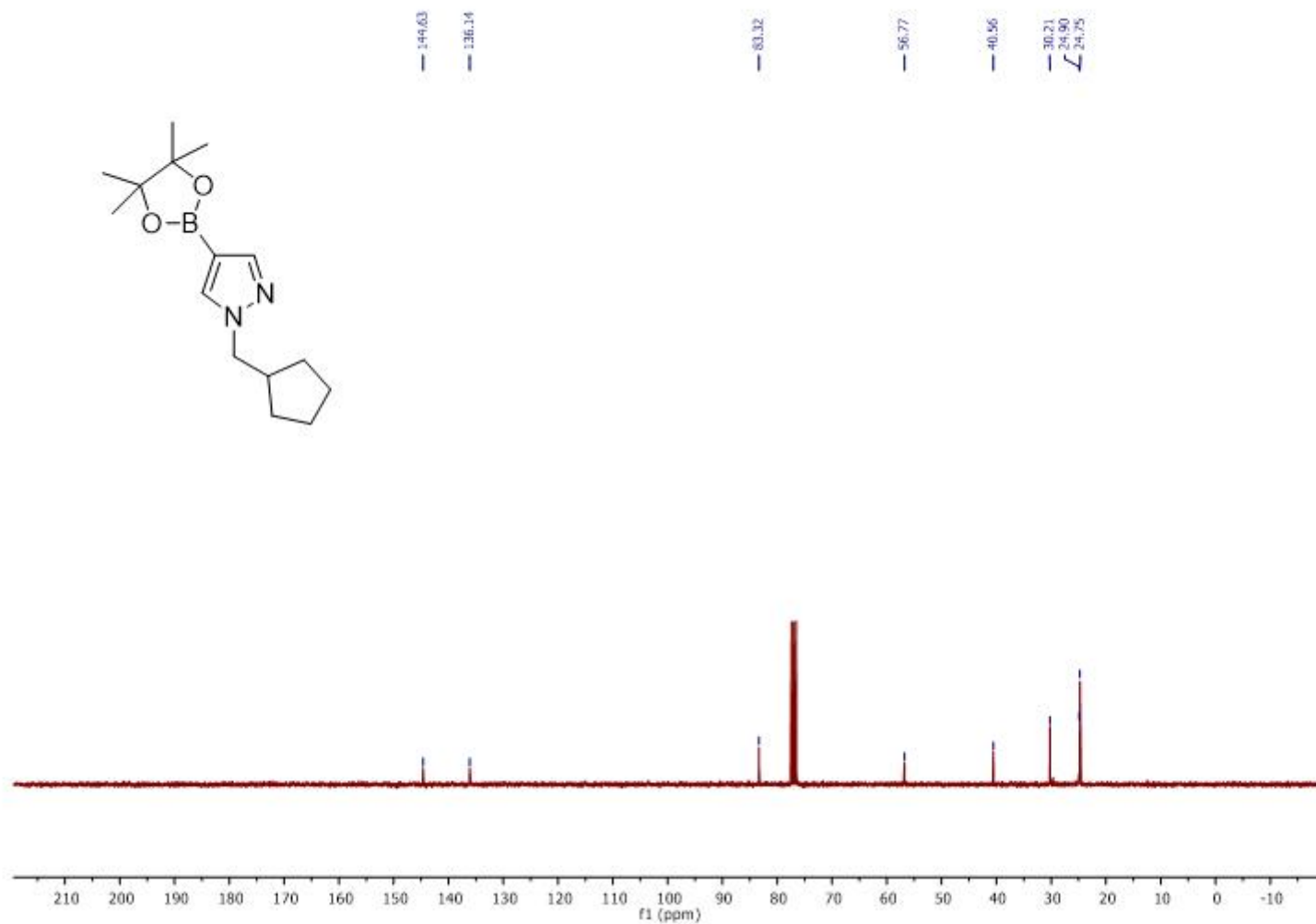
^1H spectrum of compound 2



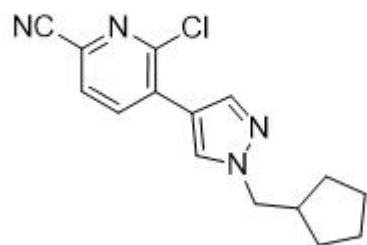
¹H spectrum of compound 4



¹³C spectrum of compound 4

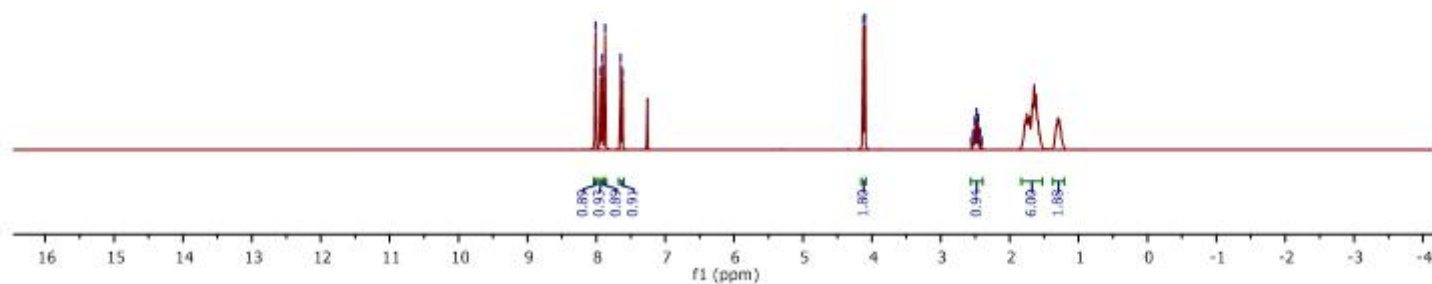


¹H spectrum of compound 6a



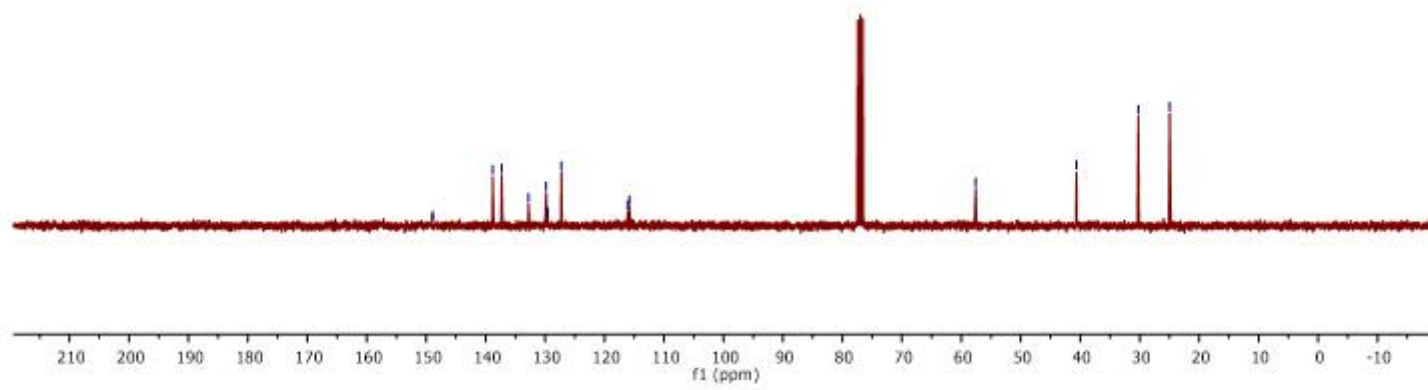
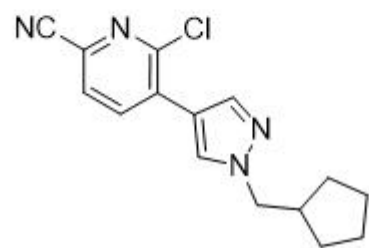
8.01, 7.94, 7.81, 7.87, 7.65, 7.62, 4.12, 4.10, 2.56, 2.53, 2.51, 2.48, 2.46, 2.43, 2.40

A (m)
2.48

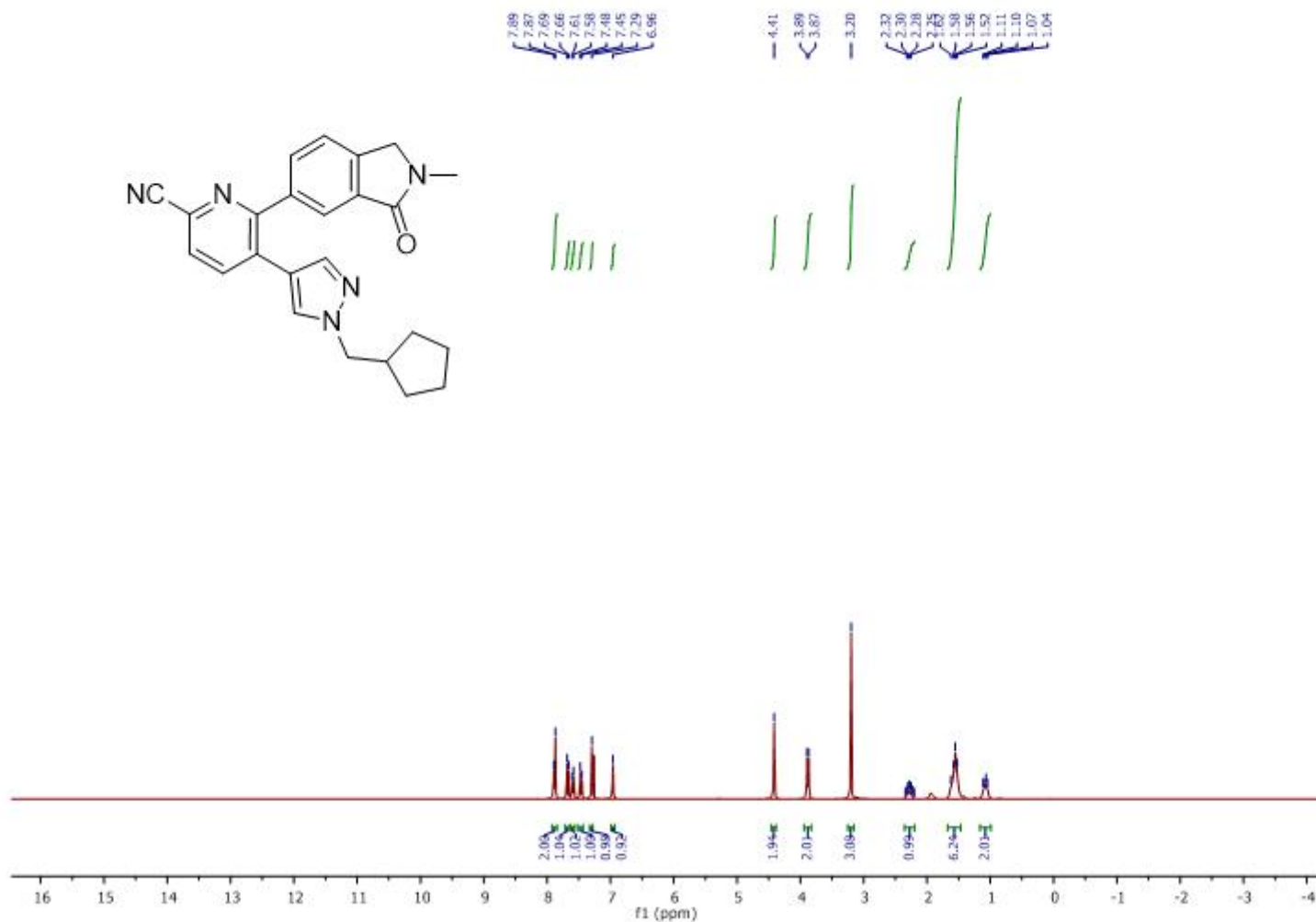
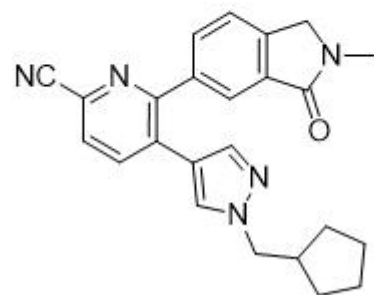


¹³C spectrum of compound **6a**

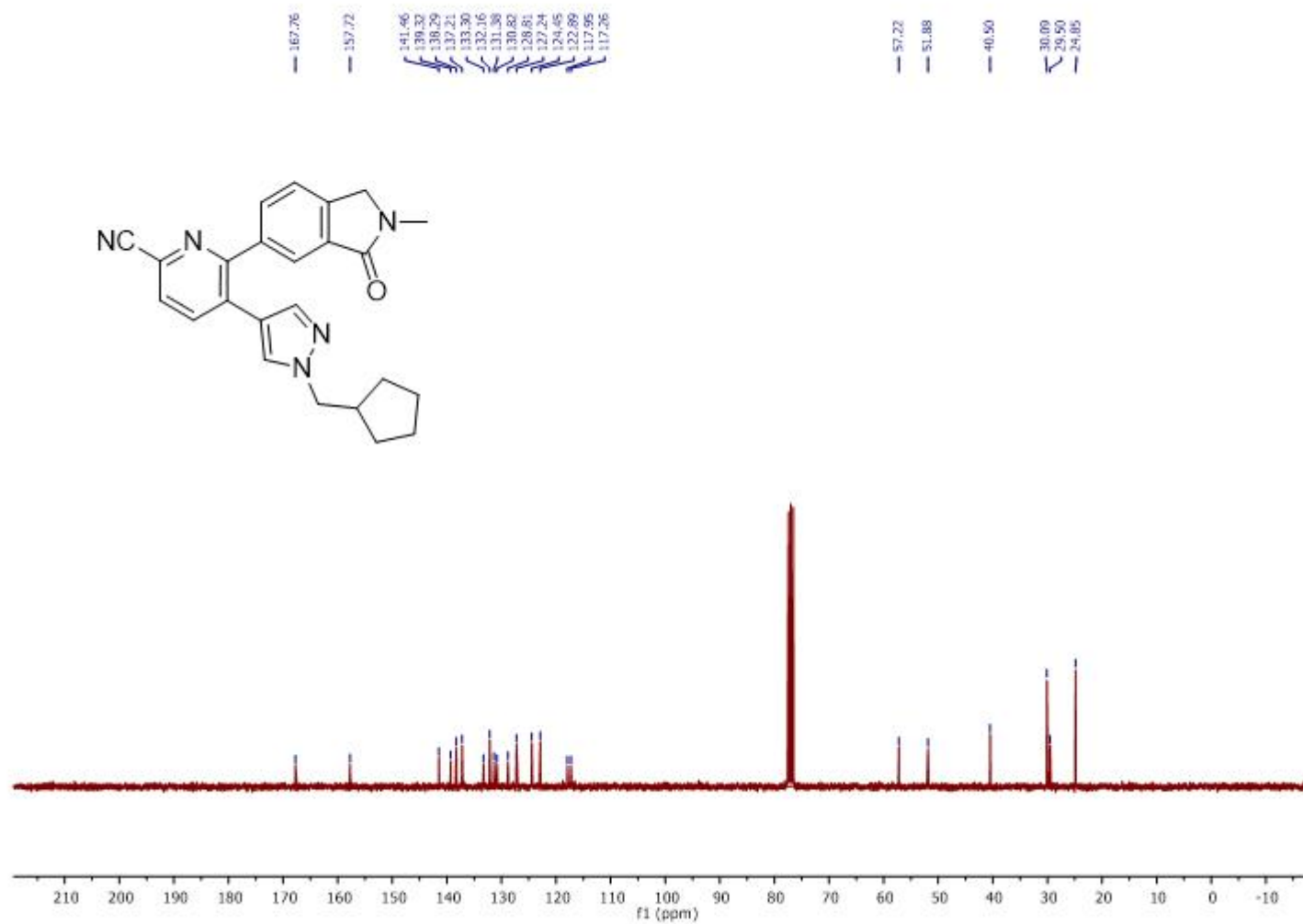
- 148.94
- 138.83
- 137.30
- 132.81
- 129.84
- 129.57
- 127.26
- 116.14
- 115.83
- 57.58
- 40.63
- 30.25
- 24.96



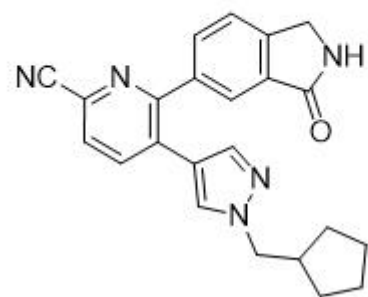
^1H spectrum of compound **8**



¹³C spectrum of compound 8



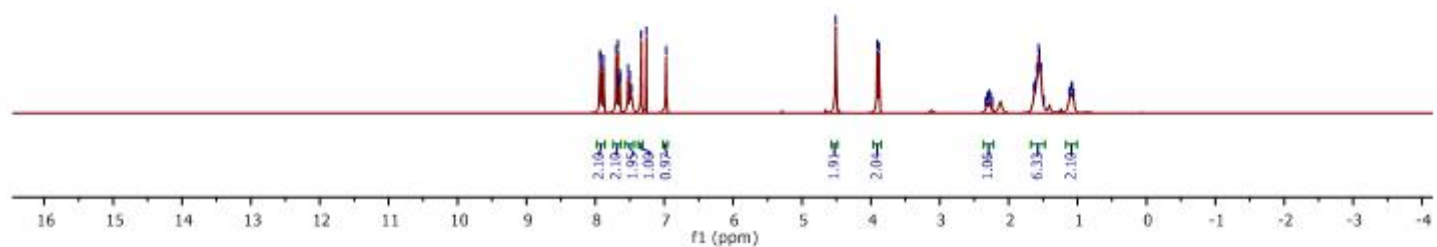
¹H spectrum of compound 9



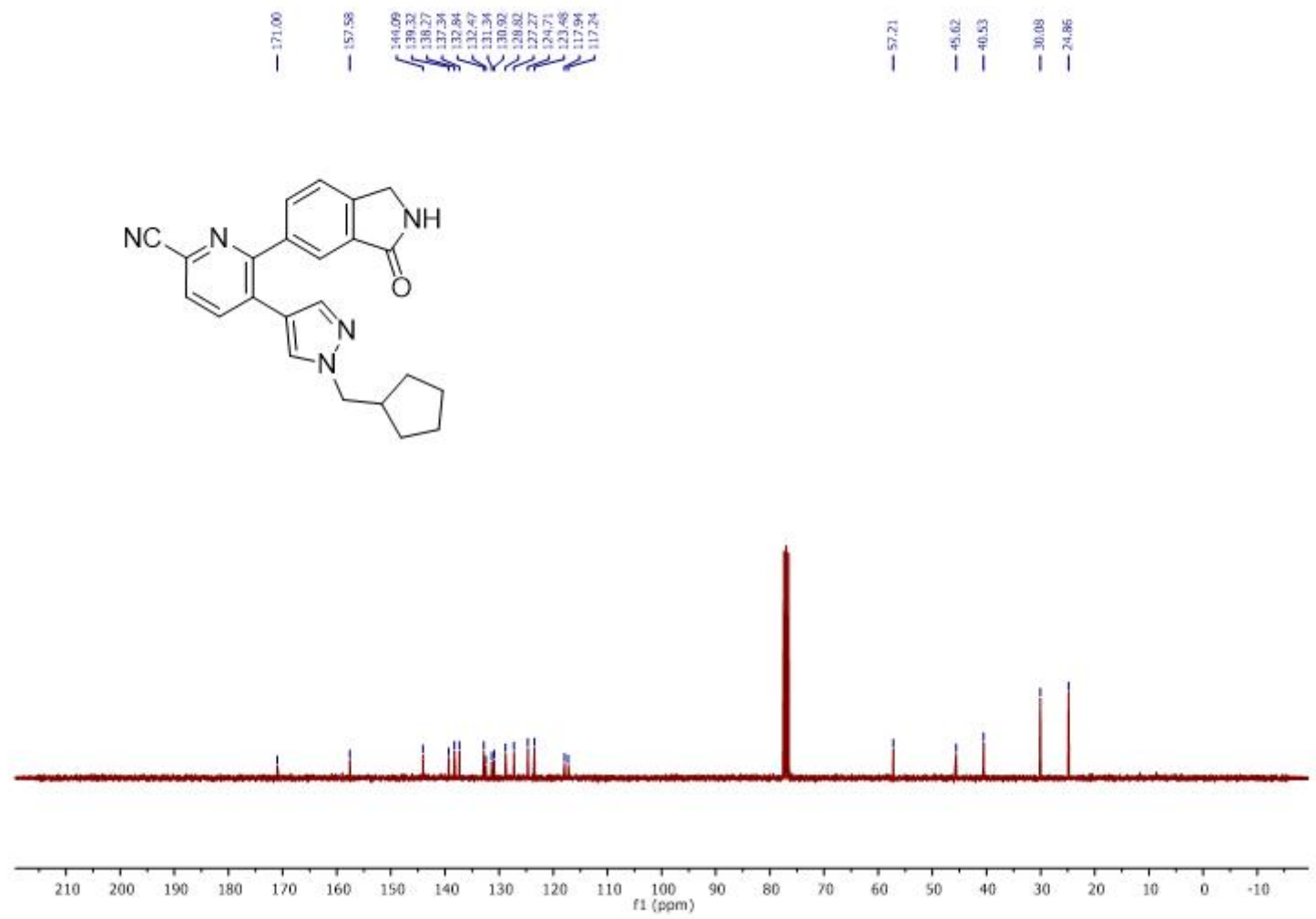
7.93
7.92
7.91
7.88
7.70
7.67
7.65
7.64
7.53
7.50
7.47
7.33
7.26
6.97

4.51
3.91
3.88

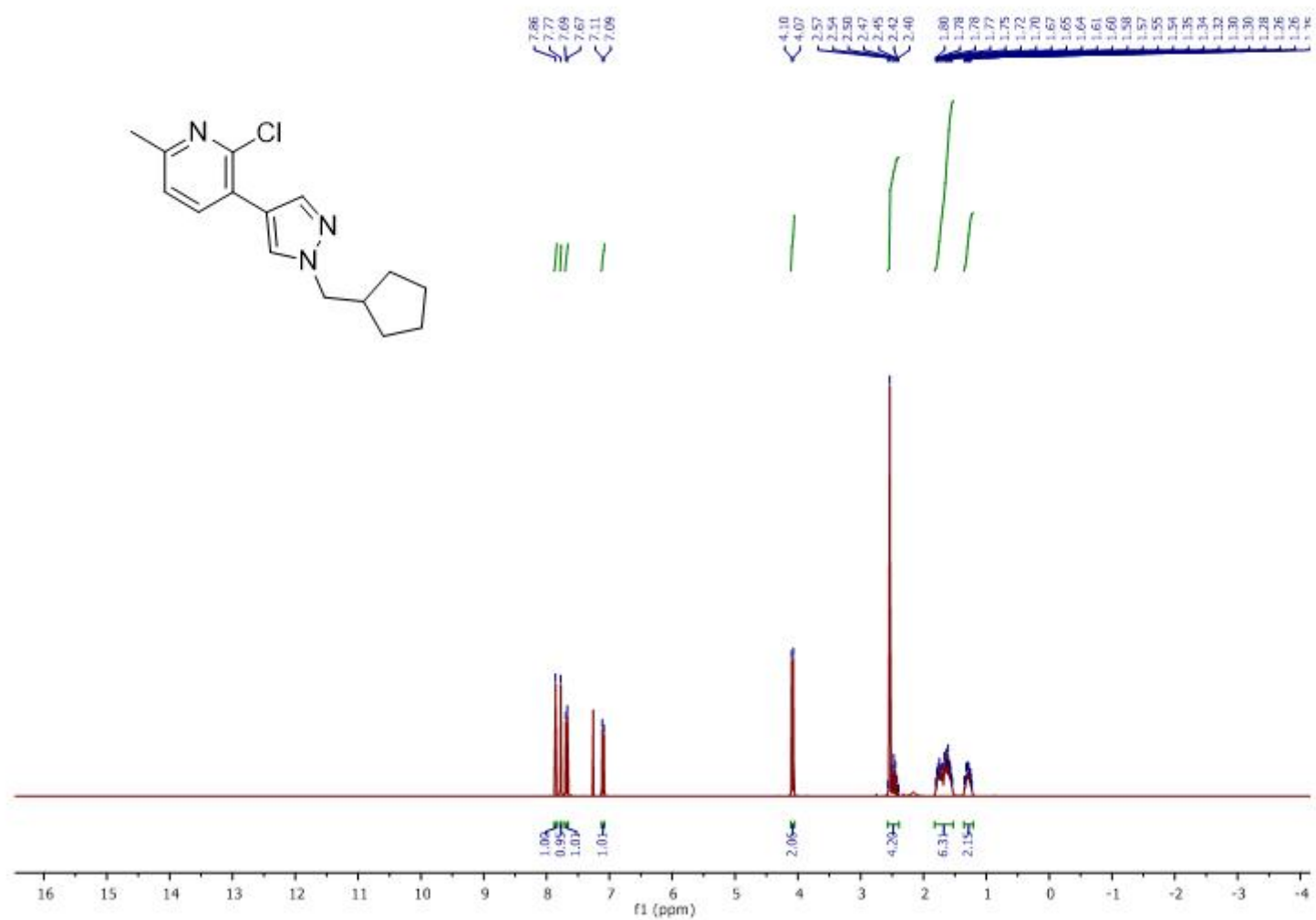
2.33
2.31
2.29
2.26
2.24
1.63
1.62
1.59
1.57
1.55
1.49
1.12
1.09
1.08
1.06



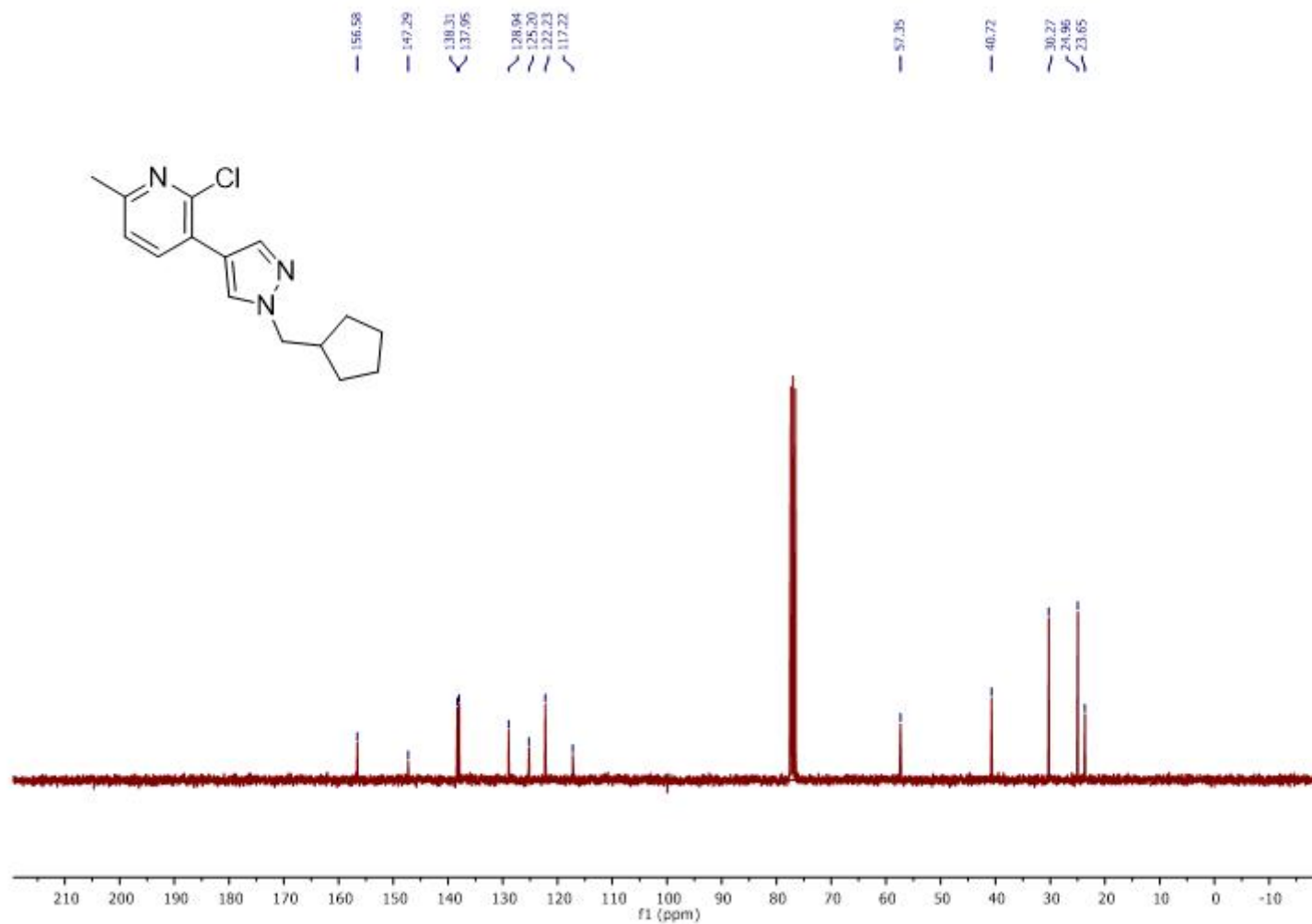
¹³C spectrum of compound 9



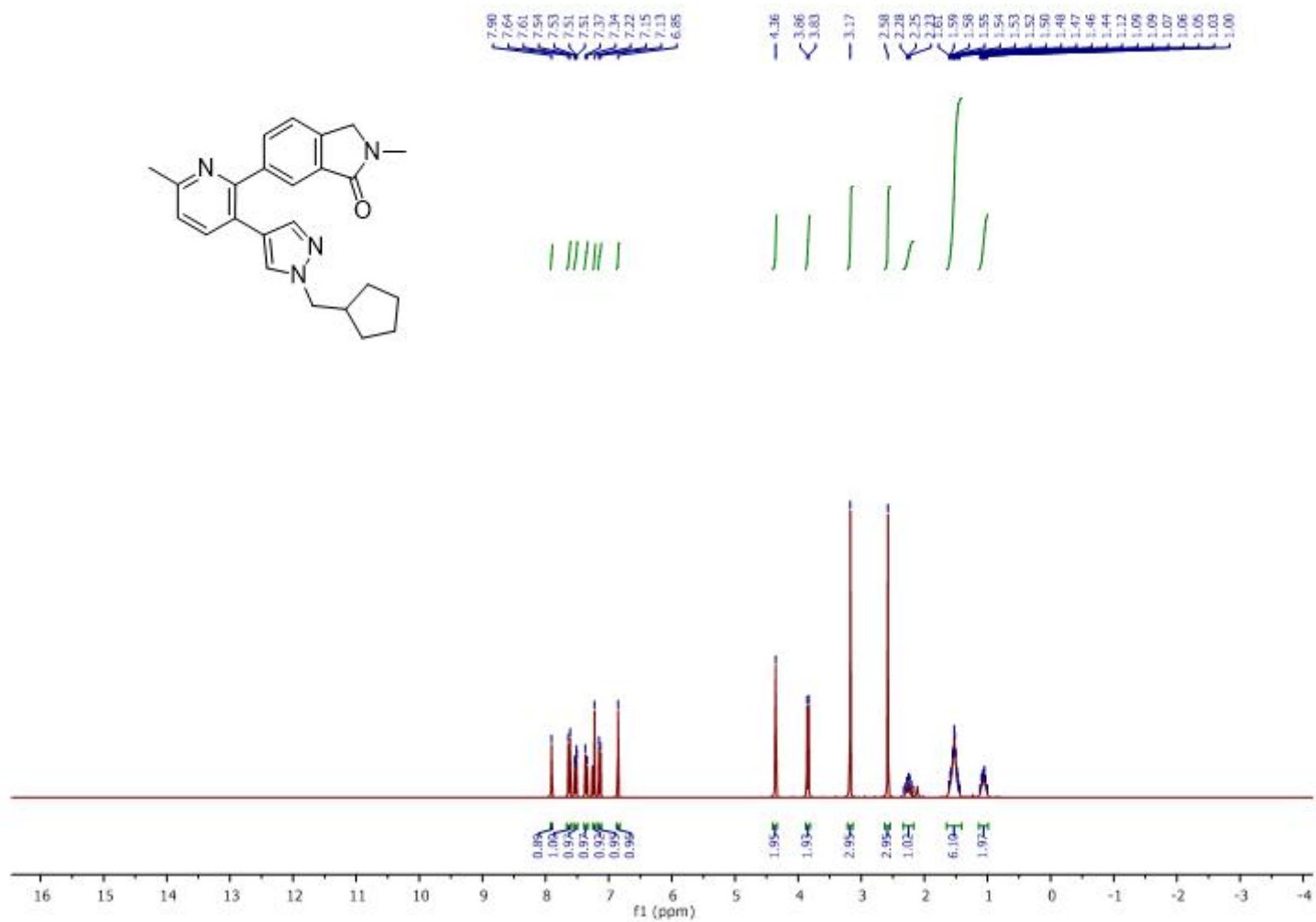
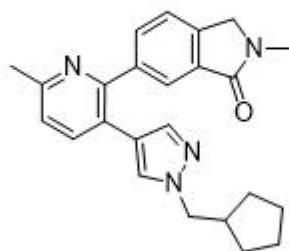
¹H spectrum of compound **6b**



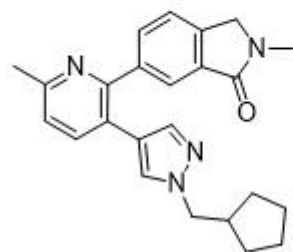
¹³C spectrum of compound **6b**



¹H spectrum of compound 10

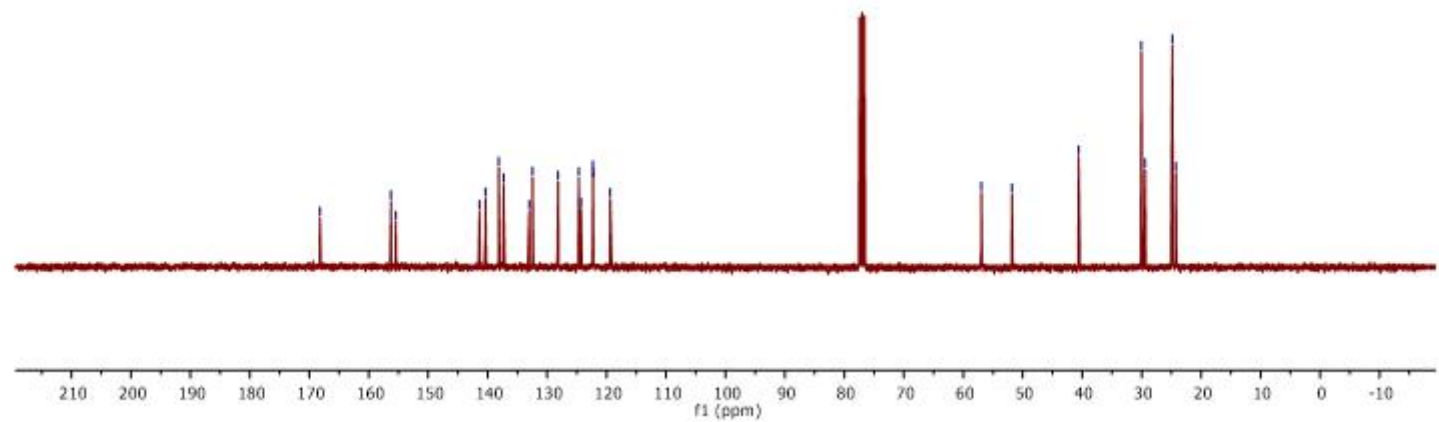


¹³C spectrum of compound 10

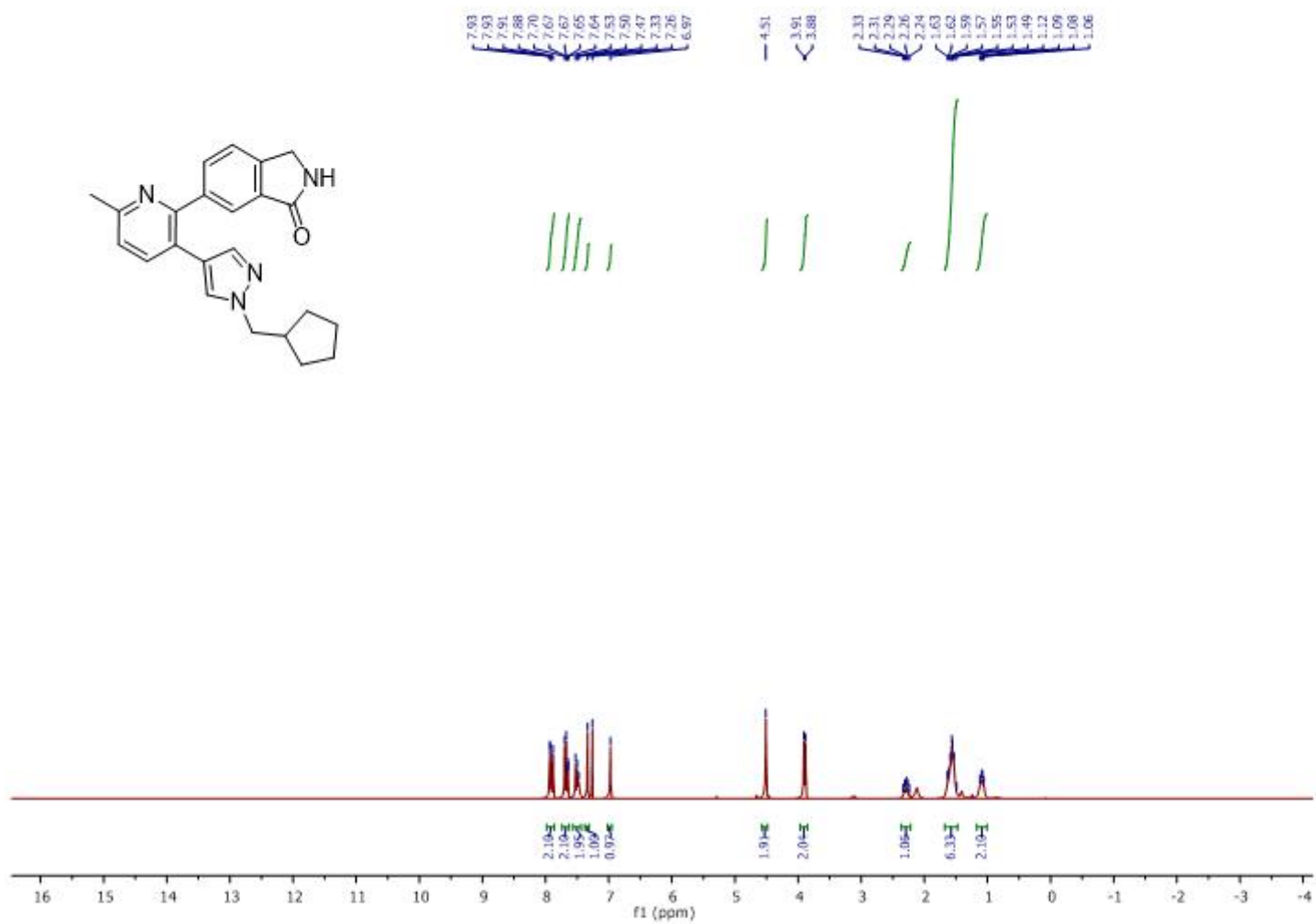
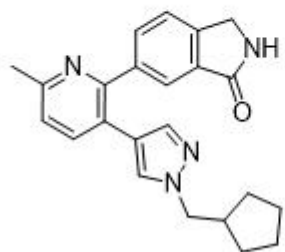


168.22
156.27
155.47
141.39
140.37
138.14
137.31
133.01
132.45
128.14
124.68
124.30
122.30
122.22
119.39

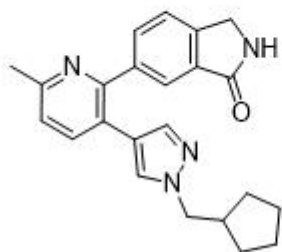
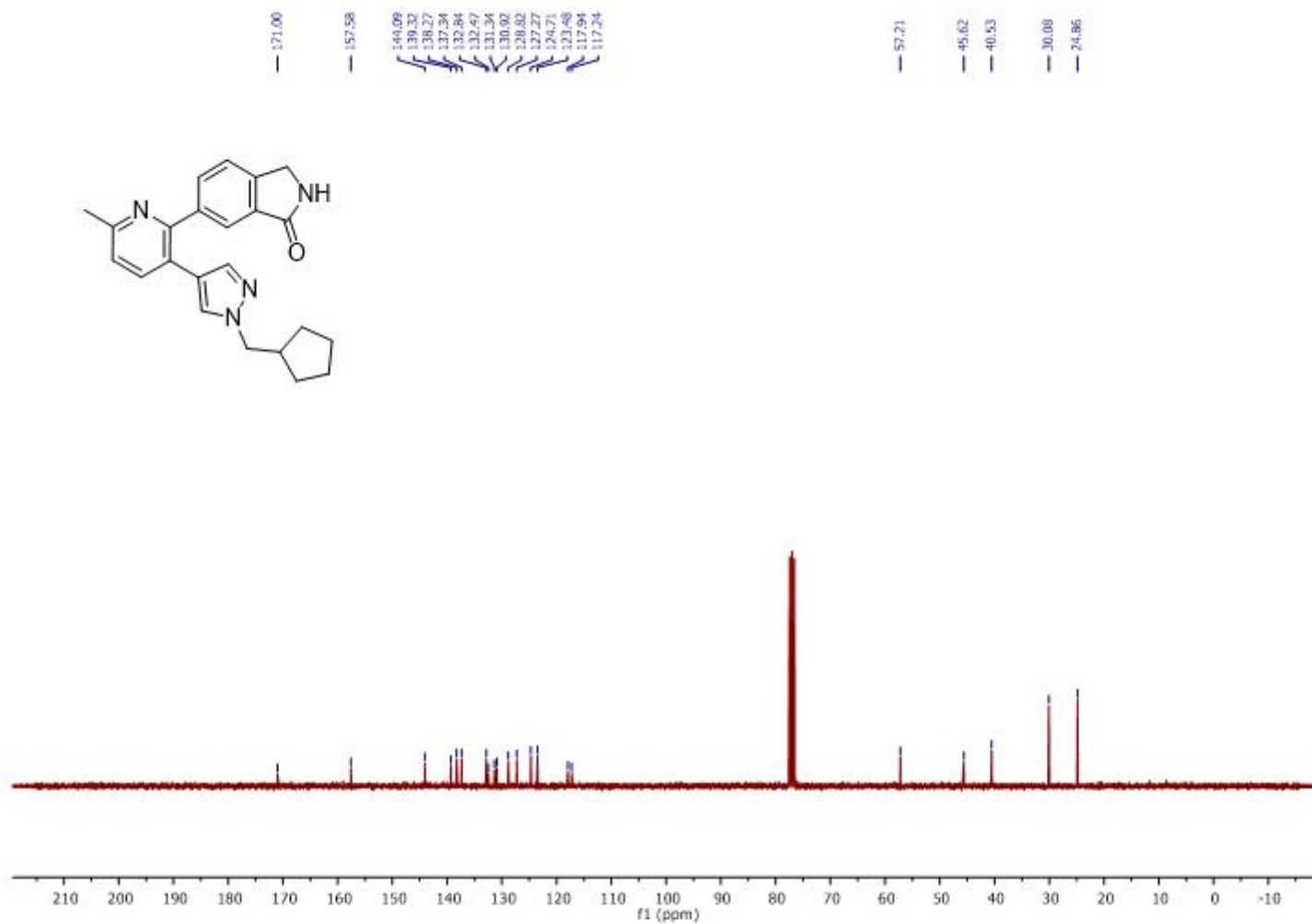
56.95
51.83
40.60
30.06
29.43
24.85
24.23



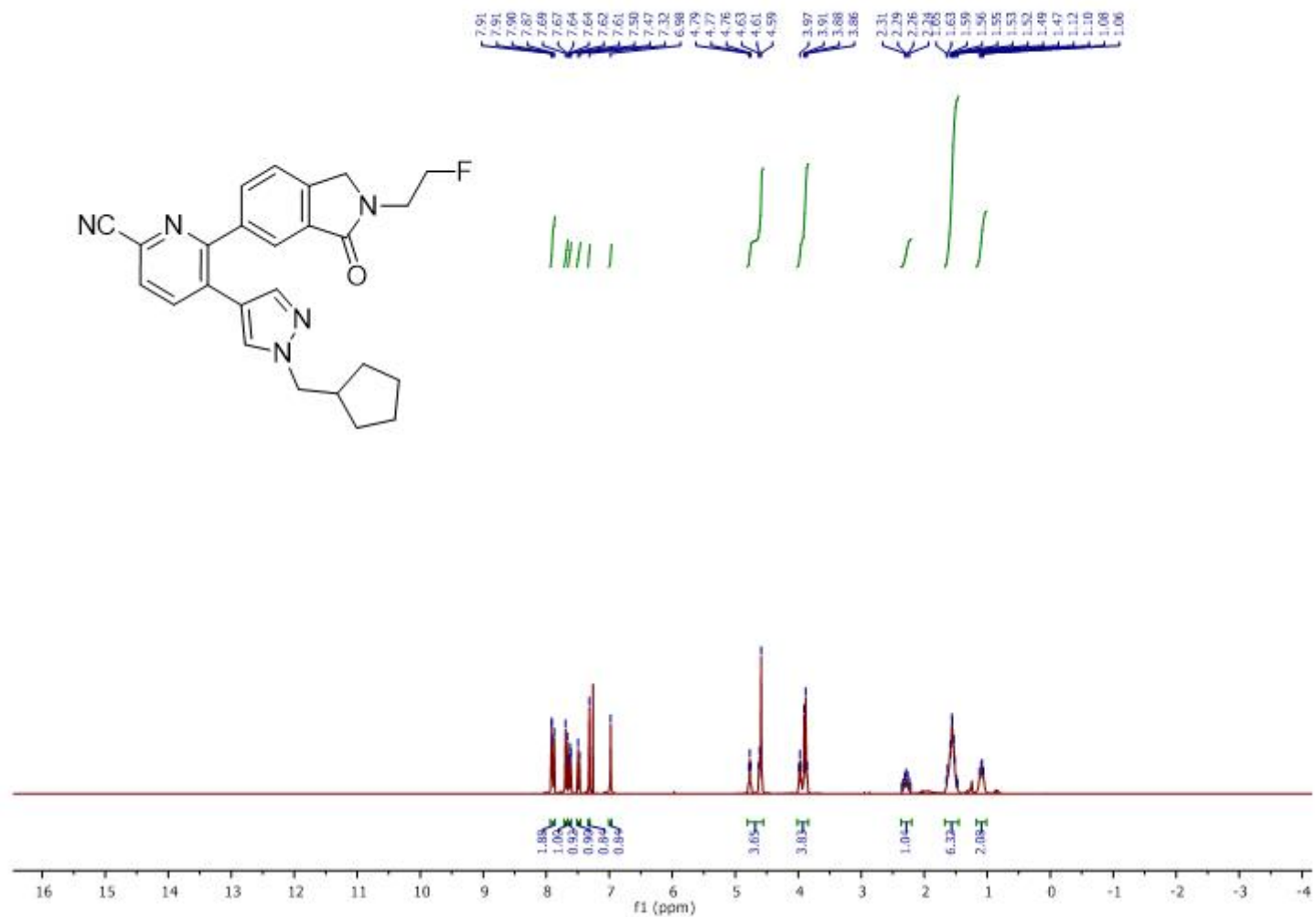
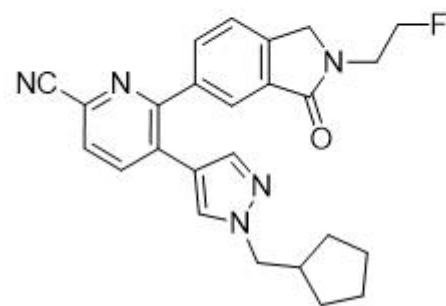
^1H spectrum of compound 11



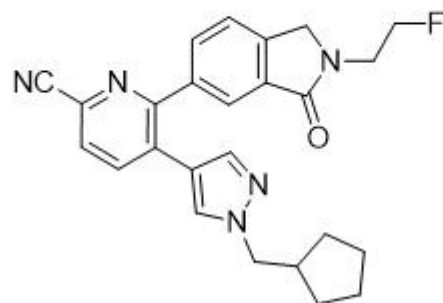
¹³C spectrum of compound **11**



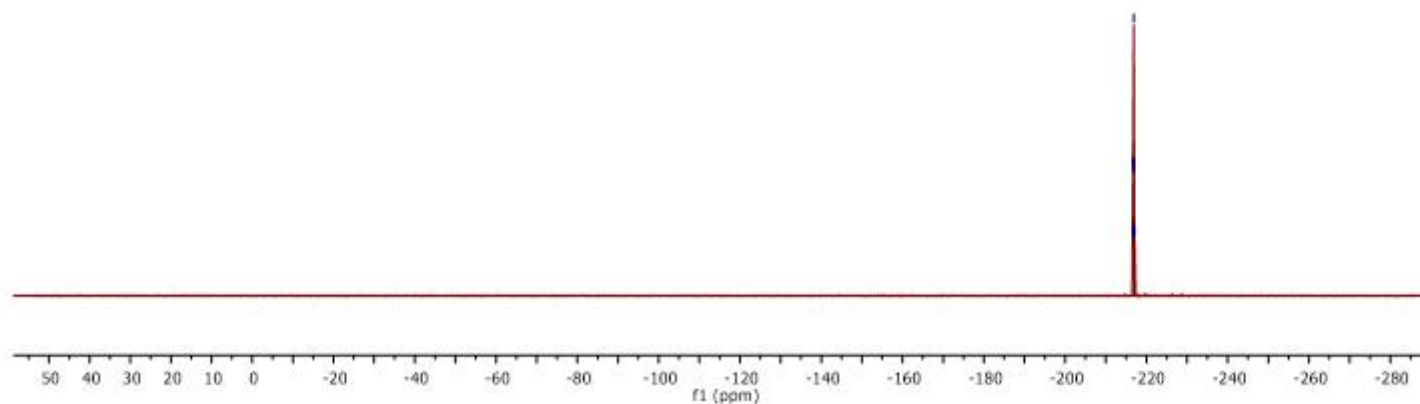
¹H spectrum of compound 12



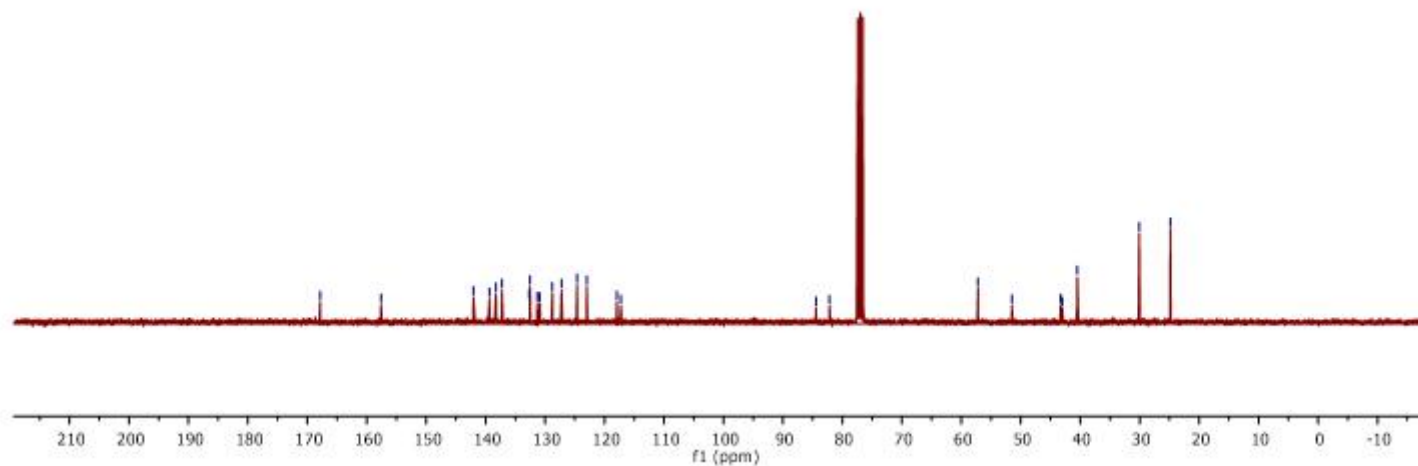
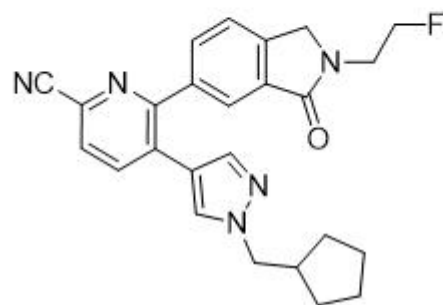
^{19}F spectrum of compound **12**



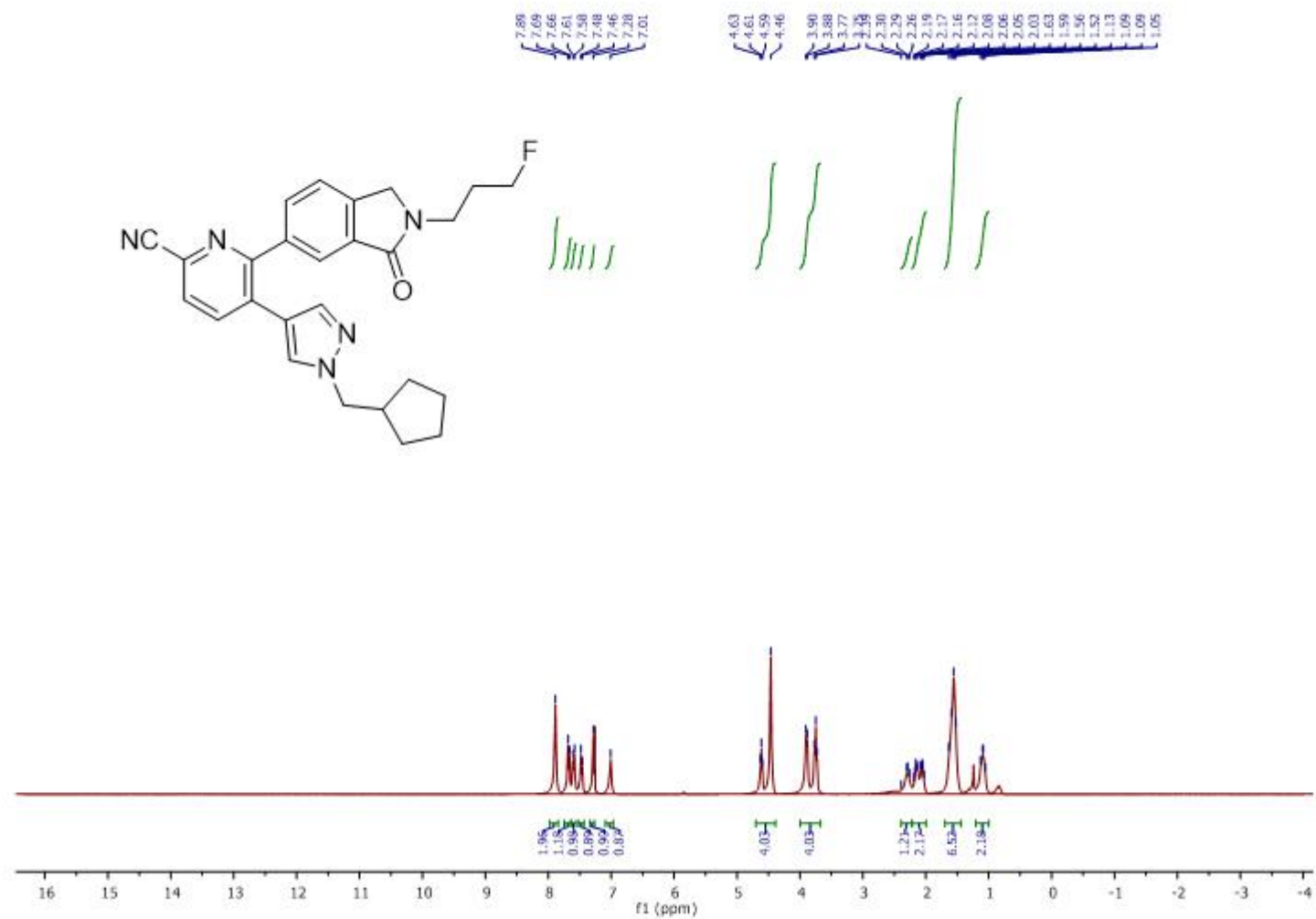
-216.60
-216.70
-216.76
-216.90
-216.87
-216.93
-216.89
-217.03
-217.14



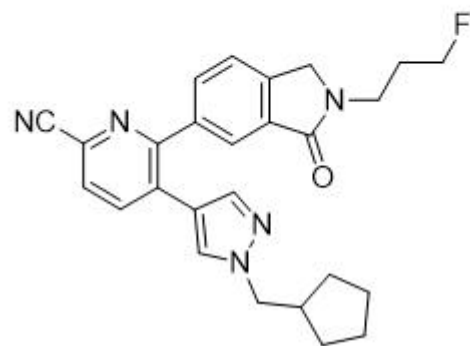
¹³C spectrum of compound 12



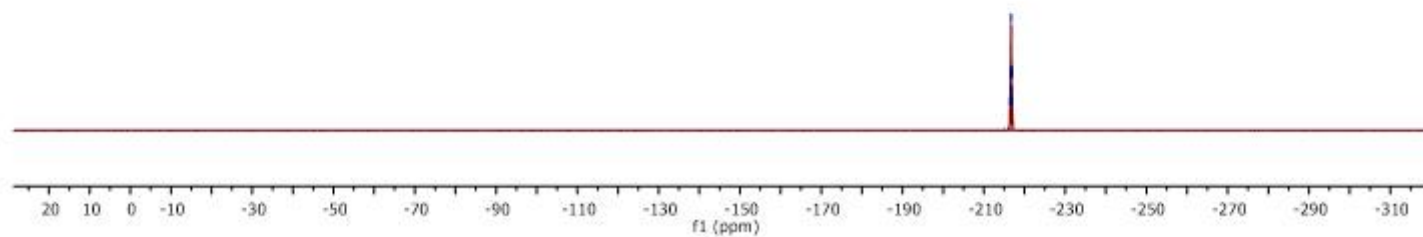
¹H spectrum of compound 13



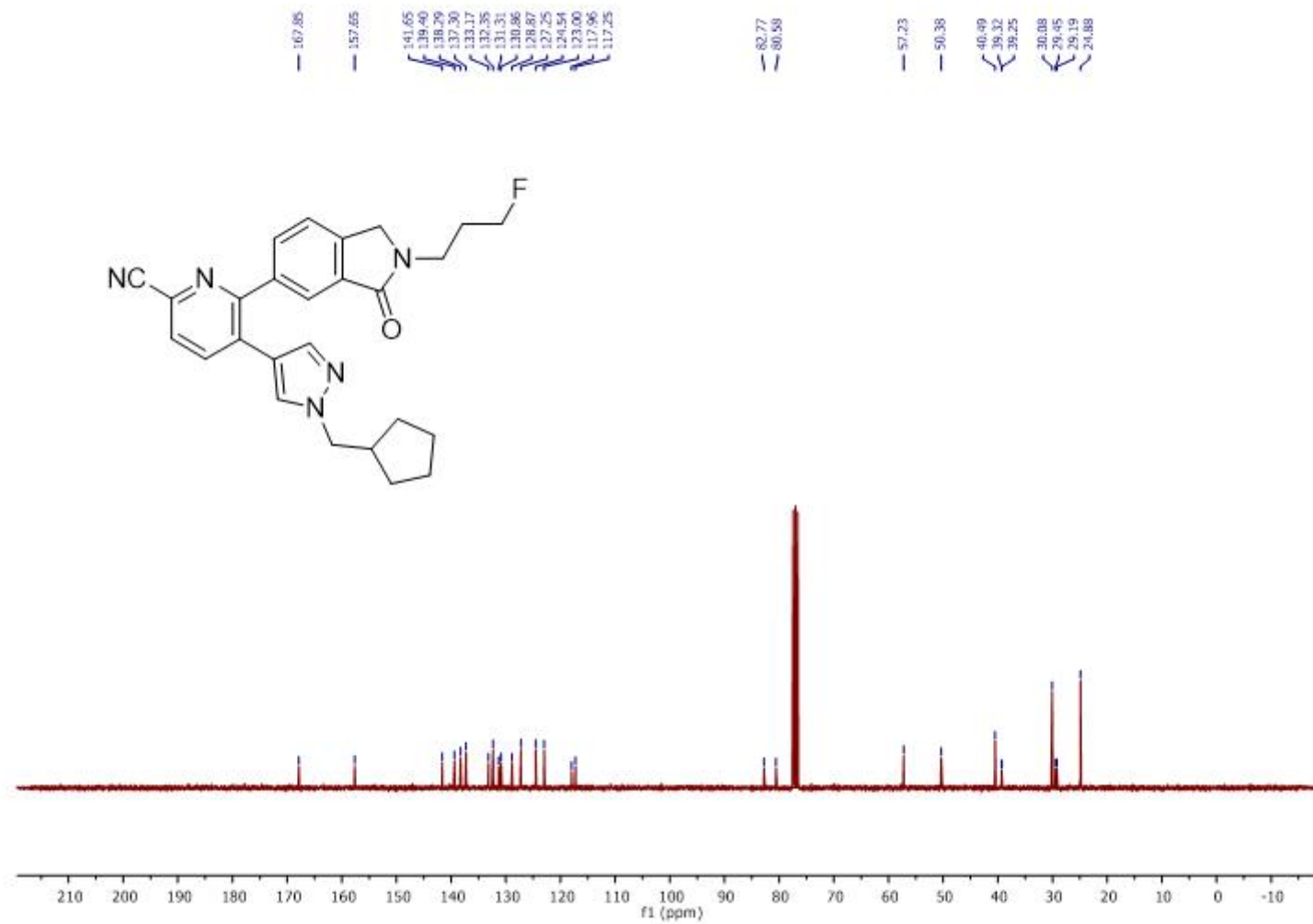
^{19}F spectrum of compound **13**



-216.45
-216.35
-216.62
-216.64
-216.71
-216.79
-216.81
-216.88
-216.97

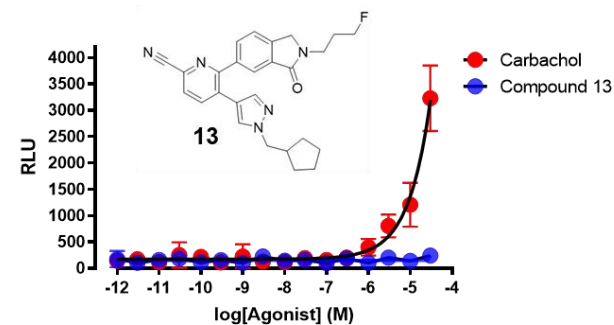
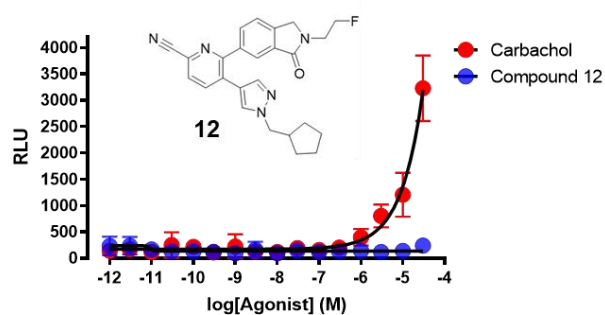
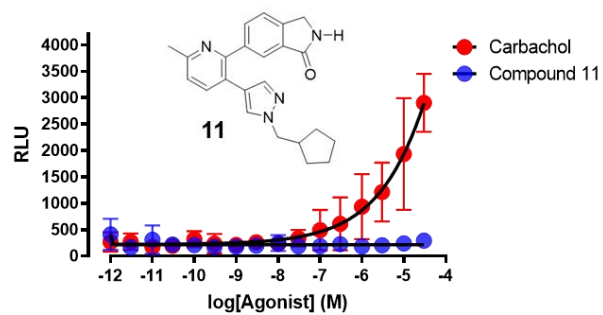
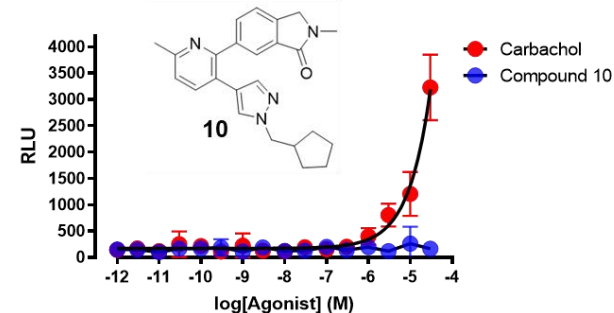
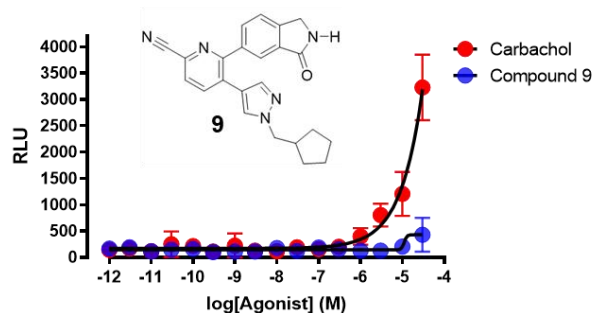
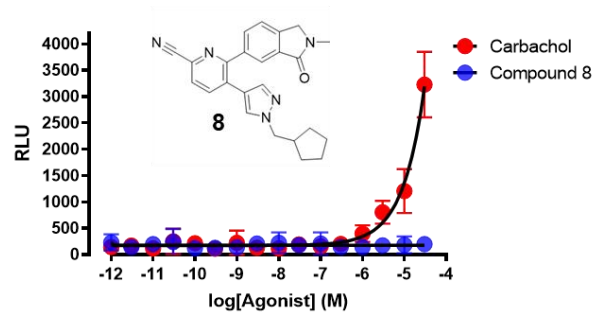


¹³C spectrum of compound **13**



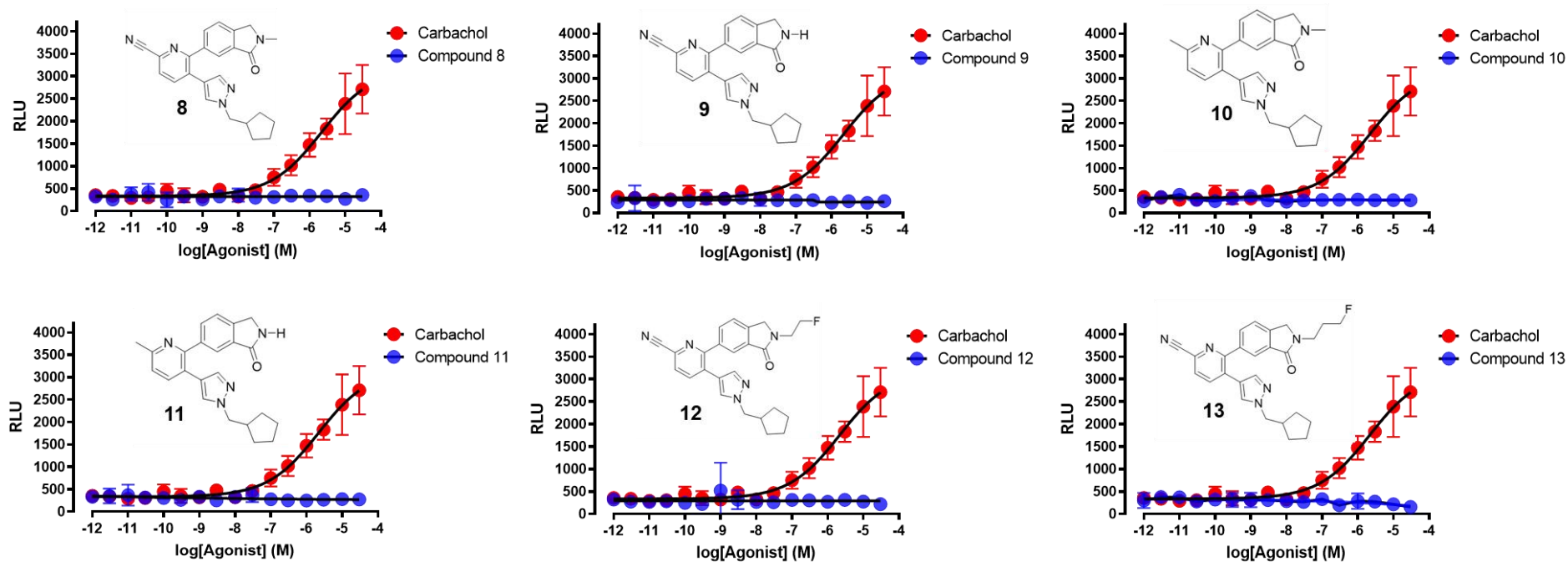
M1 Receptor

Supplemental Figure 1



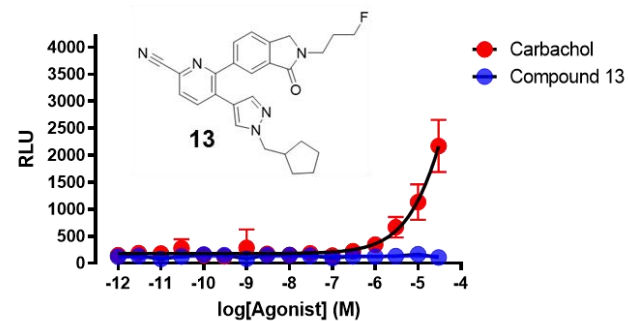
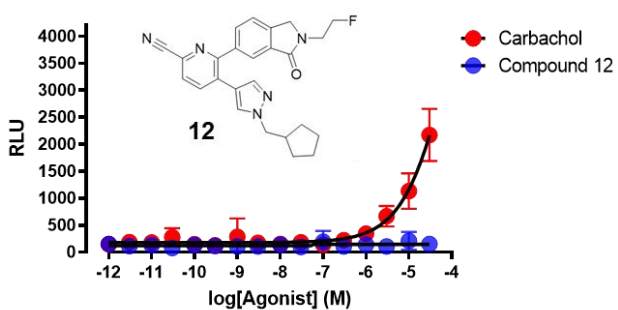
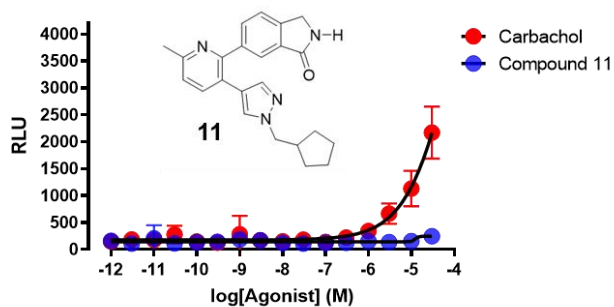
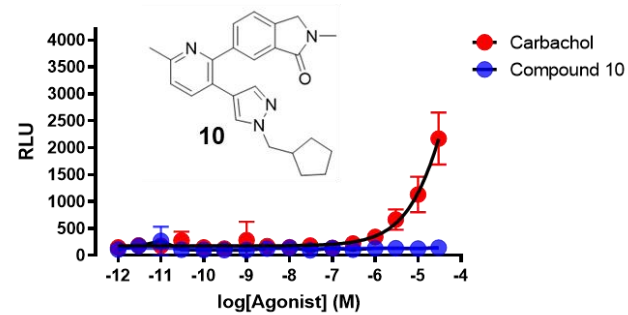
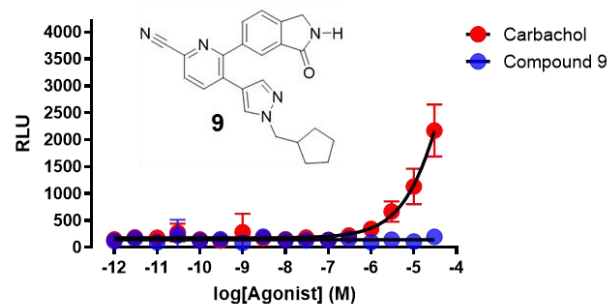
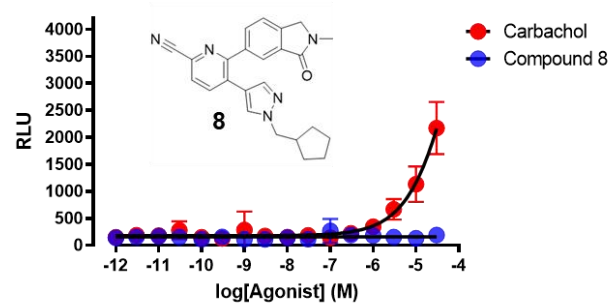
M2 Receptor

Supplemental Figure 2



M3 Receptor

Supplemental Figure 3



M5 Receptor

Supplemental Figure 4

