Electronic Supplementary Material (ESI) for RSC Advances.

Novel thiohydantoin analogues bearing 1-hydroxyl-2,2,2-trifluoro-1-ethyl moiety as androgen receptor inhibitors for the potential treatment of castration resistant prostate cancer

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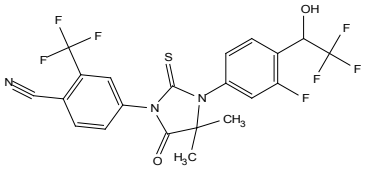
† *These authors contributed equally.*

Spectroscopic Data of Synthetic Compounds

(400.13 MHz, CDCl3)



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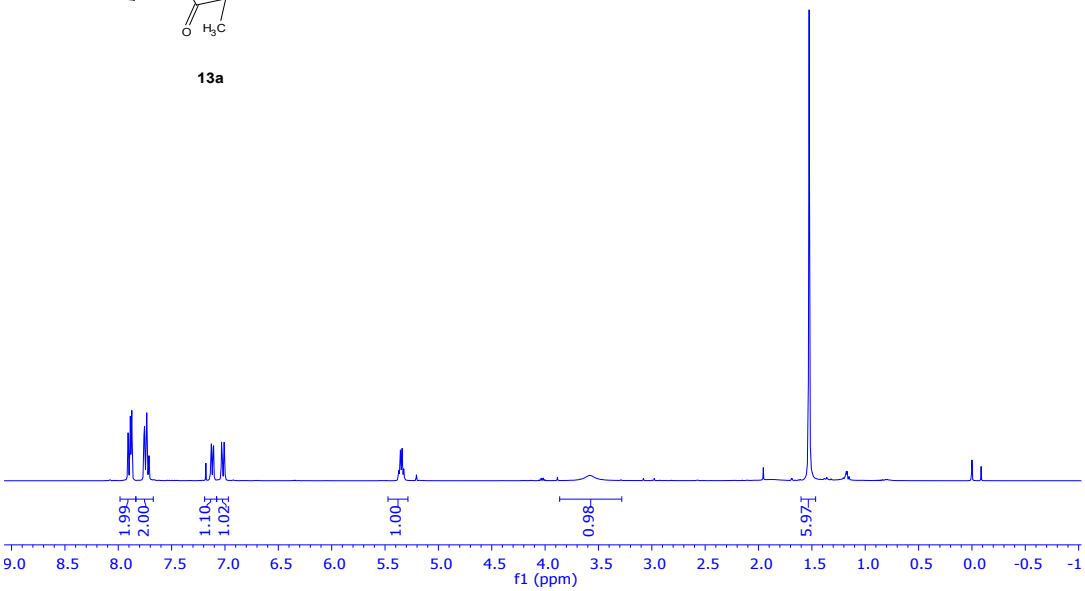

(100.61 MHz, CDCl3)

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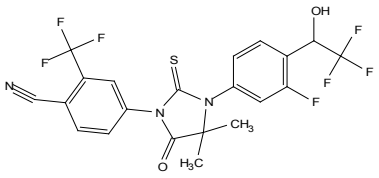

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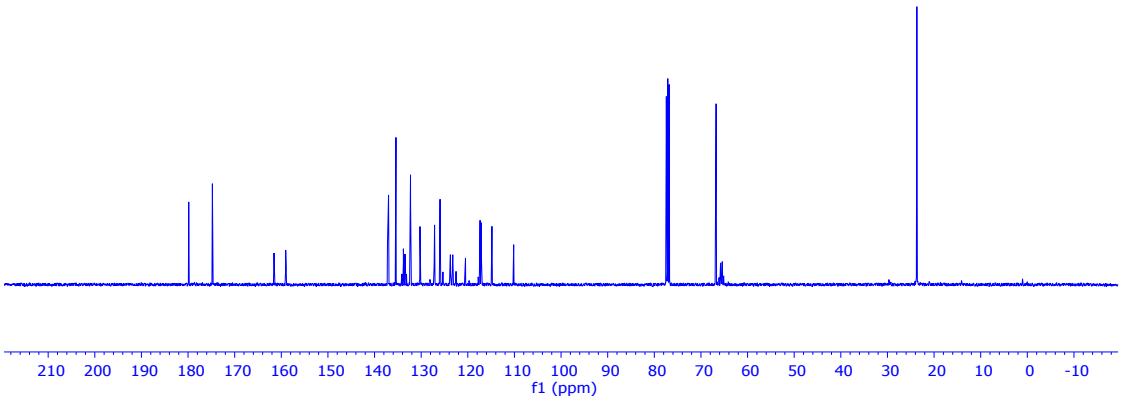
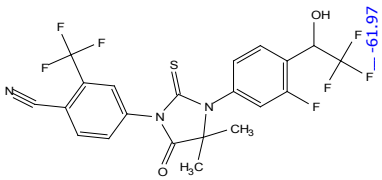


(376.50 MHz, CDCl3)

-61.97 -78.38 -113.85



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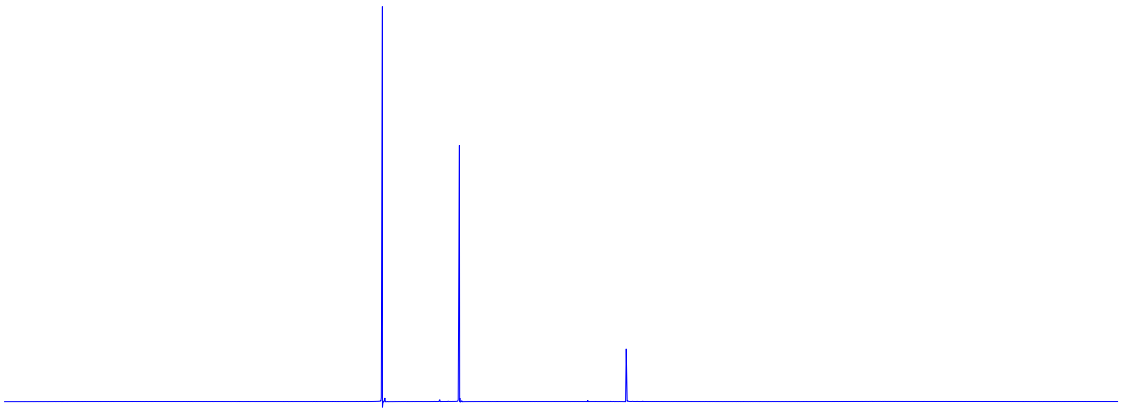

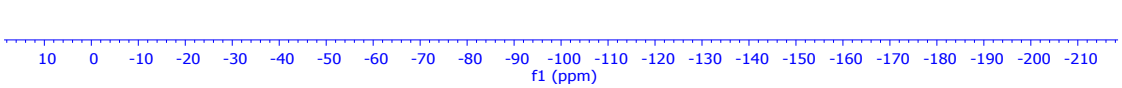

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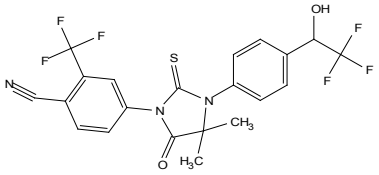

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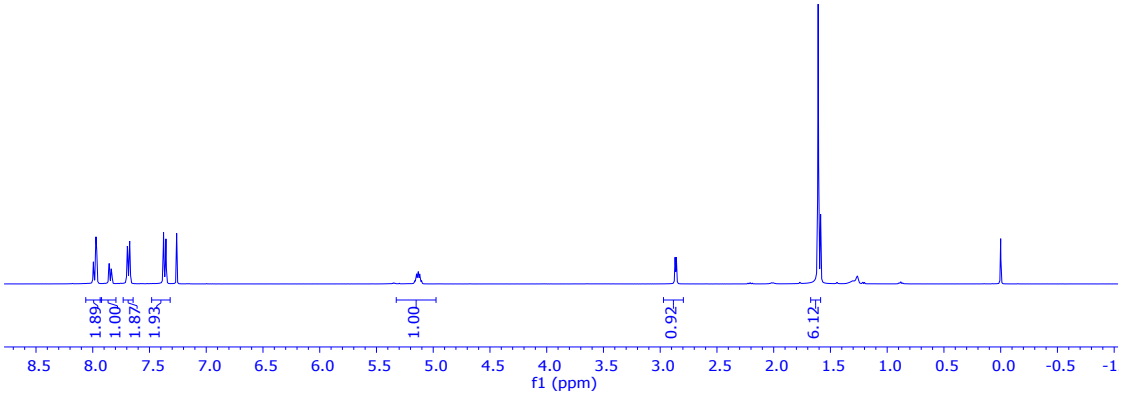

(100.61 MHz, CDCl3)

179.88
174.96
137.09
136.00
135.77
135.32
133.79
133.45
132.26
129.76
129.07
127.18
127.13
125.44
123.25
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114.83
110.19
110.17
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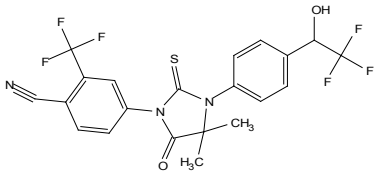
72.13
71.81
71.49
66.60
23.73



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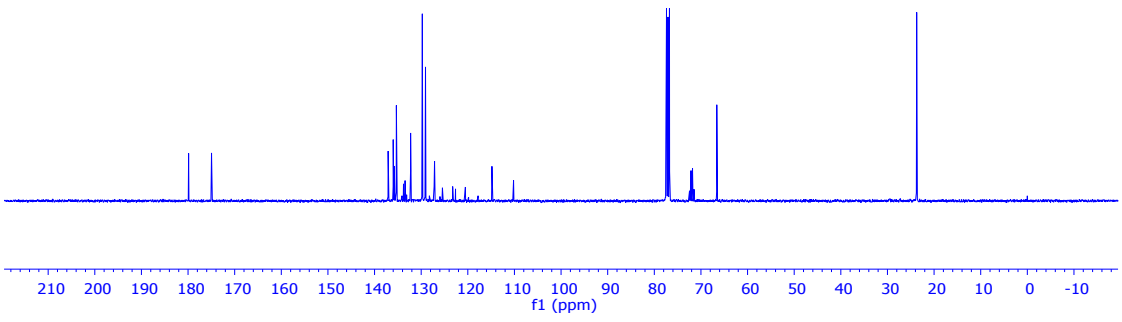

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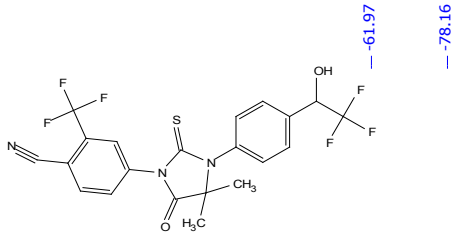

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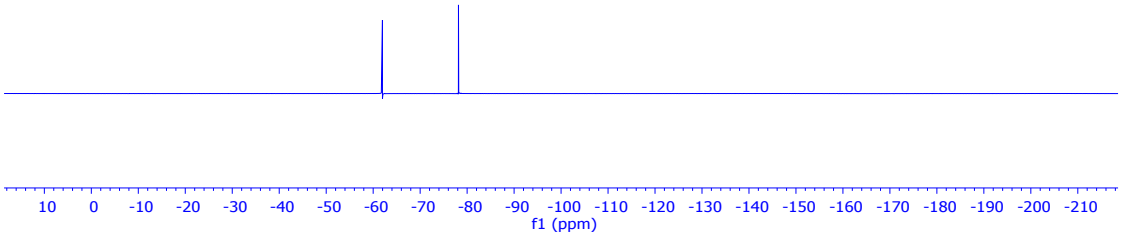

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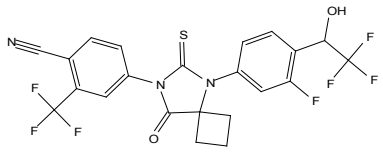

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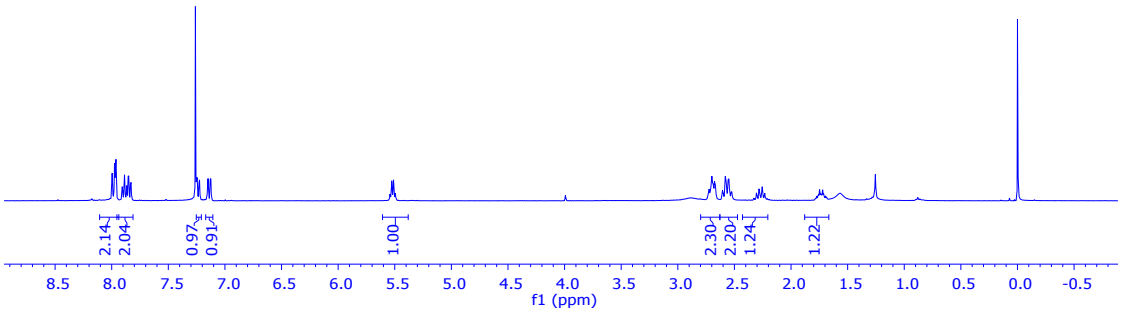

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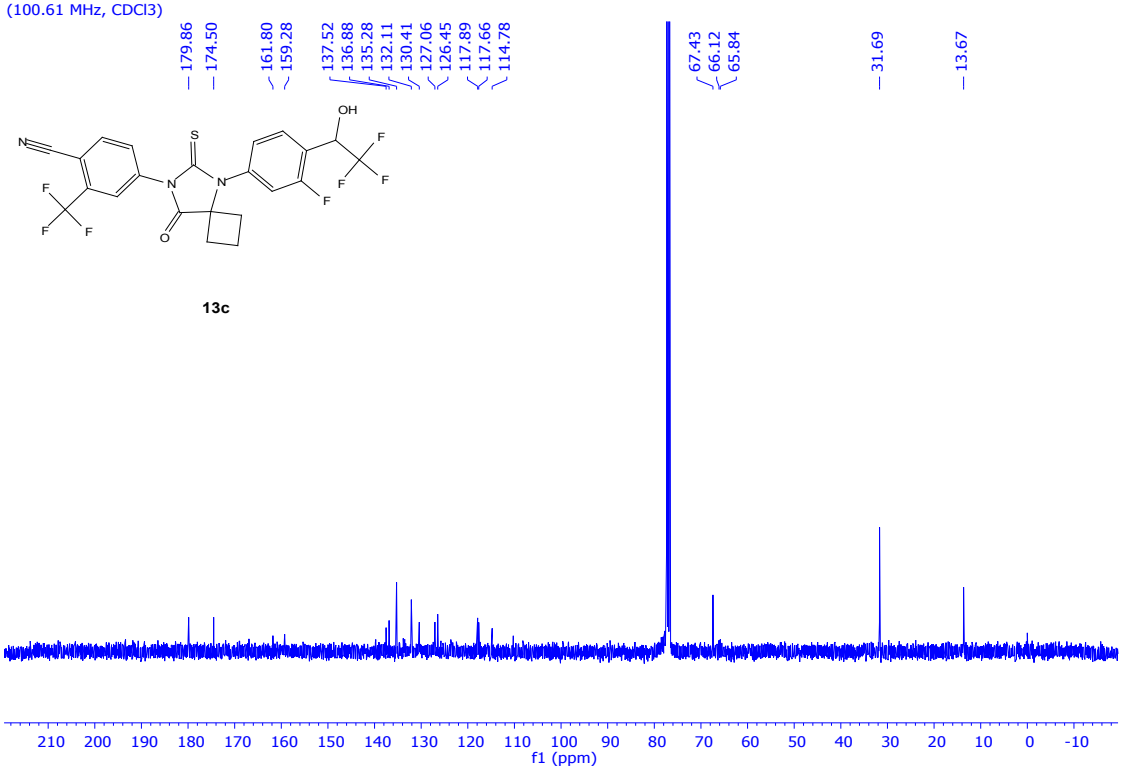

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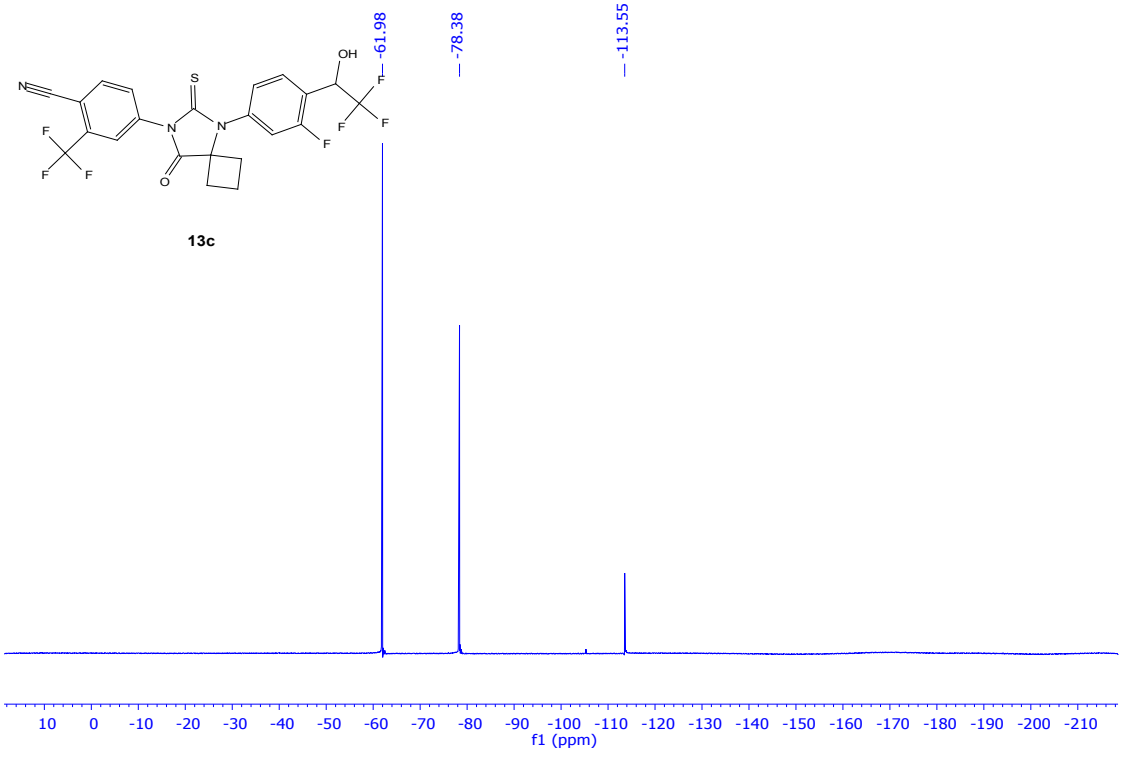
(376.50 MHz, CDCl3)



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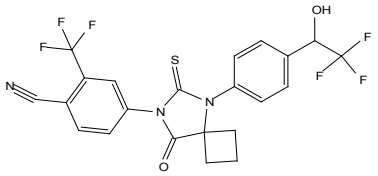

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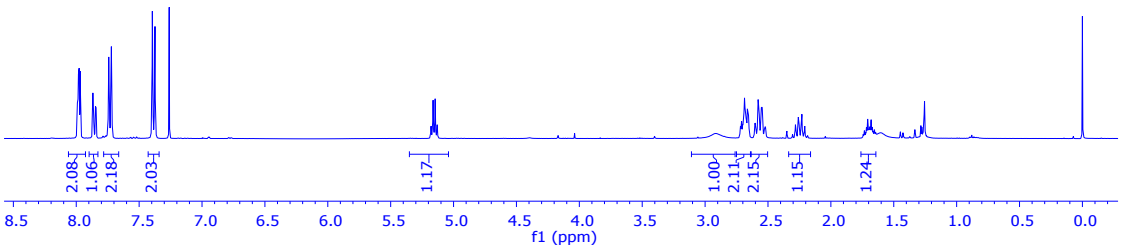

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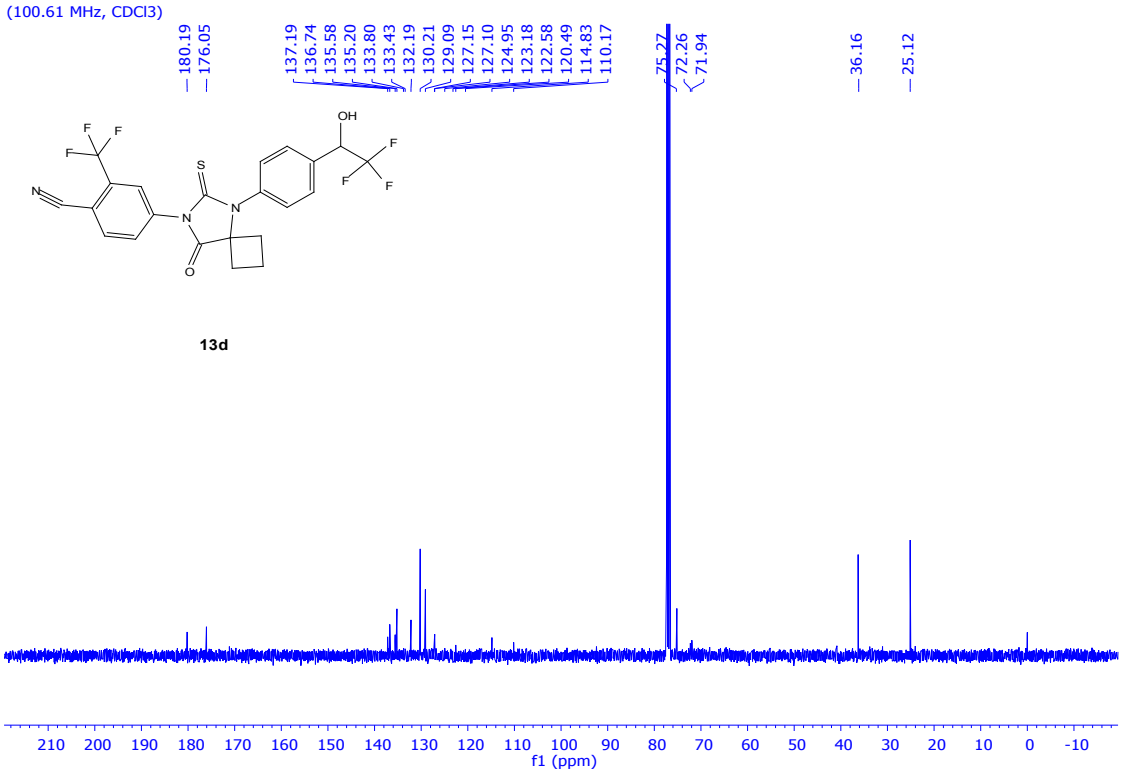

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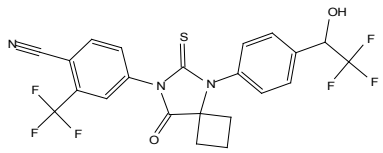

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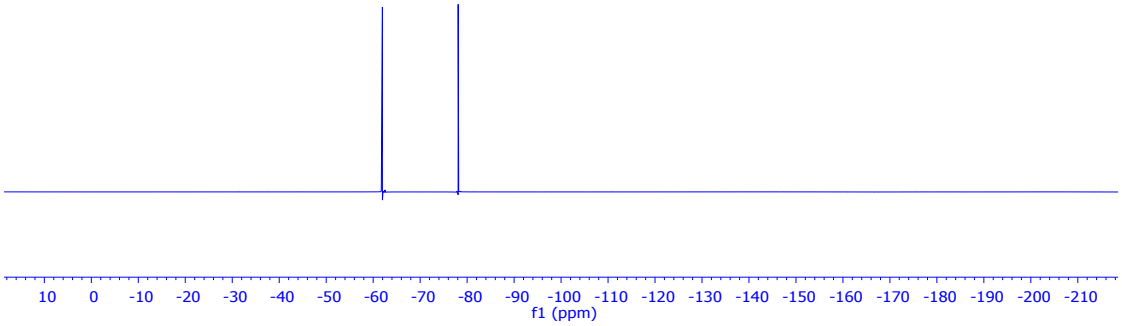
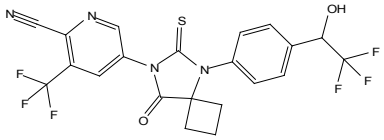


(400.13 MHz, DMSO)



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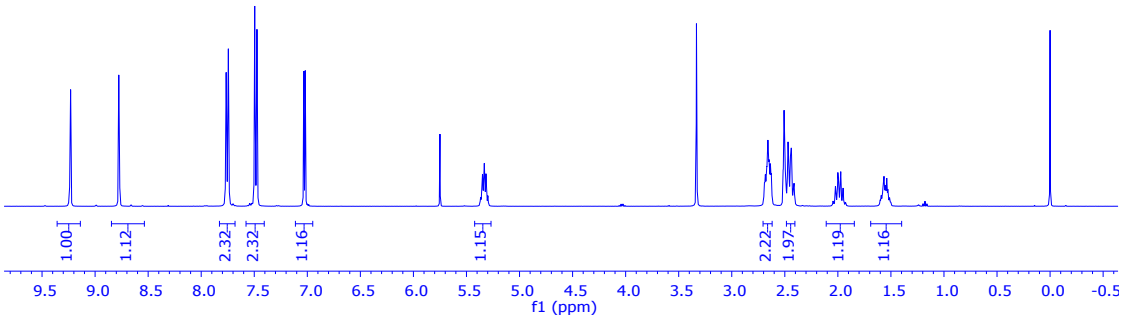
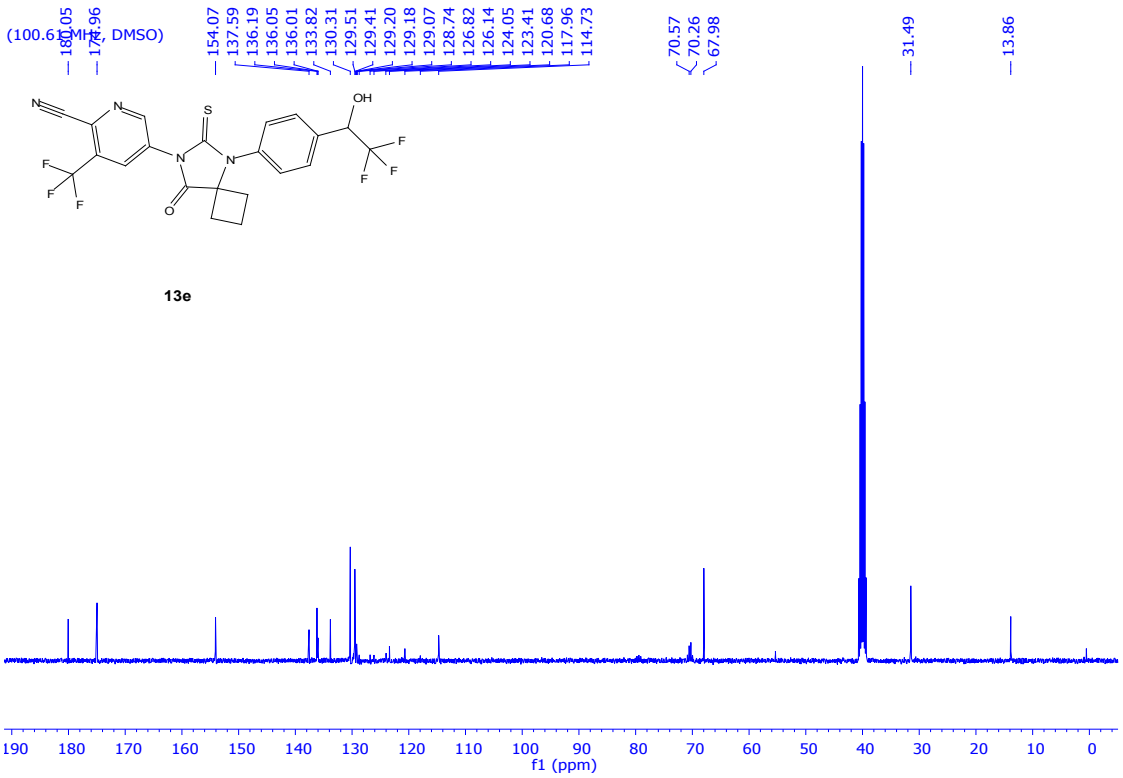
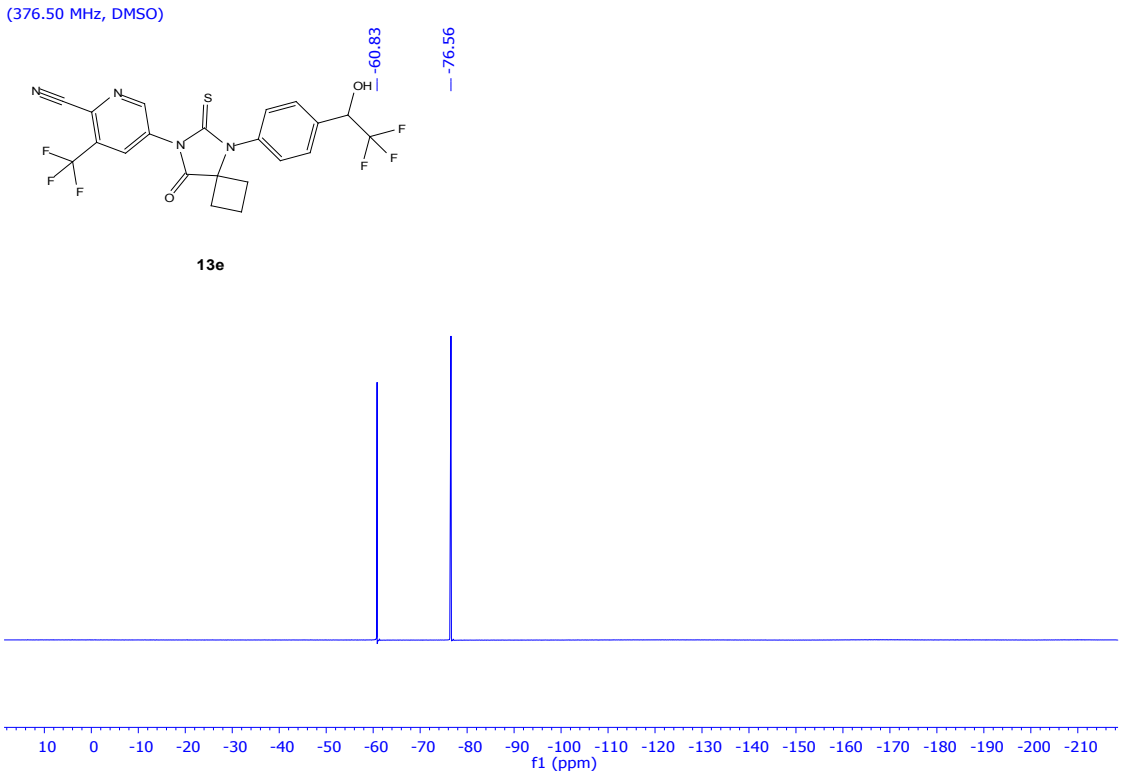
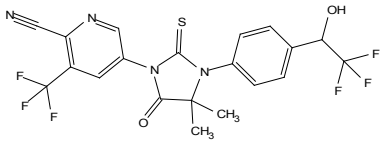



(100.61 MHz, DMSO)
180.05
174.96
154.07
137.59
136.19
136.05
136.01
133.82
130.31
129.51
129.41
129.20
129.18
129.07
128.74
126.82
126.14
124.05
123.41
120.68
117.96
114.73
70.57
70.26
67.98
31.49
13.86
13e
f1 (ppm)


(376.50 MHz, DMSO)
-60.83
-76.56
13e
f1 (ppm)

(400.13 MHz, CDCl3)



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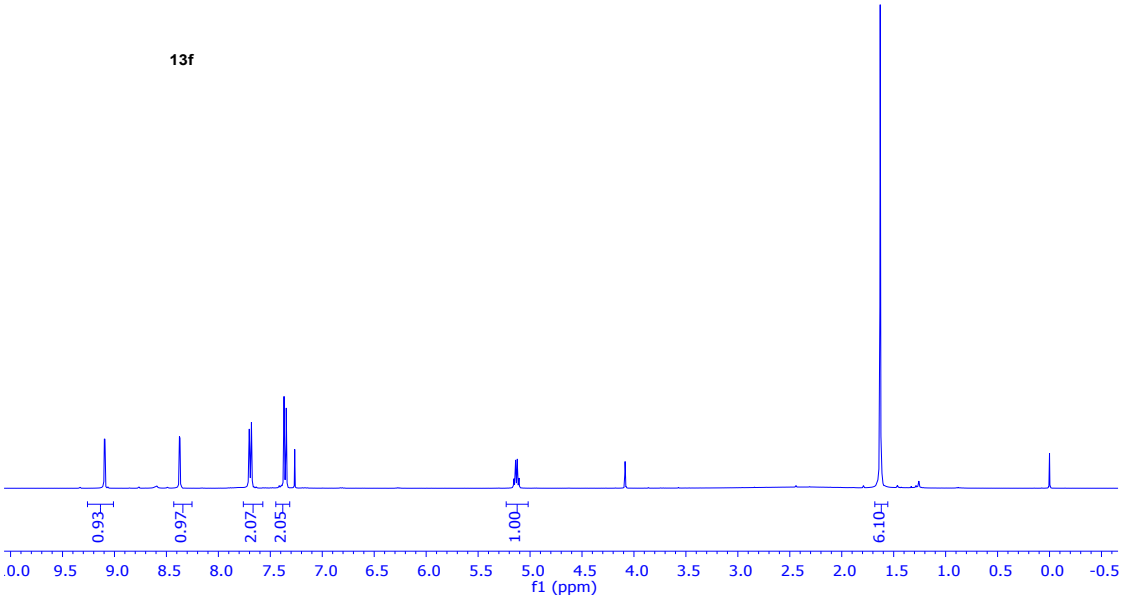
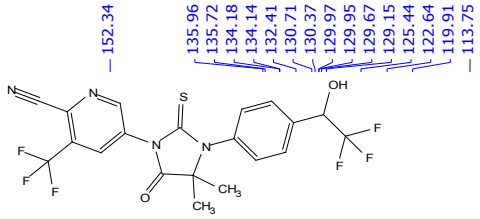
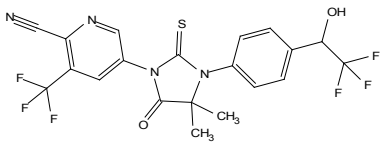


(100.61 MHz, CDCl3)



13f

(376.50 MHz, CDCl3)



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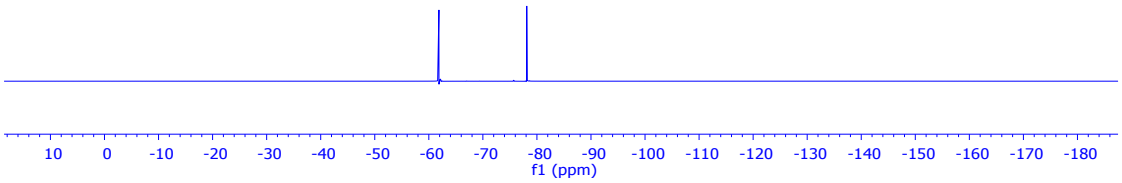
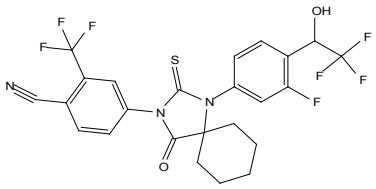


(400.13 MHz, CDCl3)



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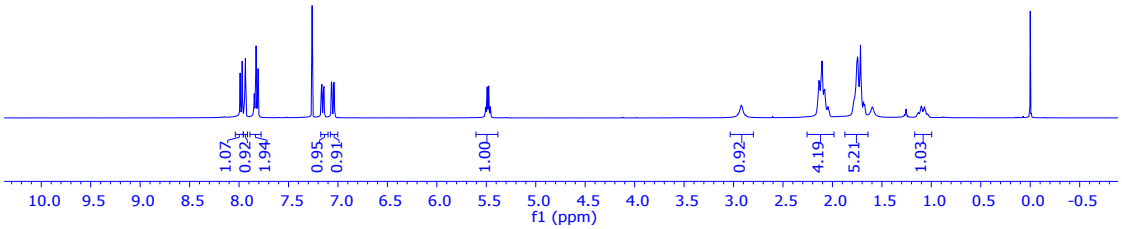

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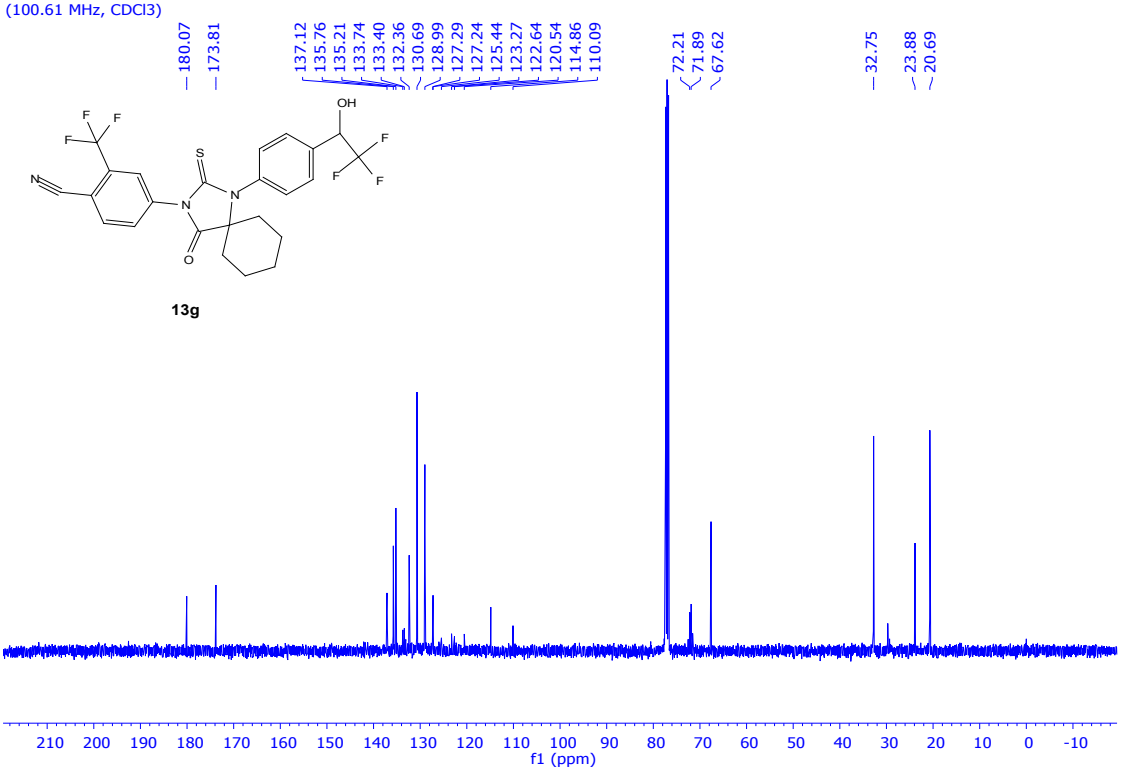

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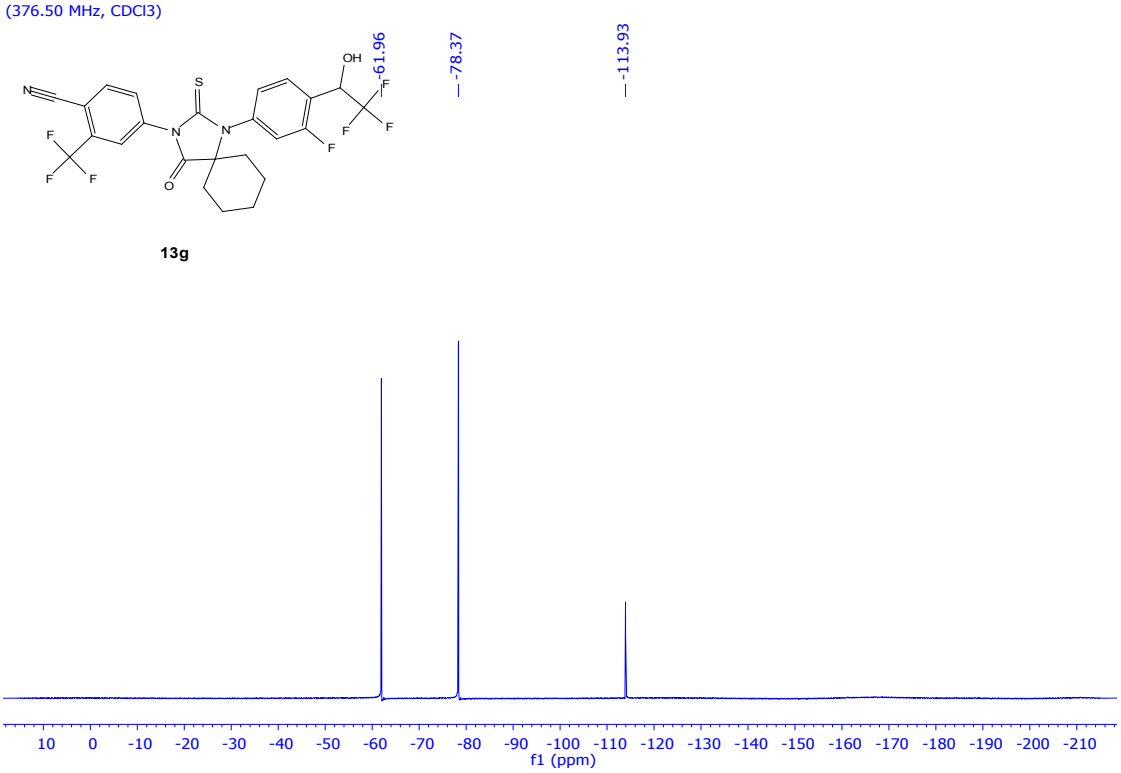

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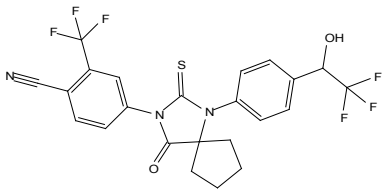

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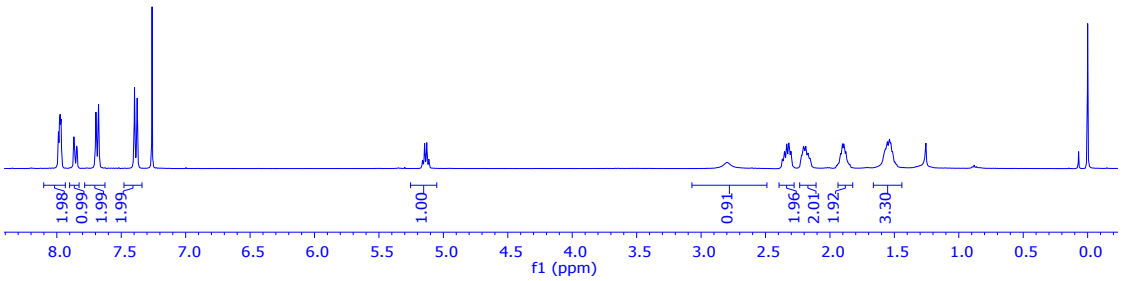

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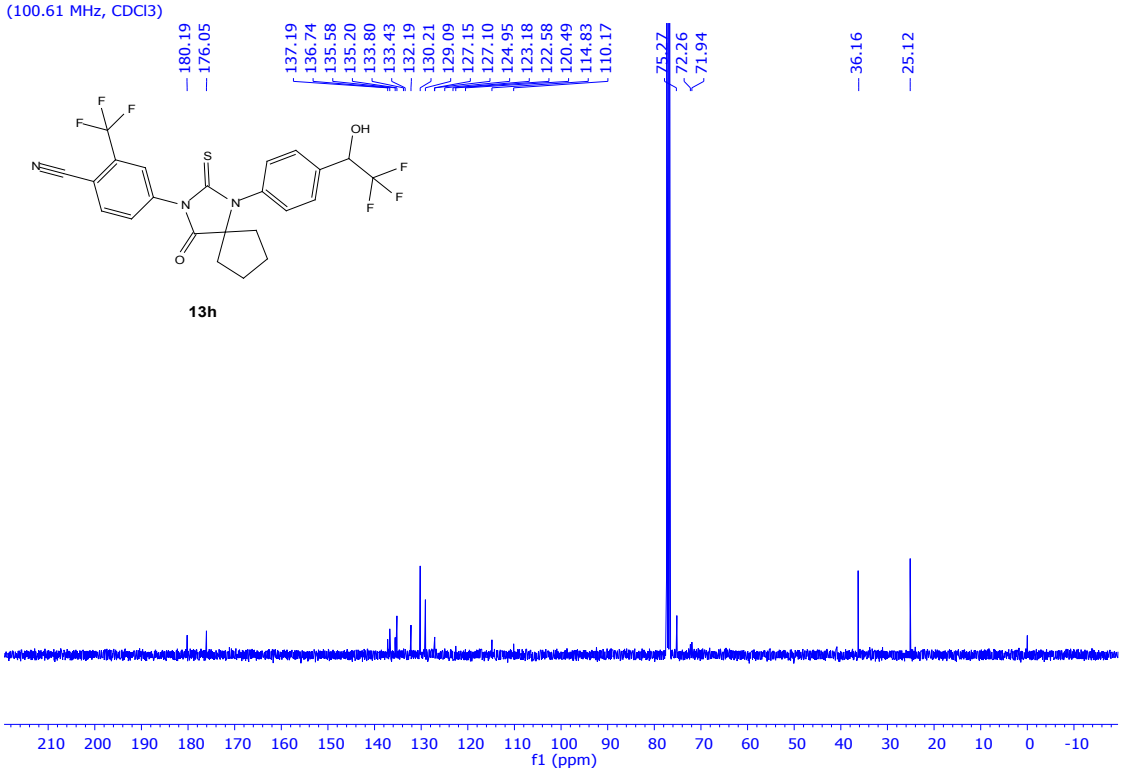

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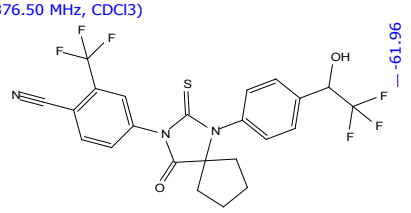

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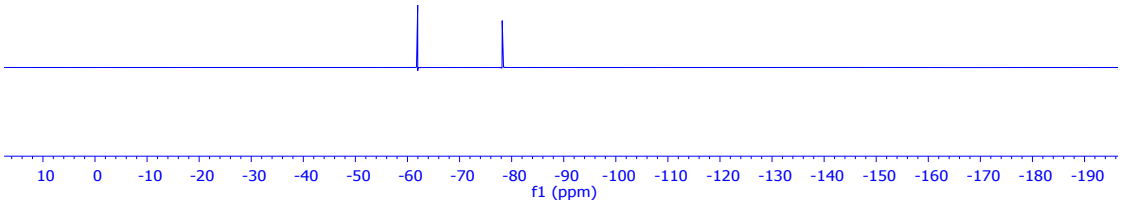

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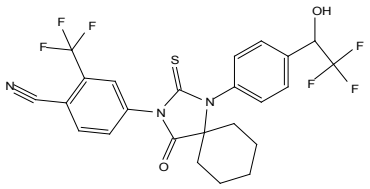

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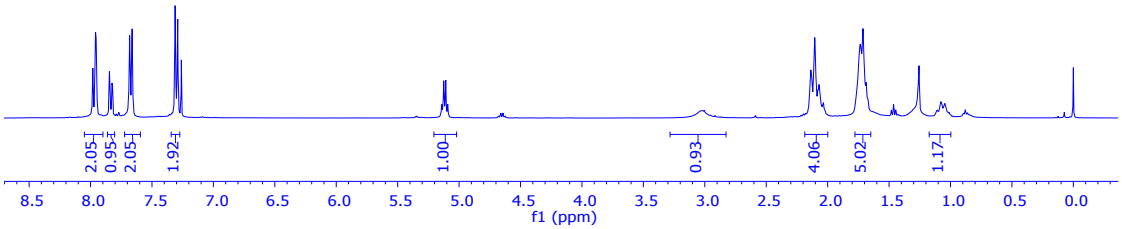

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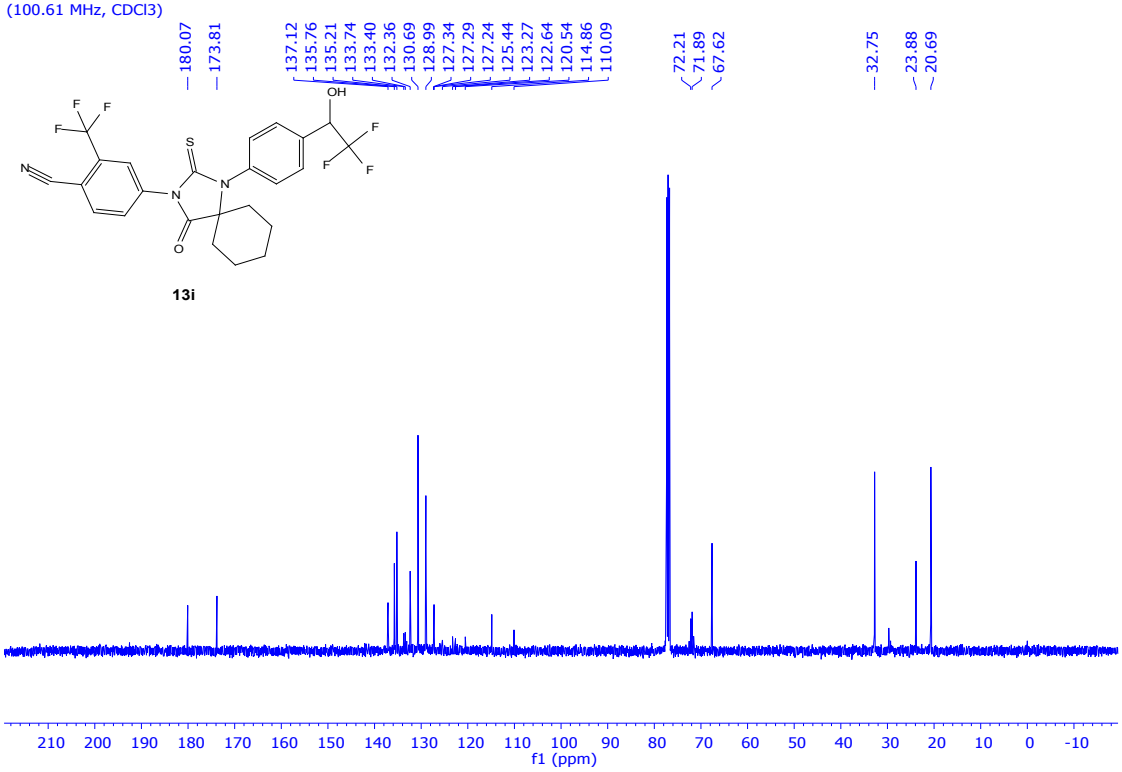

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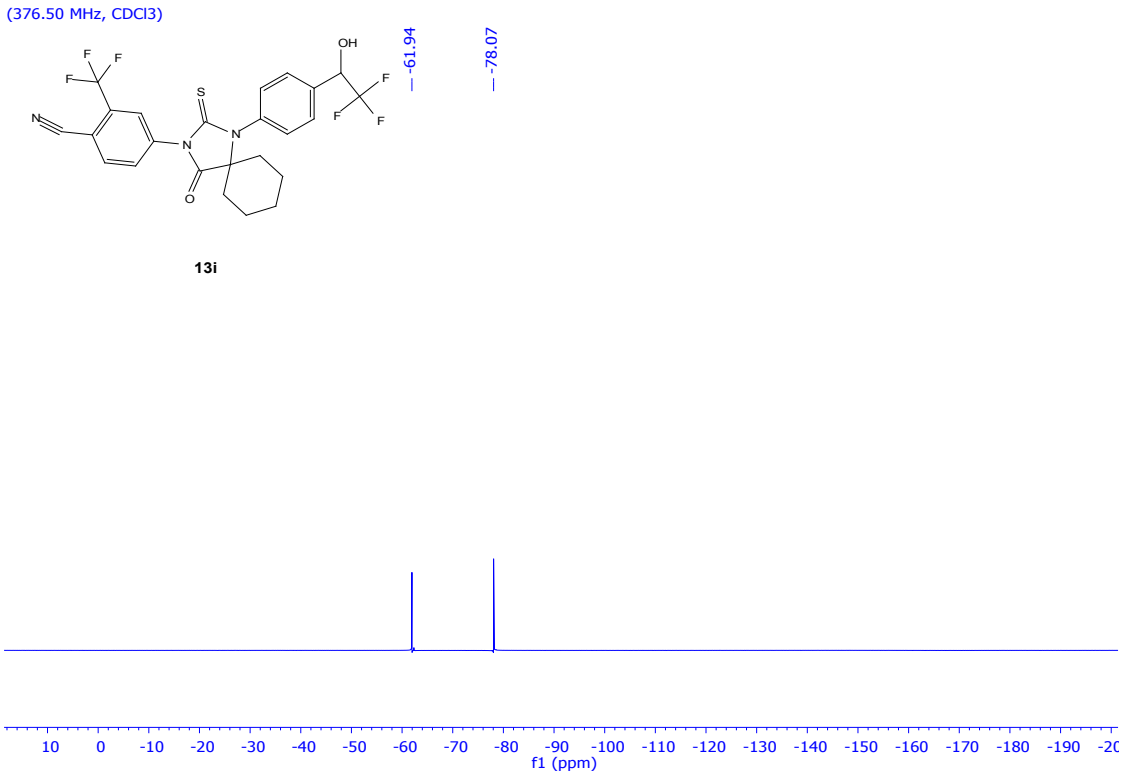
(376.50 MHz, CDCl3)



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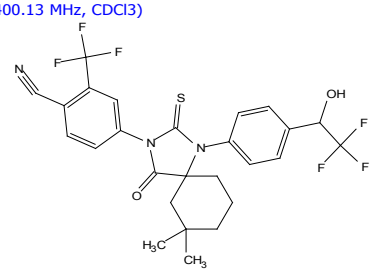
(400.13 MHz, CDCl3)



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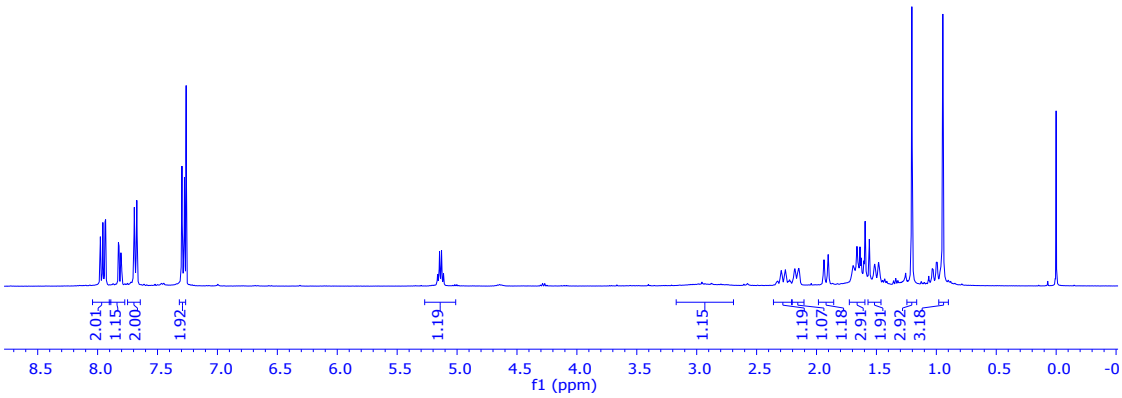

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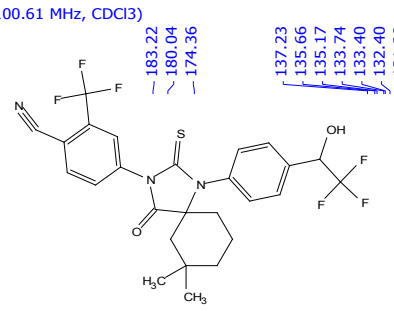

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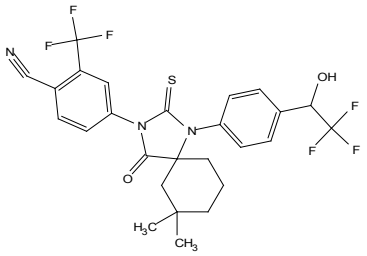
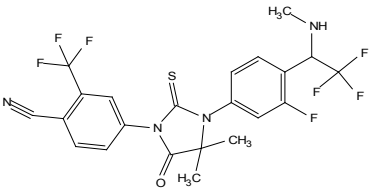
(376.50 MHz, CDCl3)



13j

(400.13 MHz, CDCl3)



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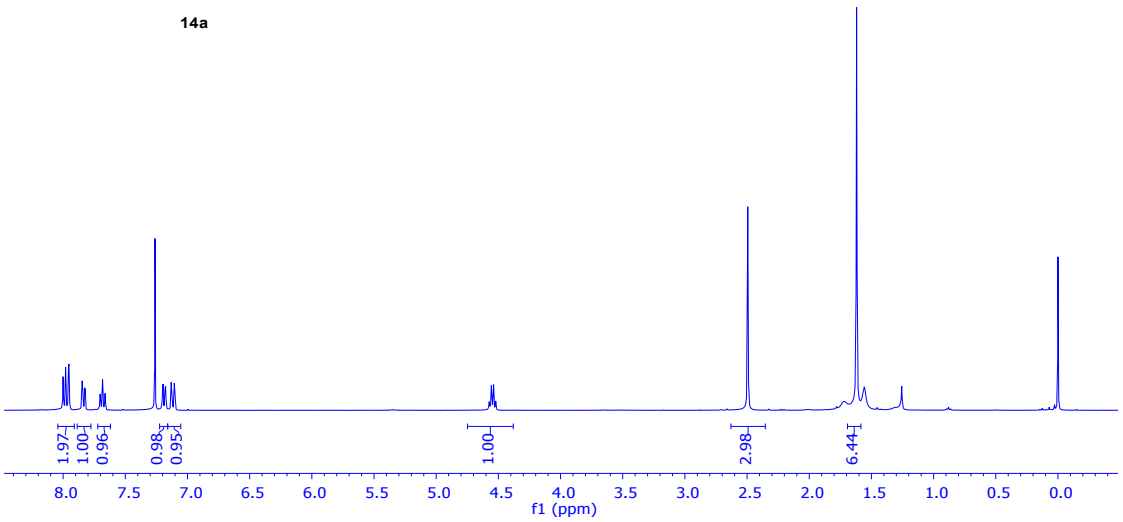
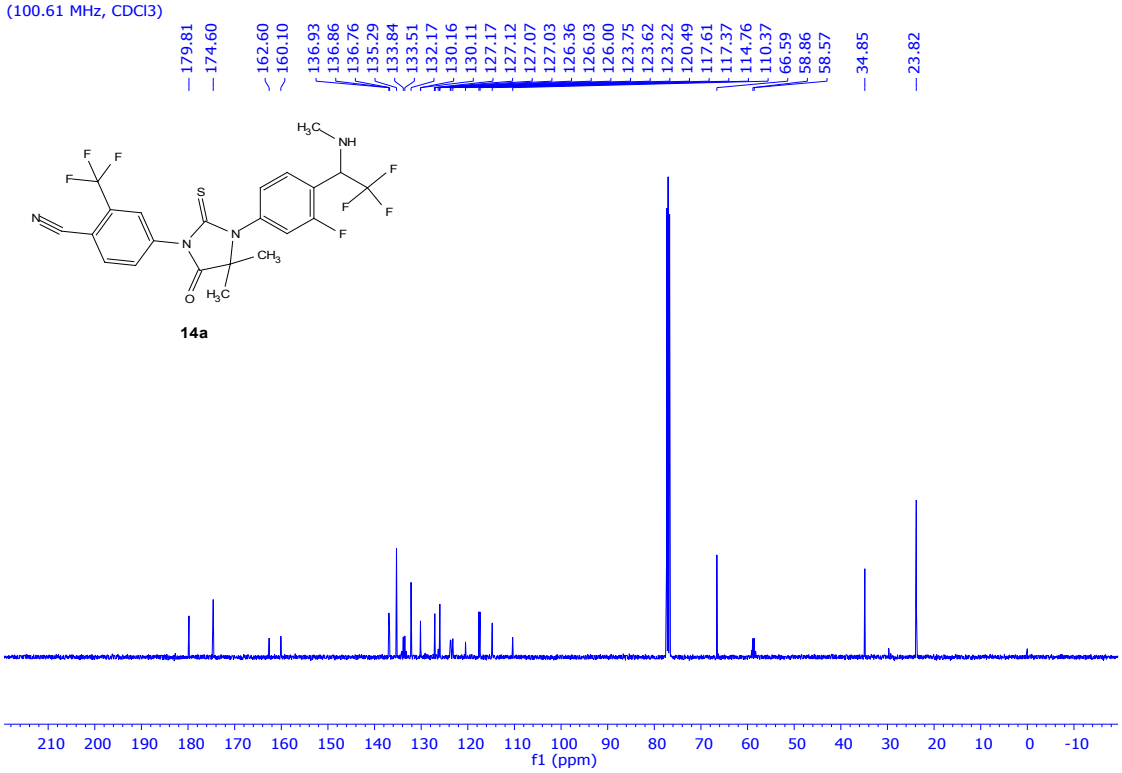


(100.61 MHz, CDCl3)



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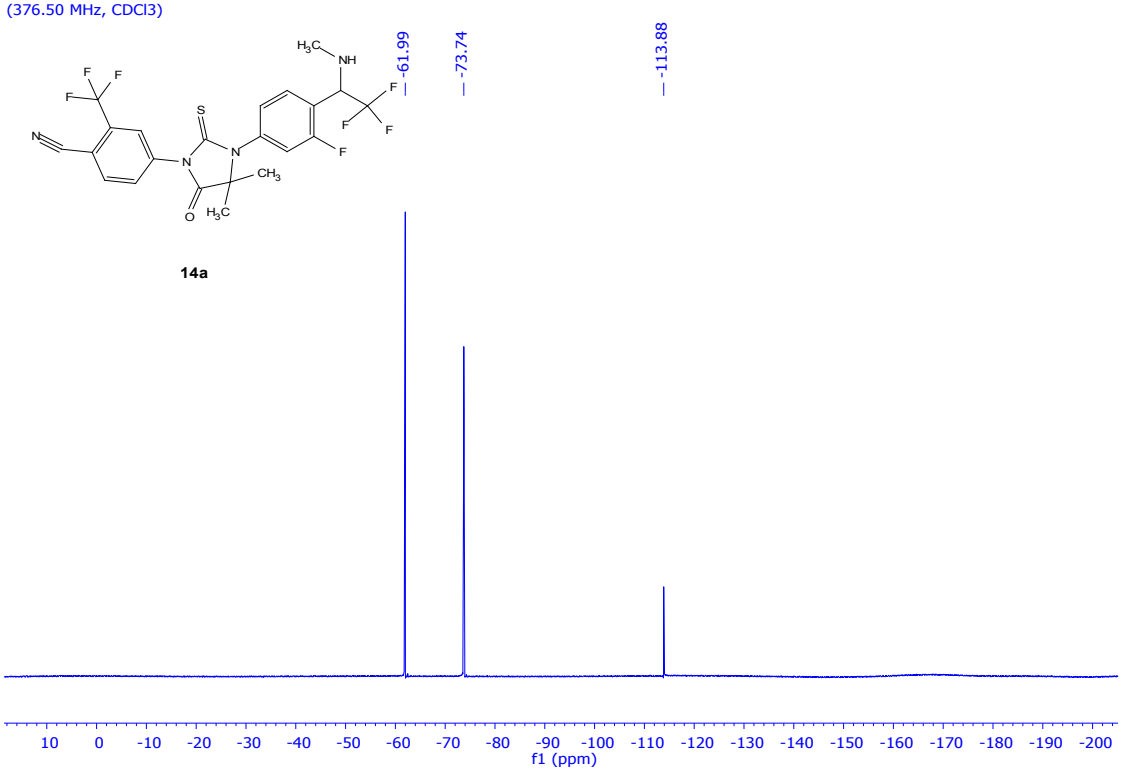

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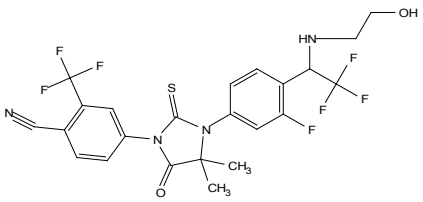
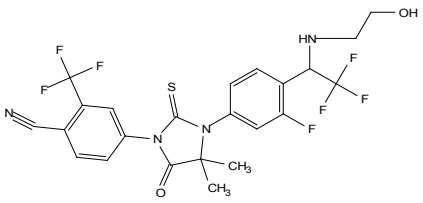
(400.13 MHz, CDCl3)



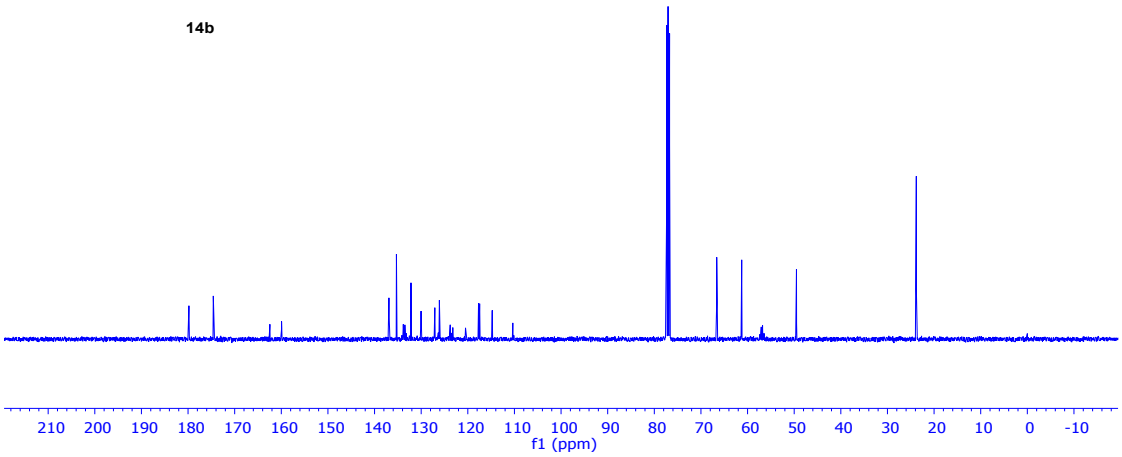
14b

(100.61 MHz, CDCl3)

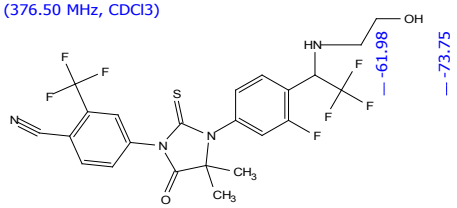
179.81
174.58
162.45
159.94
136.96
136.92
136.86
135.31
133.83
133.50
132.18
130.07
130.03
127.17
127.12
127.07
127.03
126.33
126.10
126.07
123.91
123.77
123.52
123.22
120.49
117.70
117.46
114.76
110.37
110.35
66.62
61.26
57.09
56.77
49.51
23.81



14b



(376.50 MHz, CDCl3)

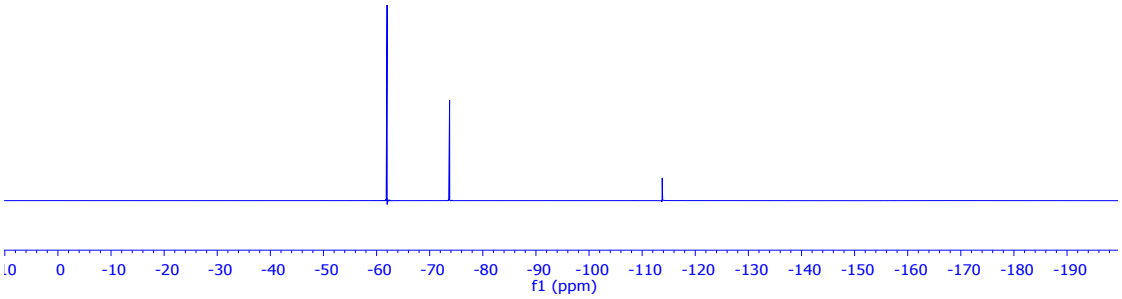


-61.98

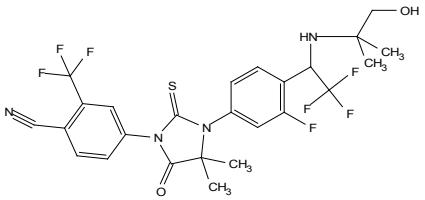
-73.75

-113.78

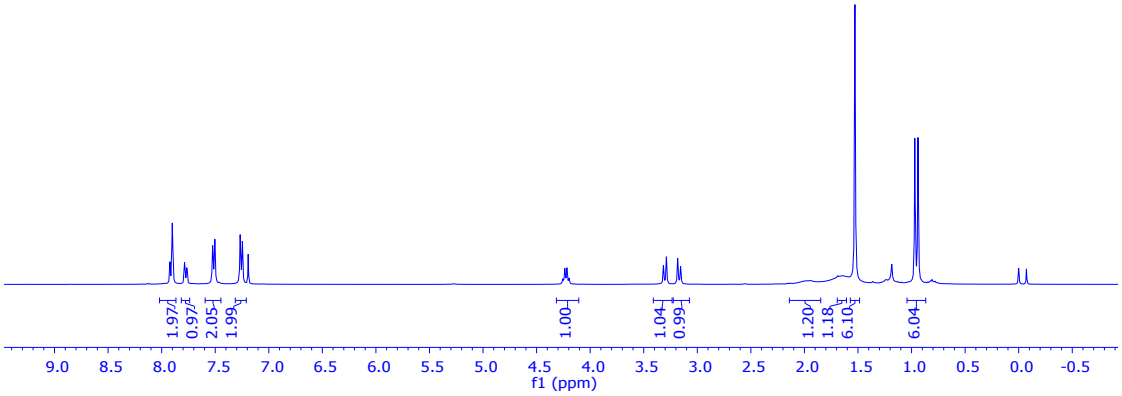
14b



(400.13 MHz, CDCl3)

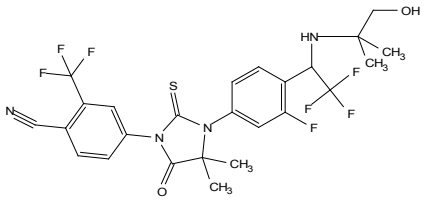


14c

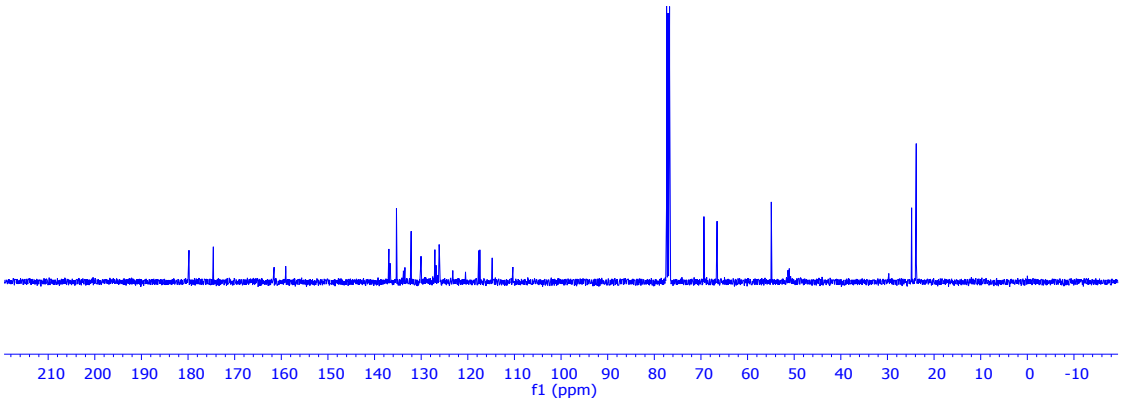


(100.61 MHz, CDCl3)

179.80
174.58
161.63
159.06
136.92
136.74
136.64
135.30
133.81
133.48
132.15
130.07
130.03
127.11
127.06
126.87
126.72
126.15
126.11
123.22
120.49
117.65
117.41
114.76
110.33
69.35
66.54
54.91
51.35
51.06
24.81
23.93
23.82



14c

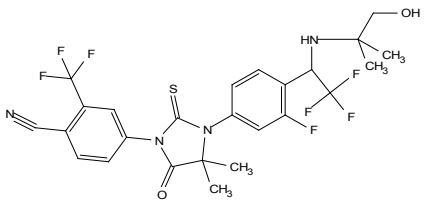


210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

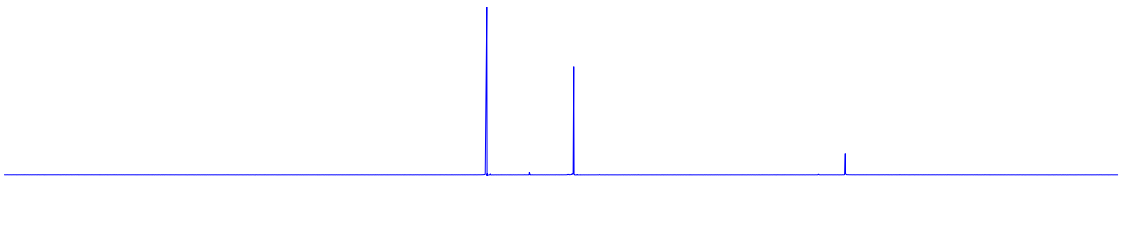
f1 (ppm)

(376.50 MHz, CDCl3)

-61.95
-74.66
-114.24



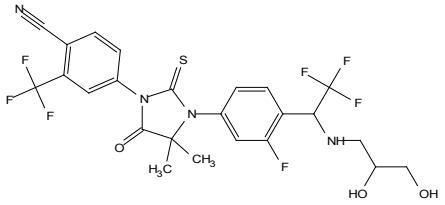
14c



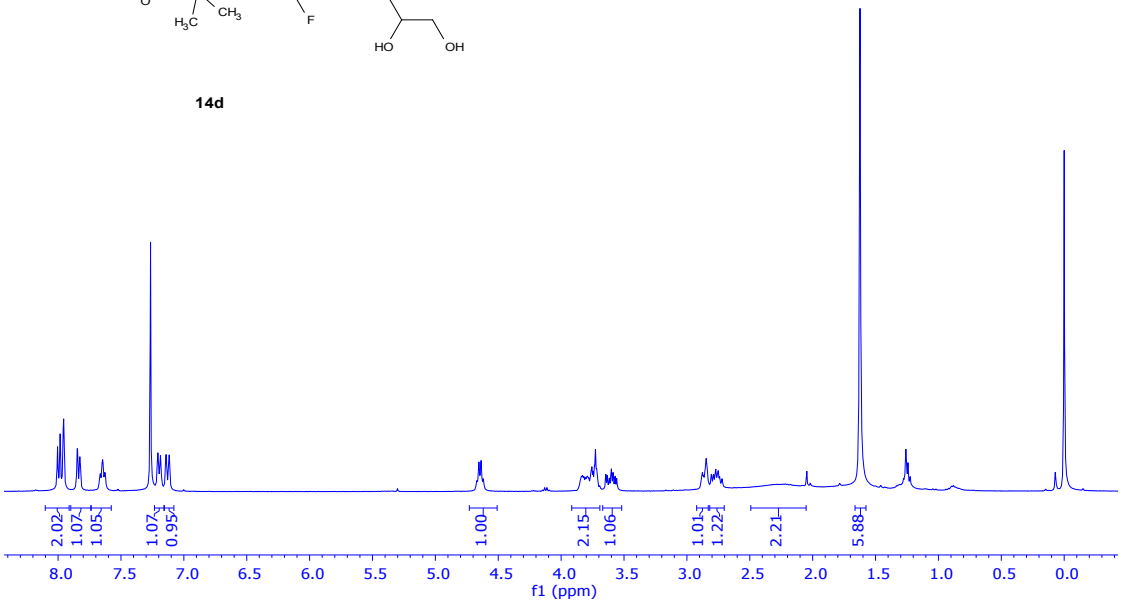
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150

f1 (ppm)

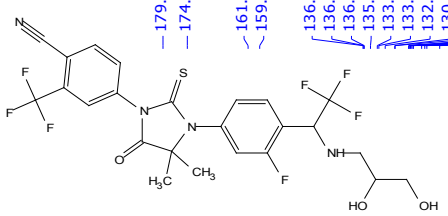
(400.16 MHz, CDCl3)



14d

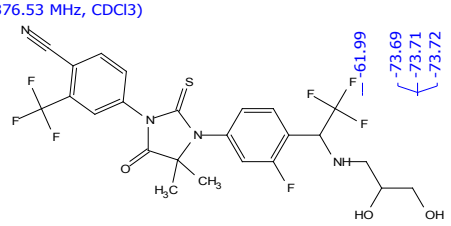


(100.62 MHz, CDCl3)



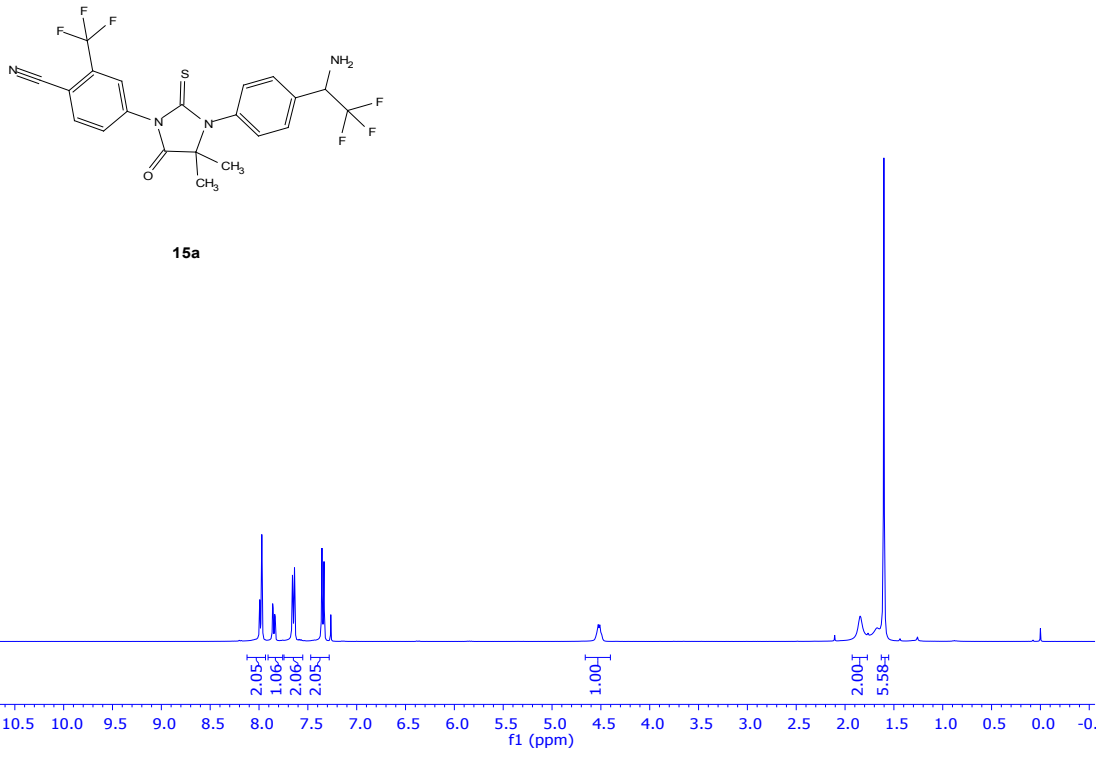
14d

(376.53 MHz, CDCl3)



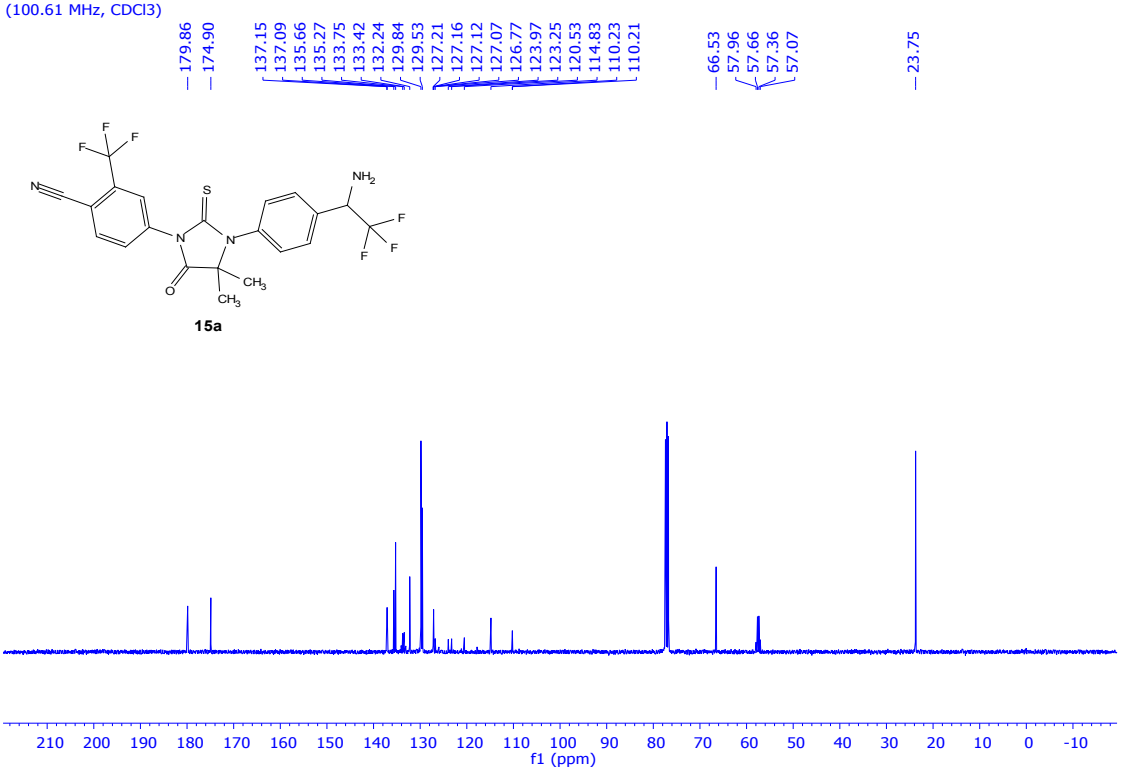
14d

(400.13 MHz, CDCl3)



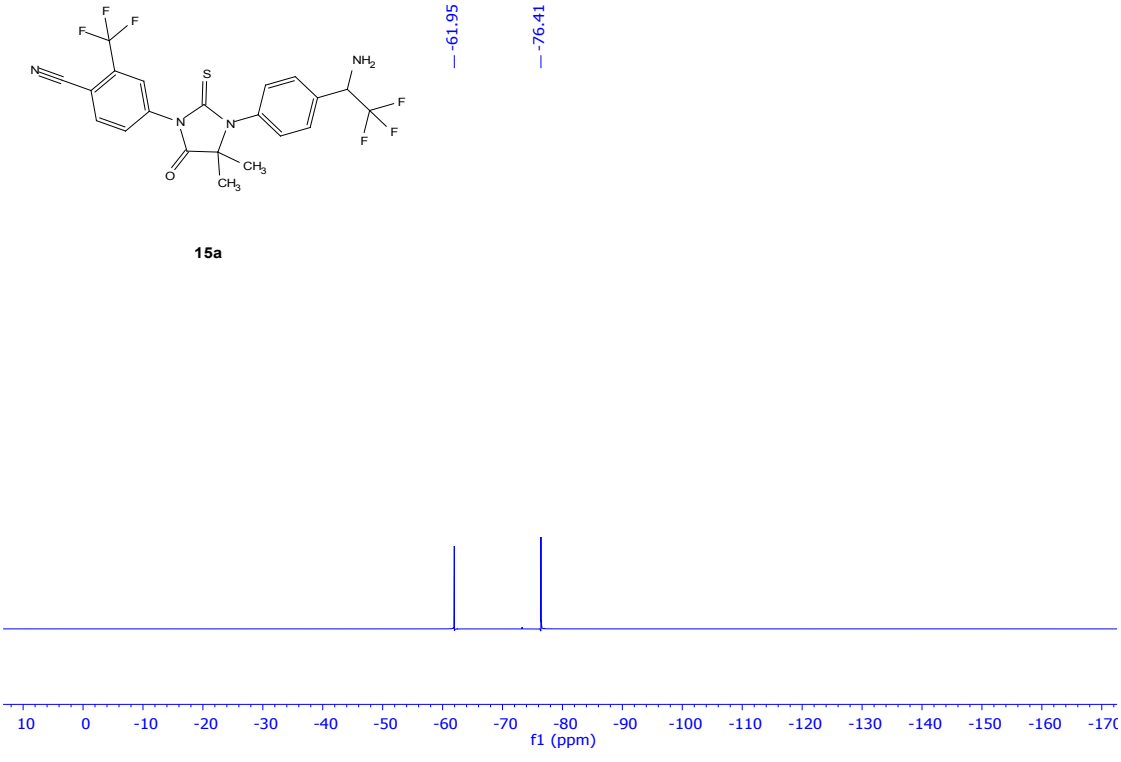
15a

(100.61 MHz, CDCl3)



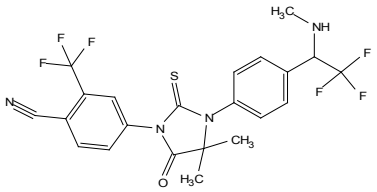
15a

(376.50 MHz, CDCl3)

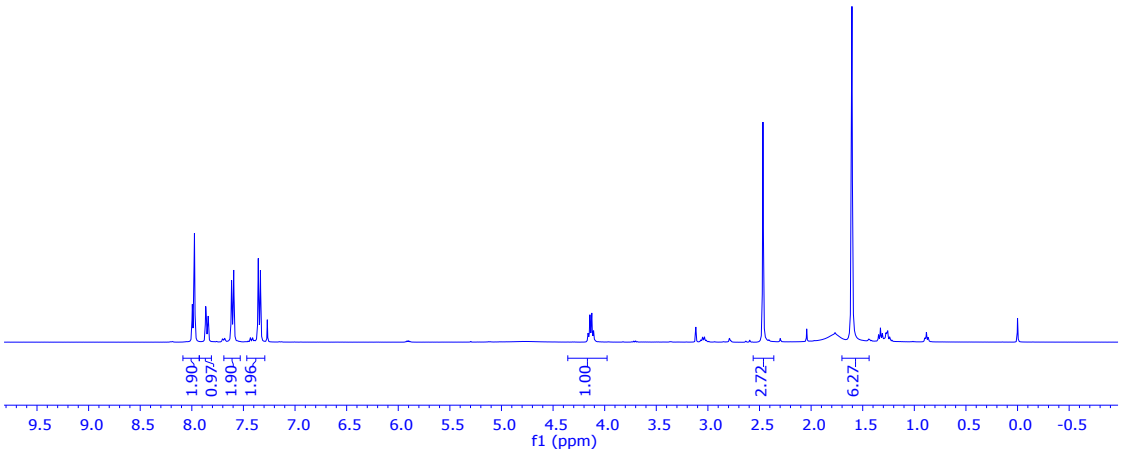


15a

(400.13 MHz, CDCl3)

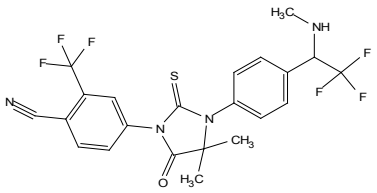


15b

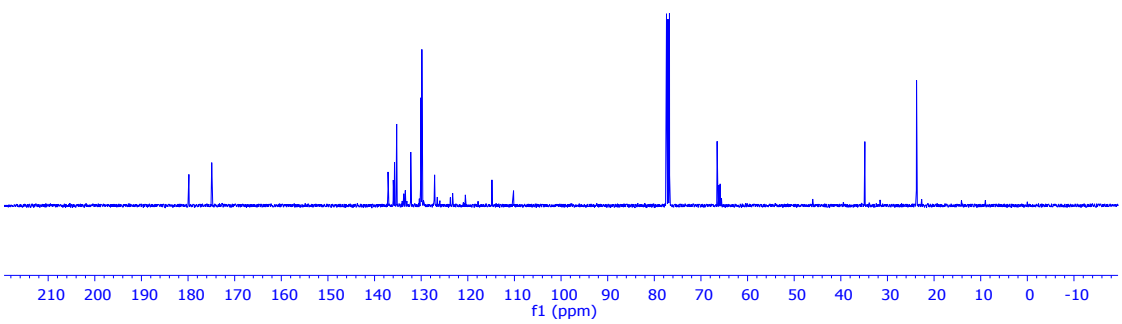


(100.61 MHz, CDCl3)

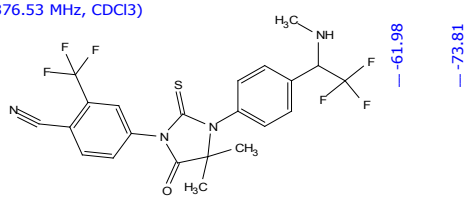
179.82
174.92
137.11
135.99
135.71
135.26
133.74
133.40
132.24
130.06
129.85
127.17
127.12
127.07
126.54
123.74
123.25
120.53
114.83
110.21
66.53
66.17
65.88
34.85
23.76



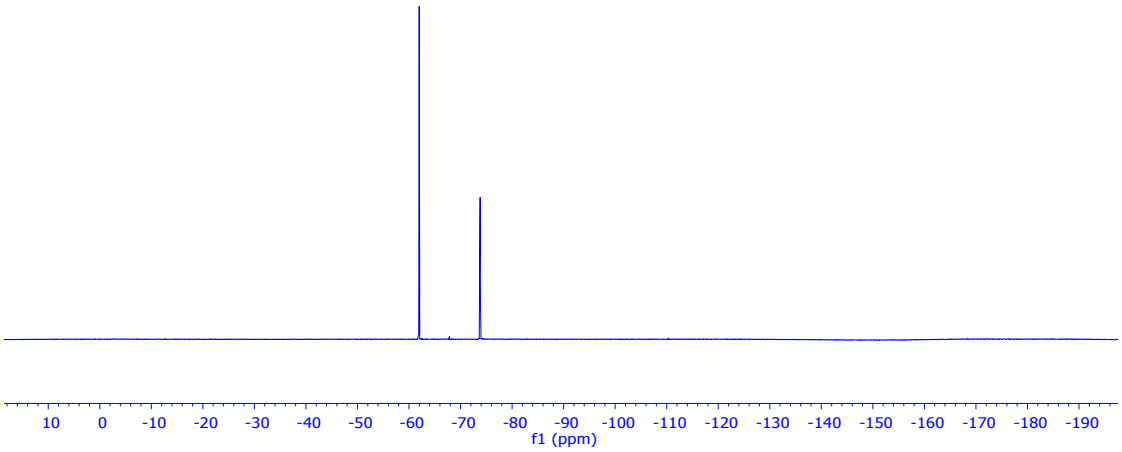
15b



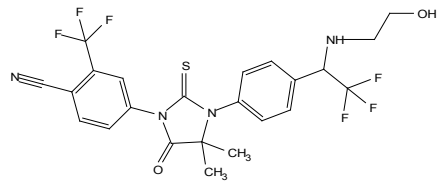
(376.53 MHz, CDCl3)



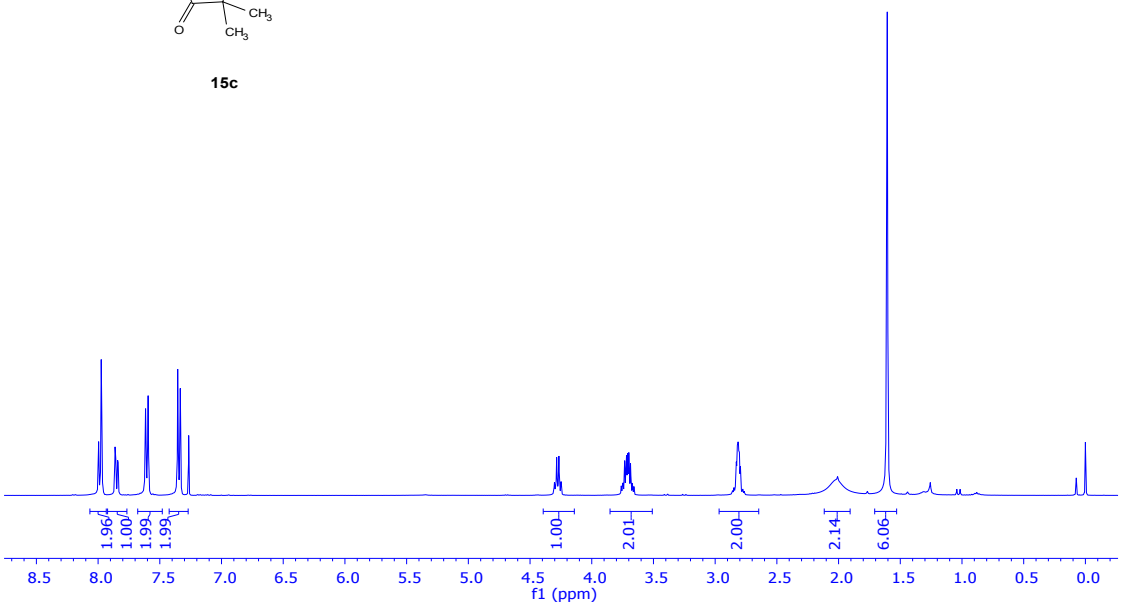
15b



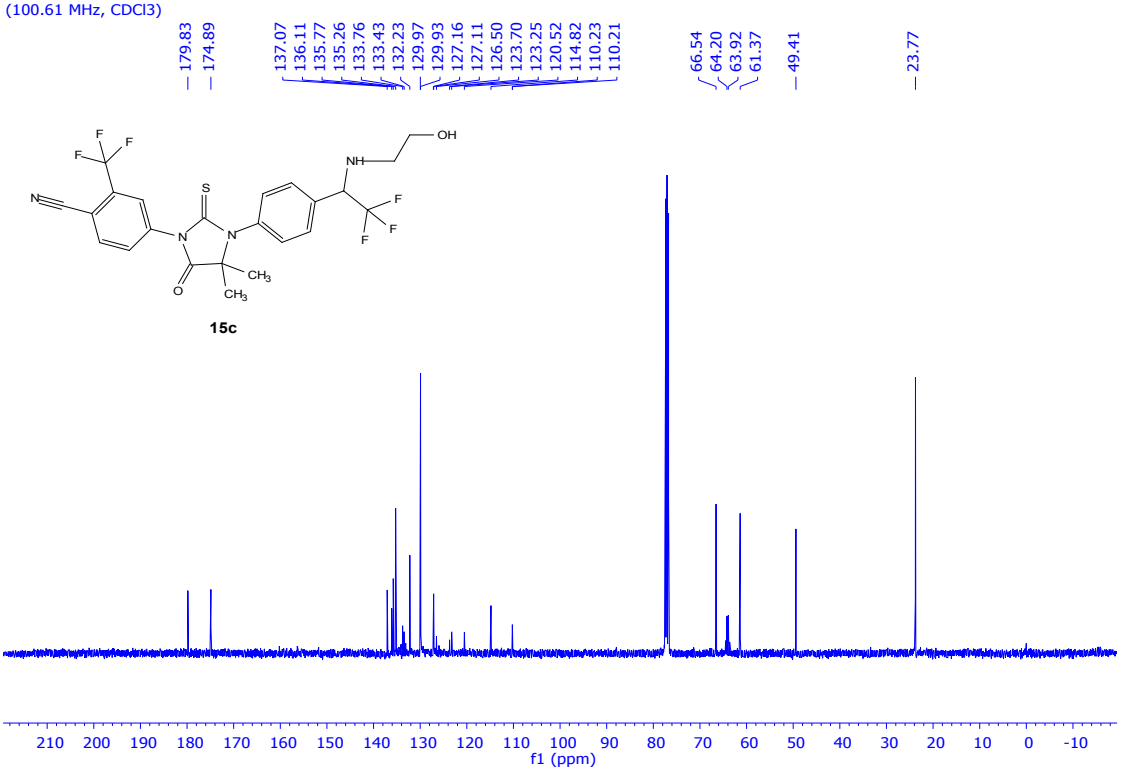
(400.13 MHz, CDCl3)



15c

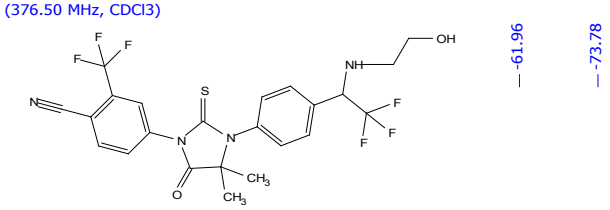


(100.61 MHz, CDCl3)



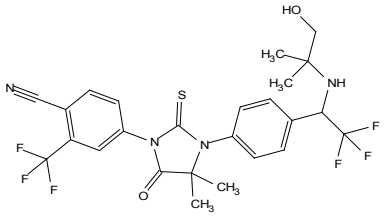
15c

(376.50 MHz, CDCl3)

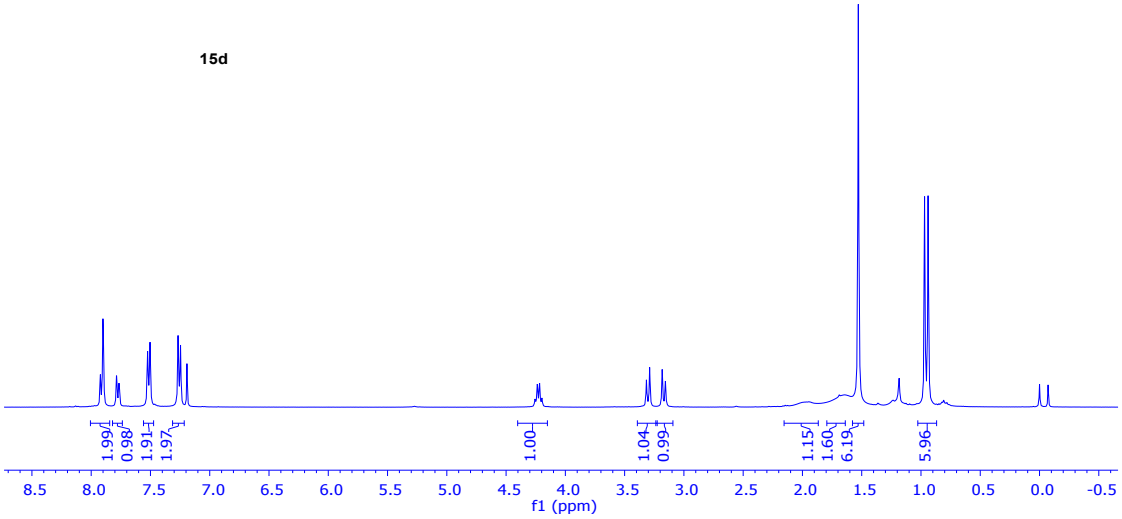


15c

(400.13 MHz, CDCl3)



15d



(100.61 MHz, CDCl3)

179.80
174.88
139.13
137.06
135.48
135.25
133.76
133.43
132.18
129.96
129.51
127.15
127.10
126.66
123.87
123.25
120.52
114.81
110.24
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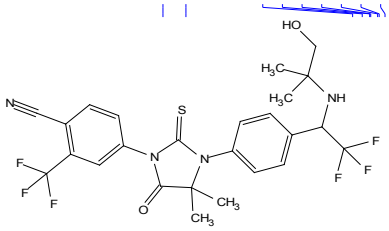
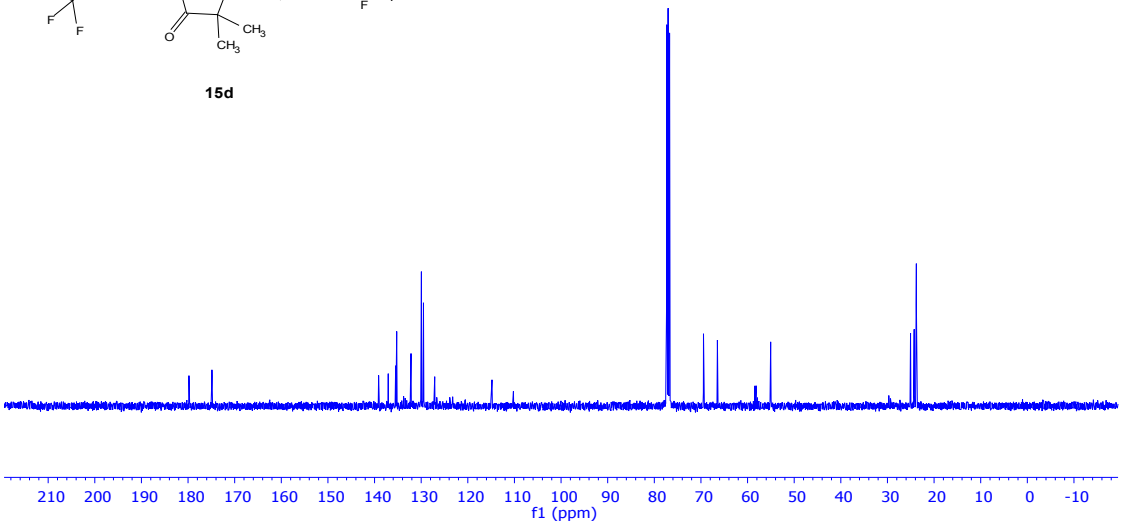
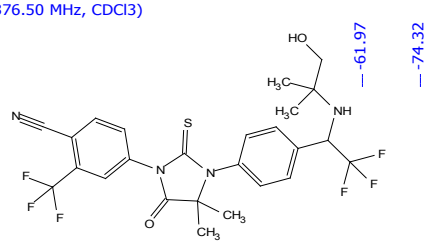
66.47
58.46
58.17
55.04
25.05
24.27
23.80



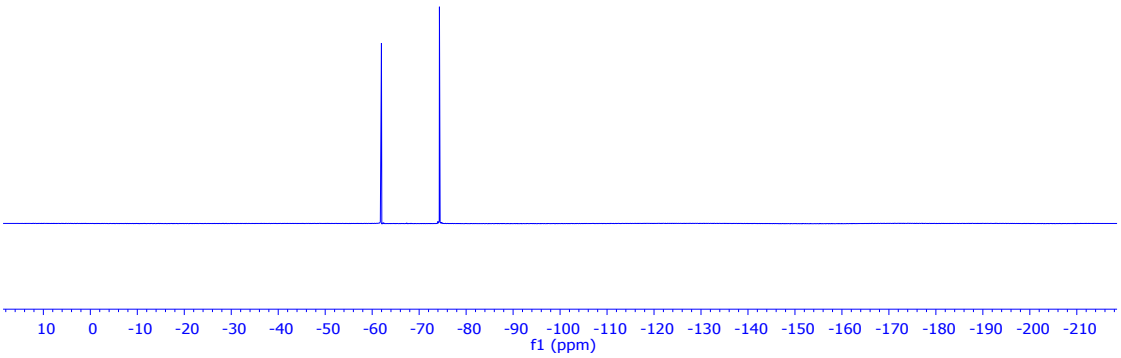
15d



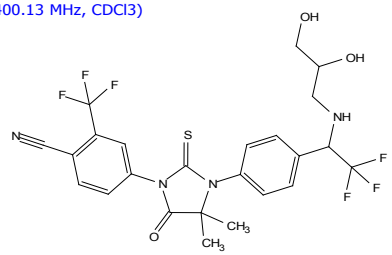
(376.50 MHz, CDCl3)



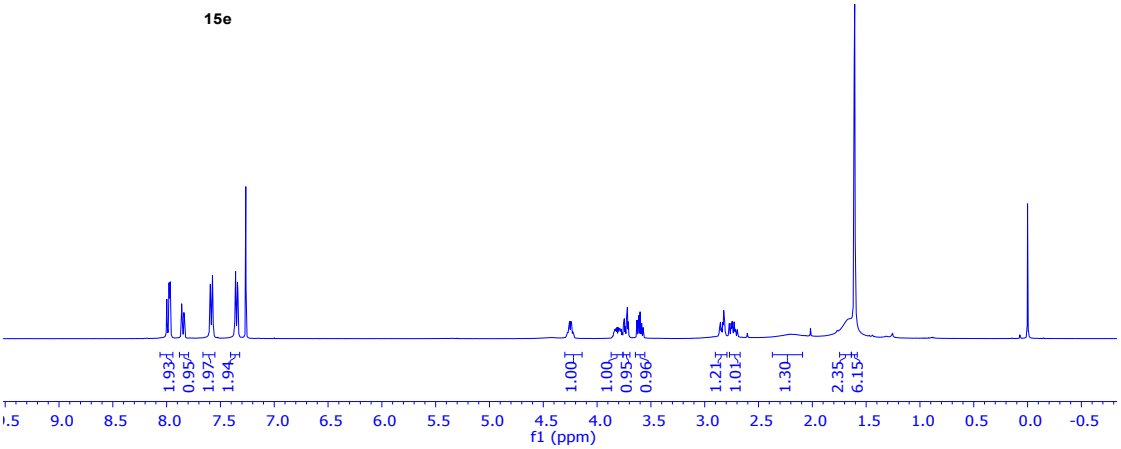
15d



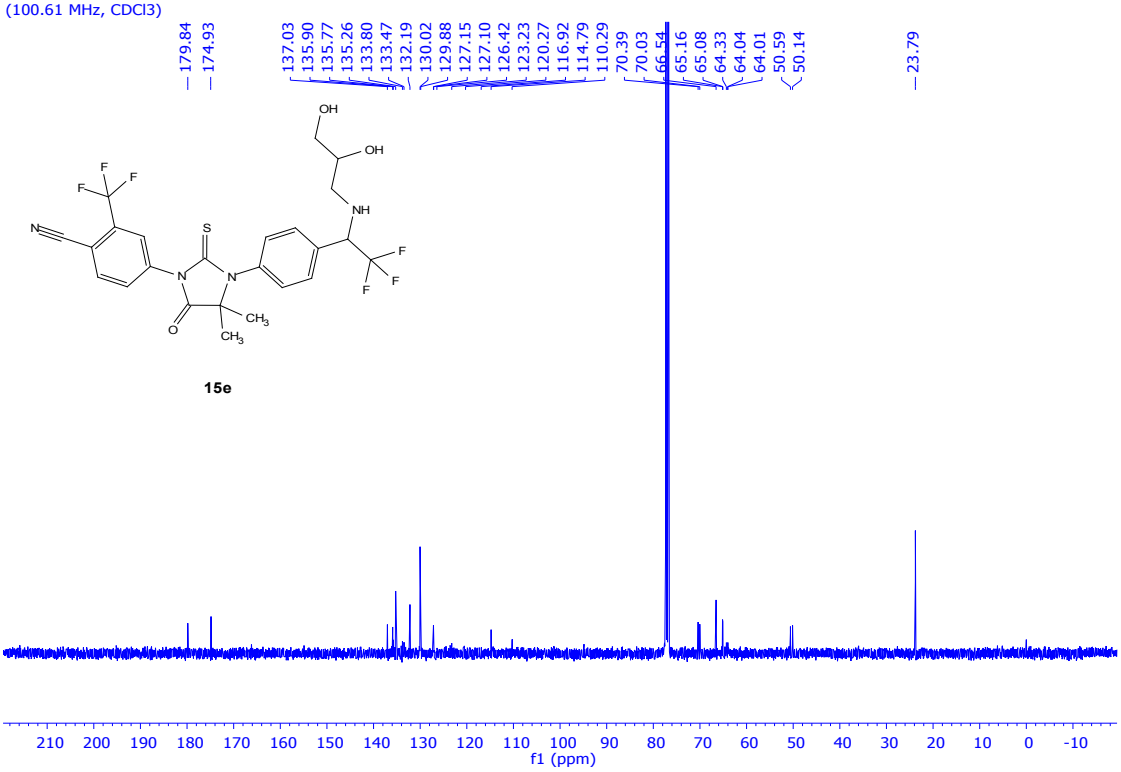
(400.13 MHz, CDCl3)



15e

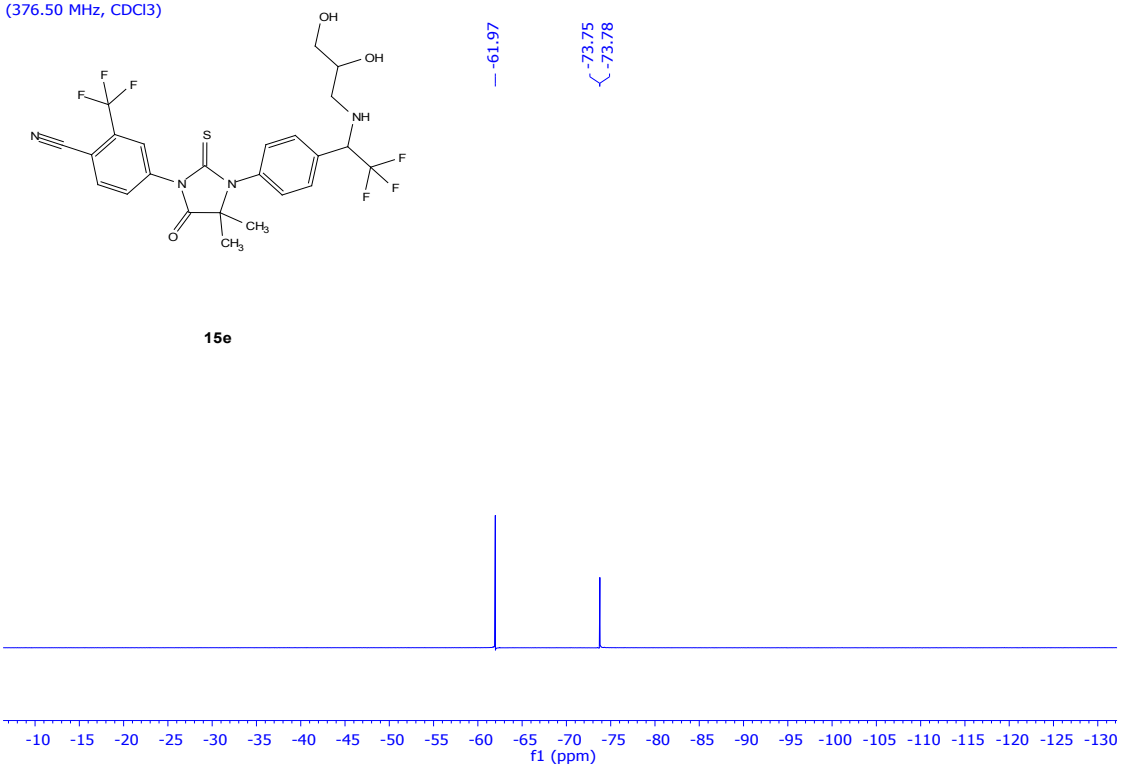


(100.61 MHz, CDCl3)



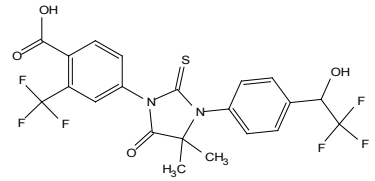
15e

(376.50 MHz, CDCl3)

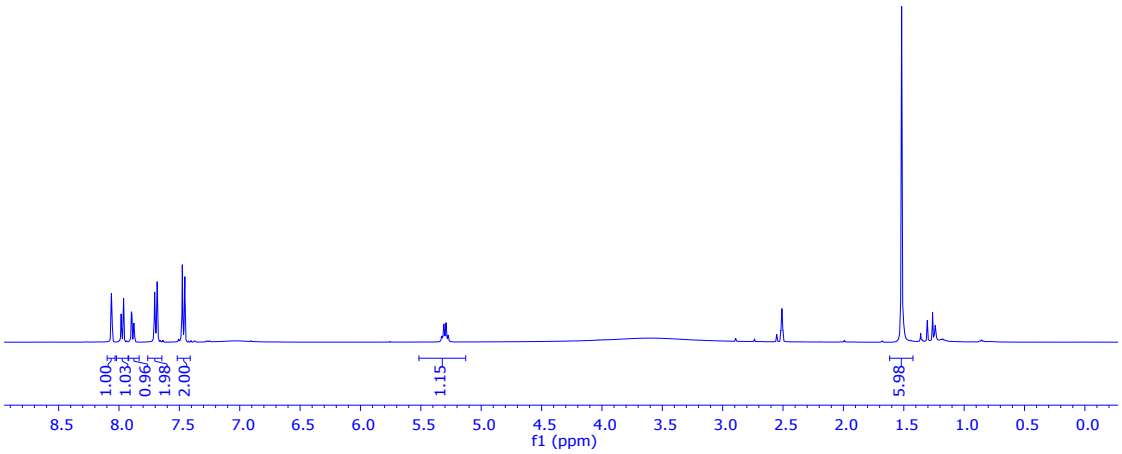


15e

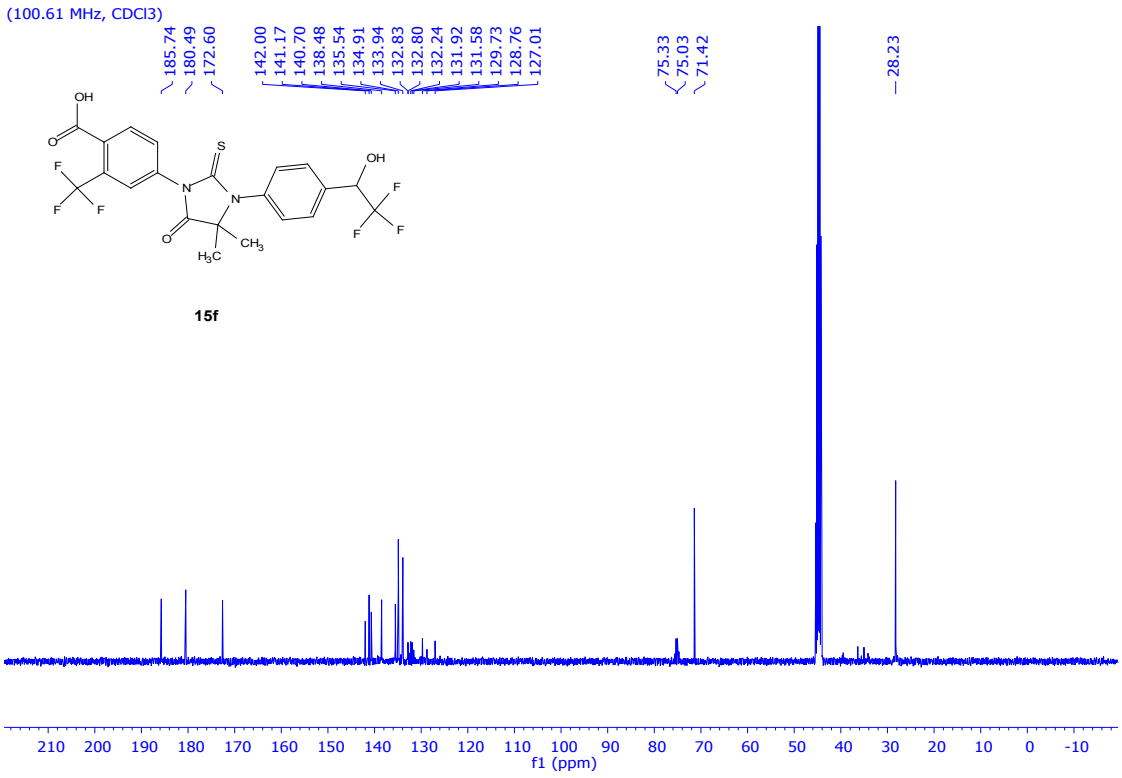
(400.13 MHz, DMSO)



15f

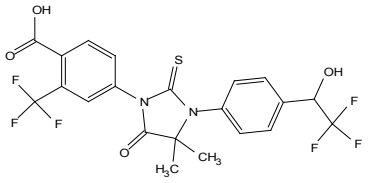


(100.61 MHz, CDCl3)



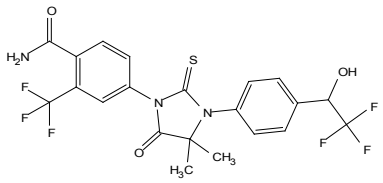
15f

(376.50 MHz, CDCl3)



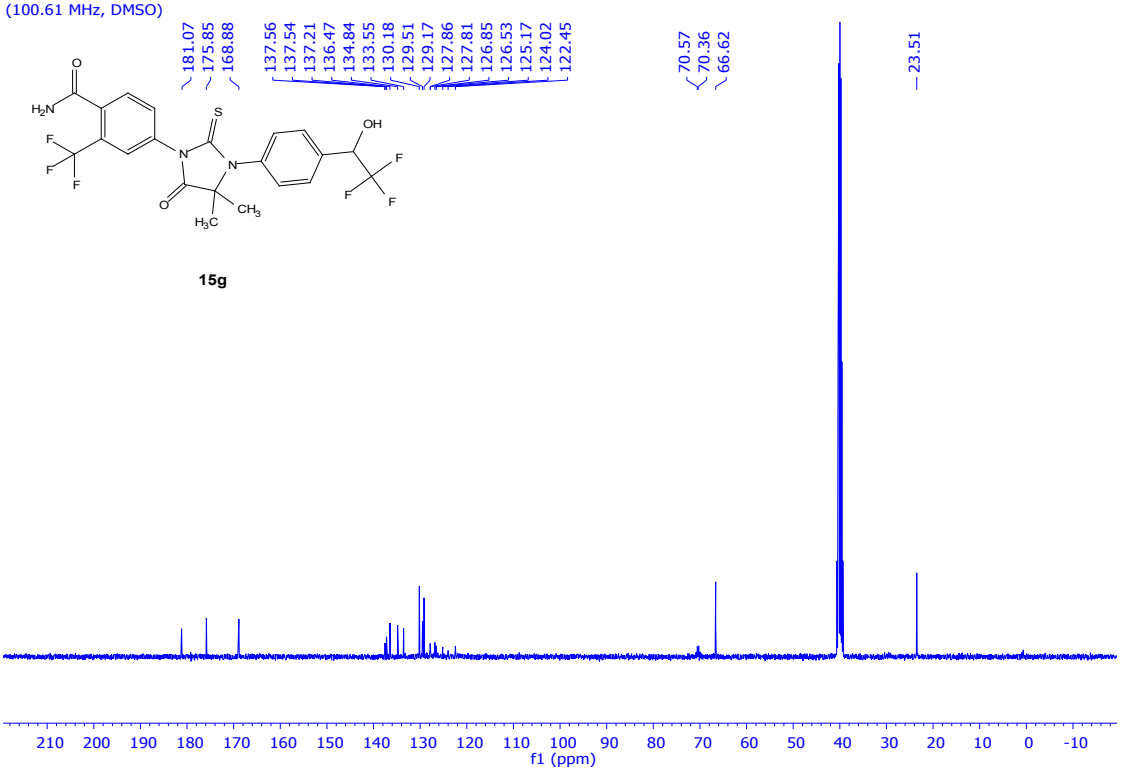
15f

(400.13 MHz, DMSO)



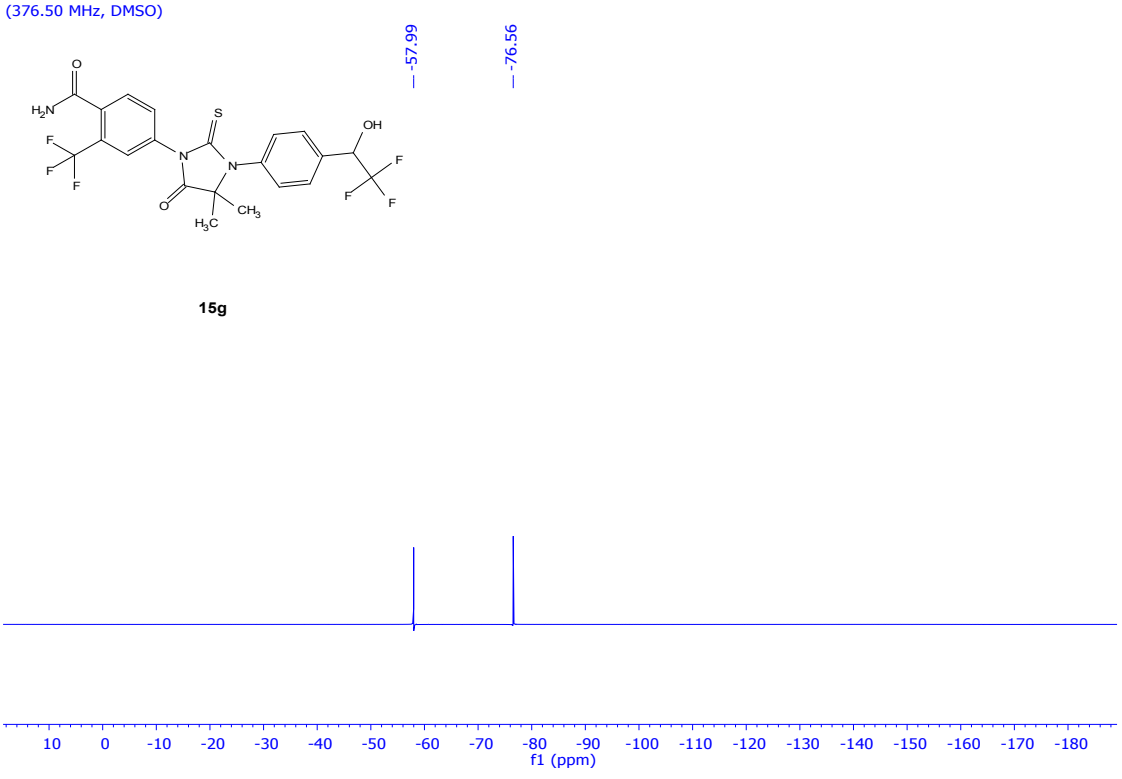
15g

(100.61 MHz, DMSO)



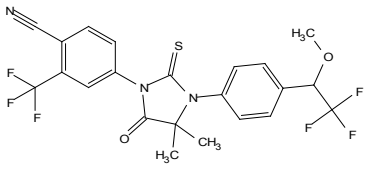
15g

(376.50 MHz, DMSO)

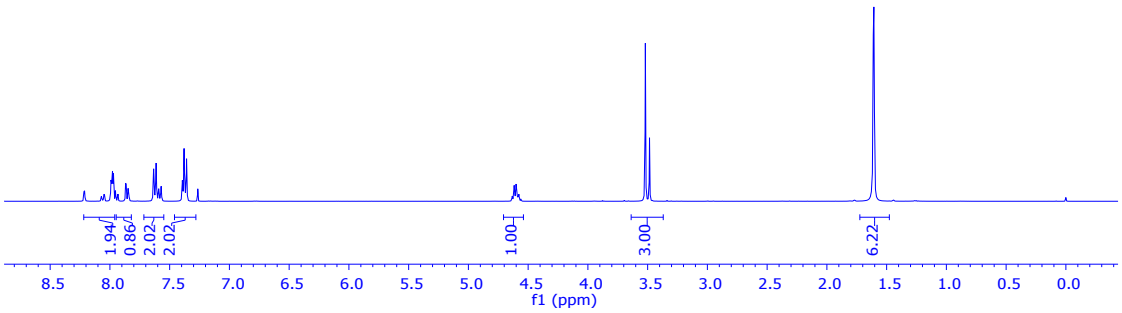


15g

(400.13 MHz, CDCl3)

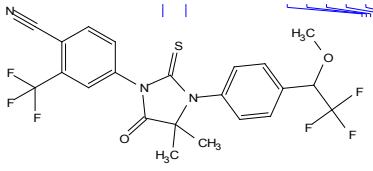


15h

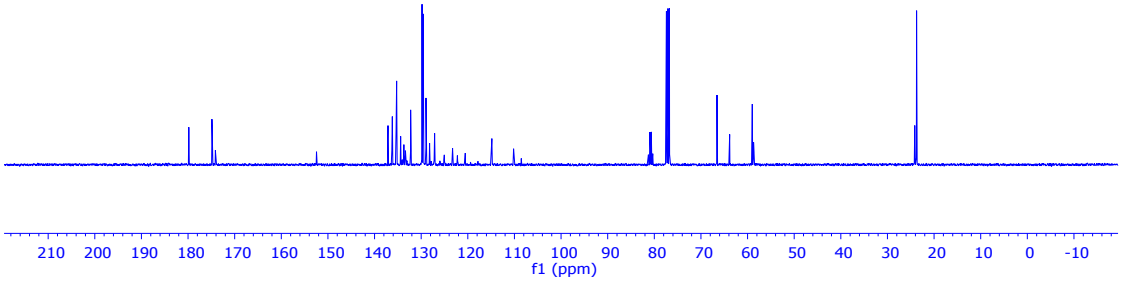


(100.61 MHz, CDCl3)

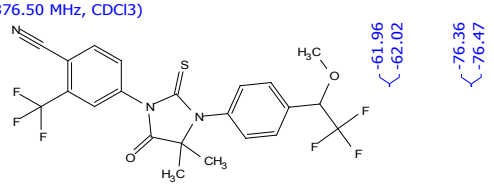
179.83
174.88
137.12
136.19
135.26
132.26
129.82
129.57
127.12
125.04
123.30
123.26
122.23
120.54
114.84
110.20
110.18
80.95
66.56
58.99
23.75



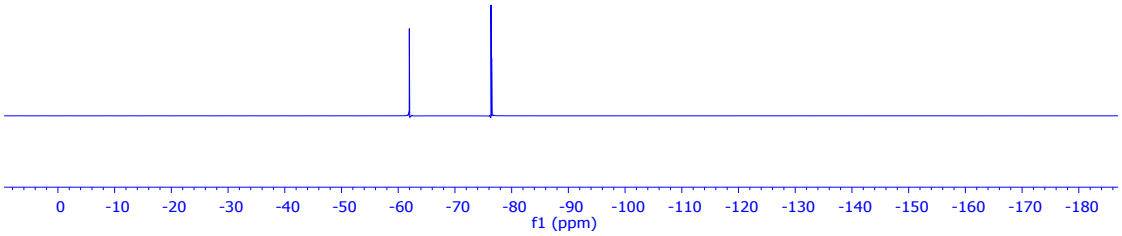
15h



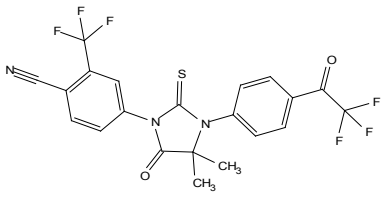
(376.50 MHz, CDCl3)



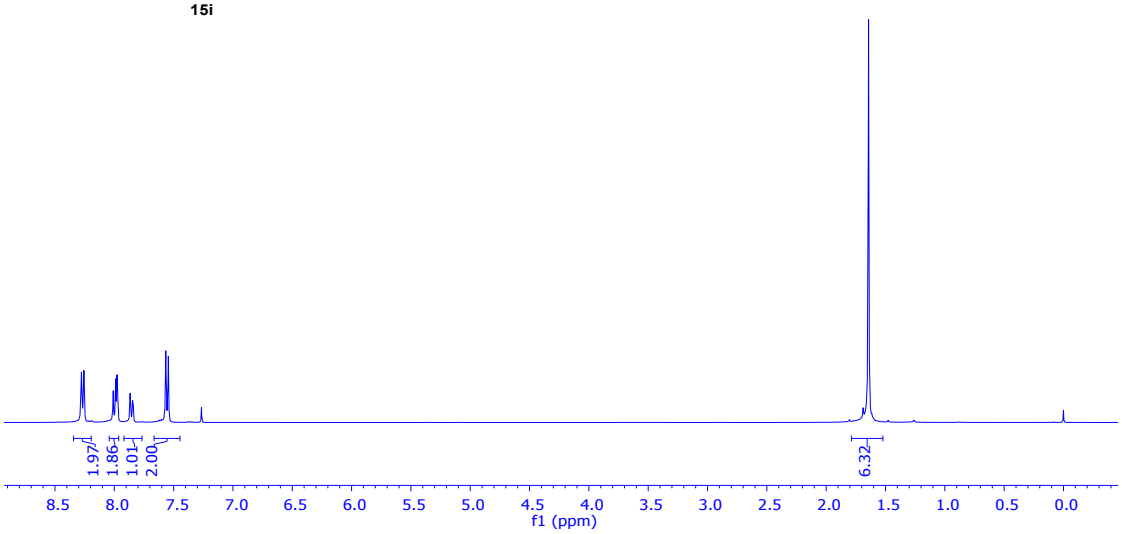
15h



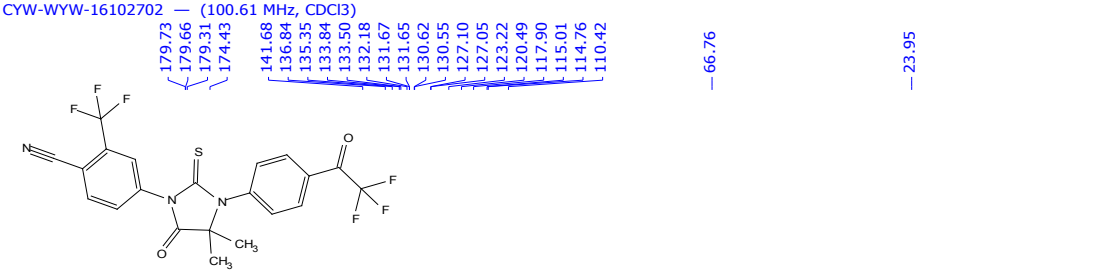
(400.13 MHz, CDCl3)



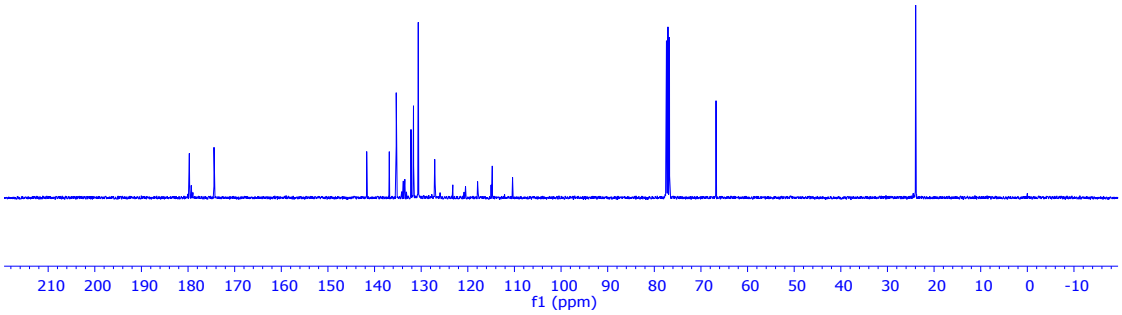
15i



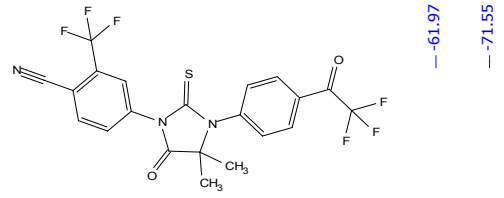
CYW-WYW-16102702 — (100.61 MHz, CDCl3)



15i



(376.50 MHz, CDCl3)



15i