

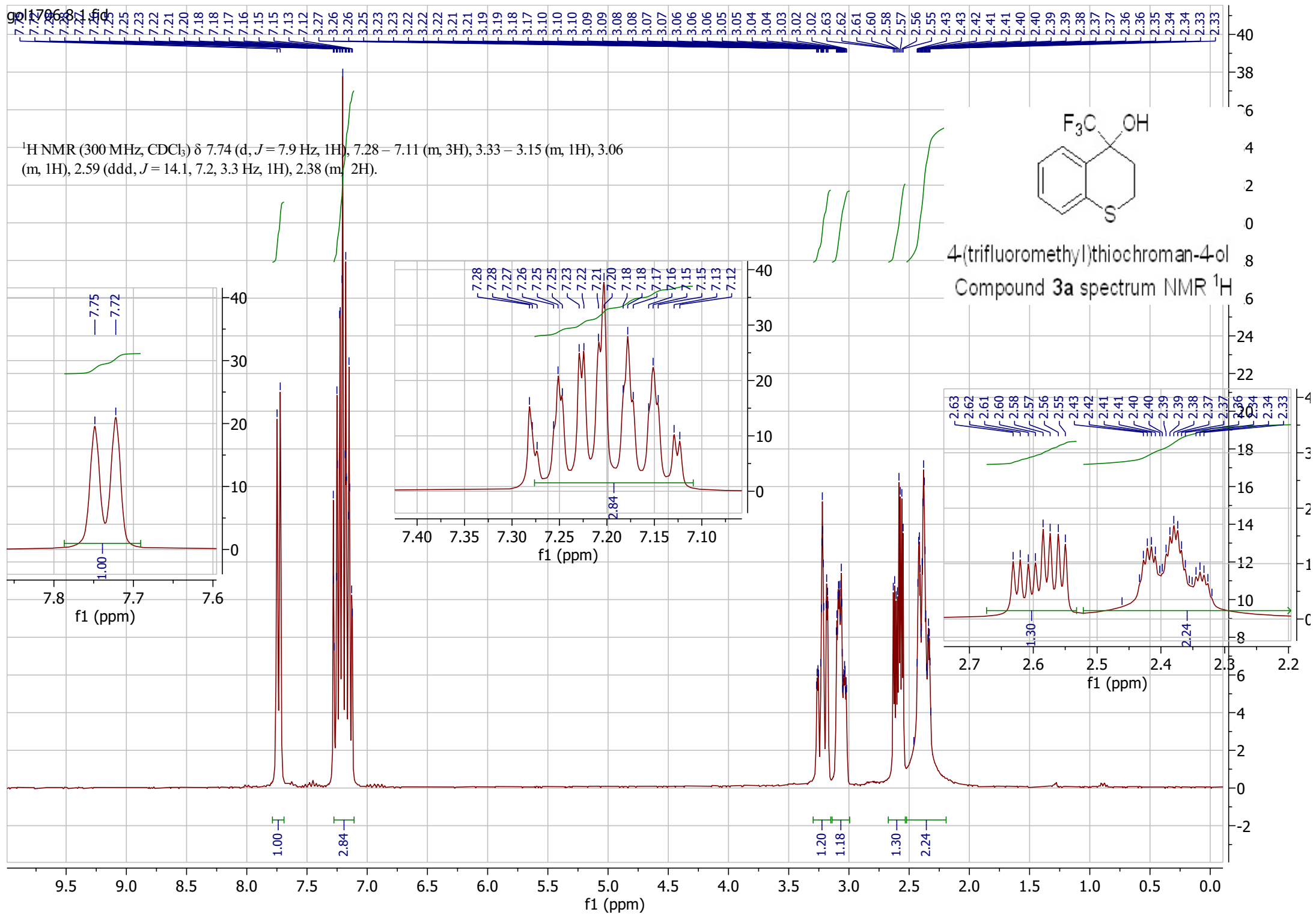
## Electronic supplementary information

### SYNTHESIS OF 4-(TRIFLUOROMETHYL)- 2H-THIOCHROMENES

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R. U. Takazova,<sup>a</sup> and N. D. Chkanikov<sup>a</sup>

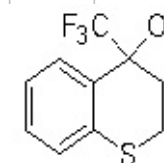
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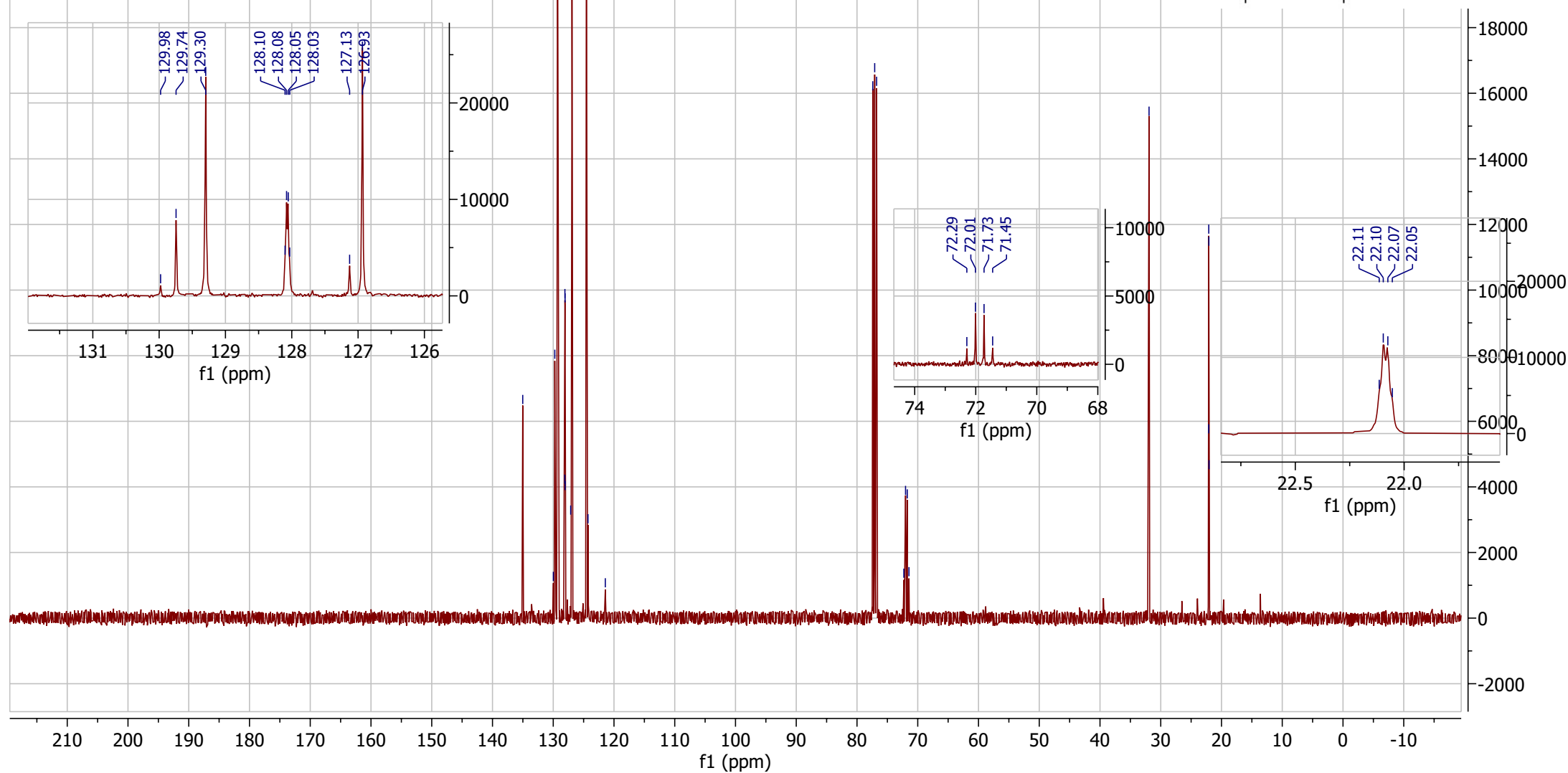
gol1706.4.13.fid

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  135.02, 129.74, 129.30, 128.07 (q,  $J = 2.3$  Hz), 126.93, 125.70 (q,  $J = 286.6$  Hz), 124.54, 71.87 (q,  $J = 28.4$  Hz), 31.93, 22.08 (q,  $J = 2.0$  Hz).



4-(trifluoromethyl)thiochroman-4-ol

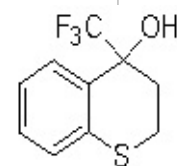
Compound **3a** spectrum NMR  $^{13}\text{C}$



gol1706.8.19.fid  
F19CPD

$^{19}\text{F}$  NMR (282 MHz,  $\text{CDCl}_3$ )  $\delta$  -77.40.

-77.40



4-(trifluoromethyl)thiochroman-4-ol

Compound **3a** spectrum NMR  $^{19}\text{F}$

-60

-65

-70

-75

f1 (ppm)

-80

-85

-90

-95

-100

180

170

160

150

140

130

120

110

100

90

80

70

60

50

40

30

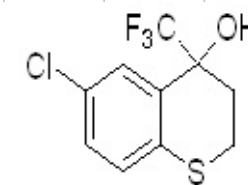
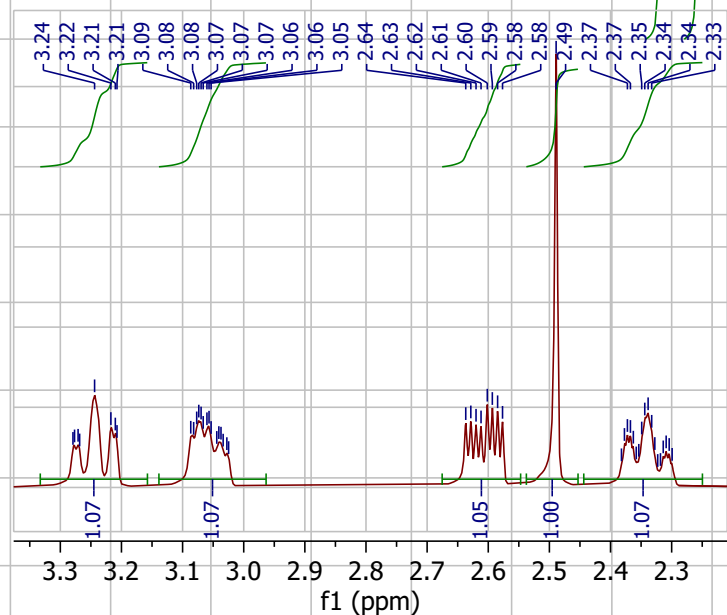
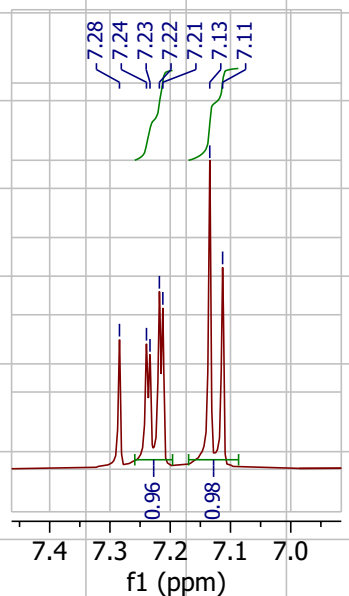
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10

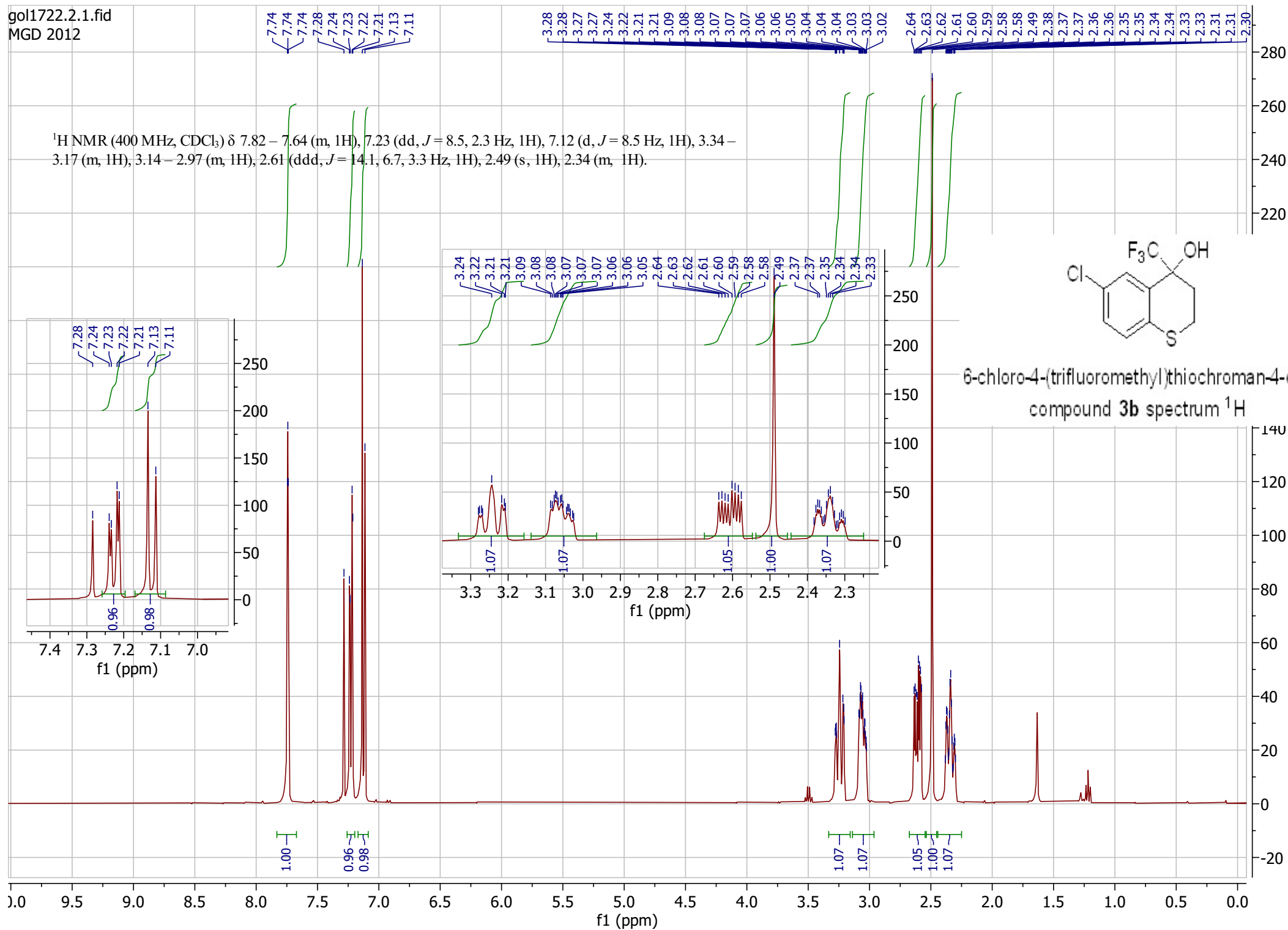
0

-10

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.82 – 7.64 (m, 1H), 7.23 (dd,  $J$  = 8.5, 2.3 Hz, 1H), 7.12 (d,  $J$  = 8.5 Hz, 1H), 3.34 – 3.17 (m, 1H), 3.14 – 2.97 (m, 1H), 2.61 (ddd,  $J$  = 14.1, 6.7, 3.3 Hz, 1H), 2.49 (s, 1H), 2.34 (m, 1H).

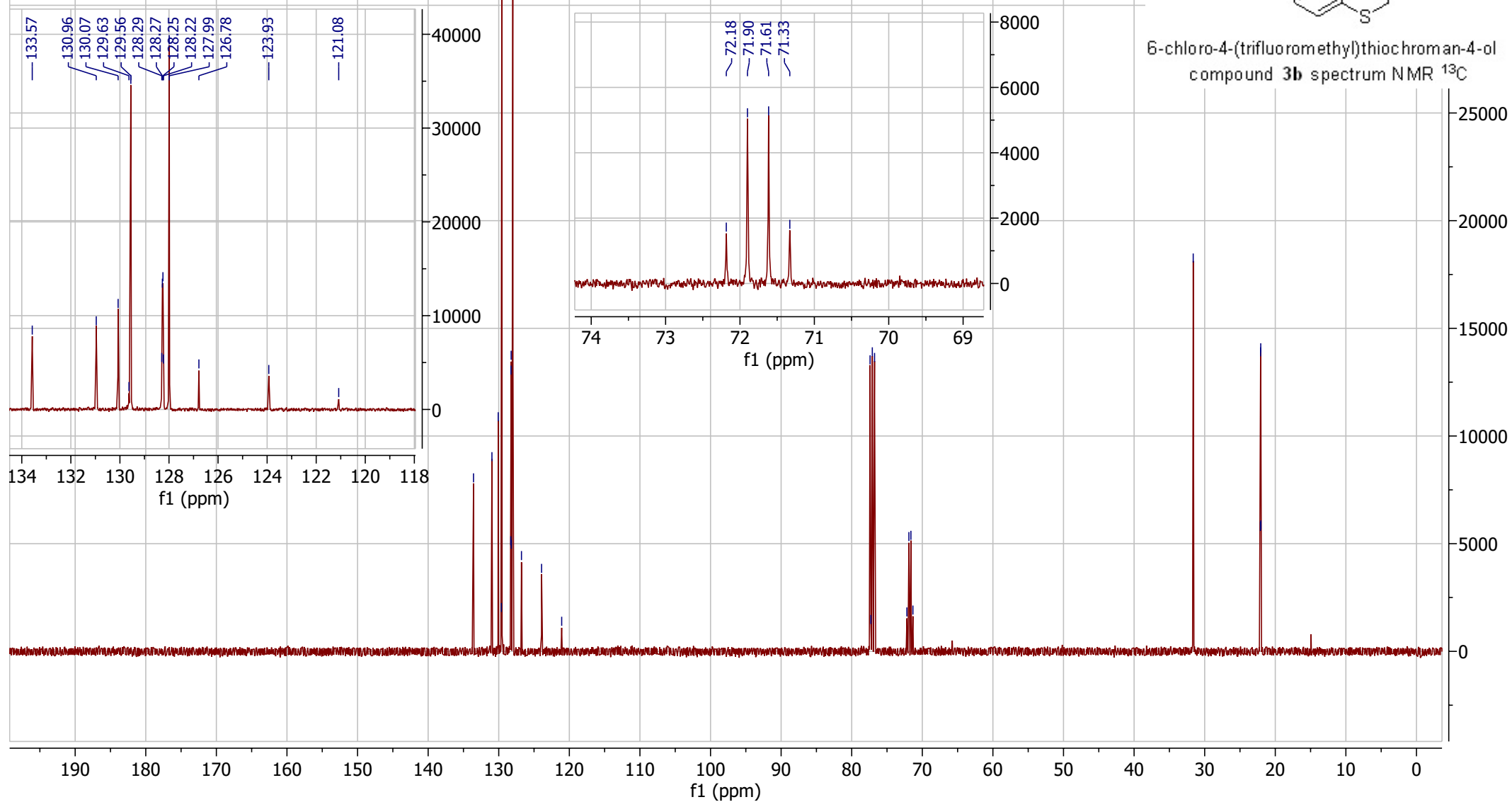


6-chloro-4-(trifluoromethyl)thiochroman-4-ol  
compound **3b** spectrum  $^1\text{H}$



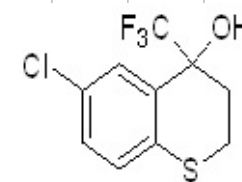
gol1722.2.13.fid

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  133.57, 130.96, 130.07, 129.56, 128.26 (q,  $J = 2.3$  Hz), 127.99, 125.36 (q,  $J = 286.6$  Hz), 71.76 (q,  $J = 28.6$  Hz), 31.63, 22.07 (q,  $J = 2.1$  Hz).

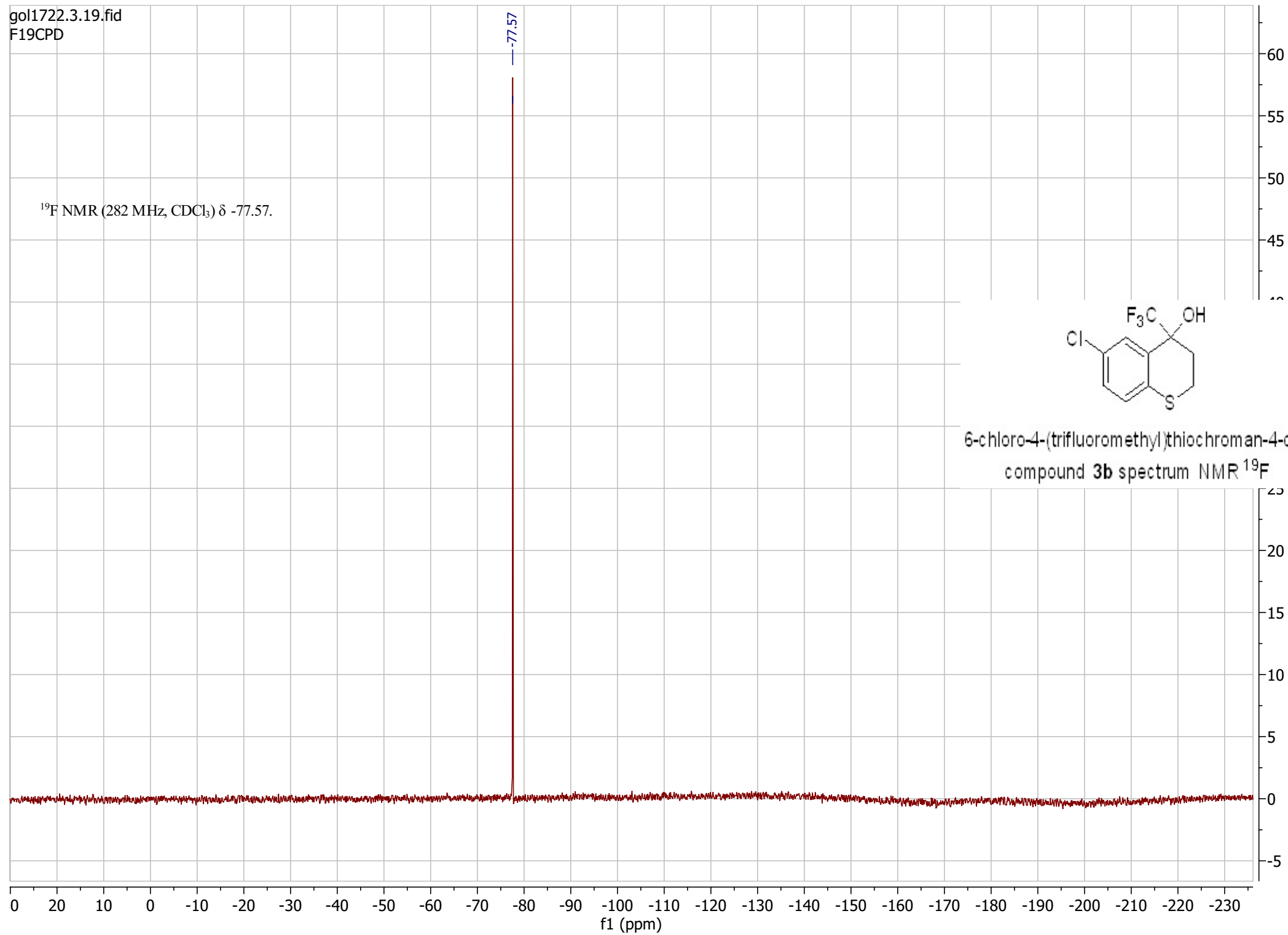


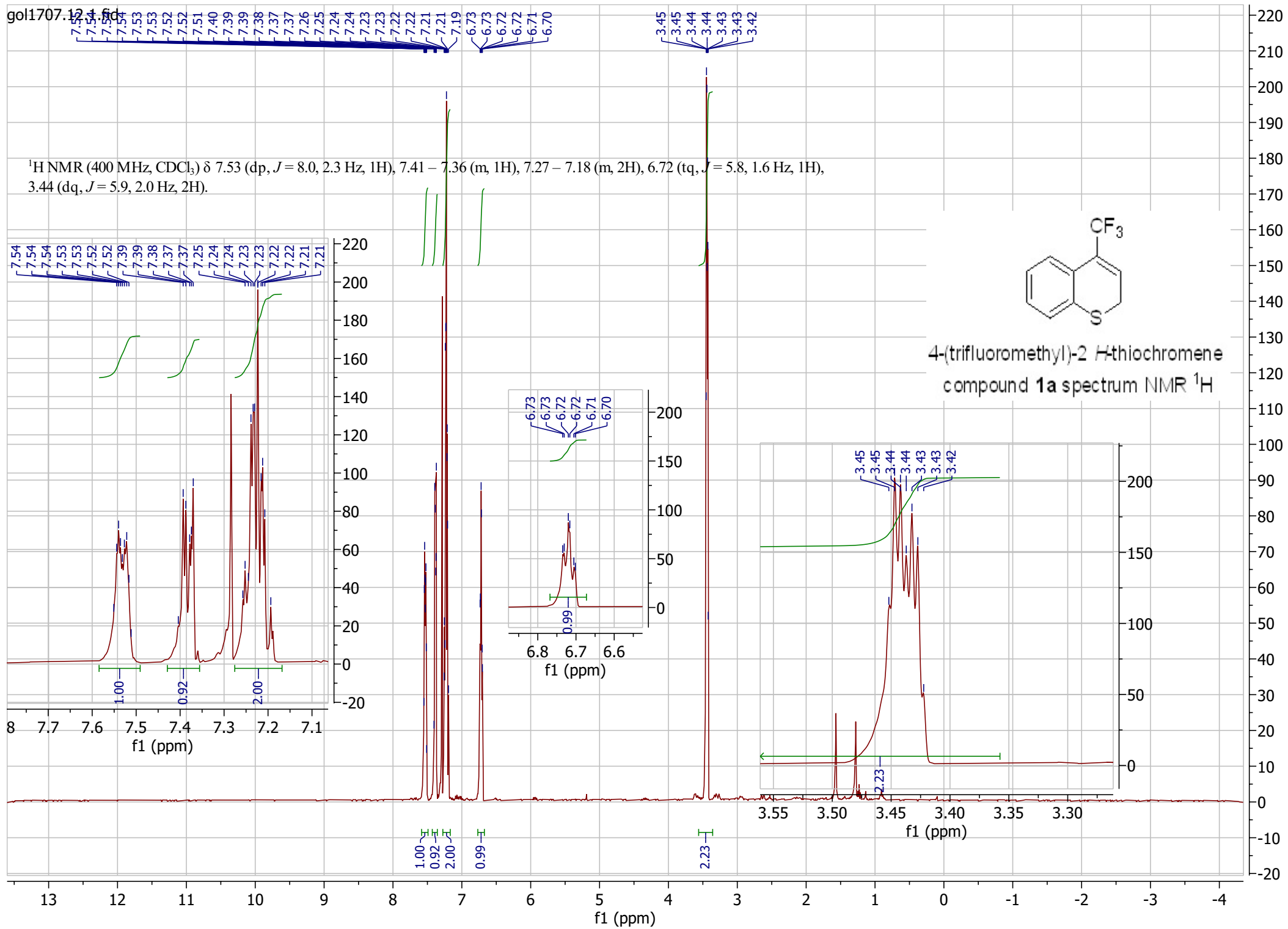
gol1722.3.19.fid  
F19CPD

$^{19}\text{F}$  NMR (282 MHz,  $\text{CDCl}_3$ )  $\delta$  -77.57.



6-chloro-4-(trifluoromethyl)thiochroman-4-ol  
compound **3b** spectrum NMR  $^{19}\text{F}$

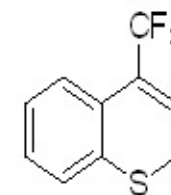
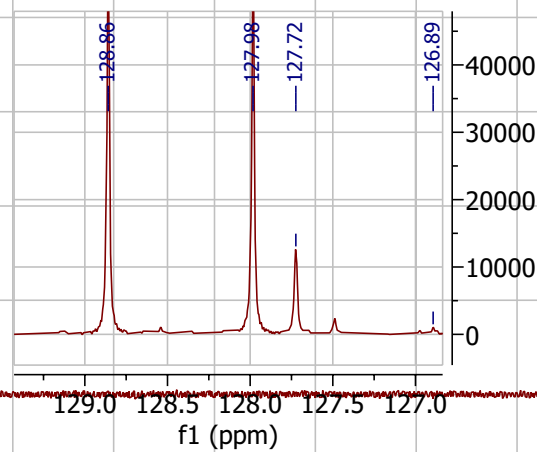
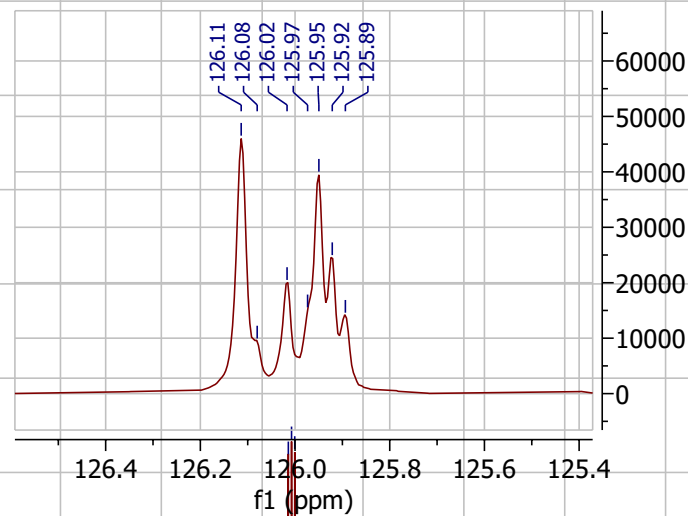
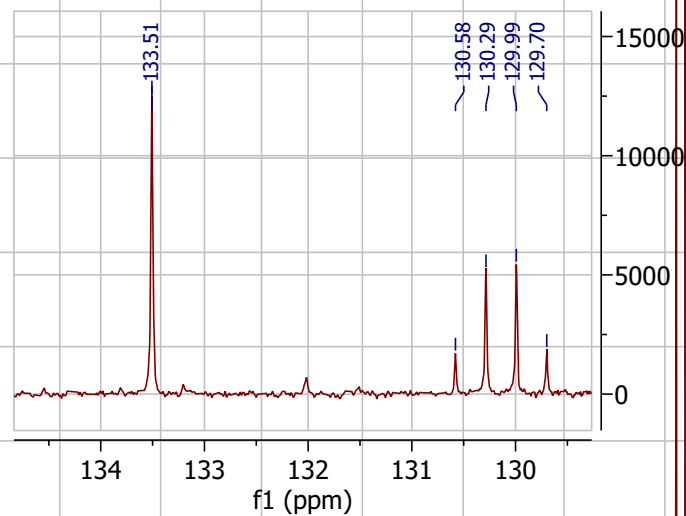




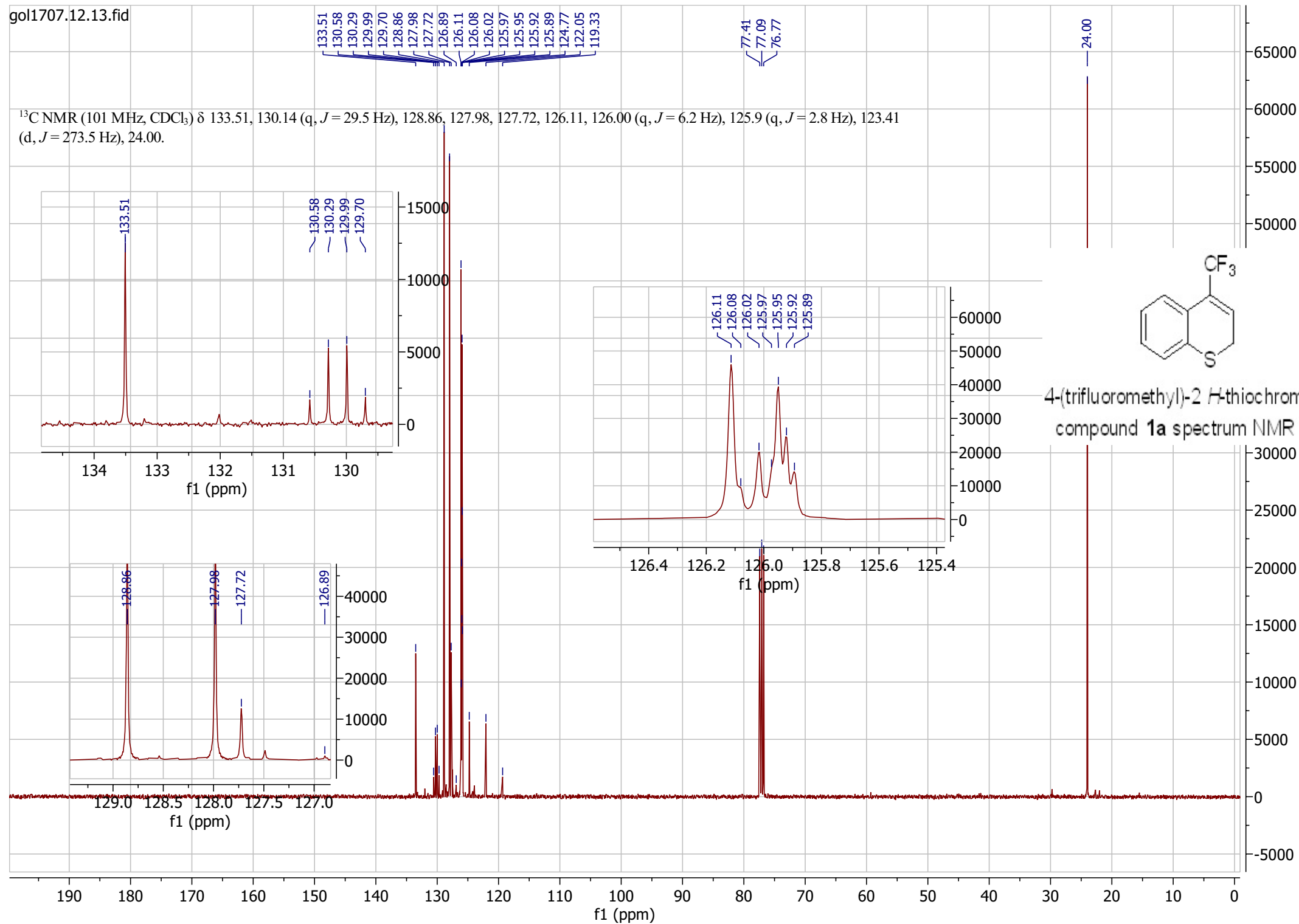


gol1707.12.13.fid

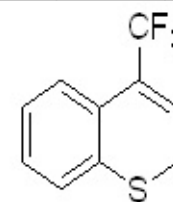
$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  133.51, 130.14 (q,  $J = 29.5$  Hz), 128.86, 127.98, 127.72, 126.11, 126.00 (q,  $J = 6.2$  Hz), 125.9 (q,  $J = 2.8$  Hz), 123.41 (d,  $J = 273.5$  Hz), 24.00.



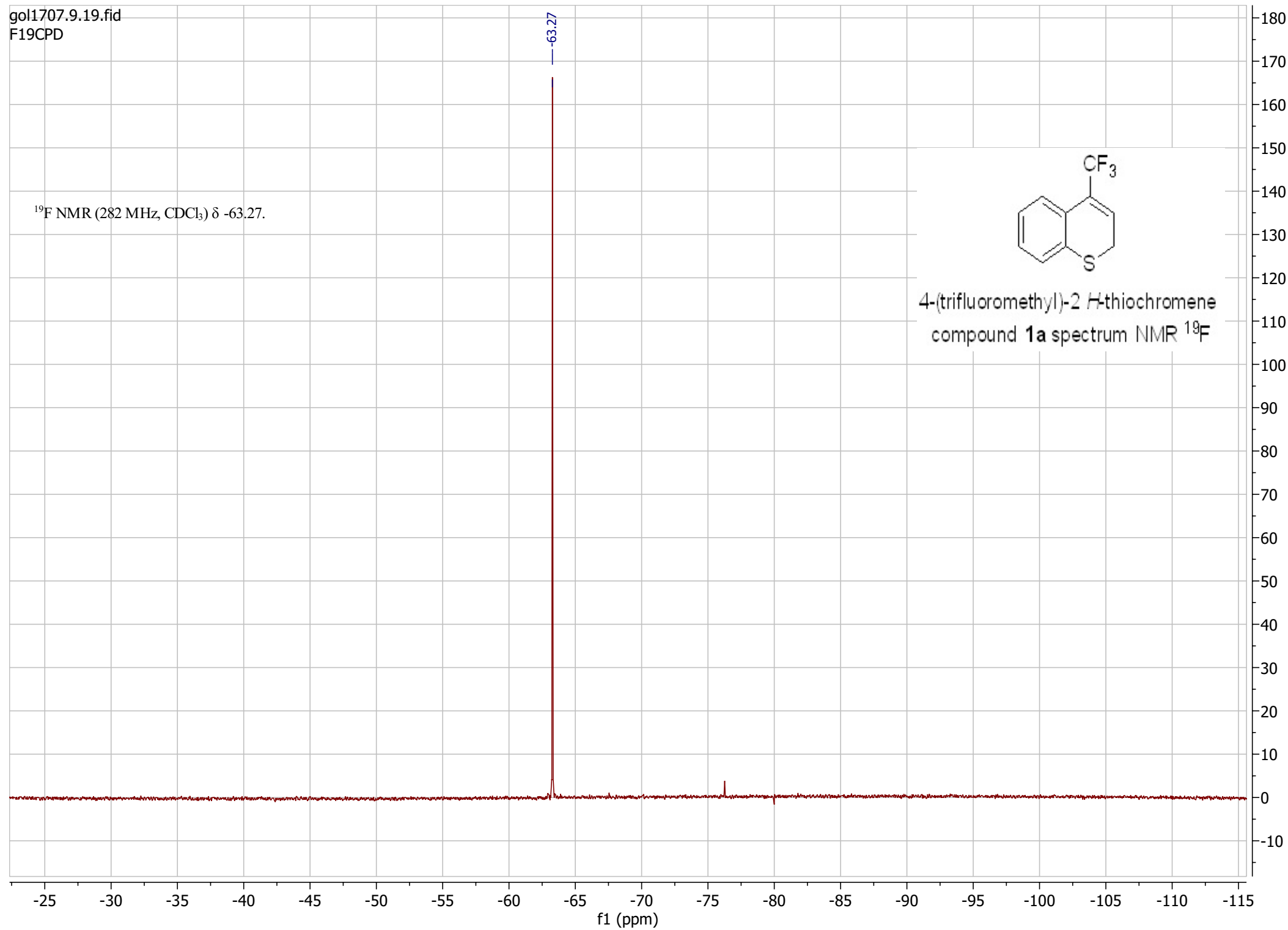
4-(trifluoromethyl)-2 *H*-thiochromene  
compound **1a** spectrum NMR  $^{13}\text{C}$



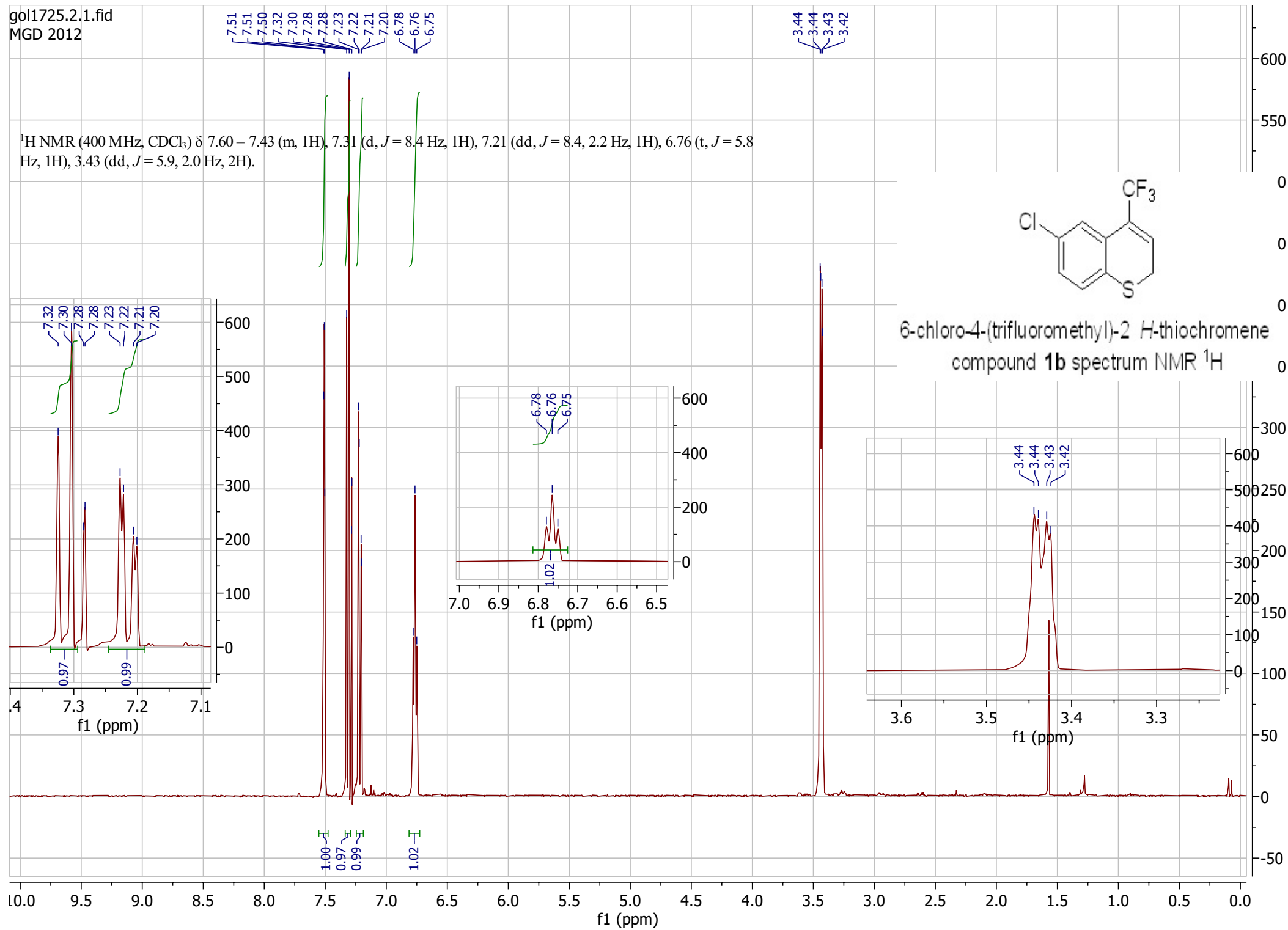
$^{19}\text{F}$  NMR (282 MHz,  $\text{CDCl}_3$ )  $\delta$  -63.27.



4-(trifluoromethyl)-2 *H*-thiochromene  
compound **1a** spectrum NMR  $^{19}\text{F}$

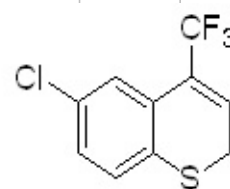


$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.60 – 7.43 (m, 1H), 7.31 (d,  $J = 8.4$  Hz, 1H), 7.21 (dd,  $J = 8.4, 2.2$  Hz, 1H), 6.76 (t,  $J = 5.8$  Hz, 1H), 3.43 (dd,  $J = 5.9, 2.0$  Hz, 2H).

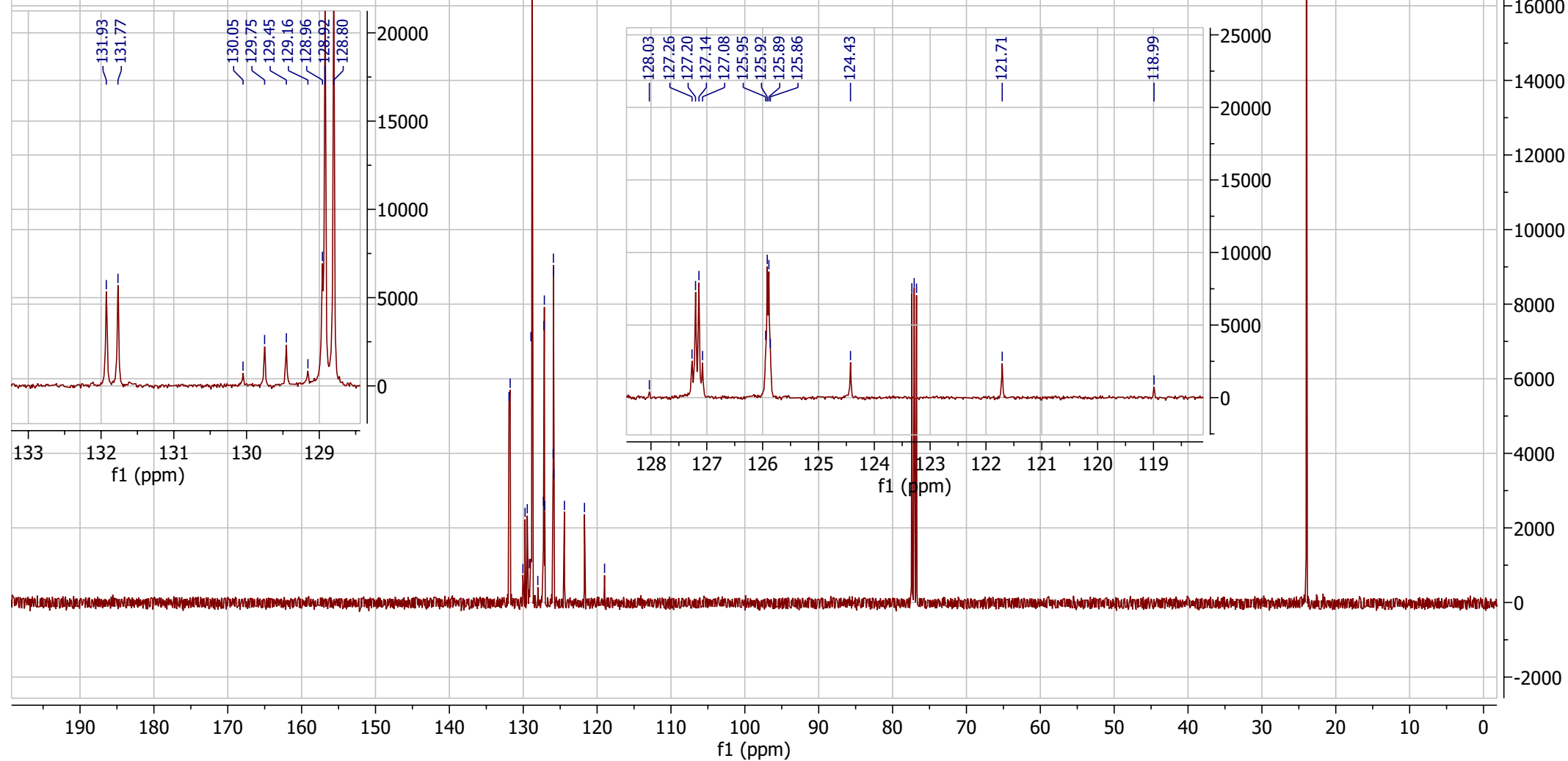


gol1725.2.13.fid

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  131.93, 131.77, 129.60 (q,  $J = 29.8$  Hz), 128.96, 128.92, 128.80, 127.17 (q,  $J = 6.4$  Hz), 125.90 (q,  $J = 2.8$  Hz), 123.07 (q,  $J = 273.4$  Hz), 23.97.

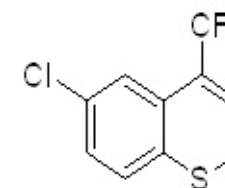


6-chloro-4-(trifluoromethyl)-2 H-thiochromene  
compound **1b** spectrum NMR  $^{13}\text{C}$

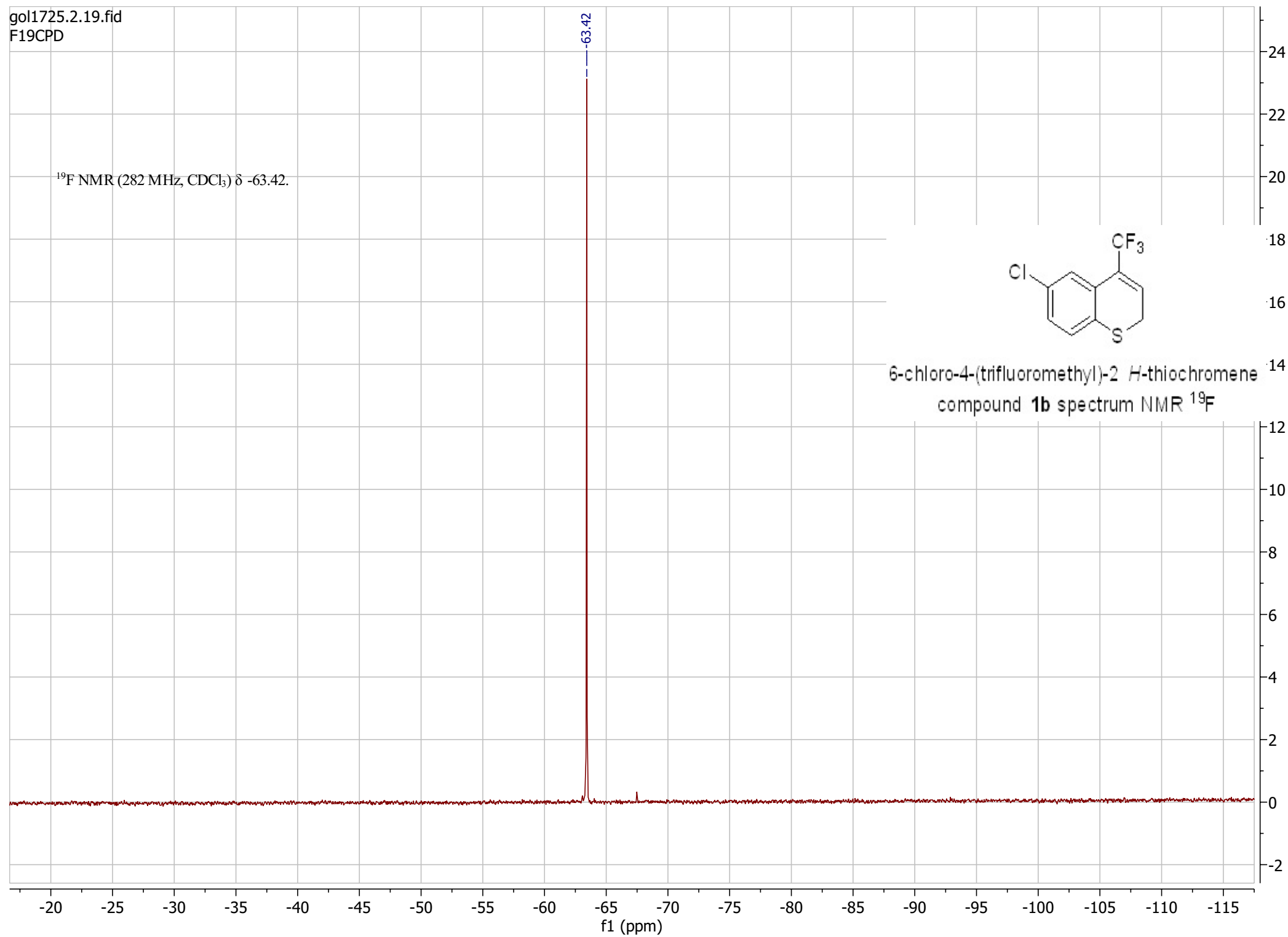


gol1725.2.19.fid  
F19CPD

$^{19}\text{F}$  NMR (282 MHz,  $\text{CDCl}_3$ )  $\delta$  -63.42.

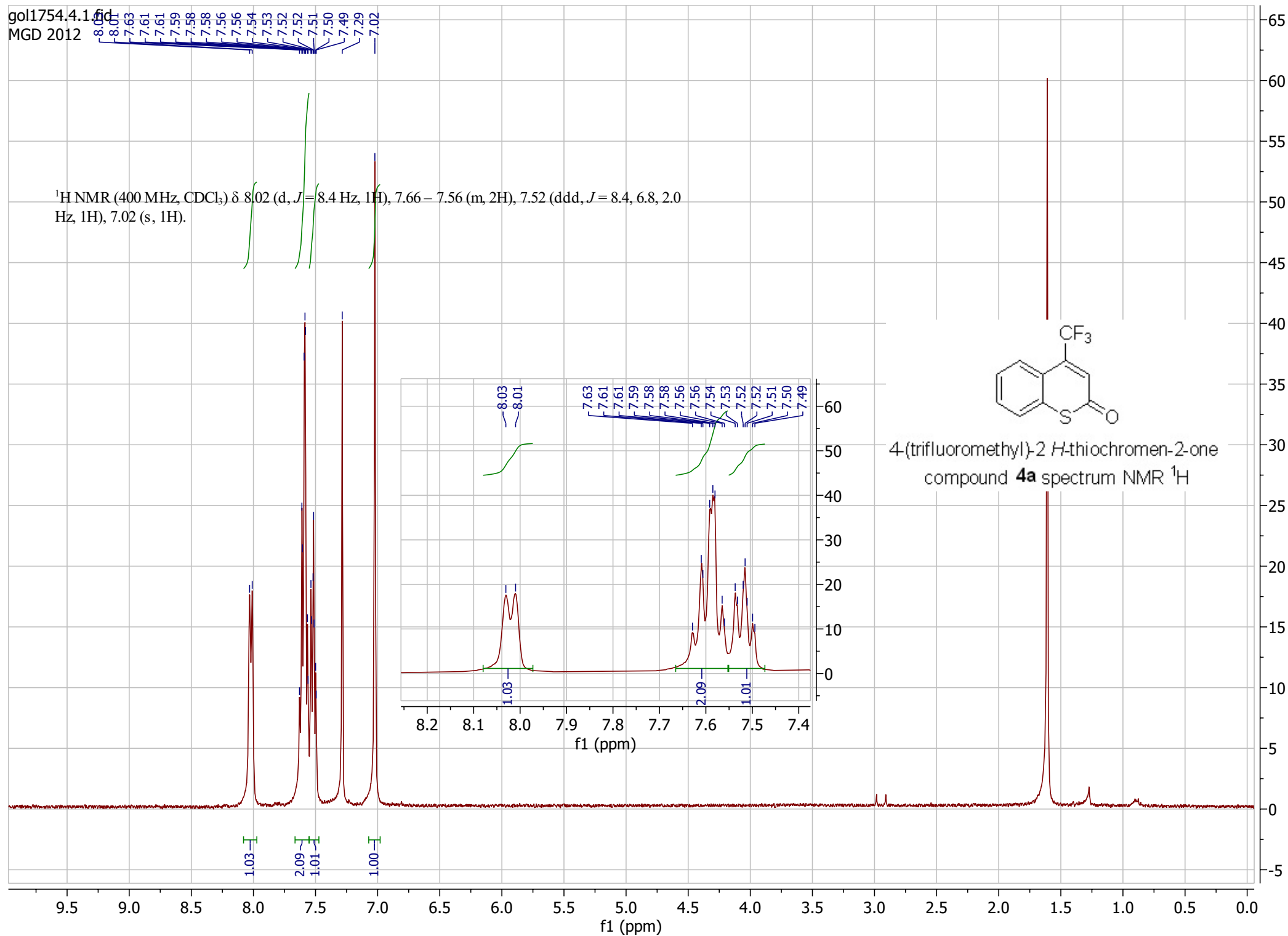


6-chloro-4-(trifluoromethyl)-2 *H*-thiochromene  
compound **1b** spectrum NMR  $^{19}\text{F}$

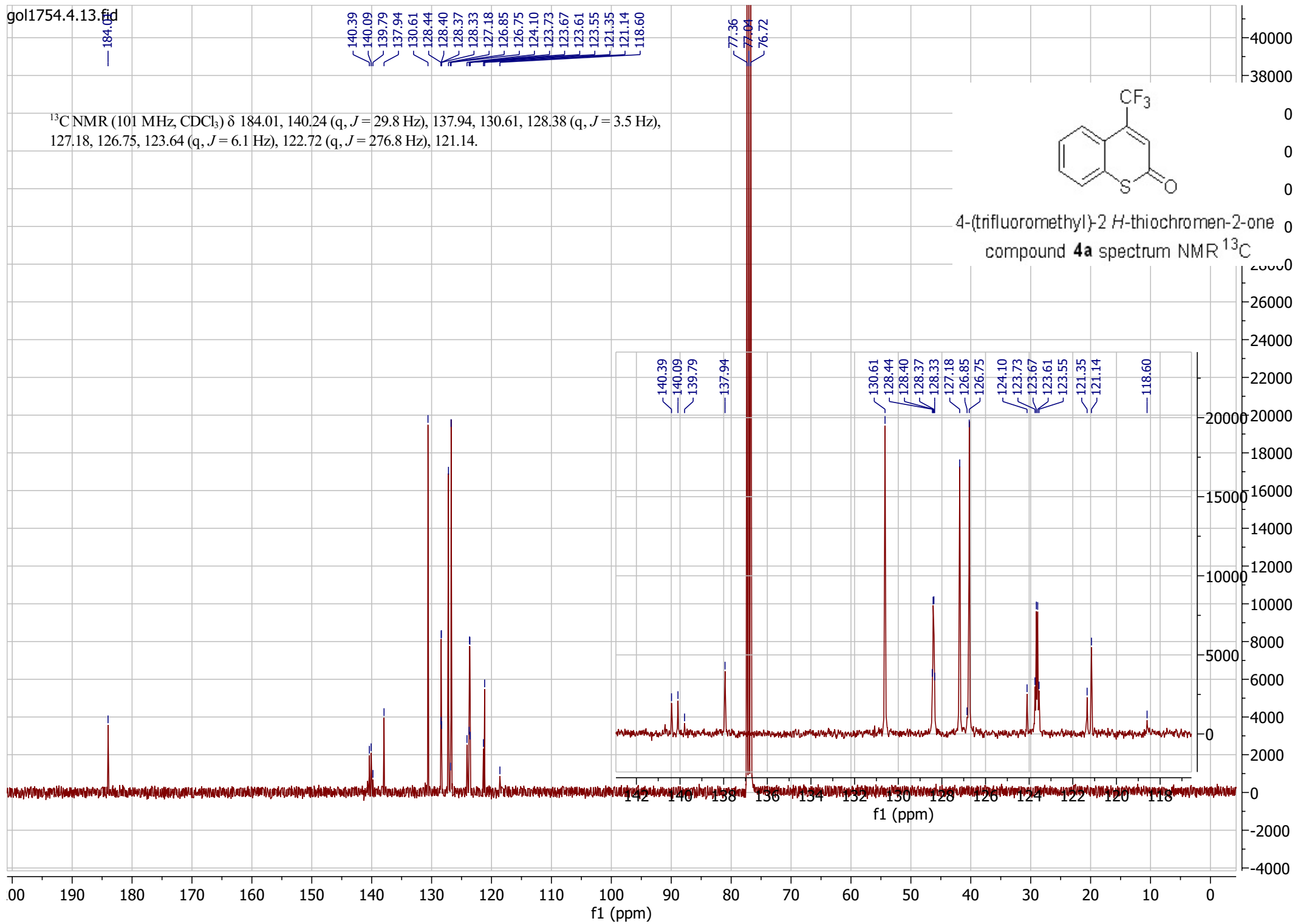


gol1754.4.1.6d  
MGD 2012

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.02 (d,  $J = 8.4$  Hz, 1H), 7.66 – 7.56 (m, 2H), 7.52 (ddd,  $J = 8.4, 6.8, 2.0$  Hz, 1H), 7.02 (s, 1H).

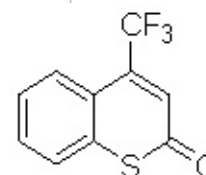


gol1754.4.13.f

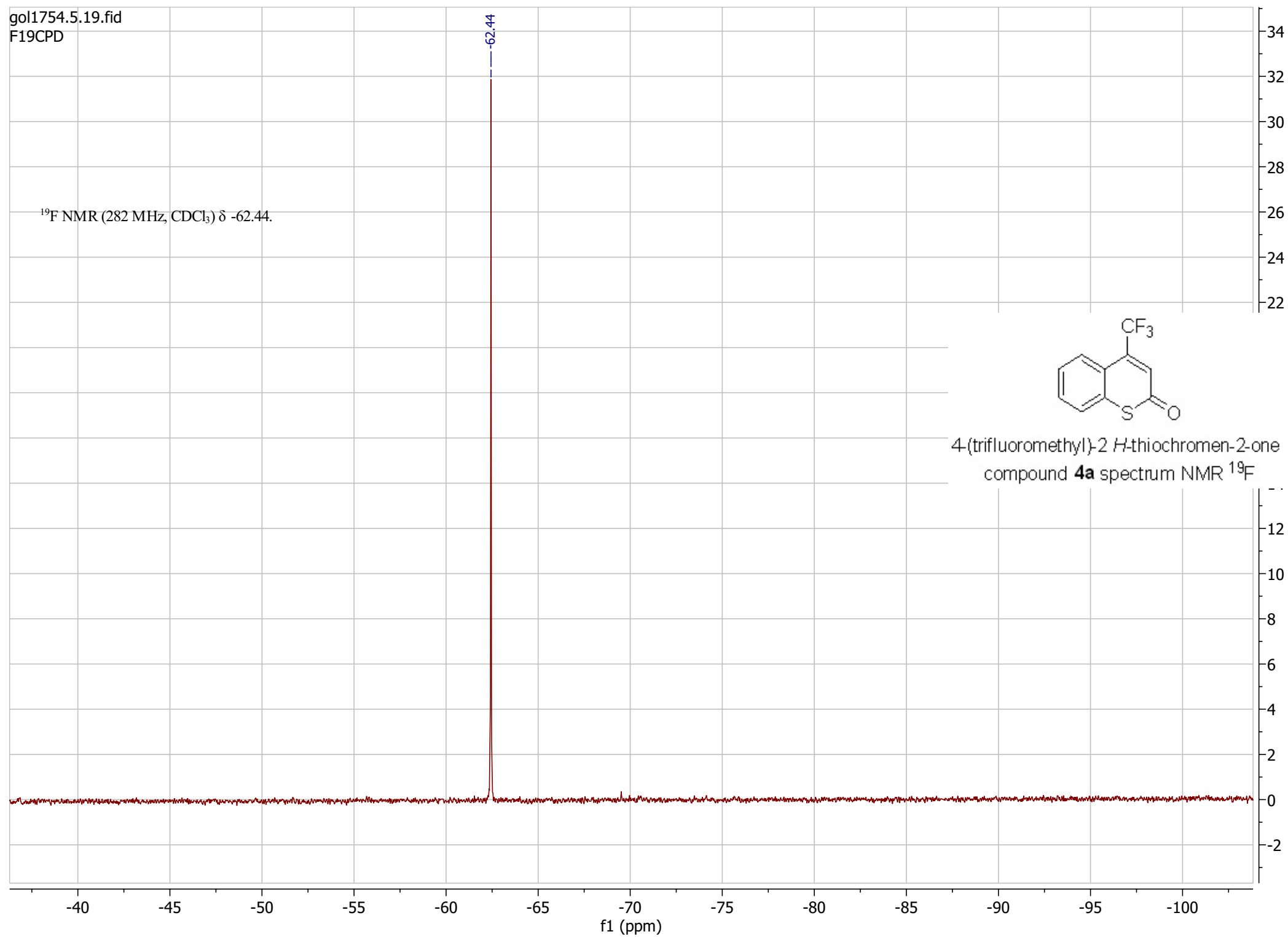


gol1754.5.19.fid  
F19CPD

$^{19}\text{F}$  NMR (282 MHz,  $\text{CDCl}_3$ )  $\delta$  -62.44.



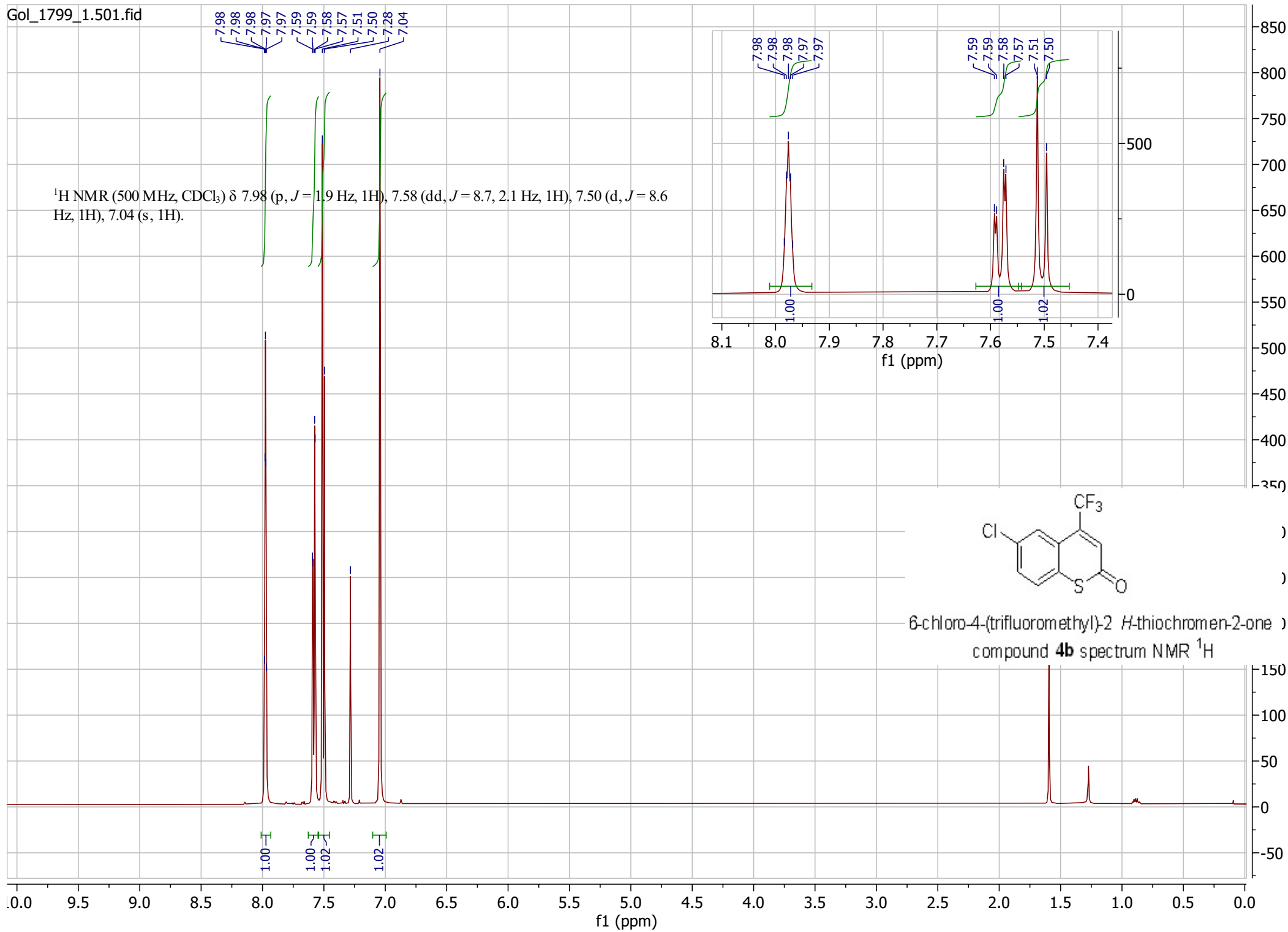
4-(trifluoromethyl)-2H-thiophene-2-one  
compound **4a** spectrum NMR  $^{19}\text{F}$





Gol\_1799\_1.501.fid

$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.98 (p,  $J = 1.9$  Hz, 1H), 7.58 (dd,  $J = 8.7, 2.1$  Hz, 1H), 7.50 (d,  $J = 8.6$  Hz, 1H), 7.04 (s, 1H).

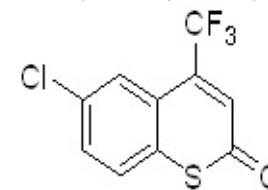


— 183.15

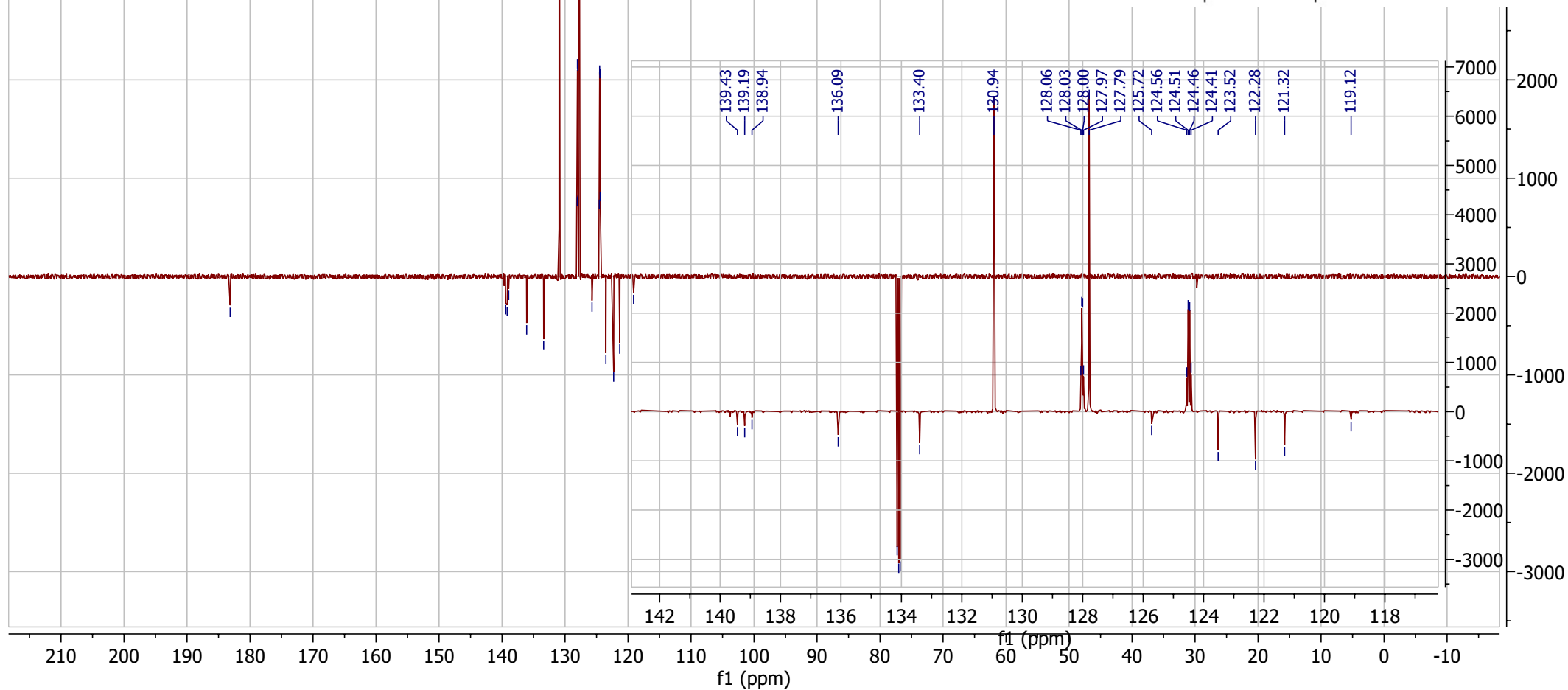
139.43  
139.19  
138.94  
136.09  
133.40  
130.94  
128.06  
128.03  
128.00  
127.97  
127.79  
125.72  
124.56  
124.51  
124.46  
124.41  
123.52  
122.28  
121.32  
119.12

77.29  
77.03  
76.78

$^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  183.15, 139.31 (q,  $J = 30.1$  Hz), 136.09, 133.40, 130.94, 128.02 (q,  $J = 3.7$  Hz), 127.79, 124.49 (q,  $J = 6.0$  Hz), 122.42 (q,  $J = 276.6$  Hz), 122.28.

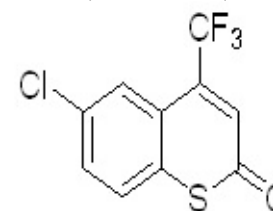


6-chloro-4-(trifluoromethyl)-2 *H*-thiochromen-2-one  
compound **4b** spectrum NMR  $^{13}\text{C}$  DEPT

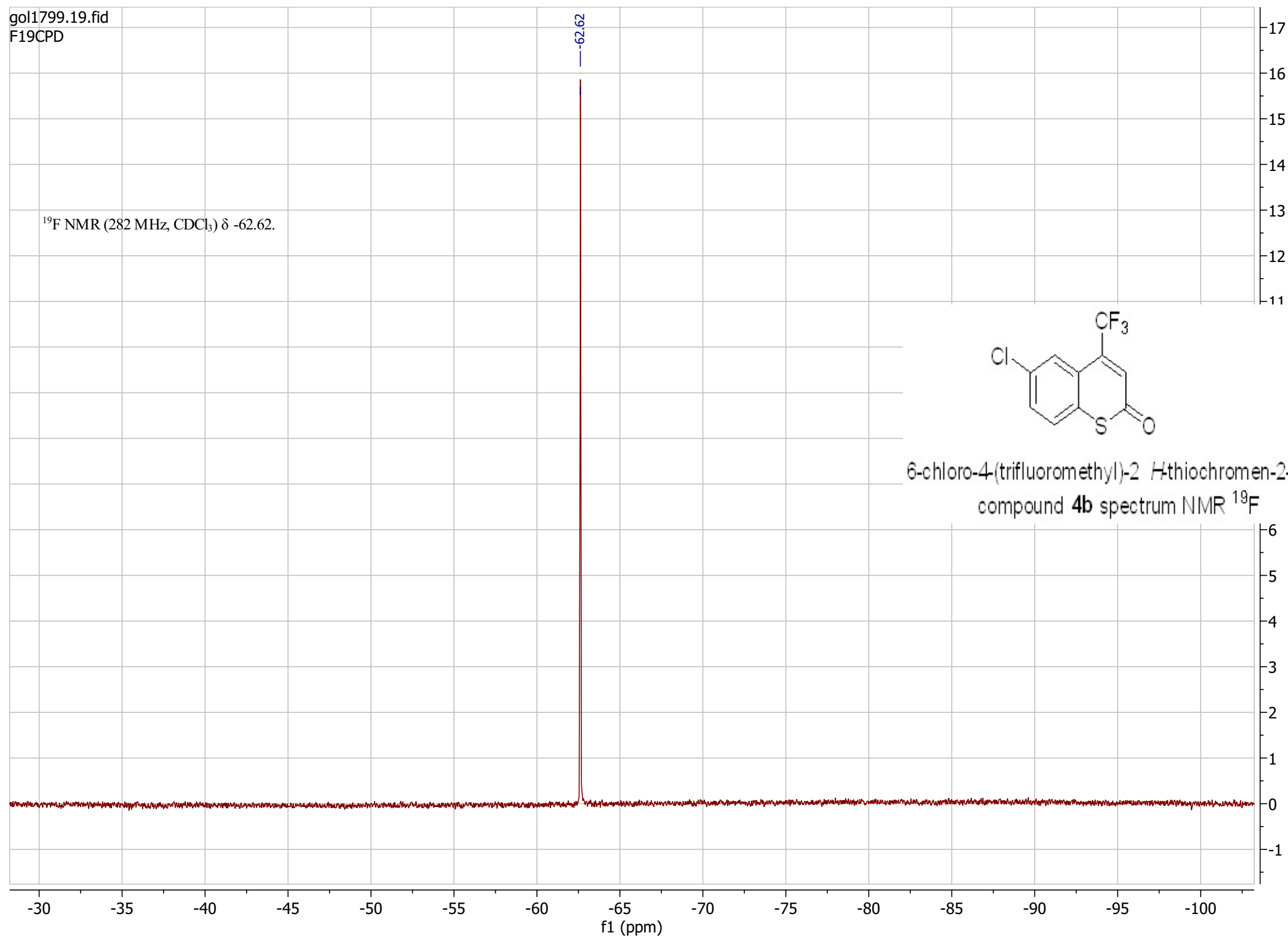


gol1799.19.fid  
F19CPD

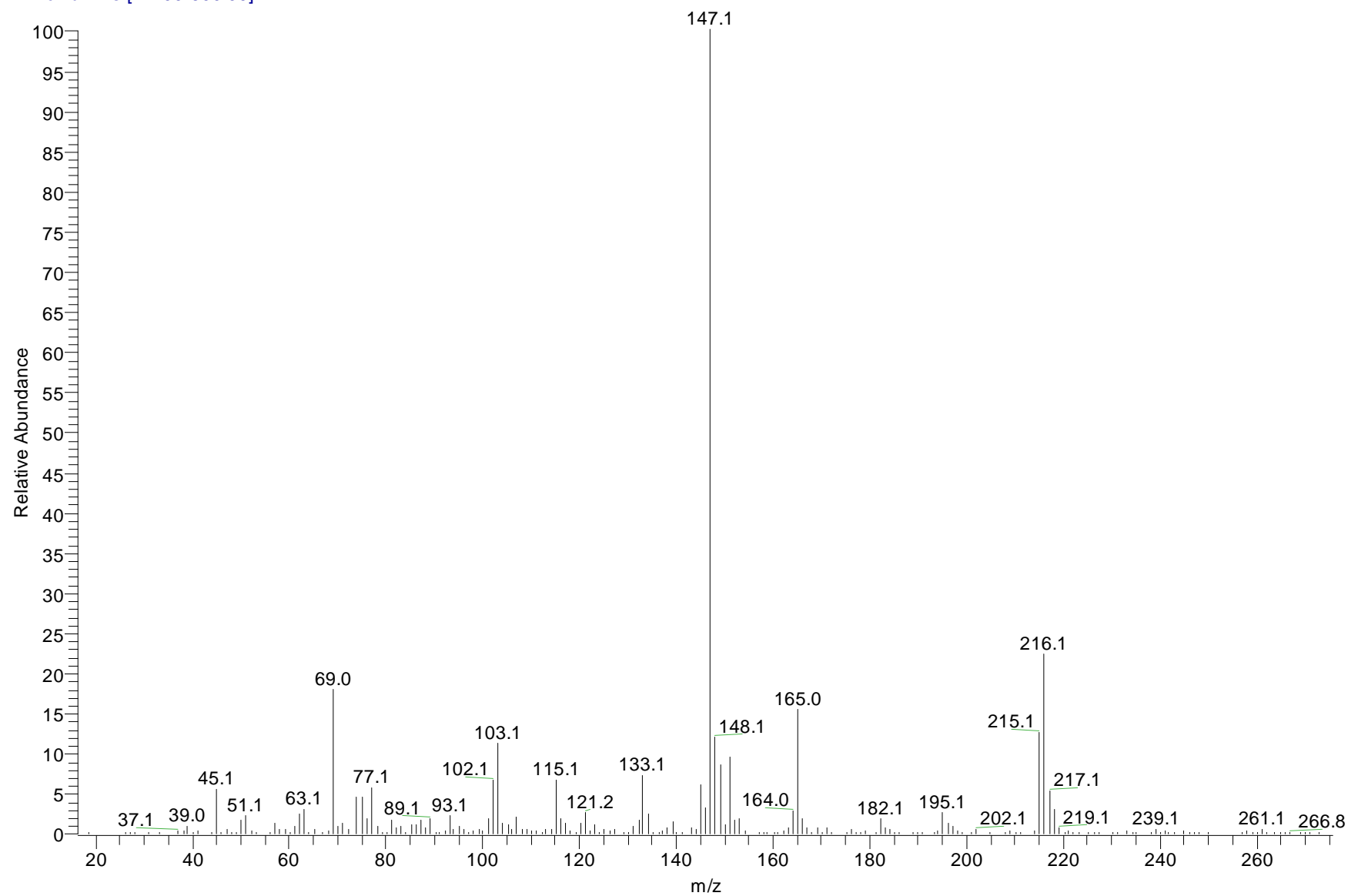
$^{19}\text{F}$  NMR (282 MHz,  $\text{CDCl}_3$ )  $\delta$  -62.62.



6-chloro-4-(trifluoromethyl)-2 *H*-thiochromen-2-one  
compound **4b** spectrum NMR  $^{19}\text{F}$



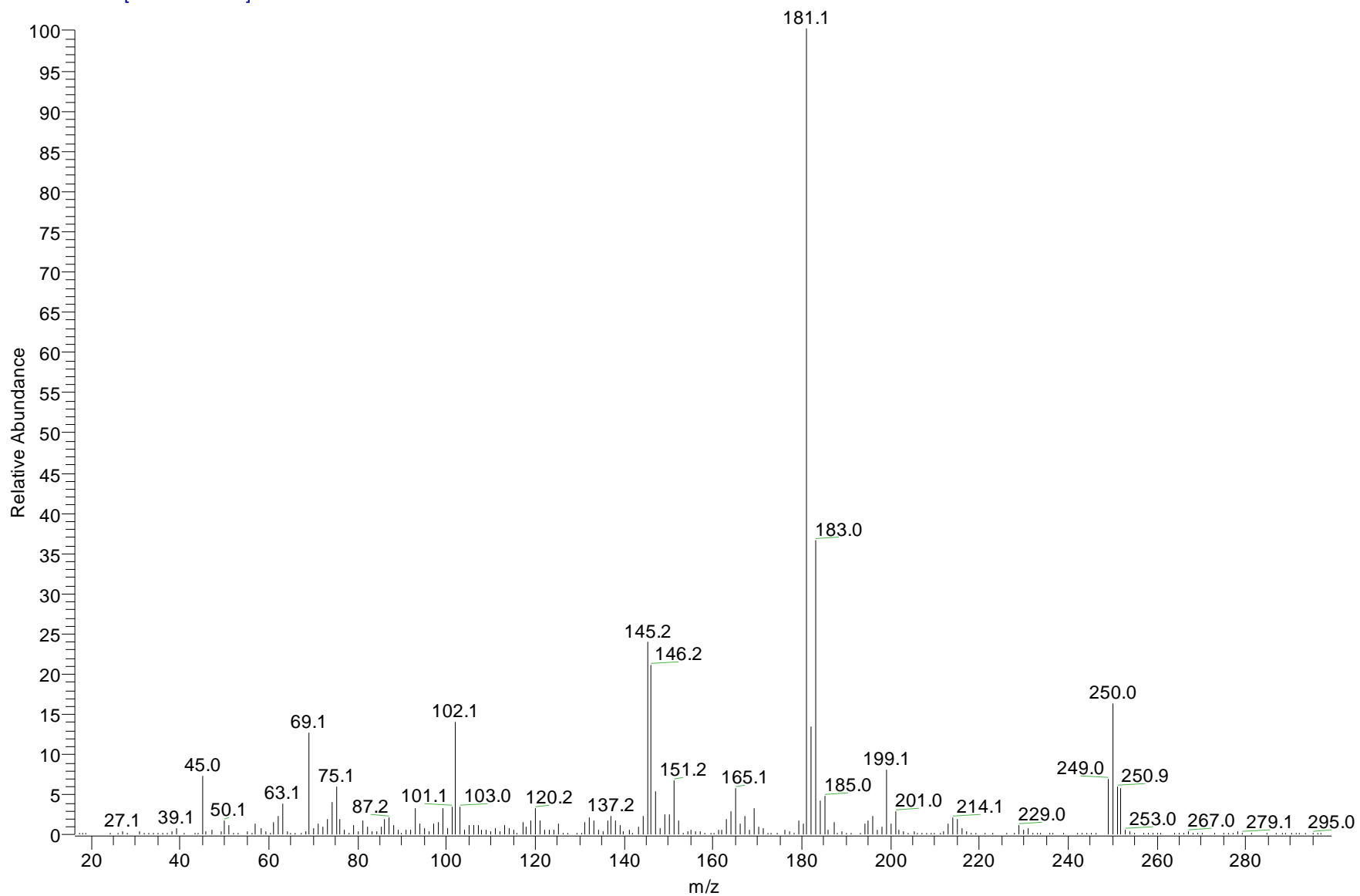
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T: + c Full ms [ 14.00-600.00]



Mass-spectrum of compounds 4-(trifluoromethyl)-2*H*-thiochromene **1a**

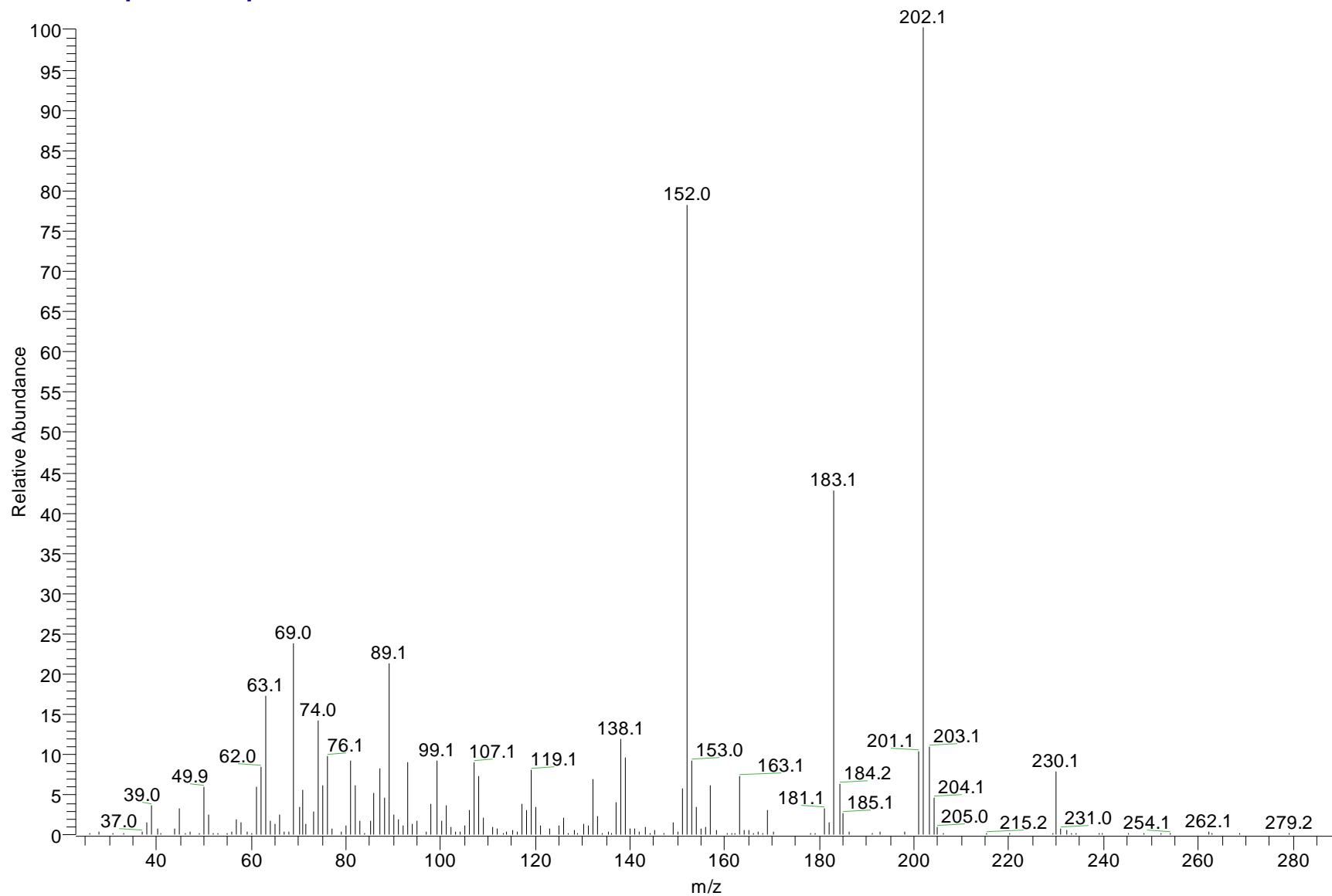
GoI\_1725 #1161 RT: 14.71 AV: 1 NL: 1.20E6

T: + c Full ms [ 14.00-600.00]



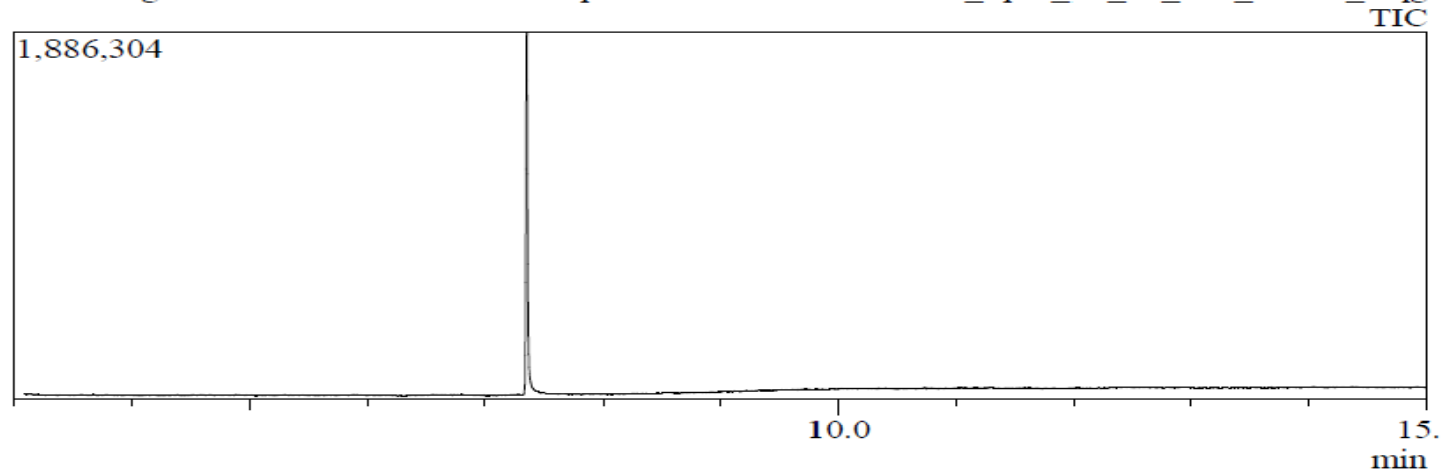
Mass-spectrum of compounds 6-chloro-4-(trifluoromethyl)-2*H*-thiochromene **1b**

Gol1716 #1112 RT: 14.11 AV: 1 NL: 3.35E5  
T: + c Full ms [20.00-600.00]



Mass-spectrum of compounds 4-(trifluoromethyl)-2*H*-thiochromen-2-one **4a**

Chromatogram 1799 Z:\Data\2024\04 April\lab 209\Khakina\1799\_Split\_50\_30\_290\_20min\_3.qg

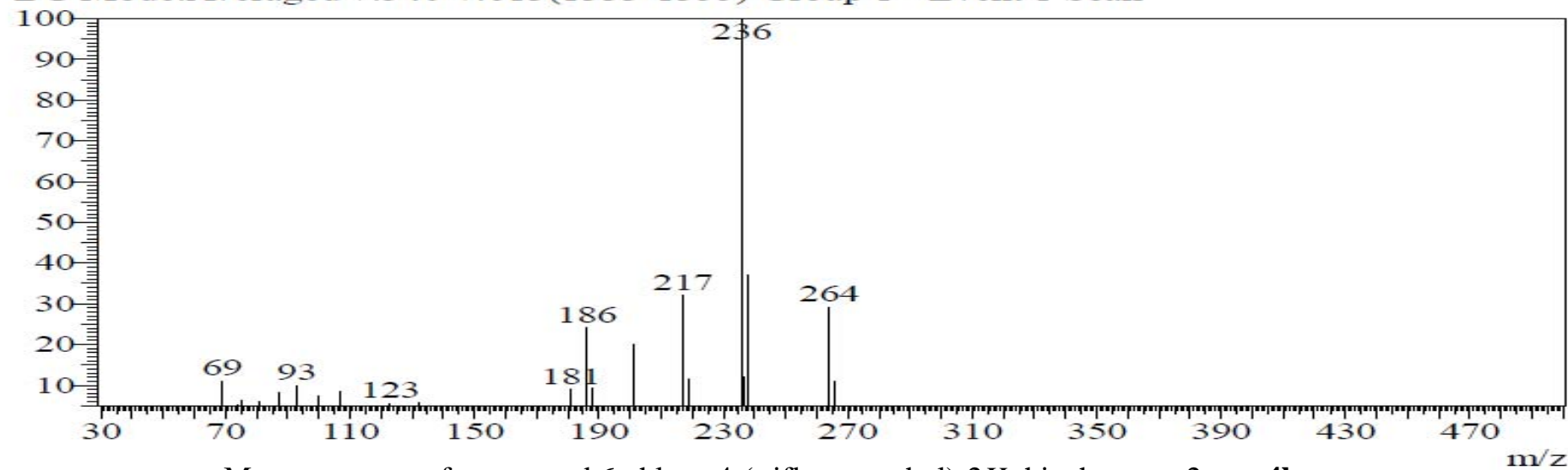


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MassPeaks:416

RawMode:Single 7.360(1279) BasePeak:236(340943)

BG Mode:Averaged 7.540-7.613(1333-1355) Group 1 - Event 1 Scan



Mass-spectrum of compound 6-chloro-4-(trifluoromethyl)-2H-thiochromen-2-one **4b**