

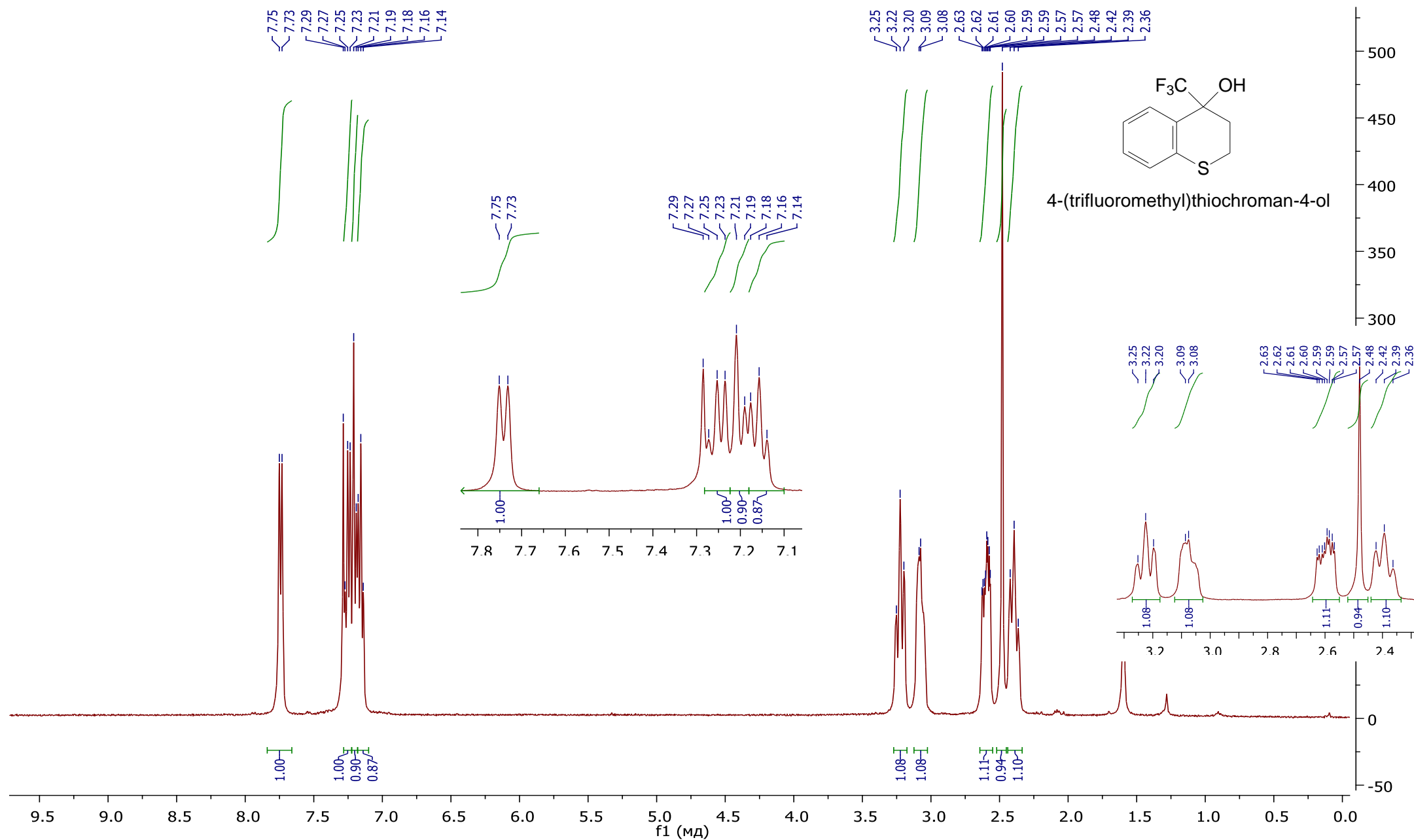
Electronic supplementary information

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

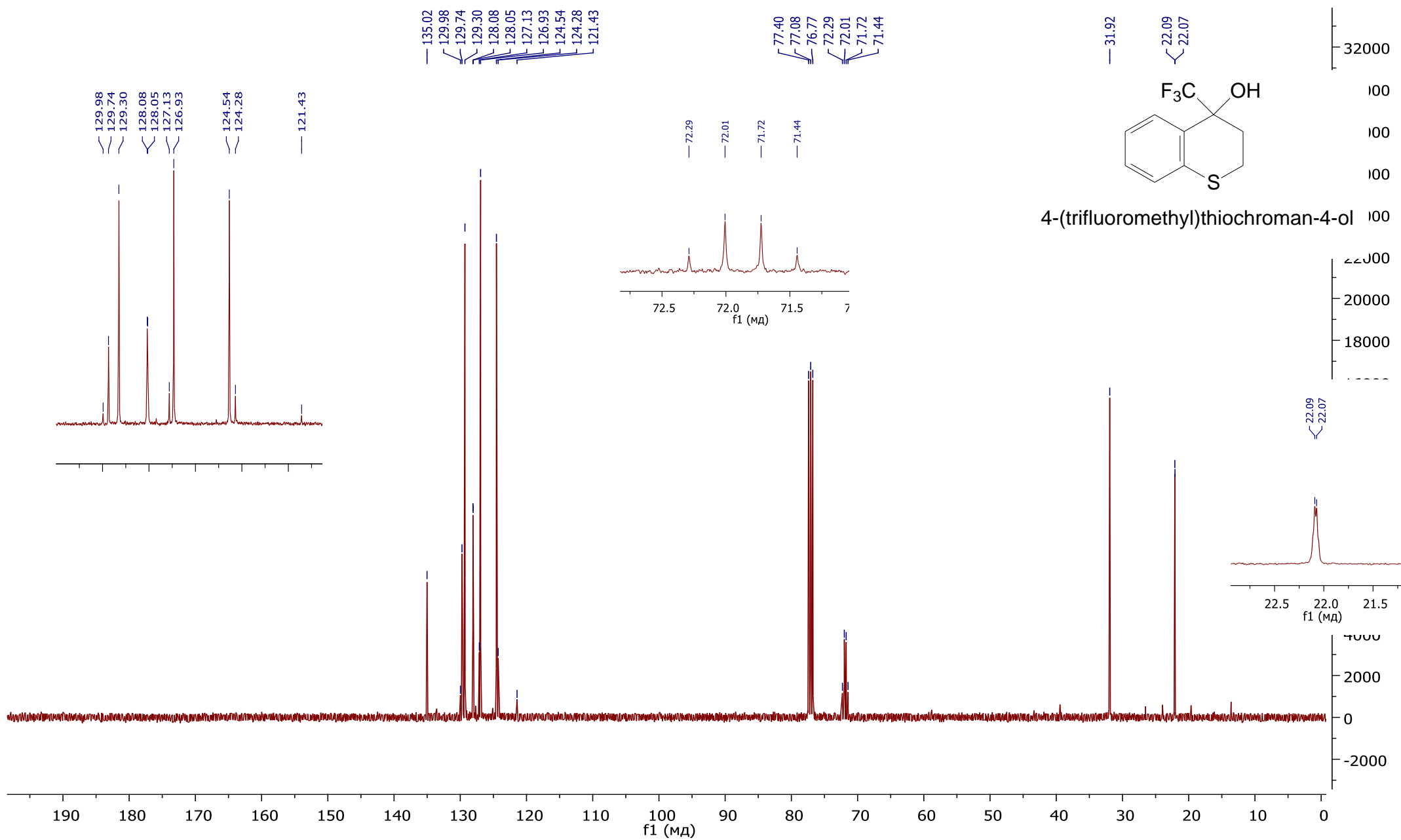
A. S. Golubev,^{*a} P. N. Ostapchuk,^b I. M. Golubev,^a N. D. Kagramanov,^a
R. U. Takazova,^a and N. D. Chkanikov^a

^a Nesmeyanov Institute of Organoelement Compounds, Russian Academy of Sciences,
ul. Vavilova 28, str. 1, Moscow, 119334 Russia

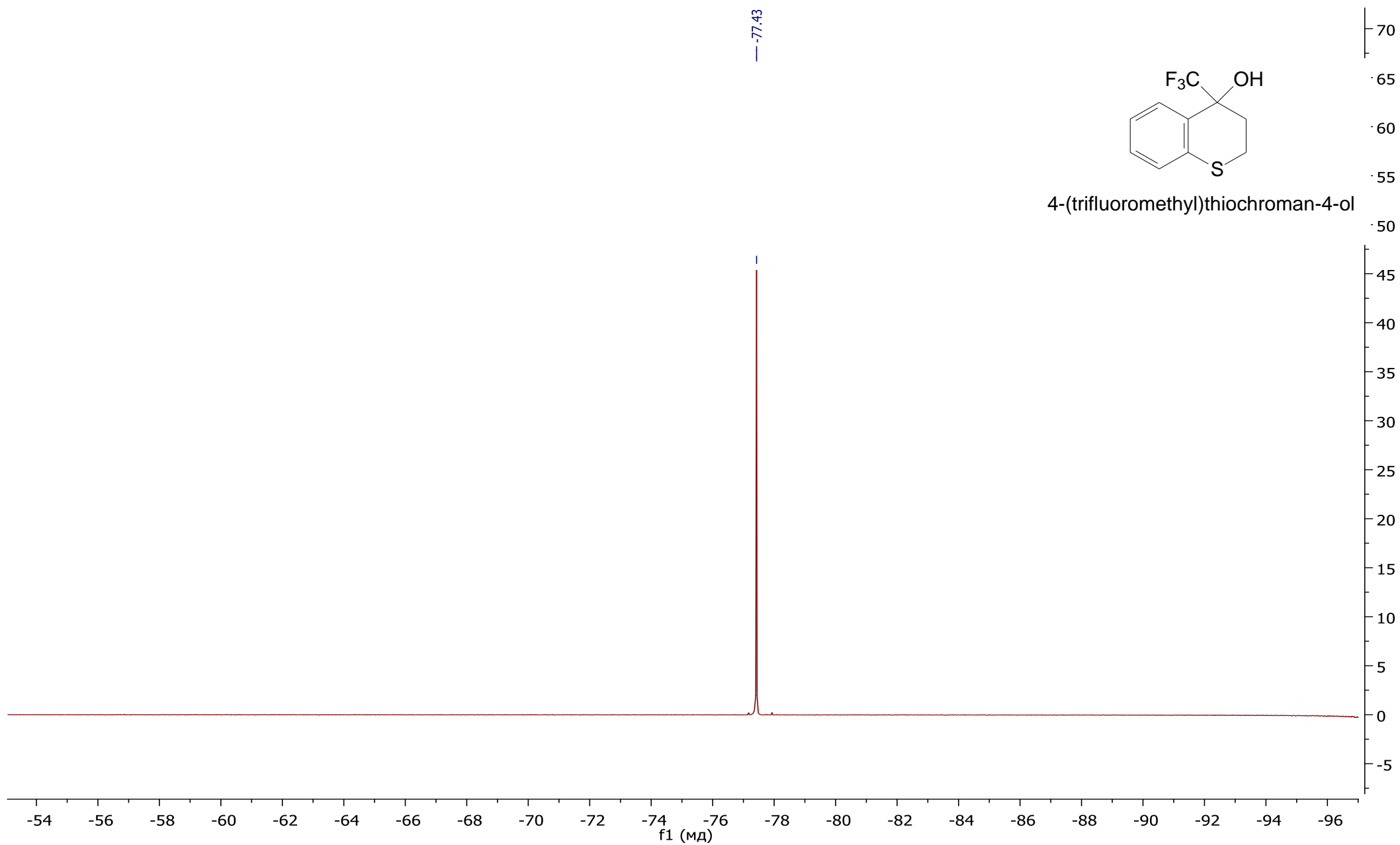
^b Zelinsky Institute of Organic Chemistry, Russian Academy of Sciences,
Leninskii pr. 47, Moscow, 119991 Russia



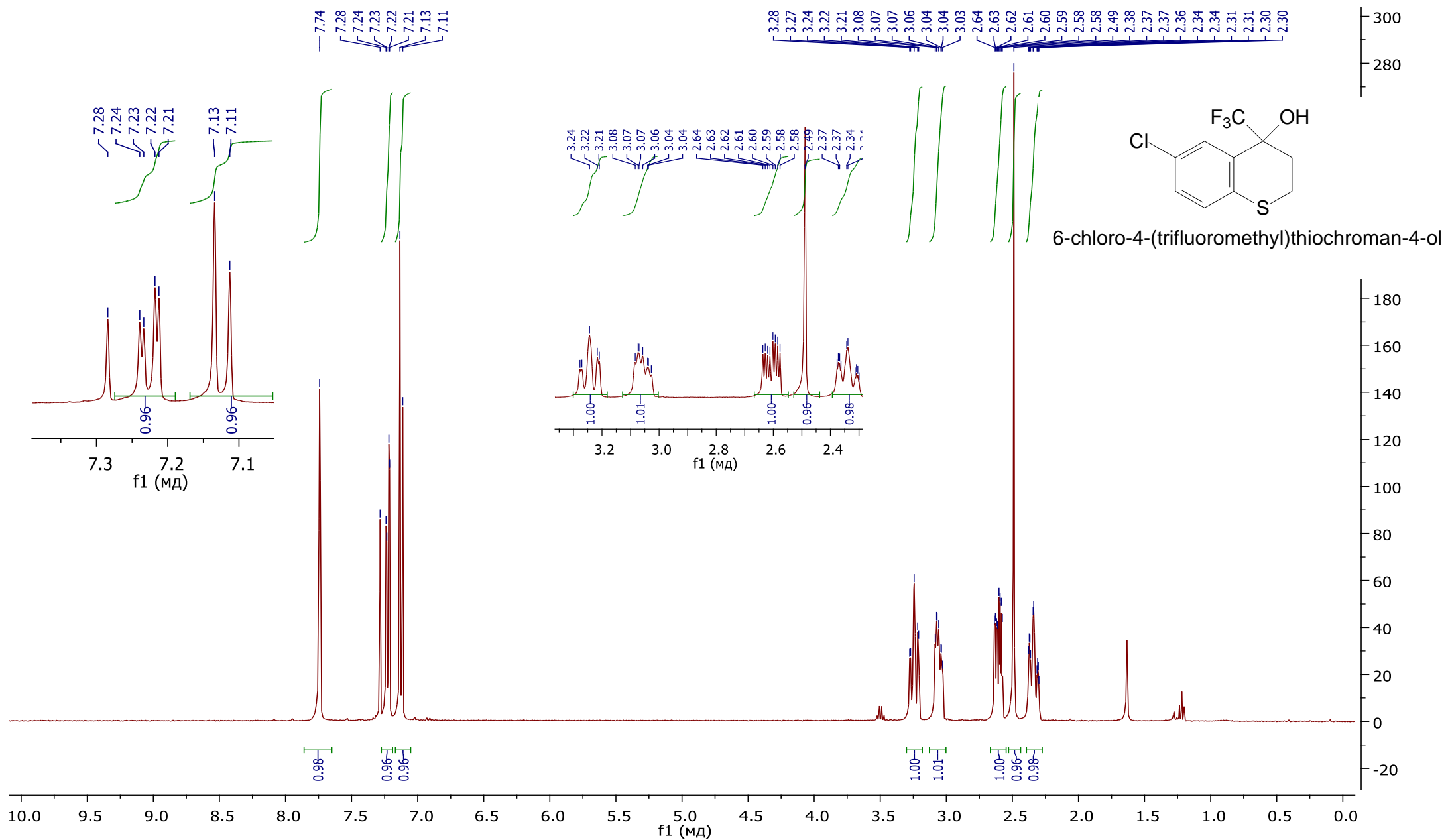
Compound **3a**. Spectrum NMR ^1H in CDCl_3



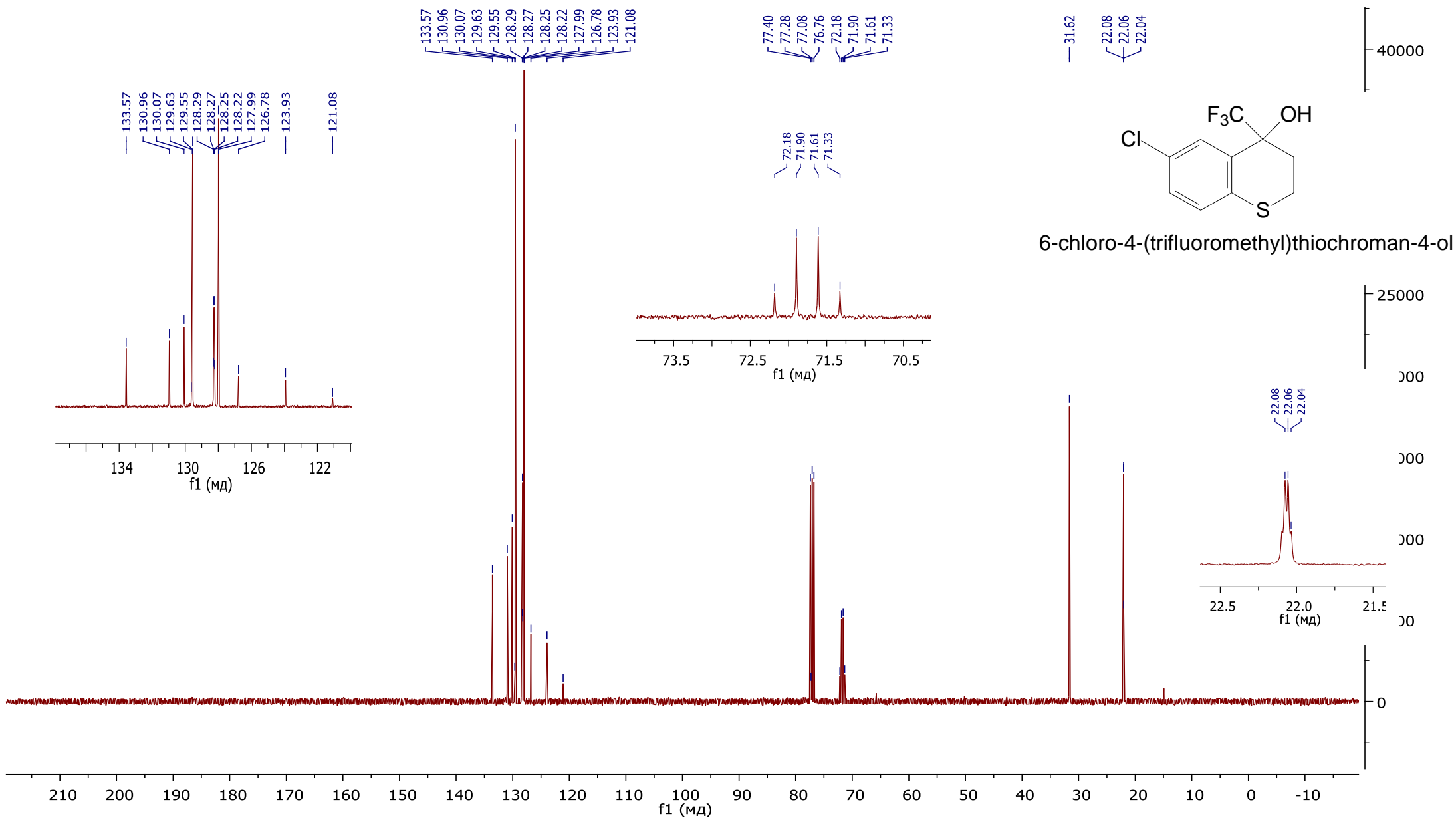
Compound **3a**. Spectrum NMR ¹³C in CDCl₃

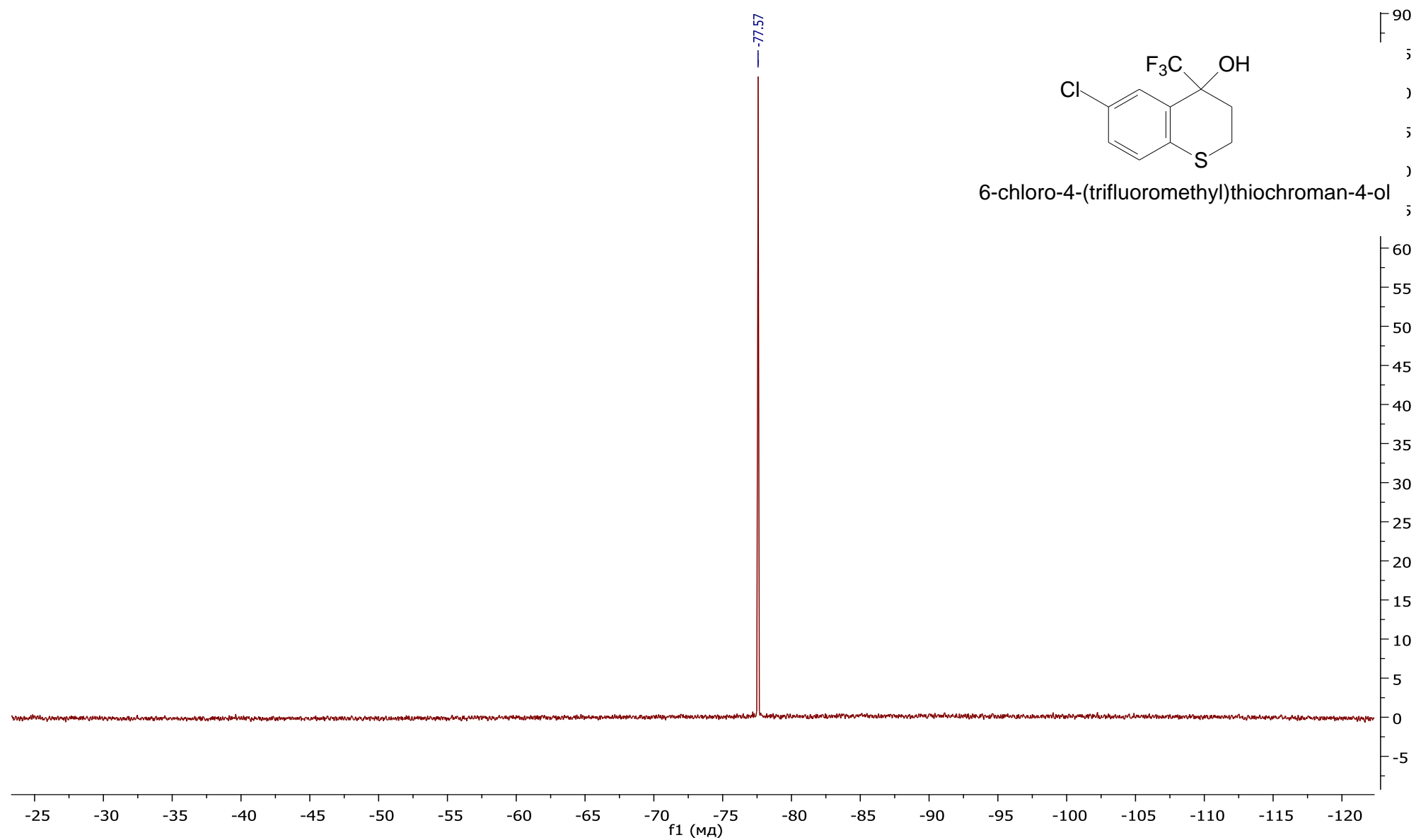


Compound **3a**. Spectrum NMR ^{19}F in CDCl_3 of

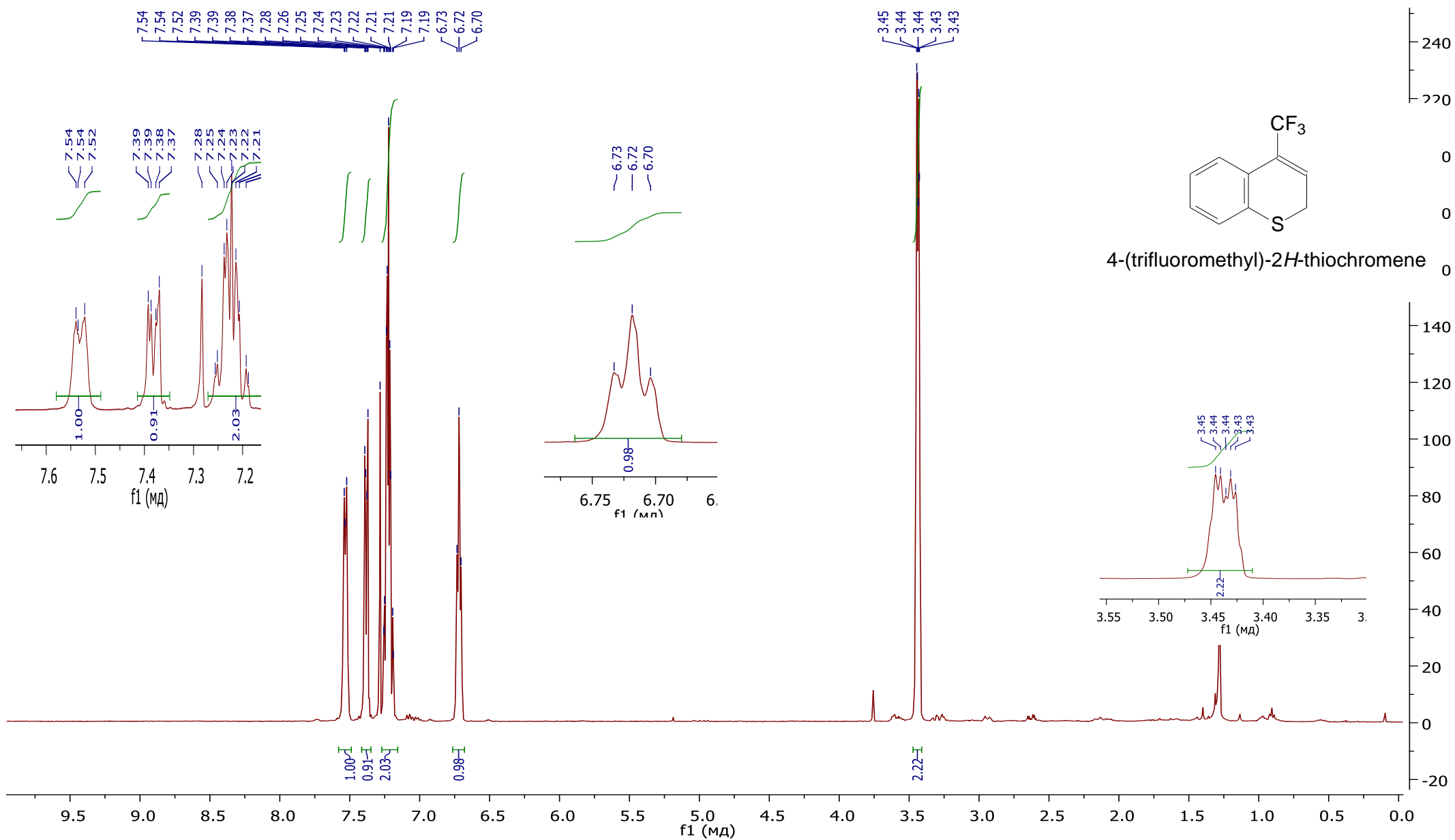


Compound **3b**. Spectrum NMR ¹H in CDCl₃

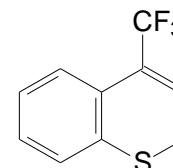
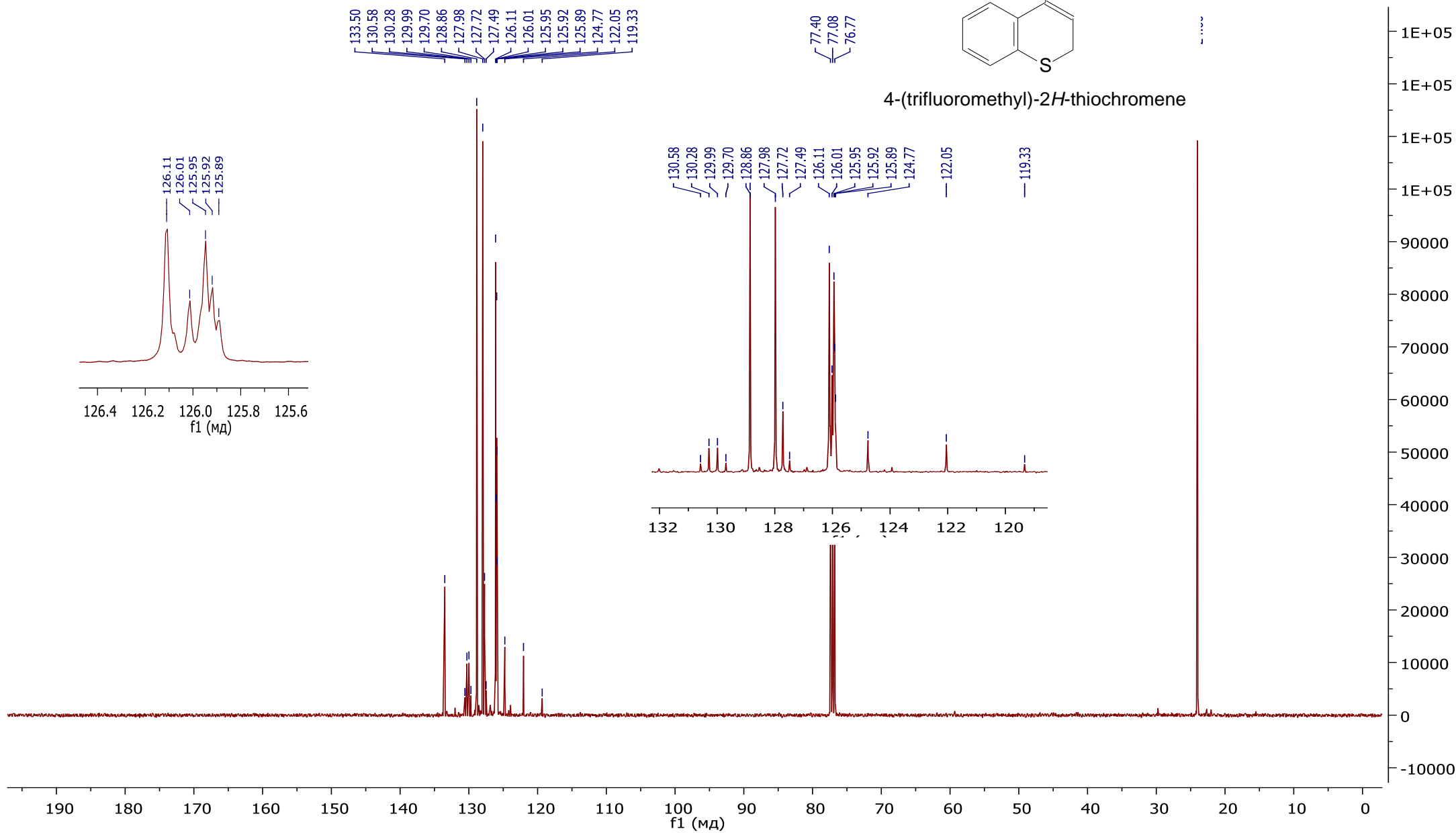


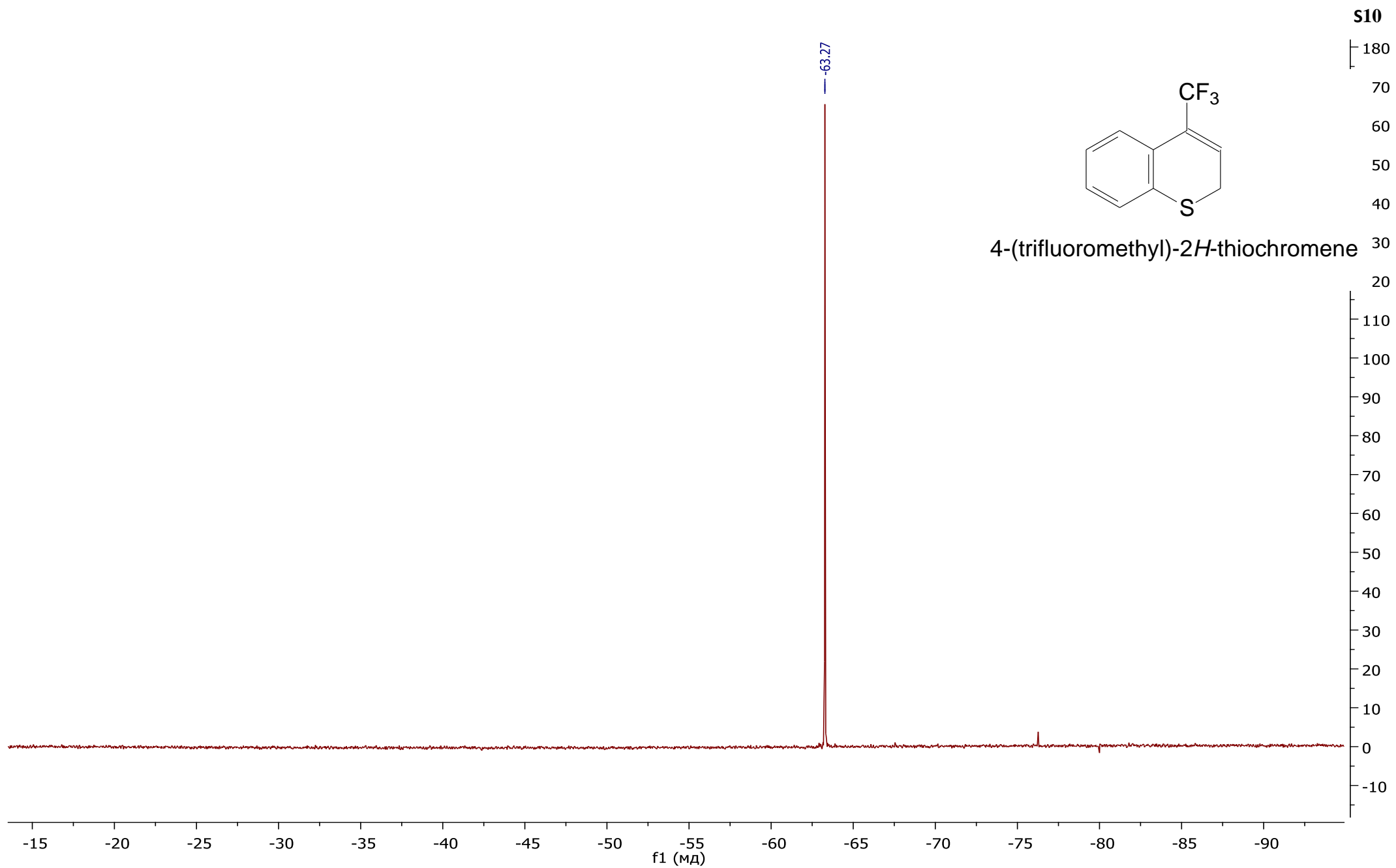


Compound **3b**. Spectrum $\text{NMR } ^{19}\text{F}$ in CDCl_3

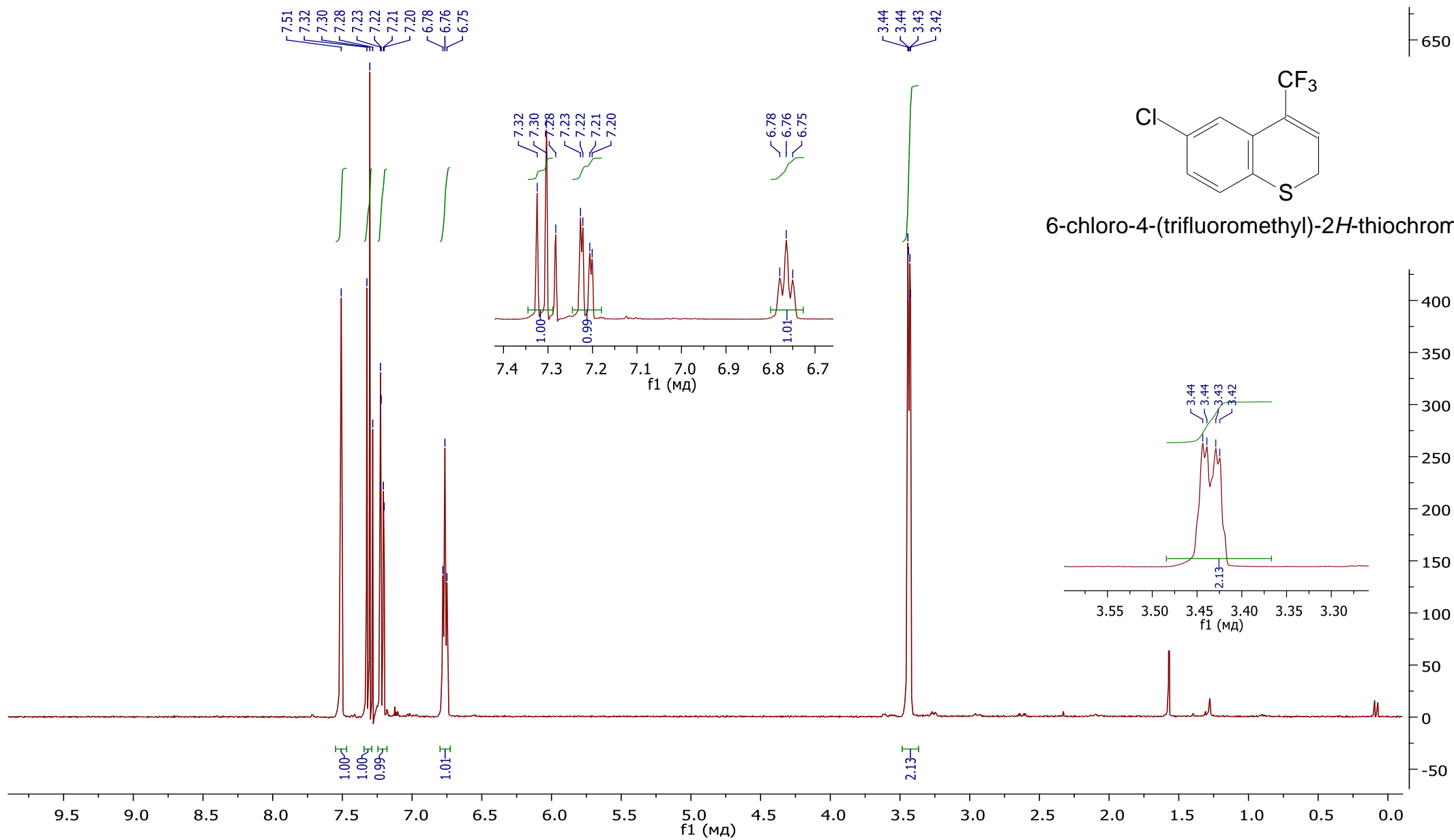


Compound **1a**. Spectrum NMR ¹H in CDCl₃

4-(trifluoromethyl)-2*H*-thiochromeneCompound *1a*. Spectrum NMR ^{13}C in CDCl_3

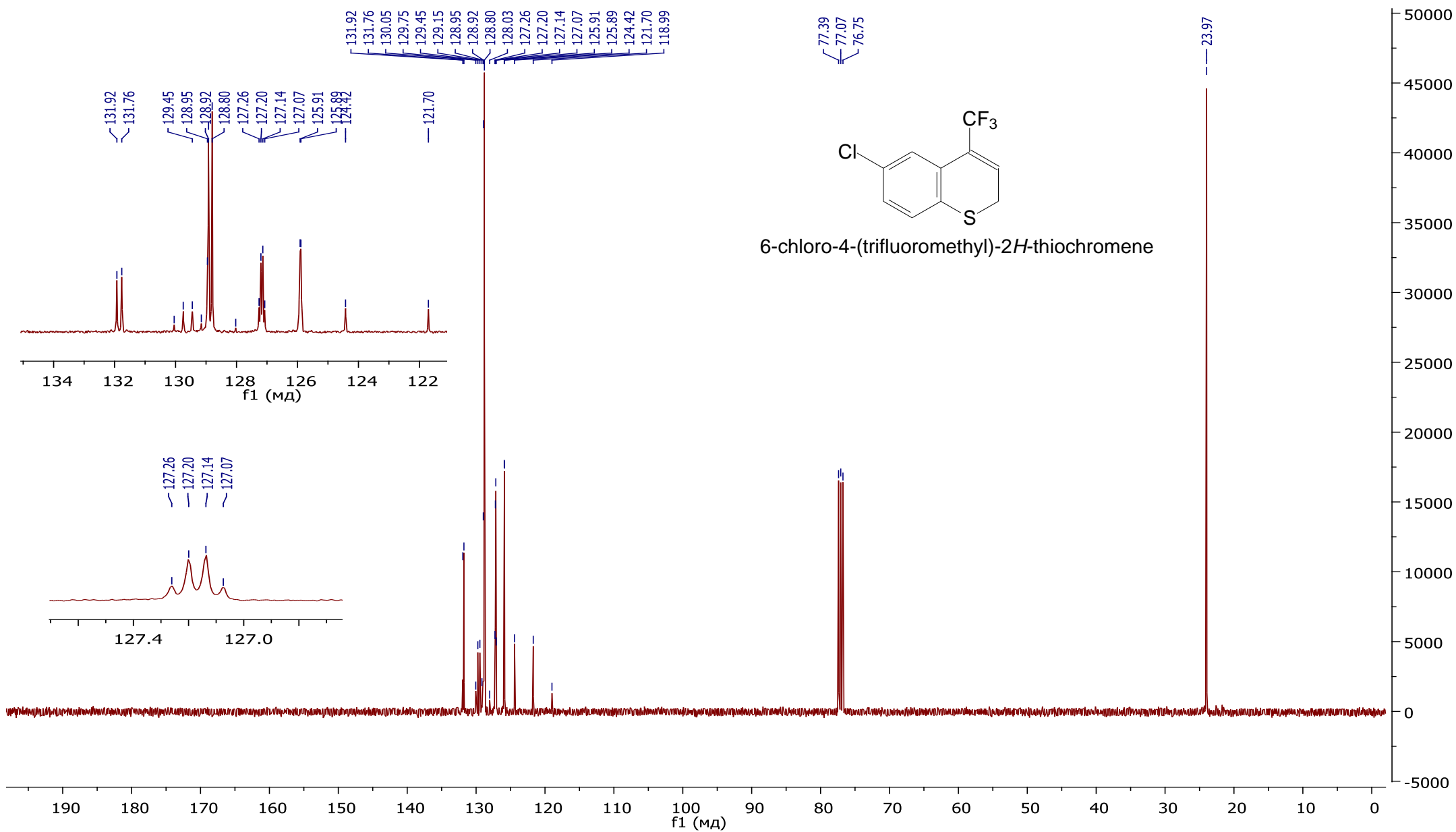


Compound **1a**. Spectrum NMR ^{19}F in CDCl_3

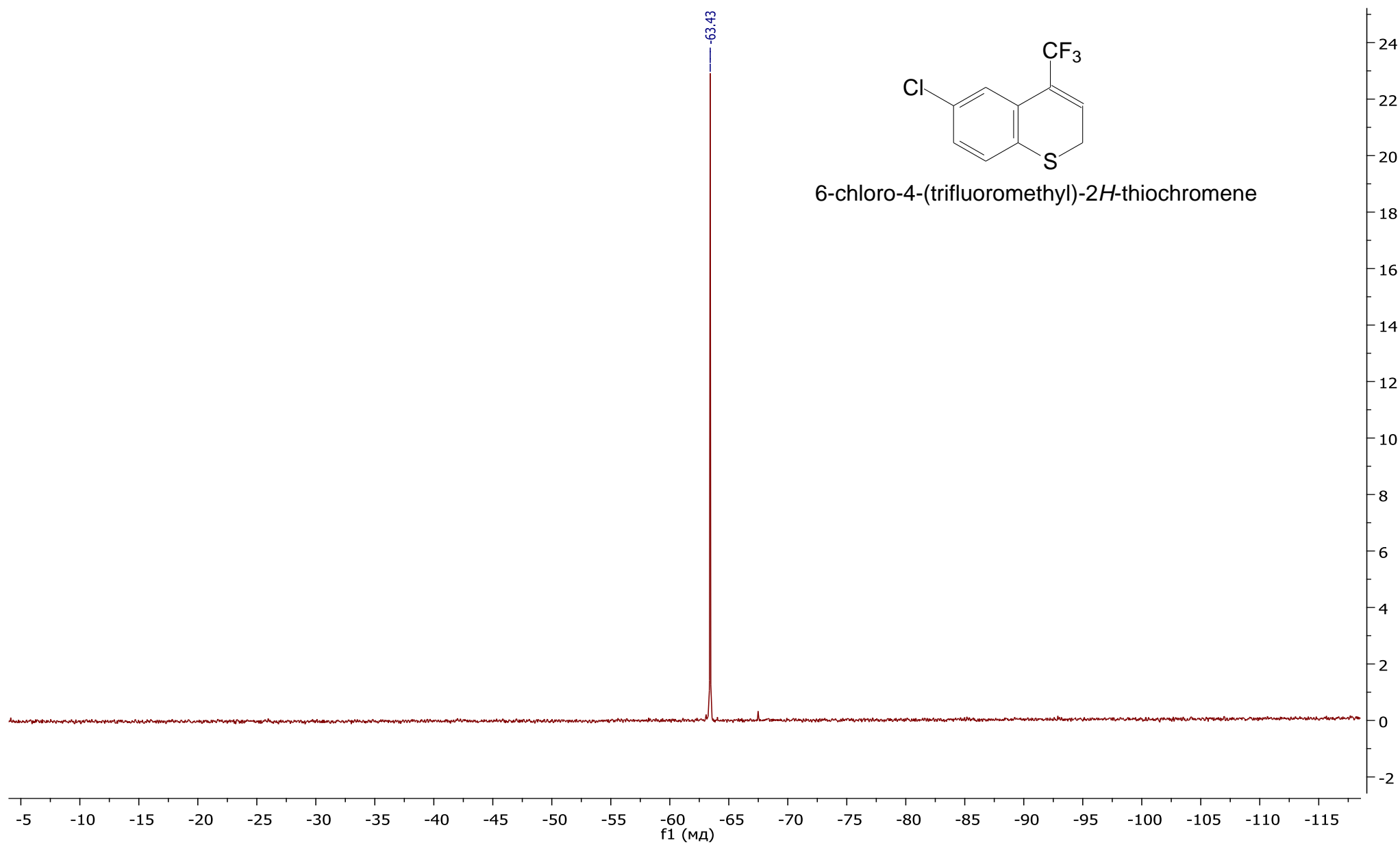


6-chloro-4-(trifluoromethyl)-2H-thiochromene

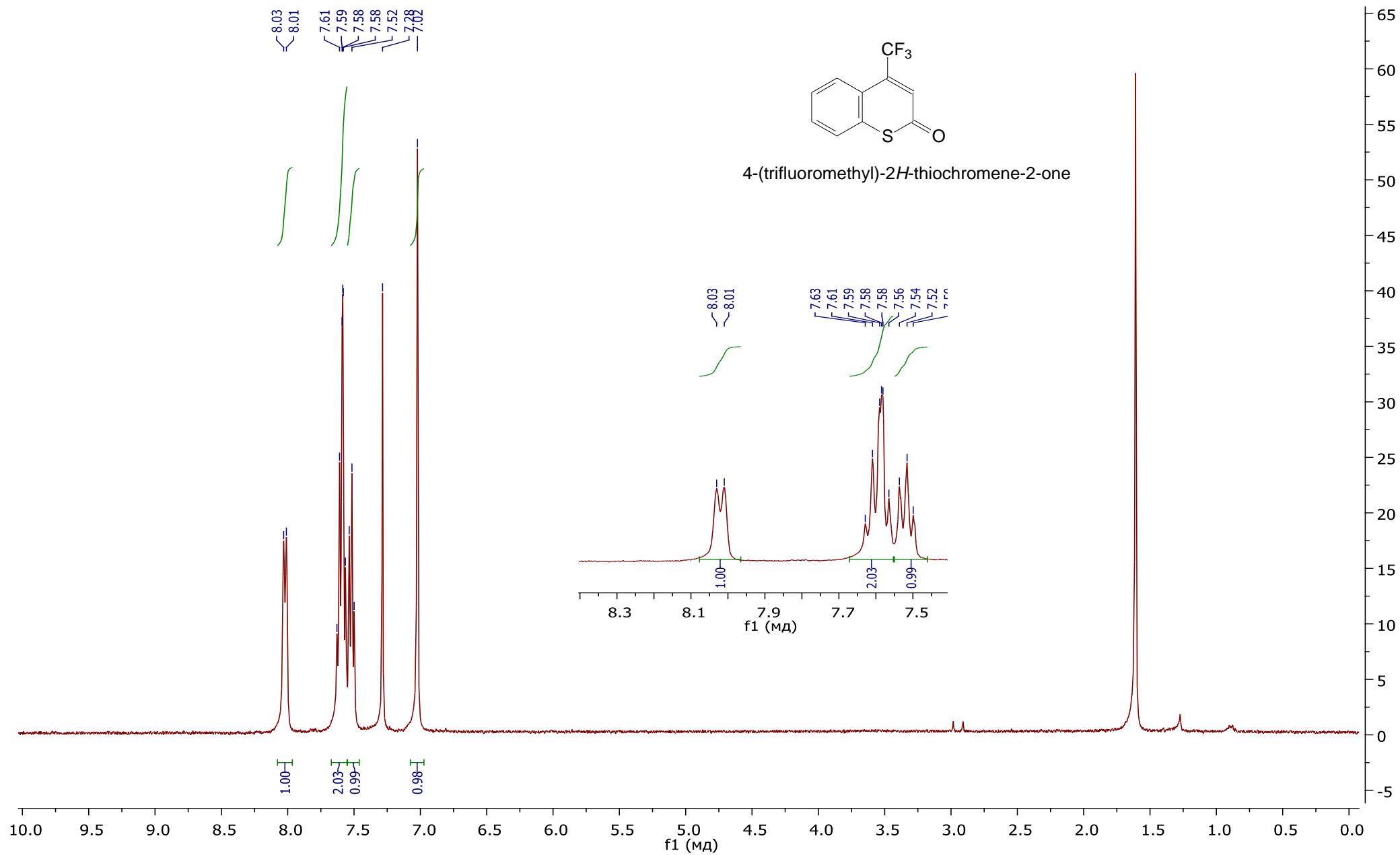
Compound **1b**. Spectrum NMR ^1H in CDCl_3



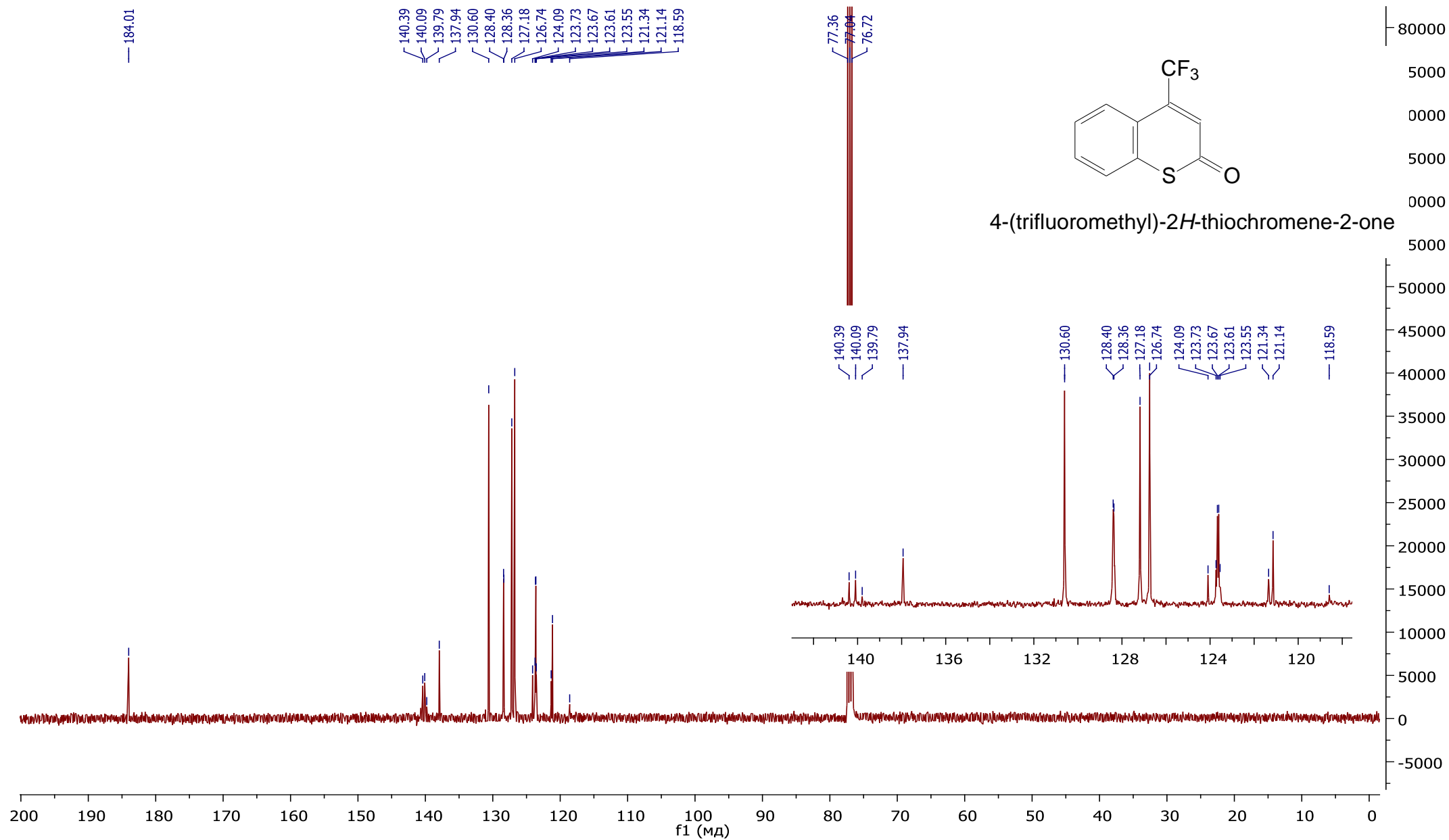
Compound **1b**. Spectrum NMR ^{13}C in CDCl_3



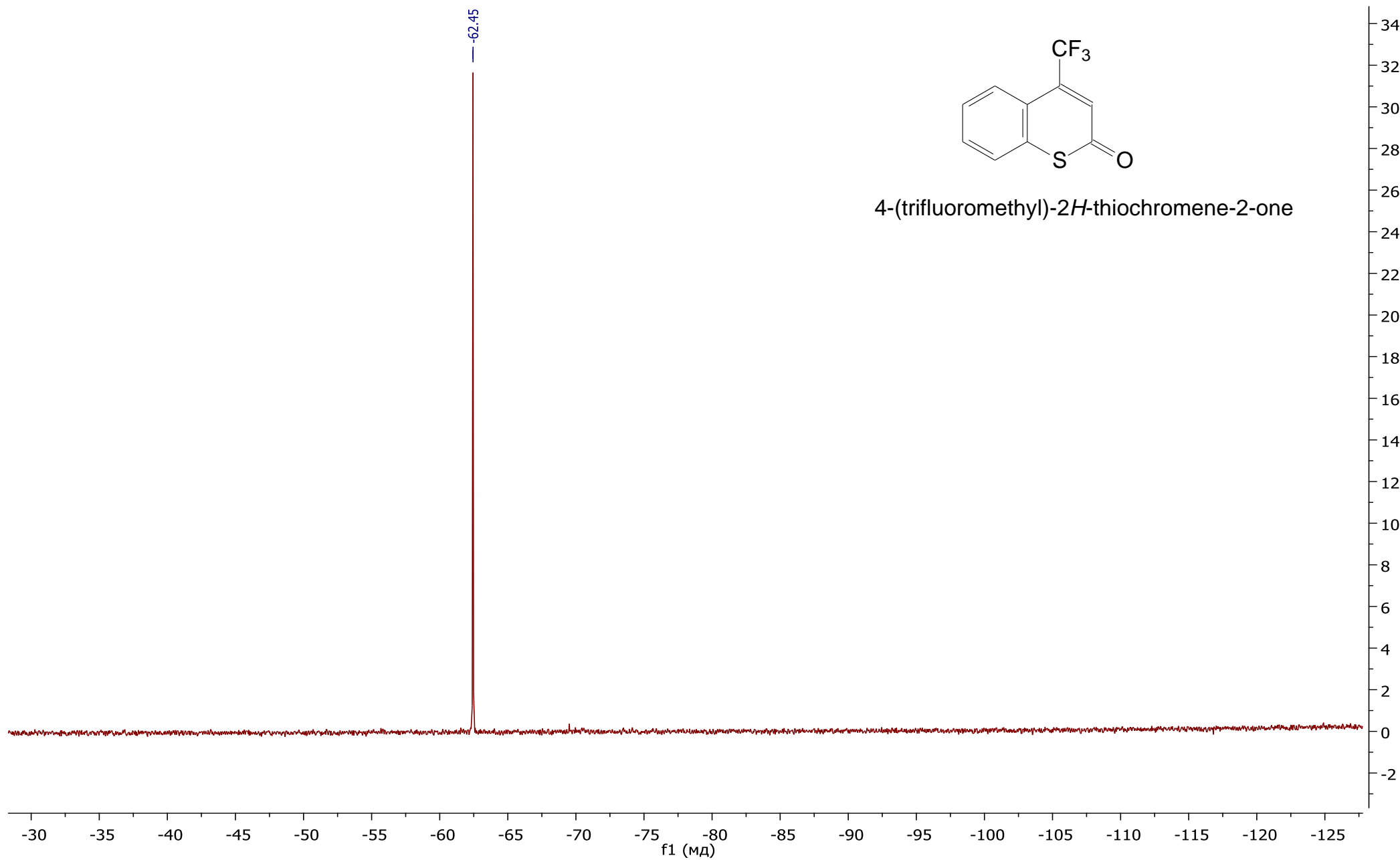
Compound **1b**. Spectrum NMR ^{19}F in CDCl_3



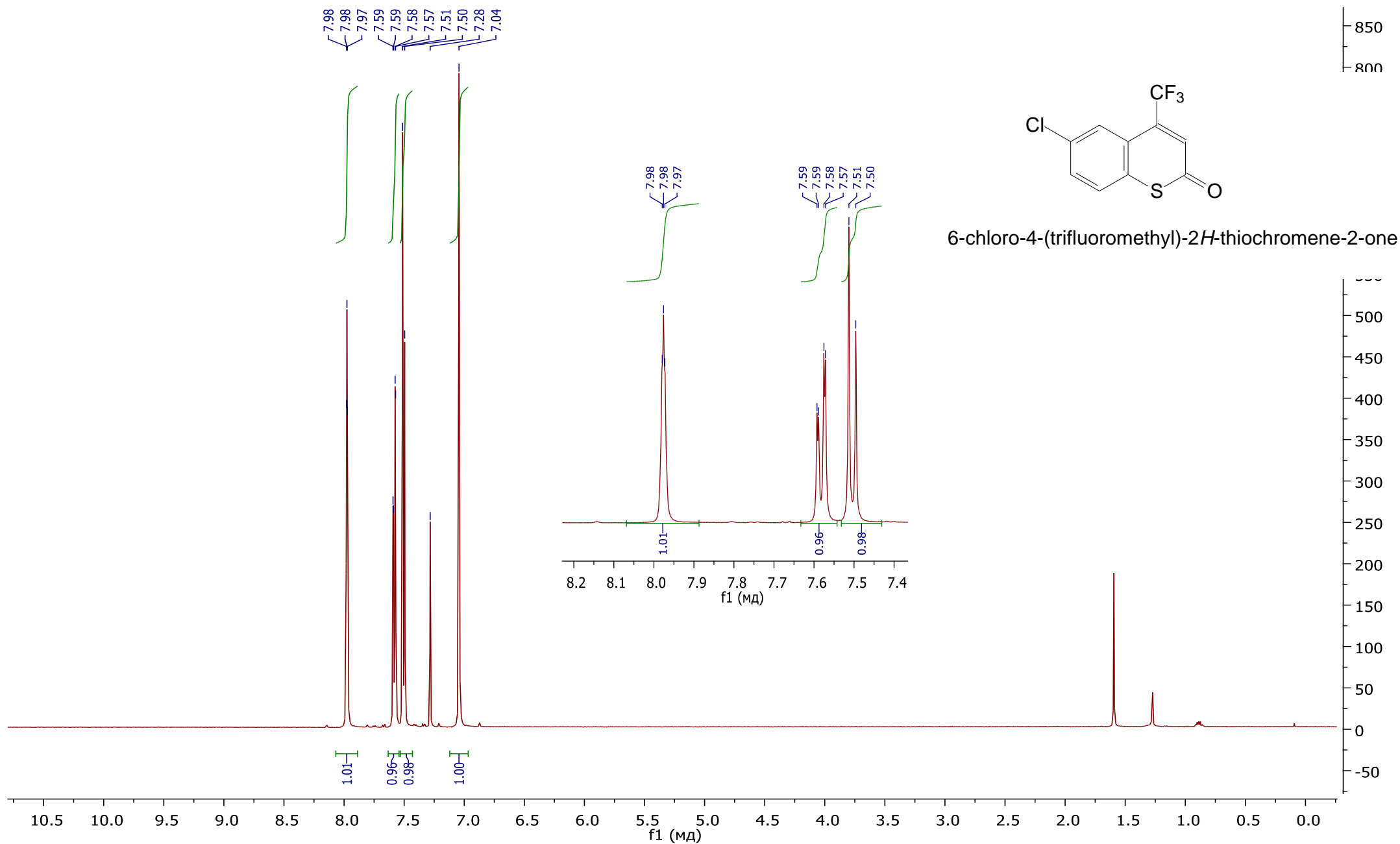
Compound 4a. Spectrum NMR ¹H in CDCl₃



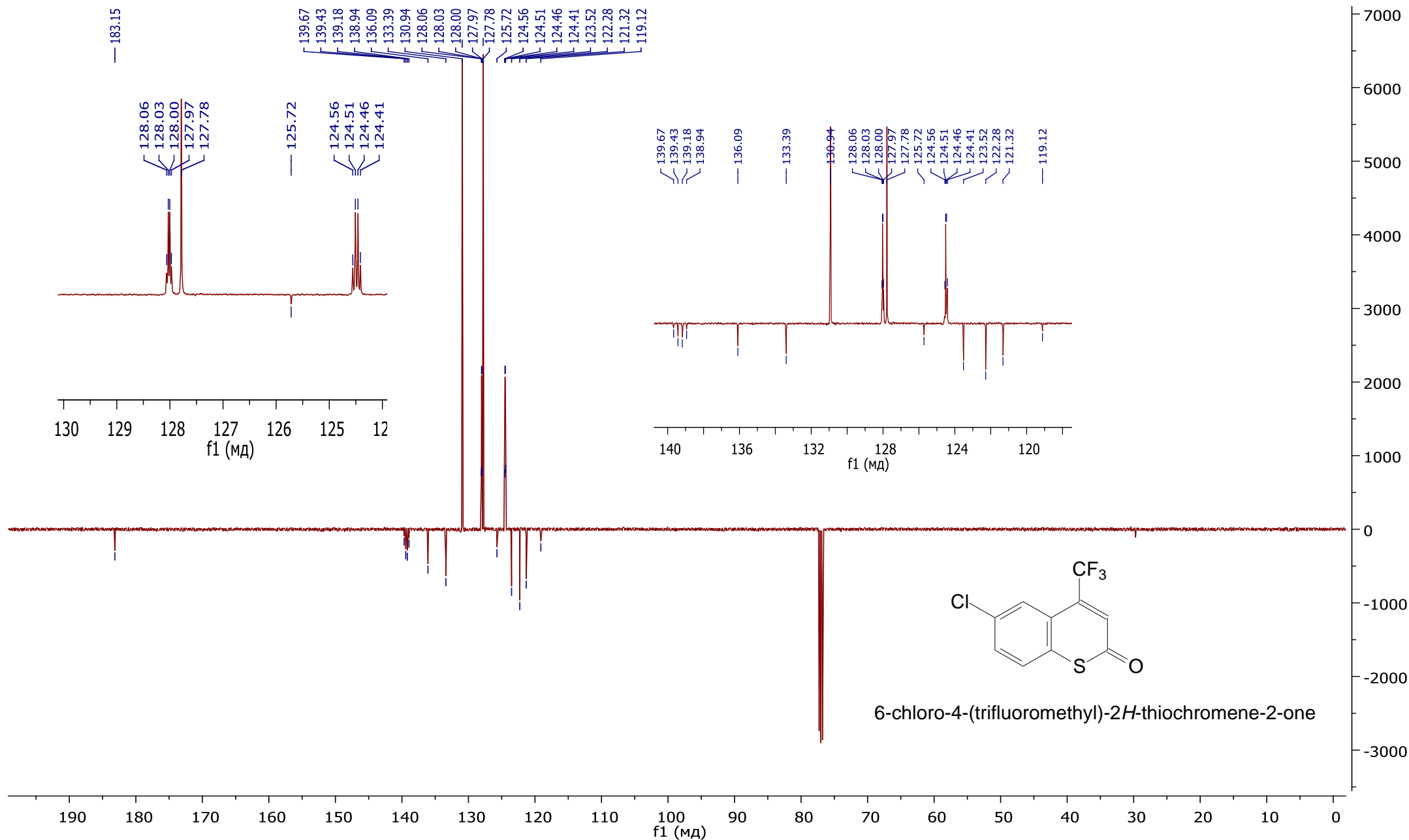
Compound **4a**. Spectrum NMR ^{13}C in CDCl_3



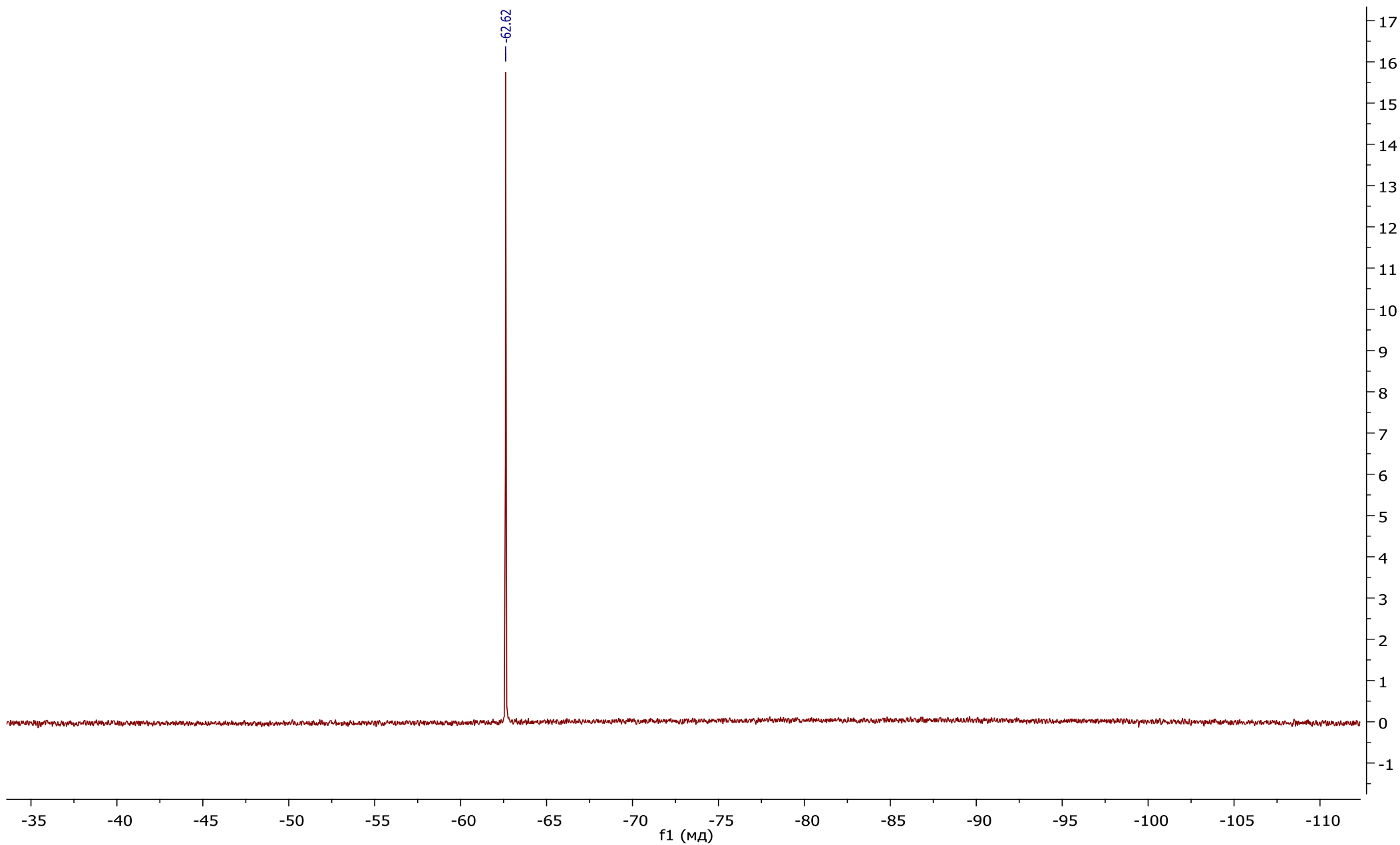
Compound **4a**. Spectrum NMR ^{19}F in CDCl_3



Compound **4b**. Spectrum NMR ¹H in CDCl₃

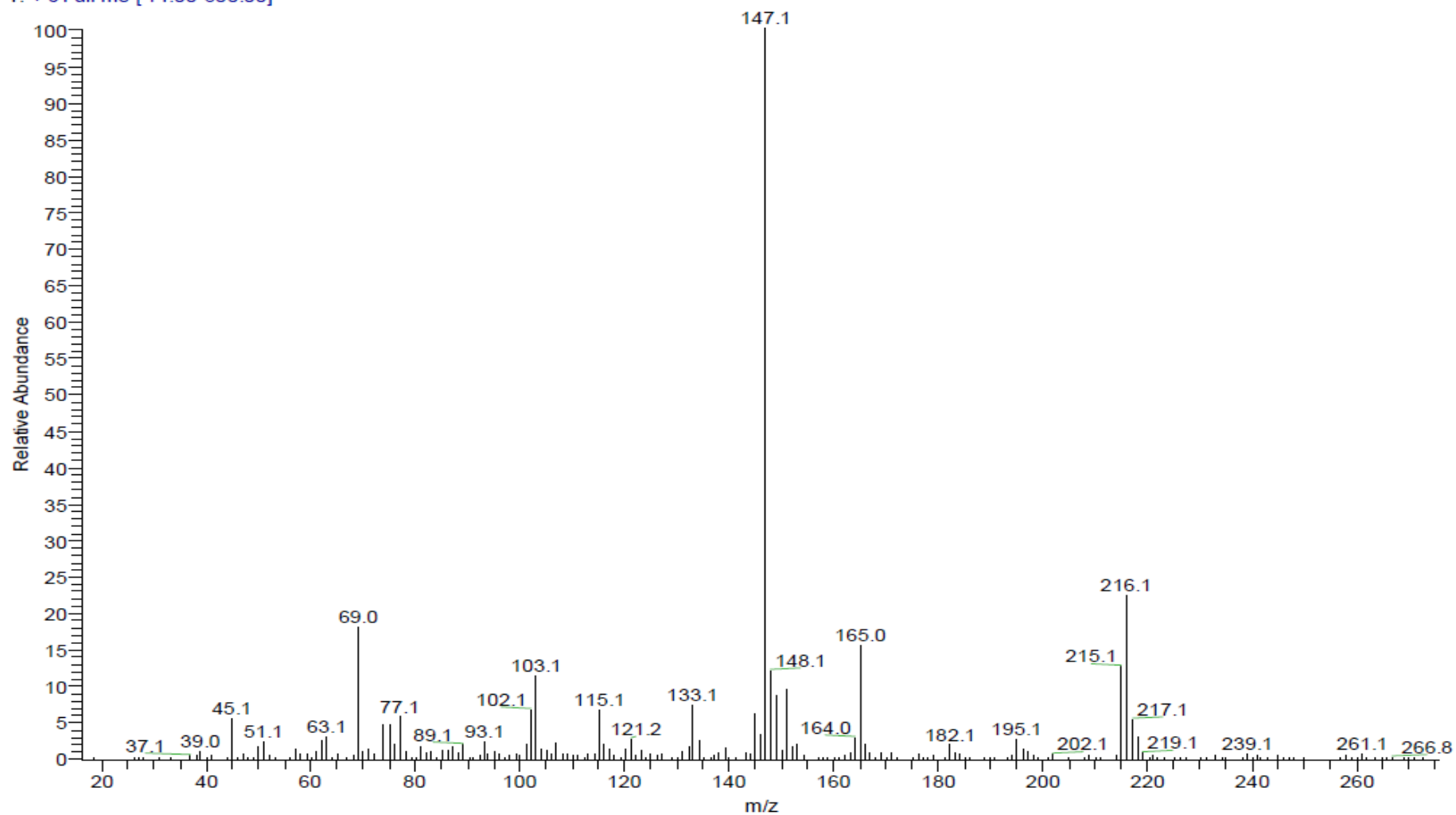


Compound **4b**. Spectrum NMR ¹³C DEPT in CDCl₃



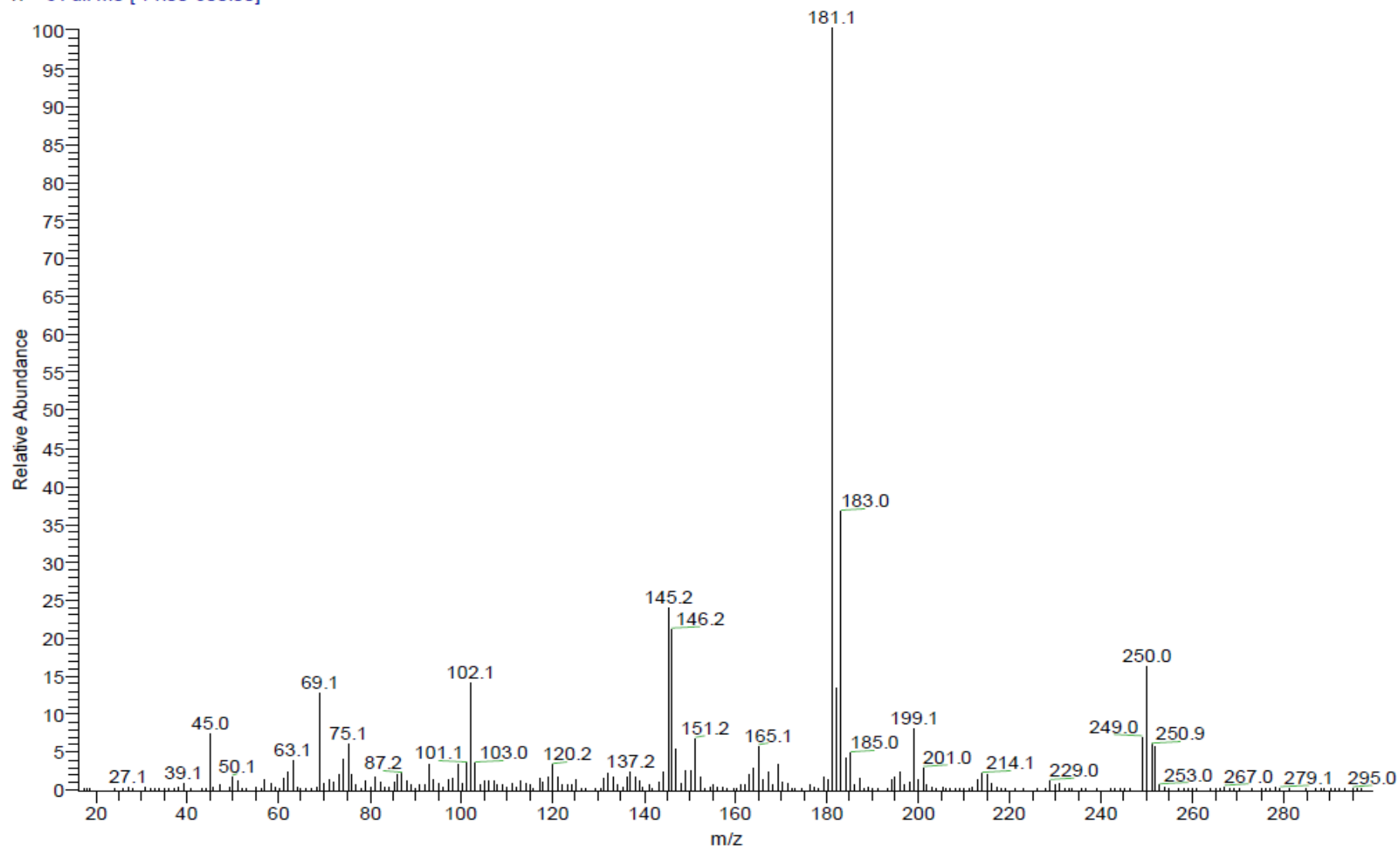
Compound **4b**. Spectrum NMR ^{19}F in CDCl_3

GoI_1707 #1031 RT: 13.34 AV: 1 NL: 4.31E6
T: + c Full ms [14.00-600.00]



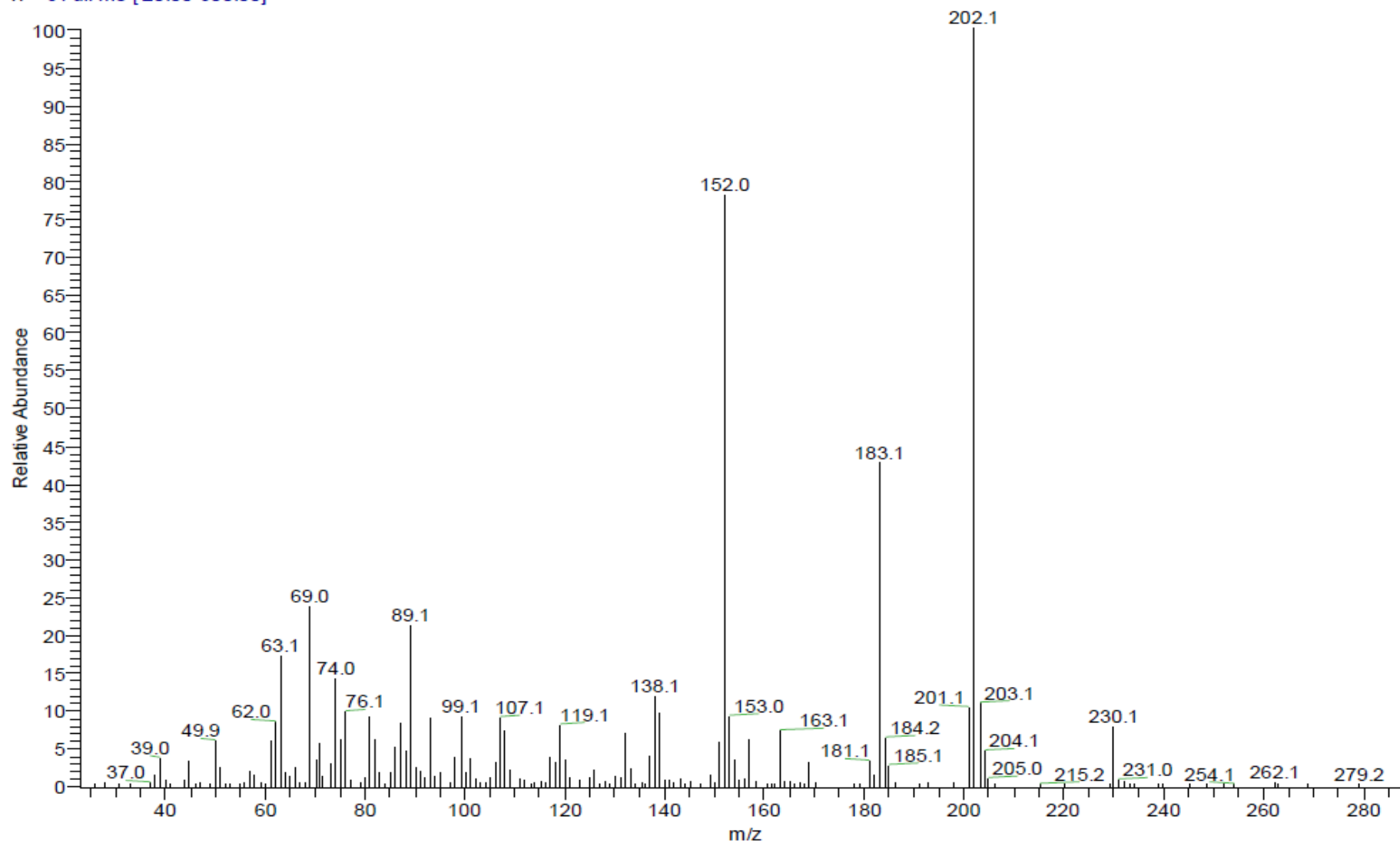
Mass spectrum of 4-(trifluoromethyl)-2H-thiochromene **1a**

GoI_1725 #1161 RT: 14.71 AV: 1 NL: 1.20E6
T: + c Full ms [14.00-600.00]



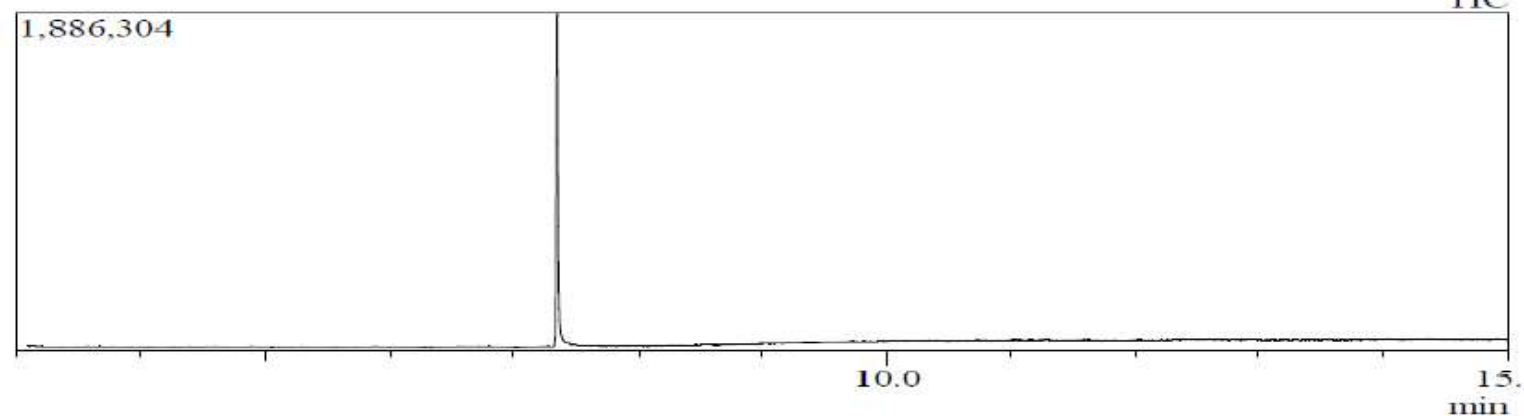
Mass spectrum of 6-chloro-4-(trifluoromethyl)-2H-thiochromene **1b**

Go1716 #1112 RT: 14.11 AV: 1 NL: 3.35E5
T: + c Full ms [20.00-600.00]

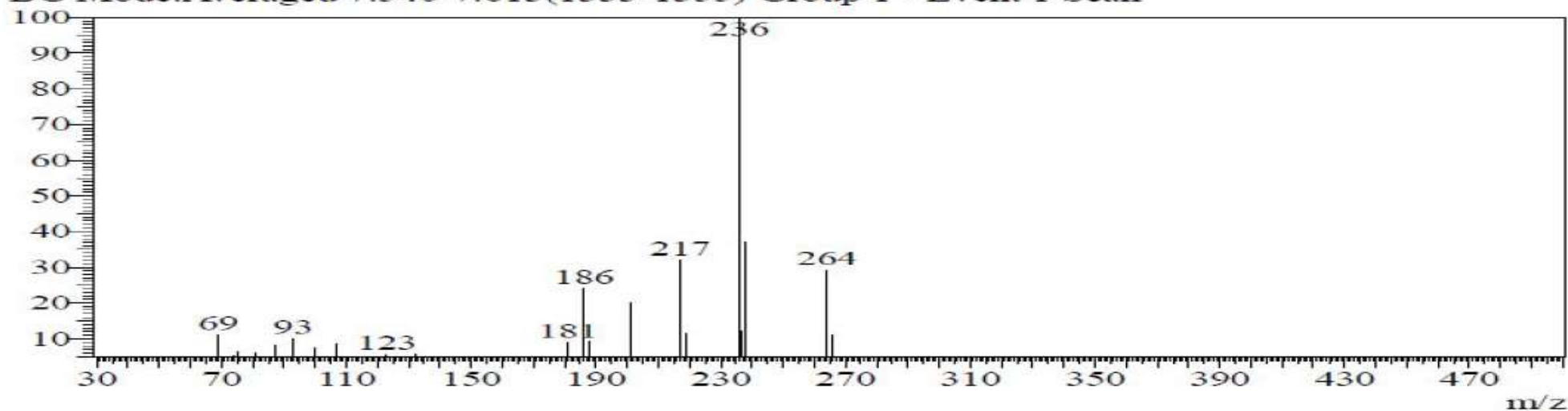


Mass spectrum of 4-(trifluoromethyl)-2H-thiochromene-2-one **4a**

Chromatogram 1799 Z:\Data\2024\04 April\lab 209\Khakina\1799_Split_50_30_290_20min_3.qg
TIC



Line#:1 R.Time:7.360(Scan#:1279)
MassPeaks:416
RawMode:Single 7.360(1279) BasePeak:236(340943)
BG Mode:Averaged 7.540-7.613(1333-1355) Group 1 - Event 1 Scan



Chromato-mass spectrum of 4-(trifluoromethyl)-2H-thiochromene-2-one **4b**