

# 1,3-Dichloroadamantyl-Containing Ureas as Potential Triple Inhibitors of Soluble Epoxide Hydrolase, p38 MAPK and c-Raf

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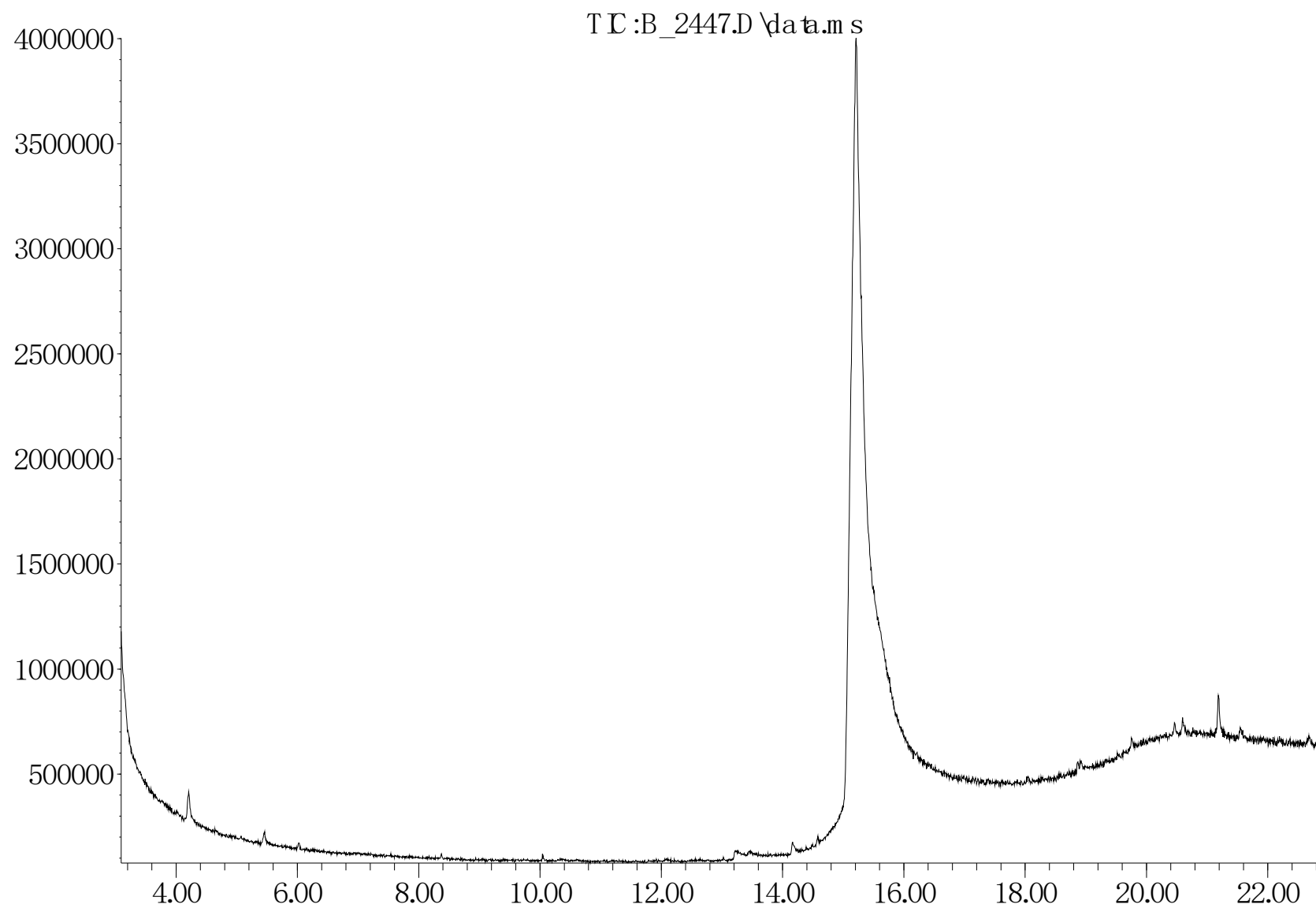
\* Correspondence: v.s.dyachenko@vstu.ru

## **Supplementary materials**

**$^1\text{H}$  NMR,  $^{13}\text{C}$  NMR and Mass spectra**

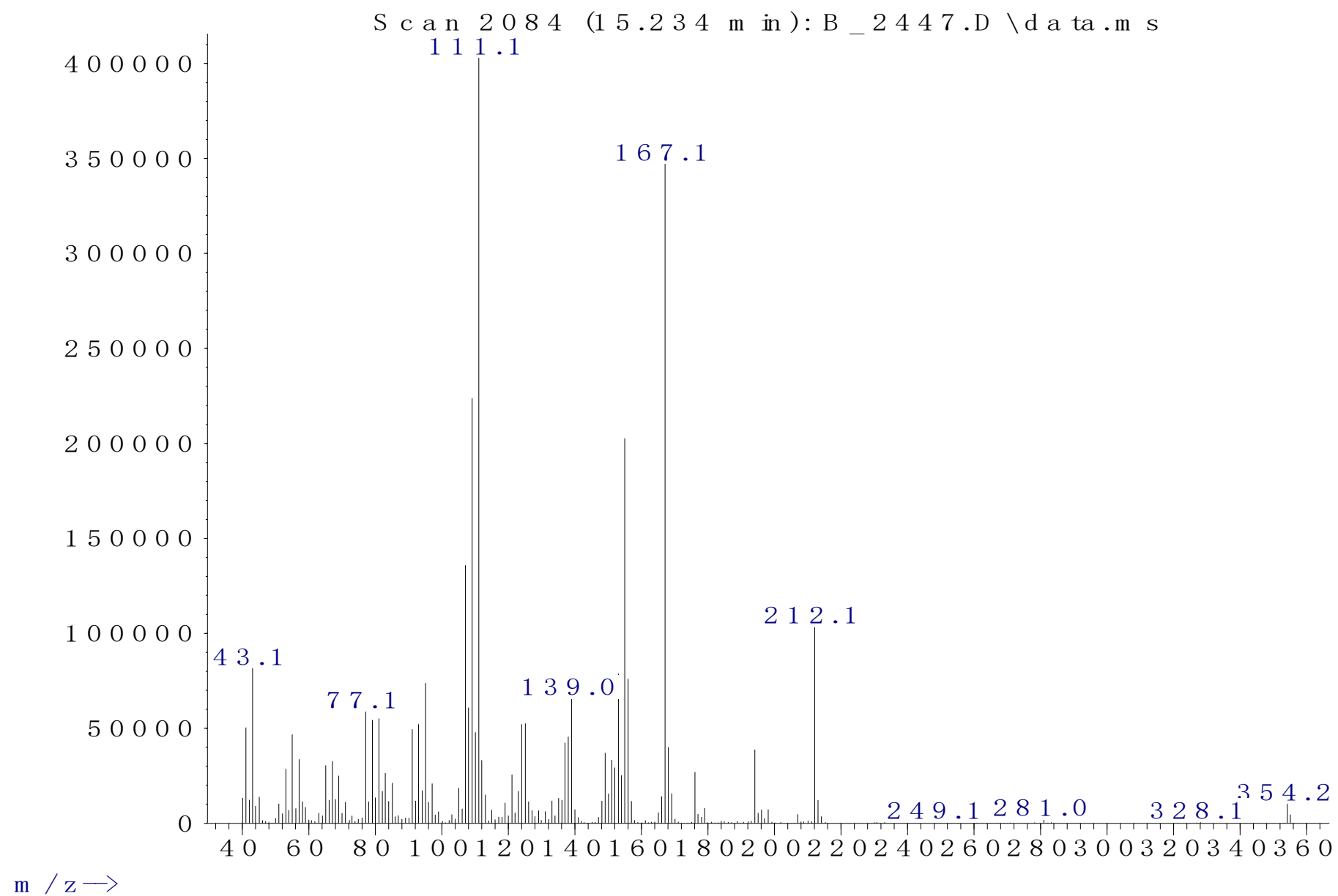
**Figure S1.** Chromatogram of compound 2

Abundance



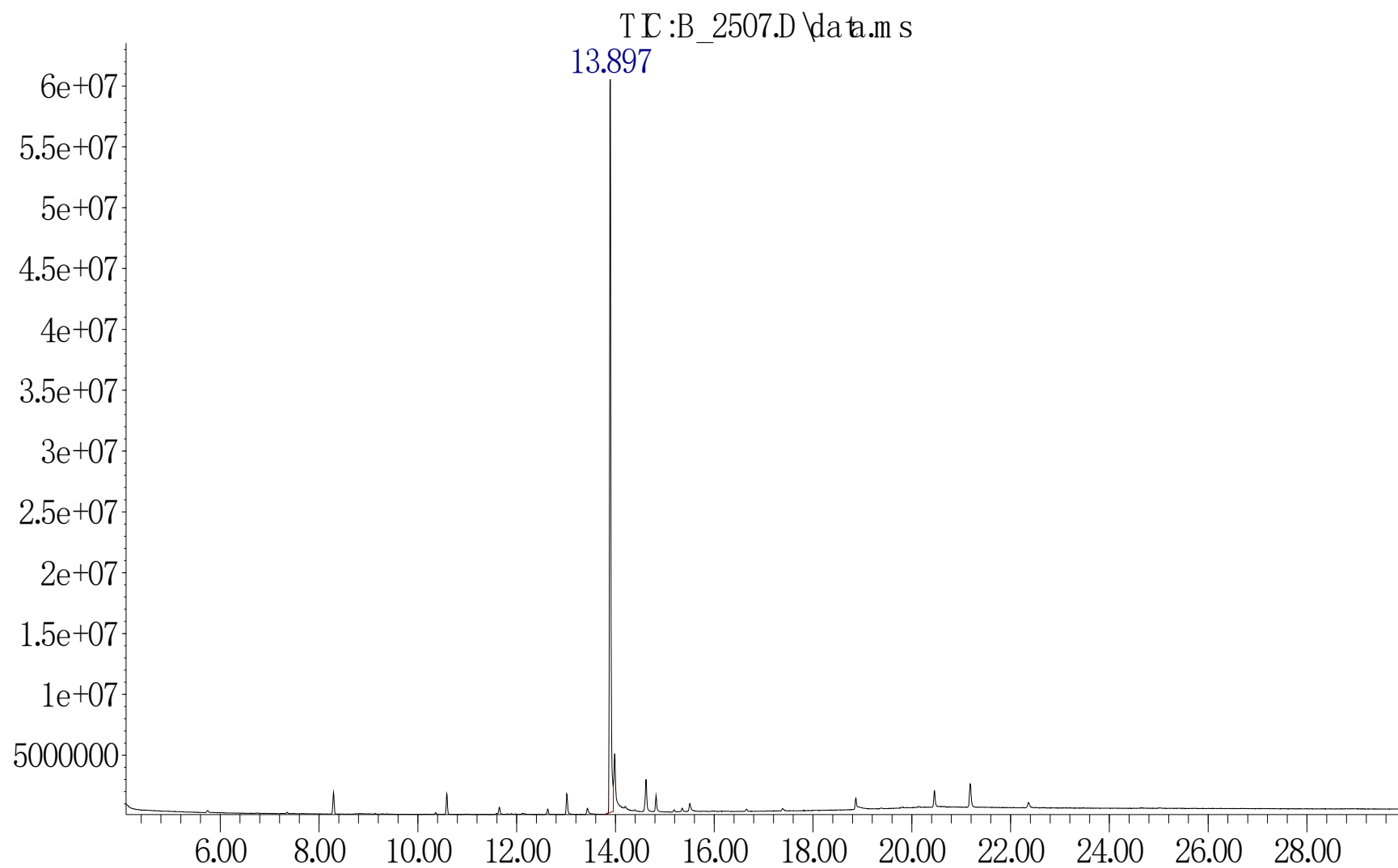
**Figure S2.** Mass spectrum of compound 2

A b u n d a n c e



**Figure S3.** Chromatogram of compound 3

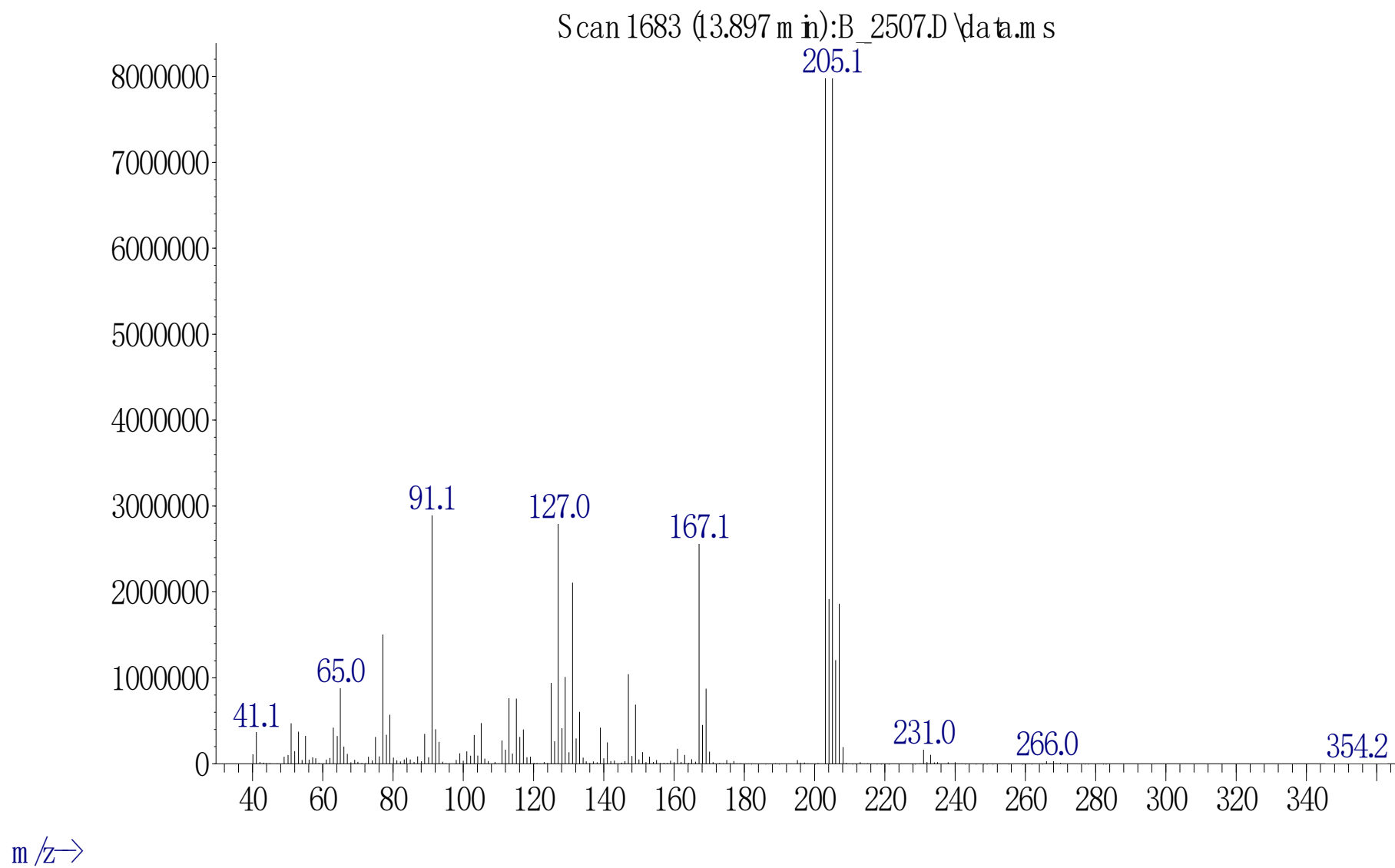
Abundance



Time→

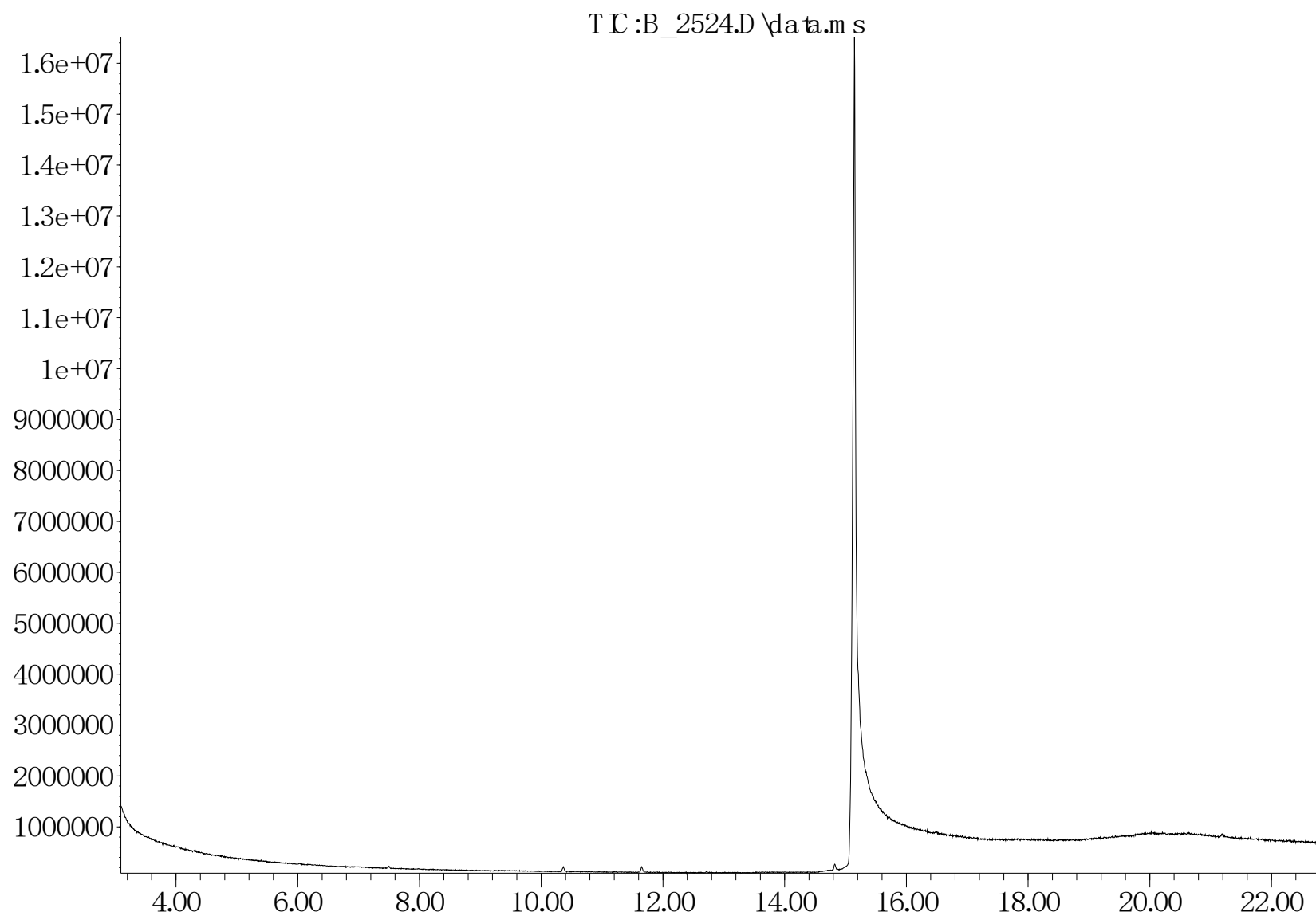
**Figure S4.** Mass spectrum of compound 3

Abundance



**Figure S5.** Chromatogram of compound **4**

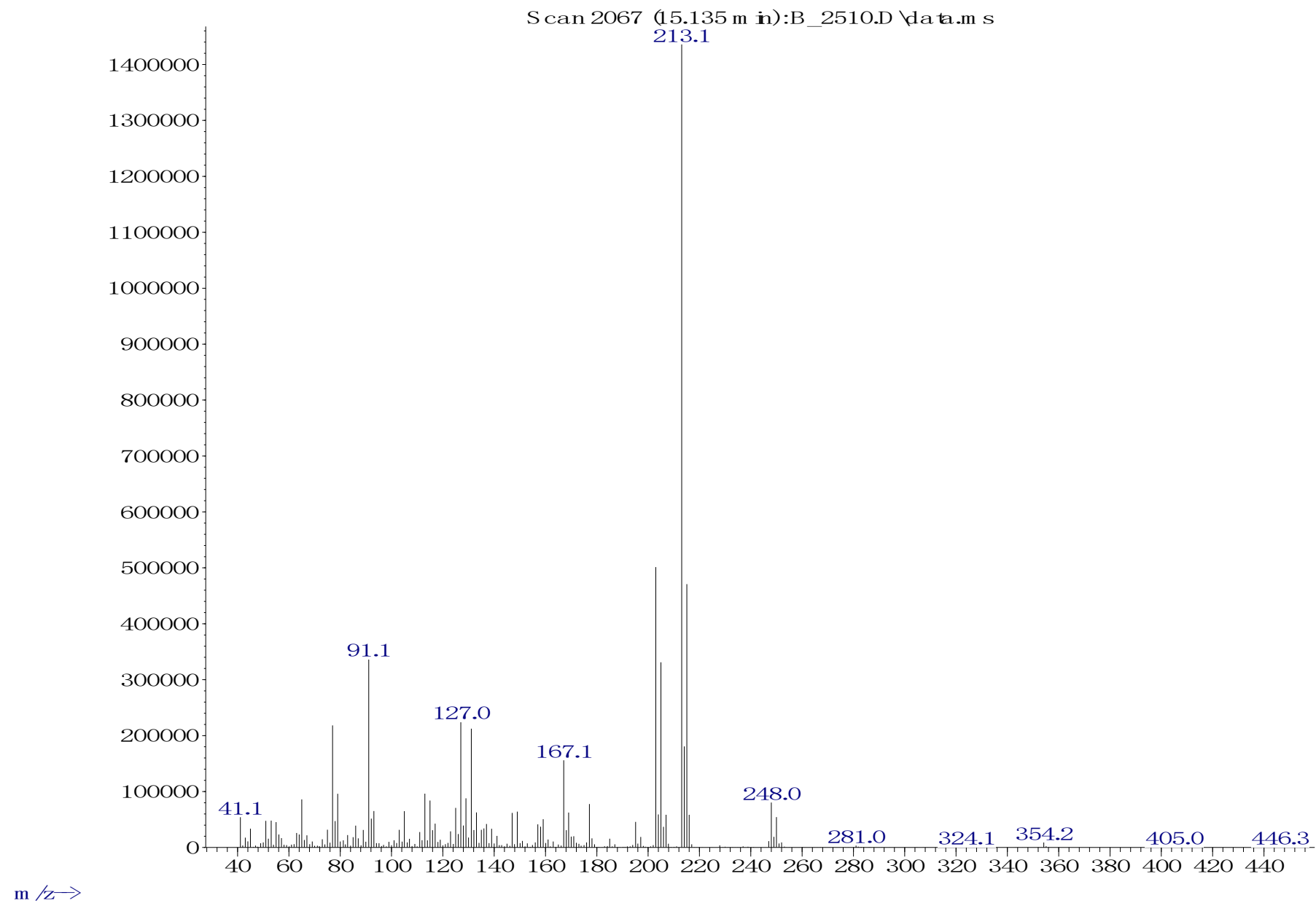
Abundance



Time→

**Figure S6.** Mass spectrum of compound **4**

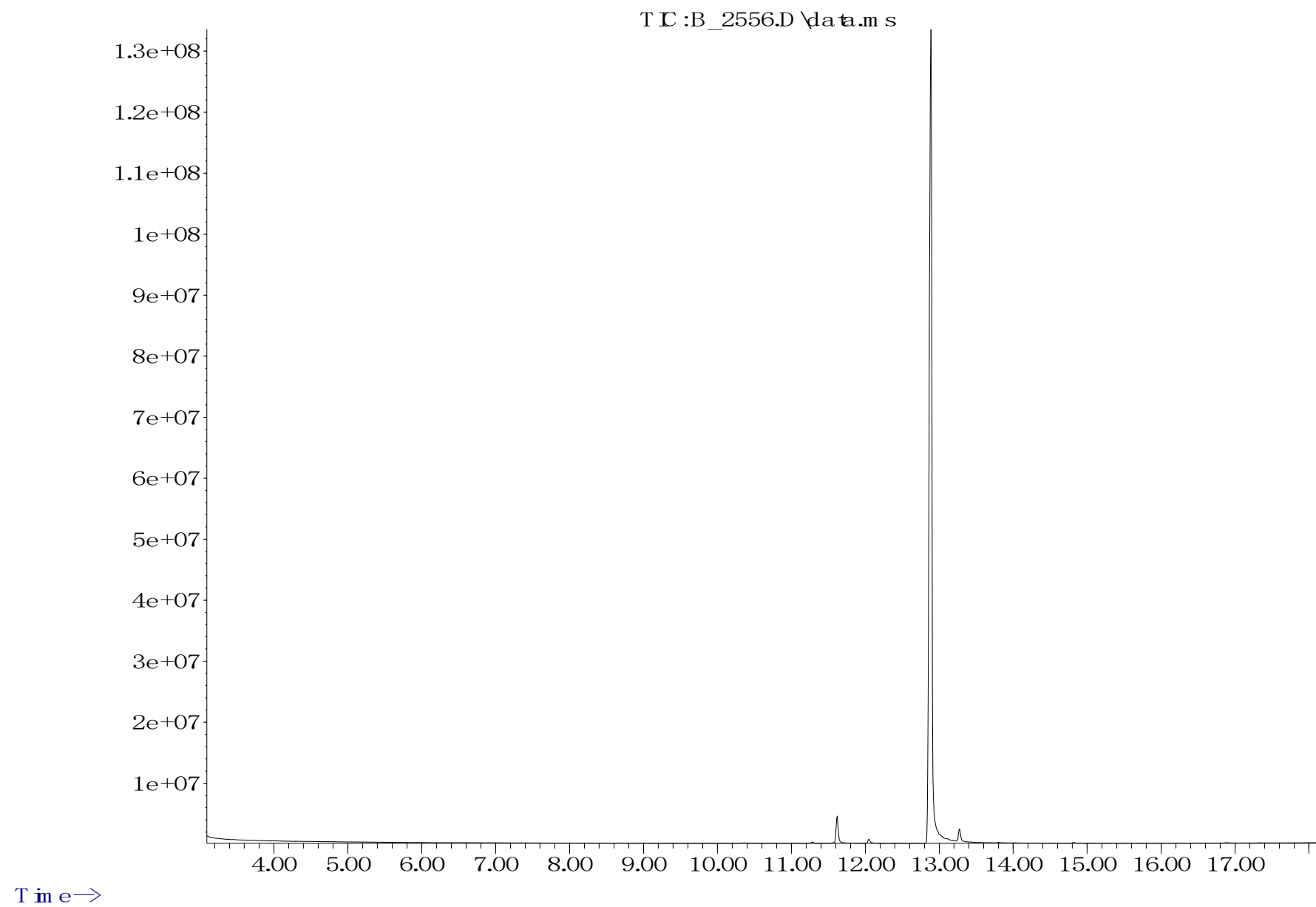
Abundance





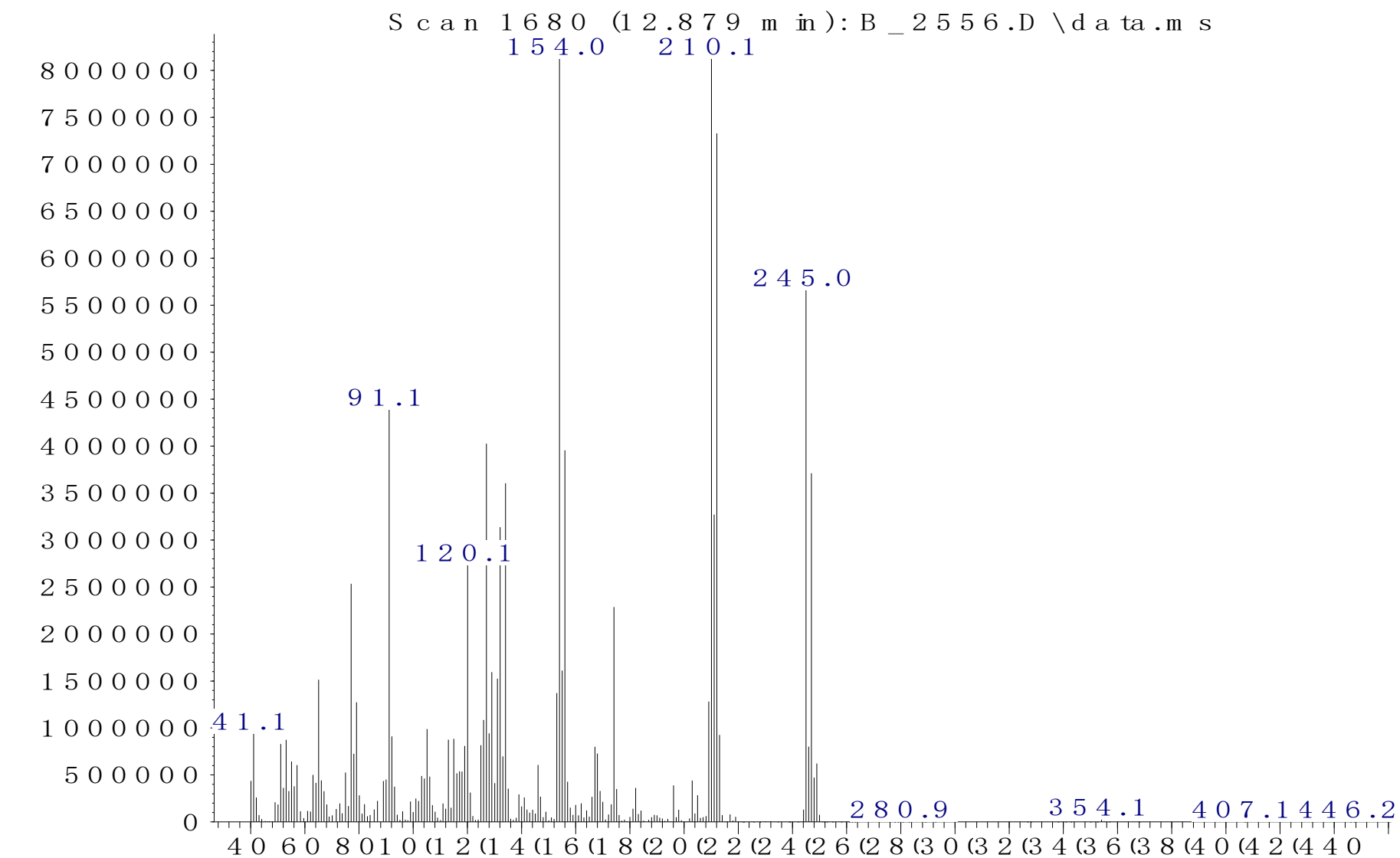
**Figure S7.** Chromatogram of compound 5

Abundance



**Figure S8.** Mass spectrum of compound 5

A b u n d a n c e



m / z →

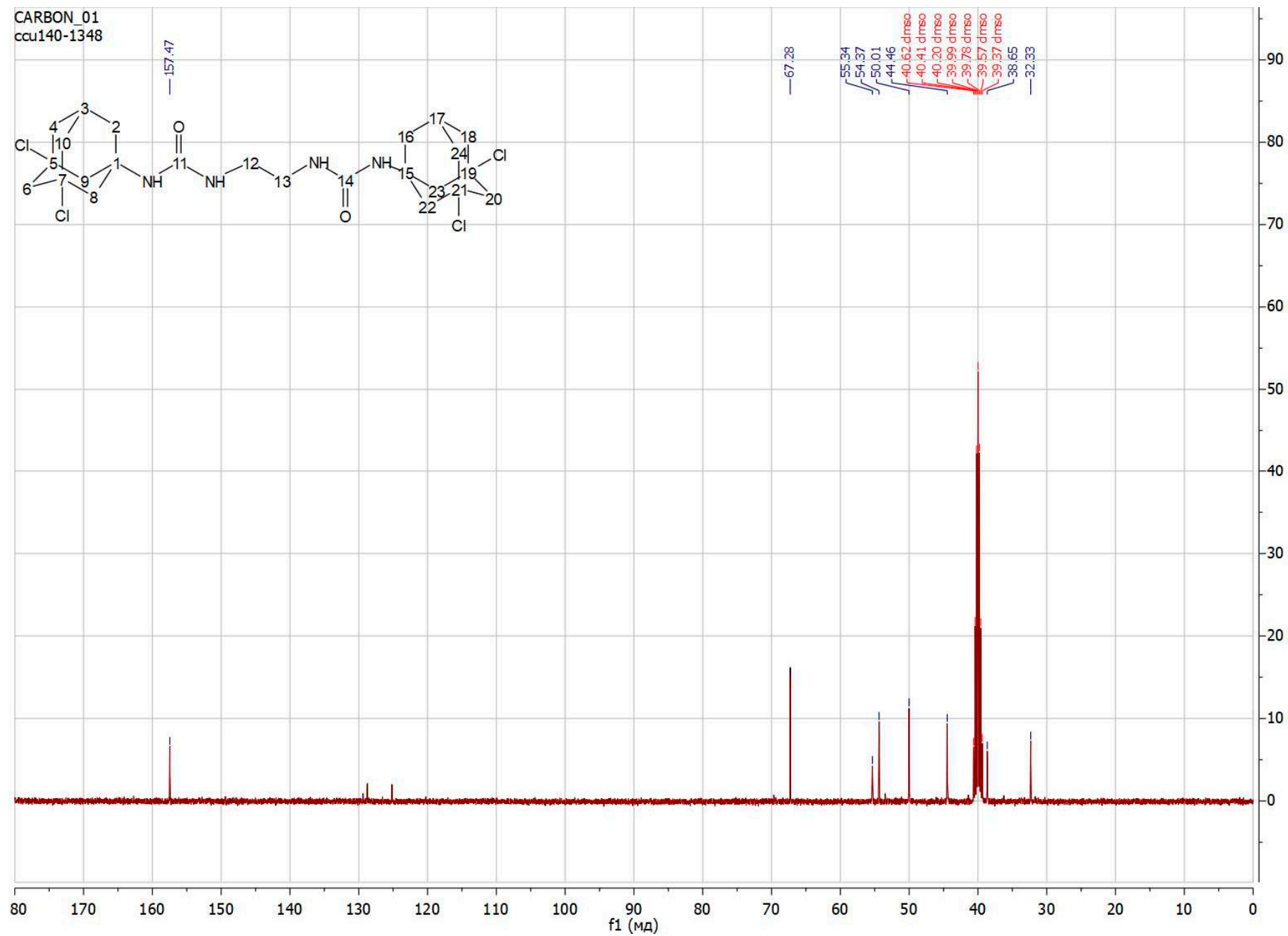
PROTON\_01  
ccu140-1348

Chemical structure: ClC1(Cl)CC2(C1)CC3(C2)CC(Cl)(Cl)C3NC(=O)NCCNC(=O)NC4(Cl)C5(Cl)CC6(C4)CC(Cl)(Cl)C6C5

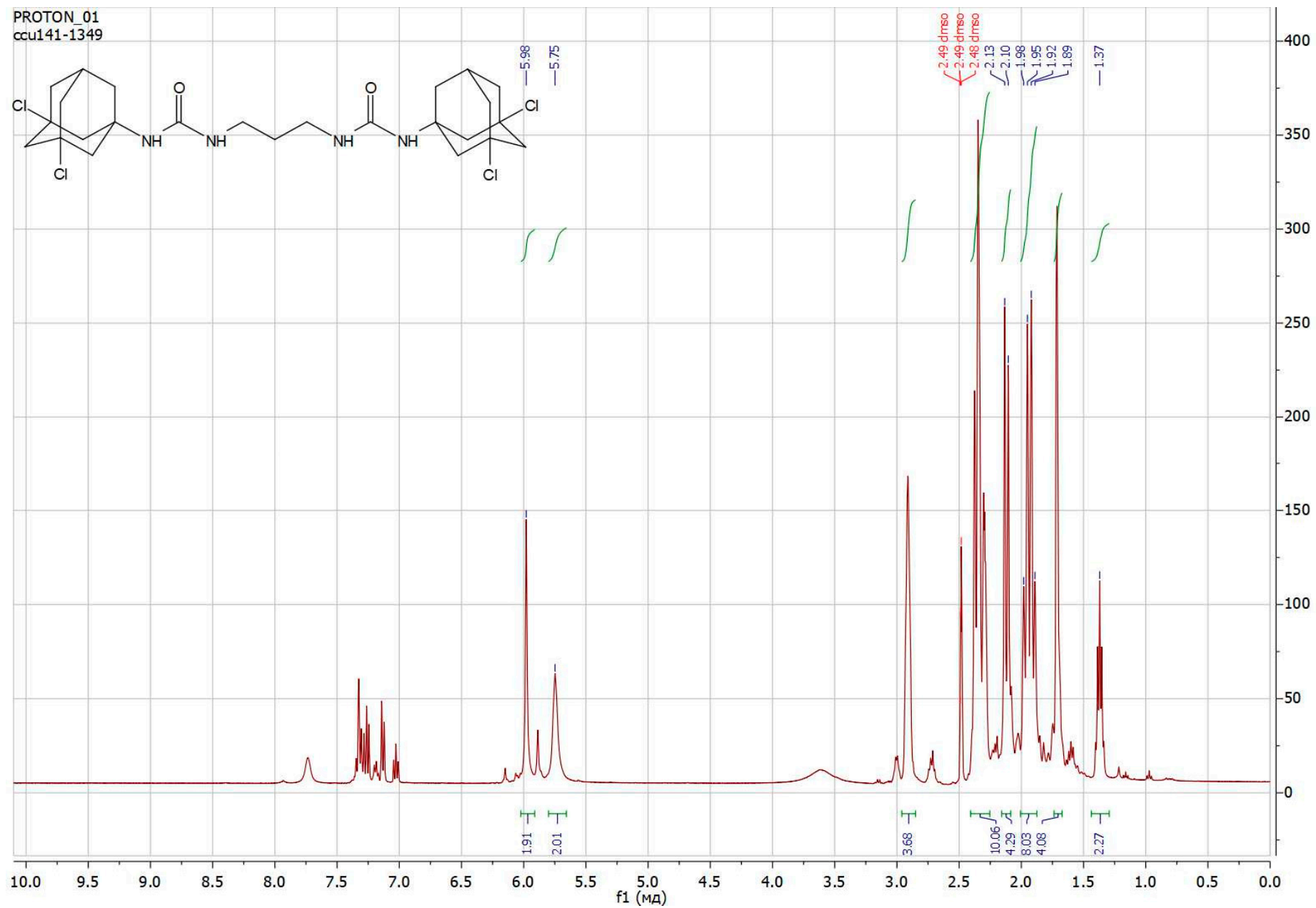
Chemical shifts (ppm): 6.01, 5.72, 3.30 (H<sub>2</sub>O), 2.48 (DMSO), 2.14, 2.11, 1.98, 1.95, 1.92, 1.89.

Integration values: 1.81, 2.00, 4.09, 9.65, 4.10, 8.04, 3.99.

**Figure S10.**  $^{13}\text{C}$  NMR of compound **7a**



**Figure S11.**  $^1\text{H}$  NMR of compound **7b**



**Figure S12.**  $^{13}\text{C}$  NMR of compound **7b**

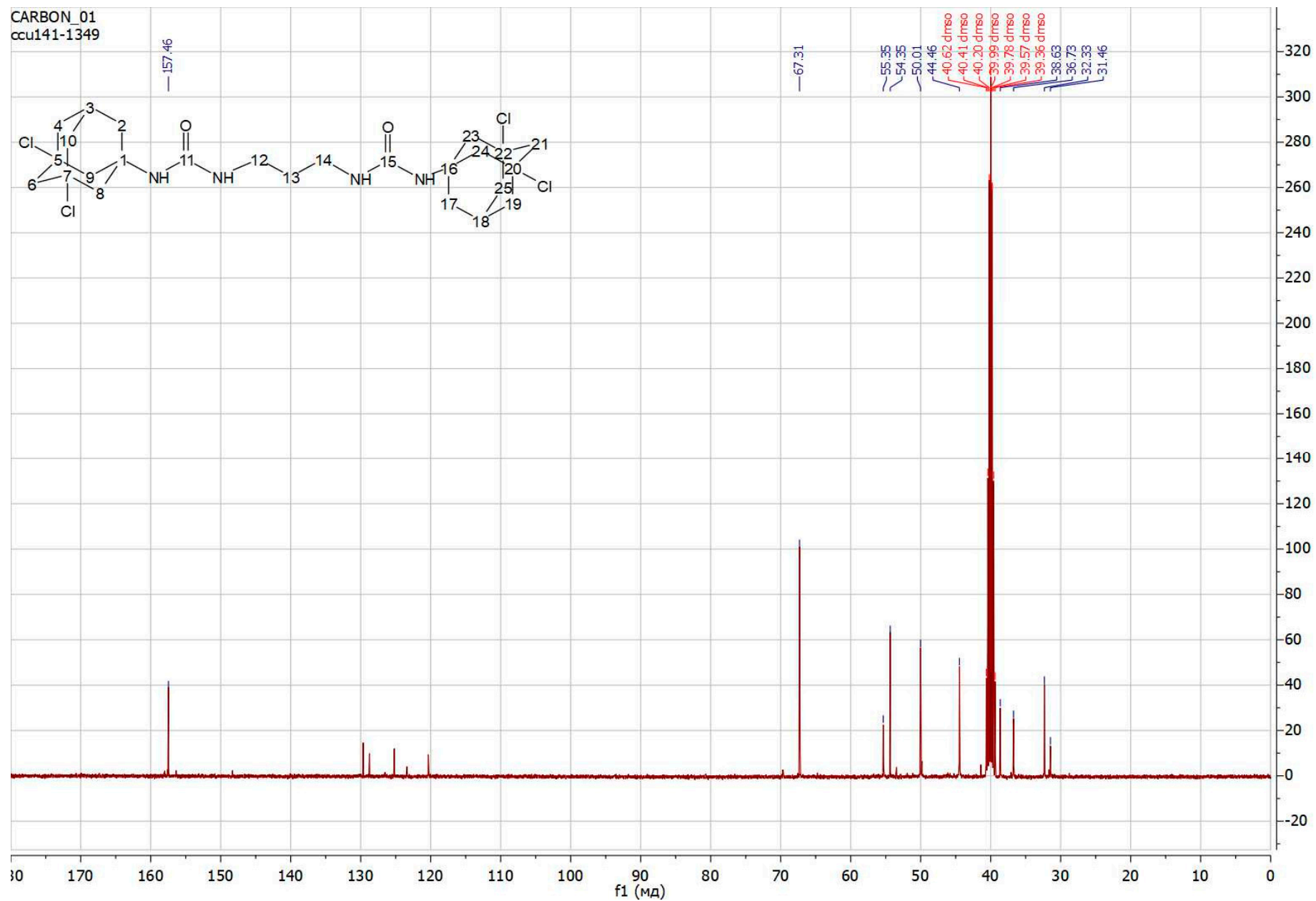
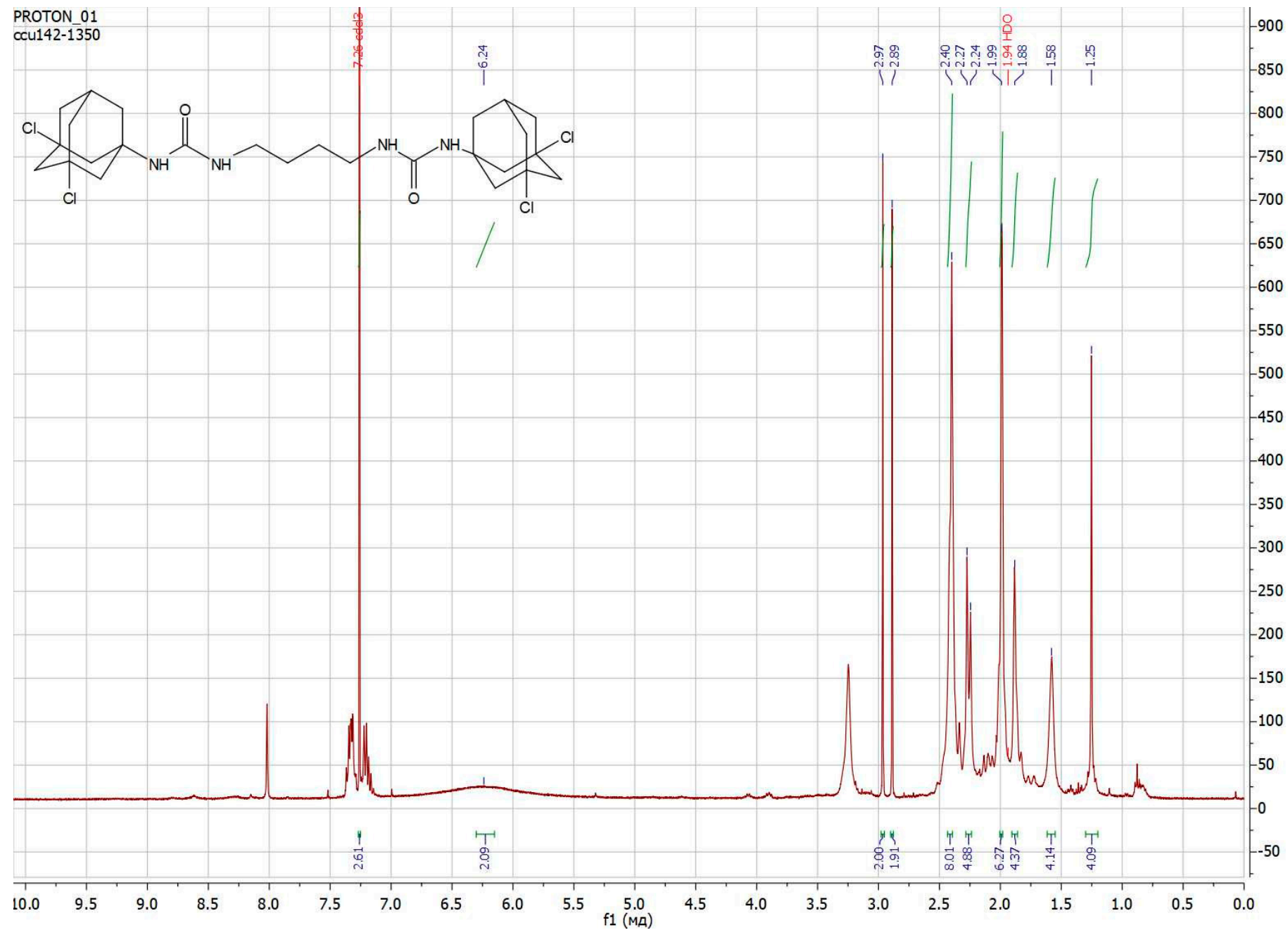
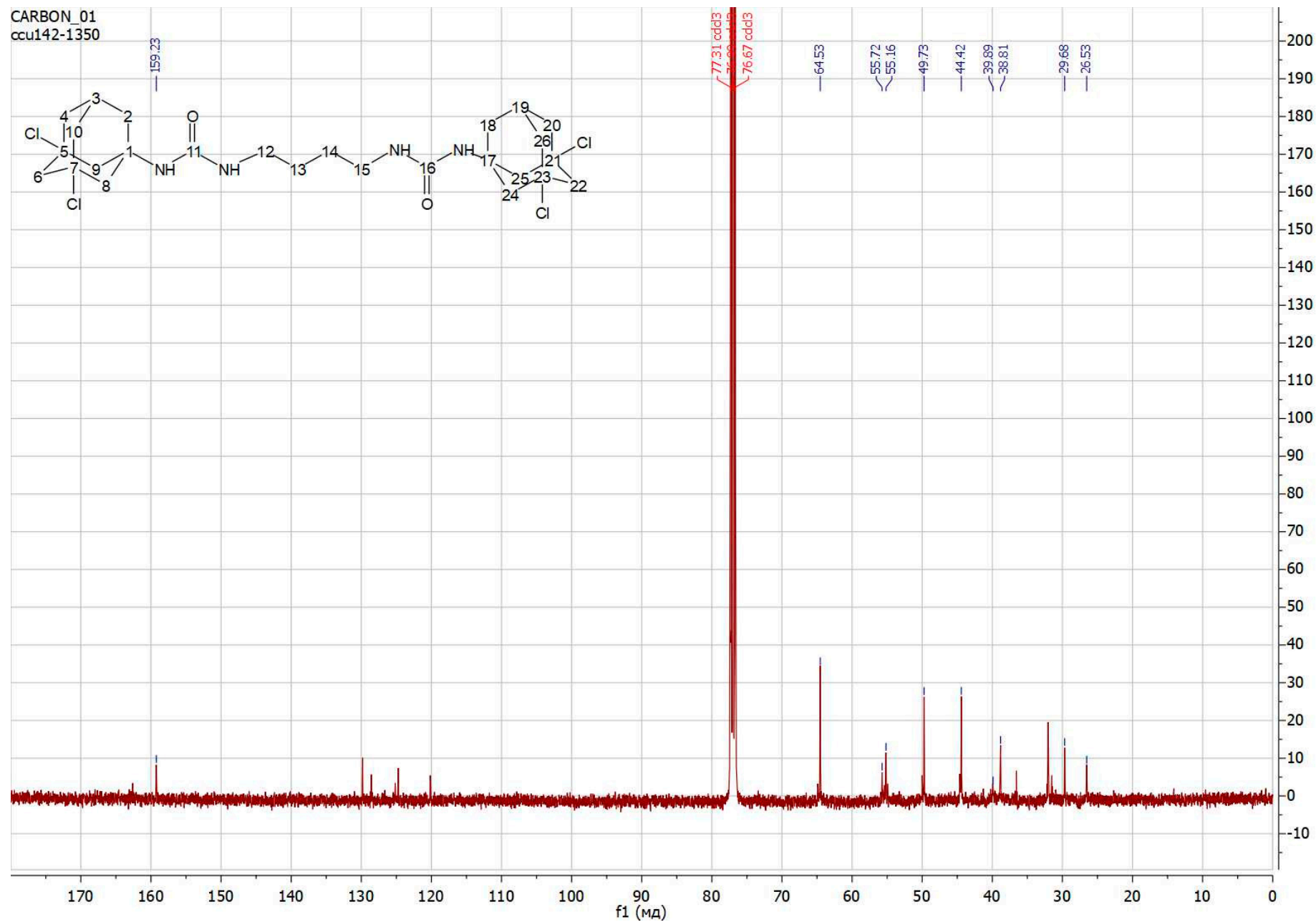


Figure S13.  $^1\text{H}$  NMR of compound 7c

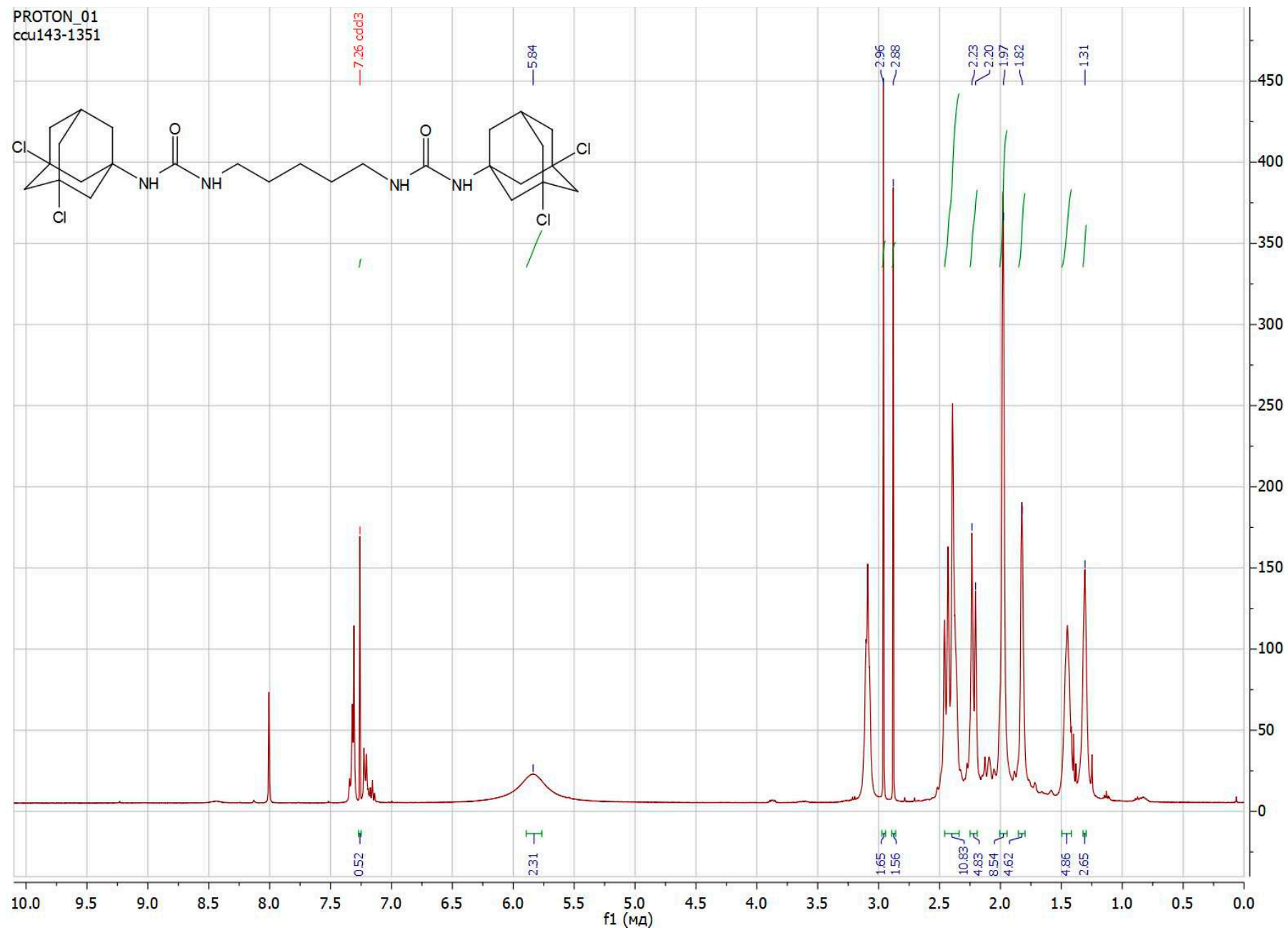


**Figure S14.**  $^{13}\text{C}$  NMR of compound **7c**





**Figure S15.**  $^1\text{H}$  NMR of compound **7d**



**Figure S16.**  $^{13}\text{C}$  NMR of compound **7d**

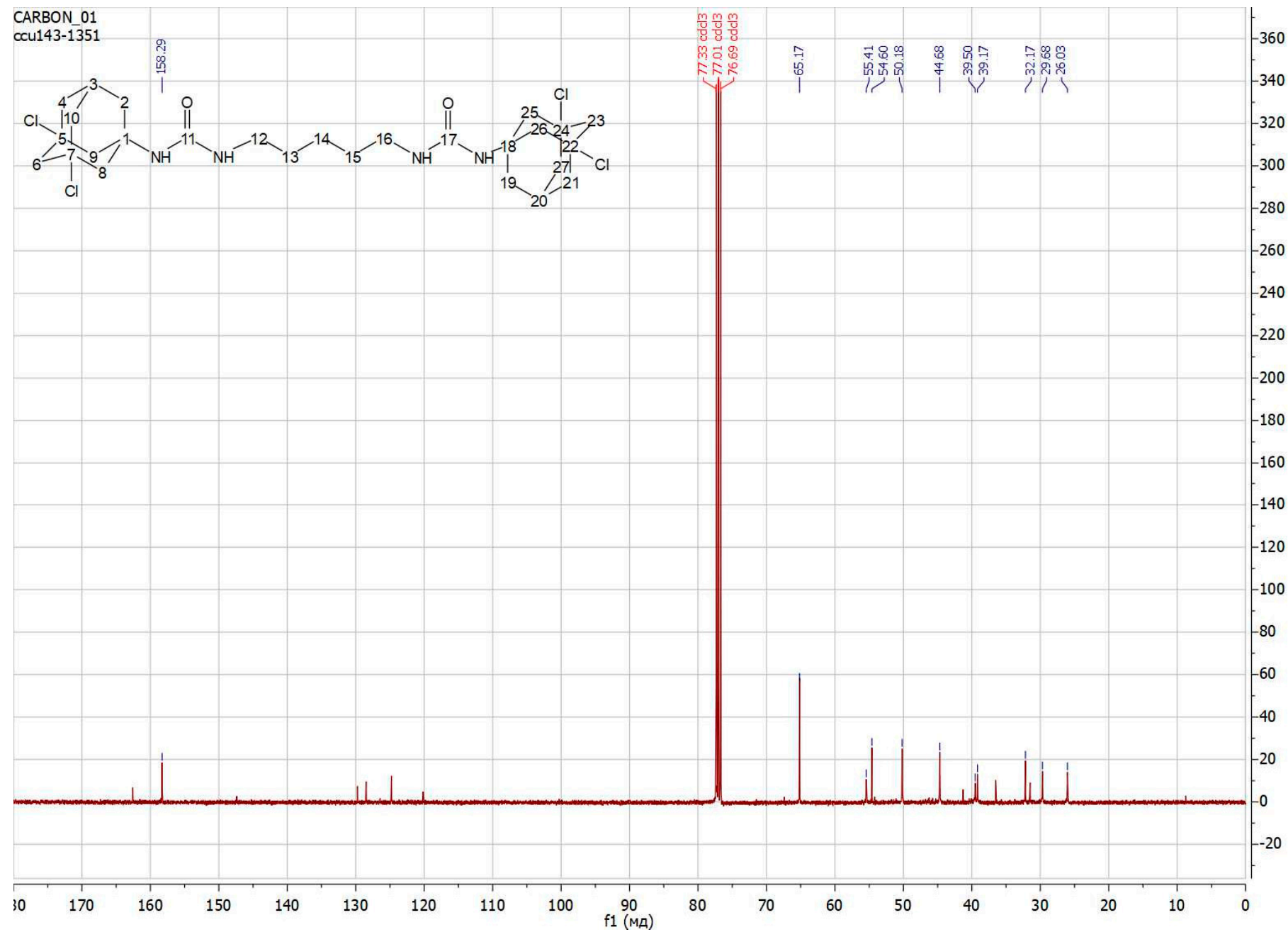
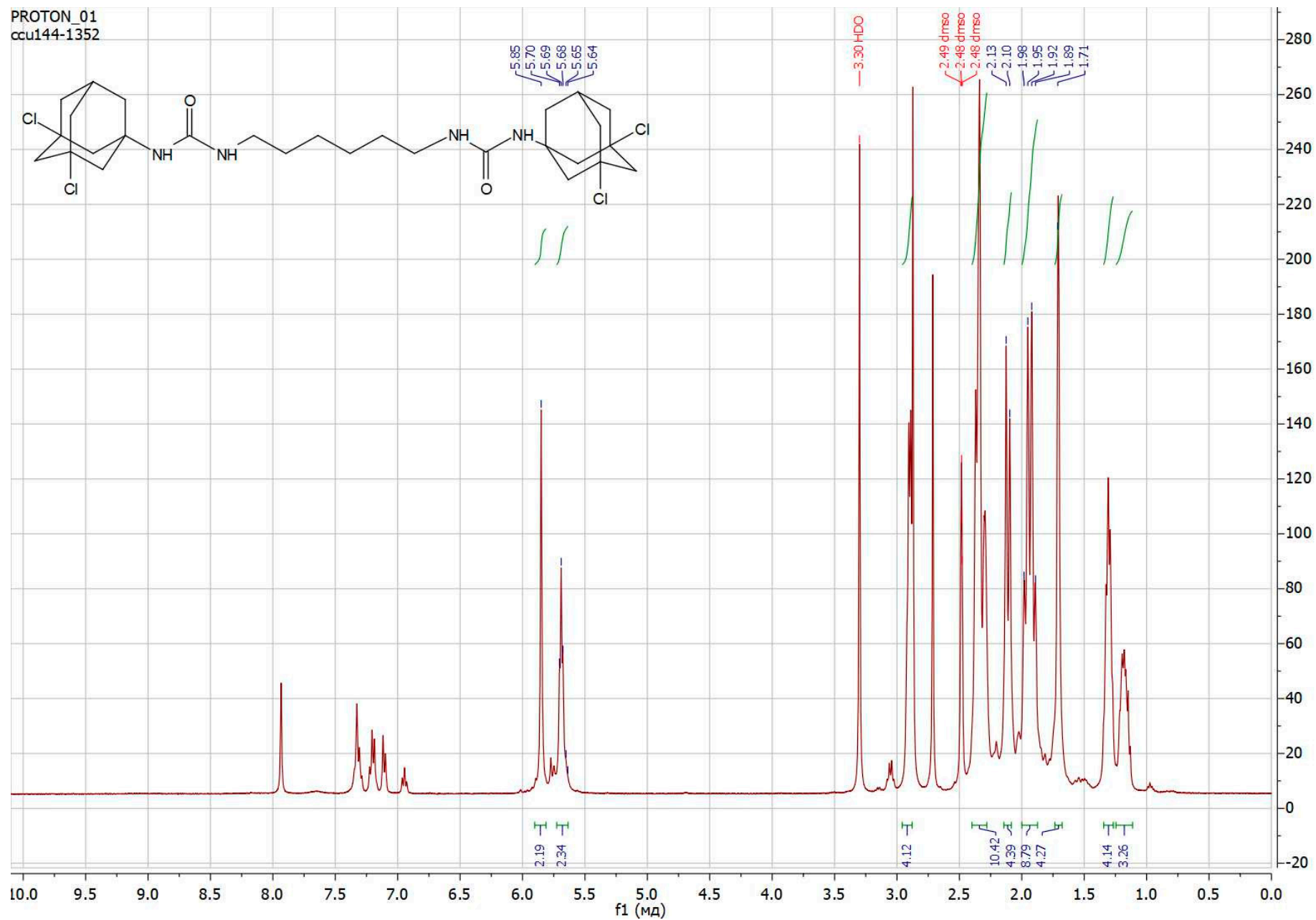
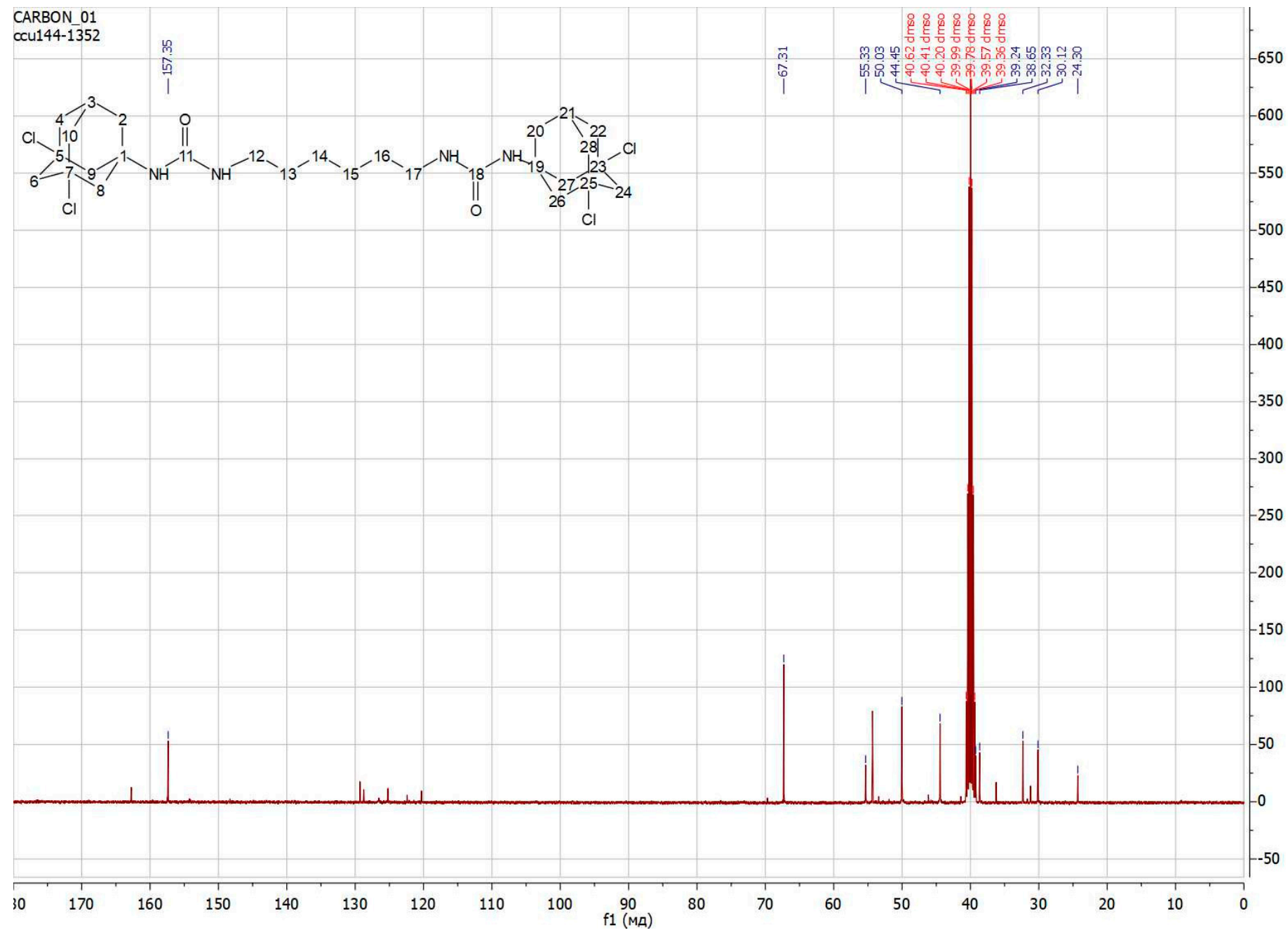


Figure S17.  $^1\text{H}$  NMR of compound 7e



**Figure S18.**  $^{13}\text{C}$  NMR of compound **7e**



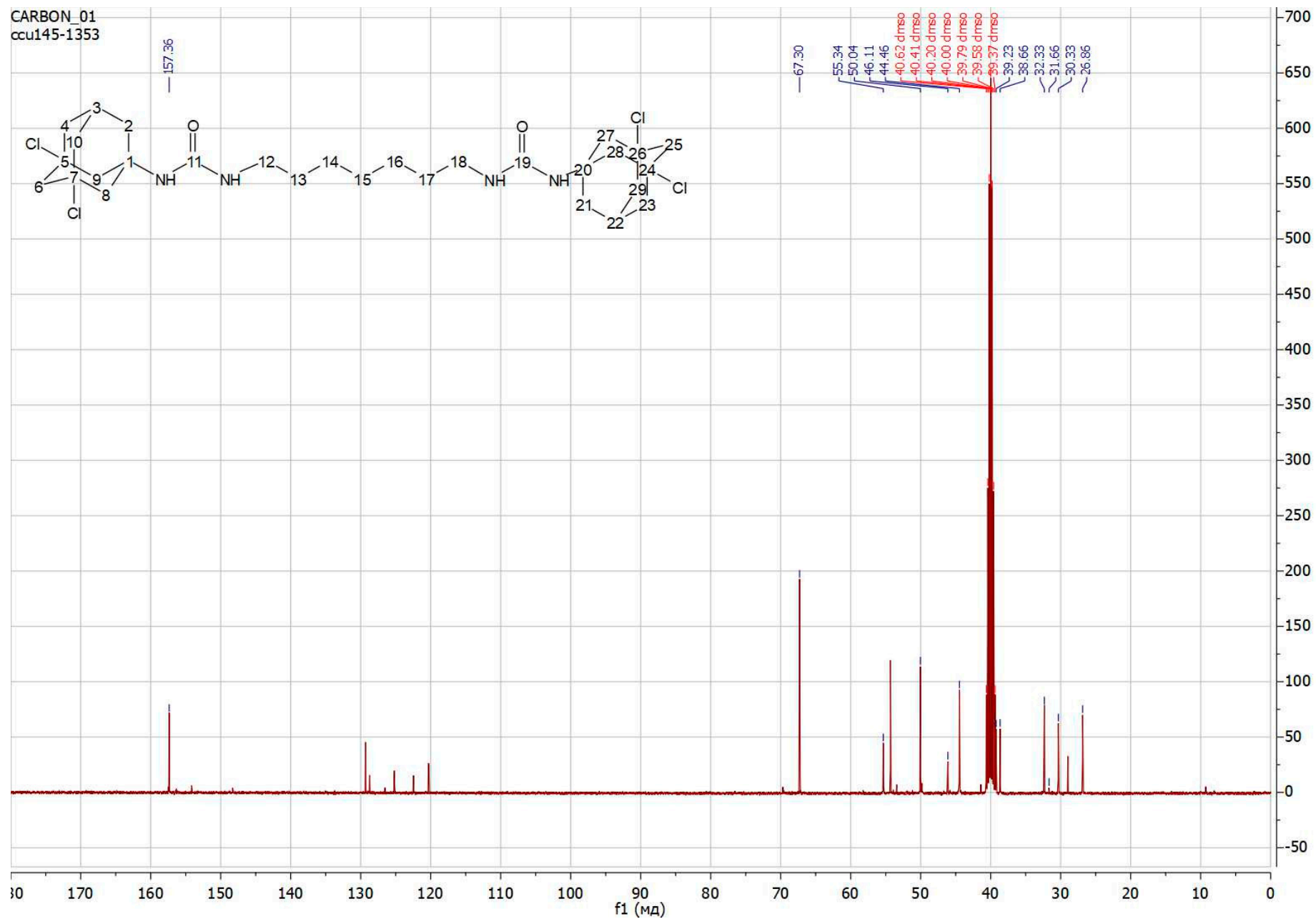
PROTON 01  
ccu145-1353

Chemical structure: ClC1(Cl)C=CC2(C)C=CC1C2NC(=O)NCCCCCCNC(=O)N3C4(C)C=CC1(C)C(Cl)C4C3

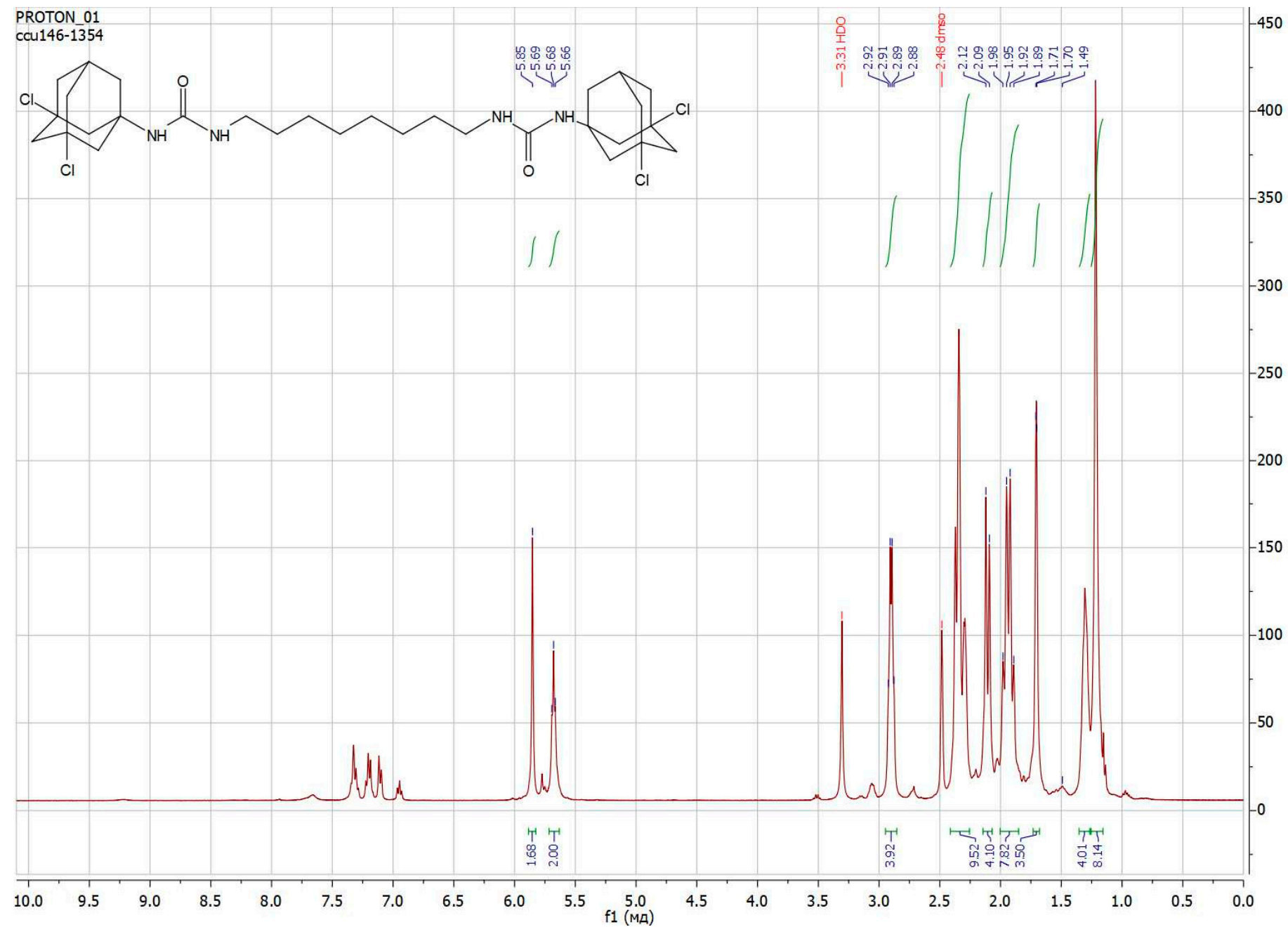
Integration values (from left to right): 1.90, 2.00, 4.27, 10.84, 4.21, 8.61, 3.50, 3.93, 6.21.

Chemical shifts (ppm) labeled above peaks: 5.86, 5.69, 3.30 (H<sub>2</sub>O), 2.92, 2.91, 2.89, 2.88, 2.49 (dms), 2.48 (dms), 2.48 (dms), 2.47 (dms), 2.12, 2.09, 1.98, 1.95, 1.92, 1.89, 1.71, 1.70.

**Figure S20.**  $^{13}\text{C}$  NMR of compound **7f**



**Figure S21.**  $^1\text{H}$  NMR of compound **7g**





**Figure S22.**  $^{13}\text{C}$  NMR of compound **7g**

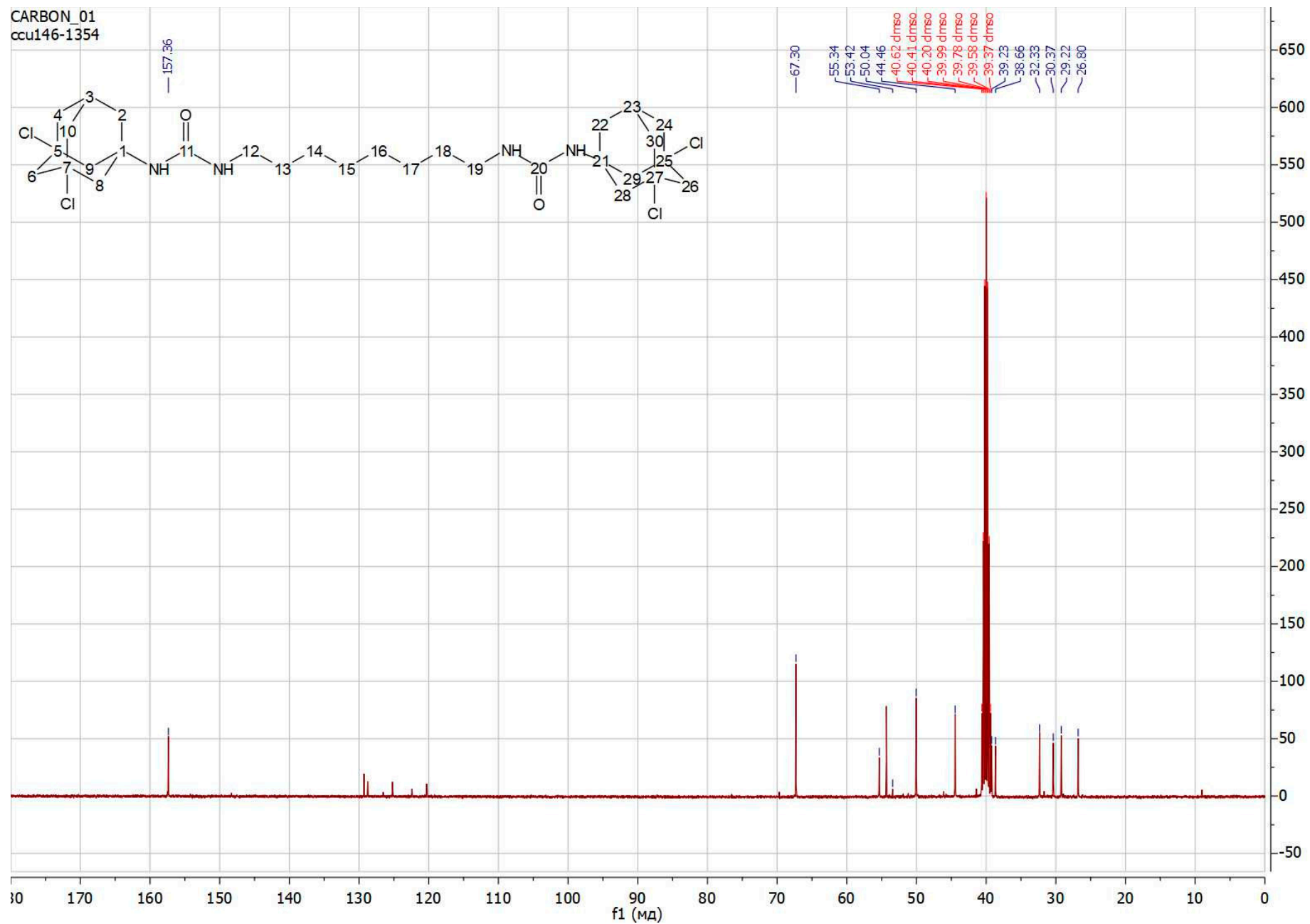
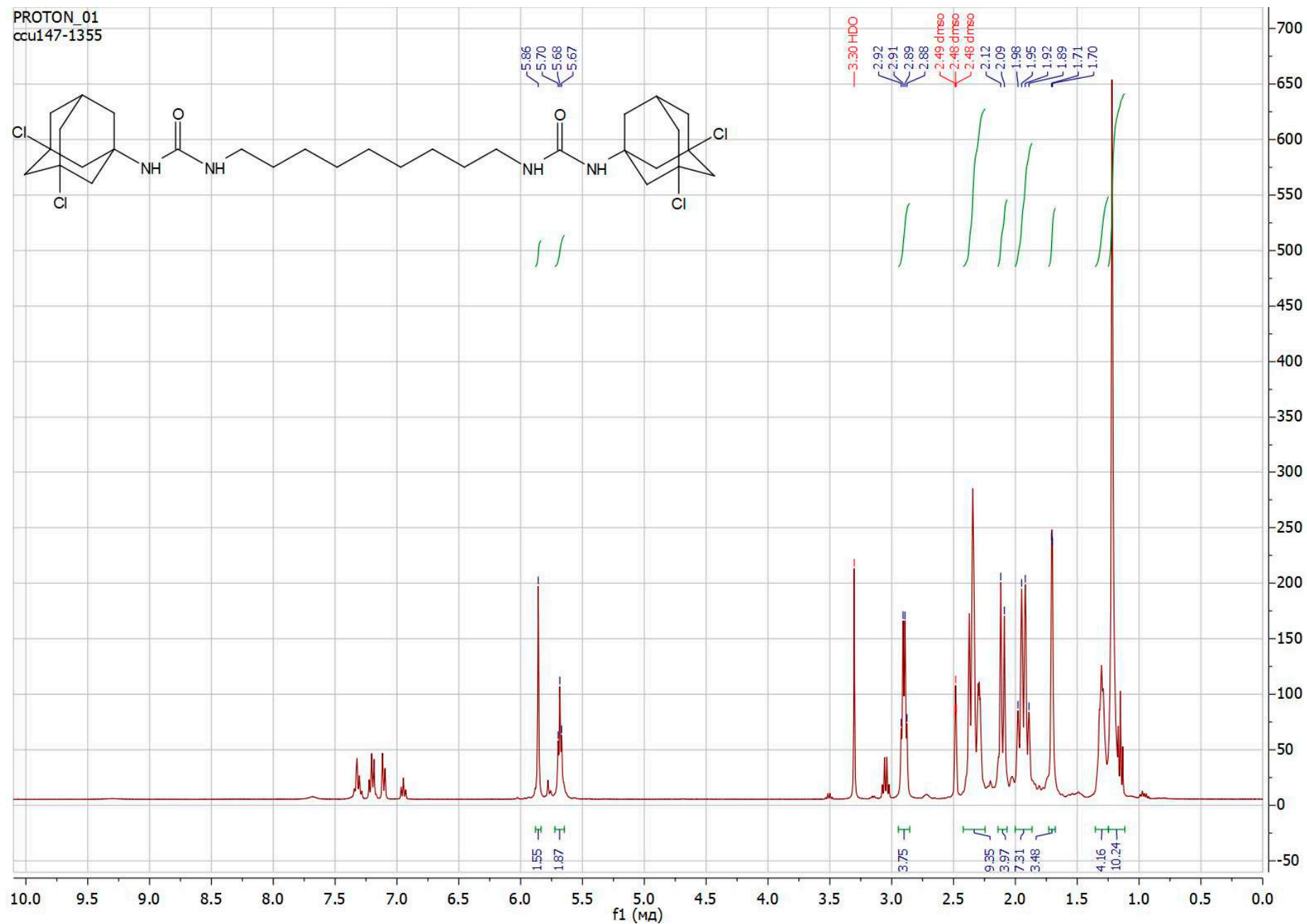




Figure S23.  $^1\text{H}$  NMR of compound 7h



**Figure S24.**  $^{13}\text{C}$  NMR of compound **7h**

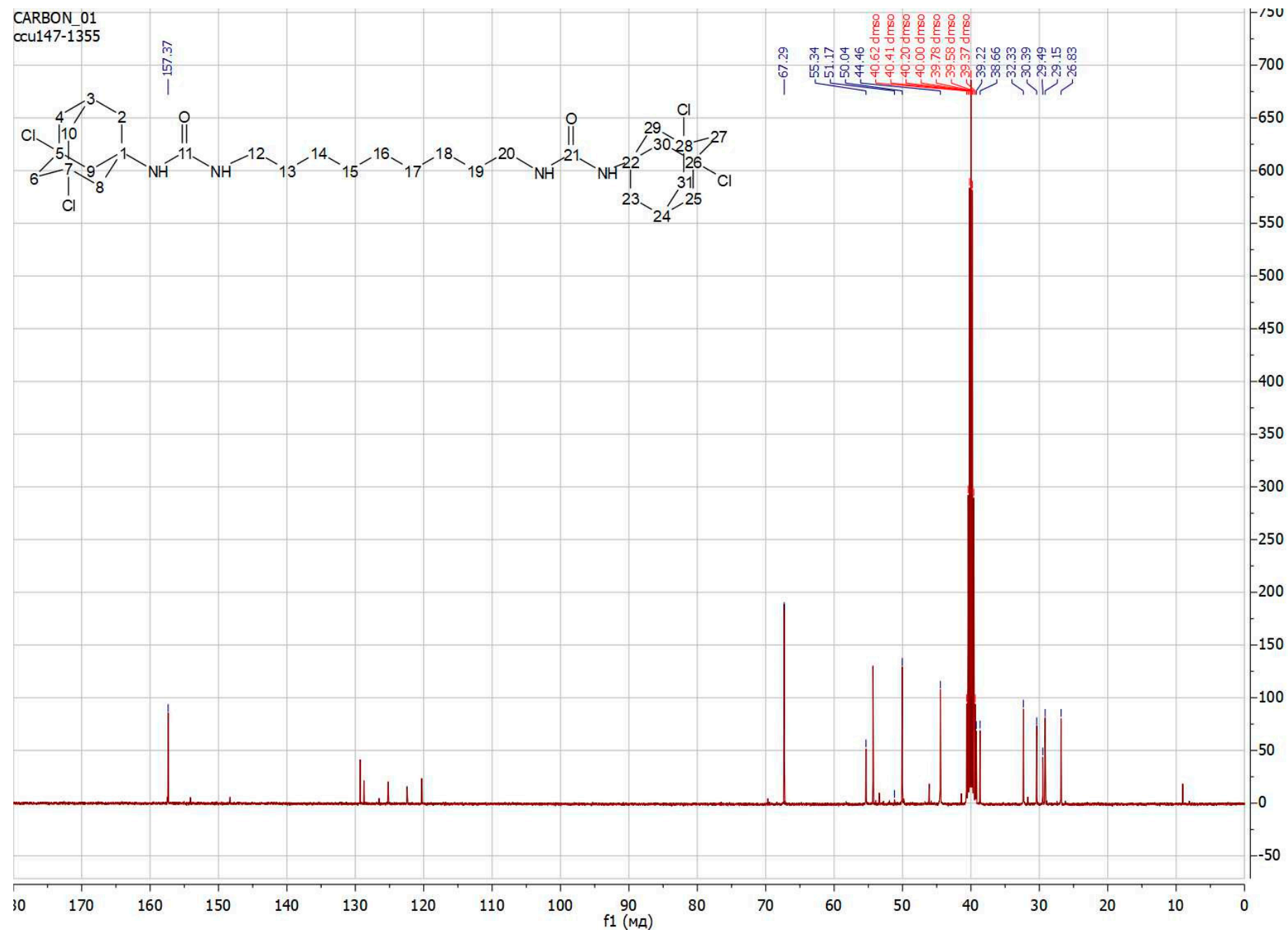
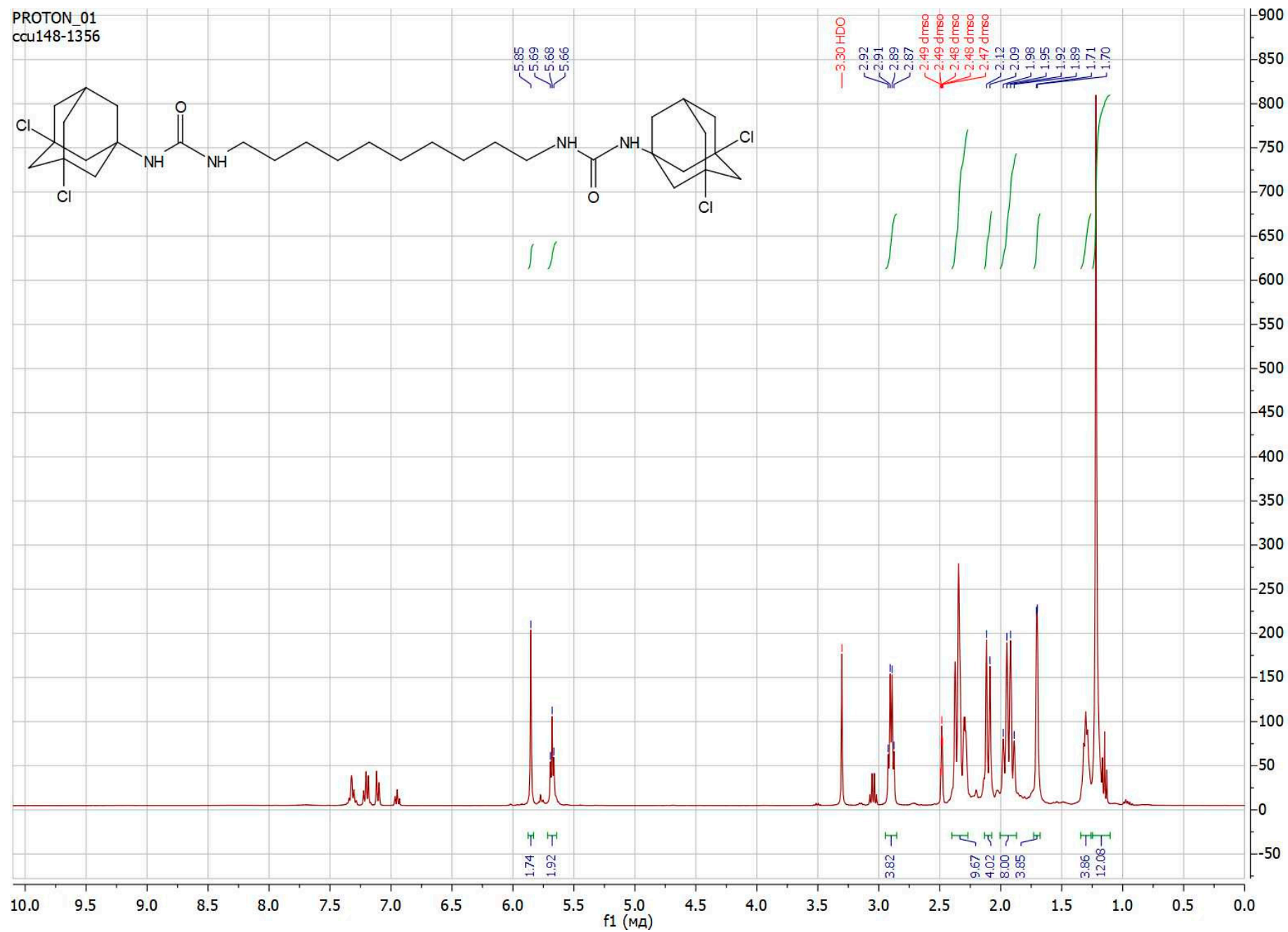


Figure S25.  $^1\text{H}$  NMR of compound 7i



CARBON 01  
ccu148-1356

Chemical structure of compound 148-1356 is shown above the spectrum. The structure is a symmetrical molecule with two 2,4-dichlorophenyl rings connected by a central chain. The carbons are numbered 1 through 32. The structure is a symmetrical molecule with two 2,4-dichlorophenyl rings connected by a central chain. The carbons are numbered 1 through 32.

Peak list (Chemical Shift in ppm):

Carbon Number	Chemical Shift (ppm)
1	157.36
2	157.36
3	157.36
4	157.36
5	157.36
6	157.36
7	157.36
8	157.36
9	157.36
10	157.36
11	157.36
12	157.36
13	157.36
14	157.36
15	157.36
16	157.36
17	157.36
18	157.36
19	157.36
20	157.36
21	157.36
22	157.36
23	157.36
24	157.36
25	157.36
26	157.36
27	157.36
28	157.36
29	157.36
30	157.36
31	157.36
32	157.36

**Figure S27.**  $^1\text{H}$  NMR of compound **9**

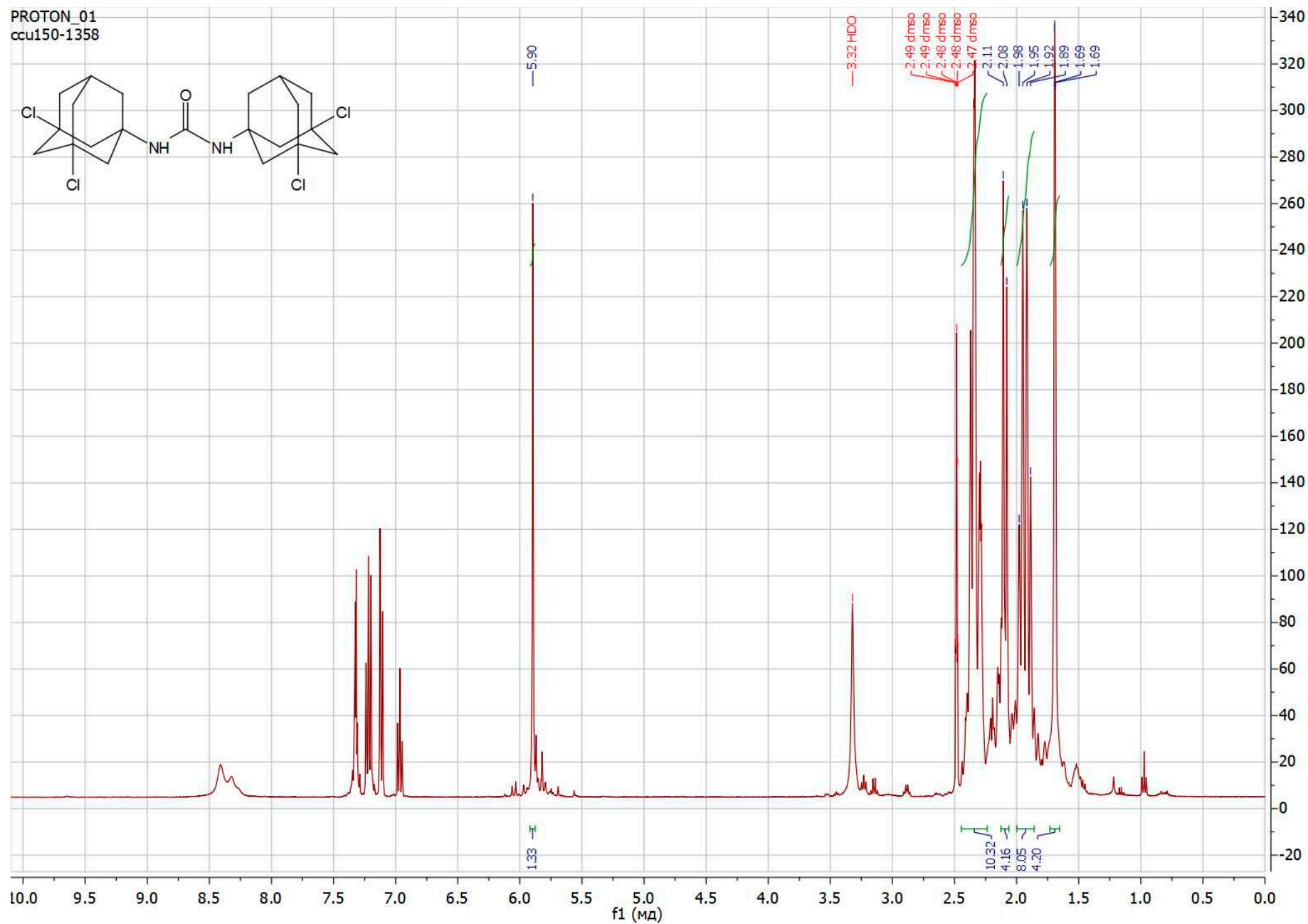
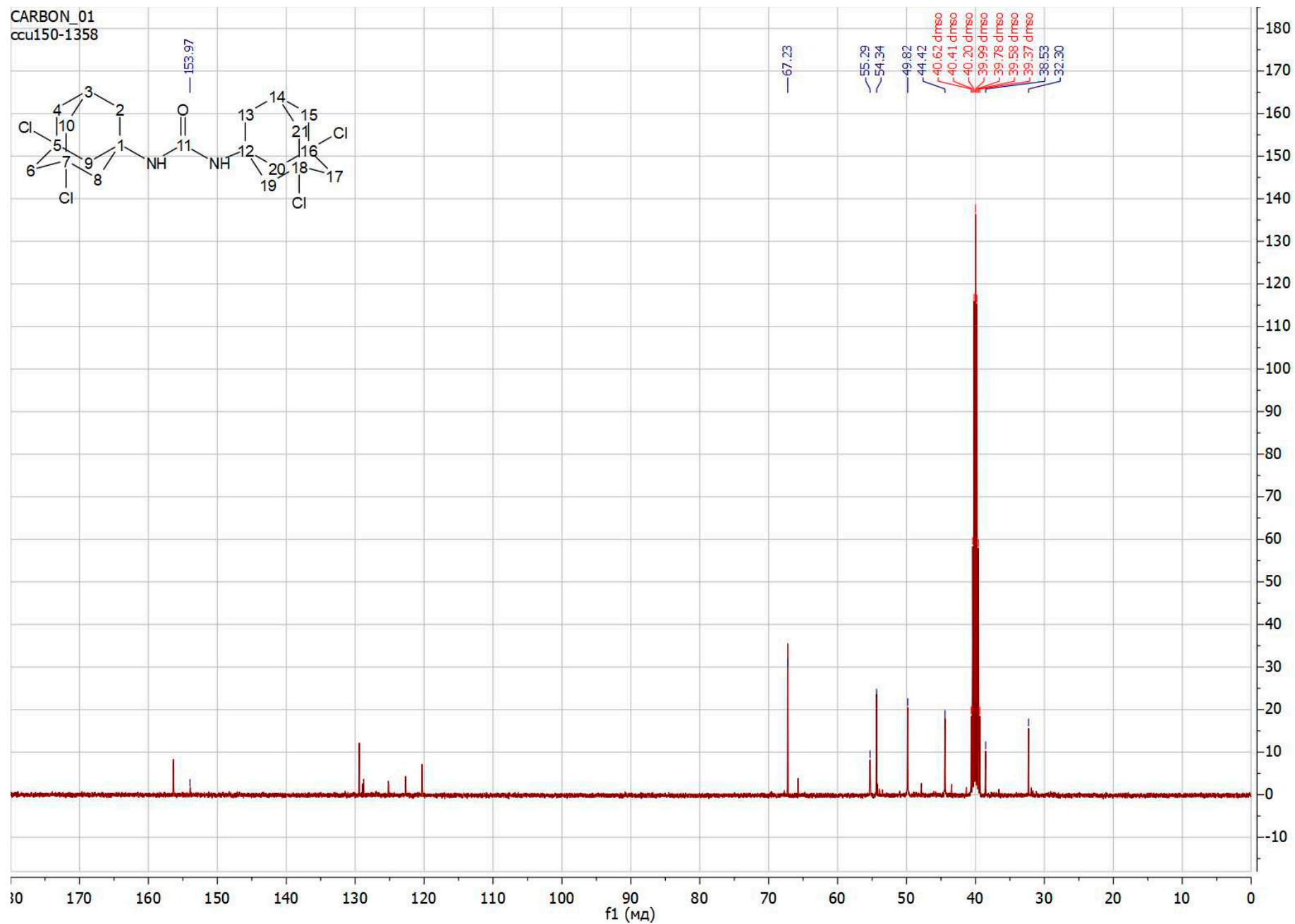


Figure S28.  $^{13}\text{C}$  NMR of compound 9



**Figure S29.**  $^1\text{H}$  NMR of compound 11

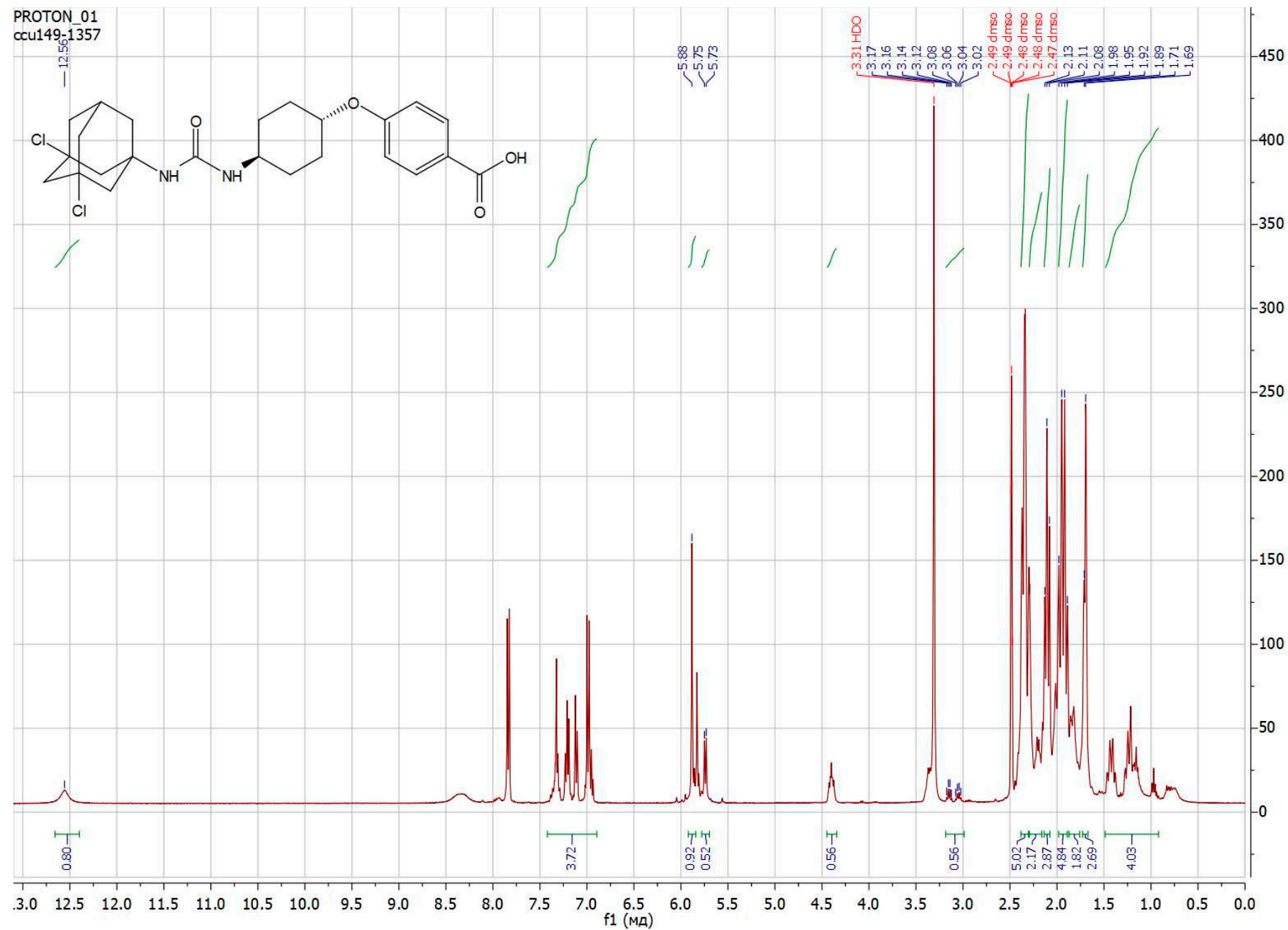




Figure S30.  $^{13}\text{C}$  NMR of compound 11

