

Domino C-H Sulfenylation and Pyrazole Annulation for Fully Substituted Pyrazole Synthesis in Water Using Hydrophilic Enaminones

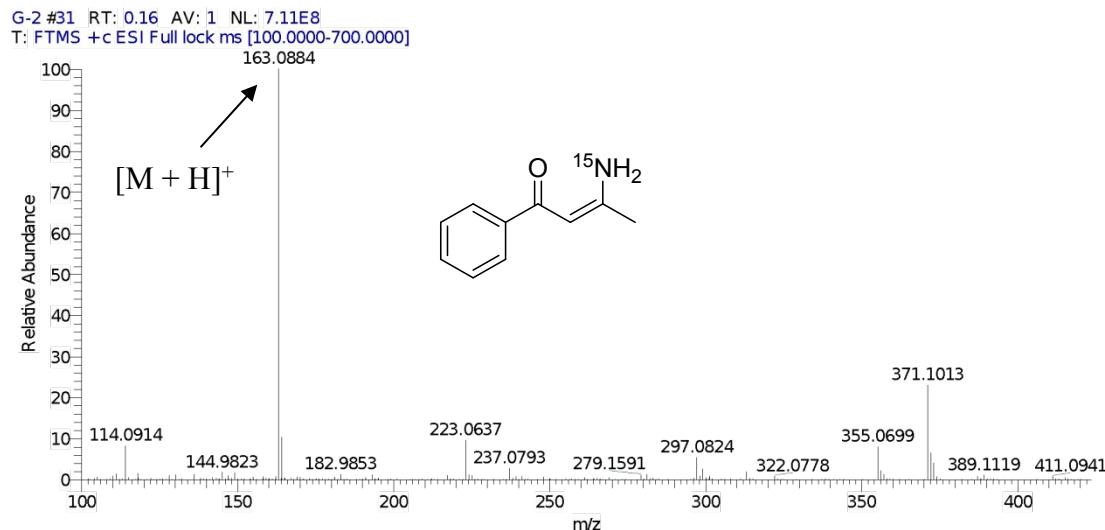
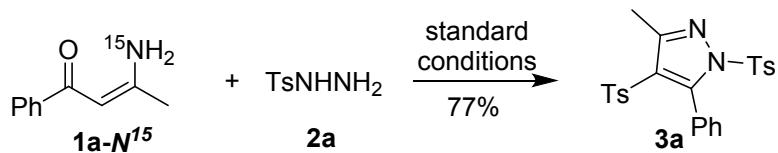
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Nanchang 330022, P. R. China. Email: wanjieping@jxnu.edu.cn

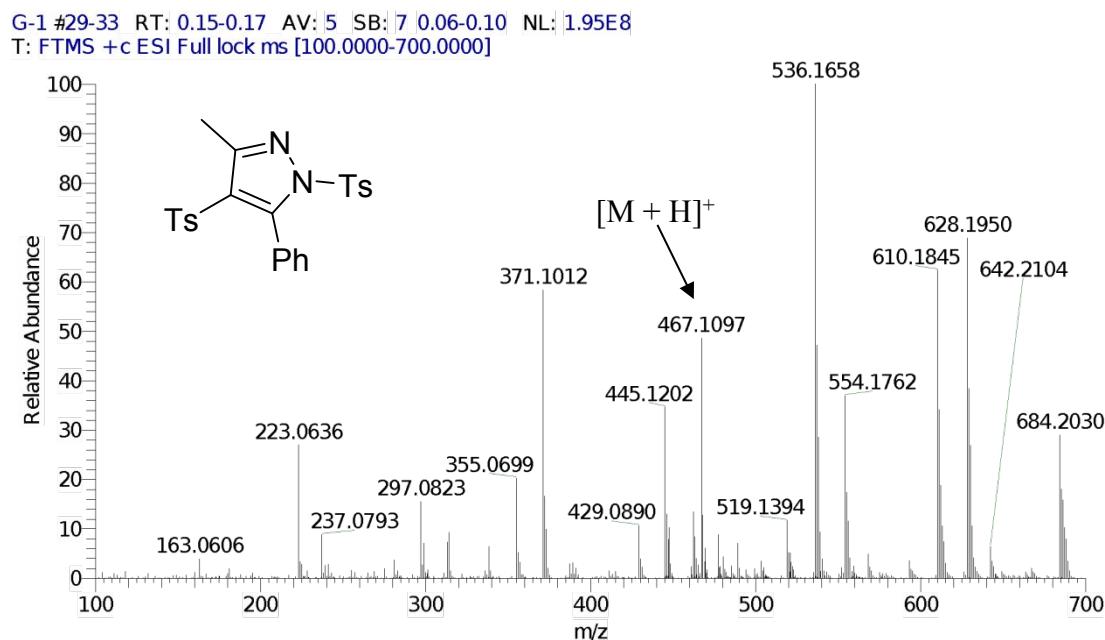
Contents

HRMS spectrum from ^{15}N -labeled control experiments.....	S2
^1H and ^{13}C NMR spectra.....	S3-S46
HMRS spectra of all new compounds.....	S47-S57

The HRMS spectrum of ^{15}N -labeled enaminone **1a and the corresponding product **3a** isolated from the isotope labeling experiment**

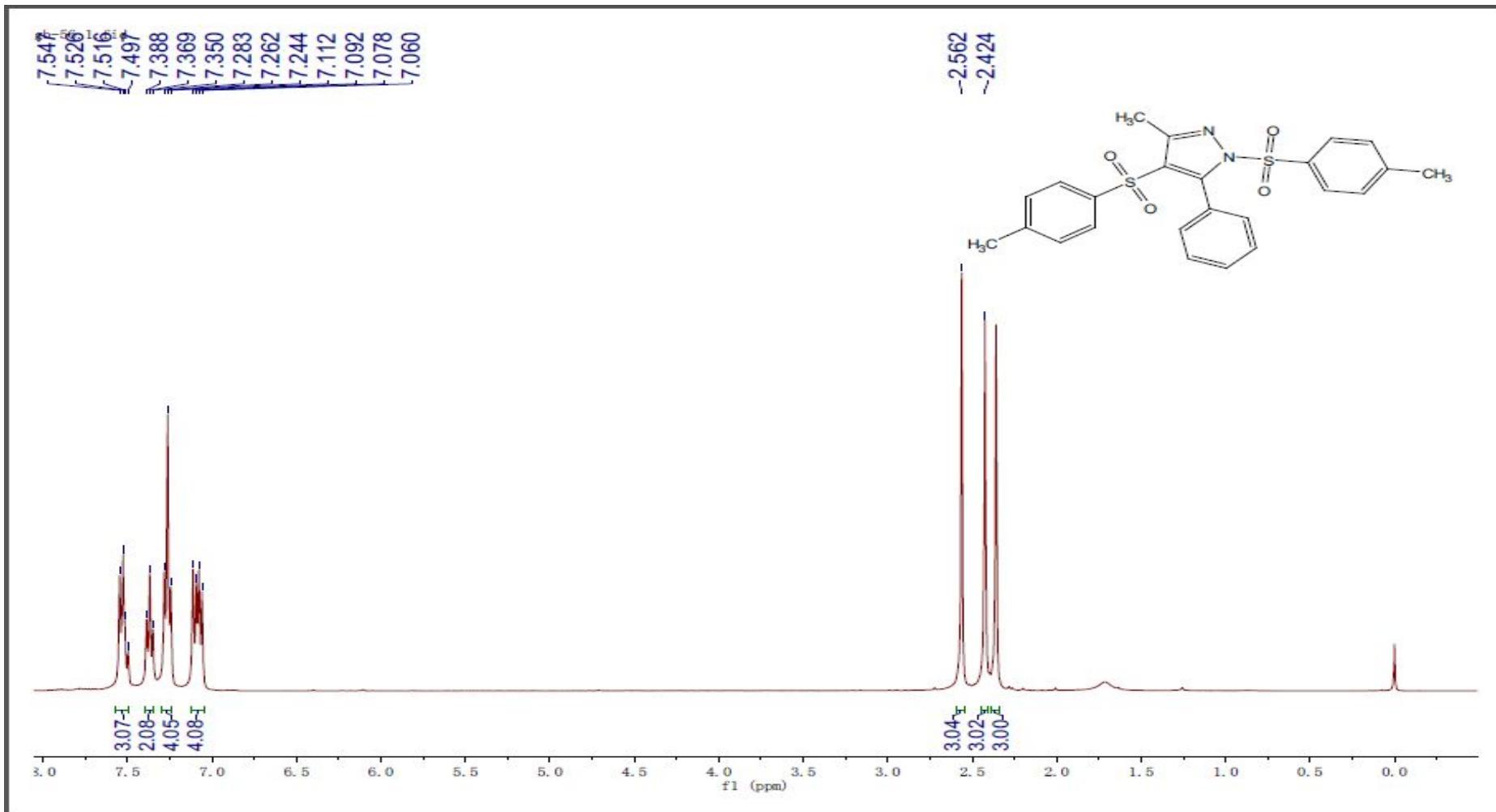


Calculated: $\text{C}_{10}\text{H}_{12}^{15}\text{NO} [\text{M} + \text{H}]^+$ 163.0884, found 163.0884.

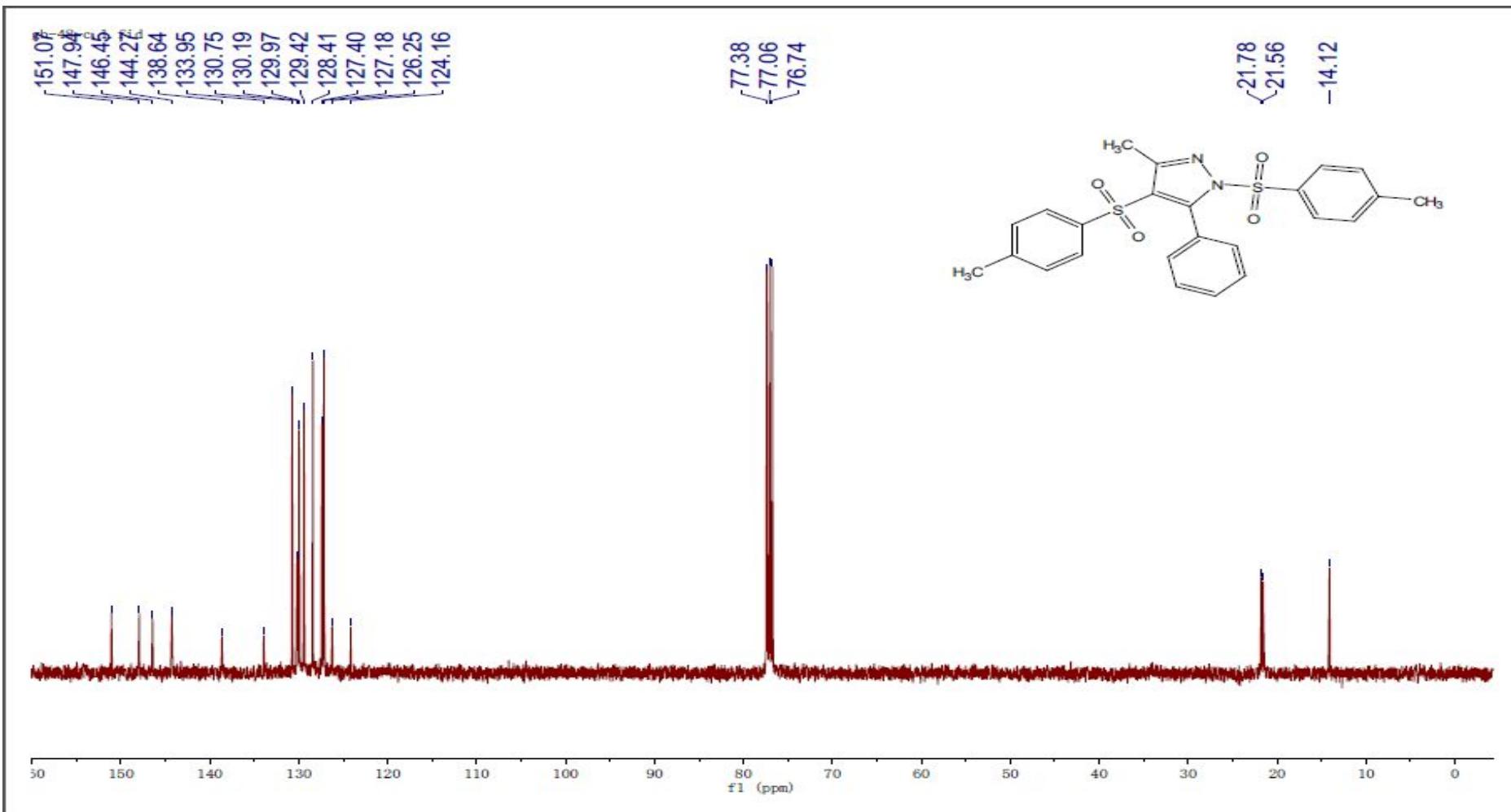


Calculated: $\text{C}_{24}\text{H}_{23}\text{N}_2\text{O}_4\text{S}_2 [\text{M} + \text{H}]^+$ 467.1094, found 467.1097.

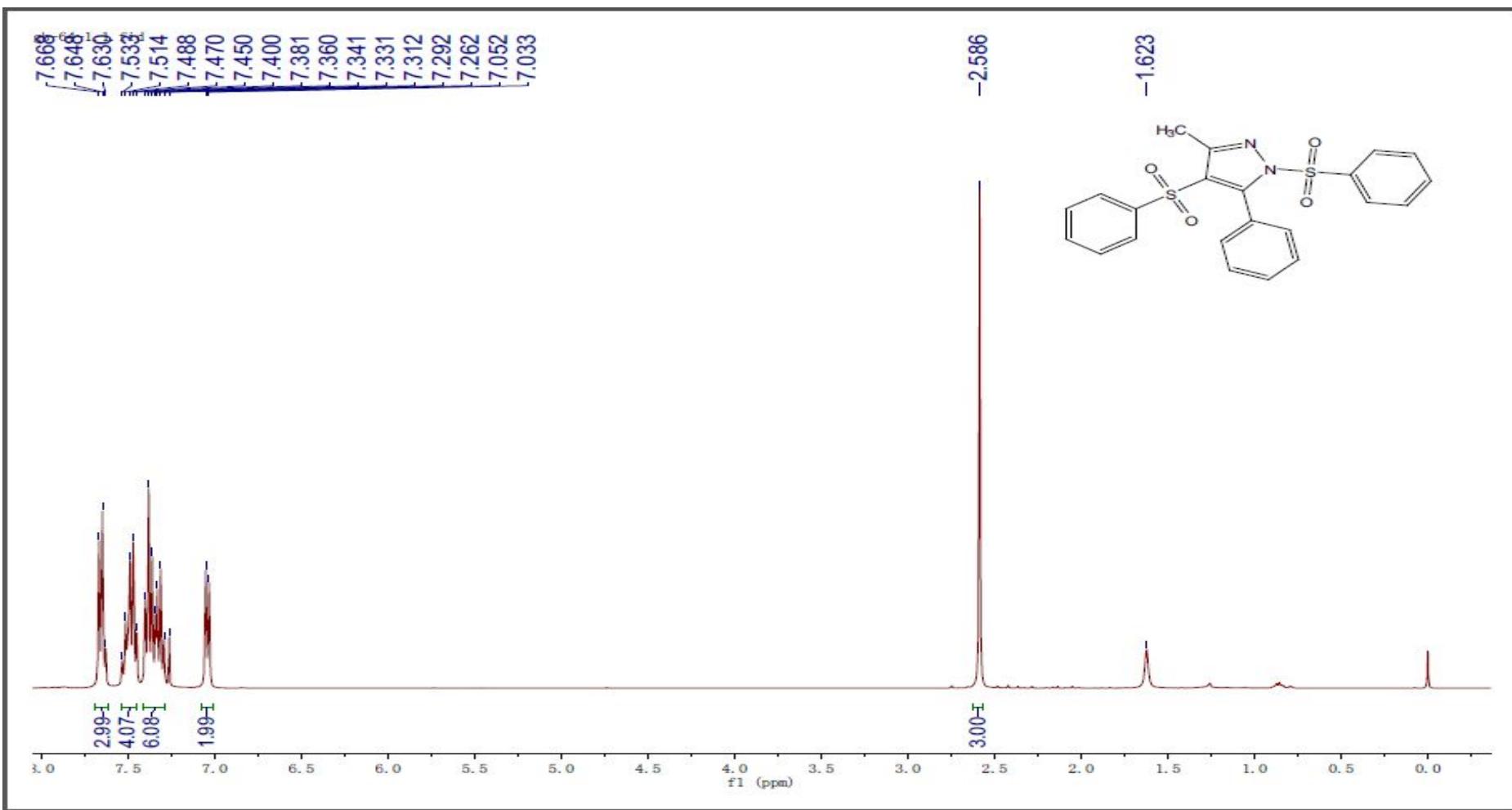
^1H and ^{13}C NMR spectra of all products



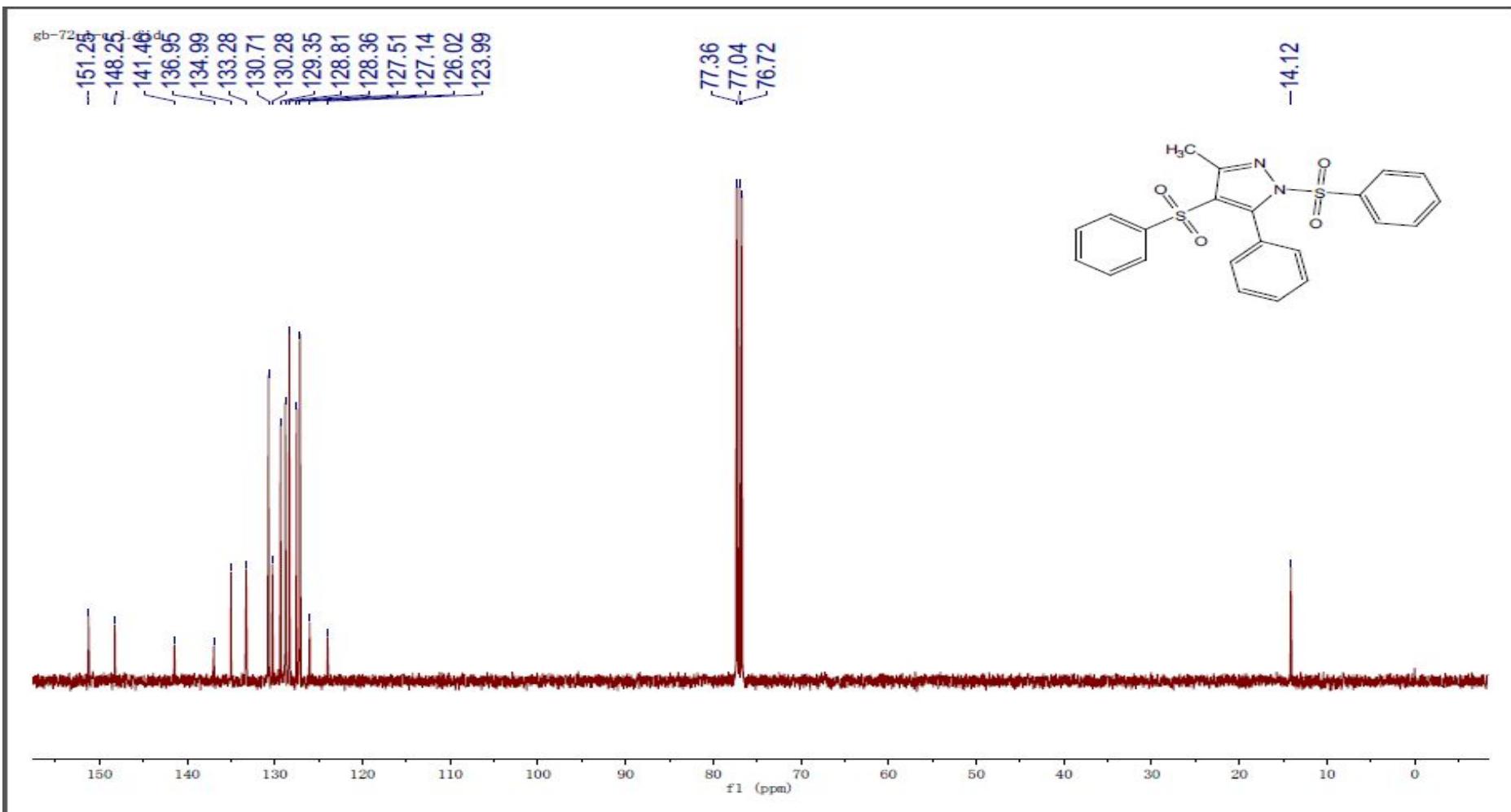
¹H NMR spectrum of 3a



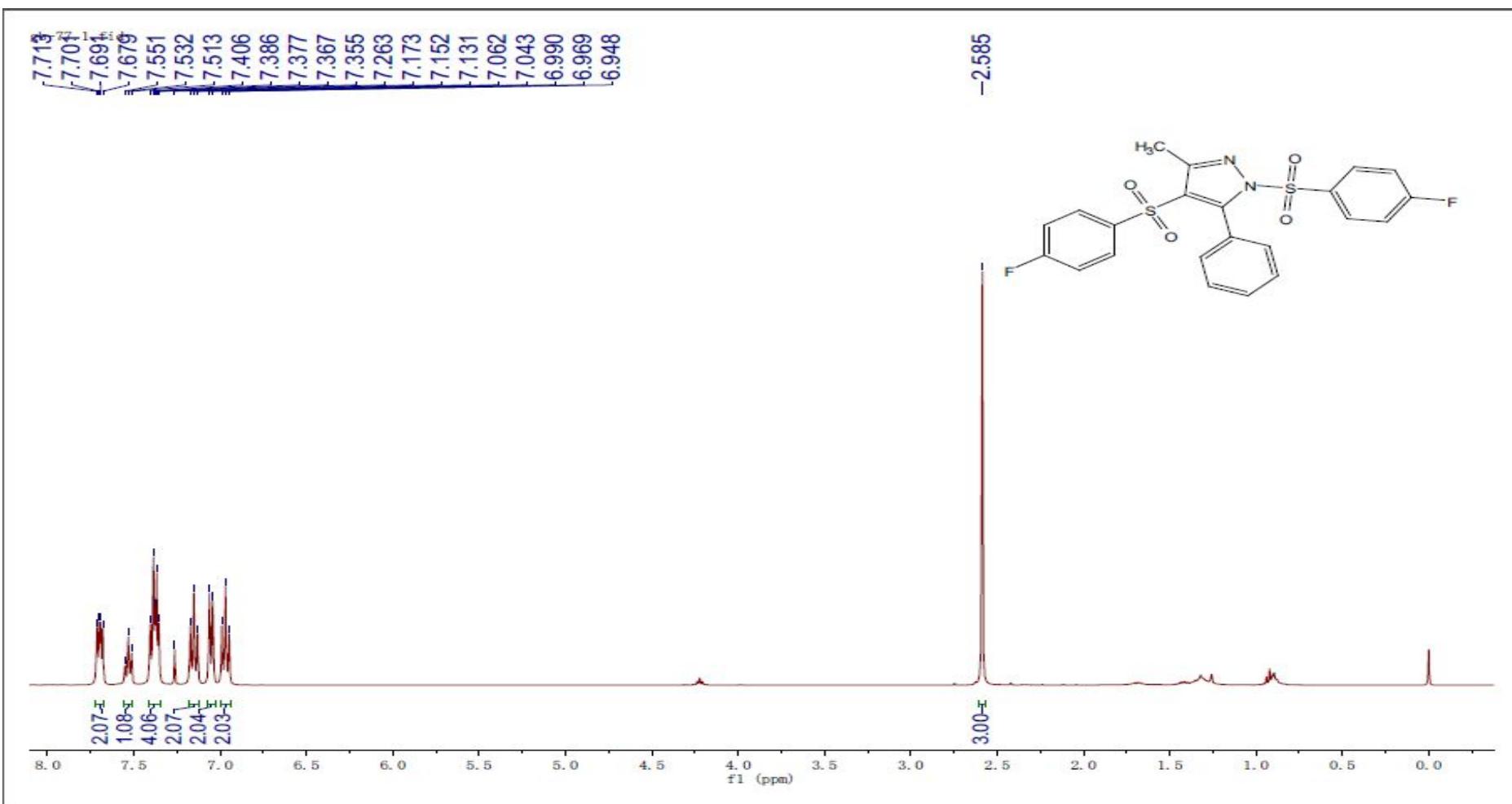
^{13}C NMR spectrum of **3a**



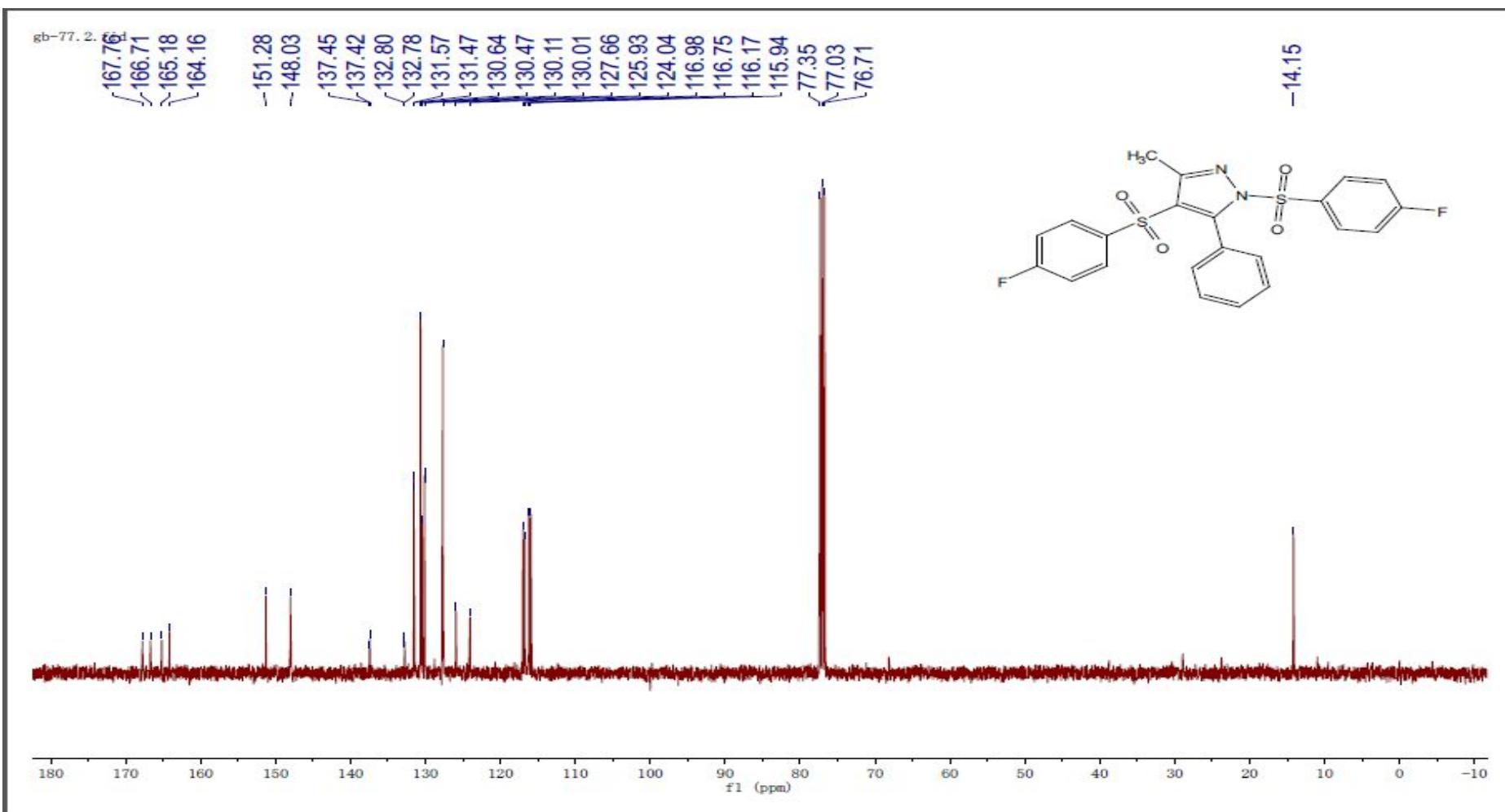
¹H NMR spectrum of **3b**



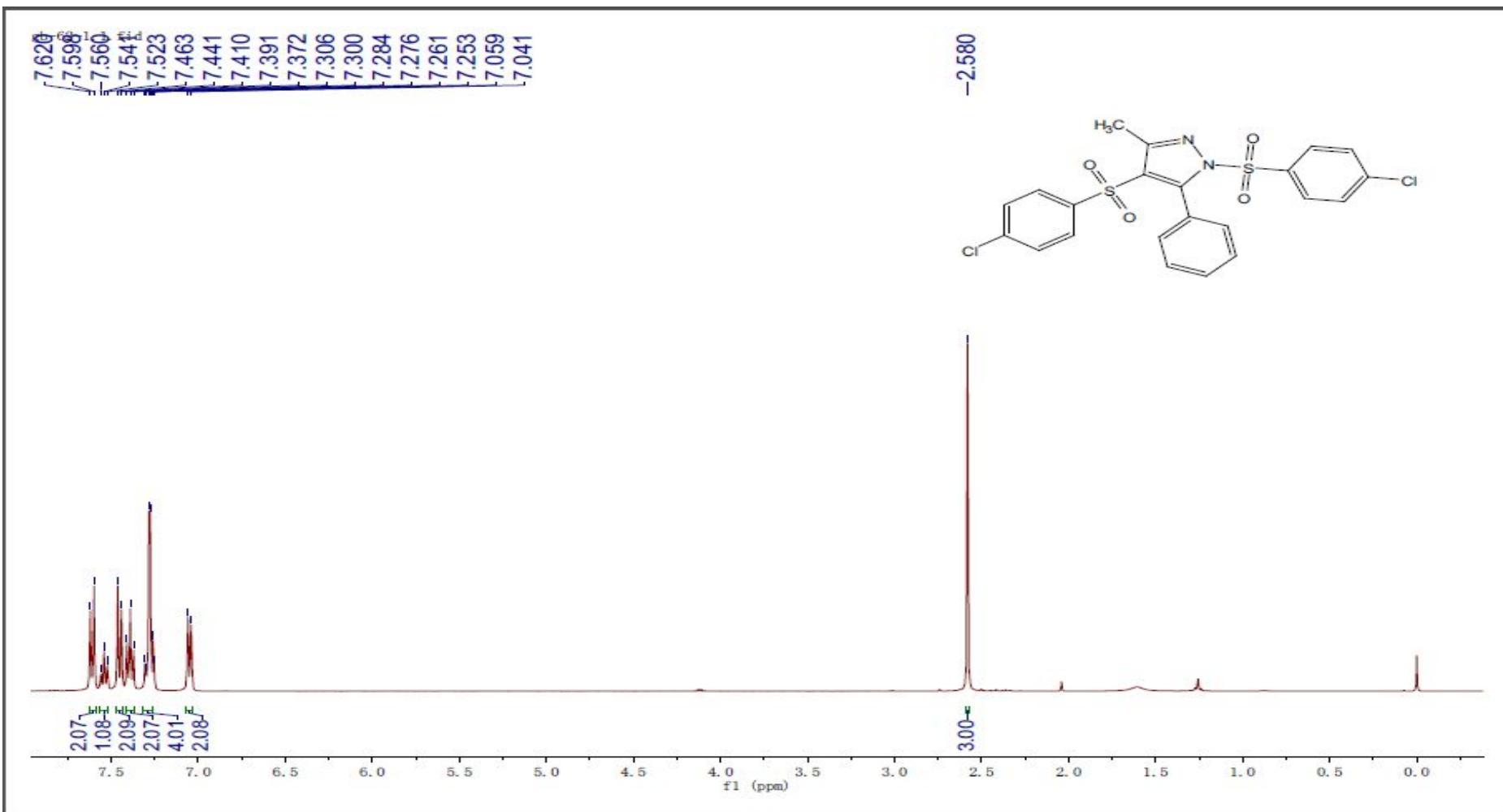
^{13}C NMR spectrum of **3b**



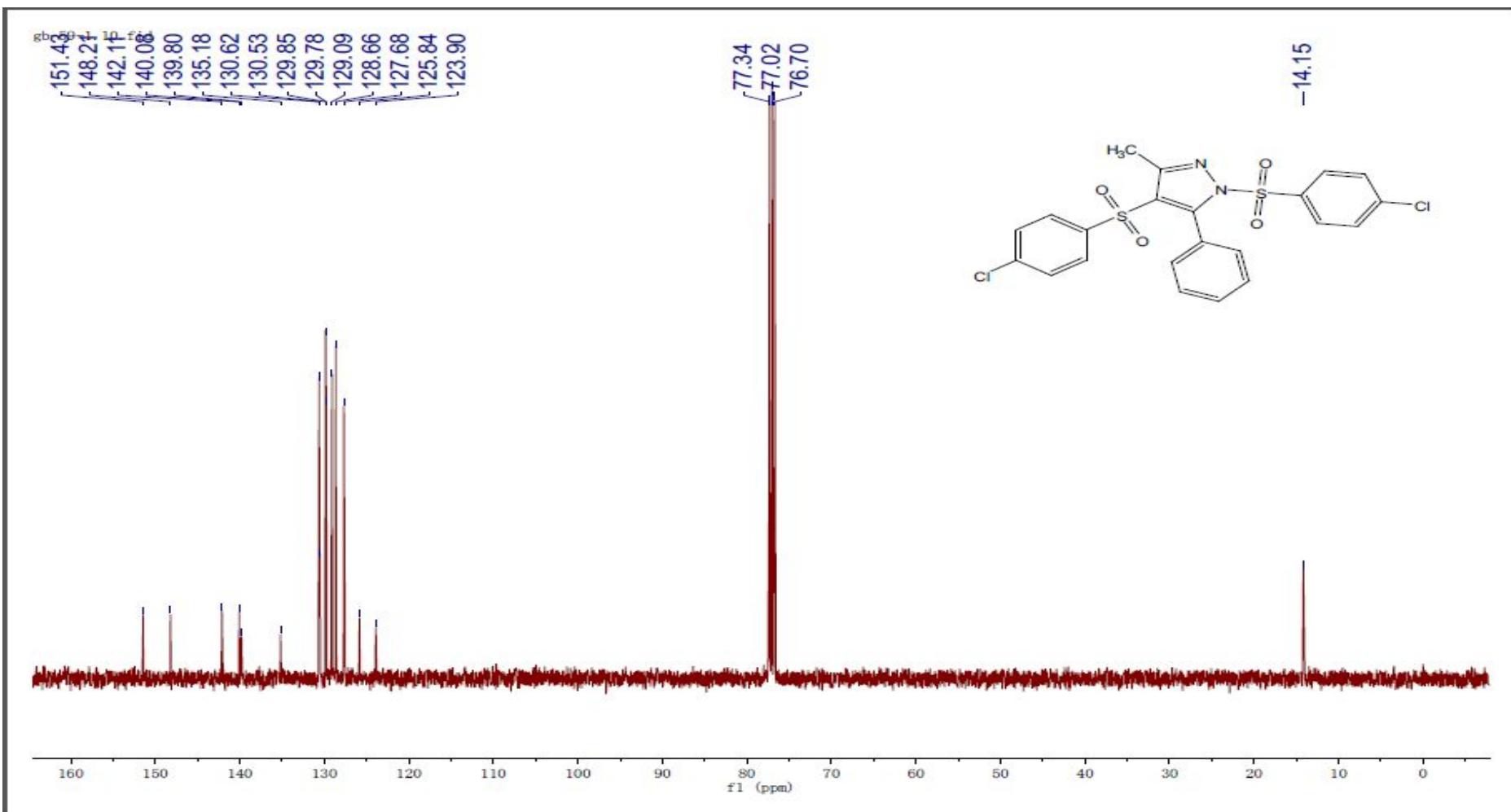
¹H NMR spectrum of **3c**



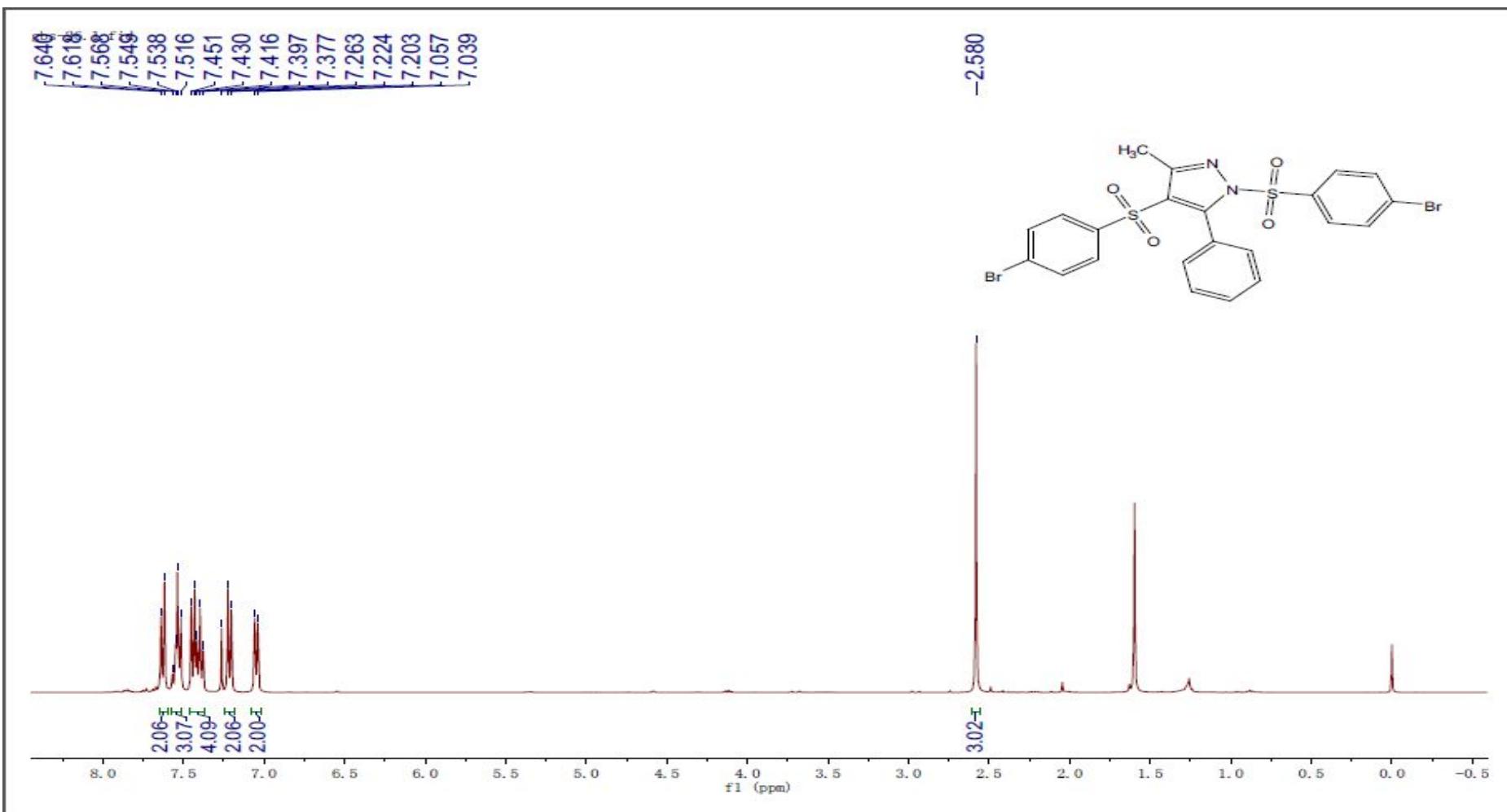
¹³C NMR spectrum of **3c**



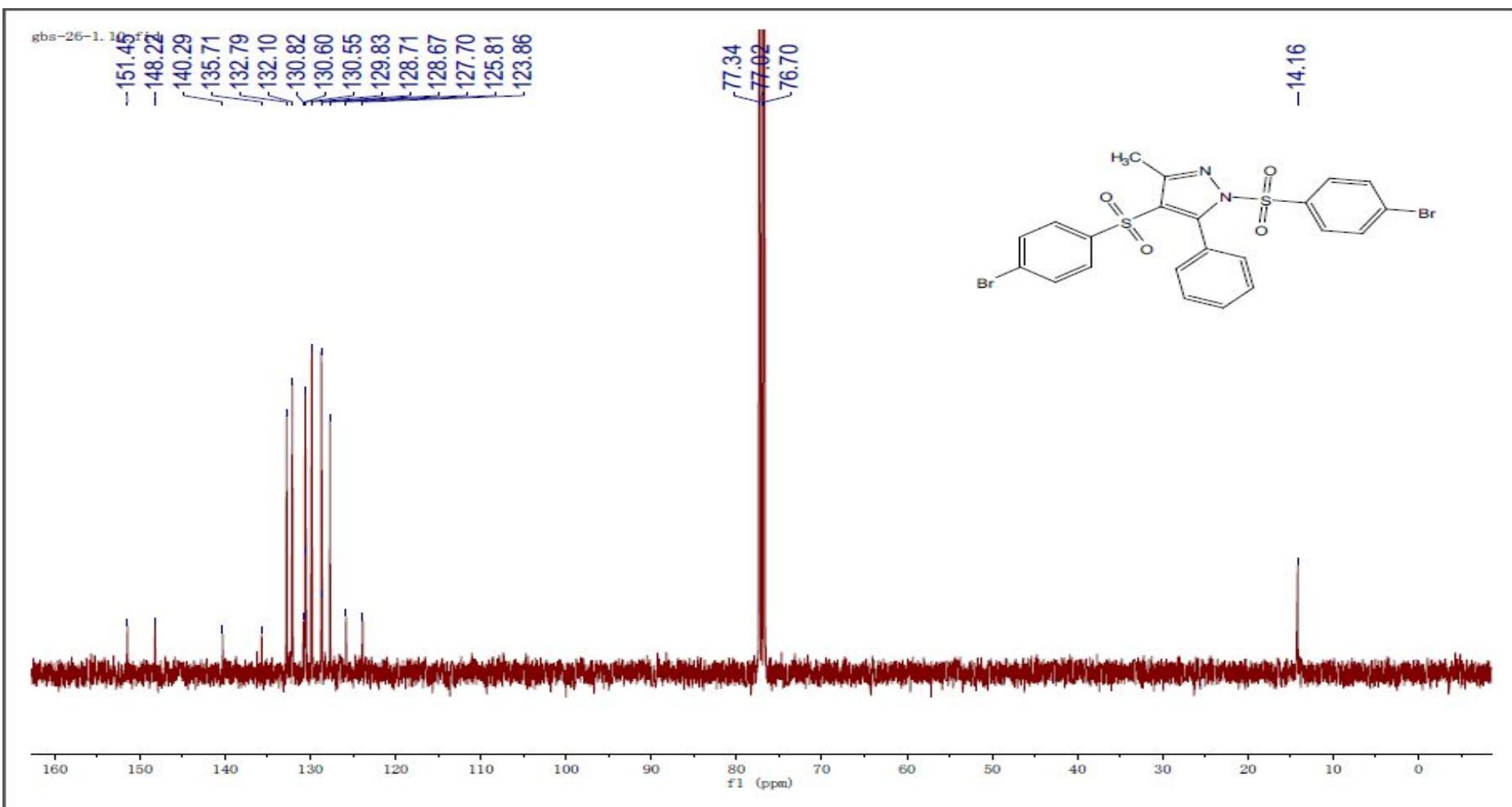
¹H NMR spectrum of **3d**



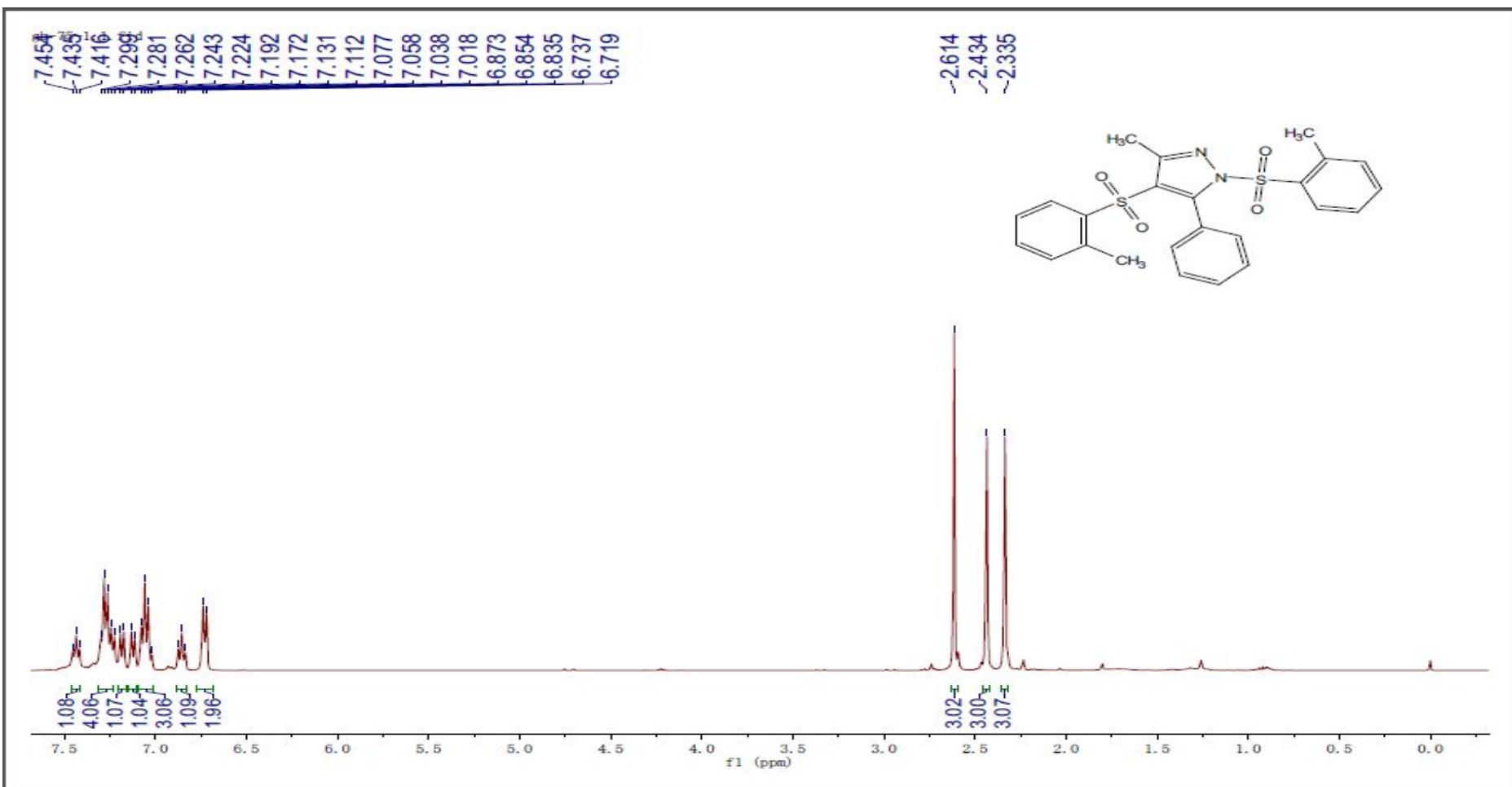
^{13}C NMR spectrum of **3d**



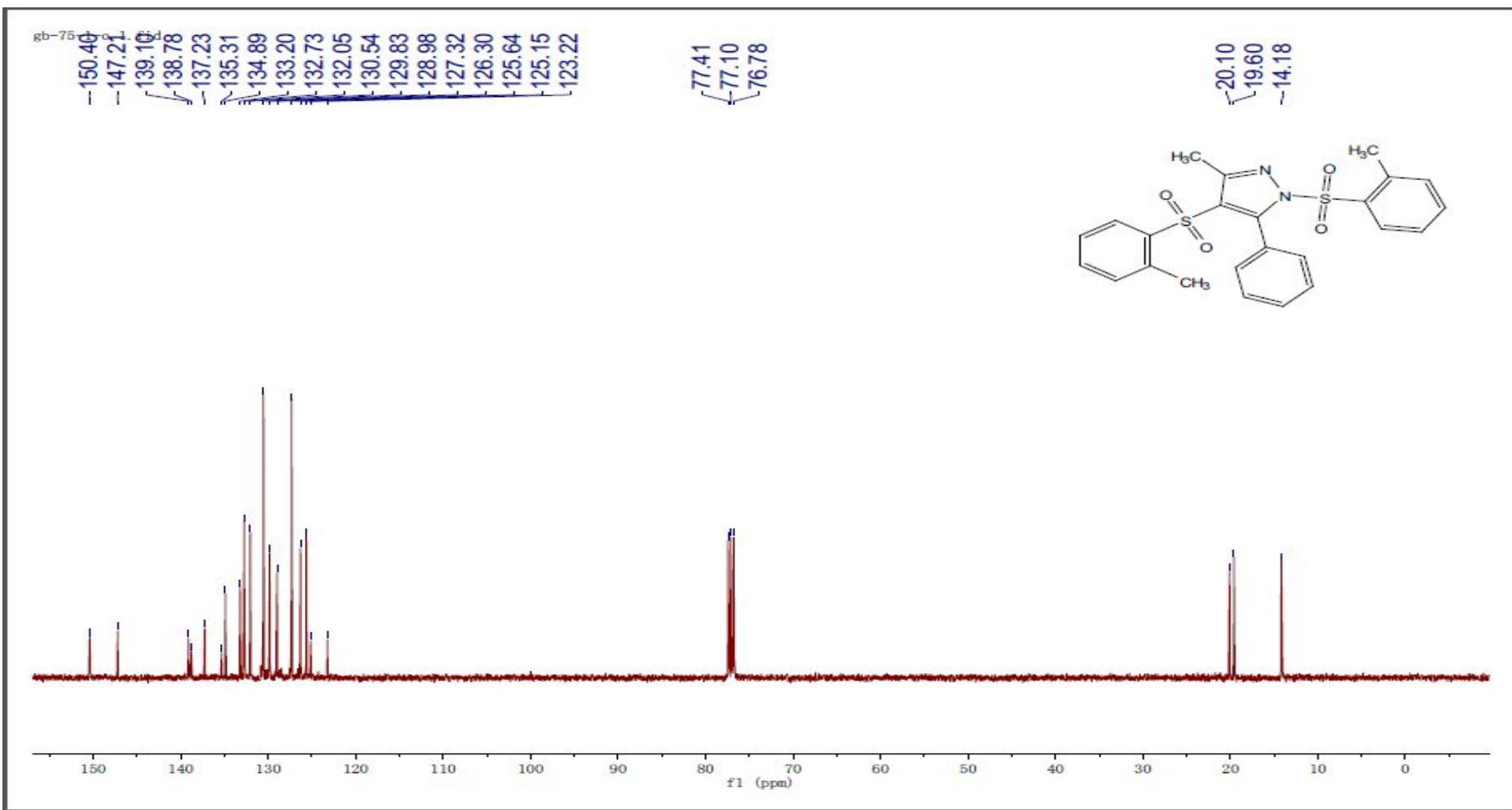
¹H NMR spectrum of 3e



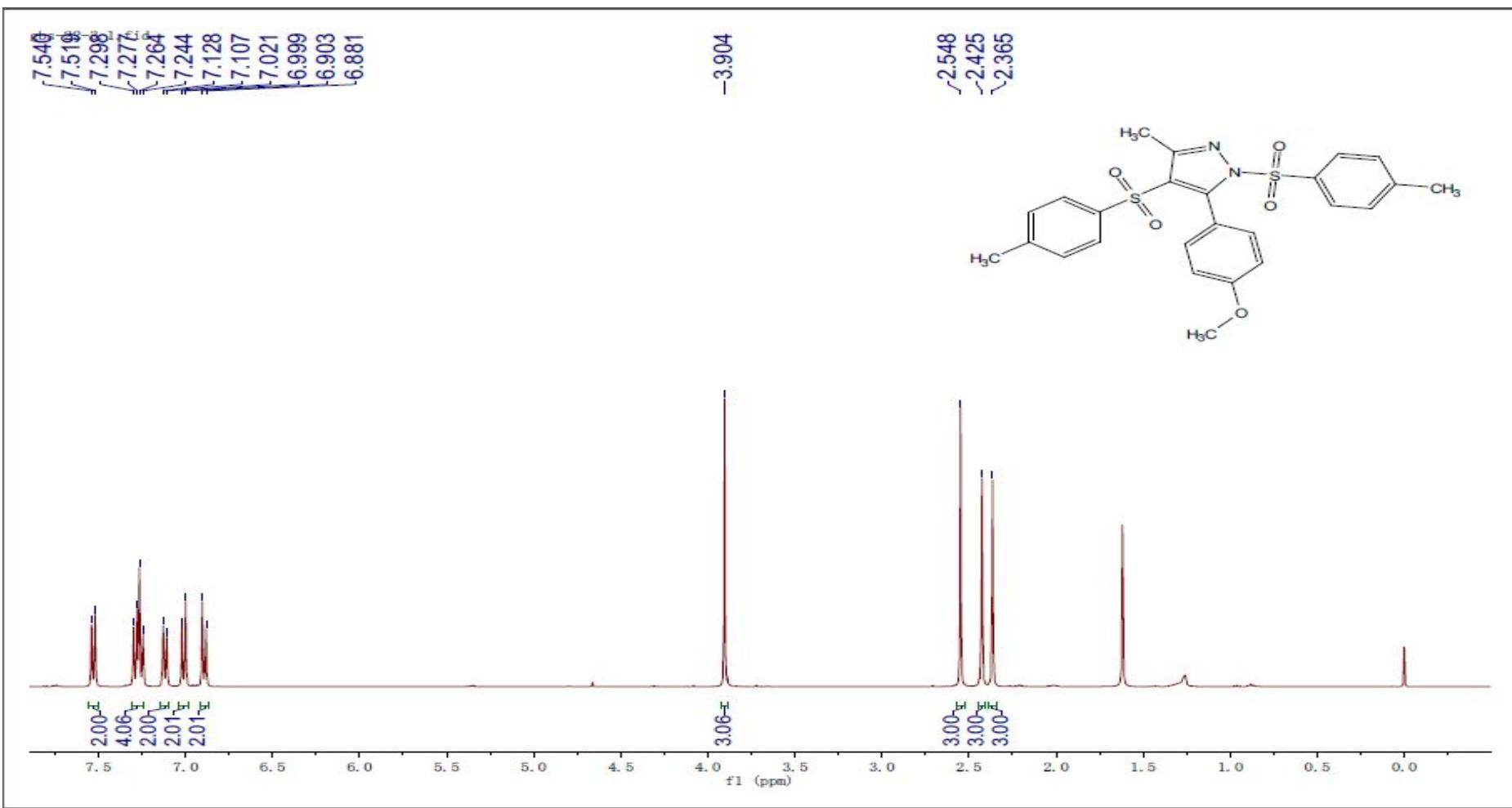
¹³C NMR spectrum of 3e



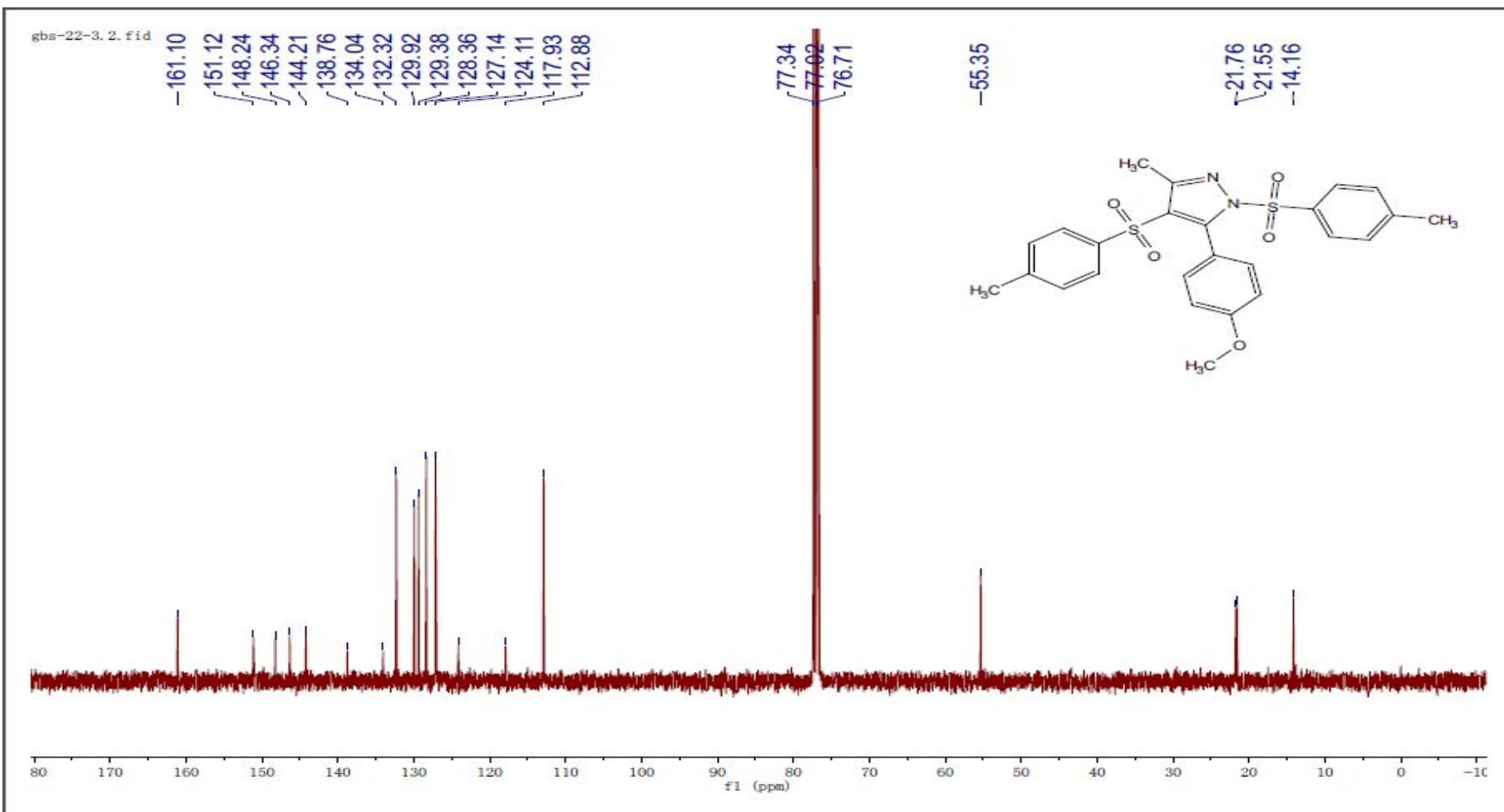
¹H NMR spectrum of 3f



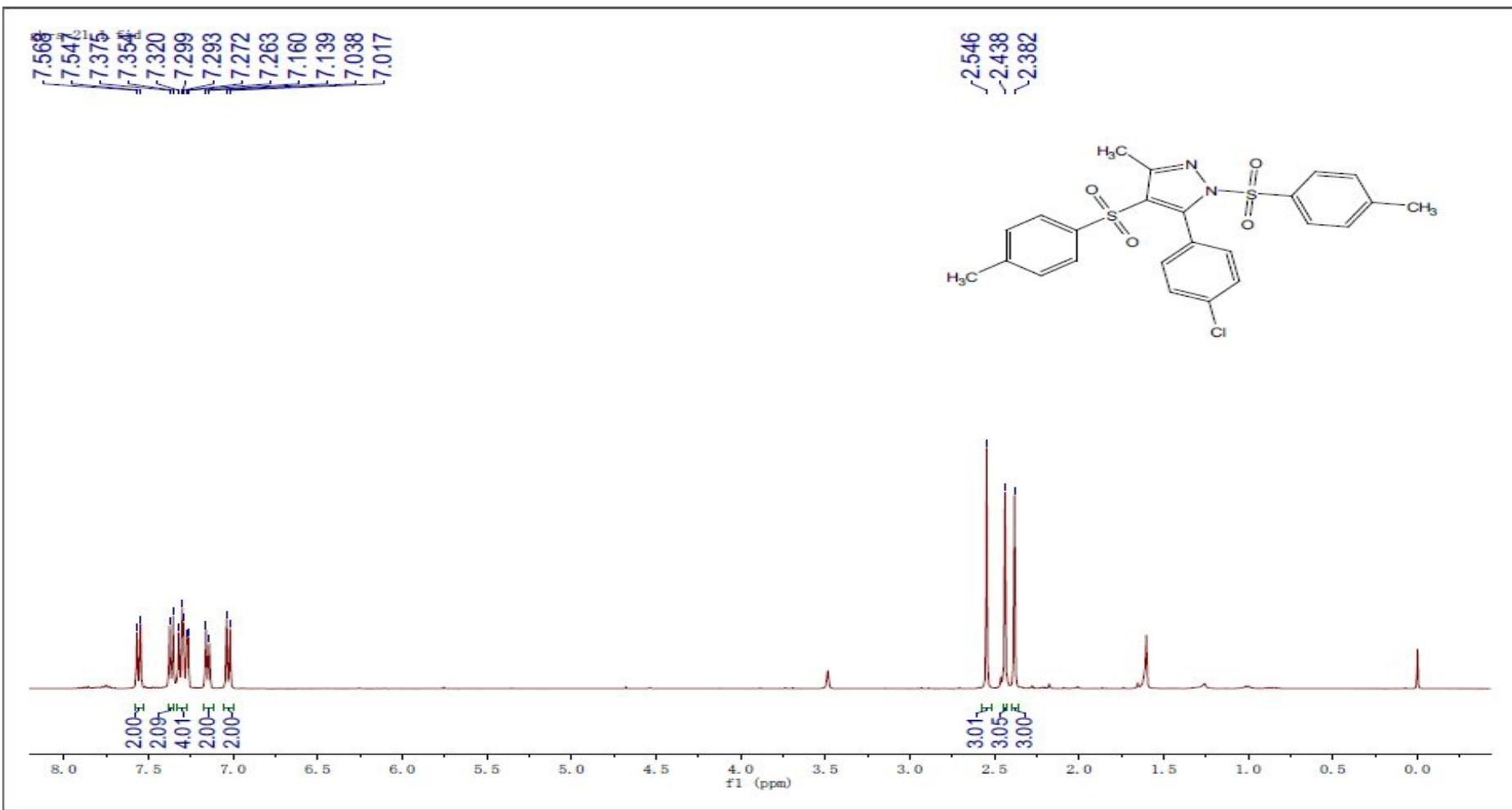
¹³C NMR spectrum of **3f**



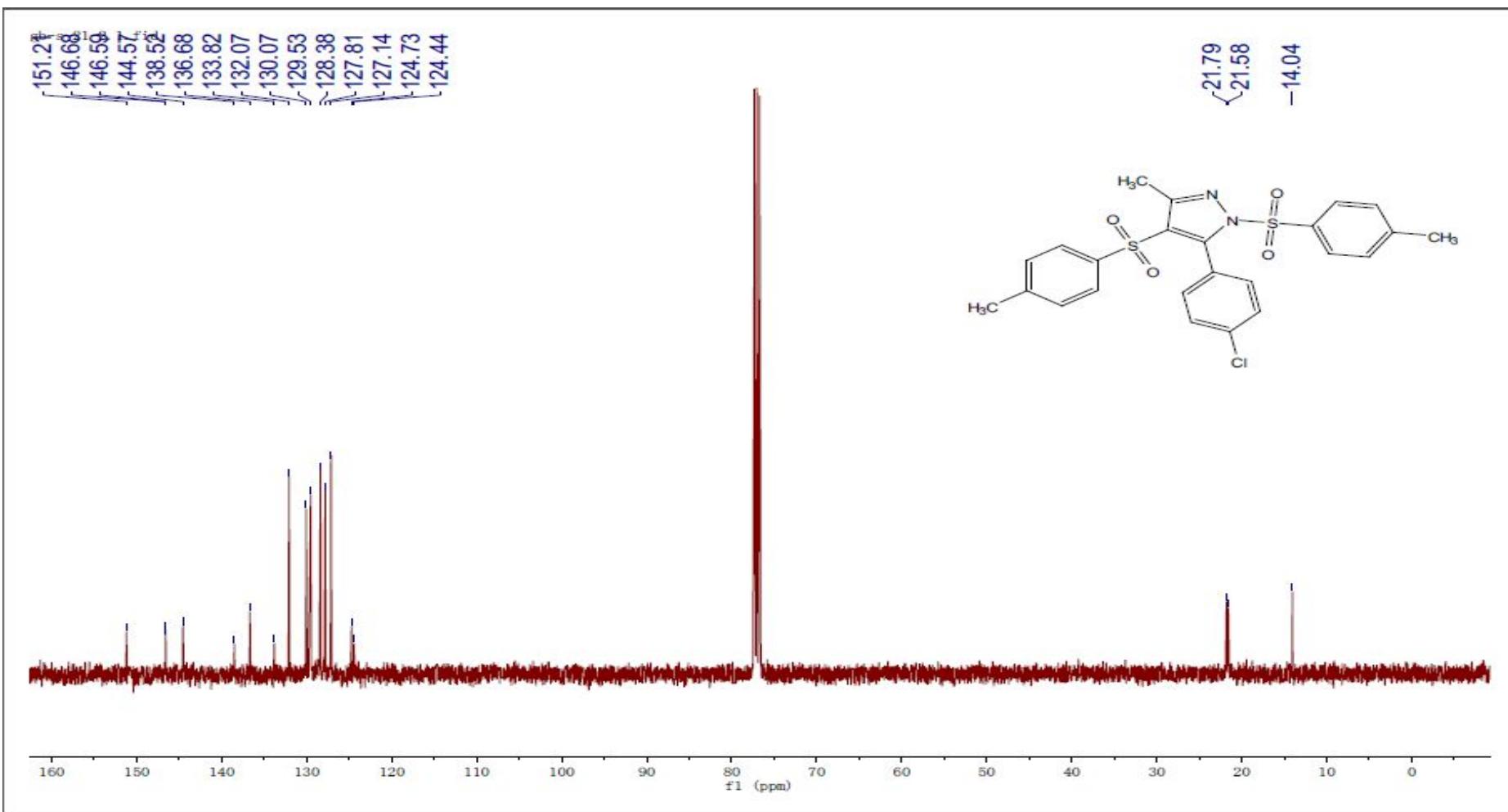
¹H NMR spectrum of 3g



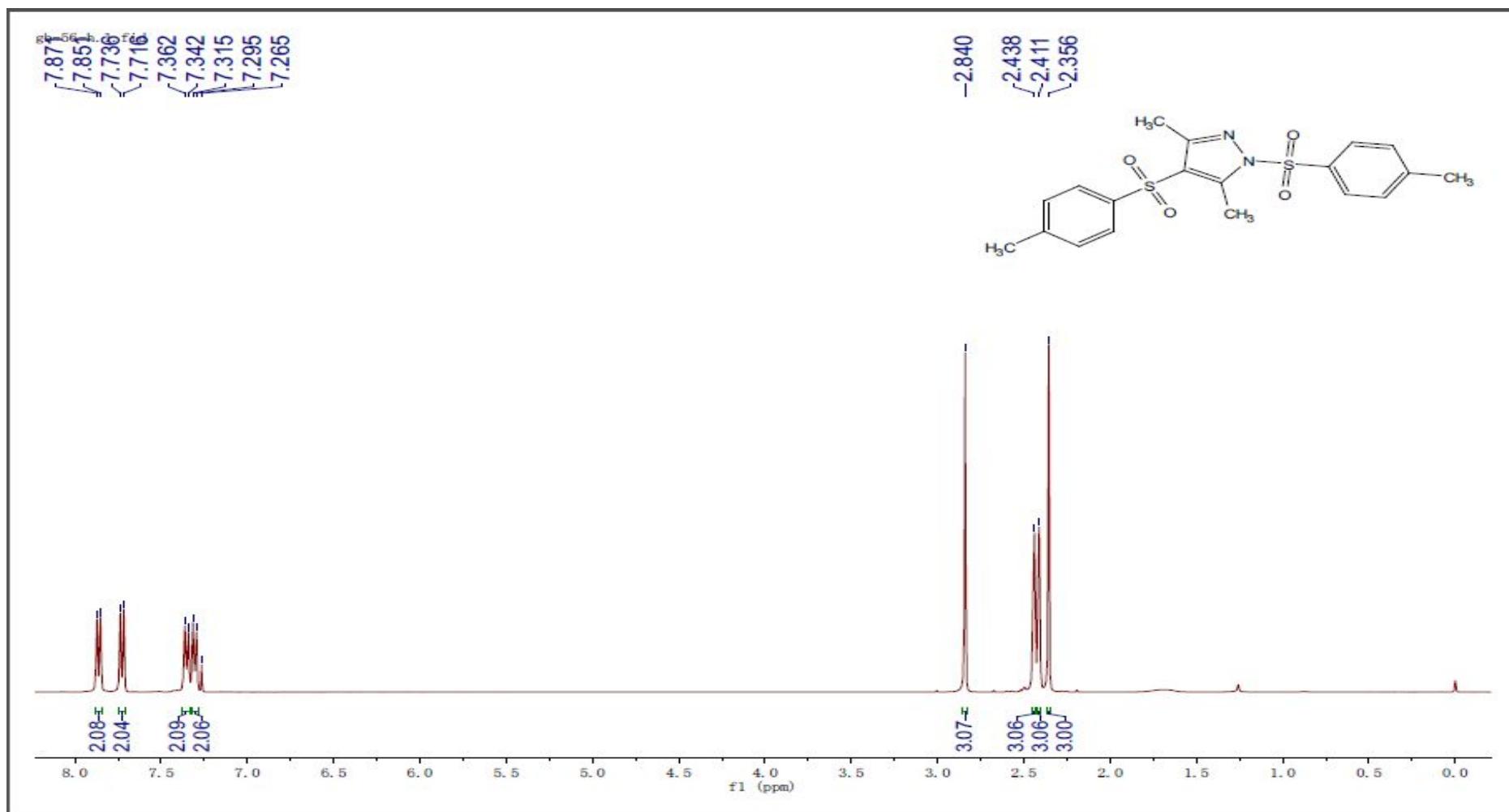
¹³C NMR spectrum of 3g



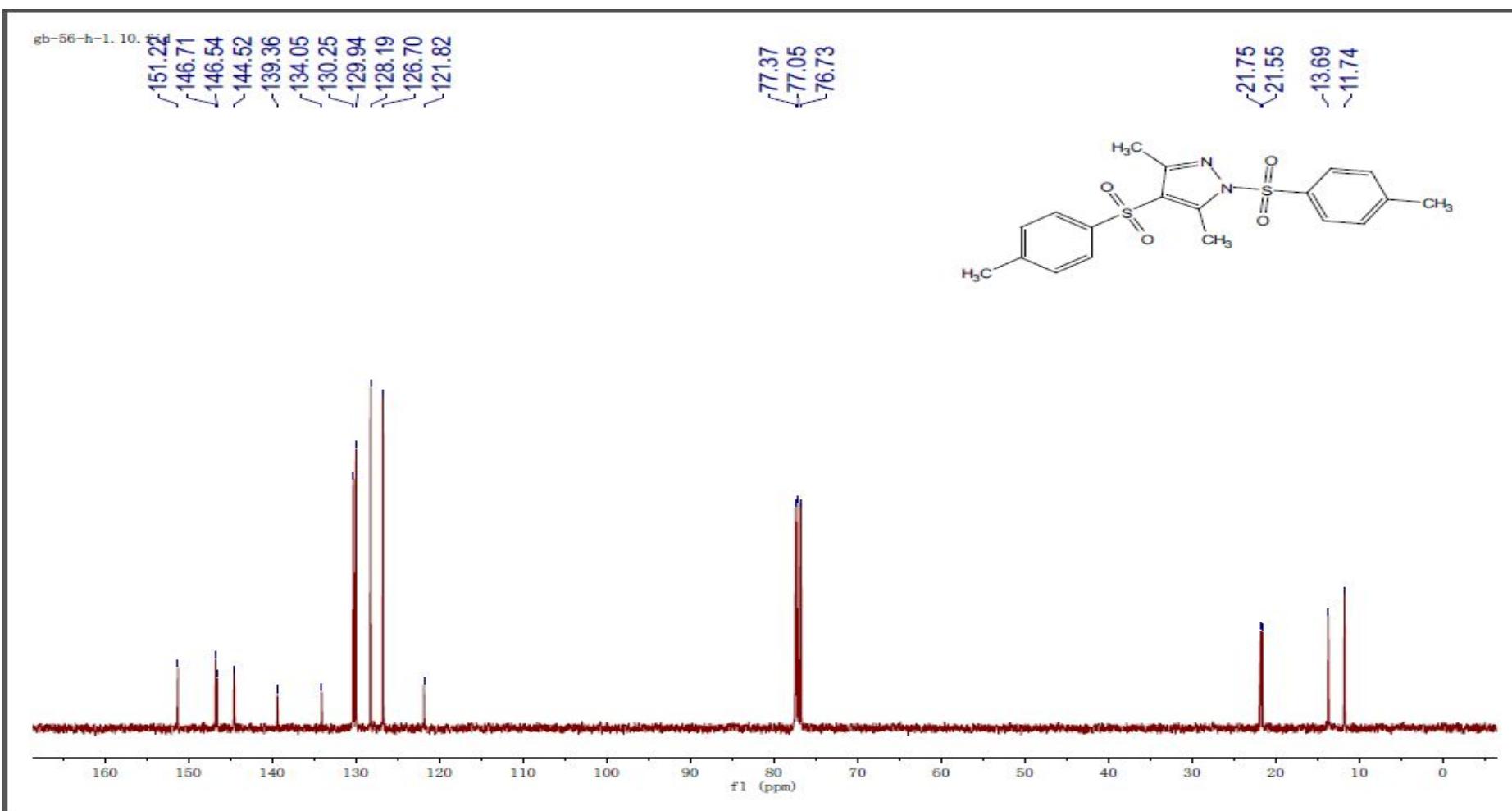
¹H NMR spectrum of **3h**



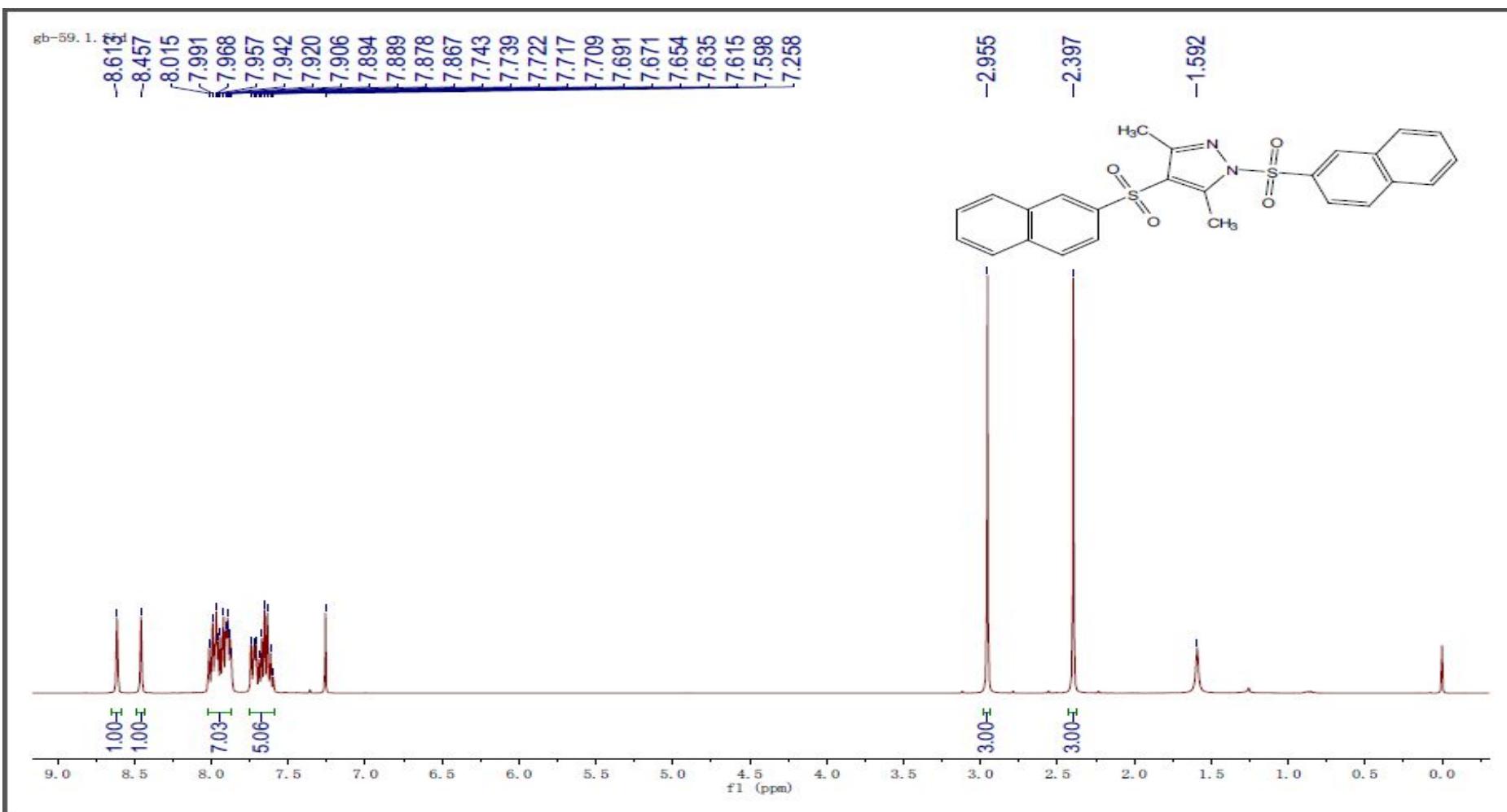
^{13}C NMR spectrum of **3h**

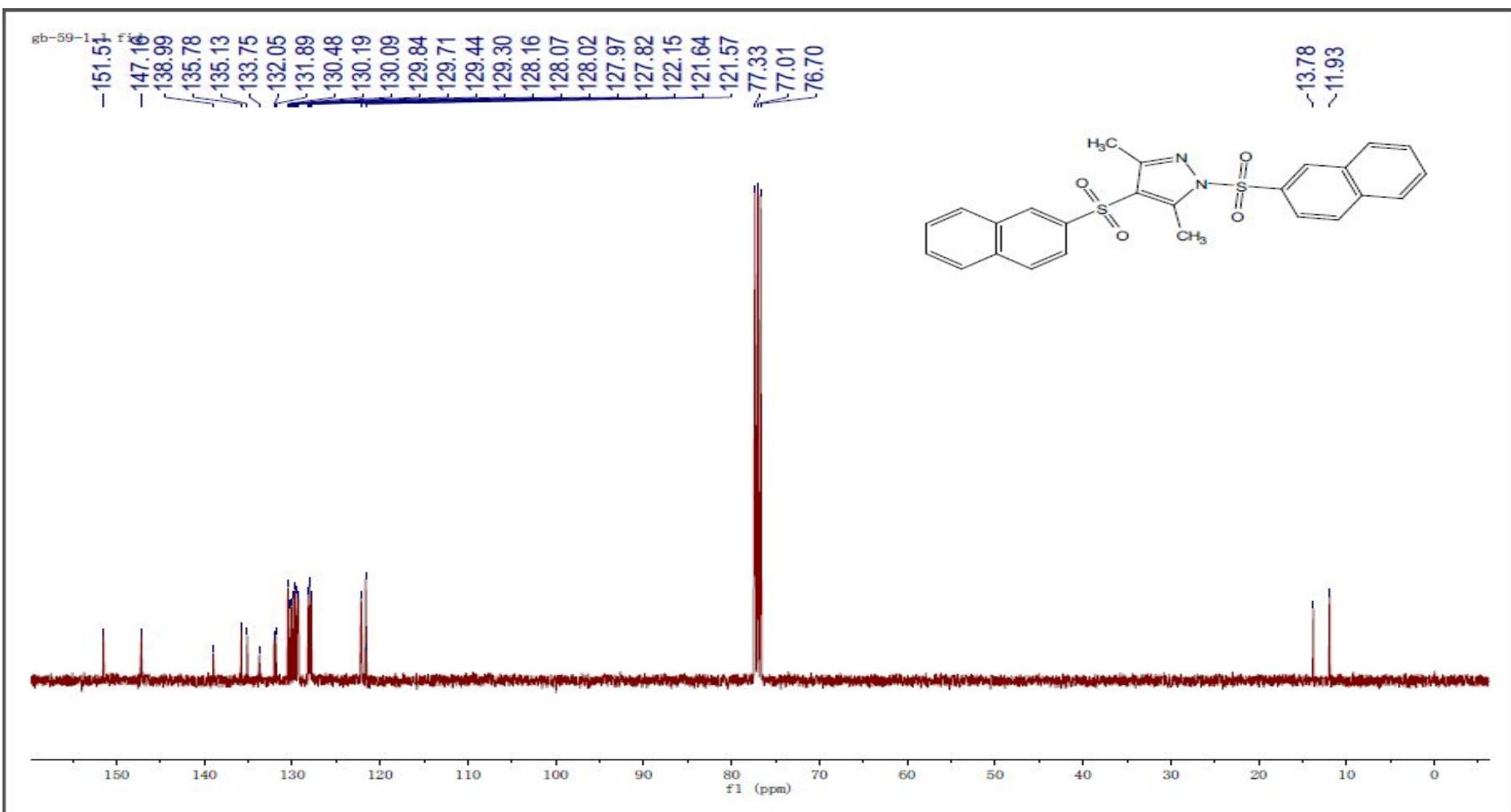


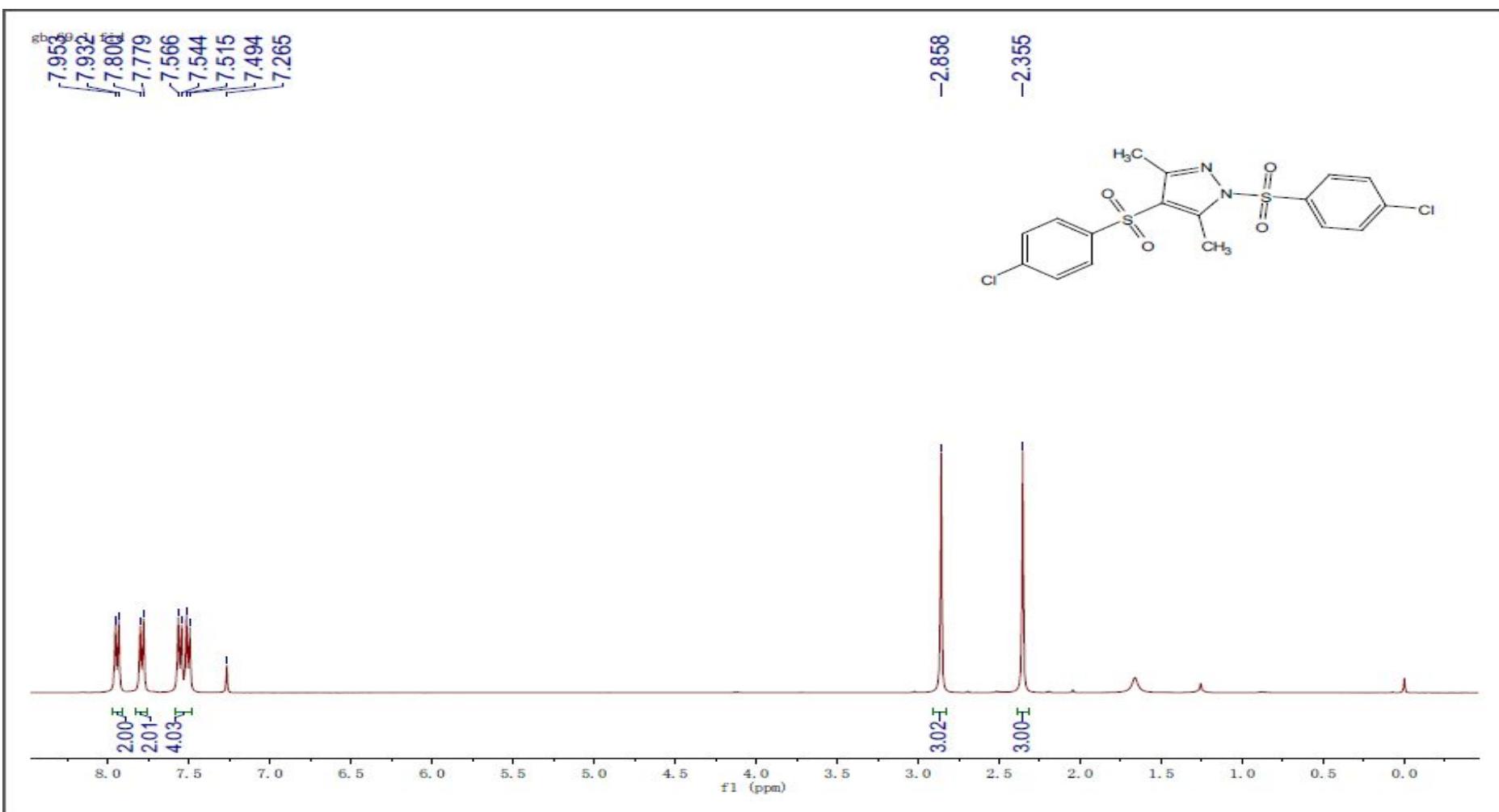
¹H NMR spectrum of 3i



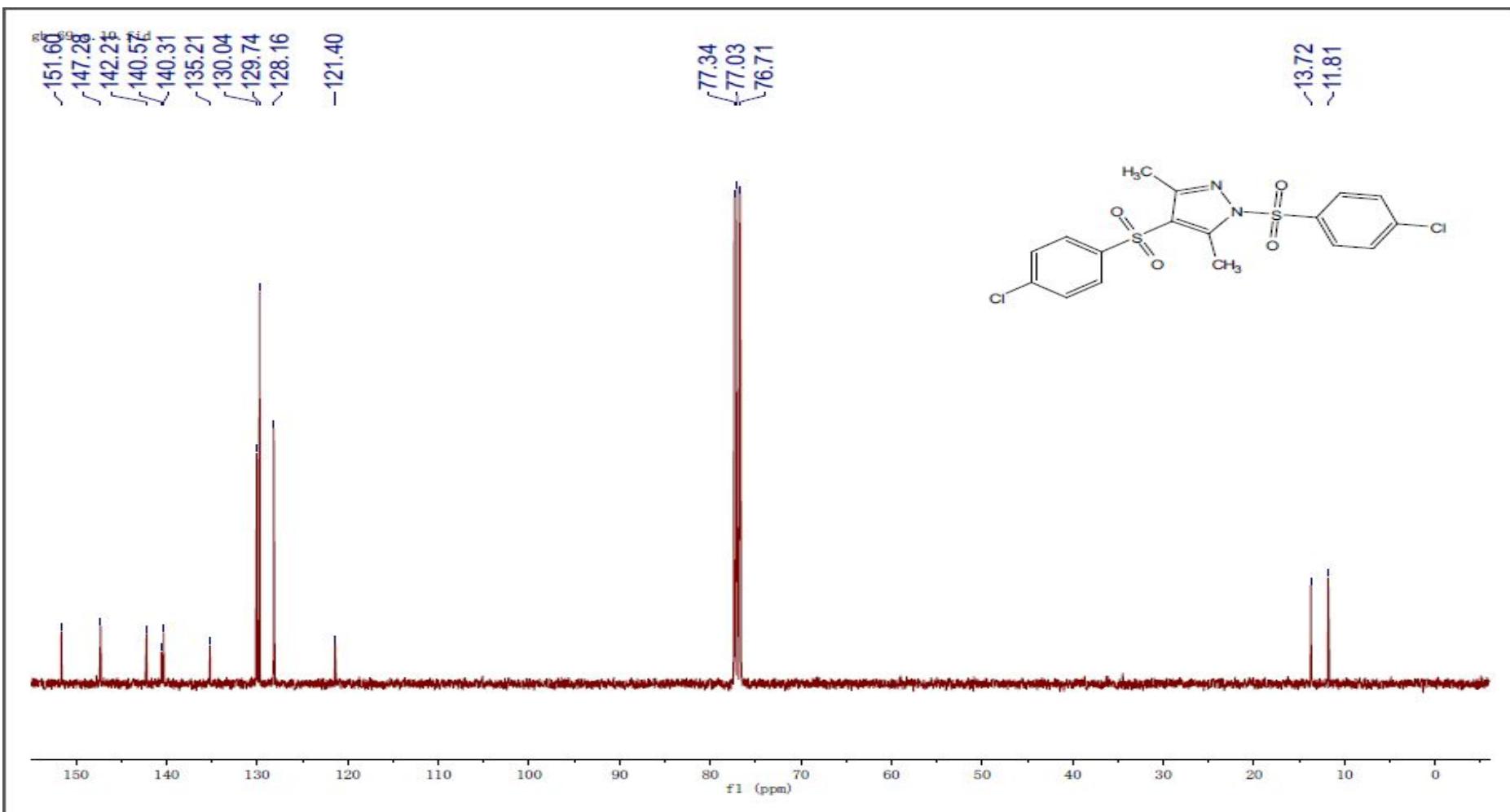
¹³C NMR spectrum of 3i



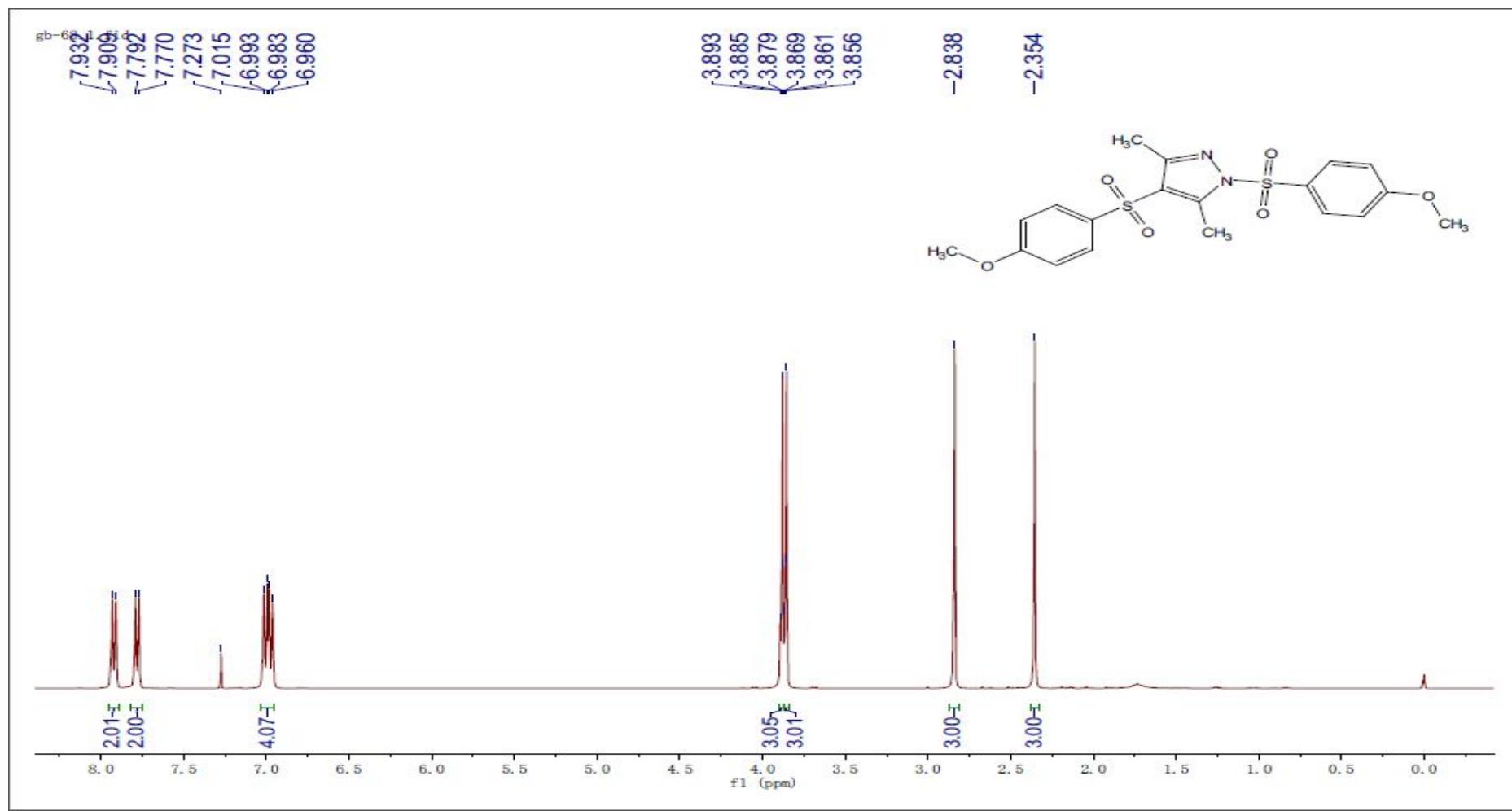




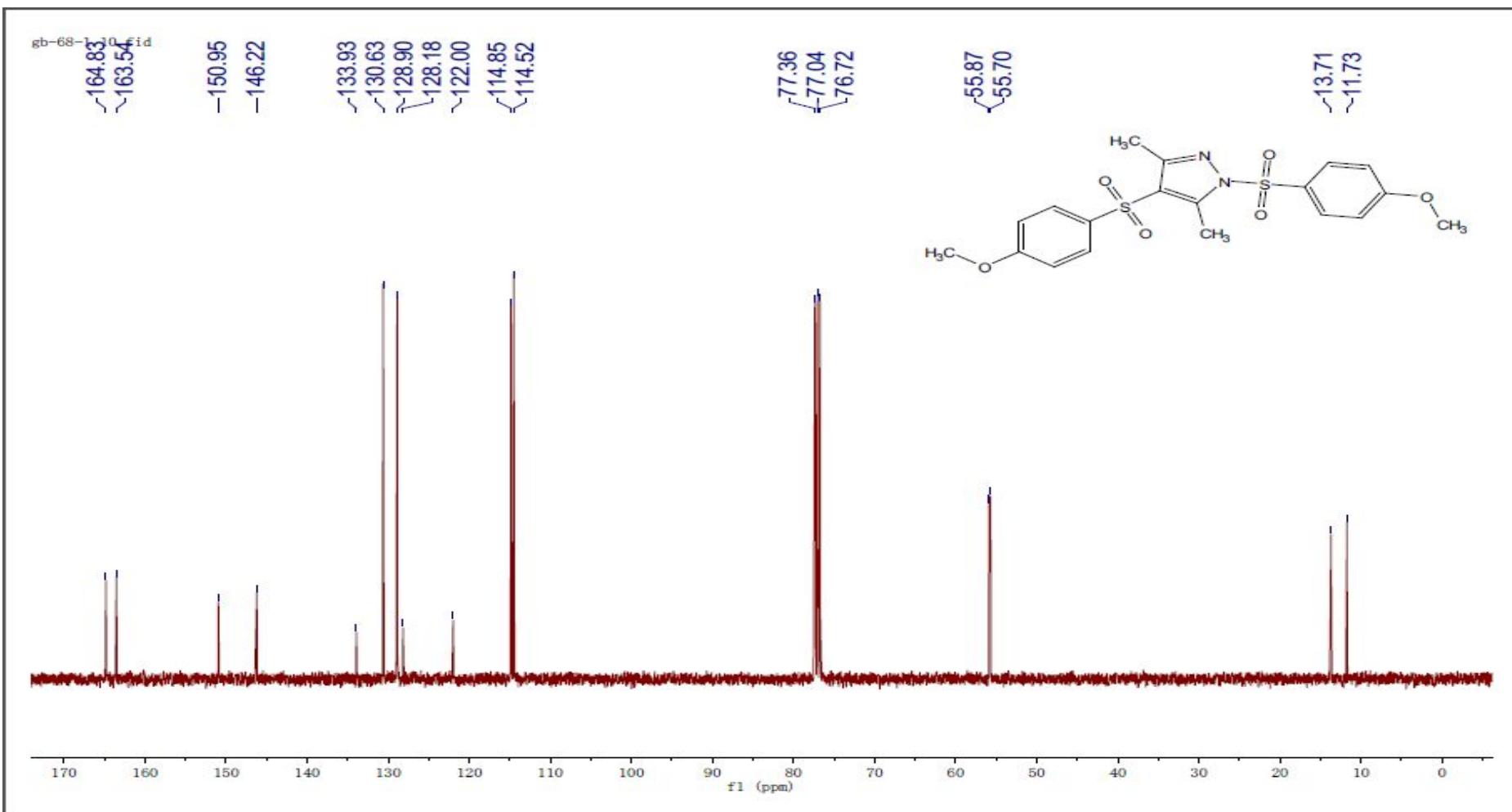
¹H NMR spectrum of **3k**



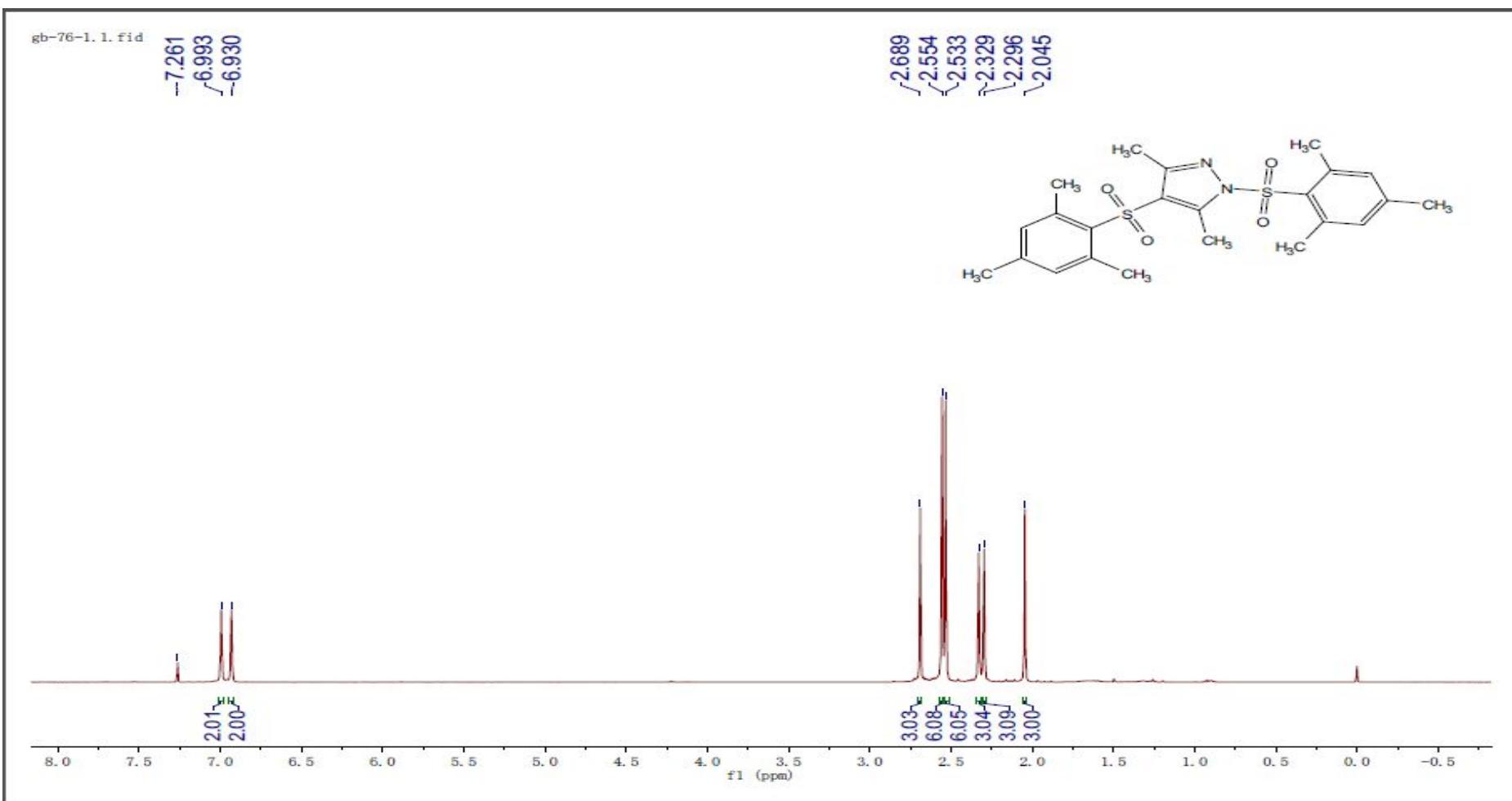
¹³C NMR spectrum of **3k**



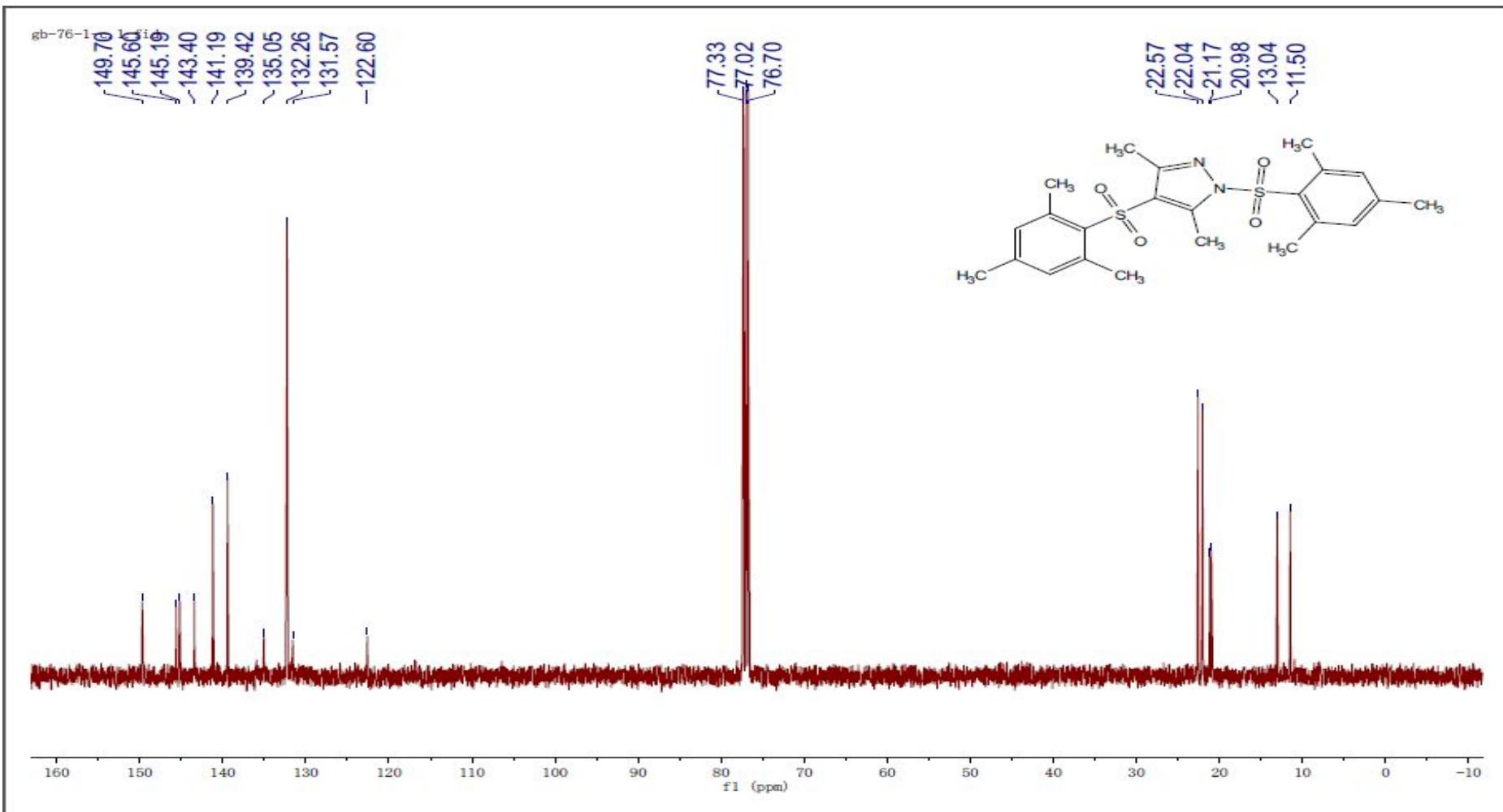
¹H NMR spectrum of 3I



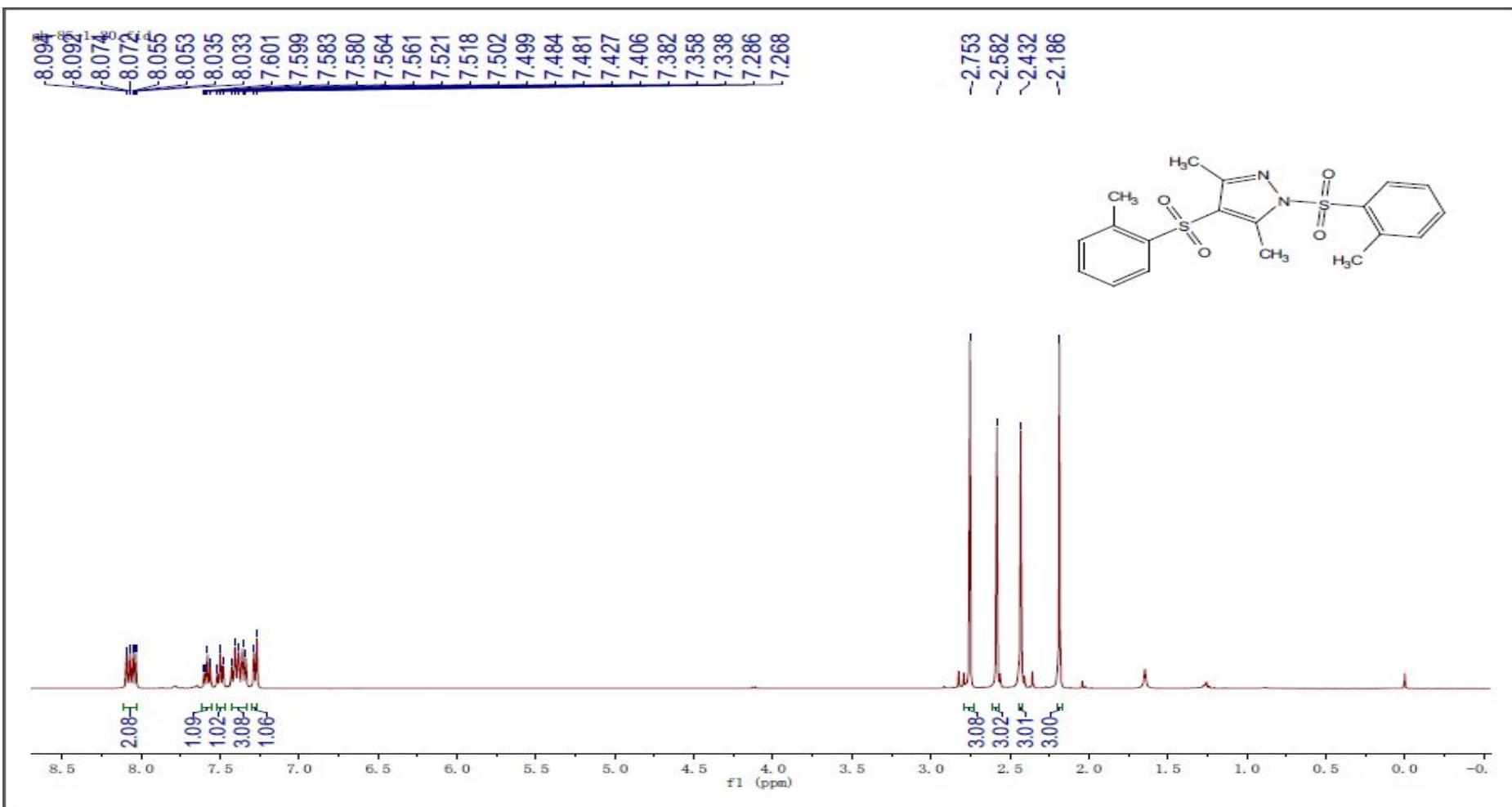
¹³C NMR spectrum of 3l



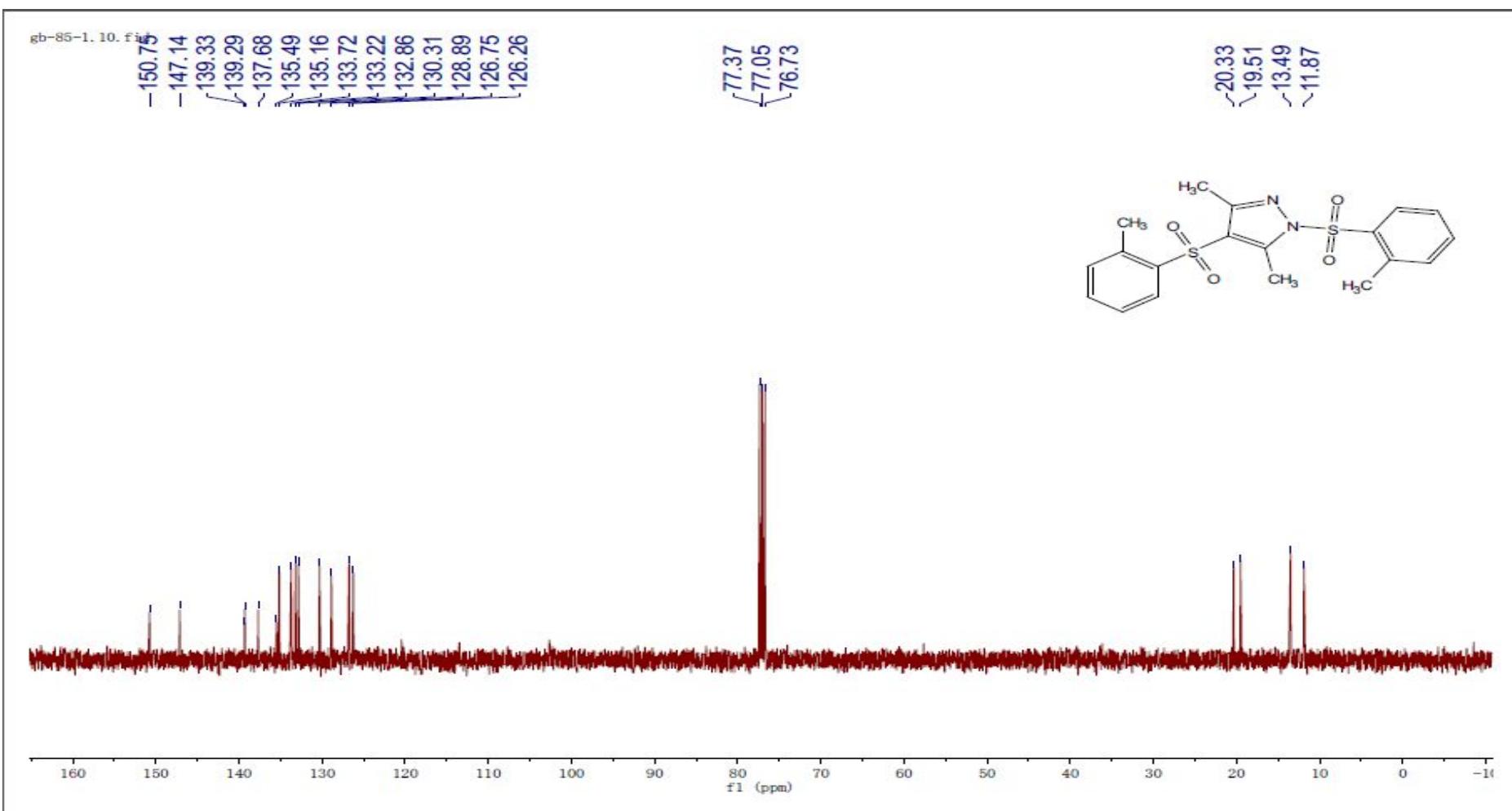
¹H NMR spectrum of 3m



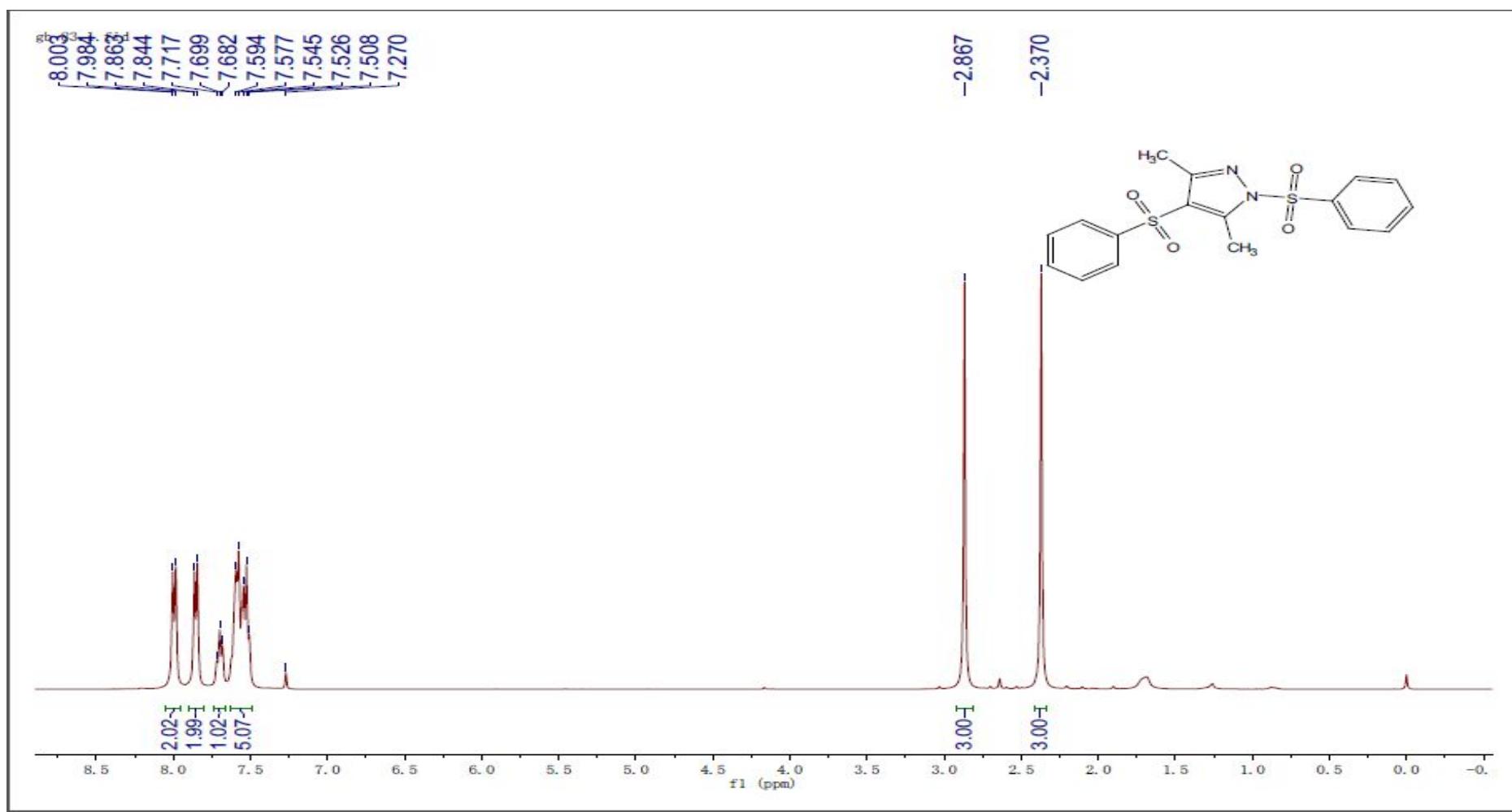
^{13}C NMR spectrum of **3m**



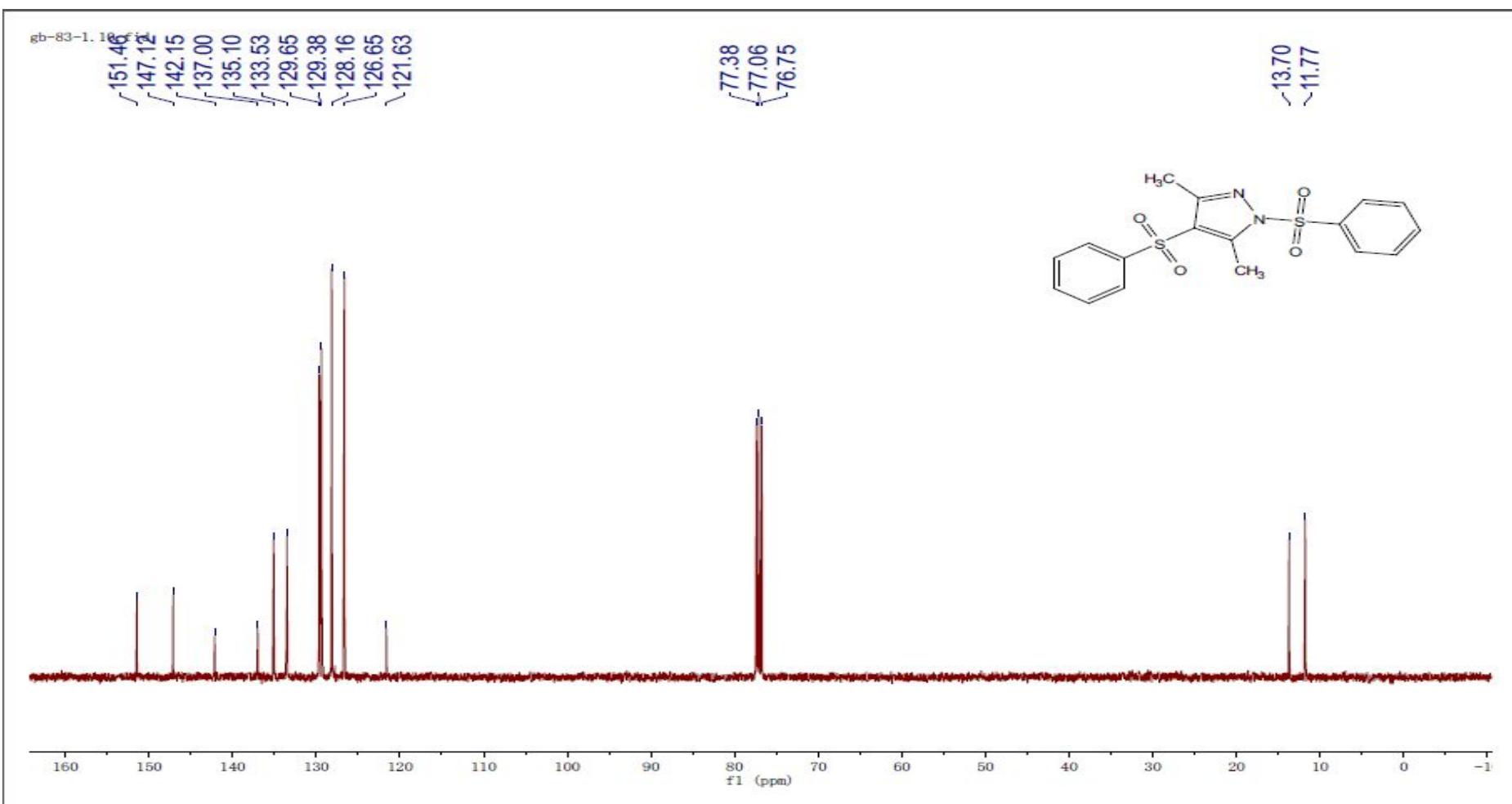
¹H NMR spectrum of **3n**



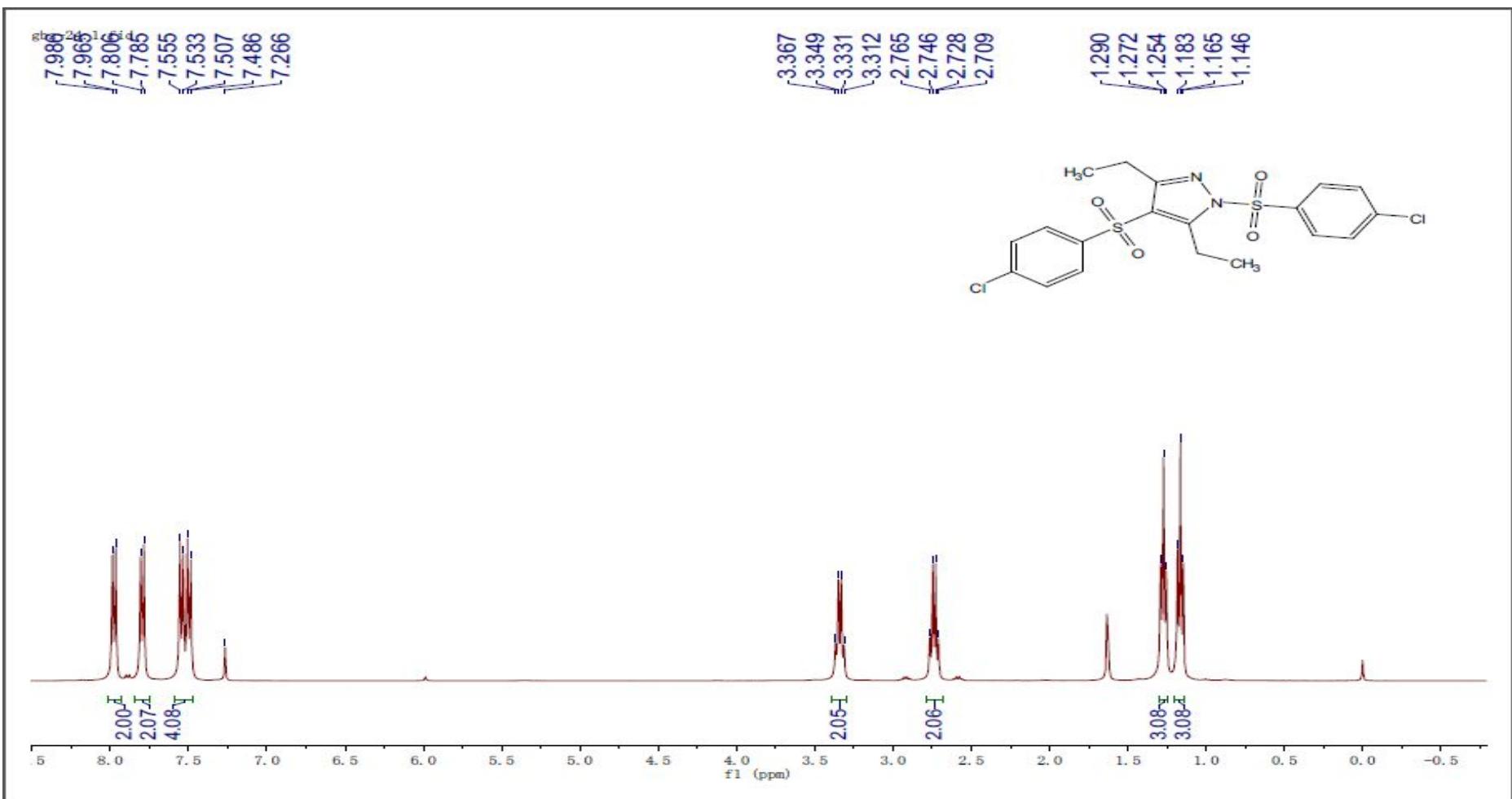
¹³C NMR spectrum of **3n**



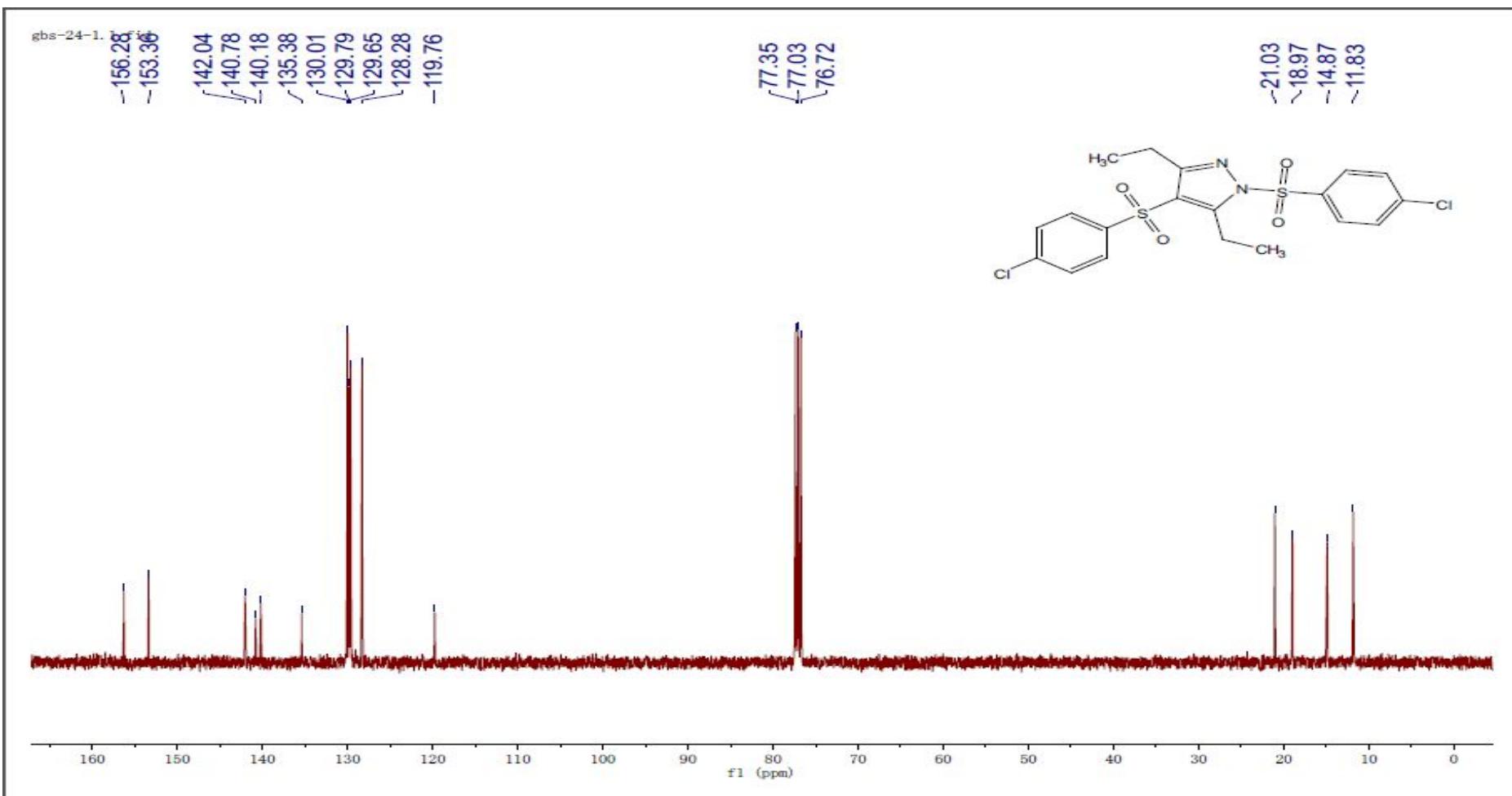
¹H NMR spectrum of **3o**



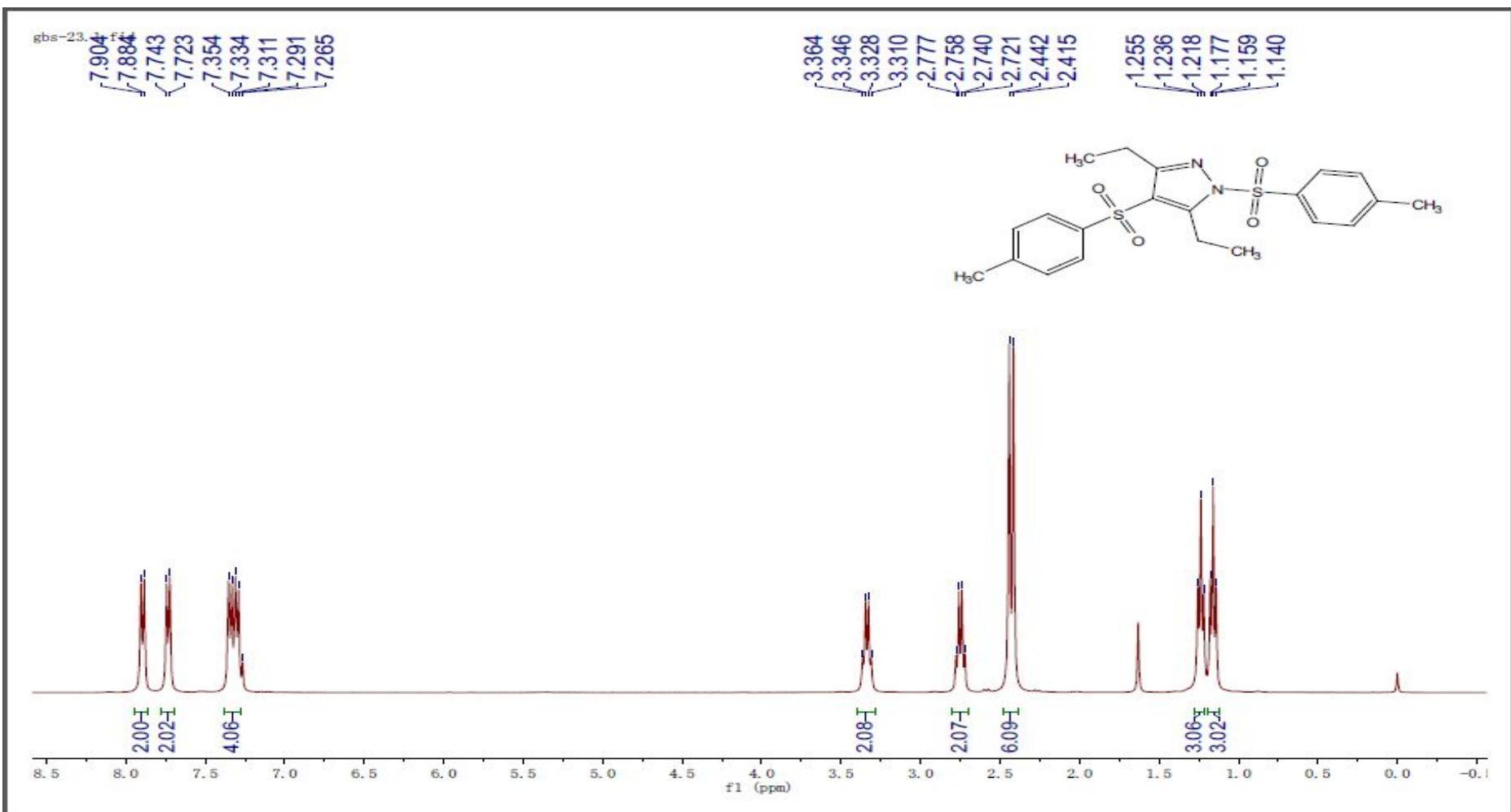
^{13}C NMR spectrum of **3o**



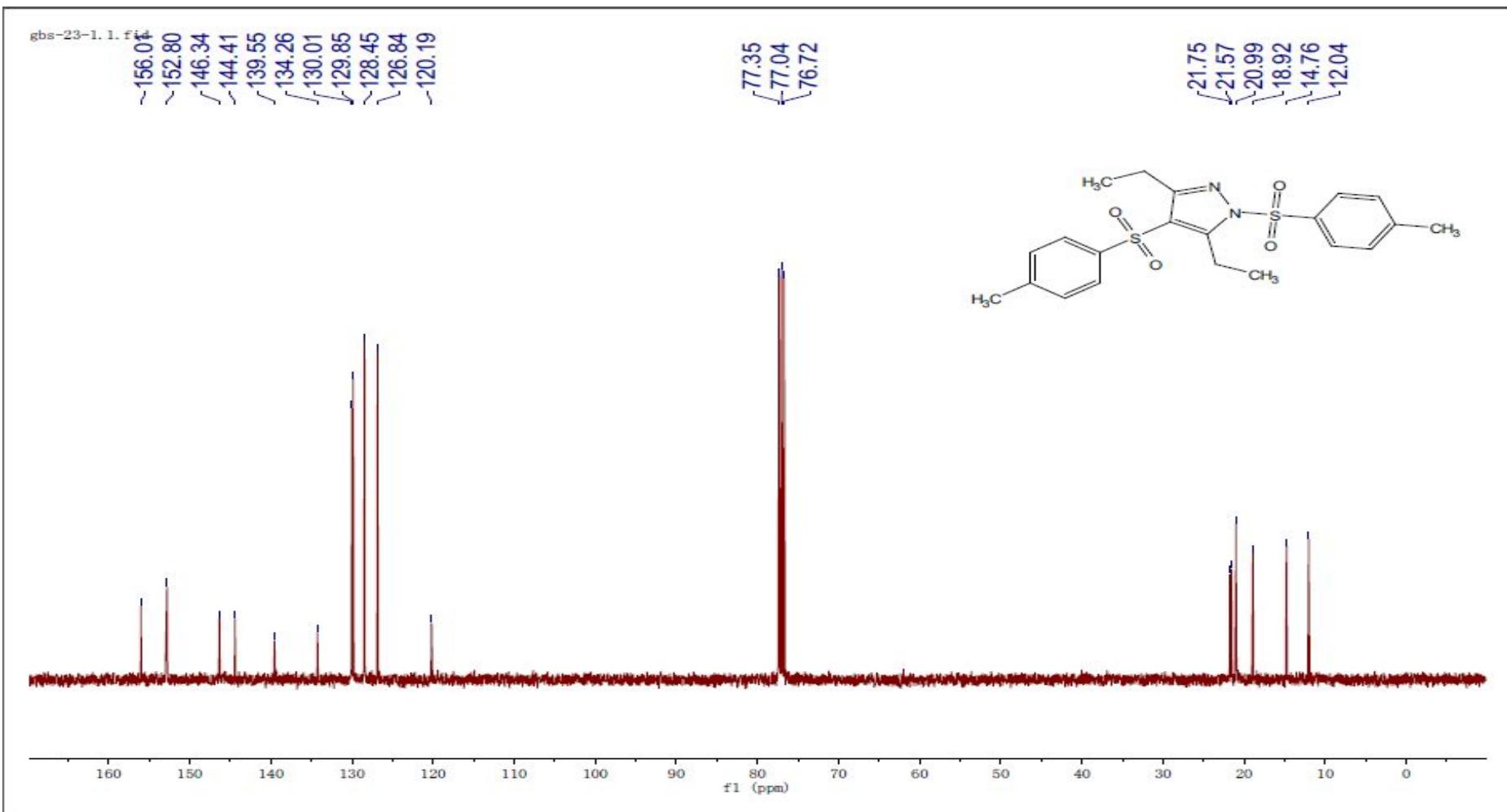
¹H NMR spectrum of 3p



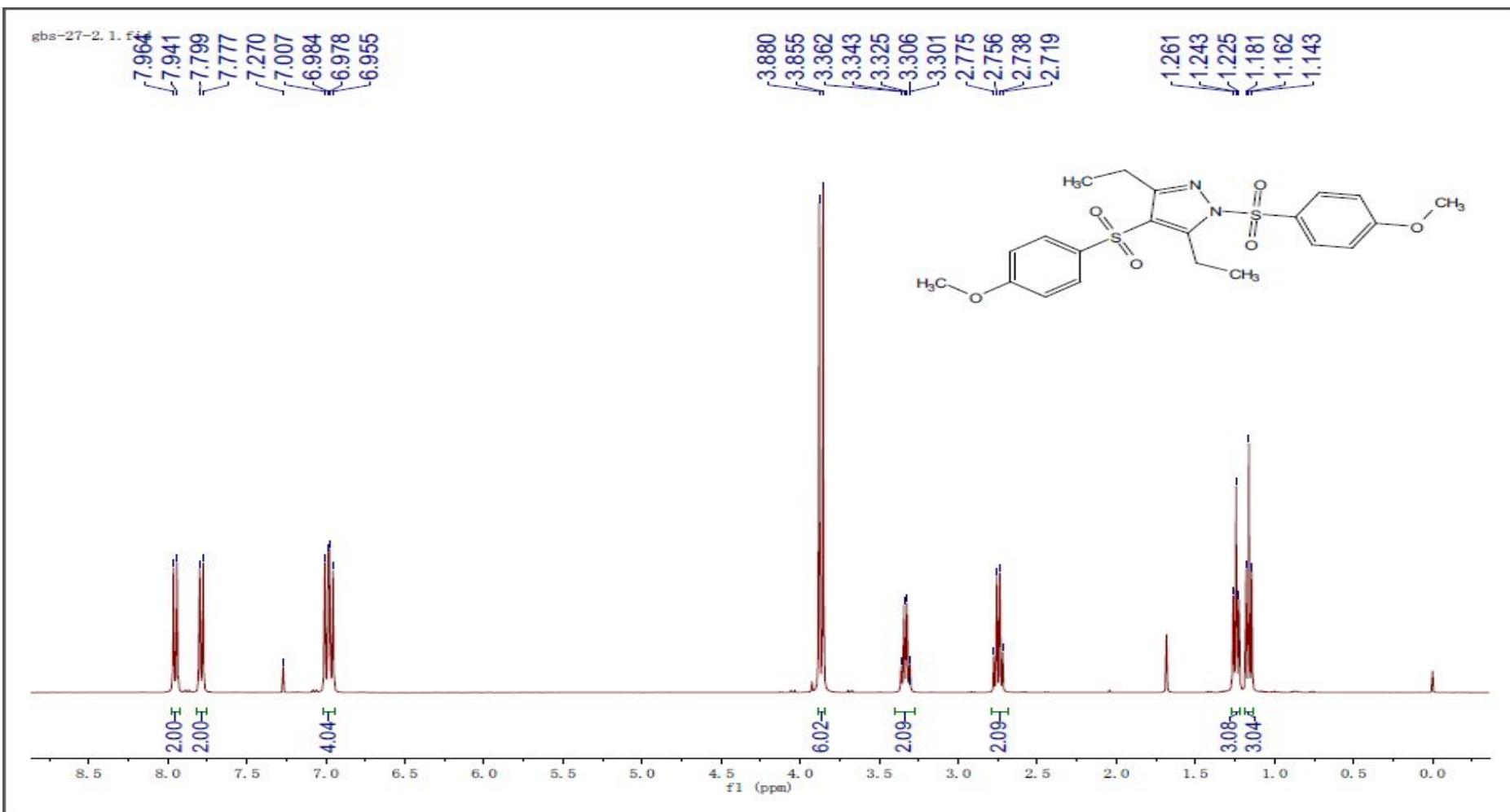
¹³C NMR spectrum of **3p**



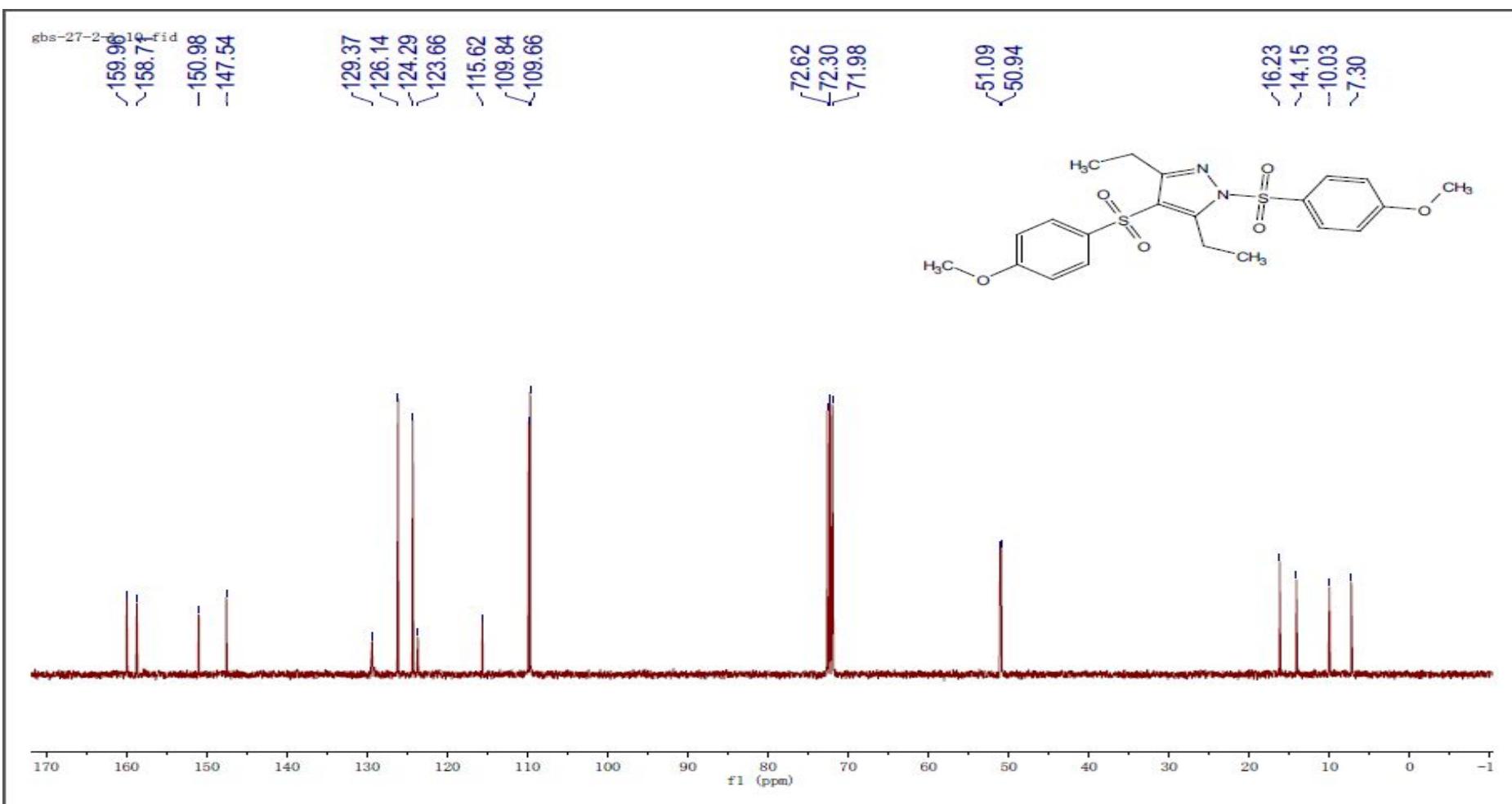
¹H NMR spectrum of 3q



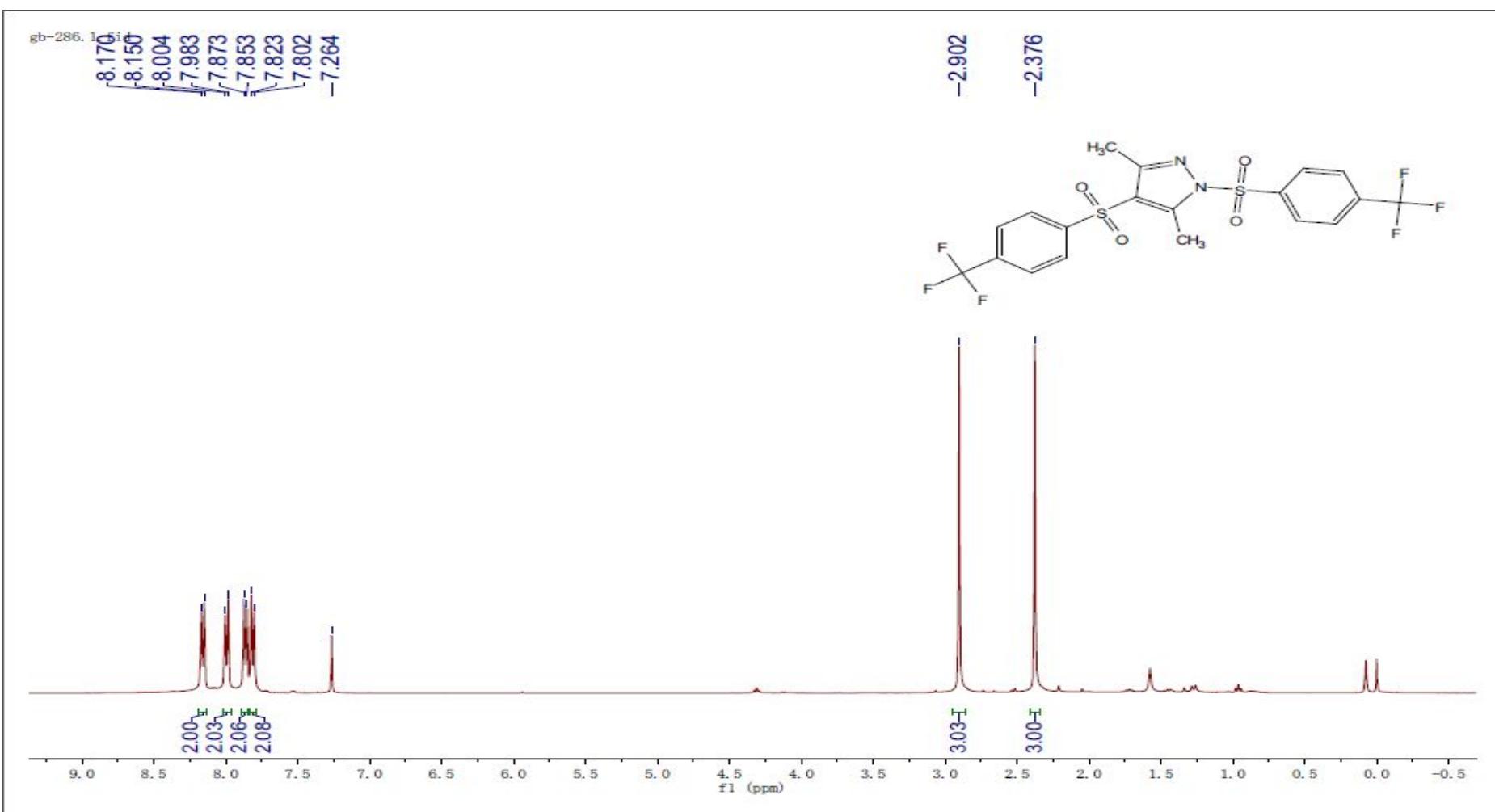
¹³C NMR spectrum of **3q**



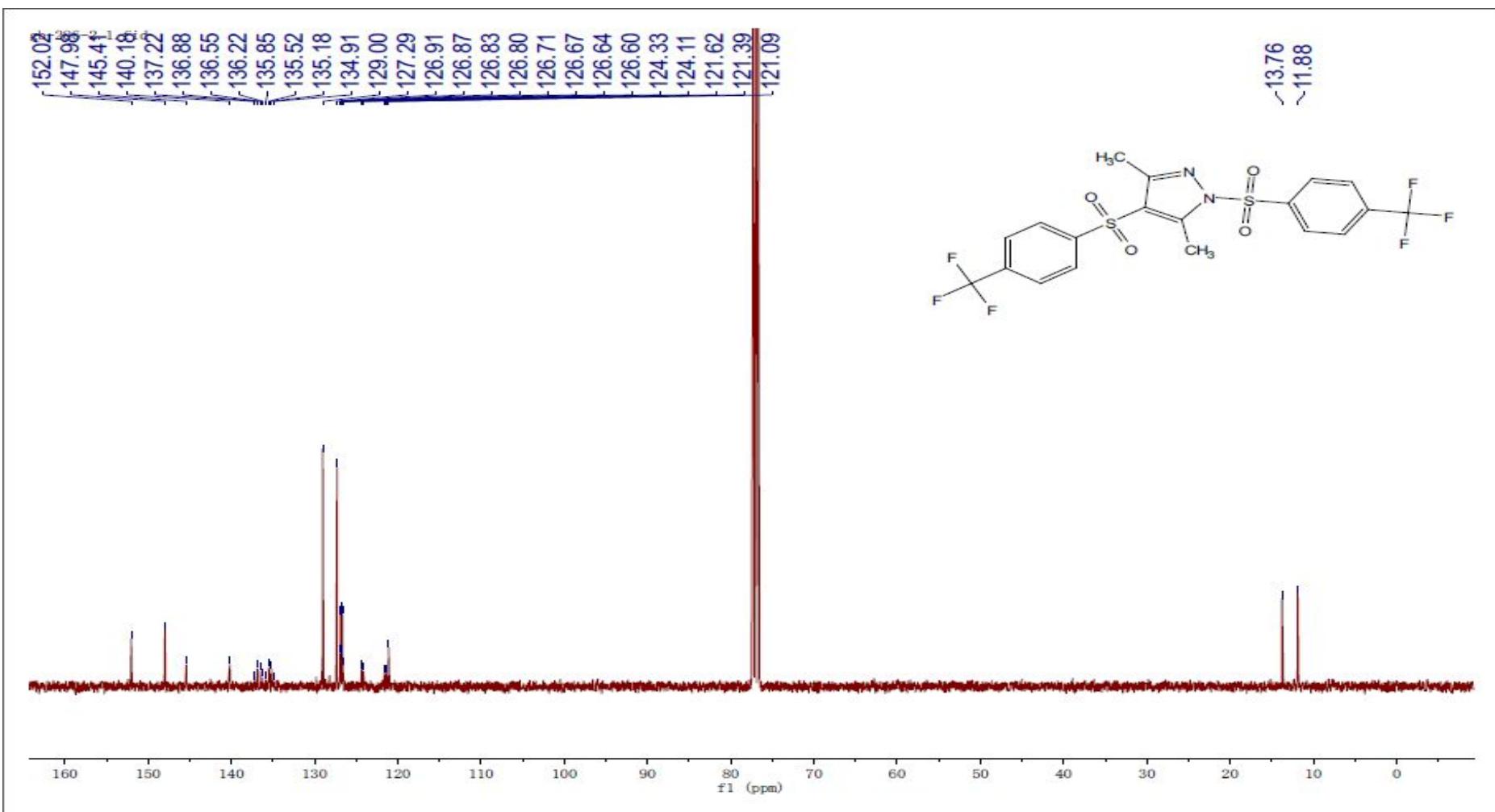
¹H NMR spectrum of 3r



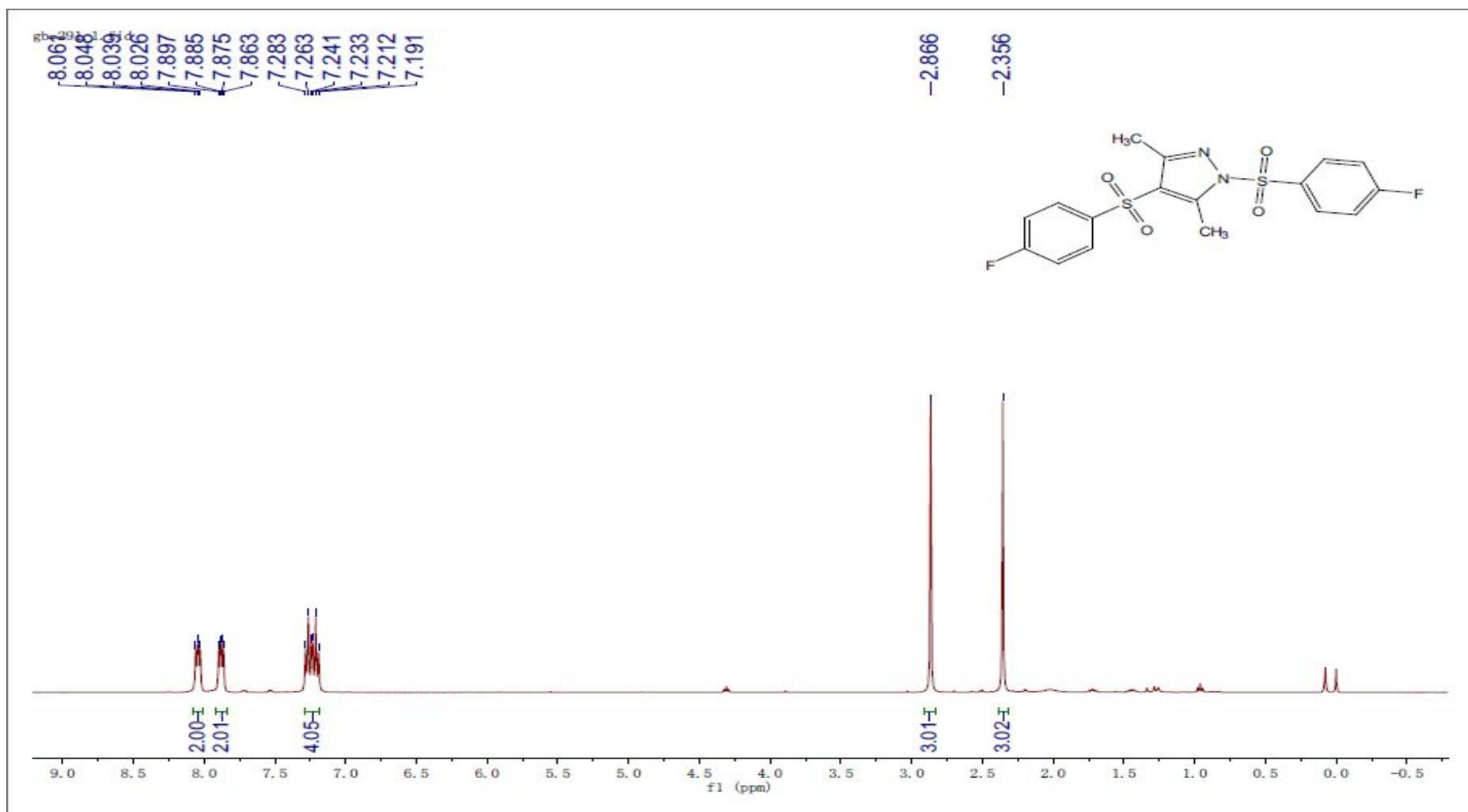
¹³C NMR spectrum of **3r**



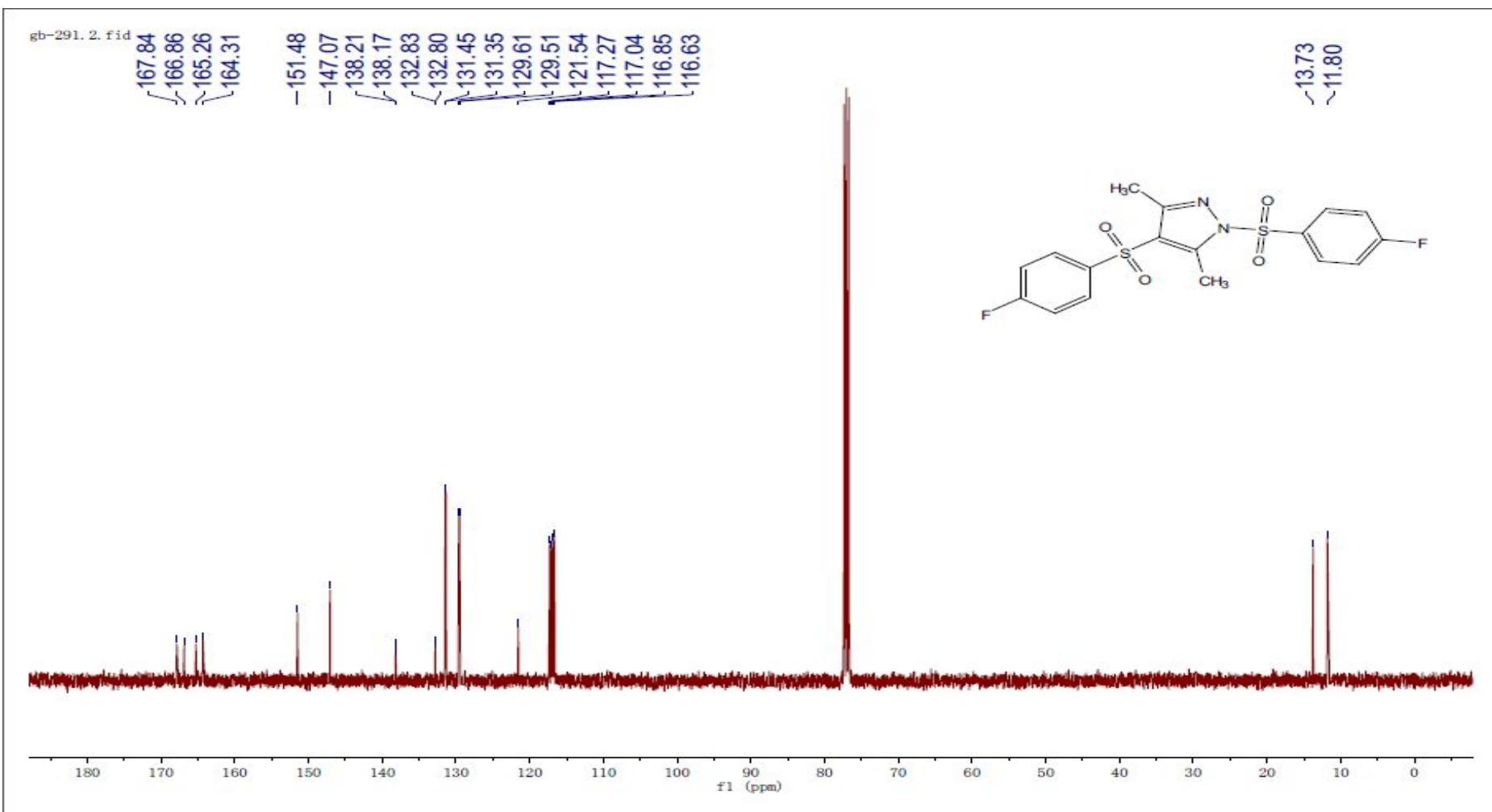
¹H NMR spectrum of 3s



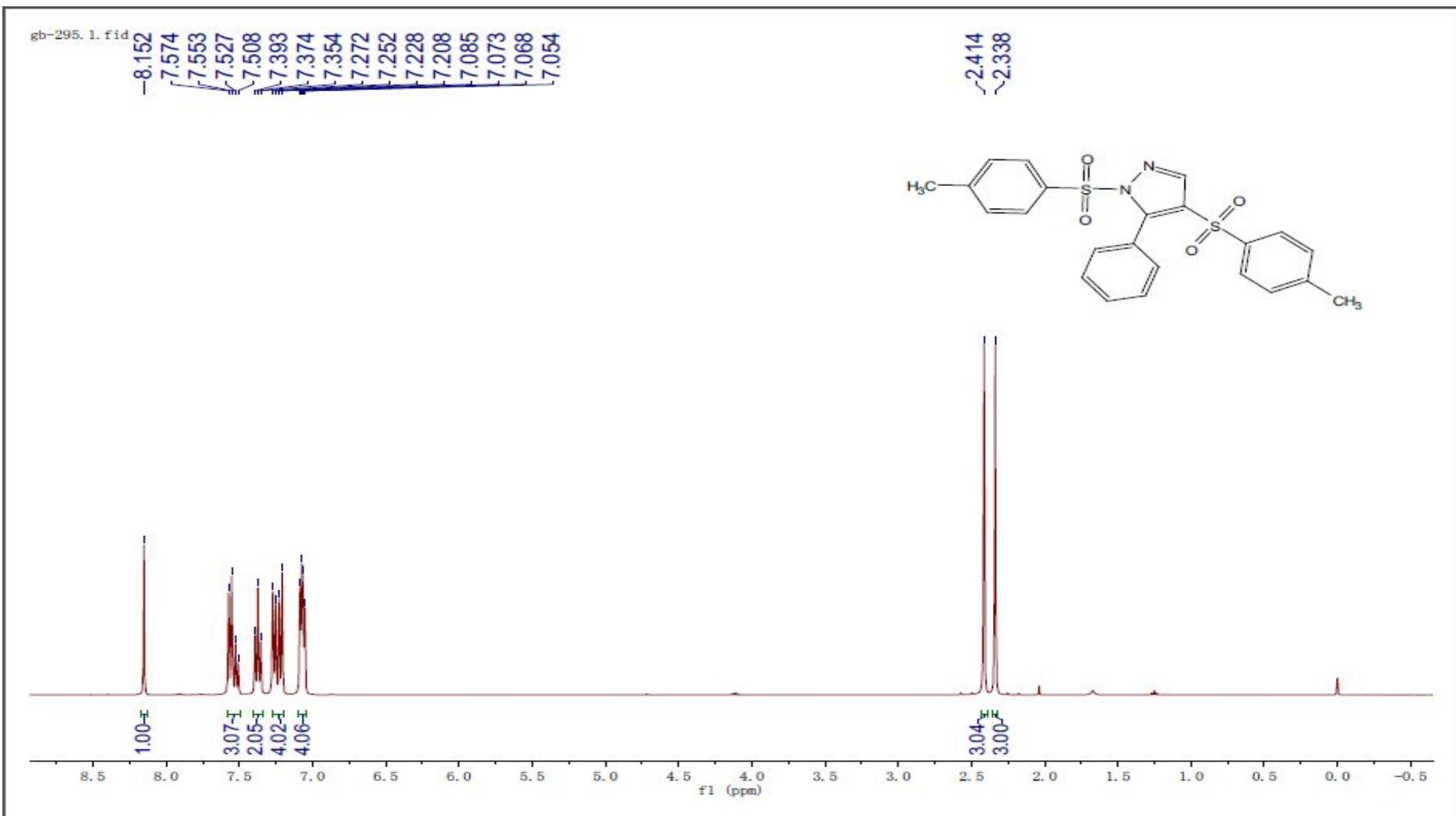
^{13}C NMR spectrum of **3s**



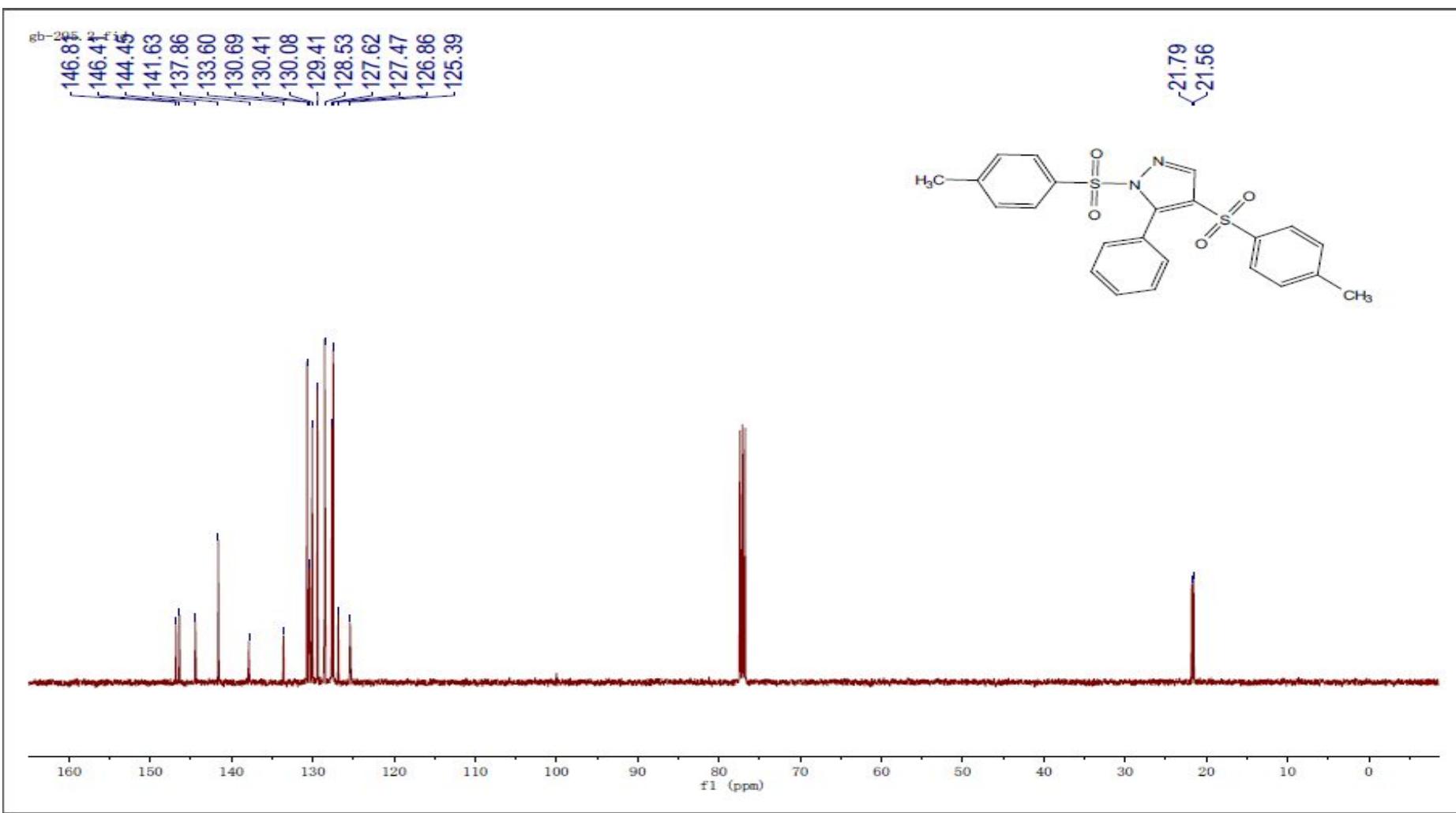
¹H NMR spectrum of **3t**



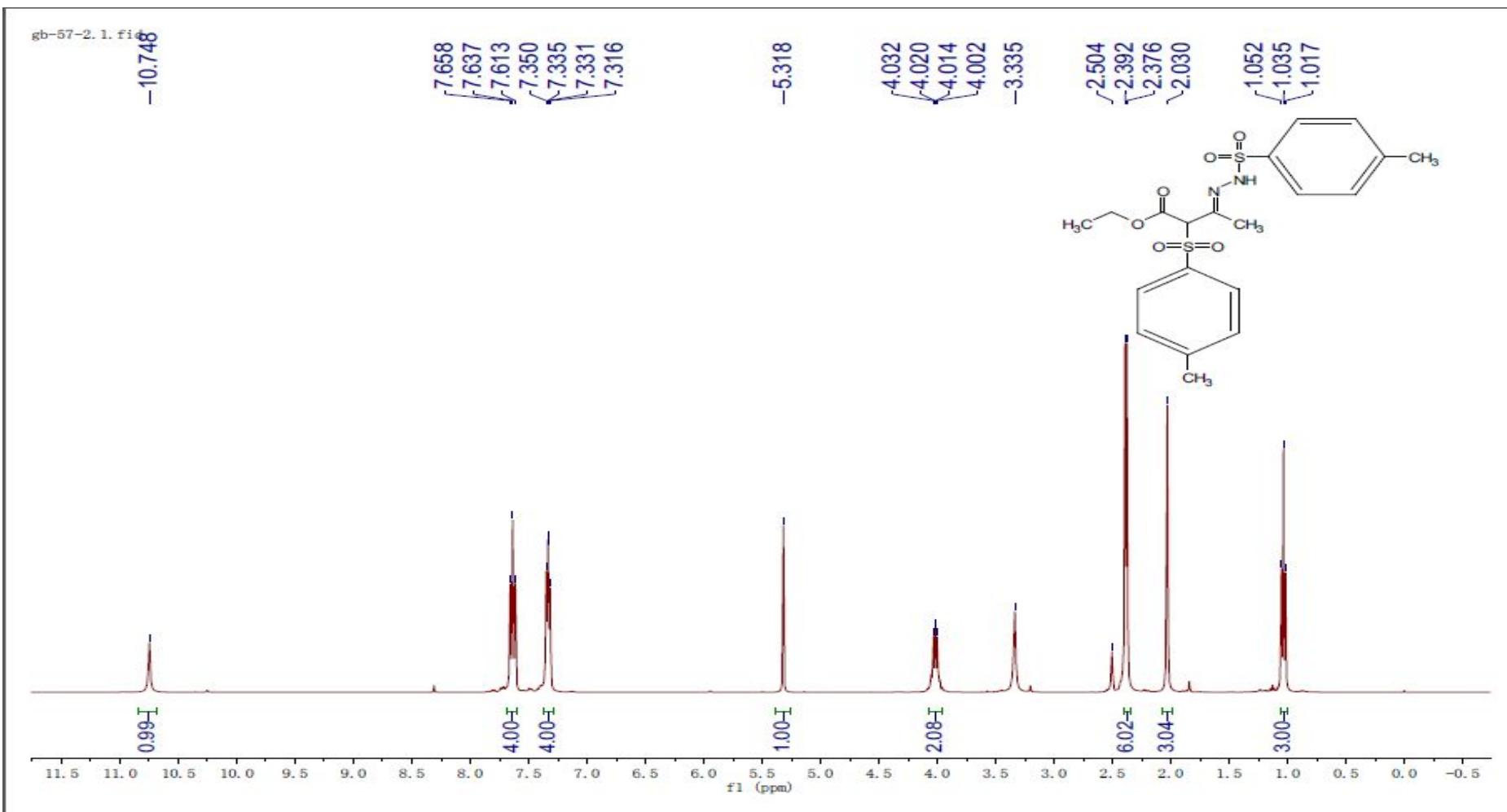
¹³C NMR spectrum of 3t



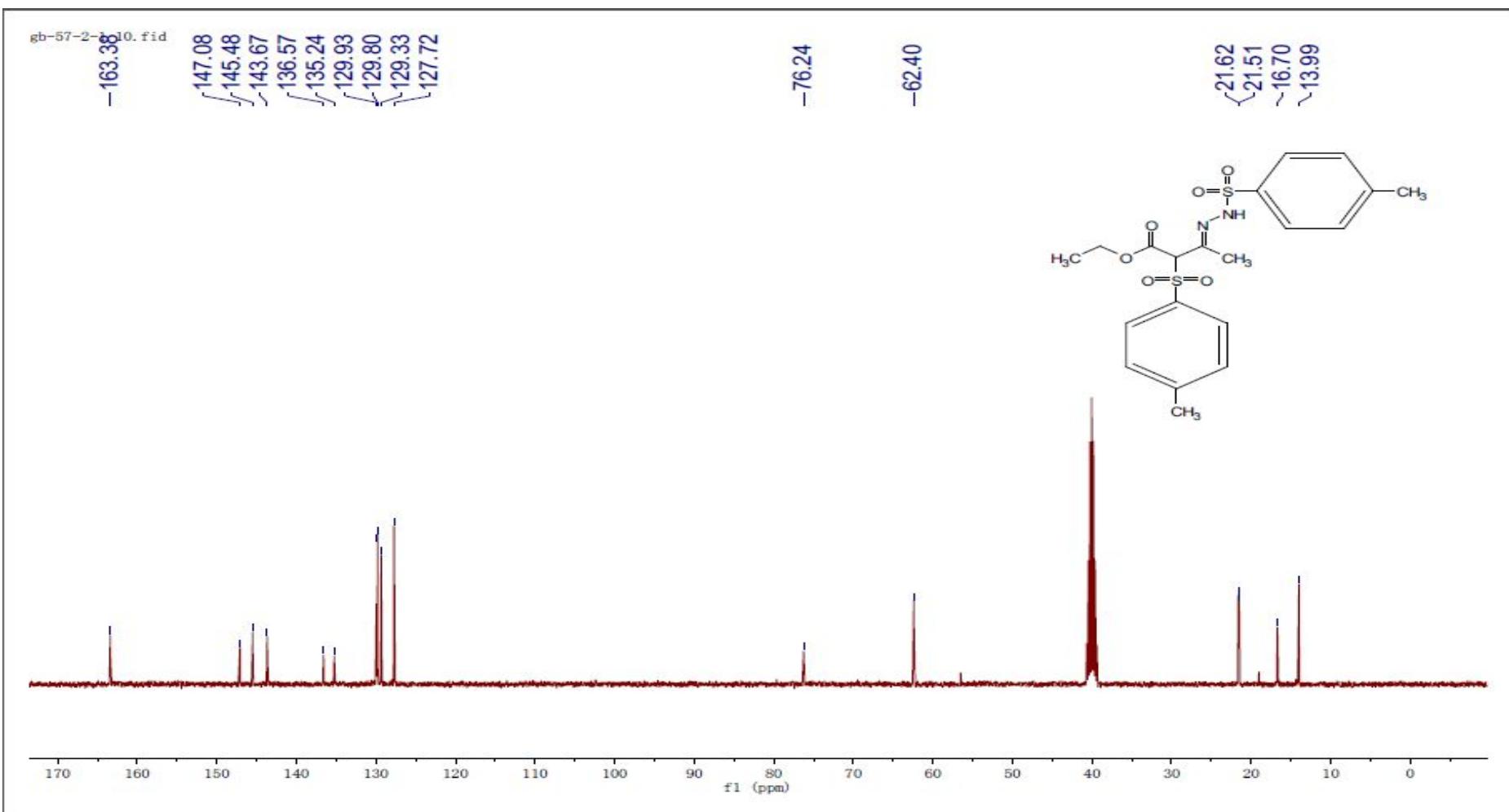
¹H NMR spectrum of 3u



^{13}C NMR spectrum of **3u**



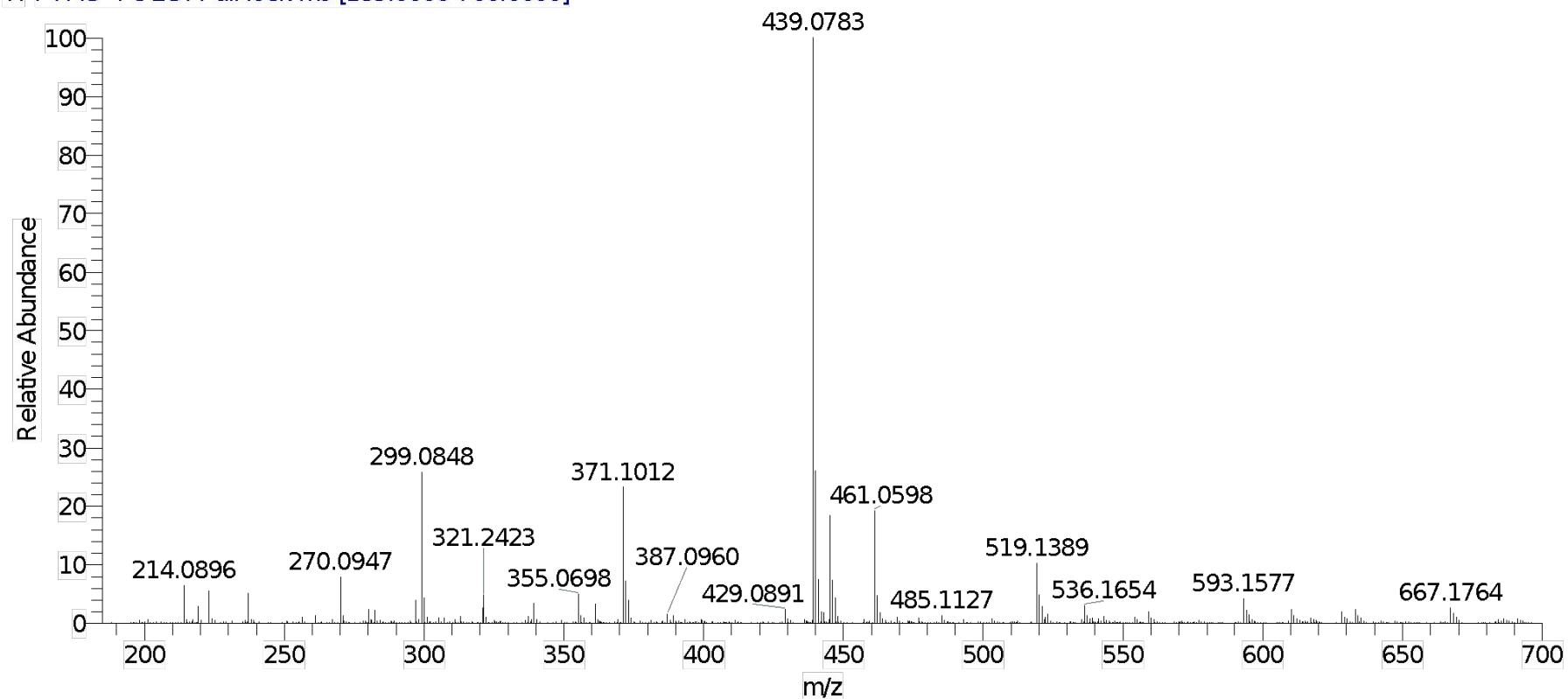
¹H NMR spectrum of **5**



^{13}C NMR spectrum of **5**

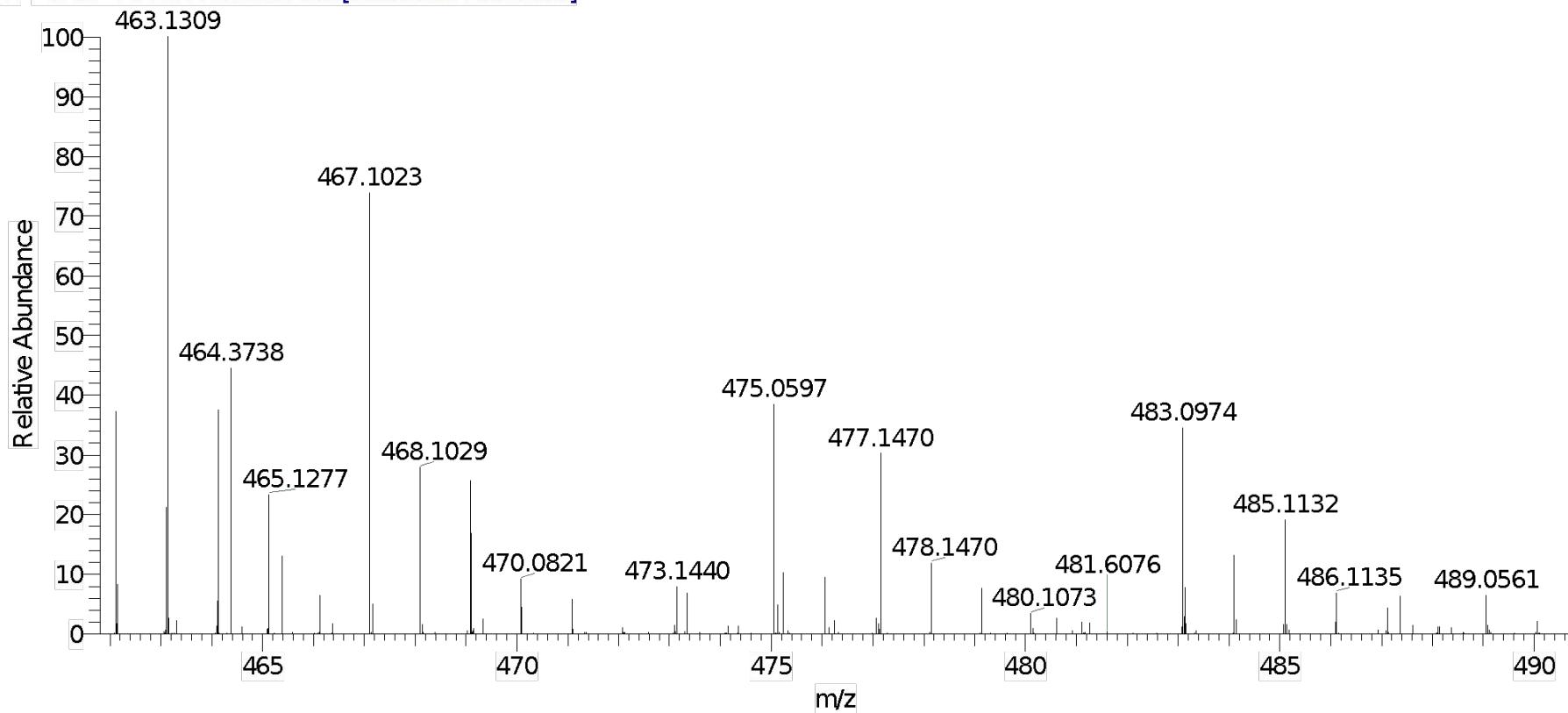
HRMS spectra all of new compounds

G3 #26-34 RT: 0.14-0.18 AV: 9 NL: 1.57E8
T: FTMS +c ESI Full lock ms [185.0000-700.0000]



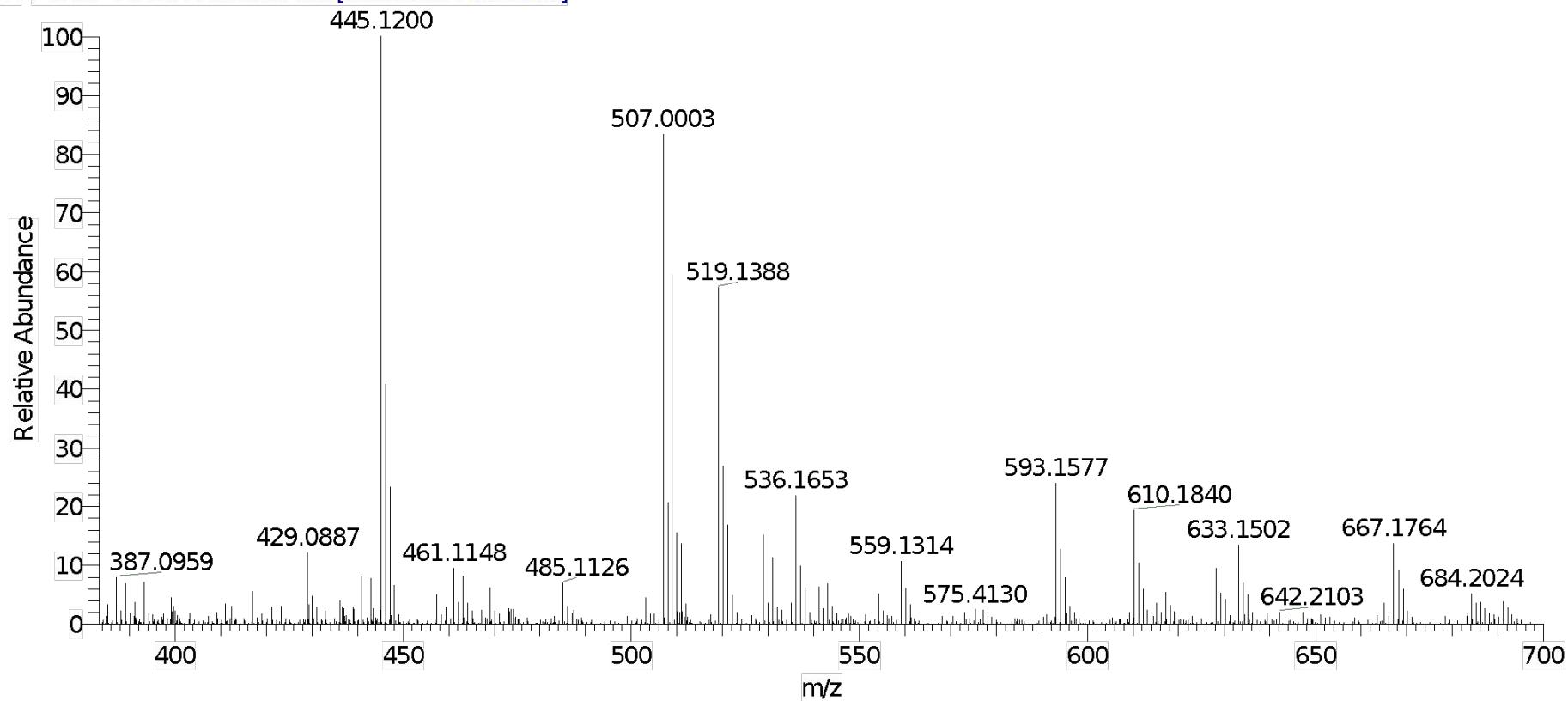
HRMS spectrum of 3b

G7 #26-38 RT: 0.14-0.20 AV: 13 NL: 1.19E7
T: FTMS +c ESI Full lock ms [185.0000-700.0000]



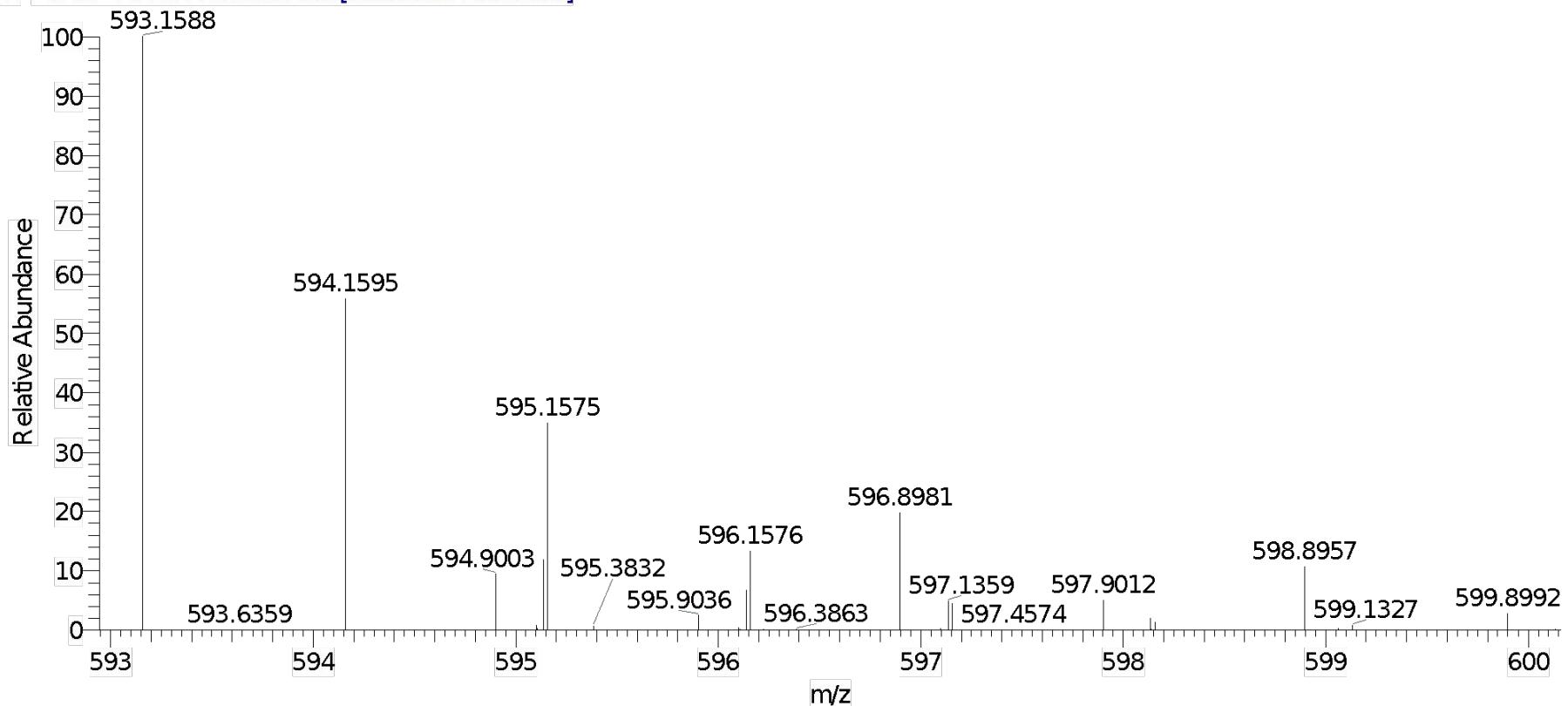
HRMS spectrum of 3c

G1 #27 RT: 0.15 AV: 1 NL: 2.13E7
T: FTMS +c ESI Full lock ms [185.0000-700.0000]



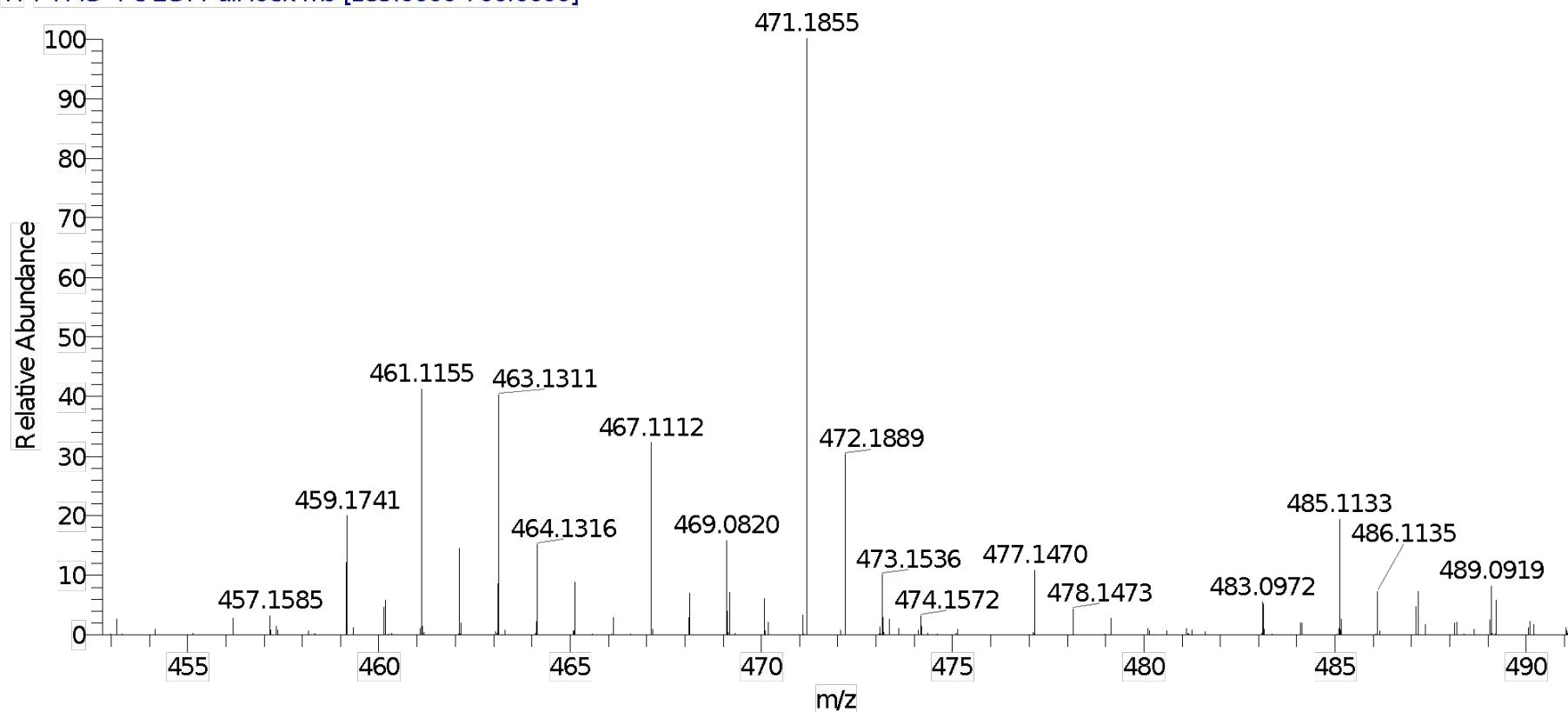
HRMS spectrum of 3d

G12 #23-40 RT: 0.13-0.21 AV: 18 NL: 9.40E7
T: FTMS +c ESI Full lock ms [185.0000-700.0000]



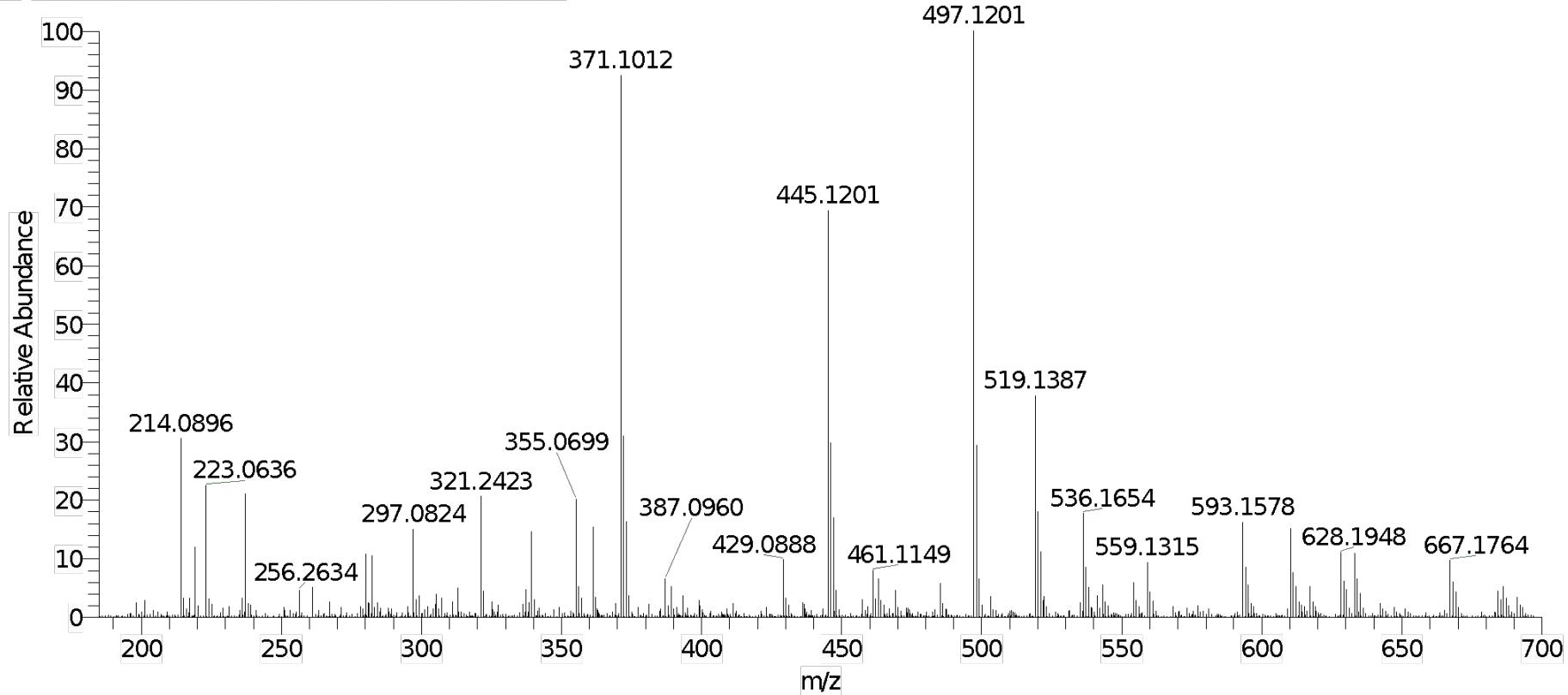
HRMS spectrum of **3e**

G5 #26-35 RT: 0.14-0.19 AV: 10 NL: 4.59E7
T: FTMS +c ESI Full lock ms [185.0000-700.0000]



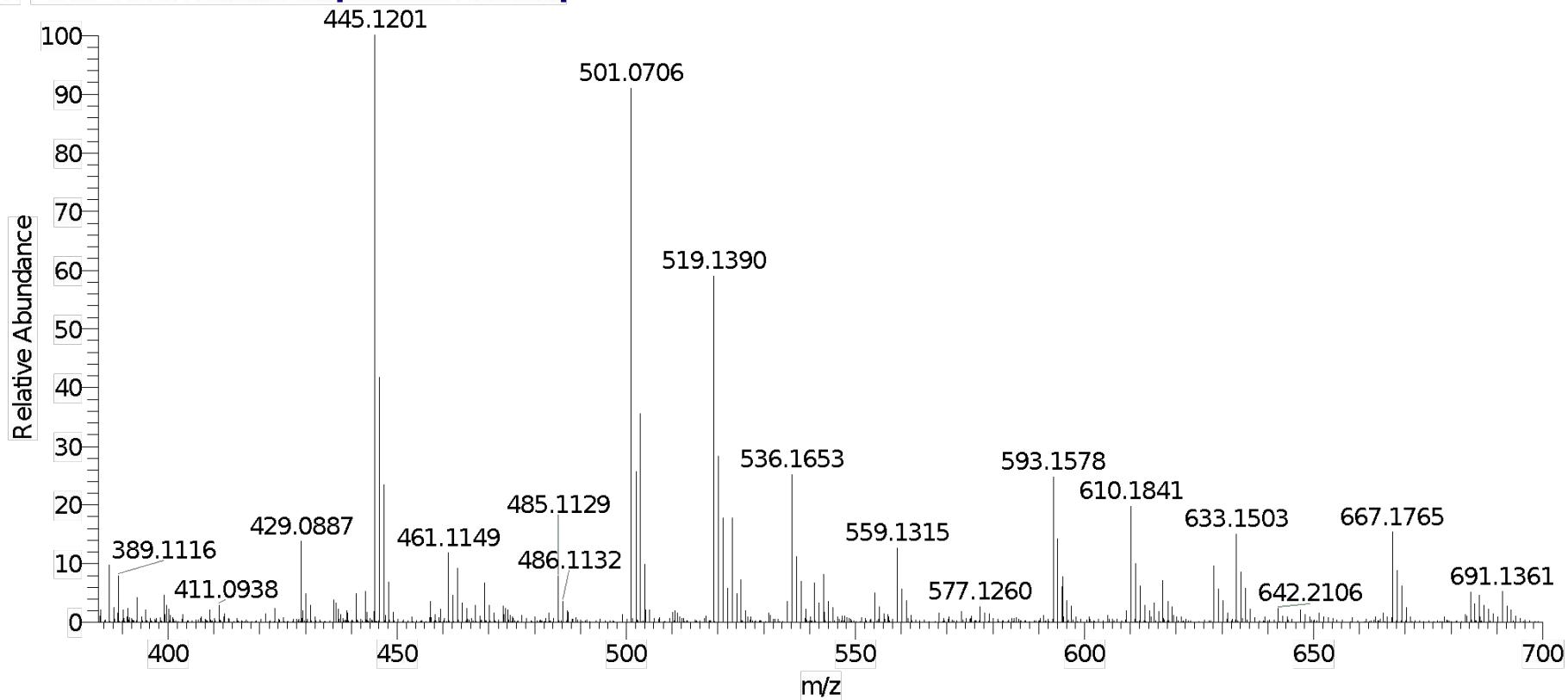
HRMS spectrum of **3f**

G9 #32 RT: 0.17 AV: 1 NL: 3.41E7
T: FTMS +c ESI Full lock ms [185.0000-700.0000]



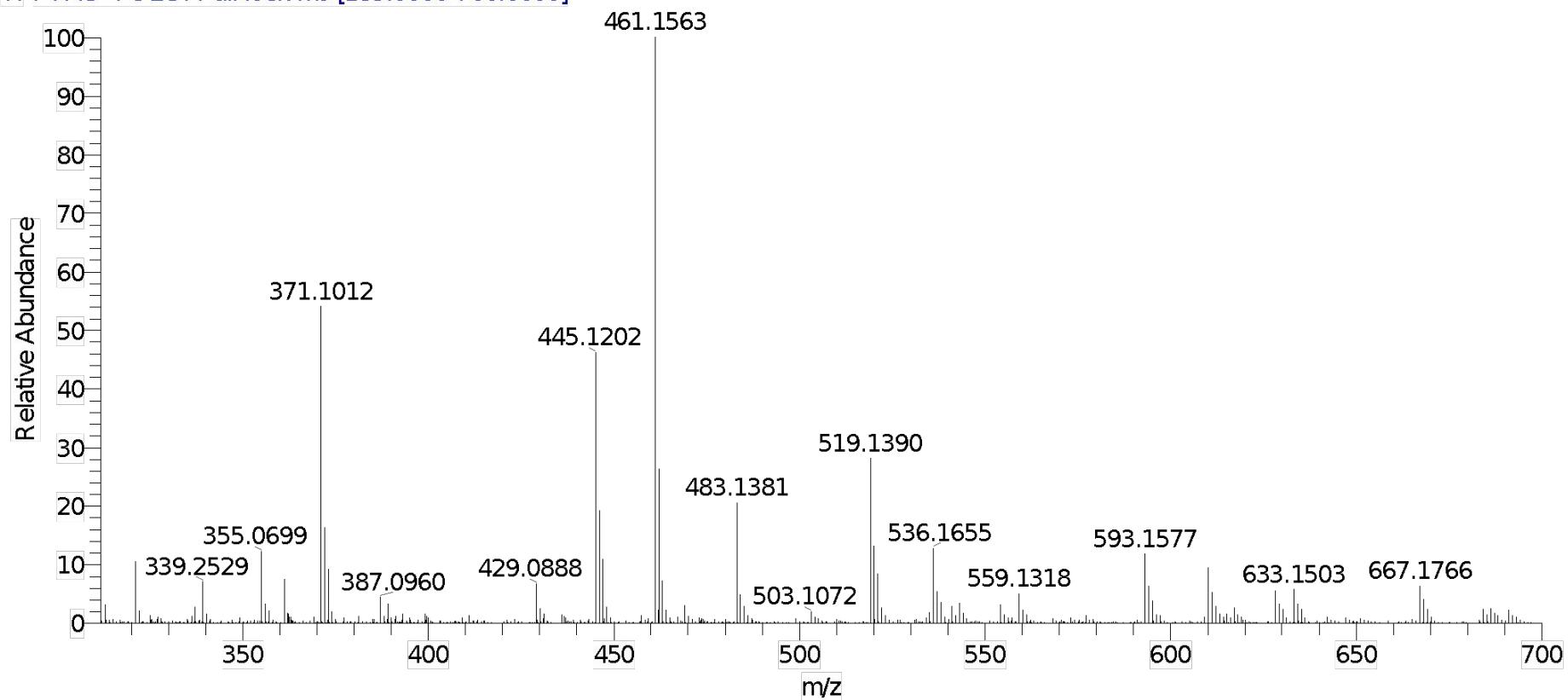
HRMS spectrum of 3g

G8 #29 RT: 0.16 AV: 1 NL: 3.03E7
T: FTMS +c ESI Full lock ms [185.0000-700.0000]



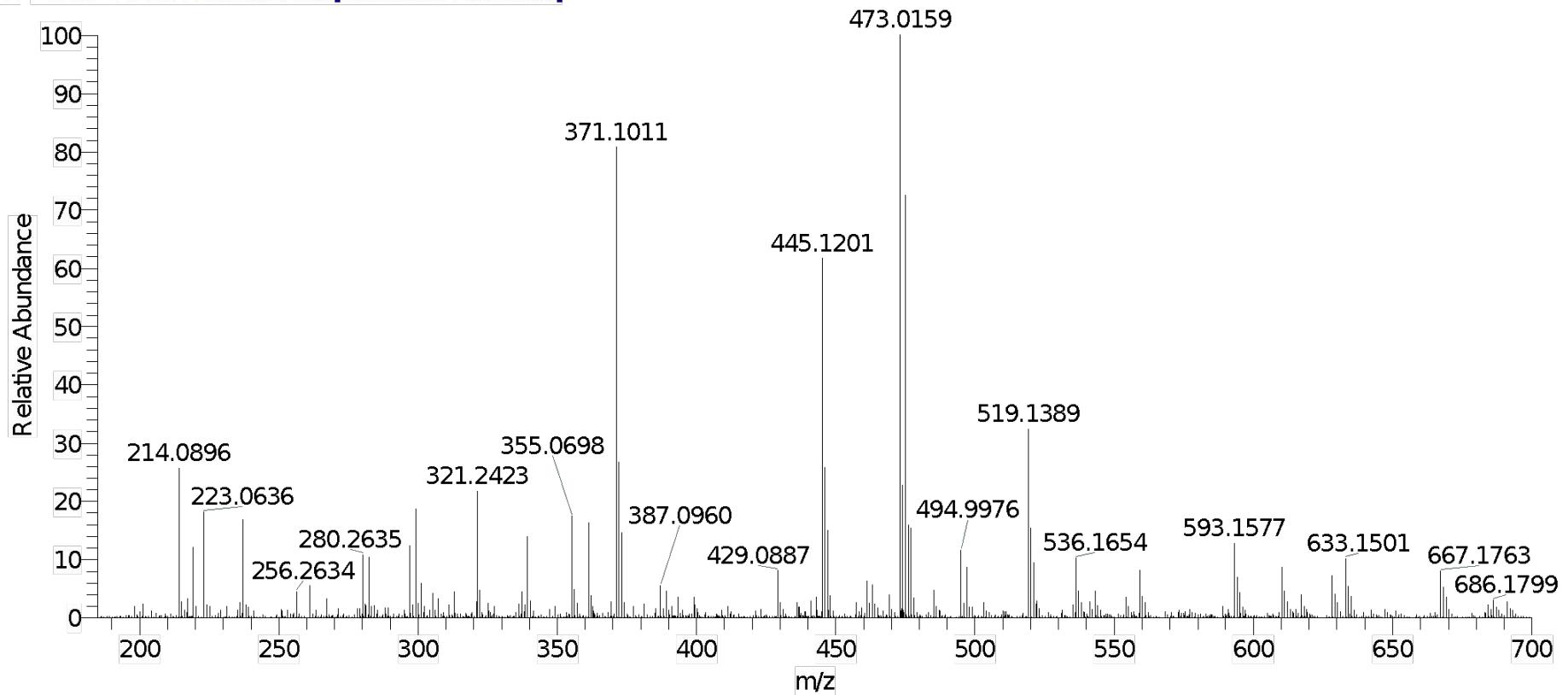
HRMS spectrum of **3h**

G6 #31 RT: 0.17 AV: 1 NL: 6.99E7
T: FTMS +c ESI Full lock ms [185.0000-700.0000]



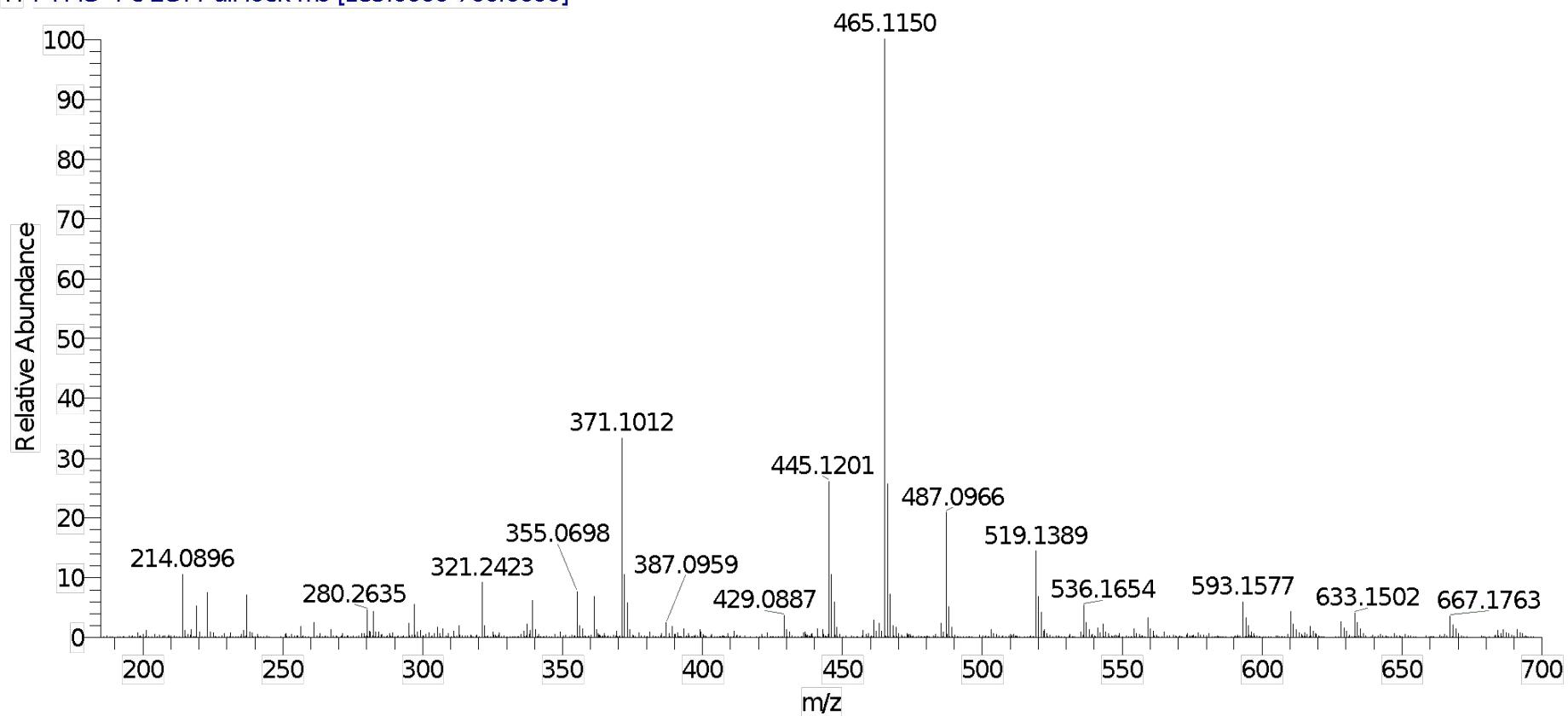
HRMS spectrum of **3m**

G10 #30 RT: 0.16 AV: 1 NL: 3.95E7
T: FTMS +c ESI Full lock ms [185.0000-700.0000]



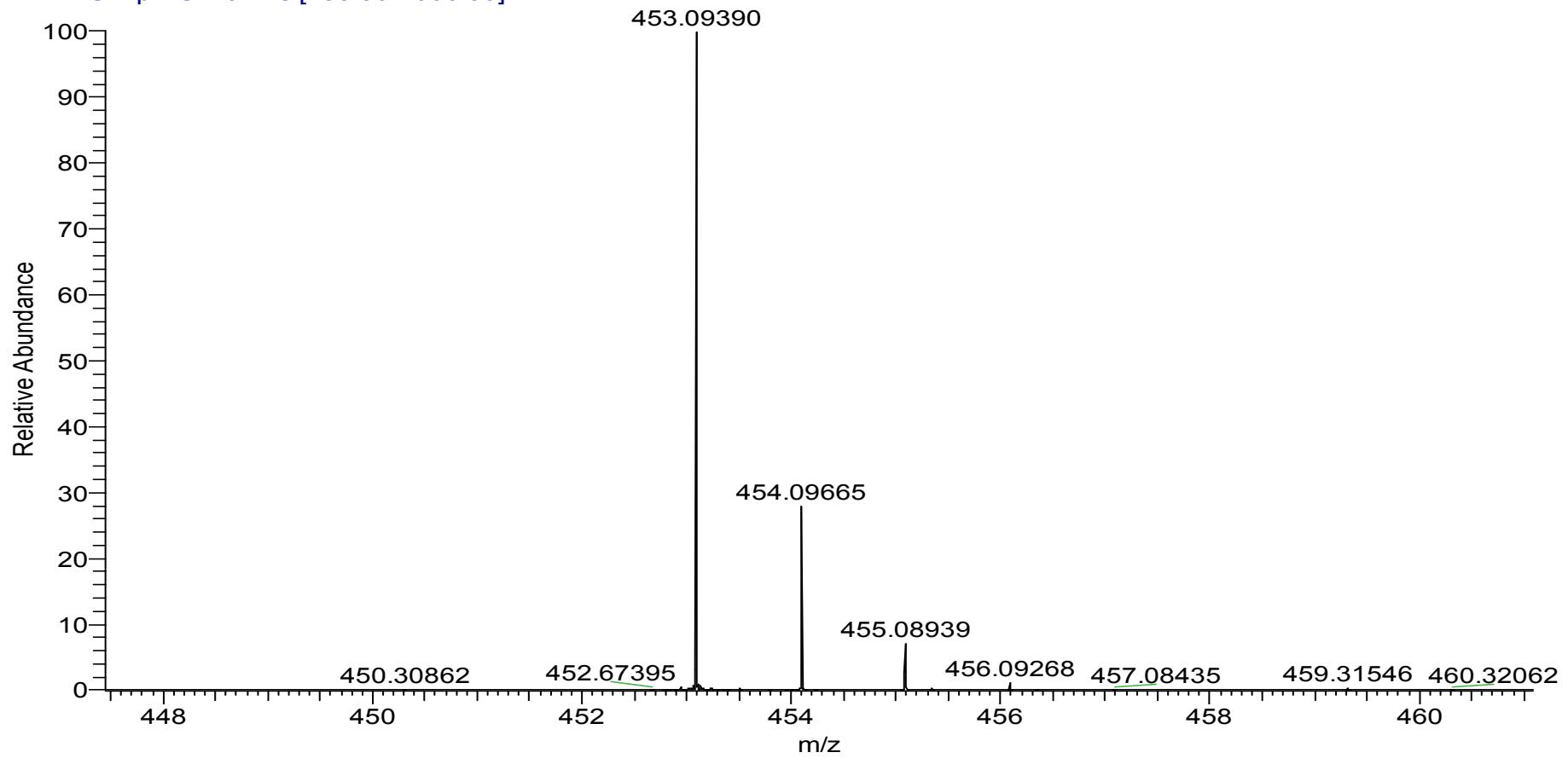
HRMS spectrum of 3p

G11 #29 RT: 0.16 AV: 1 NL: 9.47E7
T: FTMS +c ESI Full lock ms [185.0000-700.0000]



HRMS spectrum of **3r**

90 #40 RT: 0.55 AV: 1 NL: 2.81E7
T: FTMS + p ESI Full ms [150.00-2000.00]



HRMS spectrum of 3u