

Supporting Information

Coumarin–furo[2,3-d]pyrimidone hybrid molecules targeting human liver cancer cells: Synthesis, anticancer effect, EGFR inhibition and molecular docking studies

Tianshuai Wang ^{a, b, †}, Yumeng Gao ^{a, †}, Fengxu Wu, Lun Luo ^{a, b, †}, Junkai Ma ^{a, b, *}, Yanggen Hu ^{a, b, *}

^a School of Pharmaceutical Sciences and Institute of Medicinal Chemistry, Hubei University of Medicine, Shiyan 442000, China

^b Hubei Key Laboratory of Wudang Local Chinese Medicine Research, Hubei University of Medicine, Shiyan 442000, China

†These authors contributed equally to this work.

* Corresponding author. Tel.: +86-719-8891150

Yang-Gen Hu, Hubei Key Laboratory of Wudang Local Chinese Medicine Research and Institute of Medicinal Chemistry, Hubei University of Medicine, Shiyan 442000, China. Email: huyg@hbm.u.edu.cn

Junkai Ma, Hubei Key Laboratory of Wudang Local Chinese Medicine Research and Institute of Medicinal Chemistry, Hubei University of Medicine, Shiyan 442000, China. Email: majunkai17@hbm.u.edu.cn

Contents:

1. ^1H NMR of Compounds 6a-n
2. ^{13}C NMR of Compounds 6a-n
3. ESI-MS of Compounds 6a-n
4. ^1H NMR of Compounds 10a-i
5. ^{13}C NMR of Compounds 10a-i
6. ESI-MS of Compounds 10a-n

**^1H NMR of Compounds 6a-n
(Fig. S1-14)**

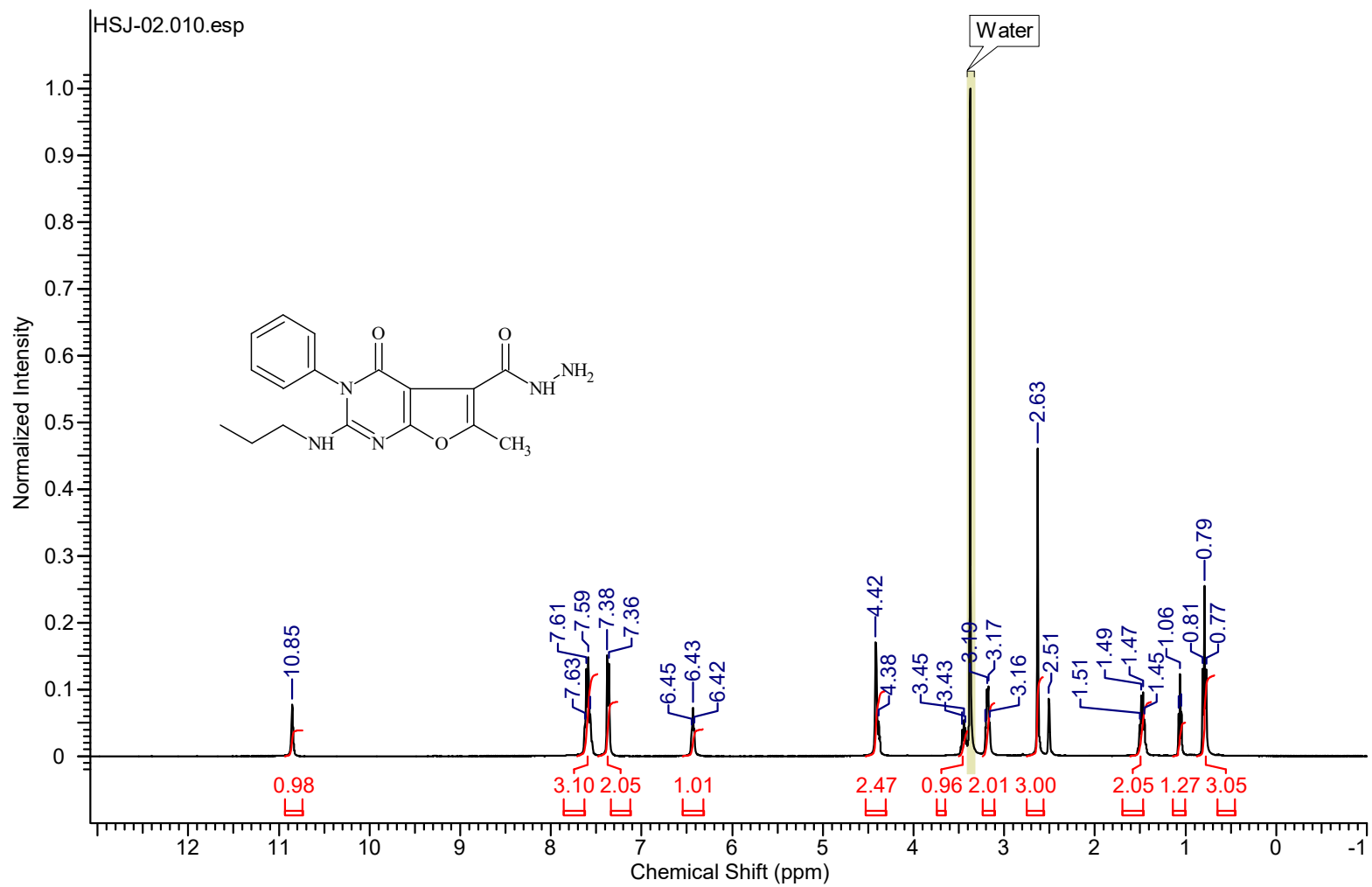


Fig.S1: ¹H NMR spectrum of compound 6a

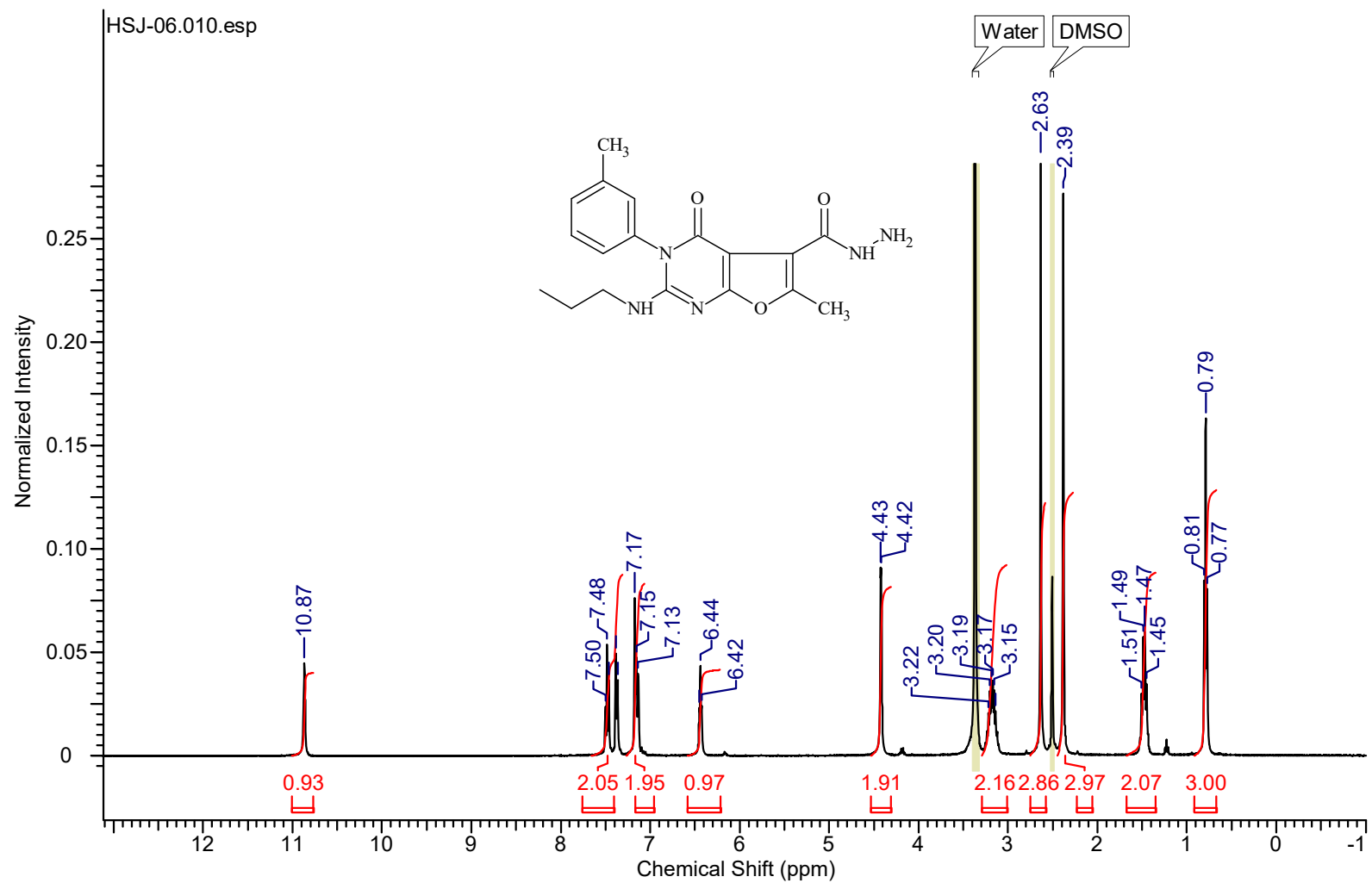


Fig.S2: ^1H NMR spectrum of compound **6b**

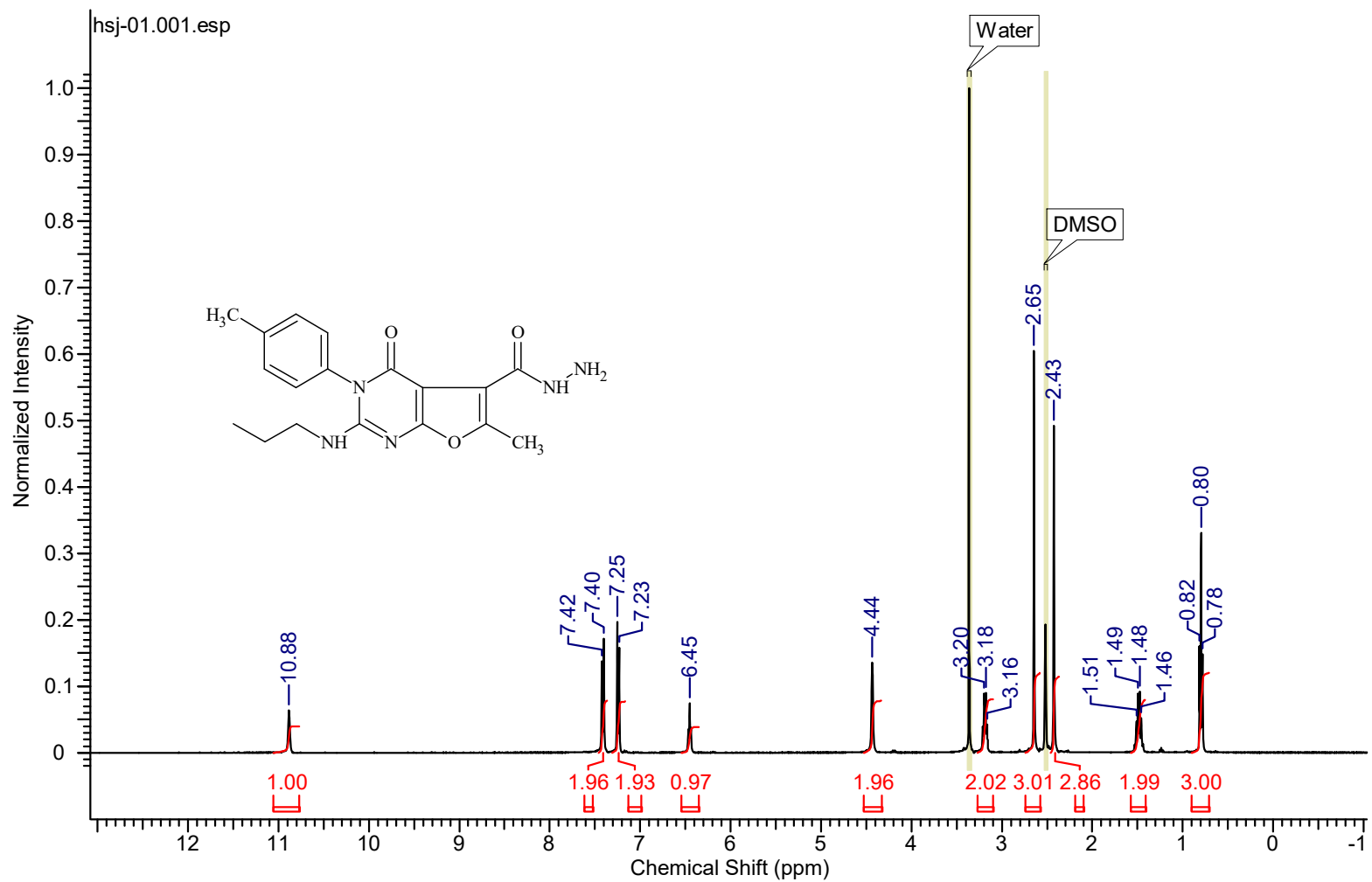


Fig.S3: ¹H NMR spectrum of compound **6c**

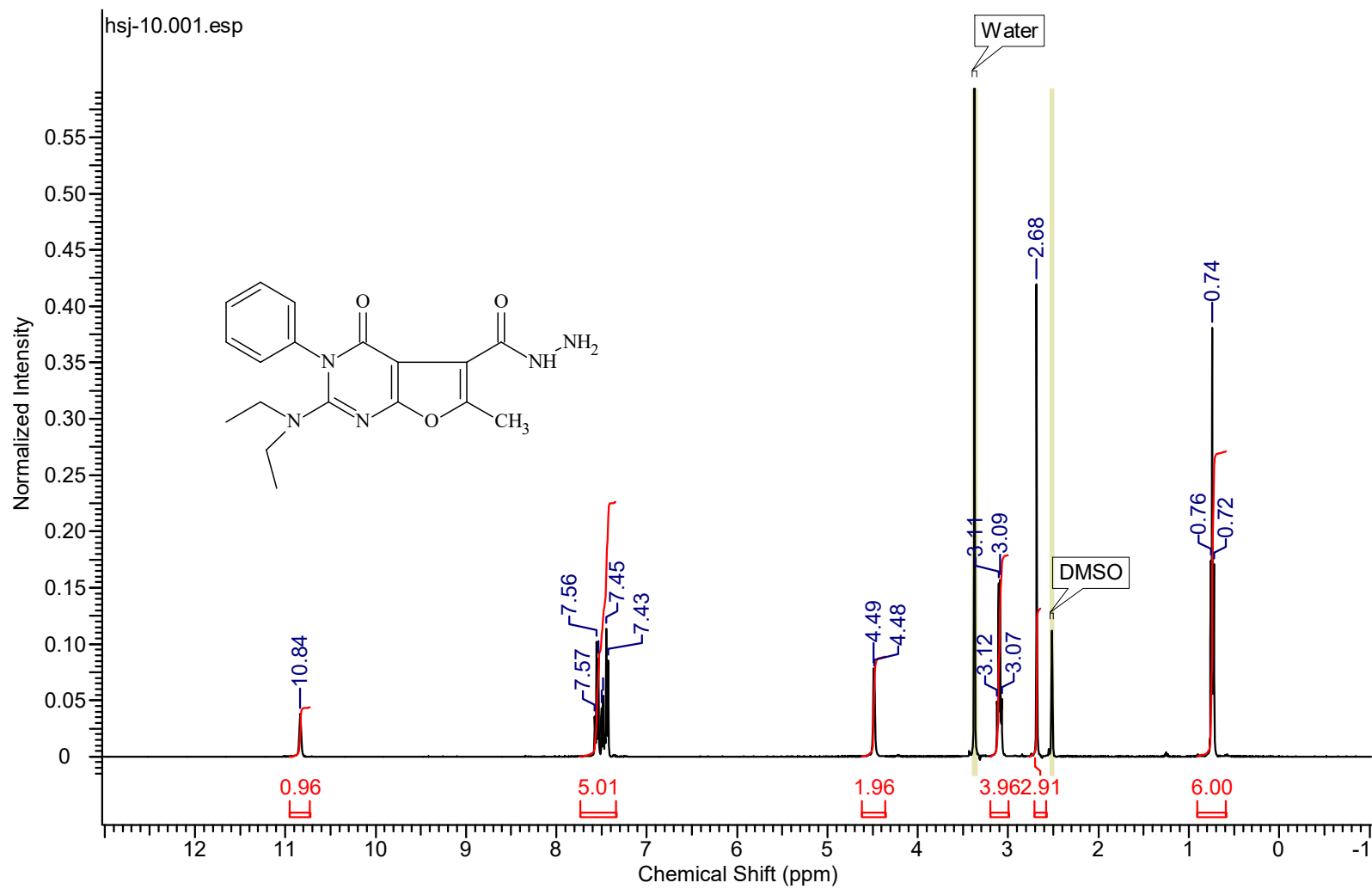


Fig.S4: ¹H NMR spectrum of compound 6d

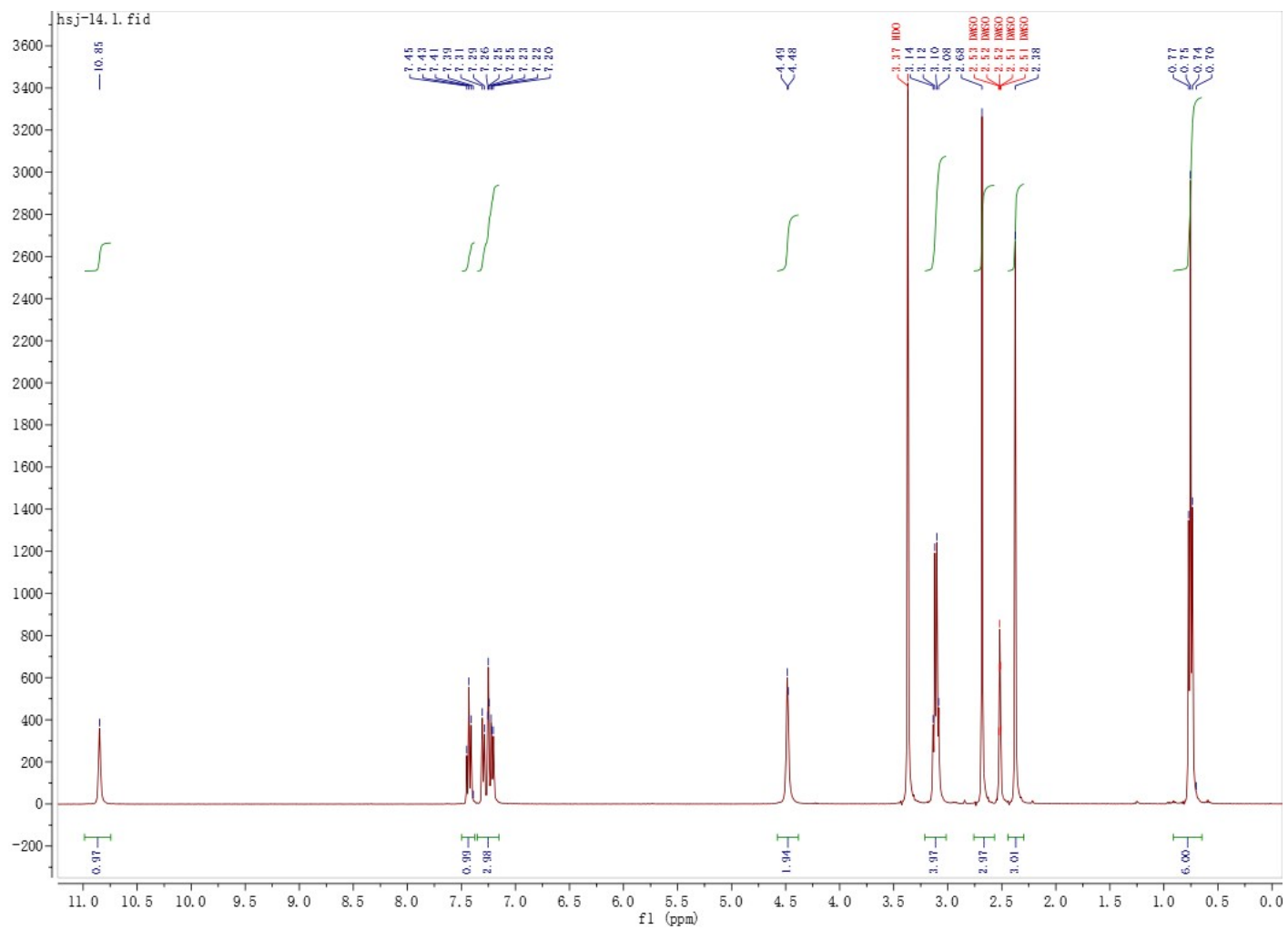


Fig.S5: ^1H NMR spectrum of compound **6e**

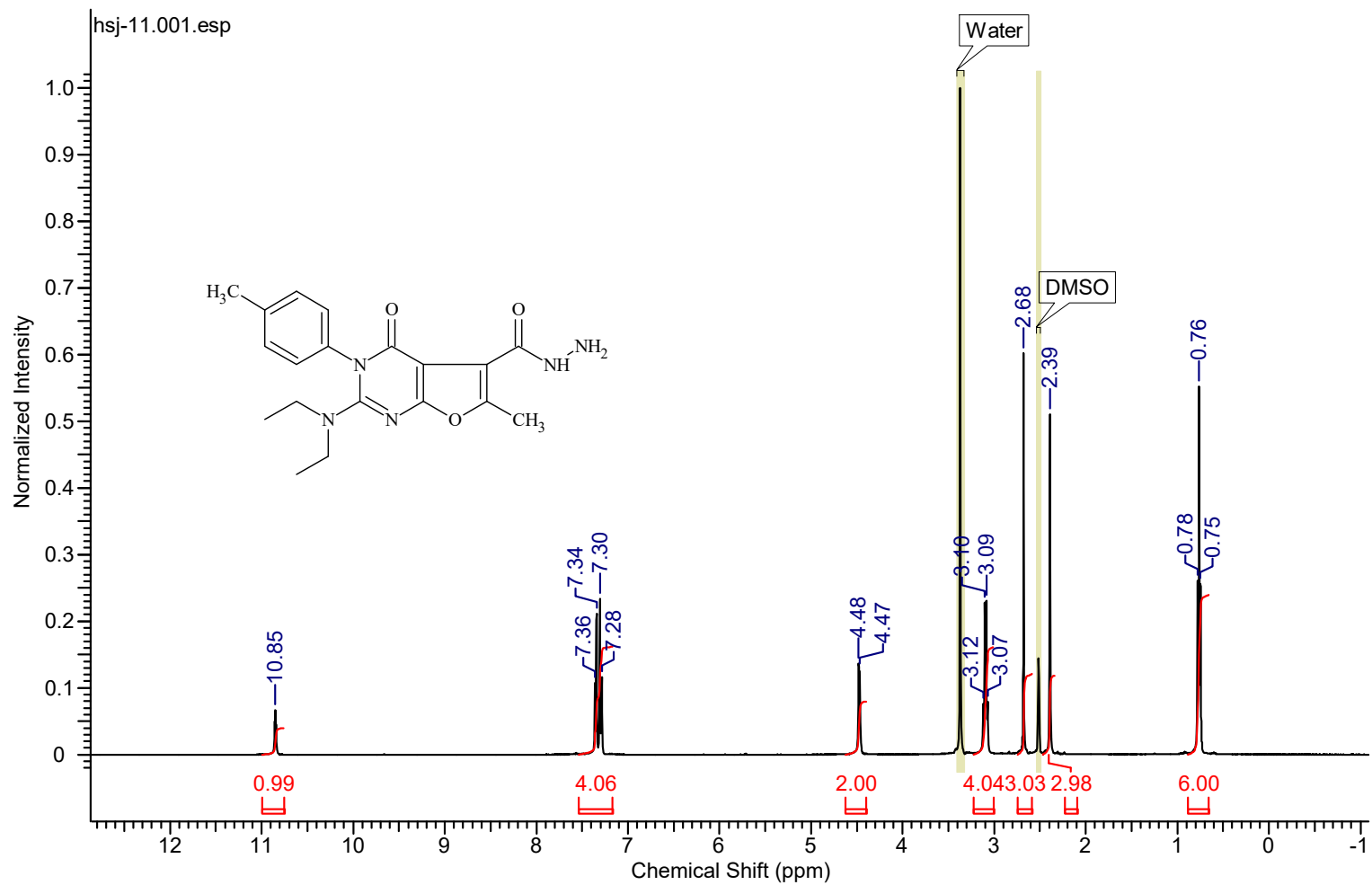


Fig.S6: ¹H NMR spectrum of compound 6f

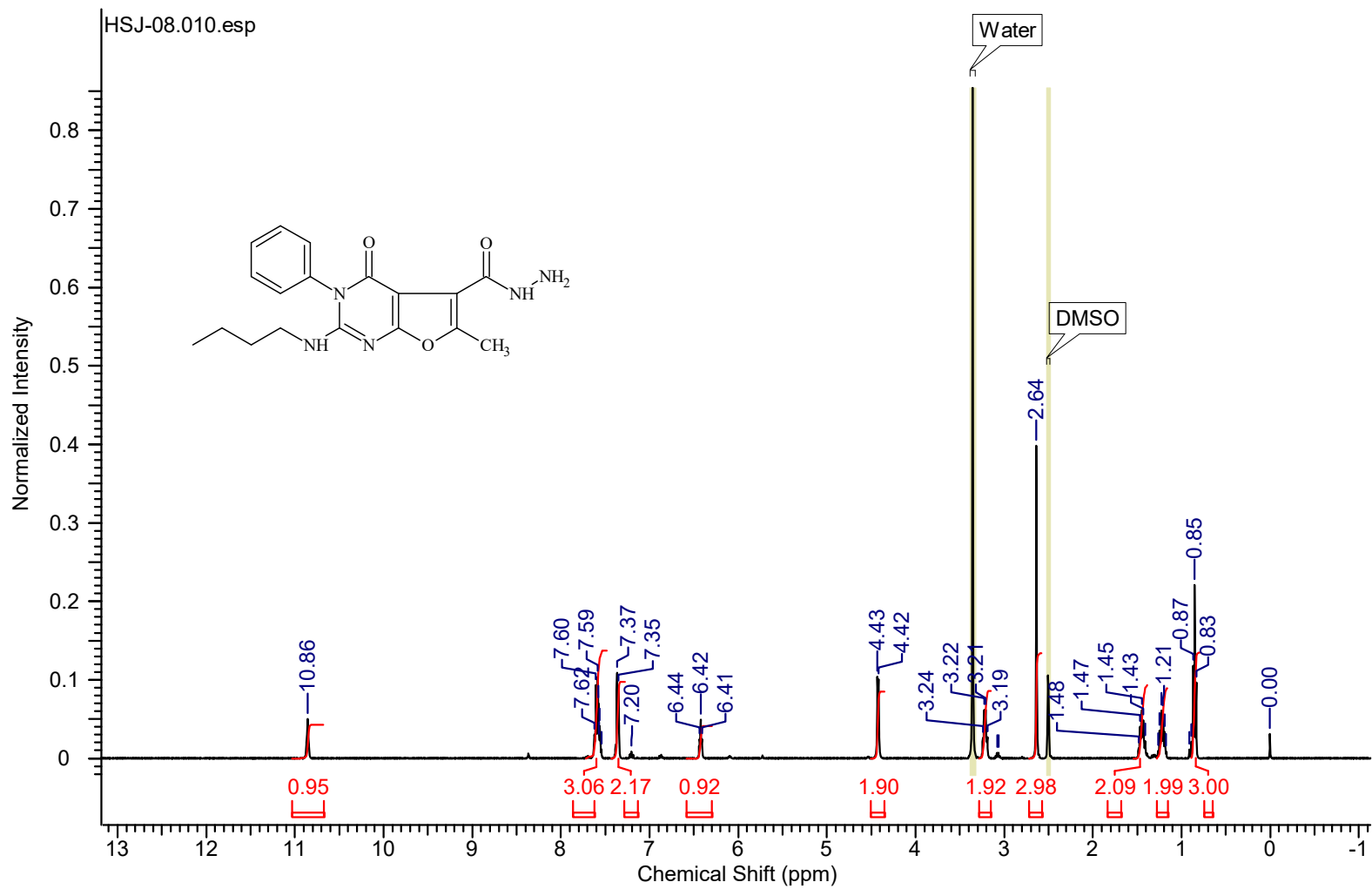


Fig.S7: ¹H NMR spectrum of compound **6g**

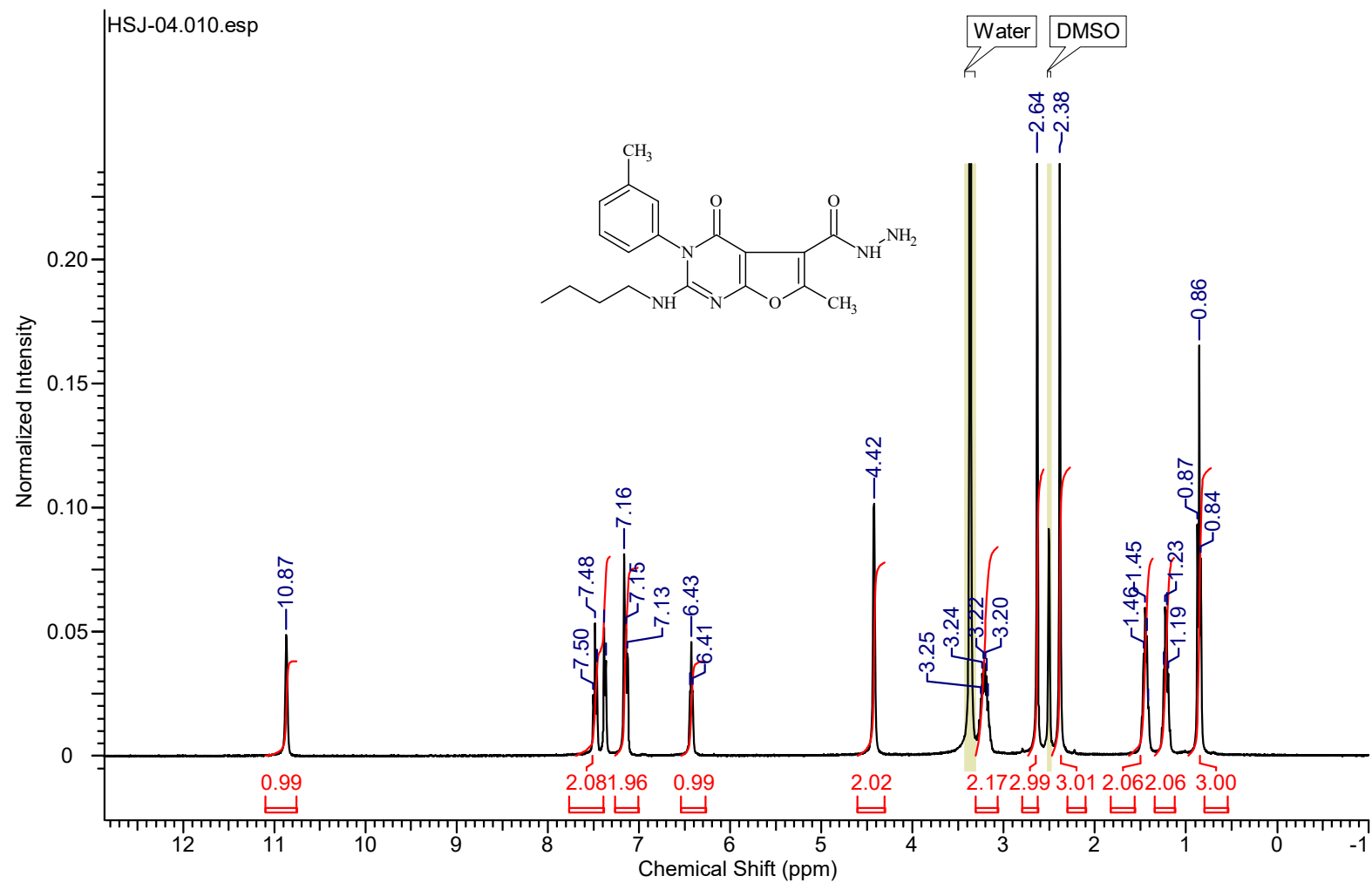


Fig.S8: ¹H NMR spectrum of compound **6h**

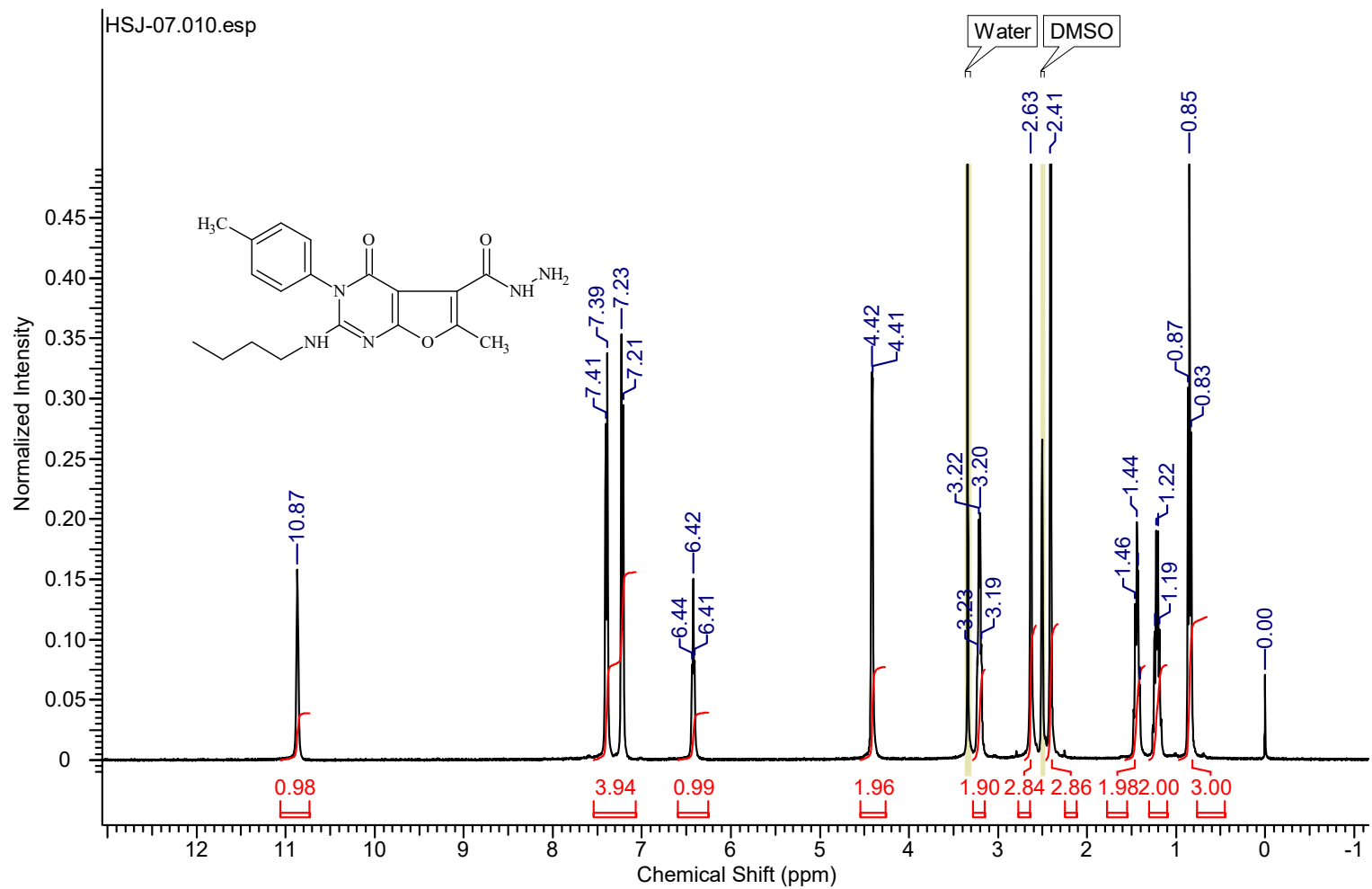


Fig.S9: ¹H NMR spectrum of compound 6i

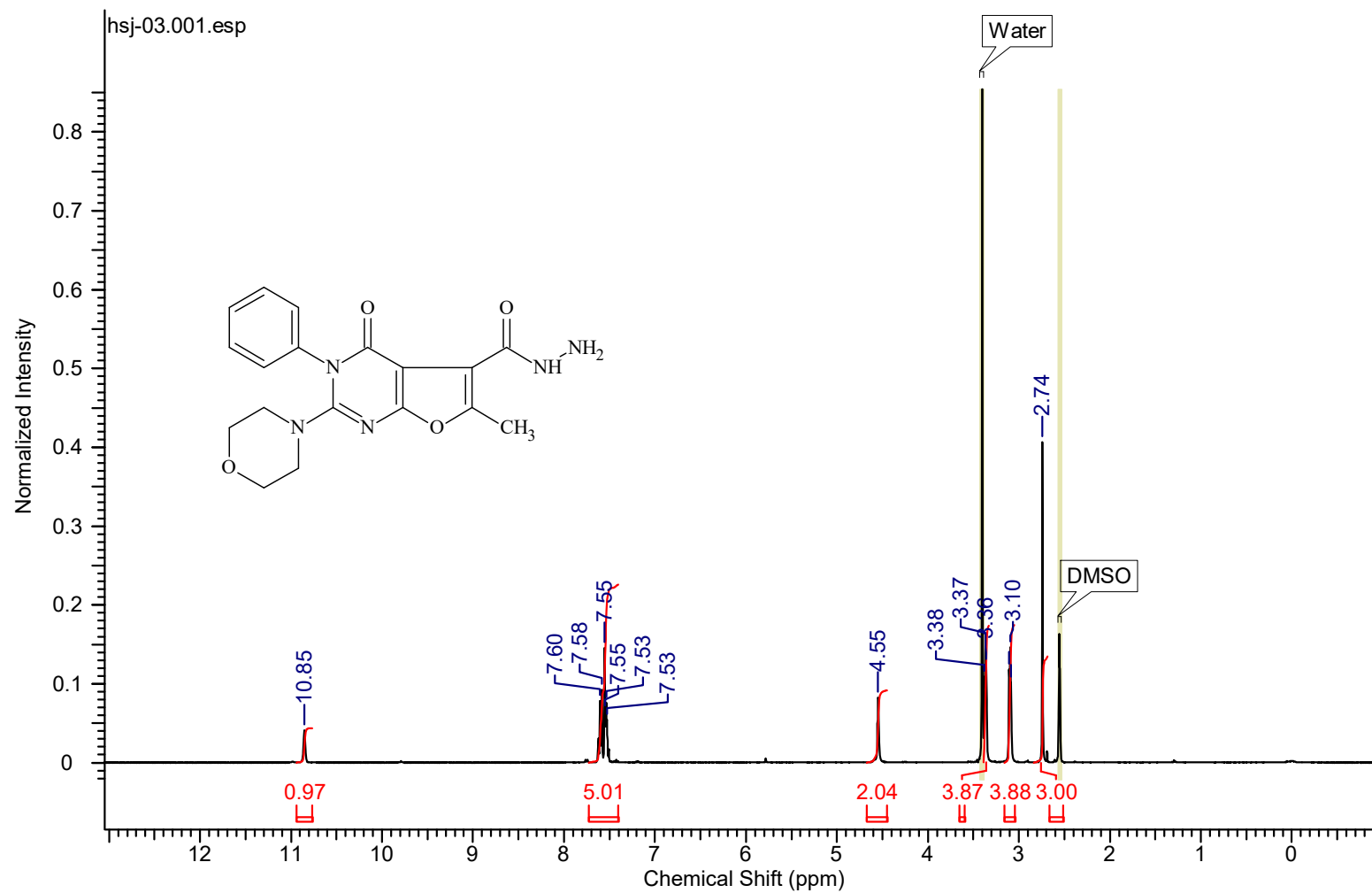


Fig.S10: ^1H NMR spectrum of compound **6j**

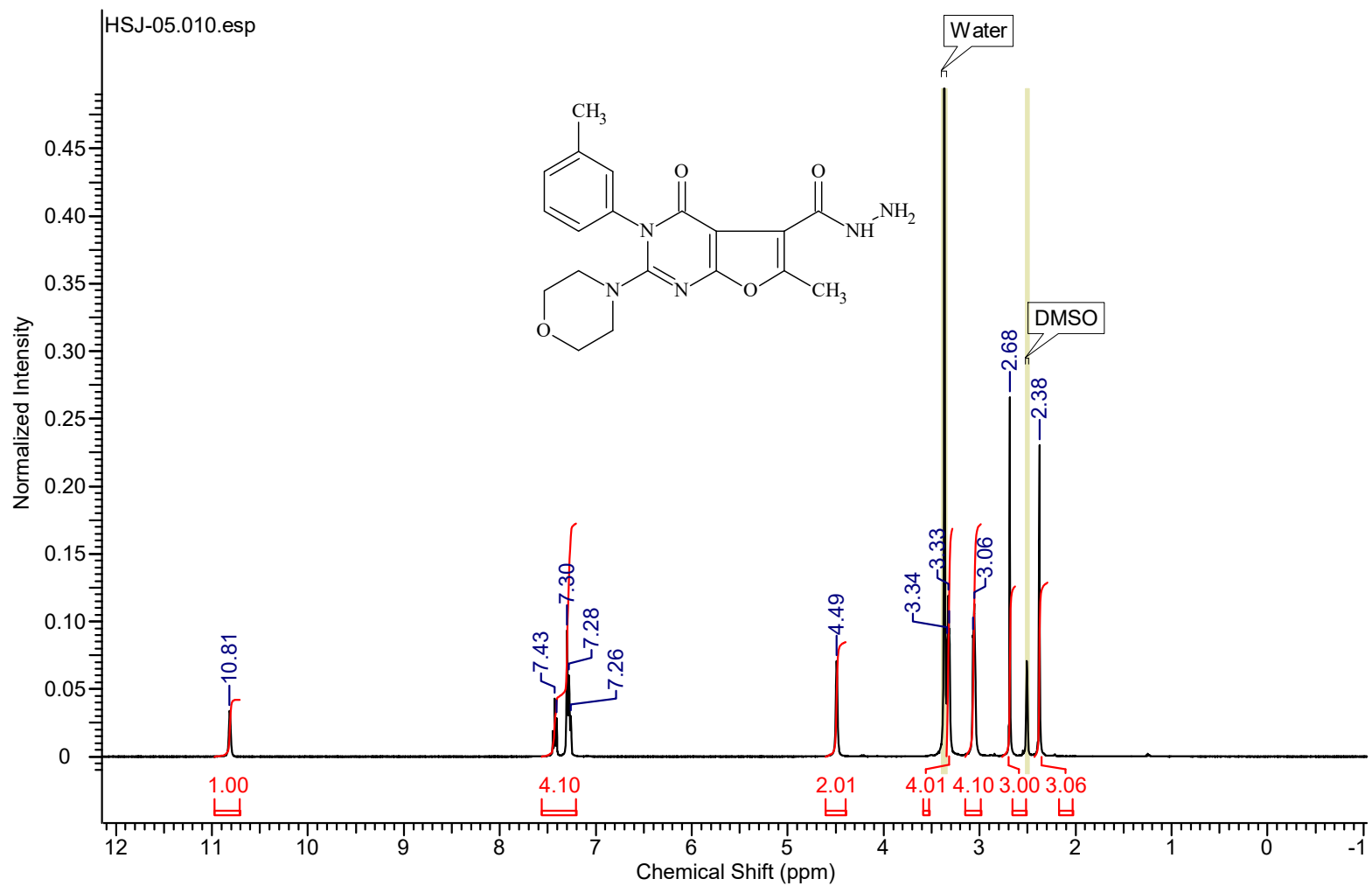


Fig.S11: ^1H NMR spectrum of compound **6k**

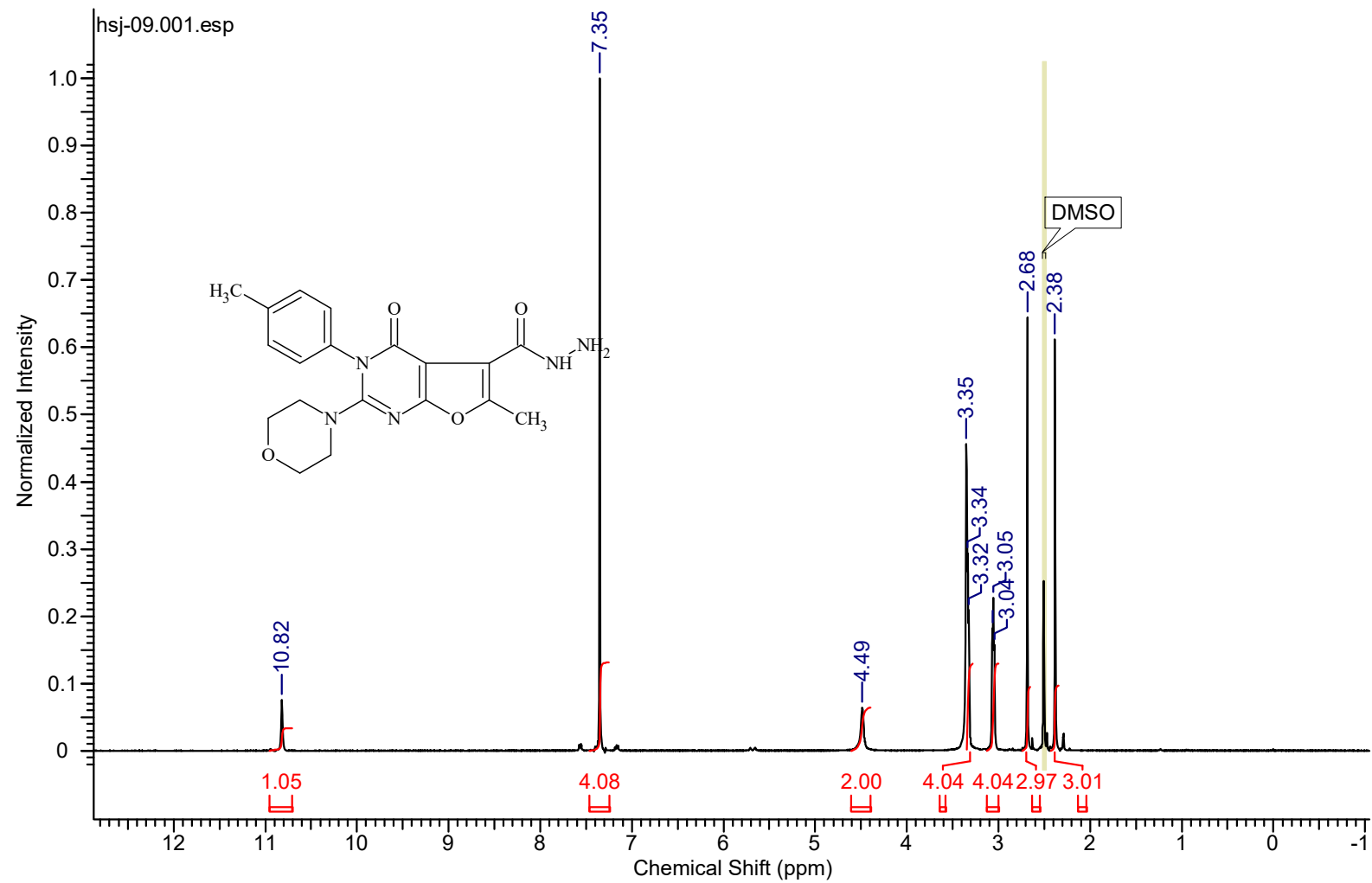


Fig.S12: ^1H NMR spectrum of compound **6l**

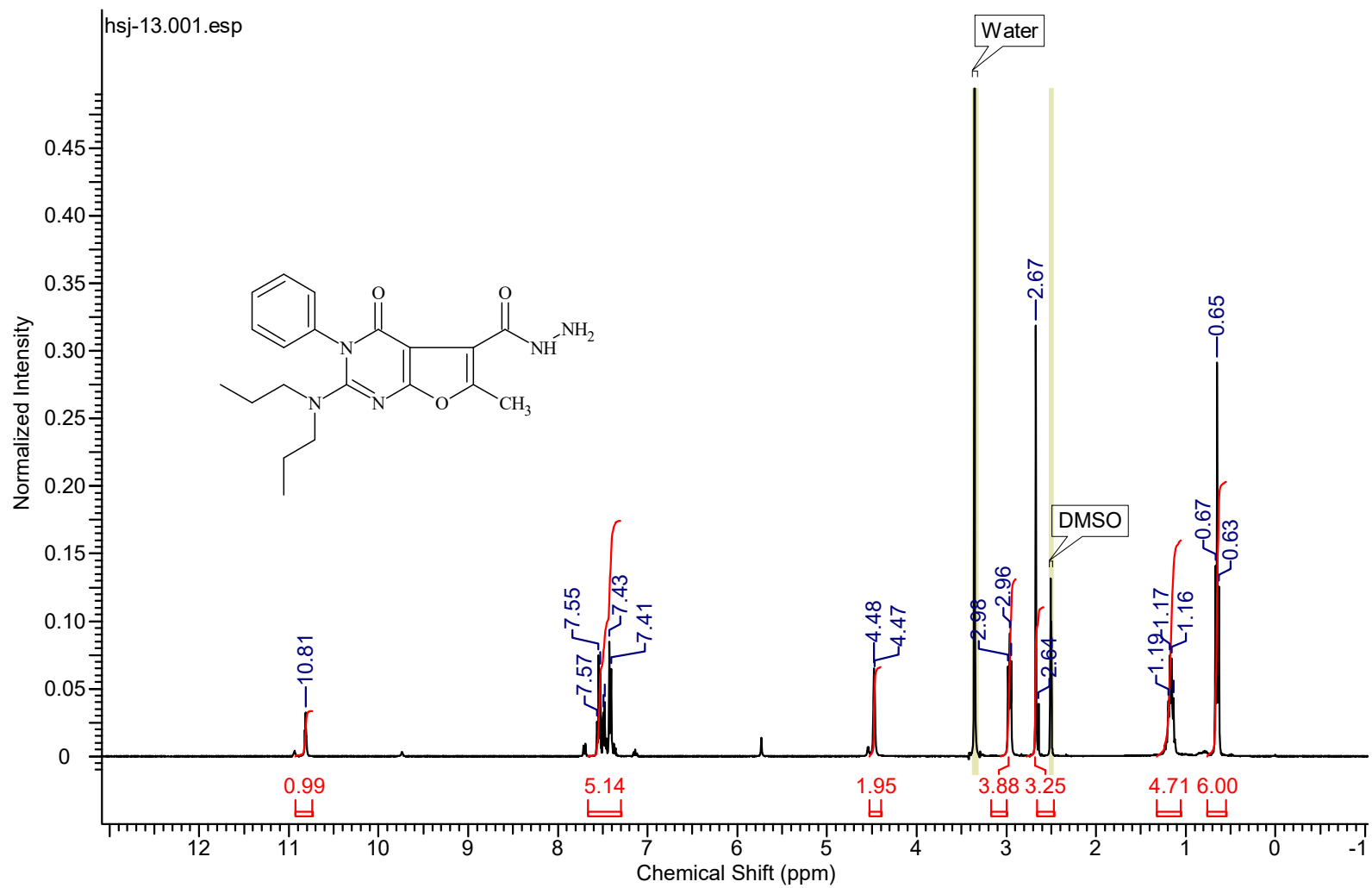


Fig.S13: ^1H NMR spectrum of compound **6m**

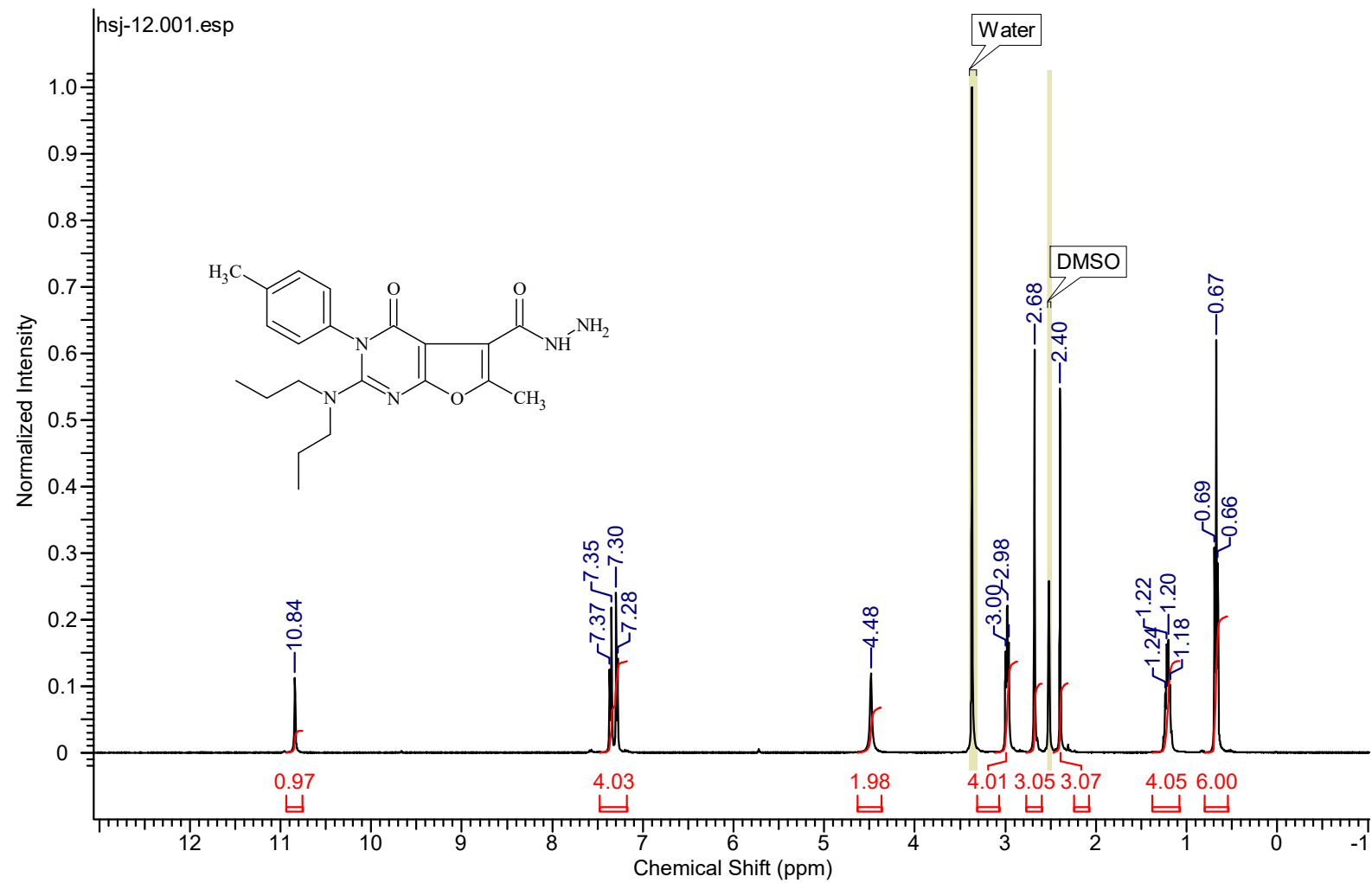


Fig.S14: ^1H NMR spectrum of compound **6n**

**^{13}C NMR of Compounds 6a-n
(Fig. S15-28)**

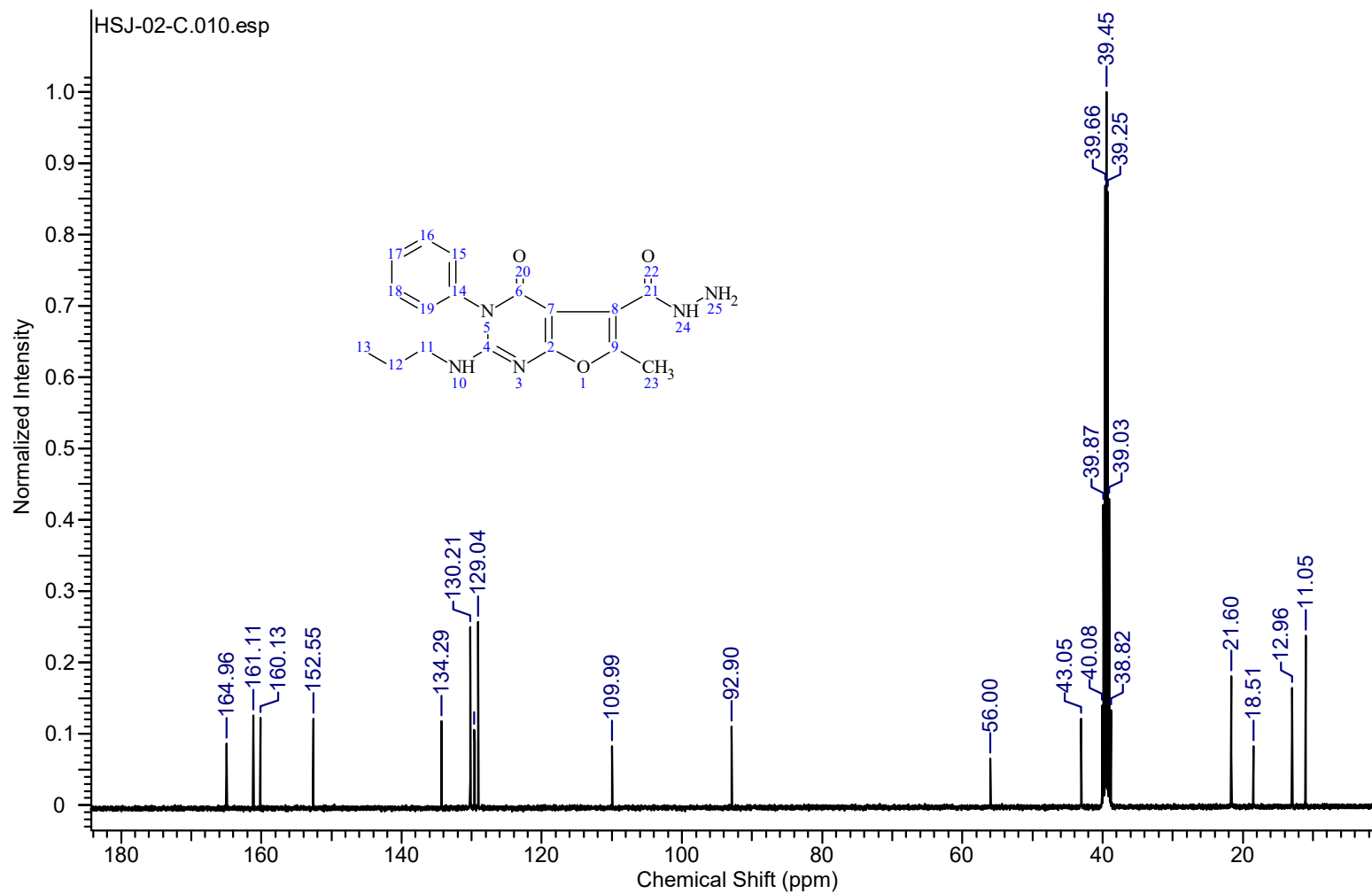


Fig.S15: ¹³C NMR spectrum of compound 6a

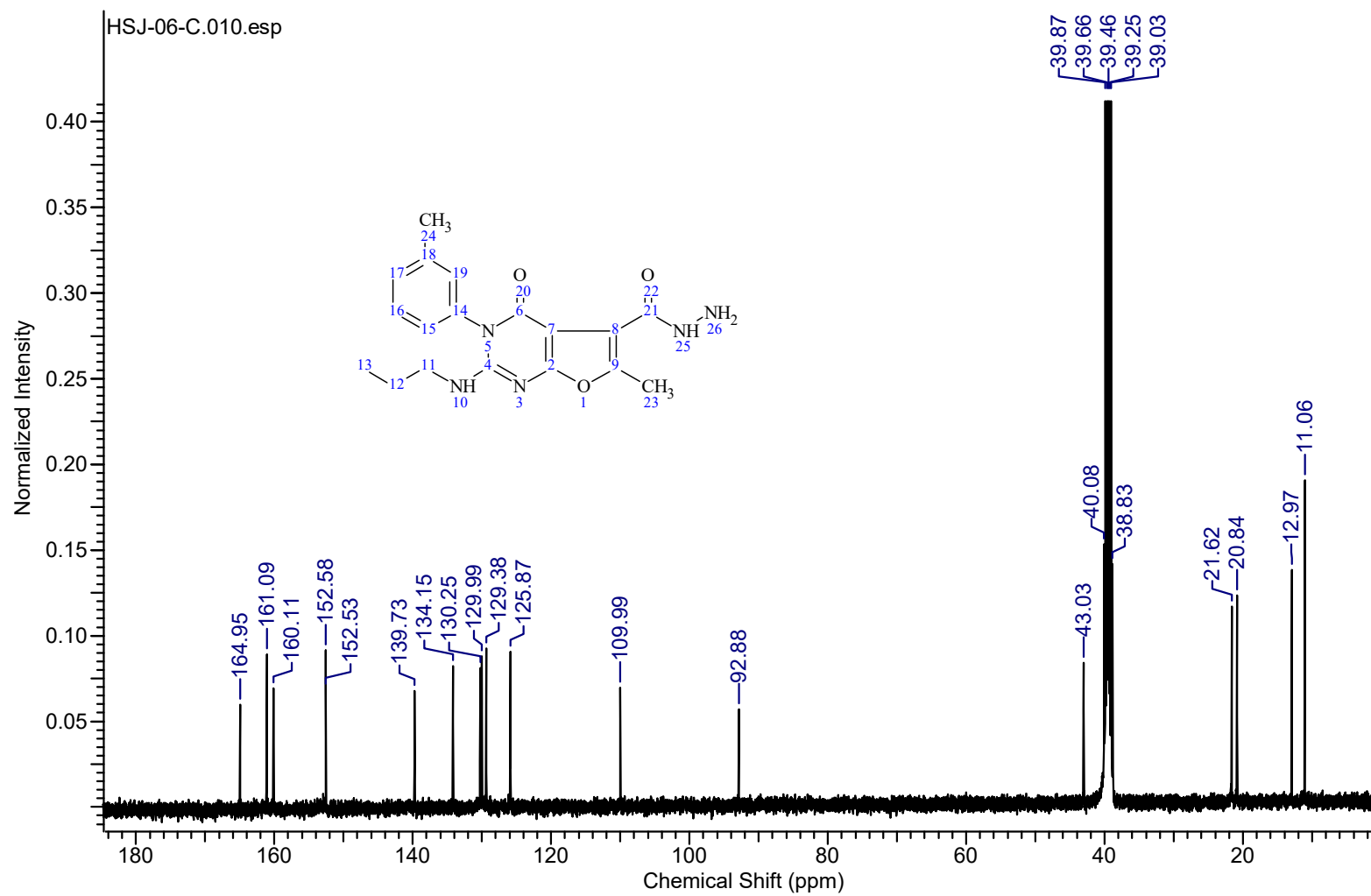


Fig.S16: ^{13}C NMR spectrum of compound **6b**

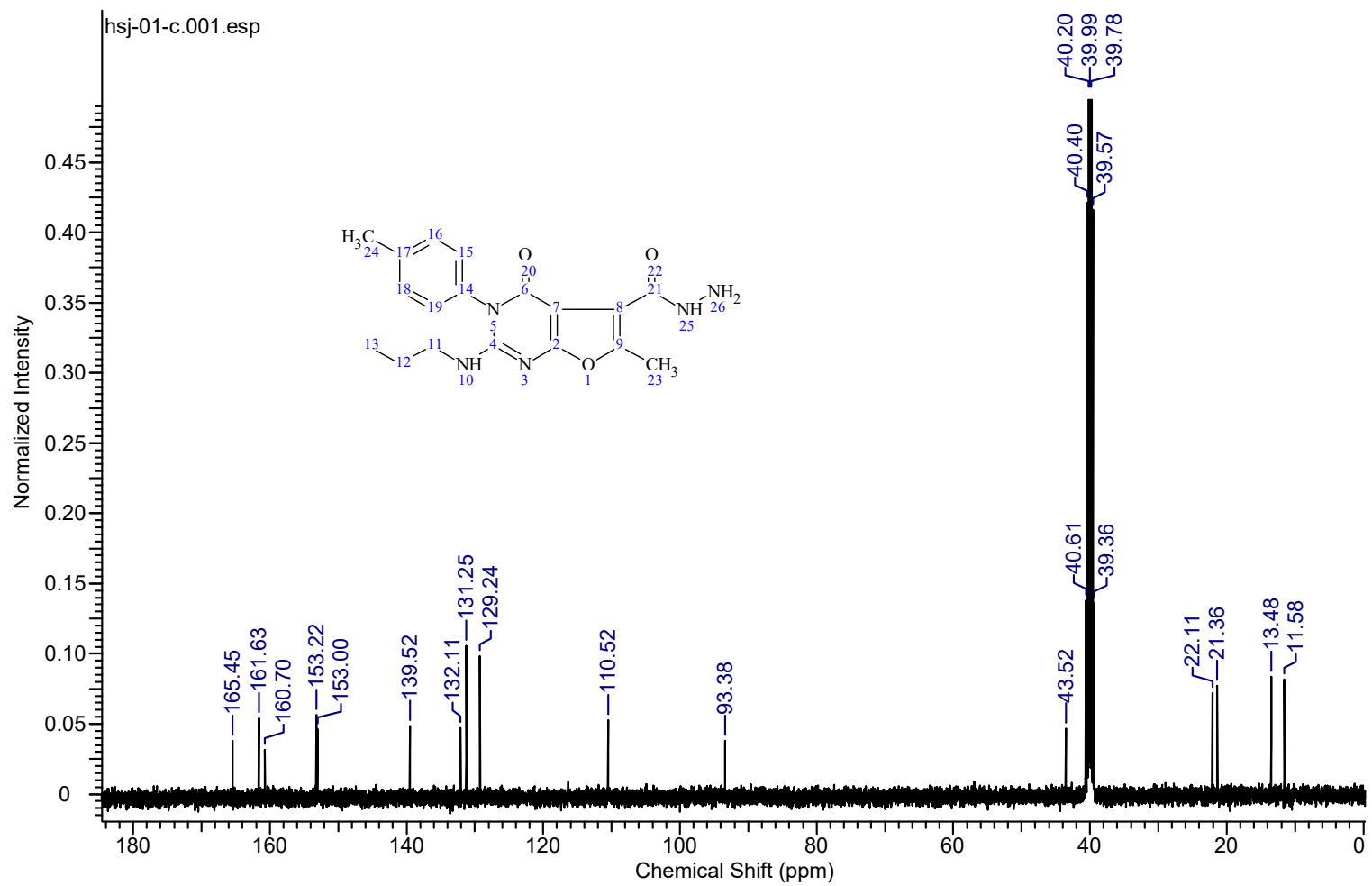


Fig.S17: ^{13}C NMR spectrum of compound **6c**

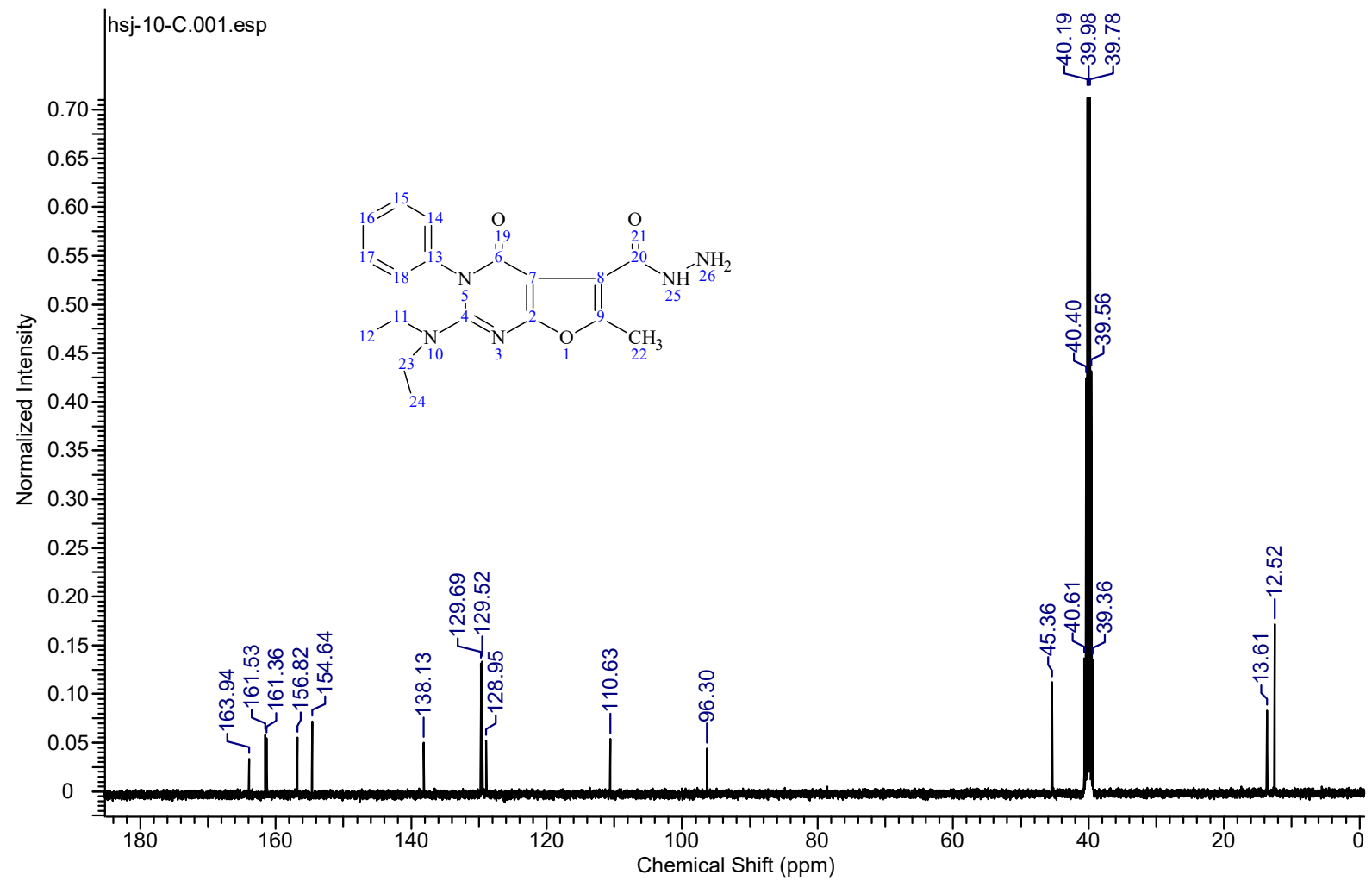


Fig.S18: ¹³C NMR spectrum of compound 6d

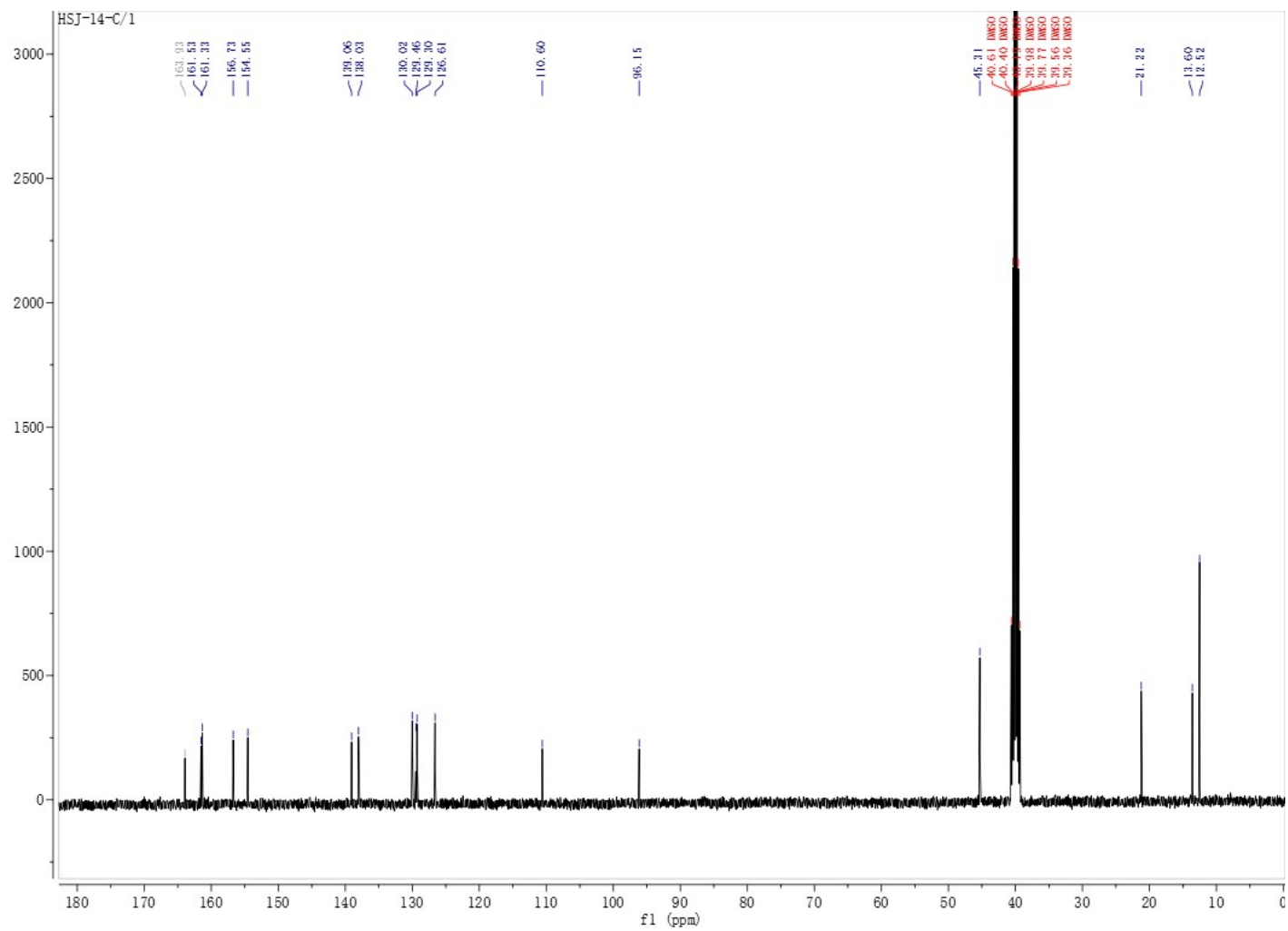


Fig.S19: ^{13}C NMR spectrum of compound **6e**

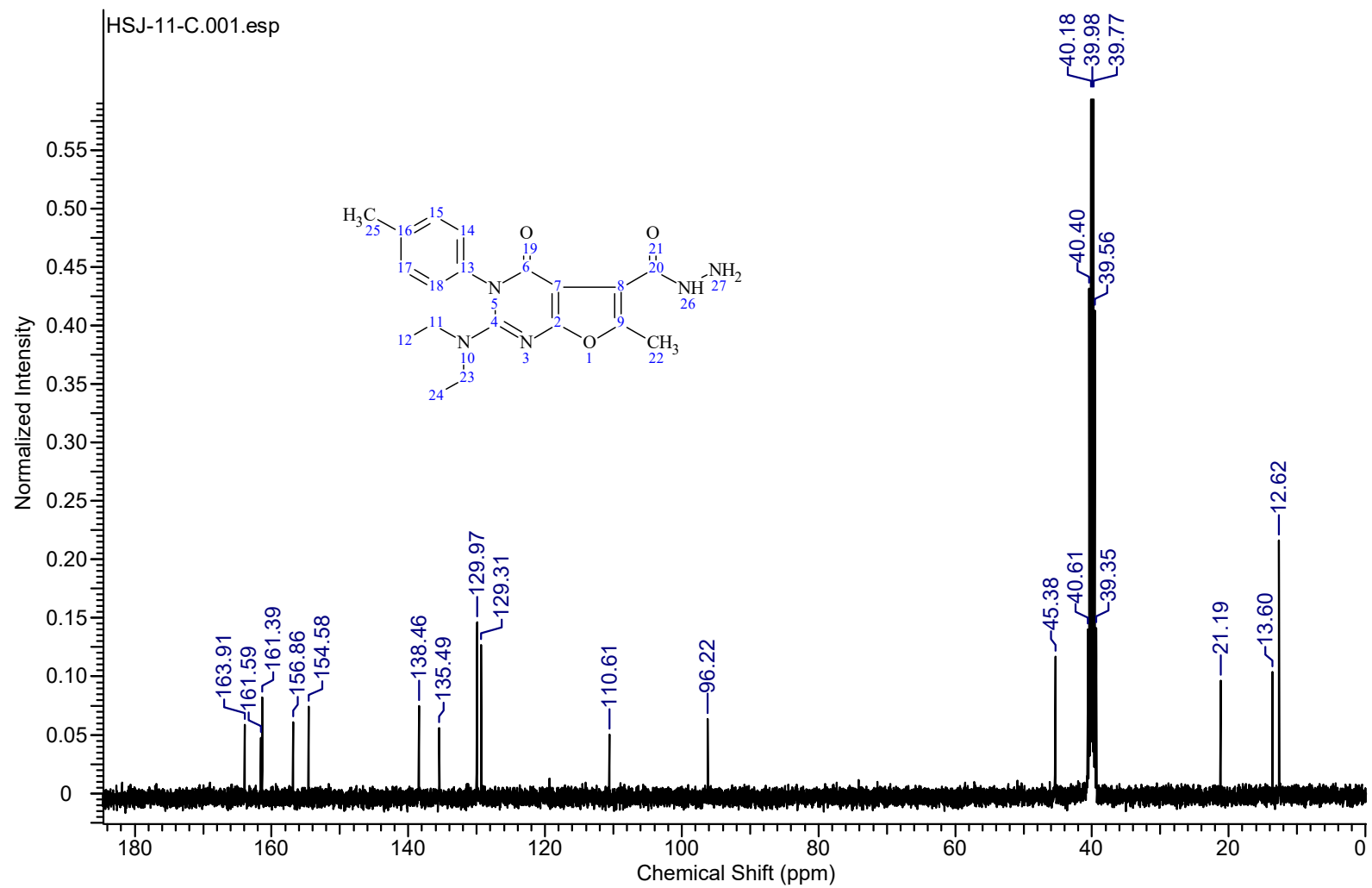


Fig.S20: ^{13}C NMR spectrum of compound 6f

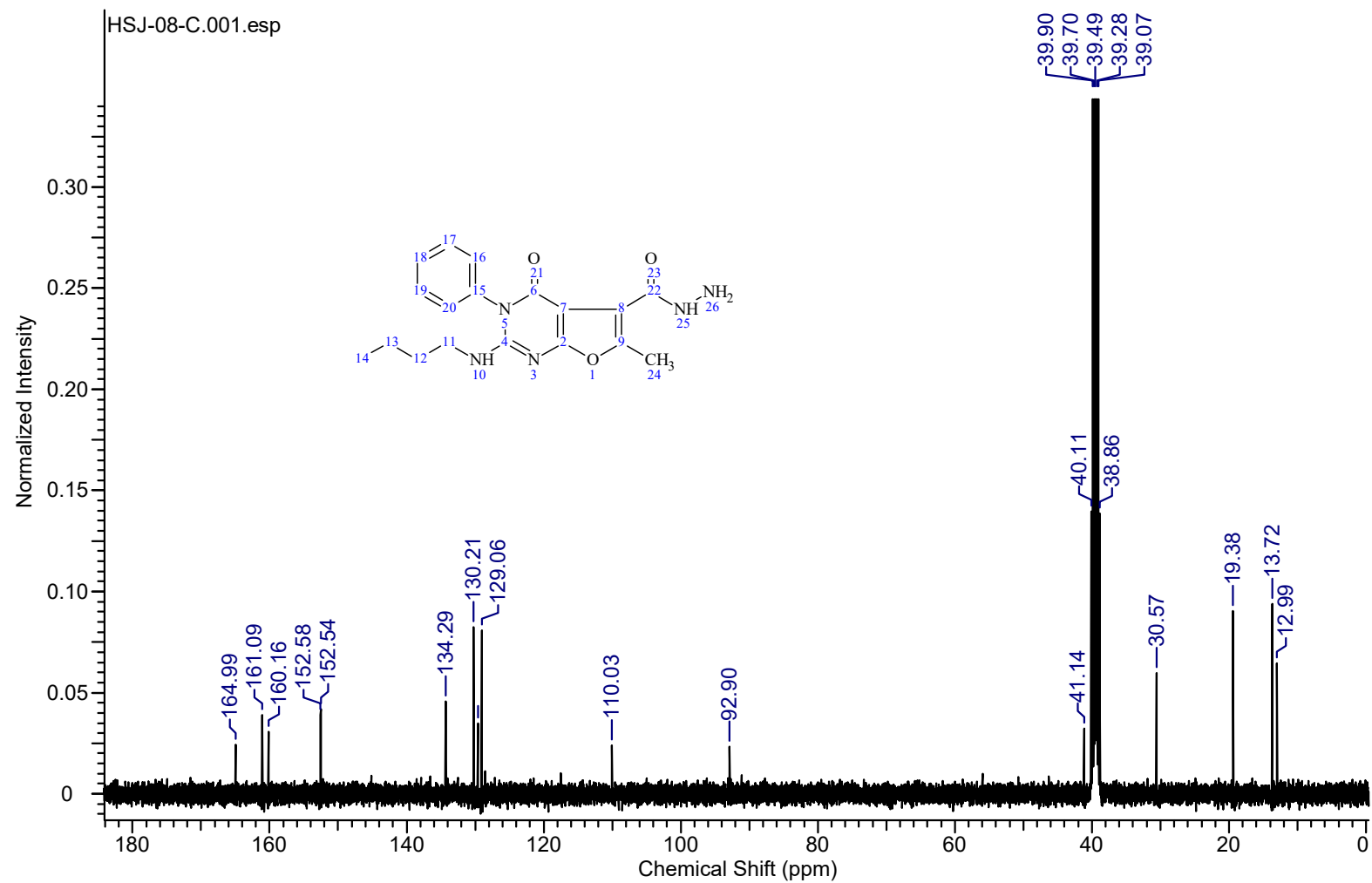


Fig.S21: ^{13}C NMR spectrum of compound 6g

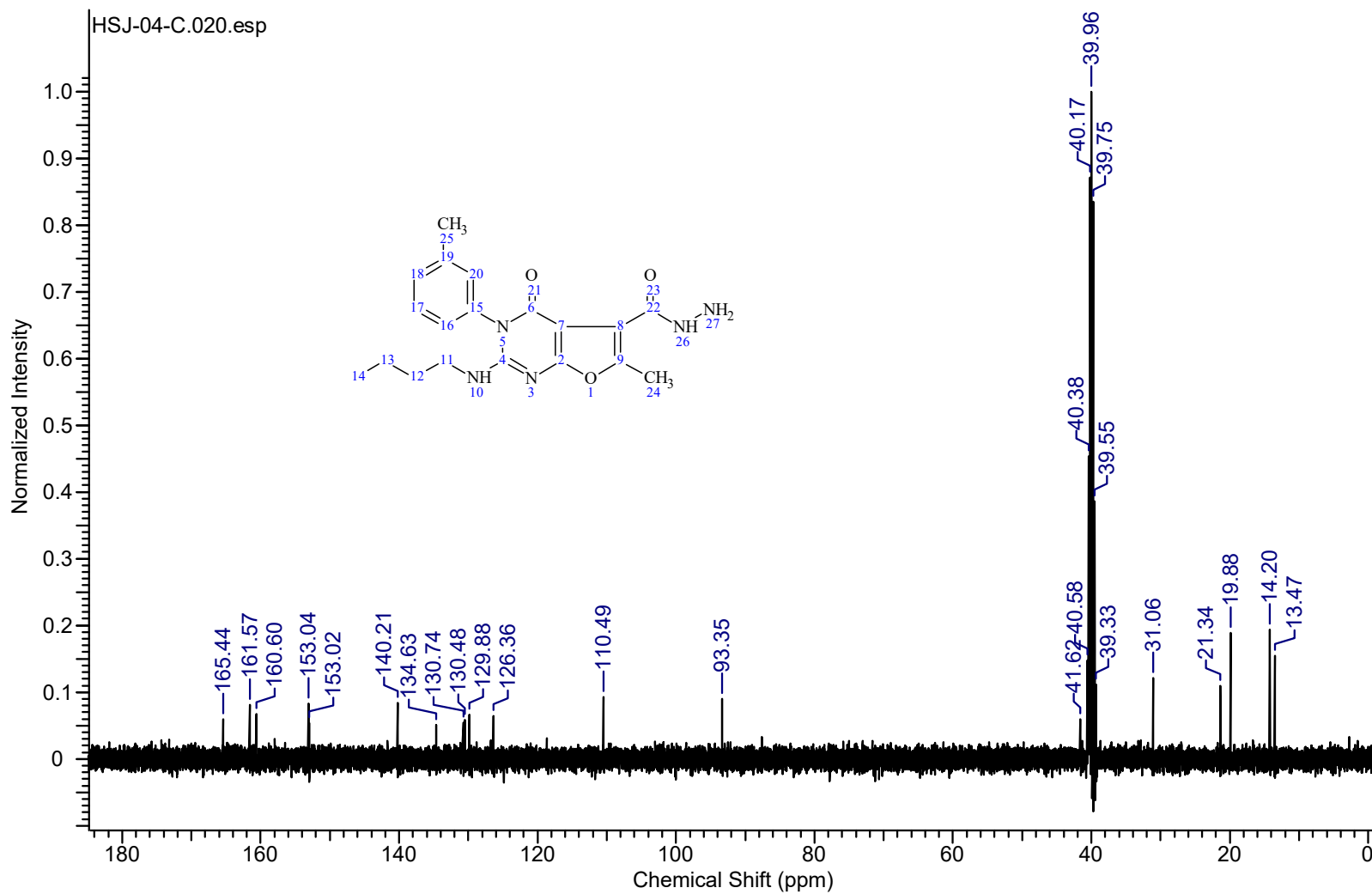


Fig.S22: ^{13}C NMR spectrum of compound 6h

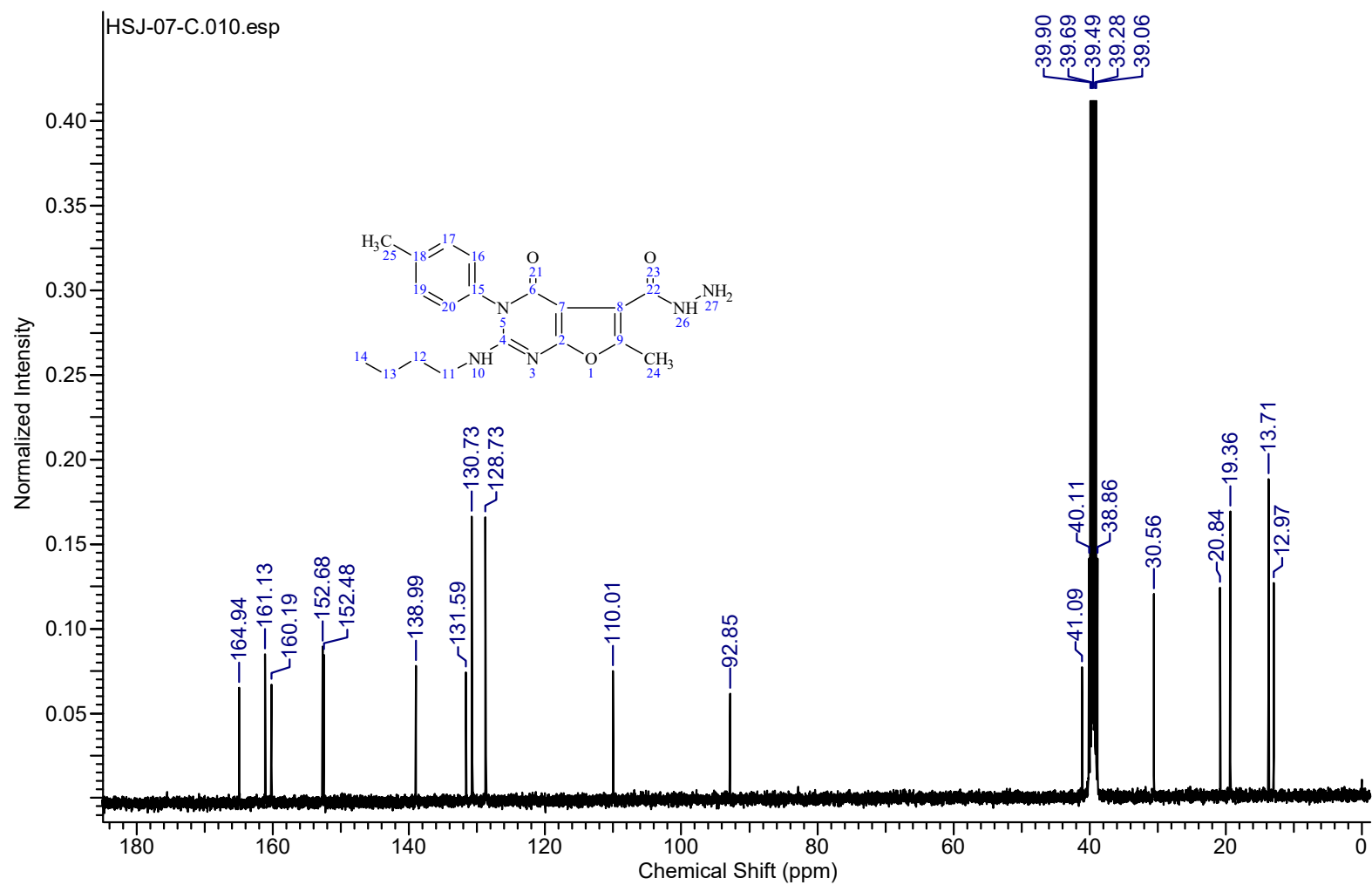


Fig.S23: ^{13}C NMR spectrum of compound 6i

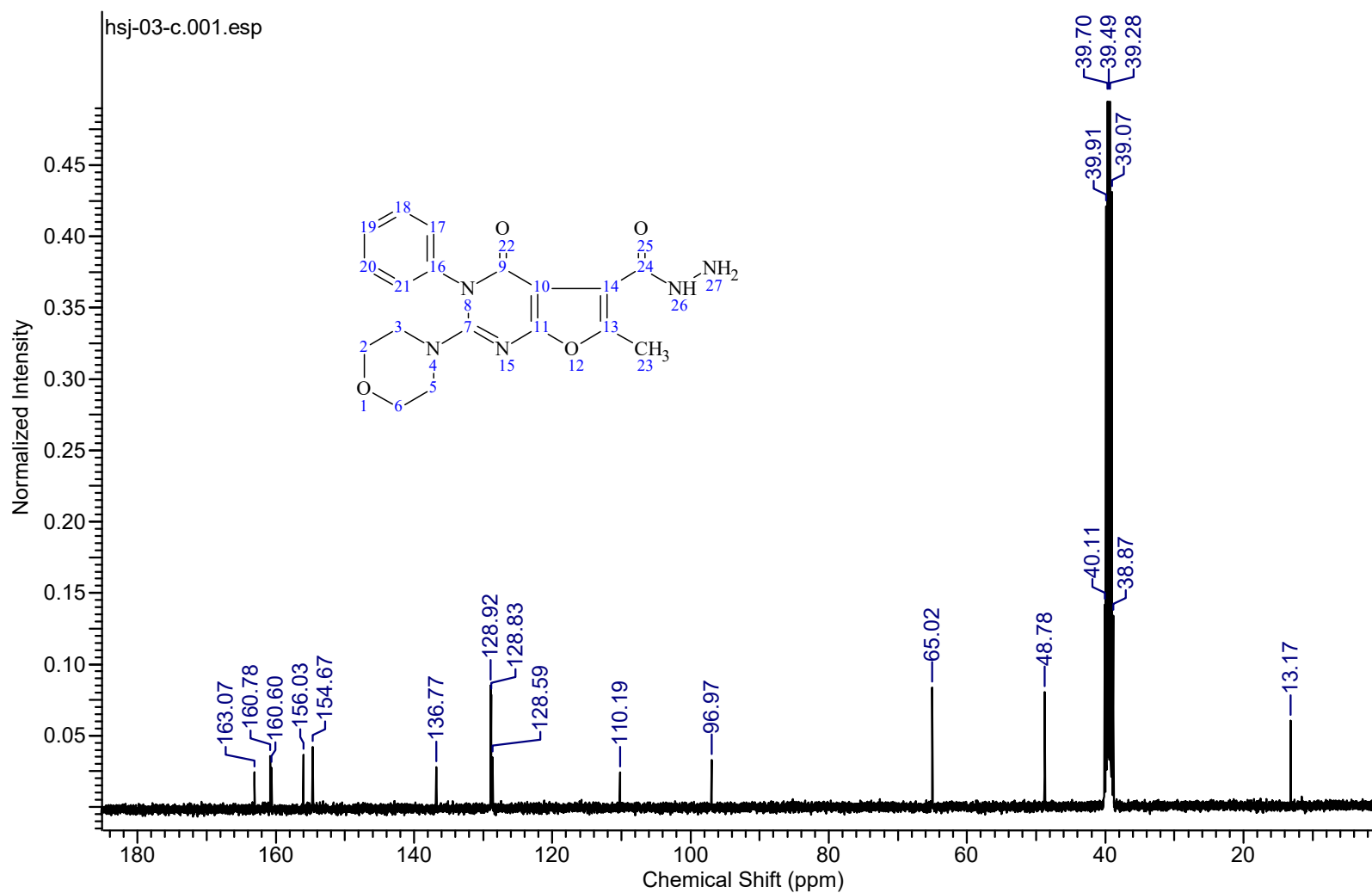


Fig.S24: ^{13}C NMR spectrum of compound 6j

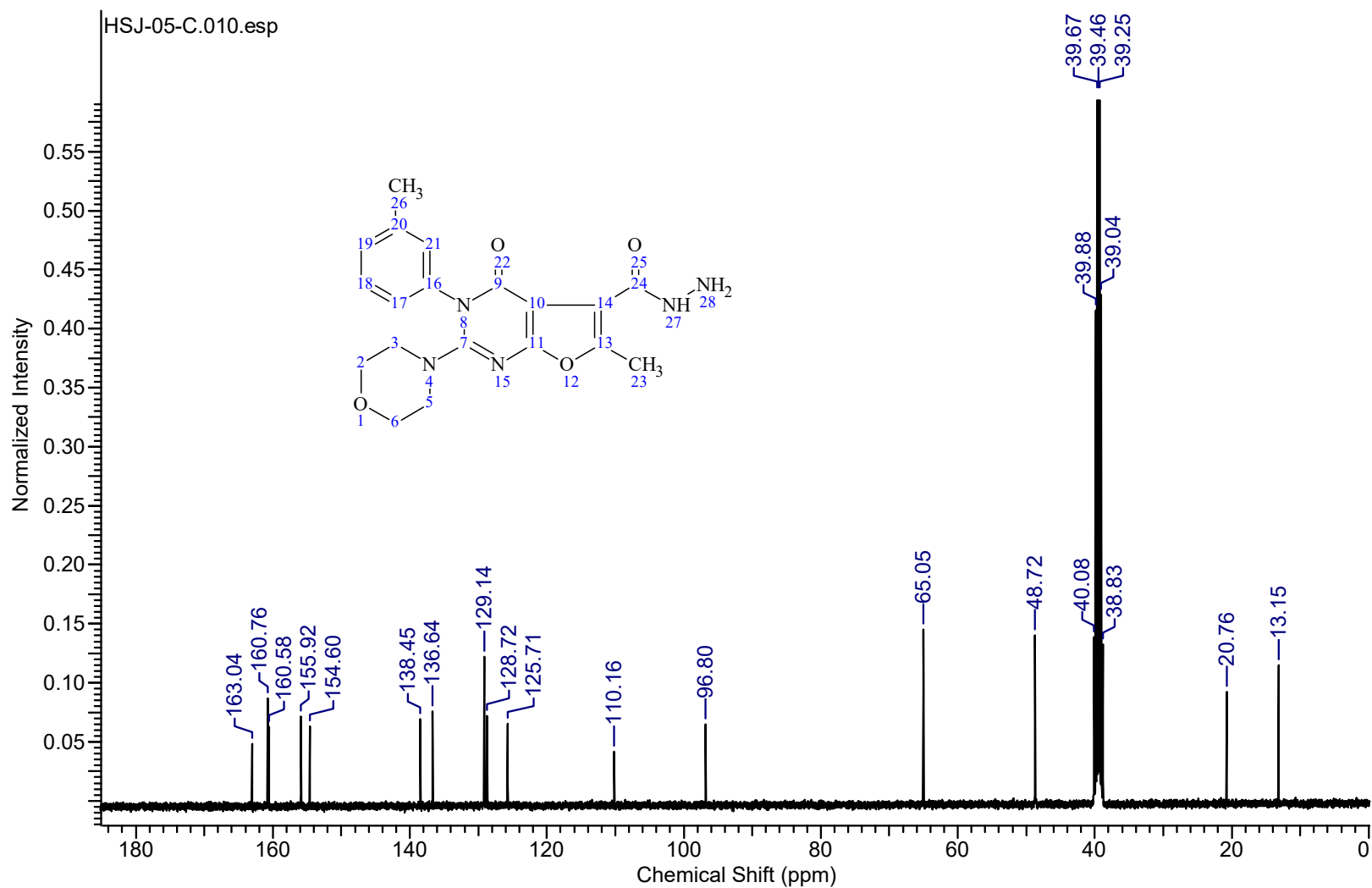


Fig.S25: ¹³C NMR spectrum of compound 6k

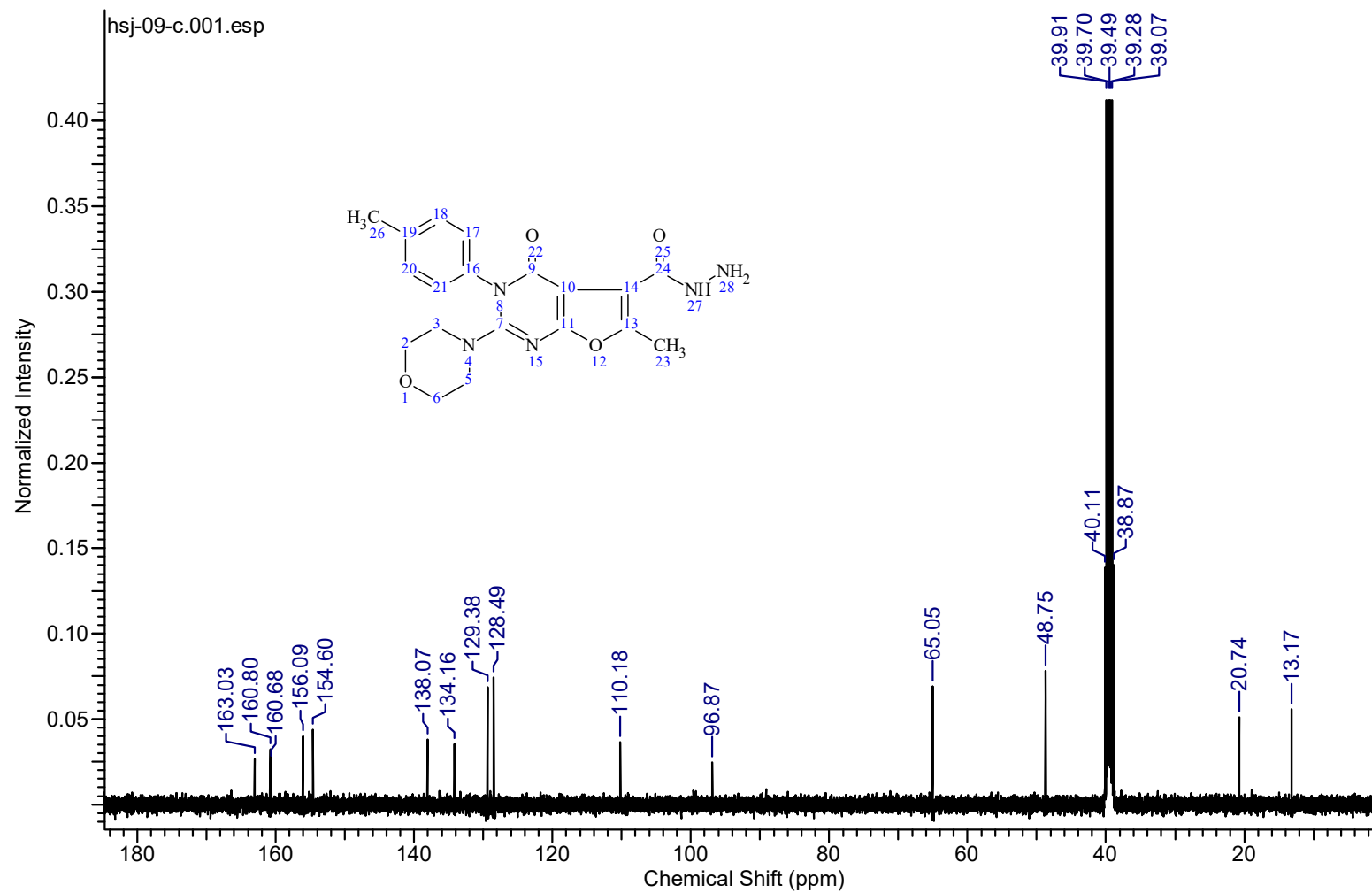


Fig.S26: ^{13}C NMR spectrum of compound 61

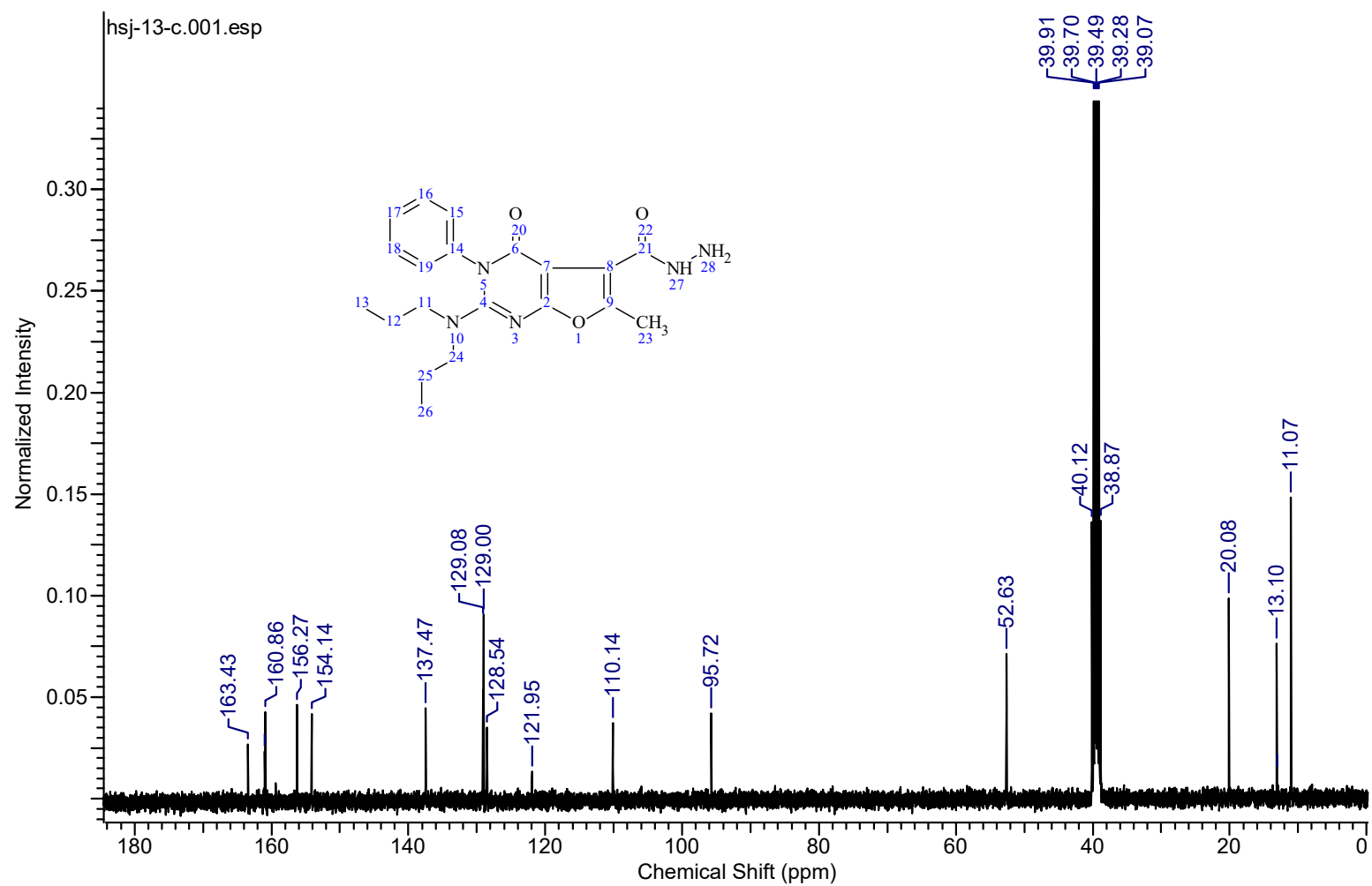


Fig.S27: ^{13}C NMR spectrum of compound 6m

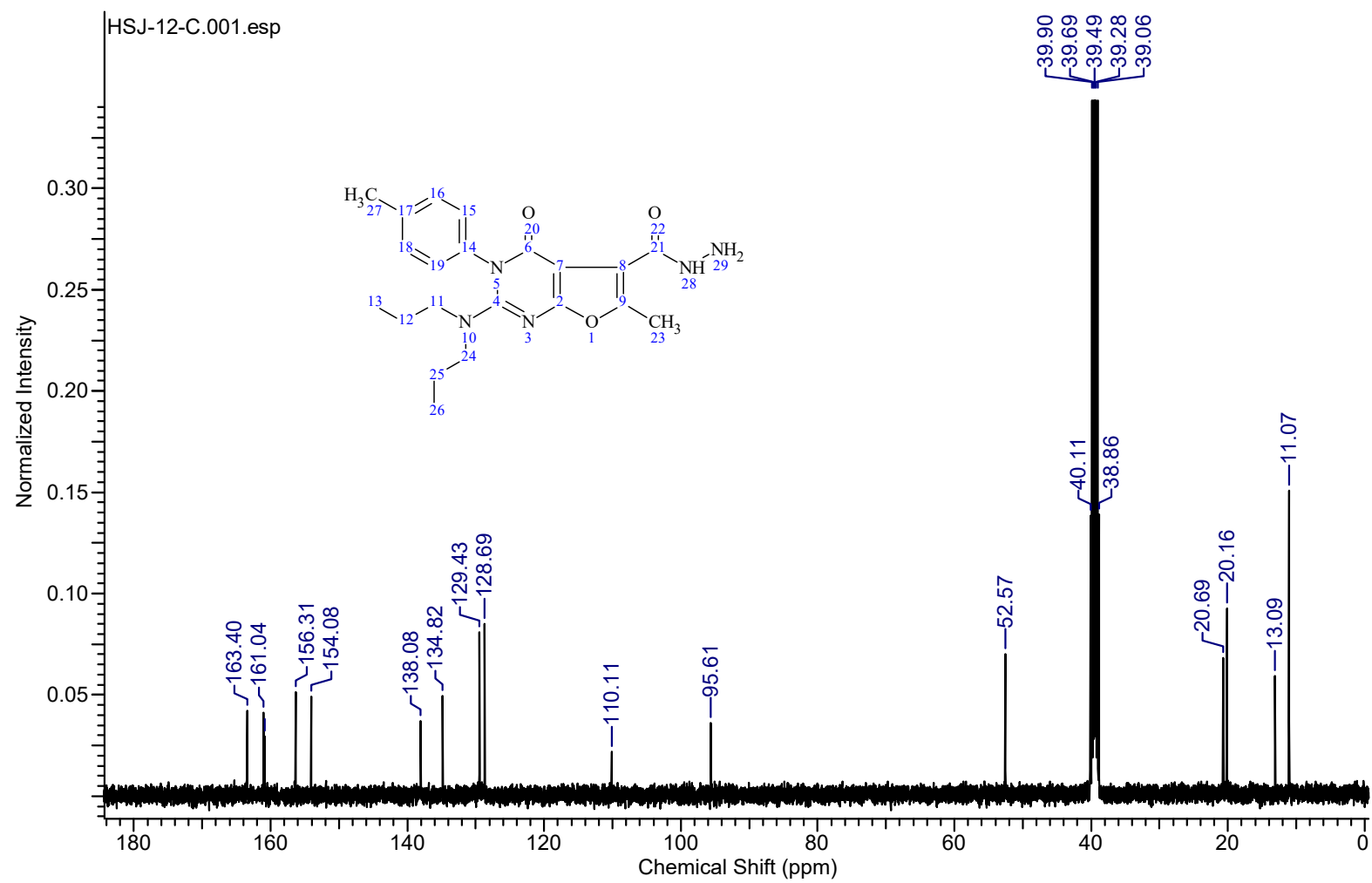


Fig.S28: ¹³C NMR spectrum of compound 6n

ESI-MS of Compounds 6a-n
(Fig. S29-39)

13_20200106043526 #21 RT: 0.13 AV: 1 NL: 2.93E7
T: +c ESI Q1MS [200.000-600.000]

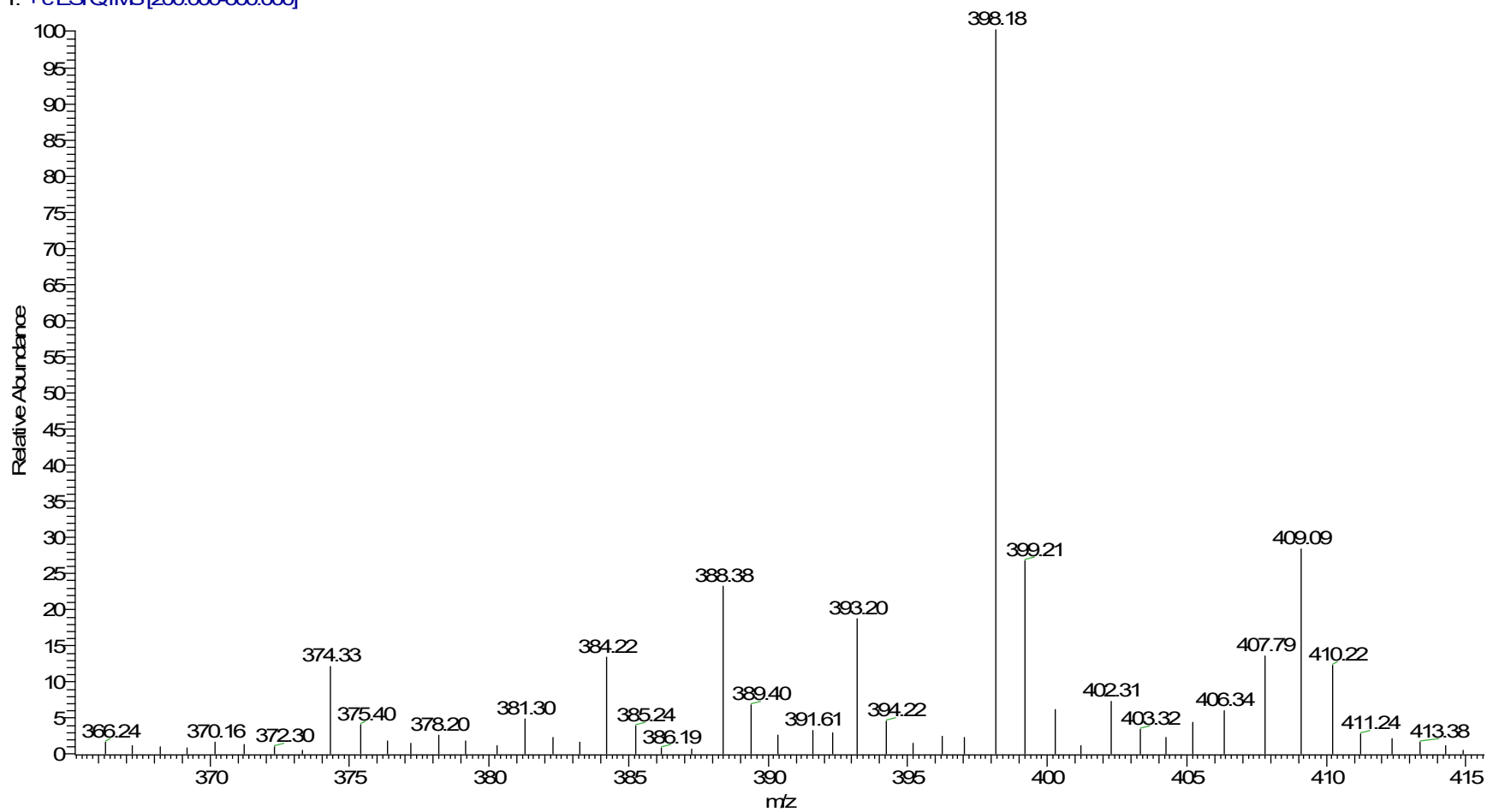


Fig.S29: ESI-MS spectrum of compound 6n

15 #9 RT: 0.04 AV: 1 NL: 5.26E6
T: +cESI Q1MS [200.000-500.000]

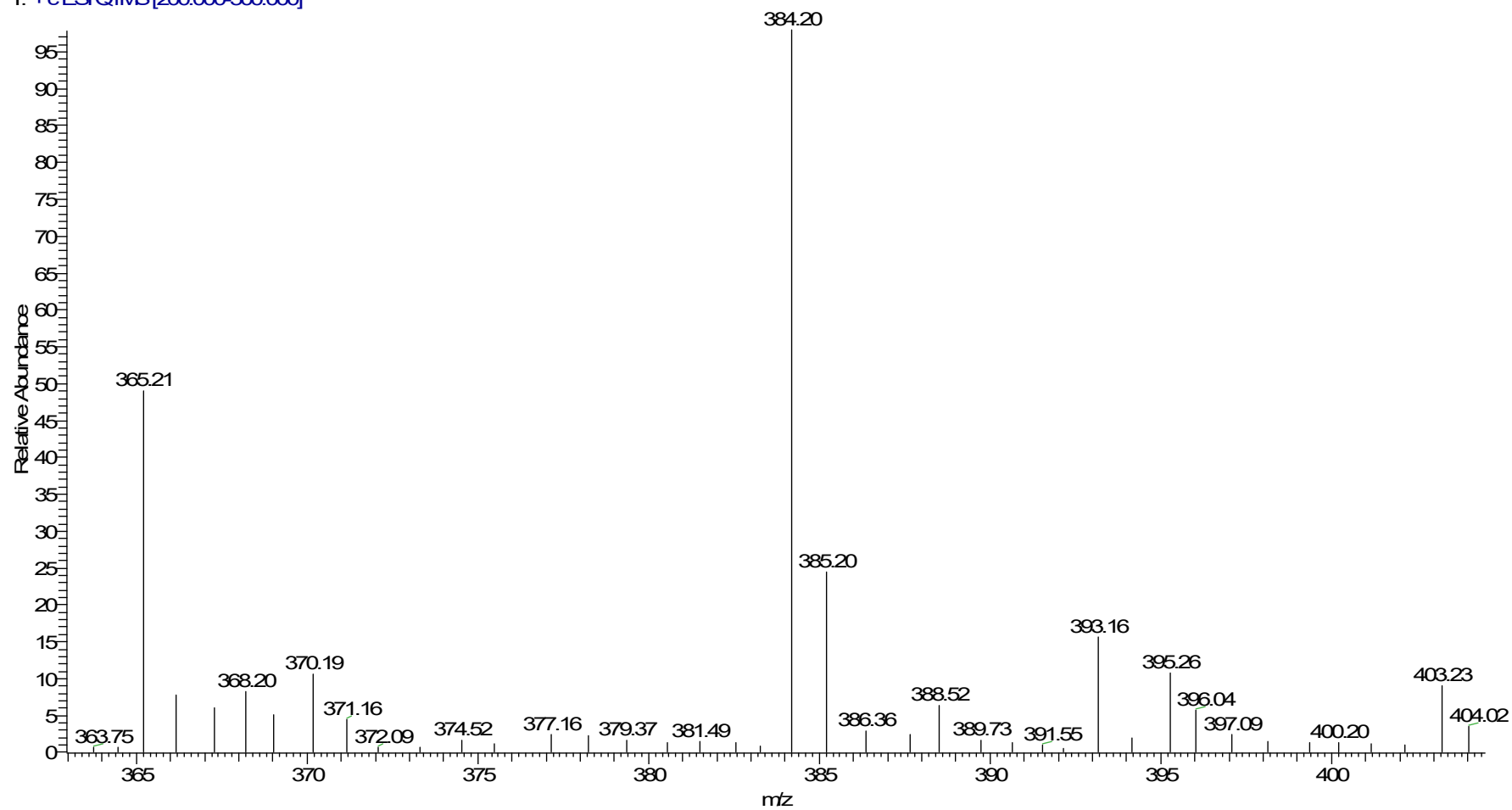


Fig.S30: ESI-MS spectrum of compound 6m

hsj-02 #3 RT: 0.01 AV: 1 NL: 8.73E7
T: +cESI Q1MS [200.000-600.000]

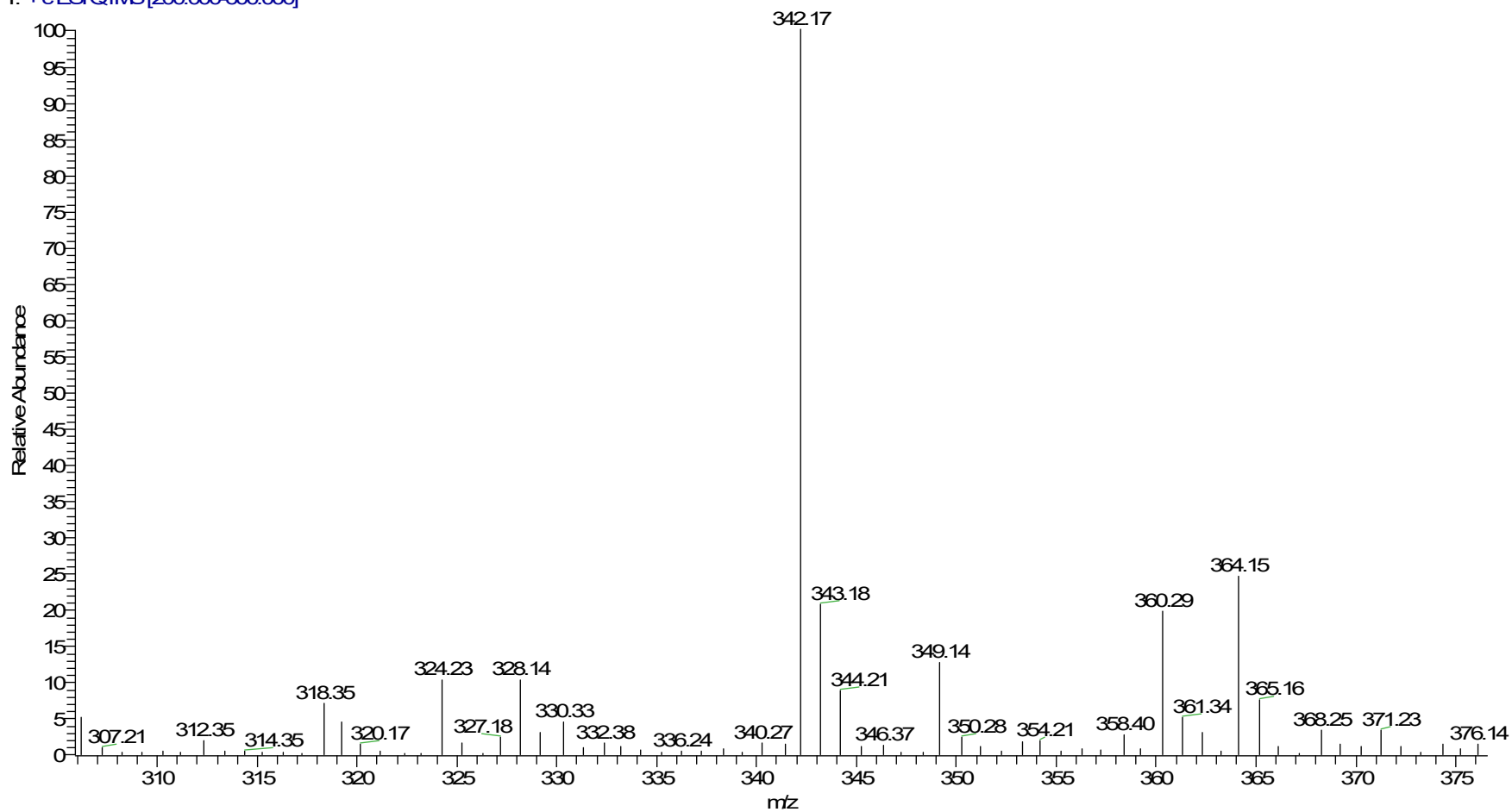


Fig.S31: ESI-MS spectrum of compound 6a

hsj-03 #18 RT: 0.11 AV: 1 NL: 1.95E6
T: -c ESI Q1MS [200.000-600.000]

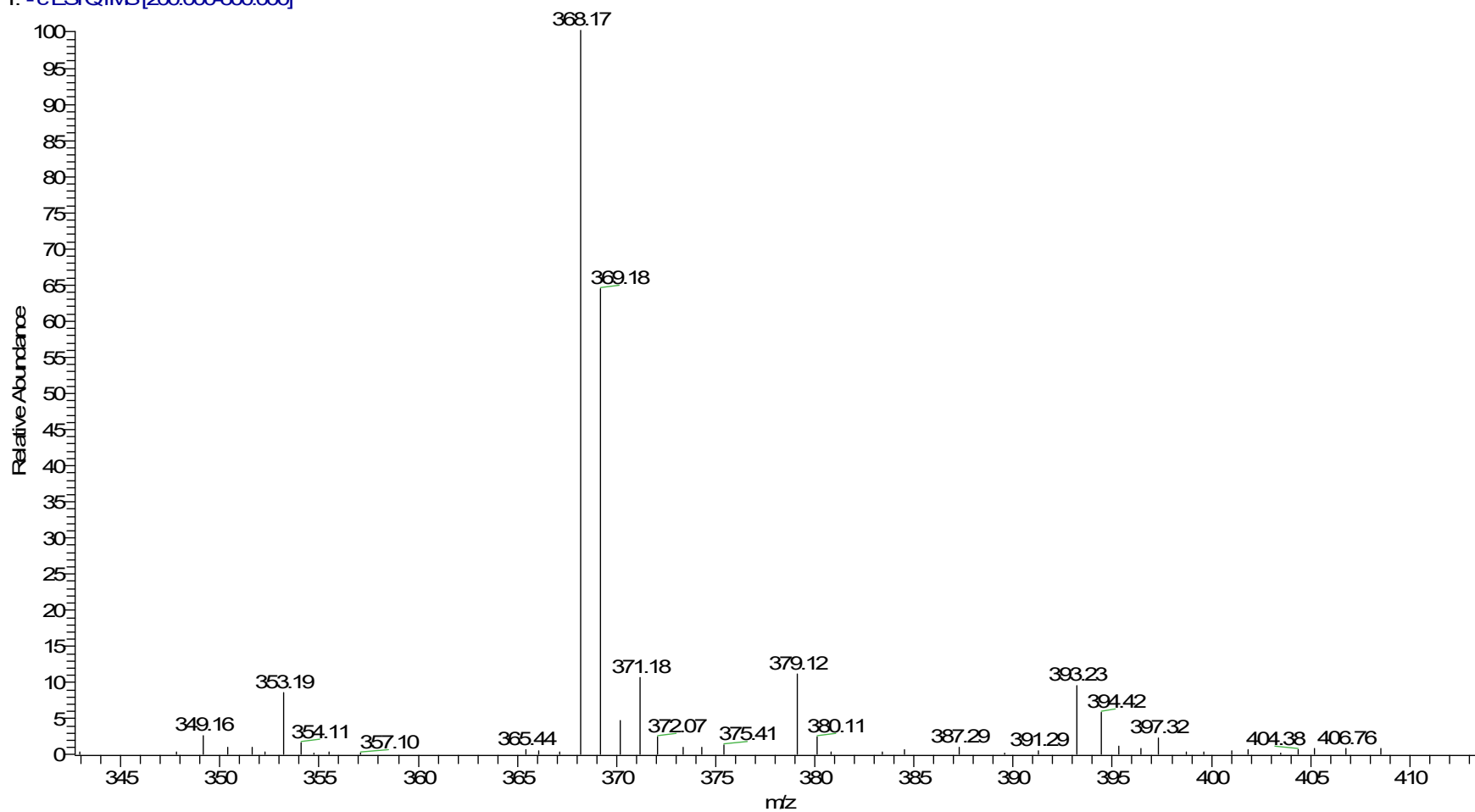


Fig.S32: ESI-MS spectrum of compound 6j

hsj-04_20191209070847 #59 RT: 0.29 AV: 1 NL: 1.35E7
T: -c ESI Q1MS [200.000-500.000]

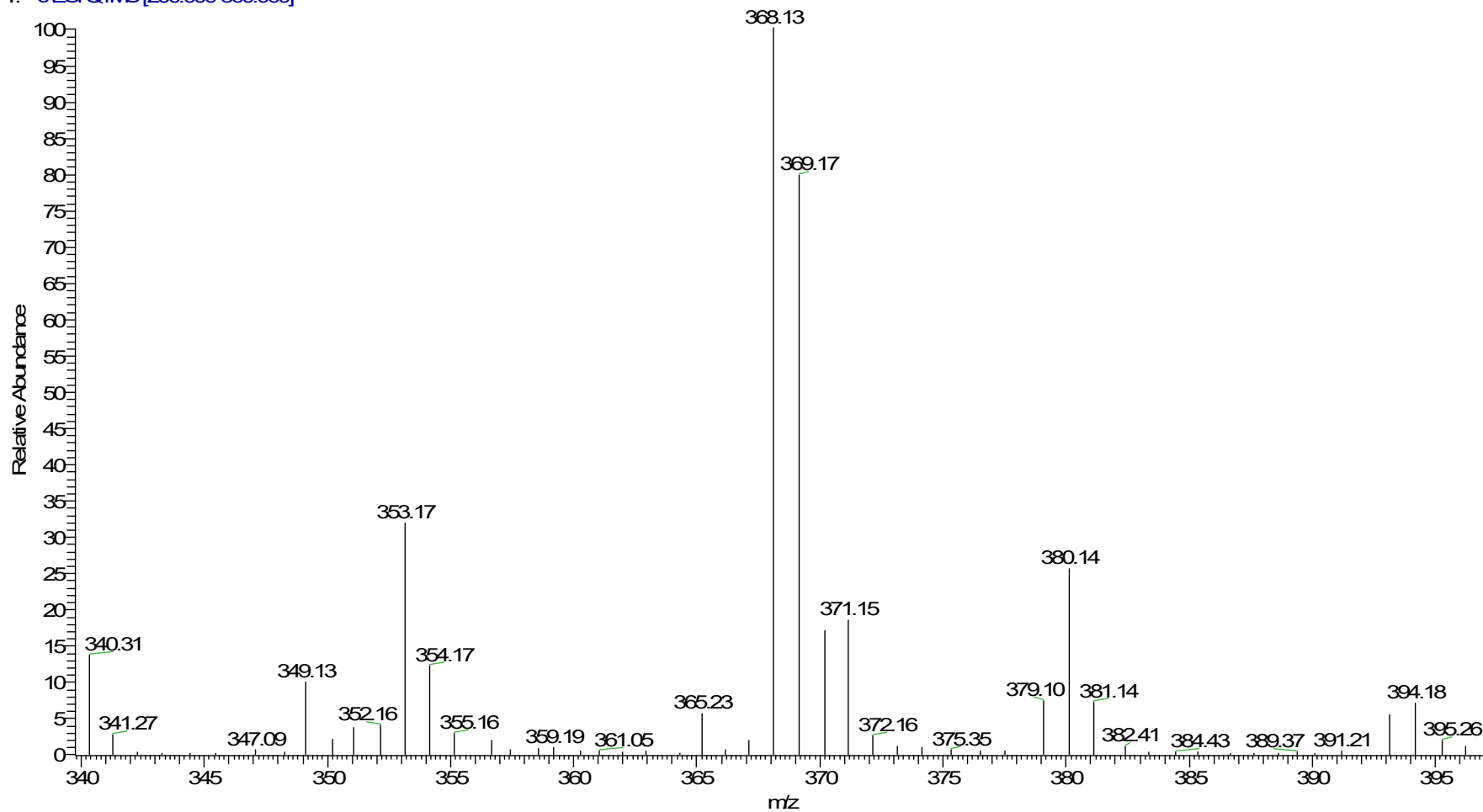


Fig.S33: ESI-MS spectrum of compound 6h

hsj-05_20191127051841#16 RT: 0.08 AV: 1 NL: 1.51E7
T: +cESI Q1MS [300.000-600.000]

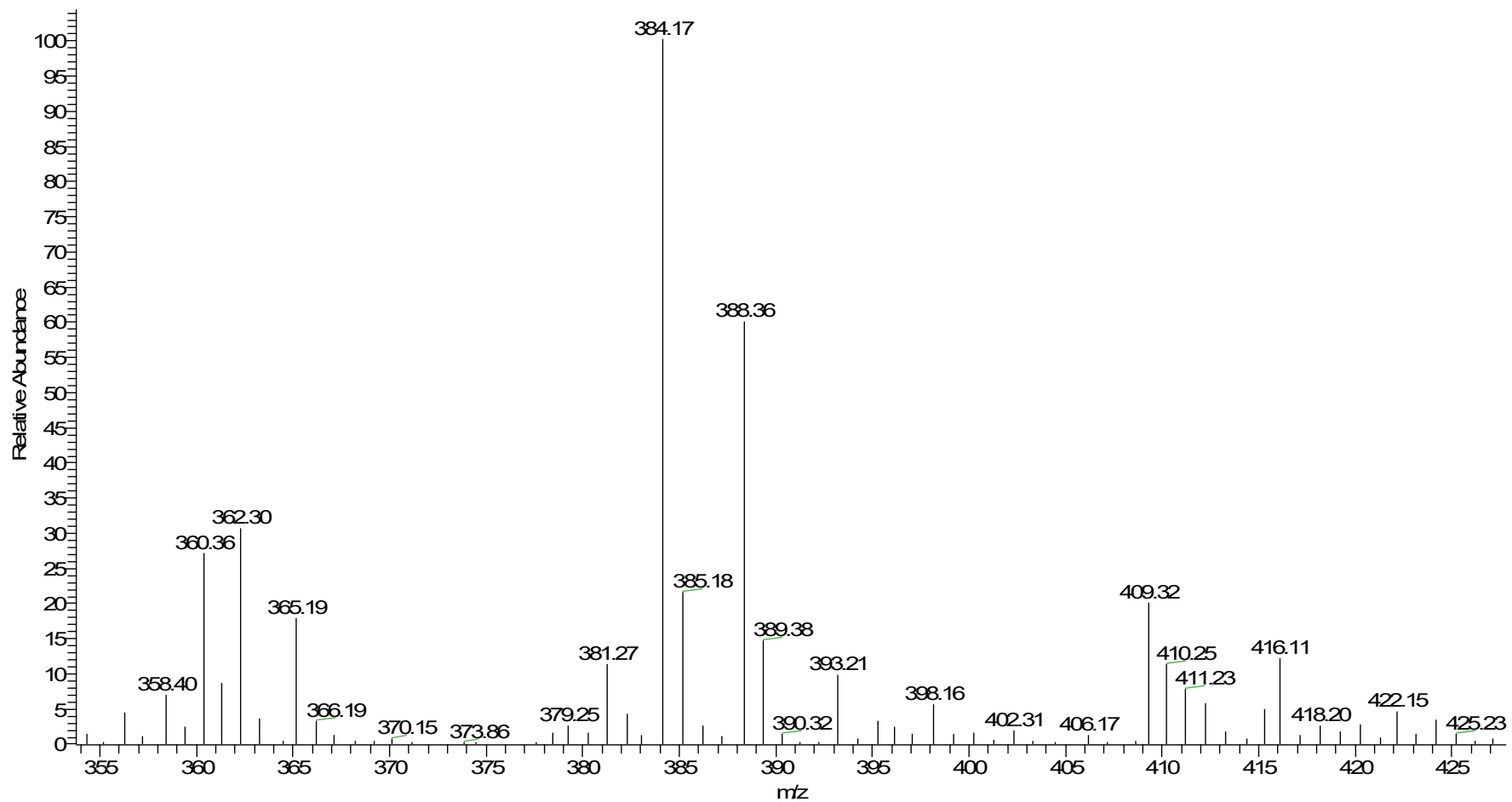


Fig.S34: ESI-MS spectrum of compound 6k

hsj-06_20191127052851#3 RT: 0.01 AV: 1 NL: 2.12E7
T: +cESI Q1MS [300.000-500.000]

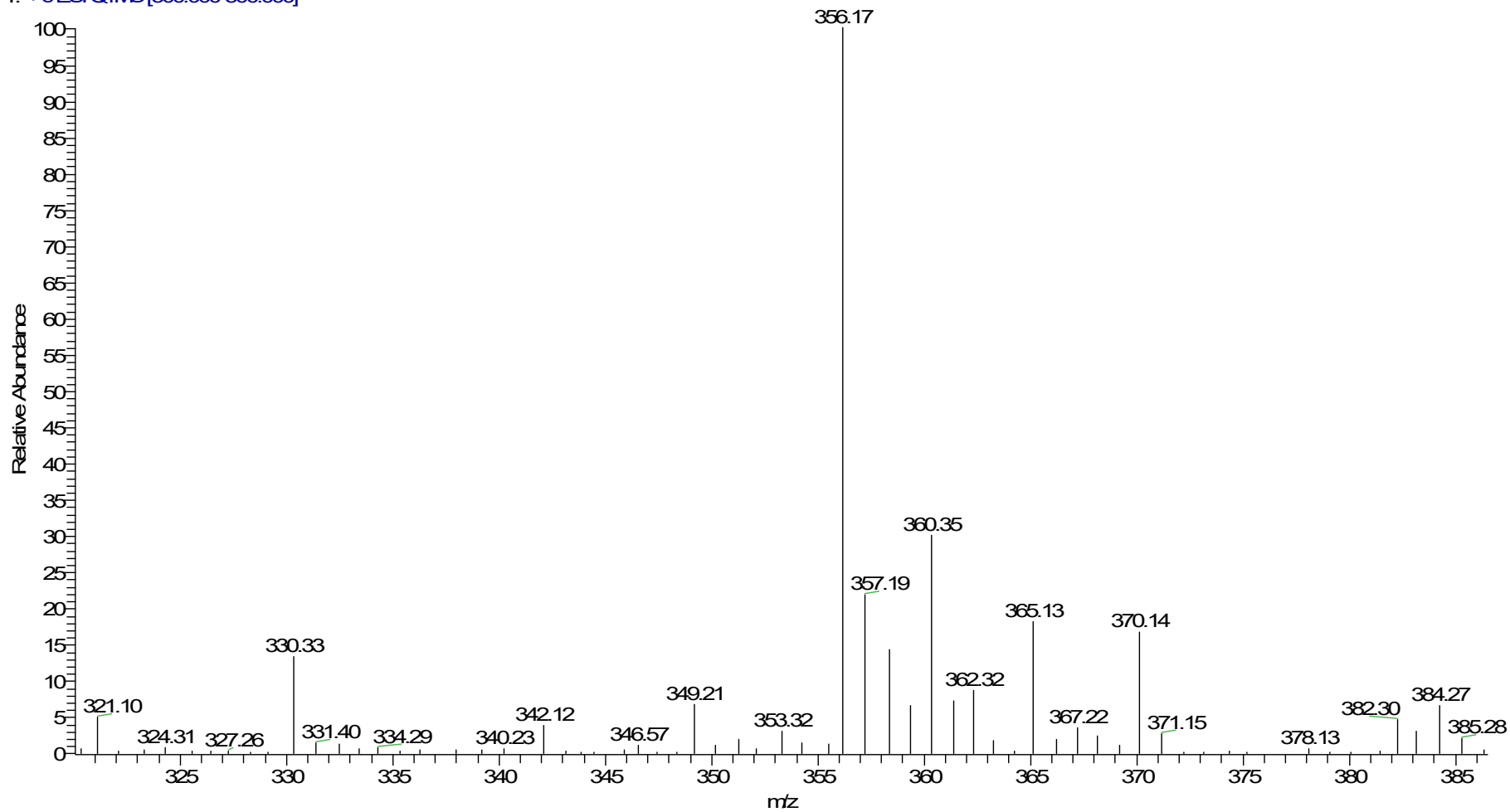


Fig.S35: ESI-MS spectrum of compound 6b

hsj-07 #1 RT: 0.00 AV: 1 NL: 2.92E7
T: +cESI Q1MS [300.000-500.000]

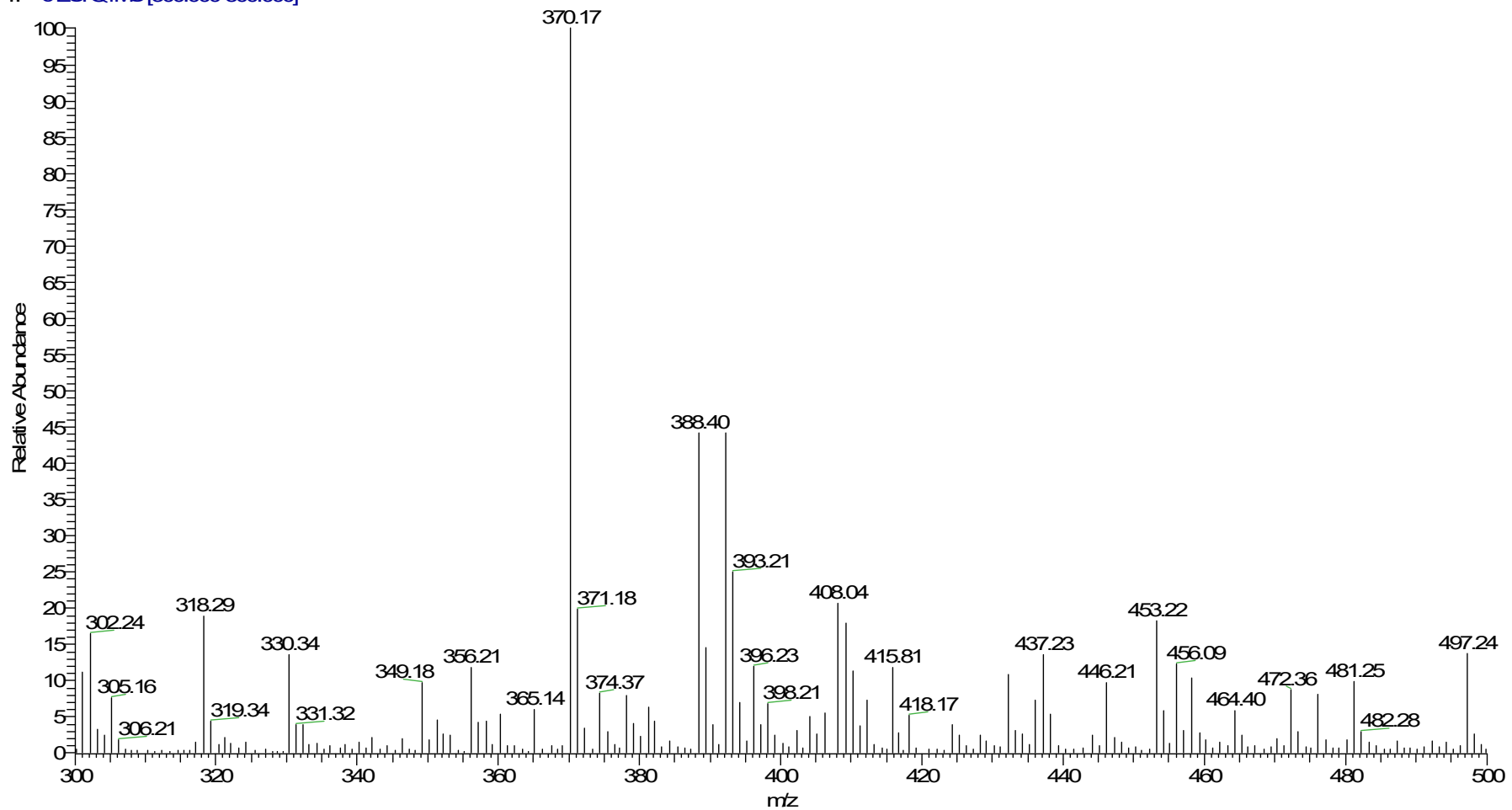


Fig.S36: ESI-MS spectrum of compound 6i

hsj-08_20191209120507 #11 RT: 0.05 AV: 1 NL: 2.10E6
T: -c ESI Q1MS [200.000-500.000]

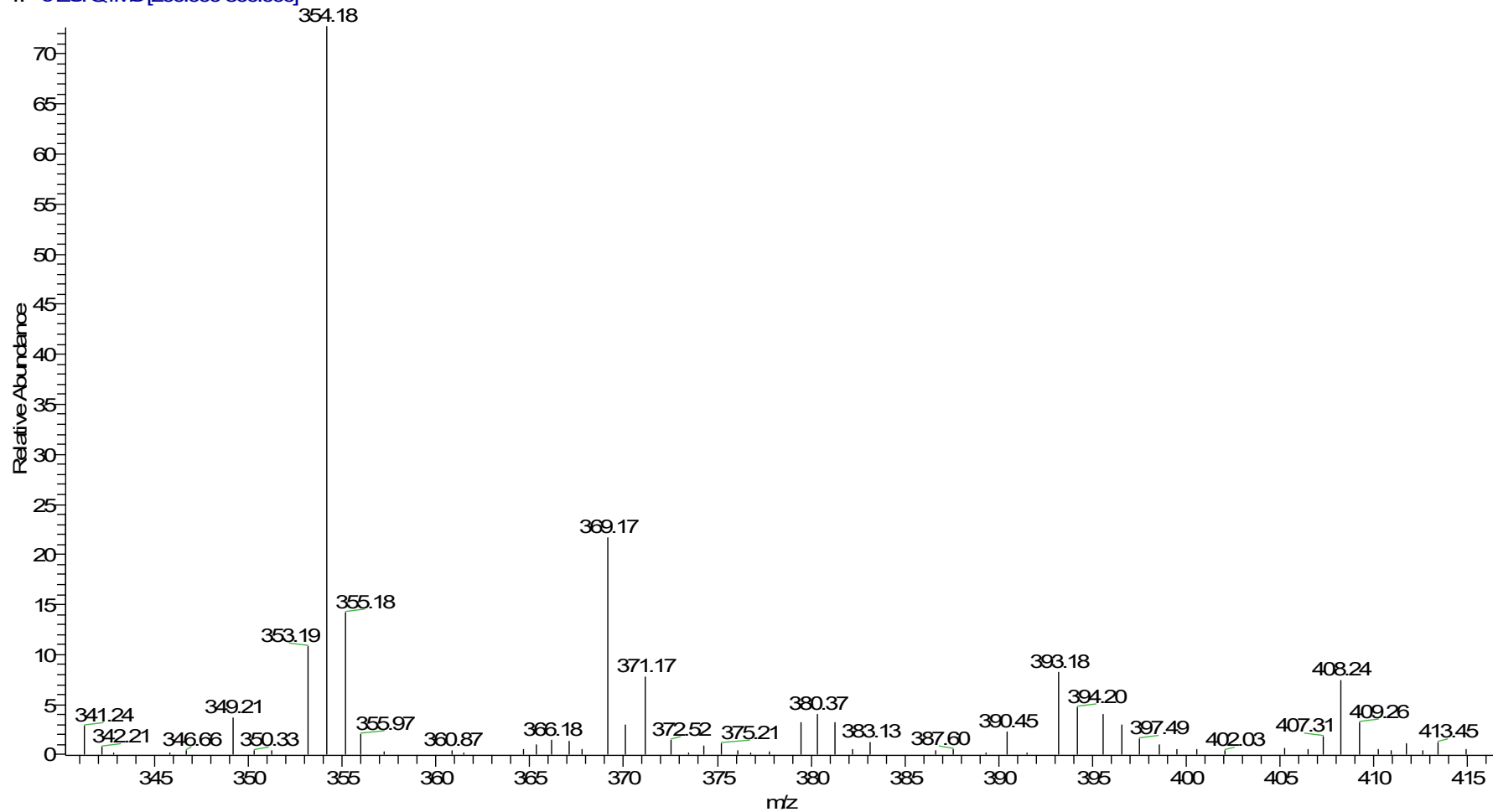


Fig.S37: ESI-MS spectrum of compound 6g

hsj-09_20191209033721#49 RT: 0.24 AV: 1 NL: 4.41E7
T: +cESI Q1MS [200.000-500.000]

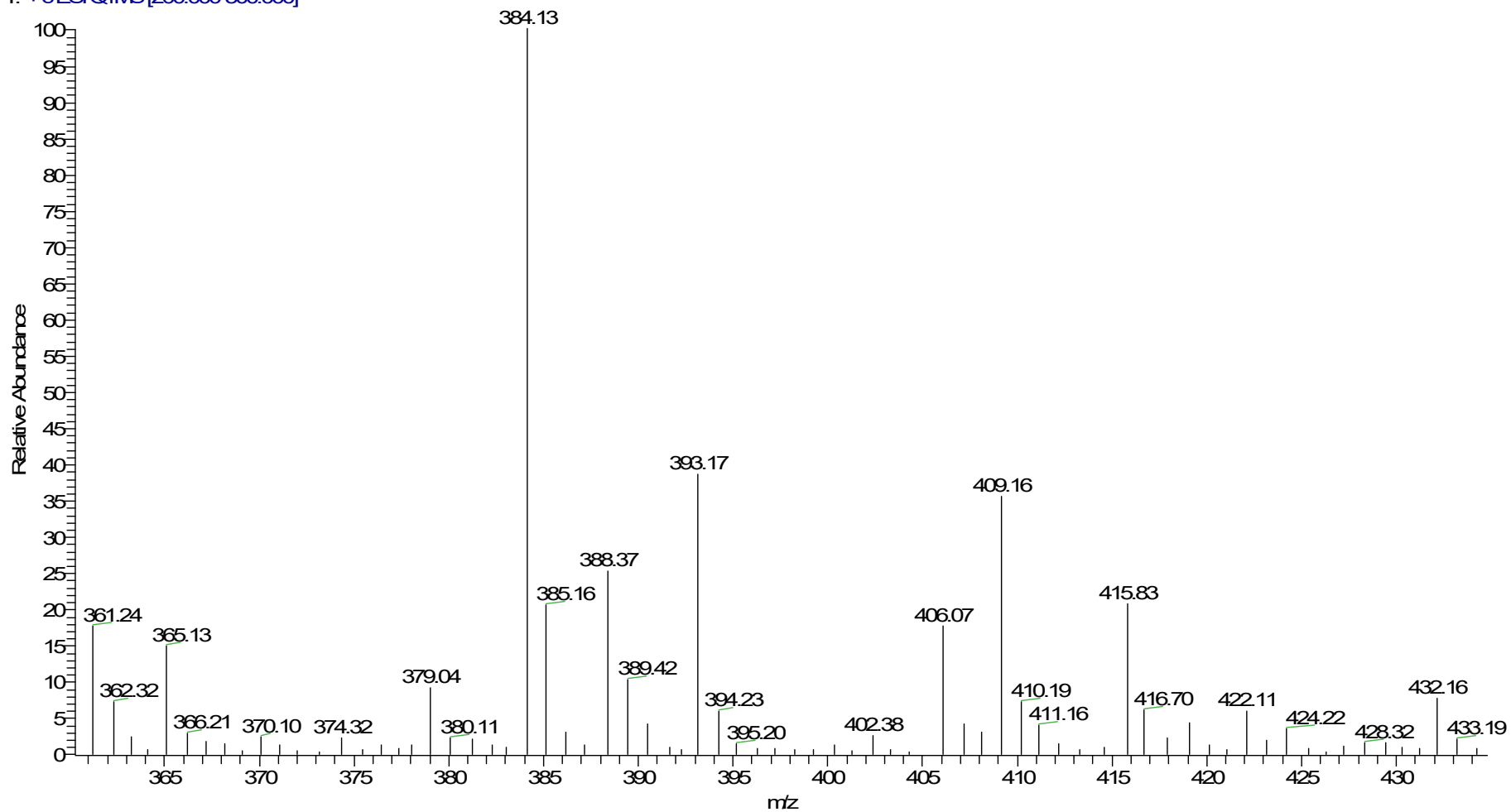


Fig.S38: ESI-MS spectrum of compound 6l

hsj-10_20191209035419 #1 RT: 0.00 AV: 1 NL: 5.13E7
T: +cESI Q1MS [200.000-500.000]

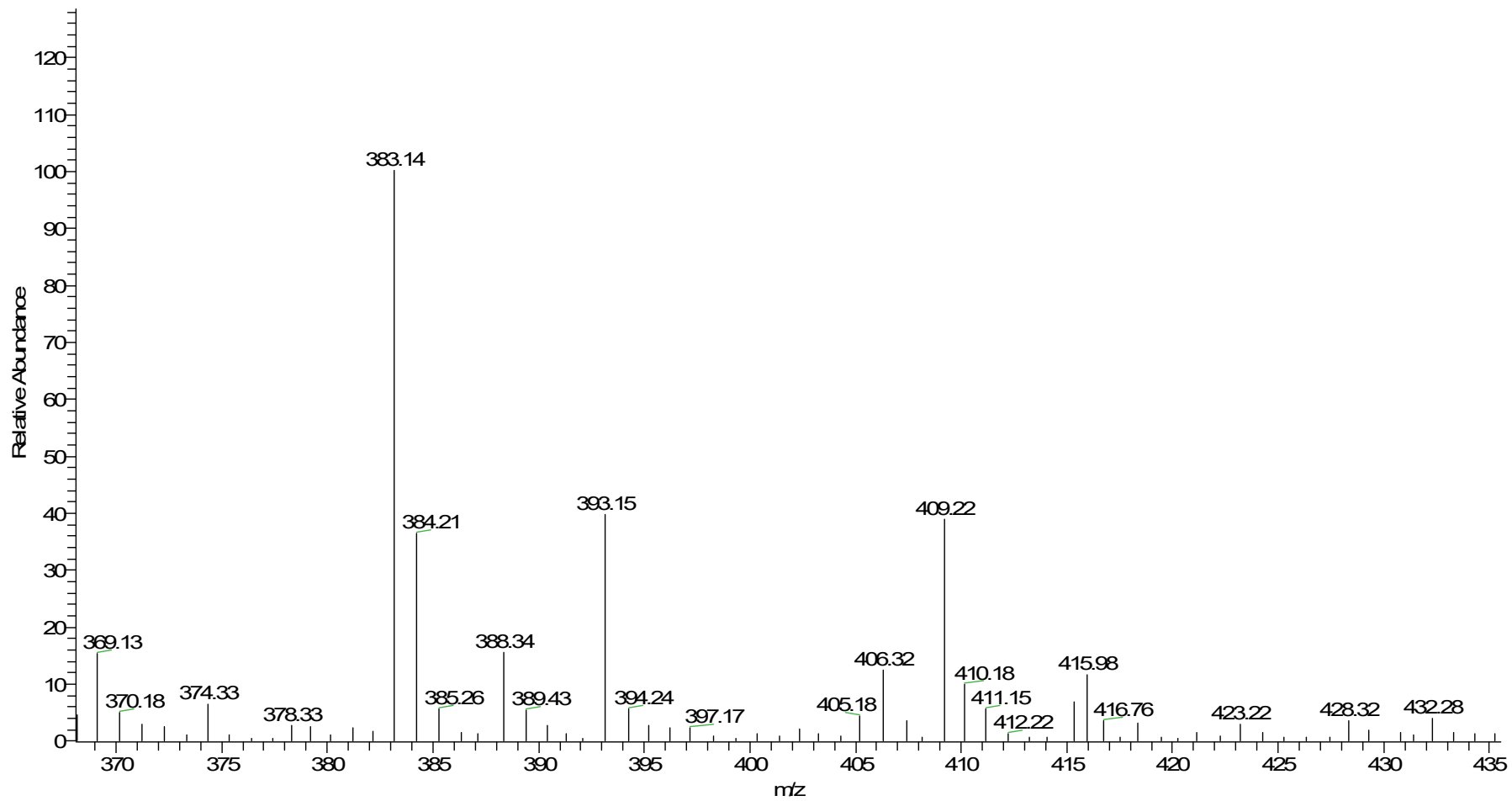


Fig.S39: ESI-MS spectrum of compound 6n

**^1H NMR of Compounds 10a-i
(Fig. S40-48)**

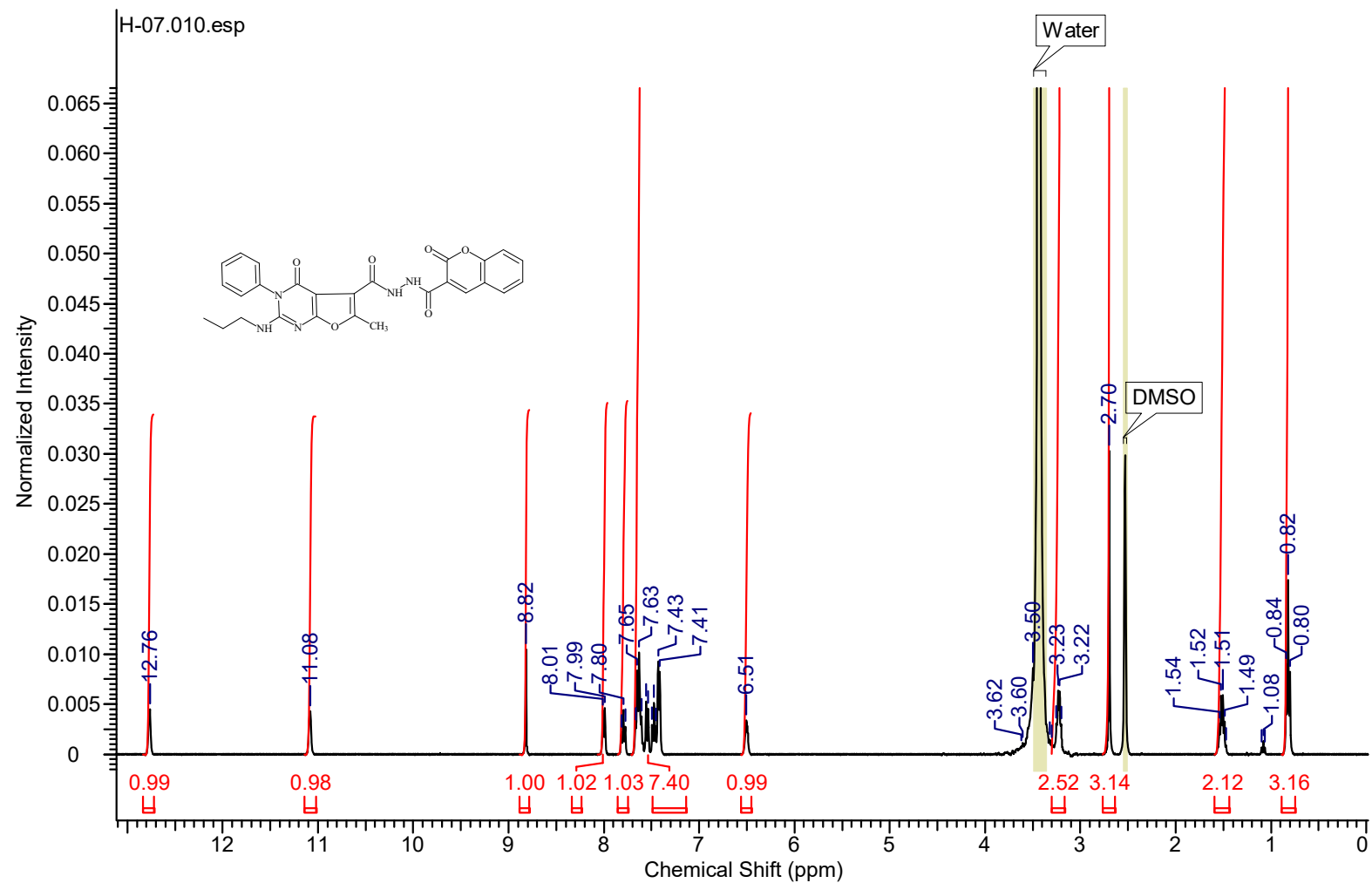


Fig.S40: ¹H NMR spectrum of compound 10a

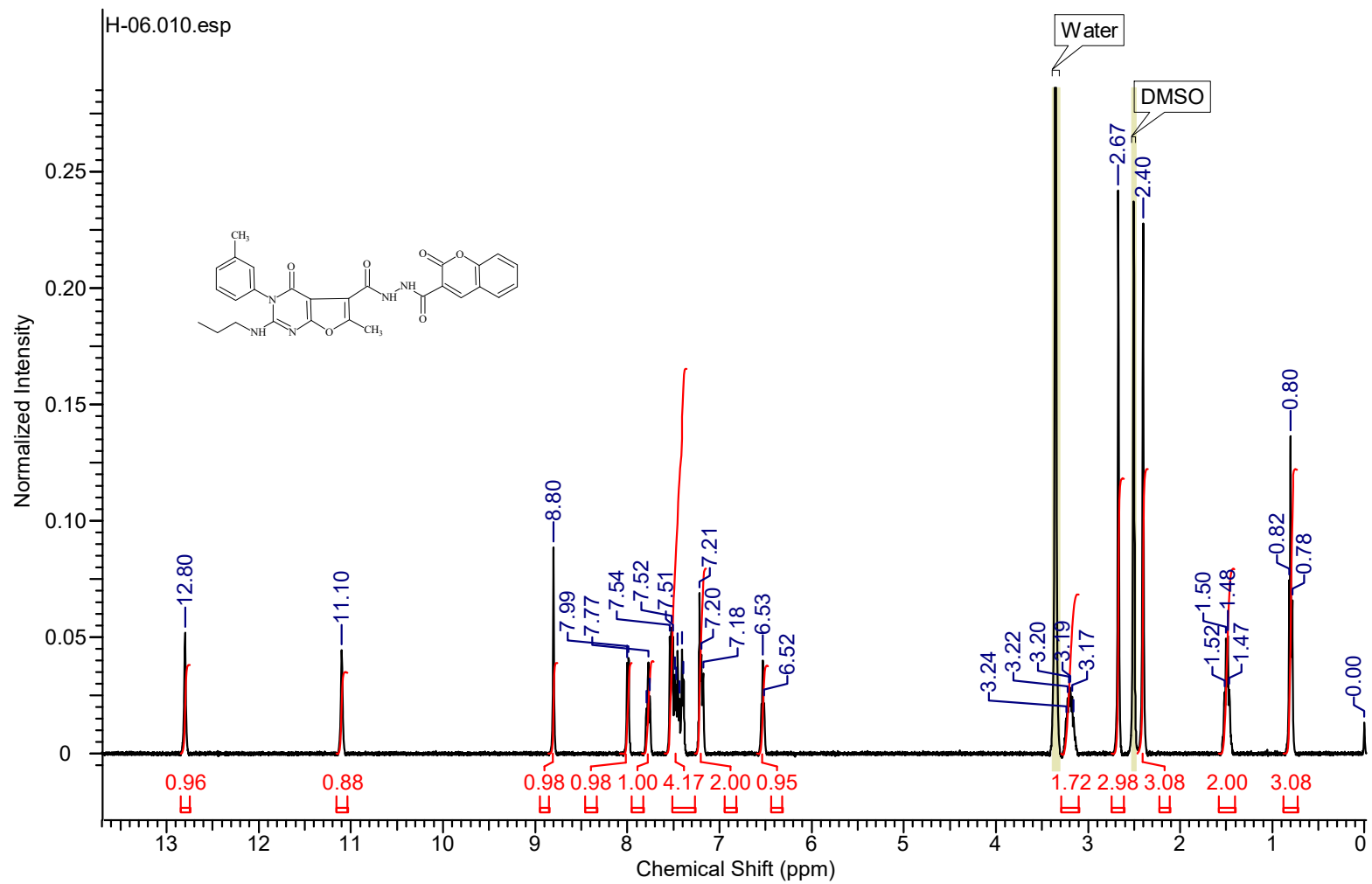


Fig.S41: ^1H NMR spectrum of compound 10b

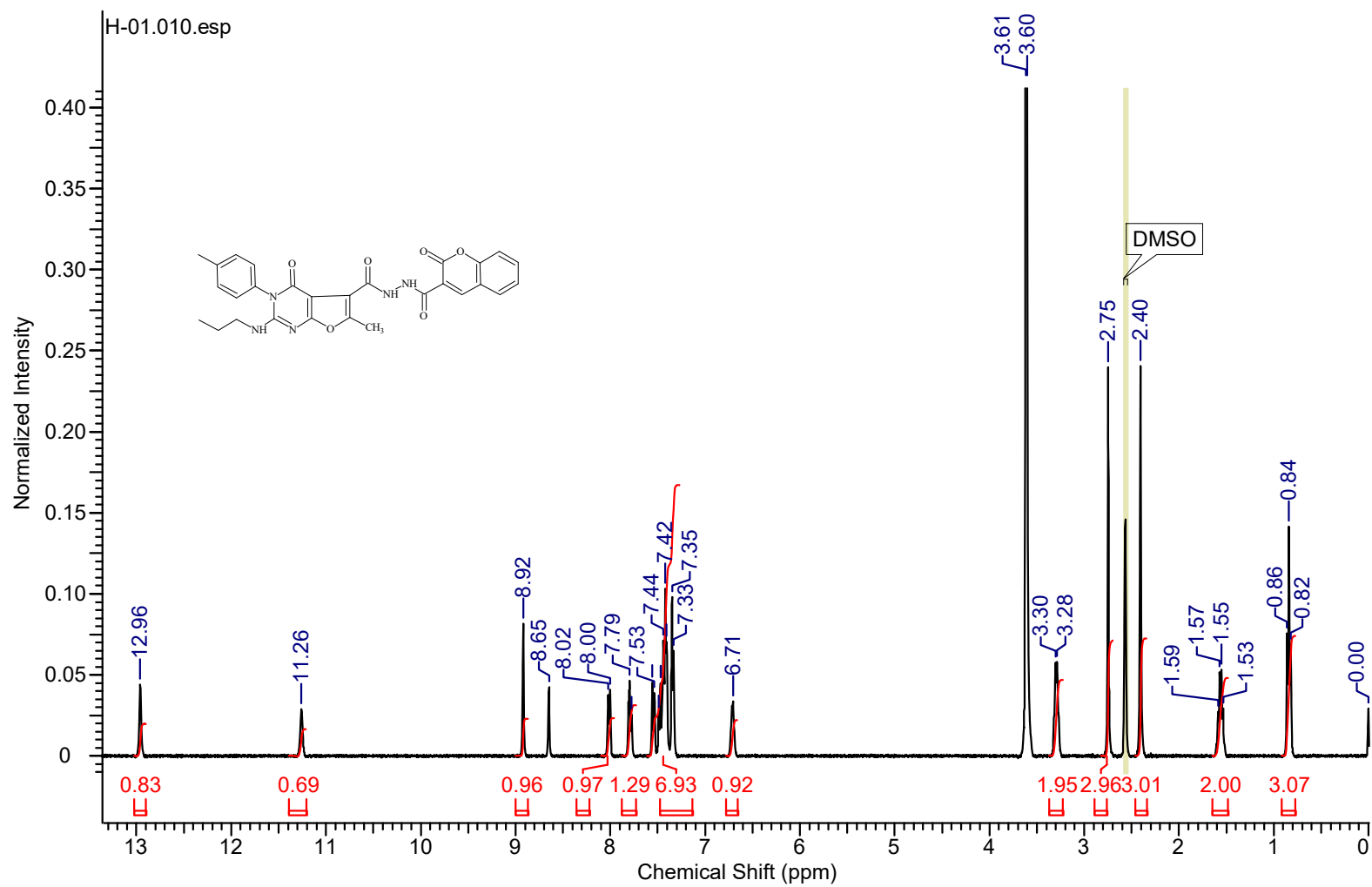


Fig.S42: ^1H NMR spectrum of compound 10c

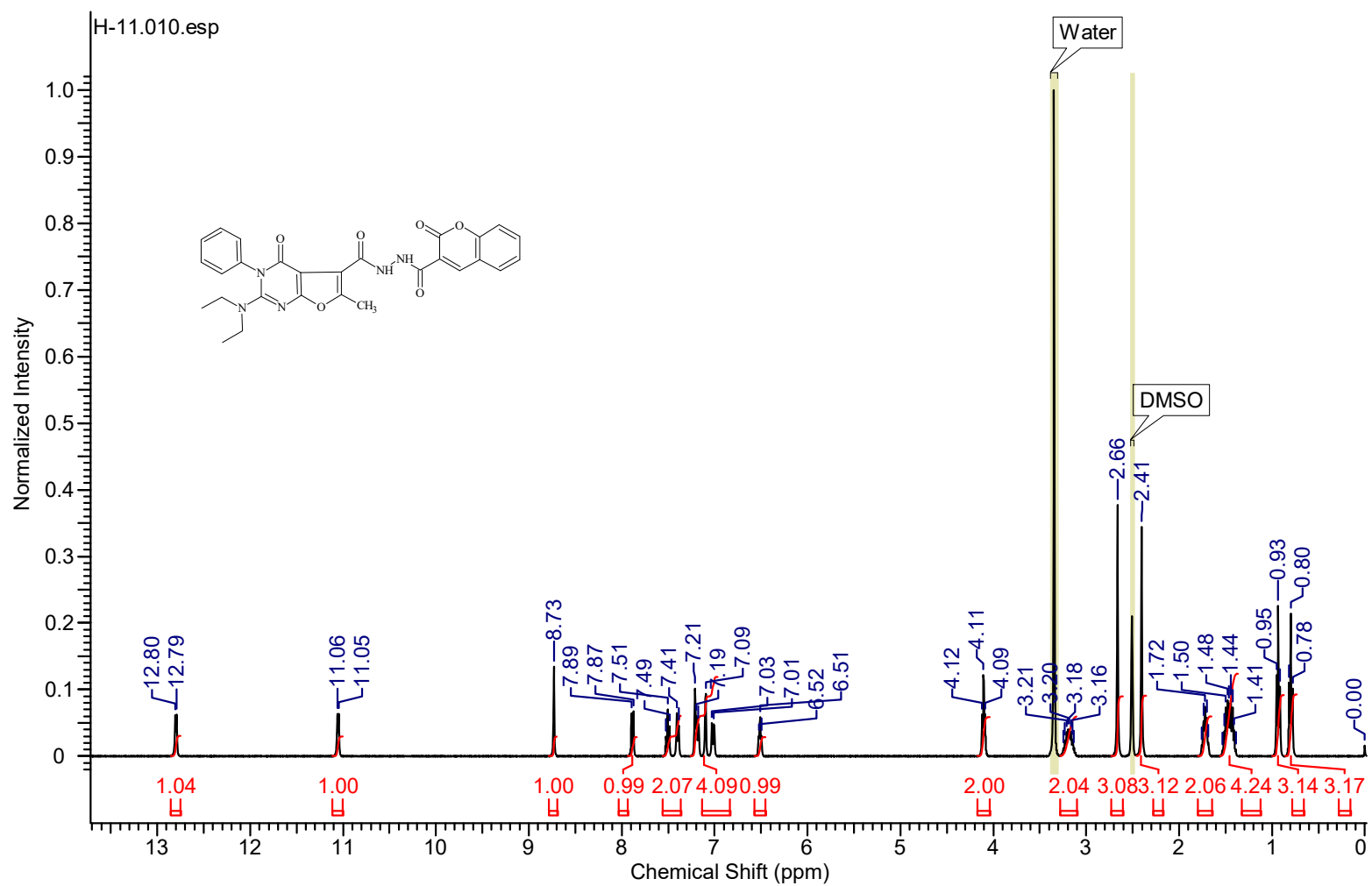


Fig.S43: ^1H NMR spectrum of compound 10d

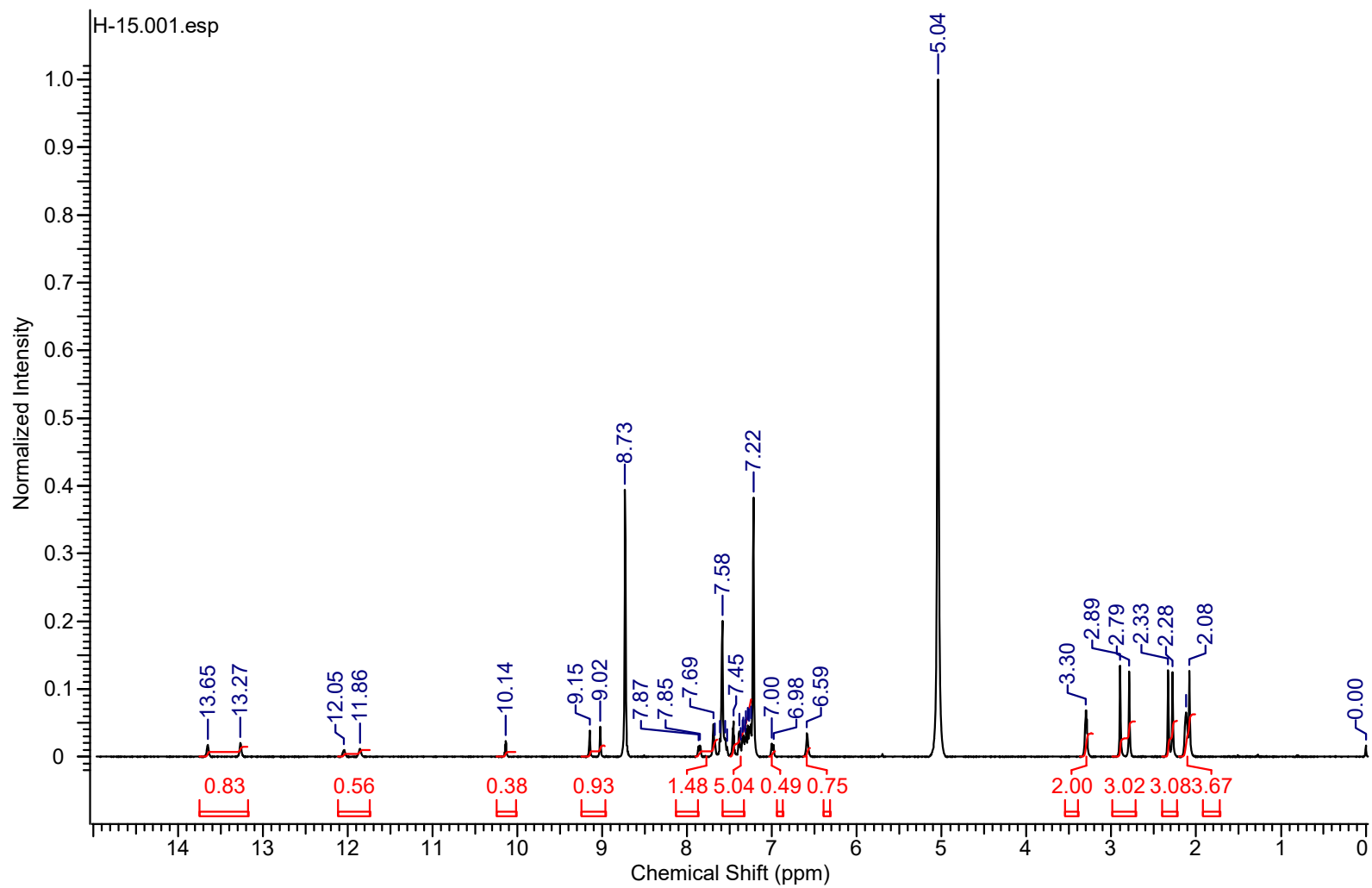


Fig.S44: ¹H NMR spectrum of compound 10e

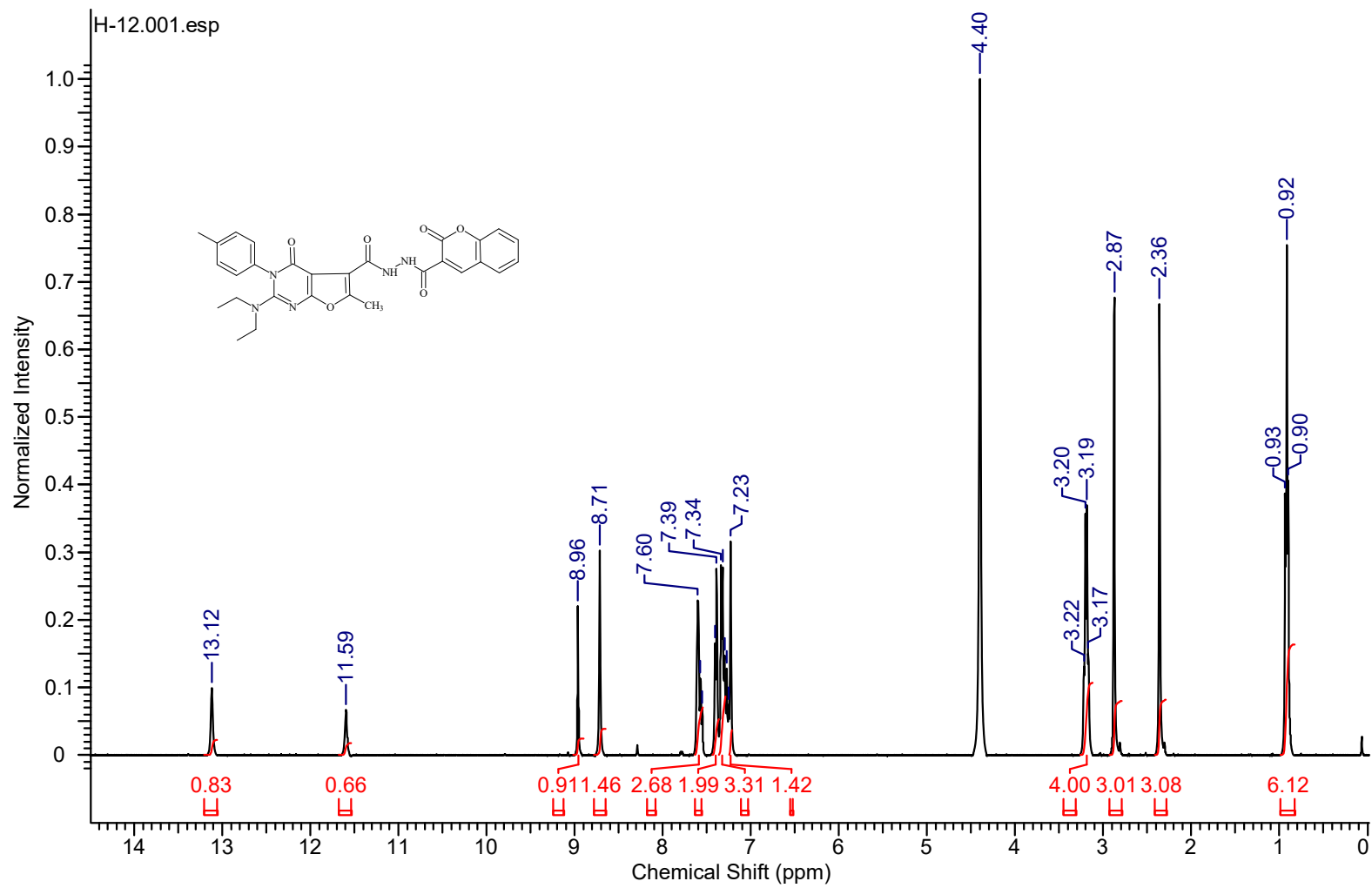


Fig.S45: ^1H NMR spectrum of compound 10f

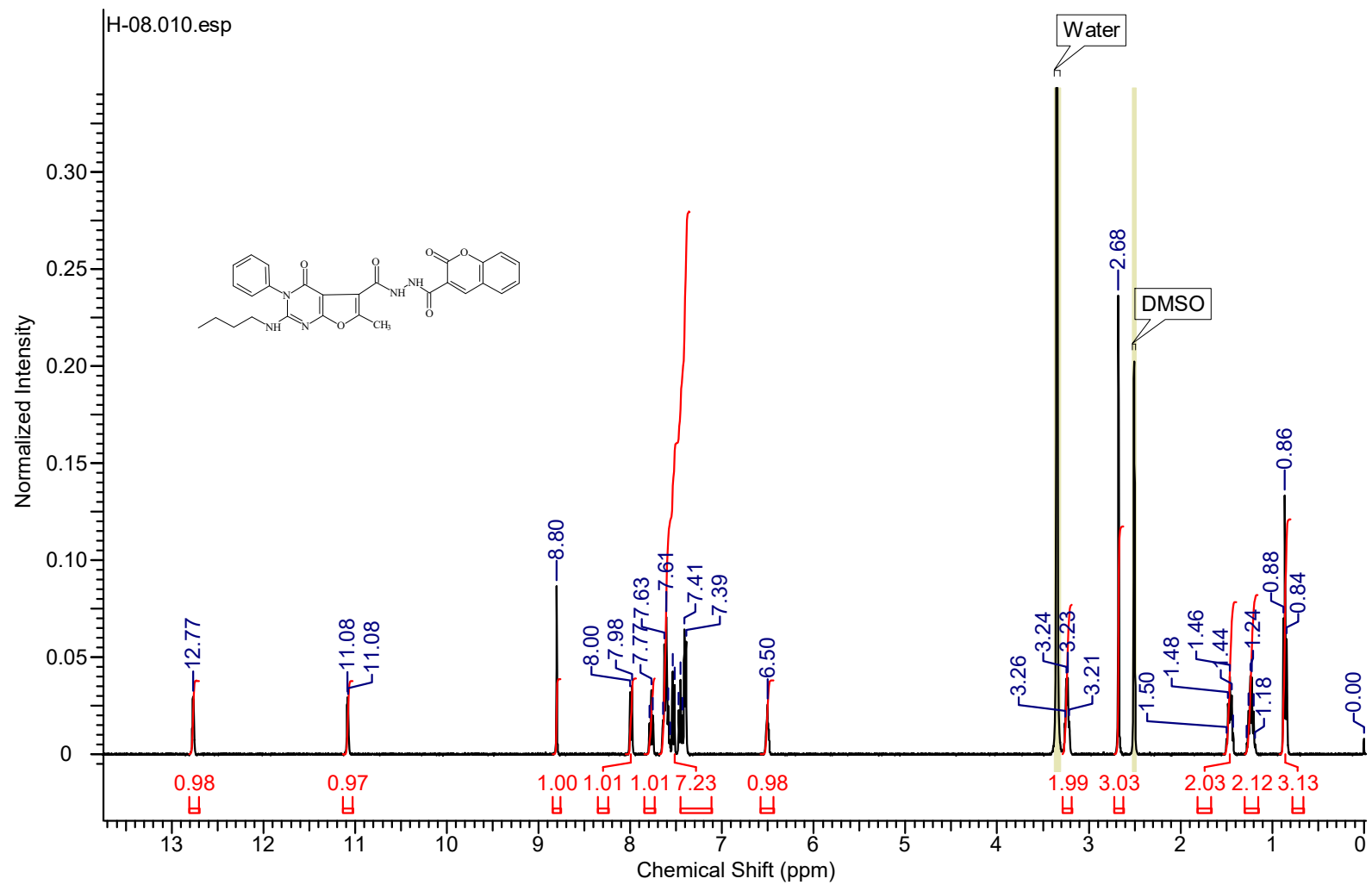


Fig.S46: ¹H NMR spectrum of compound 10g

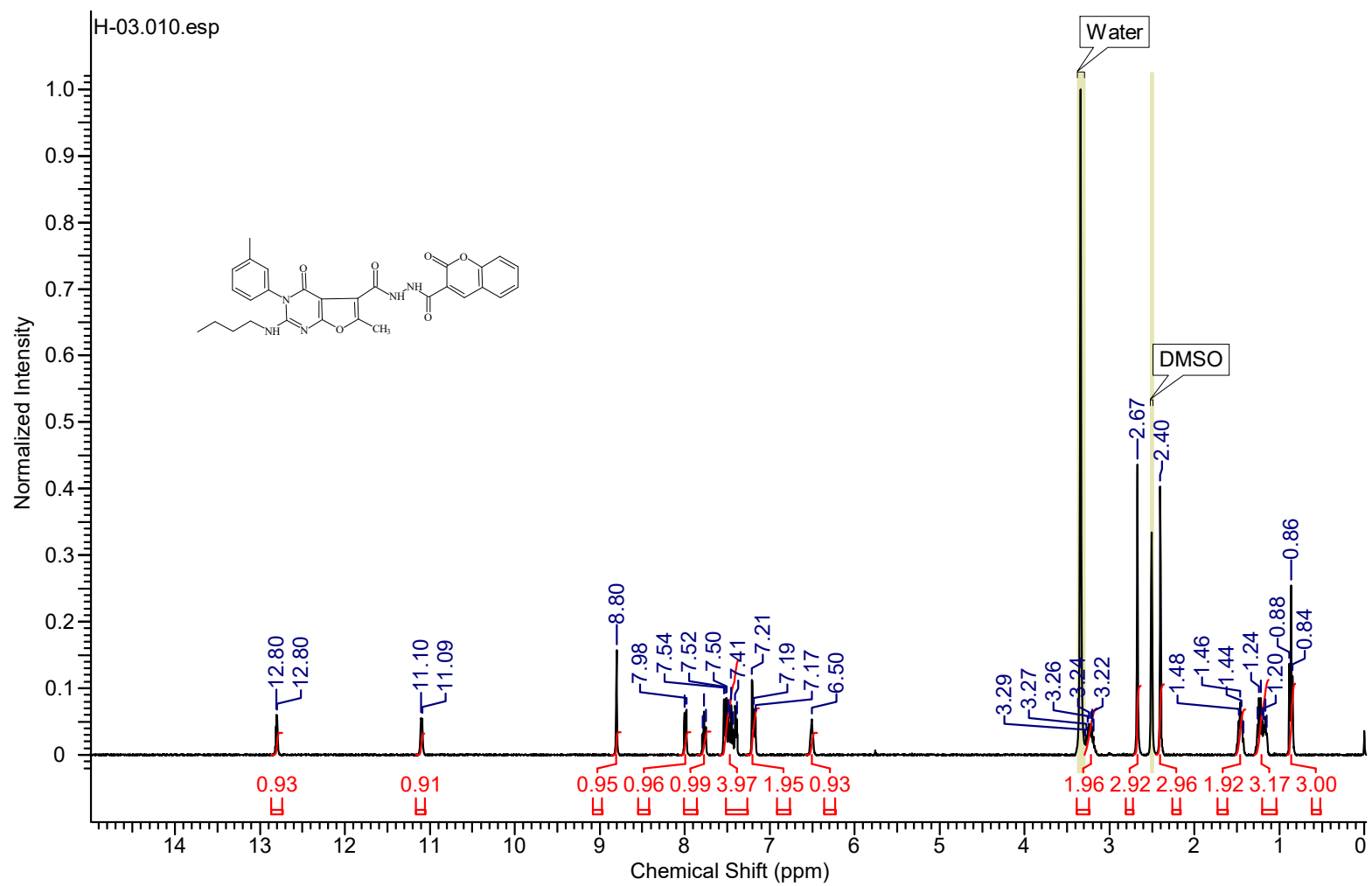


Fig.S47: ¹H NMR spectrum of compound 10h

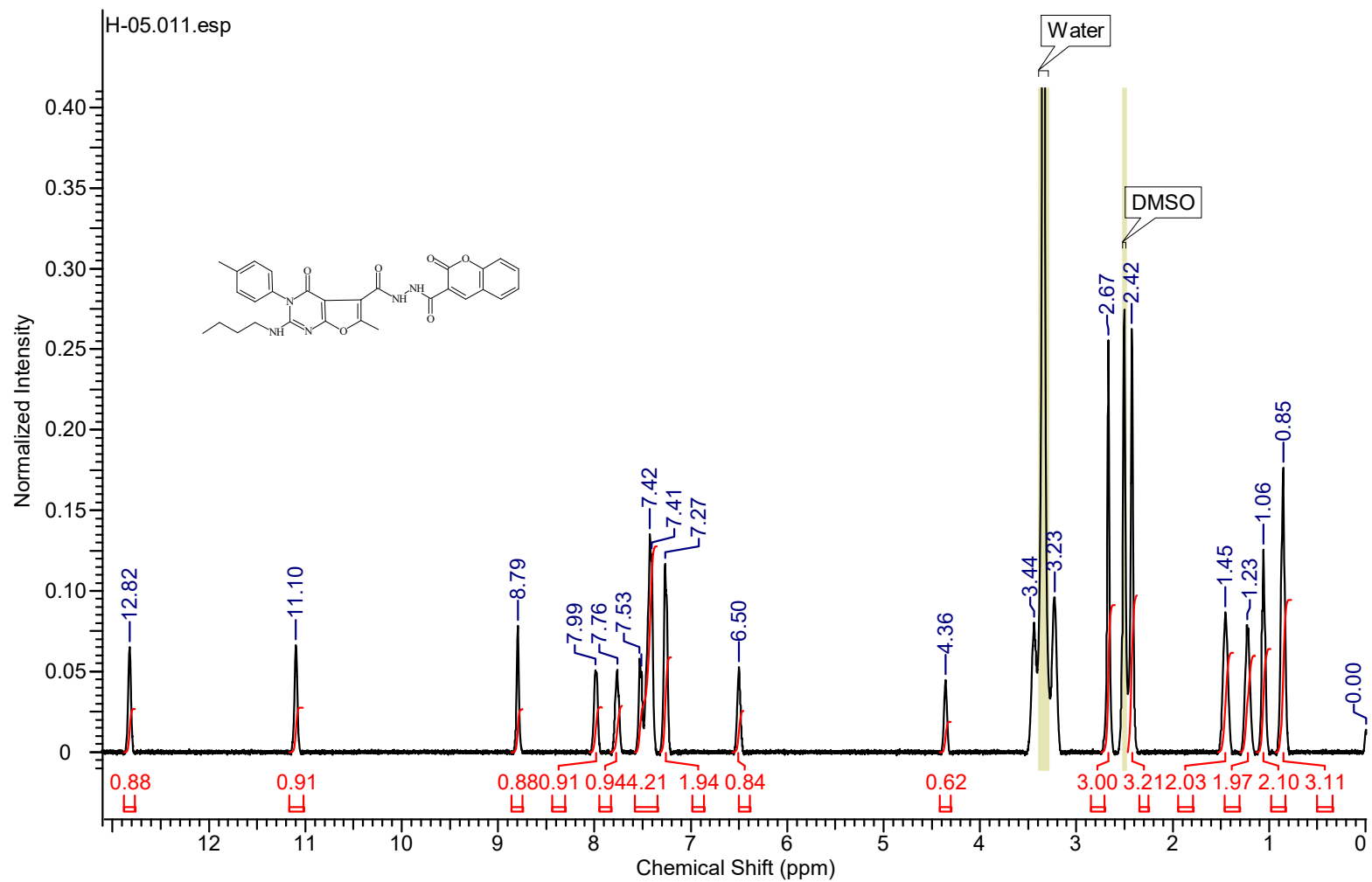


Fig.S48: ^1H NMR spectrum of compound 10i

**^{13}C NMR of Compounds 10a-i
(Fig. S49-56)**

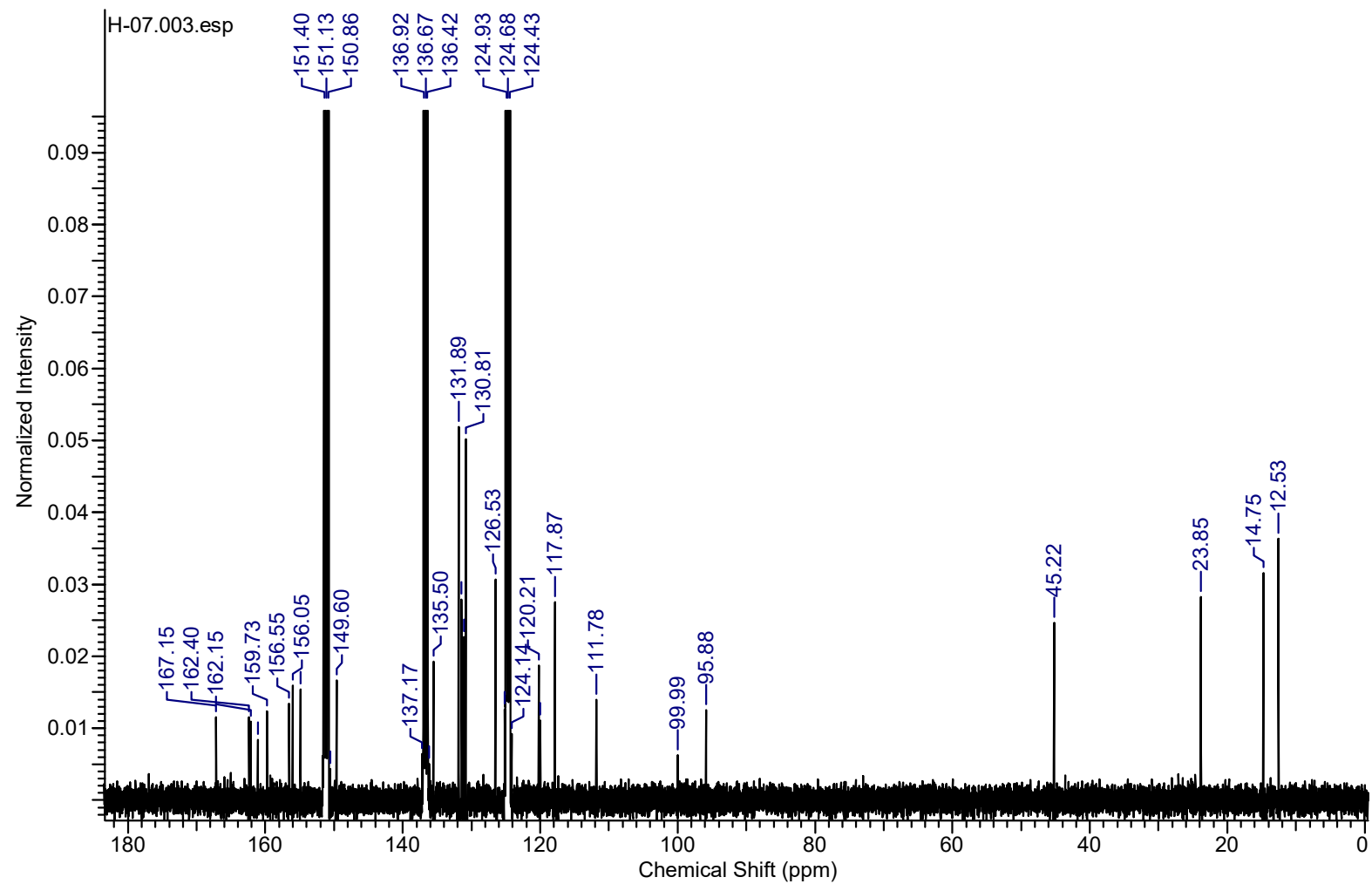


Fig.S49: ^{13}C NMR spectrum of compound **10a**

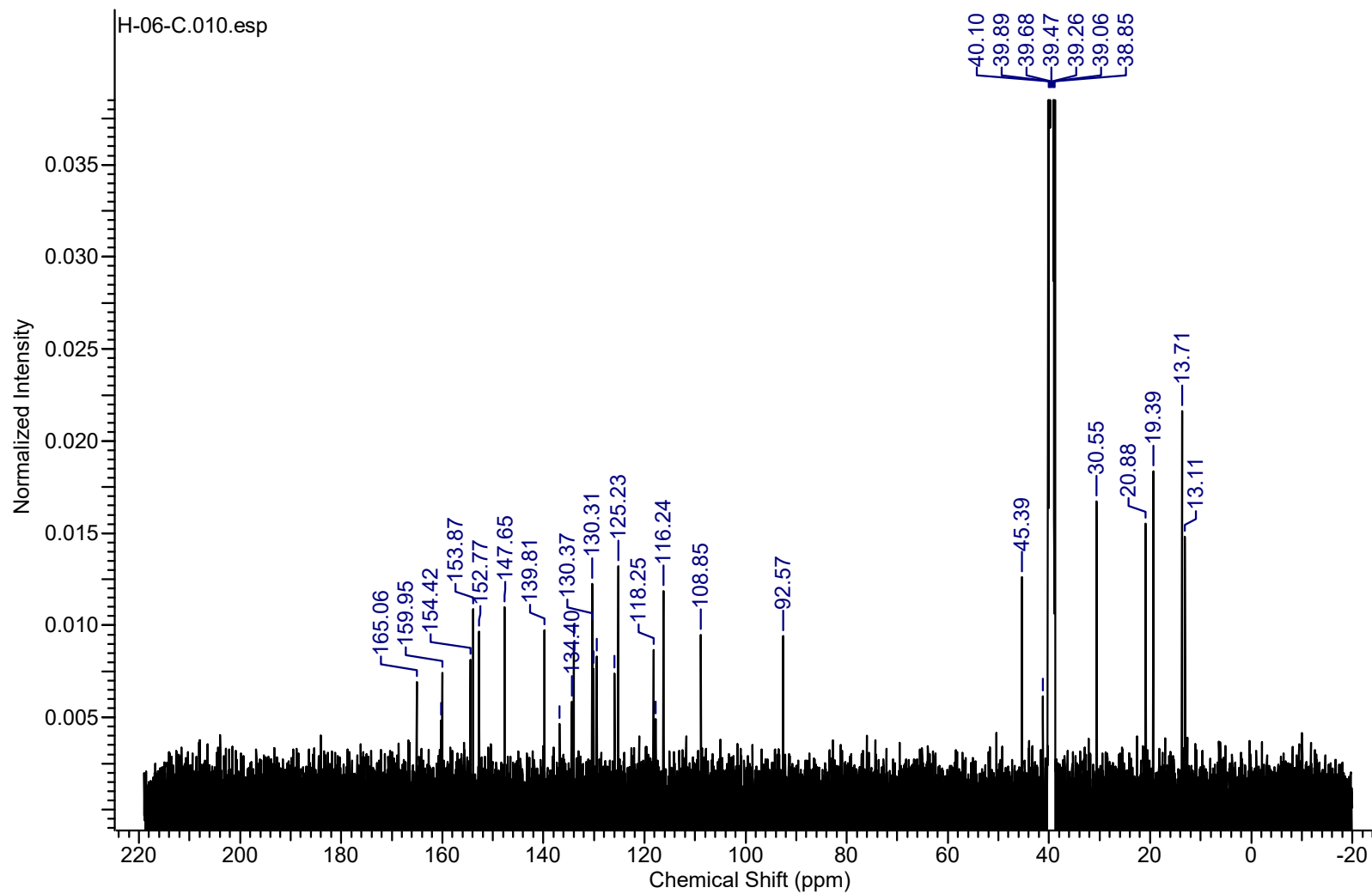


Fig.S50: ^{13}C NMR spectrum of compound **10b**

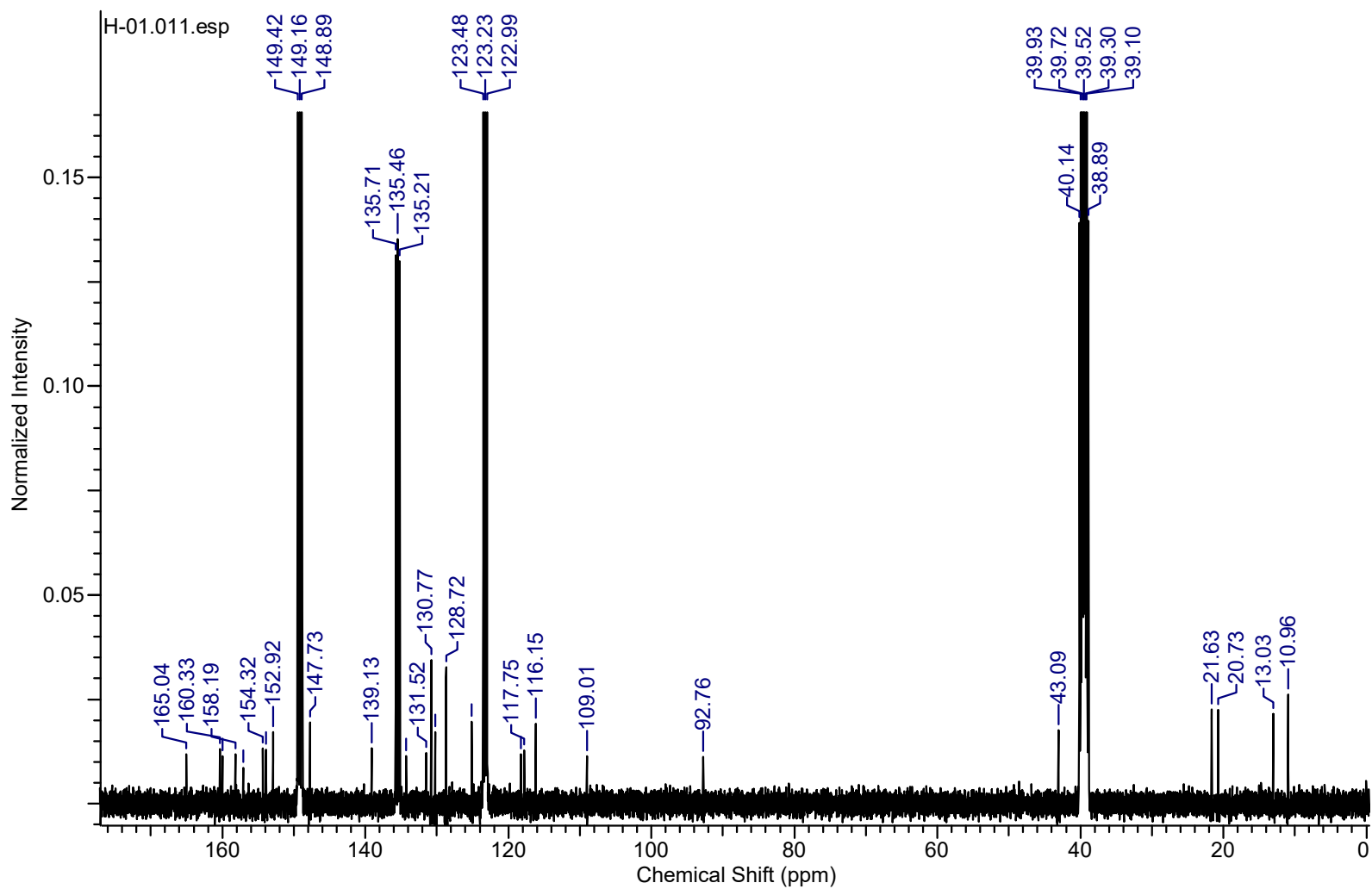


Fig.S51: ^{13}C NMR spectrum of compound **10c**

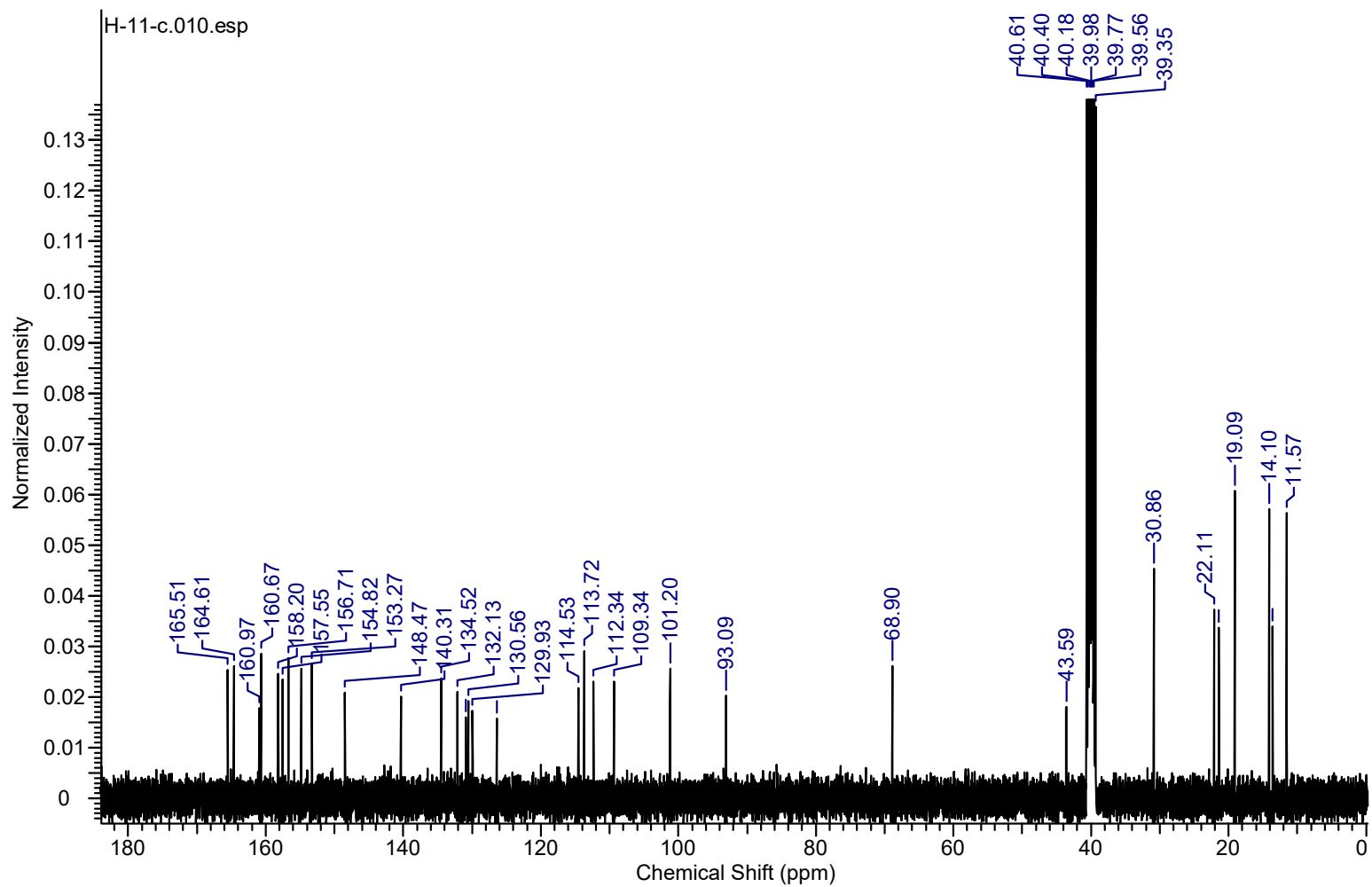


Fig.S52: ^{13}C NMR spectrum of compound 10d

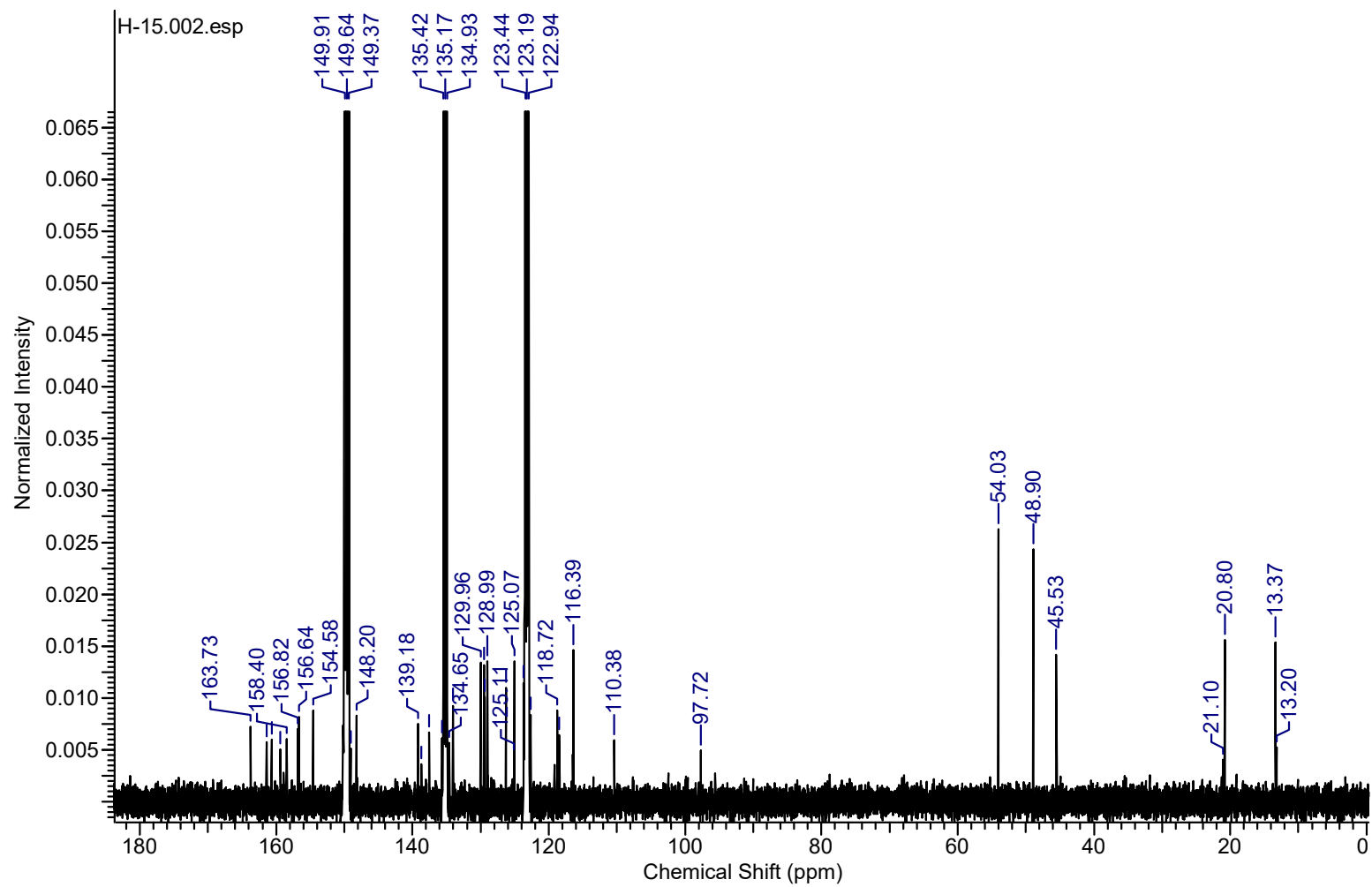


Fig.S53: ^{13}C NMR spectrum of compound **10e**

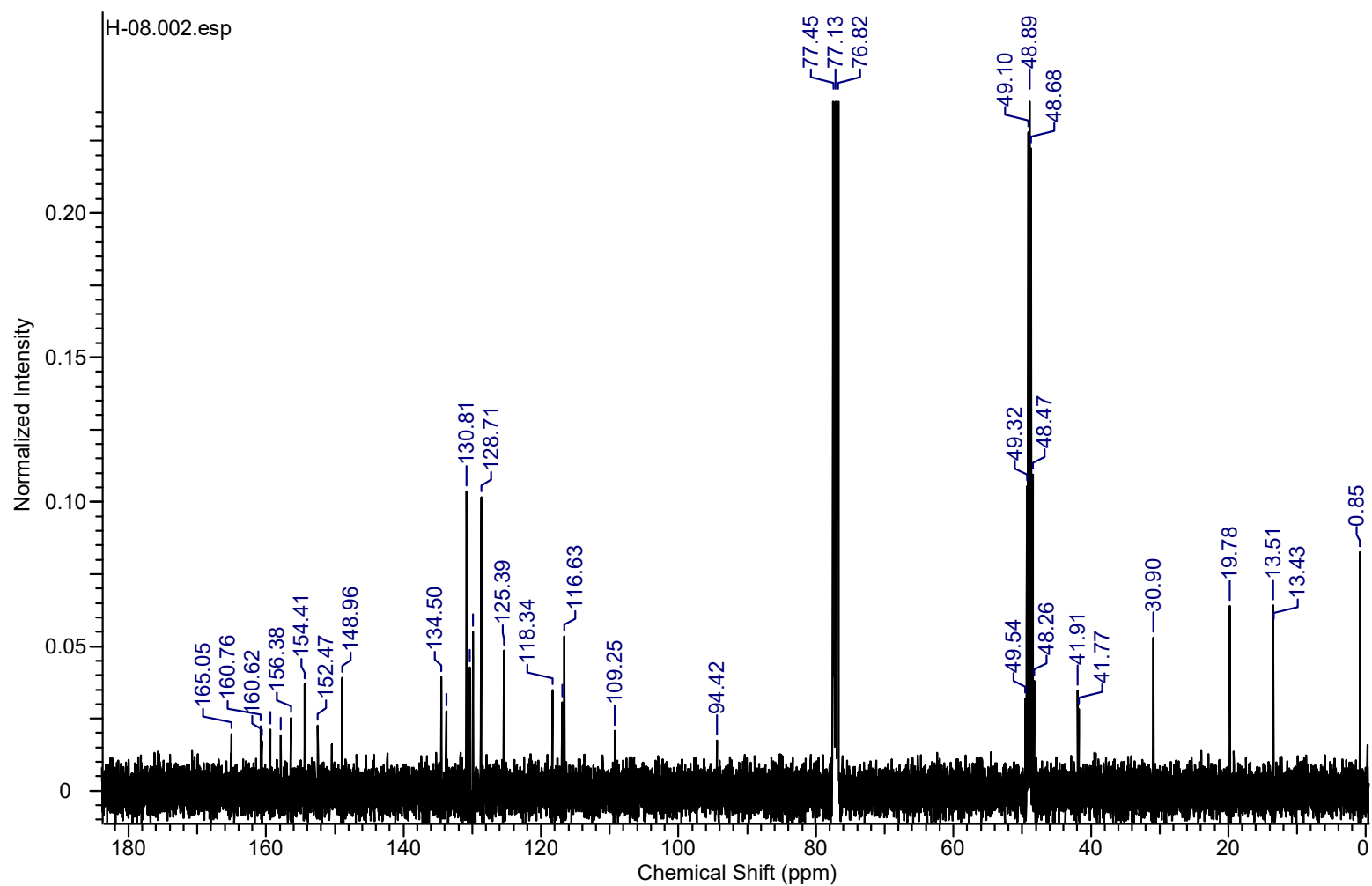


Fig.S54: ^{13}C NMR spectrum of compound **10g**

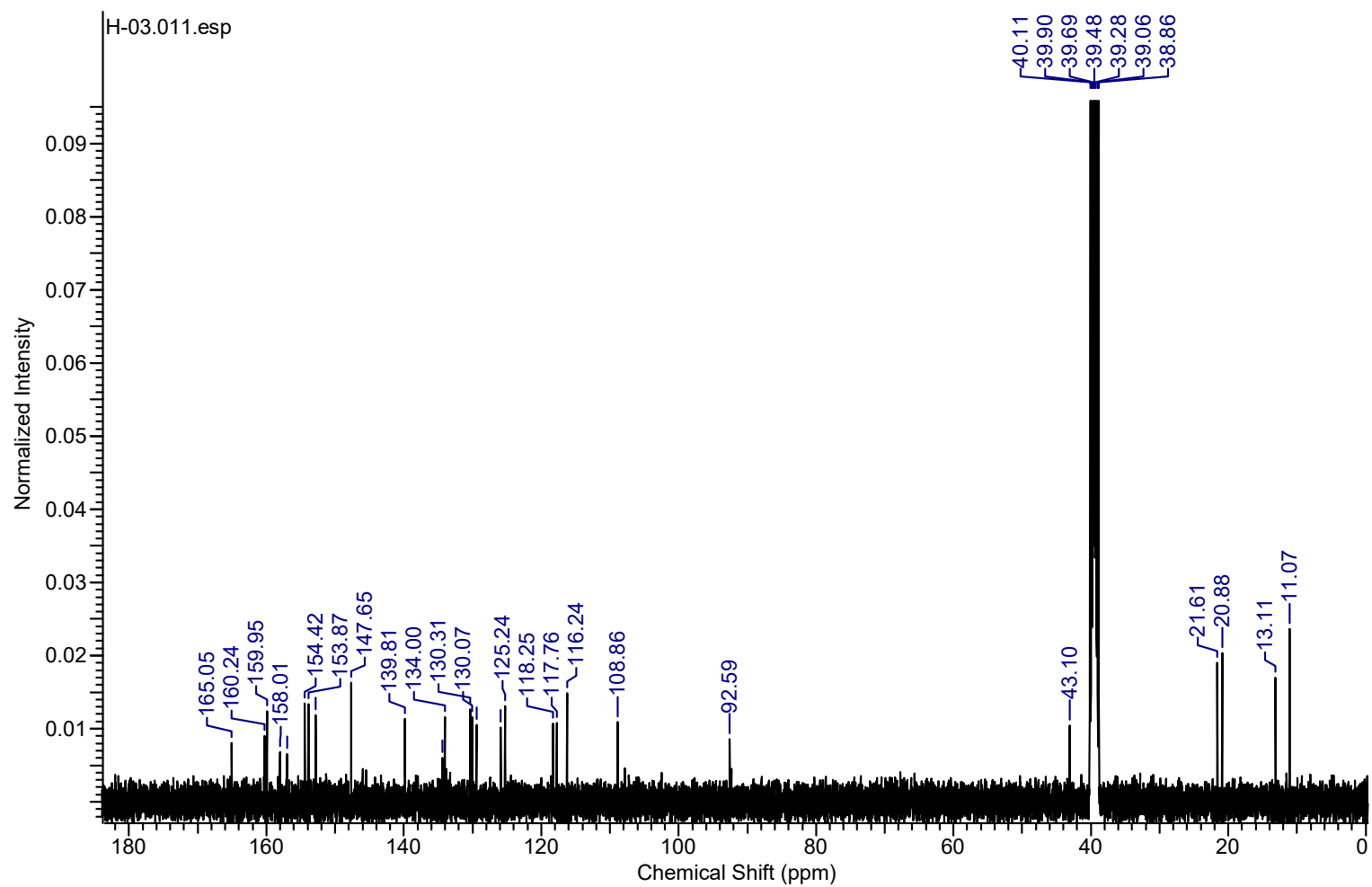


Fig.S55: ^{13}C NMR spectrum of compound 10h

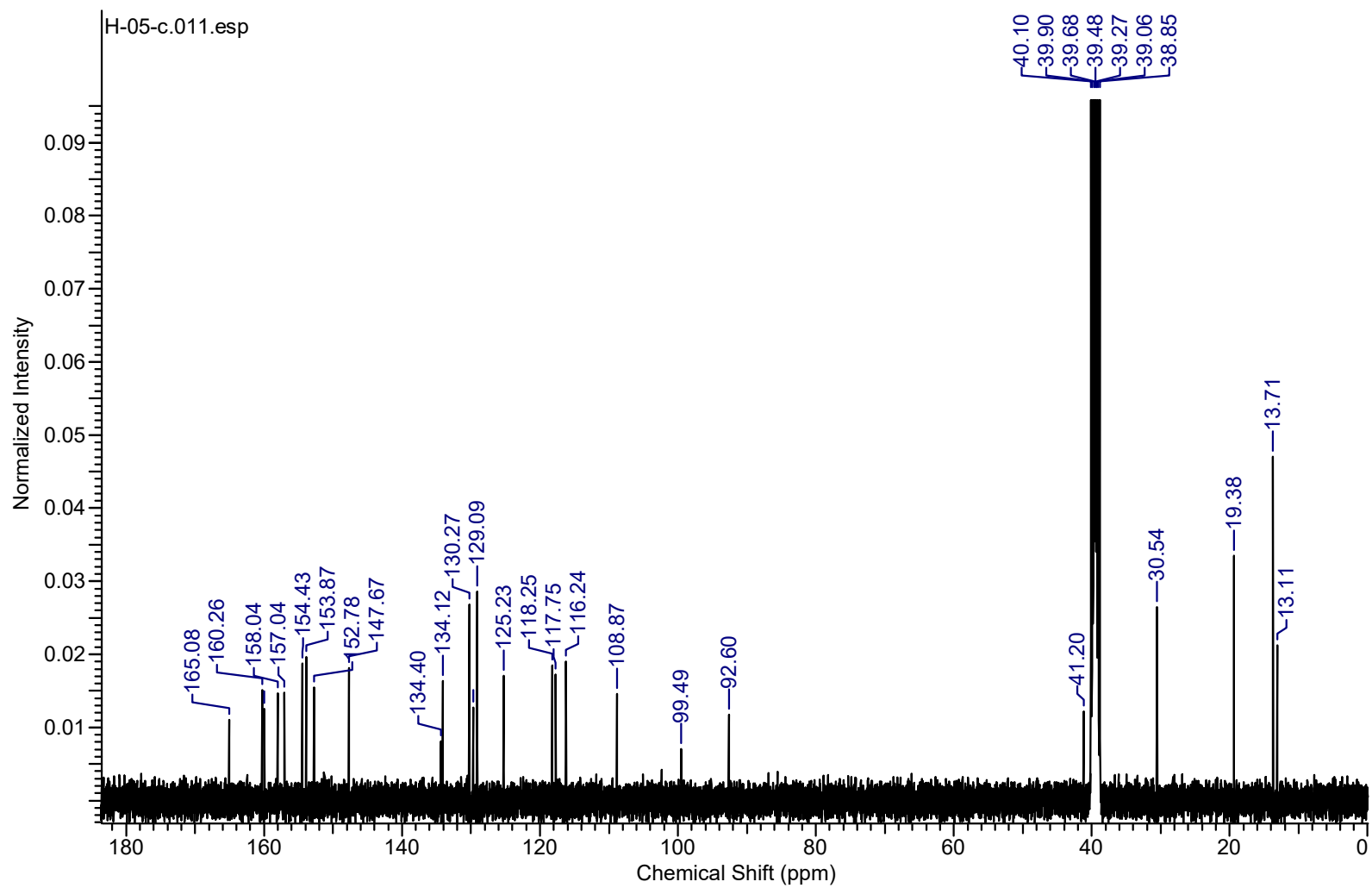


Fig.S56: ^{13}C NMR spectrum of compound **10i**

ESI-MS of Compounds 10a-n
(Fig. S57-71)

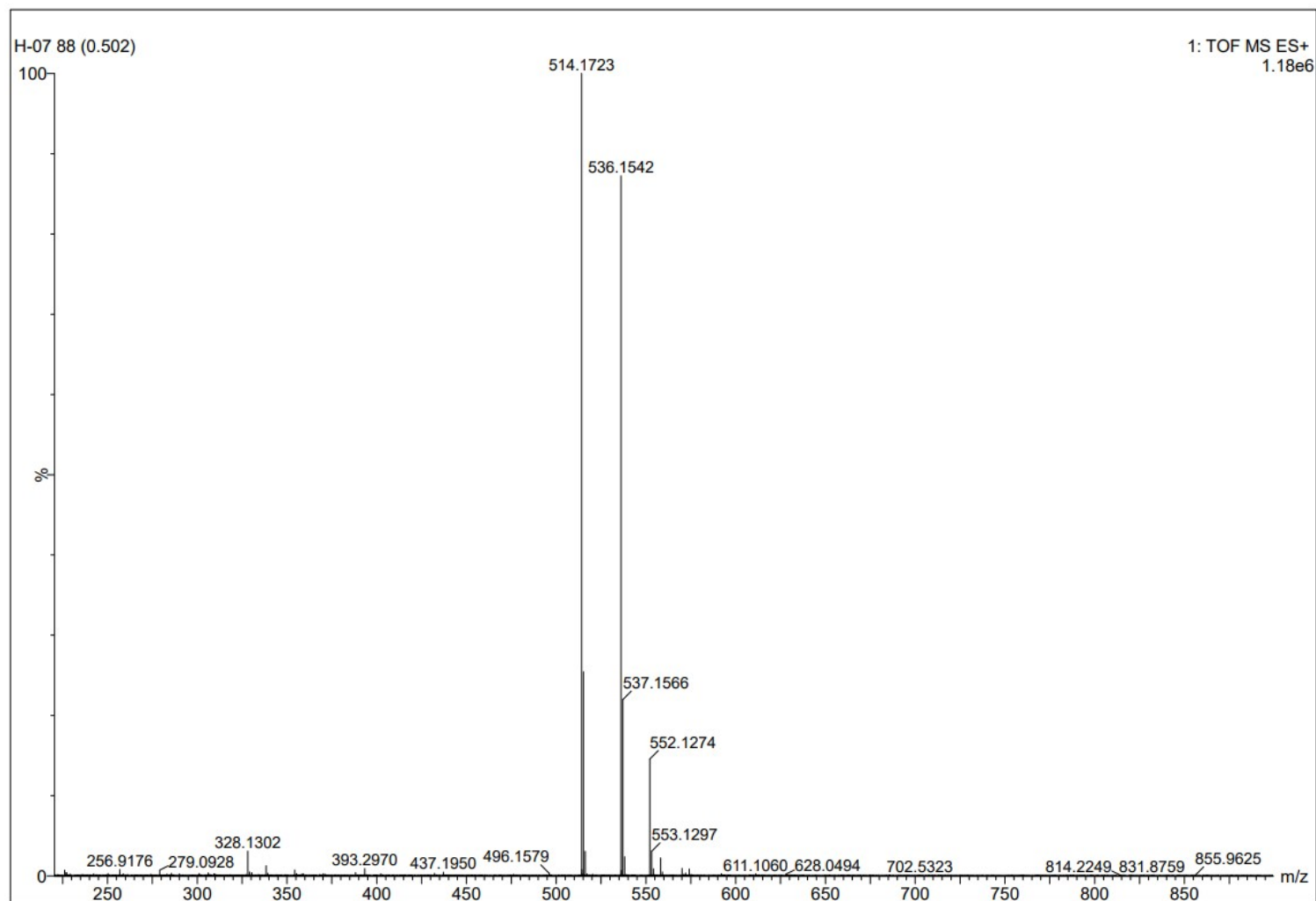


Fig.S57: HRESI-MS spectrum of compound **10a**

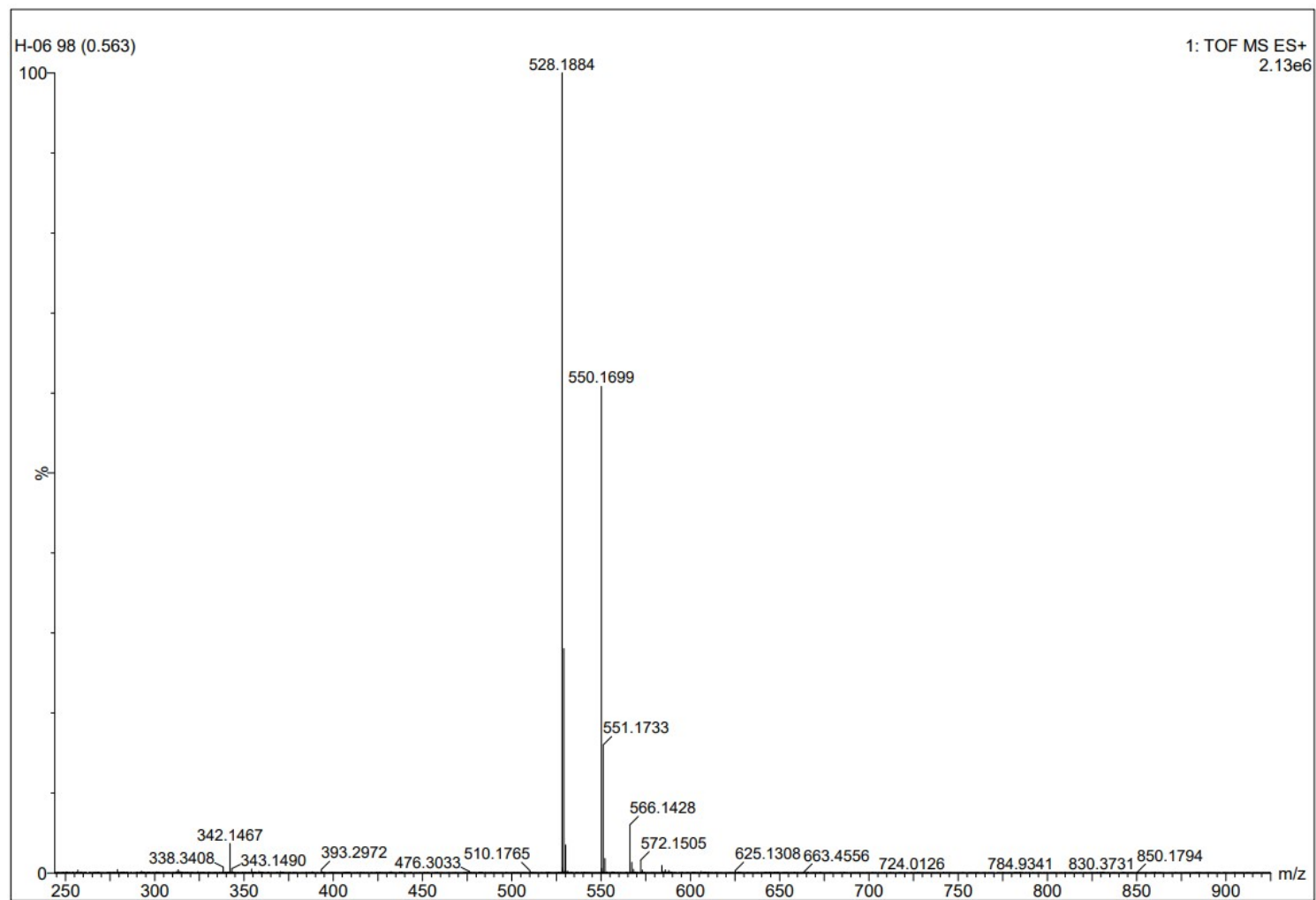


Fig.S58: HRESI-MS spectrum of compound **10b**

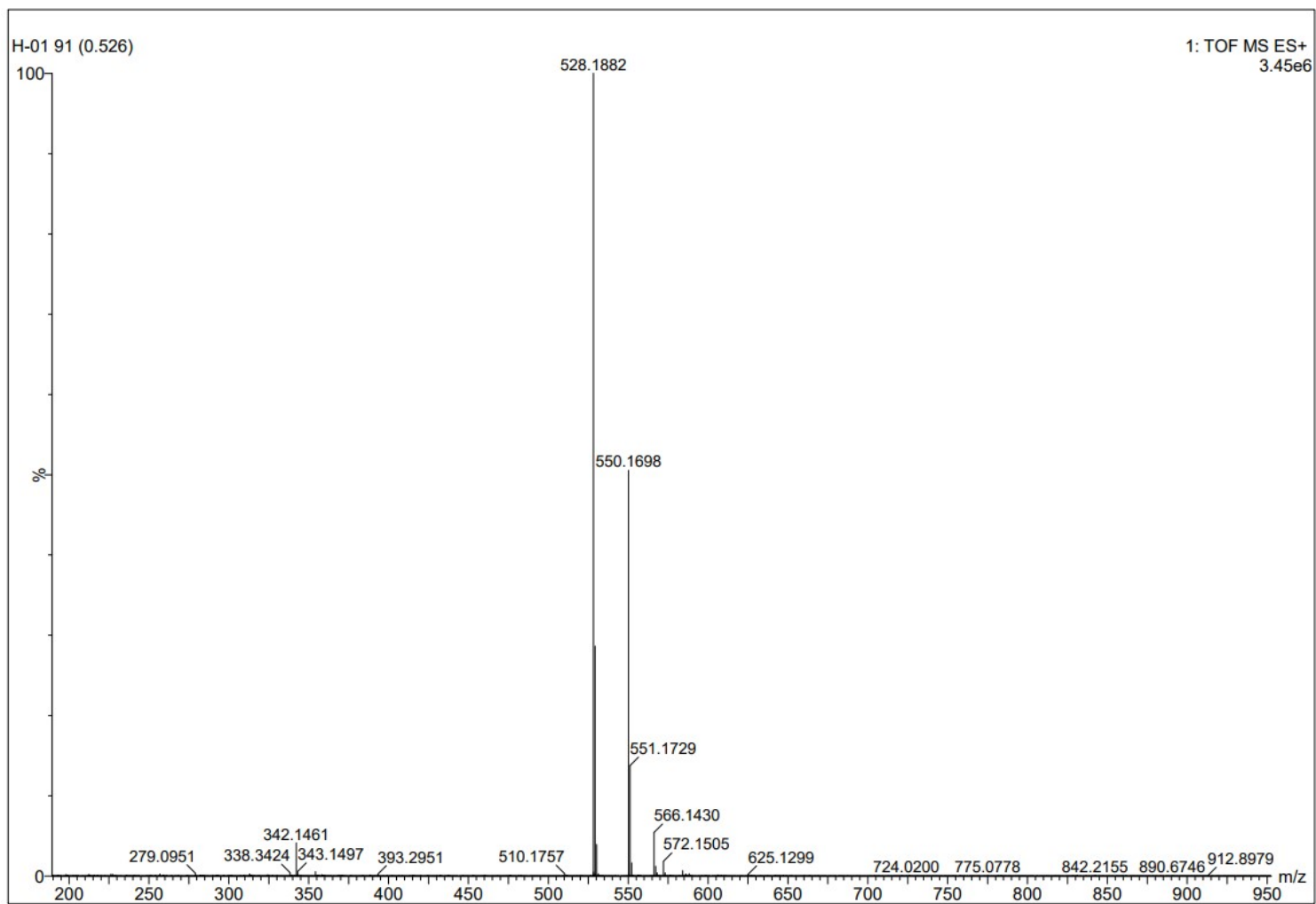


Fig.S59: HRESI-MS spectrum of compound **10c**

#33 RT: 0.16 AV: 1 NL: 6.03E6
T: -c ESI Q1MS [400.000-700.000]

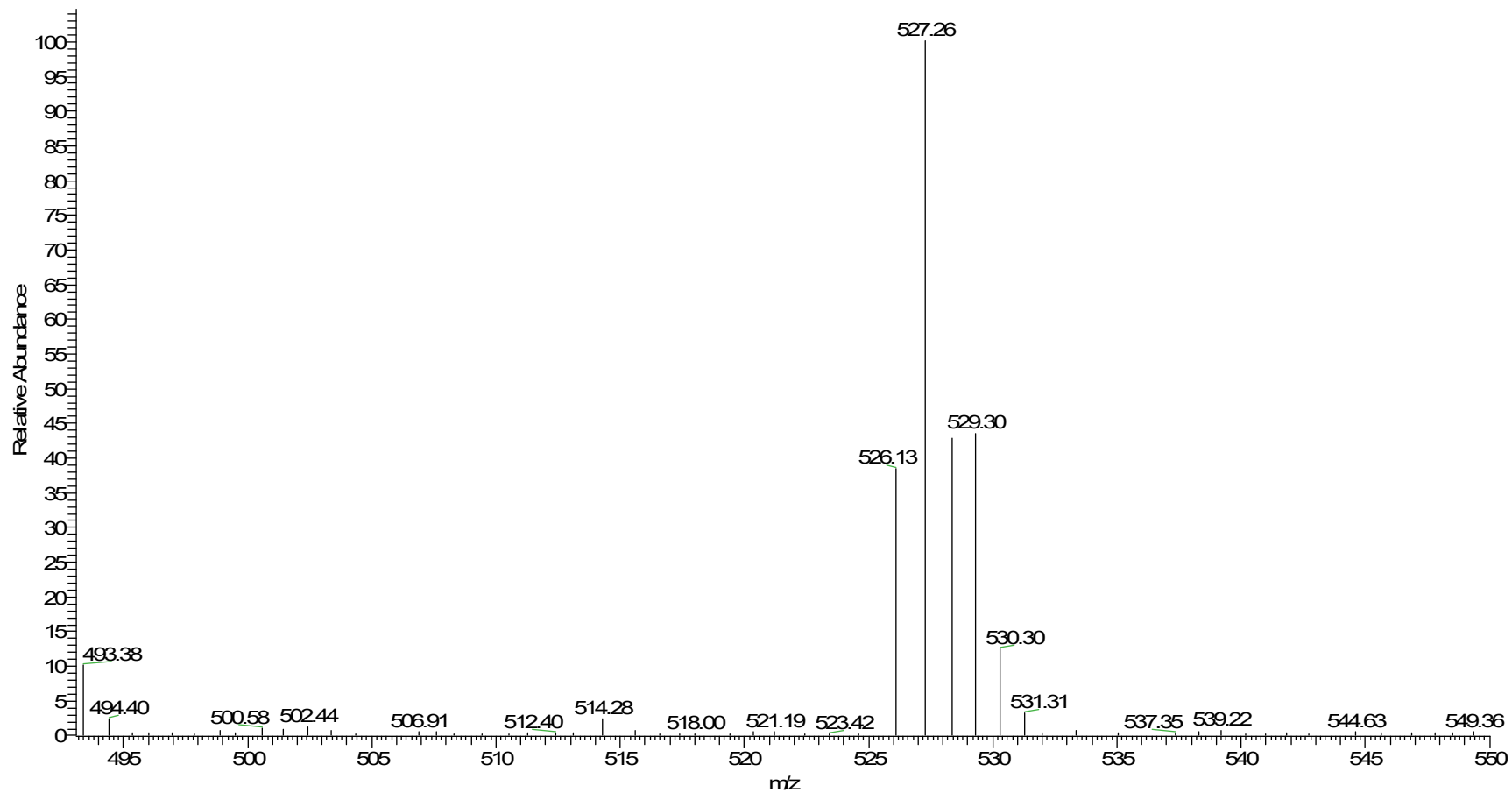


Fig.S60: ESI-MS spectrum of compound 10c

2-#8 RT: 0.04 AV: 1 NL: 3.59E6
T: -cESI Q1MS [400.000-700.000]

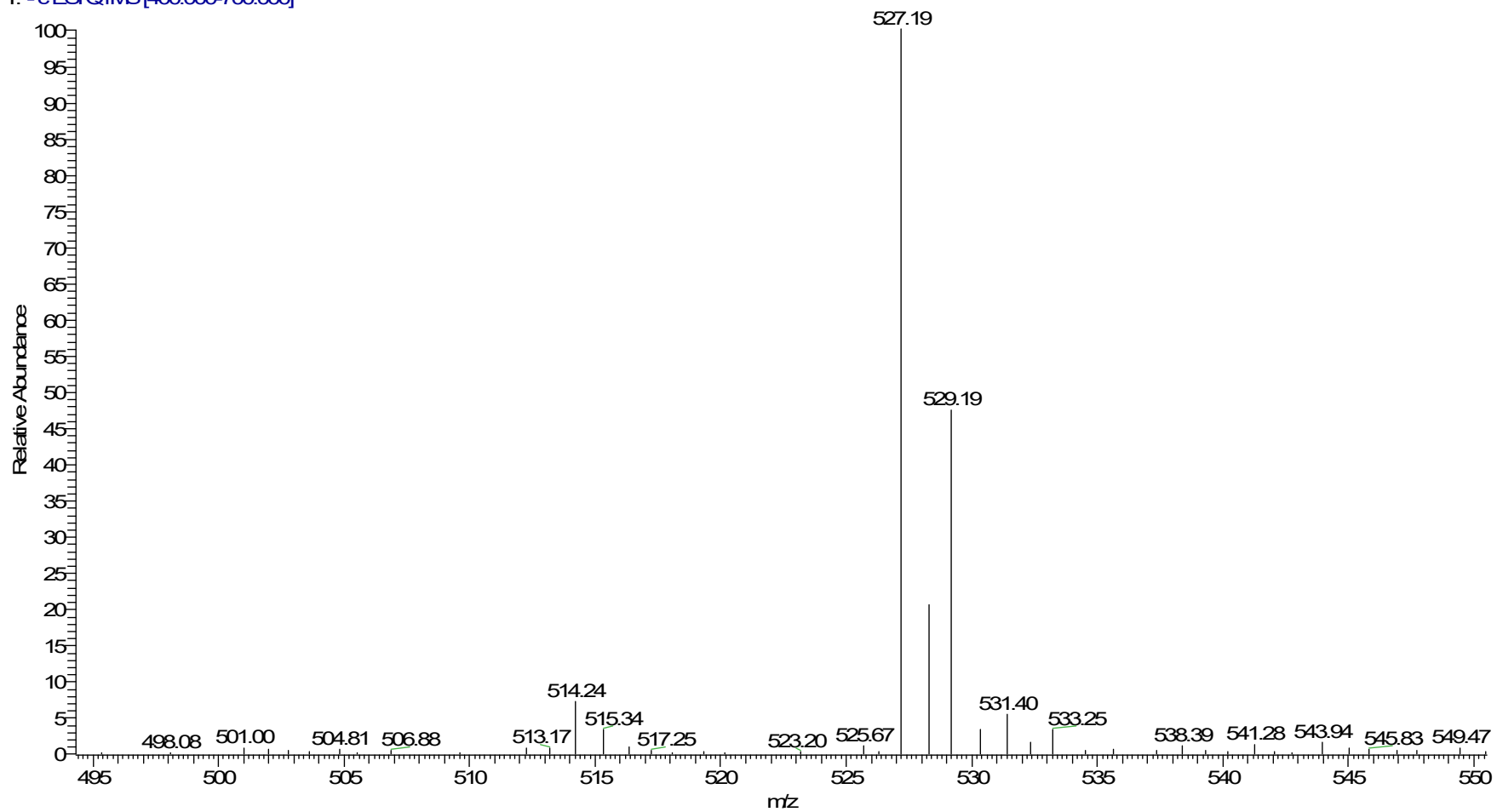


Fig.S61: ESI-MS spectrum of compound 10d

H04_20191209042033 #29 RT: 0.14 AV: 1 NL: 1.42E8
T: +c ESI Q1MS [400.000-700.000]

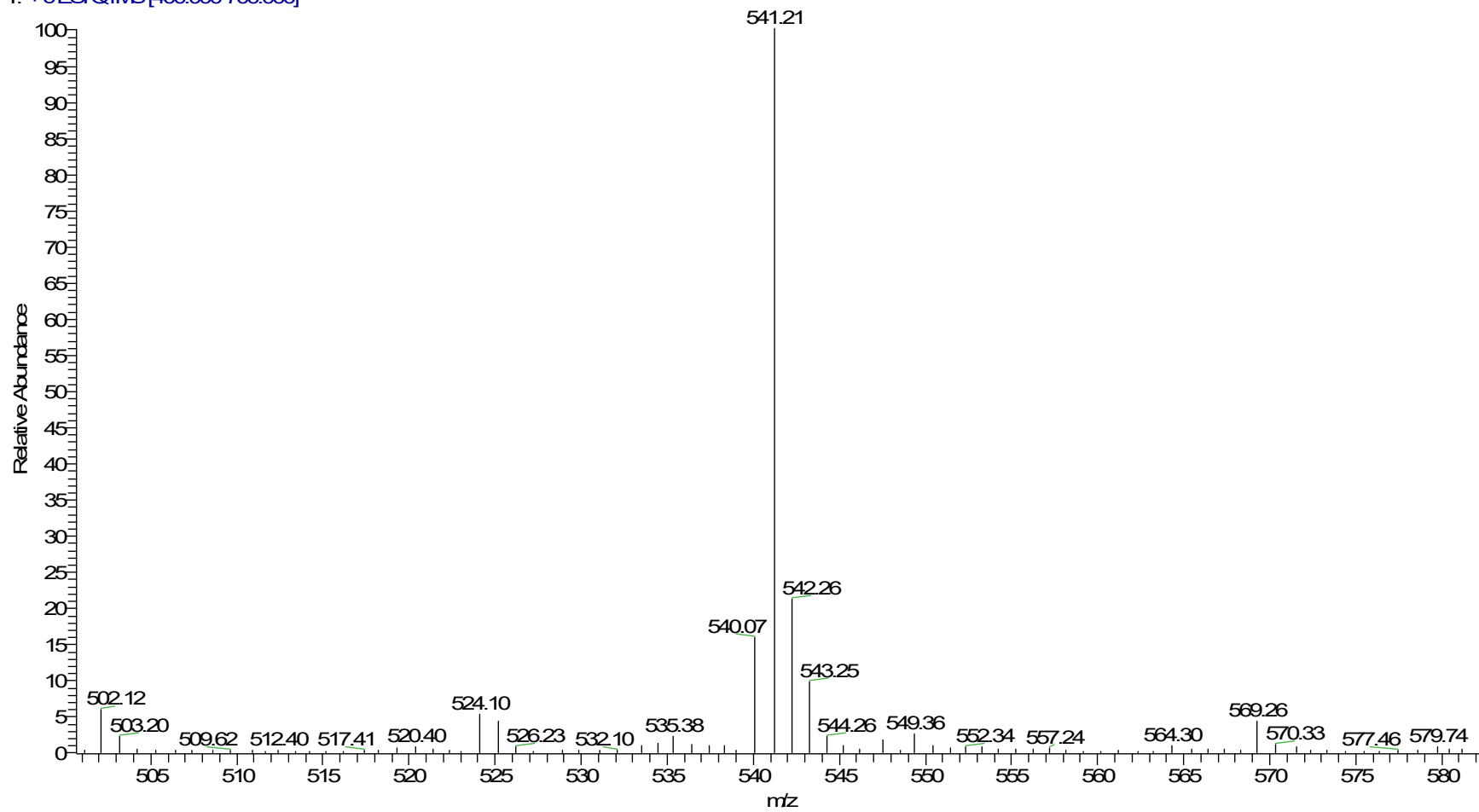


Fig.S62: ESI-MS spectrum of compound 10e

H03 #28 RT: 0.09 AV: 1 NL: 2.33E7
T: +c ESI Q1MS [450.000-650.000]

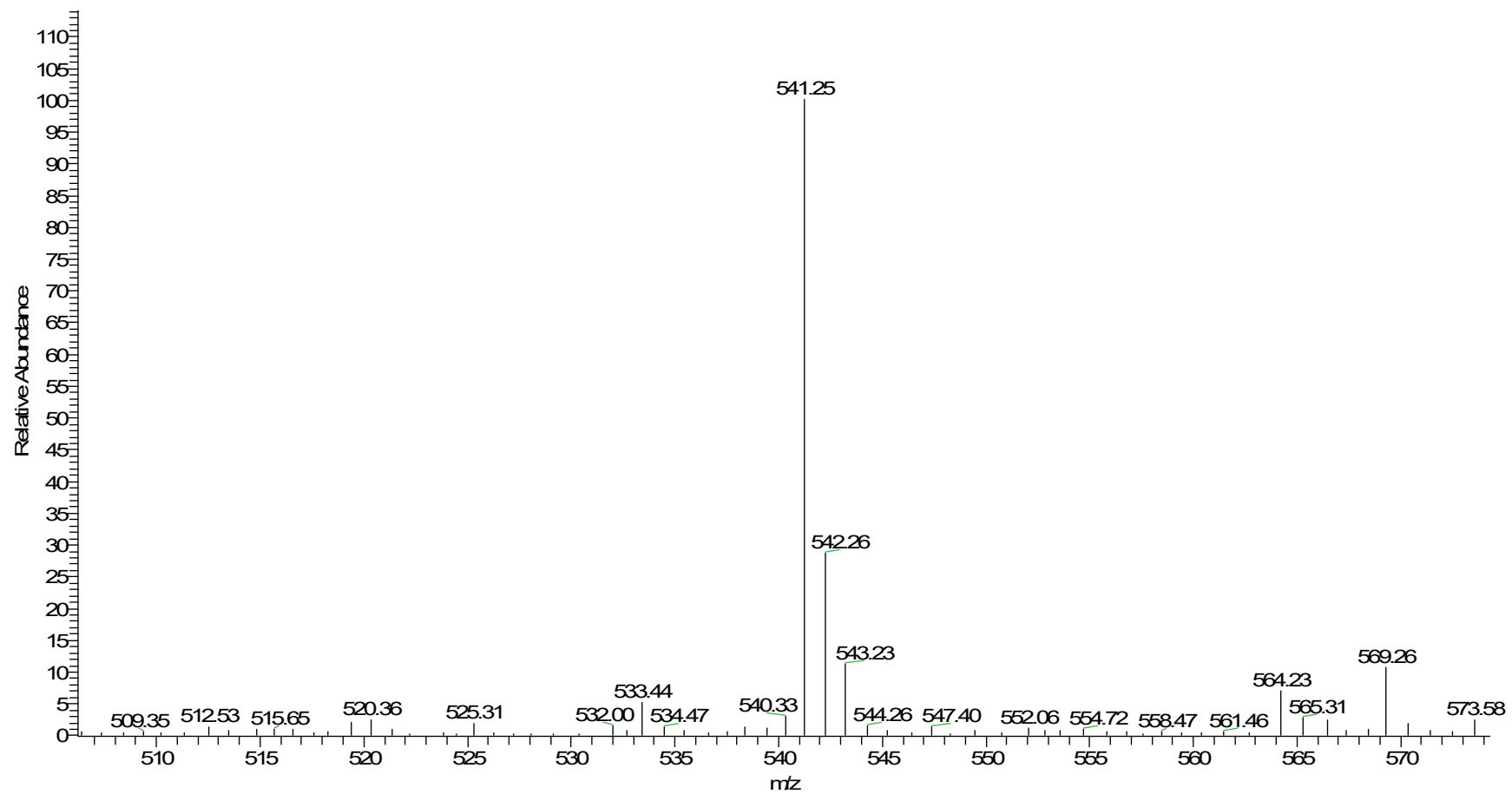


Fig.S63: ESI-MS spectrum of compound 10f

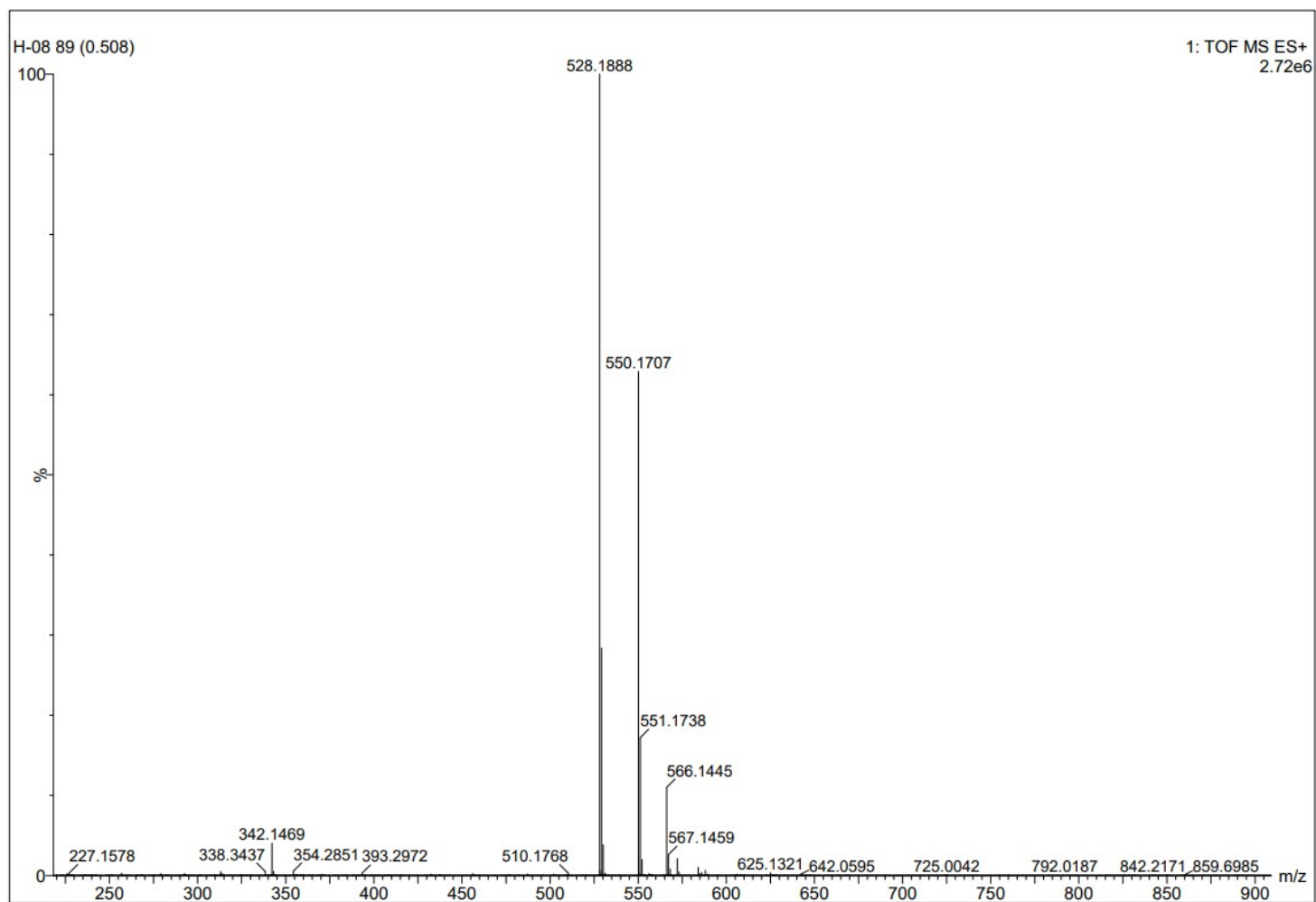


Fig.S64: HRESI-MS spectrum of compound **10g**

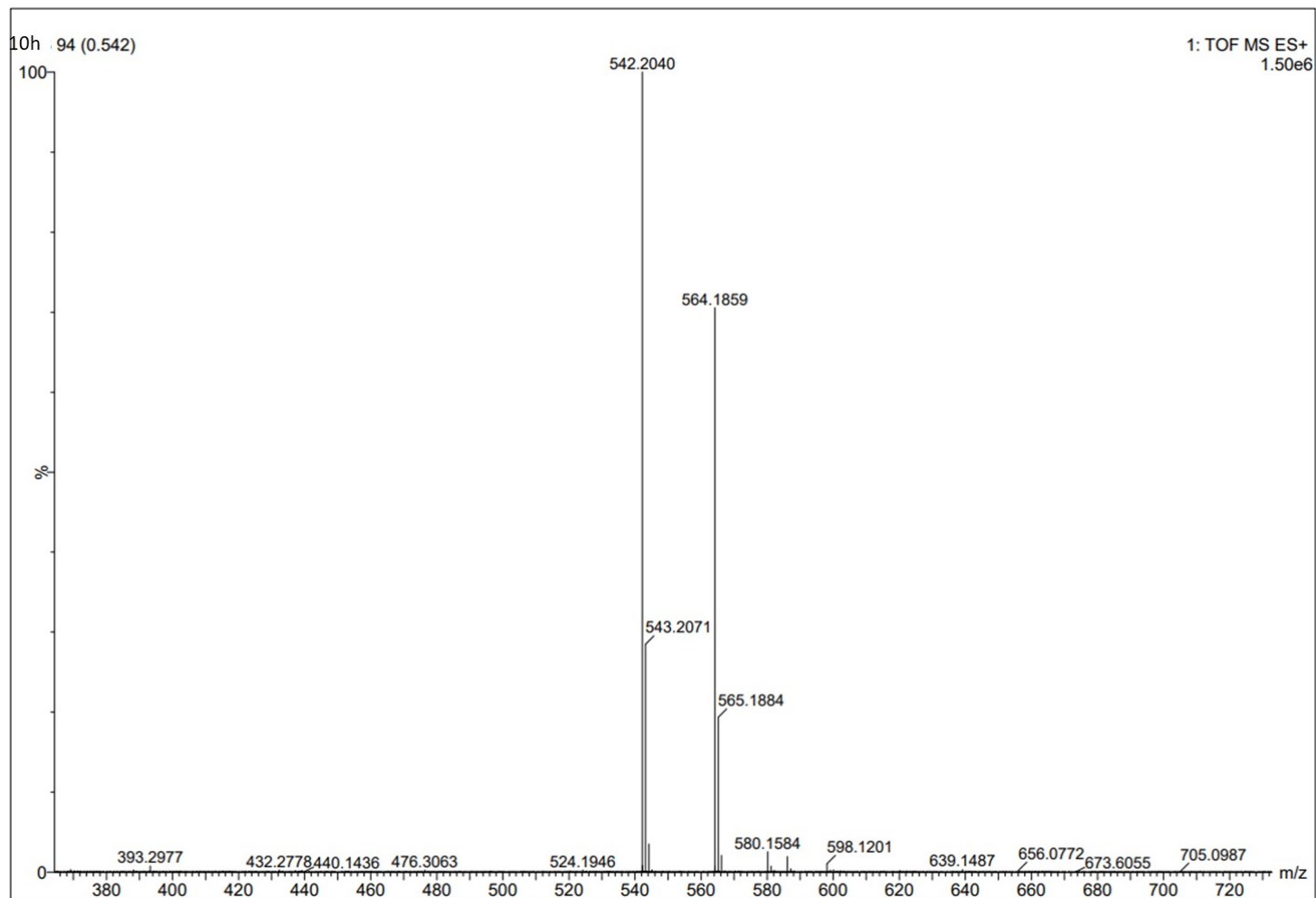


Fig.S65: HRESI-MS spectrum of compound 10h

#20 RT: 0.10 AV: 1 NL: 4.93E7
T: +cESI Q1MS [400.000-700.000]

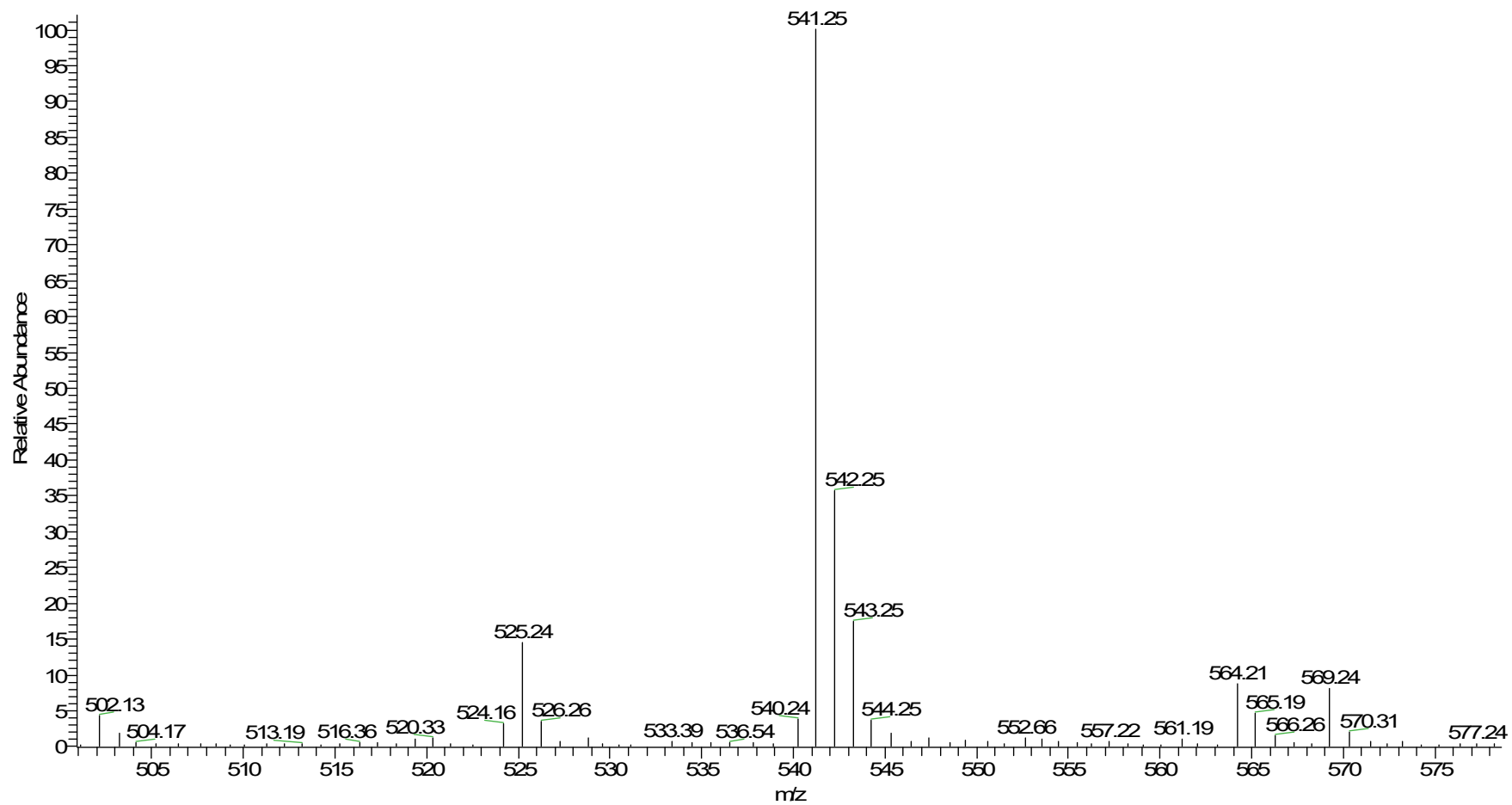


Fig.S66: ESI-MS spectrum of compound 10j

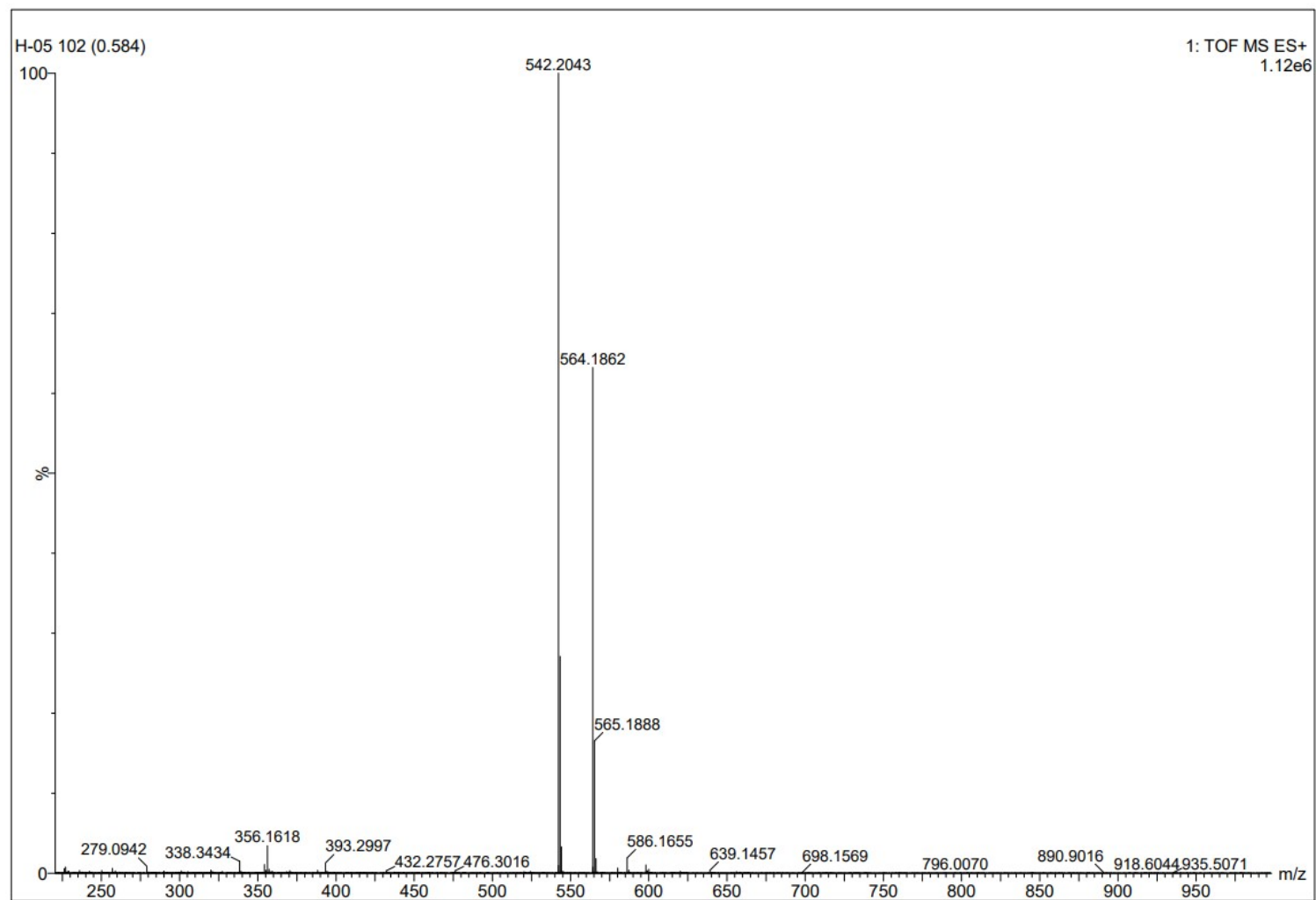


Fig.S67: HRESI-MS spectrum of compound **10i**

3-#4 RT: 0.02 AV: 1 NL: 242E7
T: +cESI Q1MS [400.000-700.000]

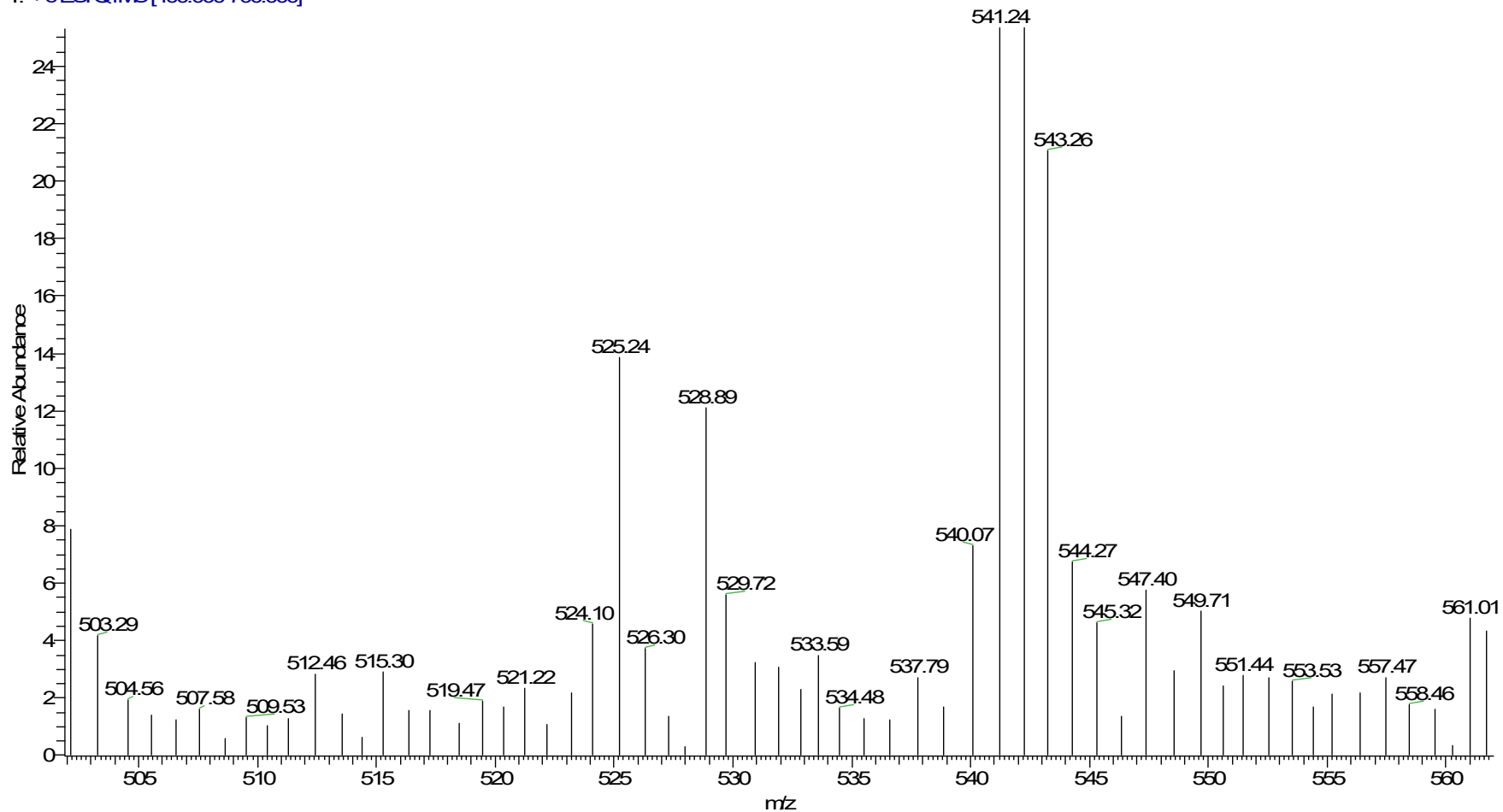


Fig.S68: ESI-MS spectrum of compound 10i

H-1C #159 RT: 0.80 AV: 1 NL: 2.77E7
T: +cESI Q1MS [400.000-700.000]

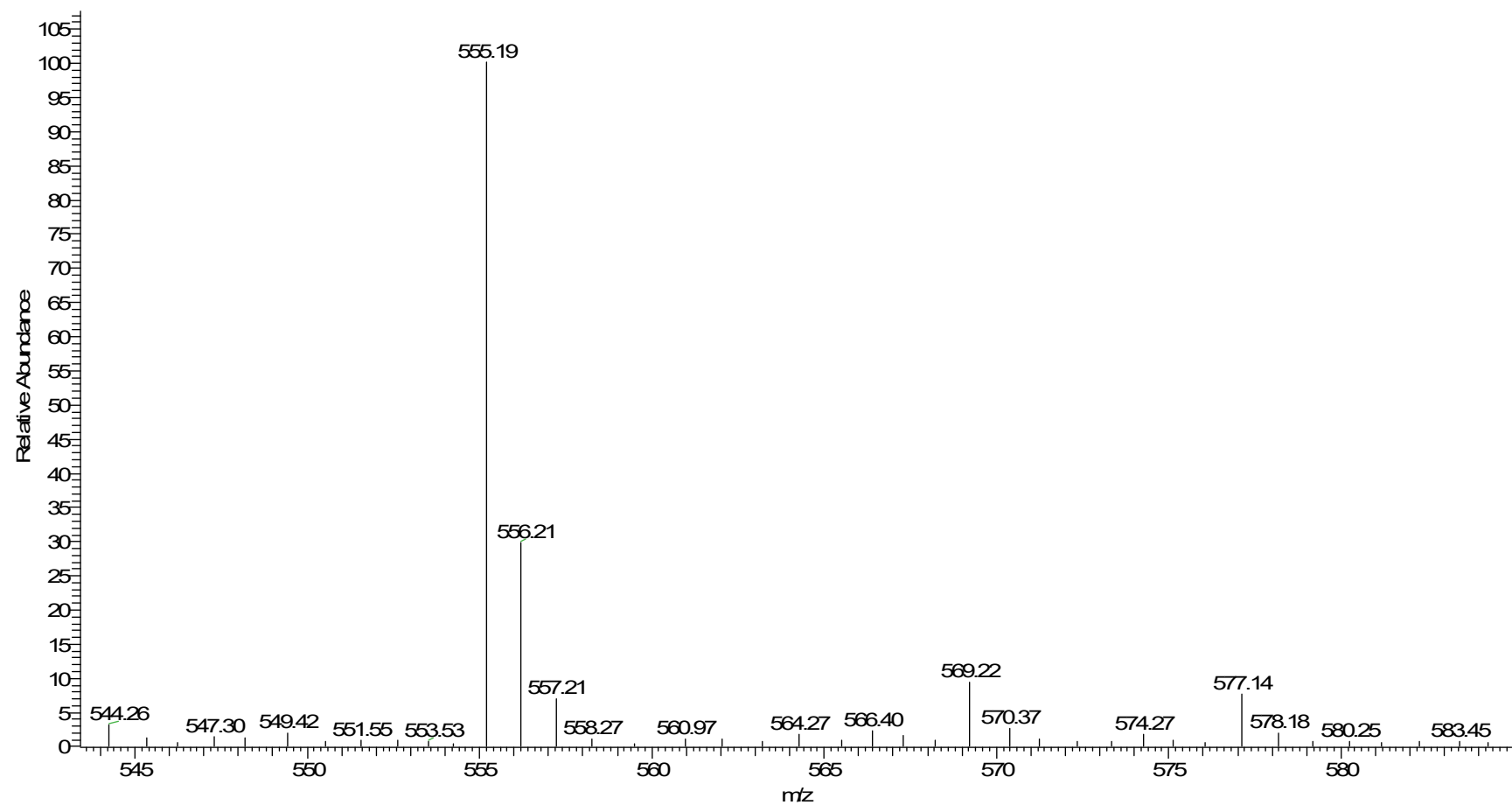


Fig.S69: ESI-MS spectrum of compound 10k

H02_20191127055723 #76 RT: 0.19 AV: 1 NL: 1.39E6
T: +cESI Q1MS [500.000-650.000]

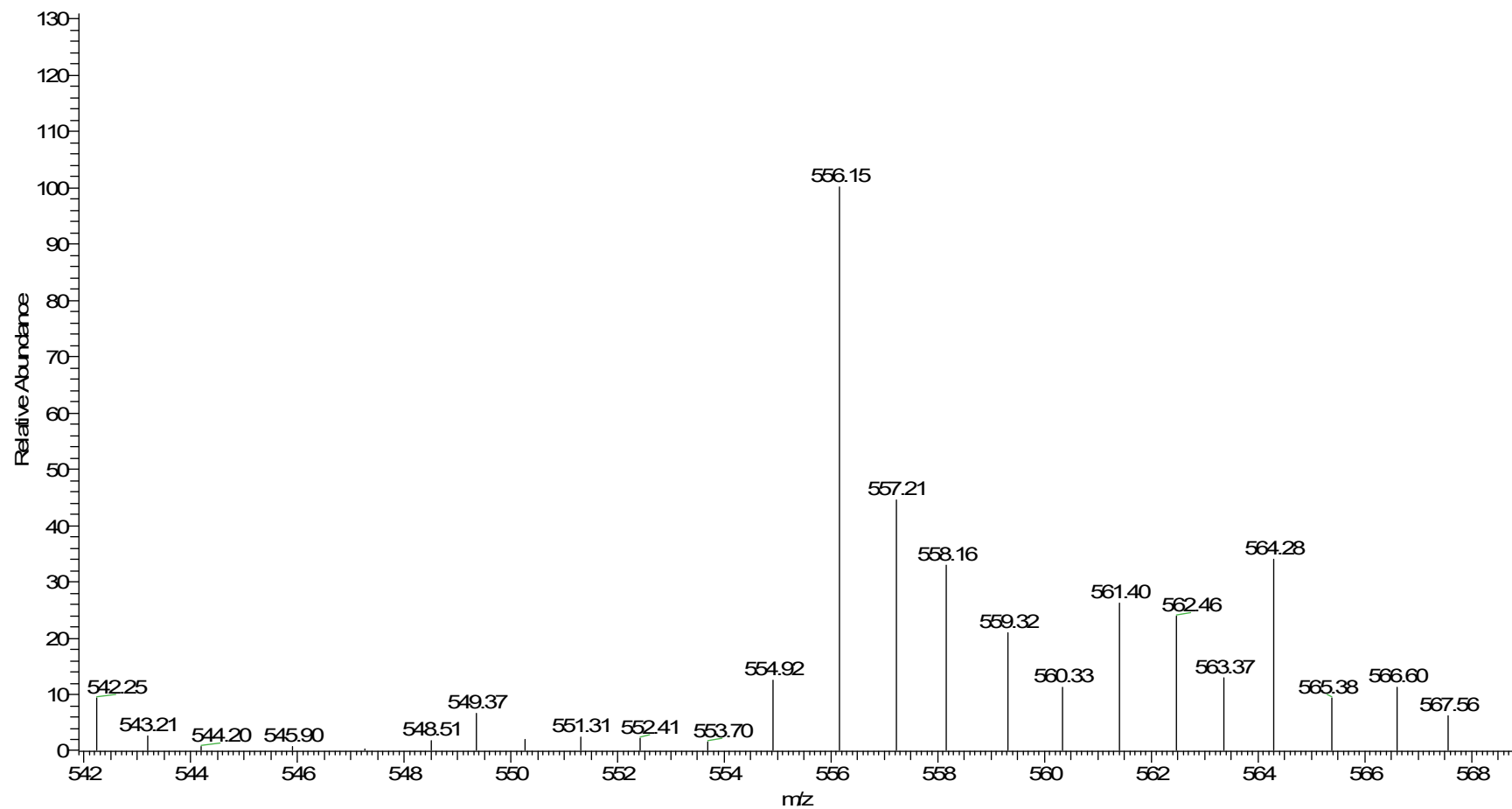


Fig.S70: ESI-MS spectrum of compound 10m

8-20200106040836 #37 RT: 0.02 AV: 1 NL: 3.57E6
T: +c ESI Q1MS [550.000-580.000]

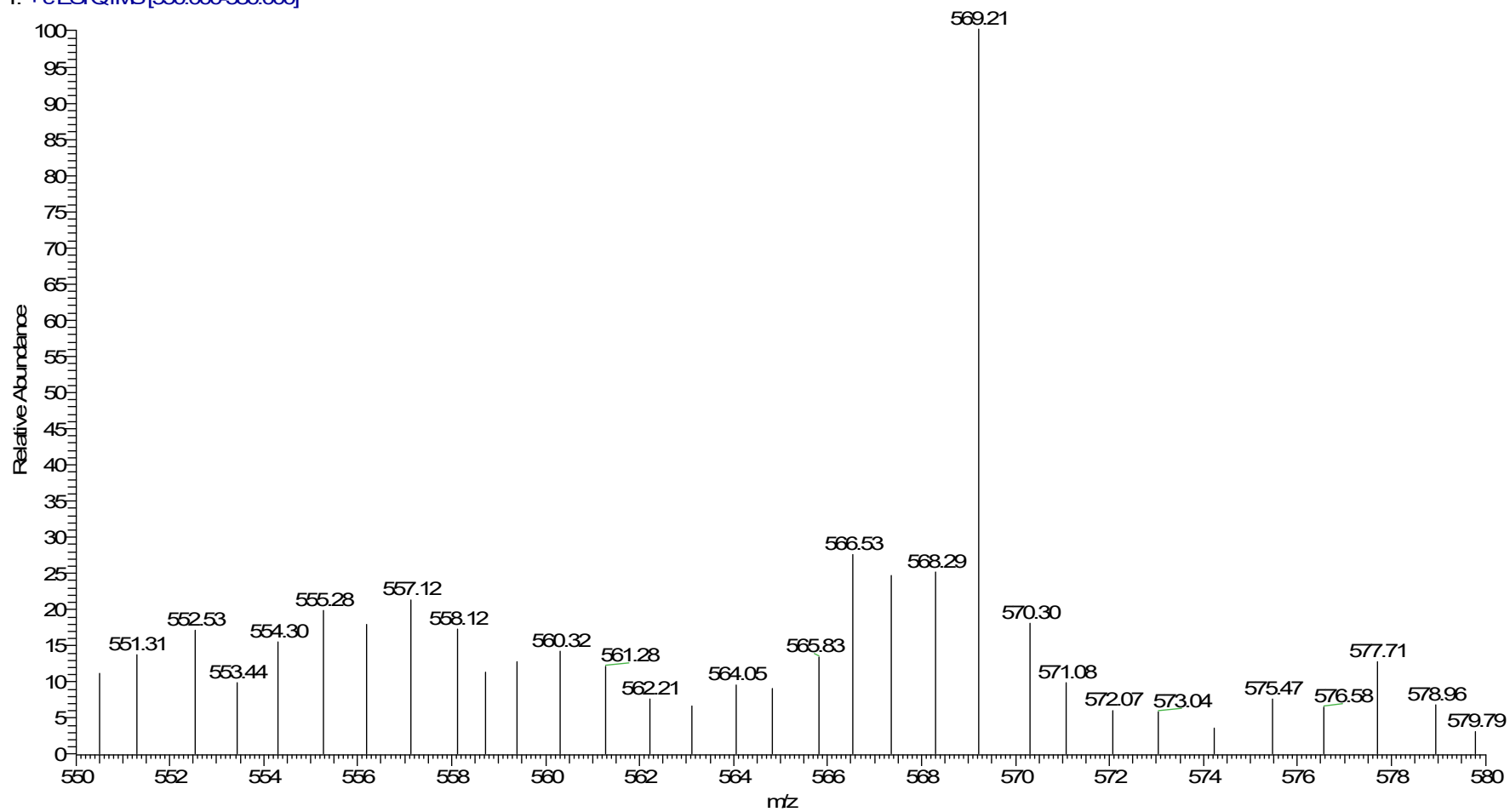


Fig.S71: ESI-MS spectrum of compound 10n