

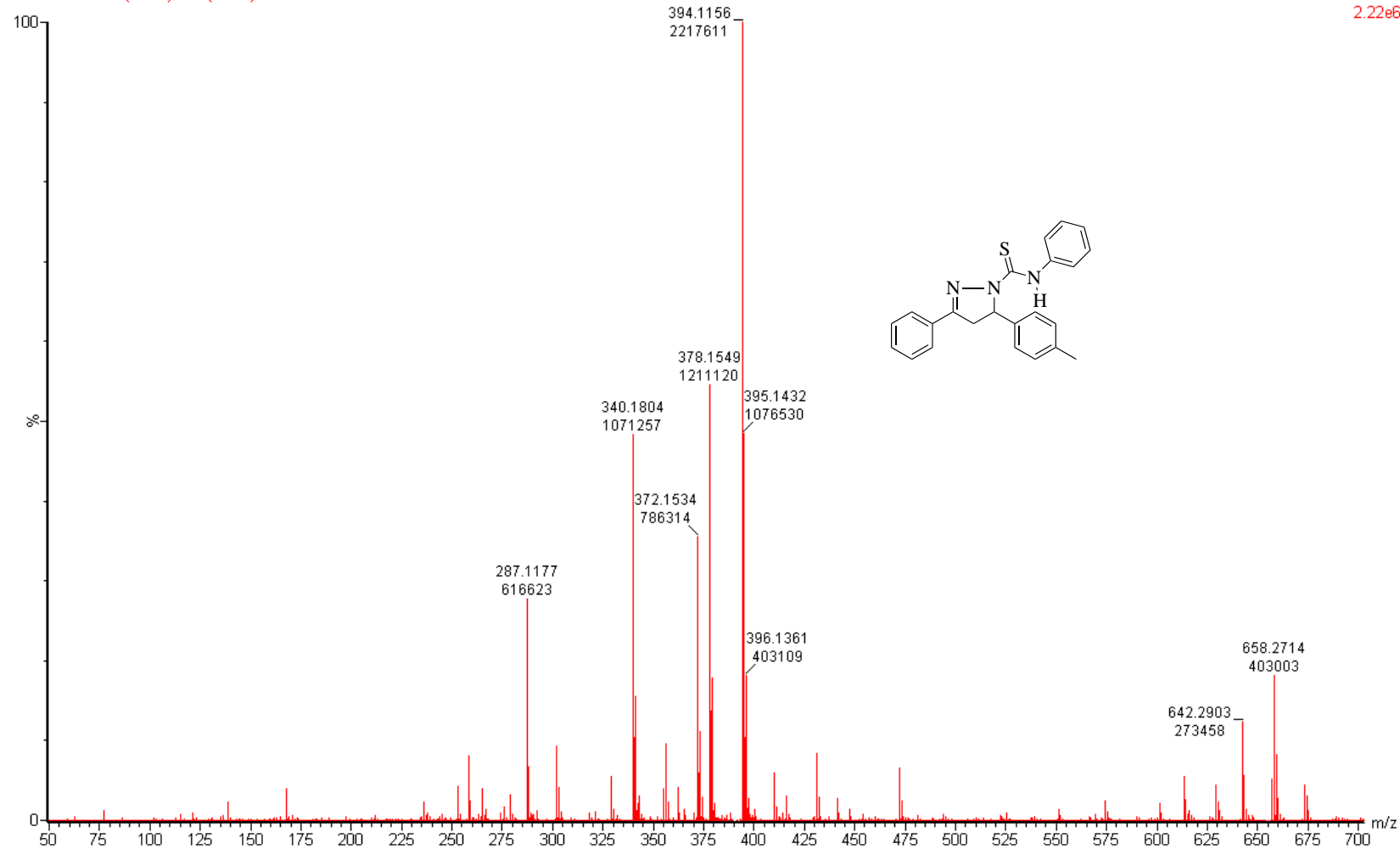
Supporting information

Synthesis, Characterisation and Biological Evaluation of New 3,5-Disubstituted-Pyrazoline Derivatives as Potential Anti-*Mycobacterium tuberculosis* H37Ra.

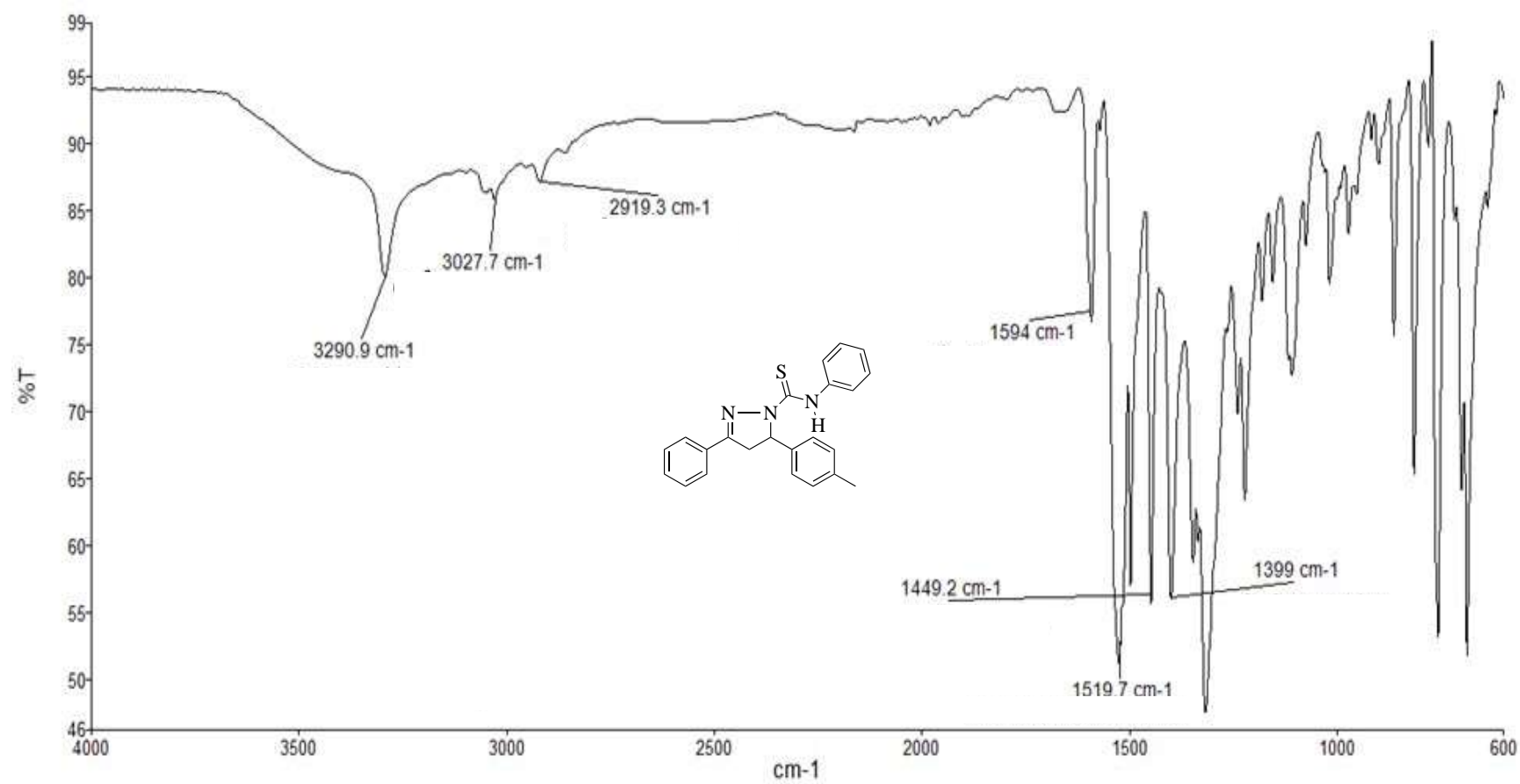
Kok Tong Wong, Hasnah Osman, Thaigarajan Parumasivam, Unang Supratman, Mohammad Tasyriq Che Omar and Mohamad Nurul Azmi*

4ME4PHNP 57 (0.986) Cm (31:57)

TOF MS ES+
2.22e6

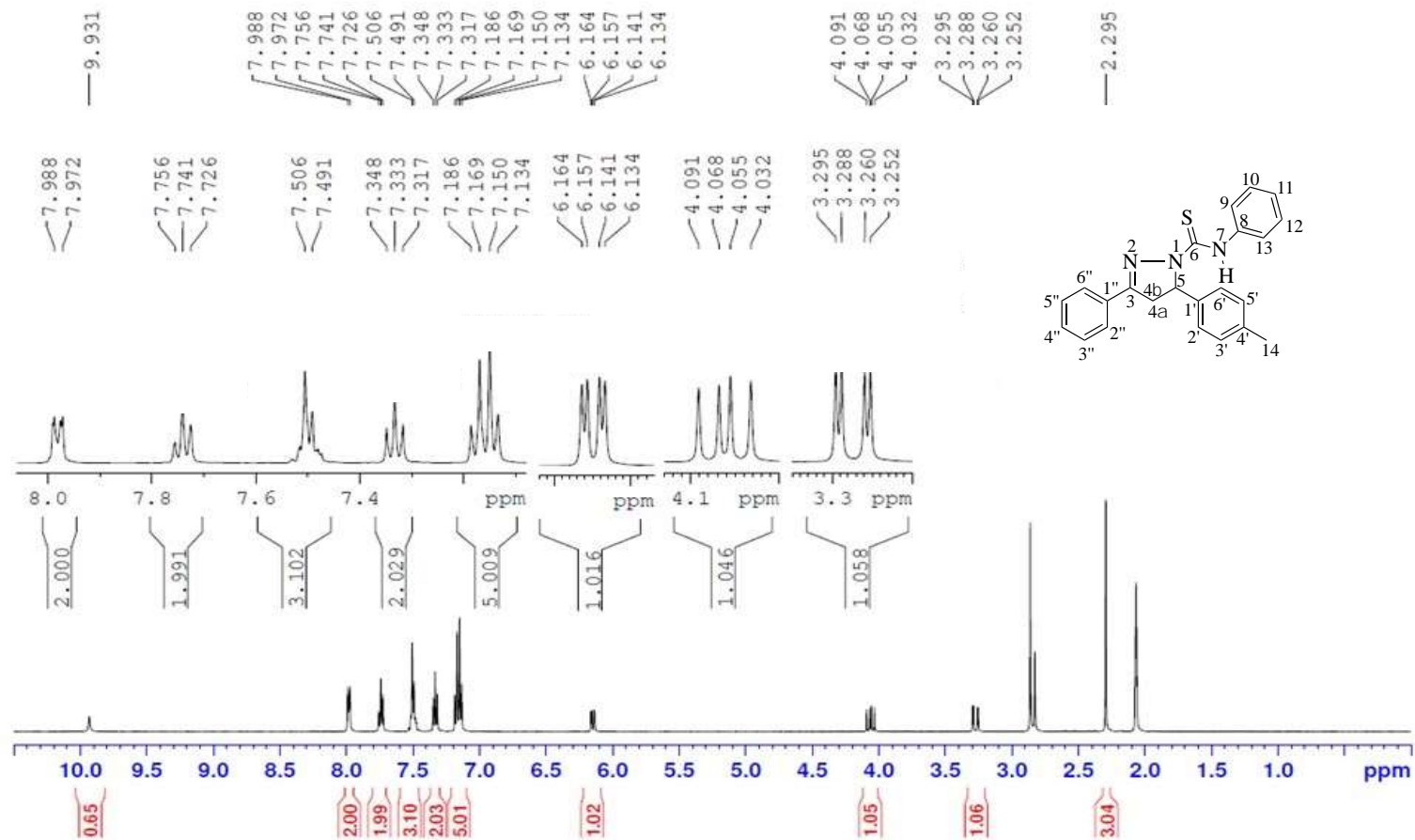


HRMS spectrum of compound 4a



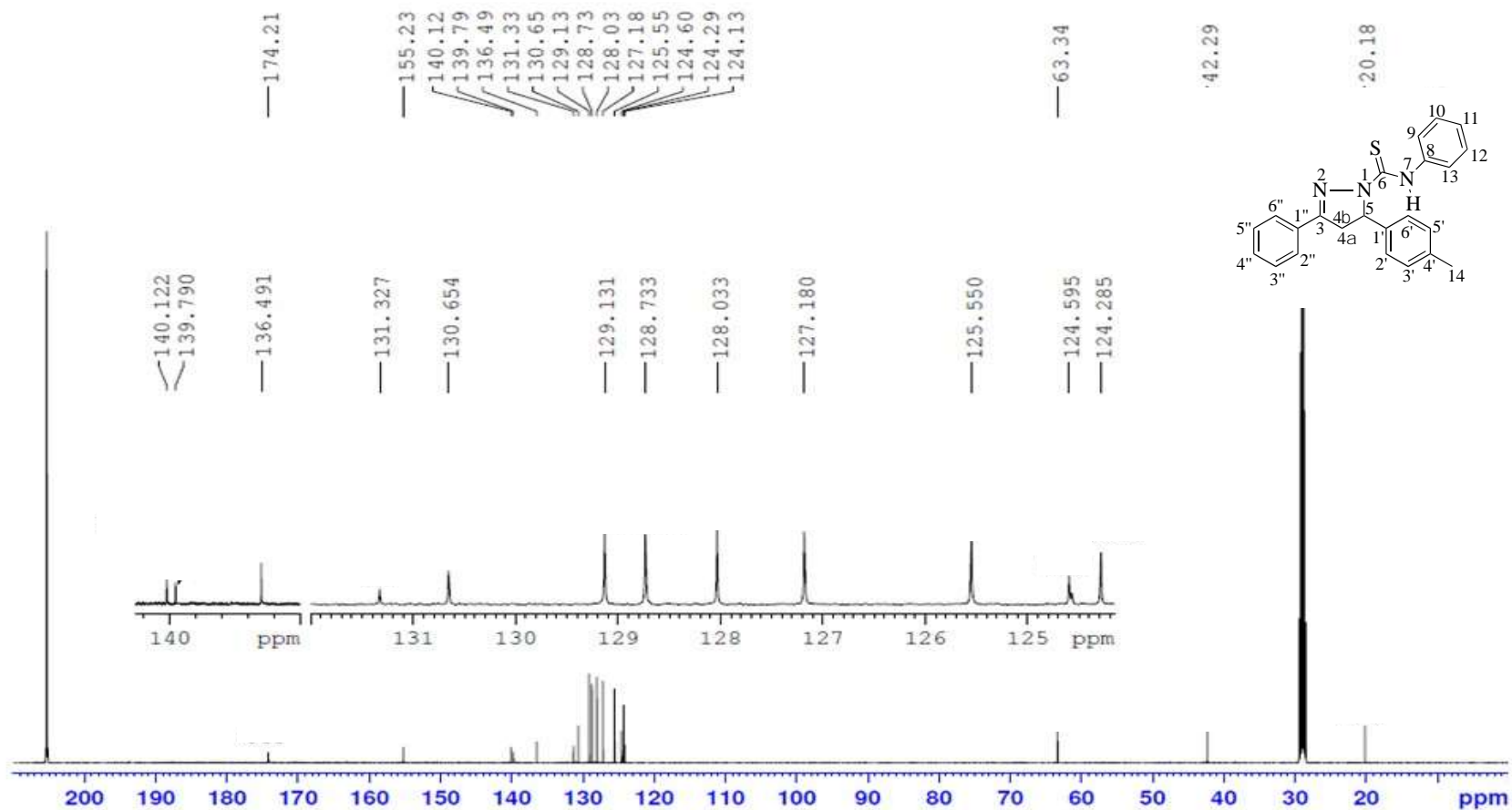
IR spectrum of compound **4a**

5-(4-methylphenyl)-N,3-diphenyl-4,5-dihydro-1H-pyrazole-1-carbothioamide_1H



¹H NMR spectrum of compound 4a

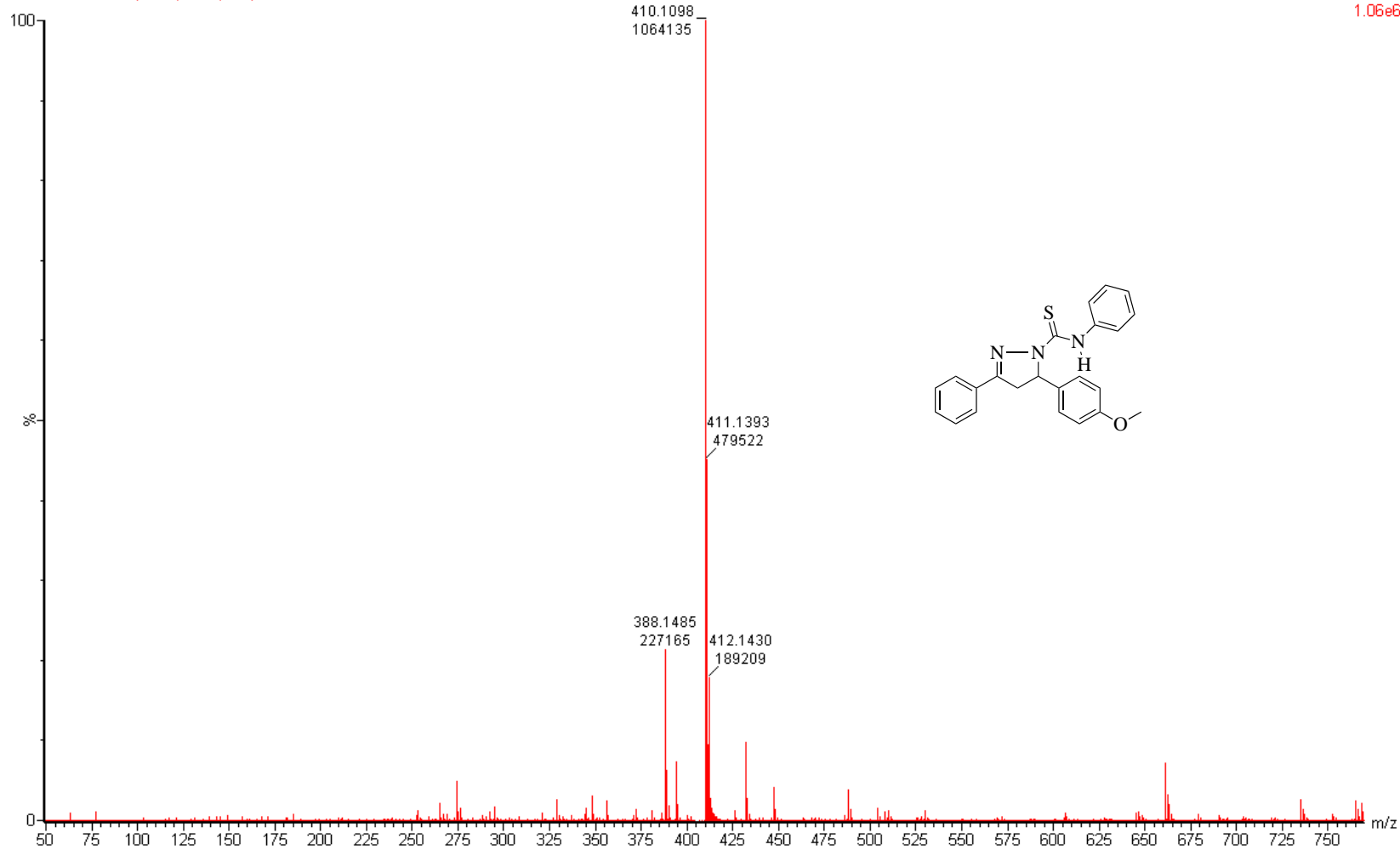
5-(4-methylphenyl)-N,3-diphenyl-4,5-dihydro-1H-pyrazole-1-carbothioamide_{13C}



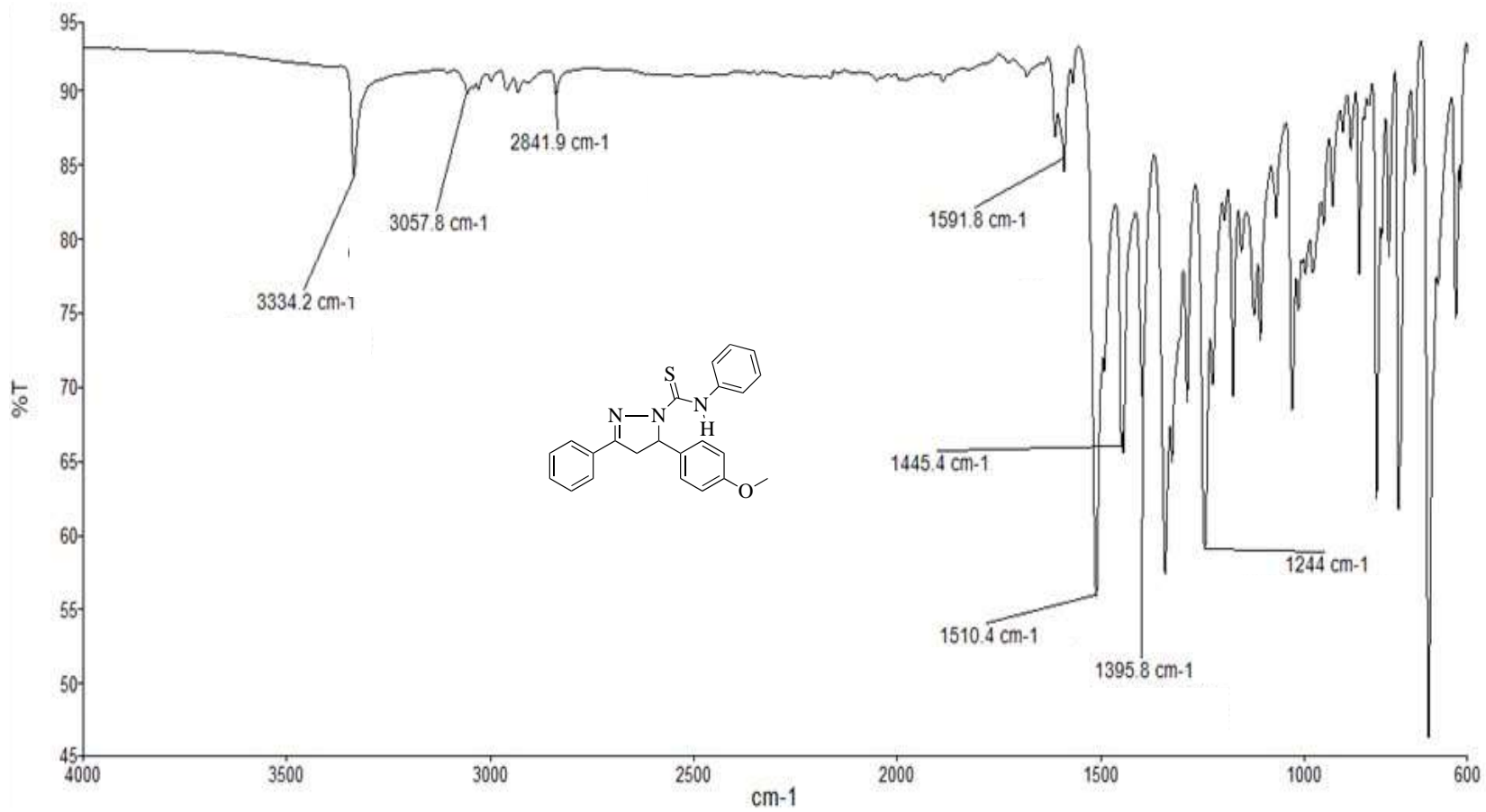
¹³C NMR spectrum of compound 4a

4MEO4PHNP 15 (0.272) Cm (3:15)

TOF MS ES+
1.06e6

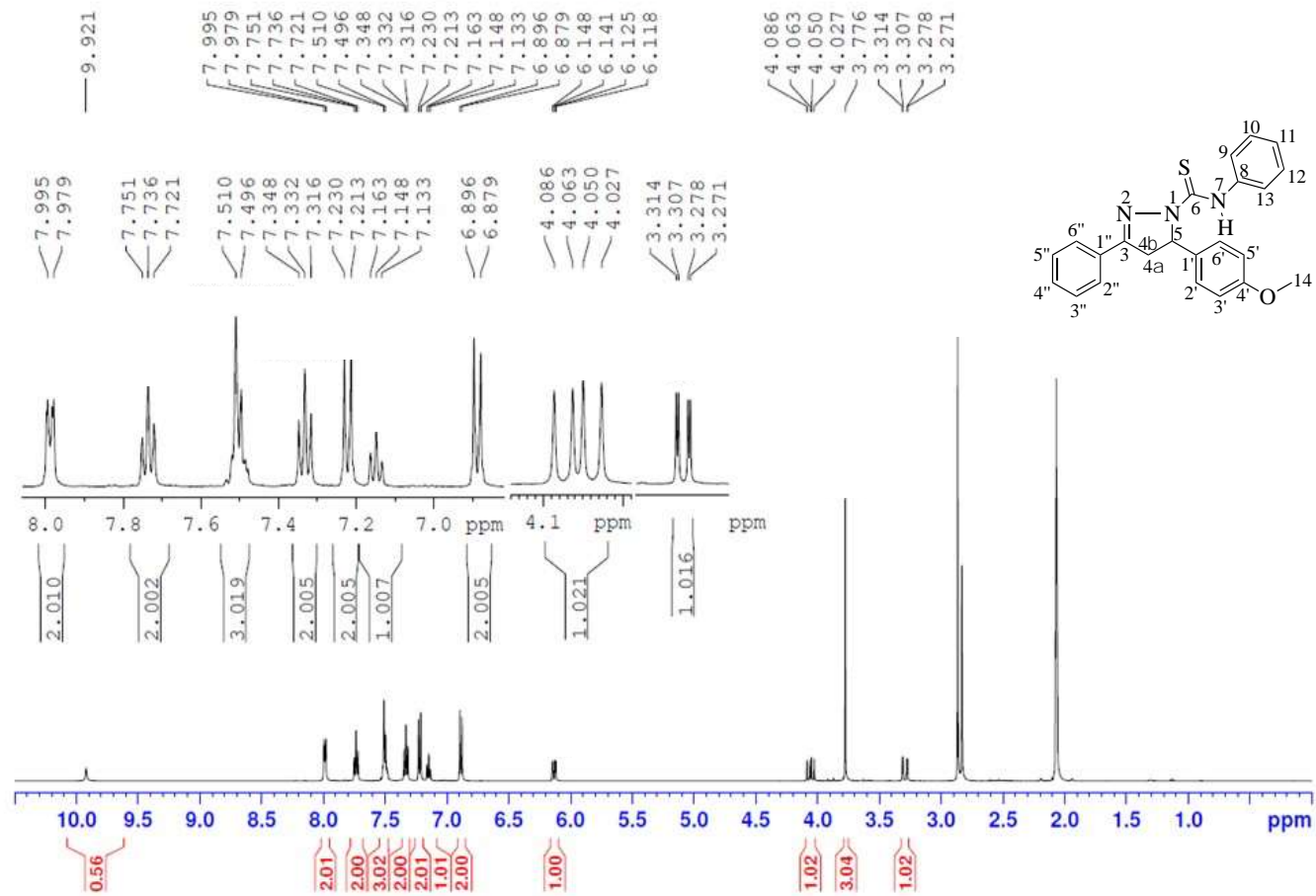


HRMS spectrum of compound **4b**



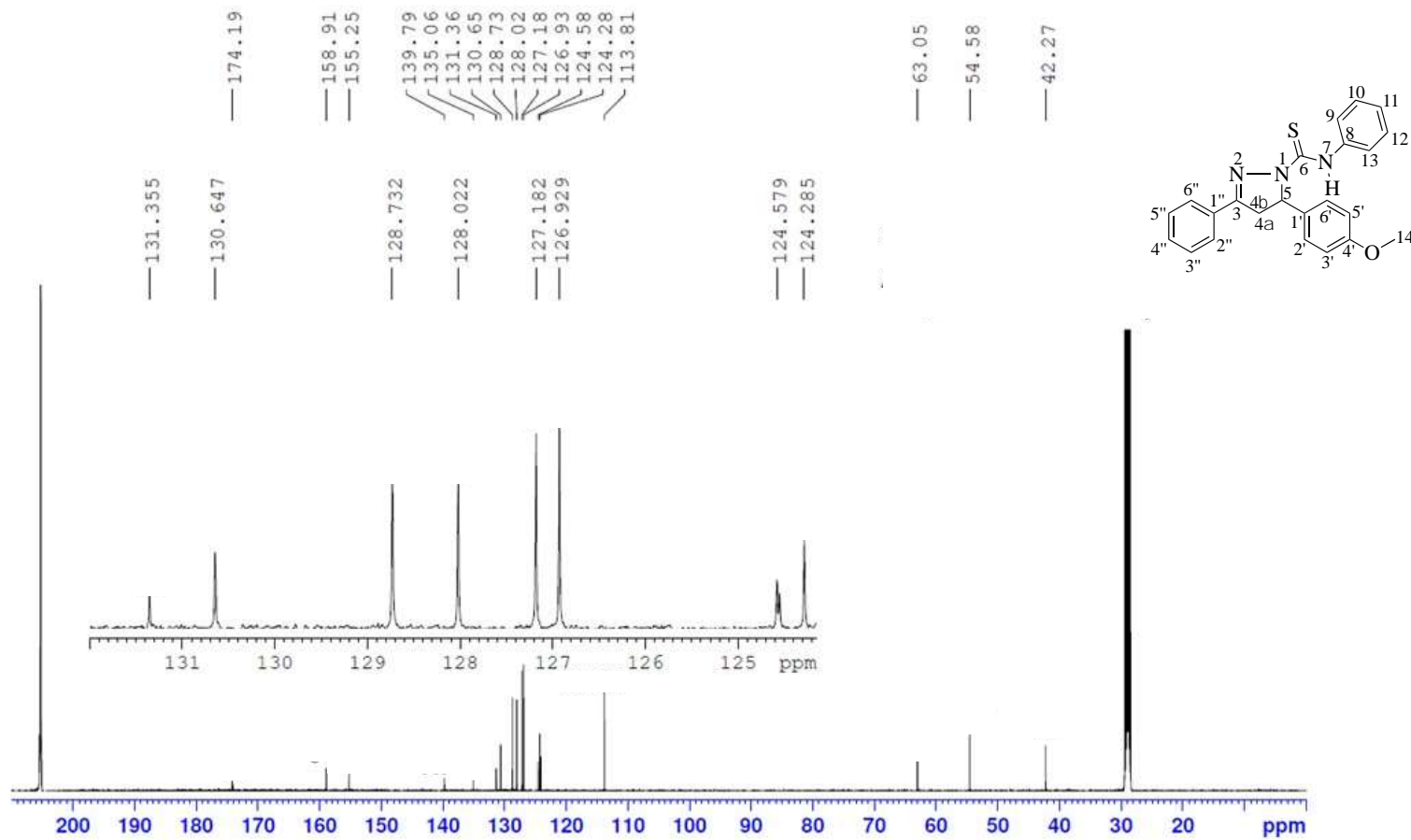
IR spectrum of compound **4b**

5-(4-methoxyphenyl)-N,3-diphenyl-4,5-dihydro-1H-pyrazole-1-carbothioamide_1H

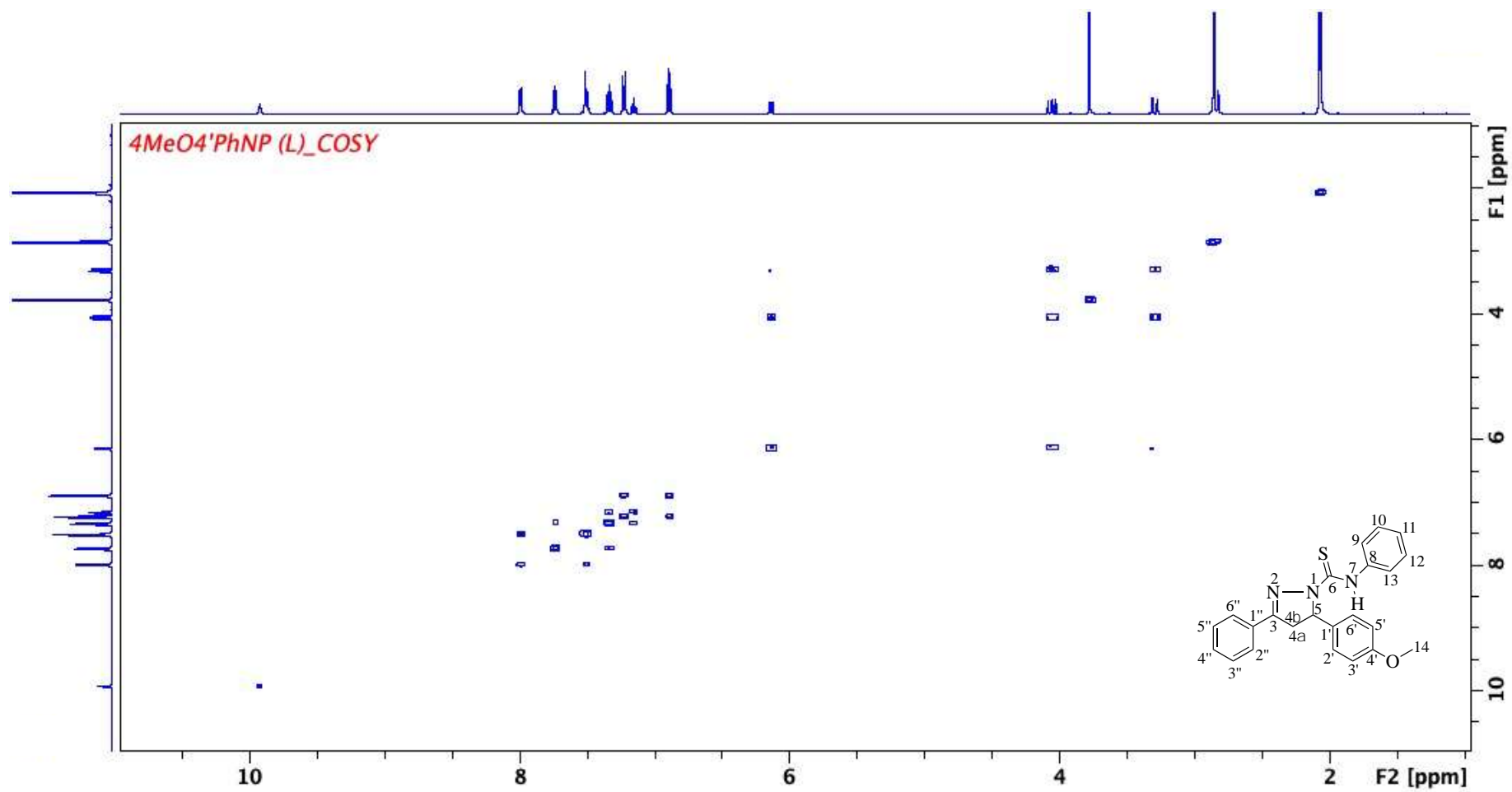


¹H NMR spectrum of compound **4b**

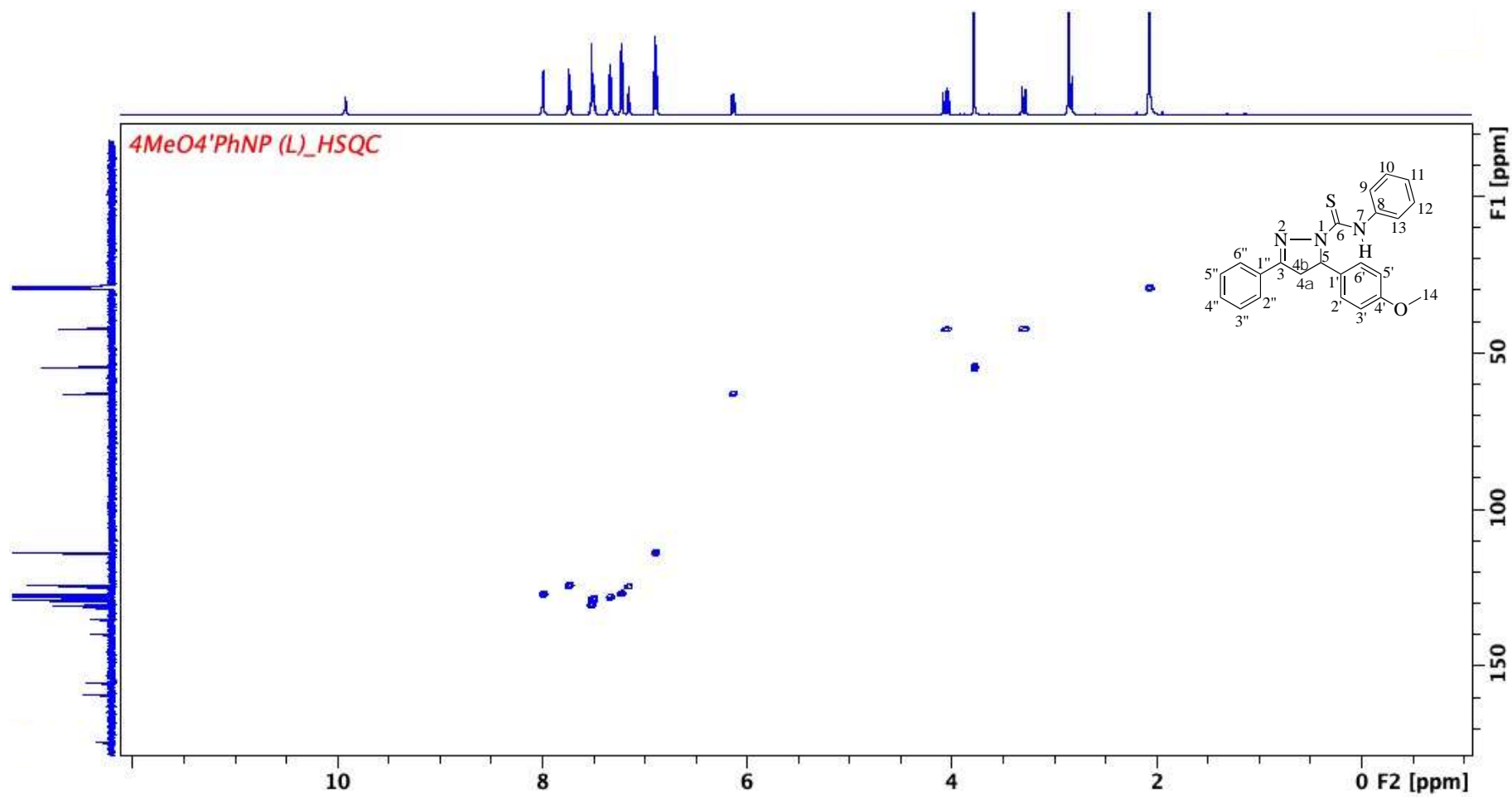
5-(4-methoxyphenyl)-N,3-diphenyl-4,5-dihydro-1H-pyrazole-1-carbothioamide_13C



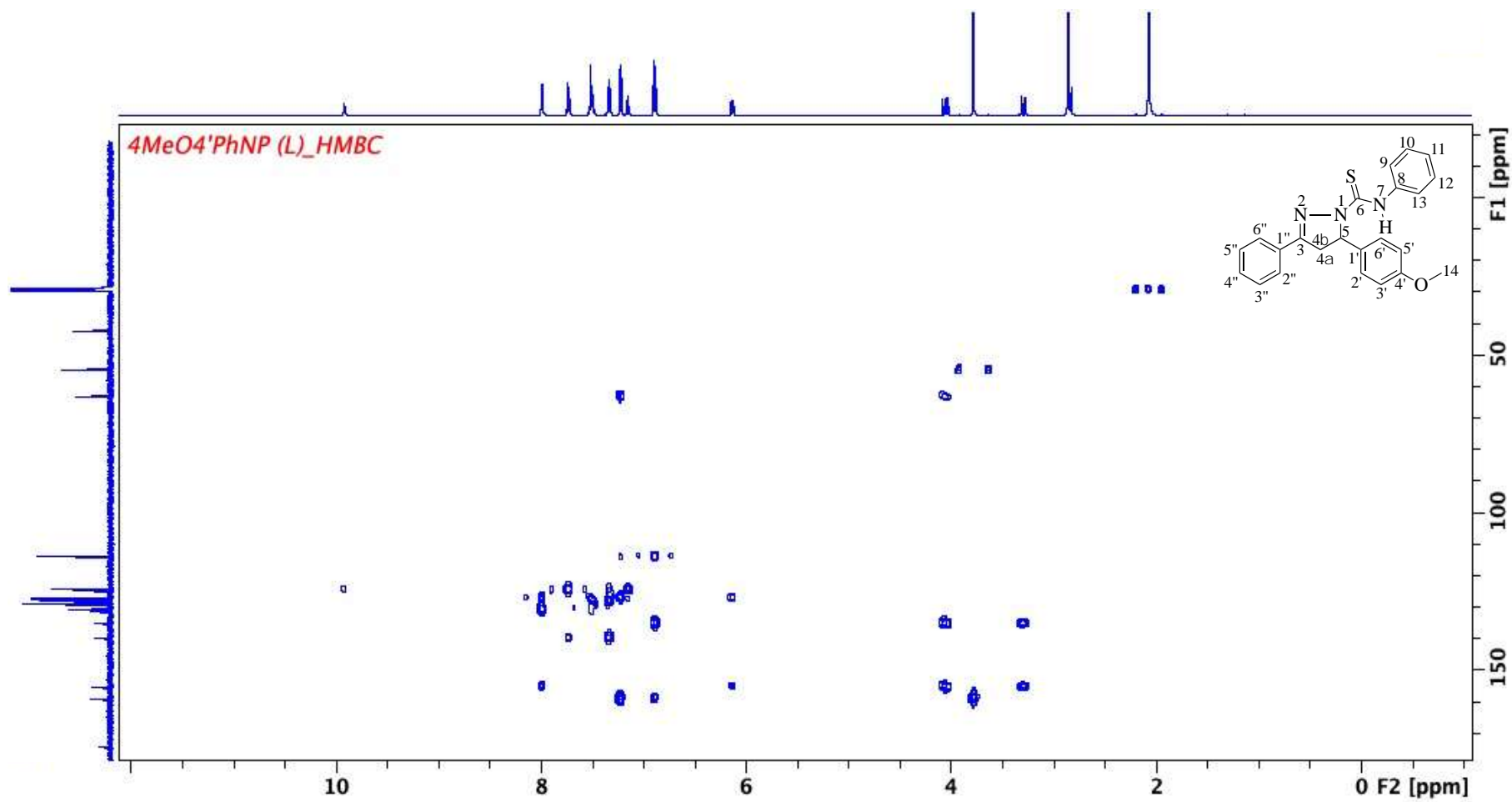
¹³C NMR spectrum of compound 4b



^1H - ^1H COSY NMR spectrum of compound 4b



^1H - ^{13}C HSQC NMR spectrum of compound 4b



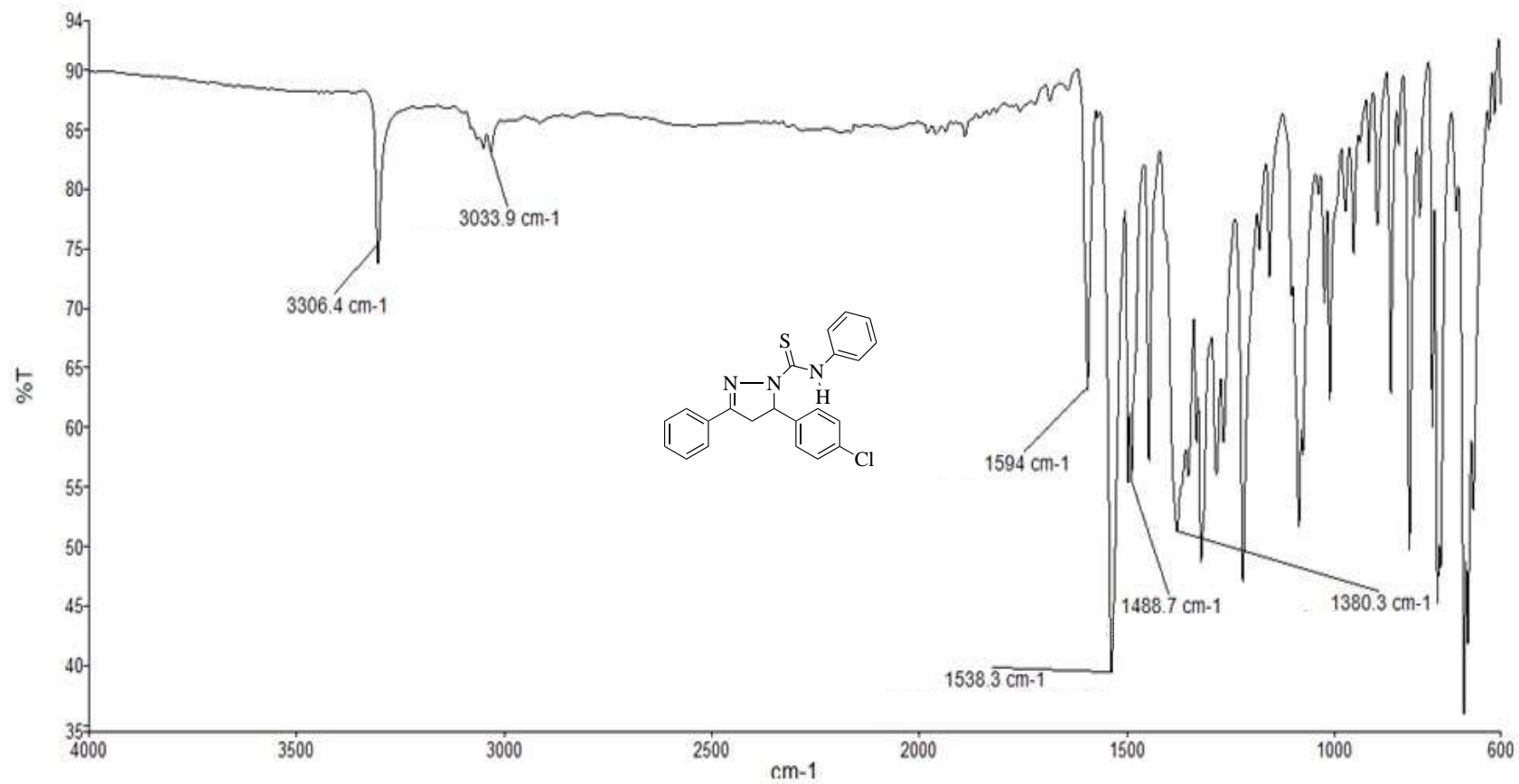
^1H - ^{13}C HMBC NMR spectrum of compound 4b

4CL4PHNP 6 (0.119) Cm (3:16)

TOF MS ES+
1.45e5

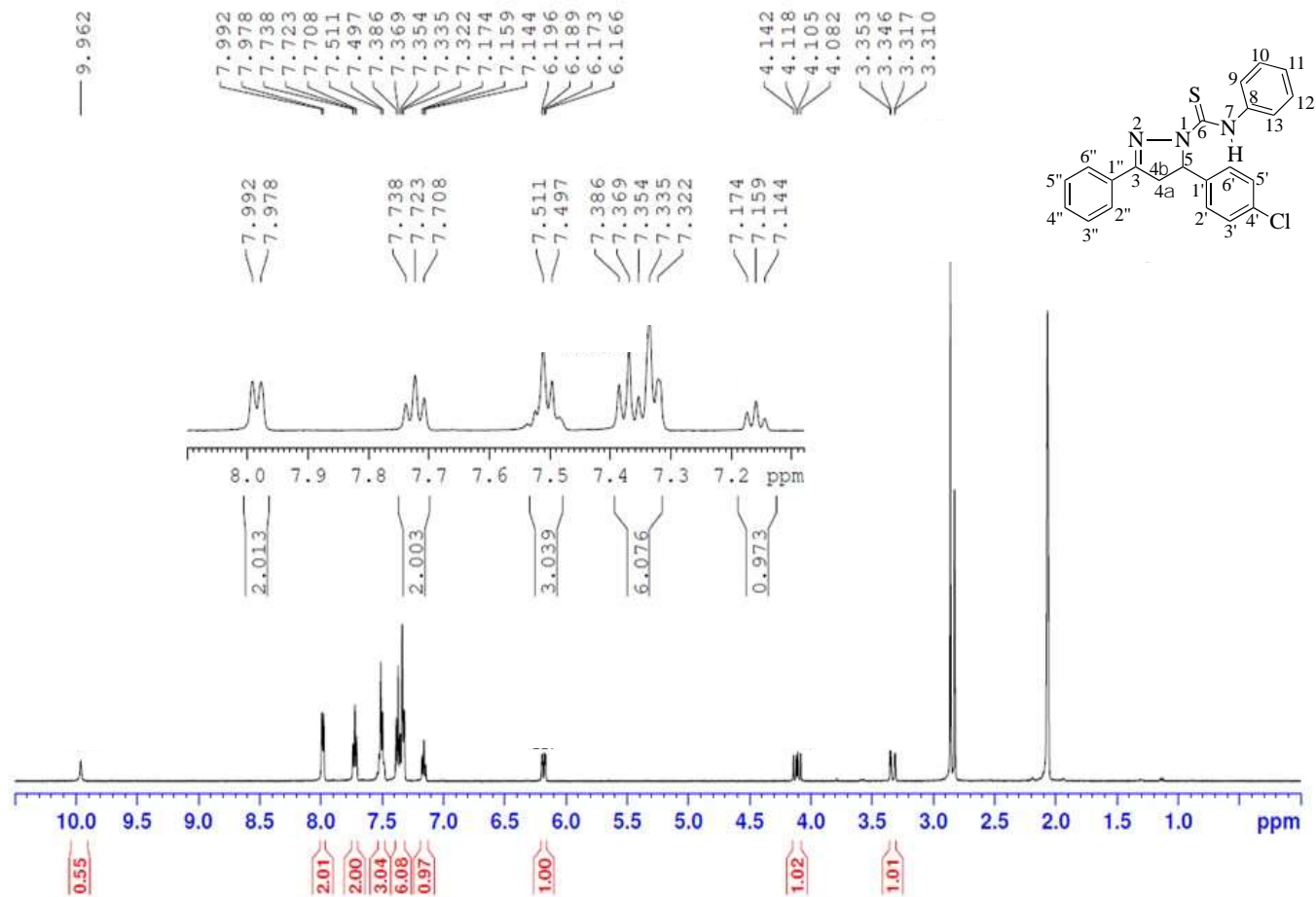


HRMS spectrum of compound 4c



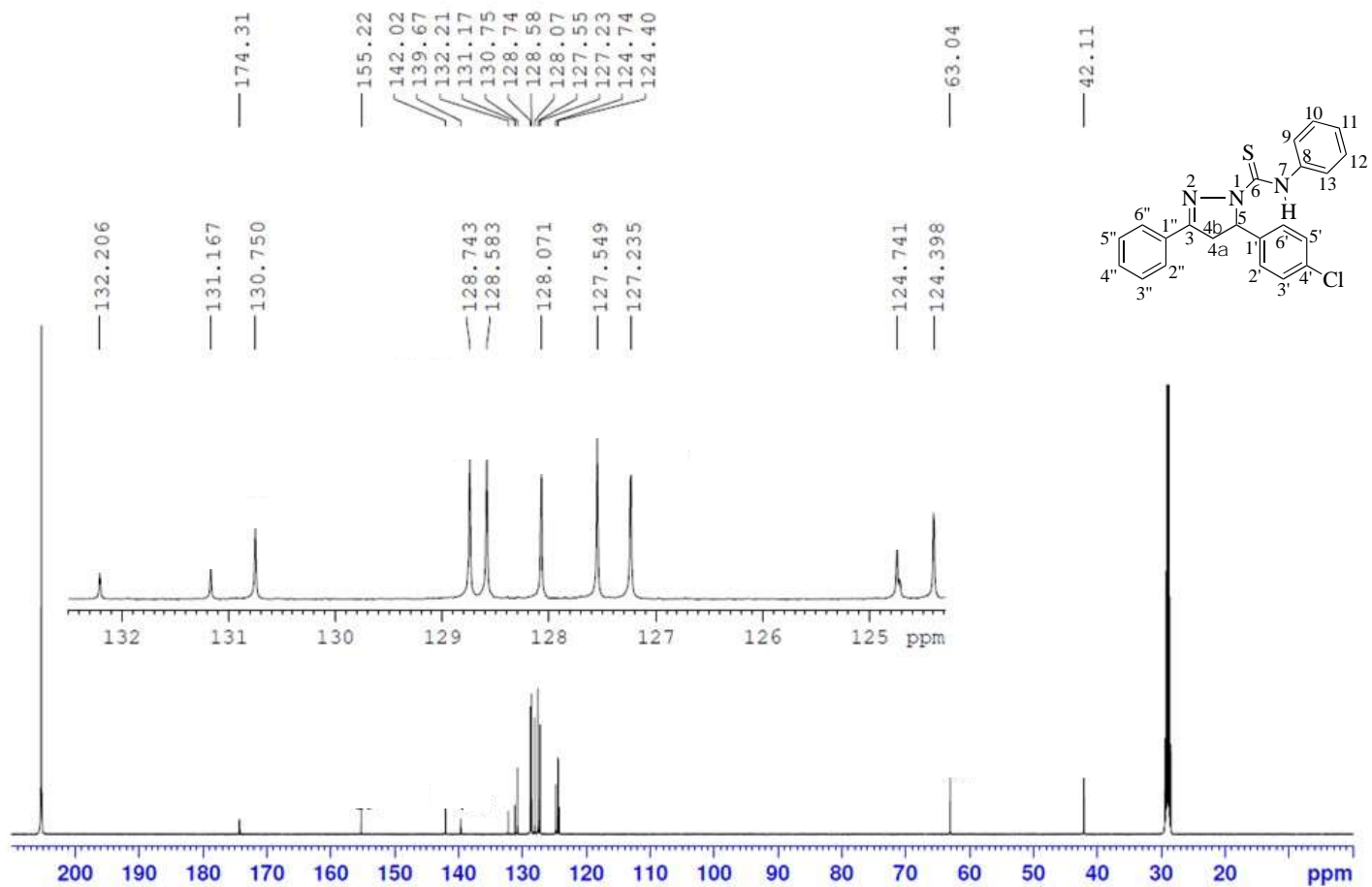
IR spectrum of compound 4c

5-(4-chlorophenyl)-N,3-diphenyl-4,5-dihydro-1H-pyrazole-1-carbothioamide_1H

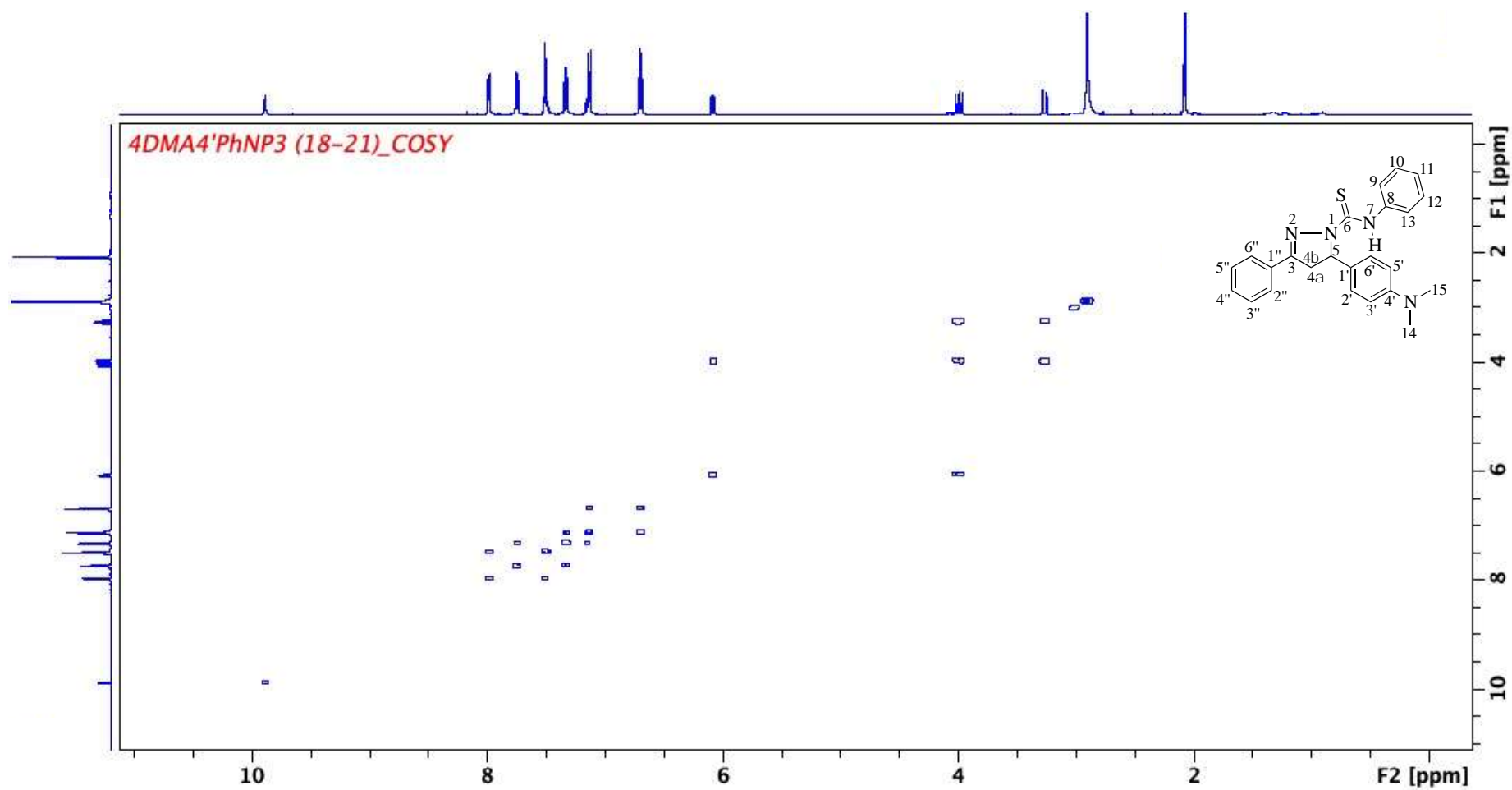


¹H NMR spectrum of compound **4c**

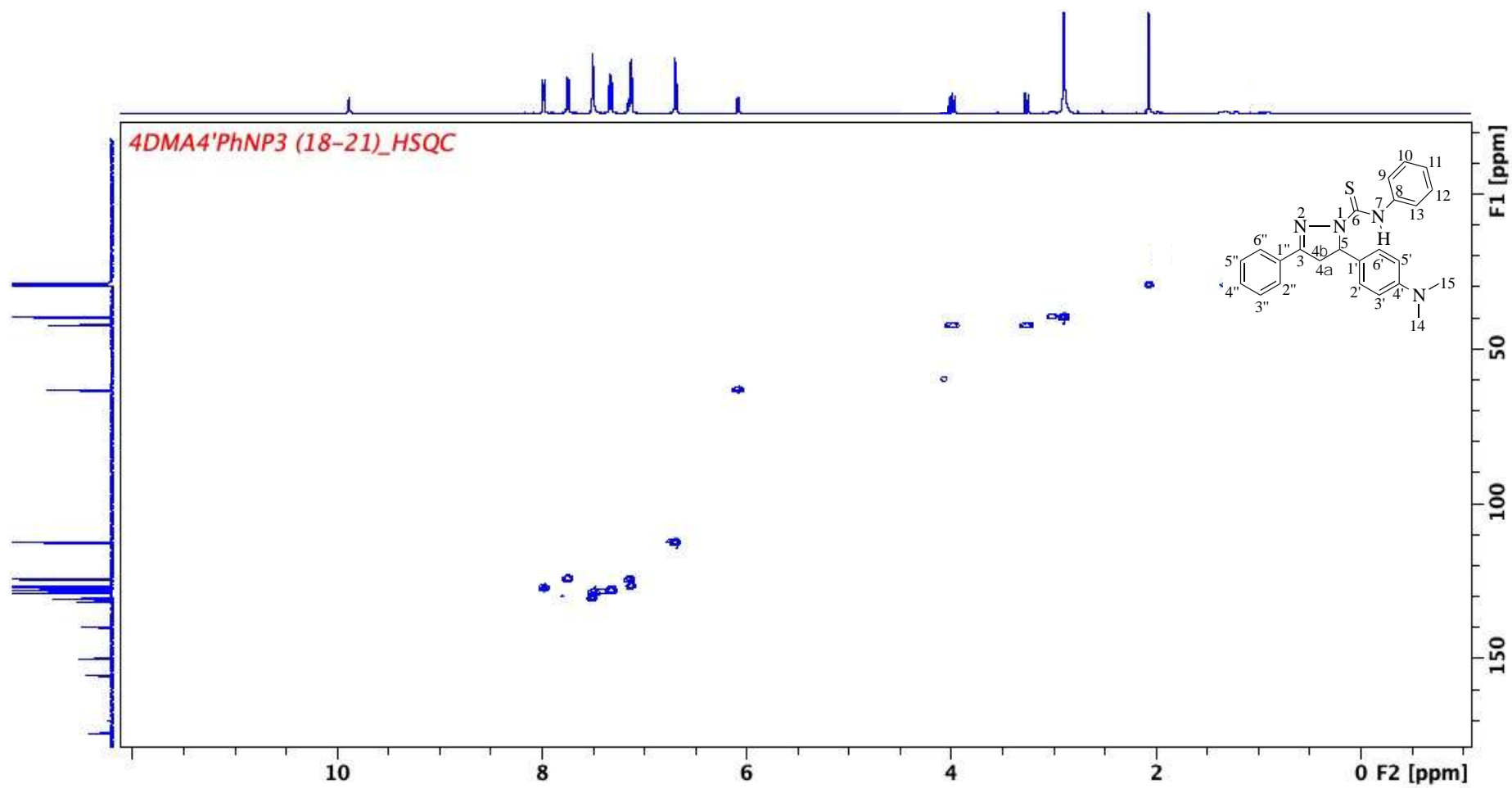
5-(4-chlorophenyl)-N,3-diphenyl-4,5-dihydro-1H-pyrazole-1-carbothioamide_13C



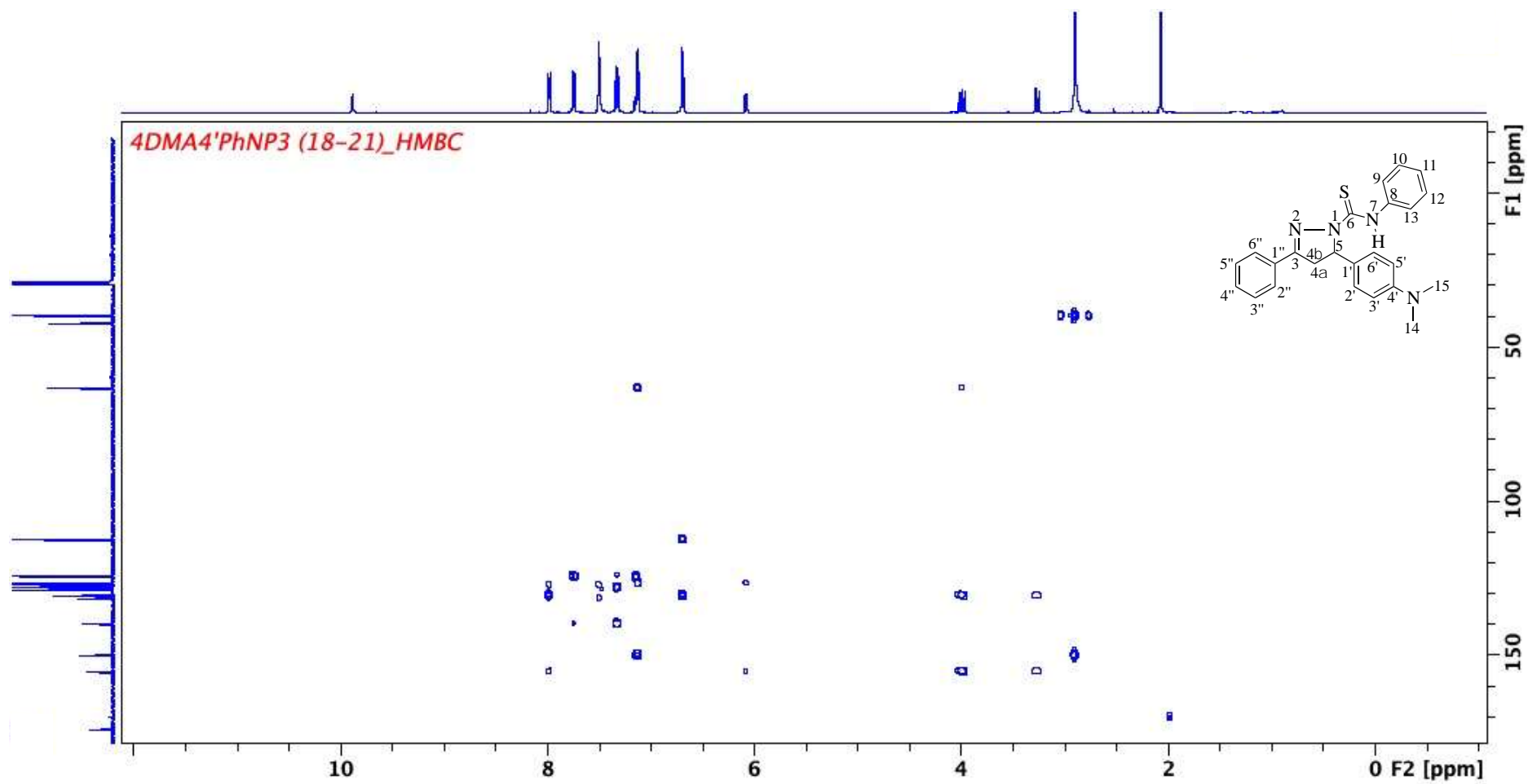
¹³C NMR spectrum of compound 4c



^1H - ^1H COSY NMR spectrum of compound 4d



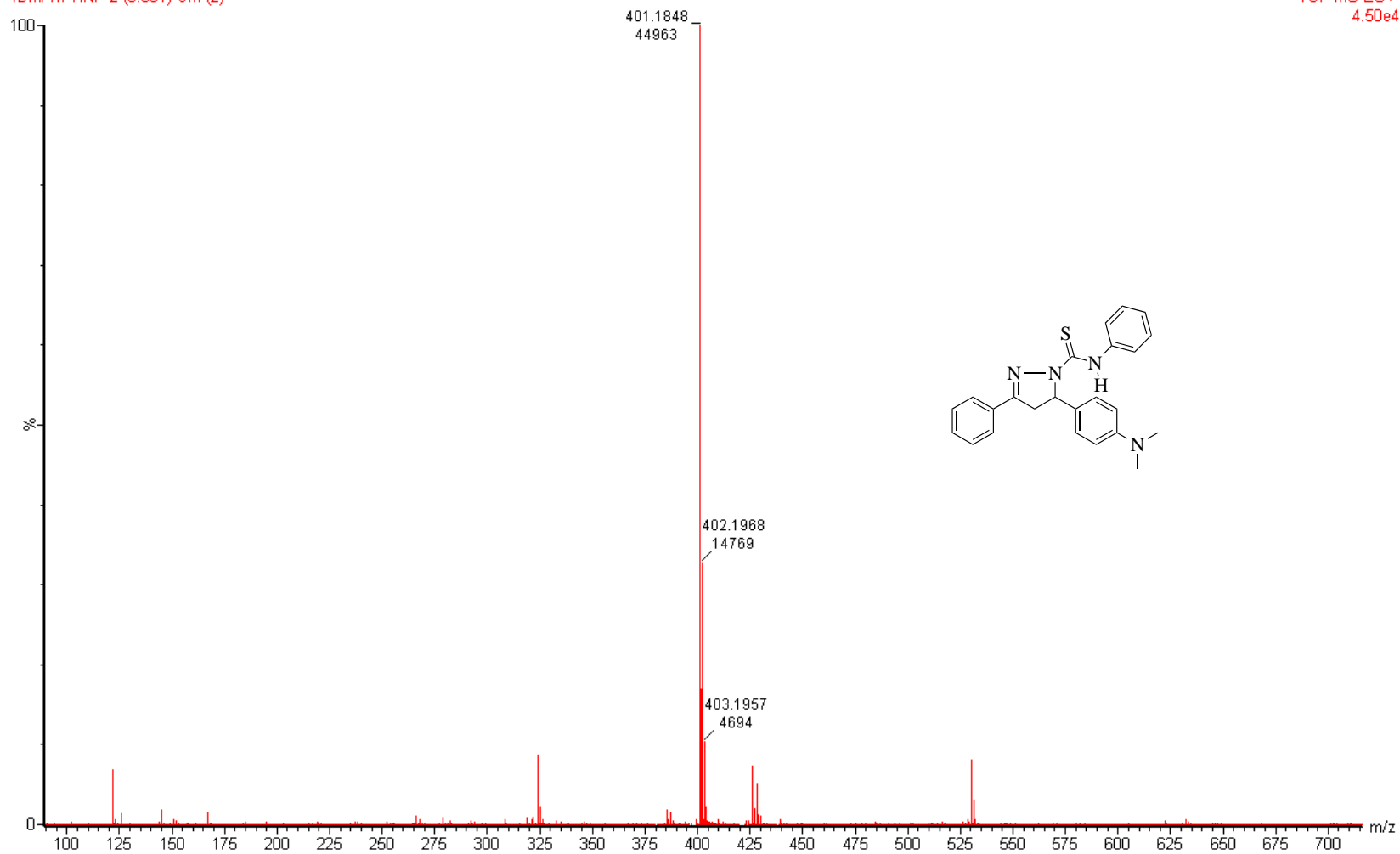
^1H - ^{13}C HSQC NMR spectrum of compound 4d



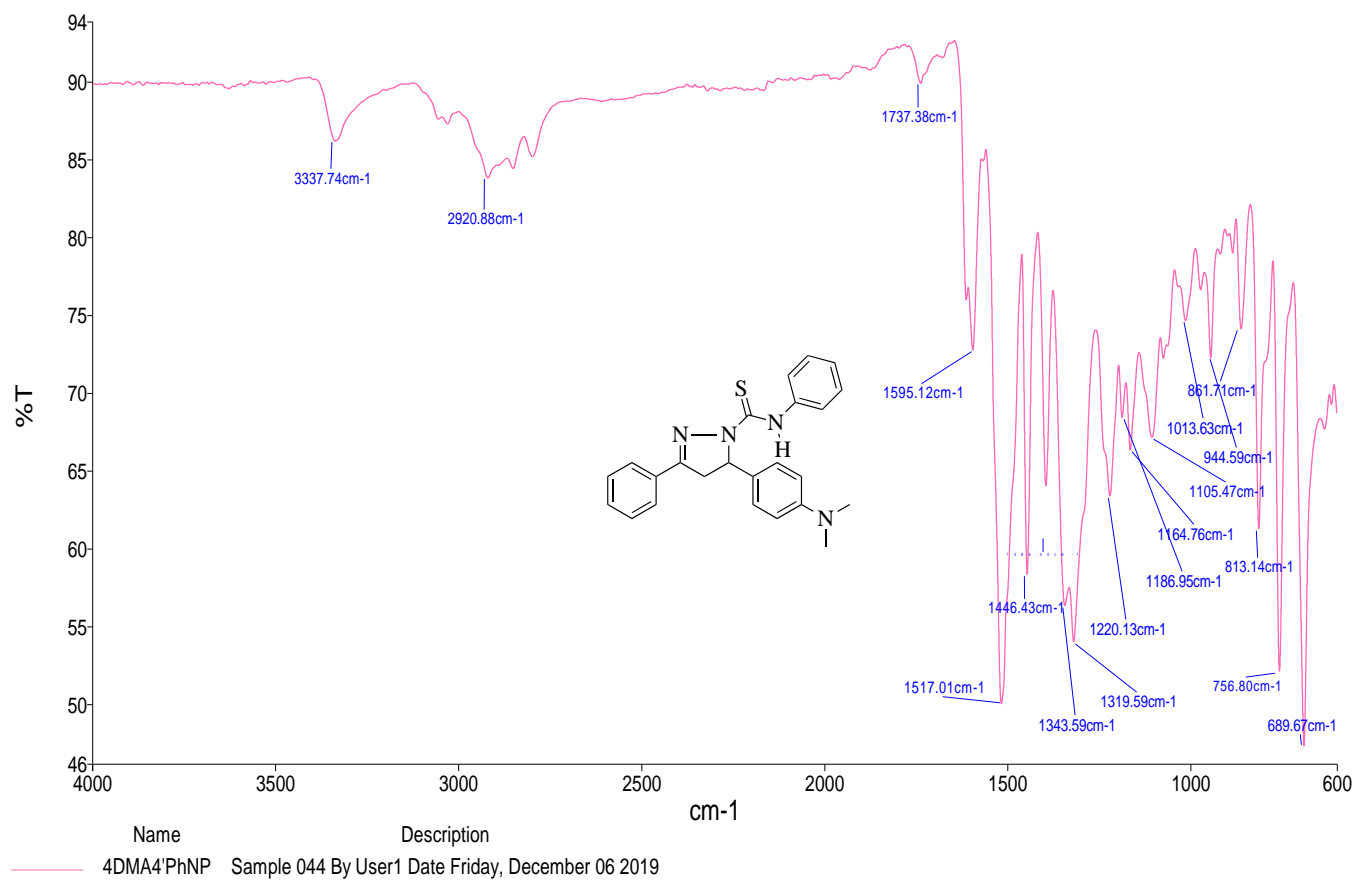
^1H - ^{13}C HMBC NMR spectrum of compound 4d

4DMA4PHNP 2 (0.051) Cm (2)

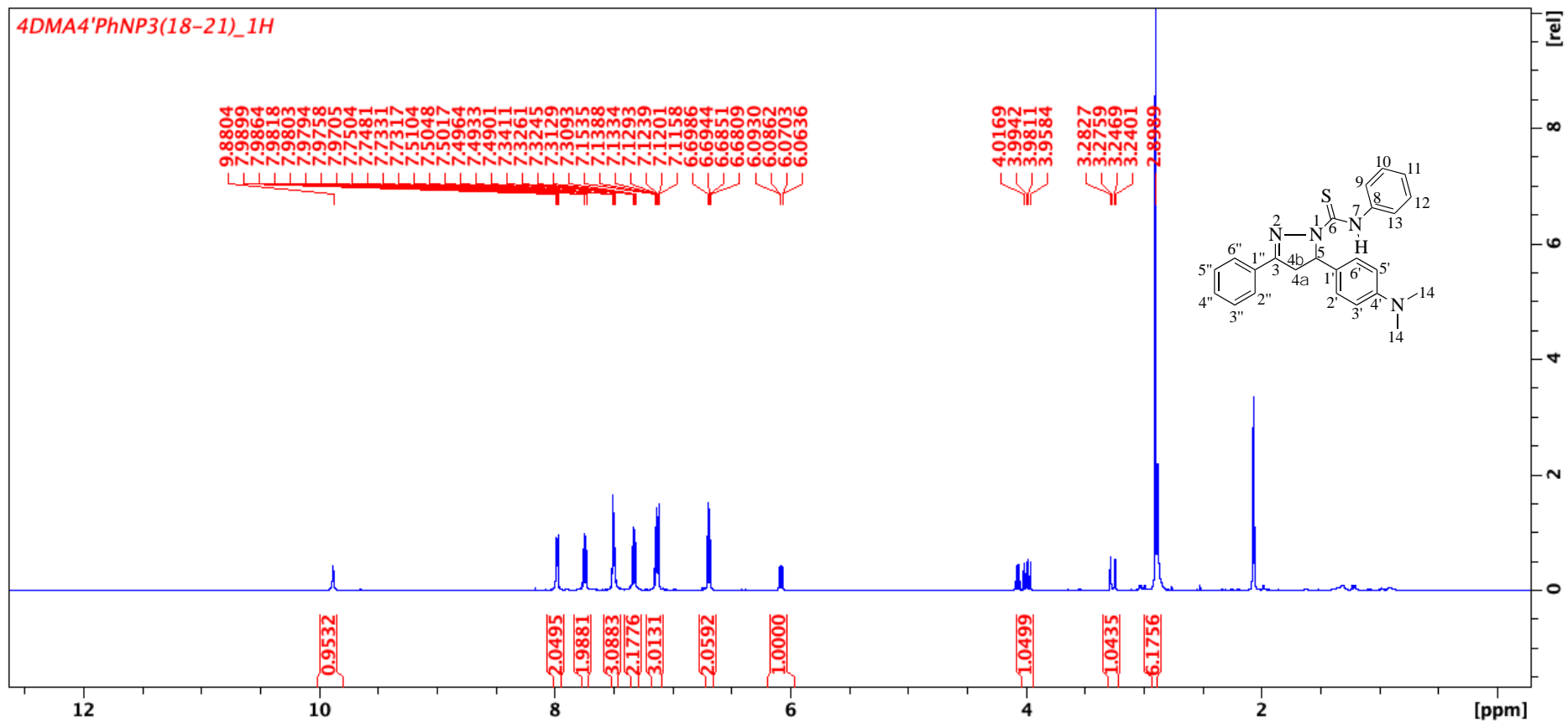
TOF MS ES+
4.50e4



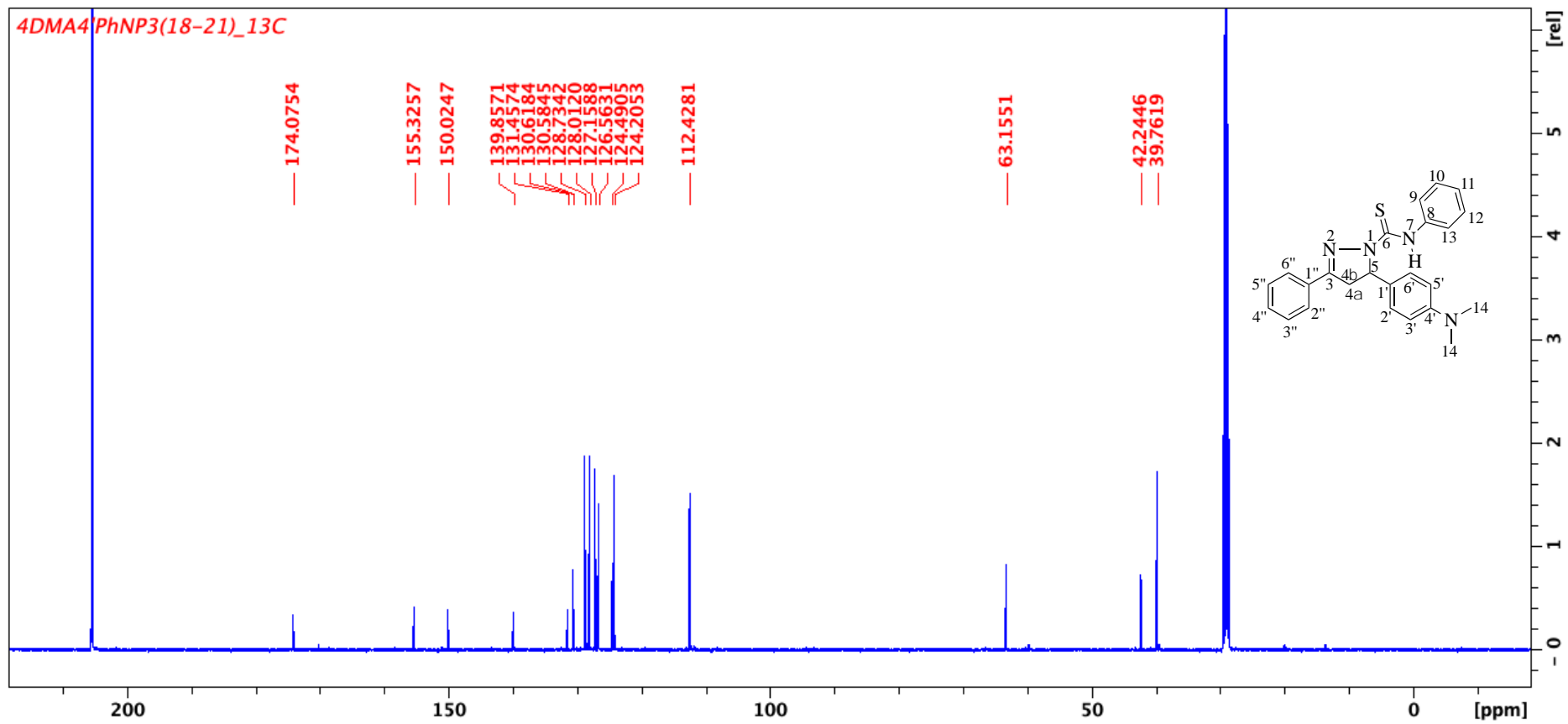
HRMS spectrum of compound **4d**



IR spectrum of compound **4d**



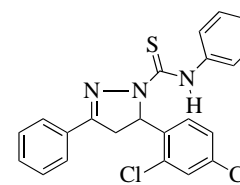
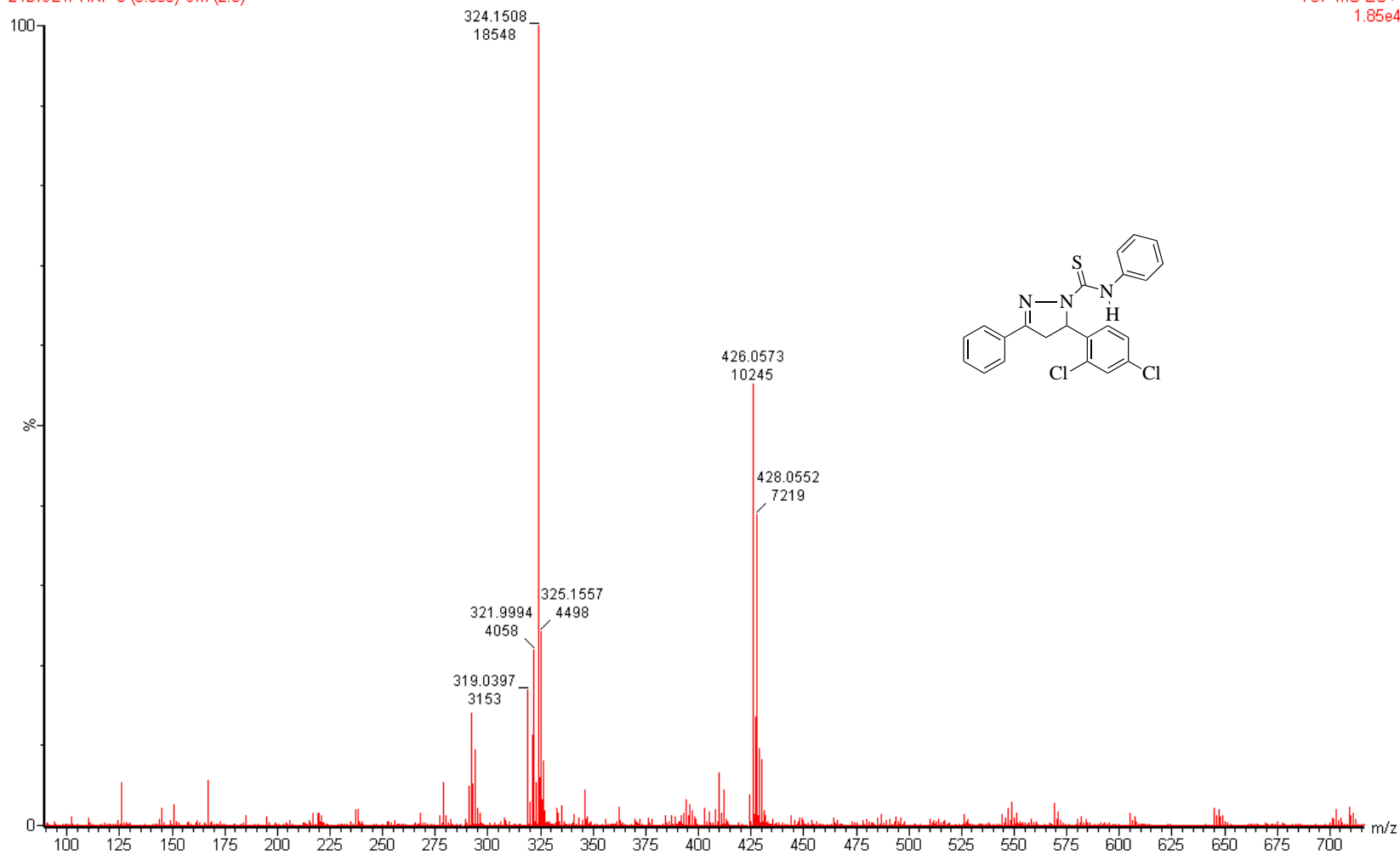
^1H NMR spectrum of compound **4d**



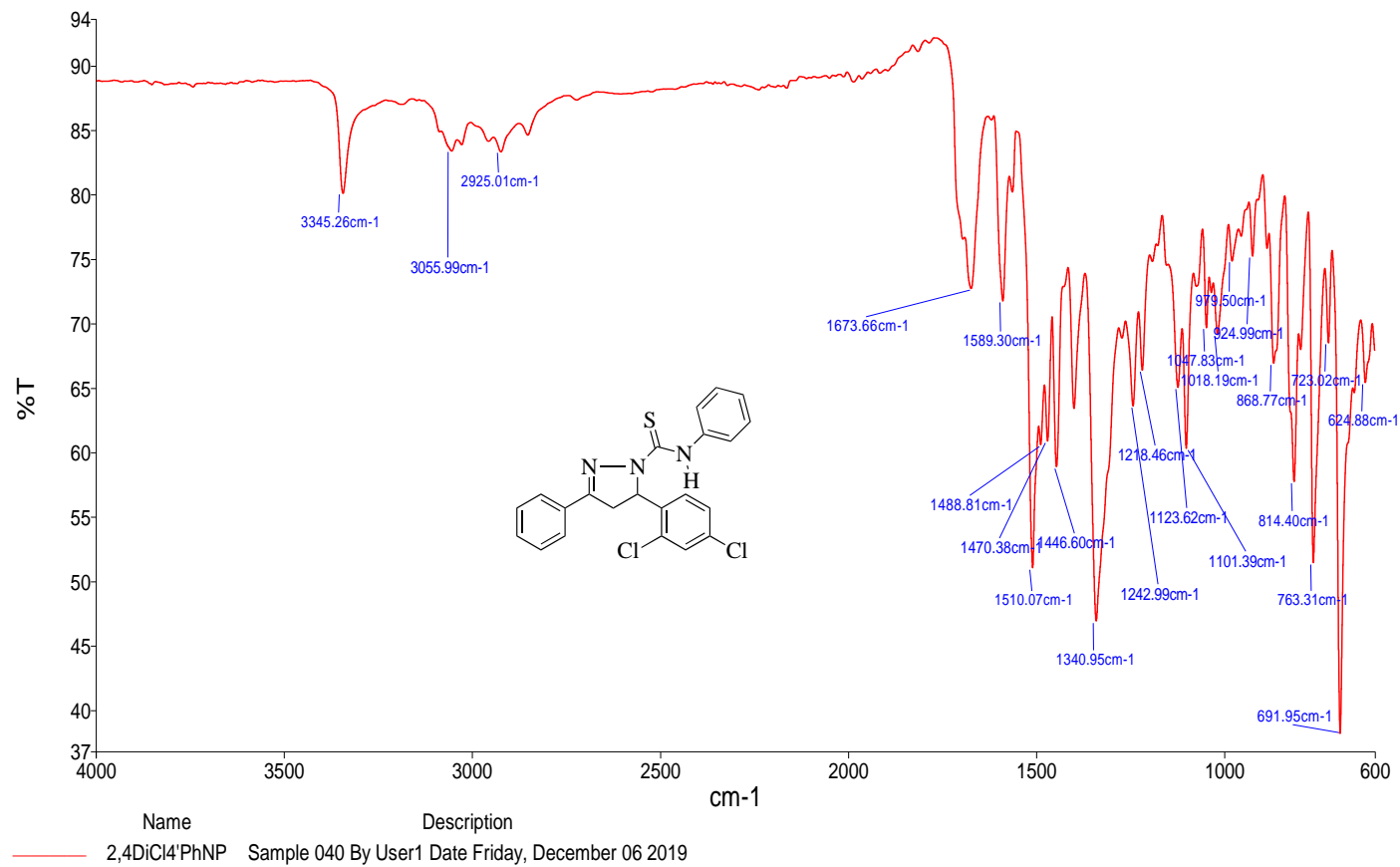
^{13}C NMR spectrum of compound **4d**

24DICL4PHNP 3 (0.068) Cm (2:3)

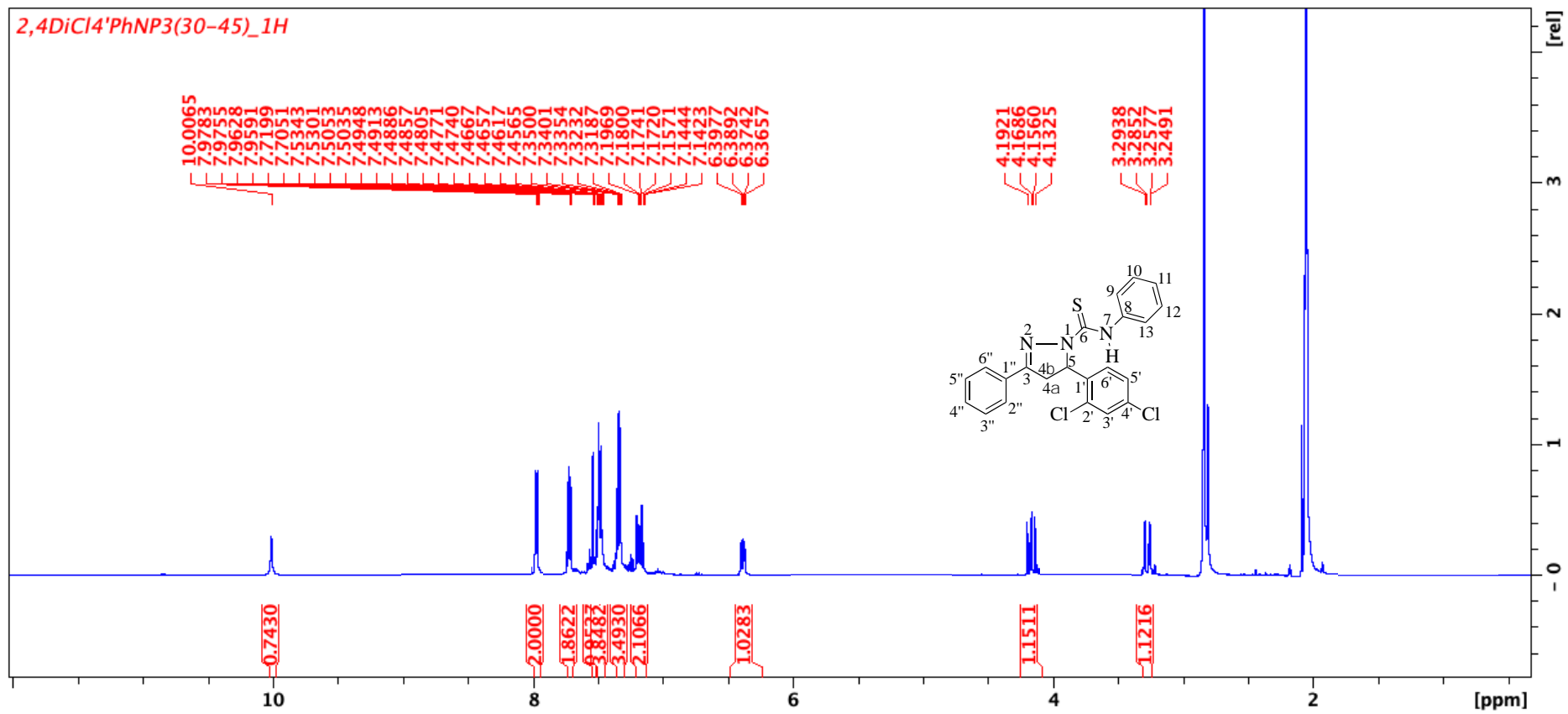
TOF MS ES+
1.85e4



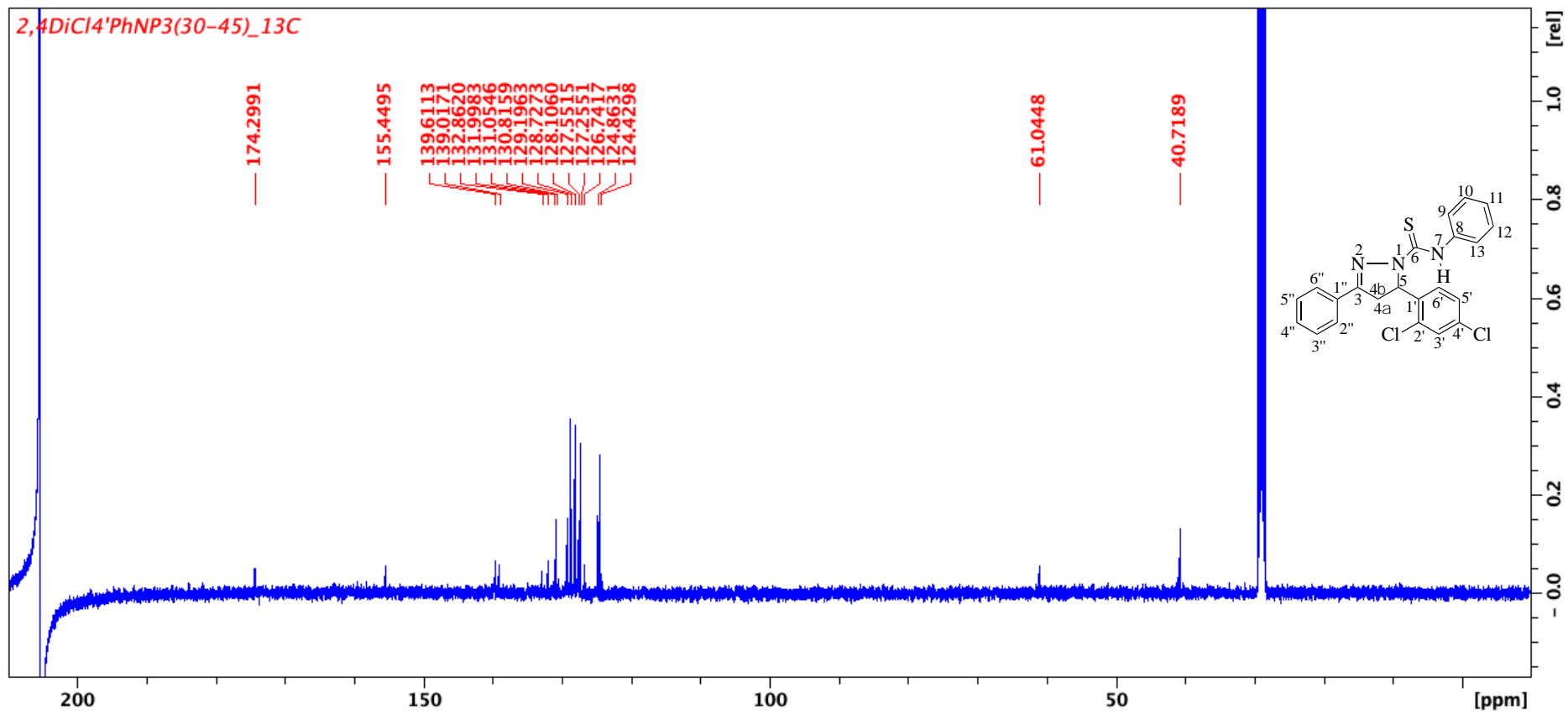
HRMS spectrum of compound 4e



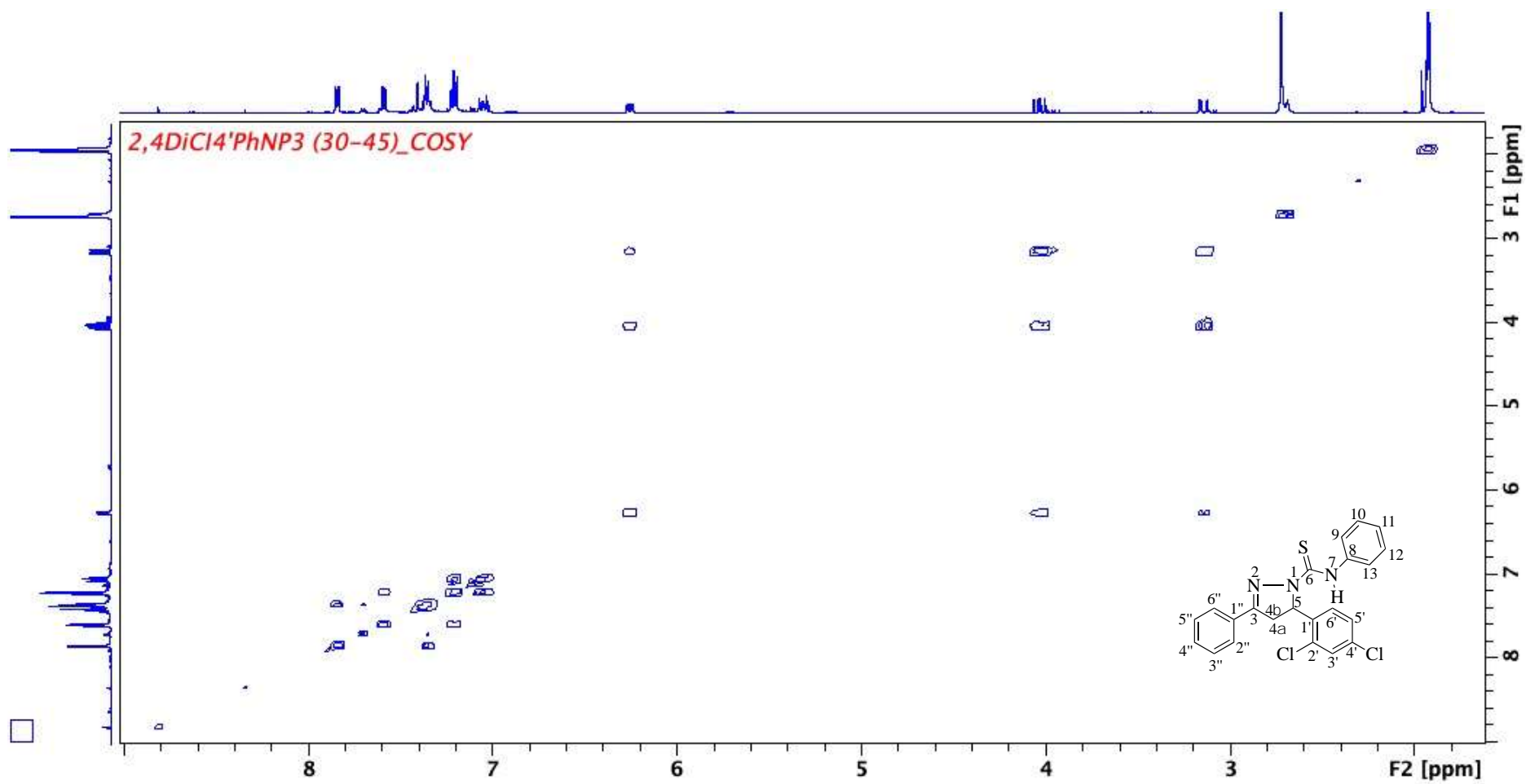
IR spectrum of compound 4e



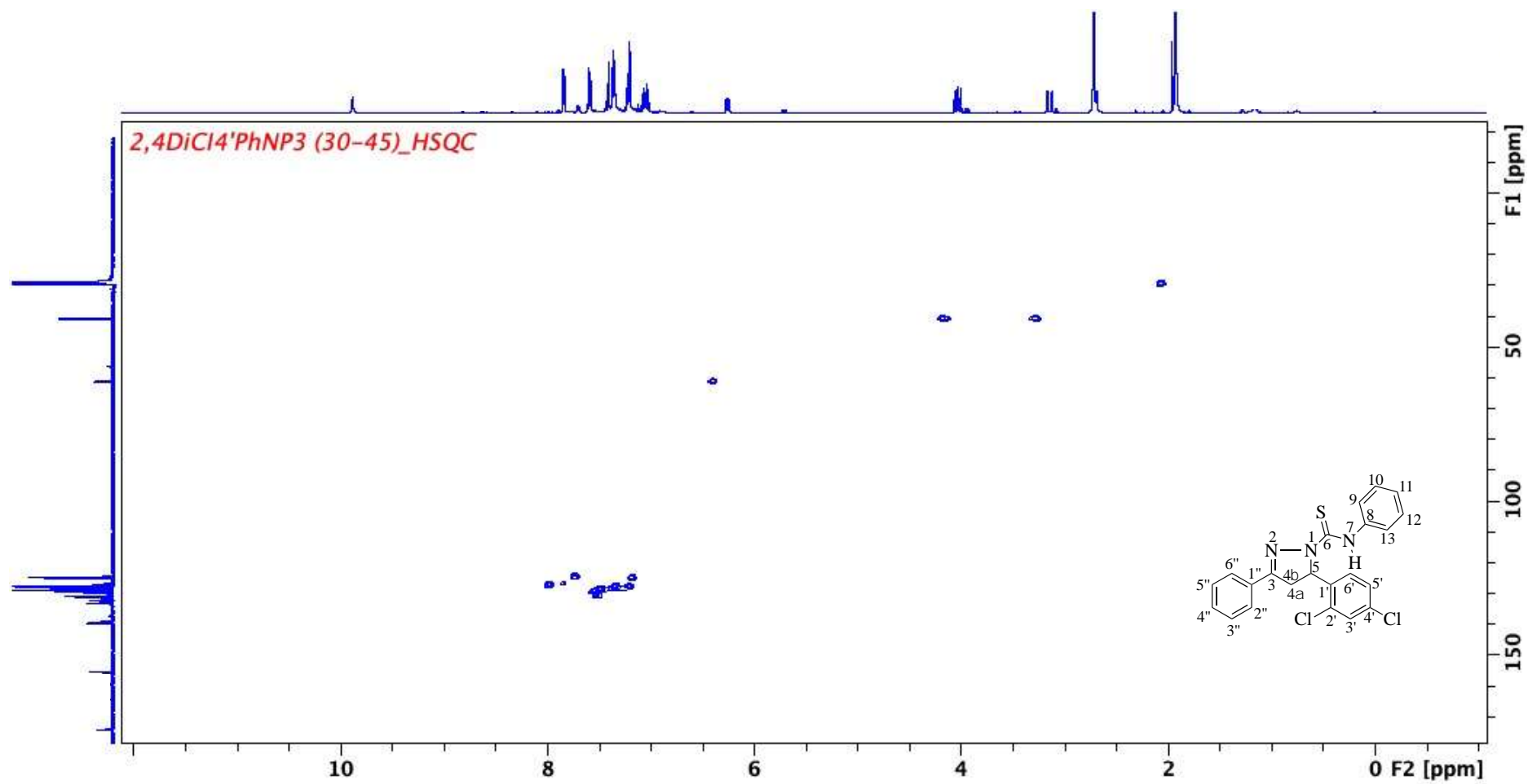
^1H NMR spectrum of compound **4e**



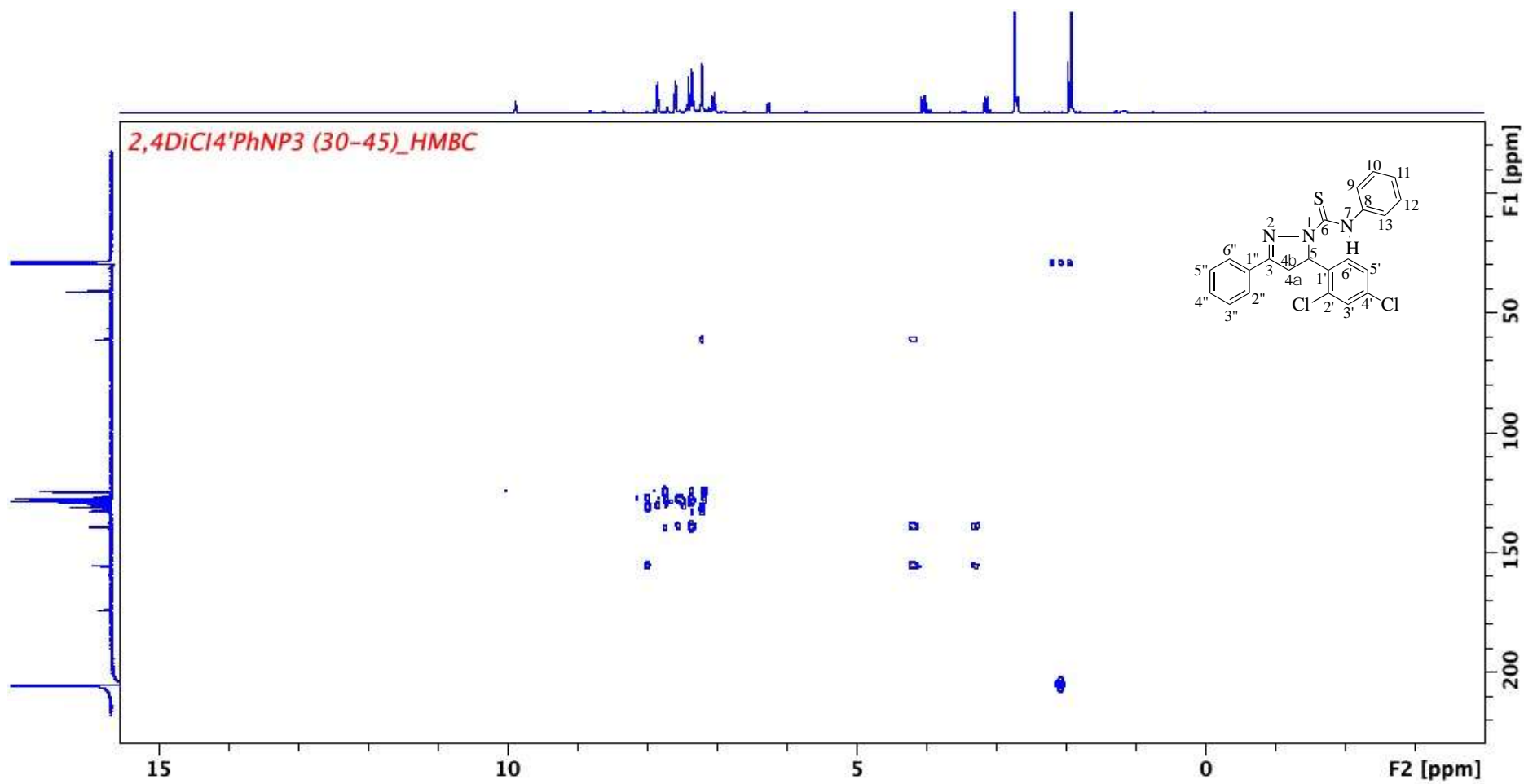
^{13}C NMR spectrum of compound 4e



^1H - ^1H COSY NMR spectrum of compound 4e



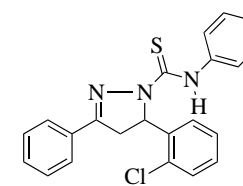
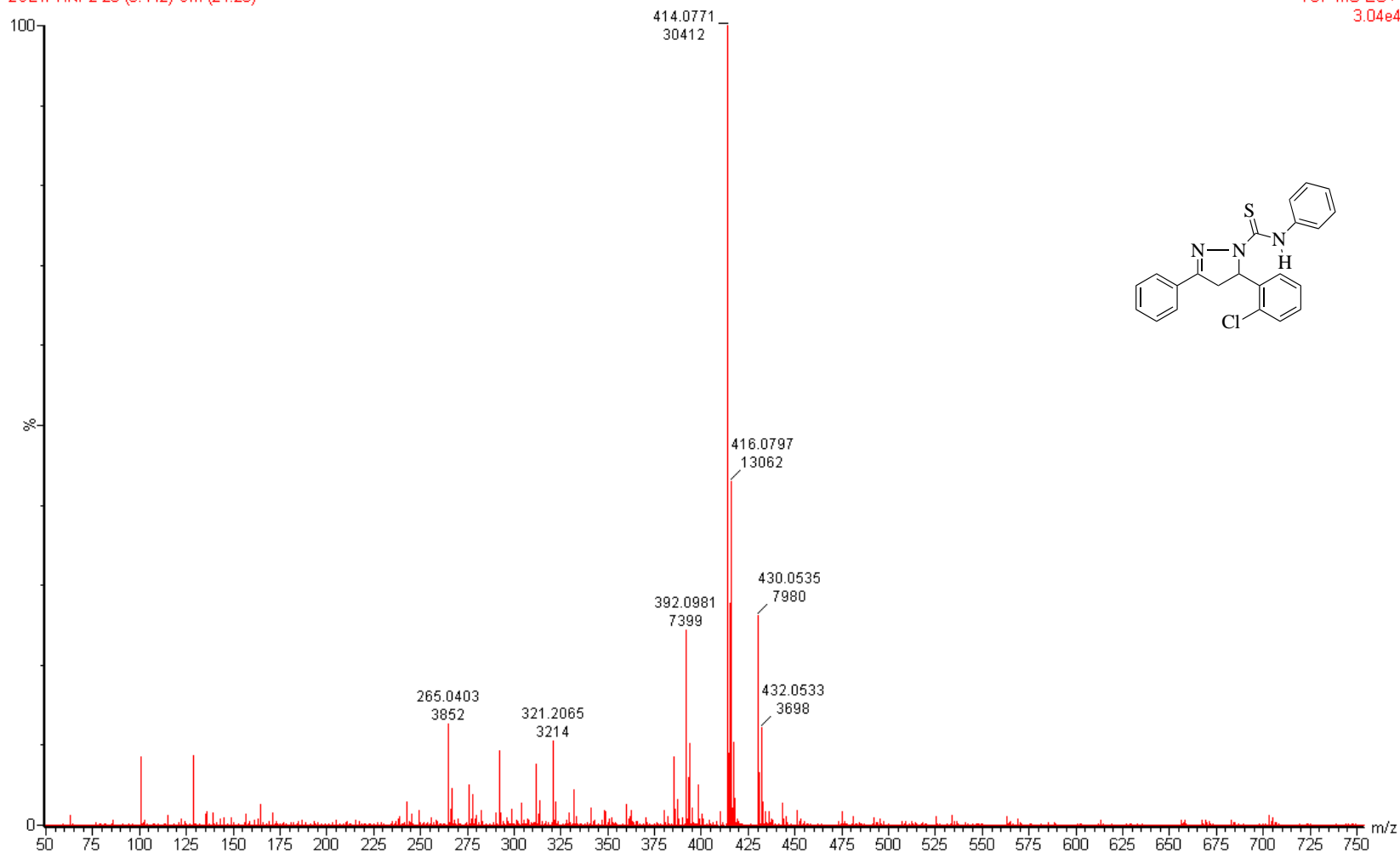
^1H - ^{13}C HSQC NMR spectrum of compound 4e



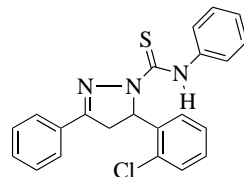
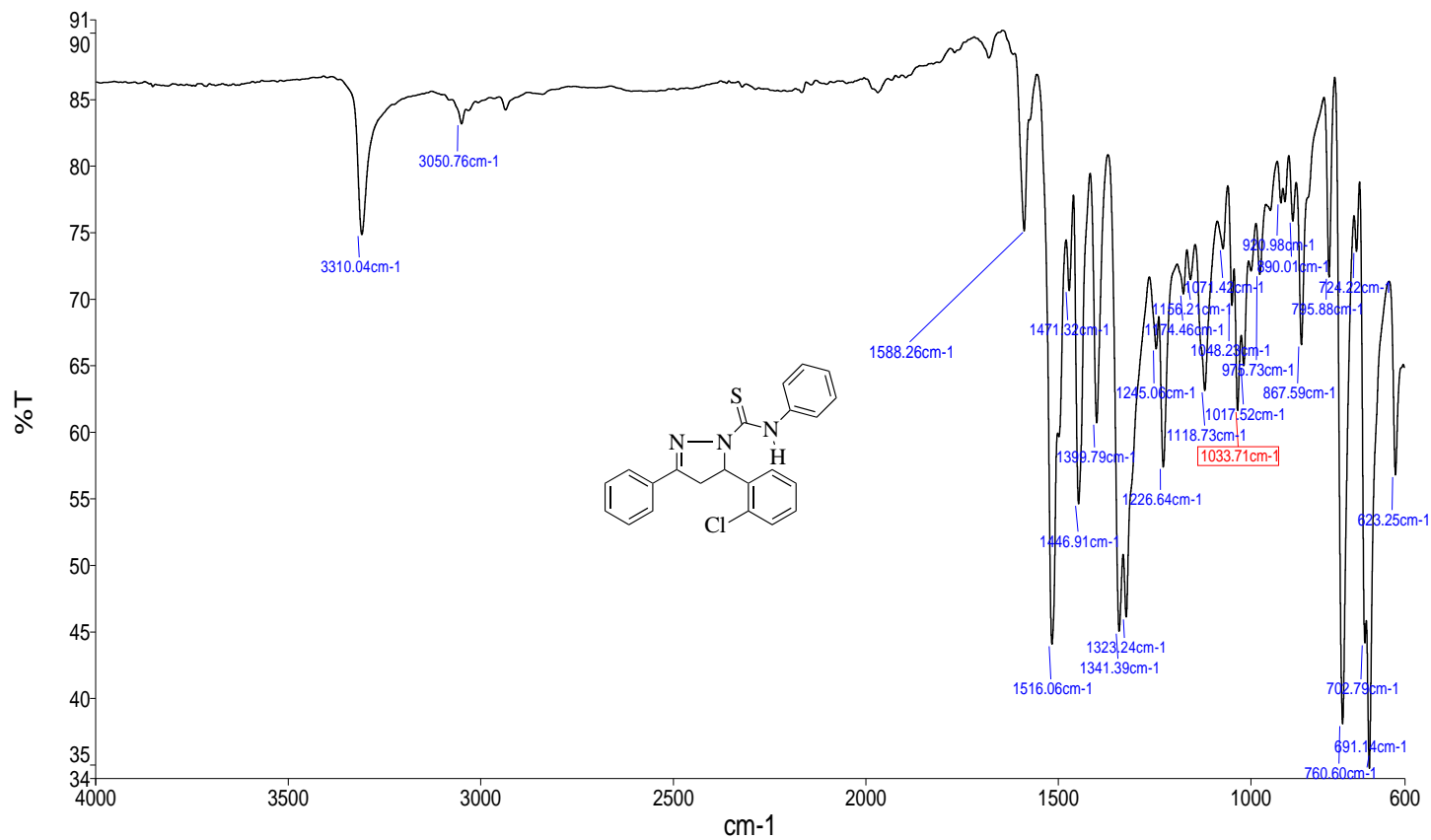
^1H - ^{13}C HMBC NMR spectrum of compound 4e

2CL4PHNP2 25 (0.442) Cm (24:25)

TOF MS ES+
3.04e4

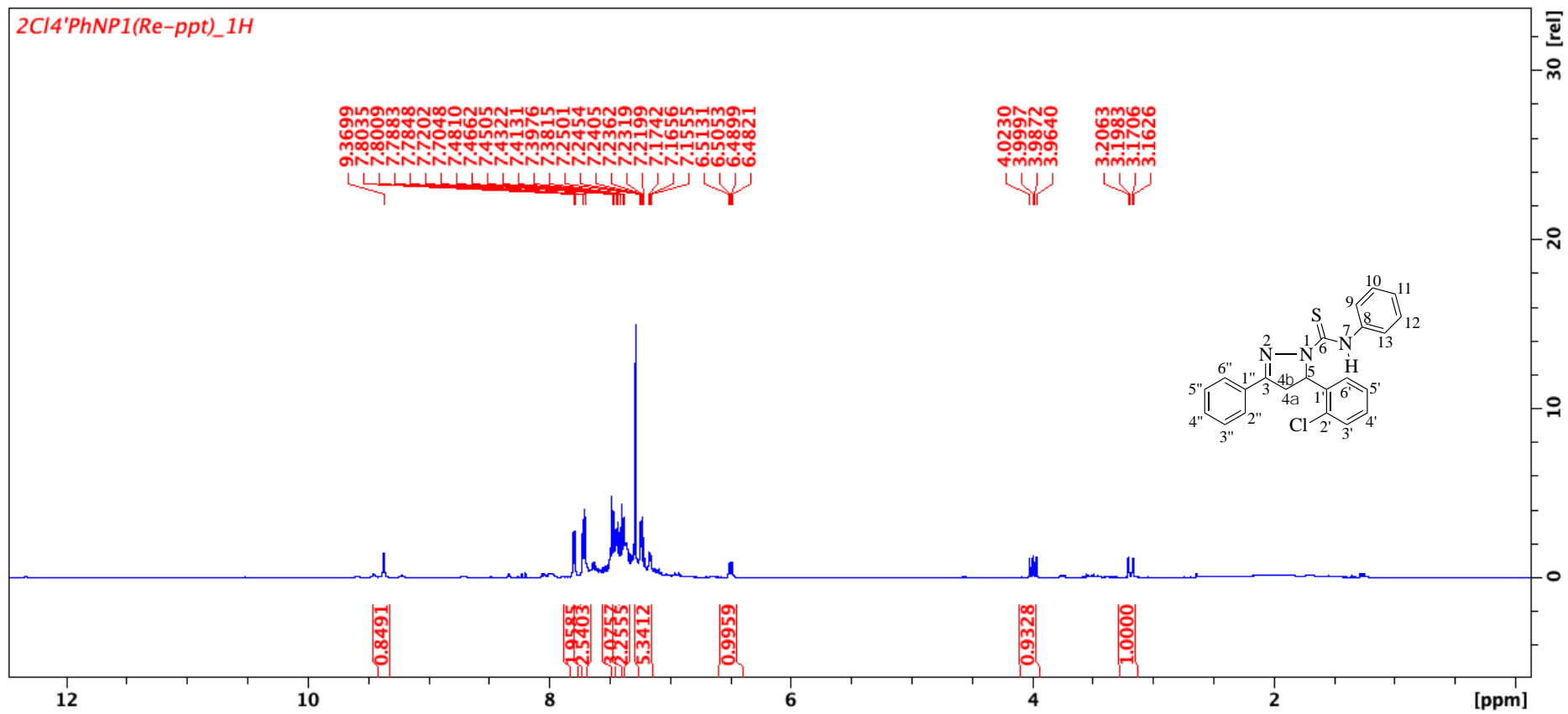


HRMS spectrum of compound 4f

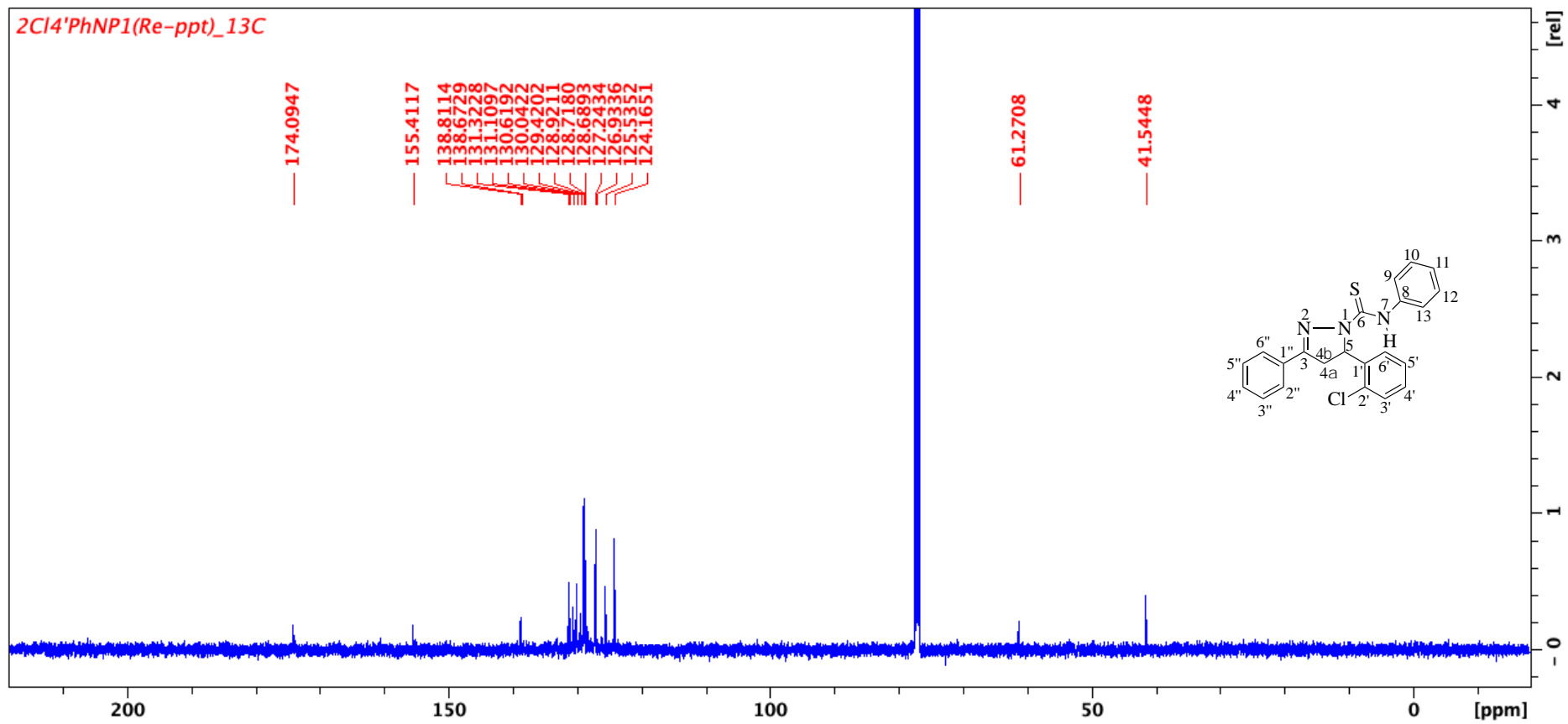


Name: 2Cl4phNP
 Description: Sample 039 By User1 Date Friday, December 06 2019

IR spectrum of compound **4f**



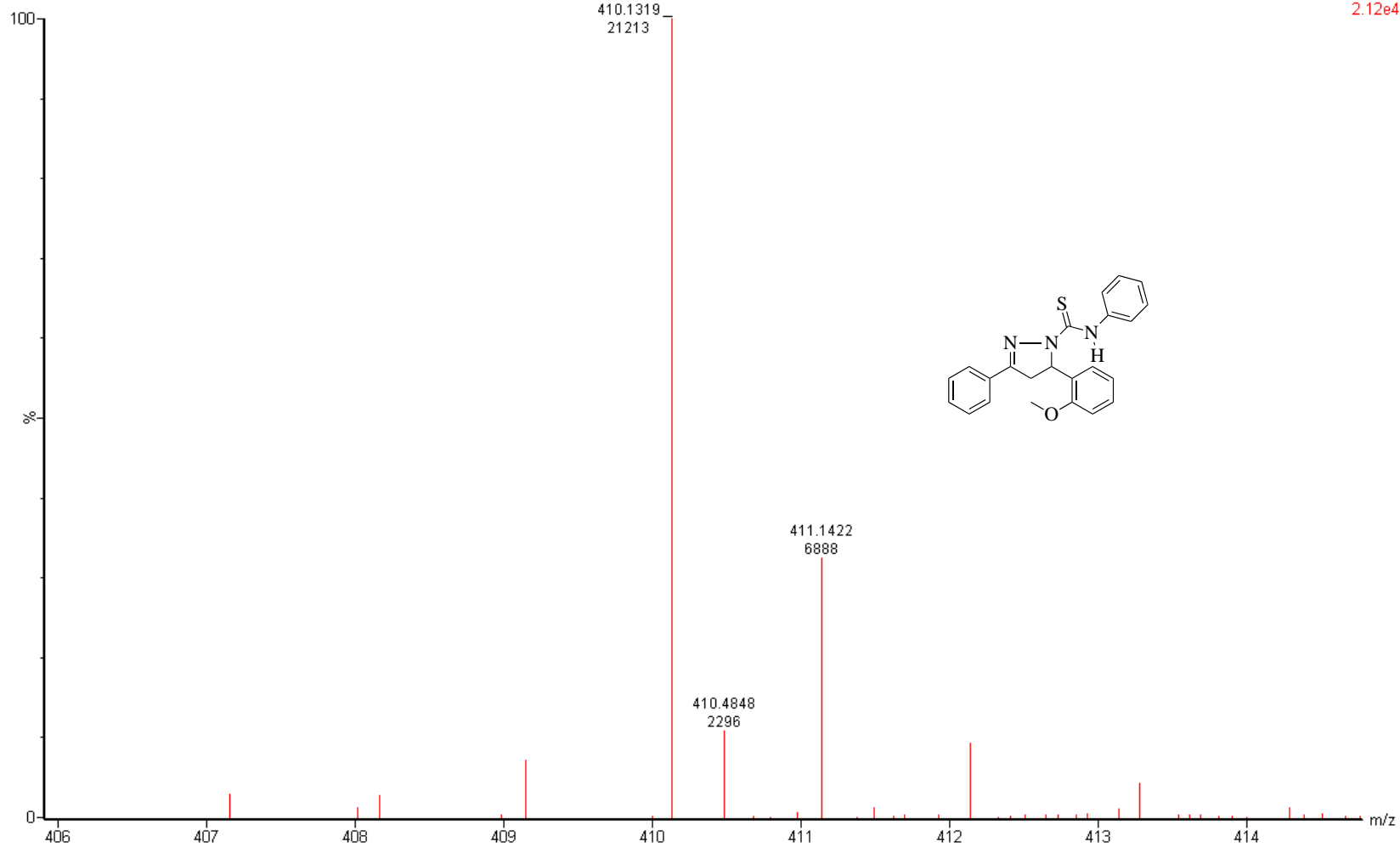
^1H NMR spectrum of compound **4f**



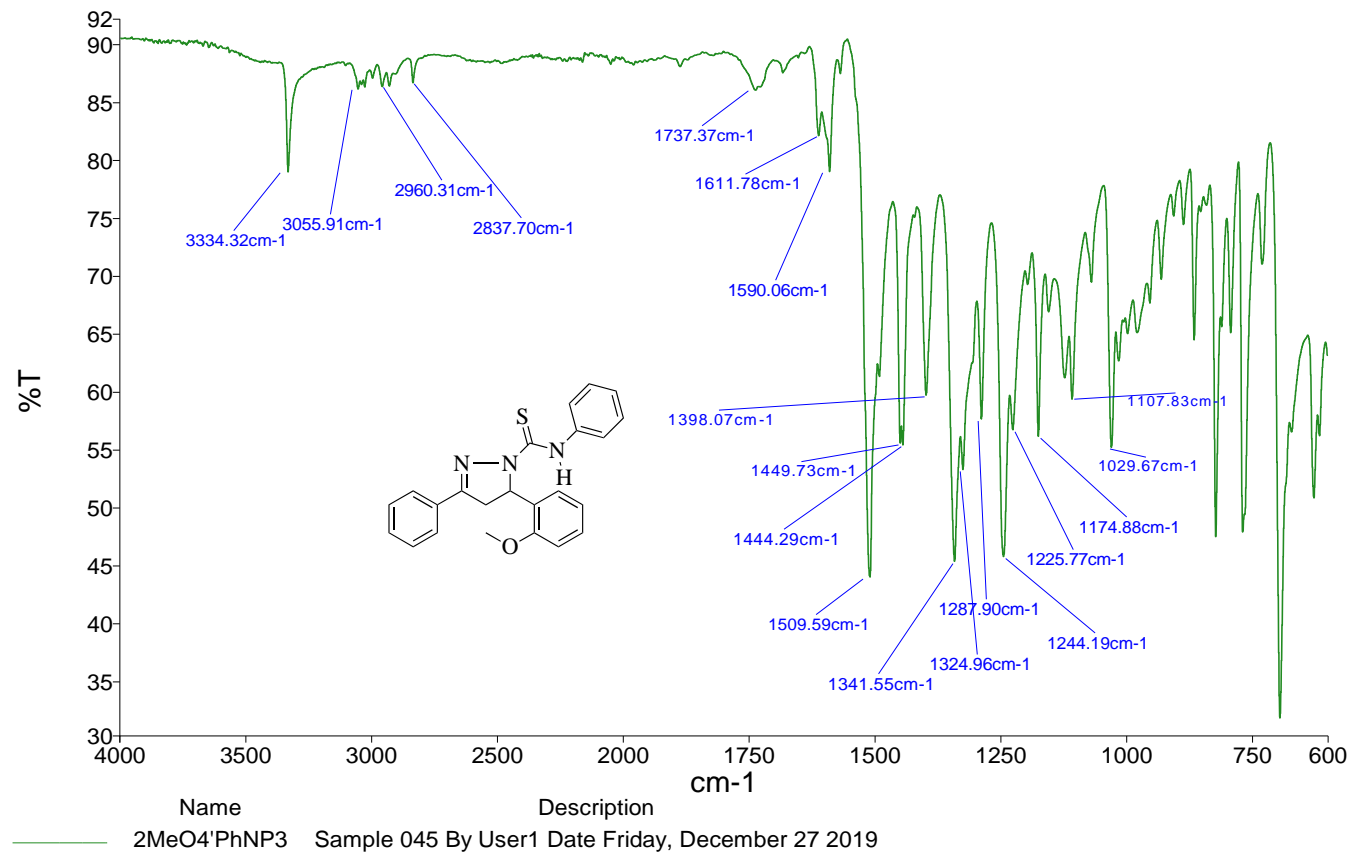
^{13}C NMR spectrum of compound **4f**

2MEO4PHNP 25 (0.442) Cm (25)

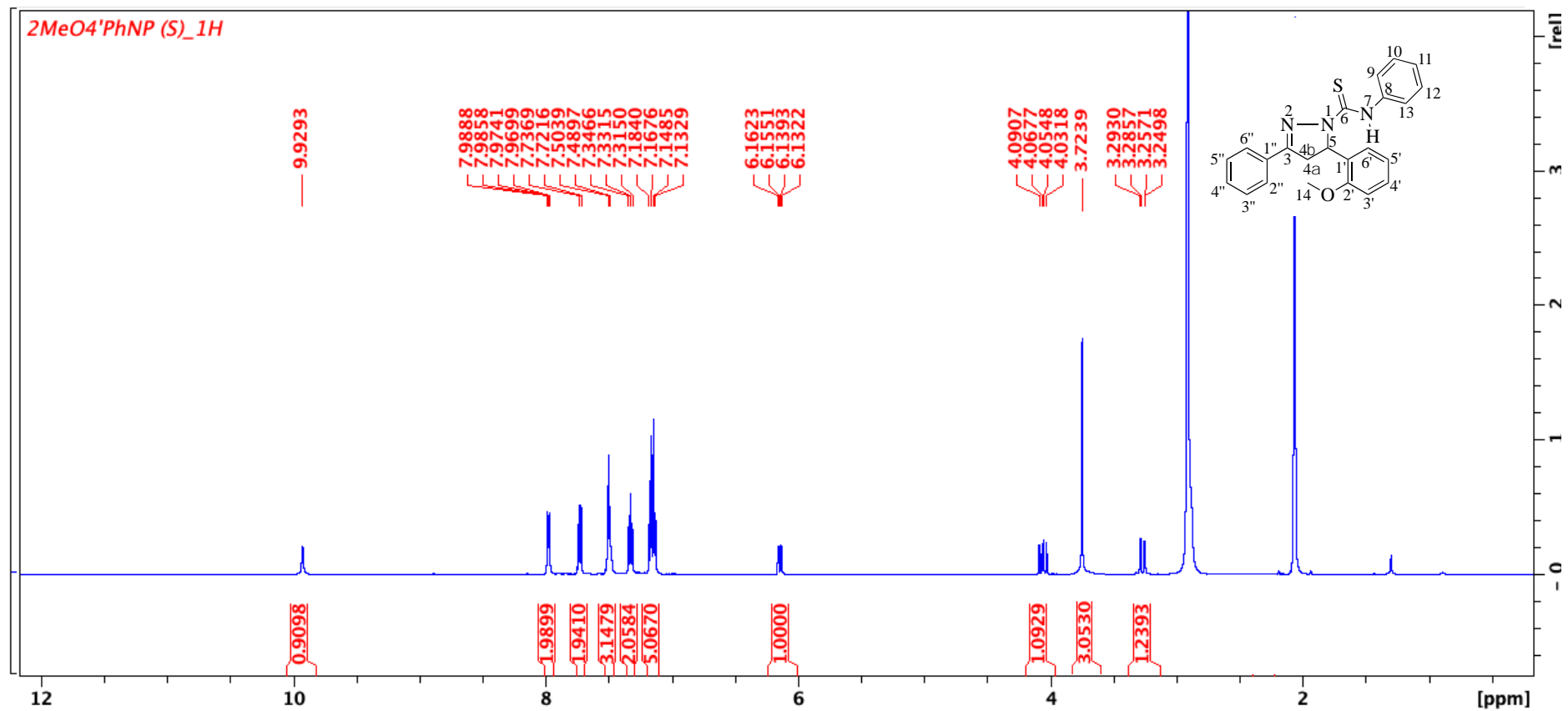
TOF MS ES+
2.12e4



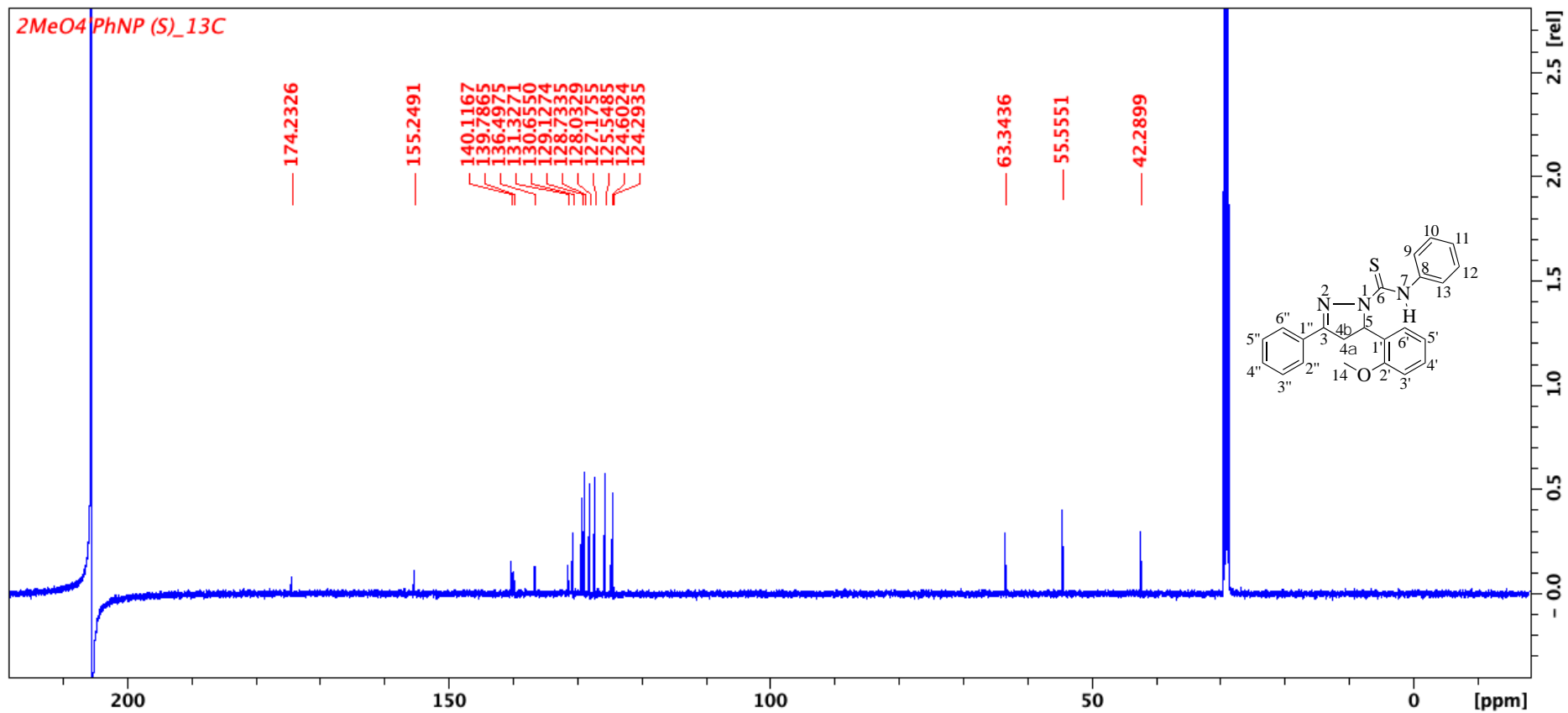
HRMS spectrum of compound **4g**



IR spectrum of compound **4g**



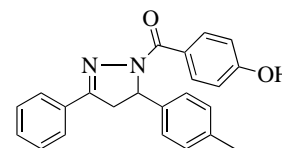
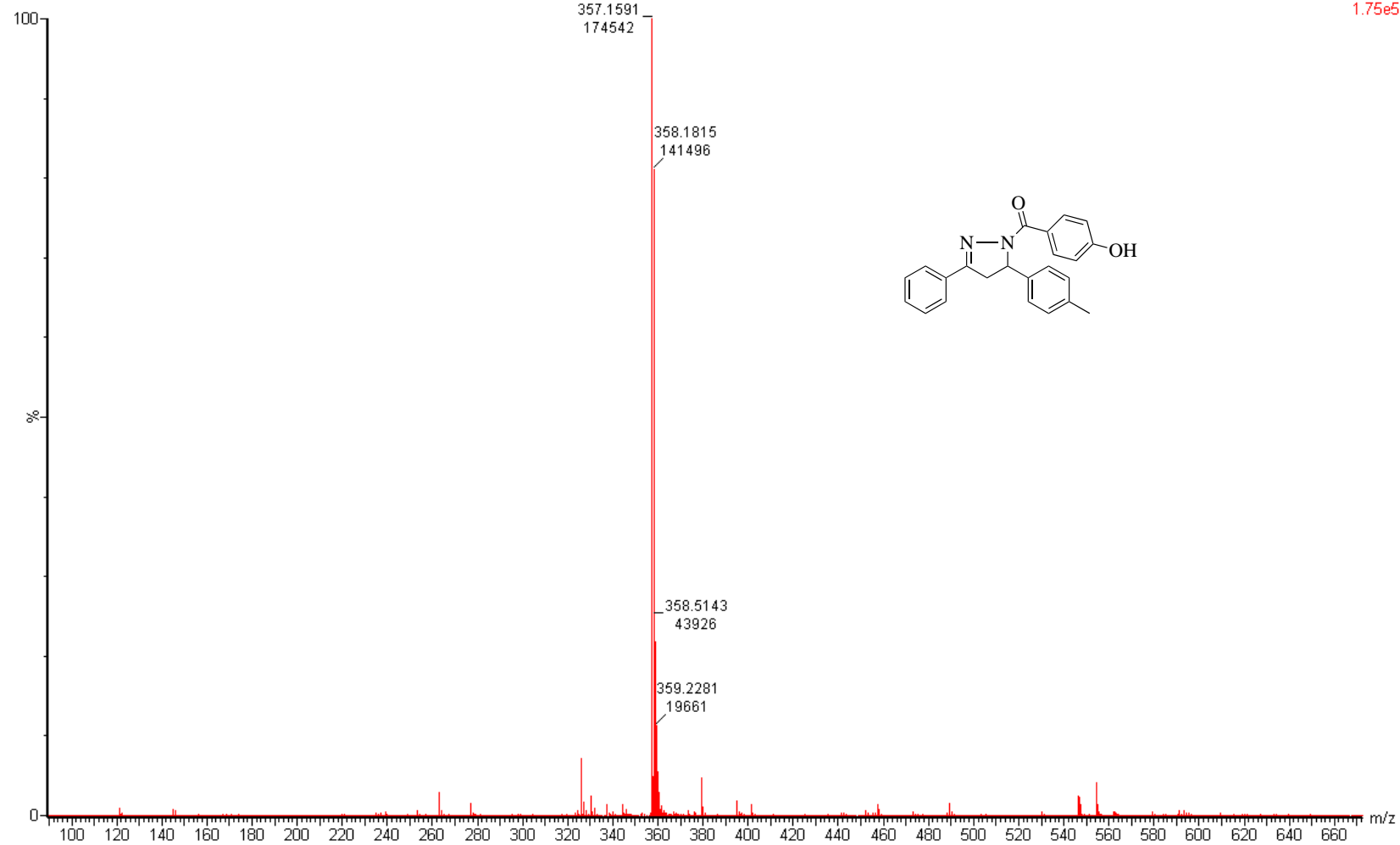
^1H NMR spectrum of compound 4g



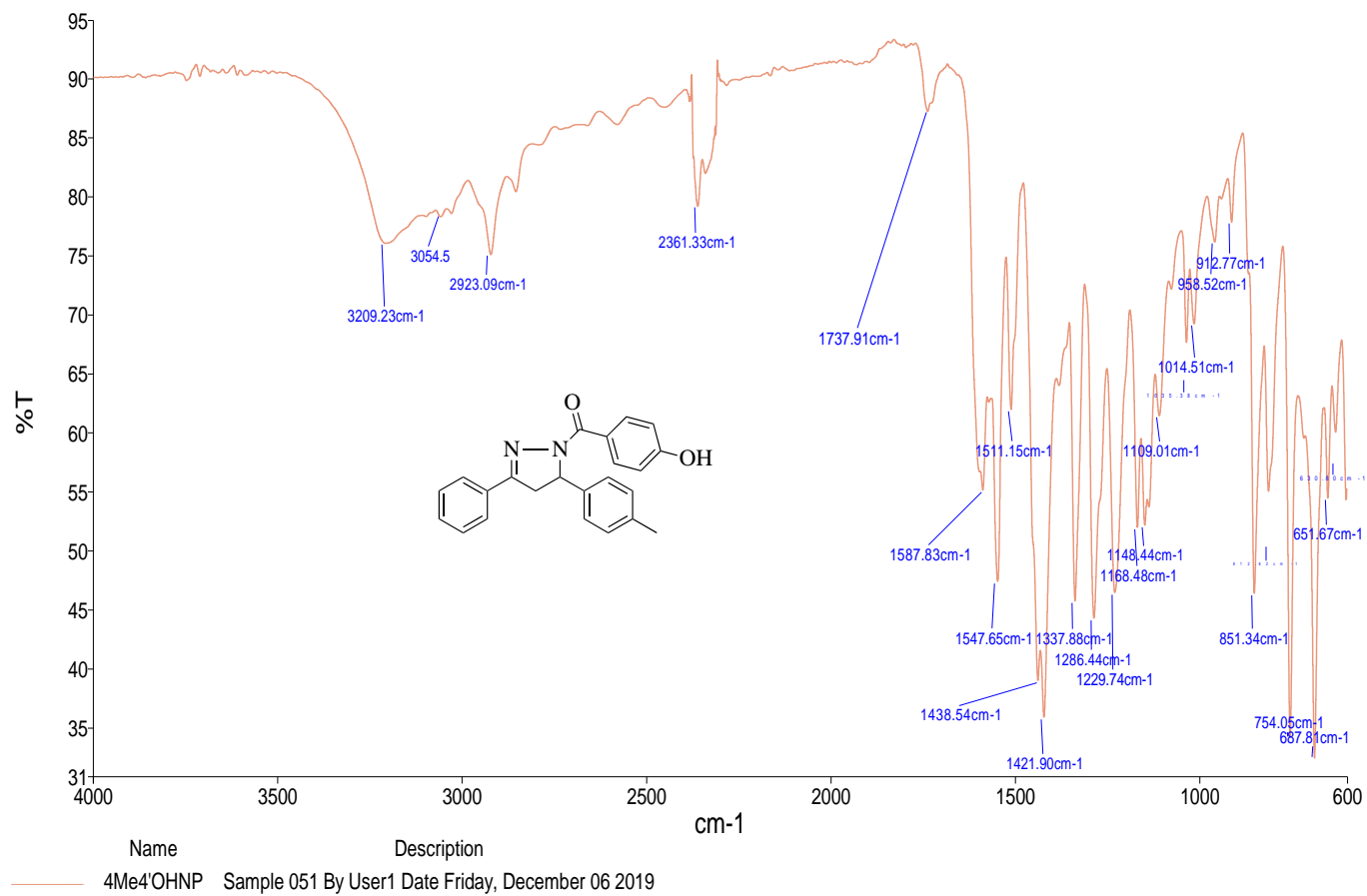
^{13}C NMR spectrum of compound **4g**

4ME4OHNP 2 (0.051) Cm (2:3)

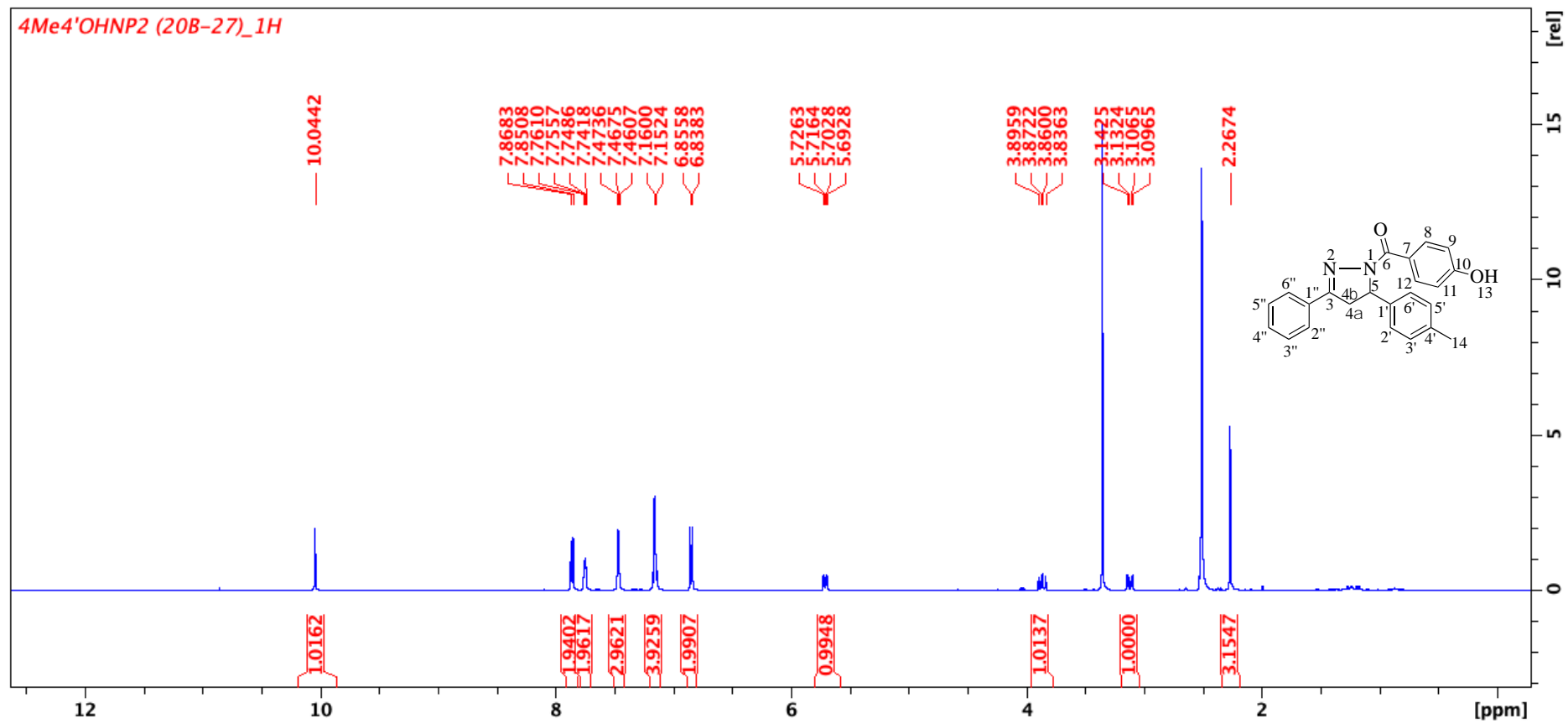
TOF MS ES+
1.75e5



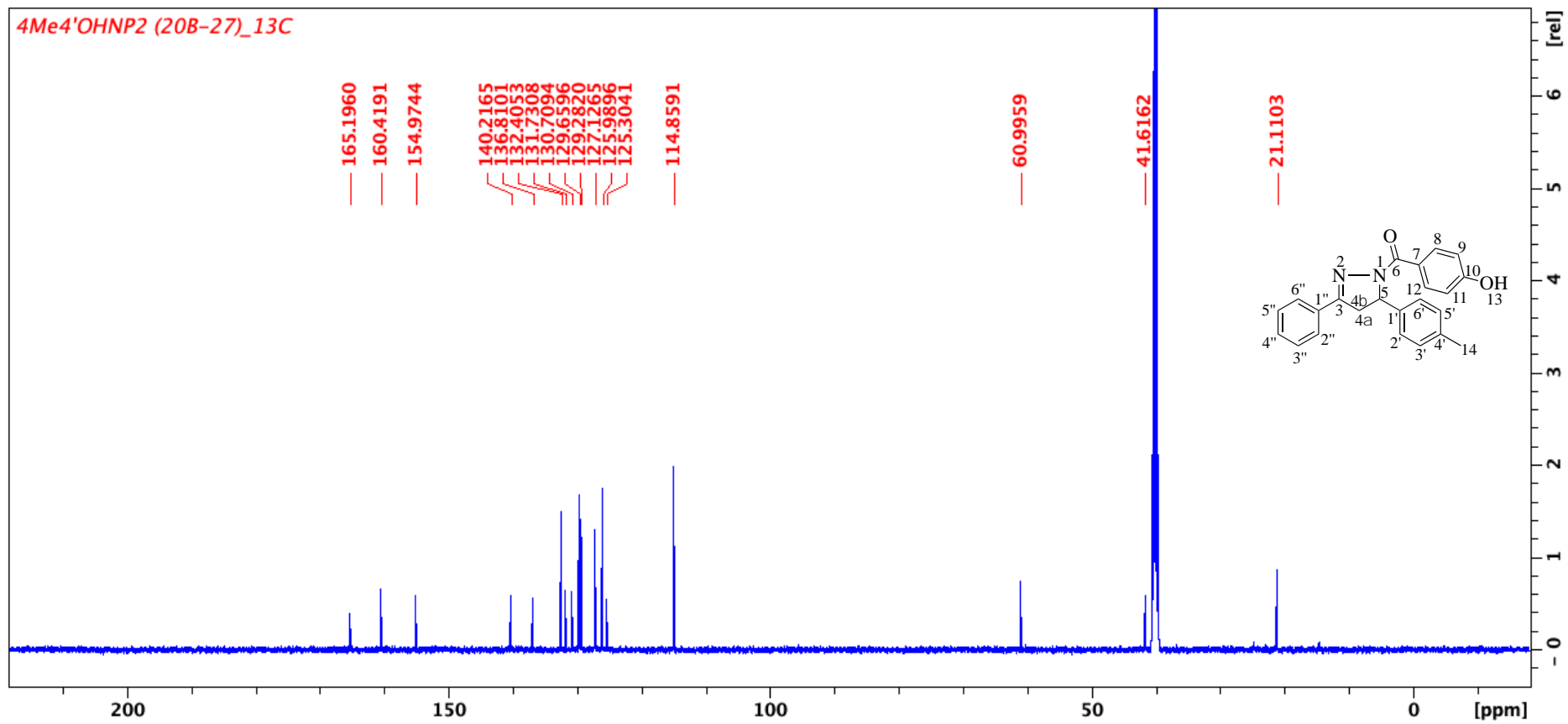
HRMS spectrum of compound 5a



IR spectrum of compound 5a



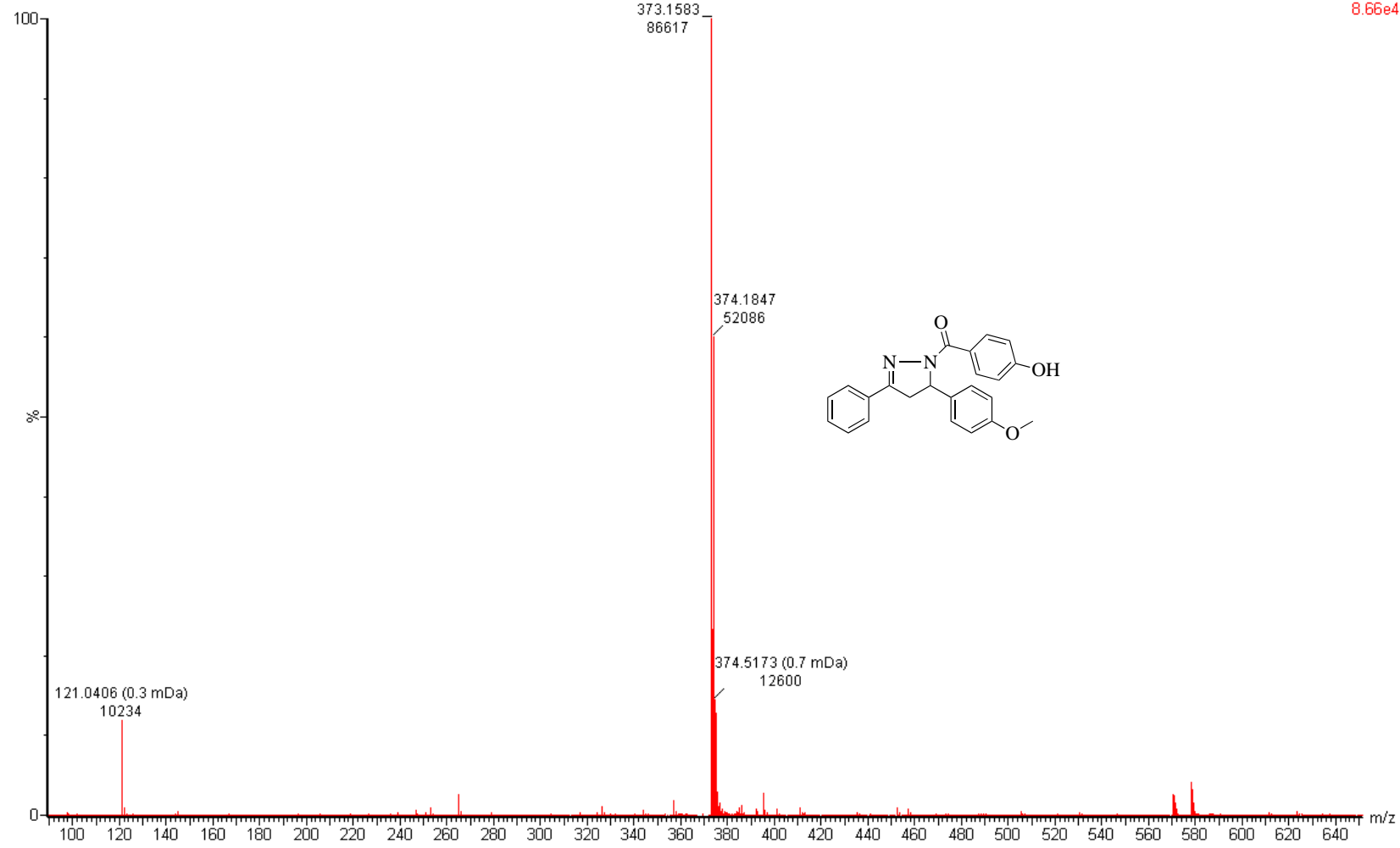
^1H NMR spectrum of compound **5a**



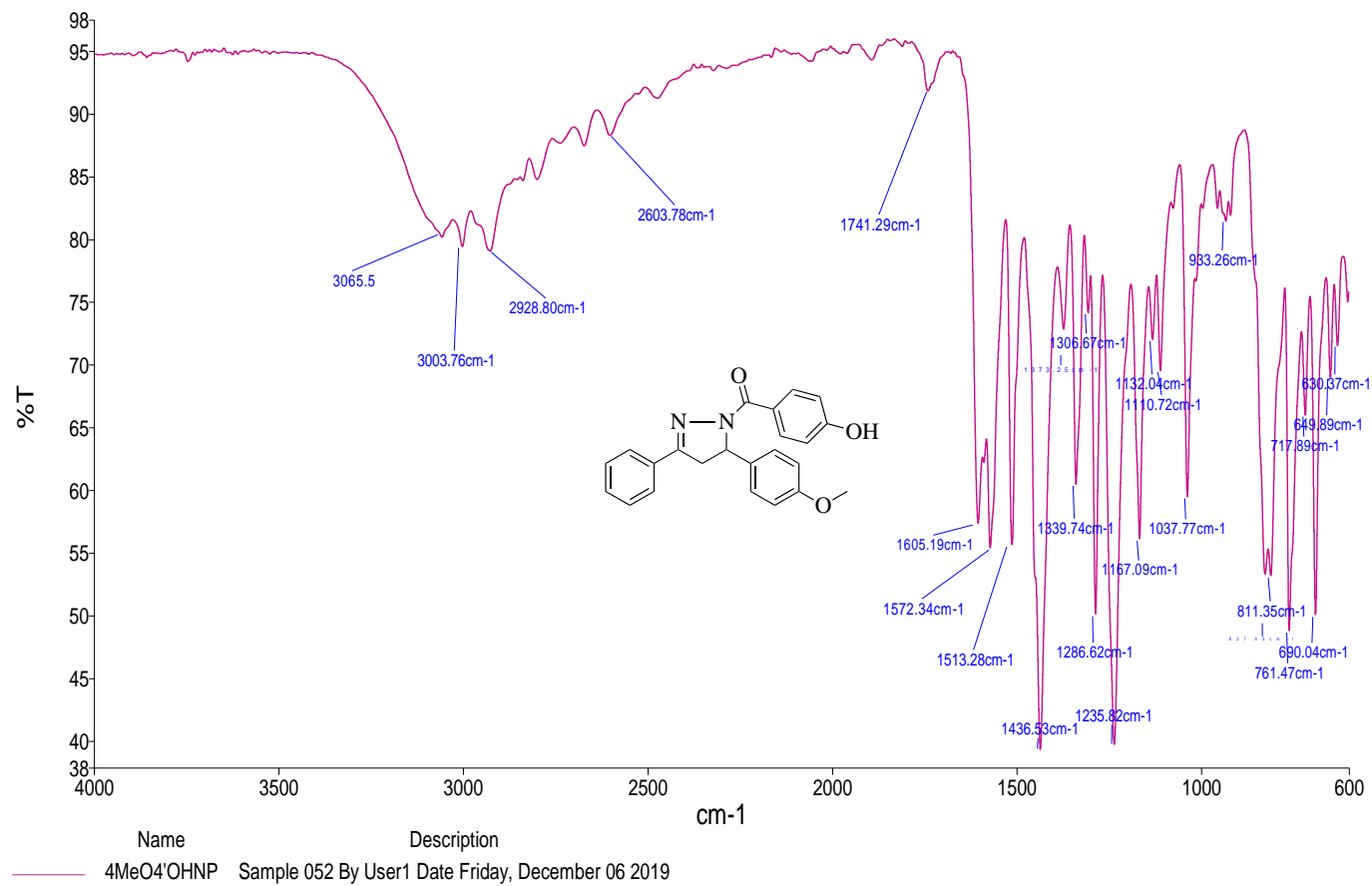
^{13}C NMR spectrum of compound 5a

4MEO4OHNP 16 (0.289)

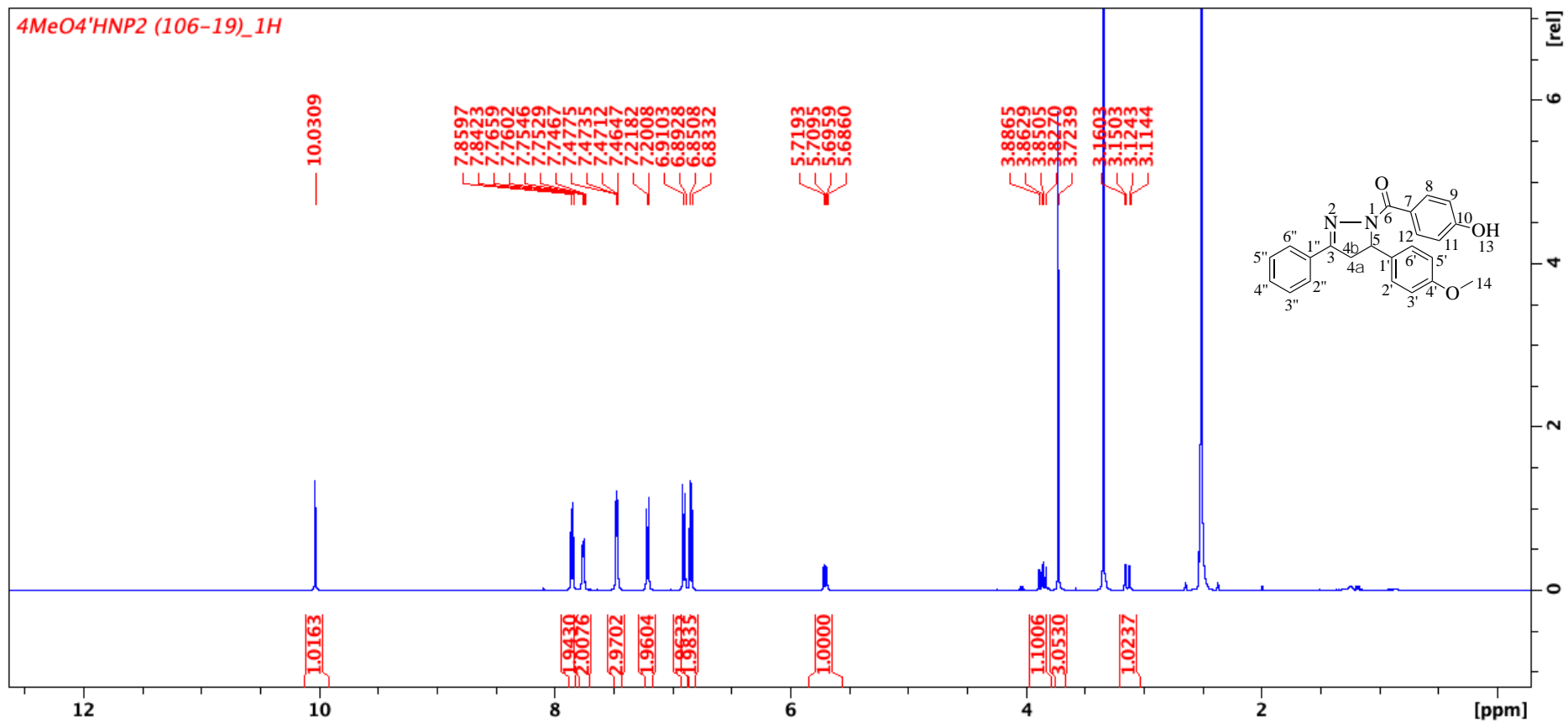
TOF MS ES+
8.66e4



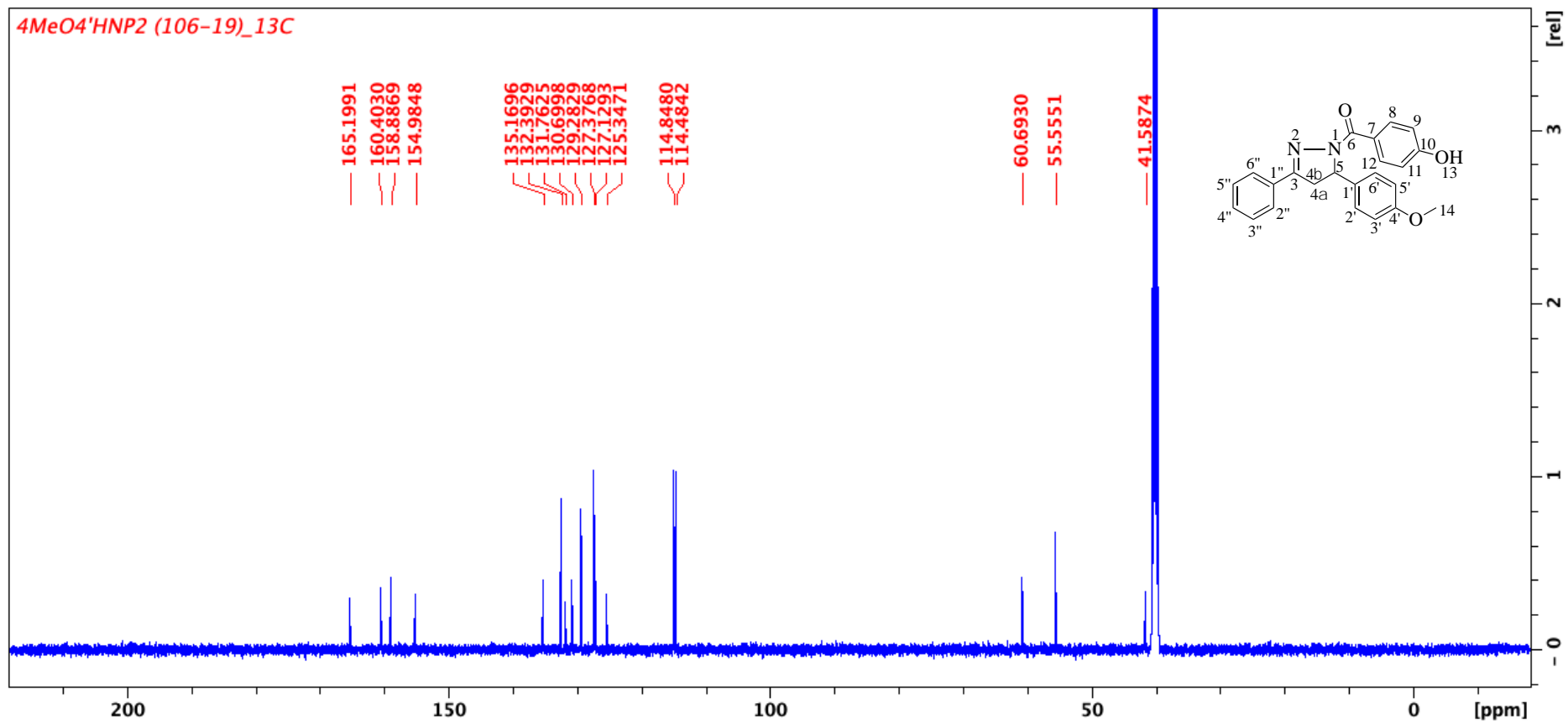
HRMS spectrum of compound **5b**



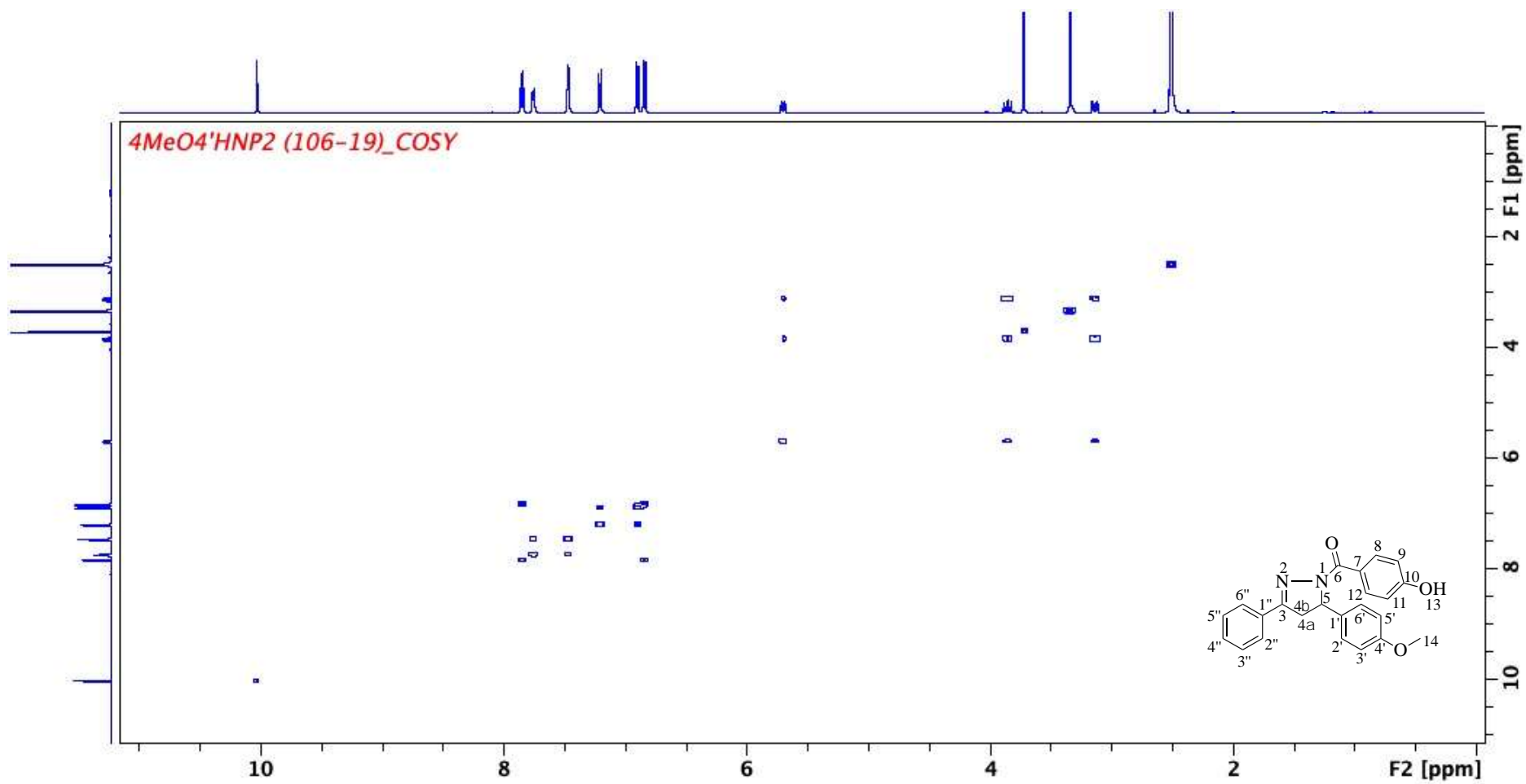
IR spectrum of compound **5b**



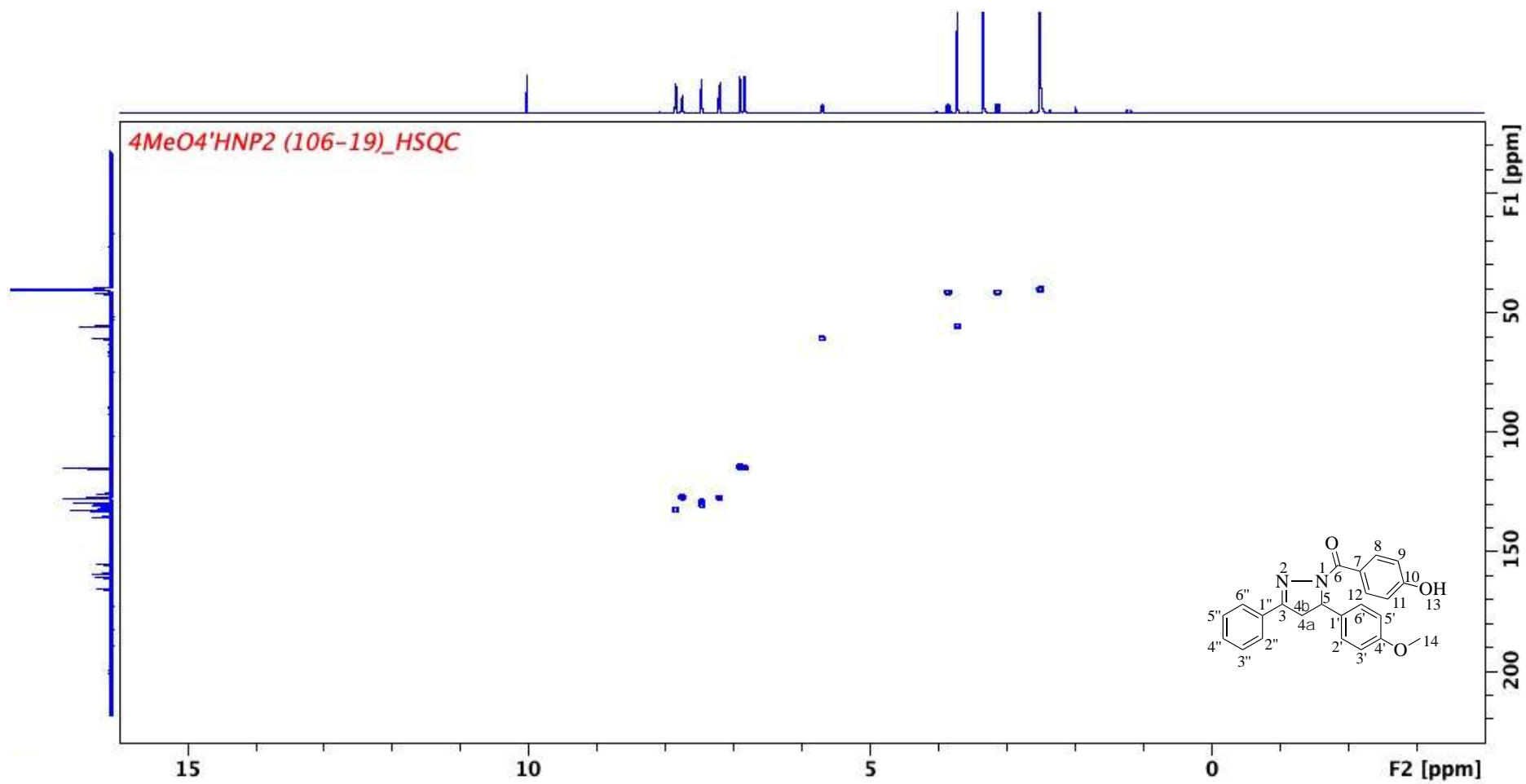
¹H NMR spectrum of compound **5b**



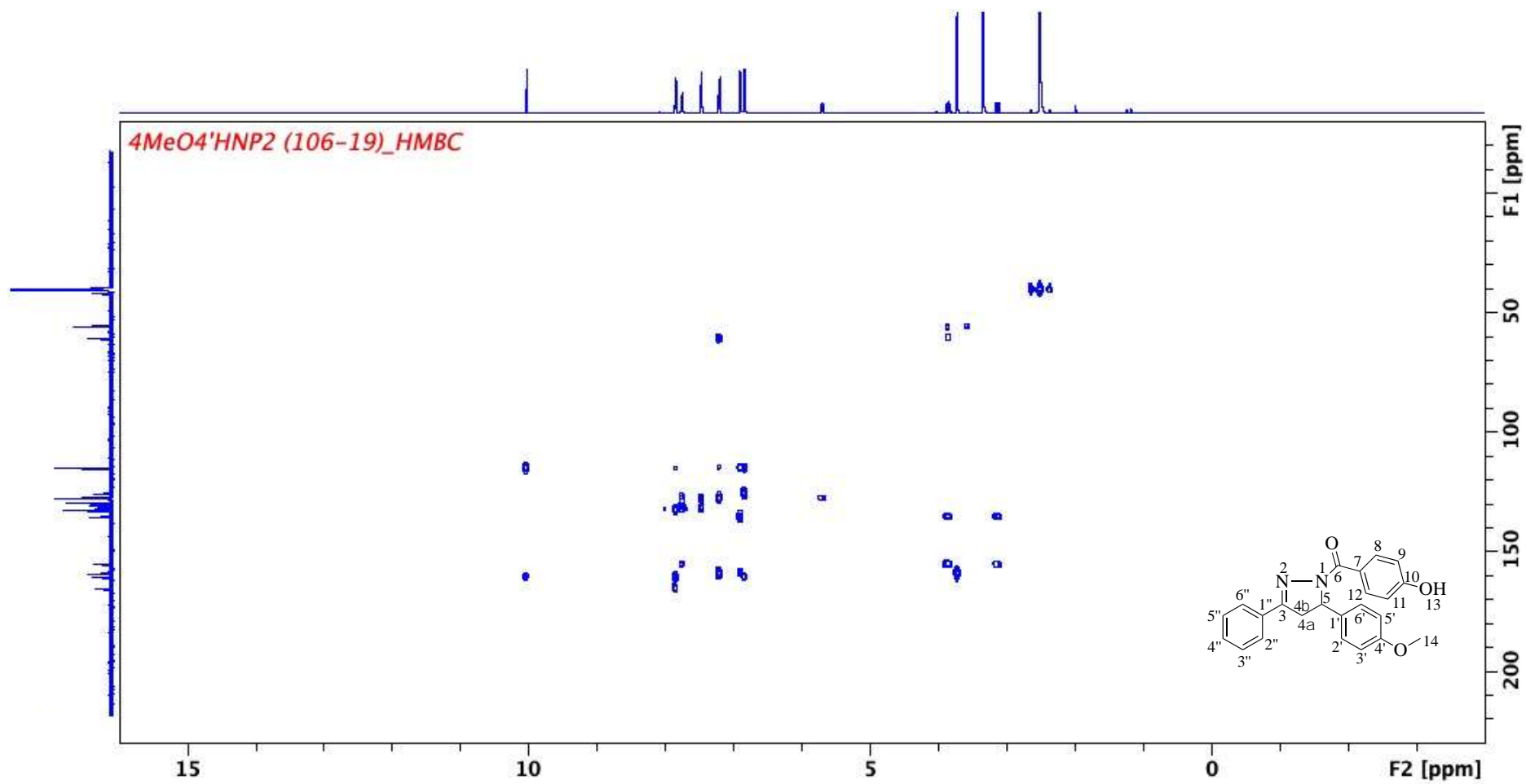
^{13}C NMR spectrum of compound **5b**



^1H - ^1H COSY NMR spectrum of compound 5b



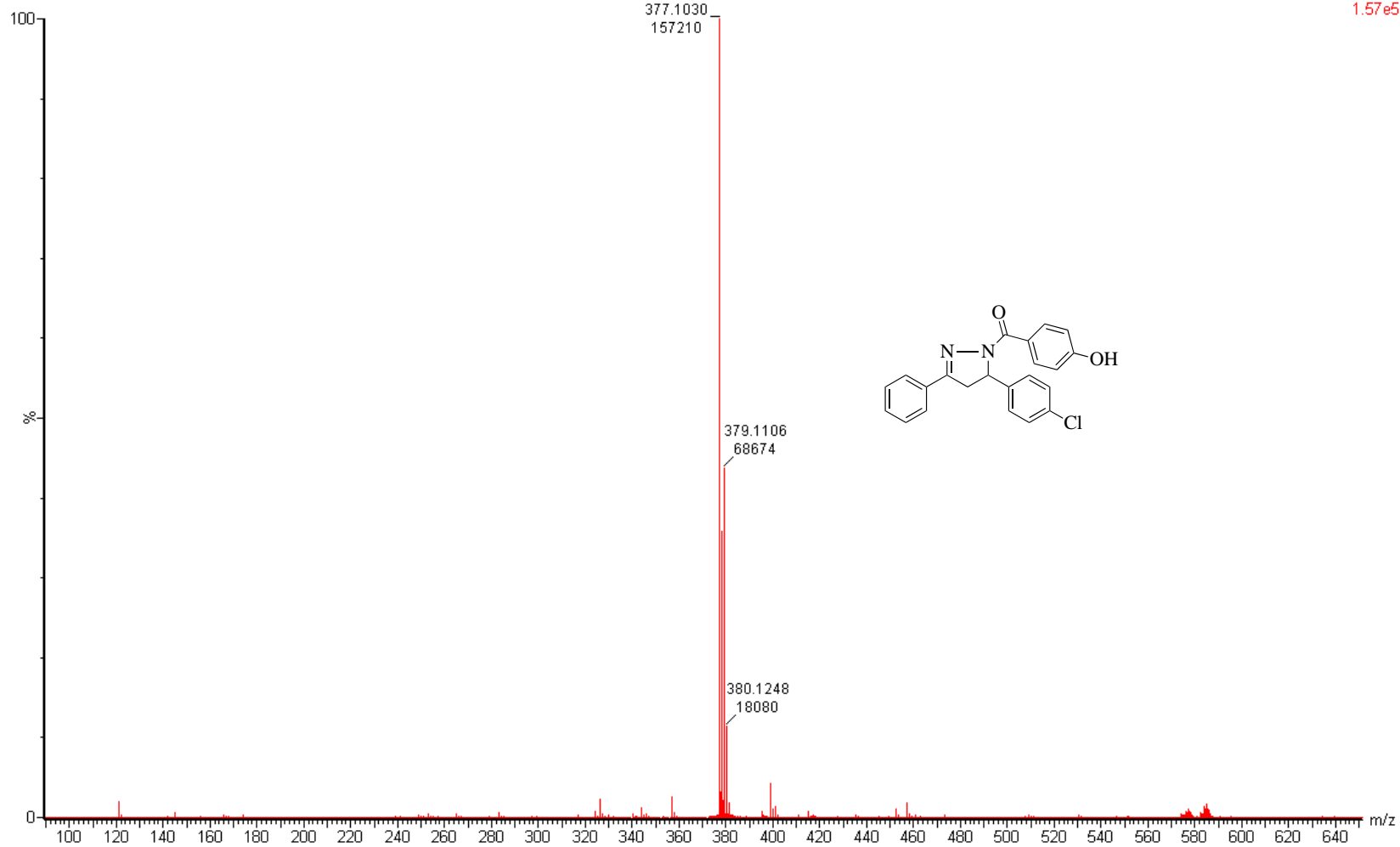
^1H - ^{13}C HSQC NMR spectrum of compound 5b



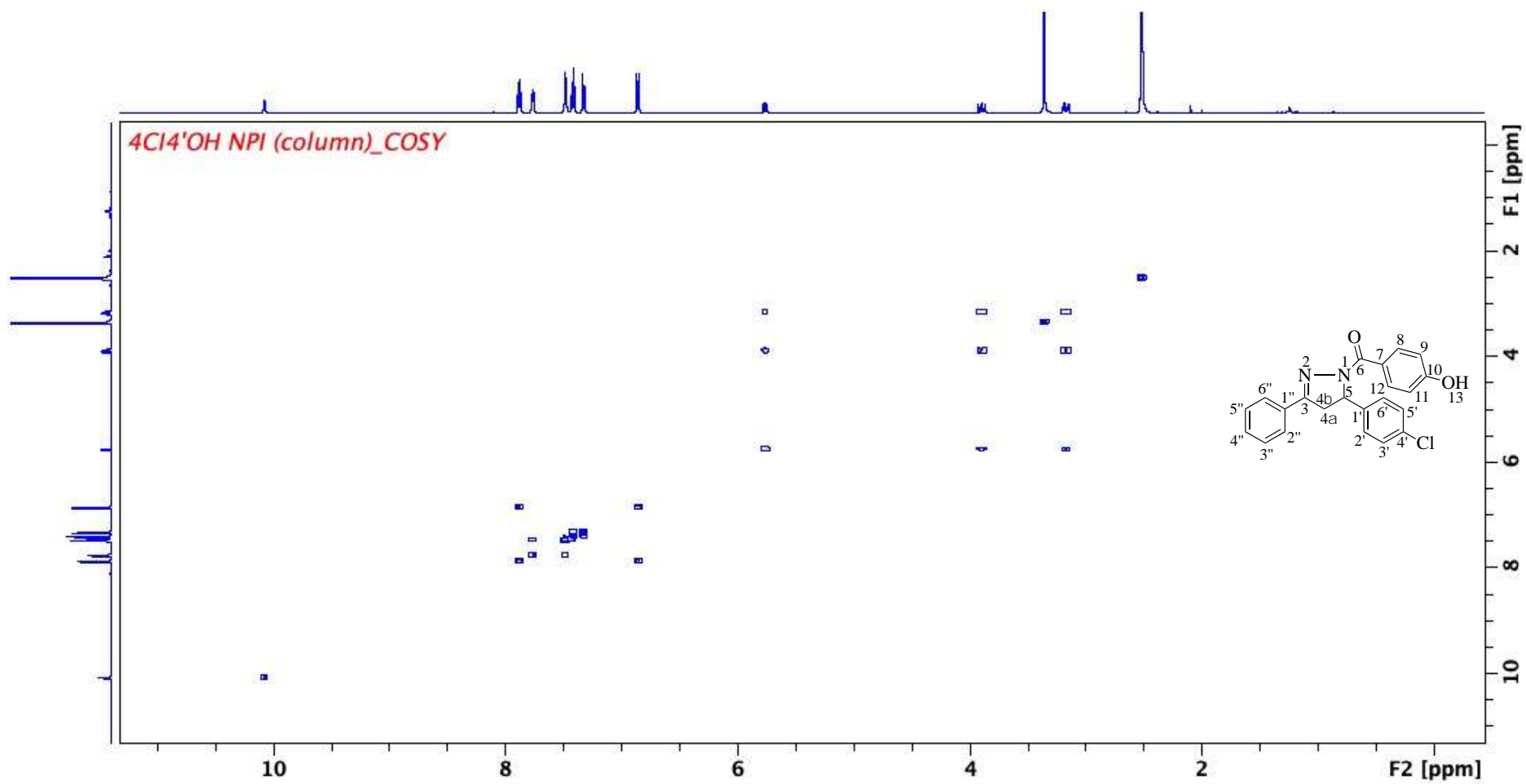
^1H - ^{13}C HMBC NMR spectrum of compound 5b

4CL4OHNP 3 (0.068) Cm (2:3)

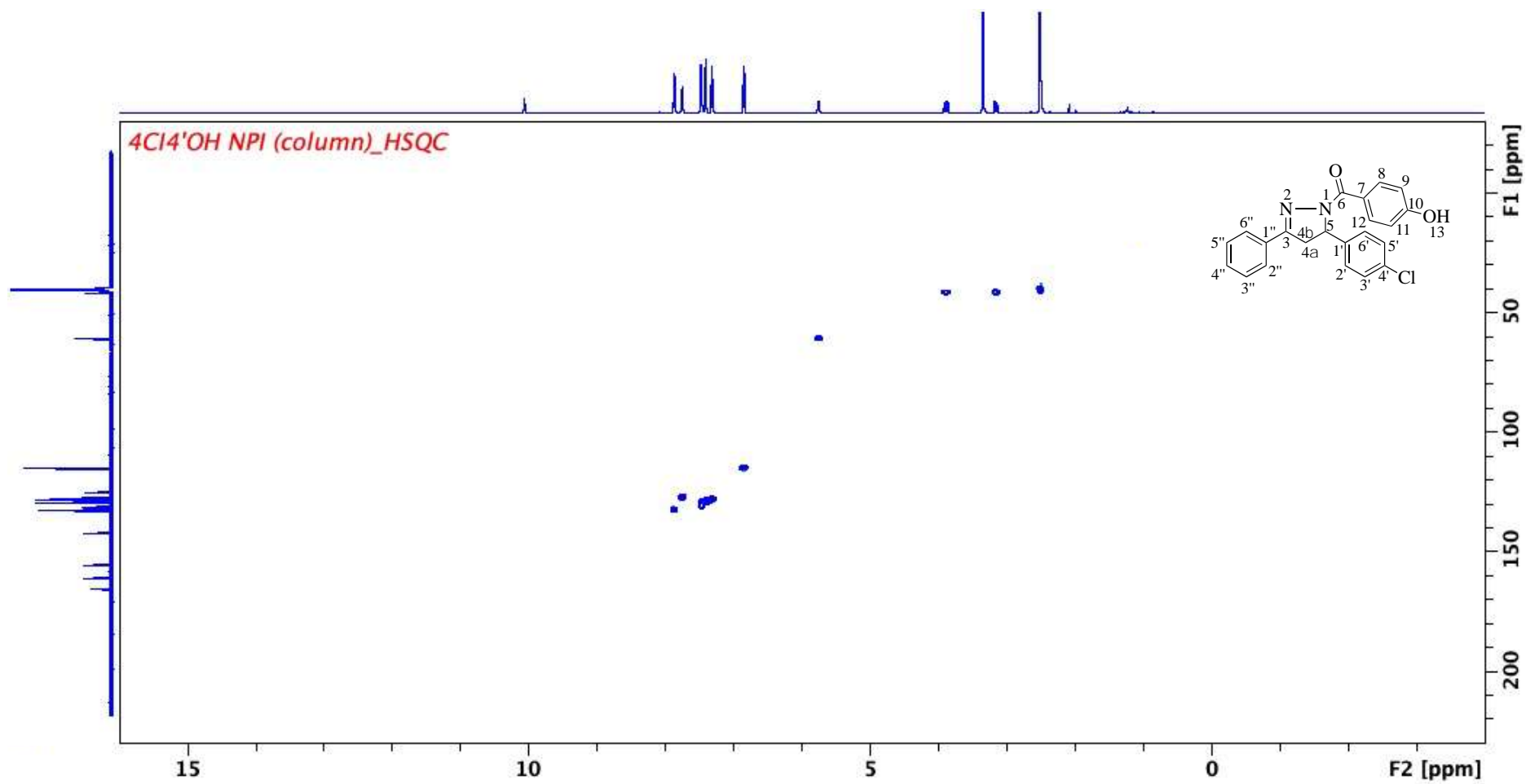
TOF MS ES+
1.57e5



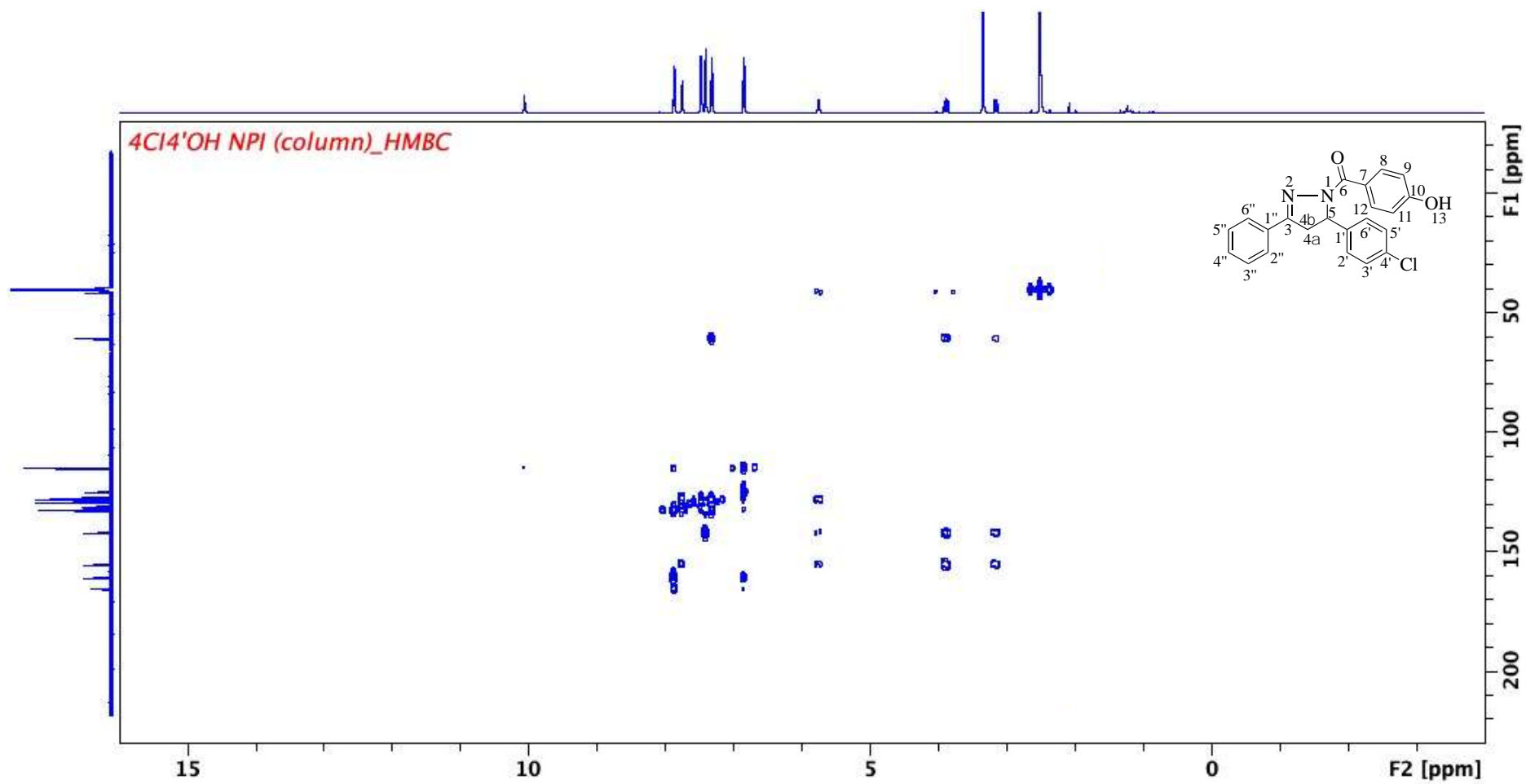
HRMS spectrum of compound 5c



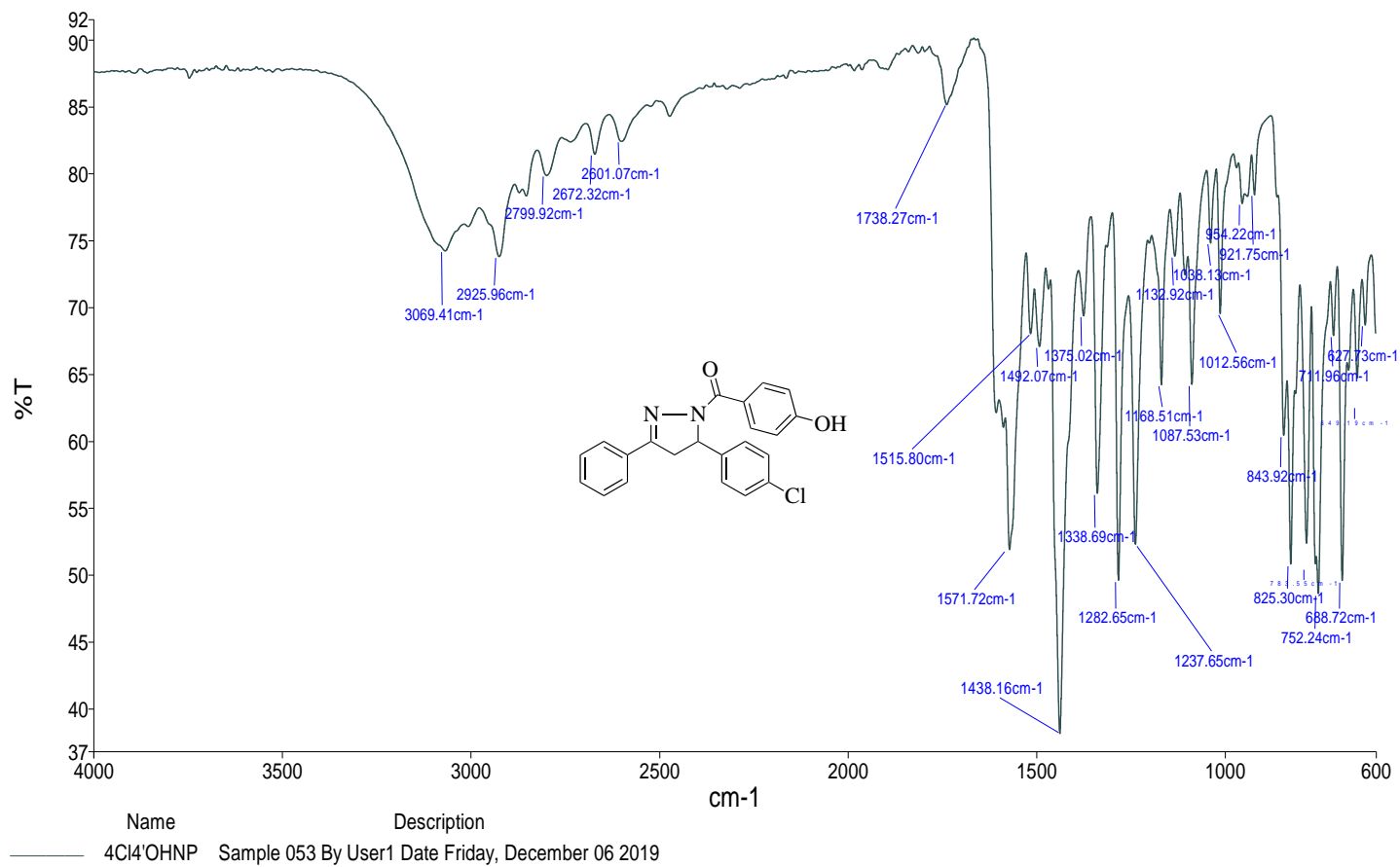
^1H - ^1H COSY NMR spectrum of compound 5c



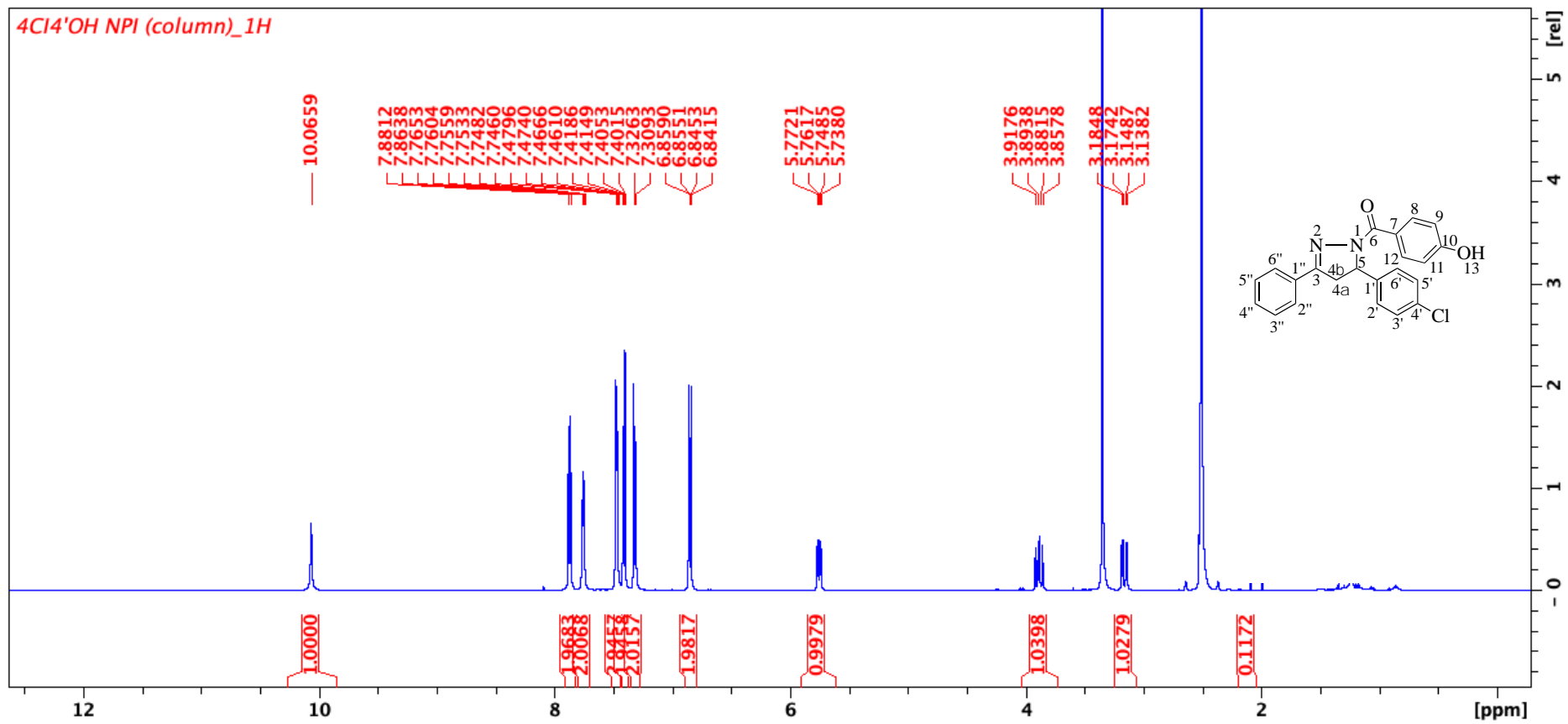
^1H - ^{13}C HSQC NMR spectrum of compound 5c



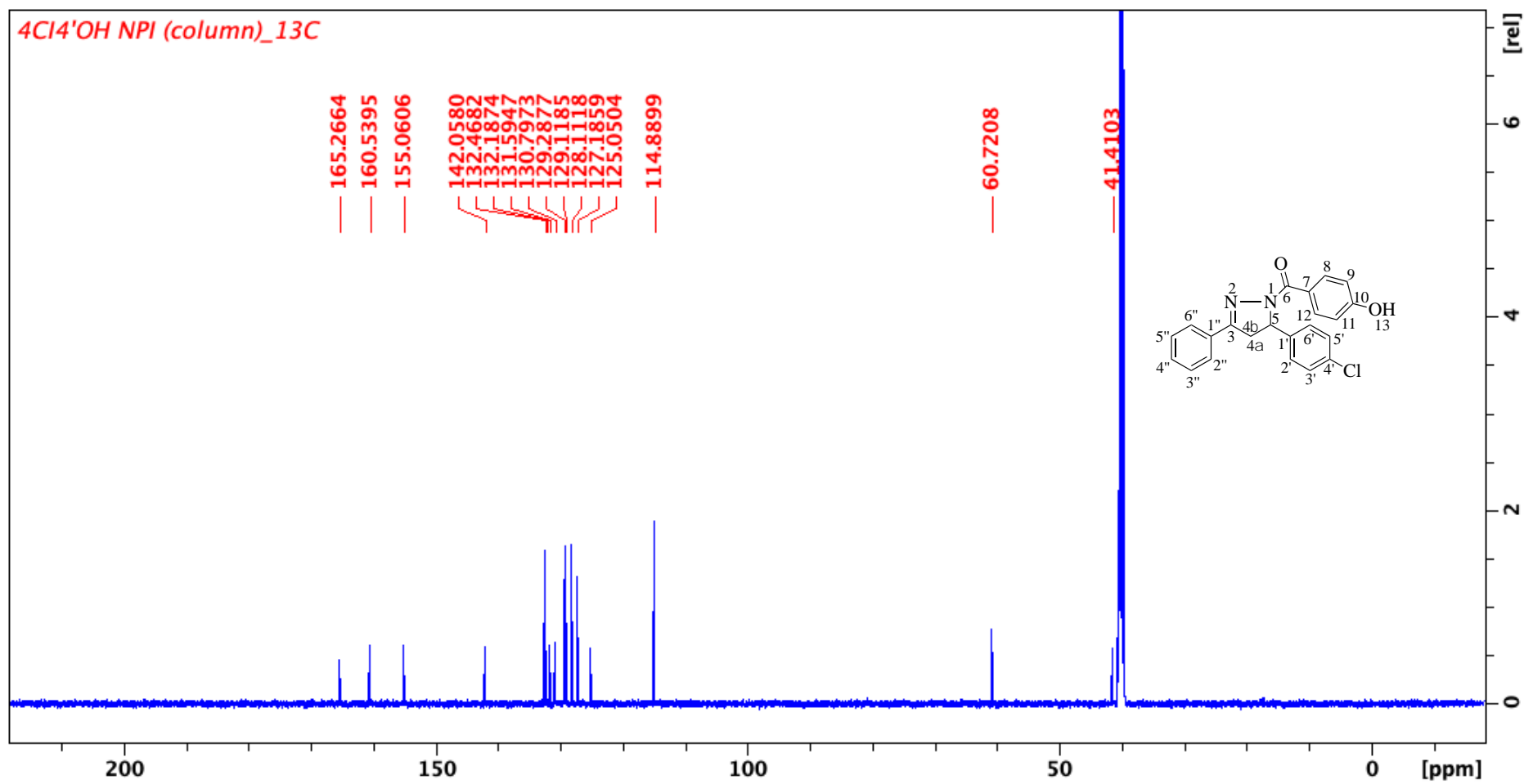
^1H - ^{13}C HMBC NMR spectrum of compound 5c



IR spectrum of compound 5c



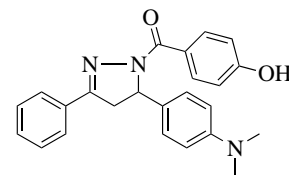
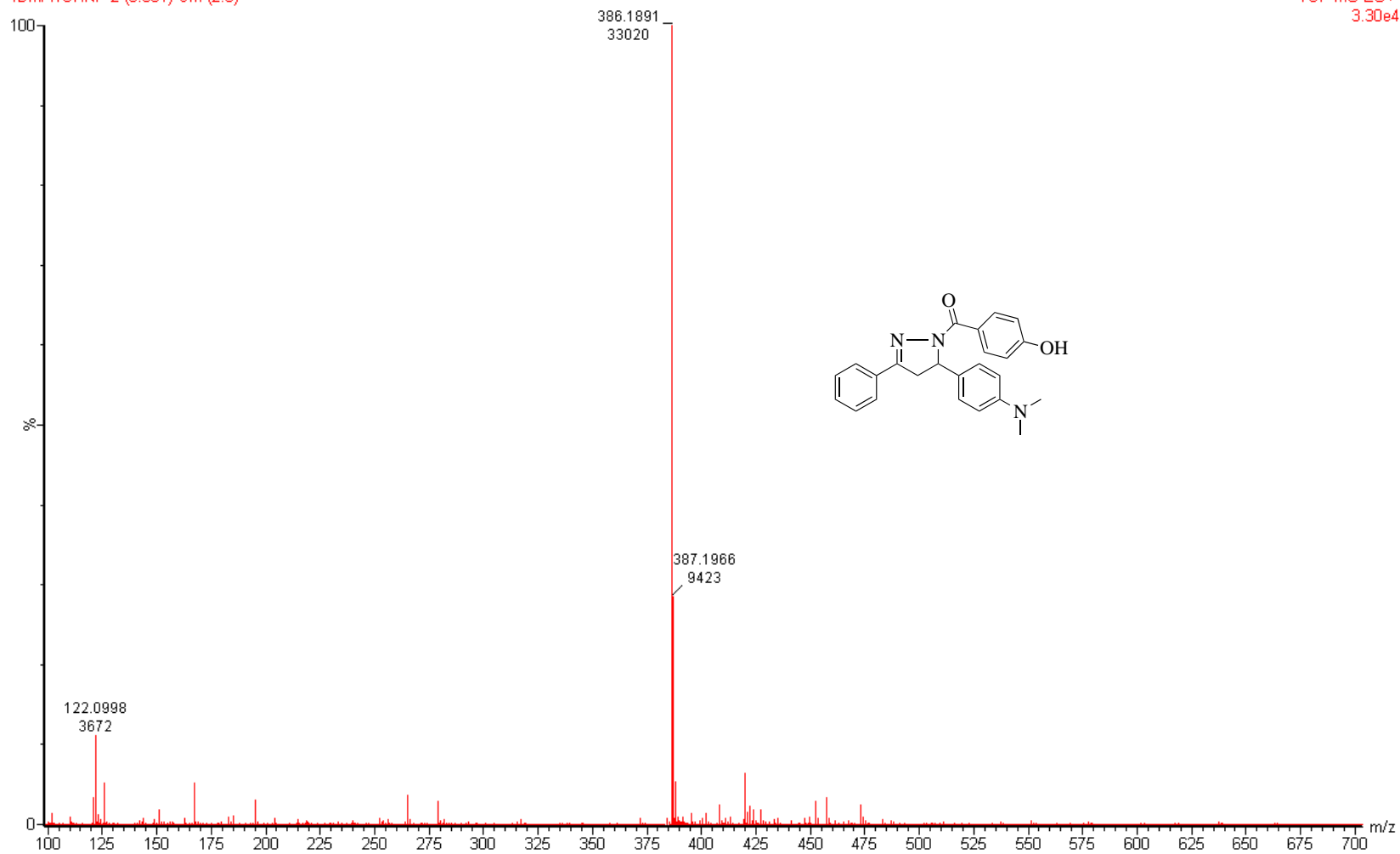
^1H NMR spectrum of compound **5c**



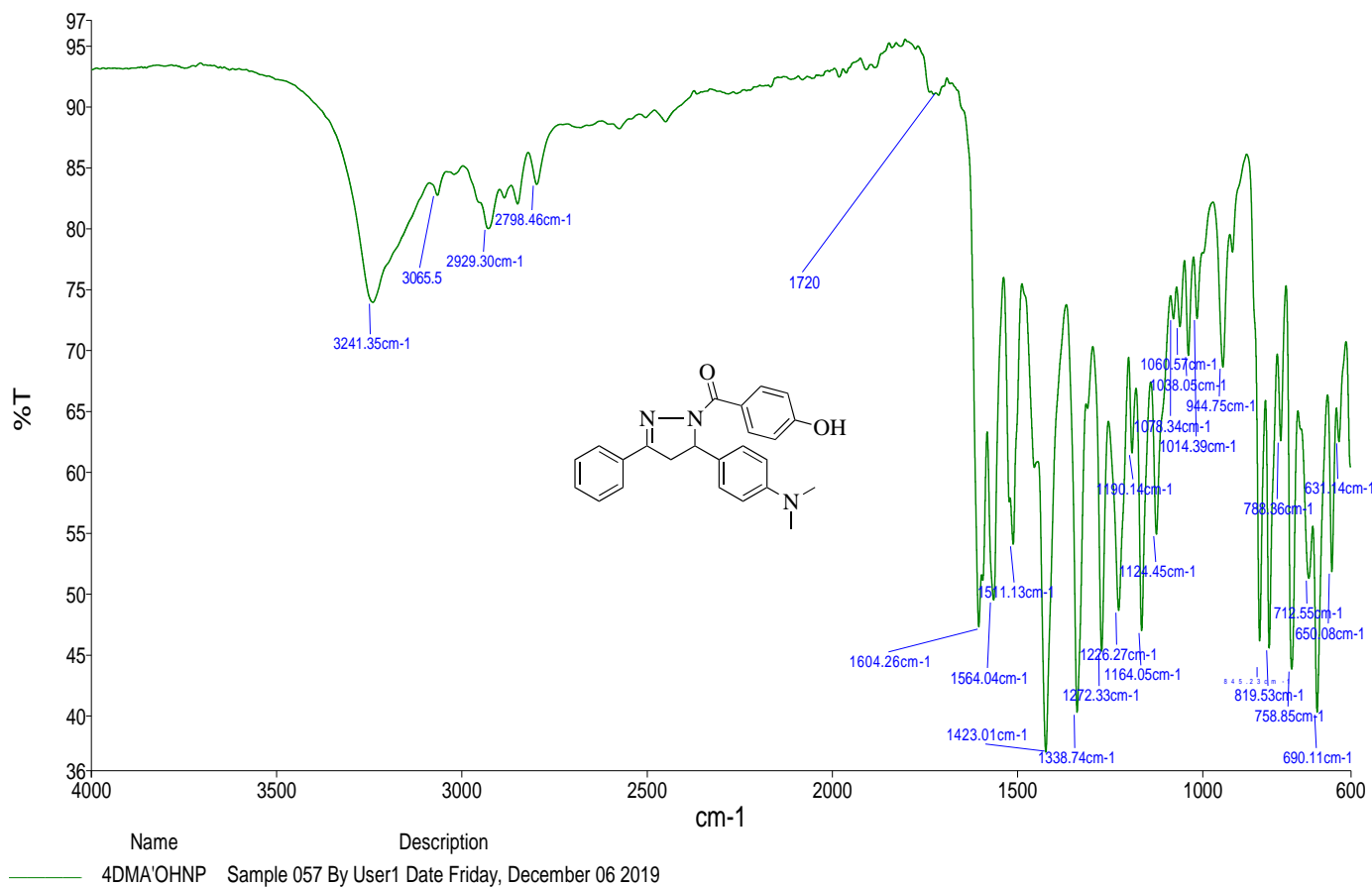
^{13}C NMR spectrum of compound 5c

4DMA4OHNP 2 (0.051) Cm (2:3)

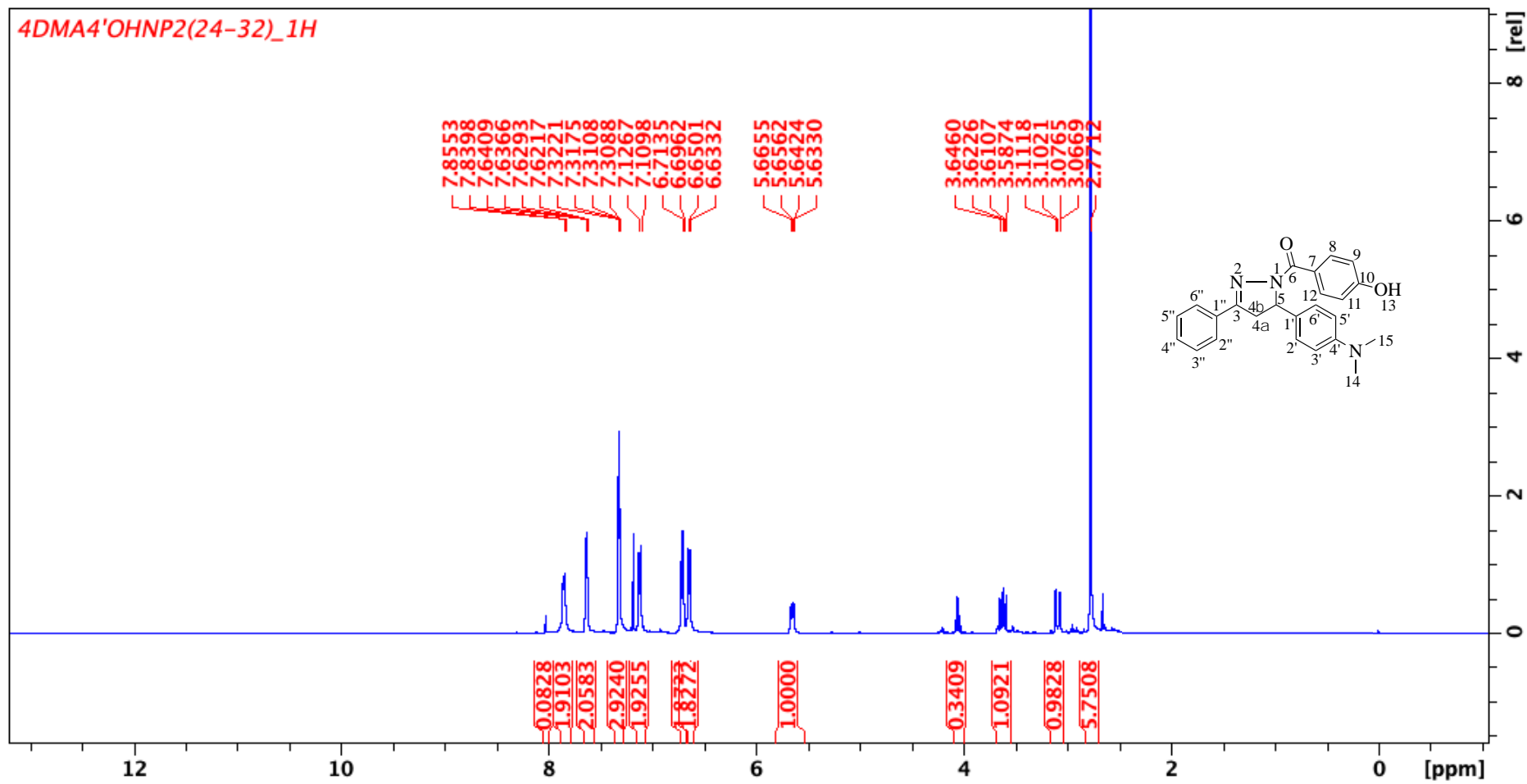
TOF MS ES+
3.30e4



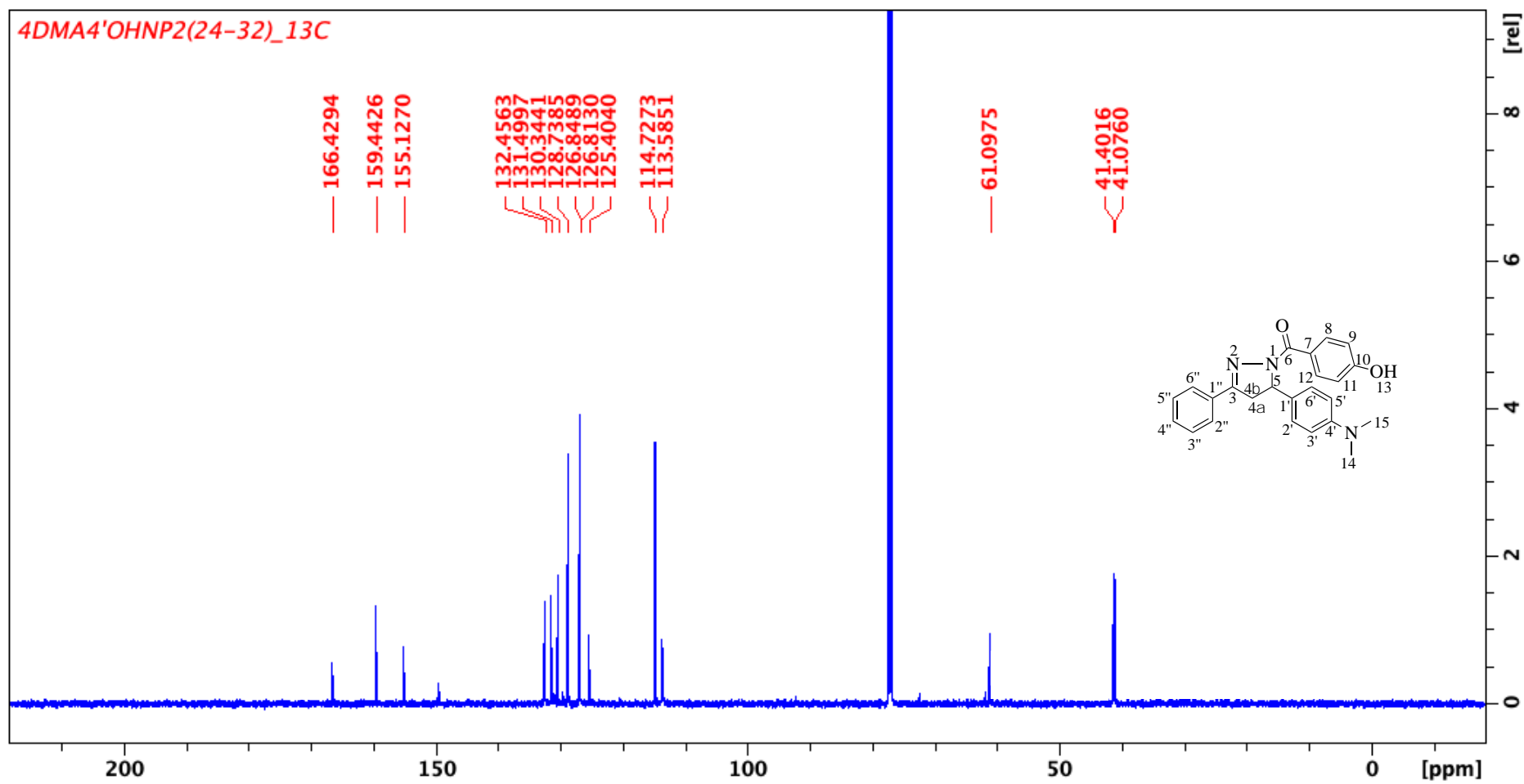
HRMS spectrum of compound **5d**



IR spectrum of compound **5d**



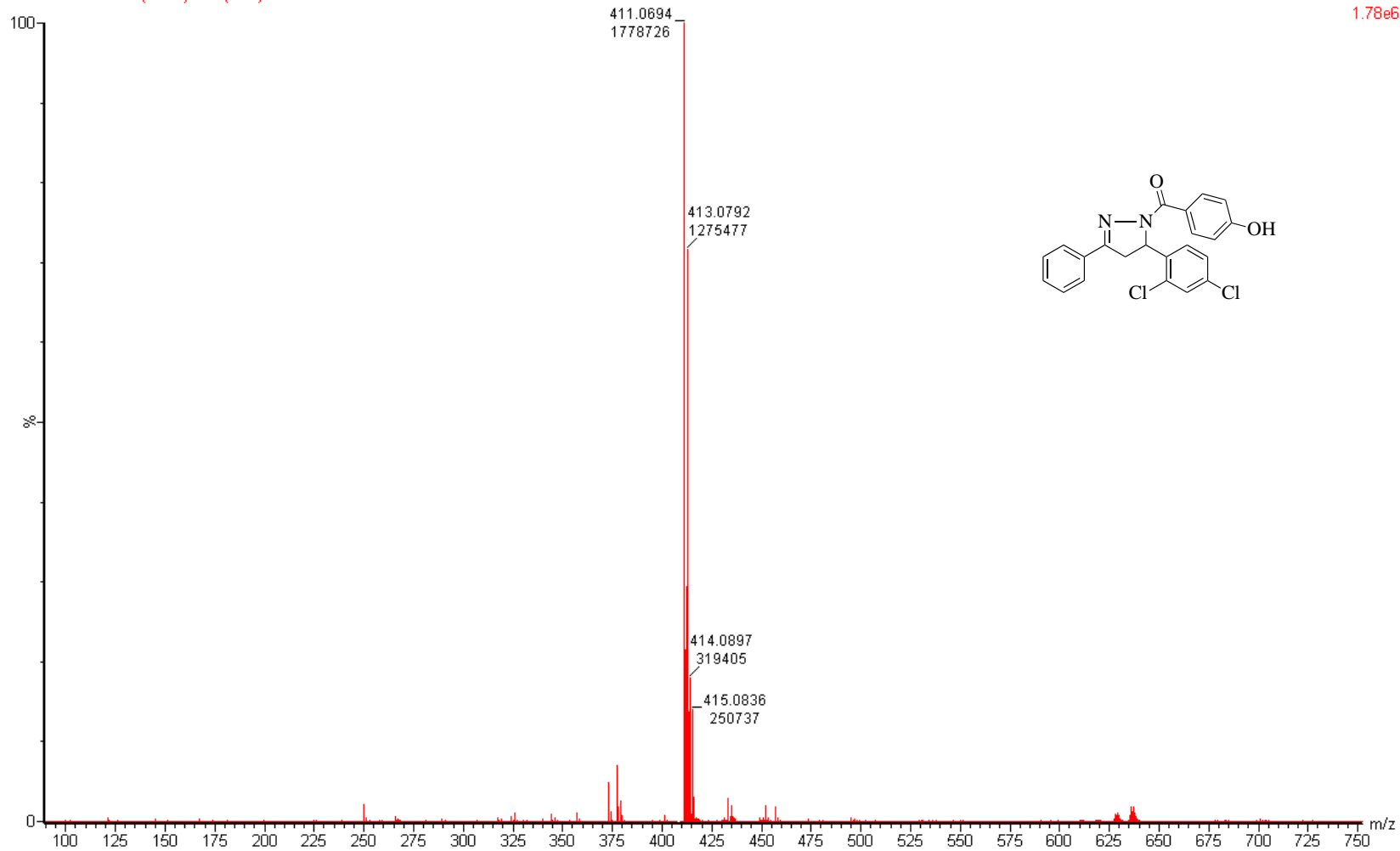
^1H NMR spectrum of compound **5d**



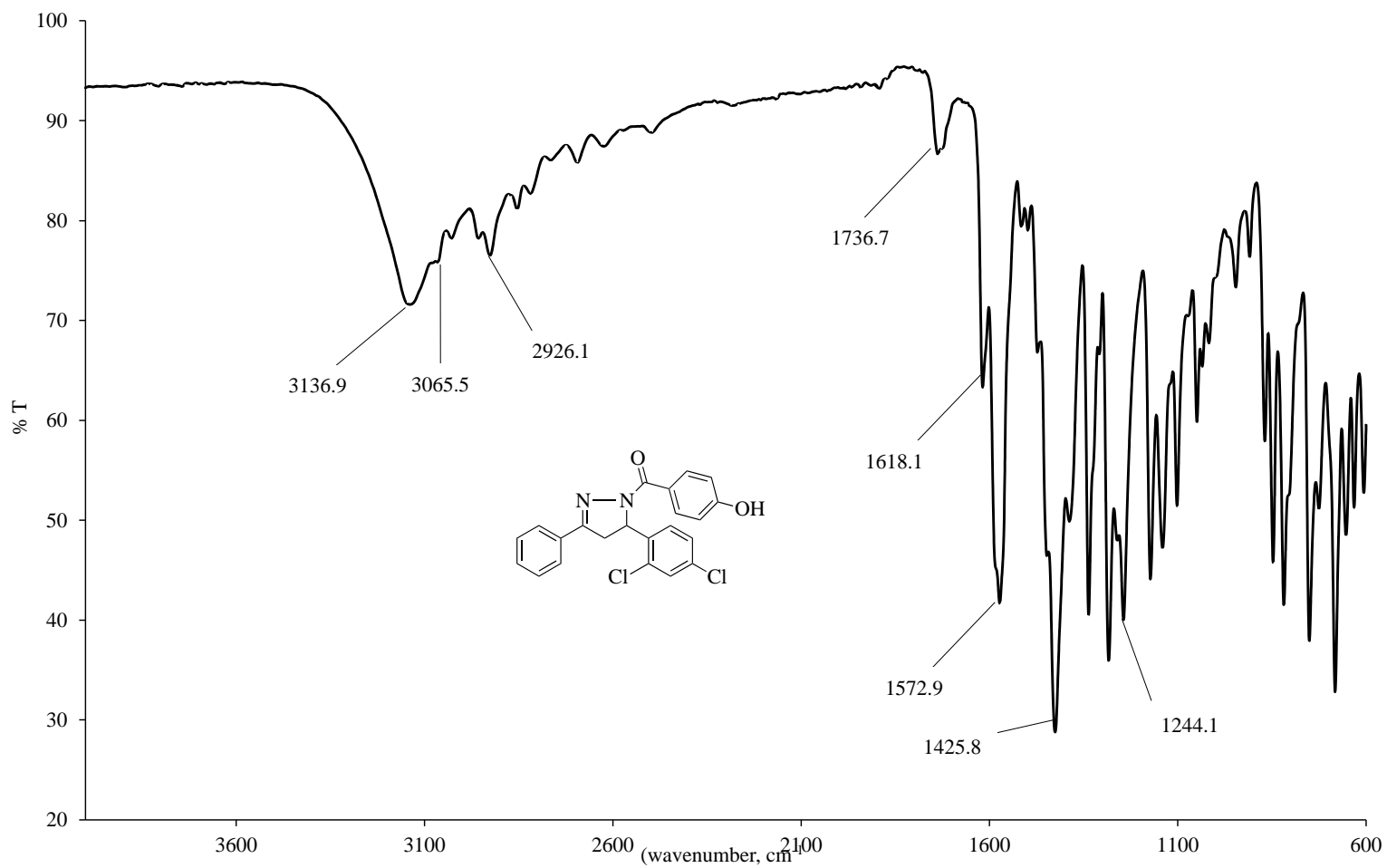
^{13}C NMR spectrum of compound **5d**

24D1CL4OHNP 28 (0.493) Cm (2:29)

TOF MS ES+
1.78e6

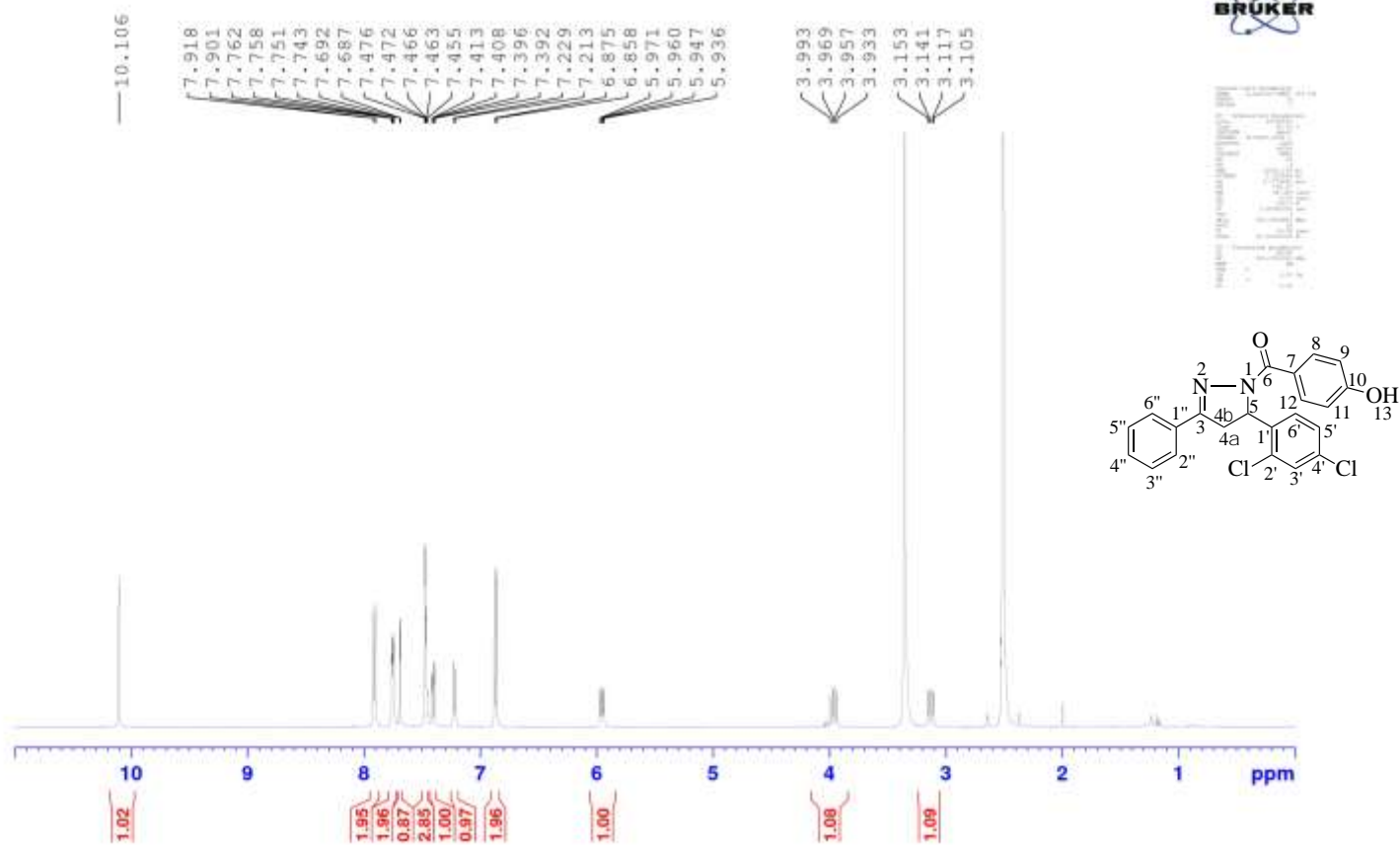


HRMS spectrum of compound 5e

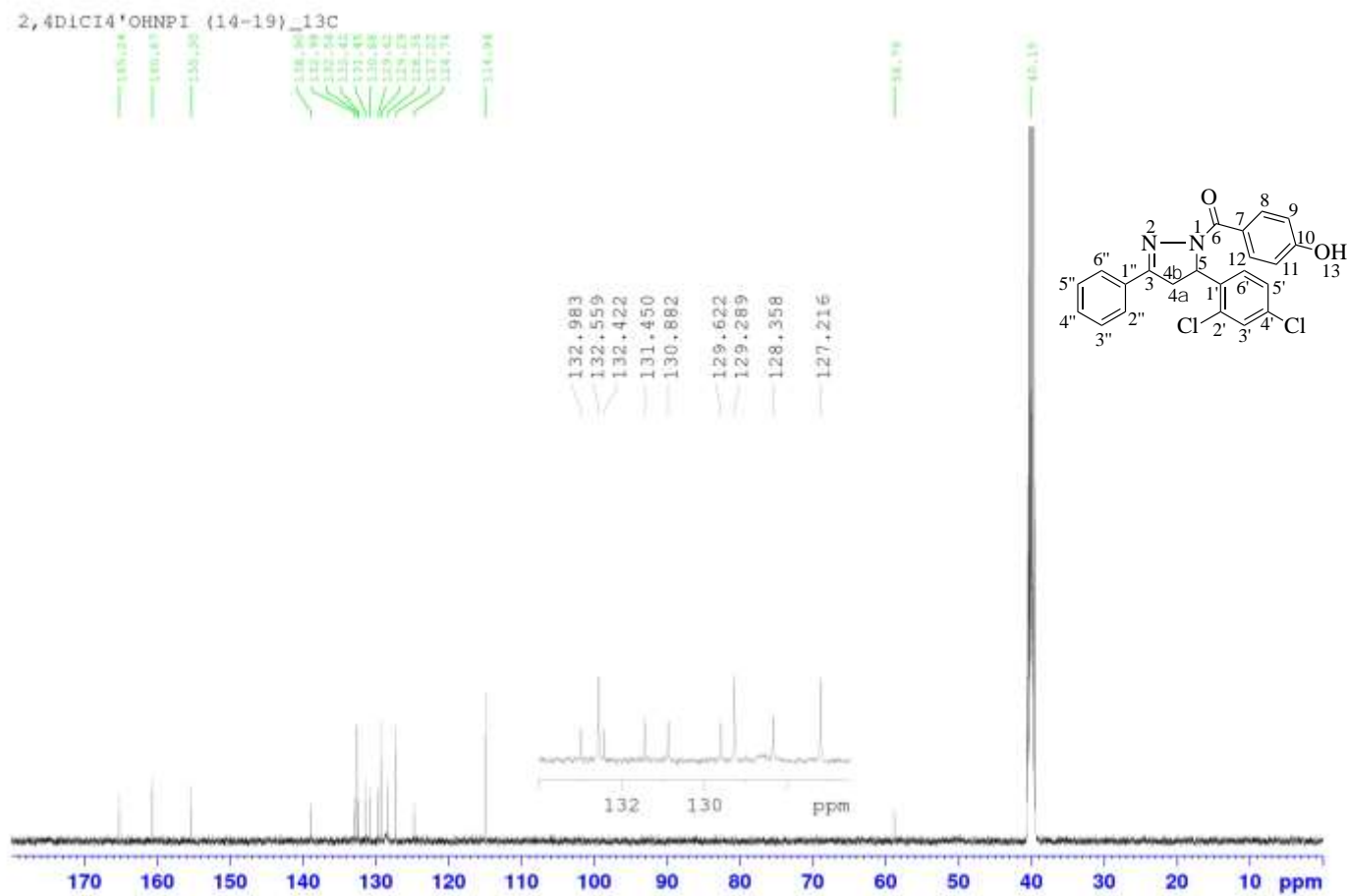


IR spectrum of compound **5e**

2,4D1CI4*OHNPI (14-19)_1H

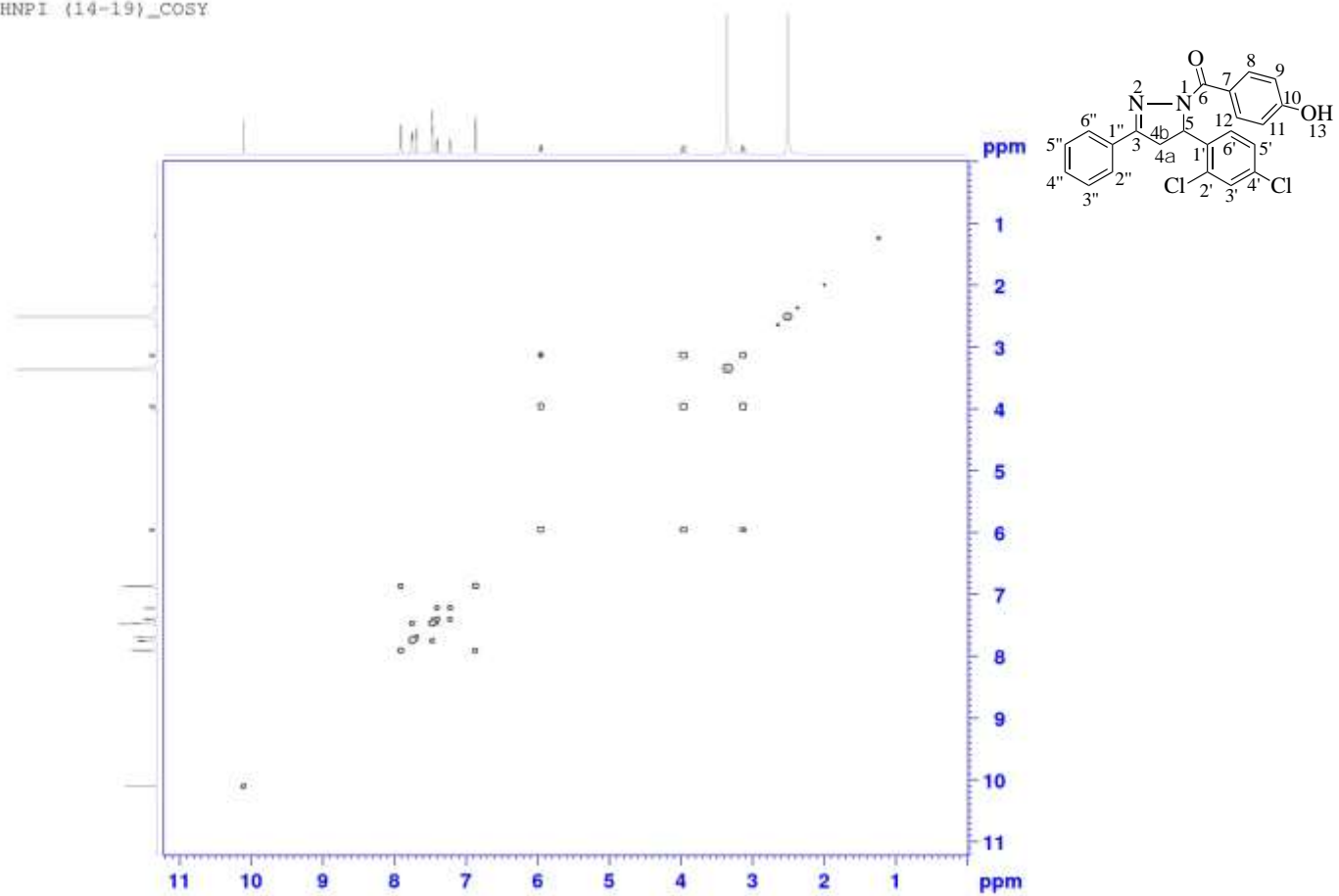


^1H NMR spectrum of compound **5e**



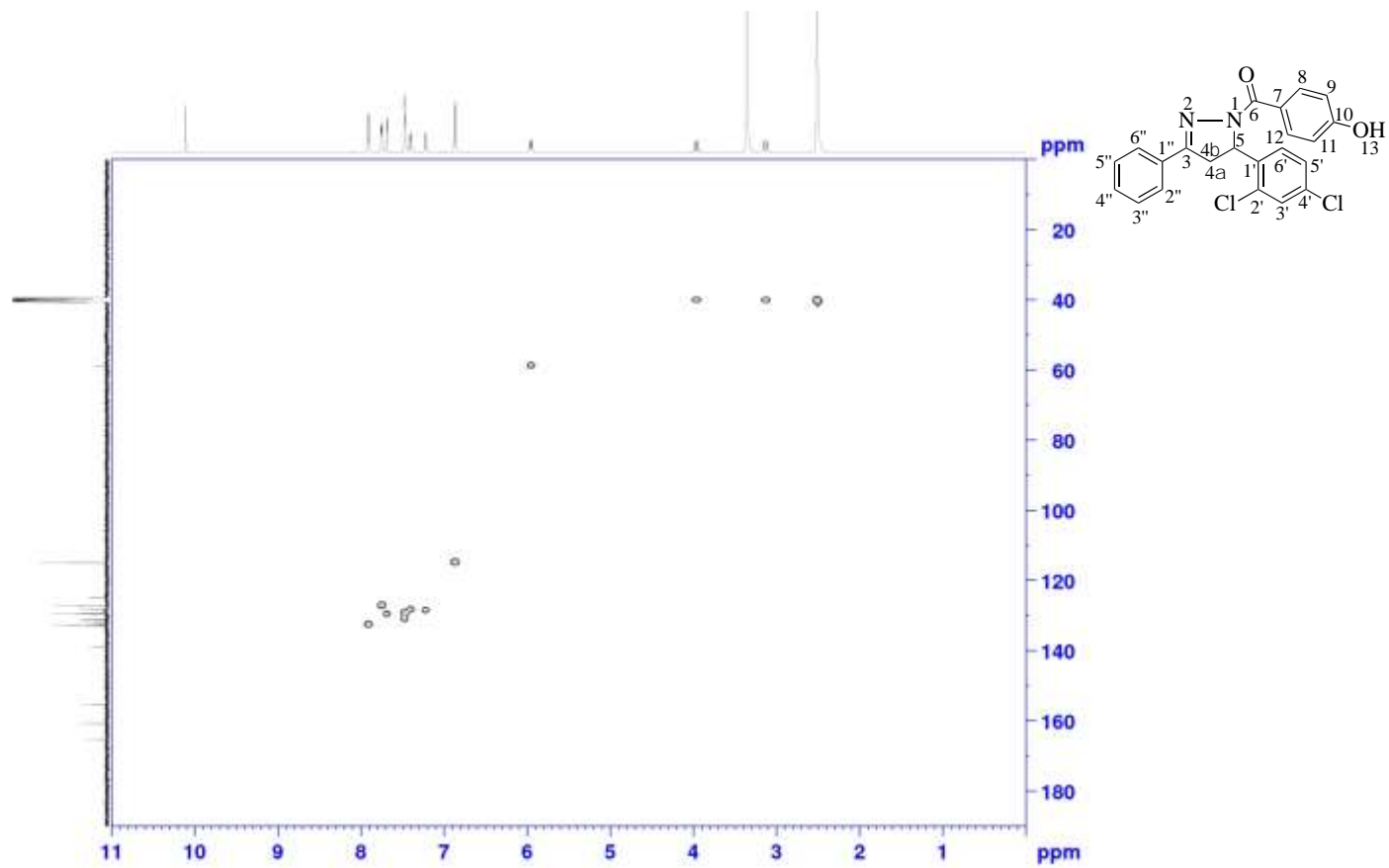
^{13}C NMR spectrum of compound **5e**

2,4D1C14'OHNPI (14-19)_COSY



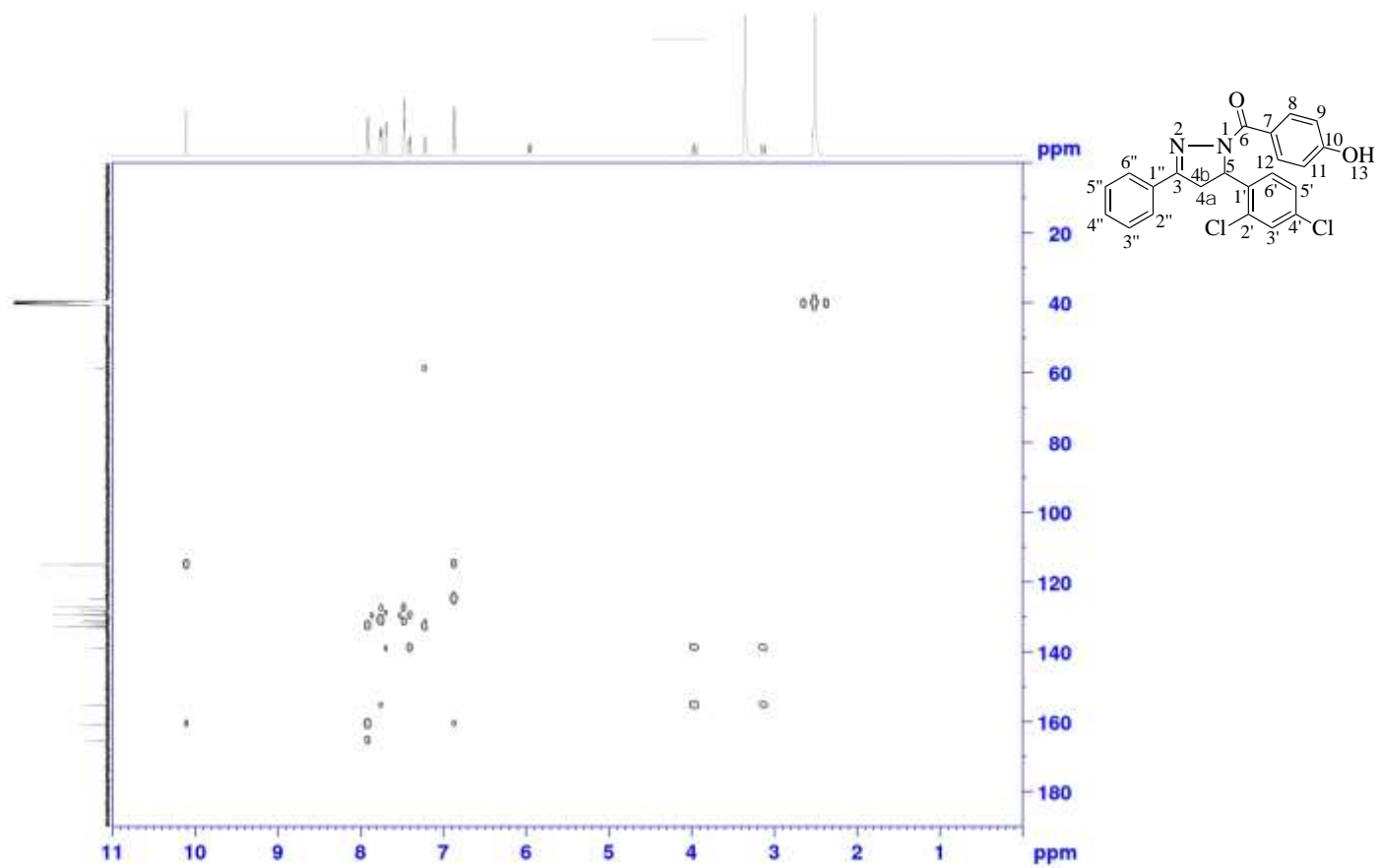
¹H-¹H COSY NMR spectrum of compound 5e

2,4D1C14*OHNPI (14-19)_HSQC



¹H-¹³C HSQC NMR spectrum of compound 5e

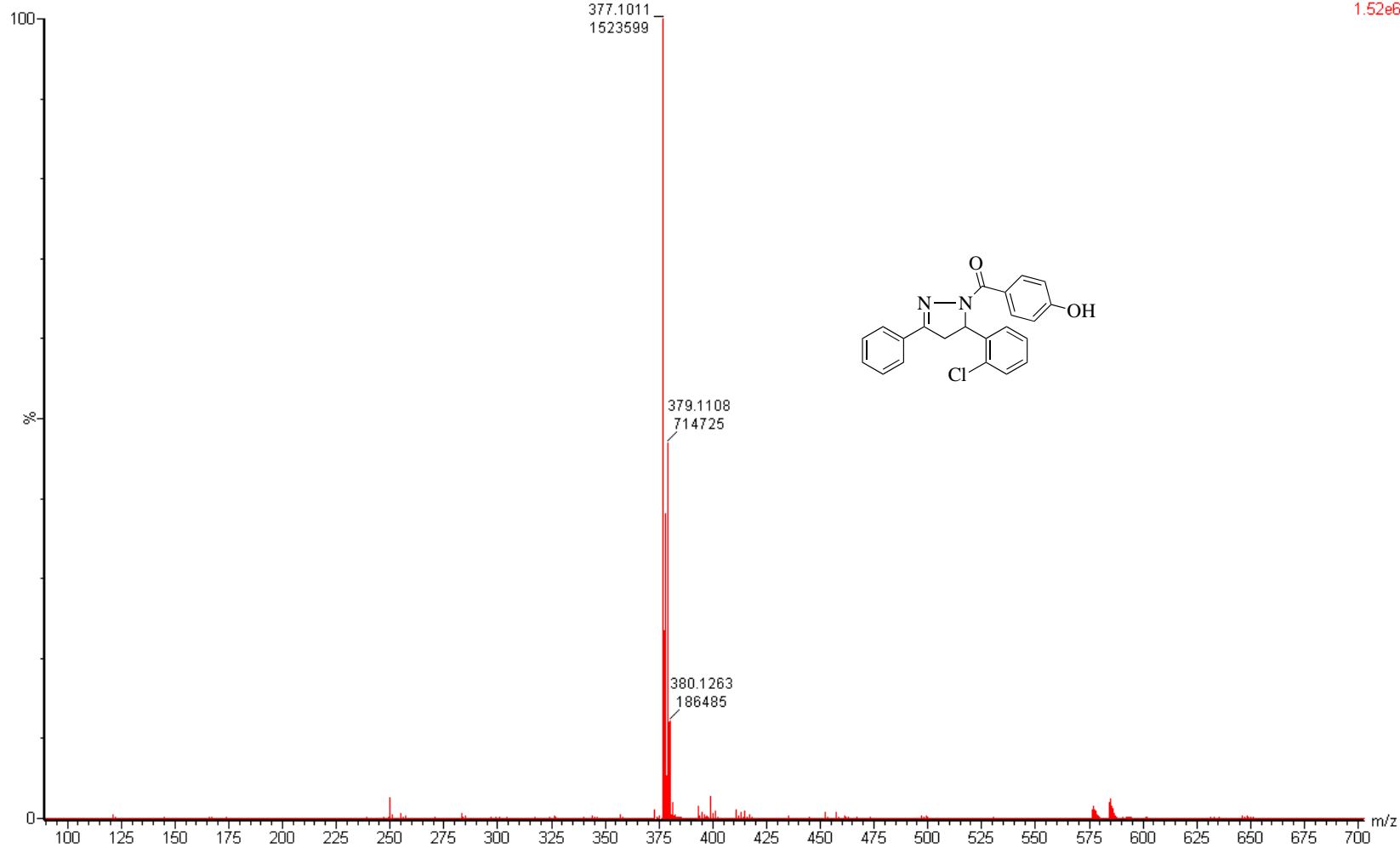
2,4D1C14'OHNPI (14-19)_HMBC



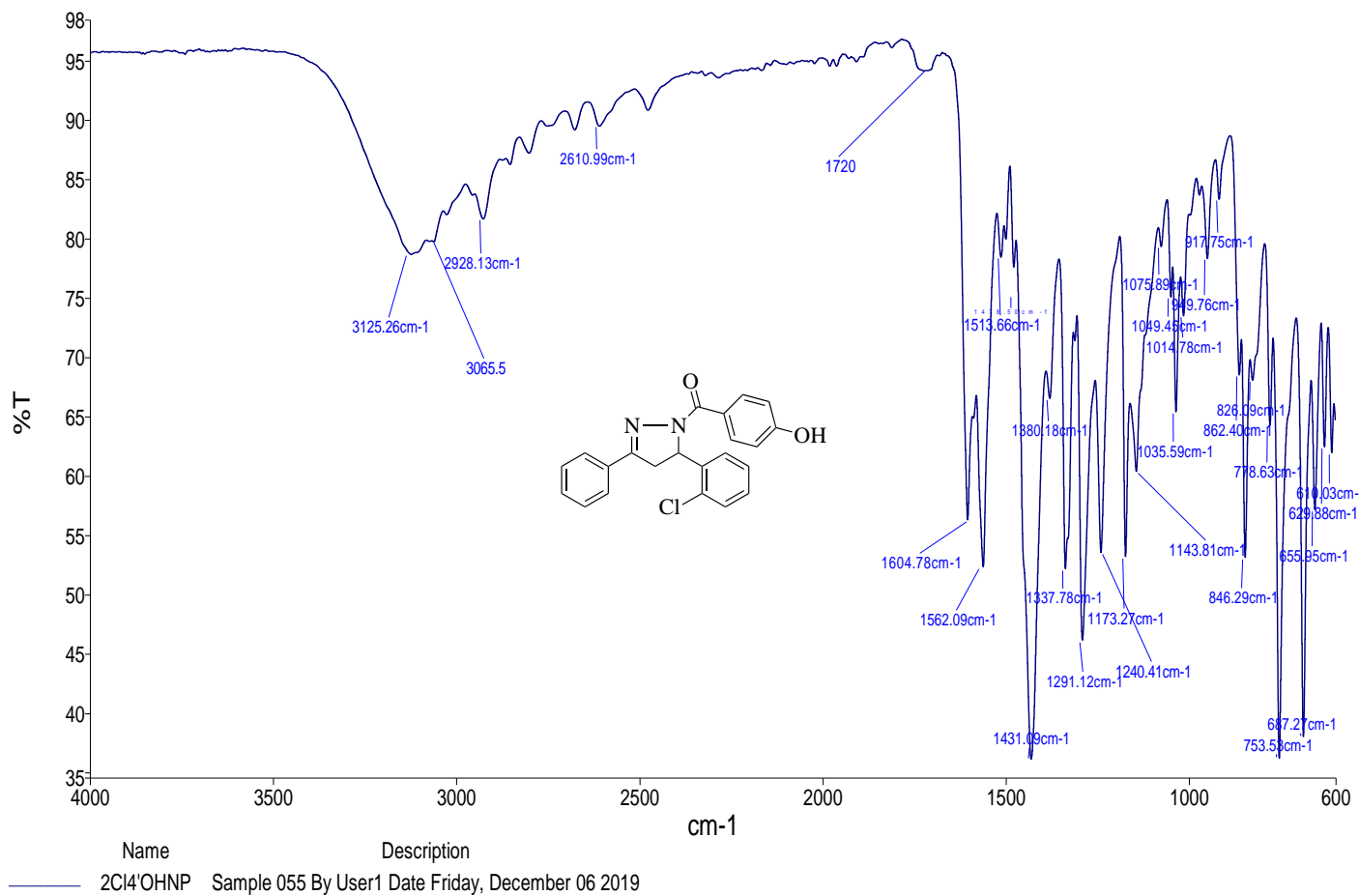
¹H-¹³C HMBC NMR spectrum of compound 5e

2CL4OHNP 20 (0.357) Cm (2:20)

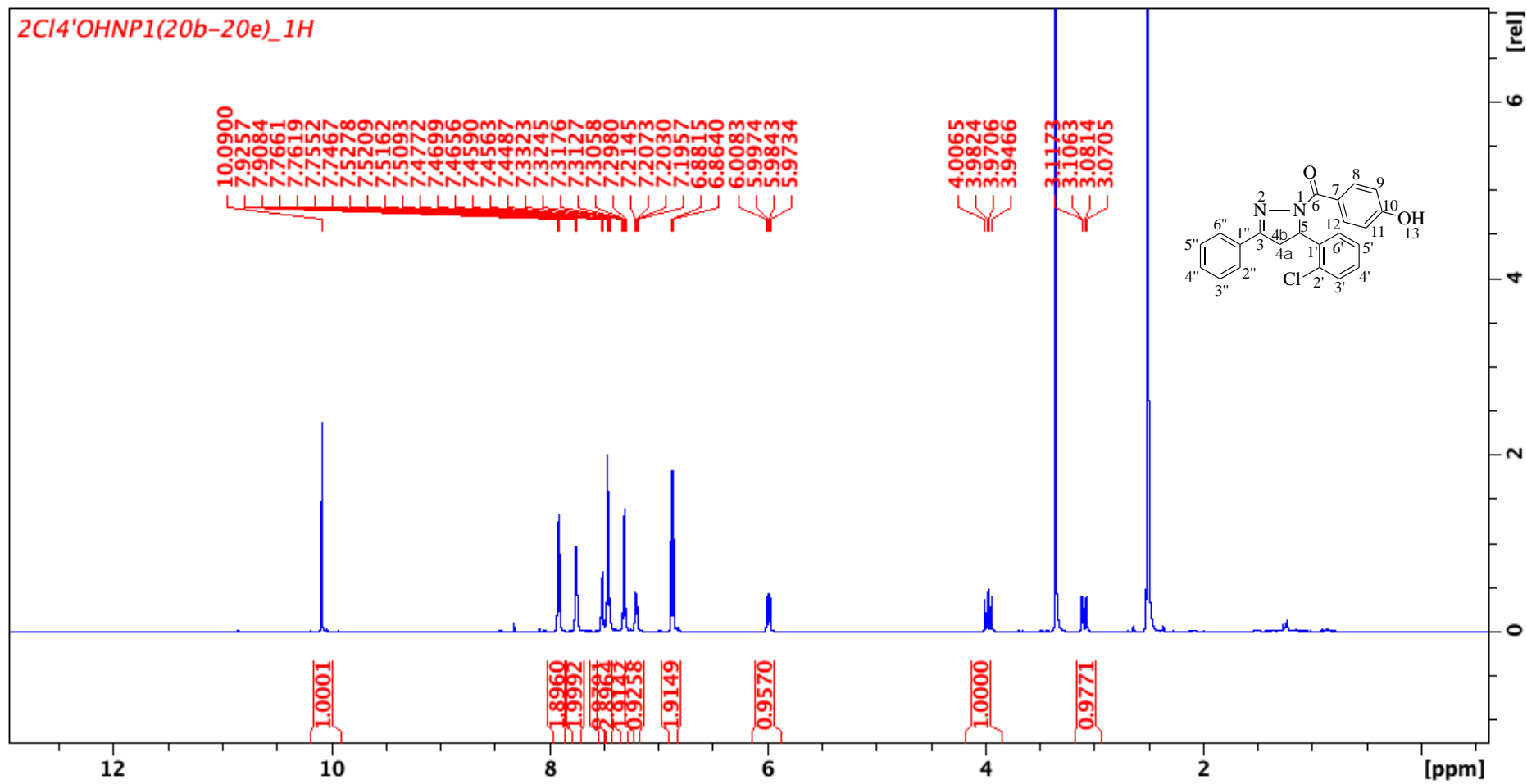
TOF MS ES+
1.52e6



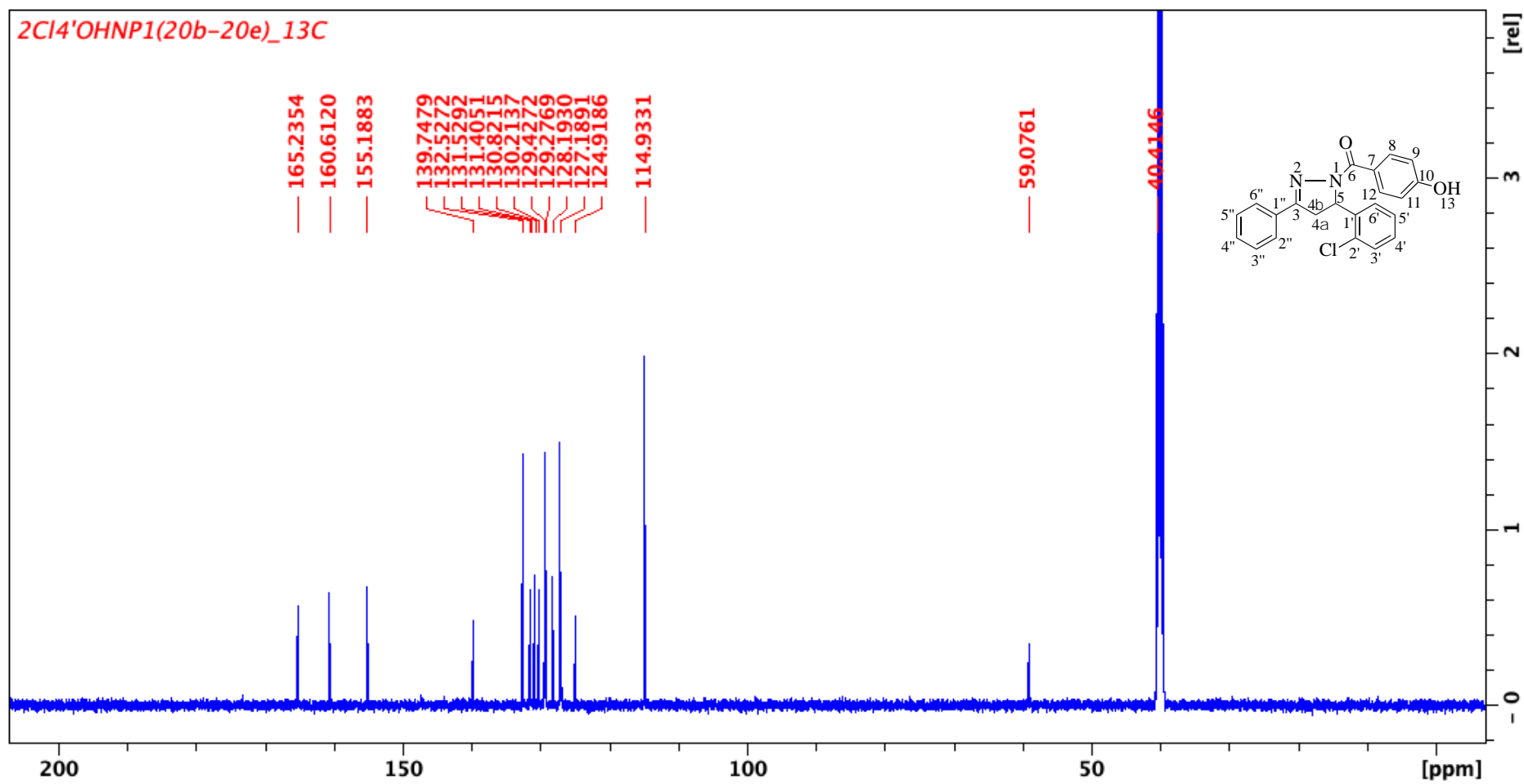
HRMS spectrum of compound **5f**



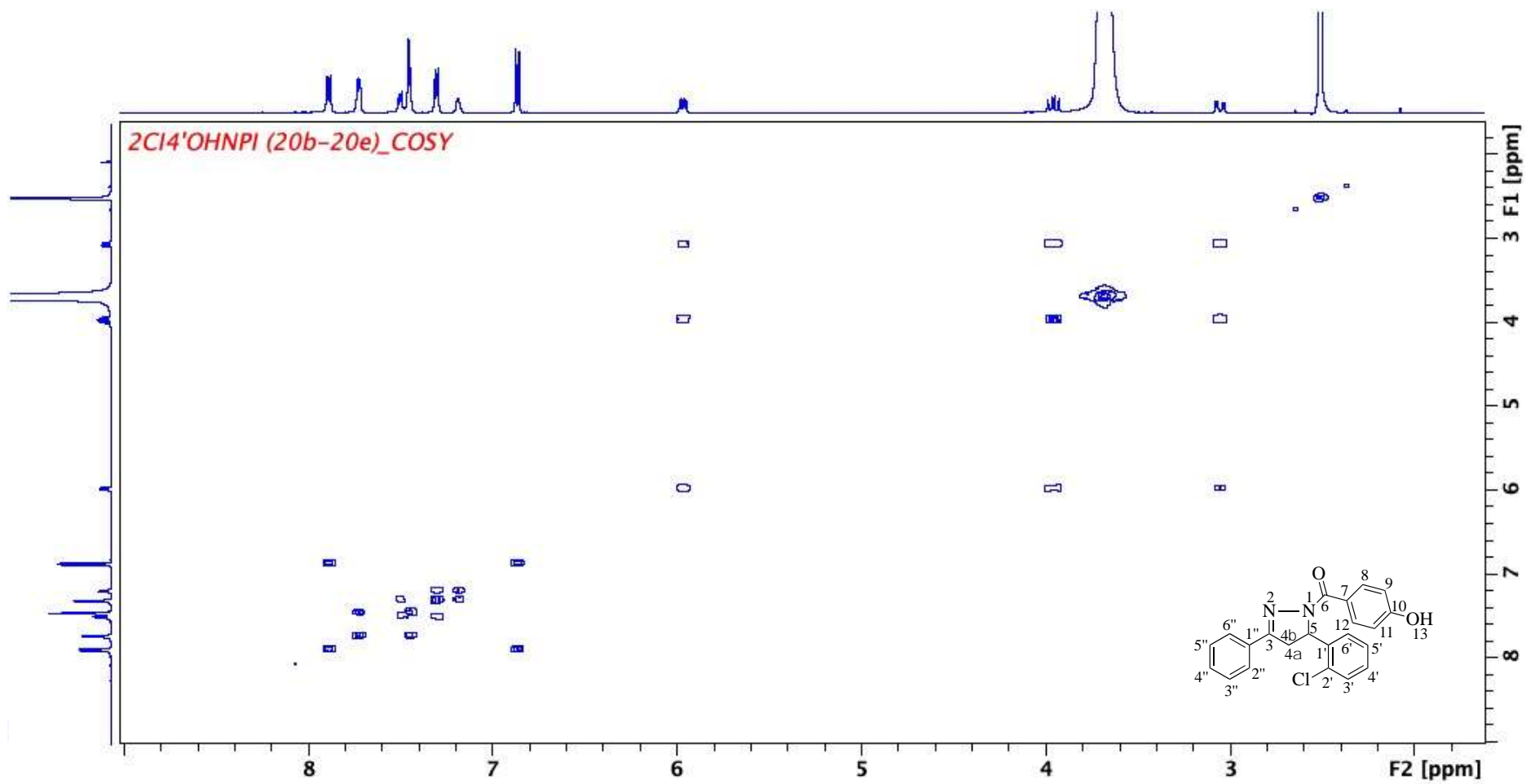
IR spectrum of compound **5f**



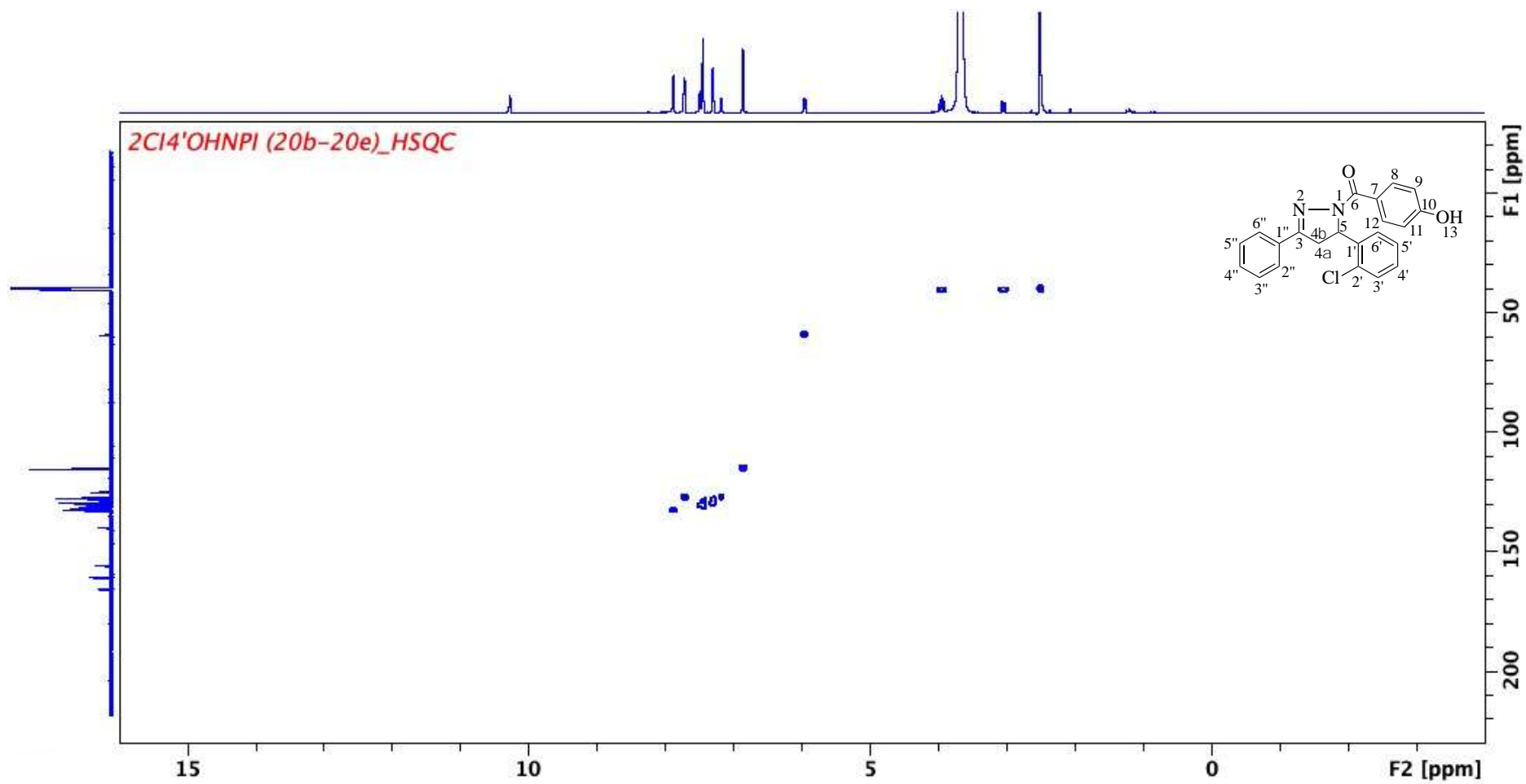
¹H NMR spectrum of compound **5f**



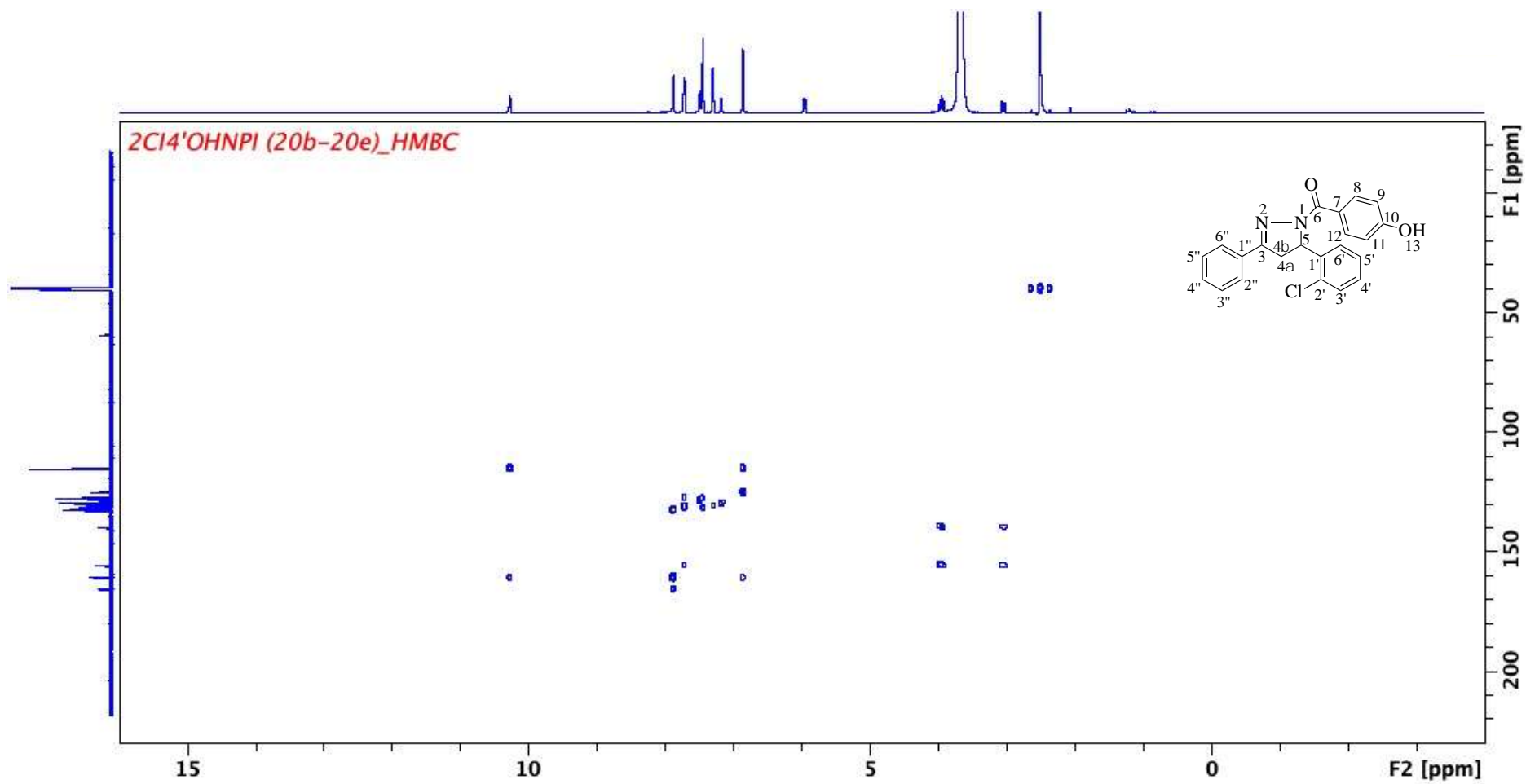
^{13}C NMR spectrum of compound **5f**



¹H-¹H COSY NMR spectrum of compound 5f



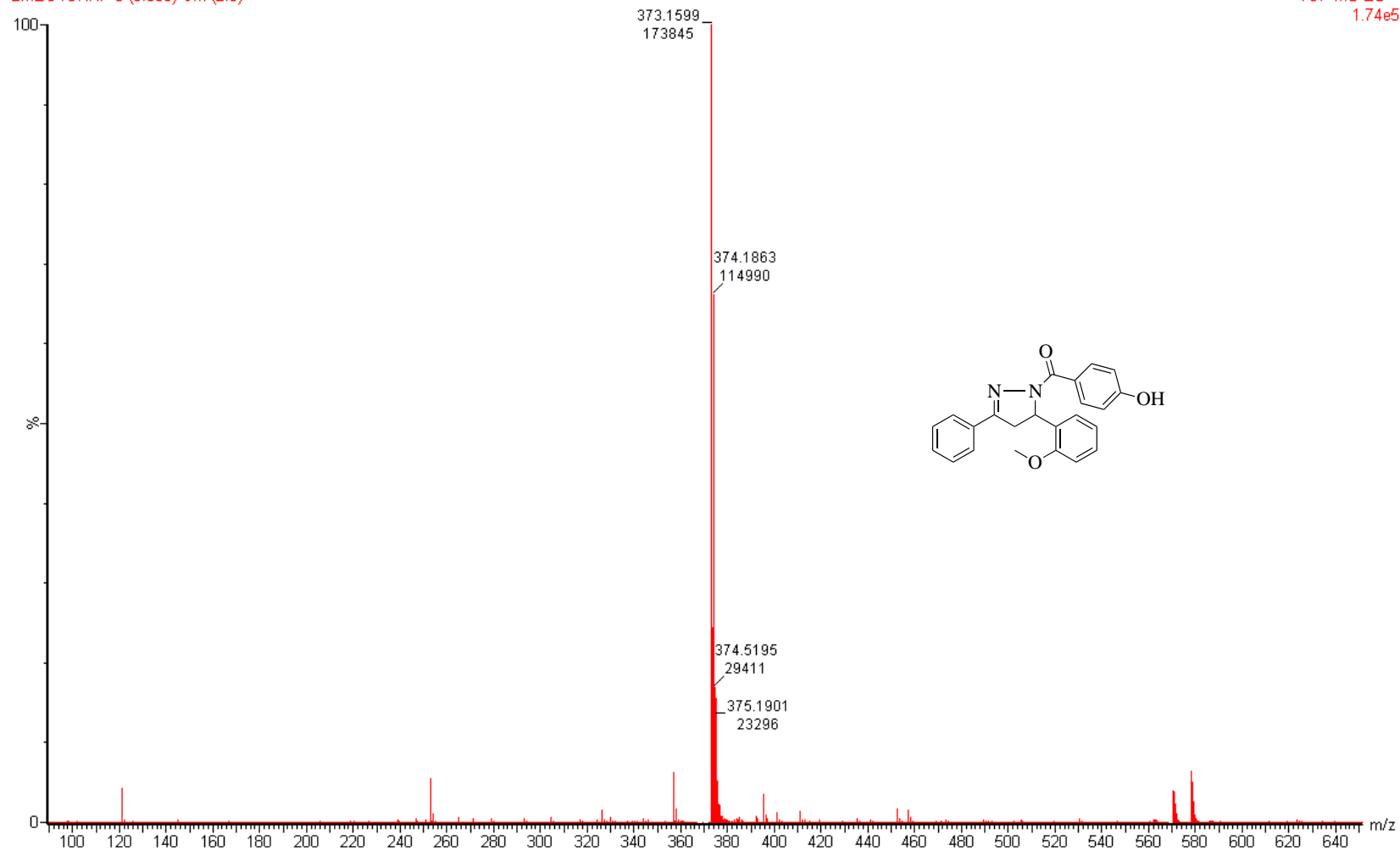
^1H - ^{13}C HSQC NMR spectrum of compound 5f



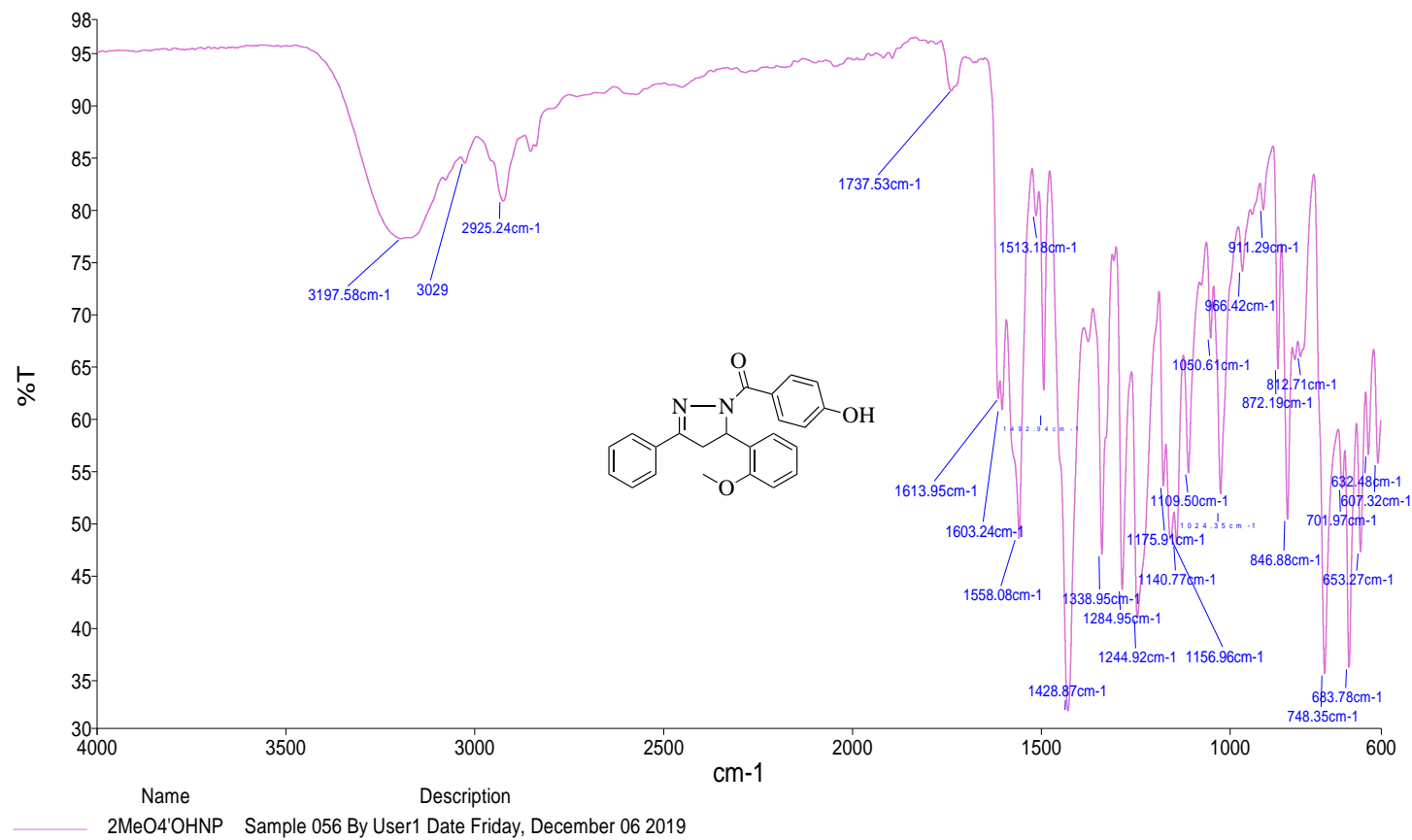
^1H - ^{13}C HMBC NMR spectrum of compound 5f

2MEO4OHNP 3 (0.068) Cm (2:3)

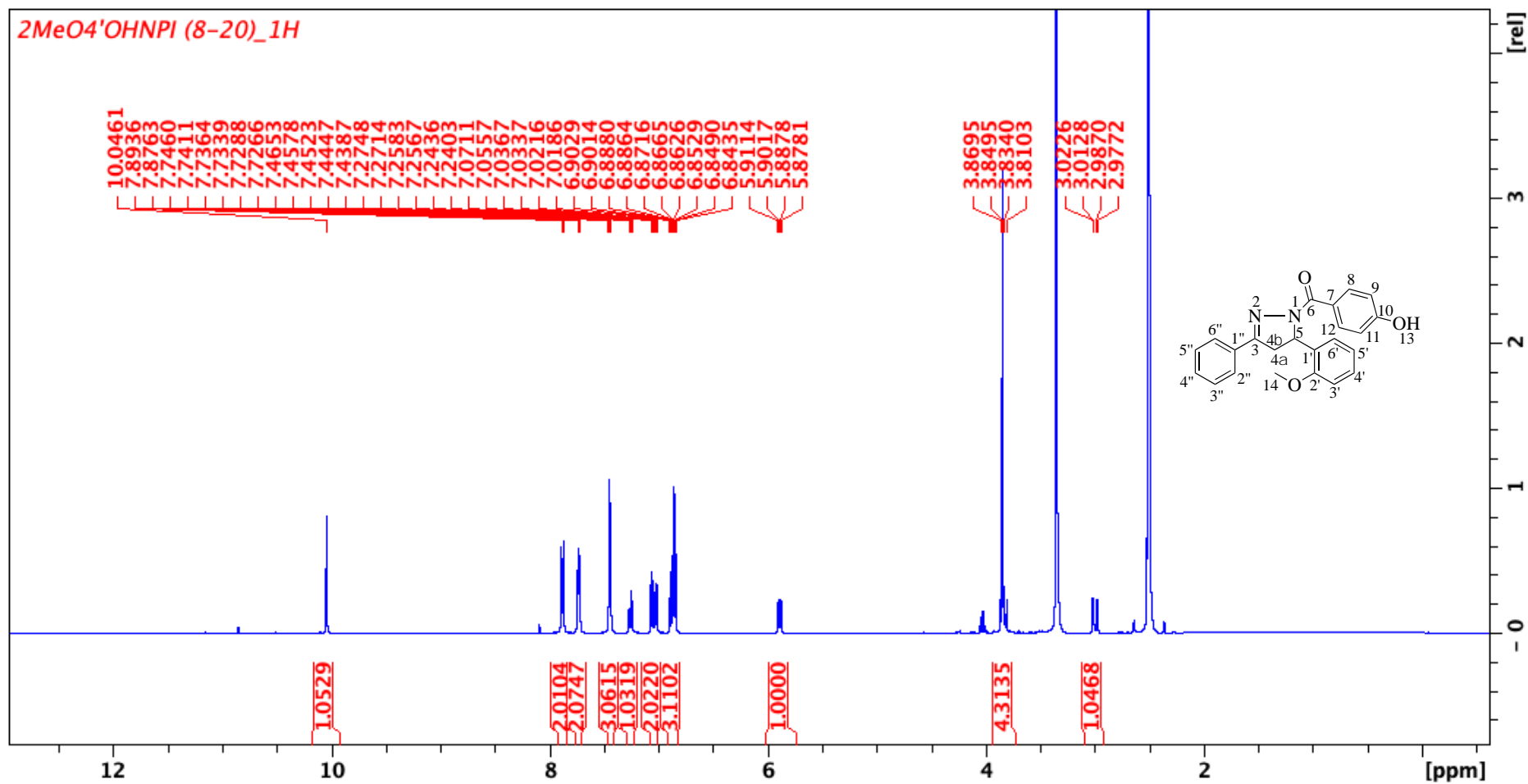
TOF MS ES+
1.74e5



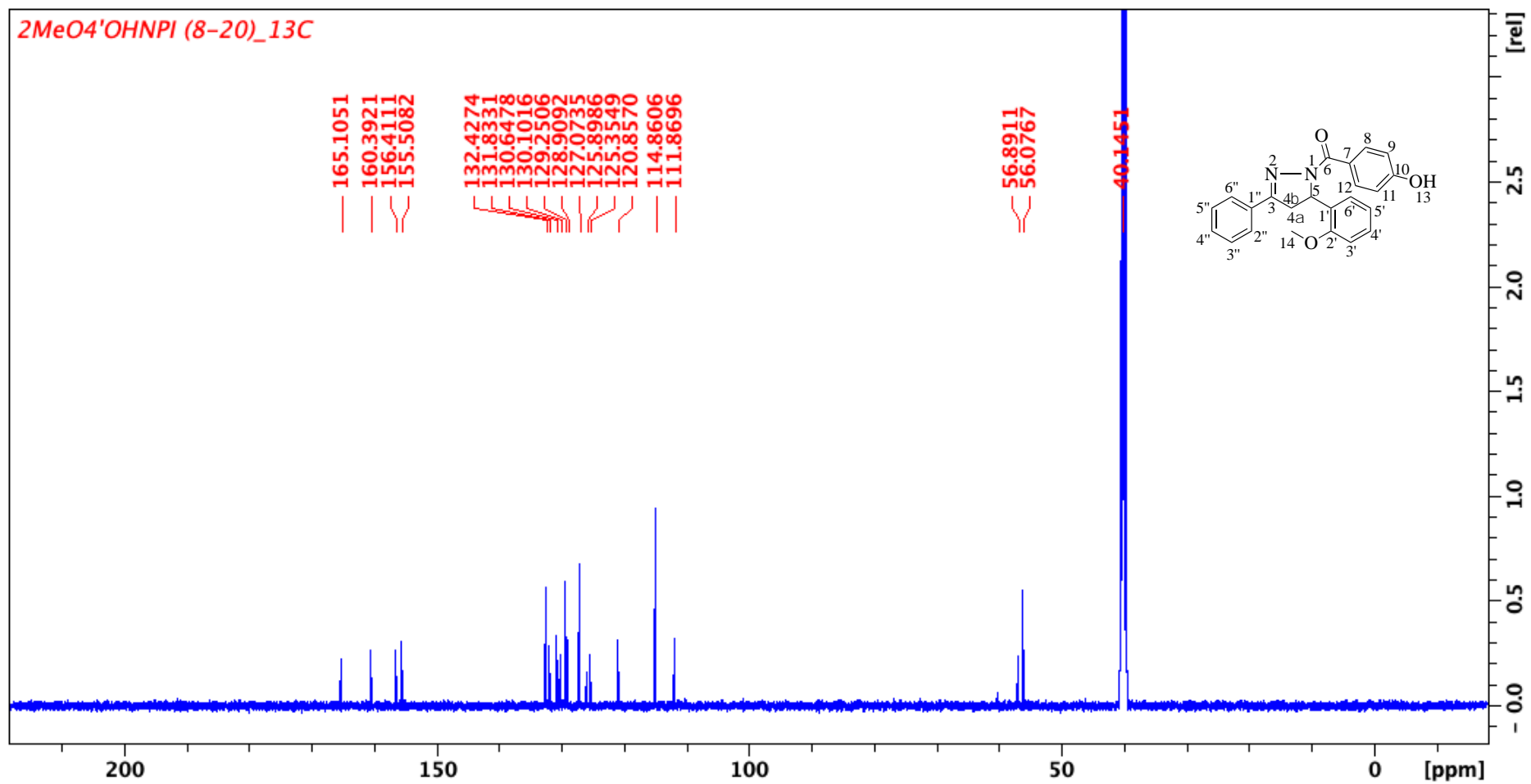
HRMS spectrum of compound **5g**



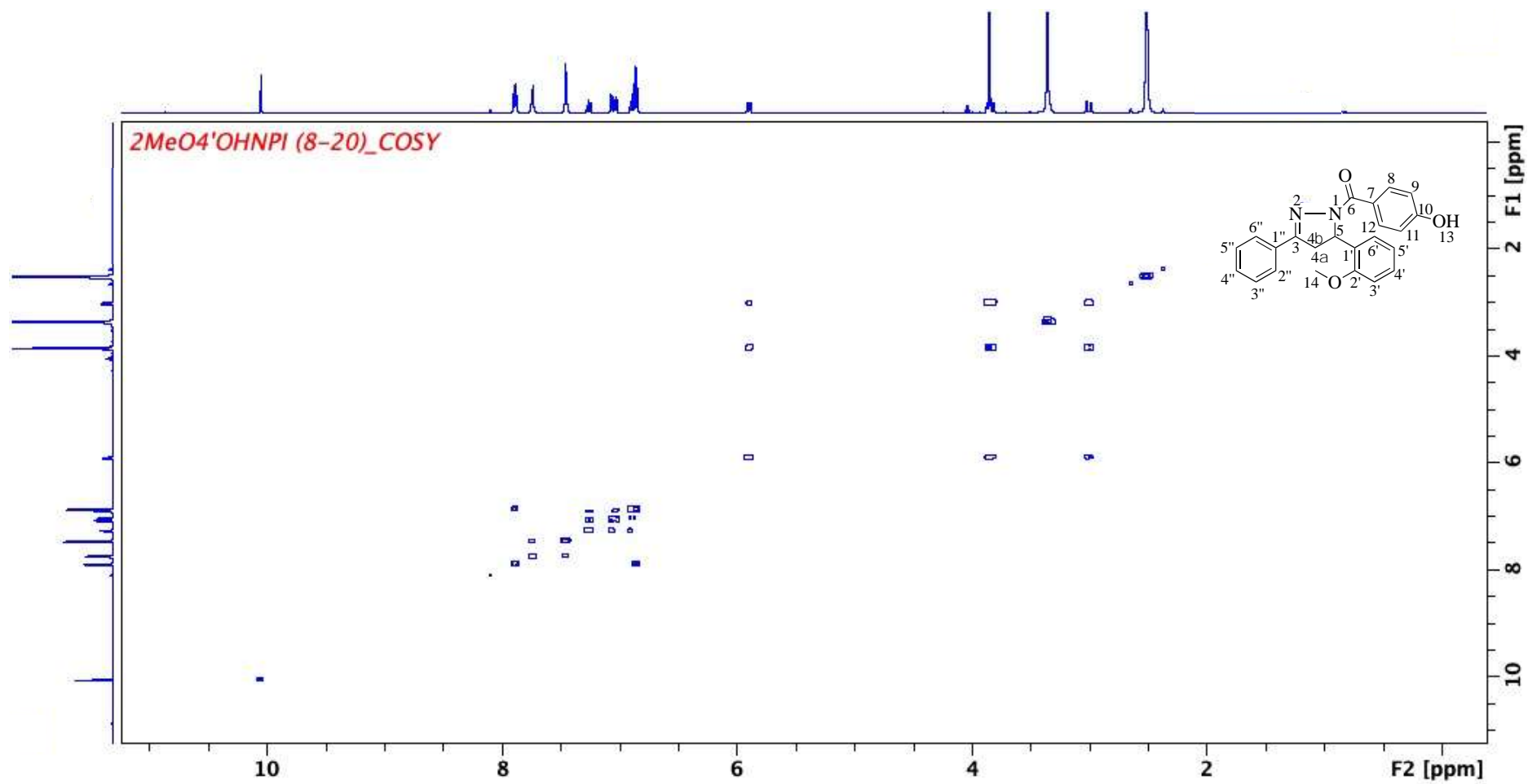
IR spectrum of compound 5g



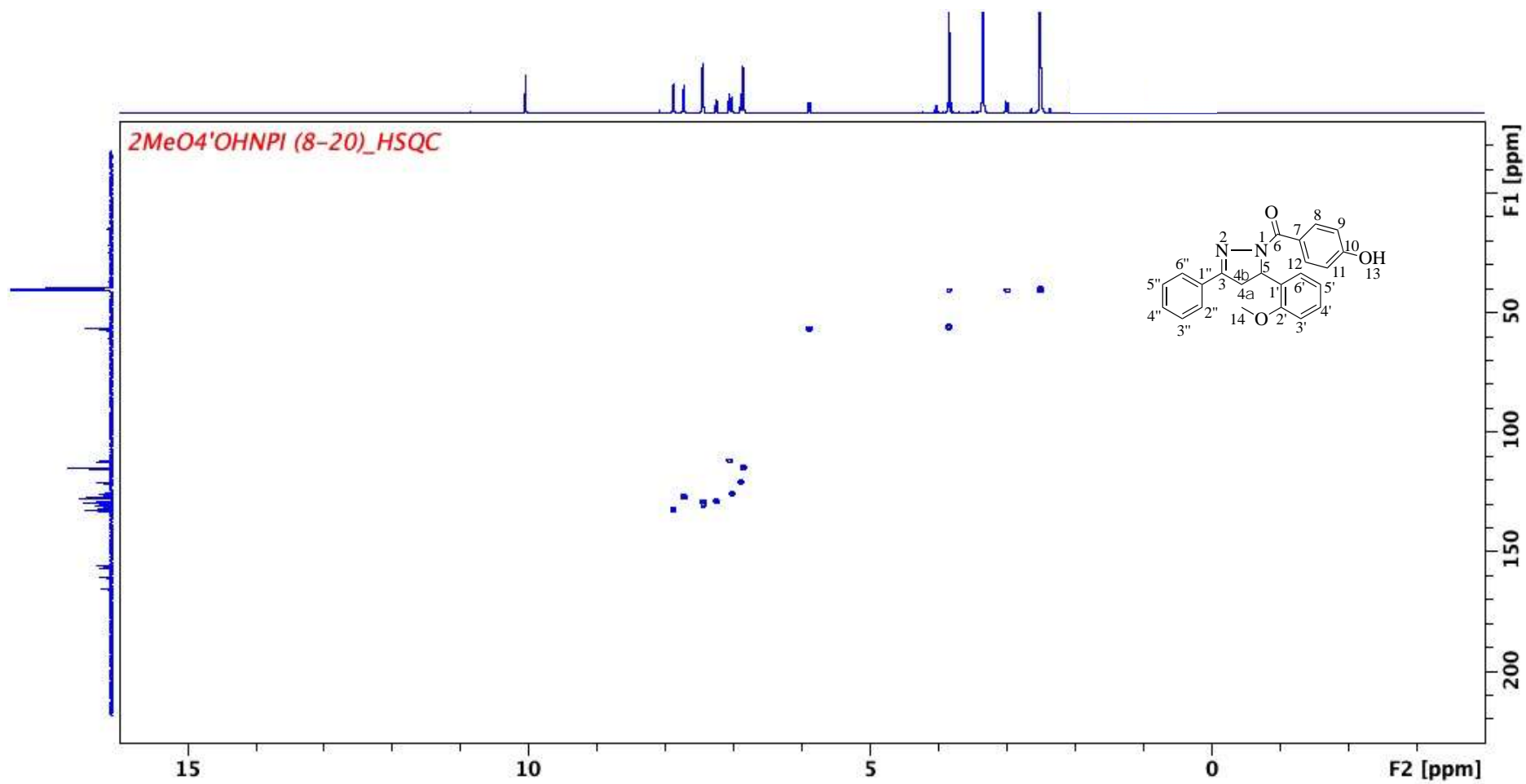
^1H NMR spectrum of compound 5g



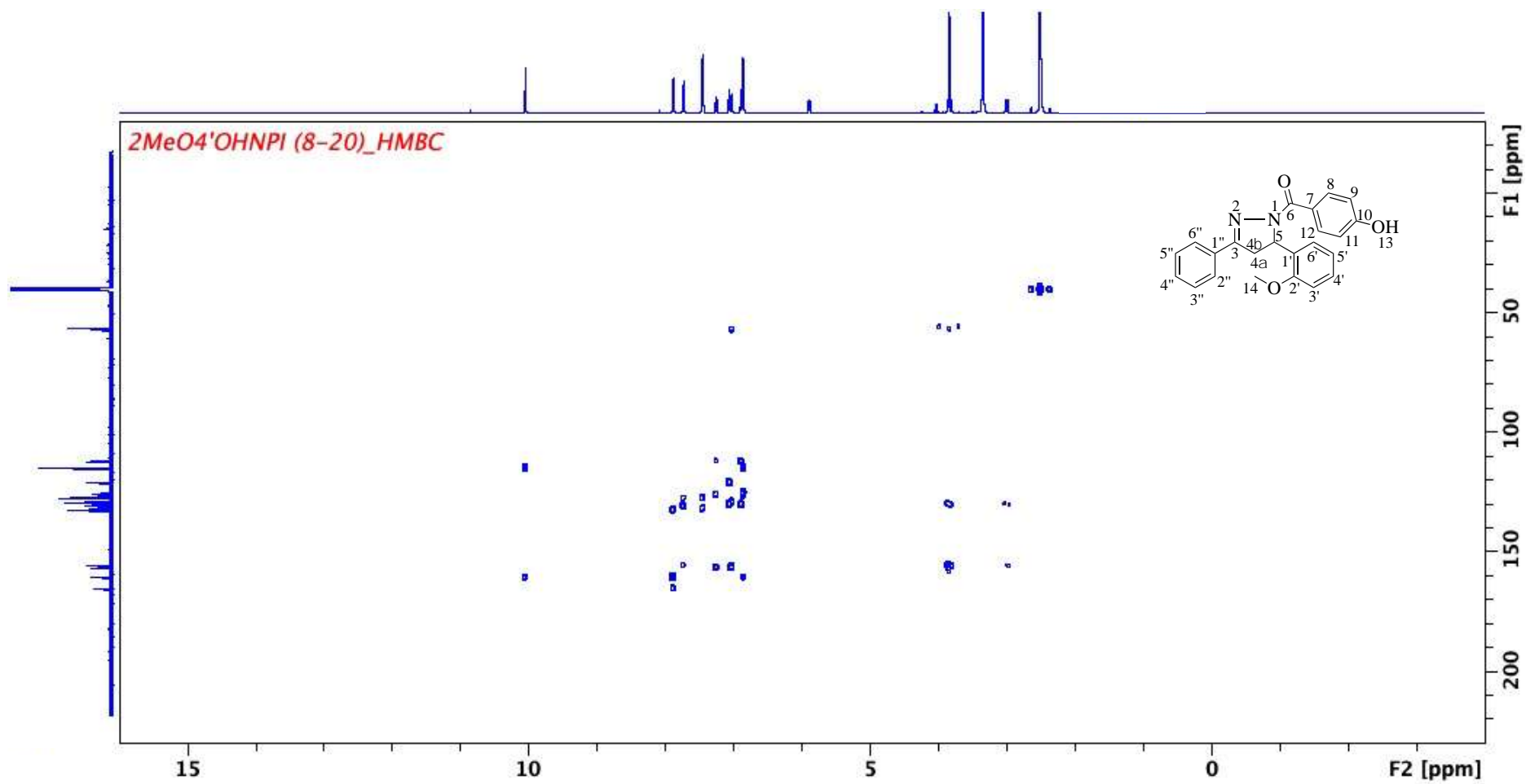
¹³C NMR spectrum of compound 5g



¹H-¹H COSY NMR spectrum of compound 5g



^1H - ^{13}C HSQC NMR spectrum of compound 5g



^1H - ^{13}C HMBC NMR spectrum of compound 5g