Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Catalyst-free, one-pot, four-component green synthesis of functionalized 1-(2-fluorophenyl)-1,4-dihydropyridines under ultrasound irradiation

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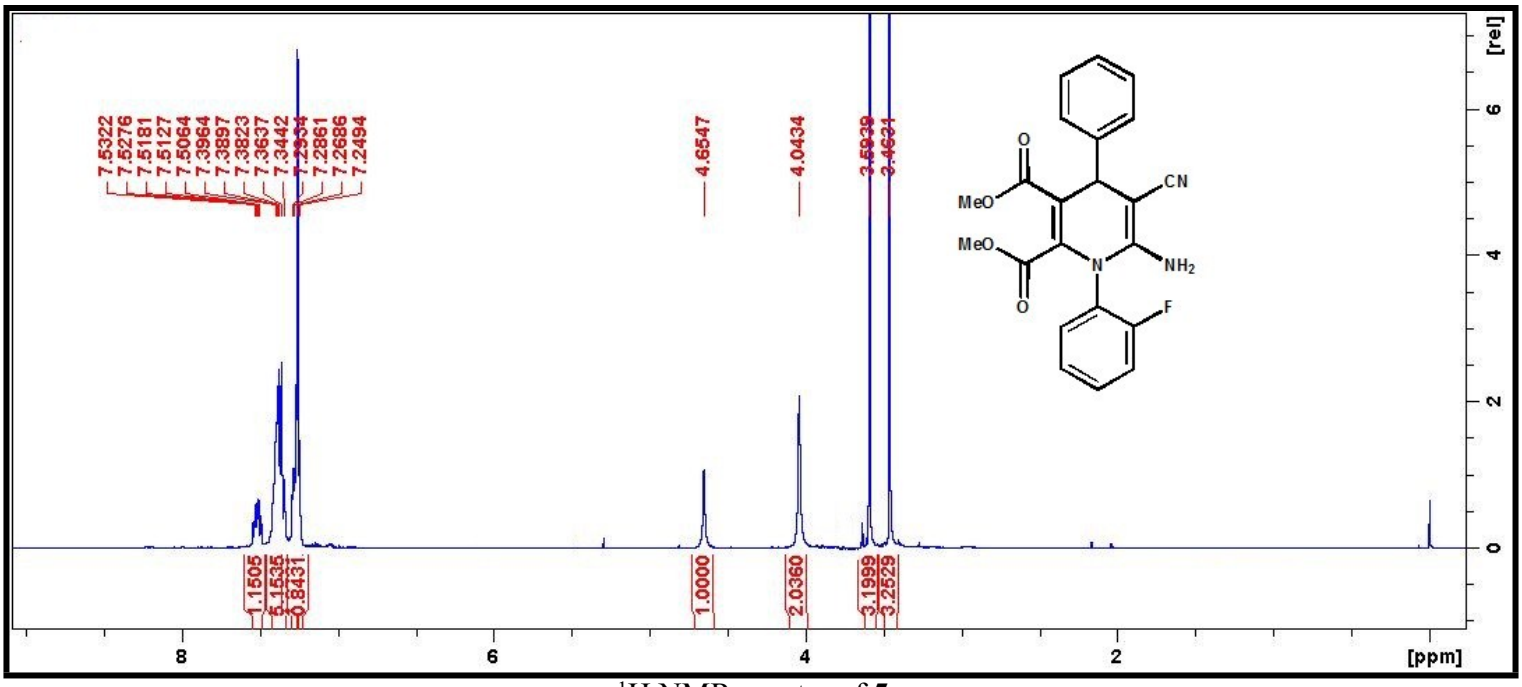
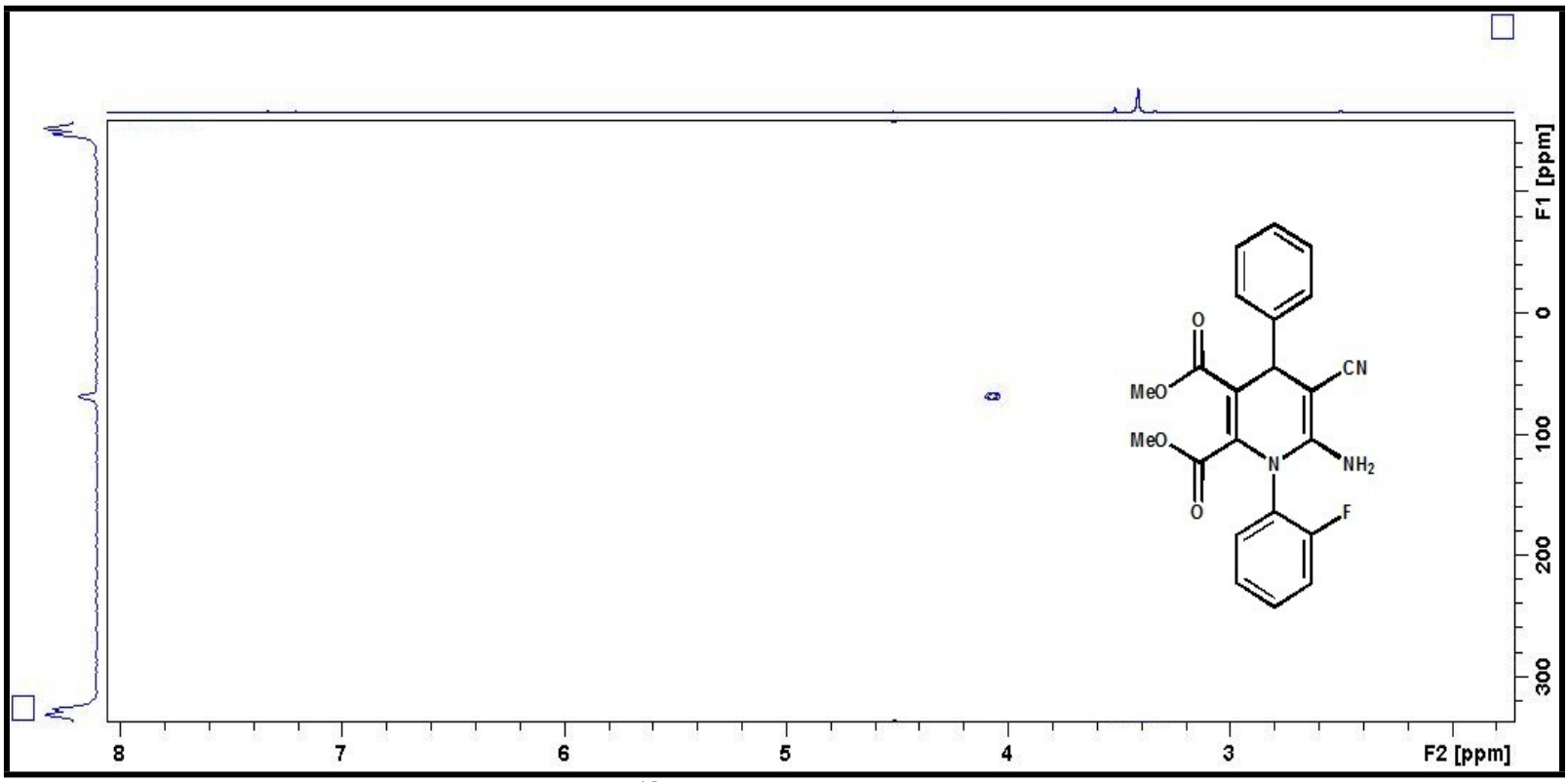
Materials, methods and instruments

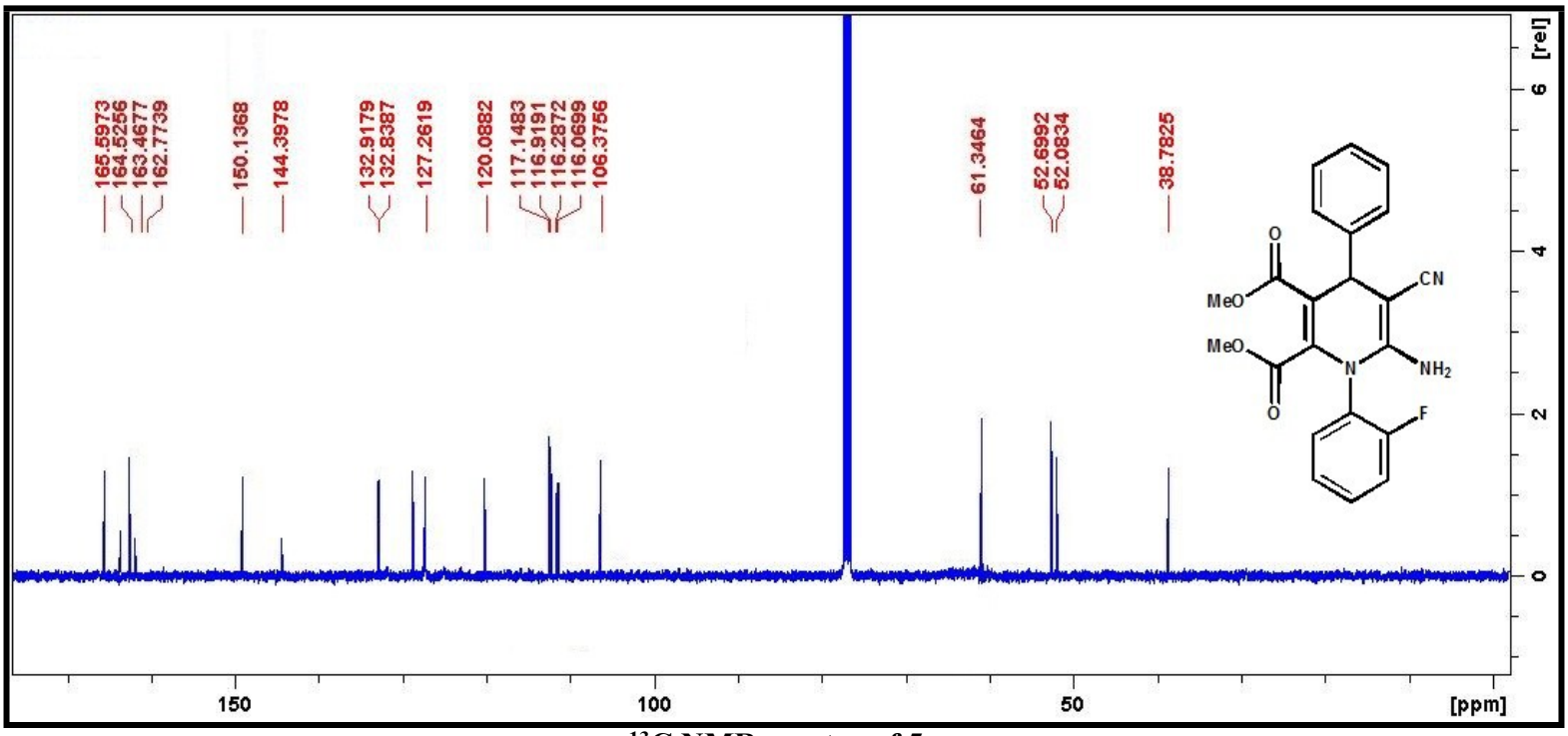
All chemicals used were reagent grade and were used as received without further purification. ^{1}H NMR, ^{13}C NMR, ^{15}N NMR and ^{19}F NMR spectra were recorded at 25 ^{o}C at 400 MHz, 100 MHz, 40.55 MHz and 376.58 MHz (Bruker Avance) instrument respectively, using TMS as internal standard. Chemical shifts are given in parts per million (ppm). The FT-IR spectroscopy of samples was carried out on a Perkin Elmer Perkin Elmer Precisely 100 FT-IR spectrometer in the 400-4000 cm^{-1} region. The HRMS were recorded on a waters micromass LCT premier mass spectrometer using electrospray ionization in the positive or negative mode. The ultrasonic assisted reactions are carried out in a ‘‘Spectralab model UMC 20 Ultrsonic cleaner” with a frequency of 40 kHz and a nominal power 250 W. Melting points were recorded on a hot stage melting point apparatus Ernst Leitz Wetzlar, Germany and were uncorrected. All the reactions and the purity of products were monitored using thin layer chromatography (TLC) on aluminum-backed plates coated with Merck Kieselgel 60 F254 silica gel, visualizing the spots under ultraviolet light and iodine chamber.



^{1}H NMR spectra of **5a**



^{15}N NMR spectra of **5a**

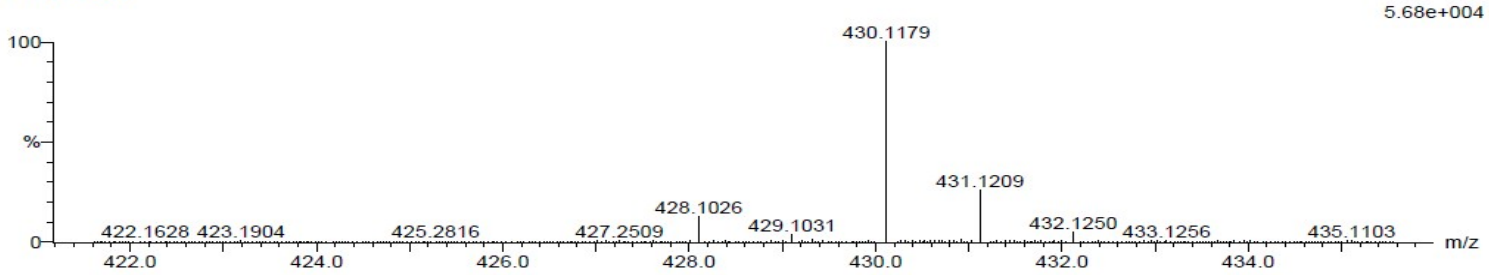


^{13}C NMR spectra of 5a

Elemental Composition Report Page 1

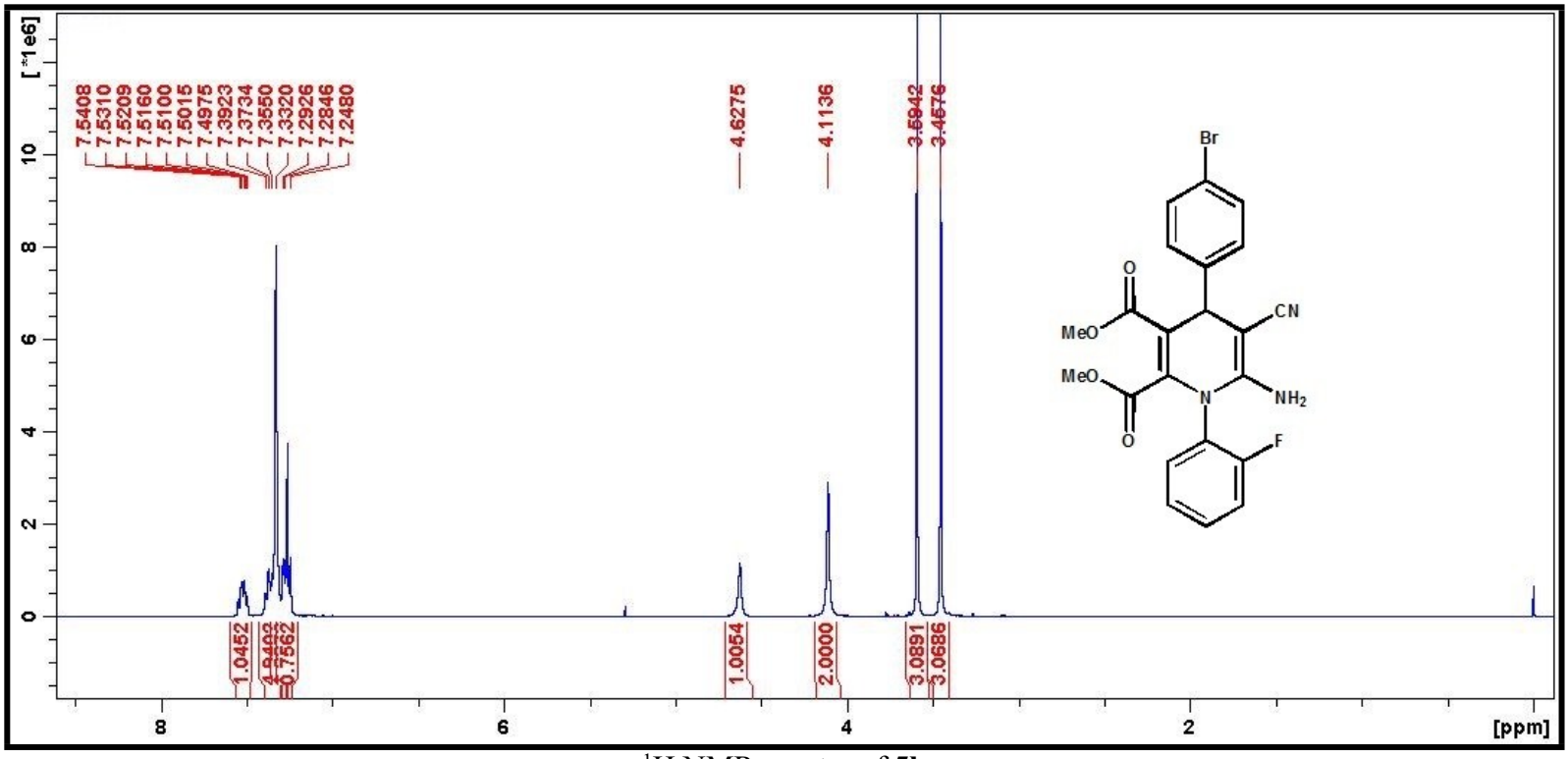
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
12 formula(e) evaluated with 1 results within limits (up to 20 closest results for each mass)
Elements Used:
C: 20-25 H: 15-20 N: 0-5 O: 0-5 F: 1-1 Na: 1-1
2FA19 44 (1.451) Cm (1:61)
TOF MS ES+



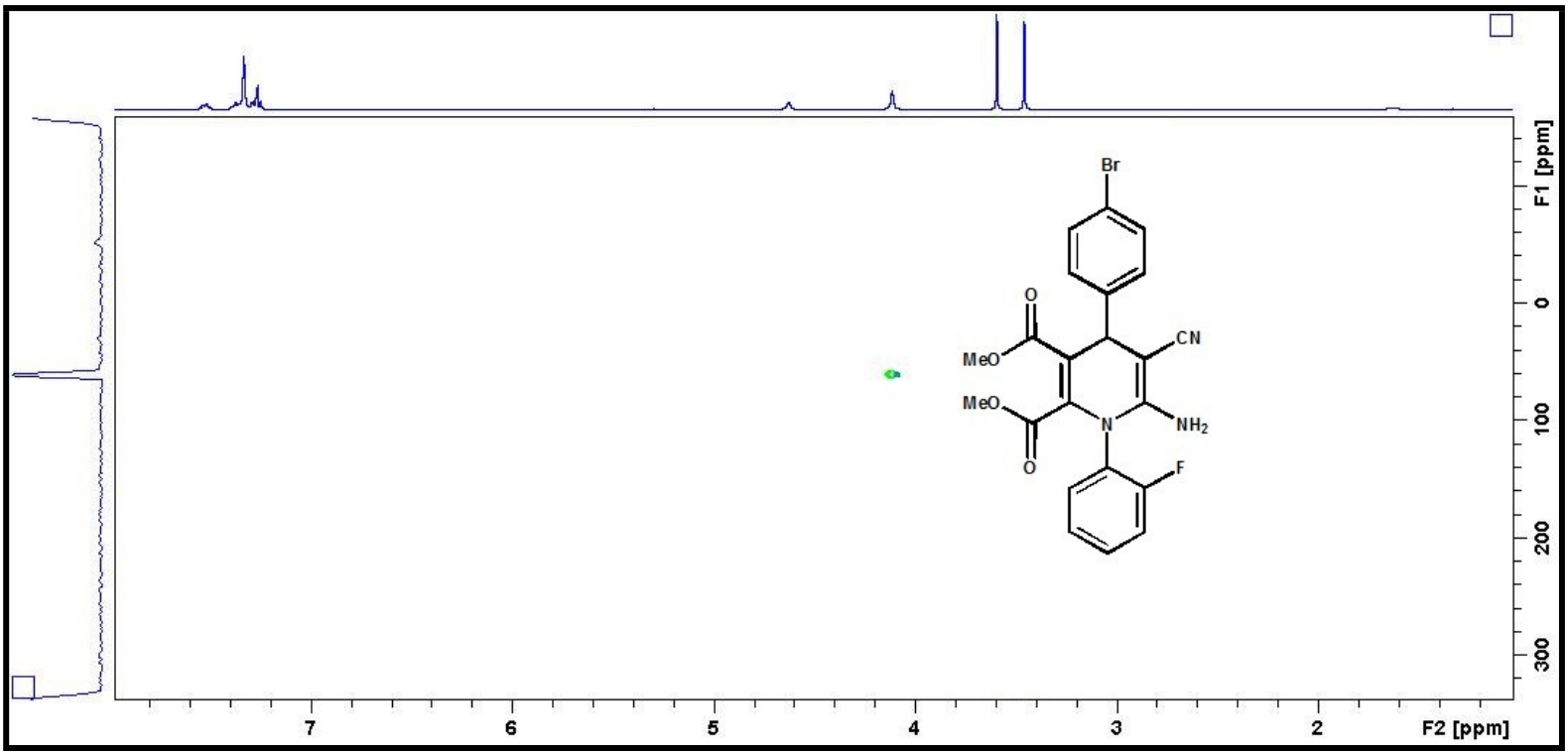
Minimum:				-1.5			
Maximum:		5.0	5.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
430.1179	430.1179	0.0	0.0	14.5	489.0	0.0	C22 H18 N3 O4 F Na

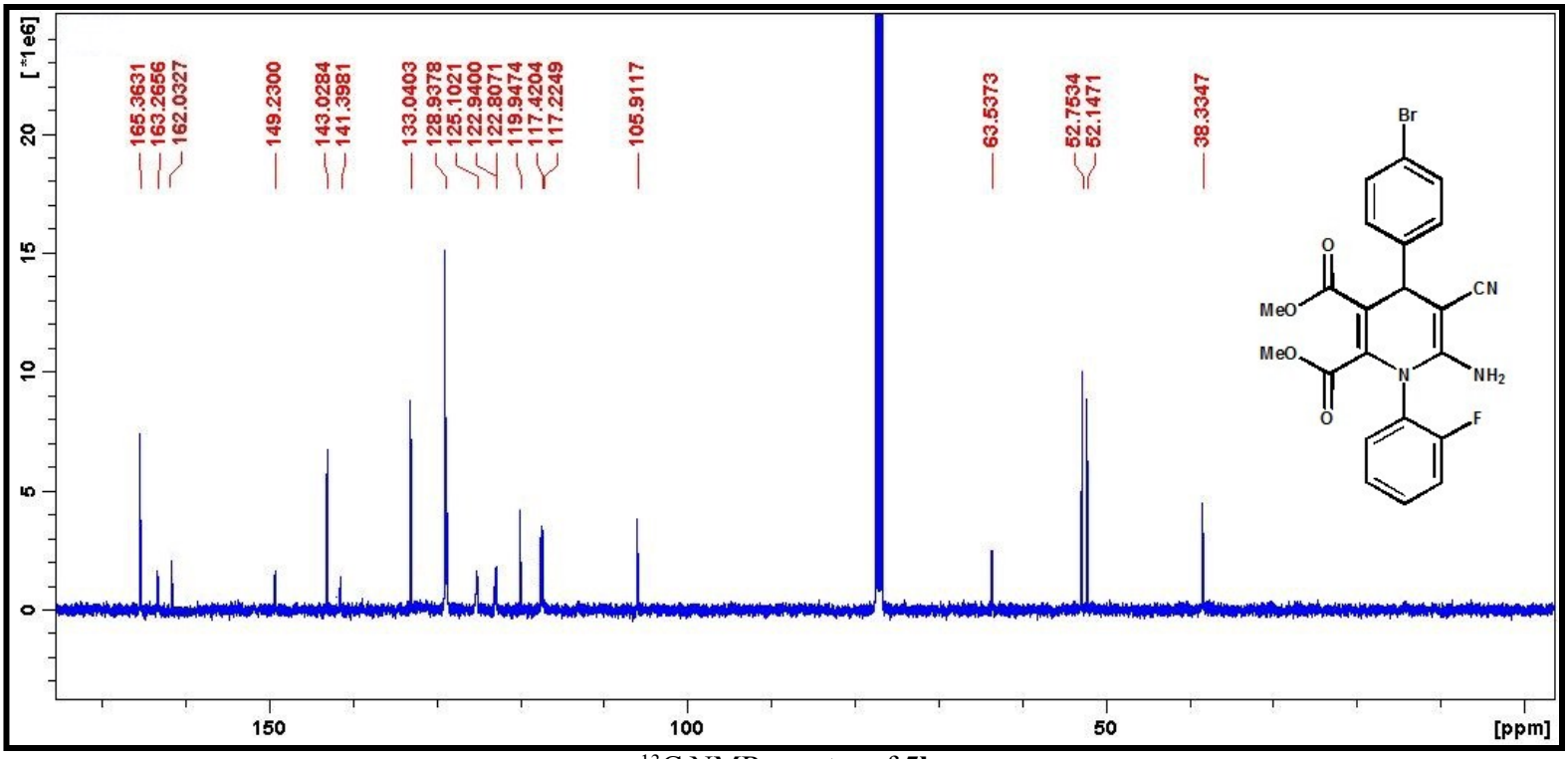
HRMS spectra of 5a



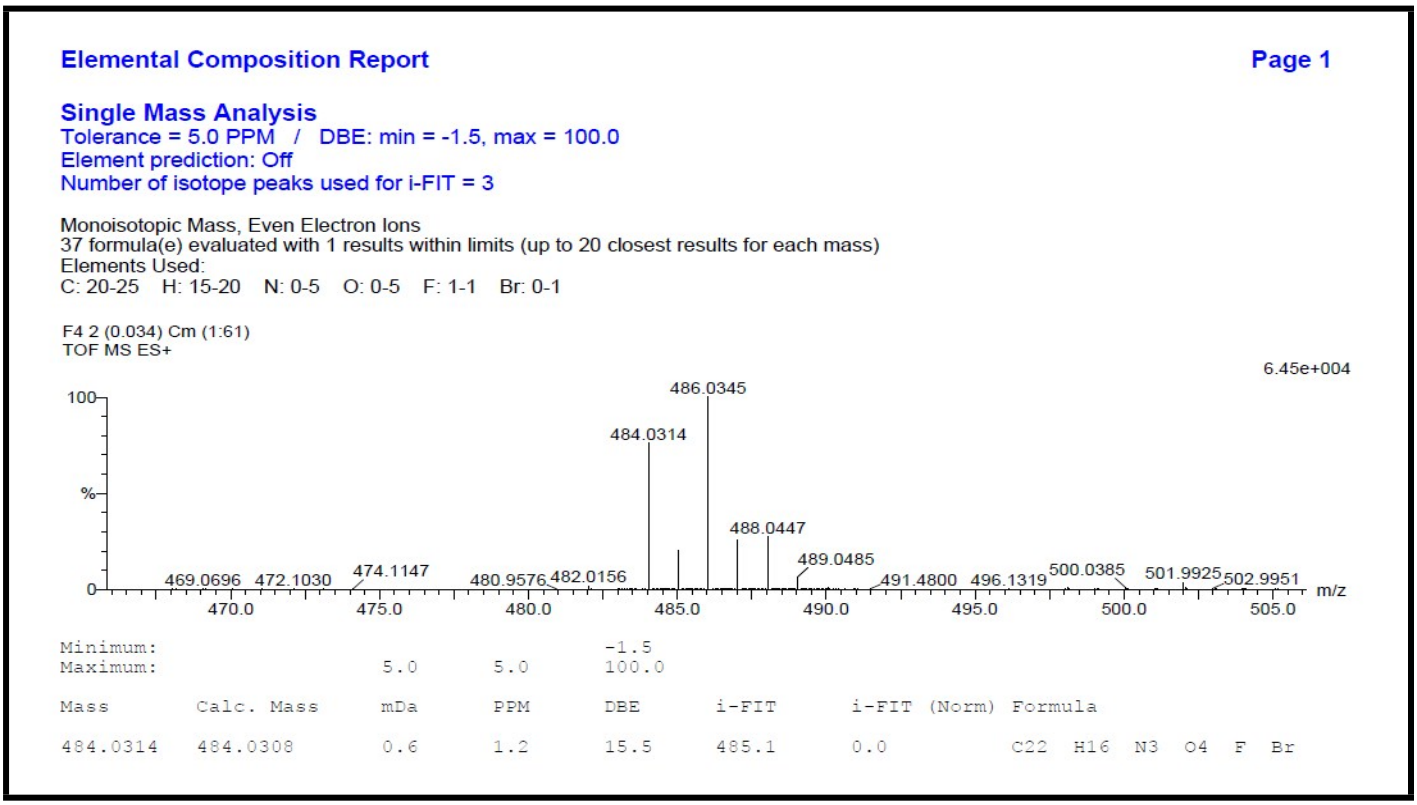
^{1}H NMR spectra of **5b**

^{15}N NMR spectra of **5b**

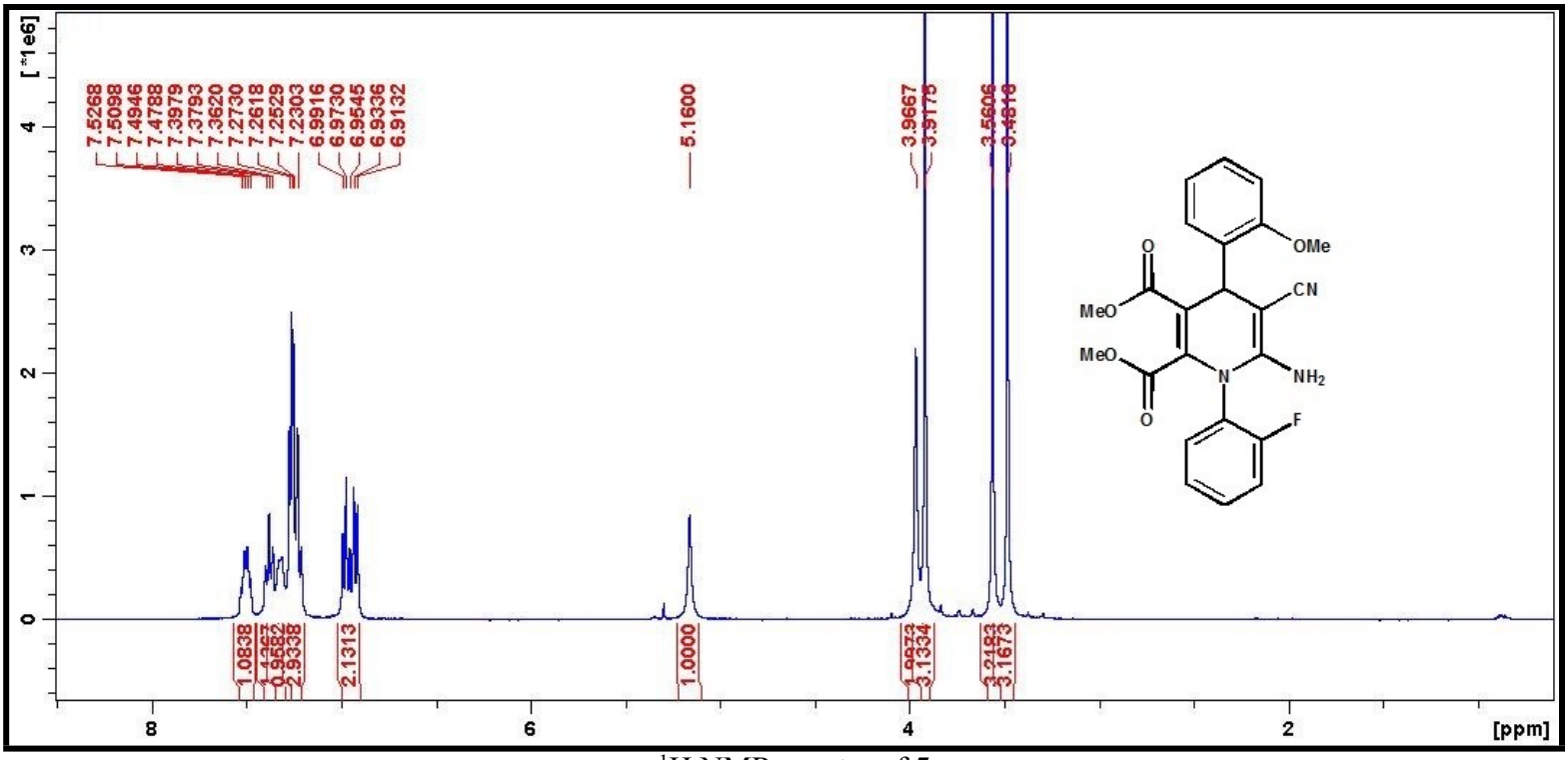




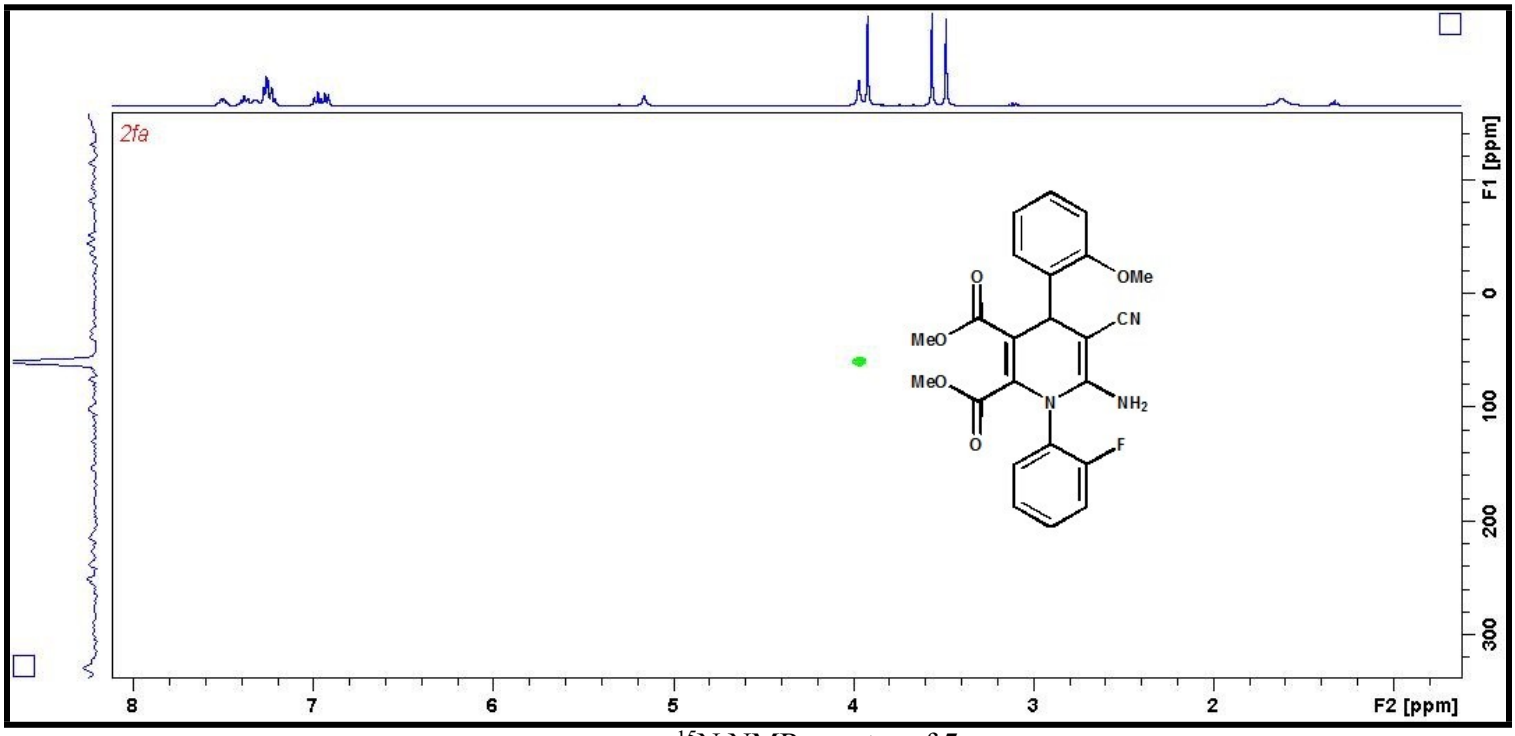
^{13}C NMR spectra of **5b**



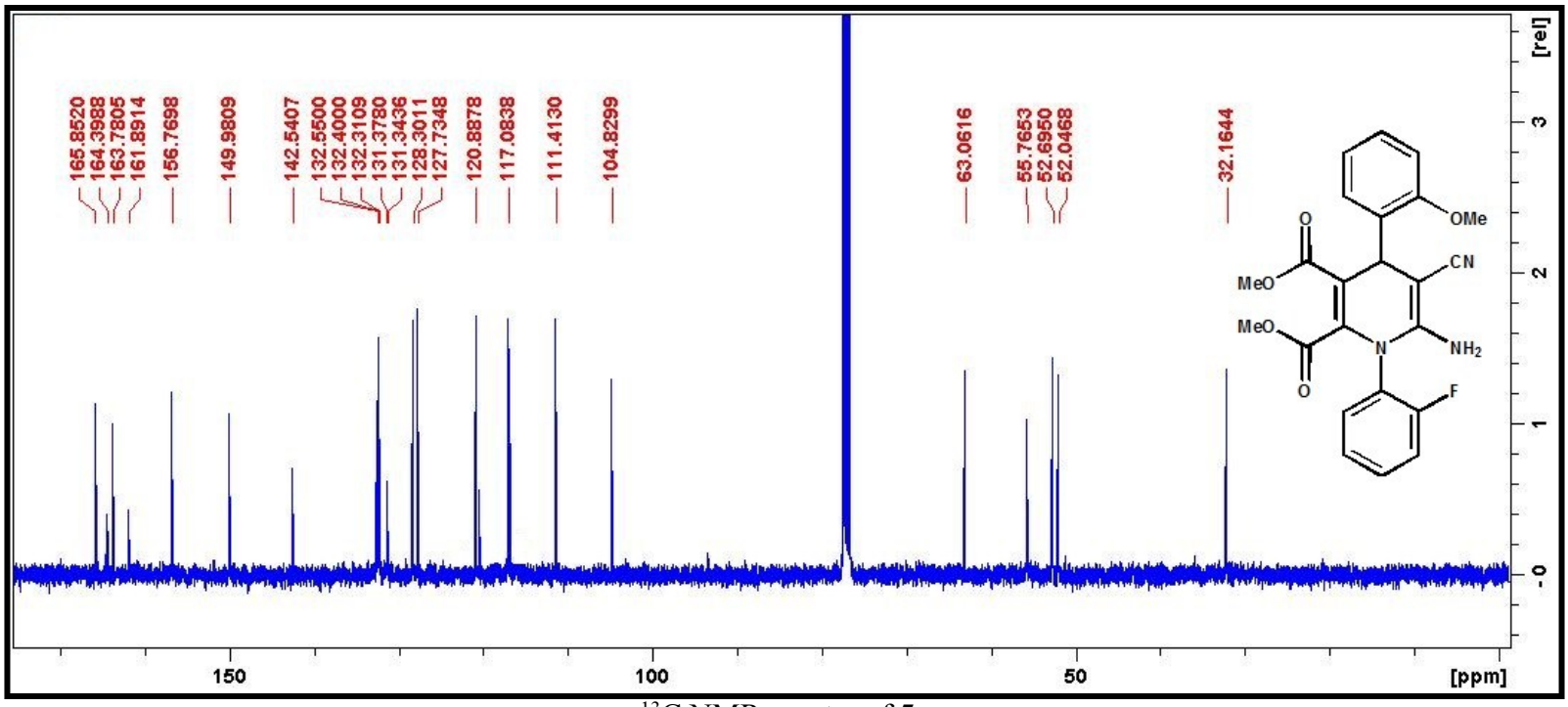
HRMS spectra of **5b**



^{1}H NMR spectra of **5c**



^{15}N NMR spectra of **5c**

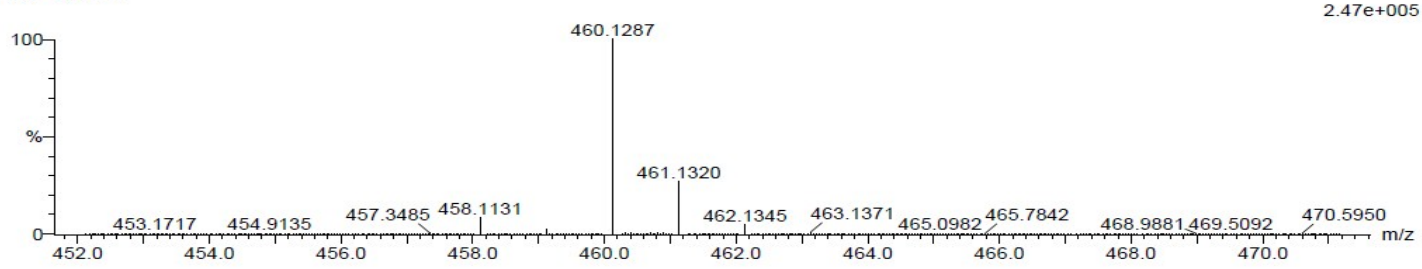


^{13}C NMR spectra of **5c**

Elemental Composition Report Page 1

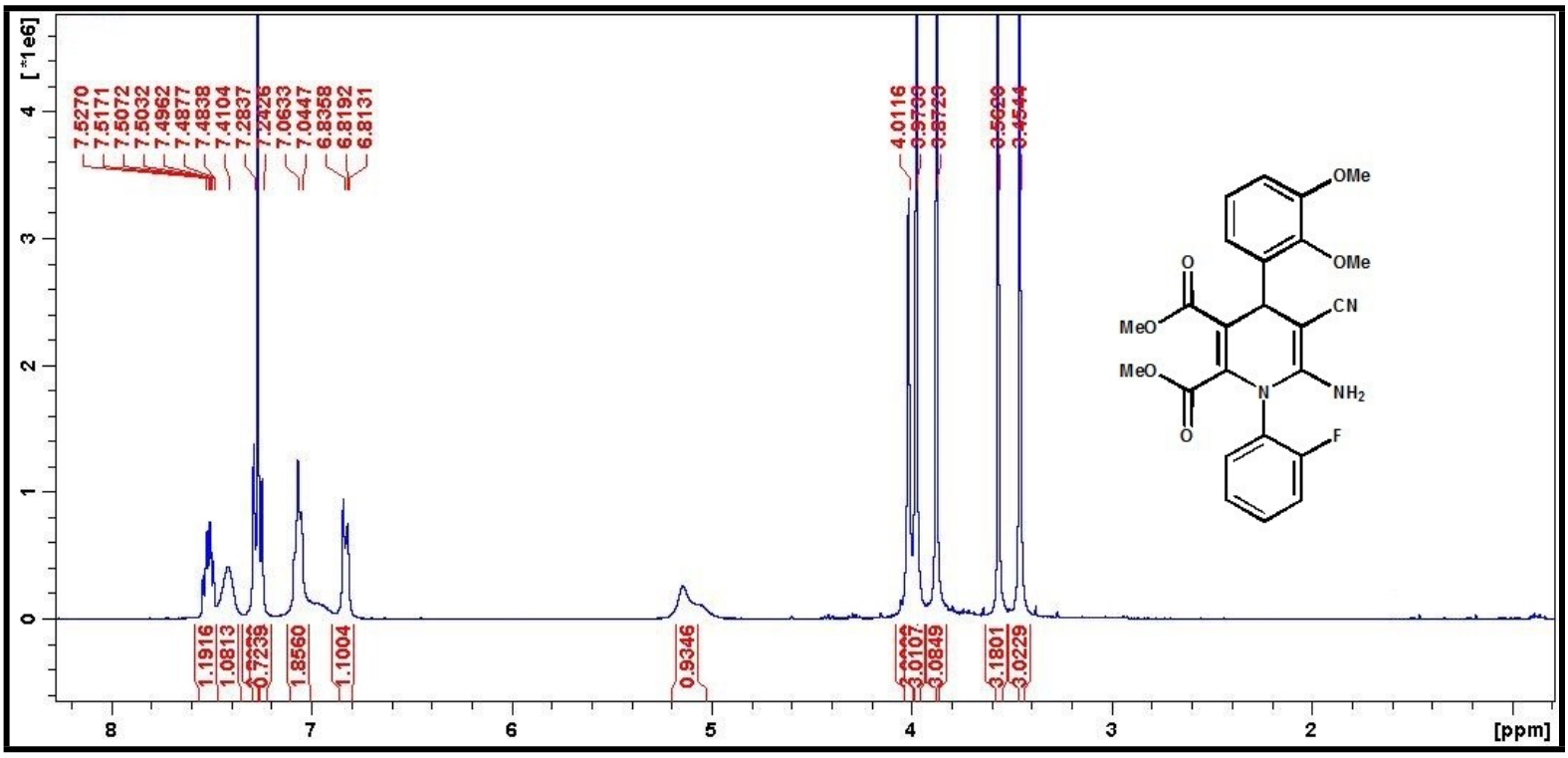
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
38 formula(e) evaluated with 1 results within limits (up to 20 closest results for each mass)
Elements Used:
C: 20-25 H: 15-25 N: 0-5 O: 0-10 F: 1-1 Na: 1-1
2FA2 14 (0.439) Cm (1:61)
TOF MS ES+

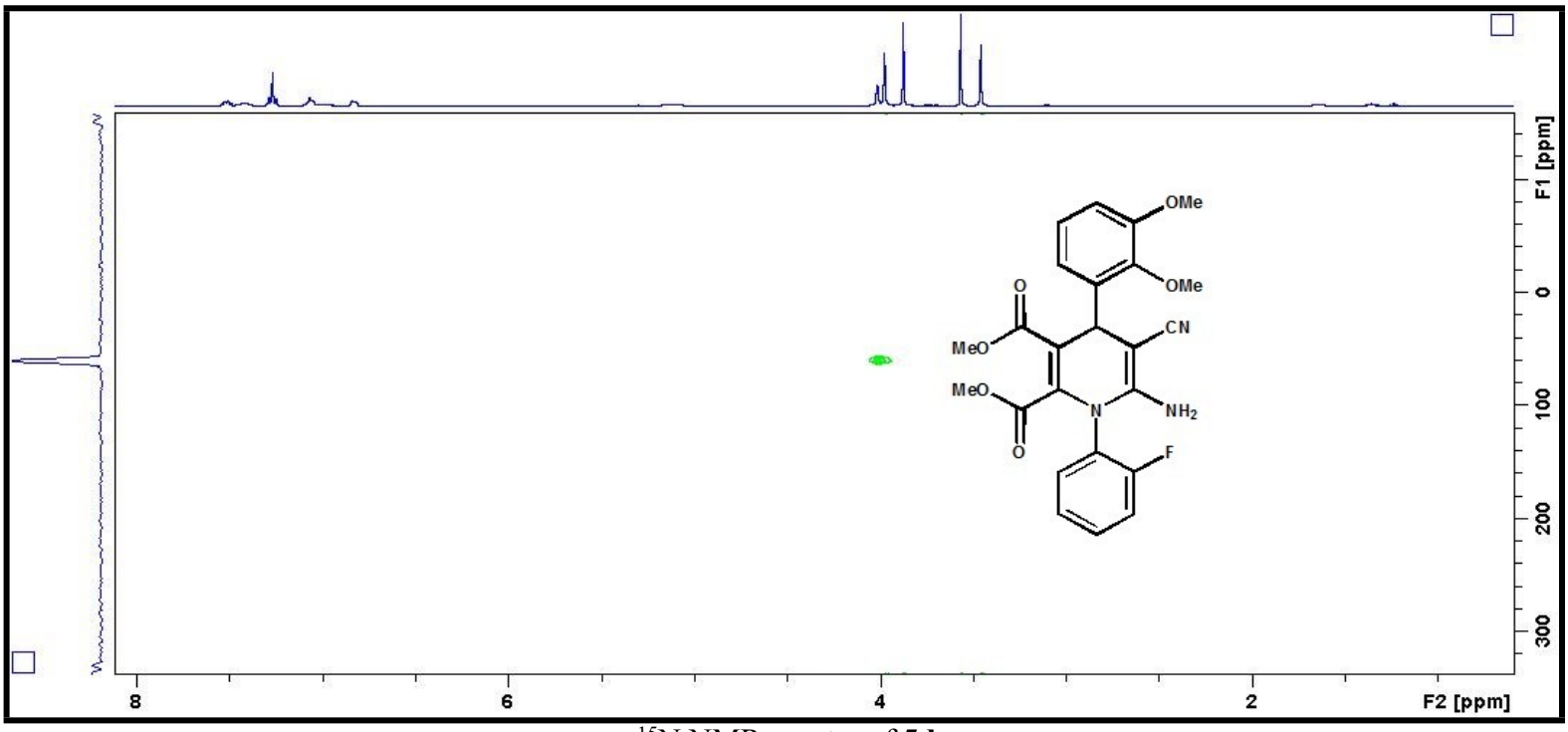


Minimum:				-1.5			
Maximum:		5.0	5.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
460.1287	460.1285	0.2	0.4	14.5	554.4	0.0	C23 H20 N3 O5 F Na

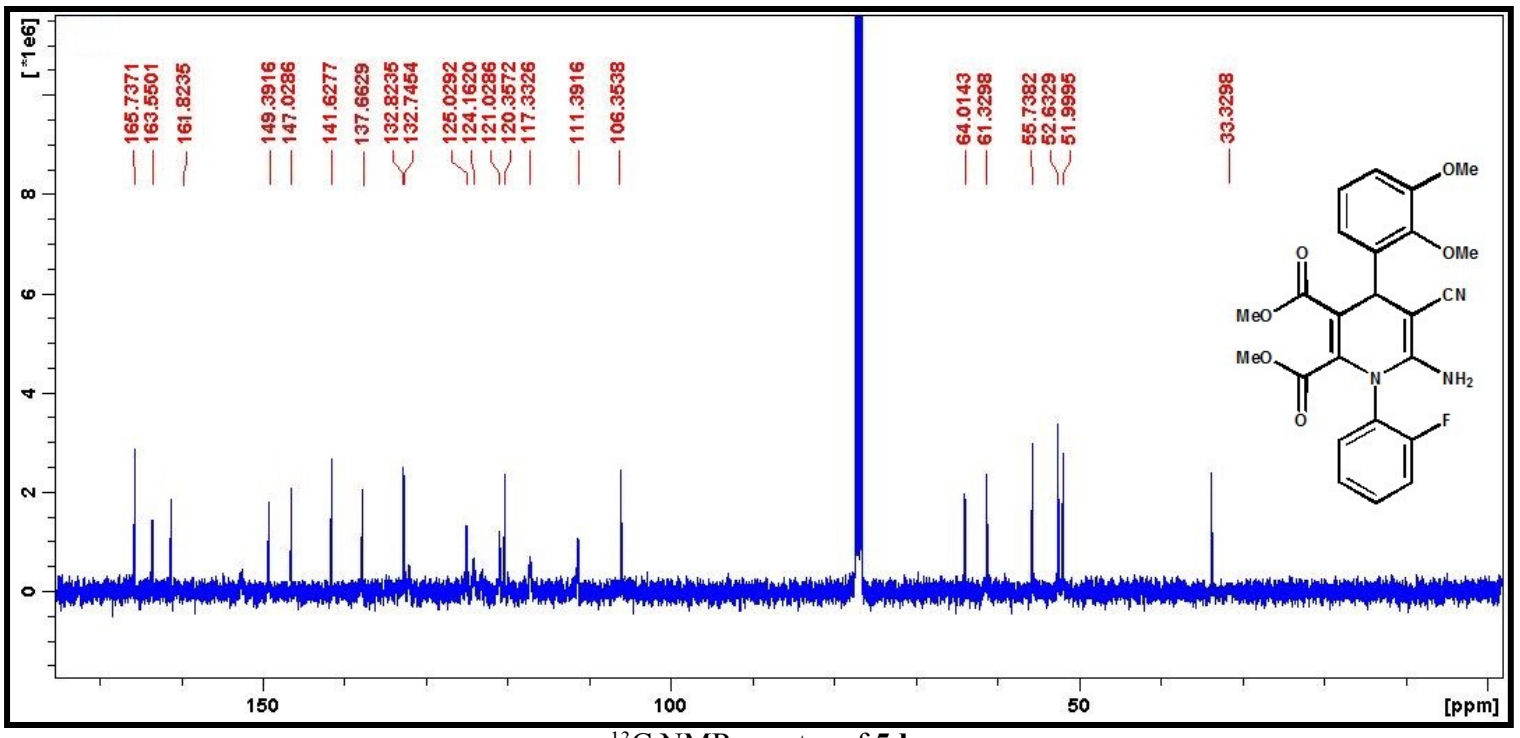
HRMS spectra of **5c**



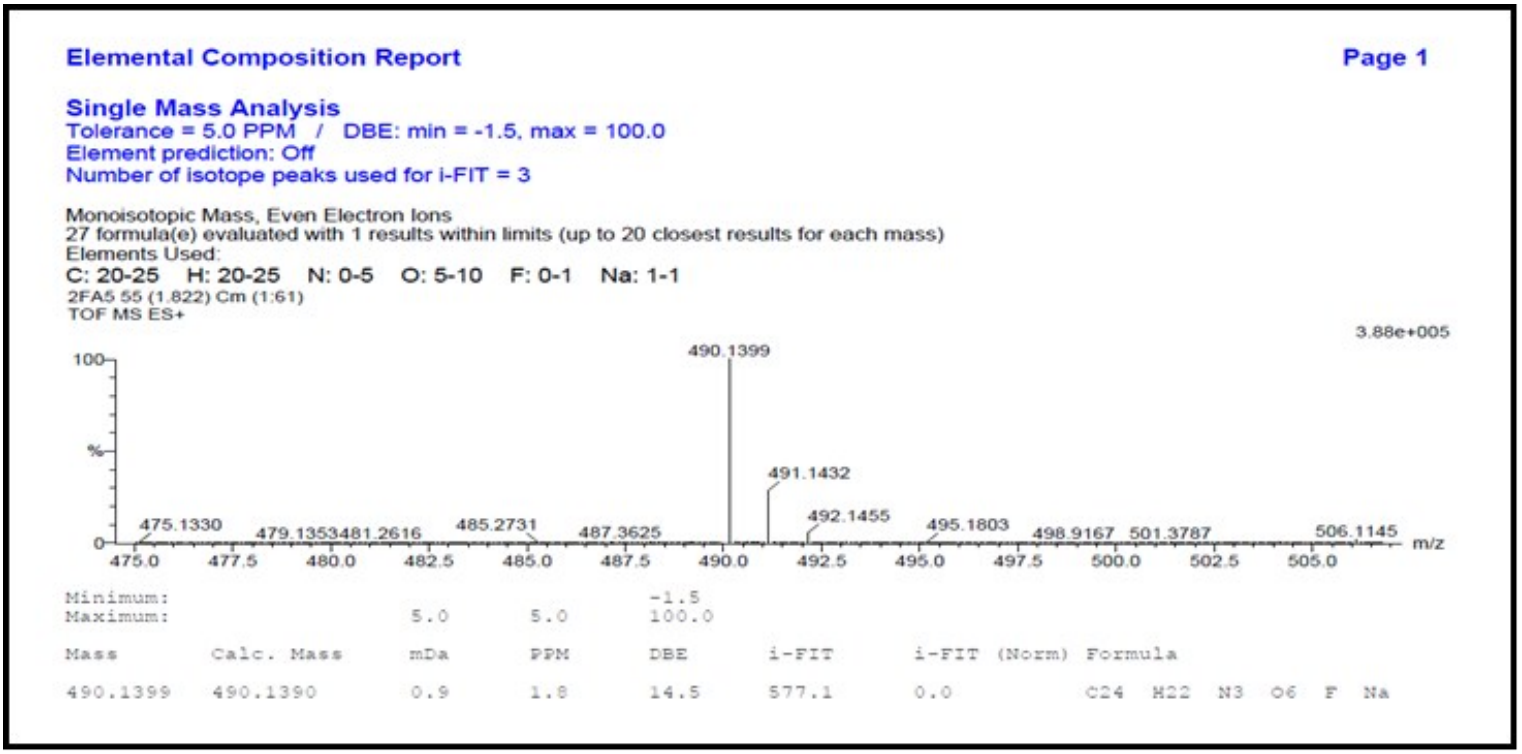
^{1}H NMR spectra of **5d**



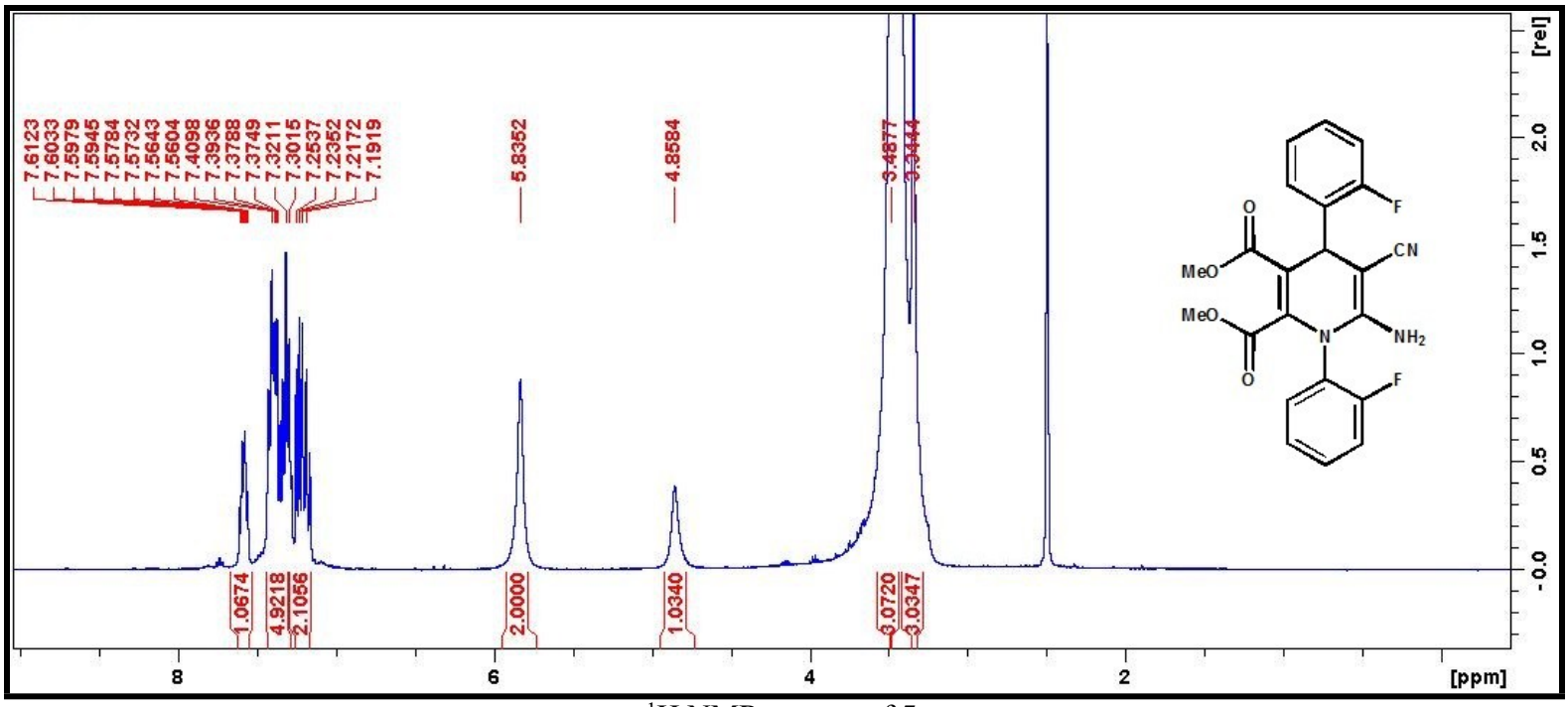
^{15}N NMR spectra of **5d**



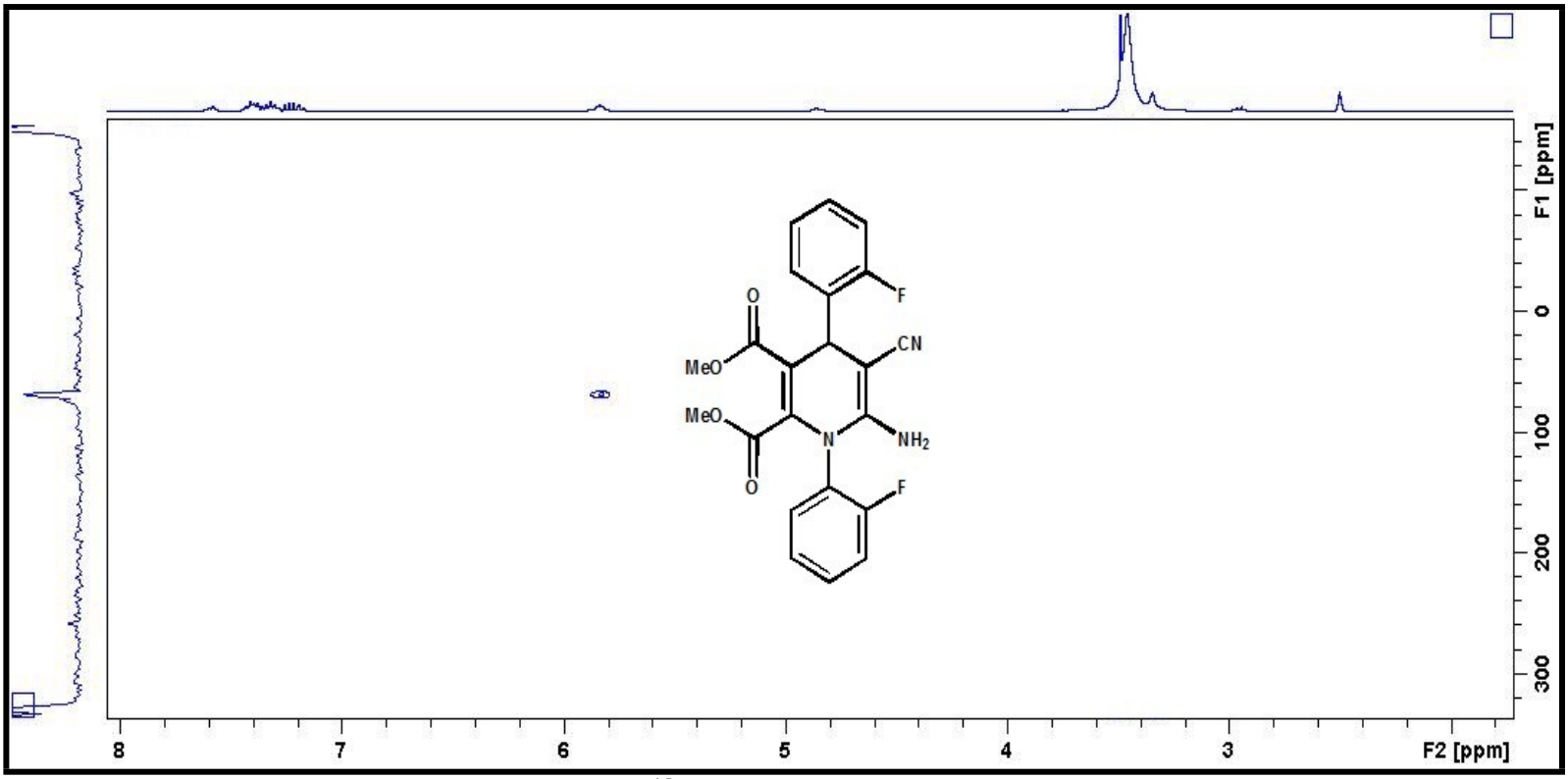
^{13}C NMR spectra of **5d**



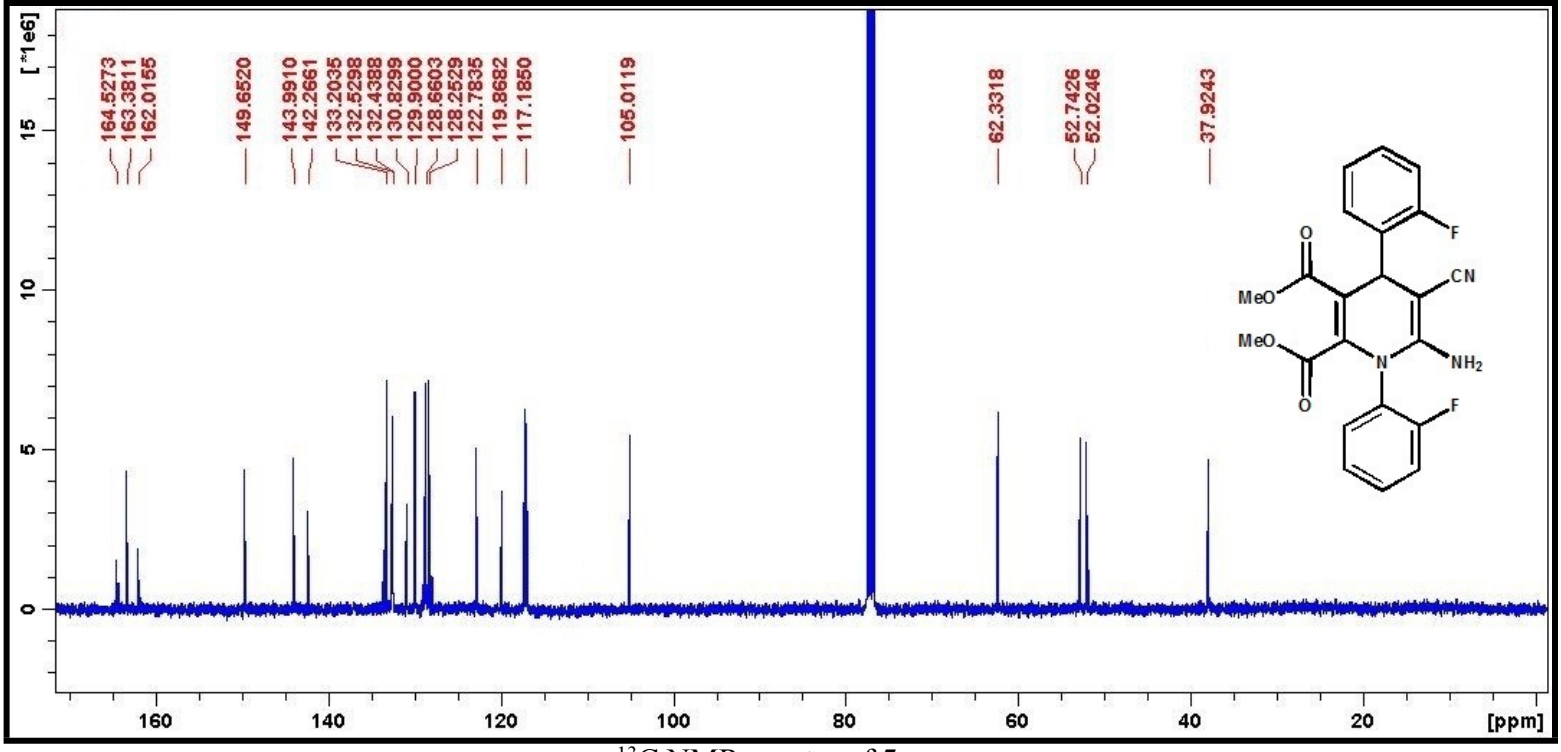
HRMS spectra of **5d**



^{1}H NMR spectra of **5e**



^{15}N NMR spectra of **5e**



^{13}C NMR spectra of **5e**

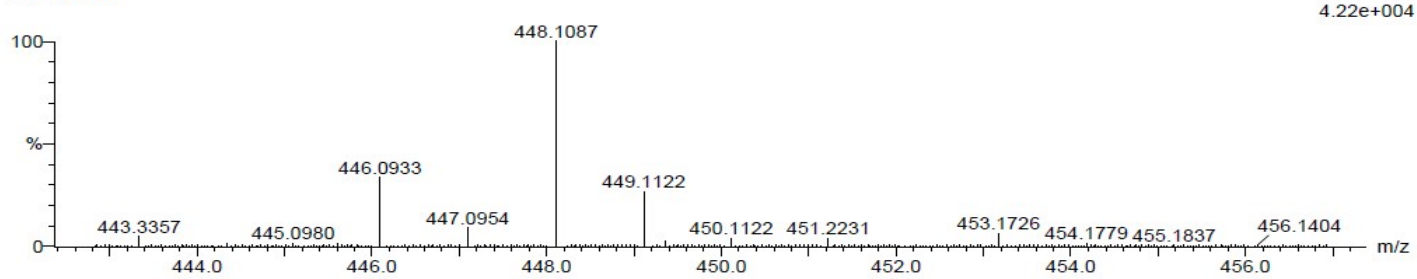
HRMS spectra of 5e

Elemental Composition Report **Page 1**

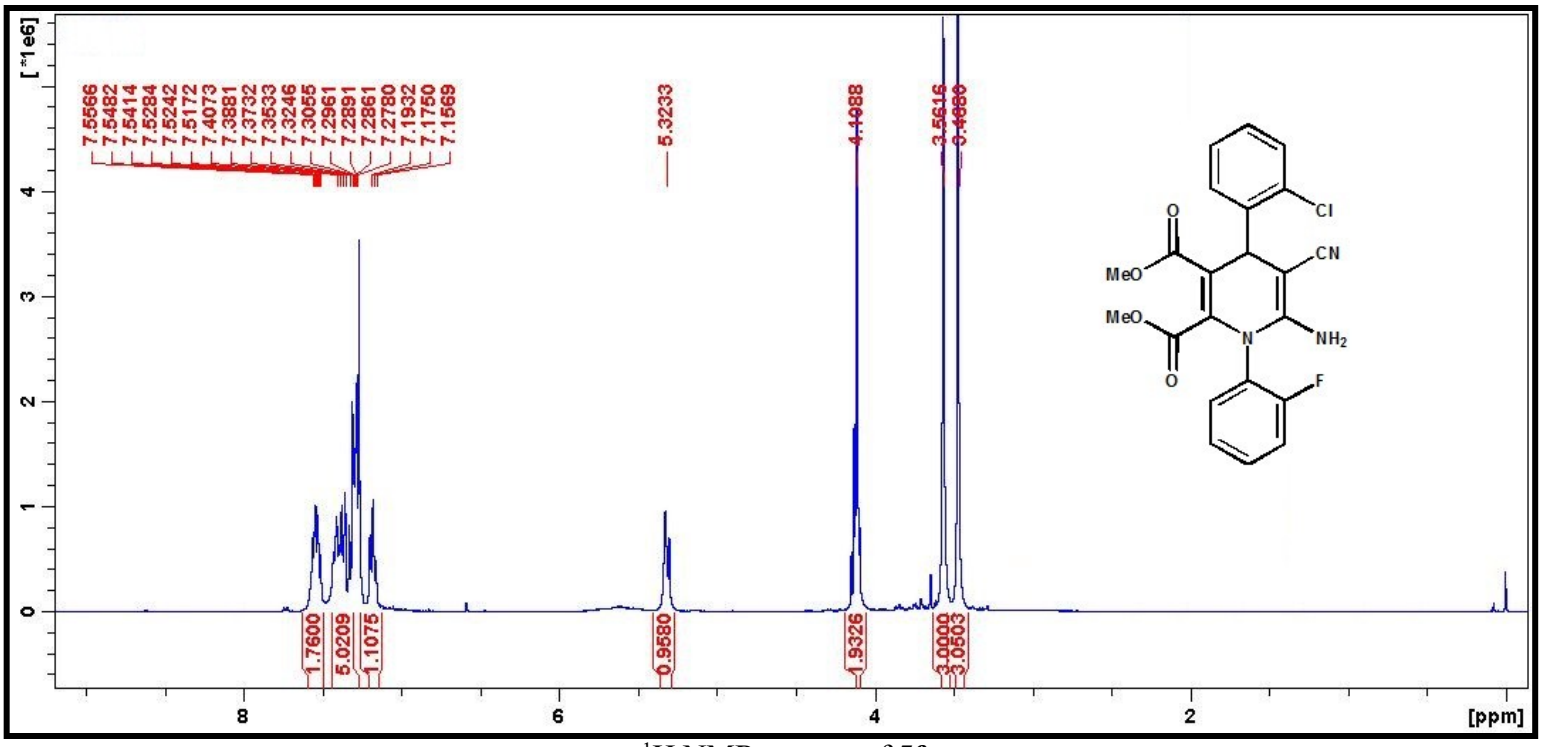
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
47 formula(e) evaluated with 1 results within limits (up to 20 closest results for each mass)
Elements Used:
C: 20-25 H: 15-25 N: 0-5 O: 0-10 F: 2-2 Na: 1-1
2FA17 61 (2.025) Cm (1:61)
TOF MS ES+

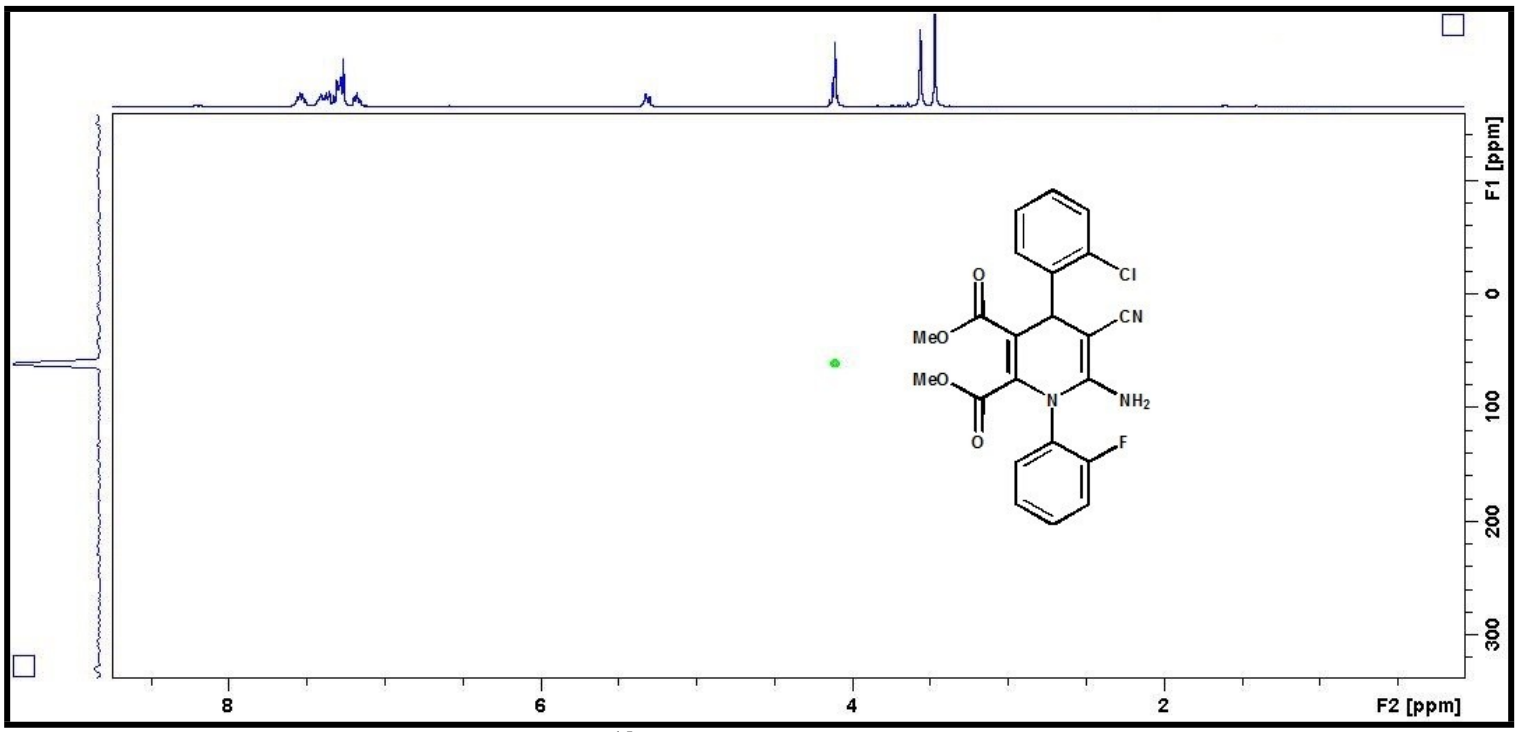
4.22e+004



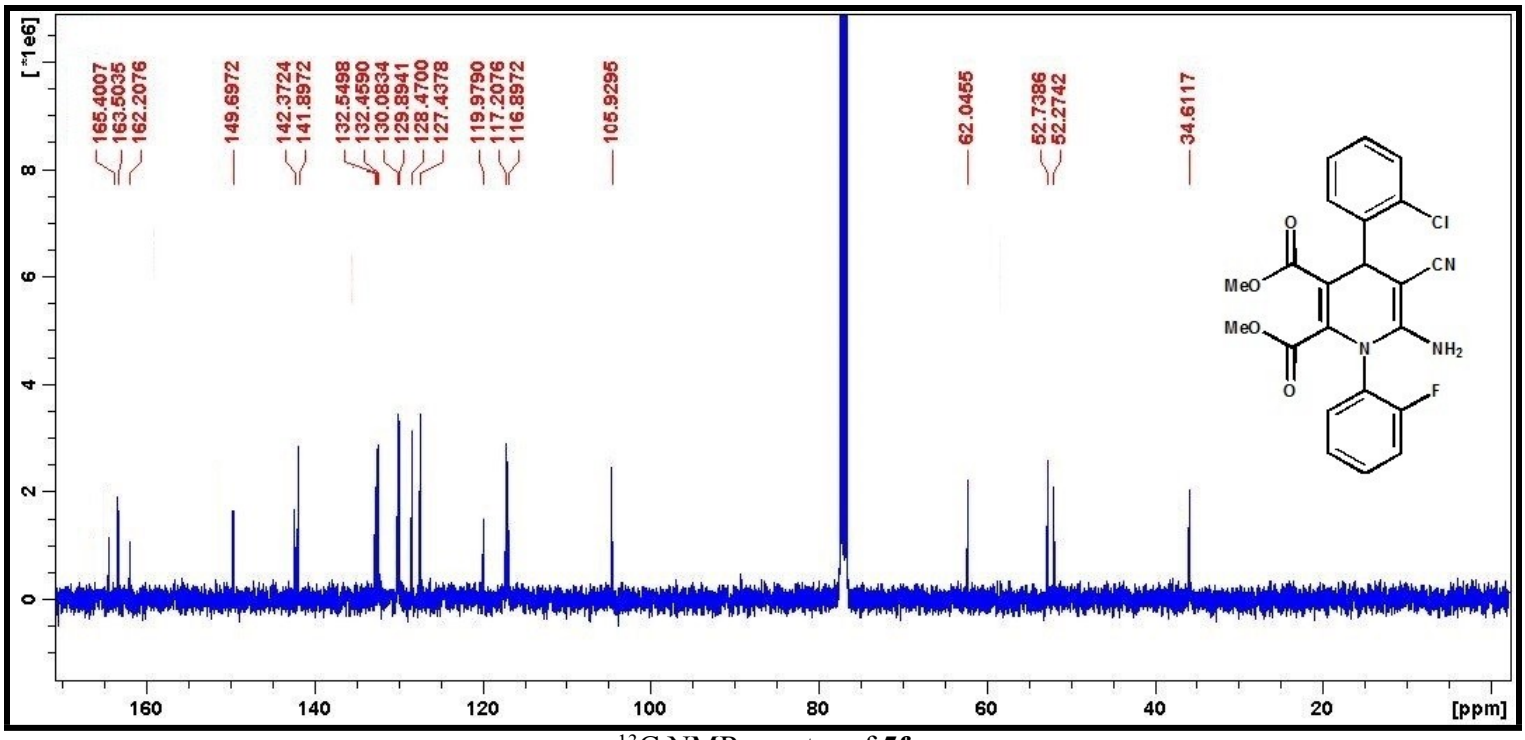
Minimum:				-1.5			
Maximum:		5.0	5.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
448.1087	448.1085	0.2	0.4	14.5	482.1	0.0	C22 H17 N3 O4 F2 Na



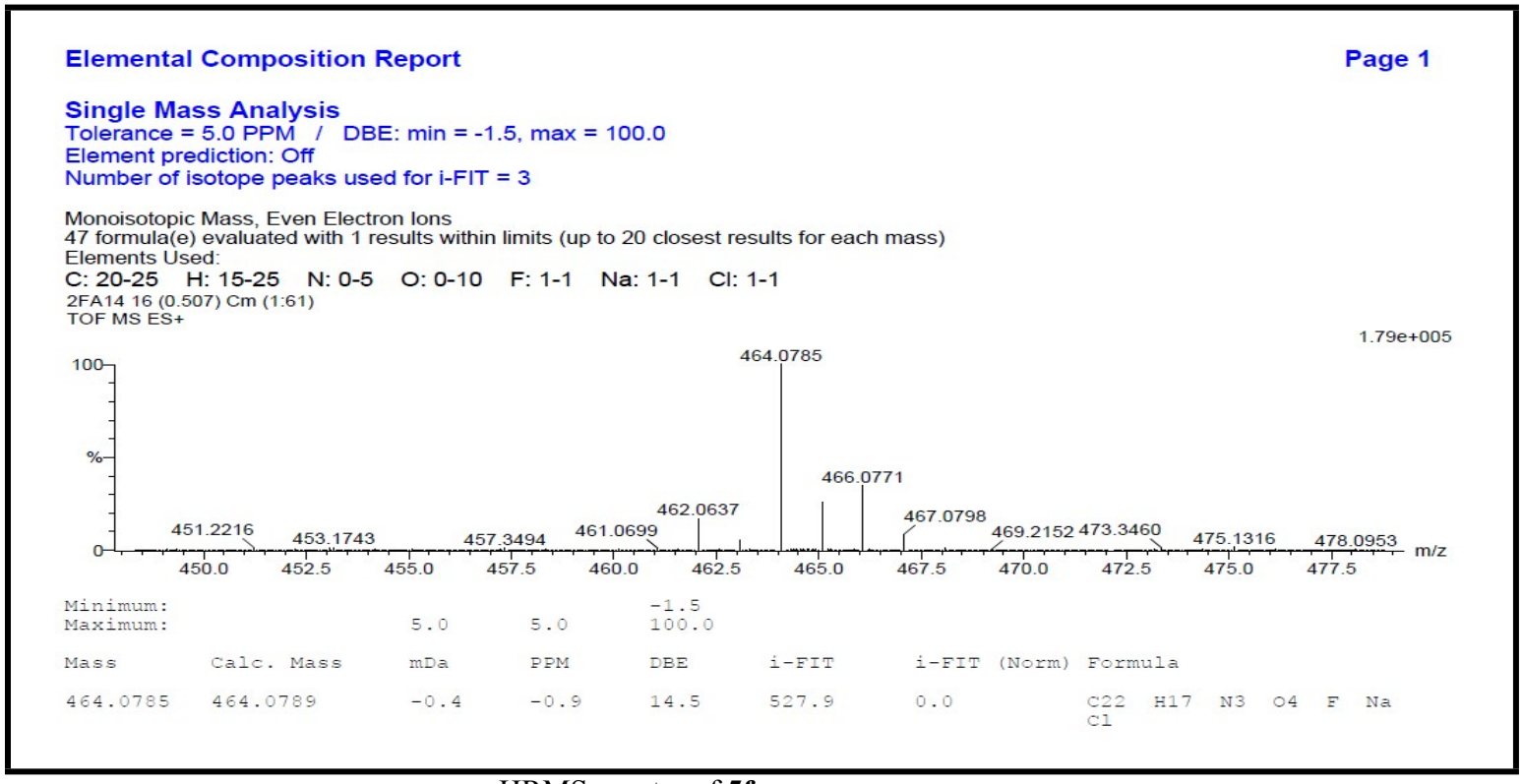
^{1}H NMR spectra of **5f**



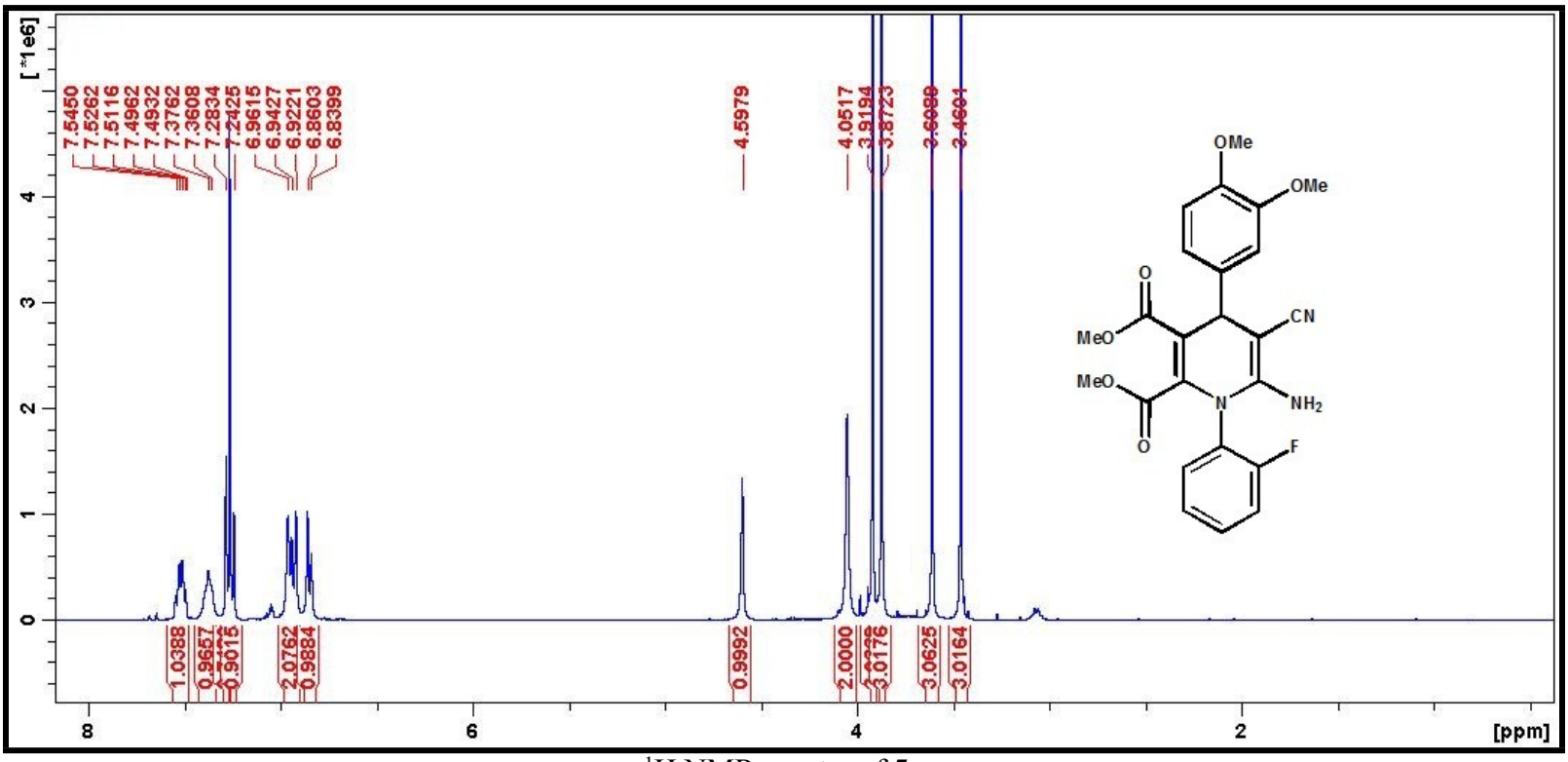
^{15}N NMR spectra of **5f**



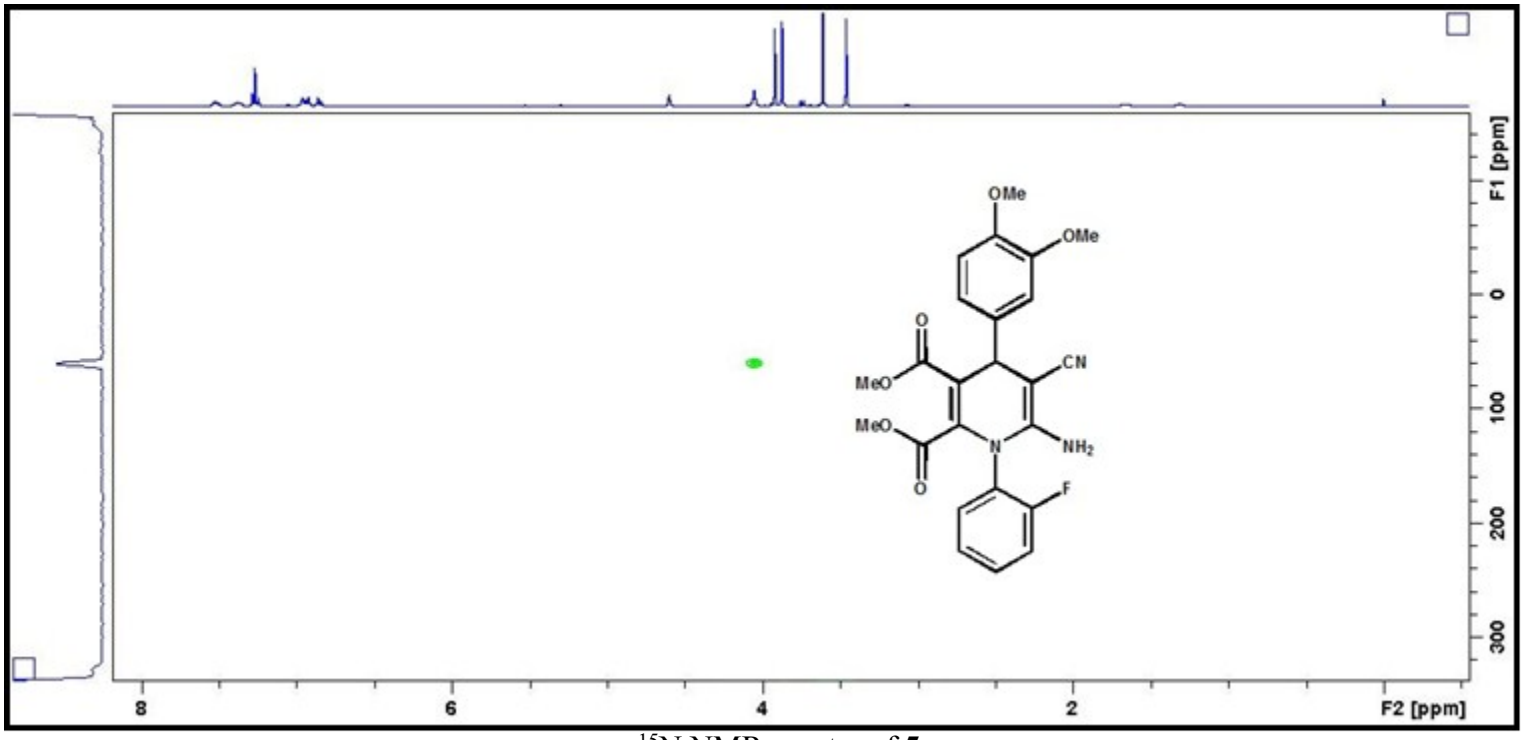
^{13}C NMR spectra of **5f**



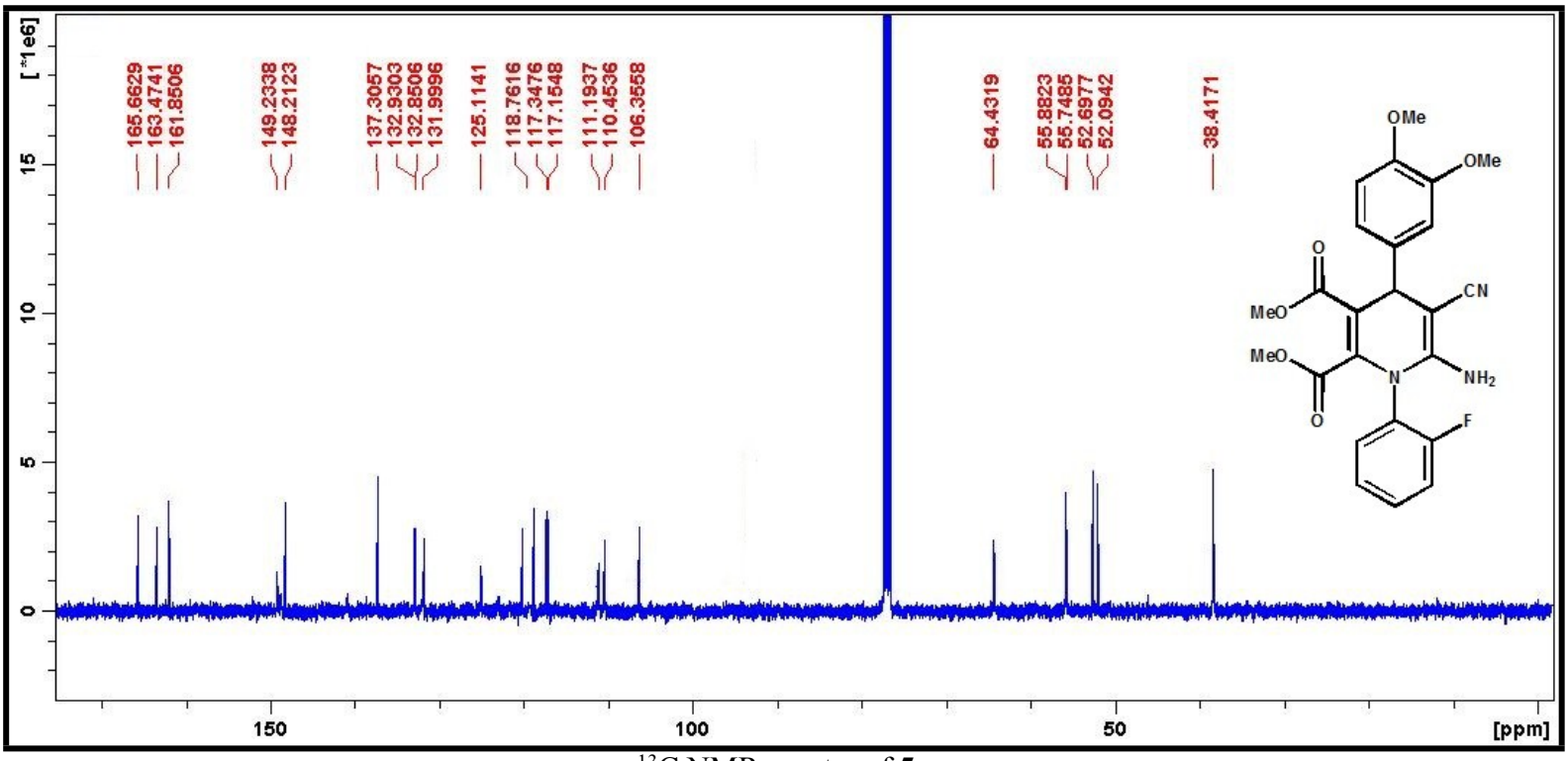
HRMS spectra of **5f**



^{1}H NMR spectra of **5g**



^{15}N NMR spectra of **5g**

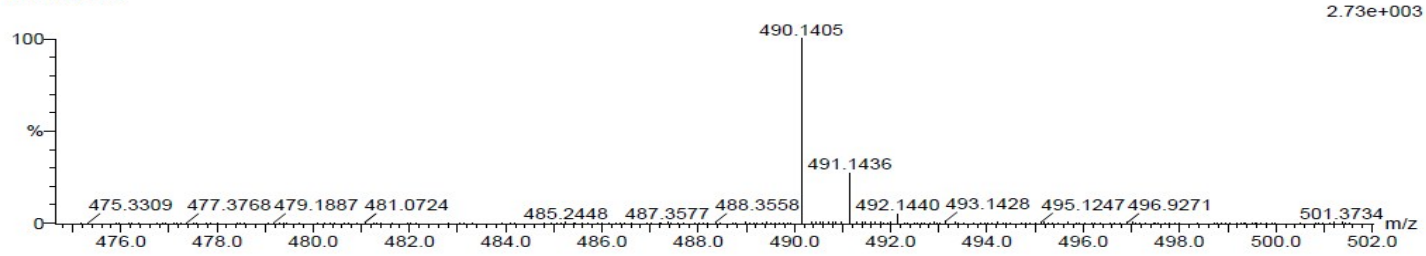


^{13}C NMR spectra of **5g**

Elemental Composition Report Page 1

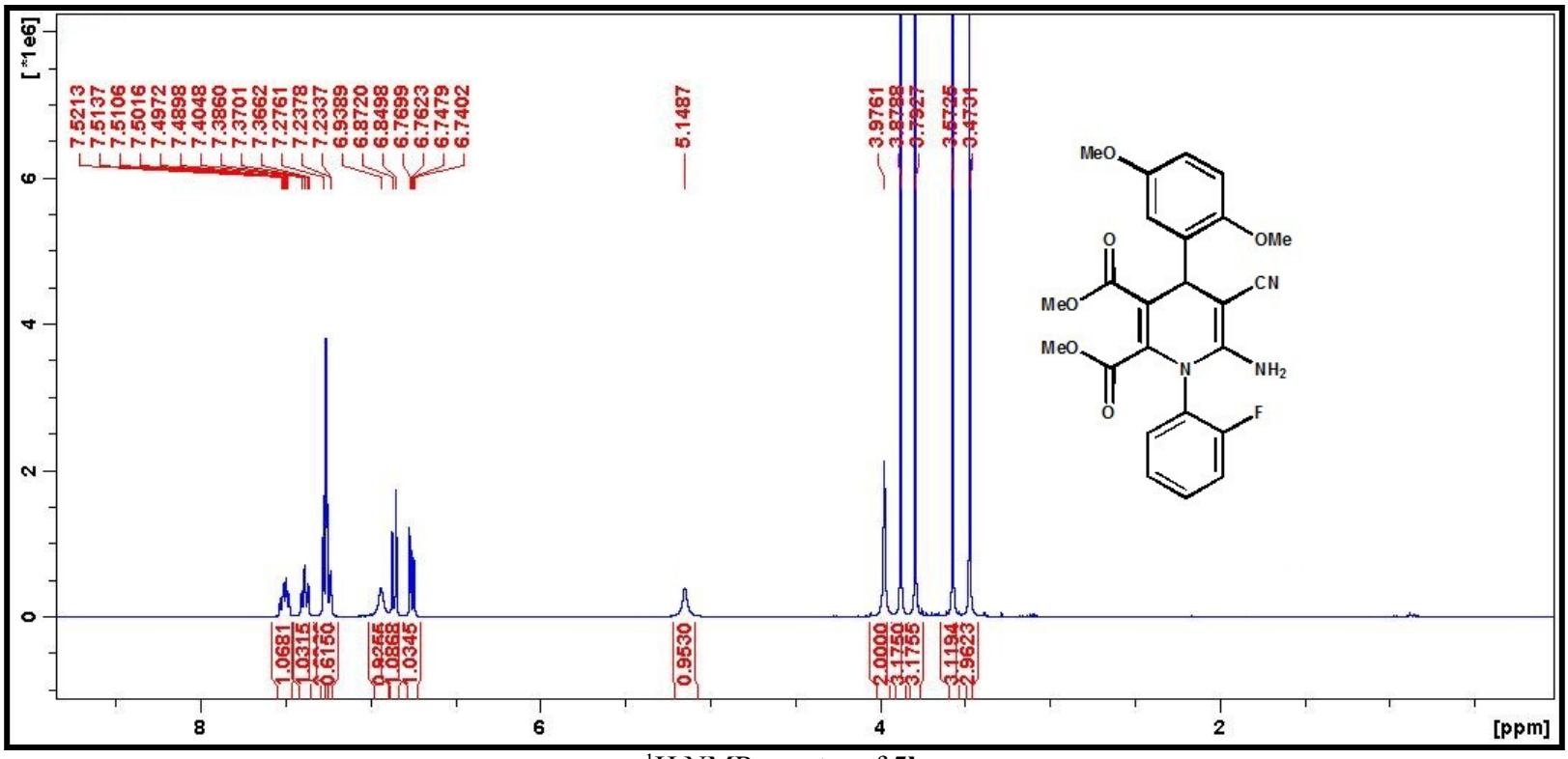
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
27 formula(e) evaluated with 1 results within limits (up to 20 closest results for each mass)
Elements Used:
C: 20-25 H: 20-25 N: 0-5 O: 5-10 F: 0-1 Na: 1-1
2FA3 6 (0.169)
TOF MS ES+

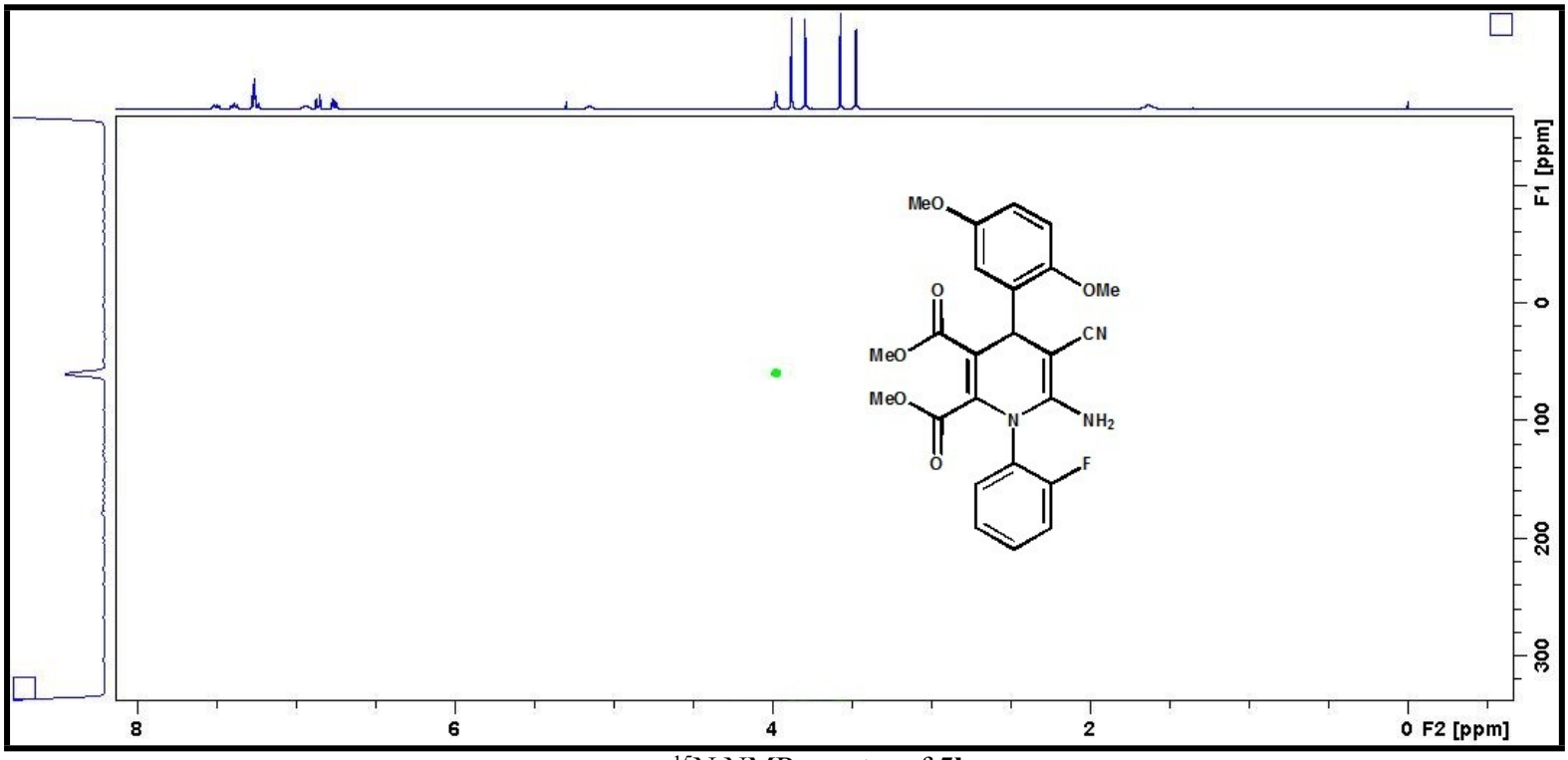


Minimum:				-1.5			
Maximum:		5.0	5.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
490.1405	490.1390	1.5	3.1	14.5	97.7	0.0	C24 H22 N3 O6 F Na

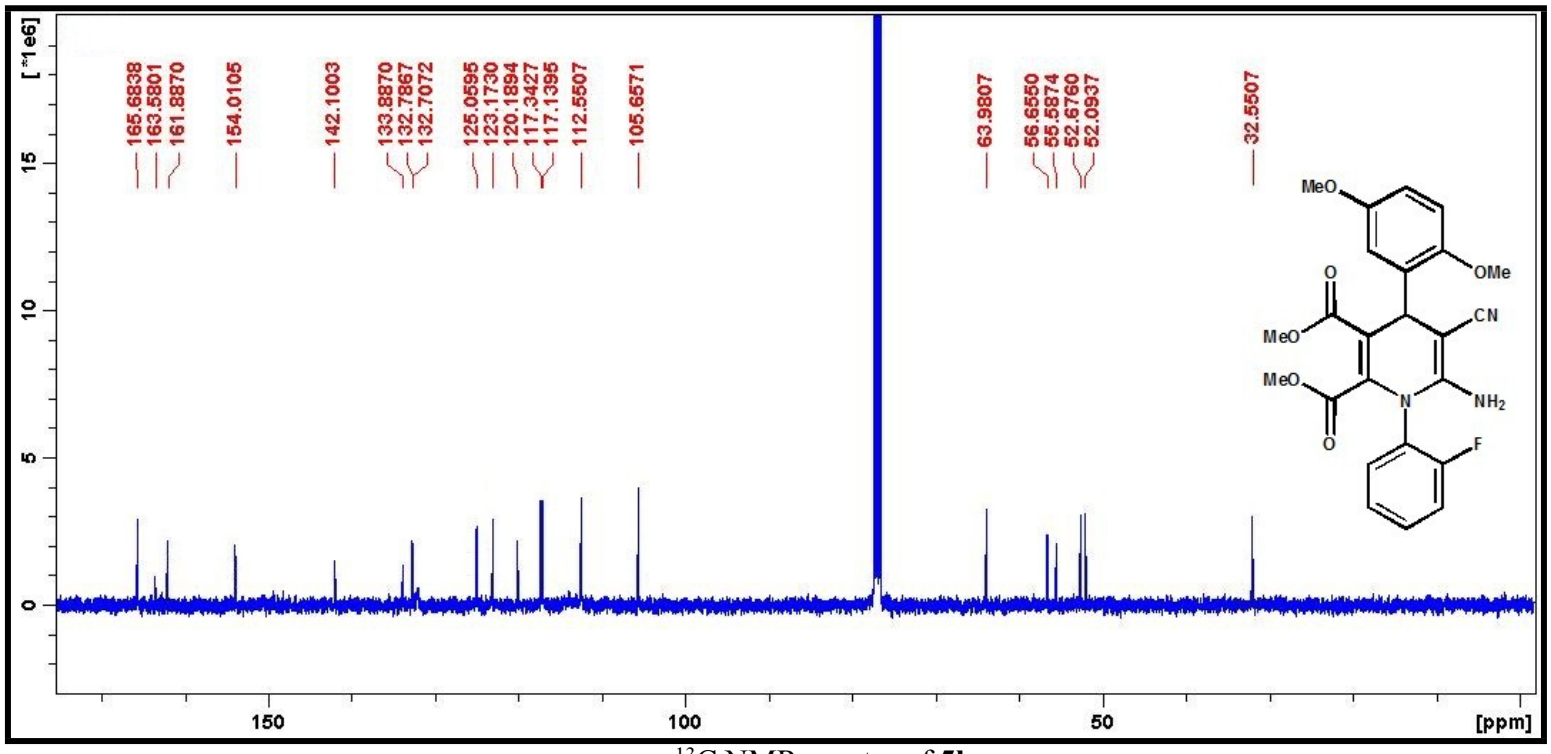
HRMS spectra of **5g**



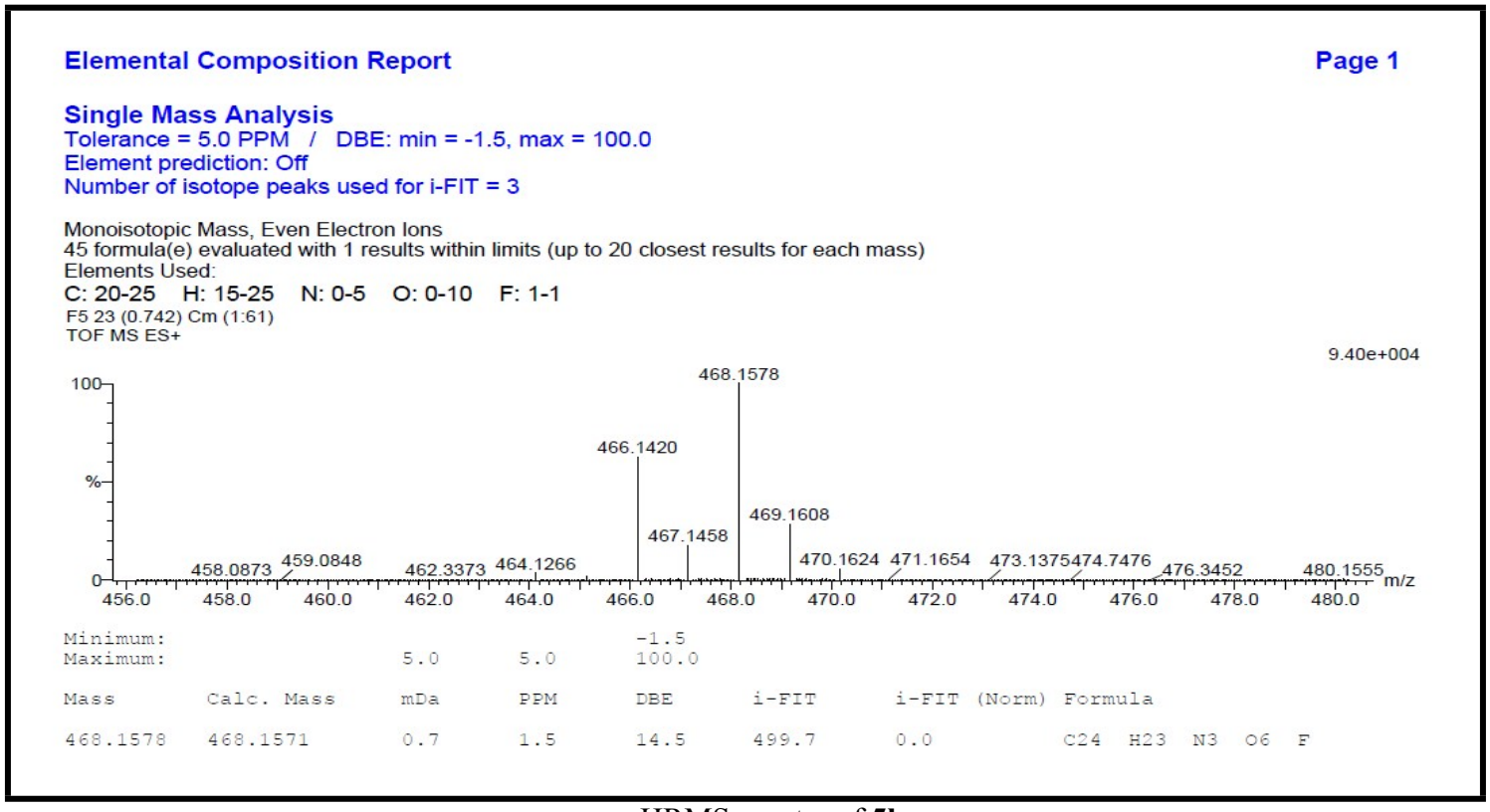
^{1}H NMR spectra of **5h**



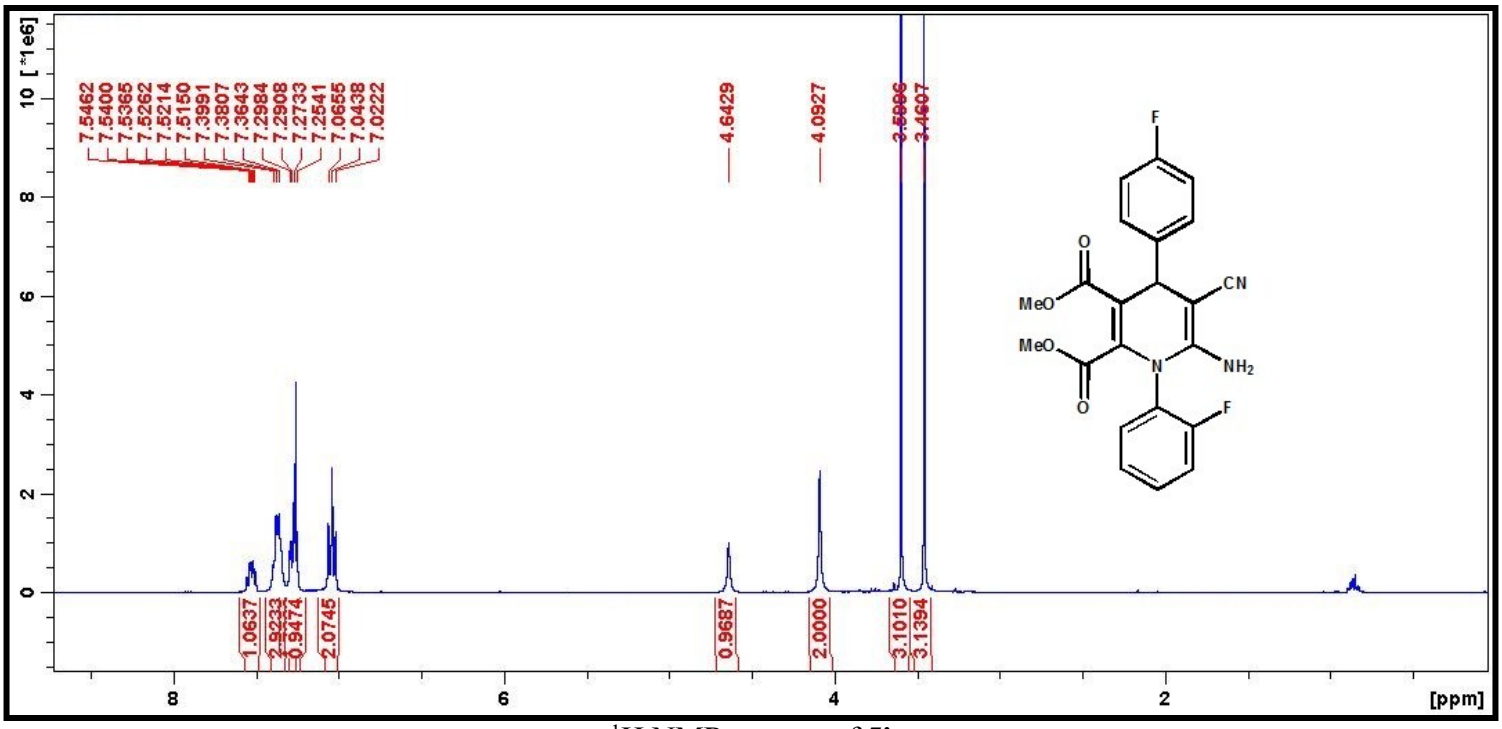
^{15}N NMR spectra of **5h**



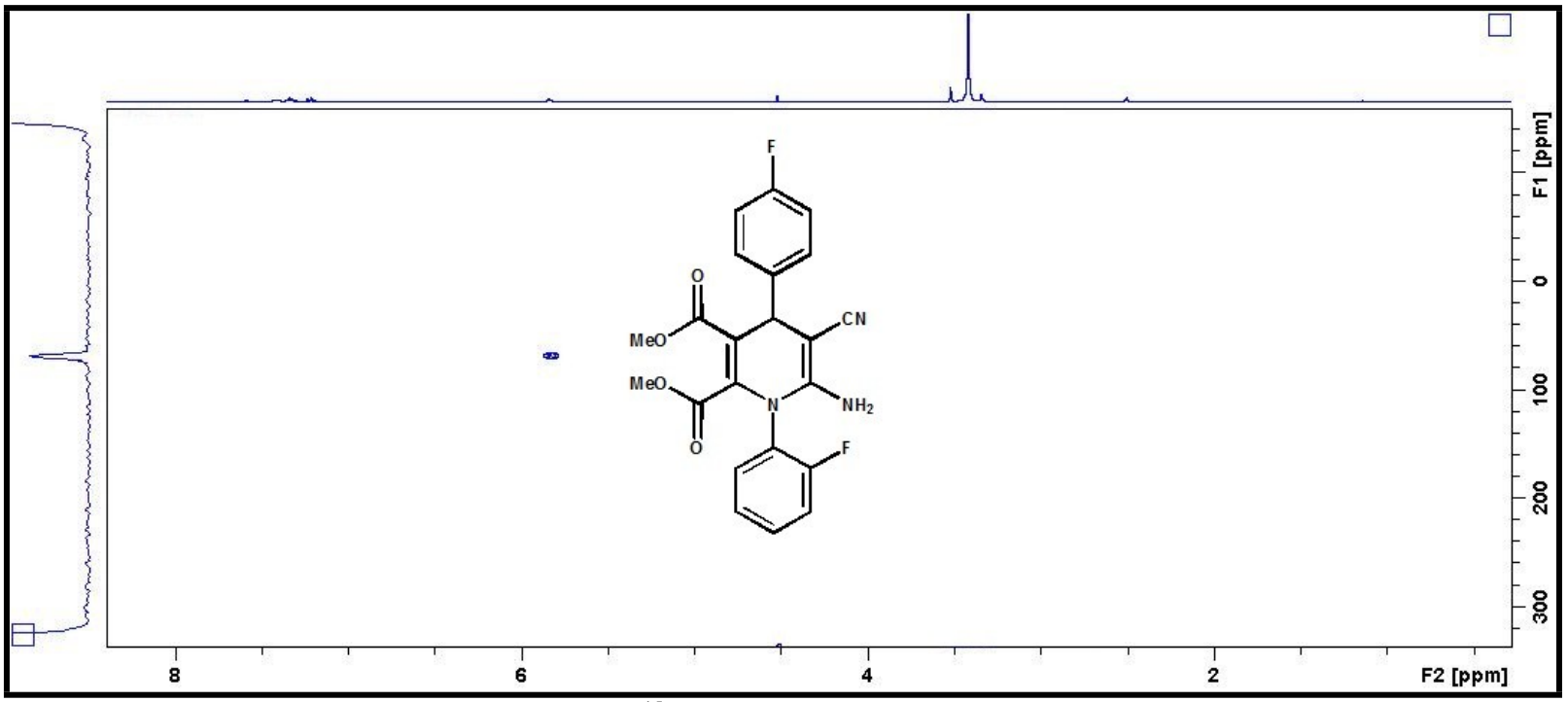
^{13}C NMR spectra of **5h**



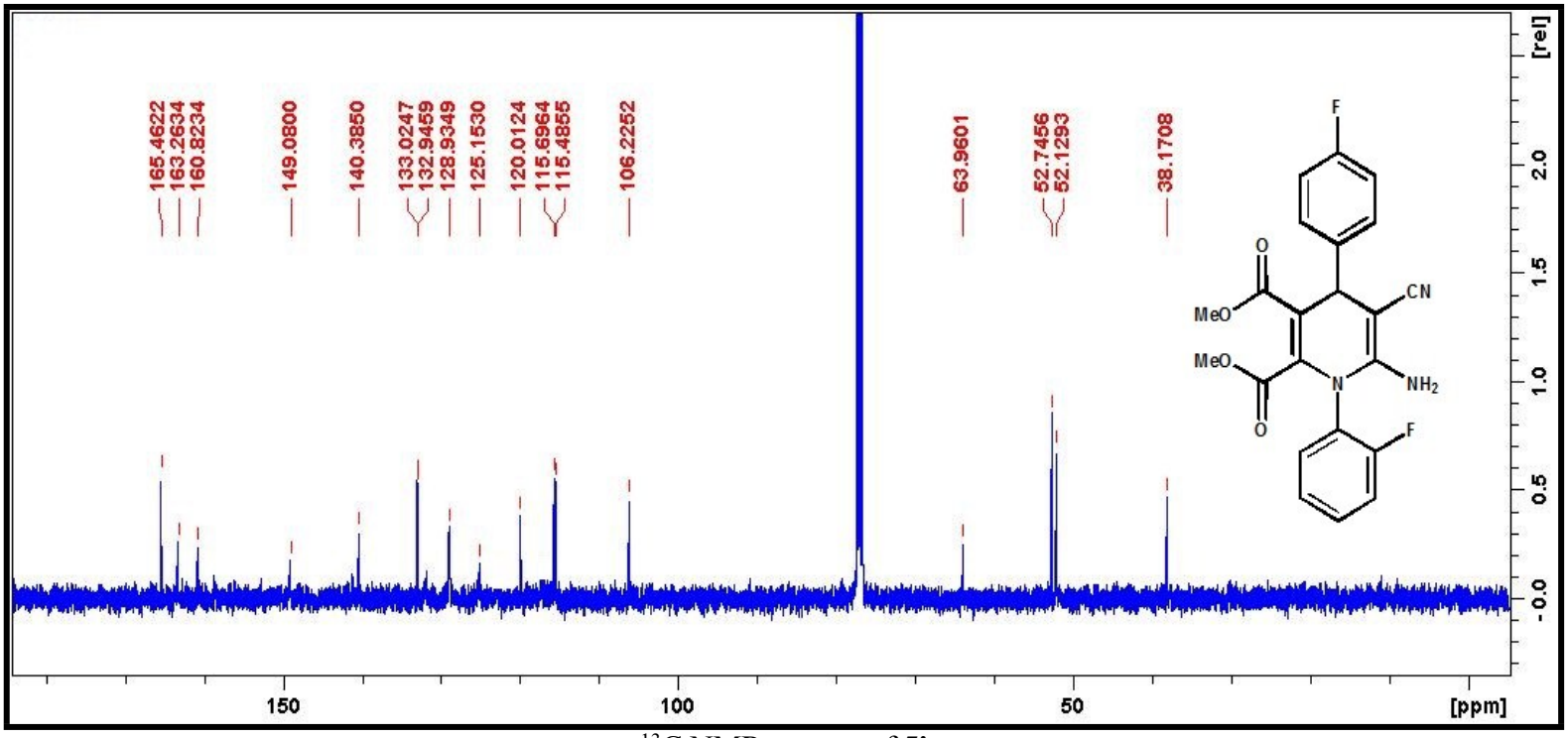
HRMS spectra of **5h**



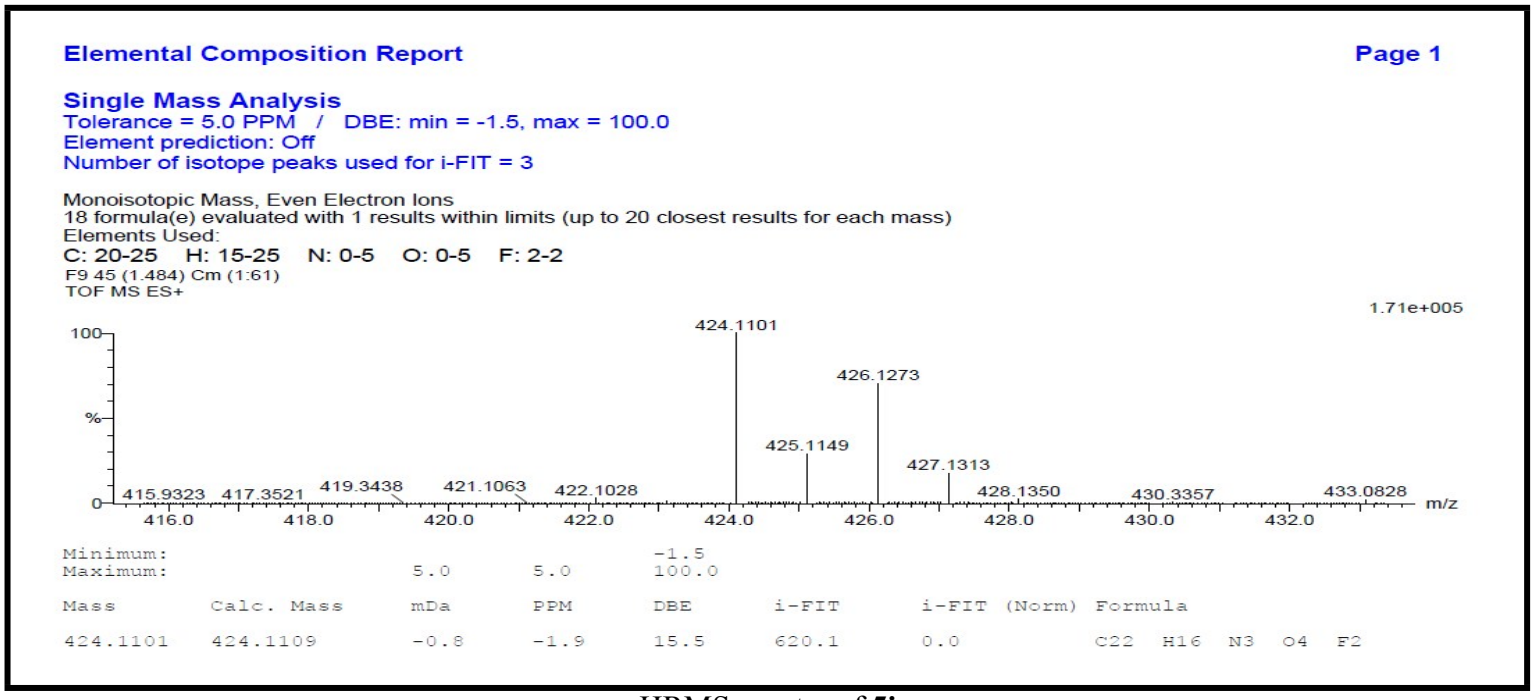
^{1}H NMR spectra of **5i**



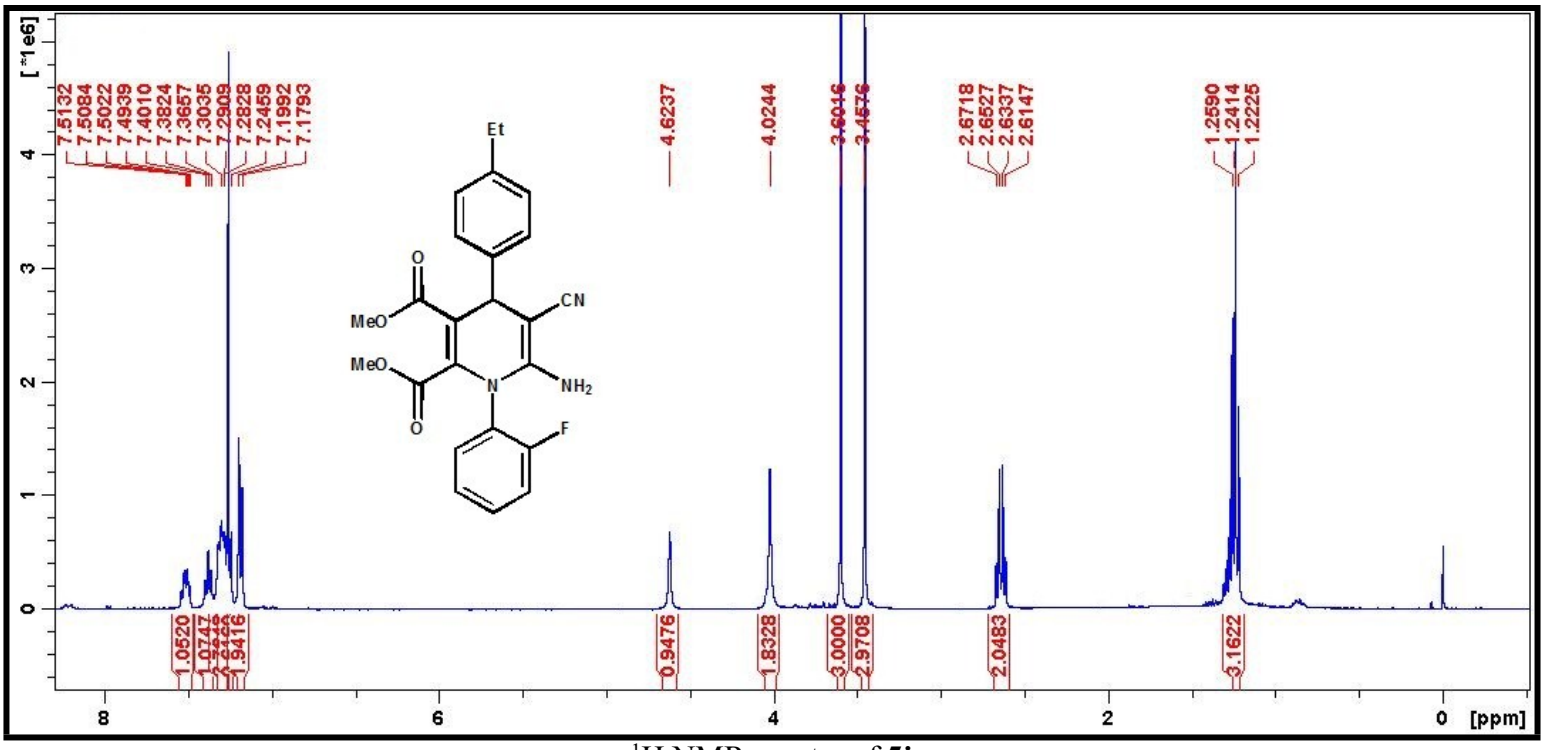
^{15}N NMR spectra of **5i**



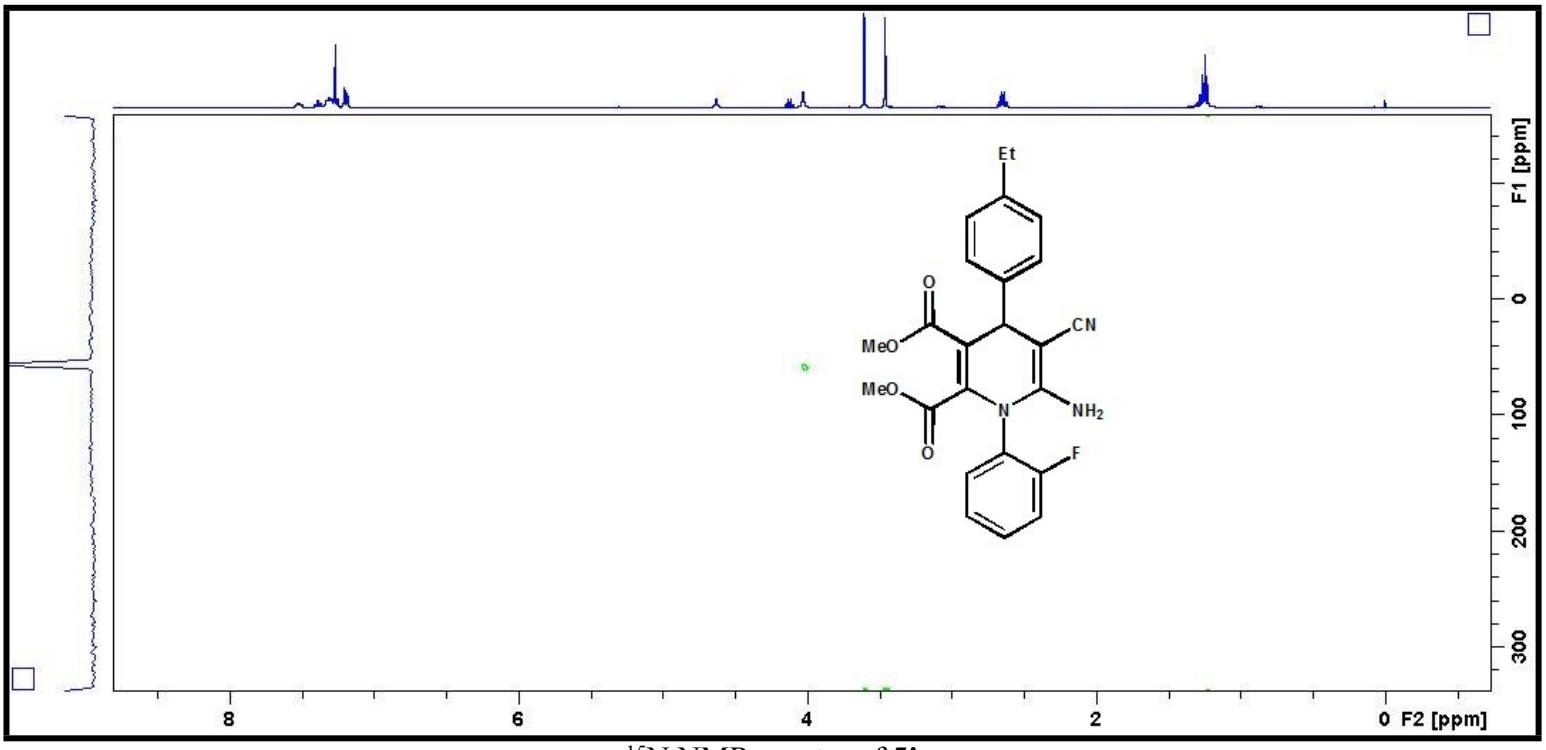
^{13}C NMR spectra of **5i**



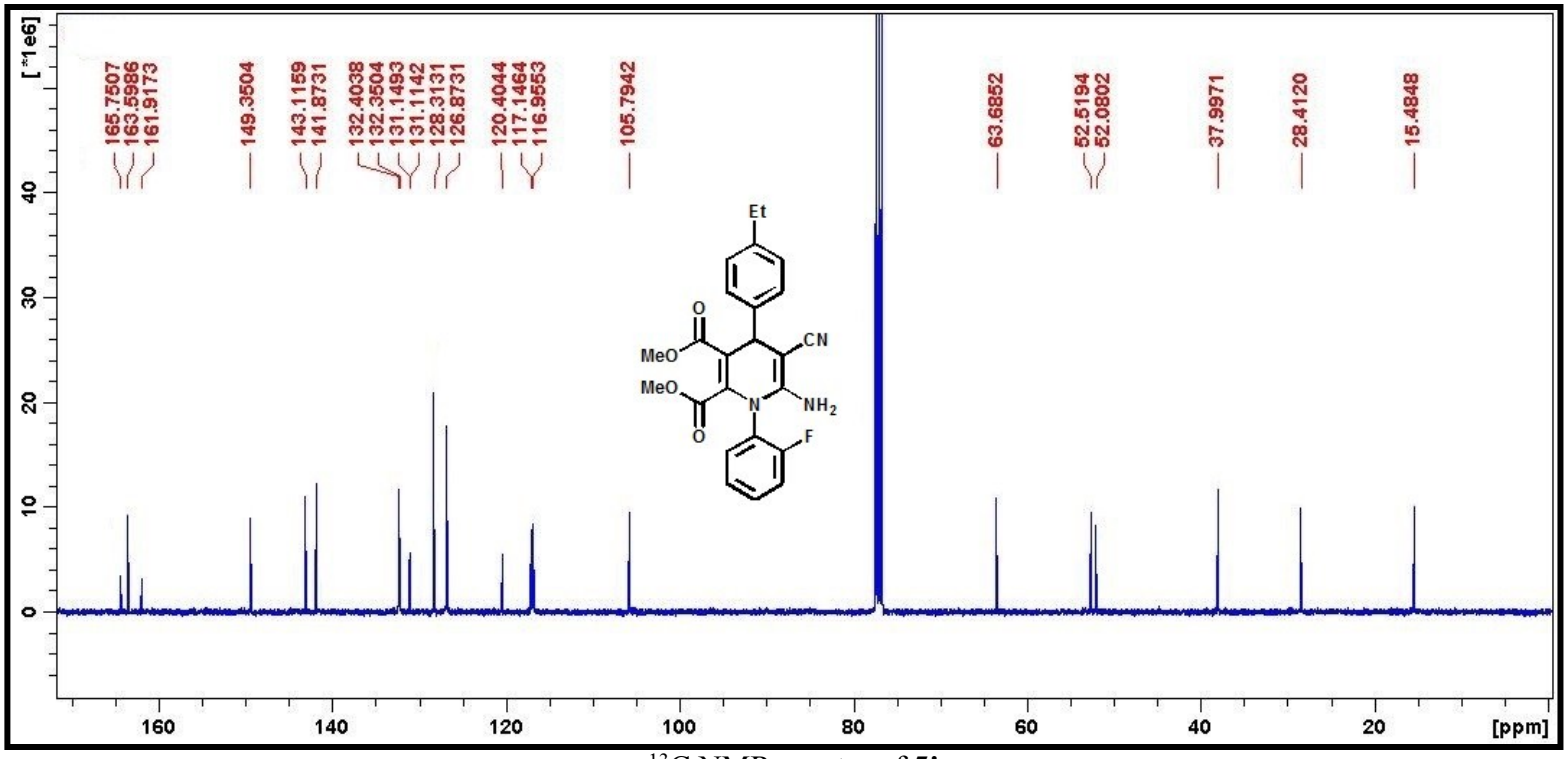
HRMS spectra of **5i**



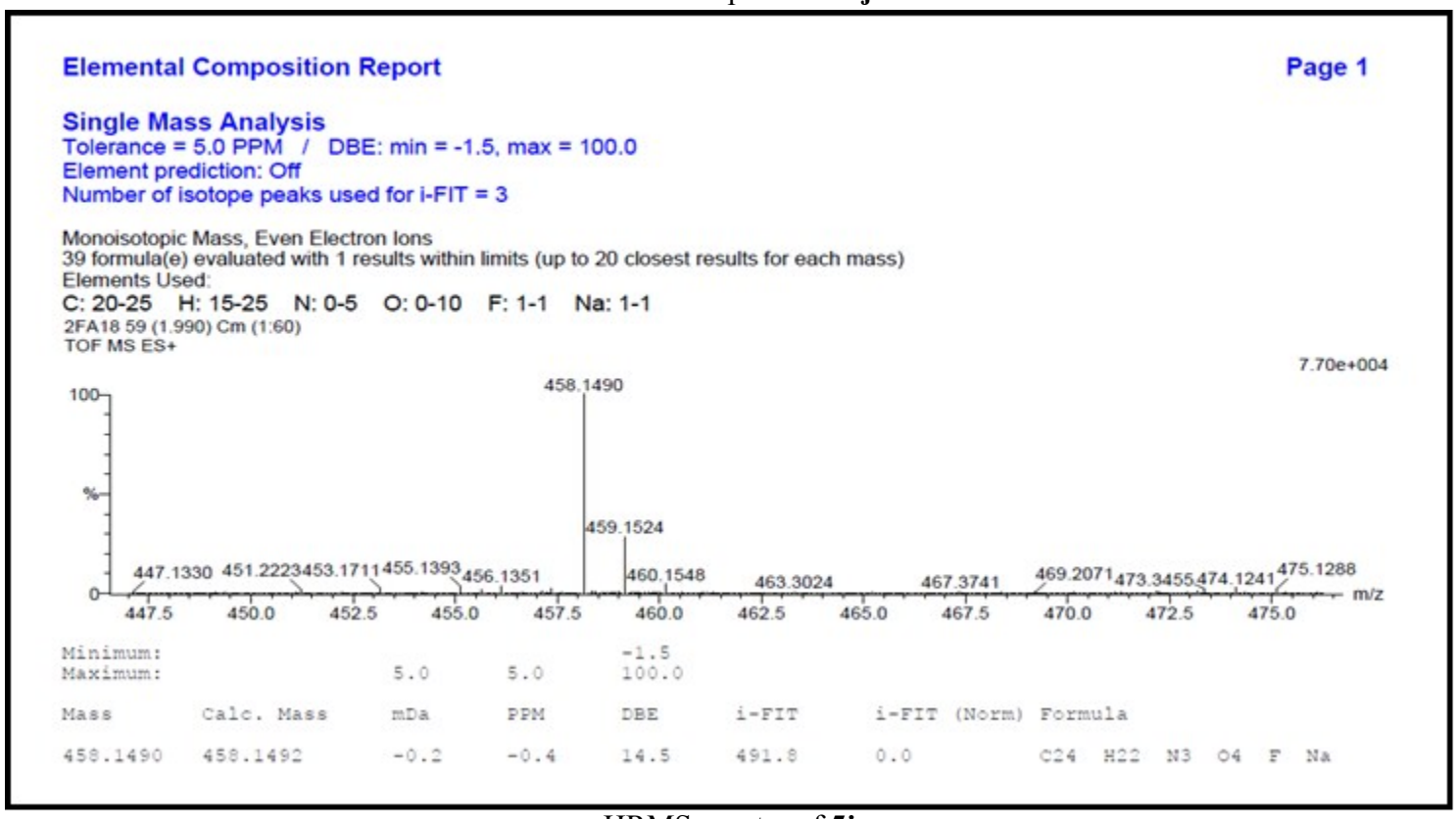
^{1}H NMR spectra of **5j**



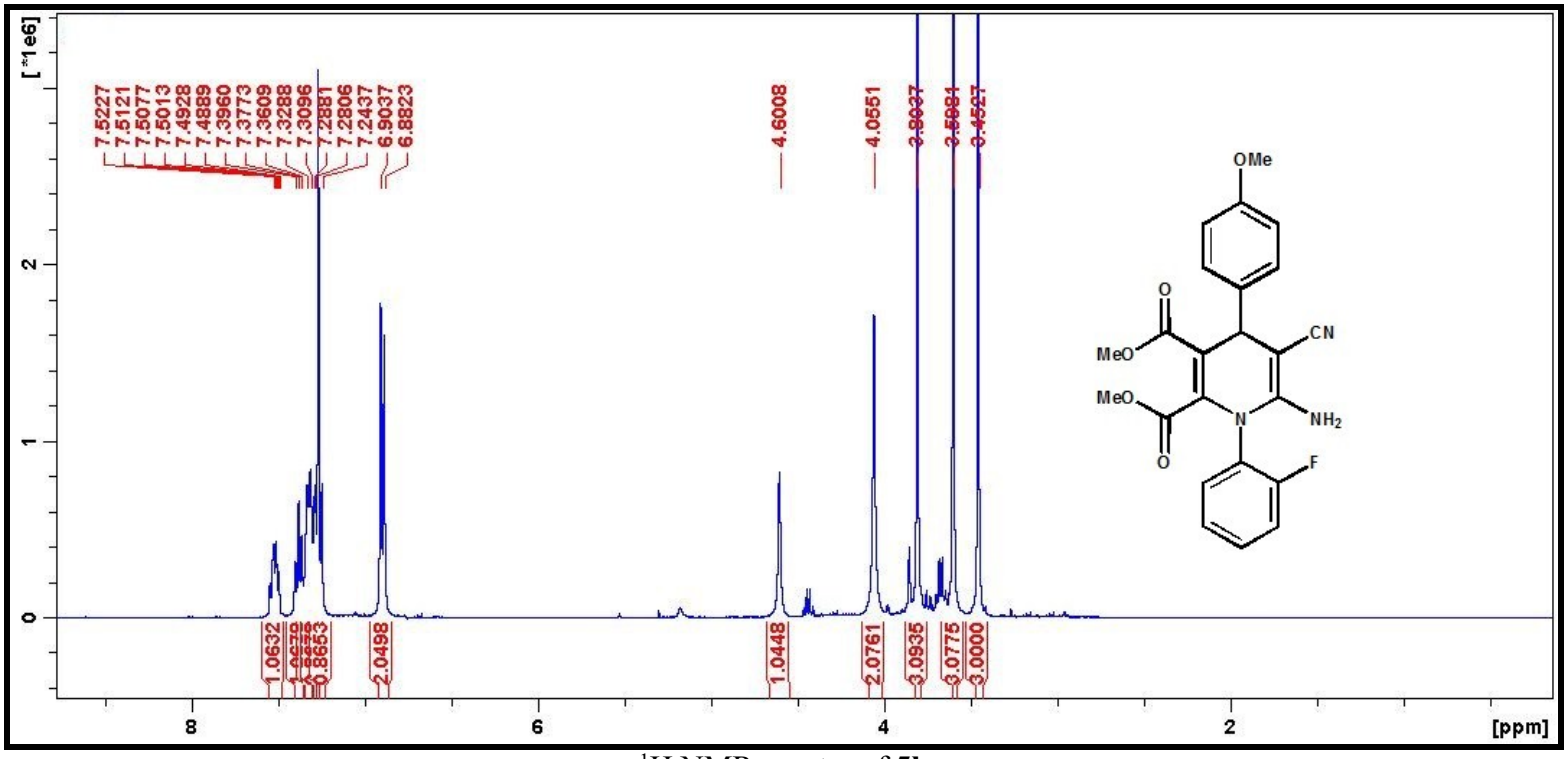
^{15}N NMR spectra of **5j**



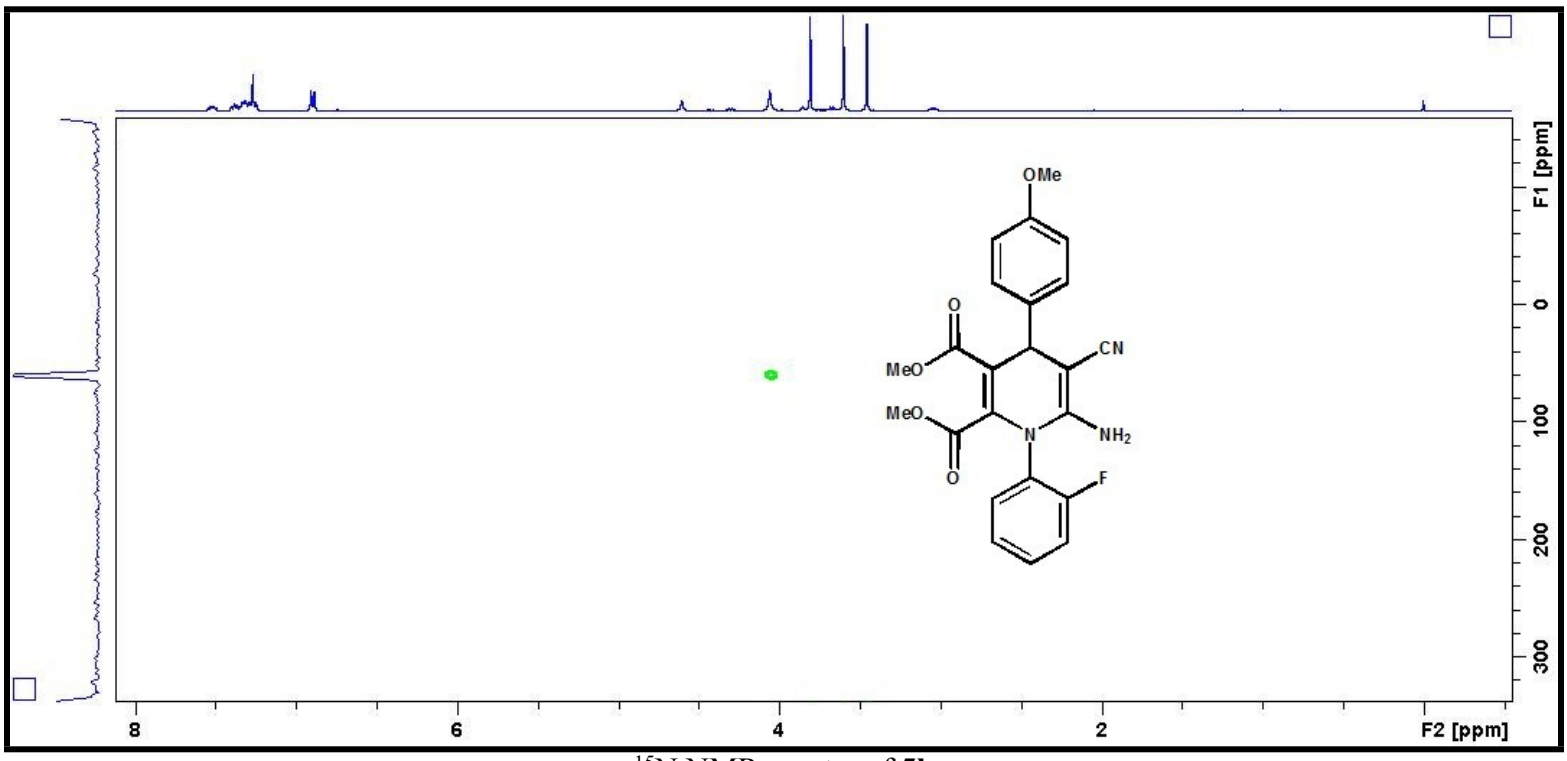
^{13}C NMR spectra of **5j**



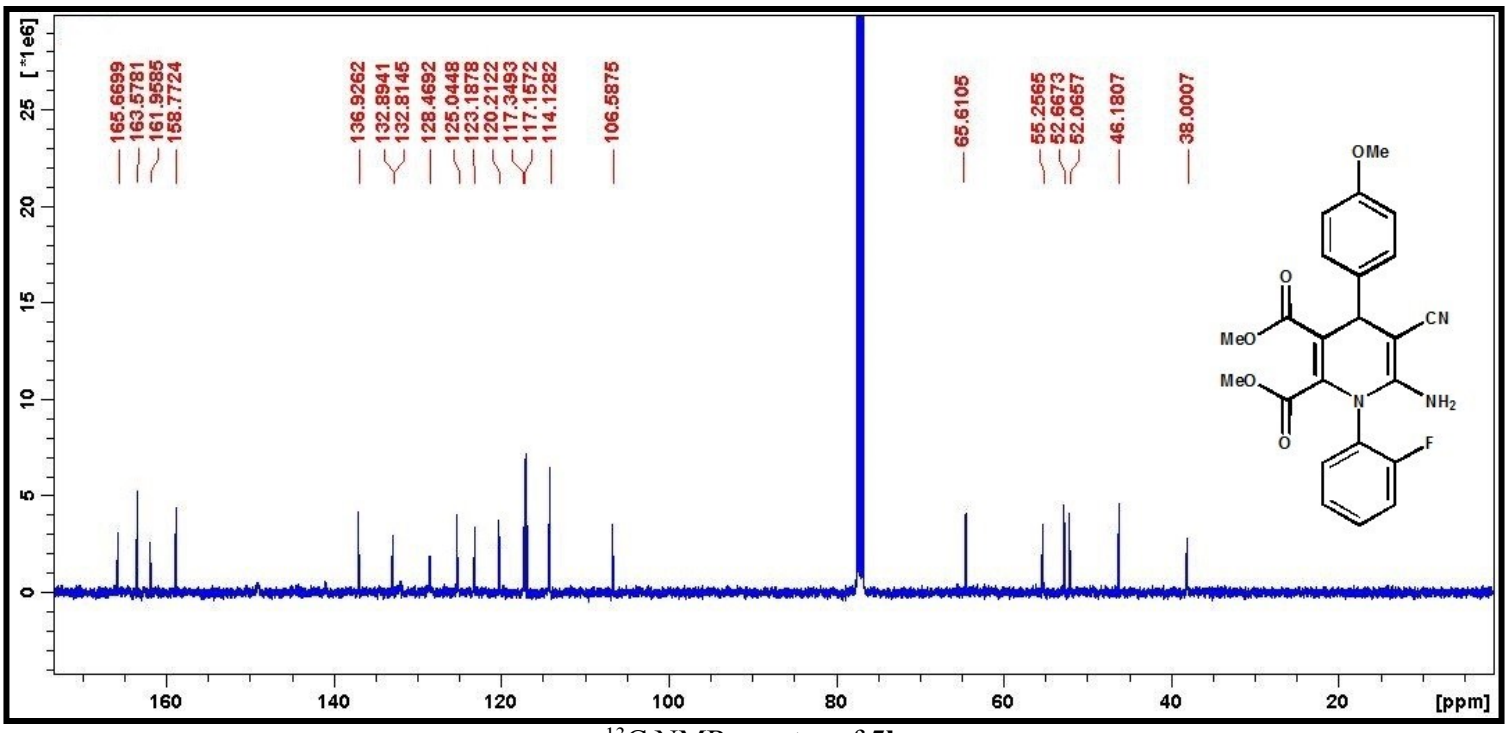
HRMS spectra of **5j**



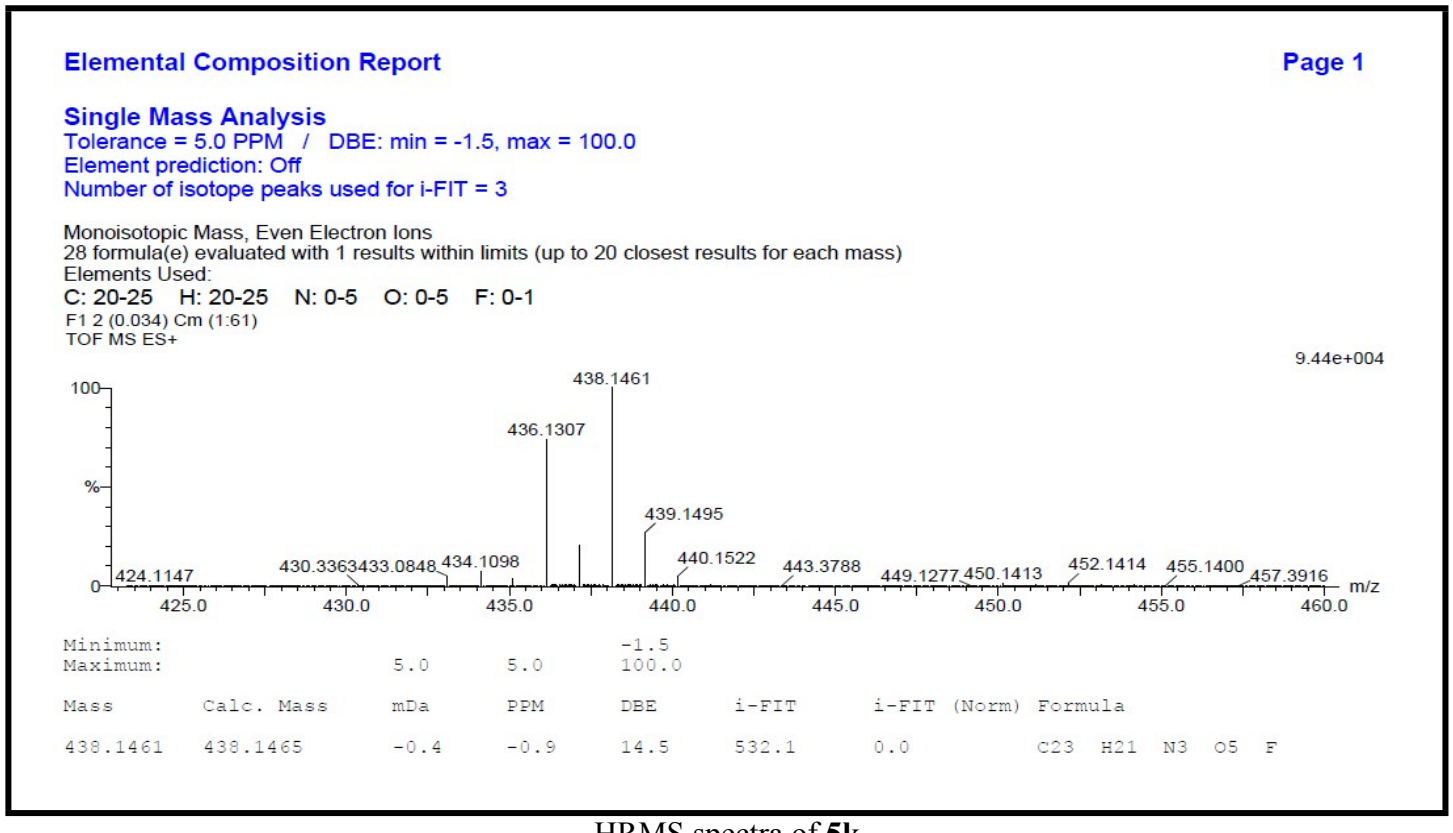
^{1}H NMR spectra of **5k**



^{15}N NMR spectra of **5k**



^{13}C NMR spectra of **5k**



HRMS spectra of **5k**