Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Electronic Supporting Information

Electronic Effect of Substituents on Anilines Favors 1,4-Addition to *trans-β*-nitrostyrenes: Access to N-Substituted 3-Arylindoles and 3-Arylindoles

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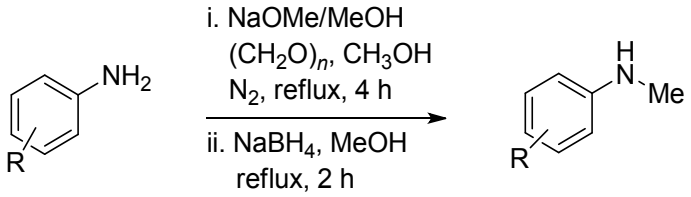
Table S1. Crystal data and structure refinement for compound **3h**

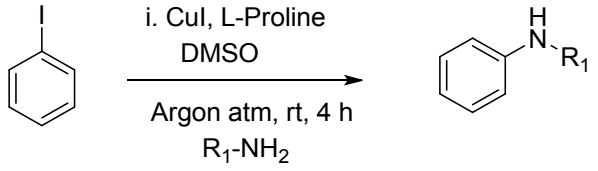
Entry	Identification code	Compound 3h
01	Empirical formula	$C_{15}H_{12}ClN$
02	Formula weight	241.71
03	Temperature	296(2) K
04	Wavelength	0.71073
05	Radiation type	MoK\a
06	Radiation source	'fine-focus sealed tube'
07	Crystal system	Triclinic
08	Space group	P-1
09	Cell length	a 9.4630(12) b 9.9221(11) c 13.5665(16)
10	Cell Angle	α 102.387(10) β 94.259(10) δ 98.976(10)
11	Cell Volume	1221.2(3)
12	Density	1.315
13	Completeness to theta	25.00° / 99.80%
14	Absorption correction	multi-scan
15	Refinement method	Full-matrix least-squares on F2
16	Index ranges	$-11 \leq h \leq 11$, $-11 \leq k \leq 11$, $-14 \leq l \leq 16$
17	Reflection number	4285
18	Theta range	3.09-25.00
19	Cell formula units Z	4
20	CCDC no	1576147

I. General Procedure for Synthesis of *N*-methylanilines[1]



To the freshly prepared solution of NaOMe (50 mmol) in MeOH (20 mL), anilines (10 mmol) and paraformaldehyde (50 mmol) were added. The mixture was allowed to reflux for 4 hours and $NaBH_4$ (15 mmol) was added portion wise at 0 °C and the mixture was refluxed for an additional 2 hours. The completion of the reaction analyzed by TLC, the mixture was cooled and solvent was evaporated on a vacuum pump to give a residue that was treated with aqueous layer (20 mL). The compound was extracted with CH_2Cl_2 (2 × 15 mL), the combined organic extracts was washed with brine solution (20 mL). The organic residue was dried over anhydrous Na_2SO_4 and solvent was removed using vacuum pump and residue that was purified through silica gel (60-120 mesh) column chromatography with petroleum ether/ethyl acetate (9.5 : 0.5 v/v) to obtain the pure product.

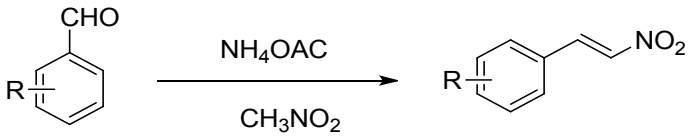
II. General Procedure for Synthesis of *N*-alkylanilines[2]



An oven-dried flask was charged with copper iodide (38 mg, 0.2 mmol) and L-proline (46 mg, 0.4 mmol); if solid, the aryl iodide (1.0 mmol) was also introduced at this stage. The flask was evacuated under high vacuum and backfilled with argon three times, then fitted with a rubber septum. The DMSO (1.0 mL) solvent was next added, as well as the aryl iodide, which was added at this stage if liquid. The resulting blue solution was stirred for 5 min before adding the amine (3.0 mmol). The resulting mixture was stirred under argon at room temperature until completion of the reaction indicated by TLC. After completion of the reaction analyzed by TLC, the mixture was cooled and solvent was evaporated on a vacuum pump to give a residue that was treated with aqueous layer (20 mL). The compound was extracted with CH_2Cl_2 (2 × 15 mL), the combined organic extracts was washed with brine solution (20 mL). The organic residue was dried over anhydrous Na_2SO_4 and solvent was removed by using vacuum pump and residue that was purified

through silica gel (60-120 mesh) column chromatography with petroleum ether/ethyl acetate (9.5 : 0.5 v/v) to obtain the pure product.

III. General Procedure for Synthesis of *trans-β*-nitrostyrene[3]

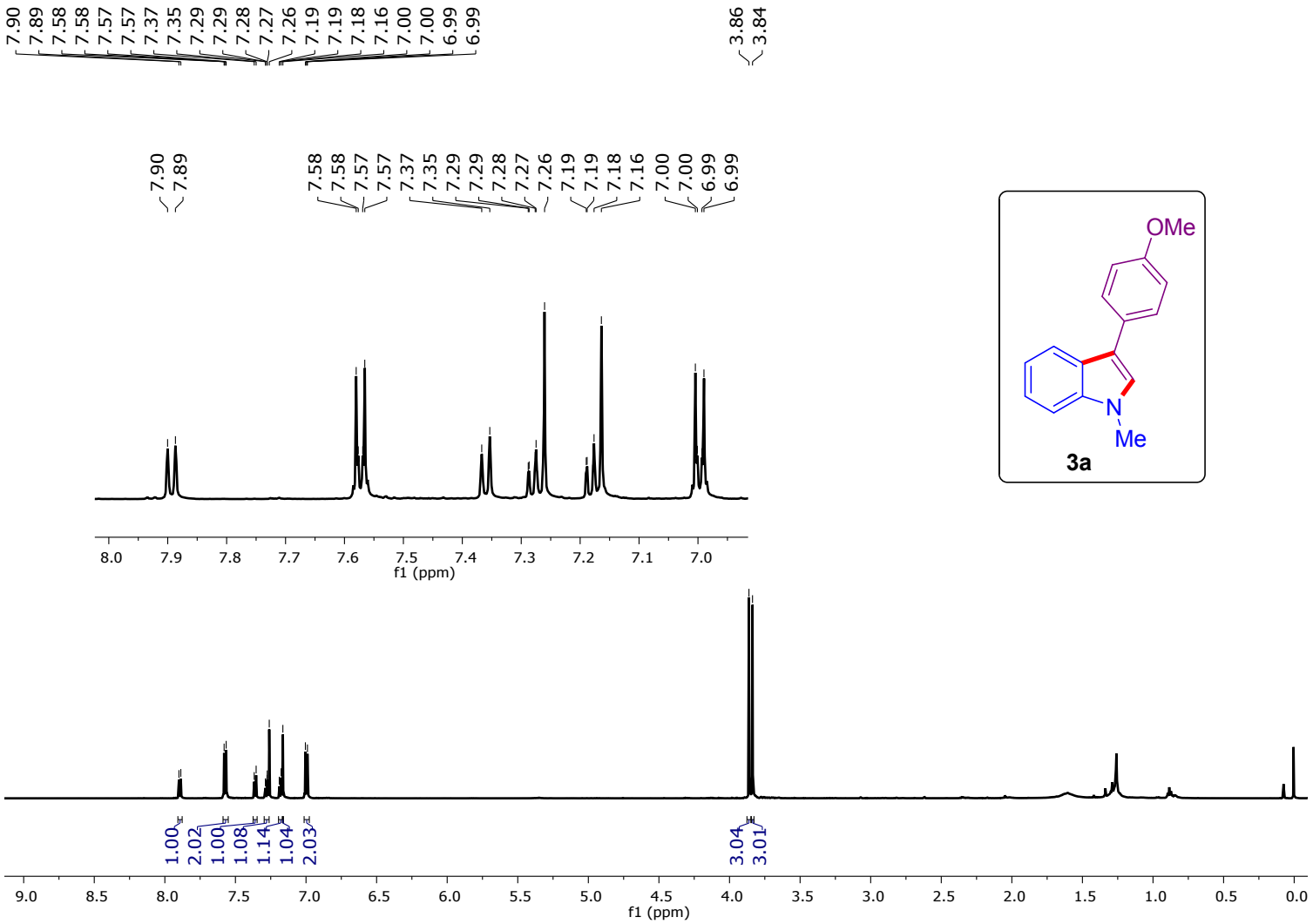


Benzaldehyde (1 mmol) reacted with nitromethane (1 mL) in the acetic acid solution (1 mL) with ammonium acetate (0.1 mmol) at 100°C for 3 hours. The completion of reaction monitored by TLC, cool down the reaction mixture to room temperature and add ice cold water to get solid product. Filter the product using Buchner funnel and dissolve in cold methanol and allow it to recrystallize. Similar procedure was followed for synthesis of other nitrostyrene derivatives.

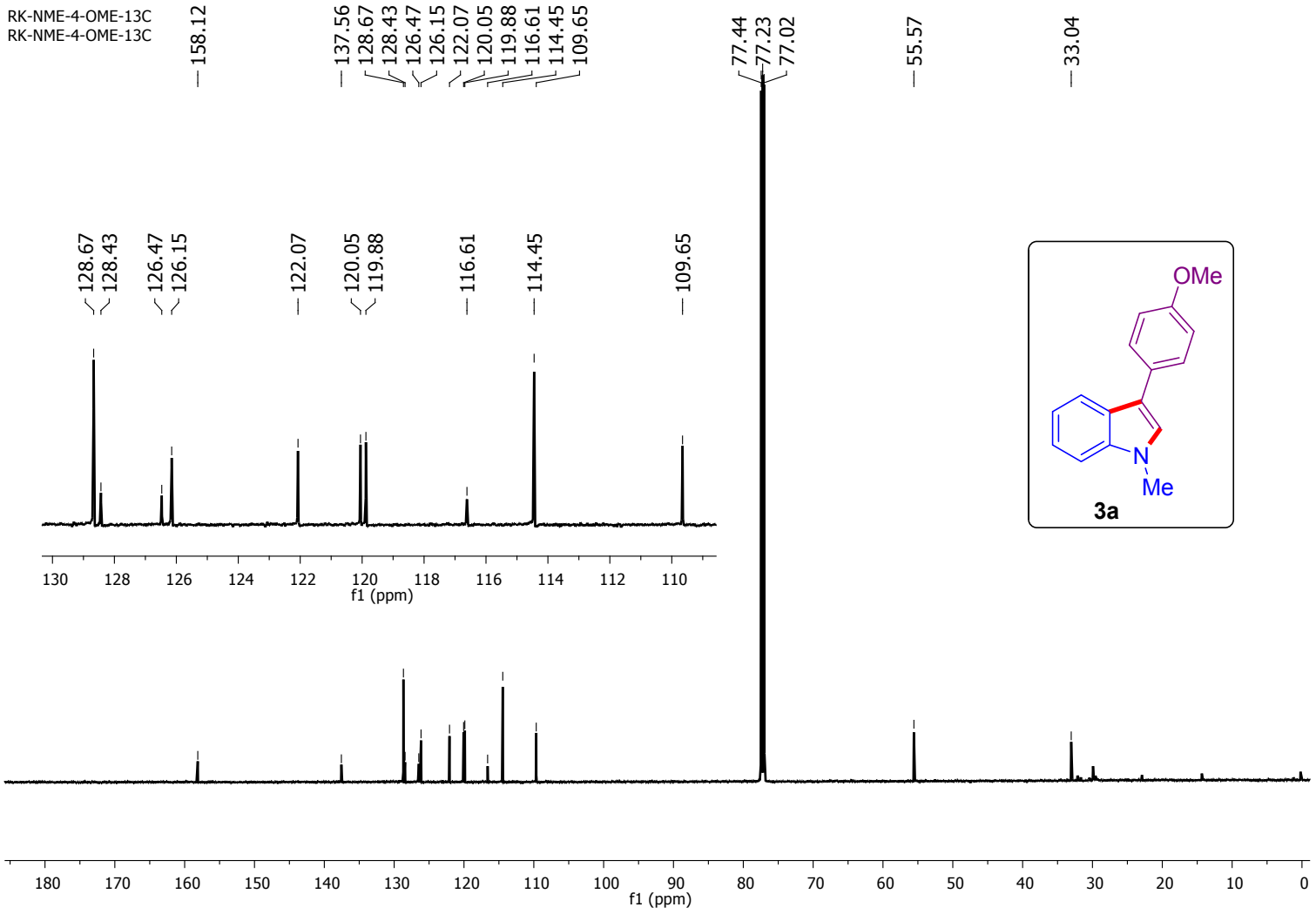
Reference

1. B. Chiranjeevi,; B. Vinayak,; T. Parsharamulu,; V. S. PhaniBabu,; B. Jagadeesh,; B. Sridhar, M. Chandrasekharam. Eur. J. Org. Chem., 2014, 7839.
2. C. Deldaele and G. Evano, ChemCatChem, 2016, **8**, 1319.
3. J. -T. Liu and C. -F. Yao, Tetrahedron Lett., 2001, **42**, 6147.

^{1}H NMR spectra of compound: 3a



^{13}C NMR spectra of compound: 3a



HRMS spectra of compound: 3a

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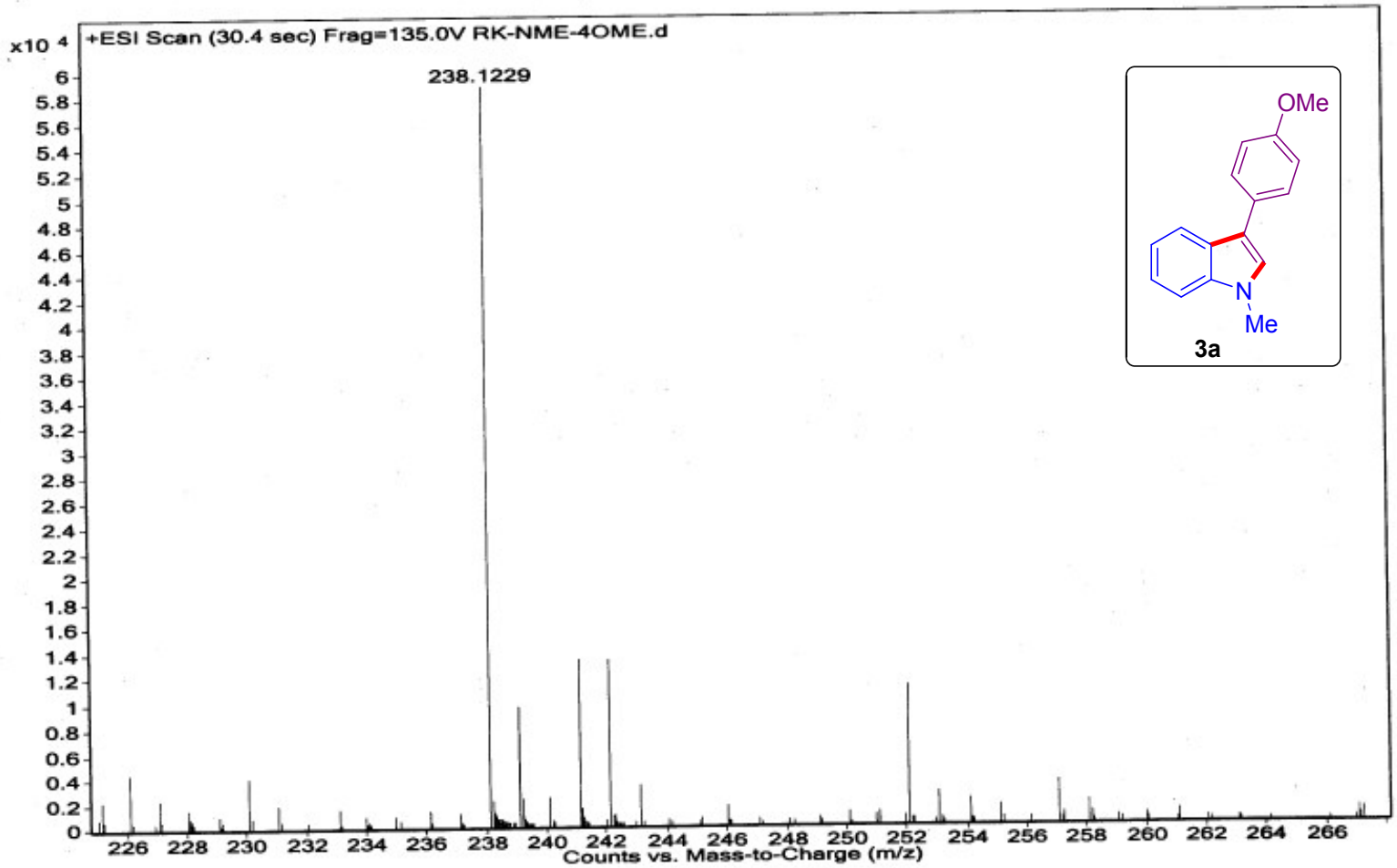
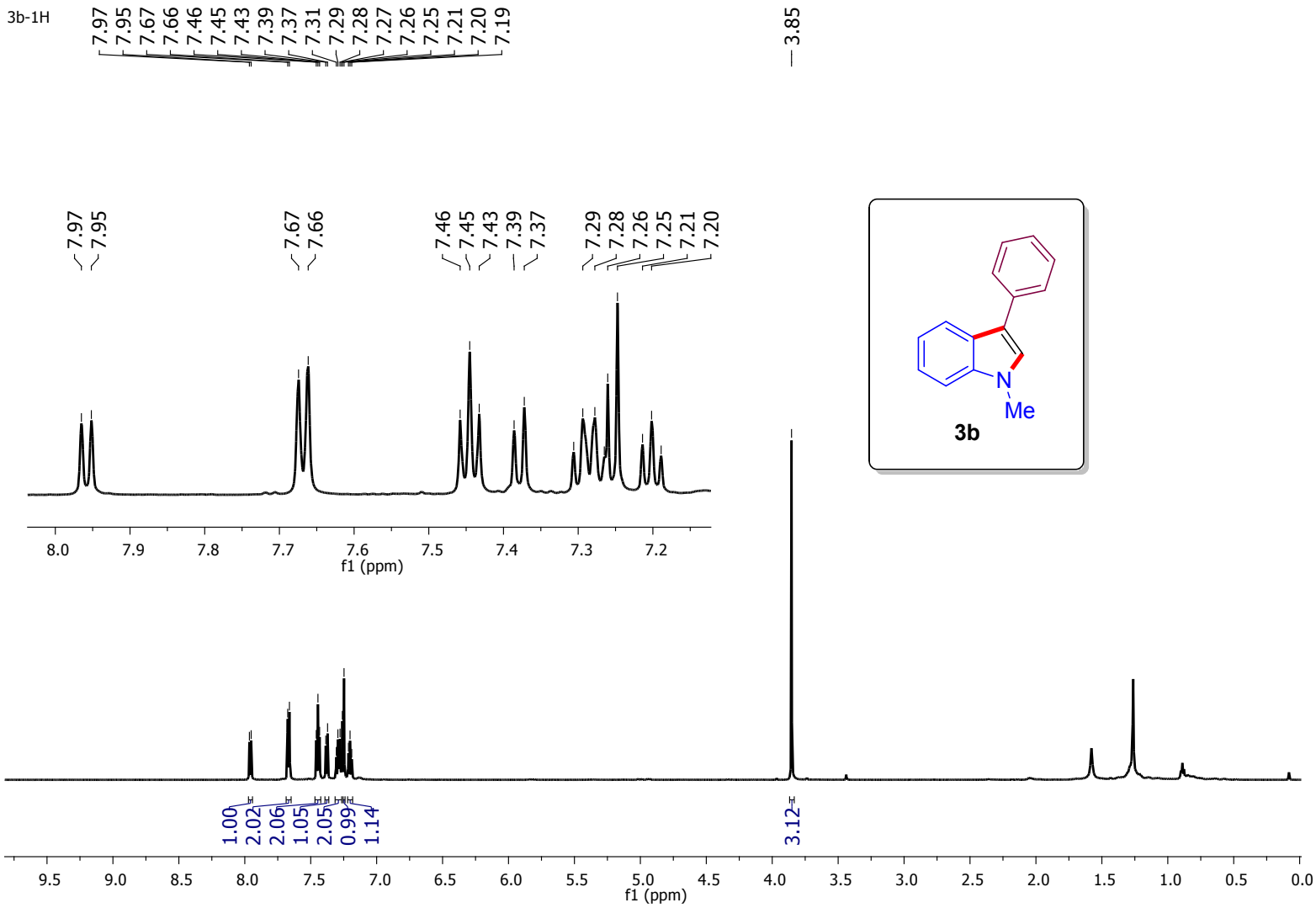
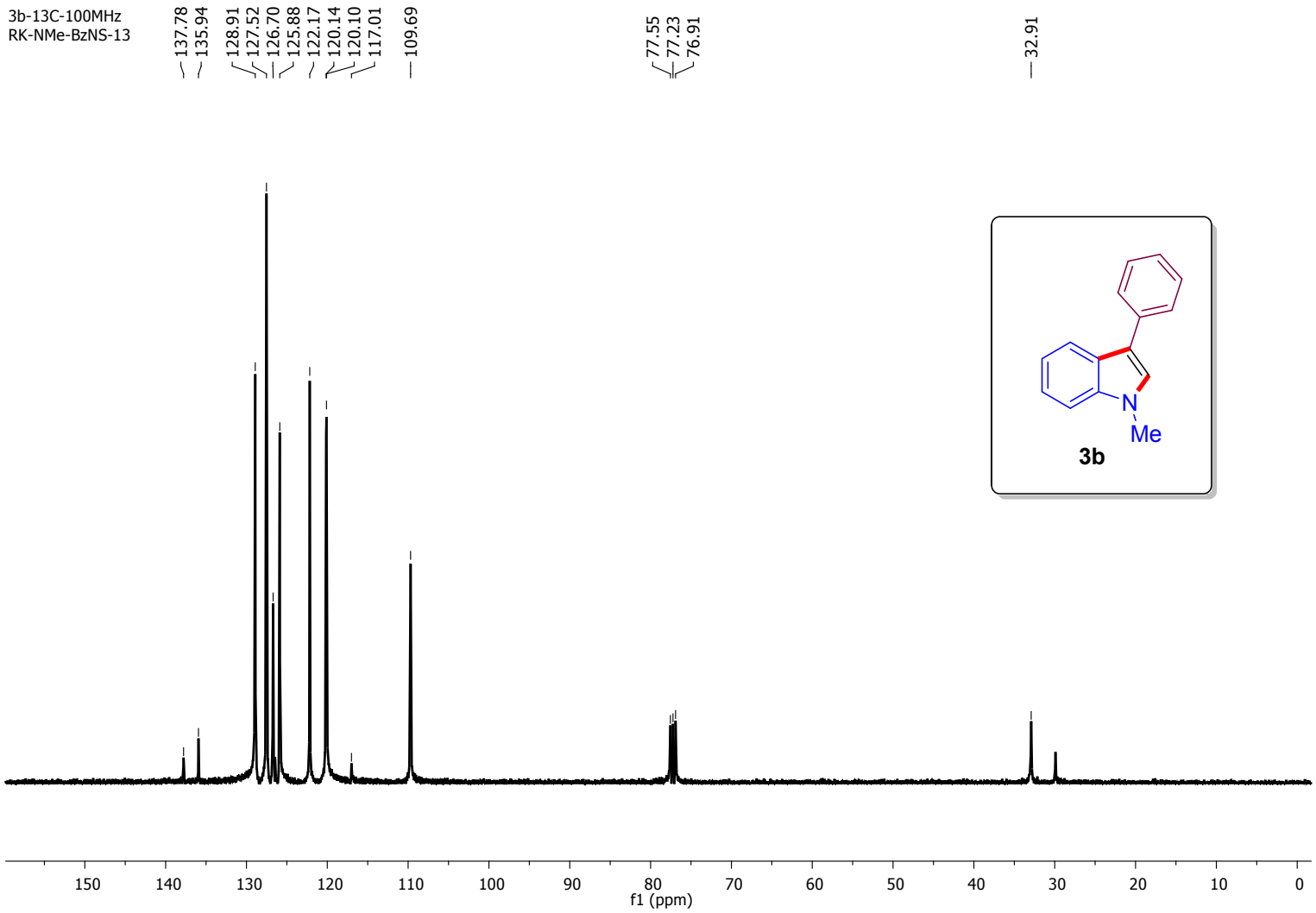


^{1}H NMR spectra of compound: 3b



^{13}C NMR spectra of compound: 3b



HRMS spectra of compound: 3b

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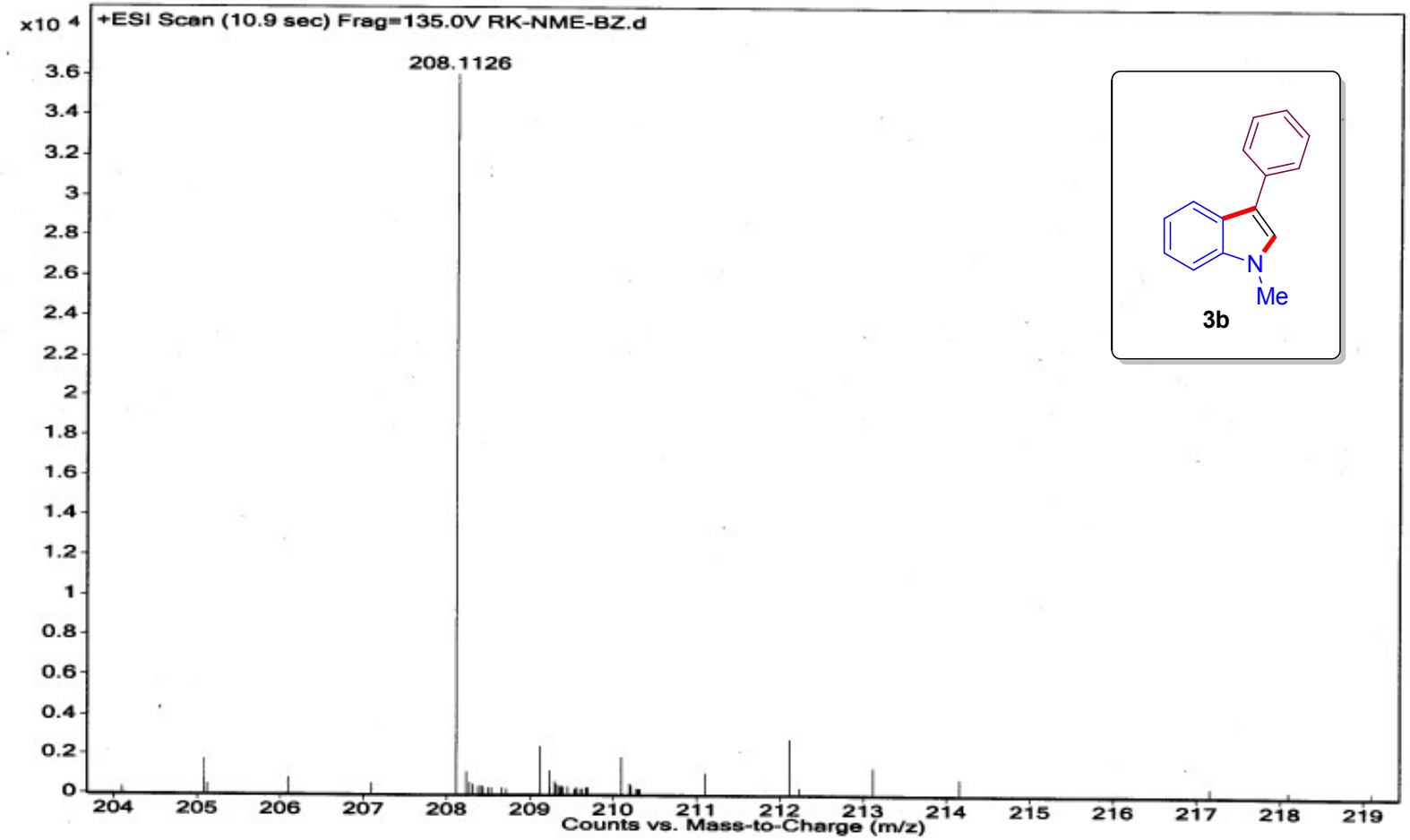
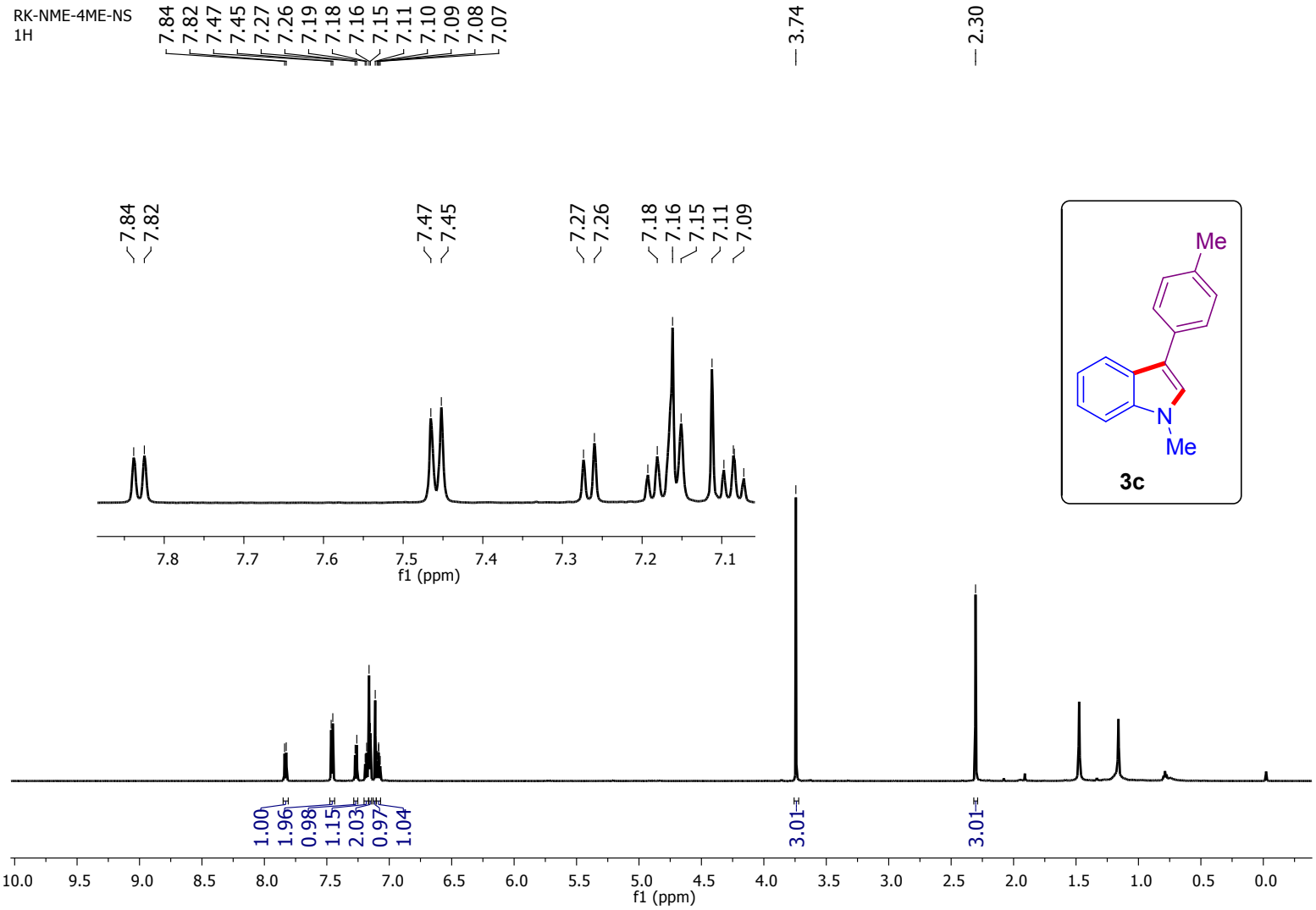
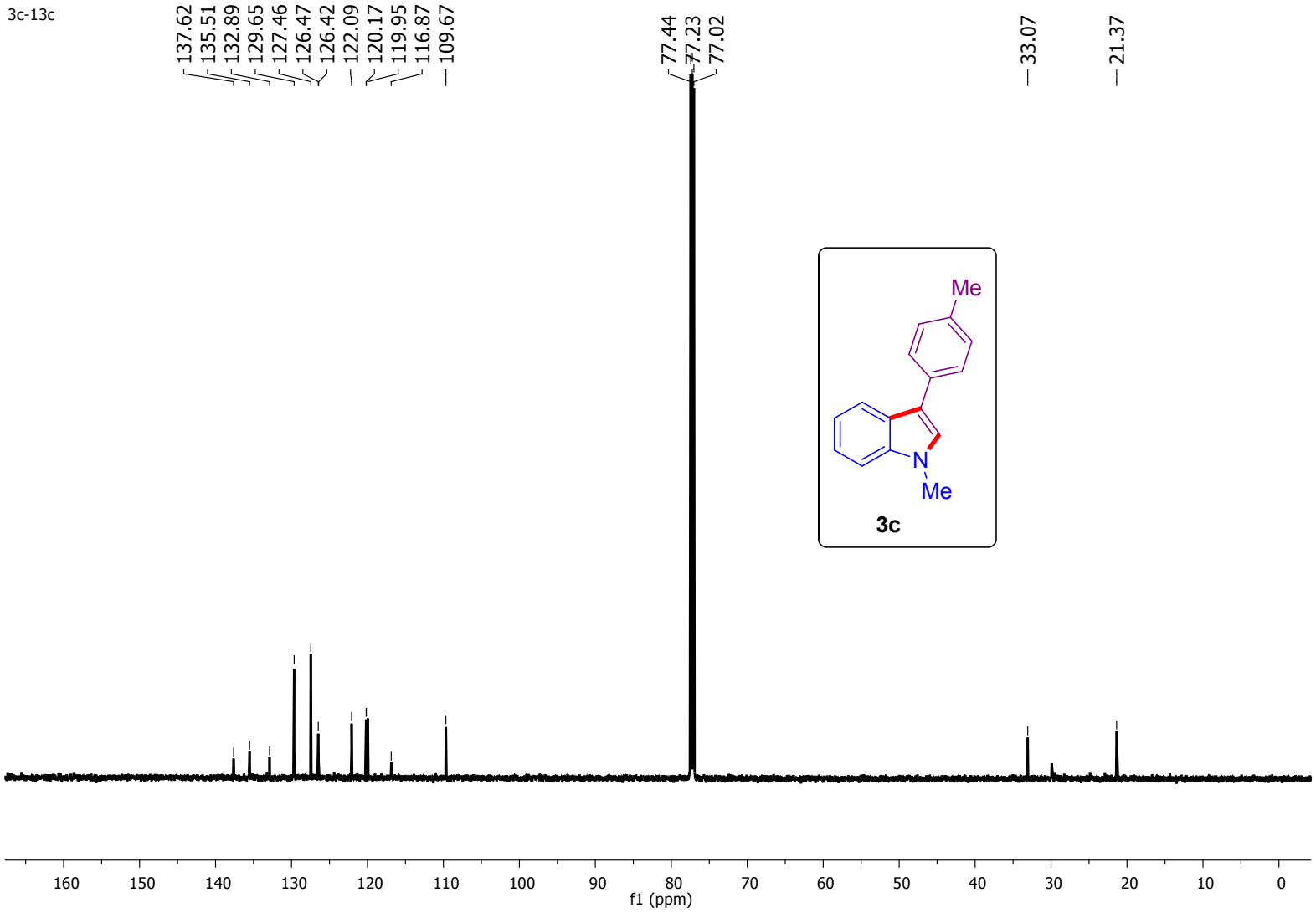


^{1}H NMR spectra of compound: 3c



^{13}C NMR spectra of compound: 3c



HRMS spectra of compound: 3c

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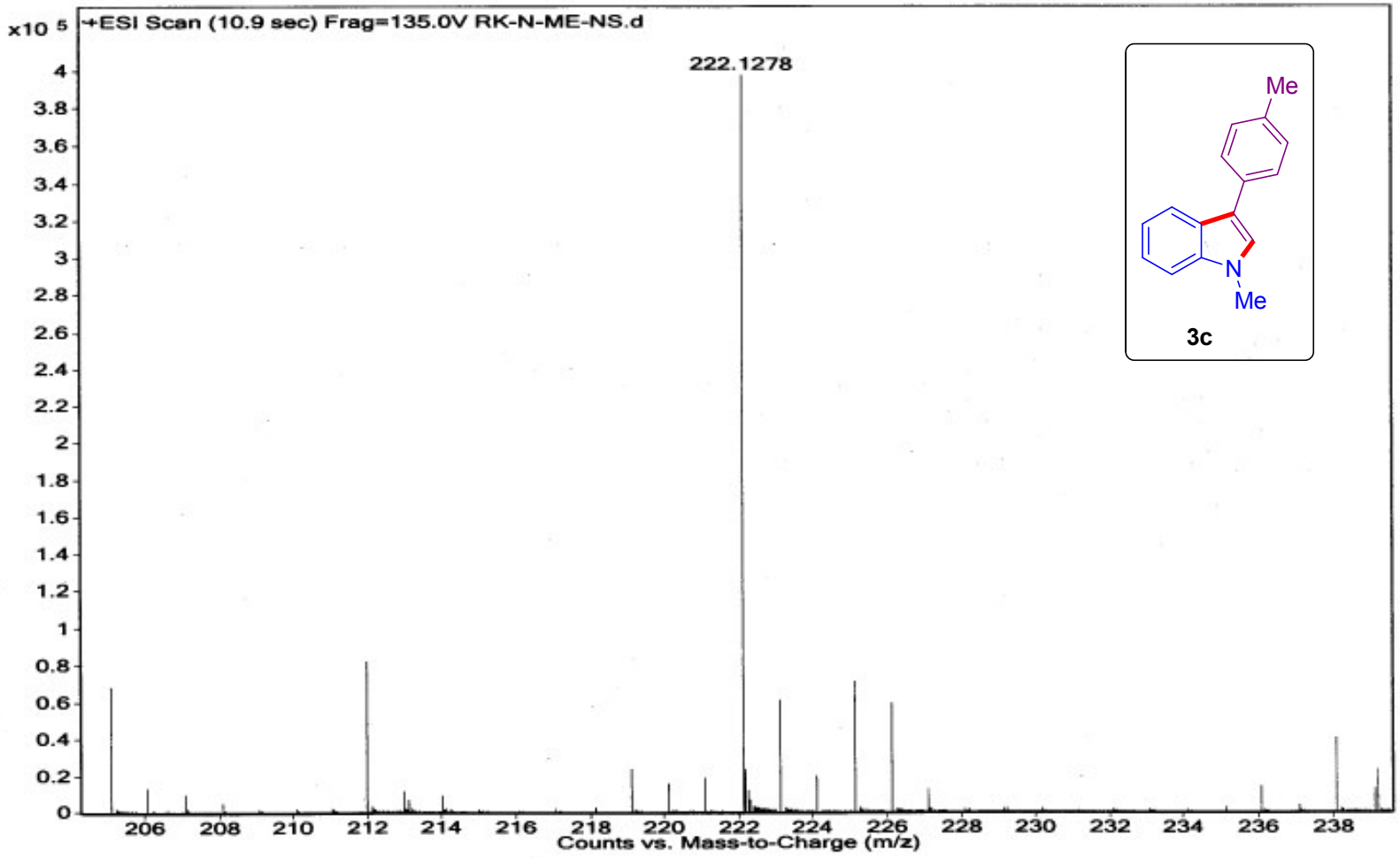
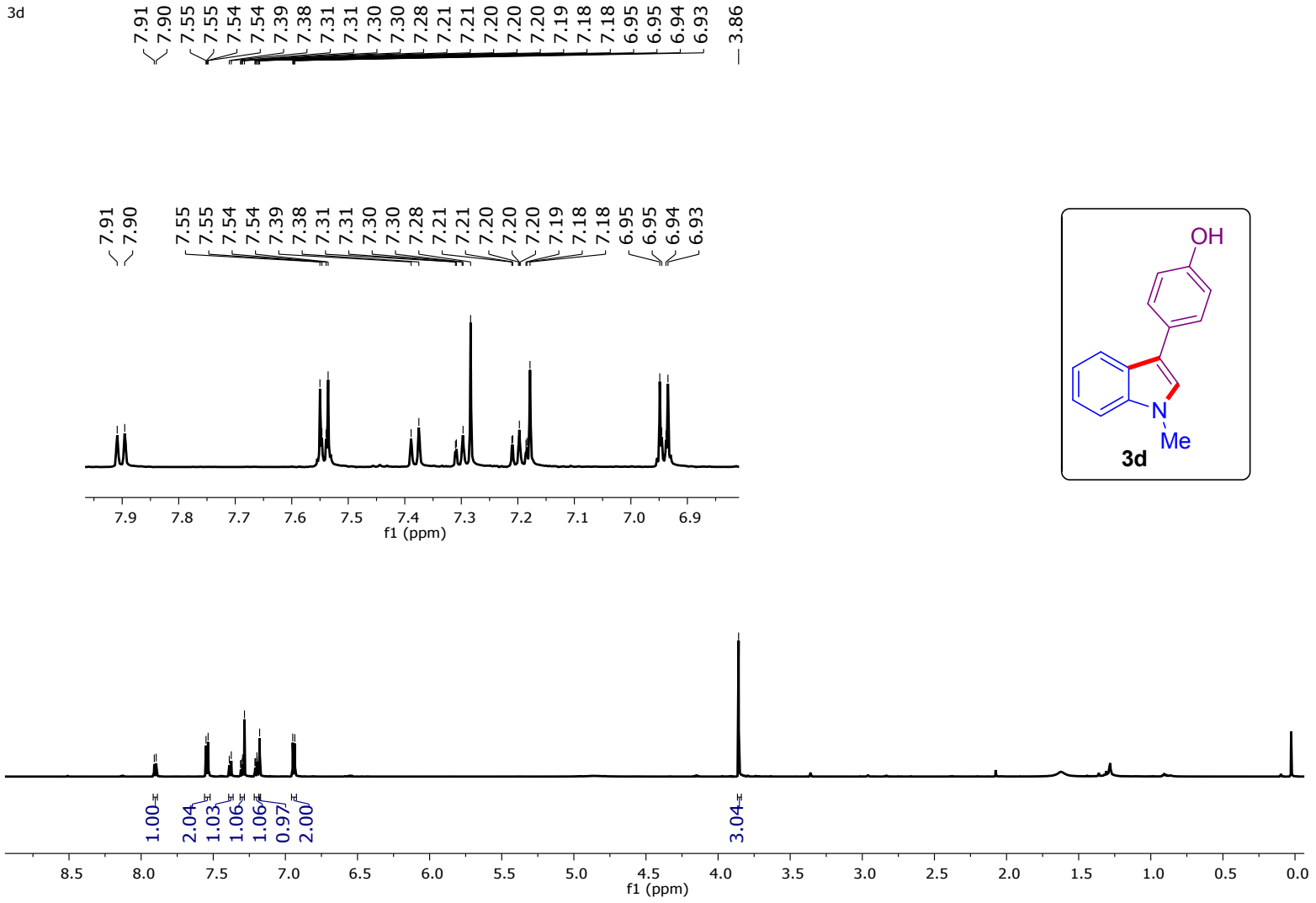
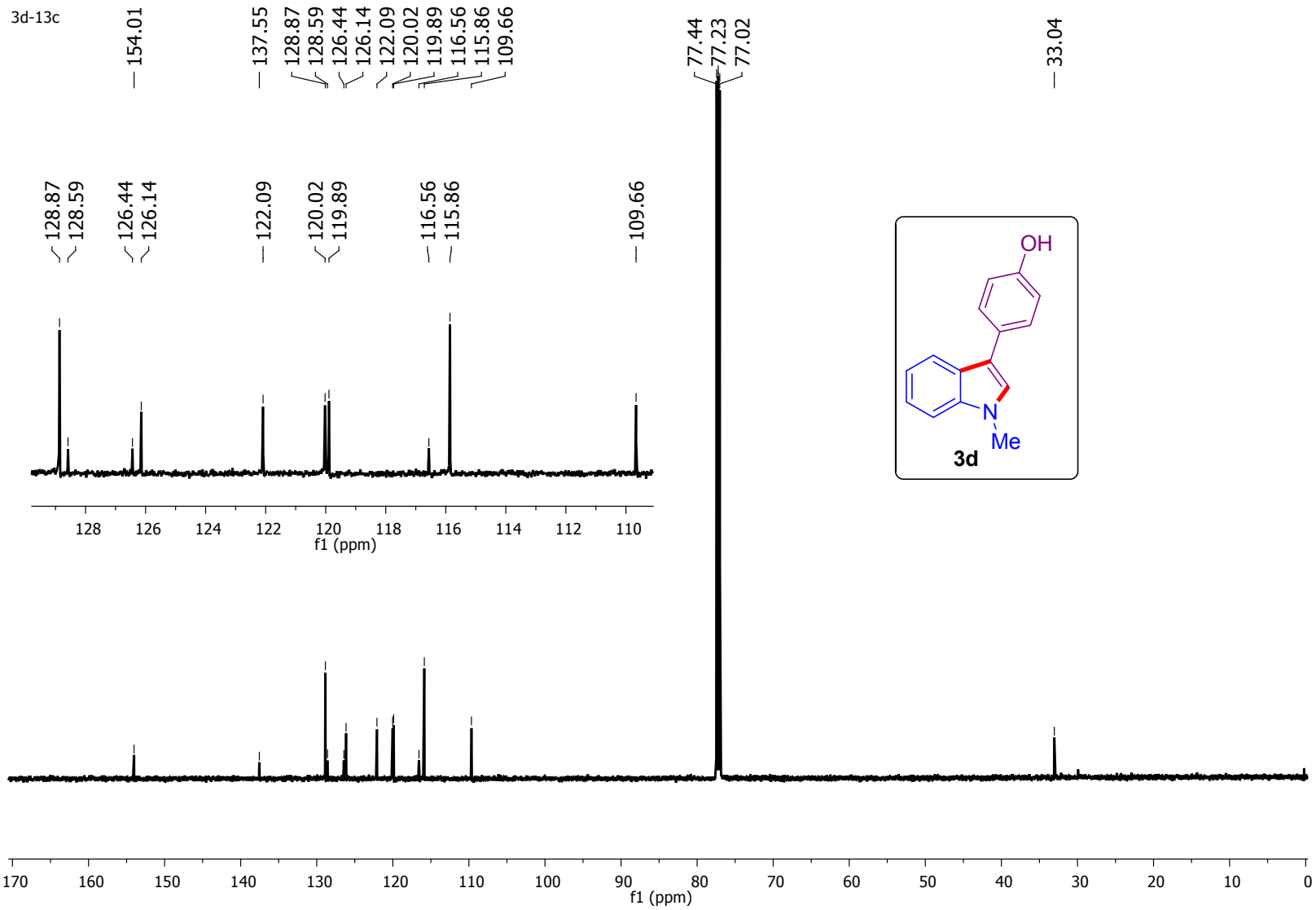


^{1}H NMR spectra of compound: 3d



^{13}C NMR spectra of compound: 3d



HRMS spectra of compound: 3d

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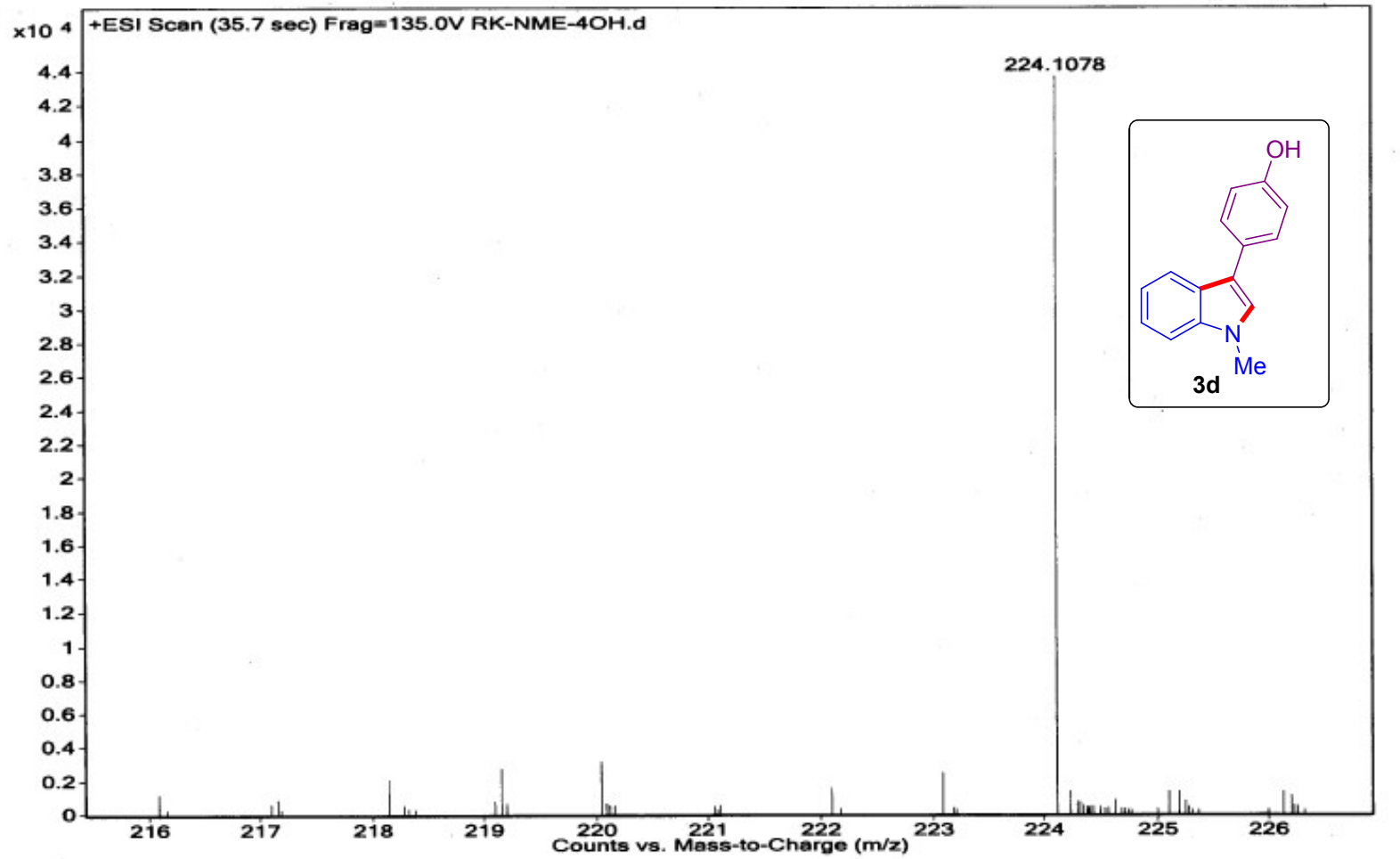
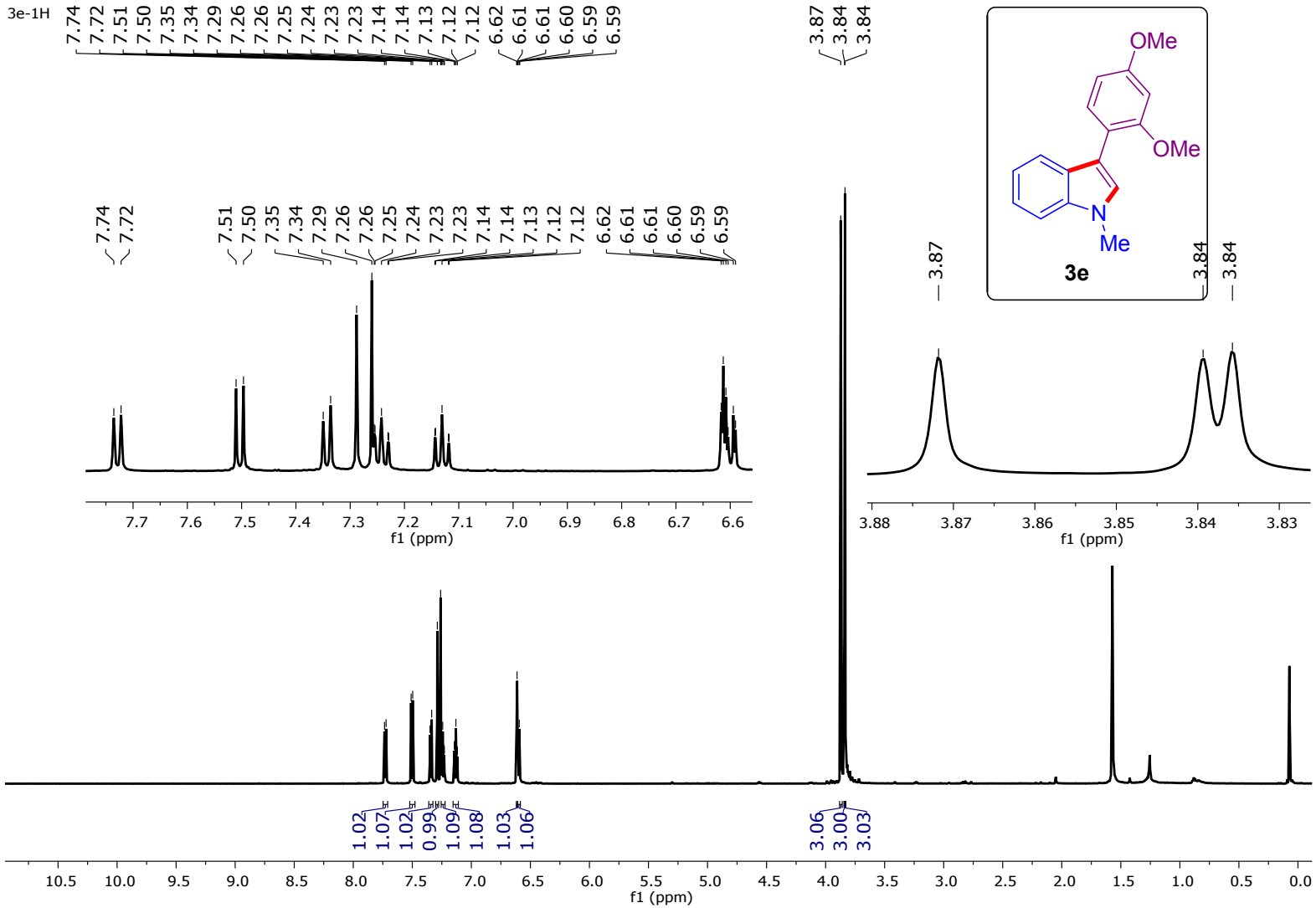
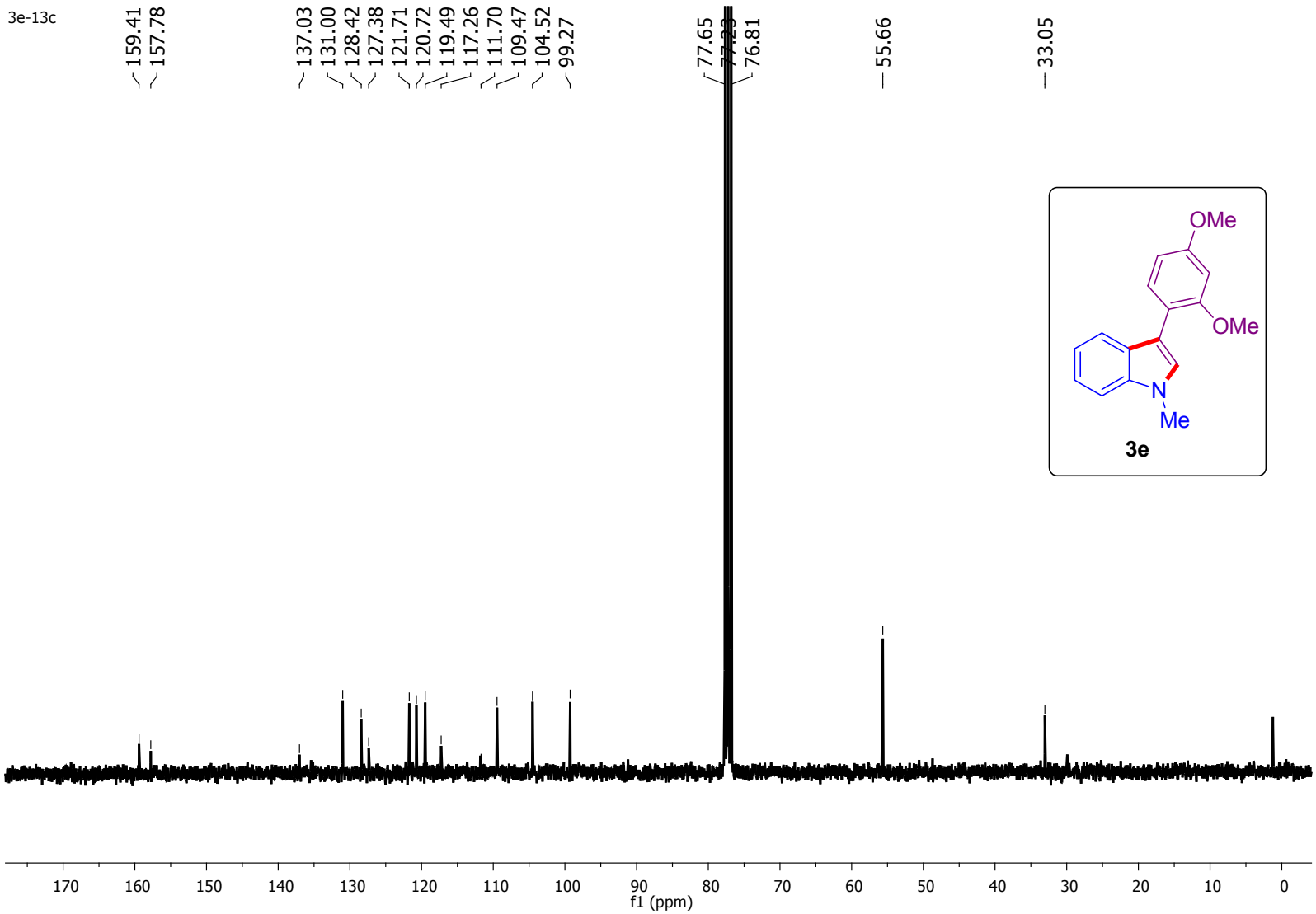


^{1}H NMR spectra of compound: 3e



^{13}C NMR spectra of compound: 3e



HRMS spectra of compound: 3e

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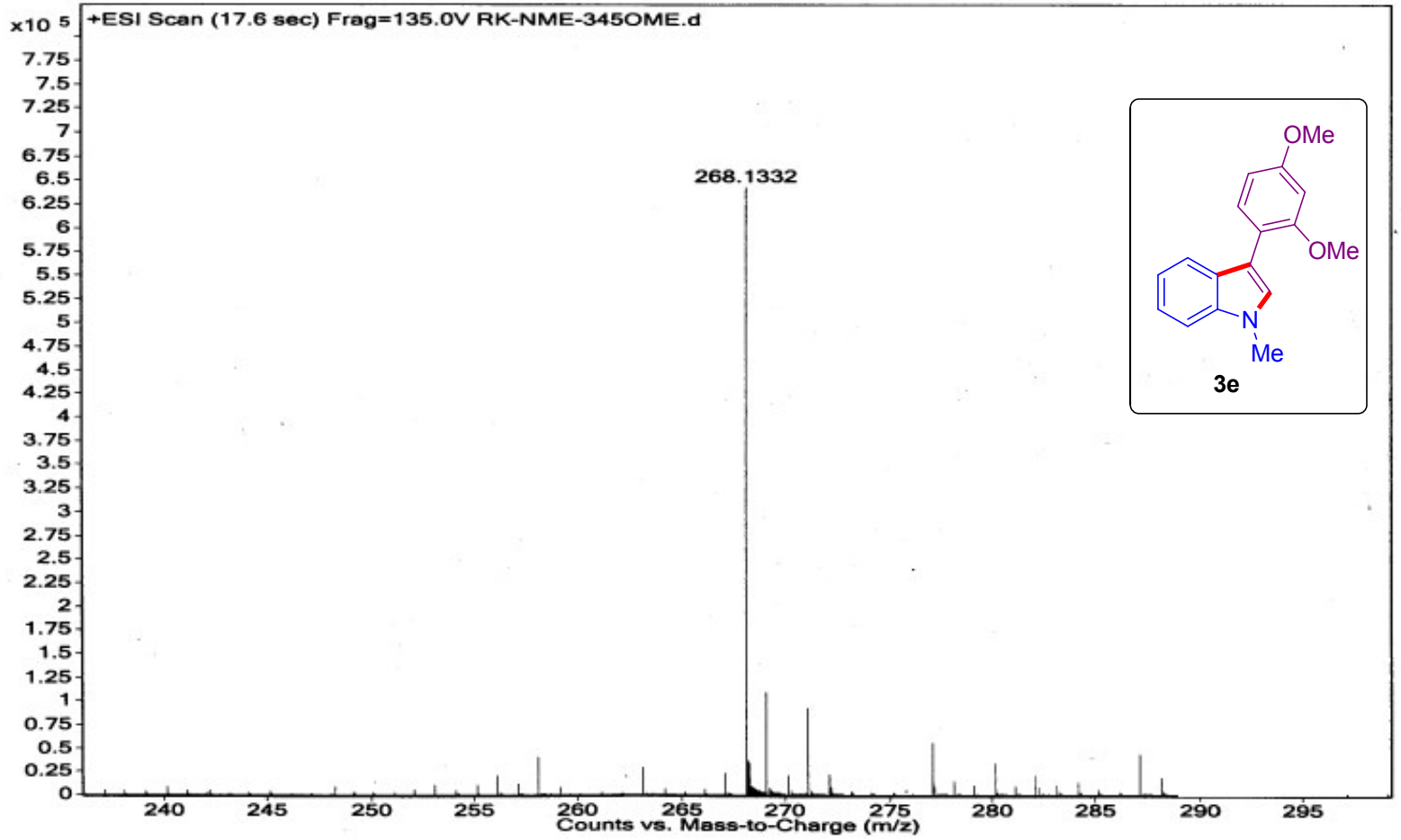
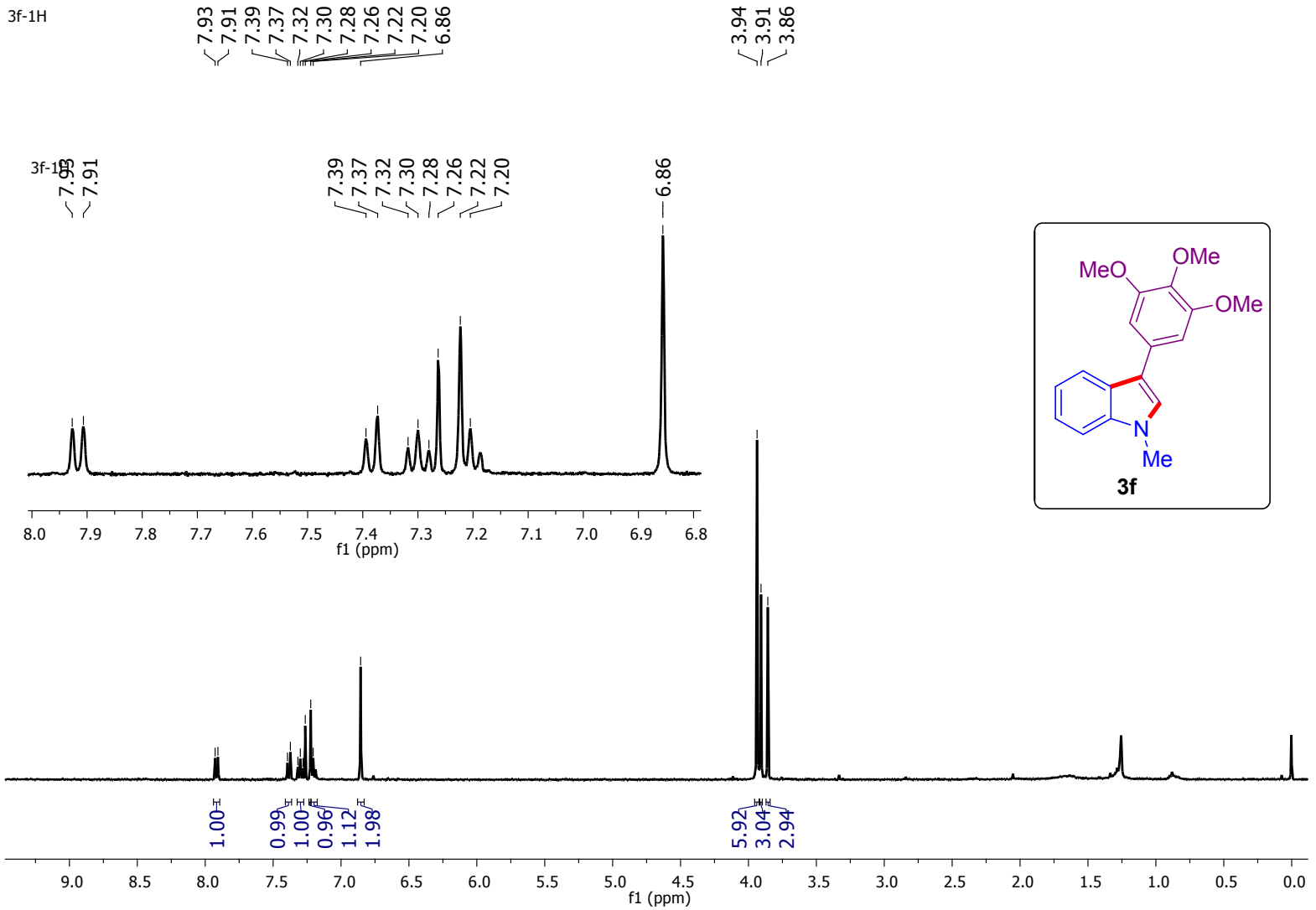
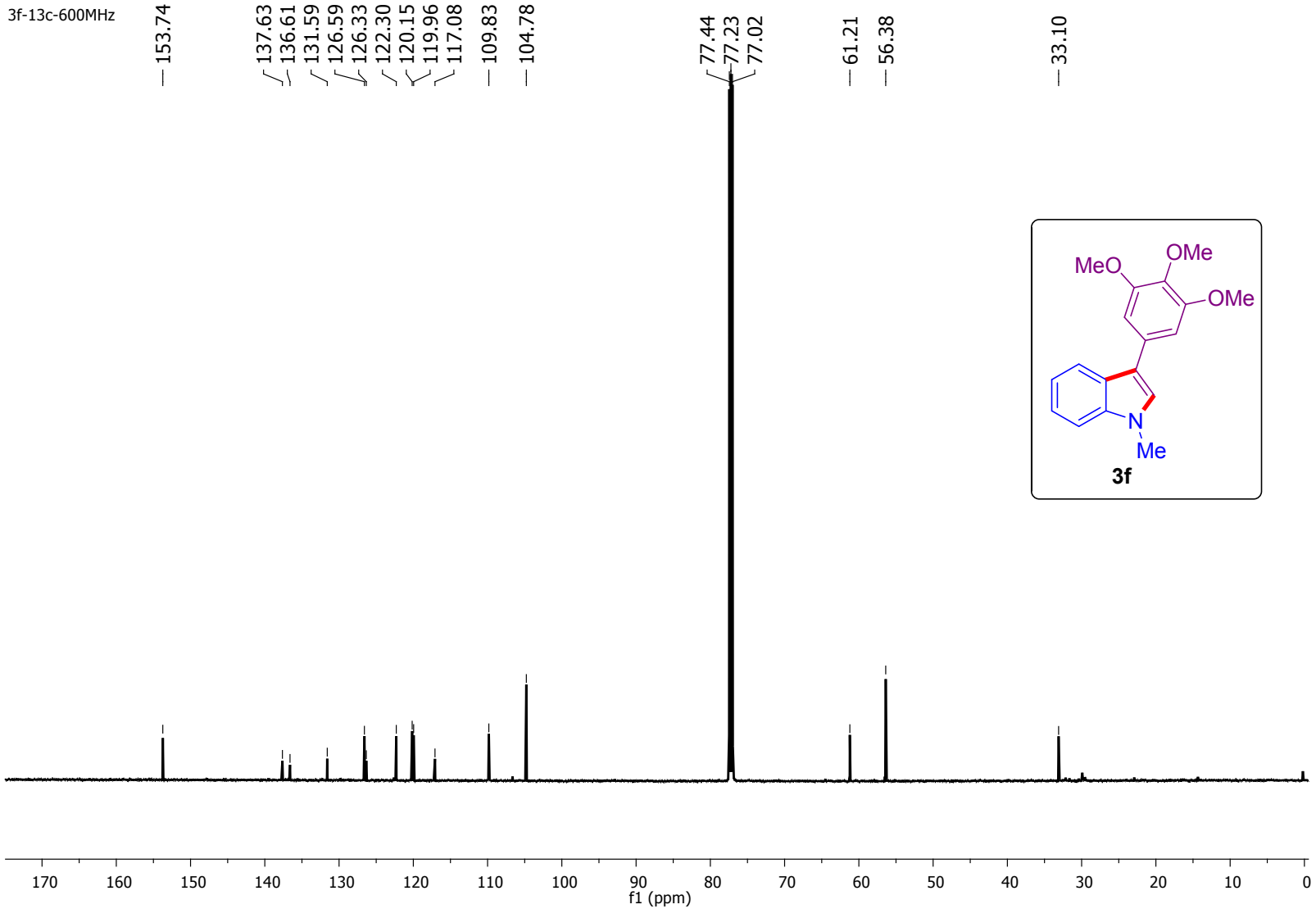


^{1}H NMR spectra of compound: 3f



^{13}C NMR spectra of compound: 3f



HRMS spectra of compound: 3f

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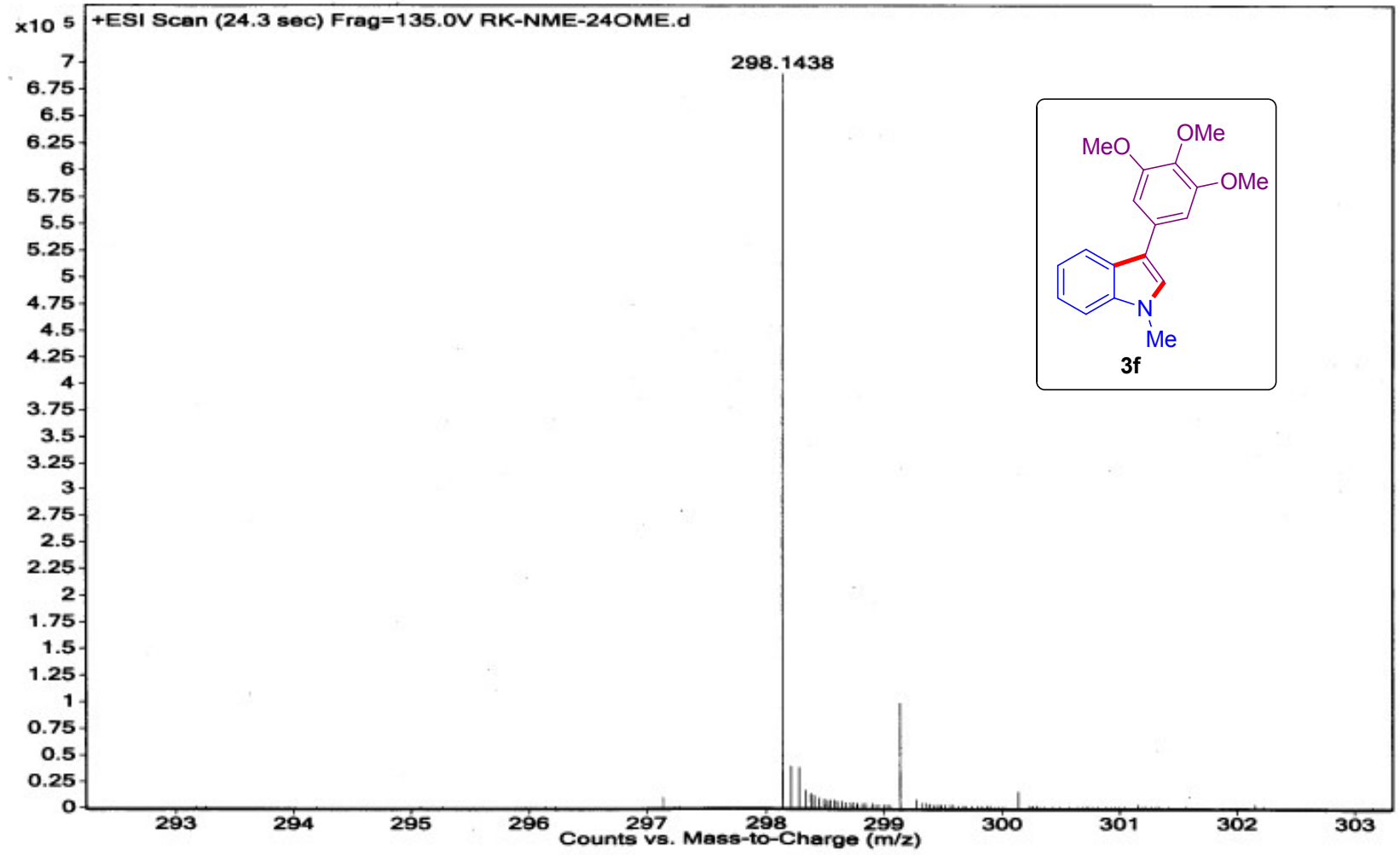
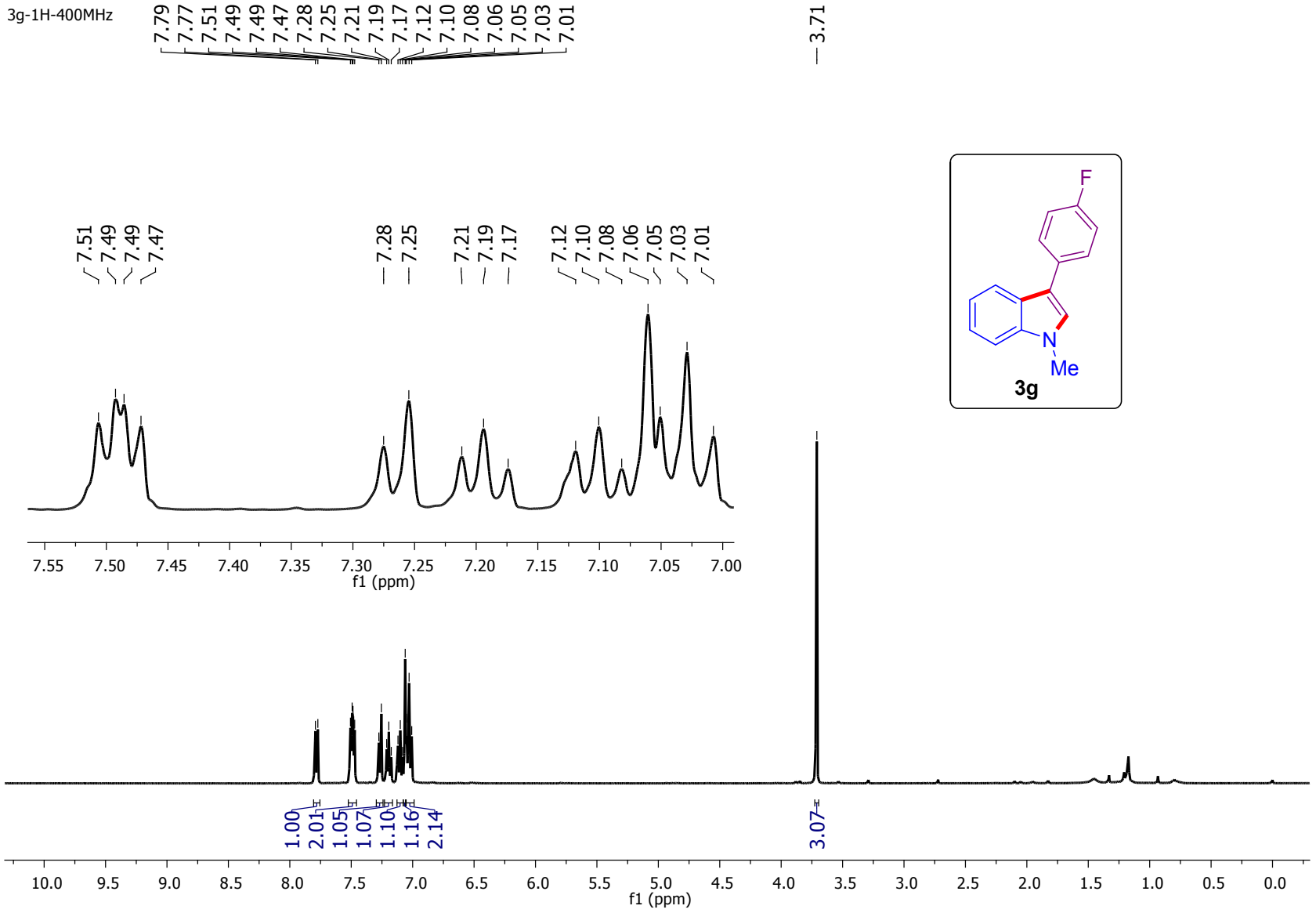
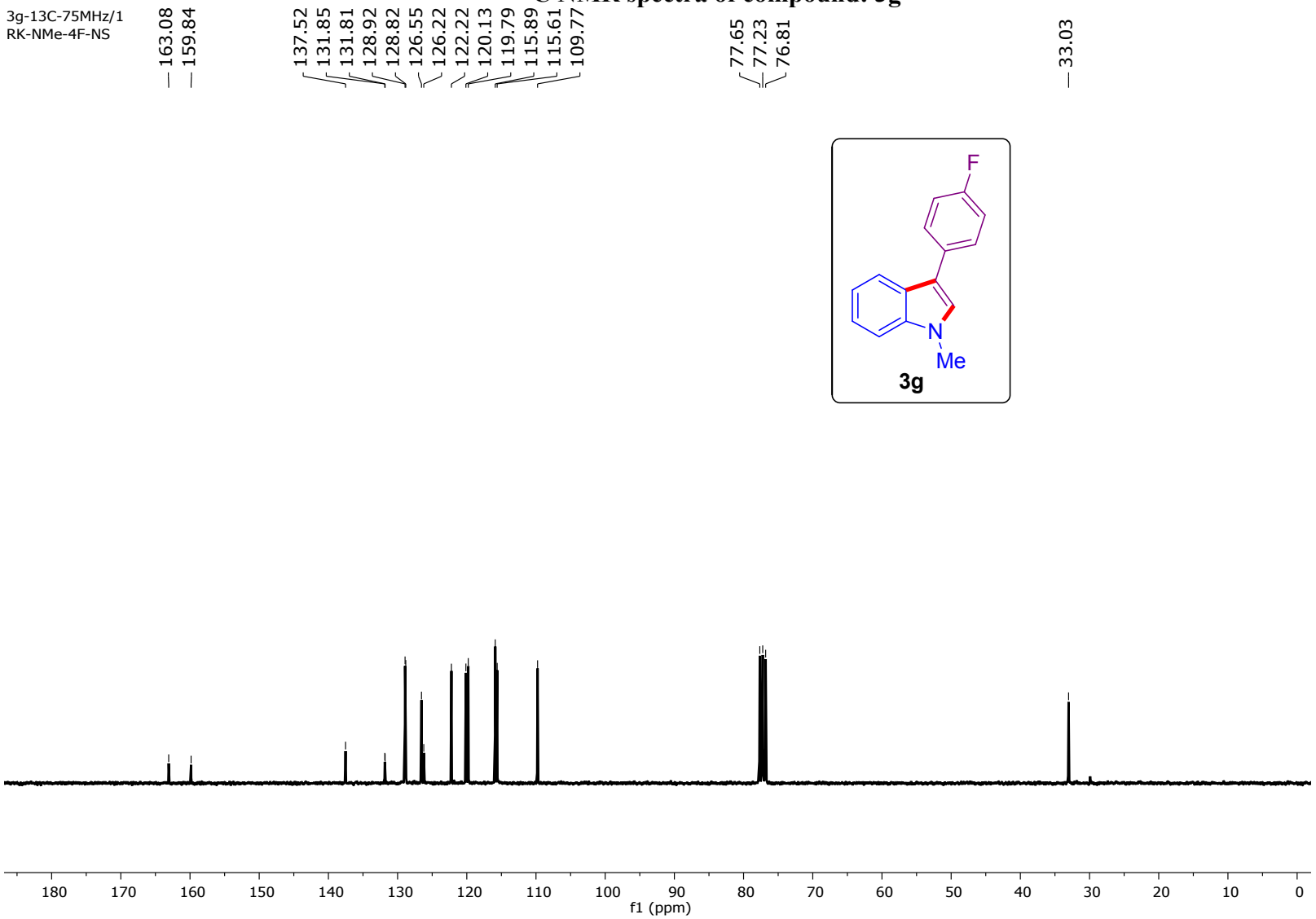


^{1}H NMR spectra of compound: 3g



^{13}C NMR spectra of compound: 3g



HRMS spectra of compound: 3g

Sample Name	RK-NME-4F	**Position**	Vial 1	**Instrument Name**	Instrument 1	**User Name**	
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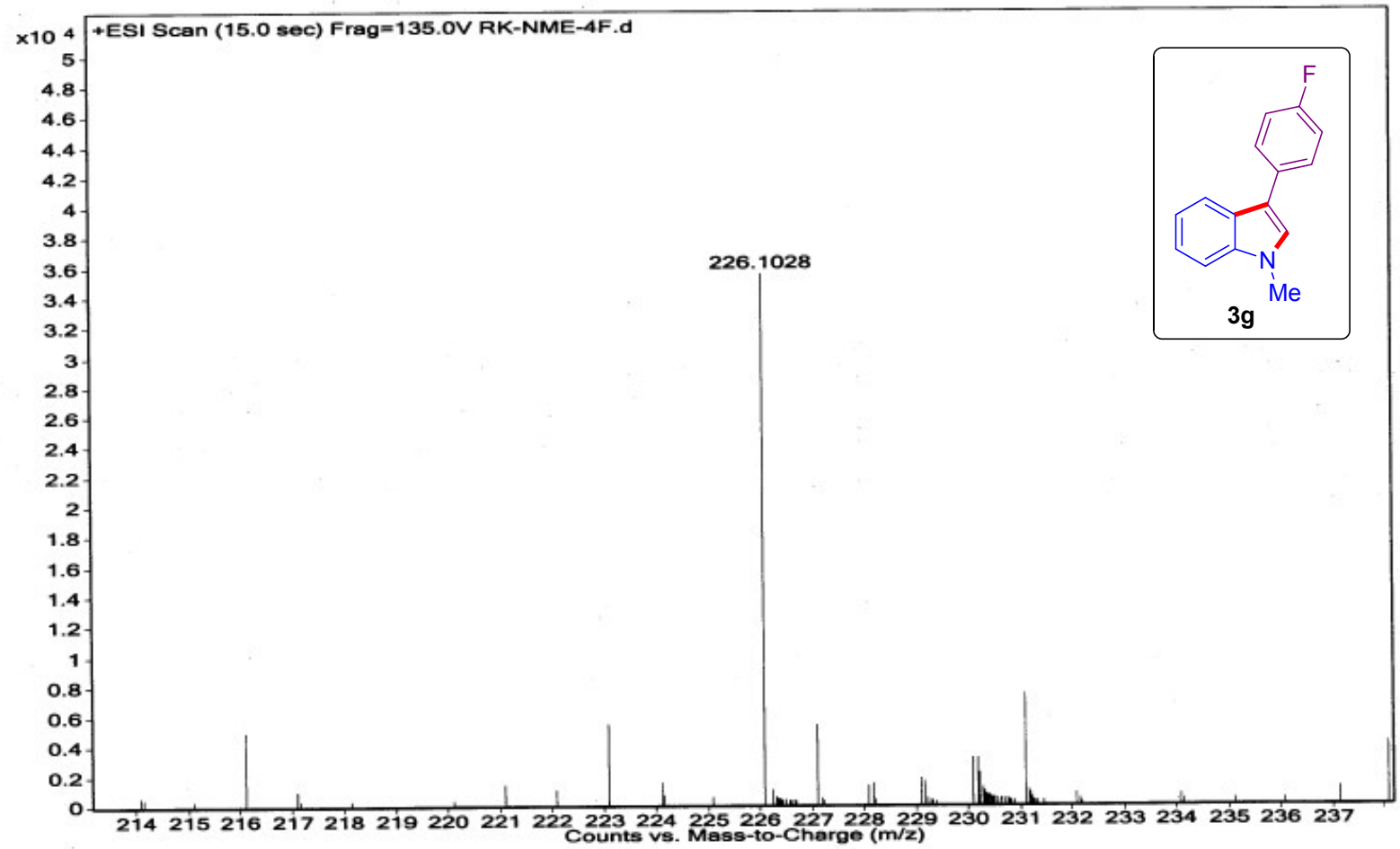
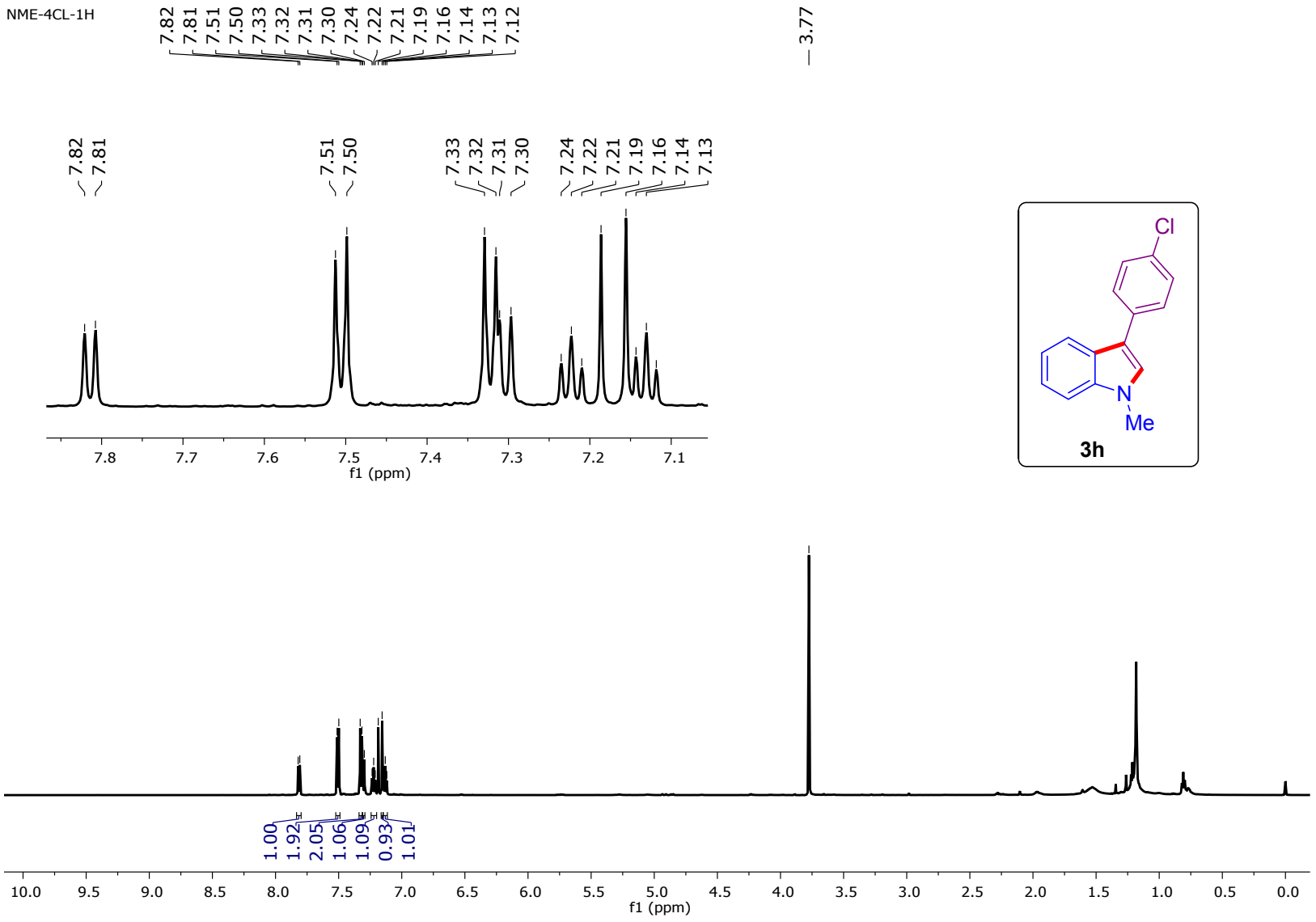


^{1}H NMR spectra of compound: 3h



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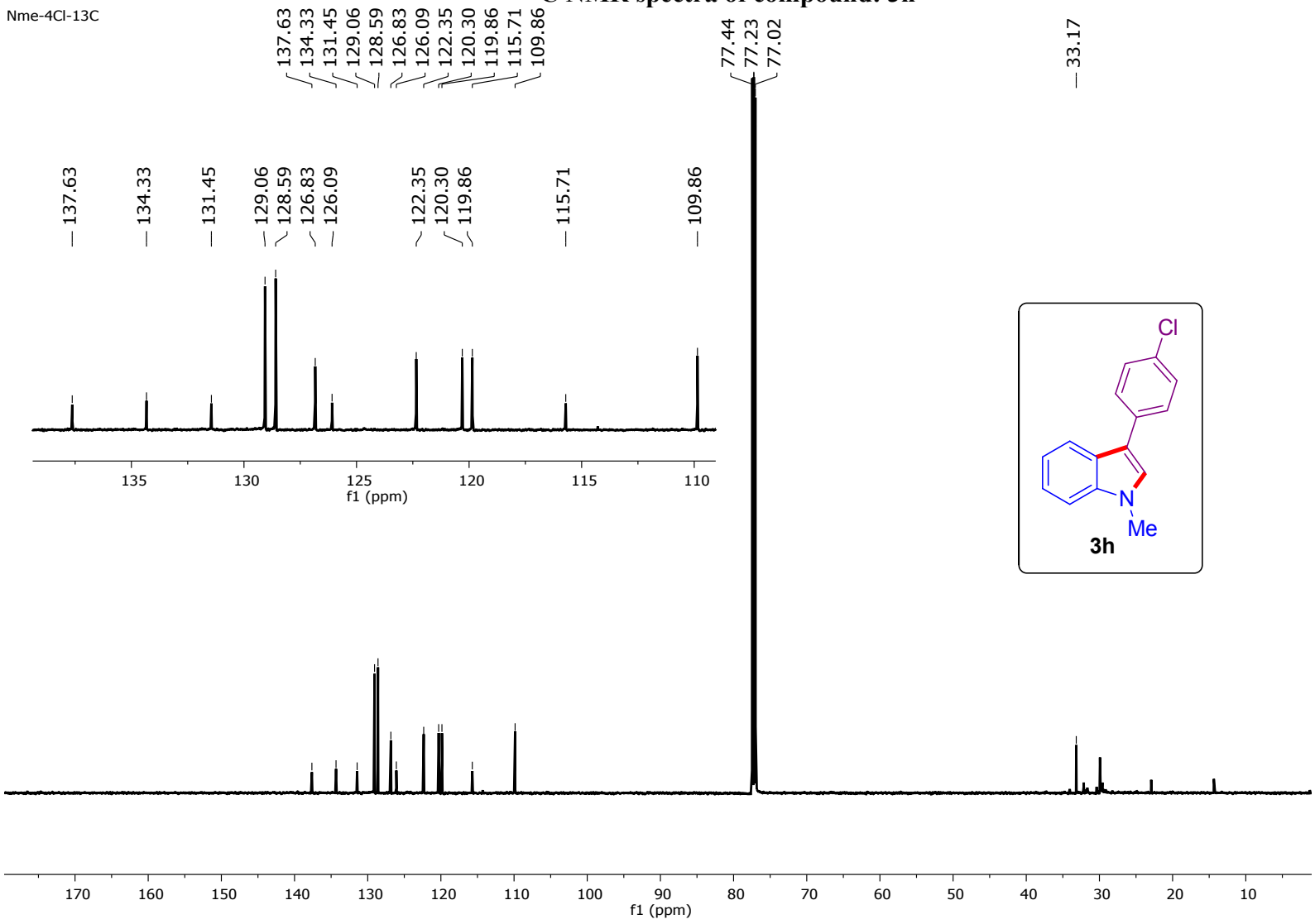
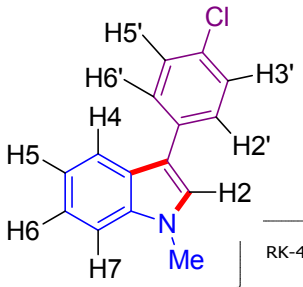
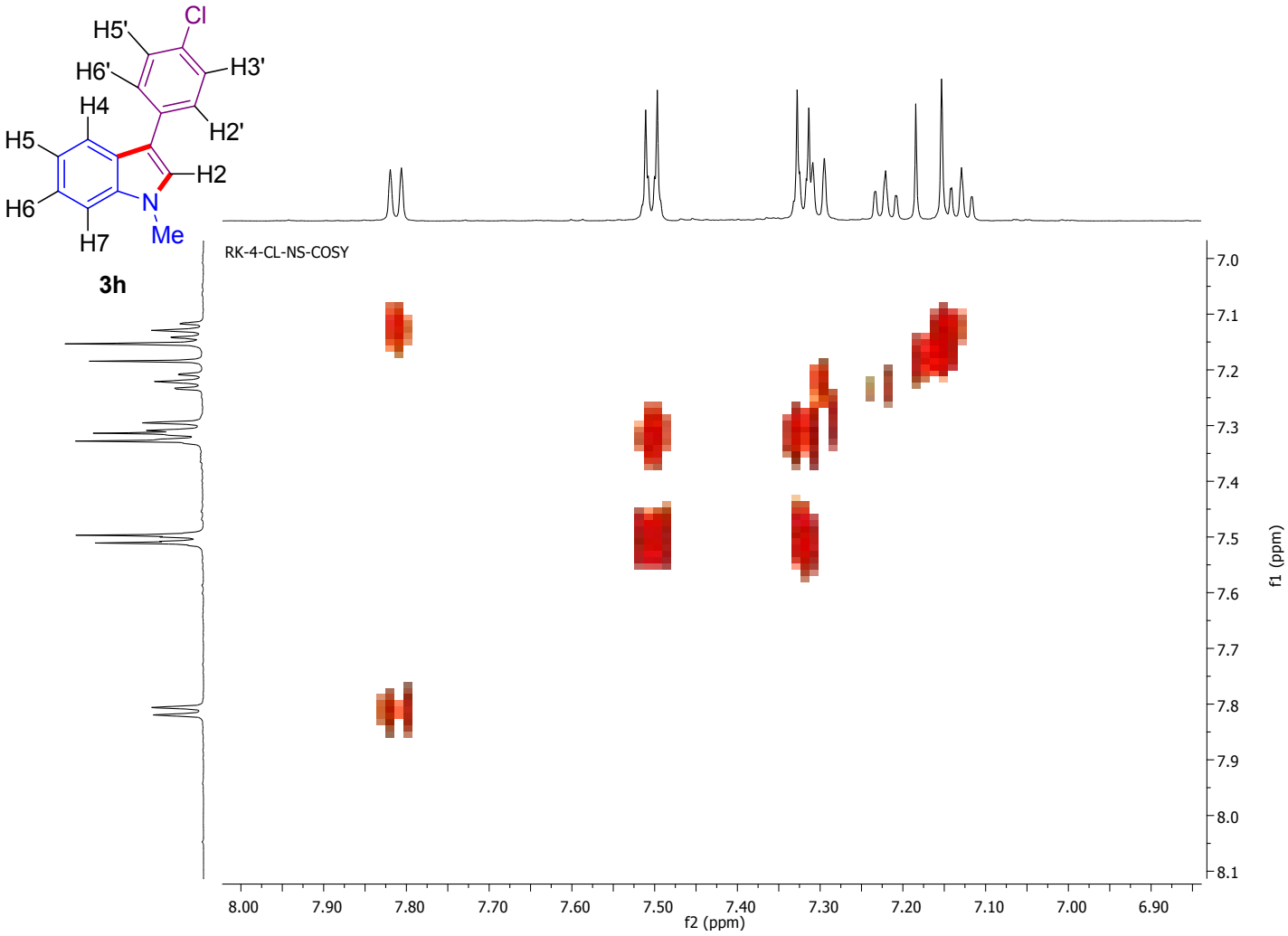


COSY spectra of compound: 3h

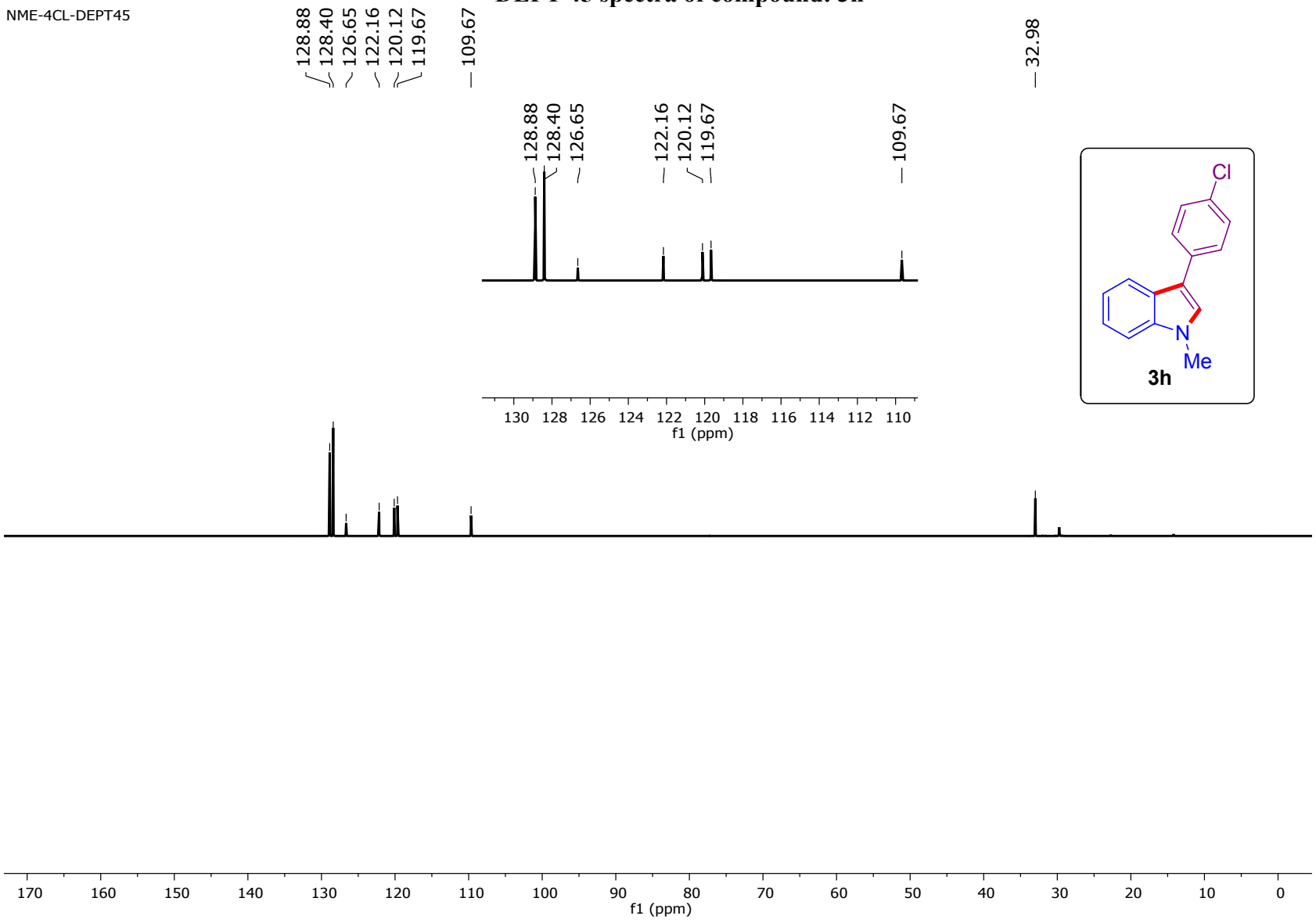


3h

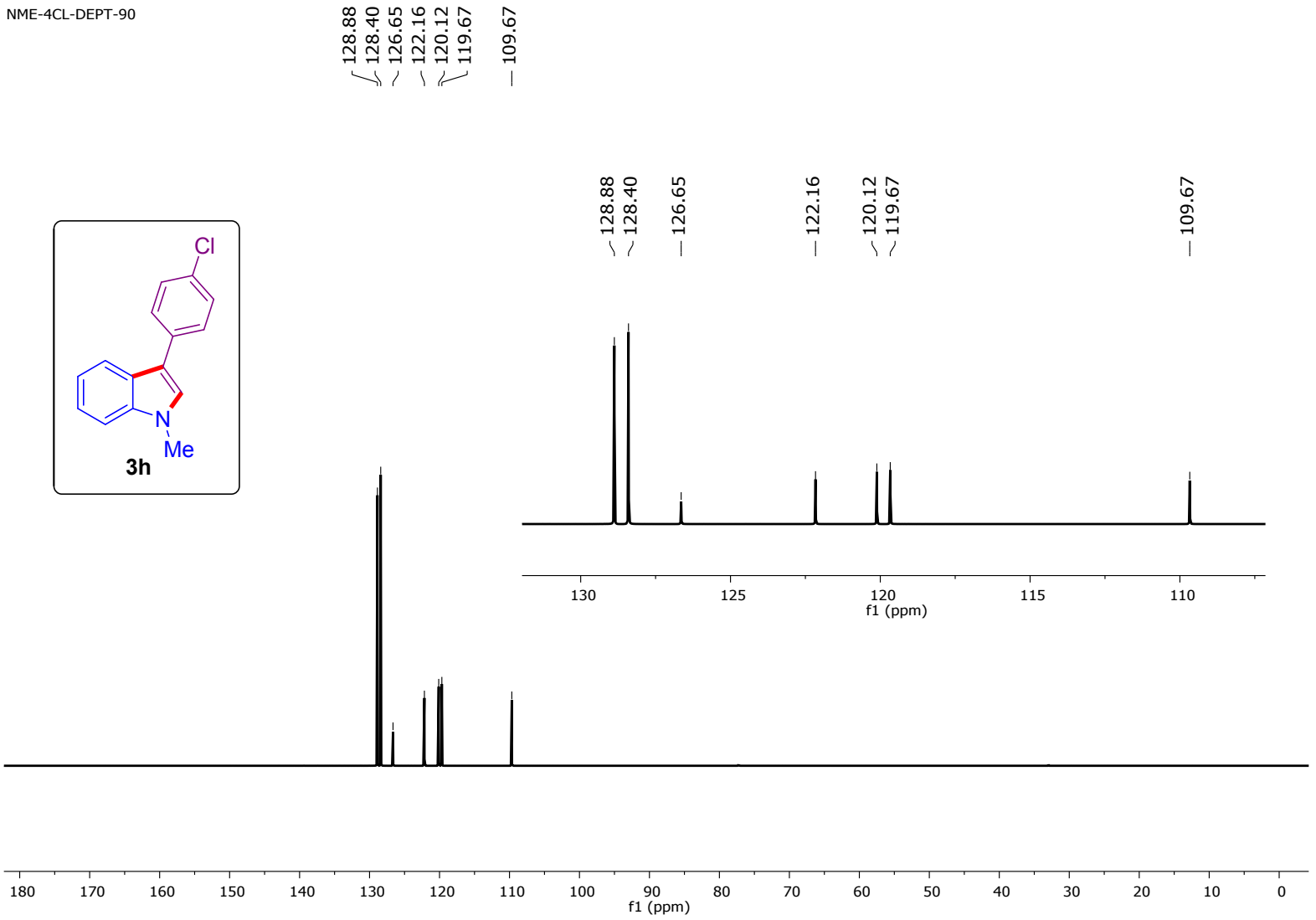
^{1}H-^{1}HCOSY spectra (Aromatic region expansion) of compound: 3h



DEPT 45 spectra of compound: 3h



DEPT 90 spectra of compound: 3h



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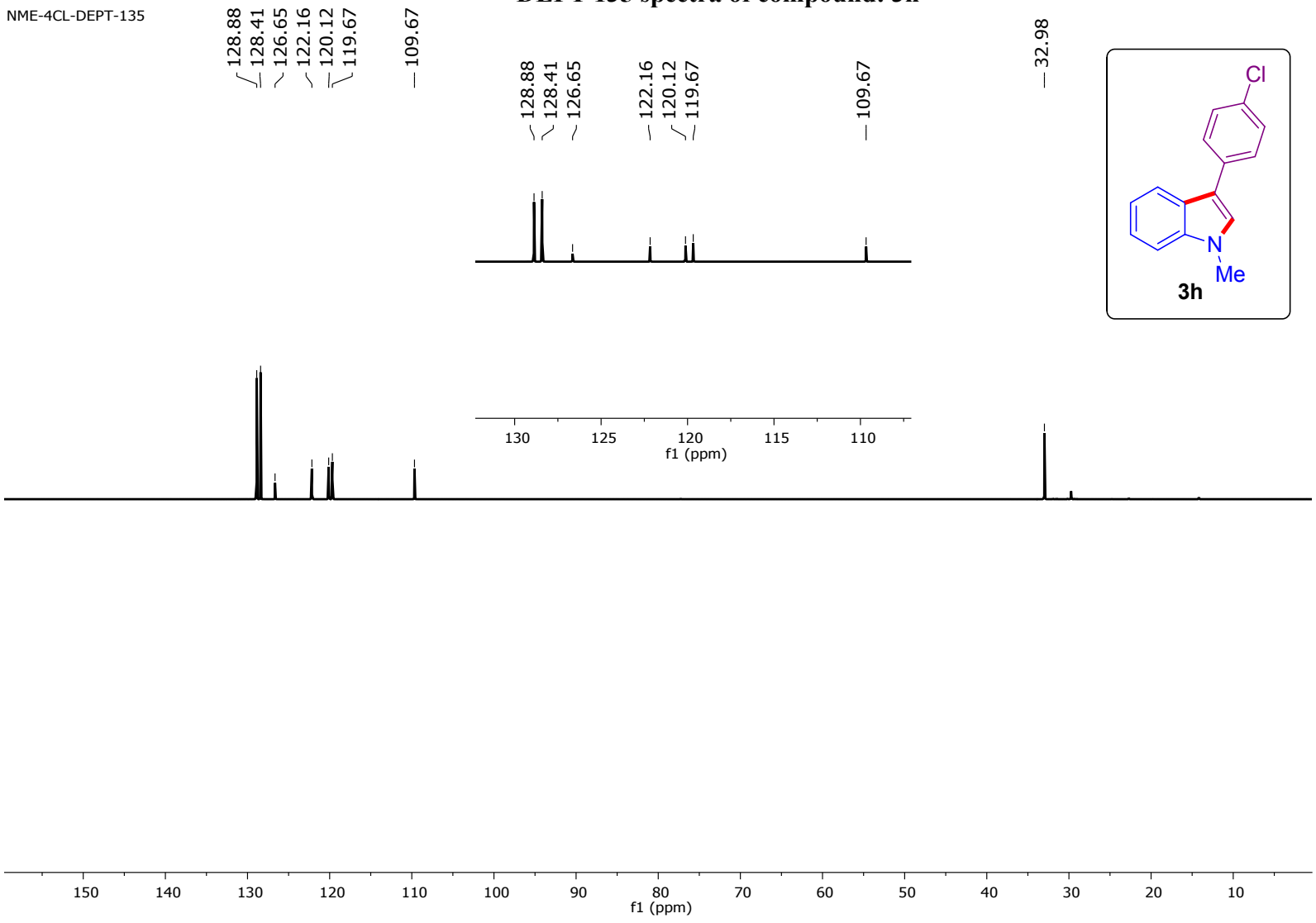
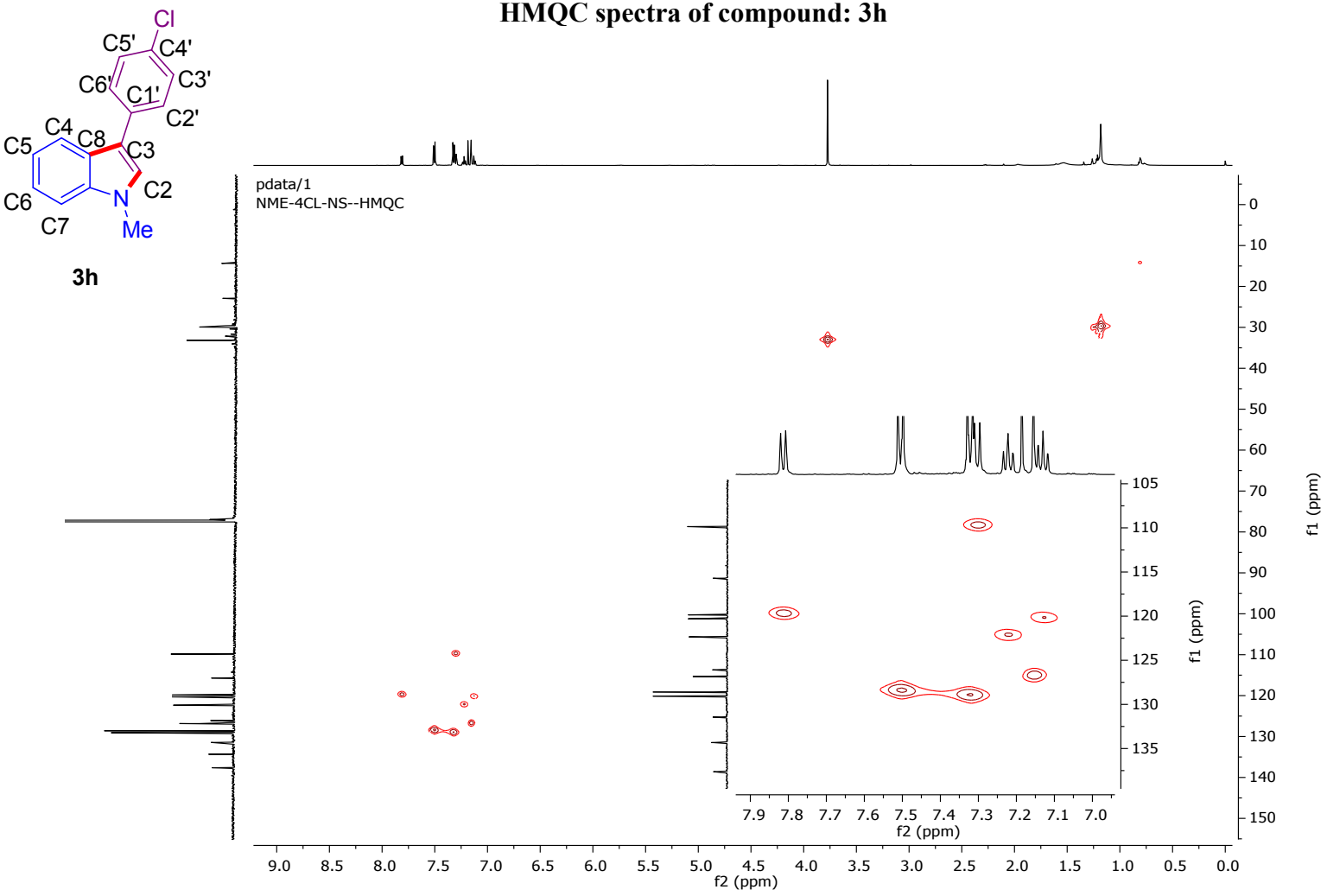
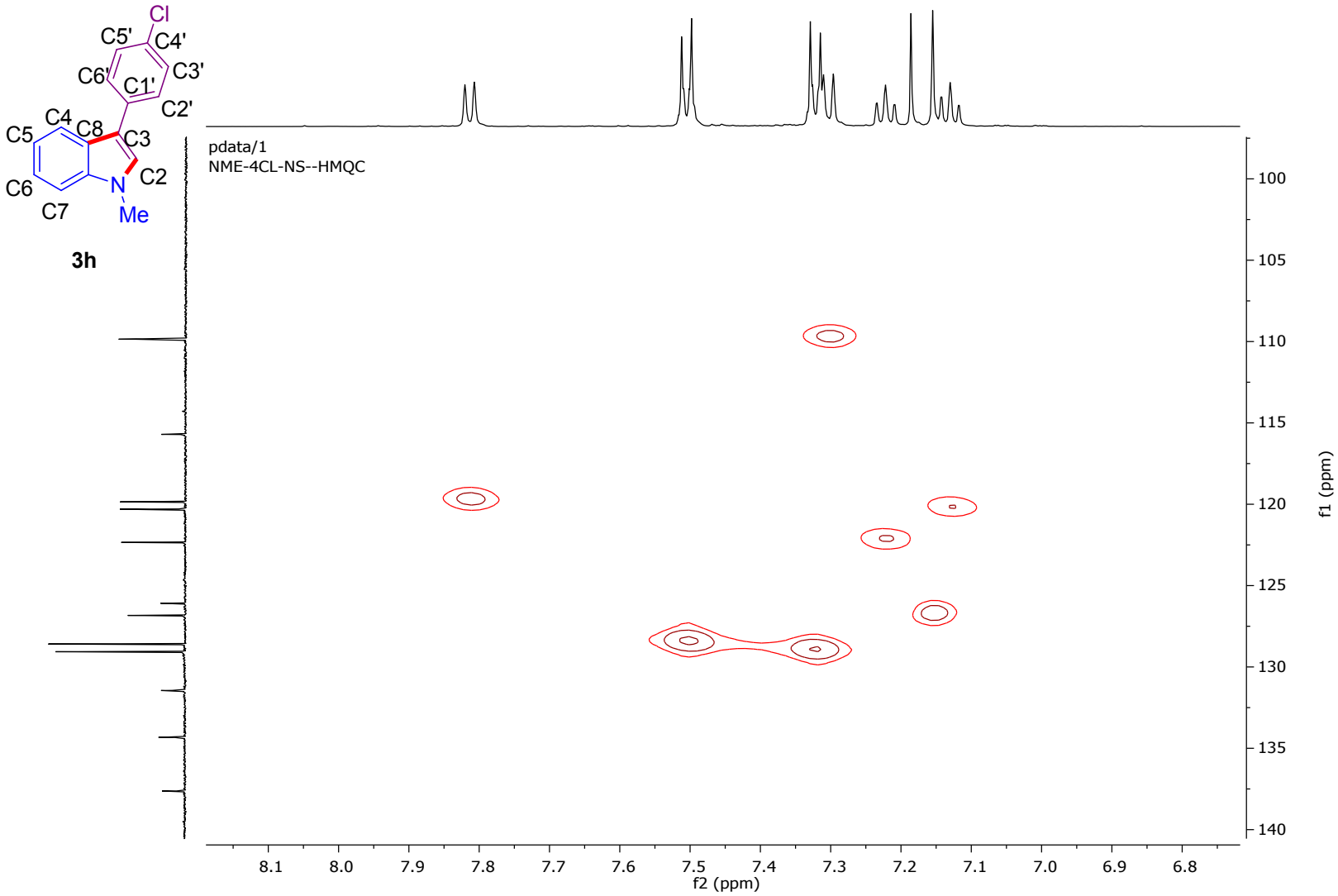


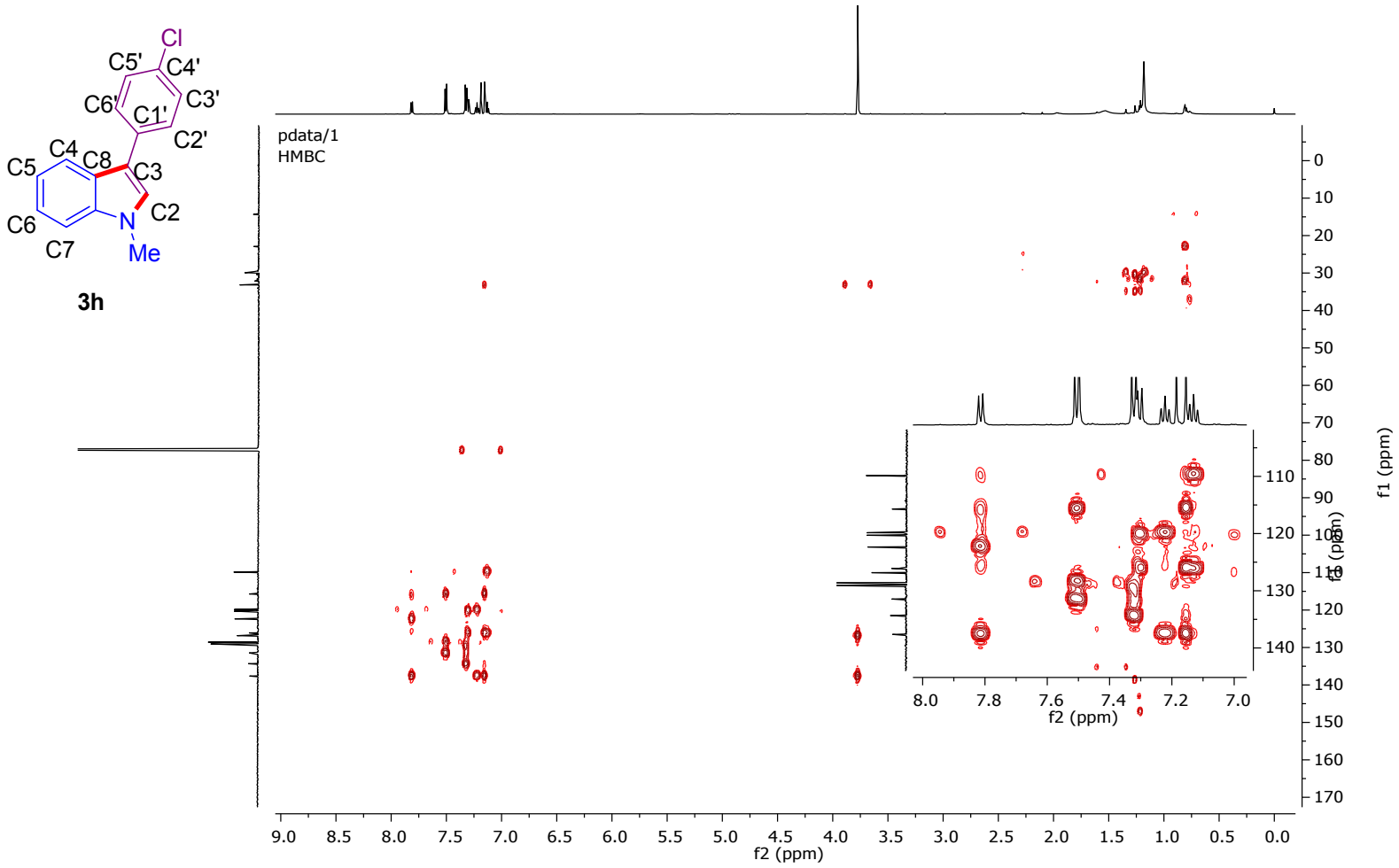
HMQC spectra of compound: 3h



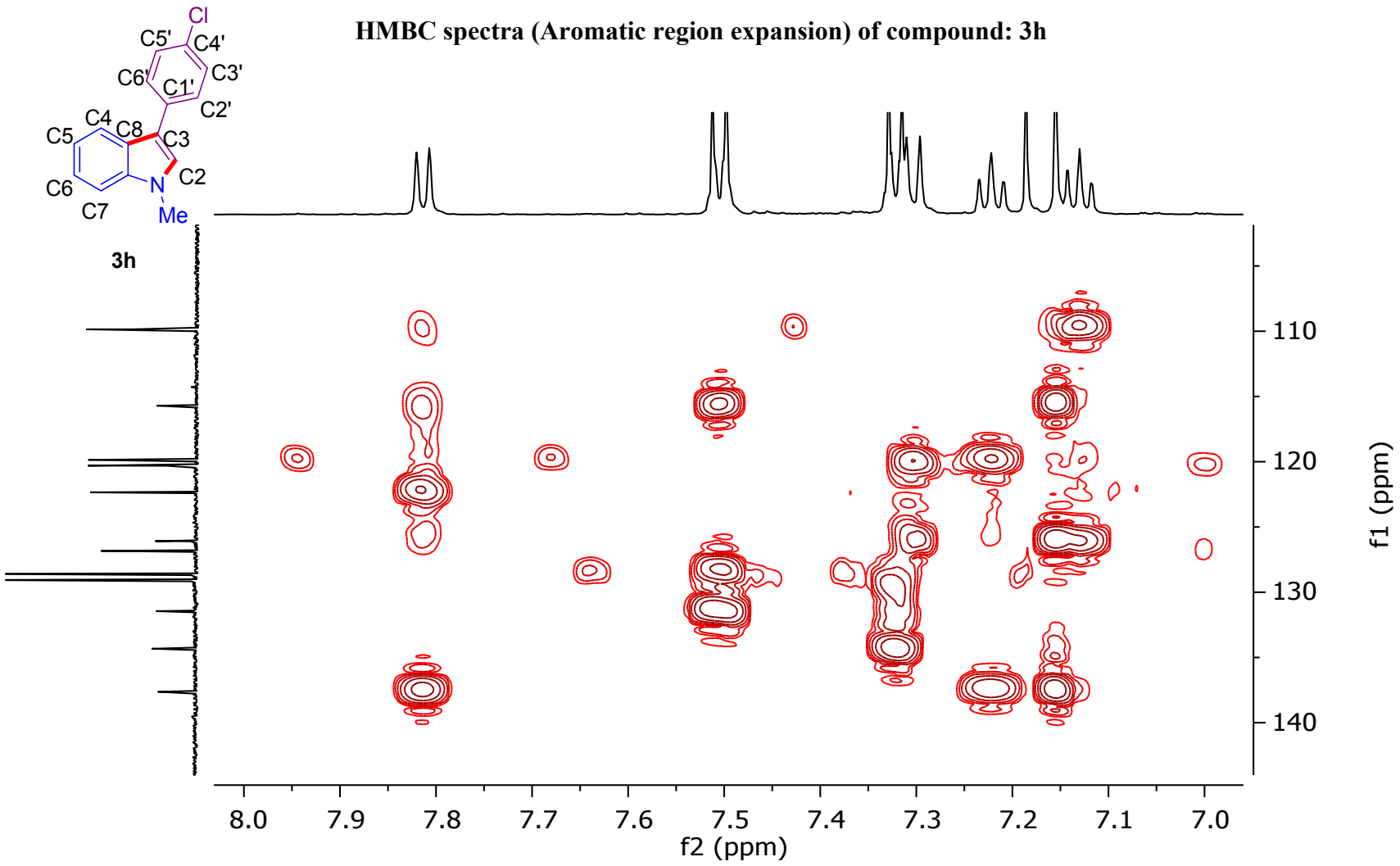
HMQC spectra (Aromatic region expansion) of compound: 3h



HMBC spectra of compound: 3h



HMBC spectra (Aromatic region expansion) of compound: 3h



HRMS spectra of compound: 3h

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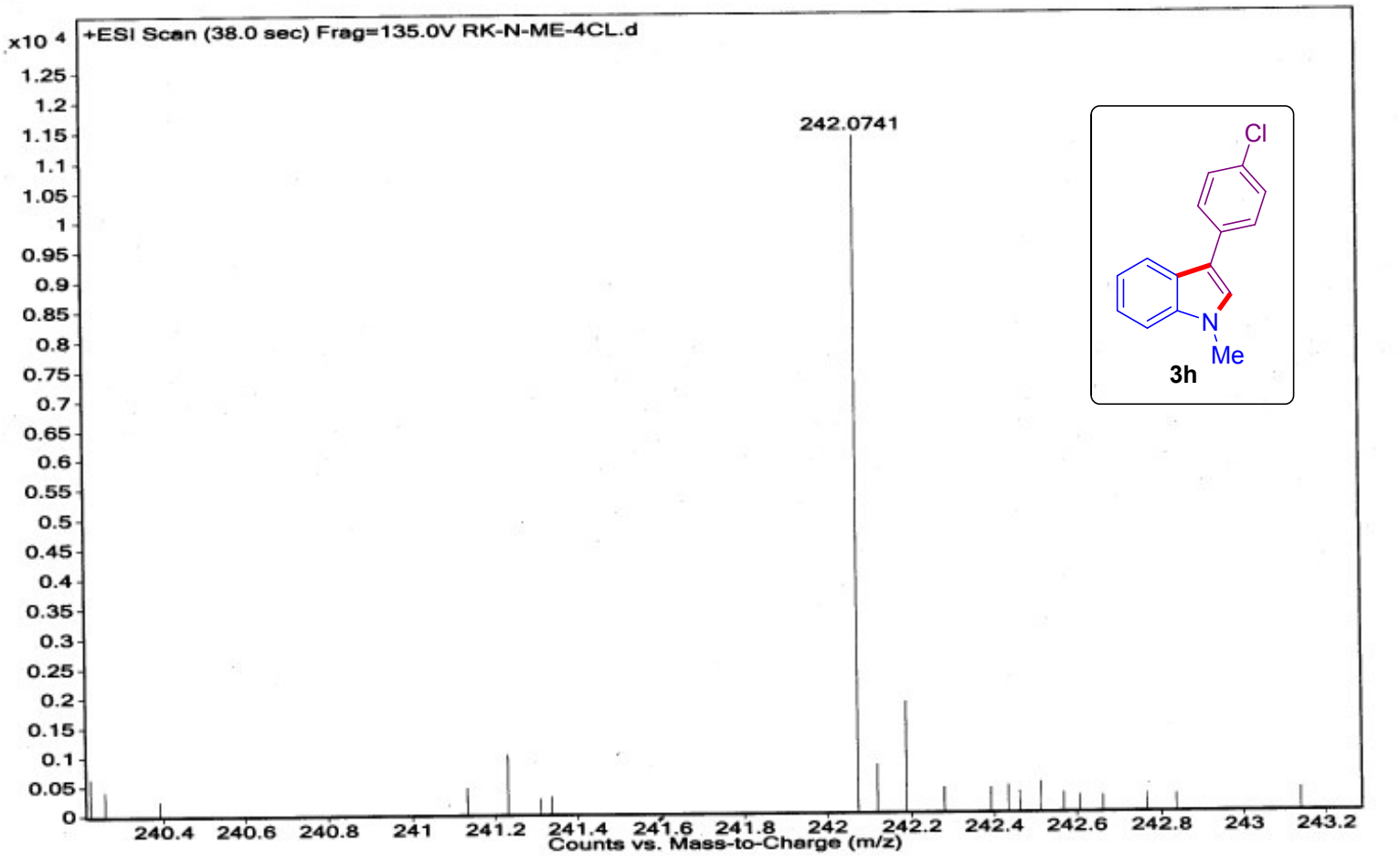
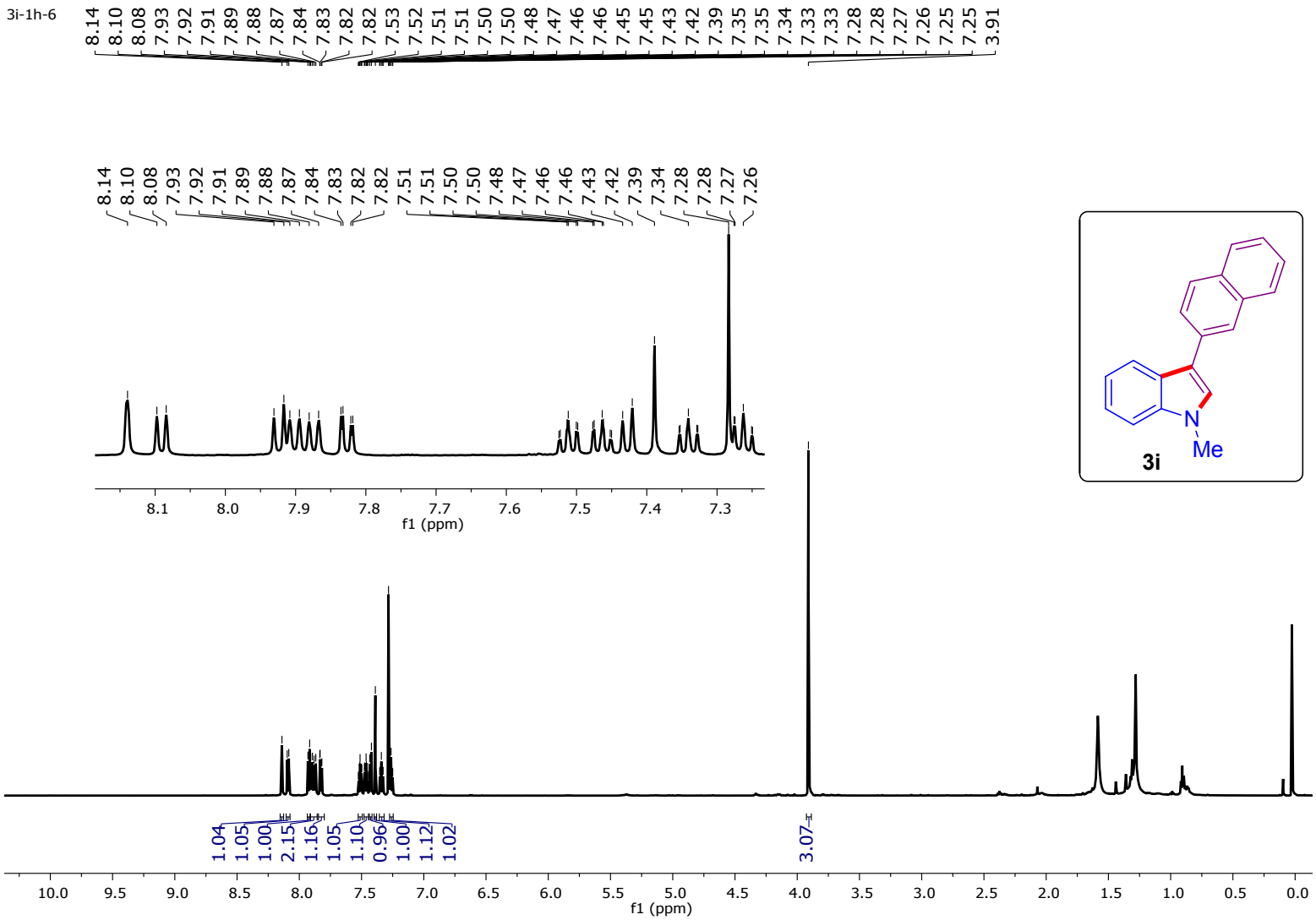
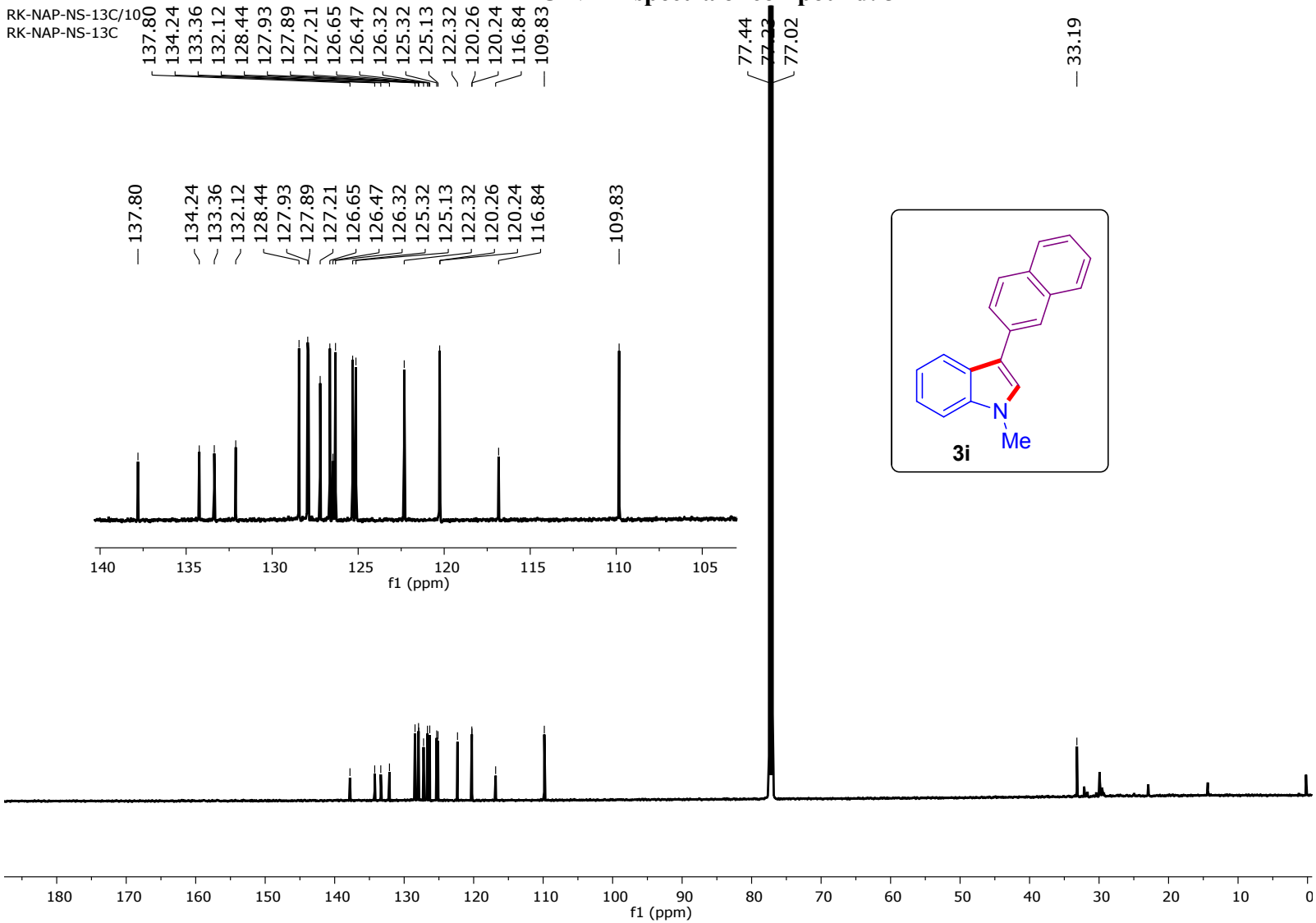


^{1}H NMR spectra of compound: 3i



^{13}C NMR spectra of compound: 3i



HRMS spectra of compound: 3i

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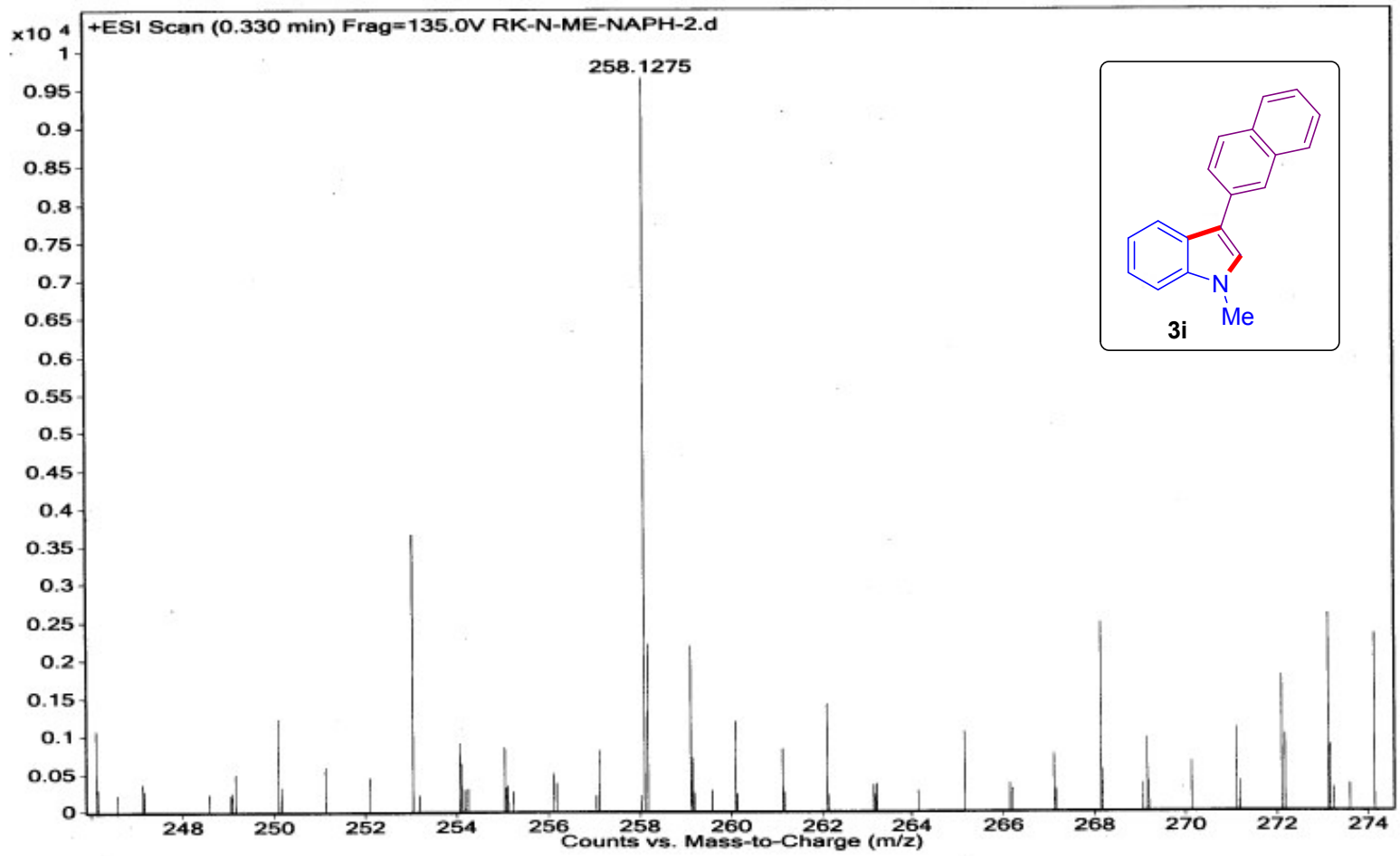
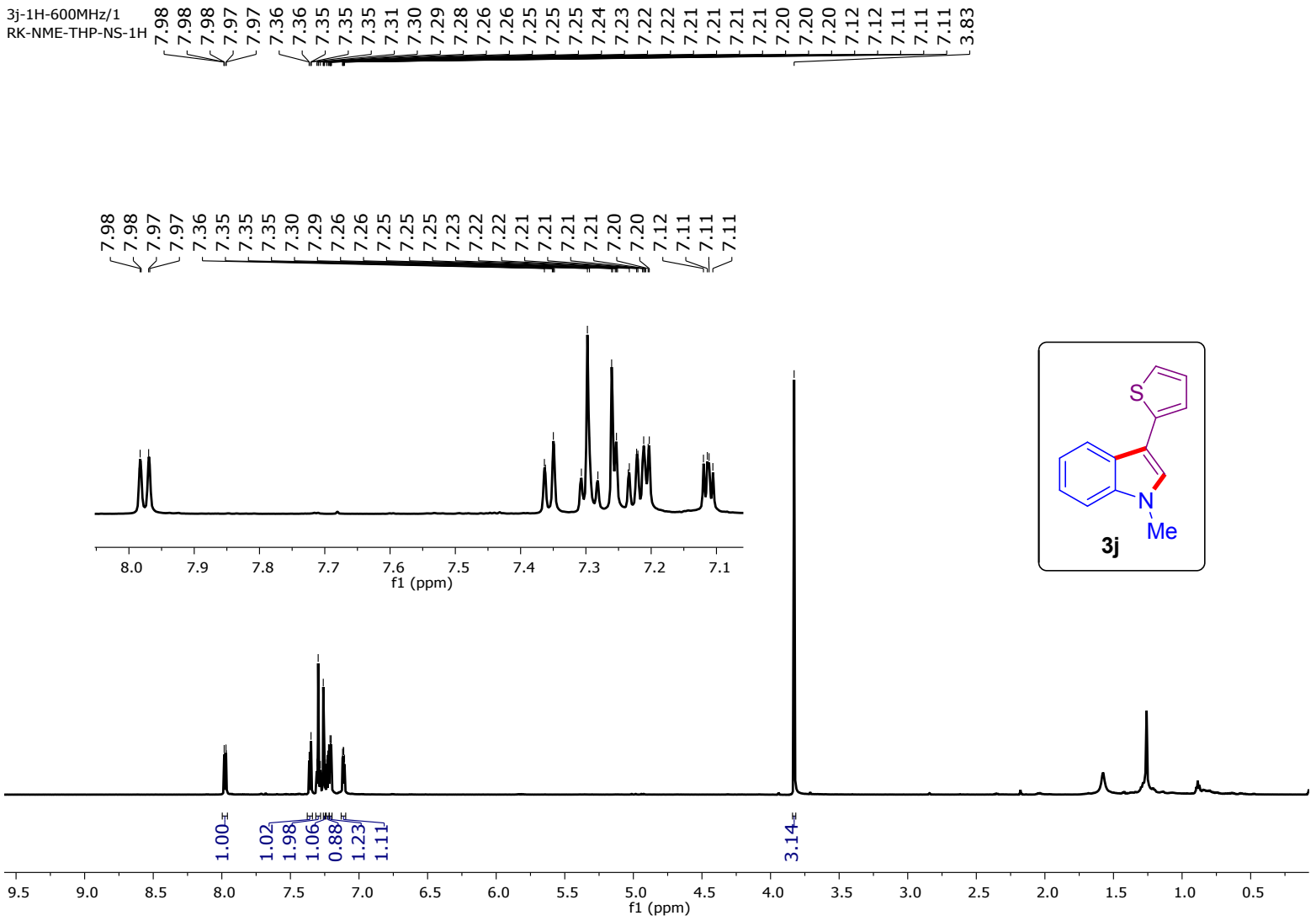
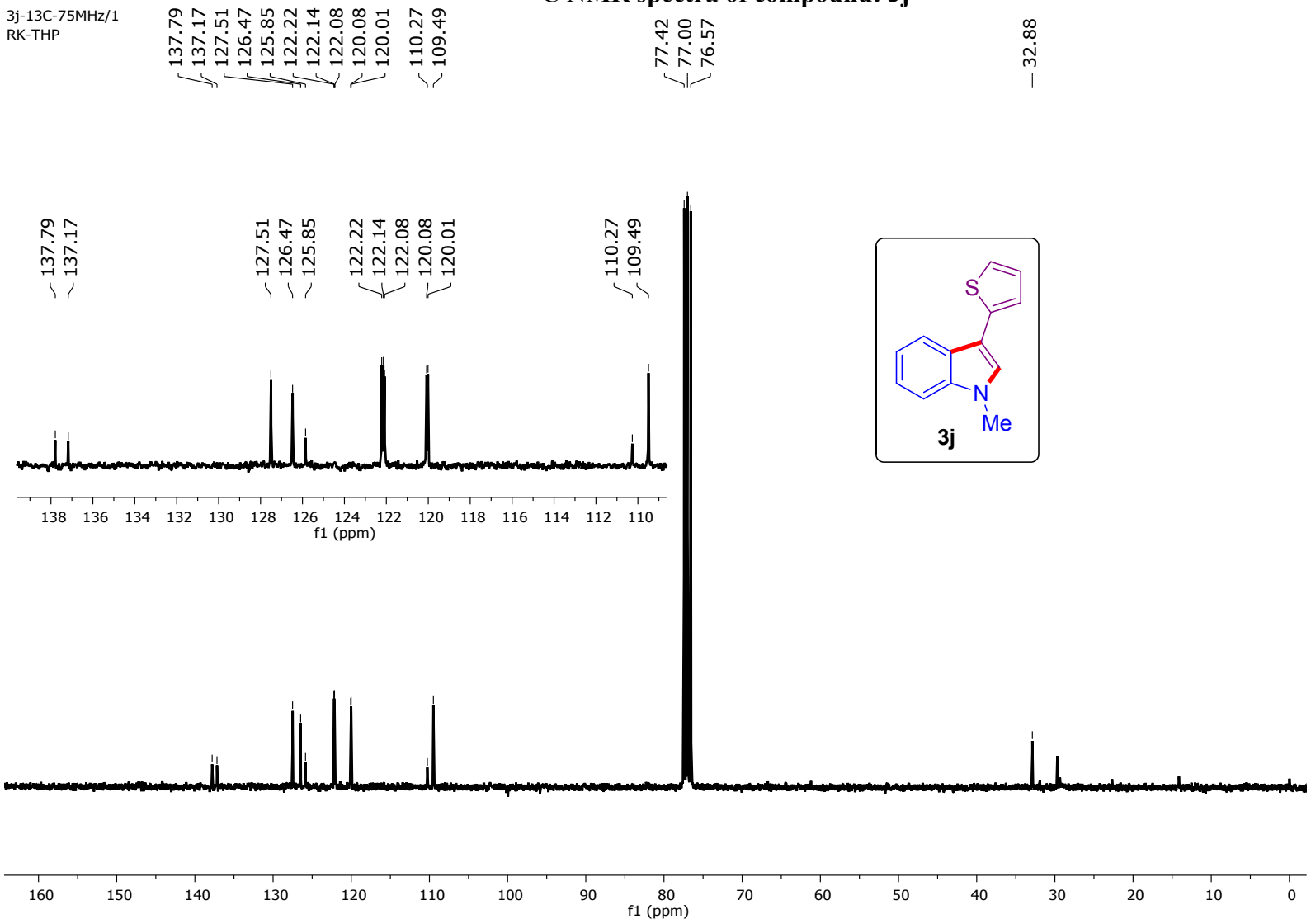


^{1}H NMR spectra of compound: 3j

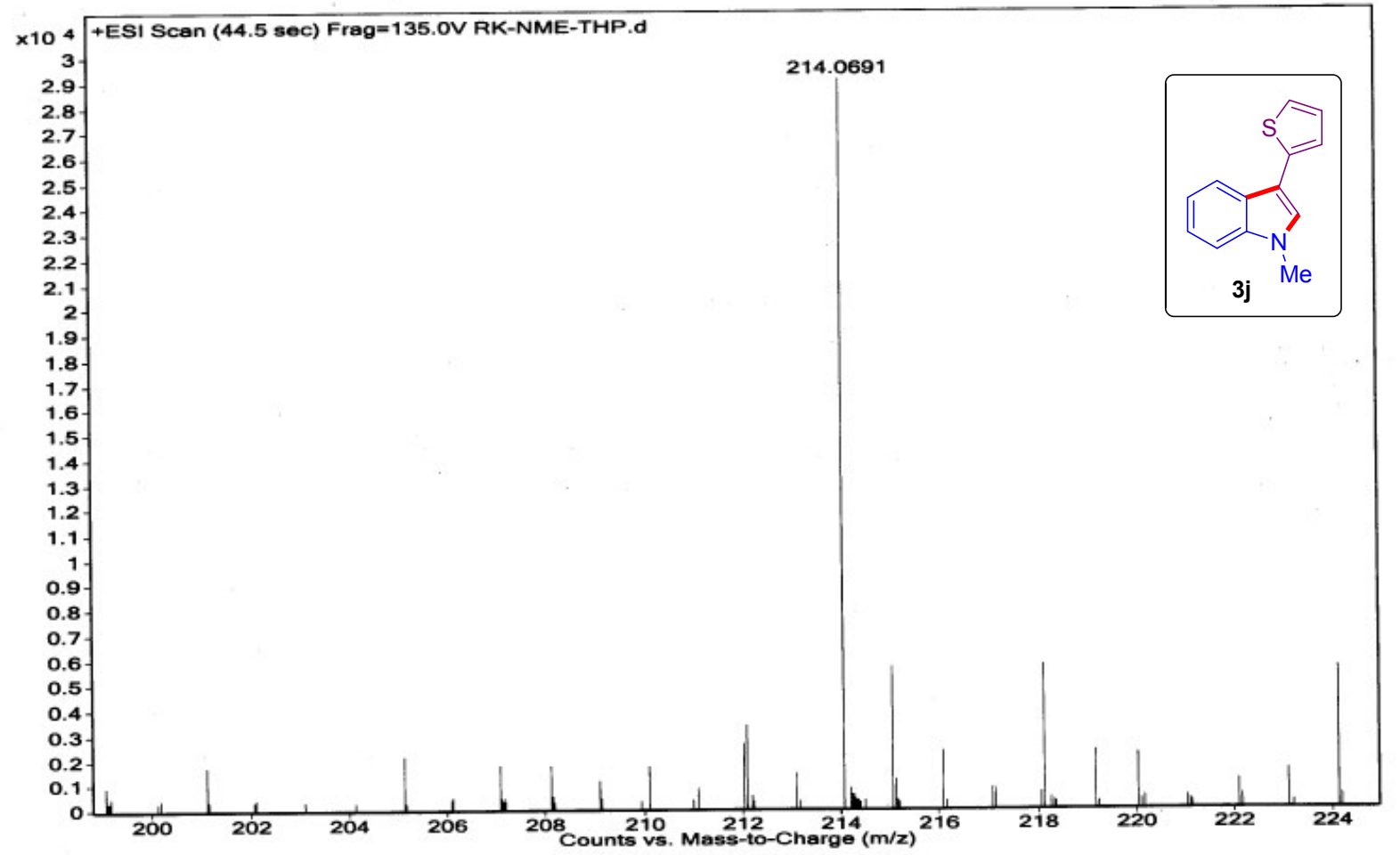


^{13}C NMR spectra of compound: 3j

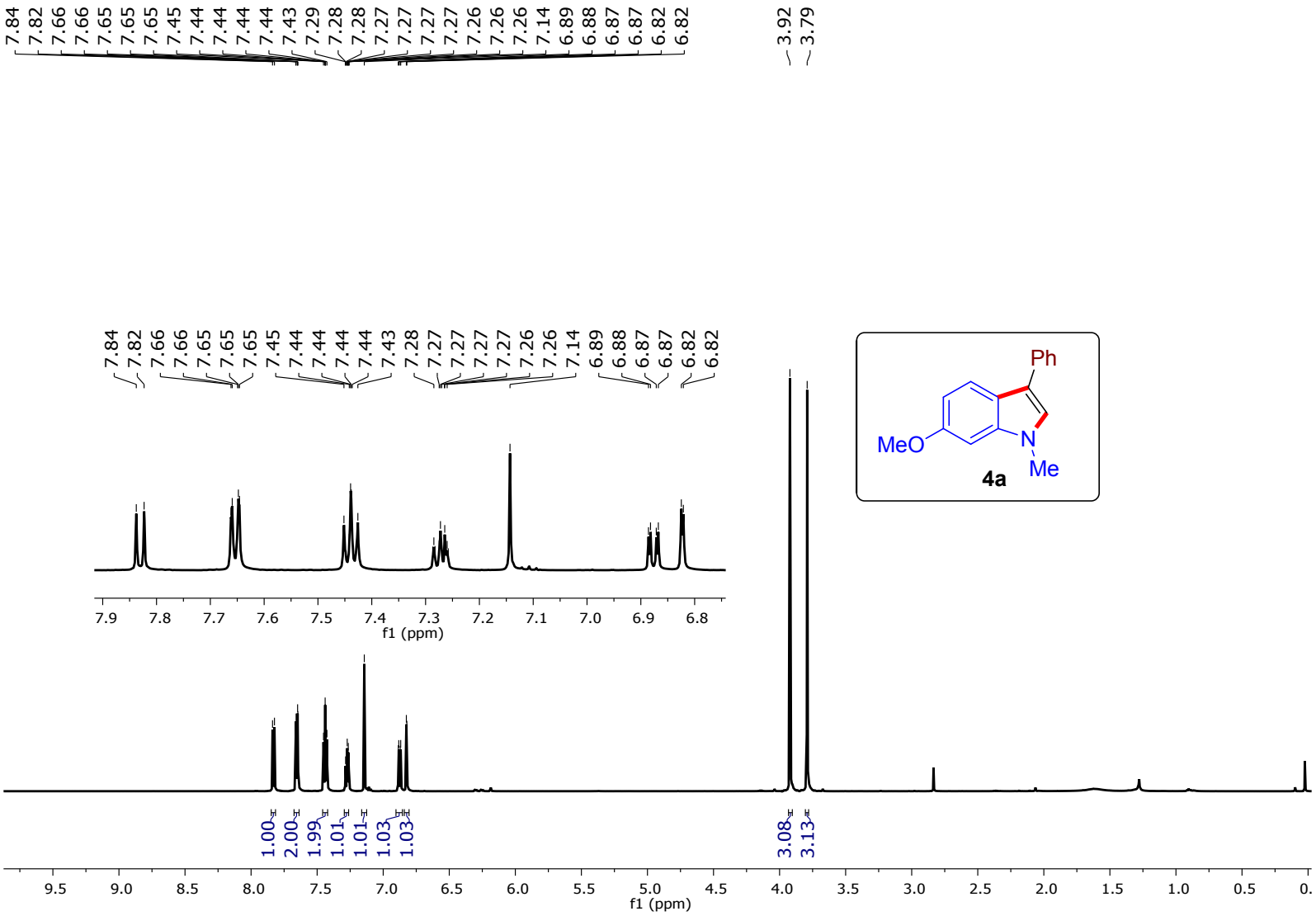


HRMS spectra of compound: 3j

Sample Name	RK-NME-THP	**Position**	Vial 1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	0	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	All Ions Missed
Data Filename	RK-NME-THP.d	**ACQ Method**		**Comment**		**Acquired Time**	8/9/2017 3:21:44 PM

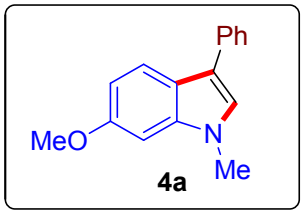


^{1}H NMR spectra of compound: 4a

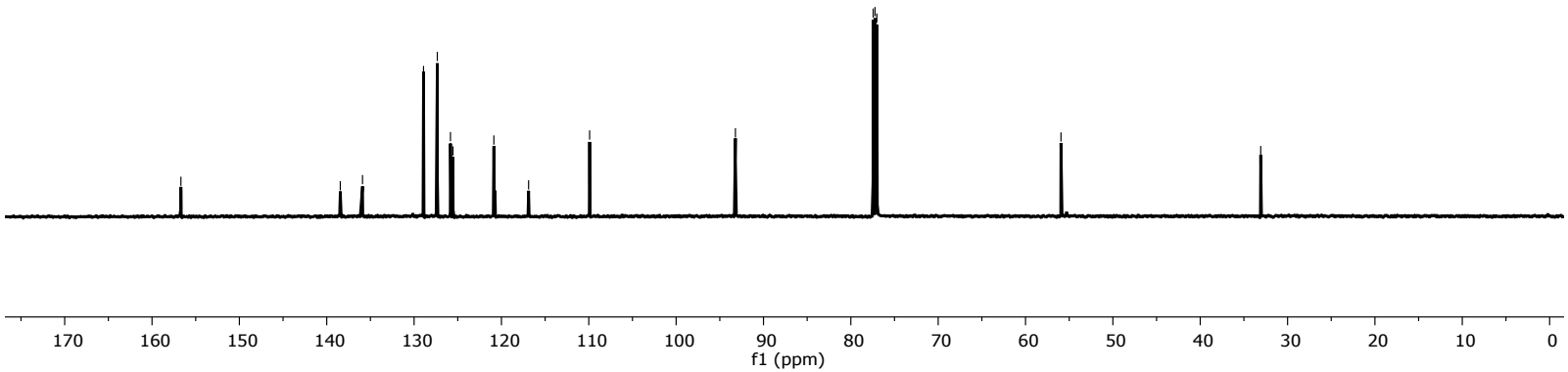


^{13}C NMR spectra of compound: 4a

156.69
138.45
135.90
128.92
127.34
125.83
125.55
120.87
120.73
116.89
109.90
93.21
77.44
77.23
77.02
55.94
33.07

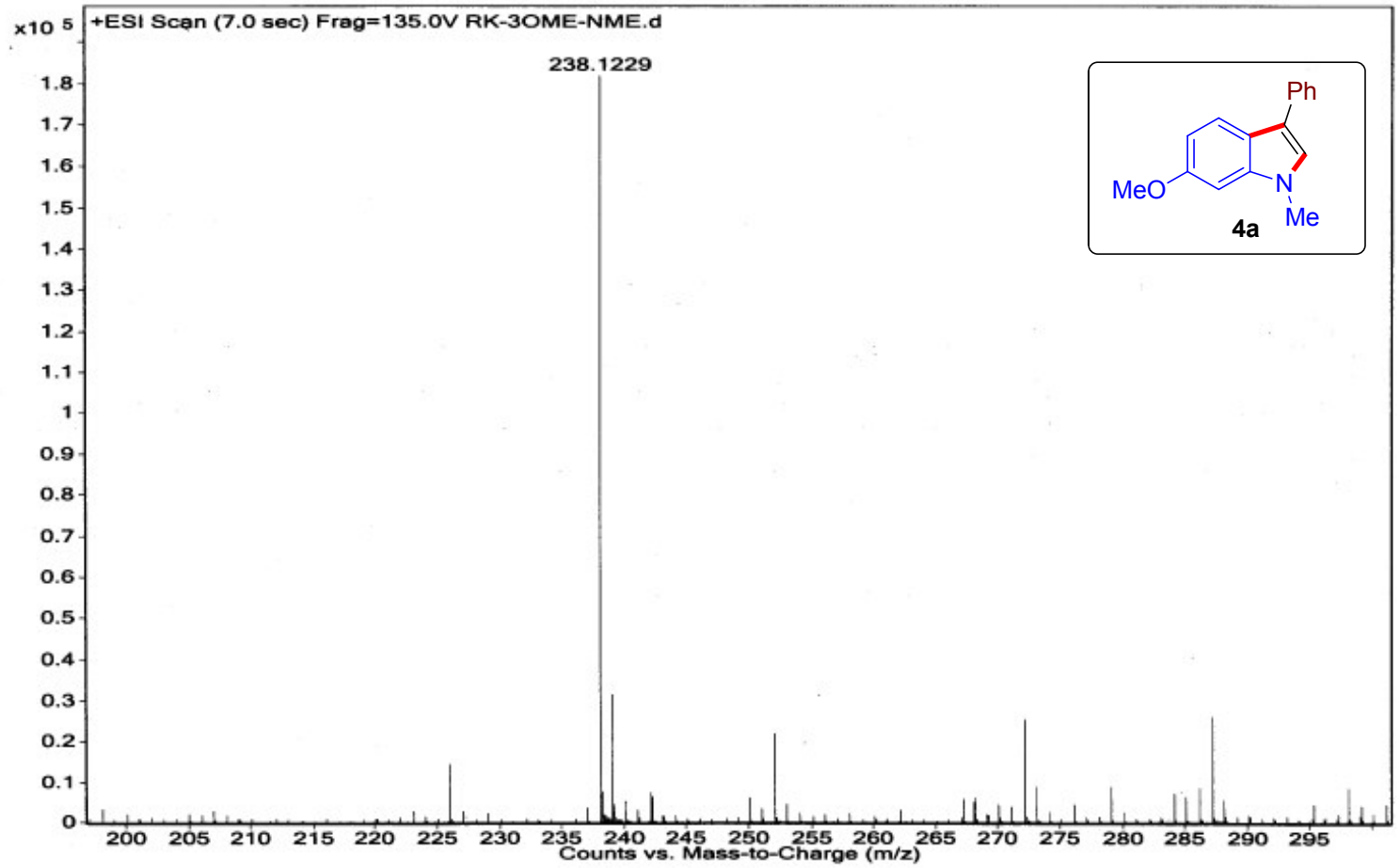


4a

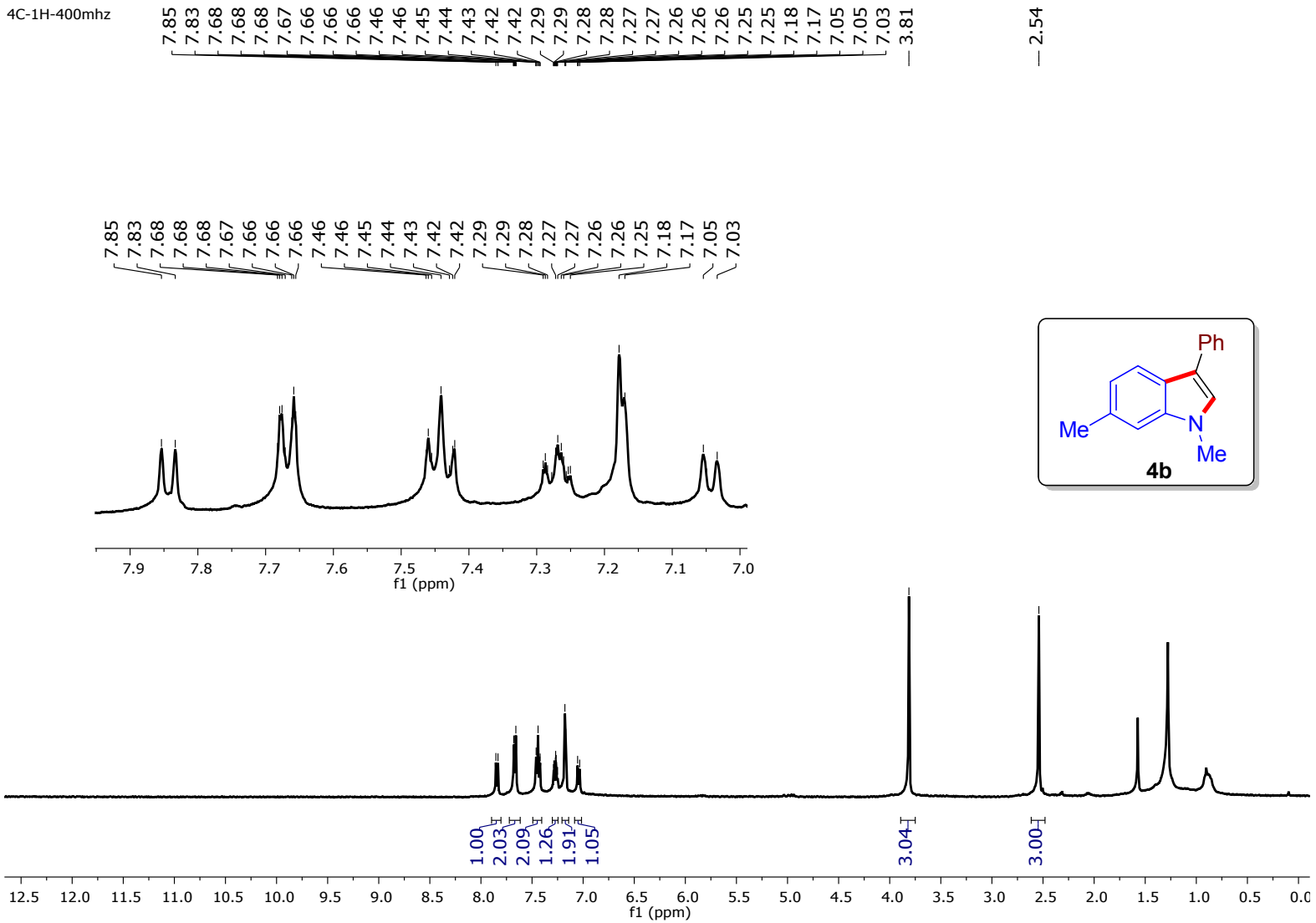


HRMS spectra of compound: 4a

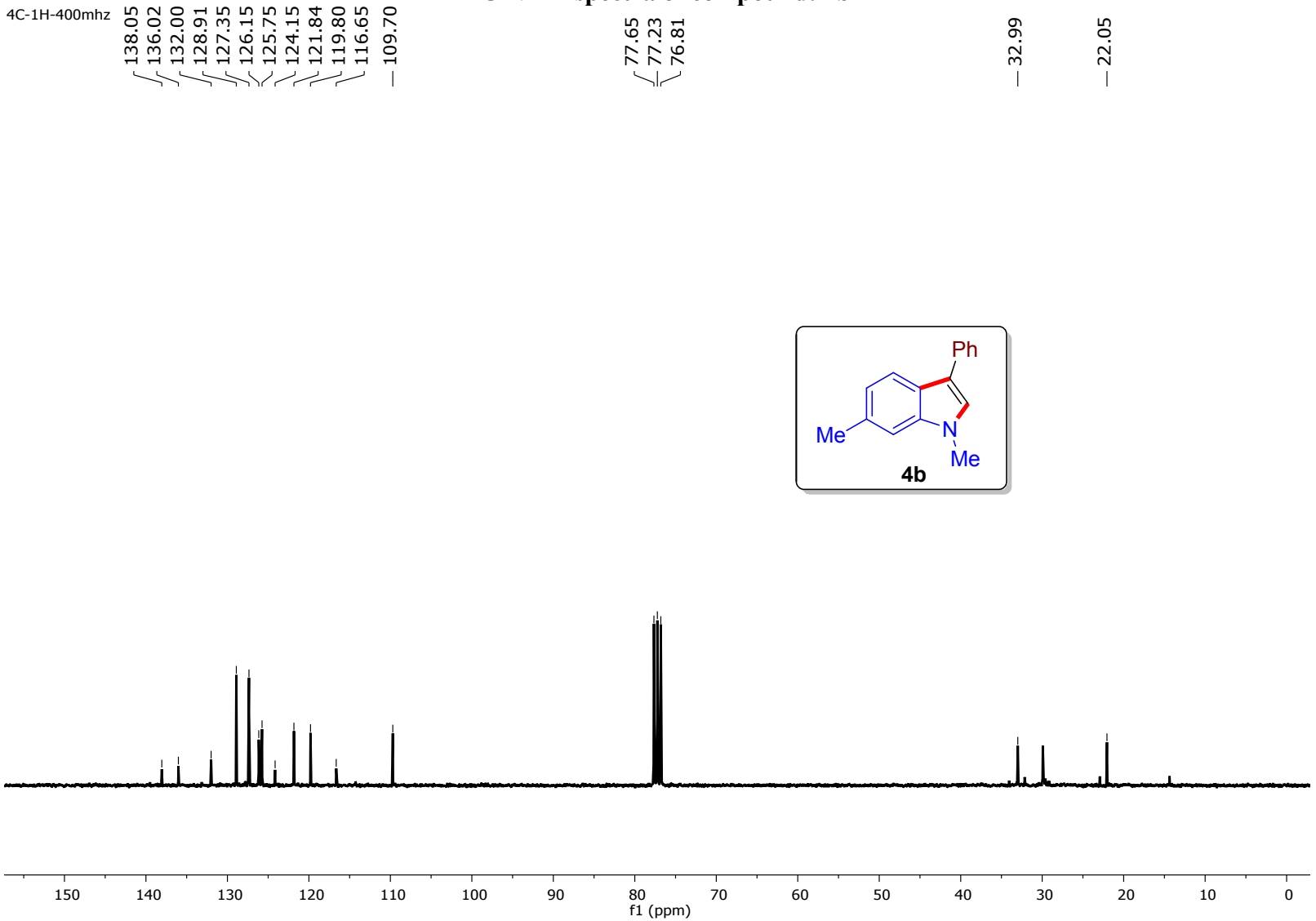
Sample Name	Unavailable	**Position**	Unavailable	**Instrument Name**	Unavailable	**User Name**	Unavailable
Inj Vol	Unavailable	**InjPosition**	Unavailable	**SampleType**	Unavailable	**IRM Calibration Status**	All Ions Missed
Data Filename	RK-3OME-NME.d	**ACQ Method**		**Comment**	Sample information is unavailable	**Acquired Time**	Unavailable



^{1}H NMR spectra of compound: 4b

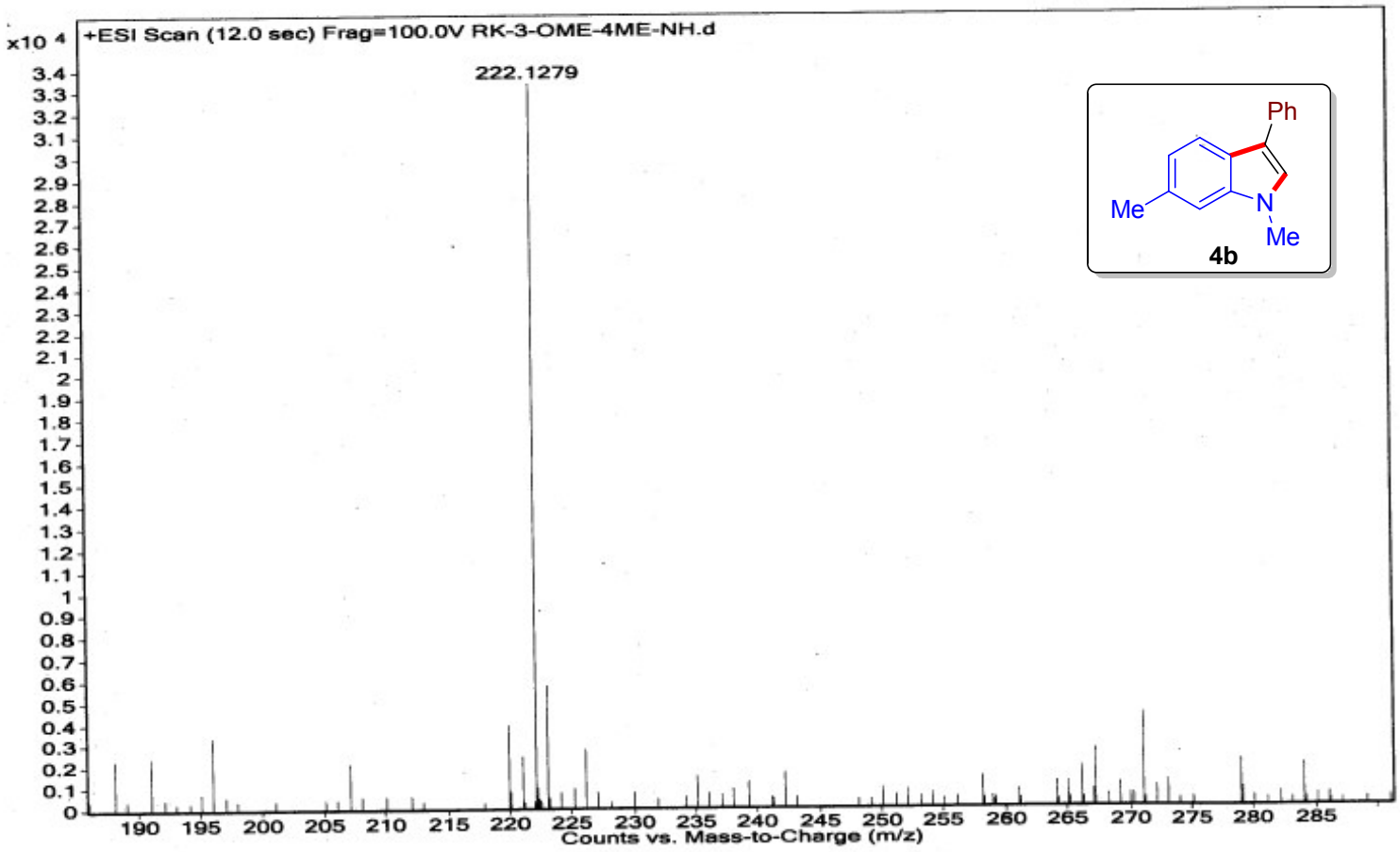


^{13}C NMR spectra of compound: 4b

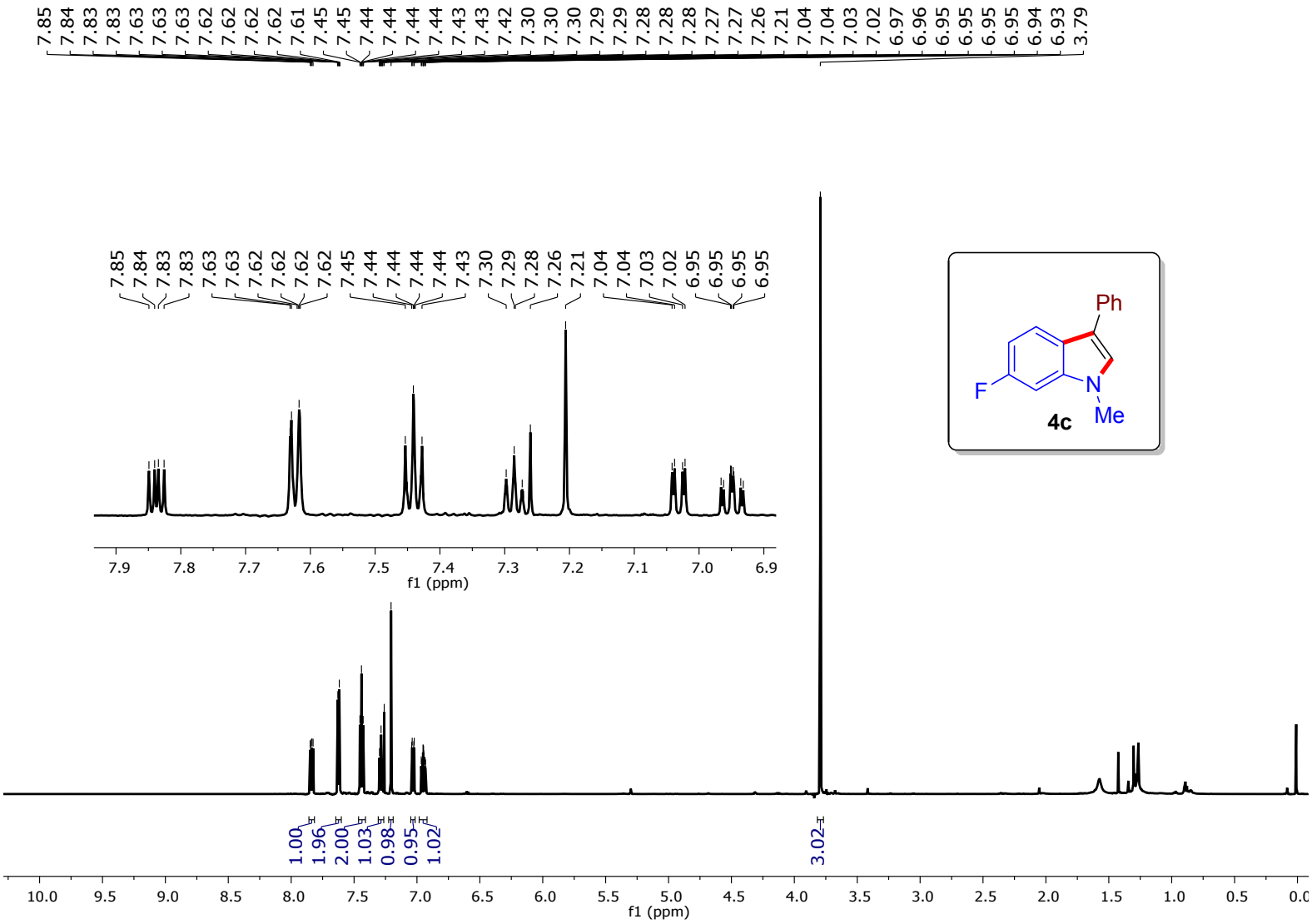


HRMS spectra of compound: 4b

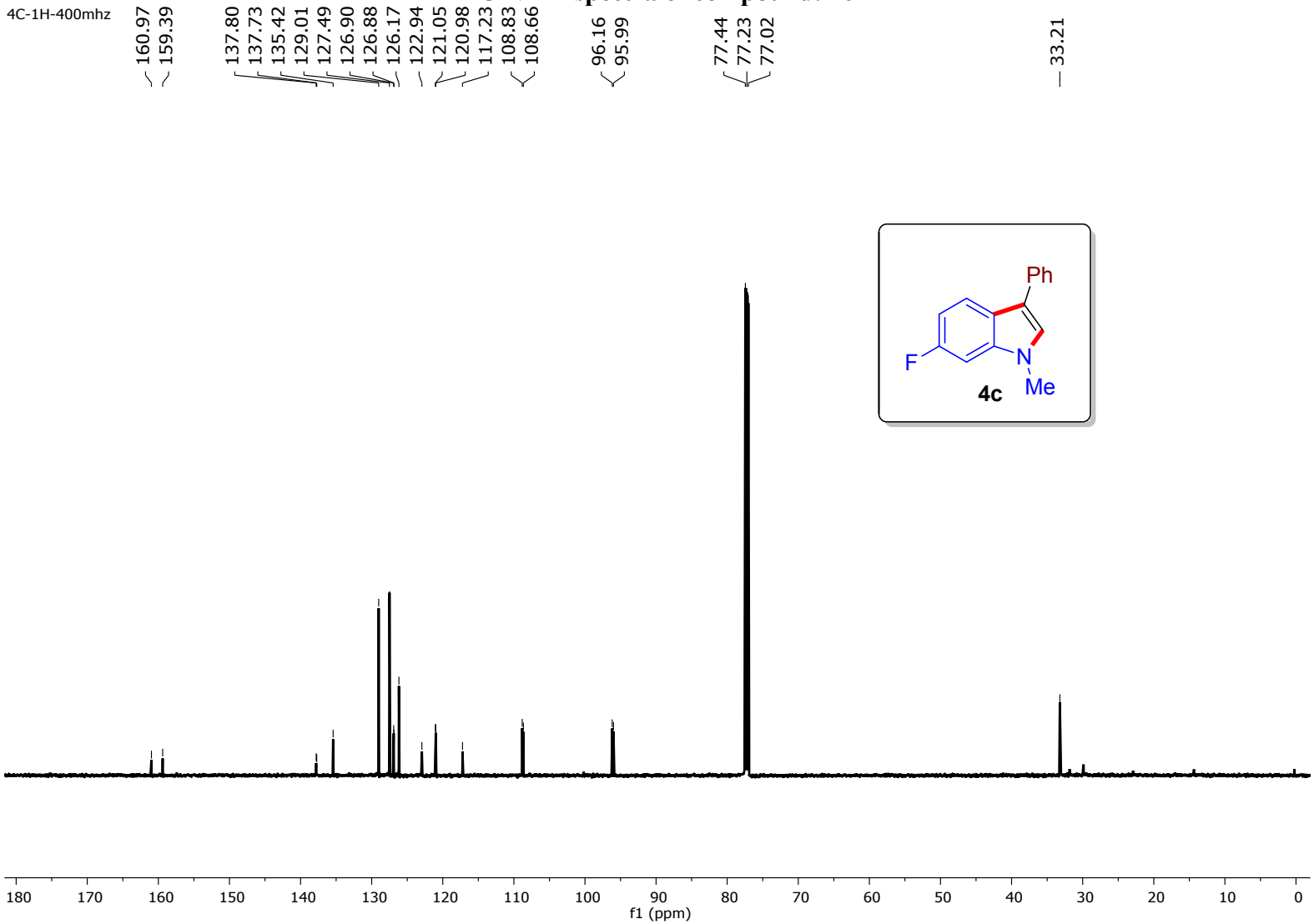
Sample Name	RK-3-OME-4ME-NH	**Position**	Vial 1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	0	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	All Ions Missed
Data Filename	RK-3-OME-4ME-NH.d	**ACQ Method**		**Comment**		**Acquired Time**	8/7/2017 1:14:29 PM



^{1}H NMR spectra of compound: 4c

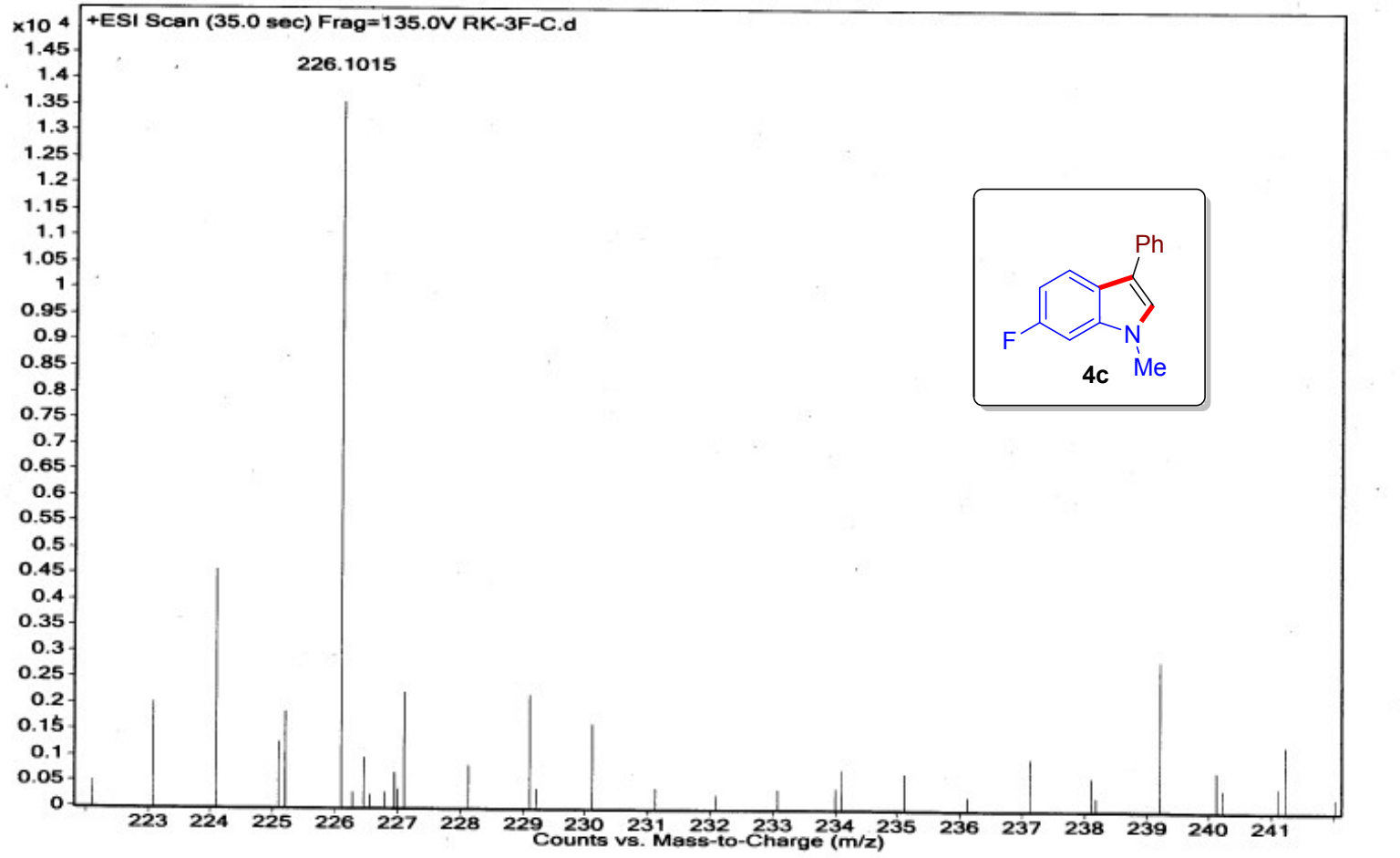


^{13}C NMR spectra of compound: 4c

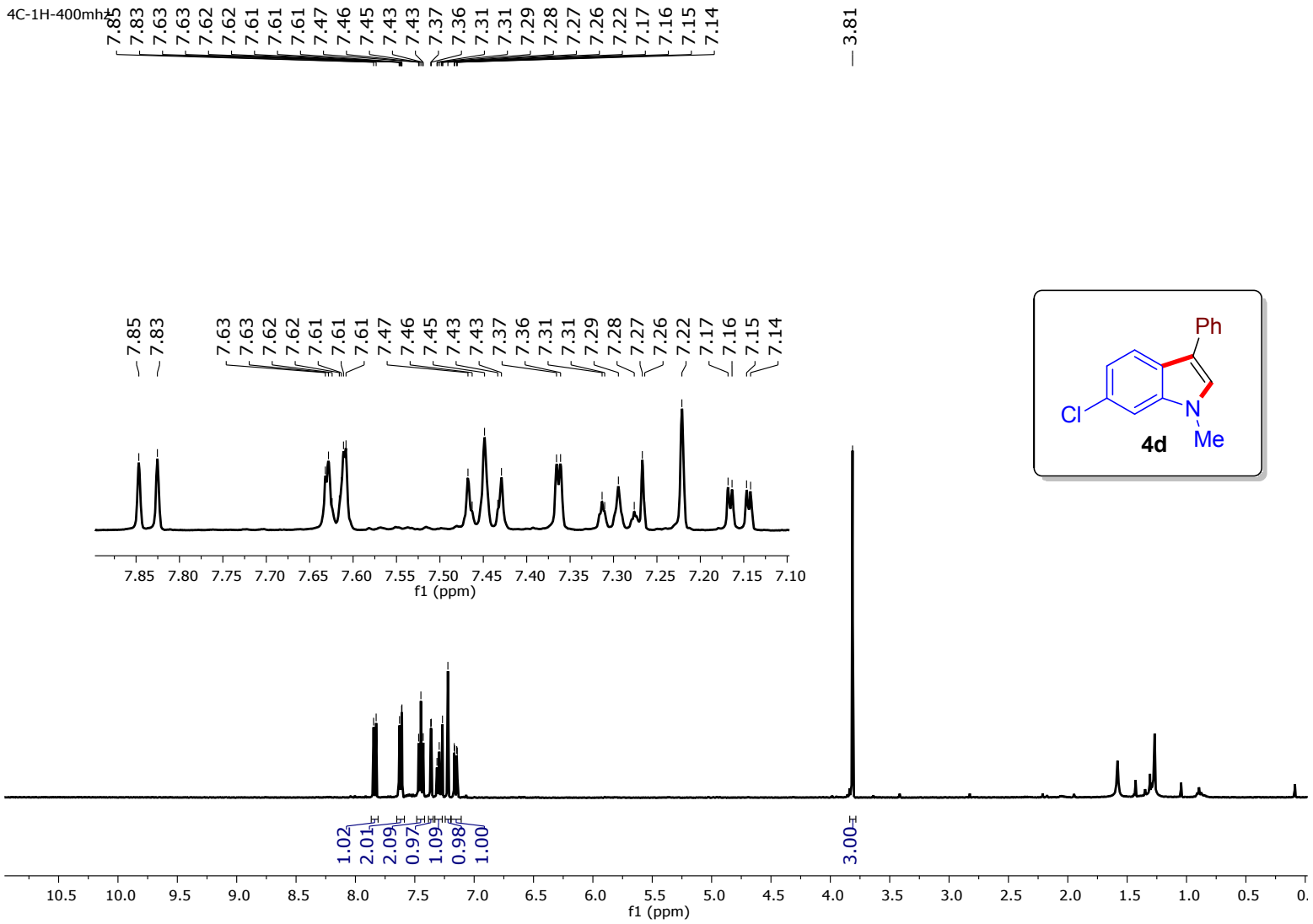


HRMS spectra of compound: 4c

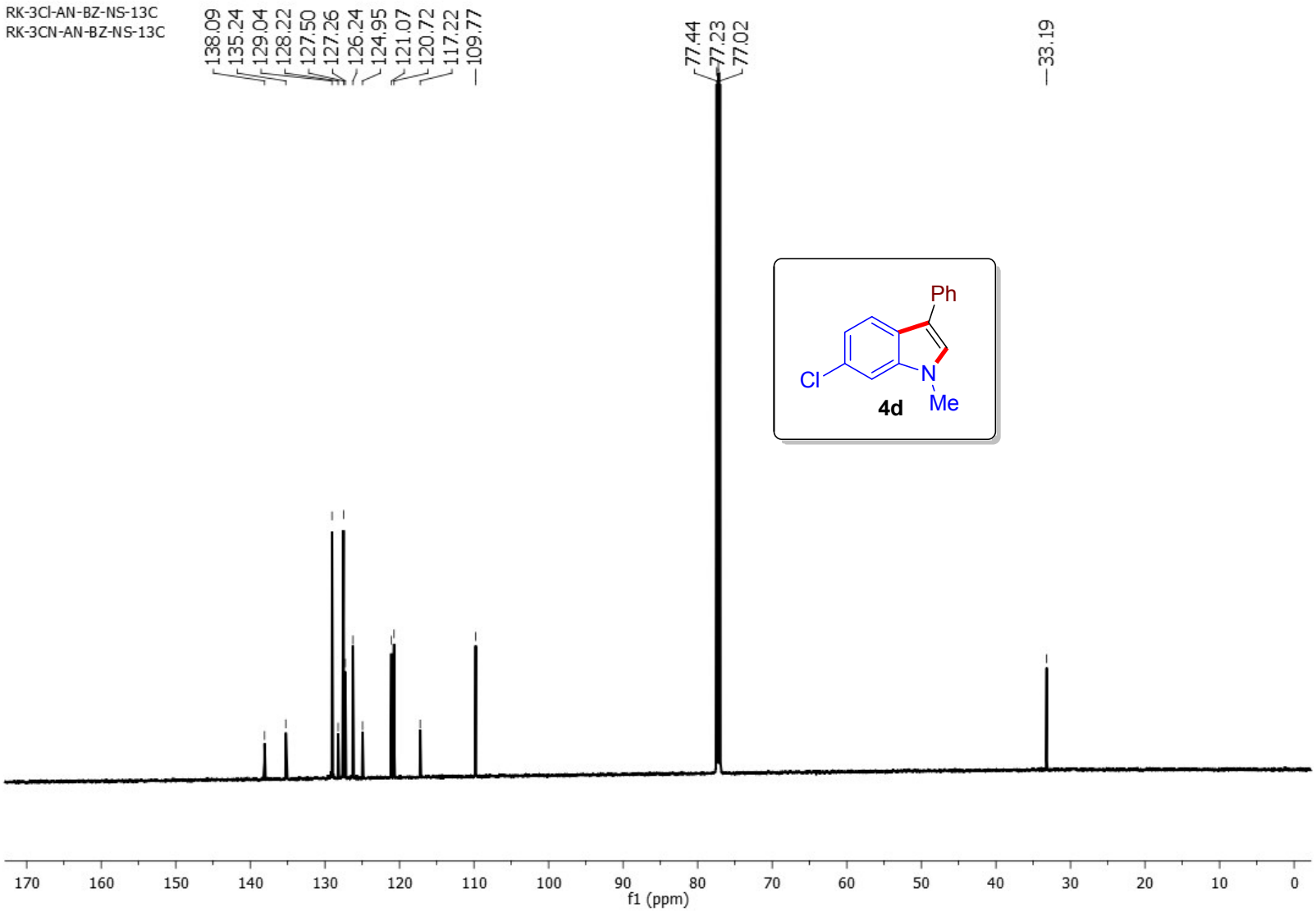
Sample Name	RK-3F-C	**Position**	Vial 1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	0	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	RK-3F-C.d	**ACQ Method**		**Comment**		**Acquired Time**	11/1/2017 4:09:40 PM



^{1}H NMR spectra of compound: 4d

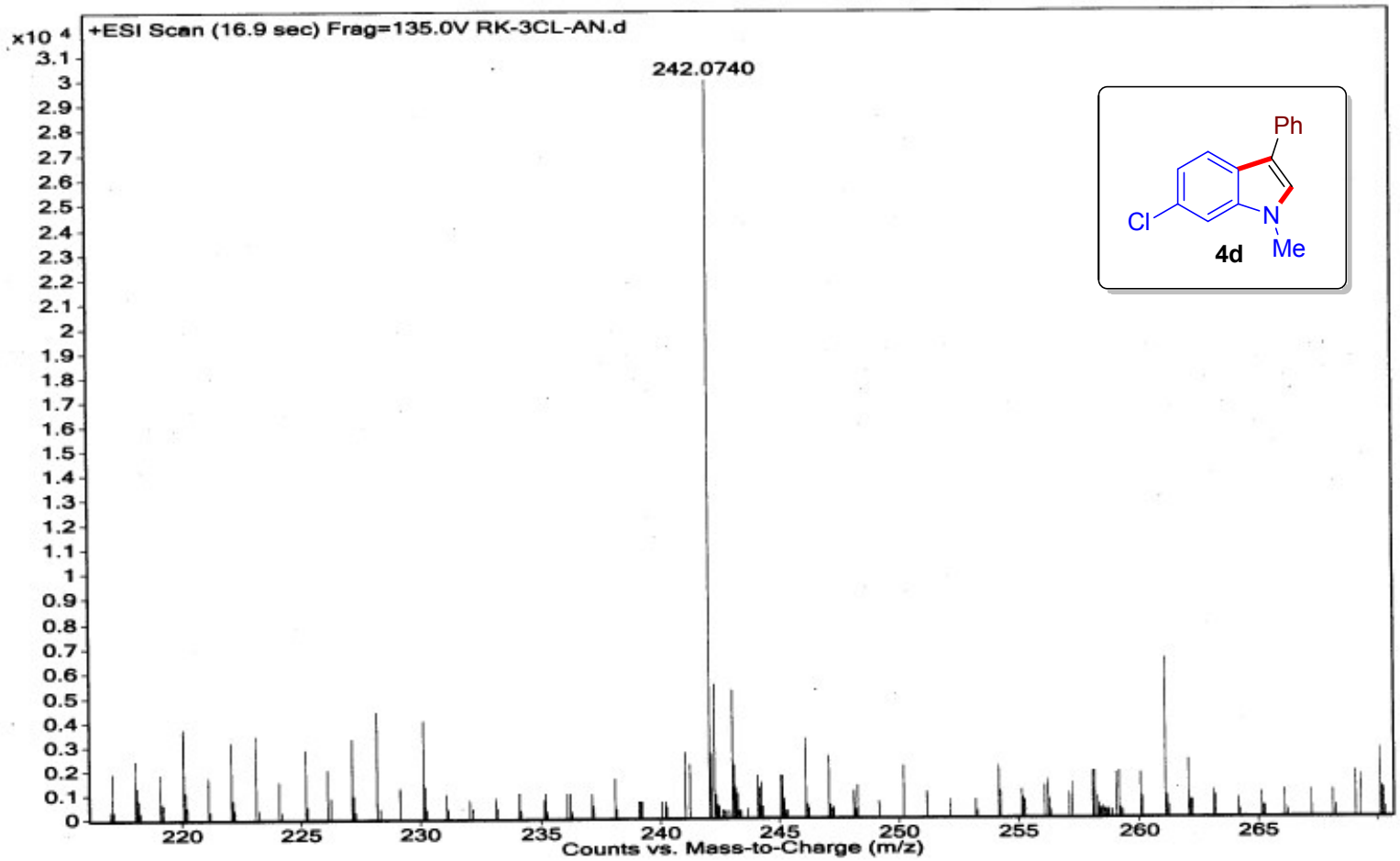


^{13}C NMR spectra of compound: 4d

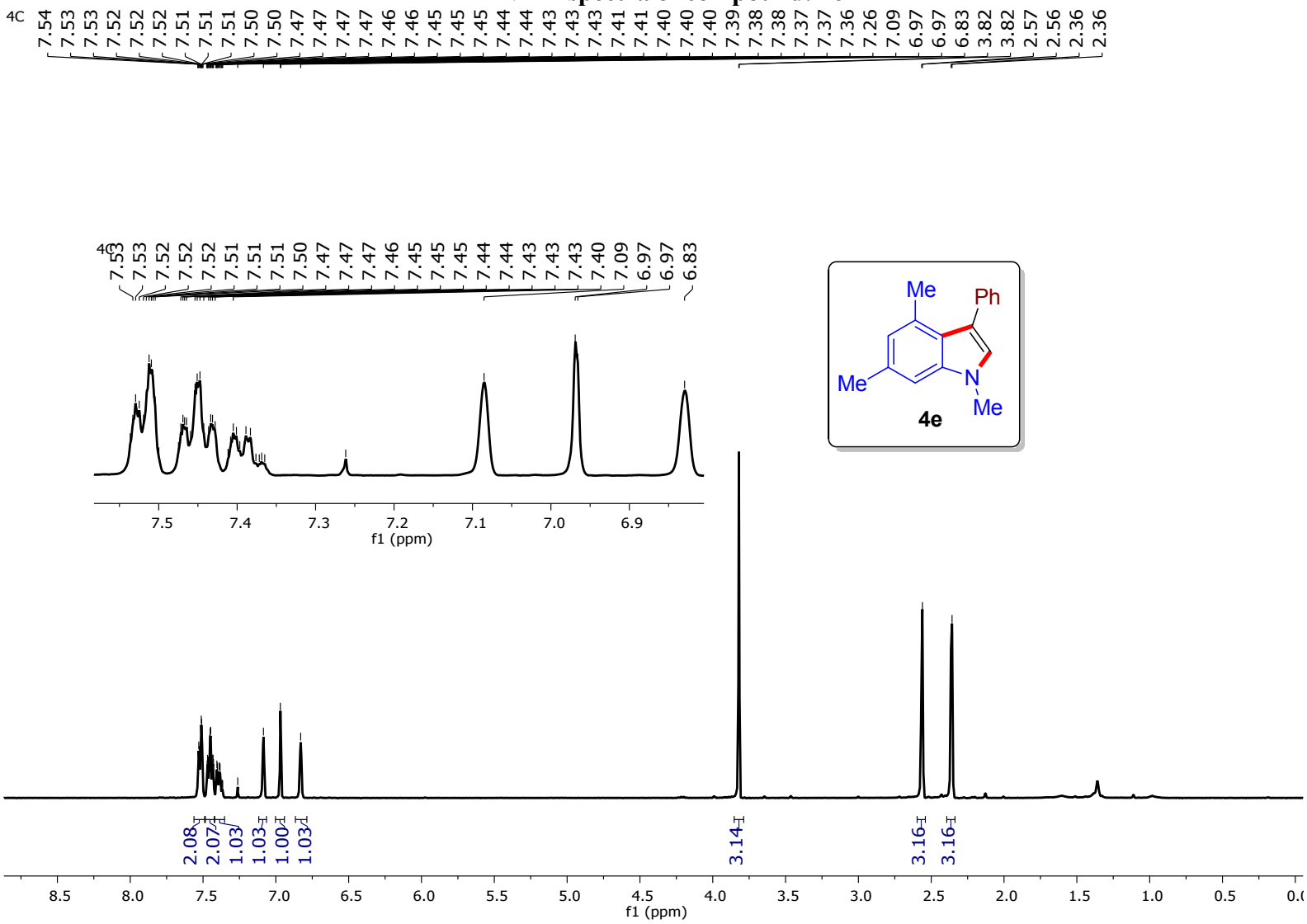


HRMS spectra of compound: 4d

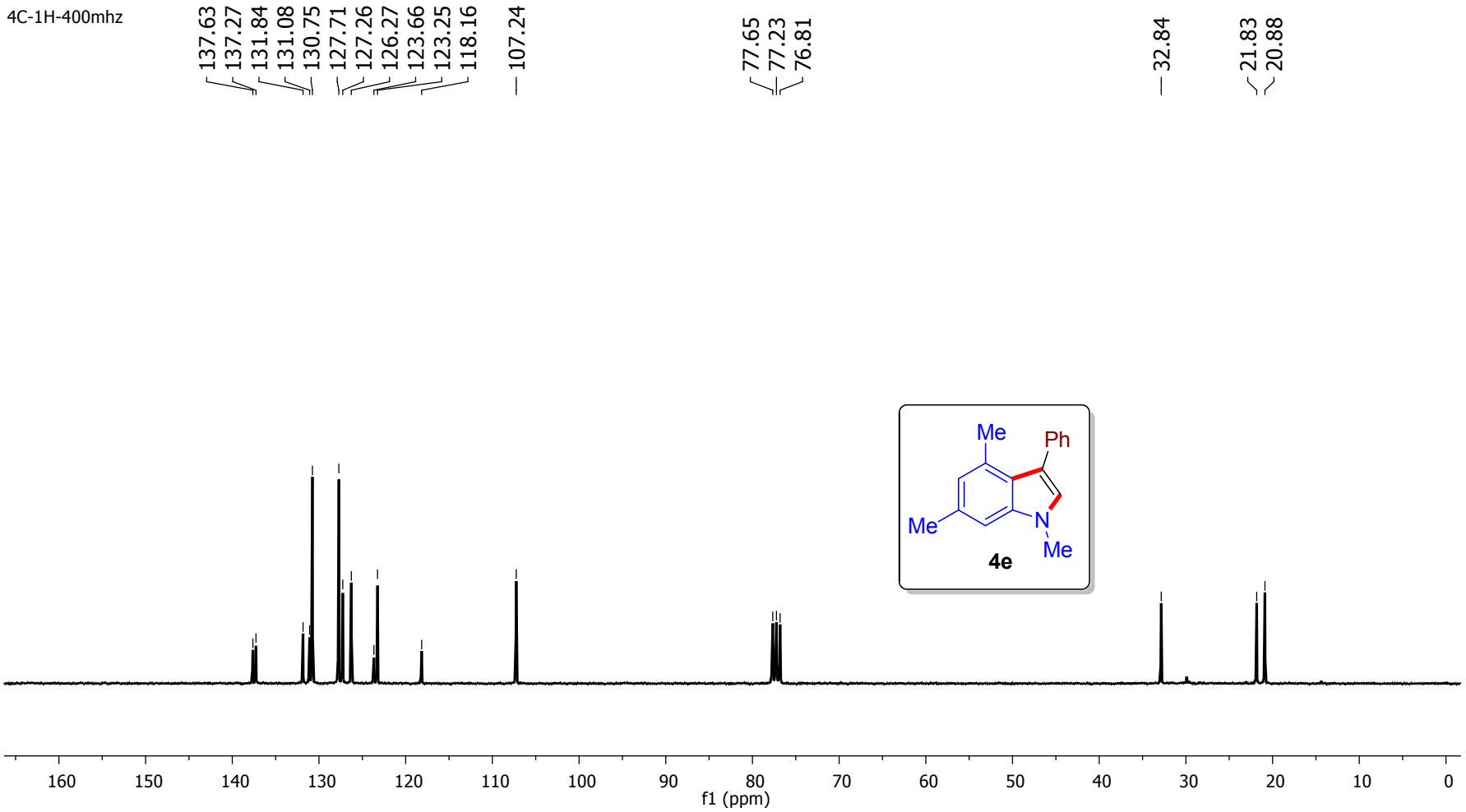
Sample Name	Unavailable	**Position**	Unavailable	**Instrument Name**	Unavailable	**User Name**	Unavailable
Inj Vol	Unavailable	**InjPosition**	Unavailable	**SampleType**	Unavailable	**IRM Calibration Status**	All Ions Missed
Data Filename	RK-3CL-AN.d	**ACQ Method**		**Comment**	Sample information is unavailable	**Acquired Time**	Unavailable



^{1}H NMR spectra of compound: 4e

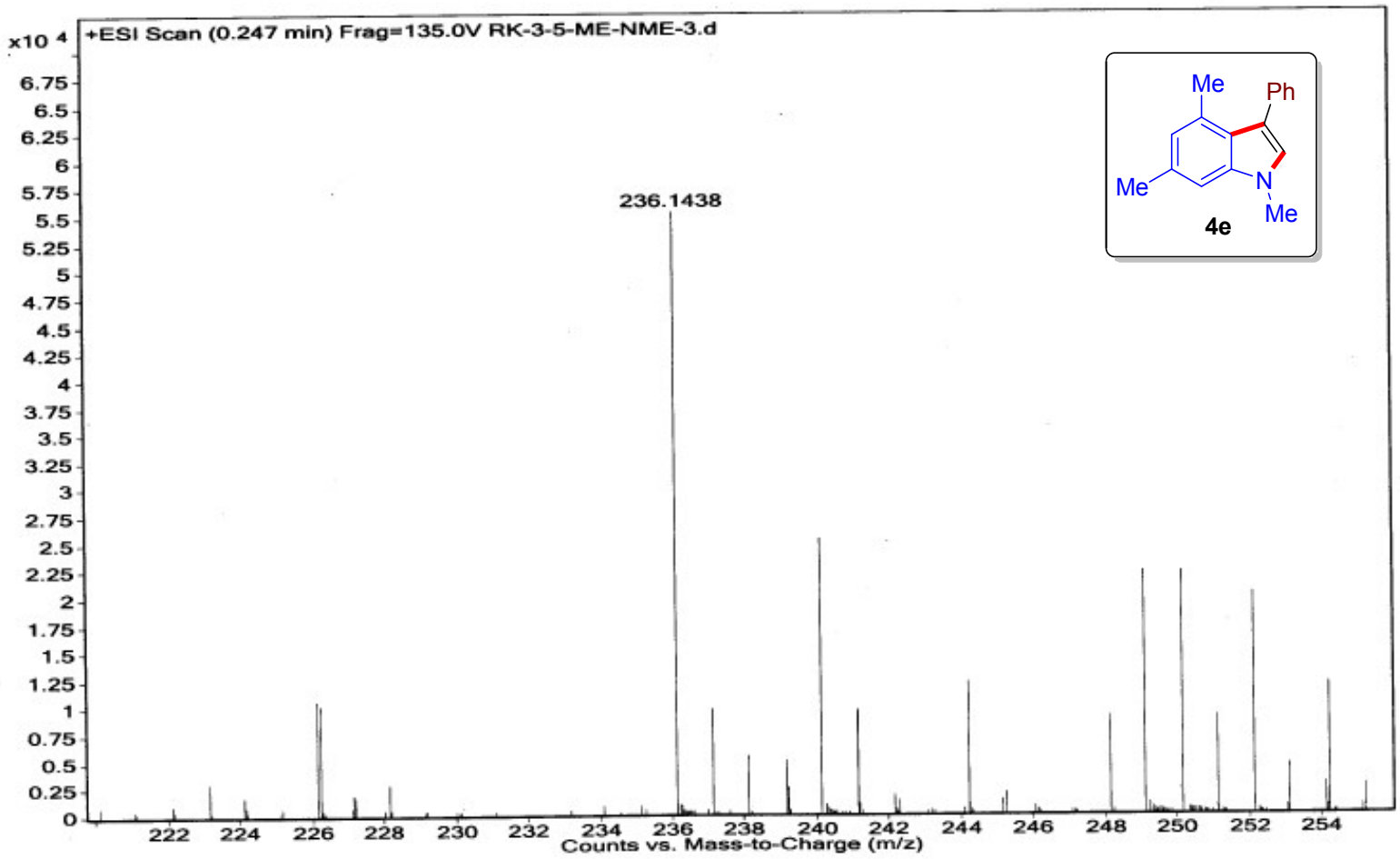


^{13}C NMR spectra of compound: 4e

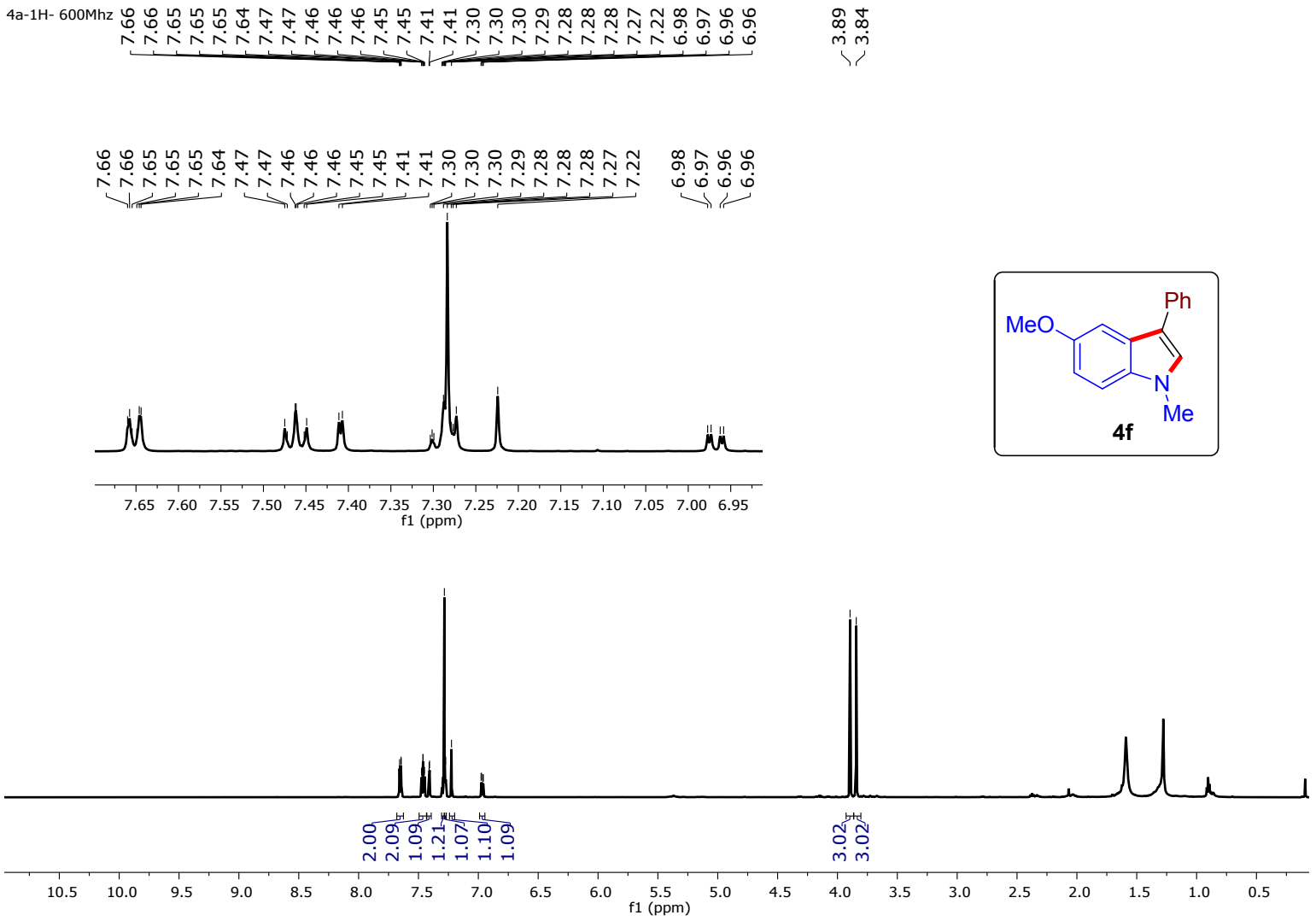


HRMS spectra of compound: 4e

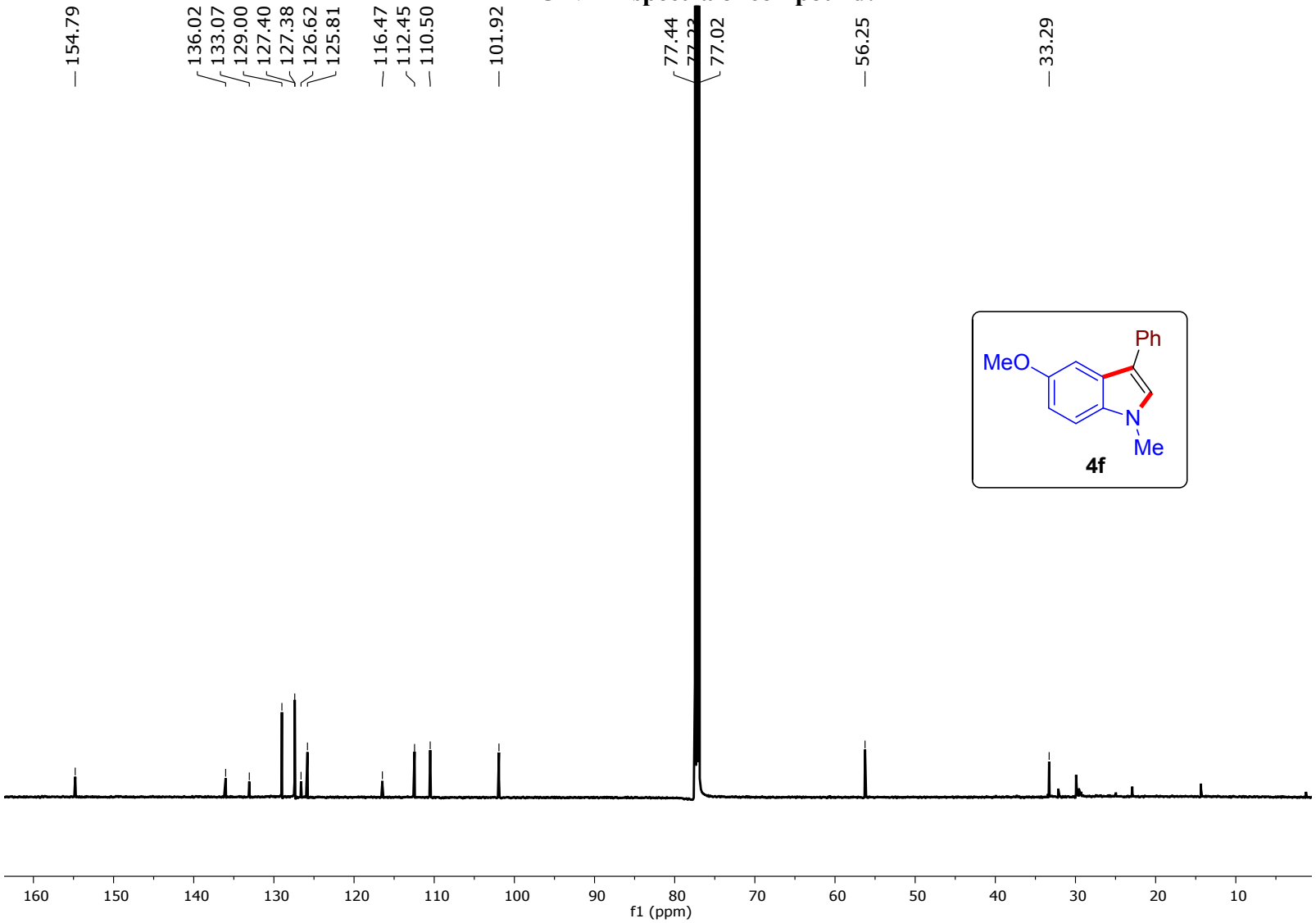
Sample Name	RK-3-5-ME-NME-3	**Position**	Vial 1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	RK-3-5-ME-NME-3.d	**ACQ Method**		**Comment**		**Acquired Time**	12/1/2017 6:31:22 PM



^{1}H NMR spectra of compound: 4f

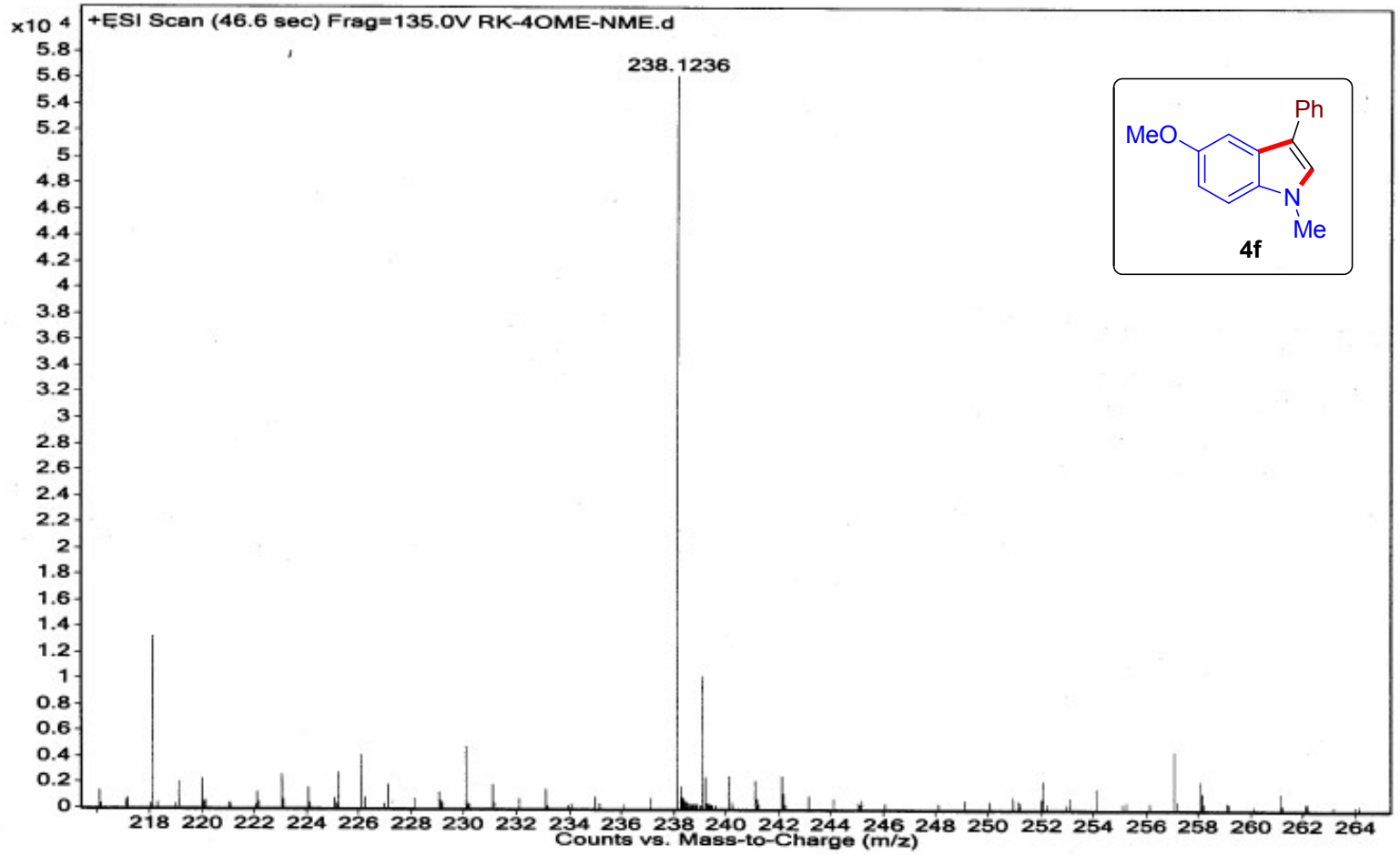


^{13}C NMR spectra of compound: 4f

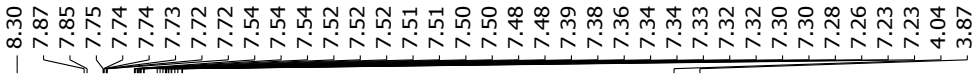


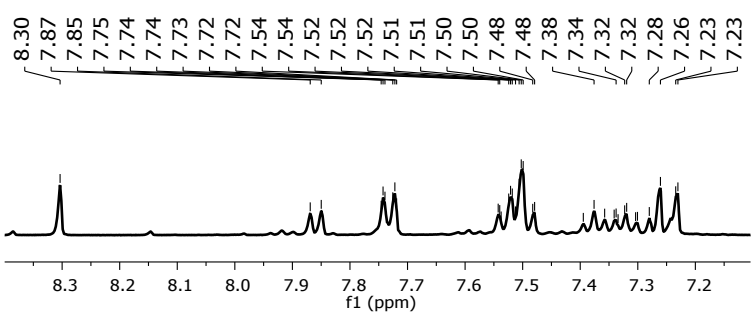
HRMS spectra of compound: 4f

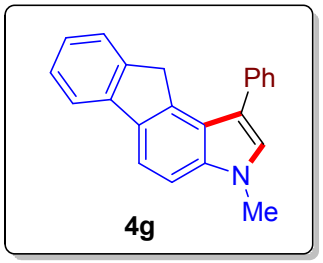
Sample Name	Unavailable	**Position**	Unavailable	**Instrument Name**	Unavailable	**User Name**	Unavailable
Inj Vol	Unavailable	**InjPosition**	Unavailable	**SampleType**	Unavailable	**IRM Calibration Status**	All Ions Missed
Data Filename	RK-4OME-NME.d	**ACQ Method**		**Comment**	Sample Information is unavailable	**Acquired Time**	Unavailable

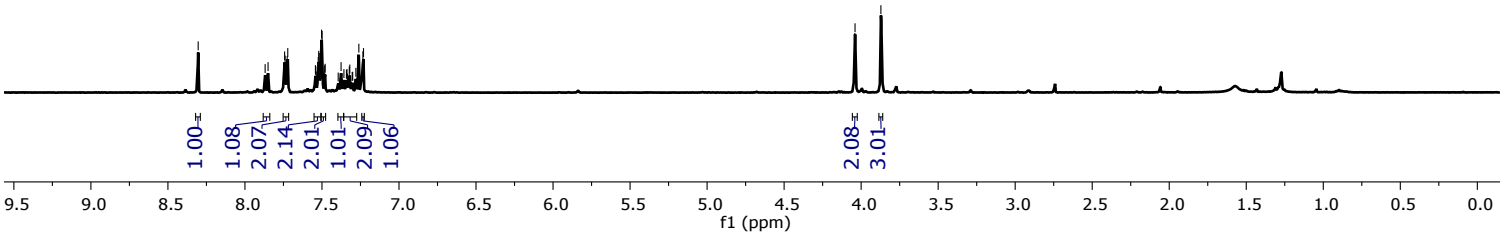


^{1}H NMR spectra of compound: 4g

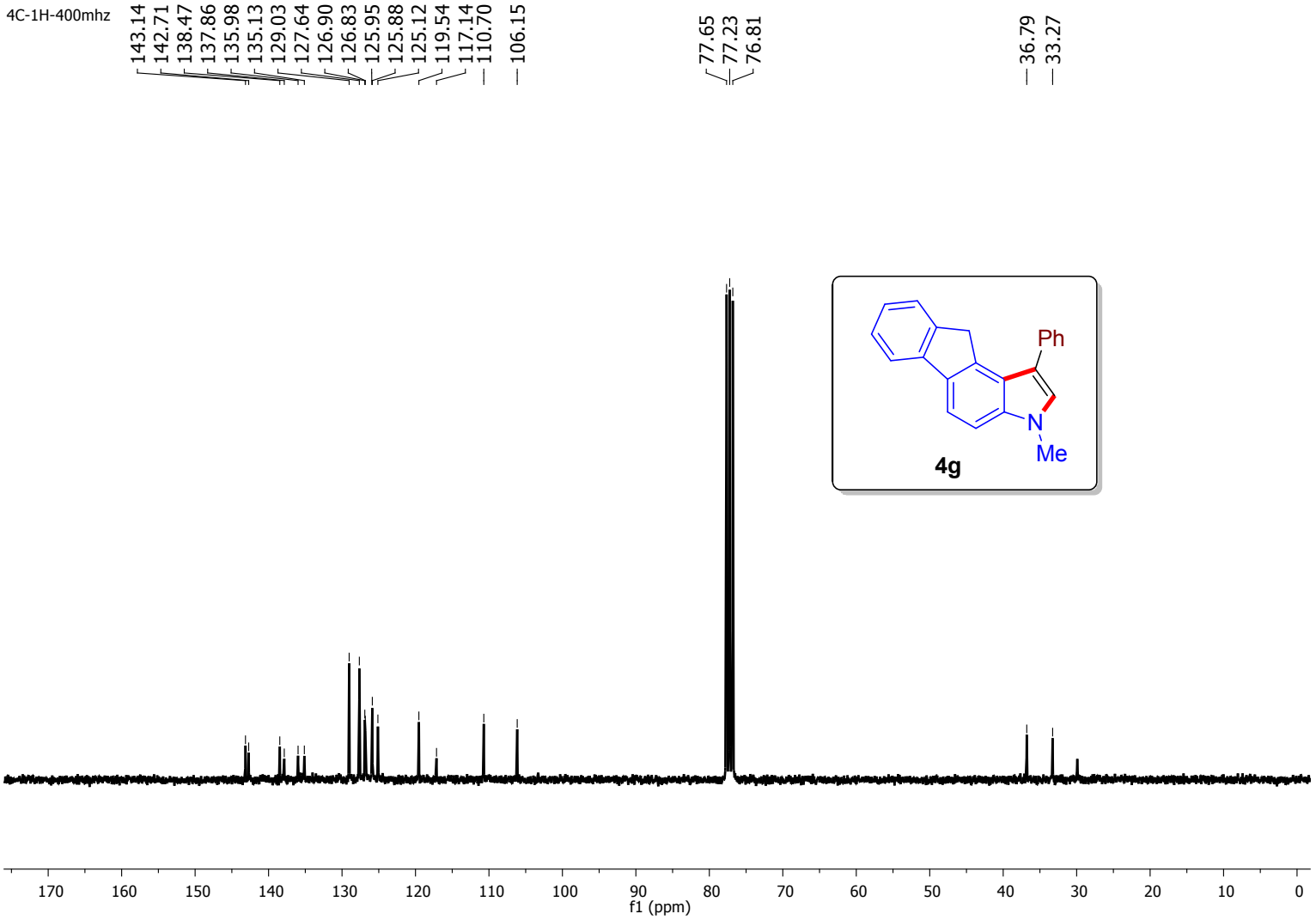




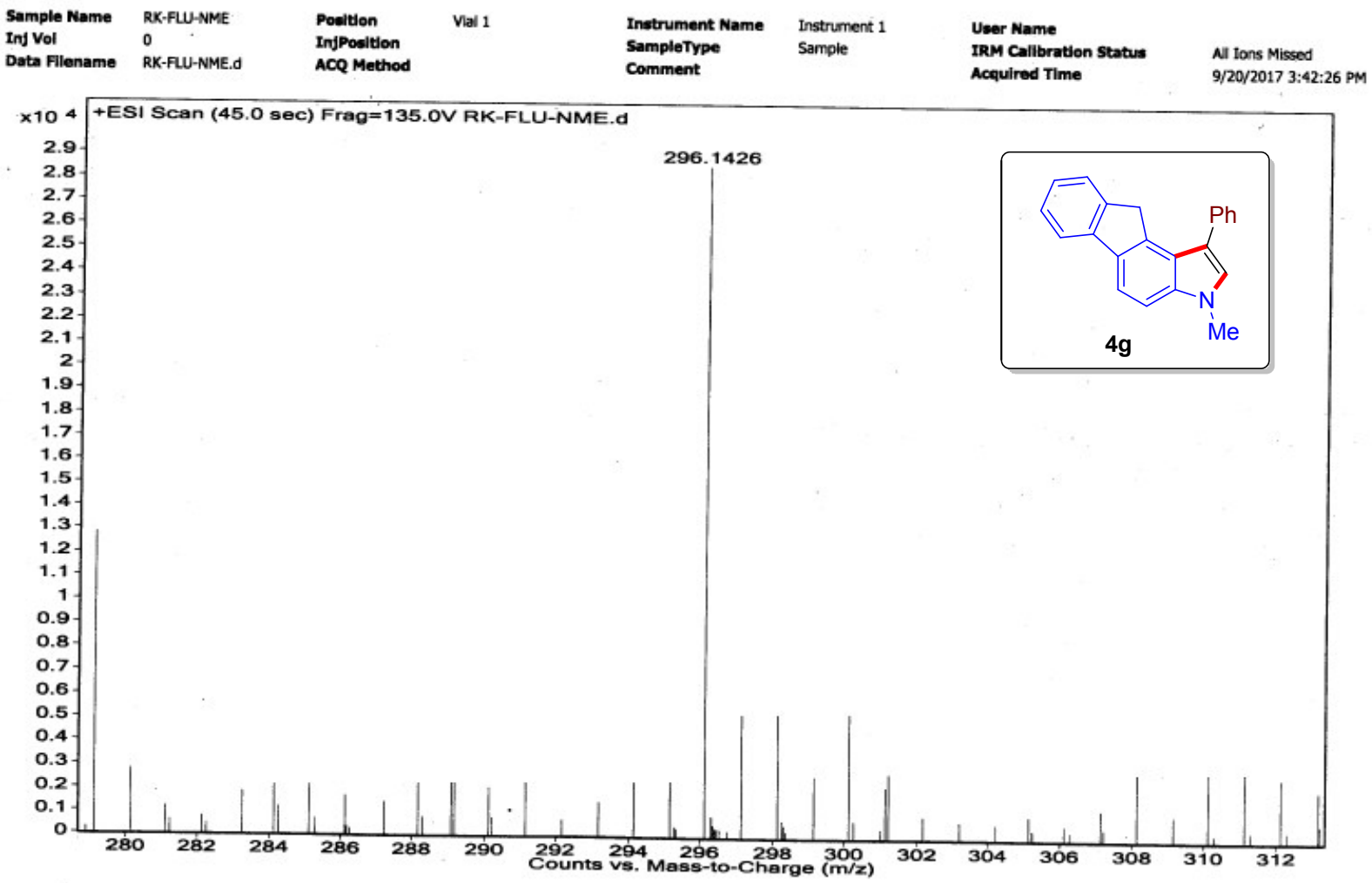




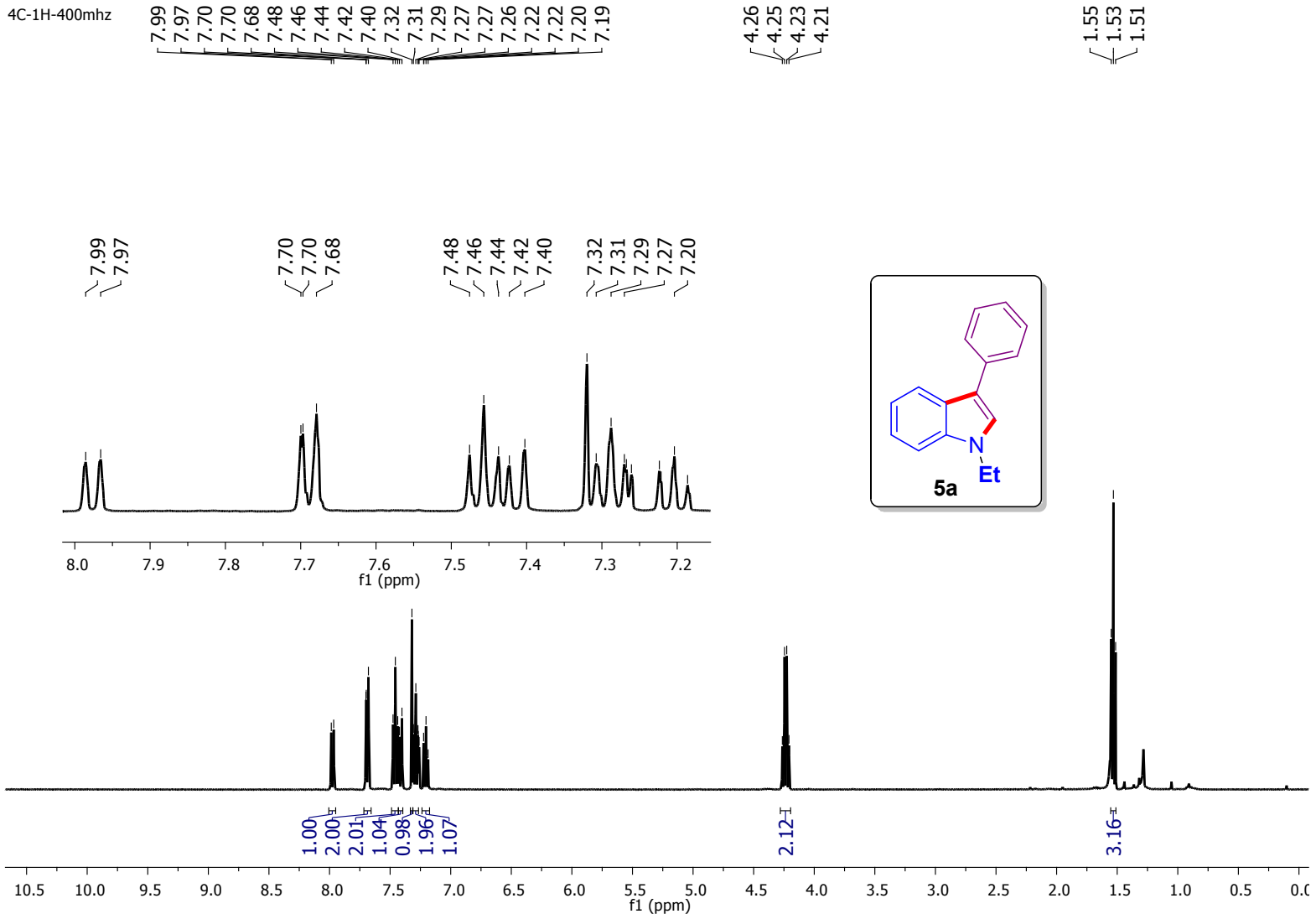
^{13}C NMR spectra of compound: 4g



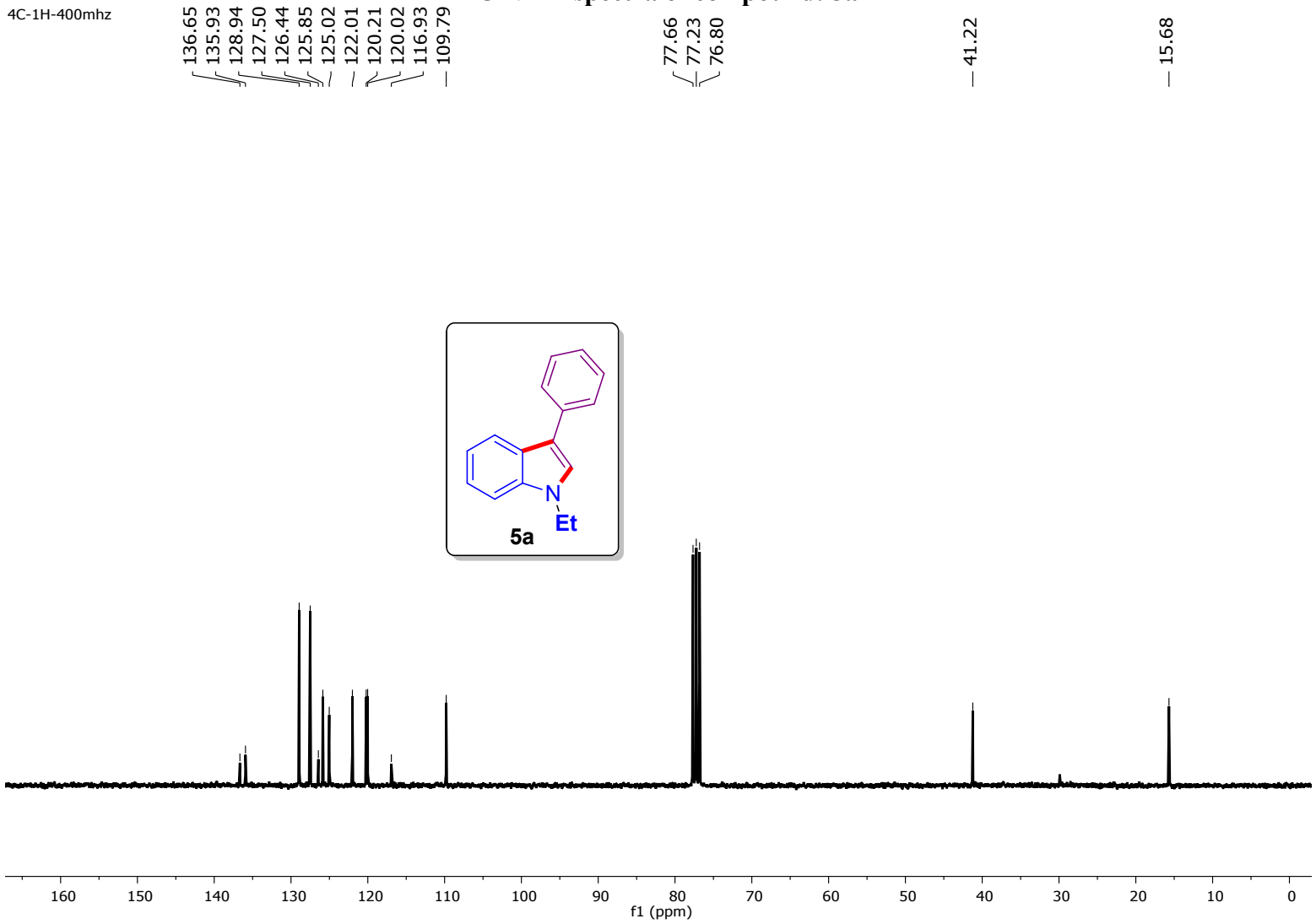
HRMS spectra of compound: 4g



^{1}H NMR spectra of compound: 5a

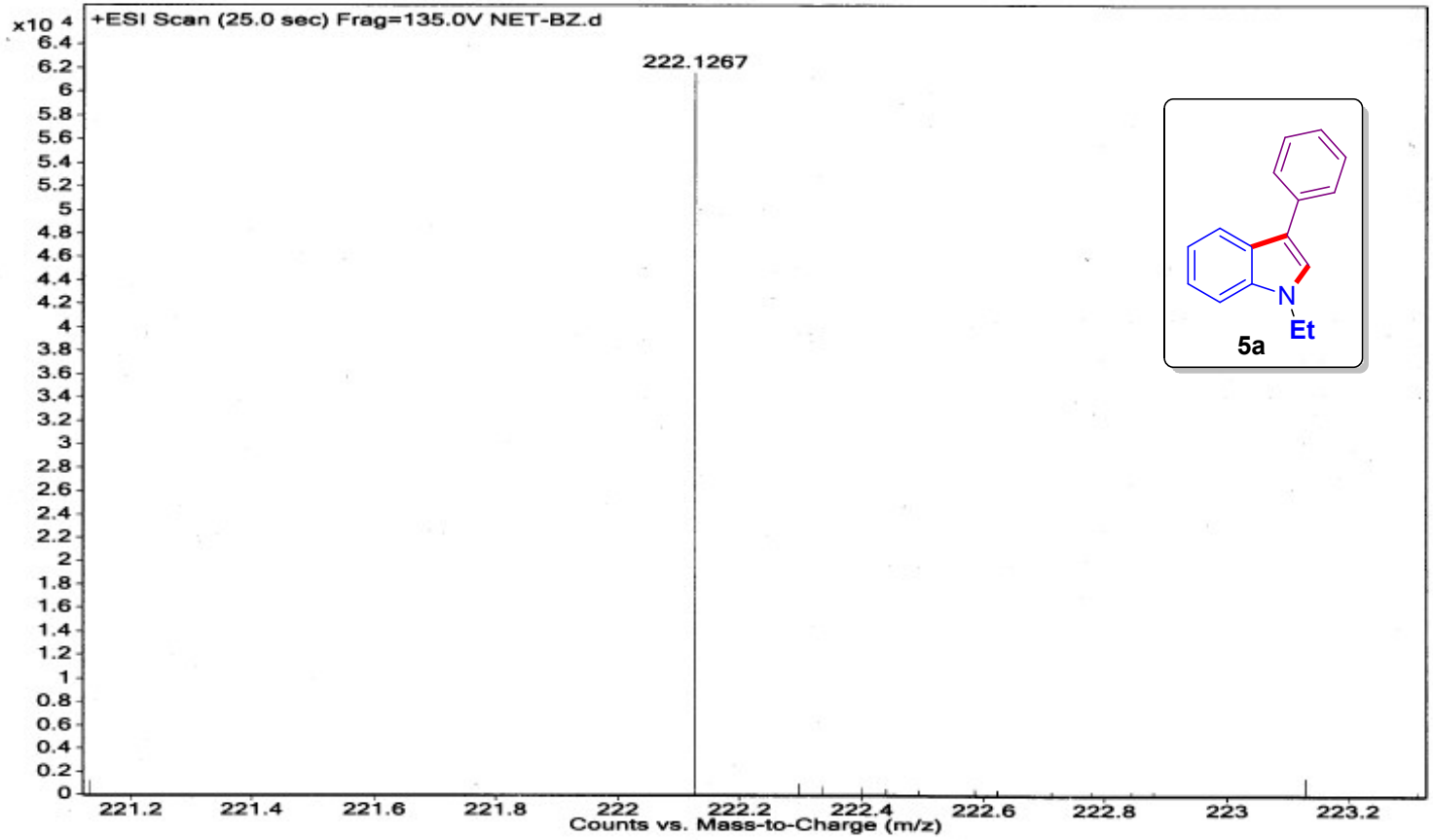


^{13}C NMR spectra of compound: 5a

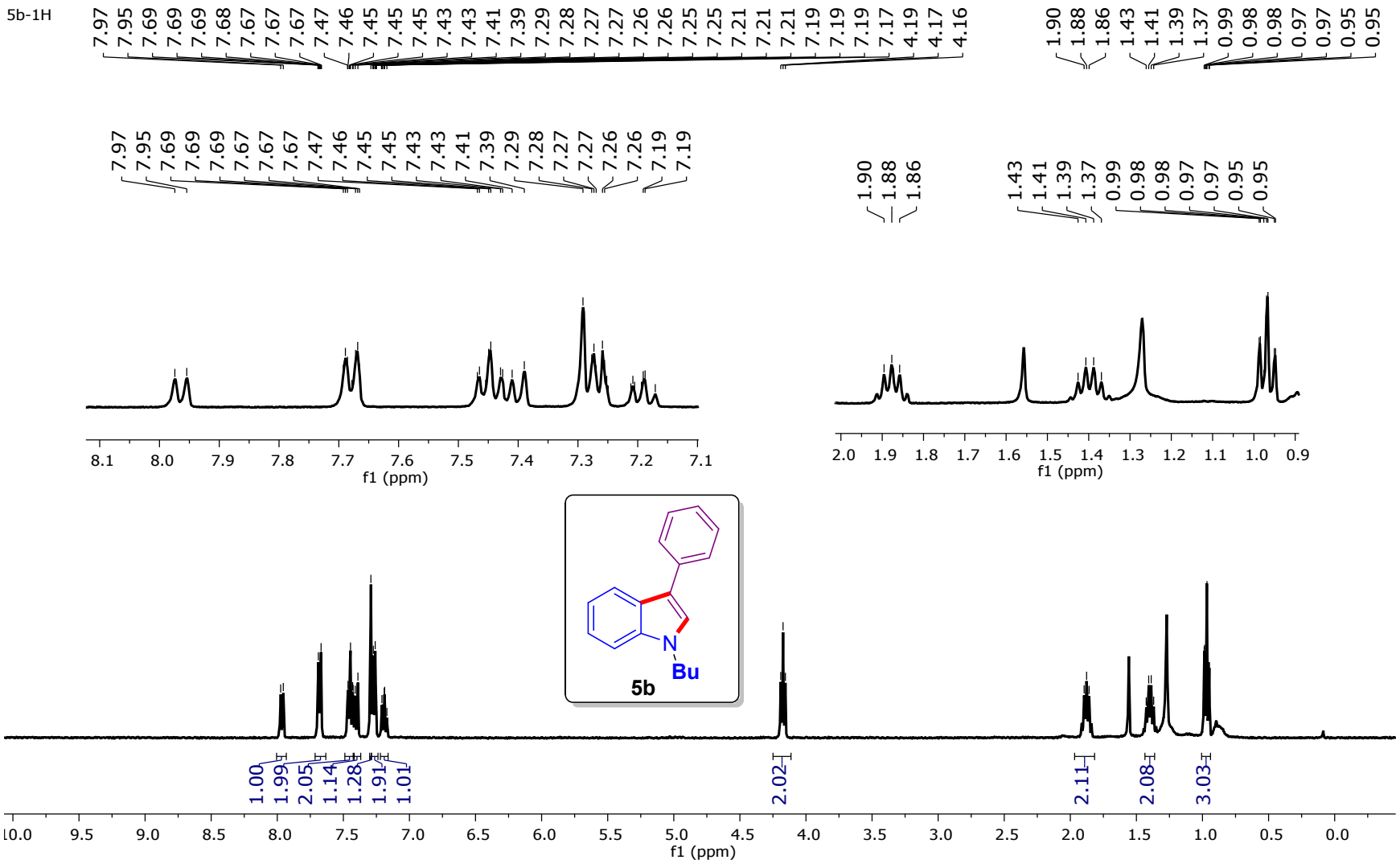


HRMS spectra of compound: 5a

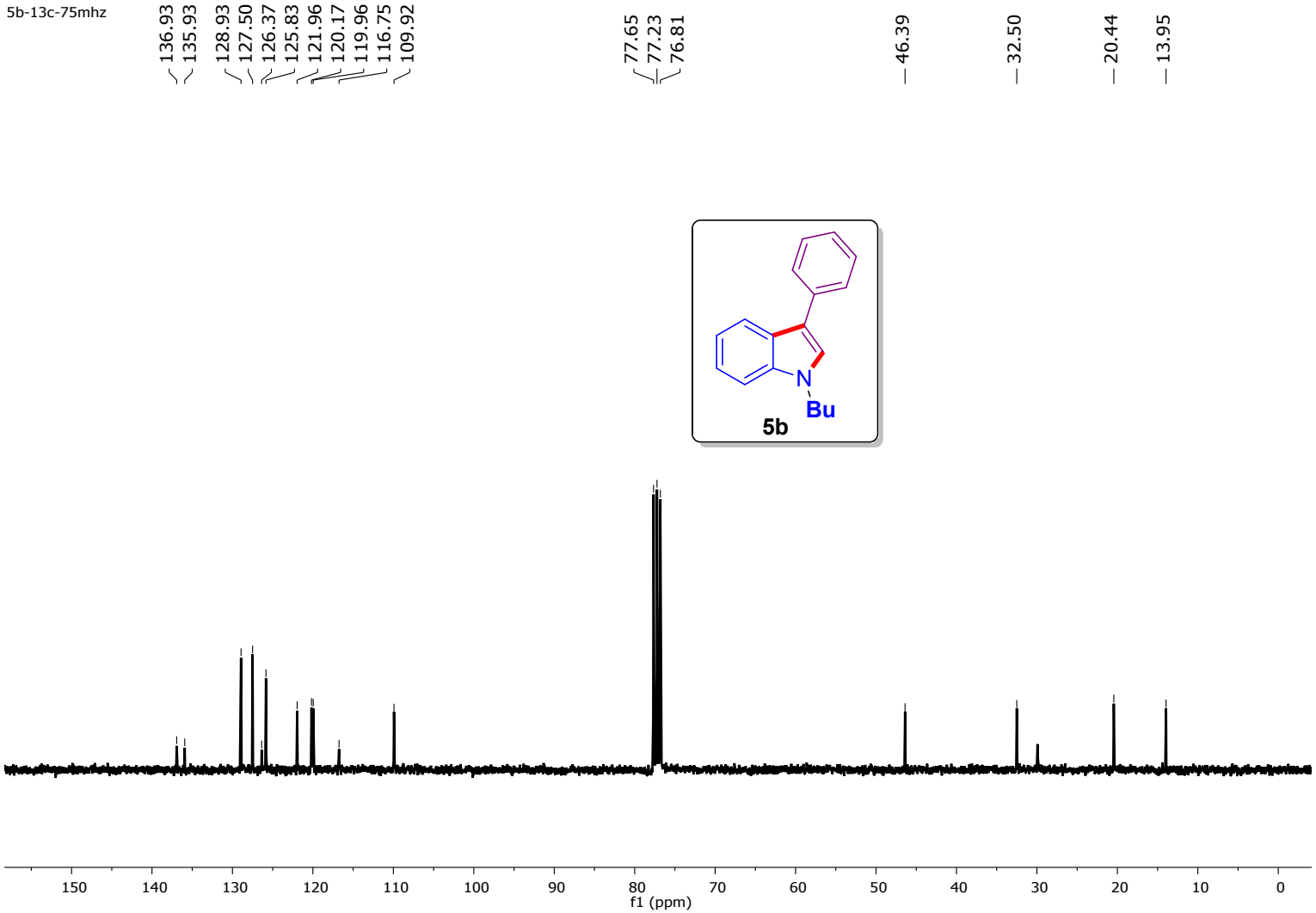
Sample Name	Unavailable	**Position**	Unavailable	**Instrument Name**	Unavailable	**User Name**	Unavailable
Inj Vol	Unavailable	**InjPosition**	Unavailable	**SampleType**	Unavailable	**IRM Calibration Status**	Some Ions Missed
Data Filename	NET-BZ.d	**ACQ Method**		**Comment**	Sample information is unavailable	**Acquired Time**	Unavailable



^{1}H NMR spectra of compound: 5b

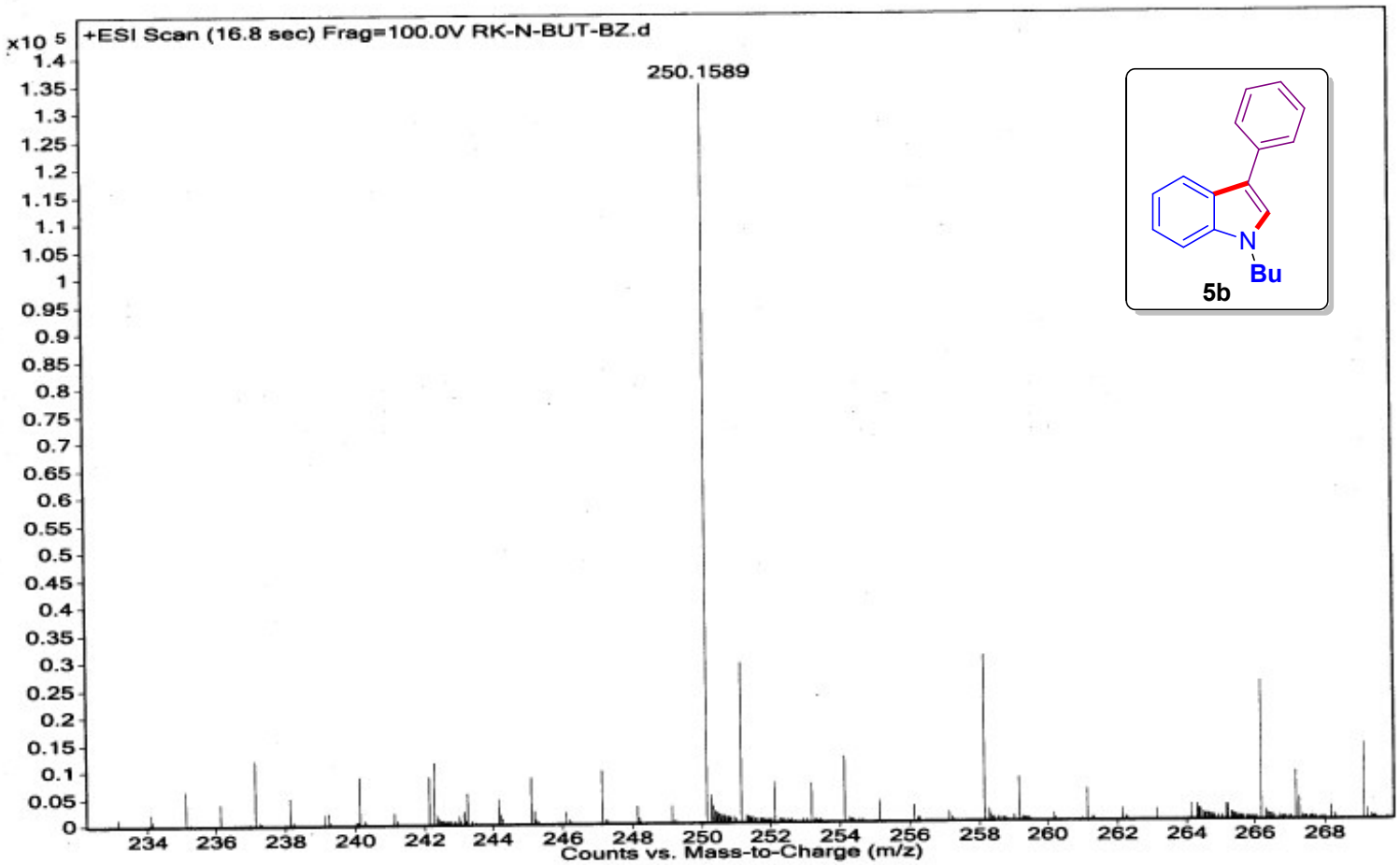


^{13}C NMR spectra of compound: 5b

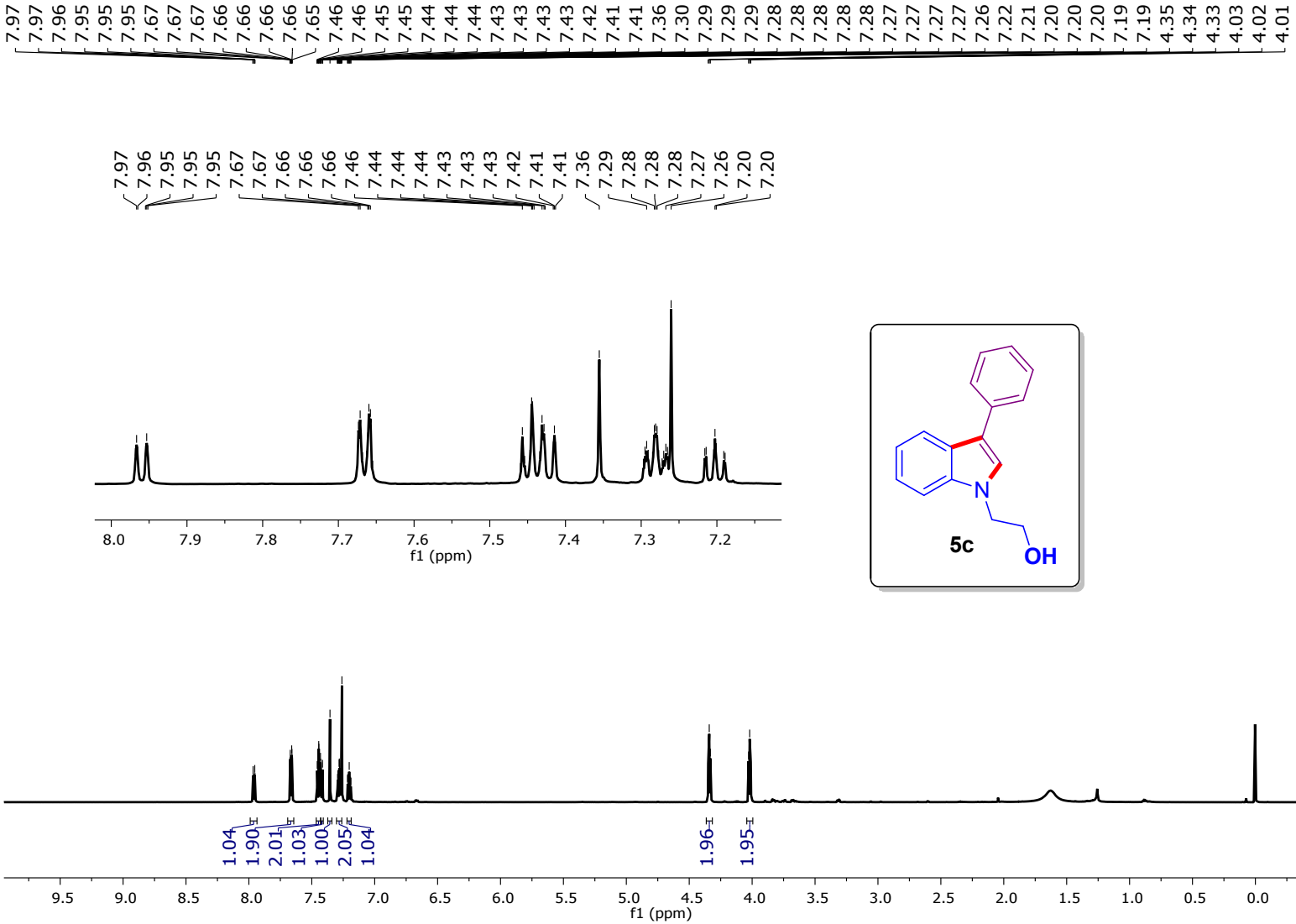


HRMS spectra of compound: 5b

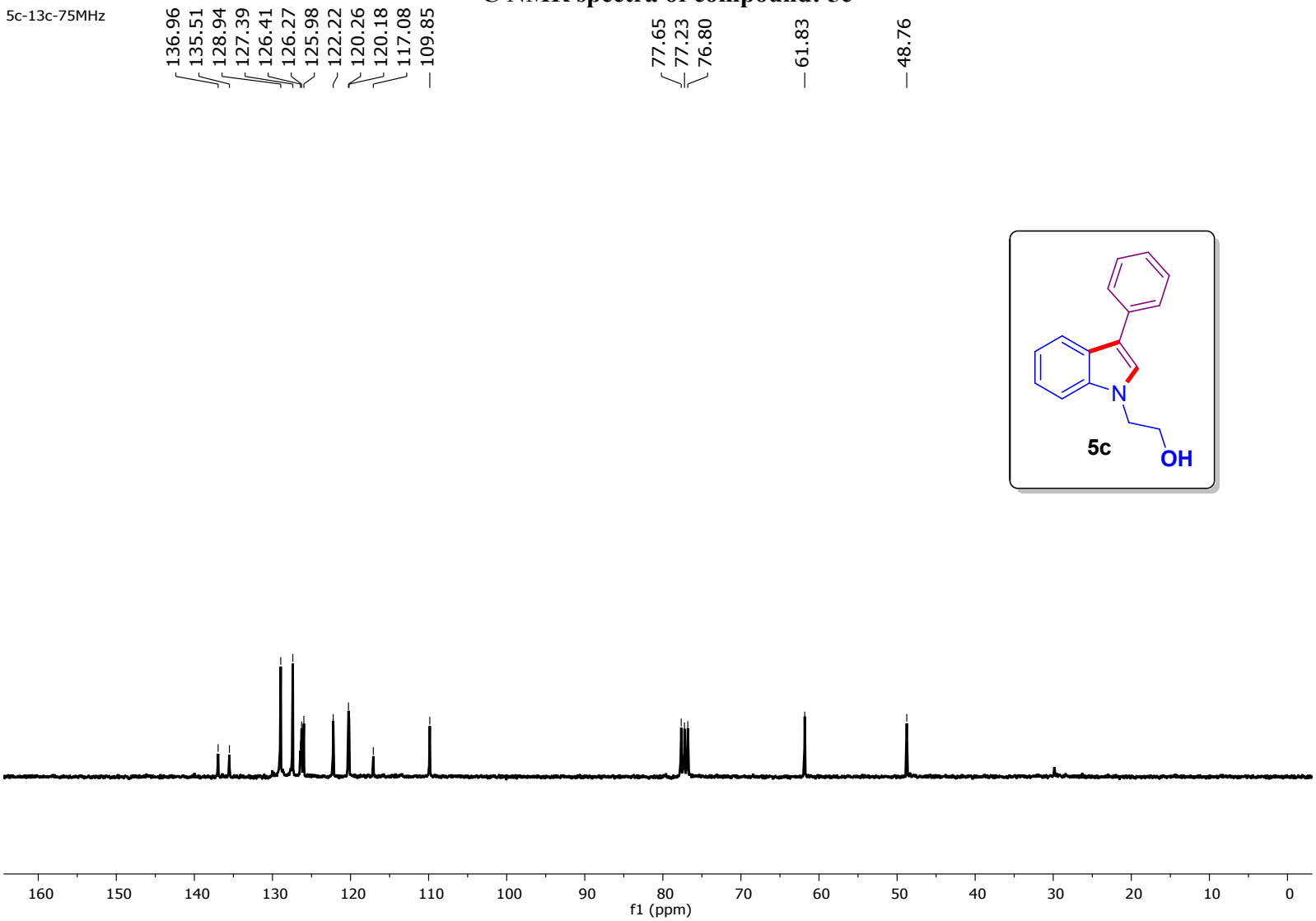
Sample Name	Unavailable	**Position**	Unavailable	**Instrument Name**	Unavailable	**User Name**	Unavailable
Inj Vol	Unavailable	**InjPosition**	Unavailable	**SampleType**	Unavailable	**IRM Calibration Status**	All Ions Missed
Data Filename	RK-N-BUT-BZ.d	**ACQ Method**		**Comment**	Sample information is unavailable	**Acquired Time**	Unavailable



^{1}H NMR spectra of compound: 5c

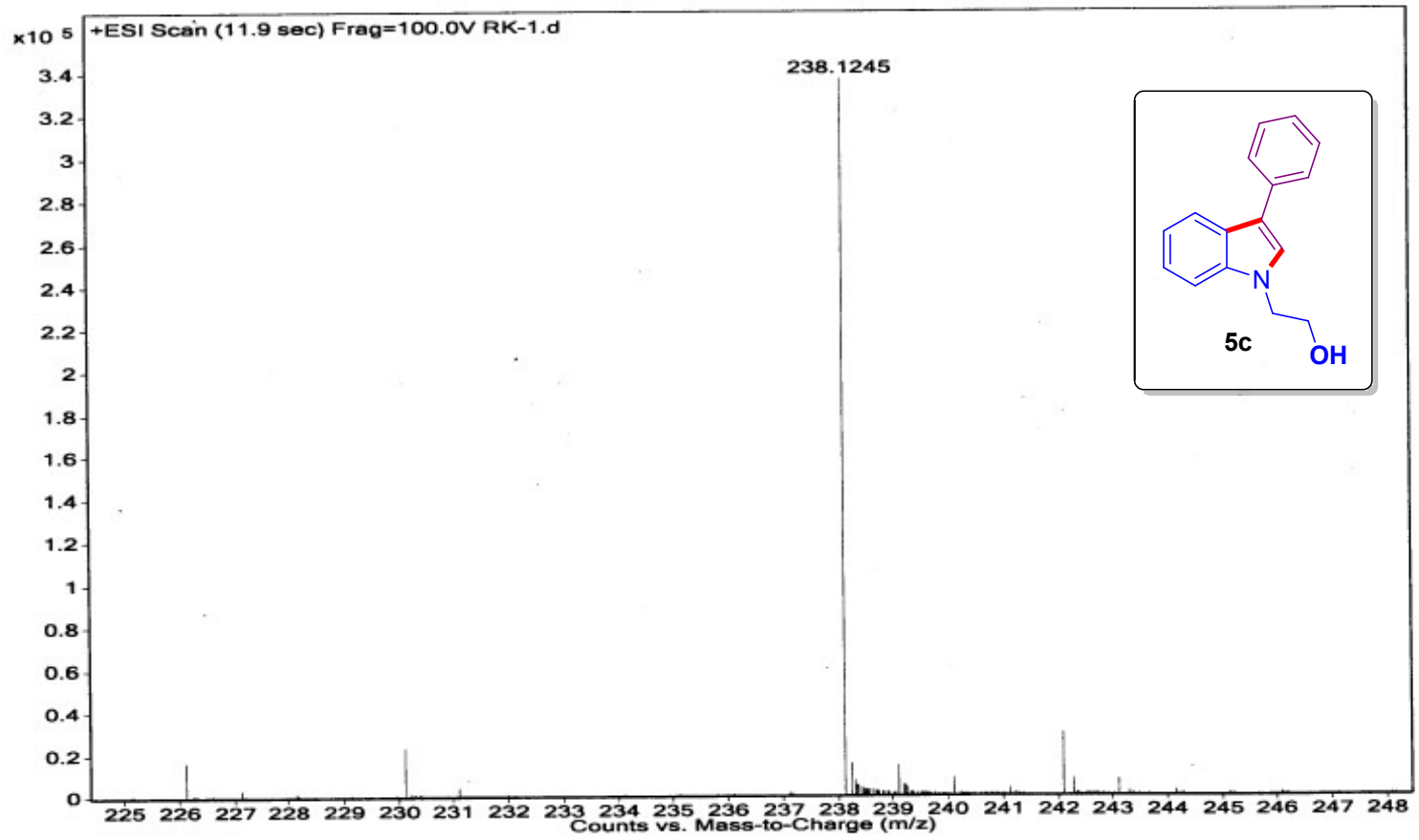


^{13}C NMR spectra of compound: 5c

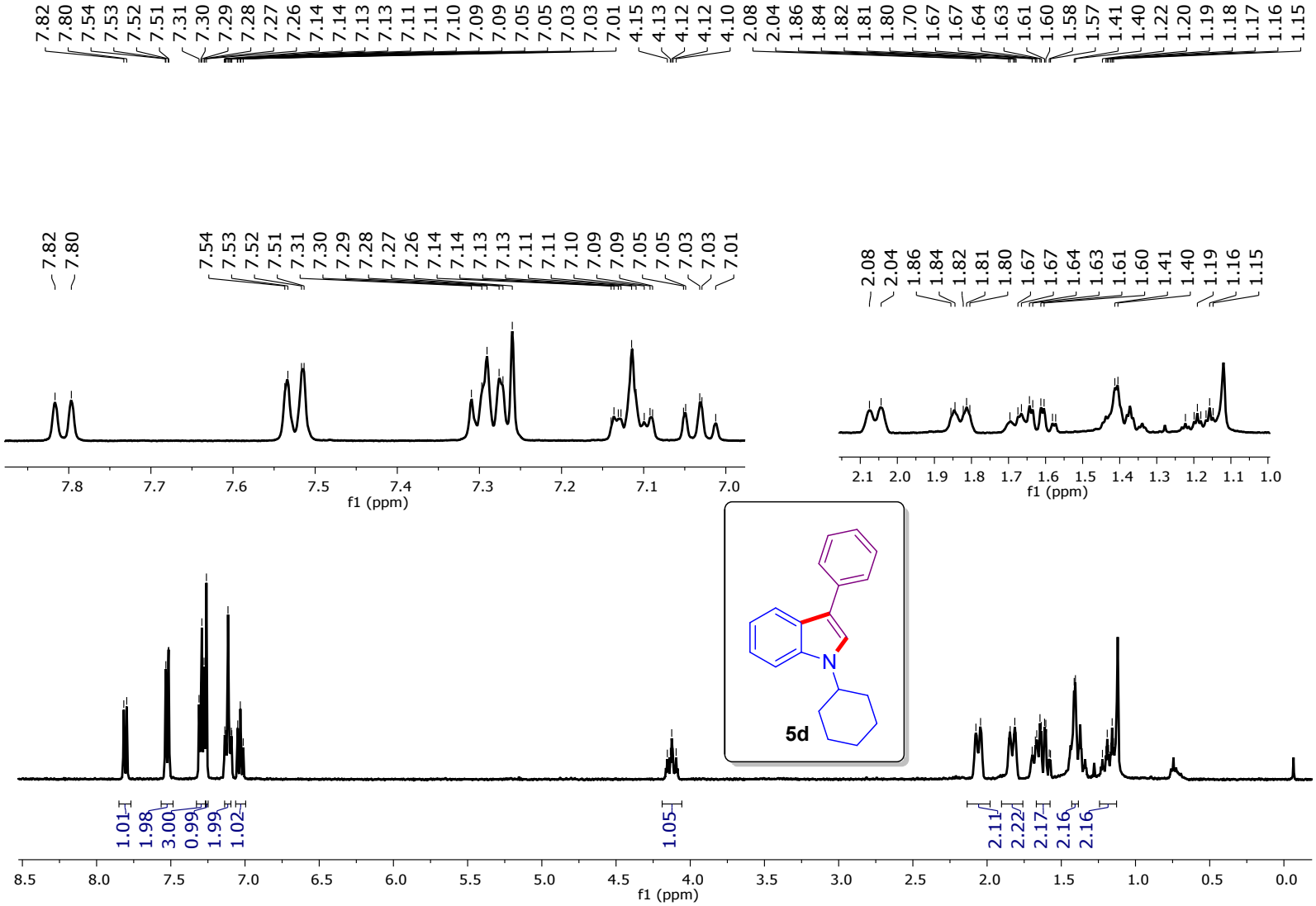


HRMS spectra of compound: 5c

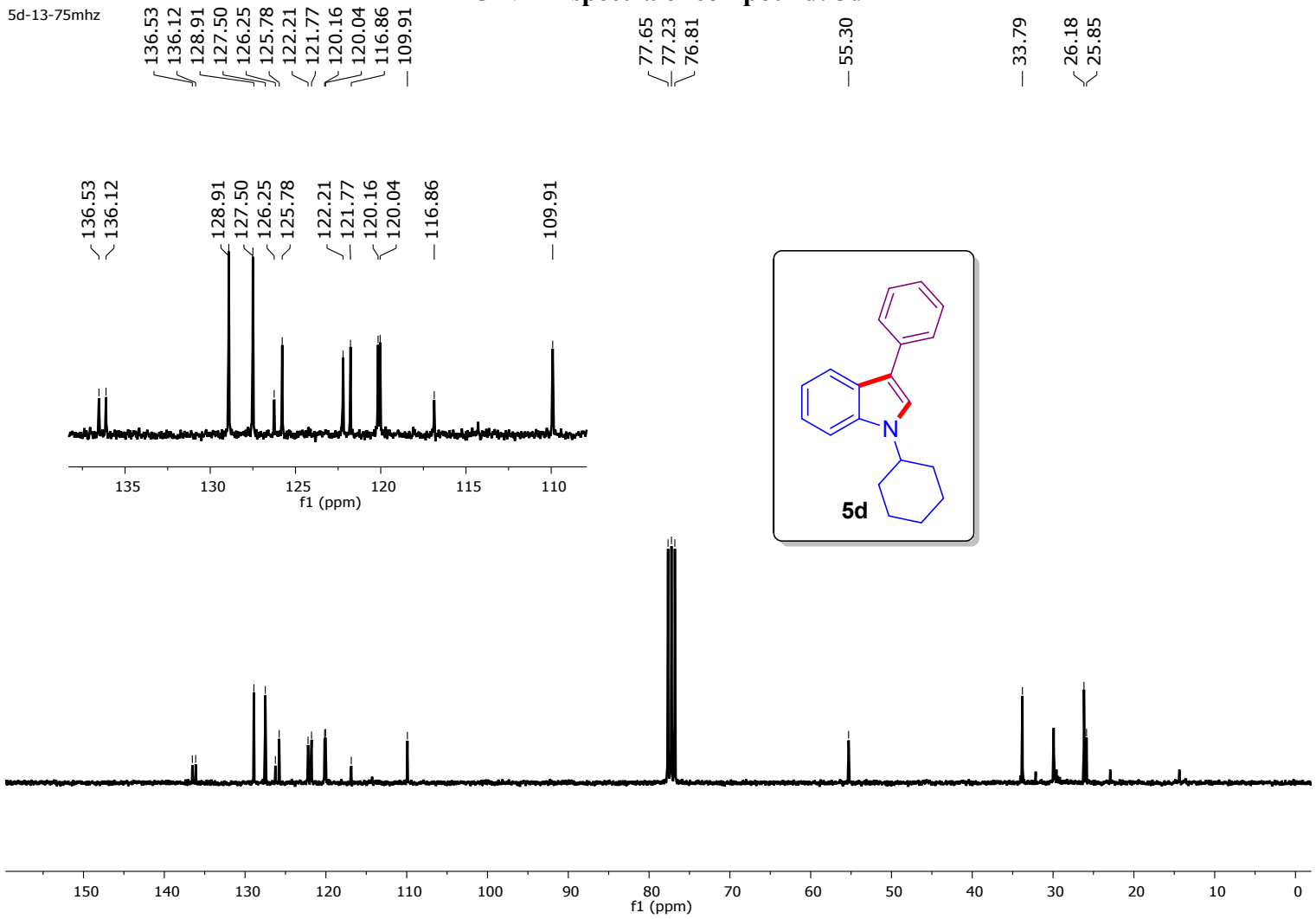
Sample Name	Unavailable	**Position**	Unavailable	**Instrument Name**	Unavailable	**User Name**	Unavailable
Inj Vol	Unavailable	**InjPosition**	Unavailable	**SampleType**	Unavailable	**IRM Calibration Status**	All Ions Missed
Data Filename	RK-1.d	**ACQ Method**		**Comment**	Sample information is unavailable	**Acquired Time**	Unavailable



^{1}H NMR spectra of compound: 5d

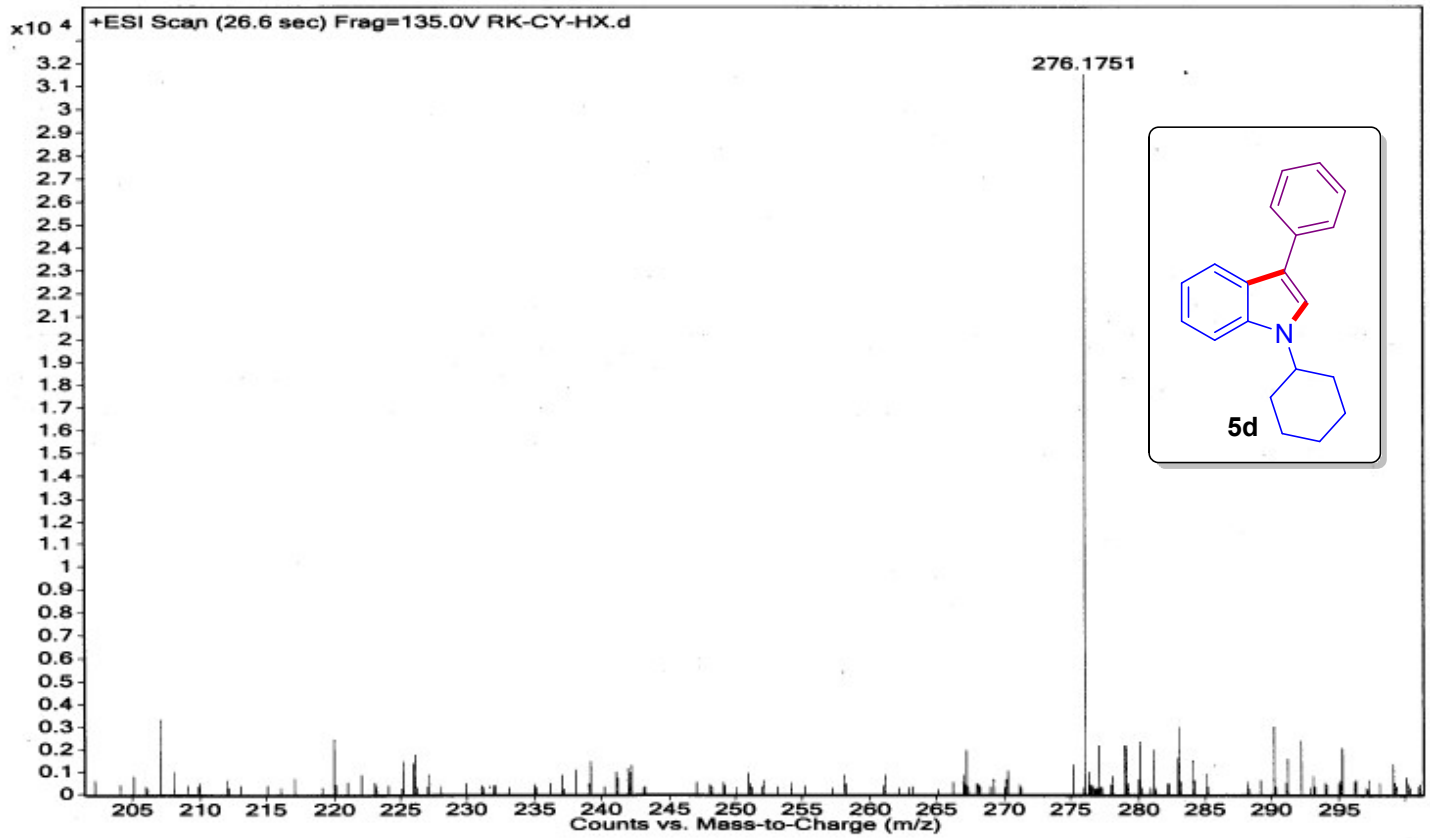


^{13}C NMR spectra of compound: 5d

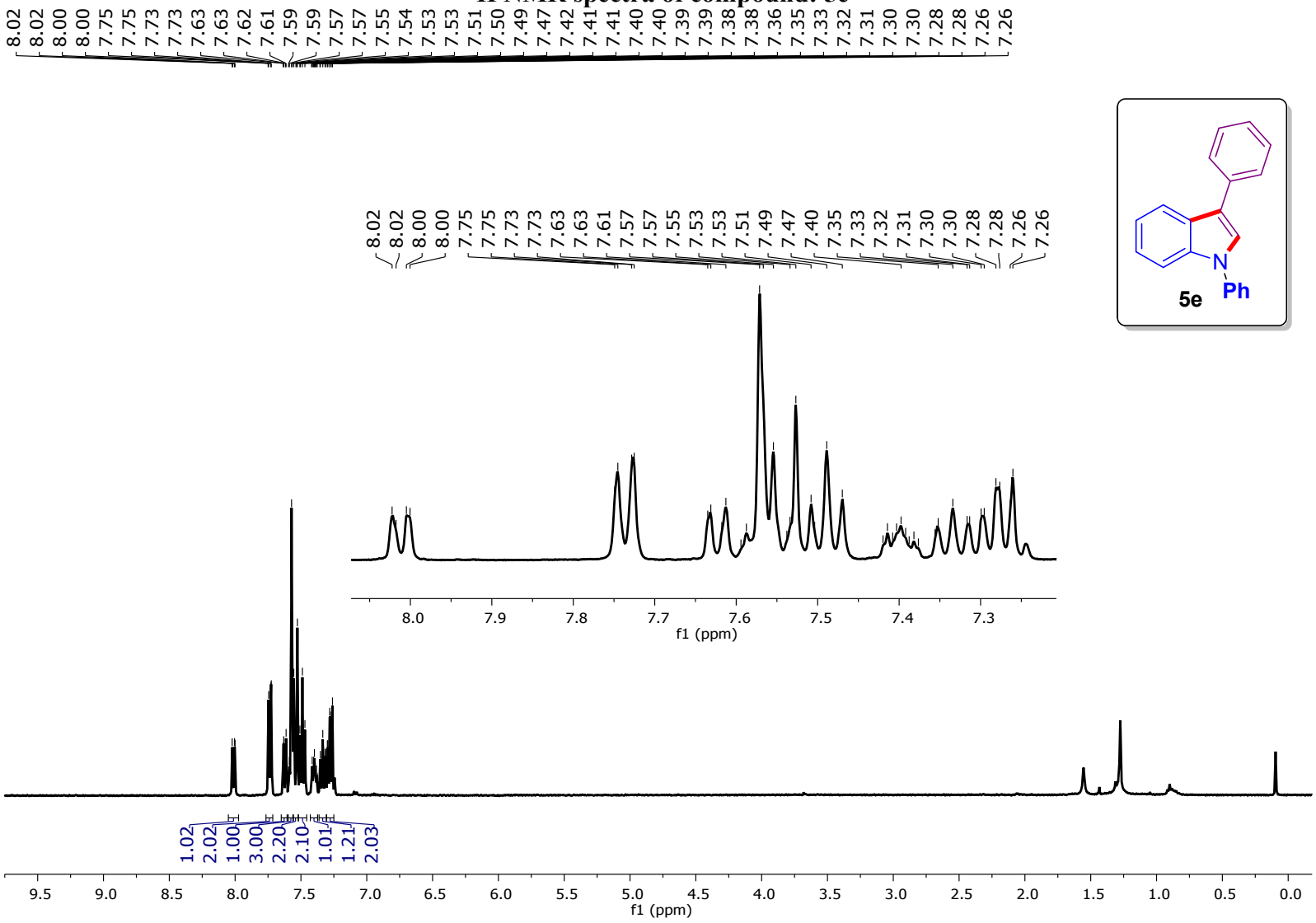


HRMS spectra of compound: 5d

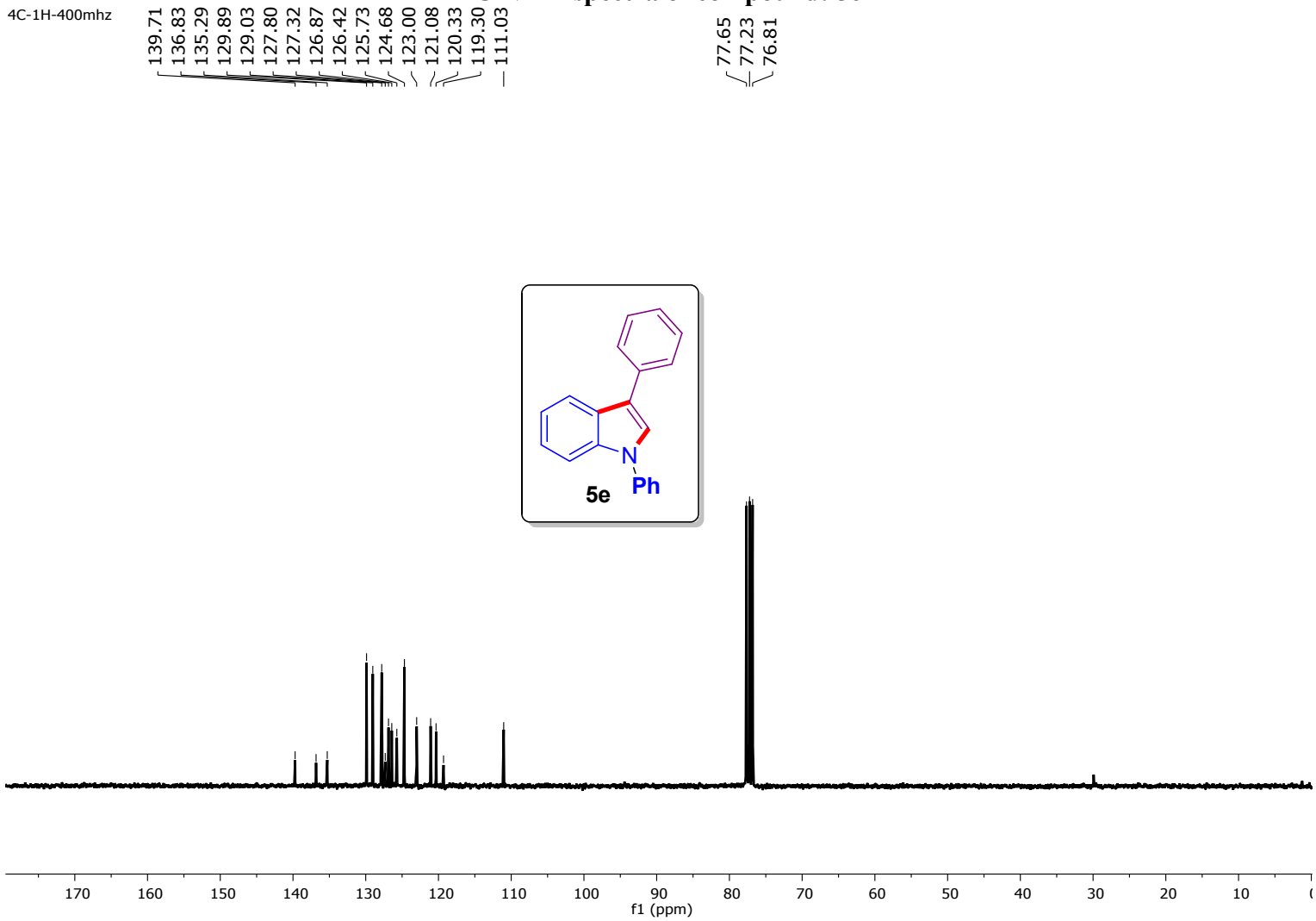
Sample Name	Unavailable	**Position**	Unavailable	**Instrument Name**	Unavailable	**User Name**	Unavailable
Inj Vol	Unavailable	**InjPosition**	Unavailable	**SampleType**	Unavailable	**IRM Calibration Status**	All Ions Missed
Data Filename	RK-CY-HX.d	**ACQ Method**		**Comment**	Sample information is unavailable	**Acquired Time**	Unavailable



^{1}H NMR spectra of compound: 5e

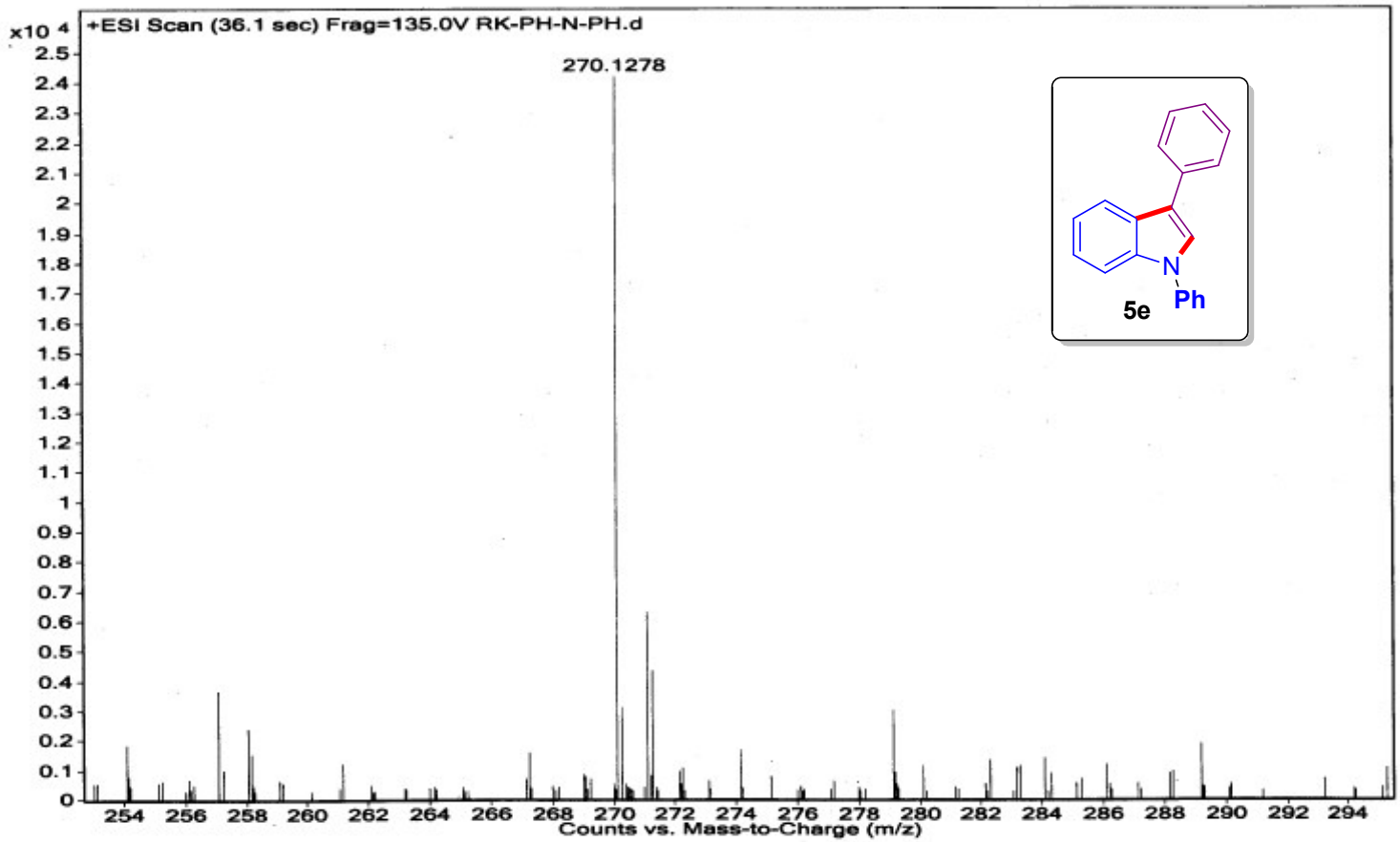


^{13}C NMR spectra of compound: 5e

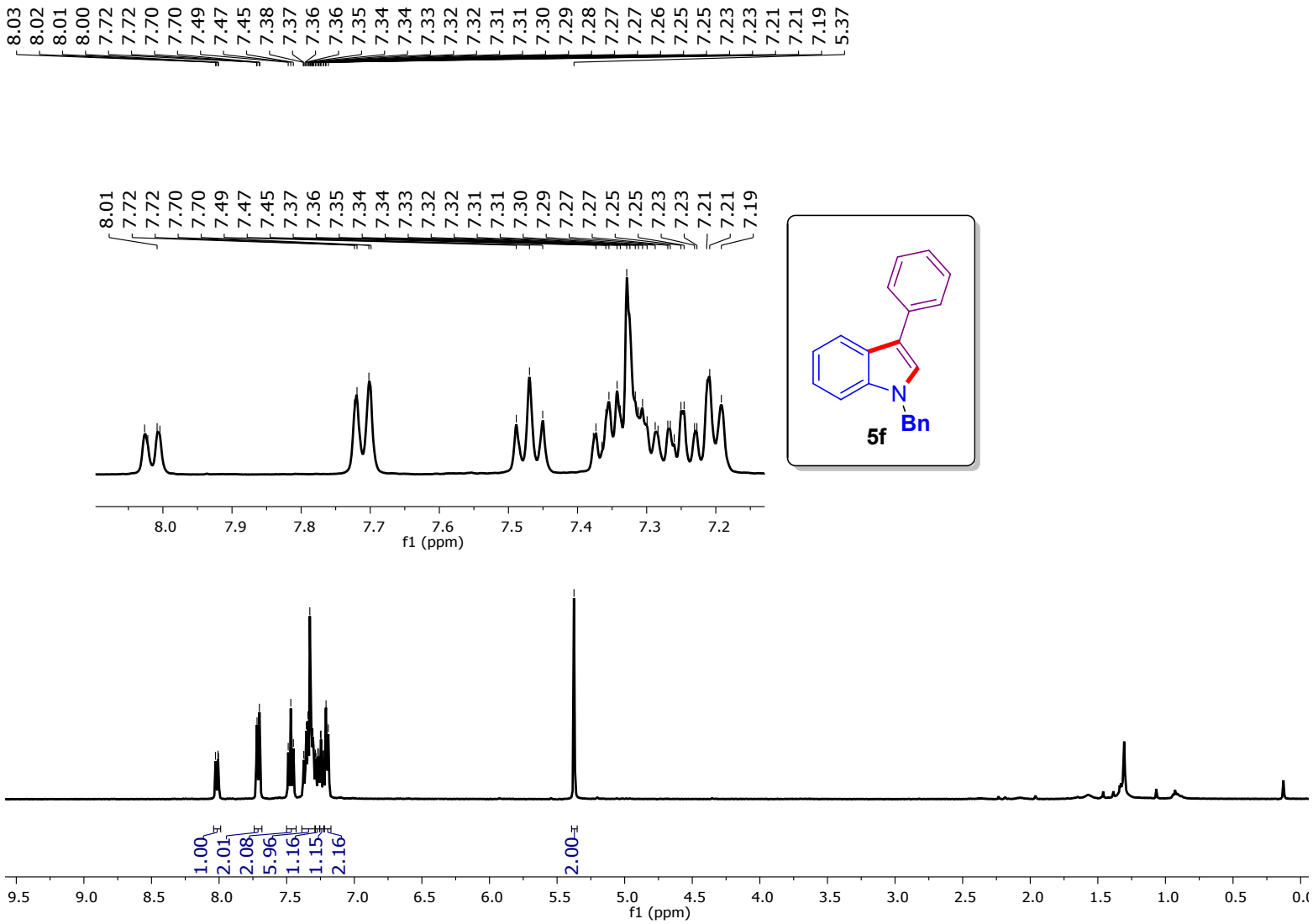


HRMS spectra of compound: 5e

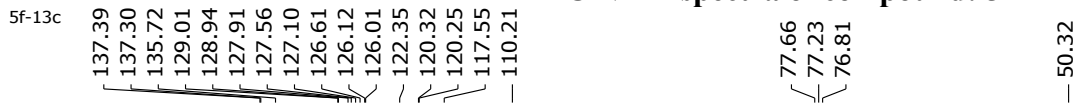
Sample Name	Unavailable	**Position**	Unavailable	**Instrument Name**	Unavailable	**User Name**	Unavailable
Inj Vol	Unavailable	**InjPosition**	Unavailable	**SampleType**	Unavailable	**IRM Calibration Status**	All Ions Missed
Data Filename	RK-PH-N-PH.d	**ACQ Method**		**Comment**	Sample information is unavailable	**Acquired Time**	Unavailable

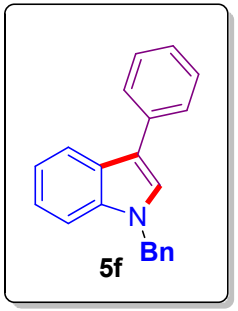


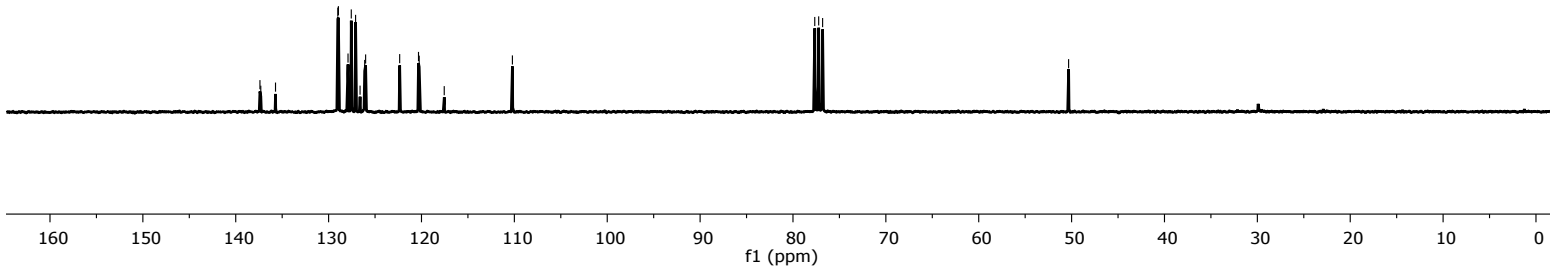
^{1}H NMR spectra of compound: 5f



^{13}C NMR spectra of compound: 5f

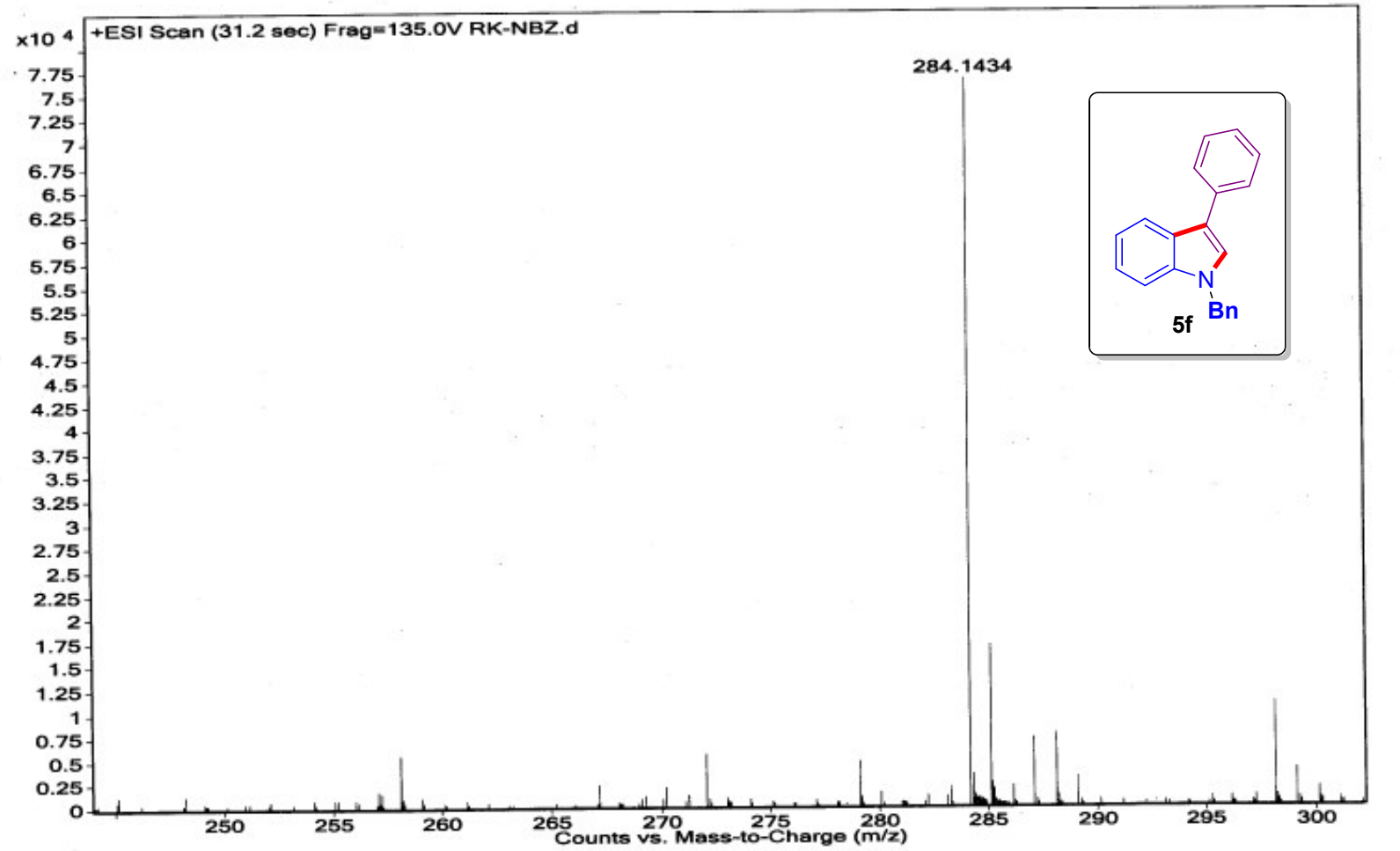




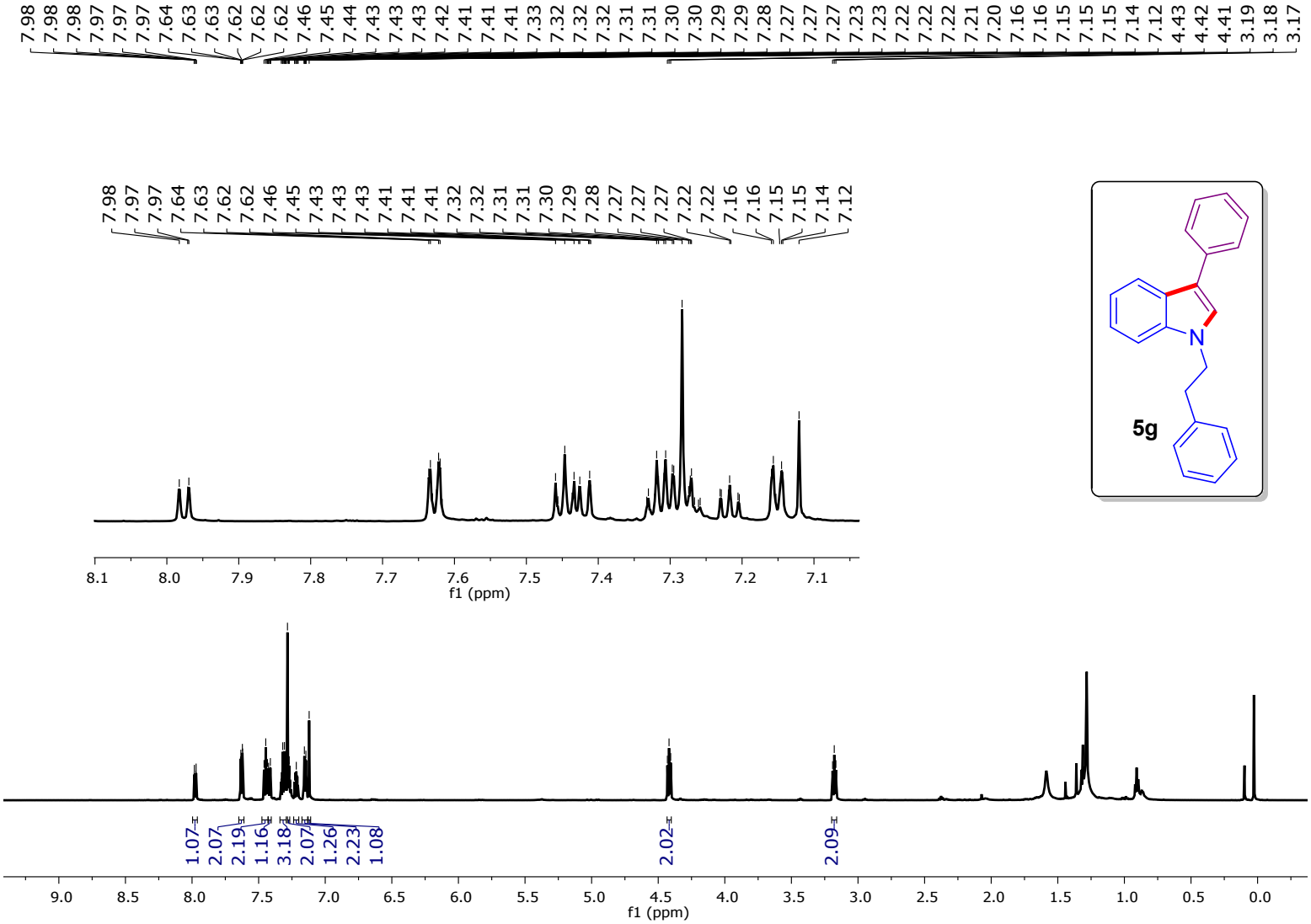


HRMS spectra of compound: 5f

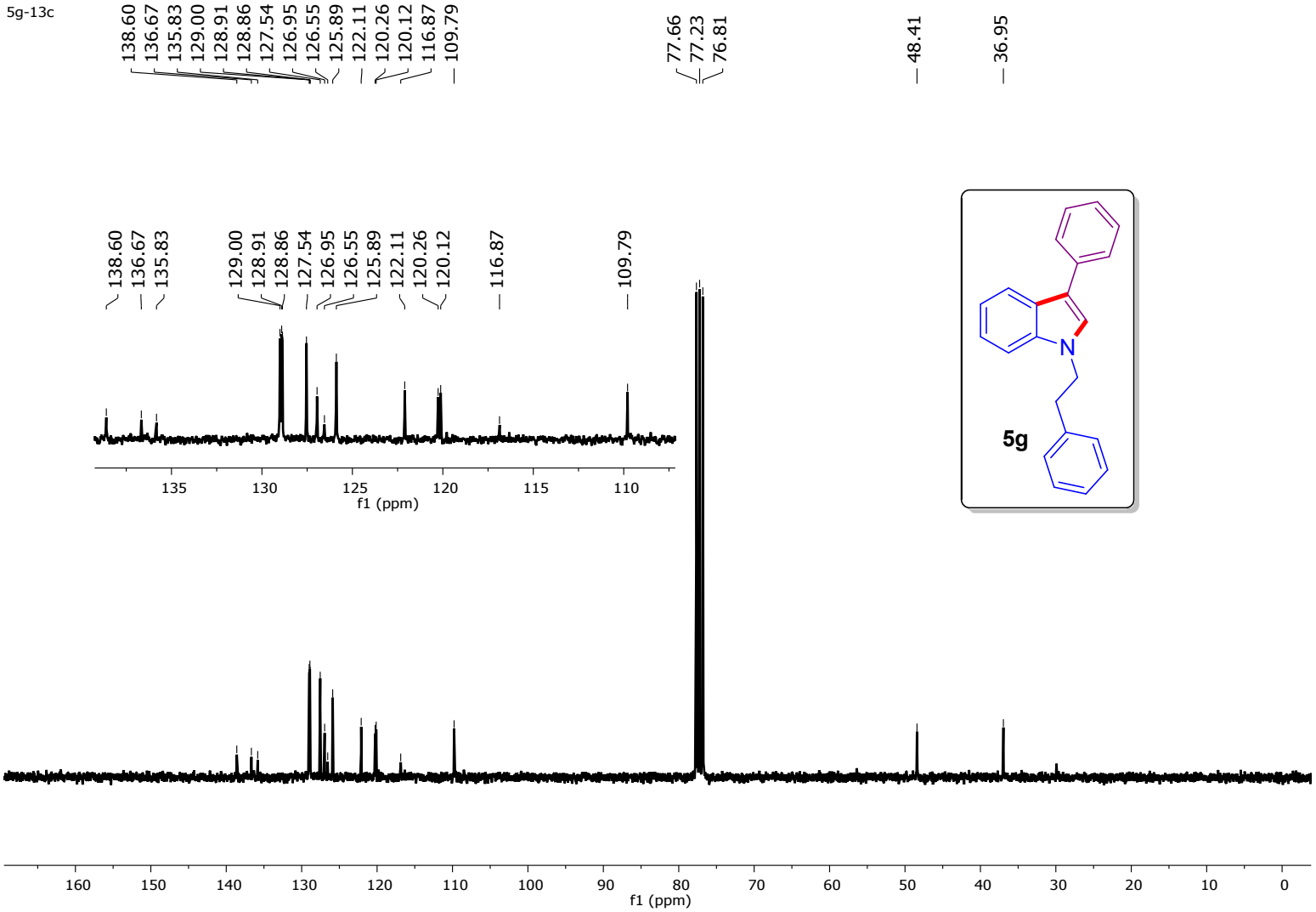
Sample Name	RK-NBZ	**Position**	Vial 1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	0	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	All Ions Missed
Data Filename	RK-NBZ.d	**ACQ Method**		**Comment**		**Acquired Time**	8/9/2017 10:49:38 AM



^{1}H NMR spectra of compound: 5g

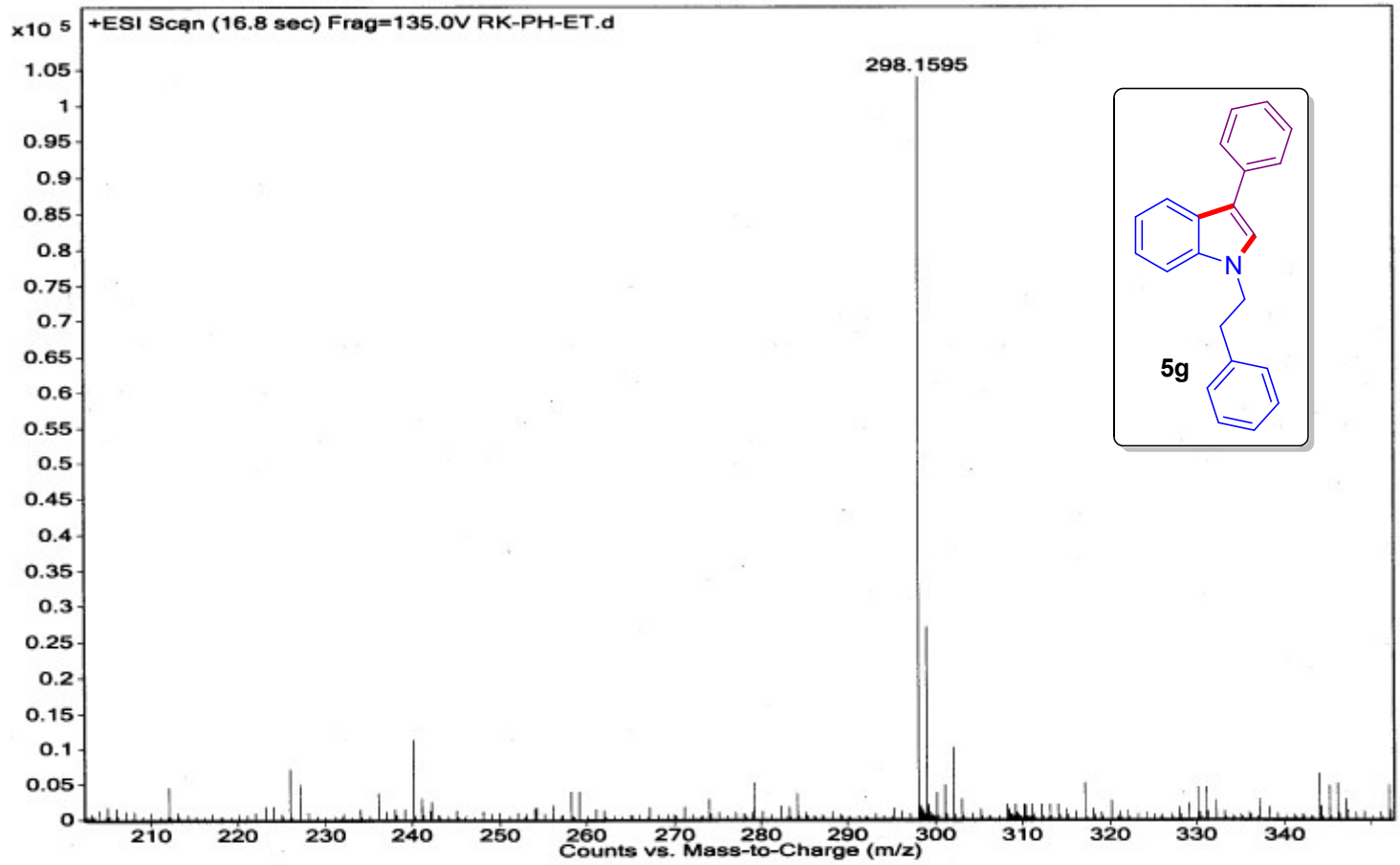


^{13}C NMR spectra of compound: 5g

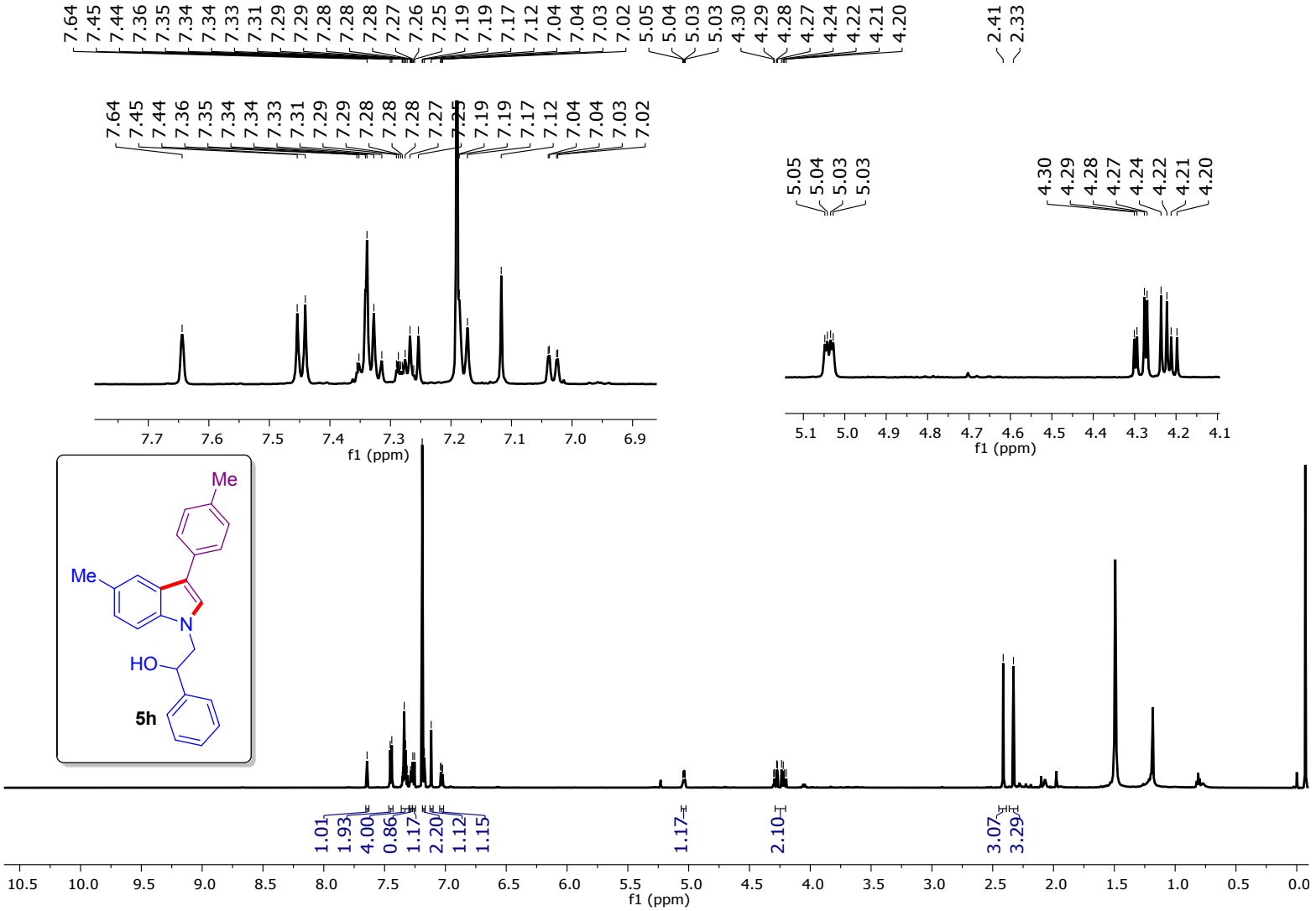


HRMS spectra of compound: 5g

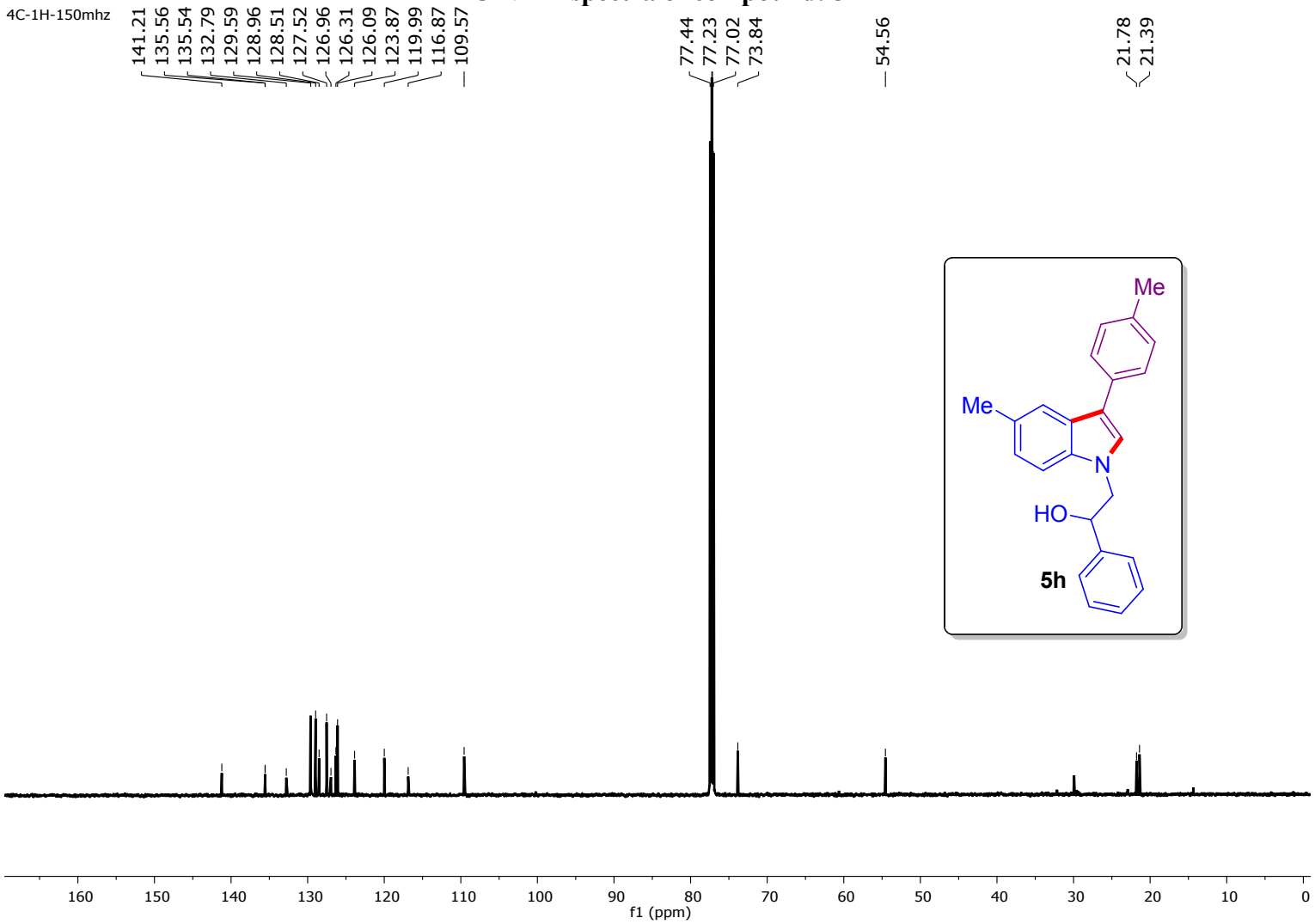
Sample Name	Unavailable	**Position**	Unavailable	**Instrument Name**	Unavailable	**User Name**	Unavailable
Inj Vol	Unavailable	**InjPosition**	Unavailable	**SampleType**	Unavailable	**IRM Calibration Status**	All Ions Missed
Data Filename	RK-PH-ET.d	**ACQ Method**		**Comment**	Sample information is unavailable	**Acquired Time**	Unavailable



^{1}H NMR spectra of compound: 5h

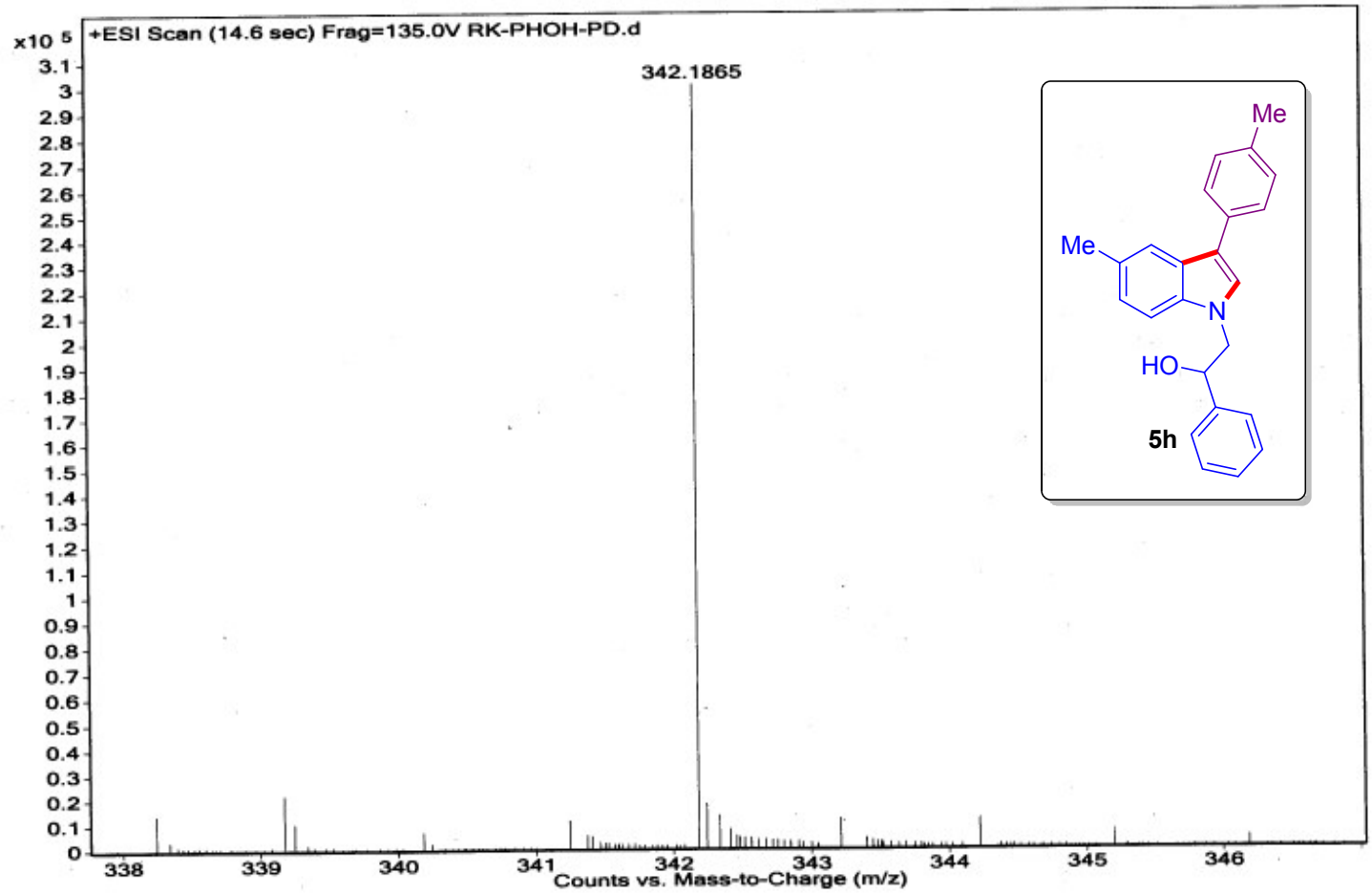


^{13}C NMR spectra of compound: 5h

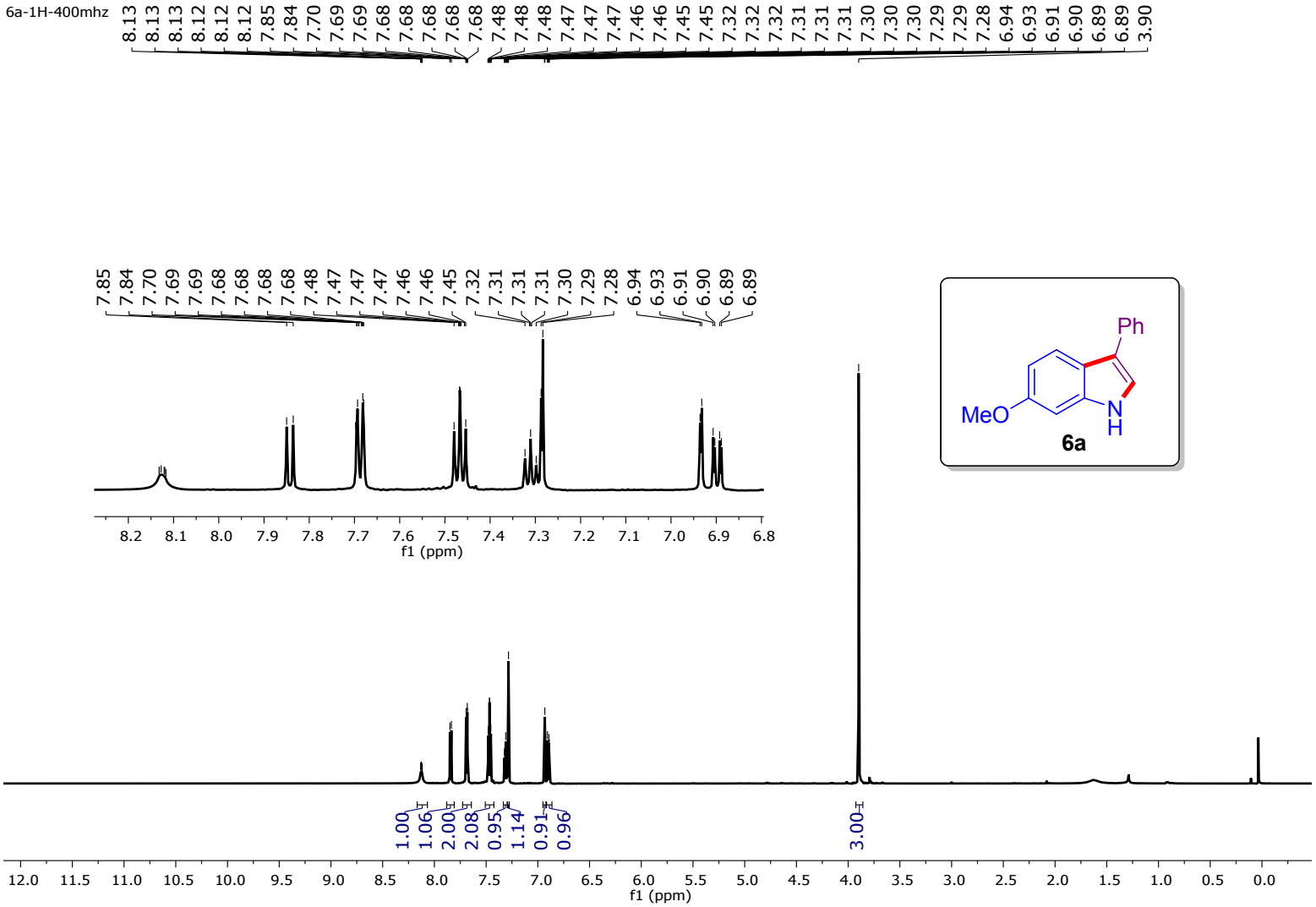


HRMS spectra of compound: 5h

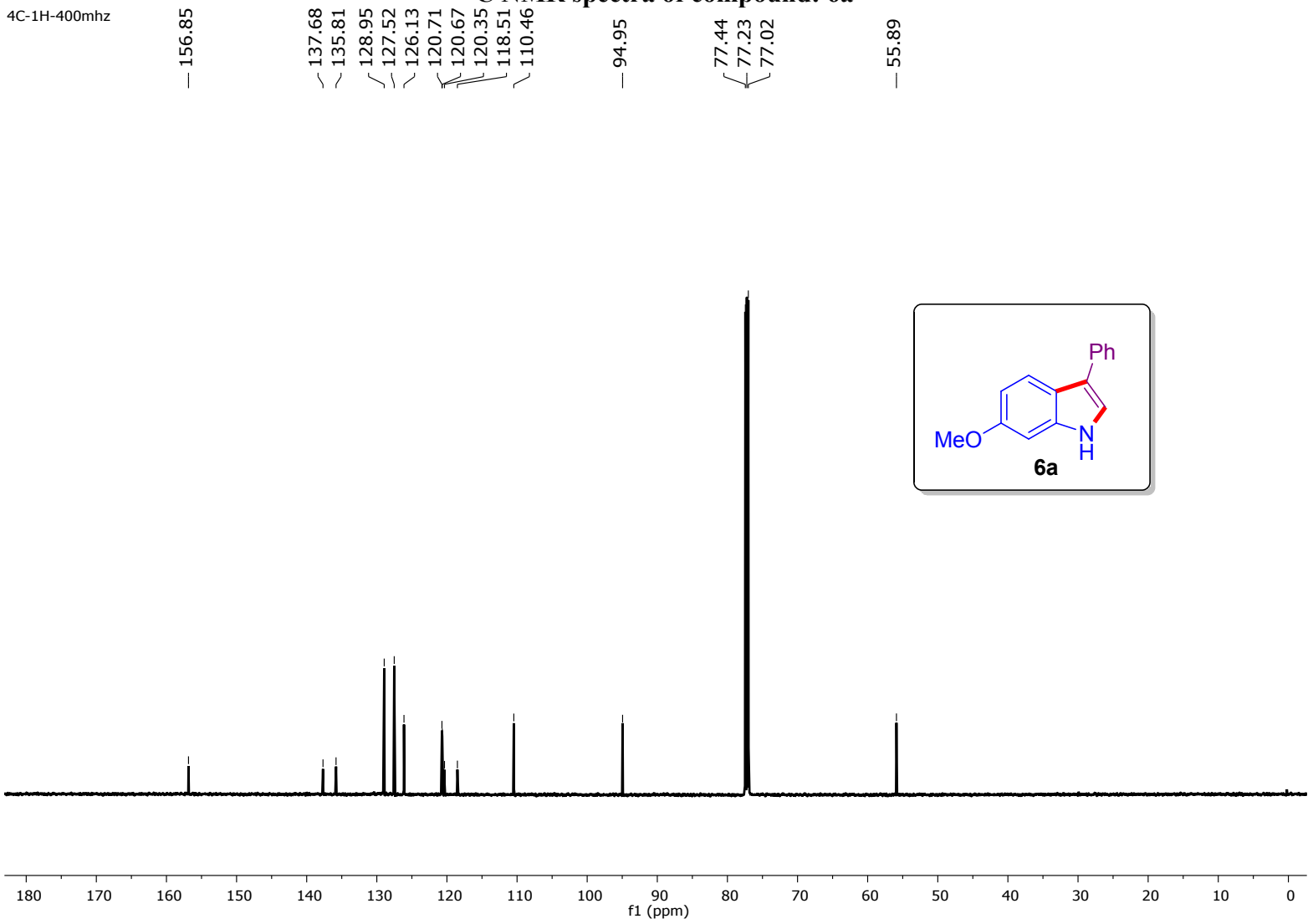
Sample Name	Unavailable	**Position**	Unavailable	**Instrument Name**	Unavailable	**User Name**	Unavailable
Inj Vol	Unavailable	**InjPosition**	Unavailable	**SampleType**	Unavailable	**IRM Calibration Status**	All Ions Missed
Data Filename	RK-PHOH-PD.d	**ACQ Method**		**Comment**	Sample information is unavailable	**Acquired Time**	Unavailable



^{1}H NMR spectra of compound: 6a

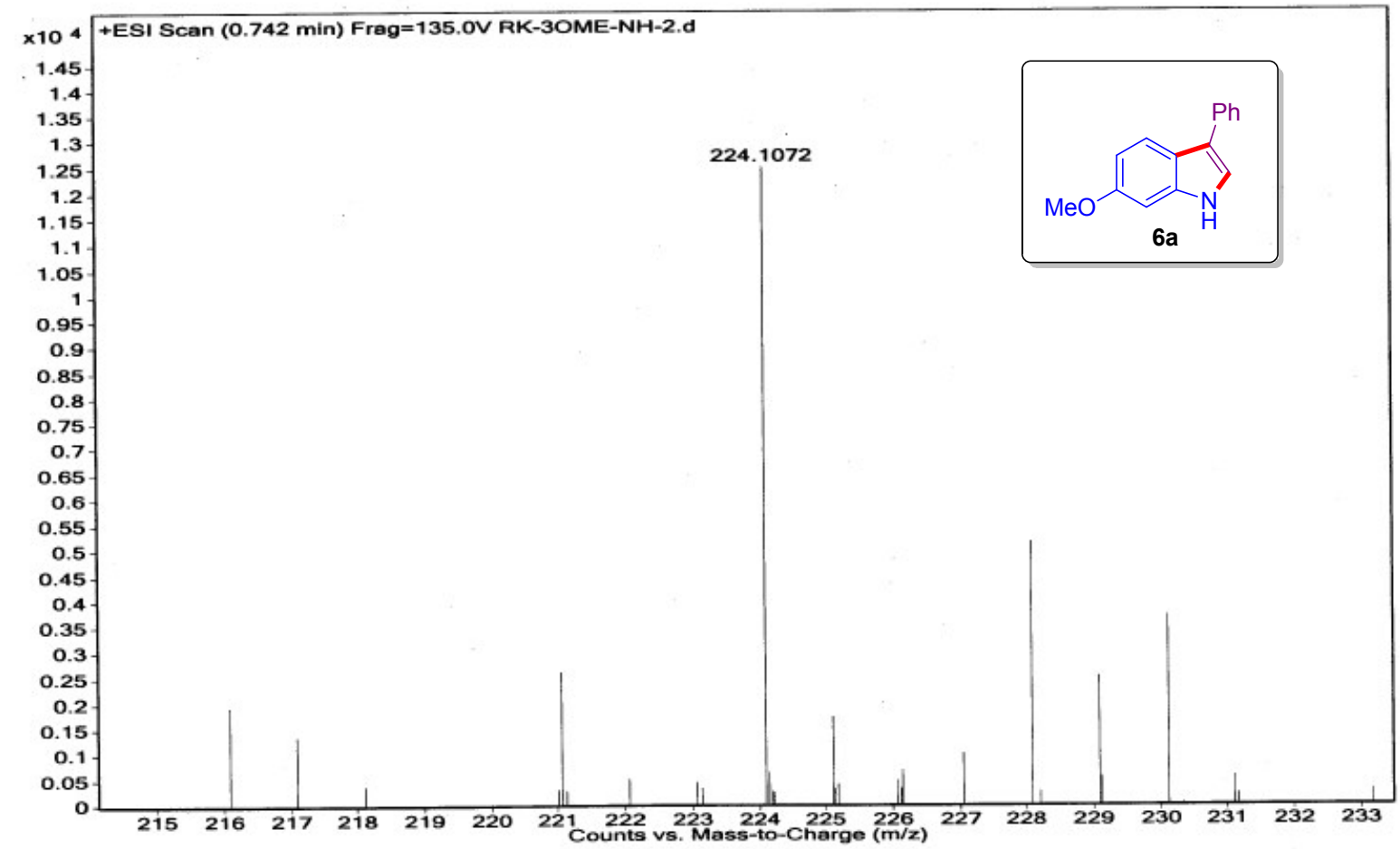


^{13}C NMR spectra of compound: 6a

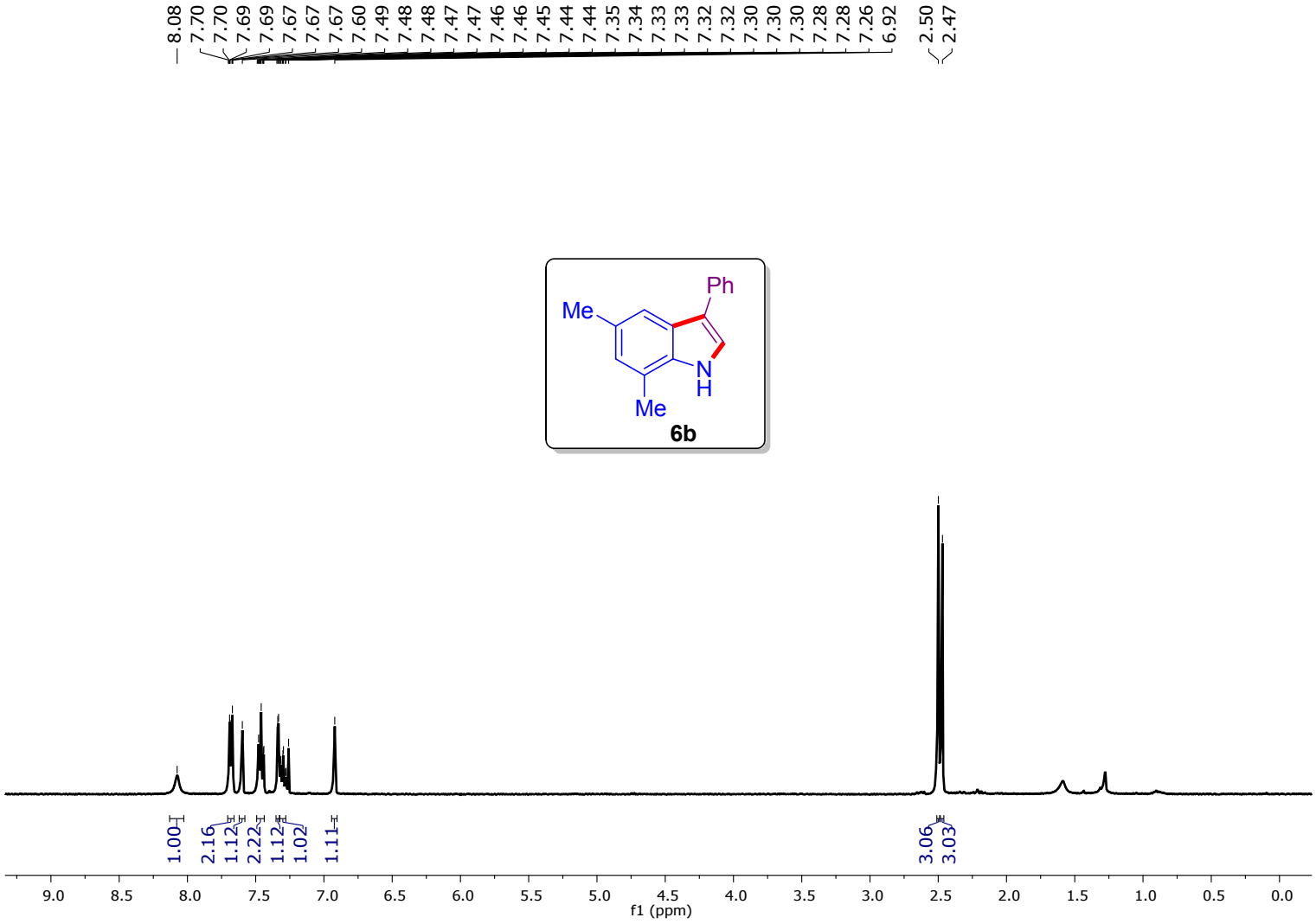


HRMS spectra of compound: 6a

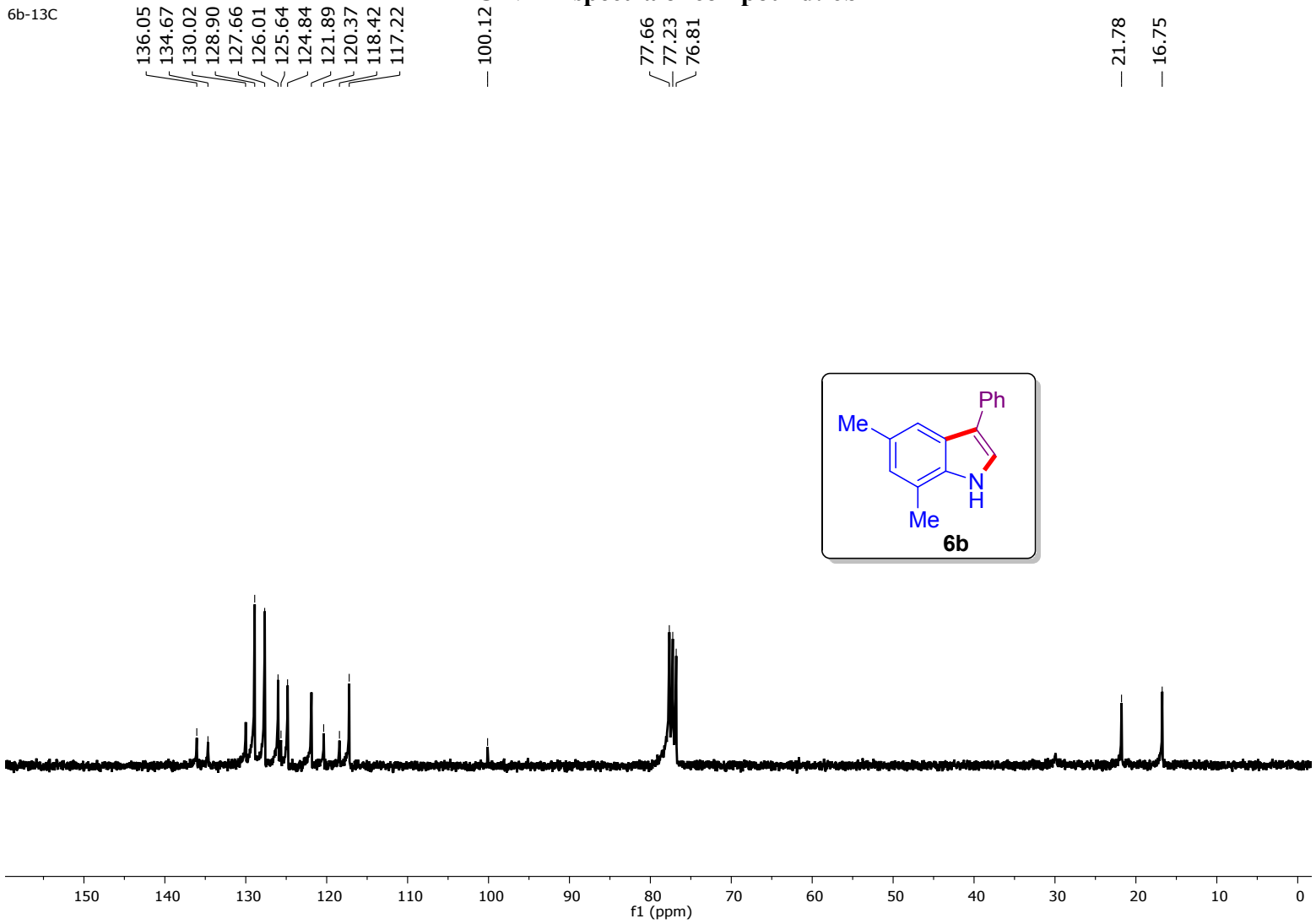
Sample Name	RK-3OME-NH-2	**Position**	Vial 1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	RK-3OME-NH-2.d	**ACQ Method**		**Comment**		**Acquired Time**	12/1/2017 6:22:39 PM



^{1}H NMR spectra of compound: 6b

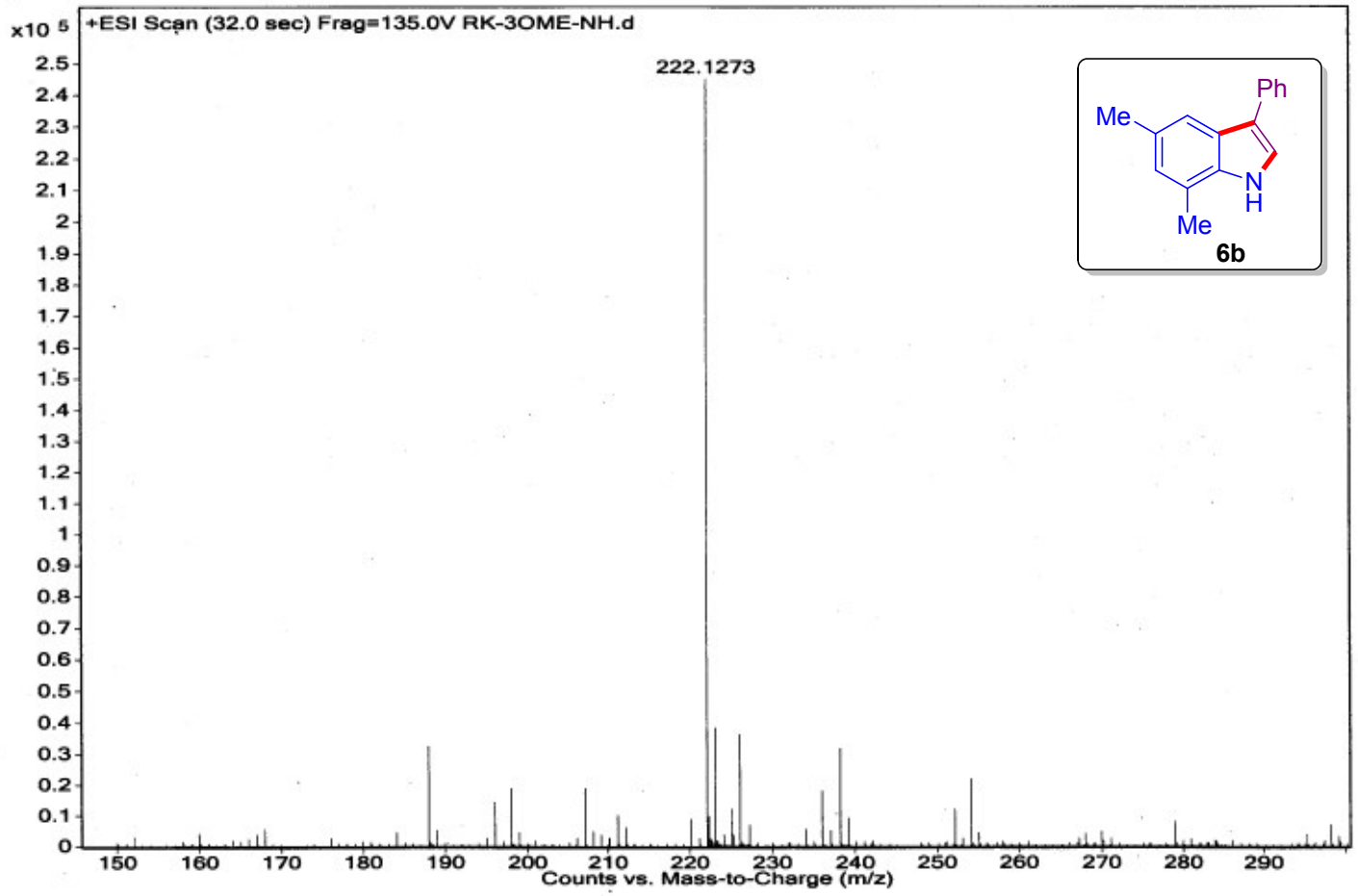


^{13}C NMR spectra of compound: 6b

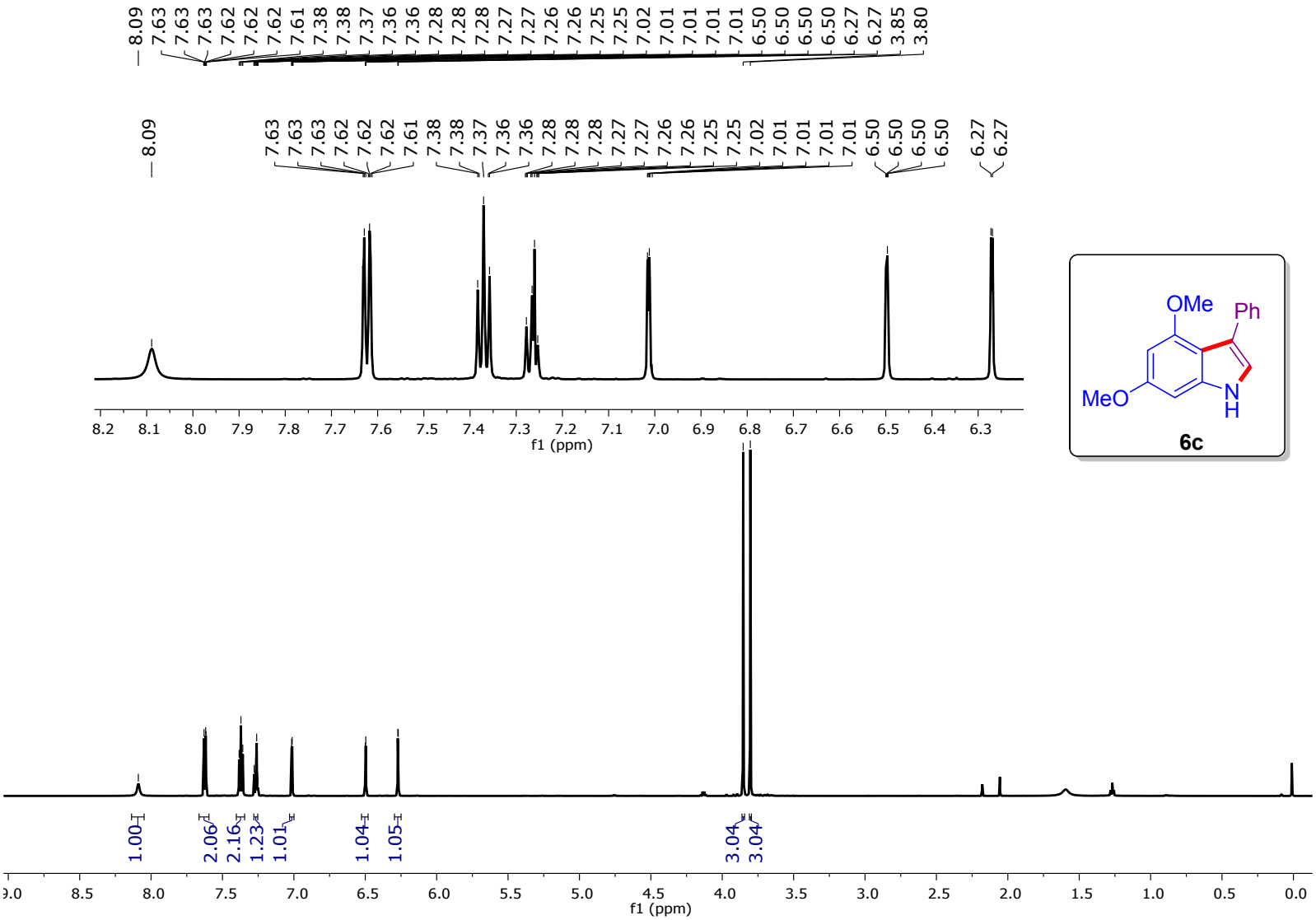


HRMS spectra of compound: 6b

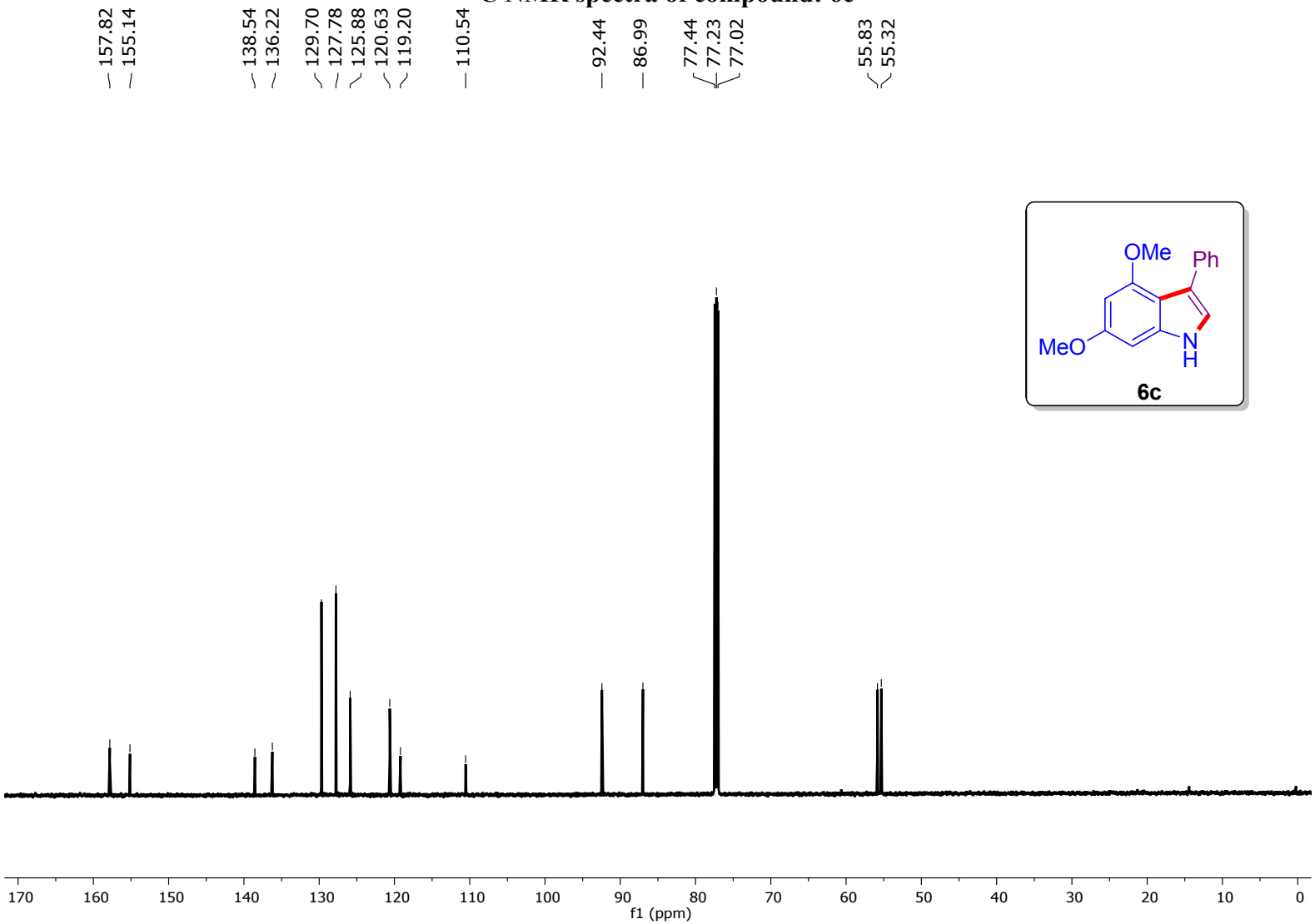
Sample Name	Unavailable	**Position**	Unavailable	**Instrument Name**	Unavailable	**User Name**	Unavailable
Inj Vol	Unavailable	**InjPosition**	Unavailable	**SampleType**	Unavailable	**IRM Calibration Status**	All Ions Missed
Data Filename	RK-3OME-NH.d	**ACQ Method**		**Comment**	Sample information is unavailable	**Acquired Time**	Unavailable



^{1}H NMR spectra of compound: 6c

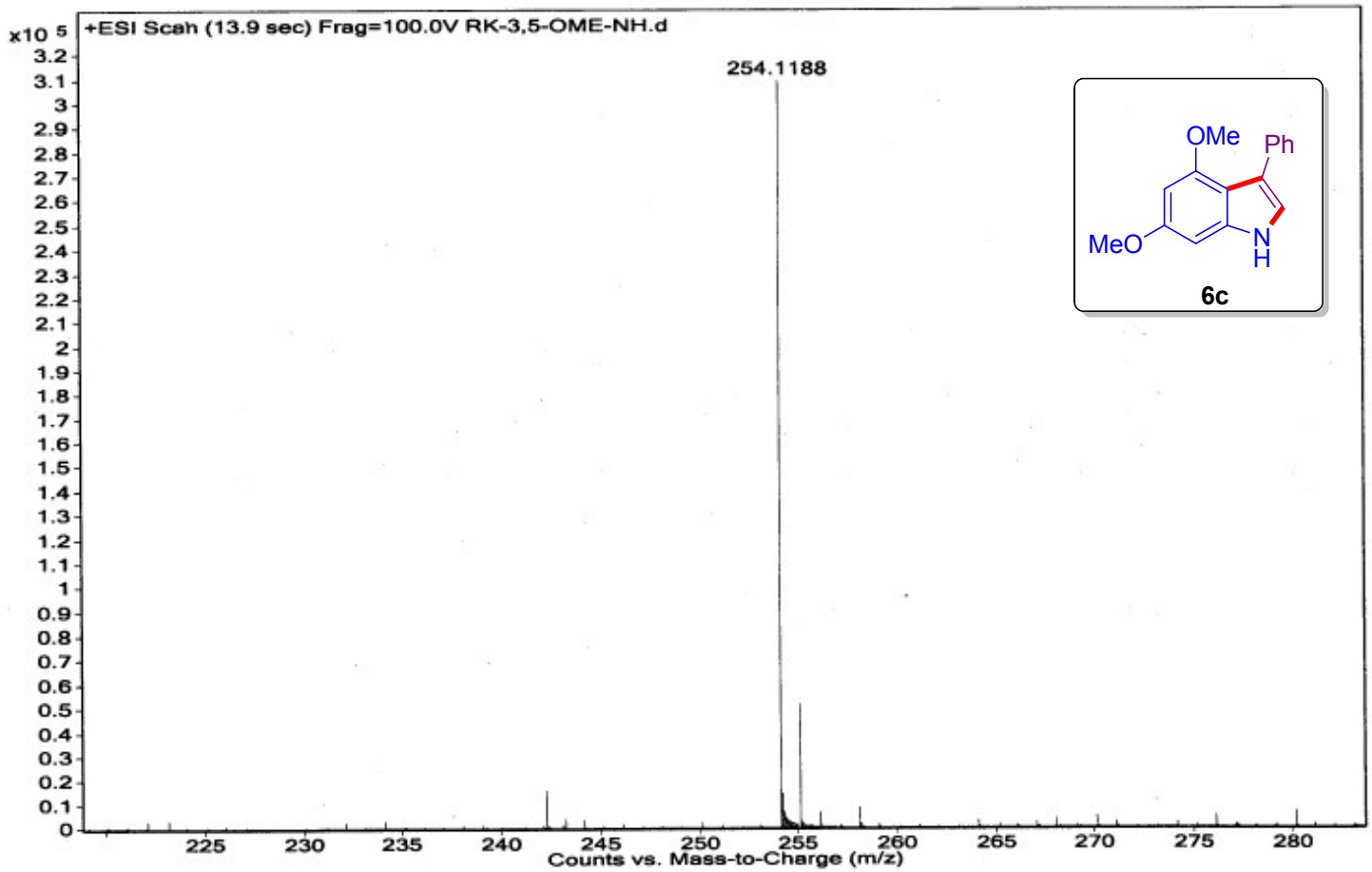


^{13}C NMR spectra of compound: 6c

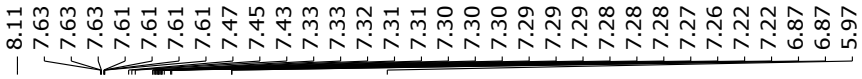


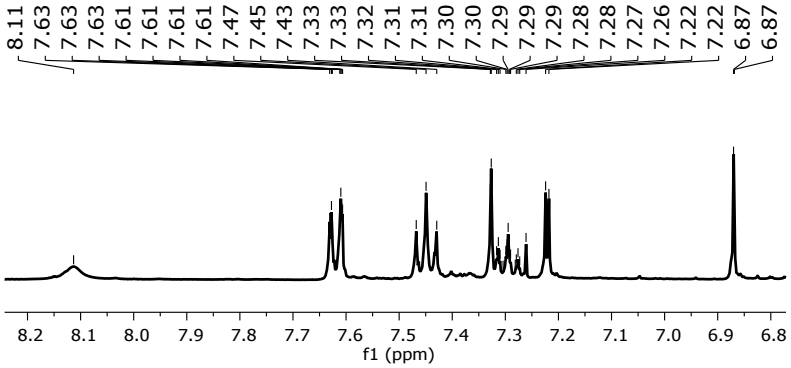
HRMS spectra of compound: 6c

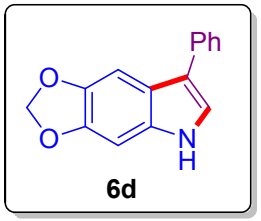
Sample Name	Unavailable	**Position**	Unavailable	**Instrument Name**	Unavailable	**User Name**	Unavailable
Inj Vol	Unavailable	**InjPosition**	Unavailable	**SampleType**	Unavailable	**IRM Calibration Status**	All Ions Missed
Data Filename	RK-3,5-OME-NH.d	**ACQ Method**		**Comment**	Sample information is unavailable	**Acquired Time**	Unavailable

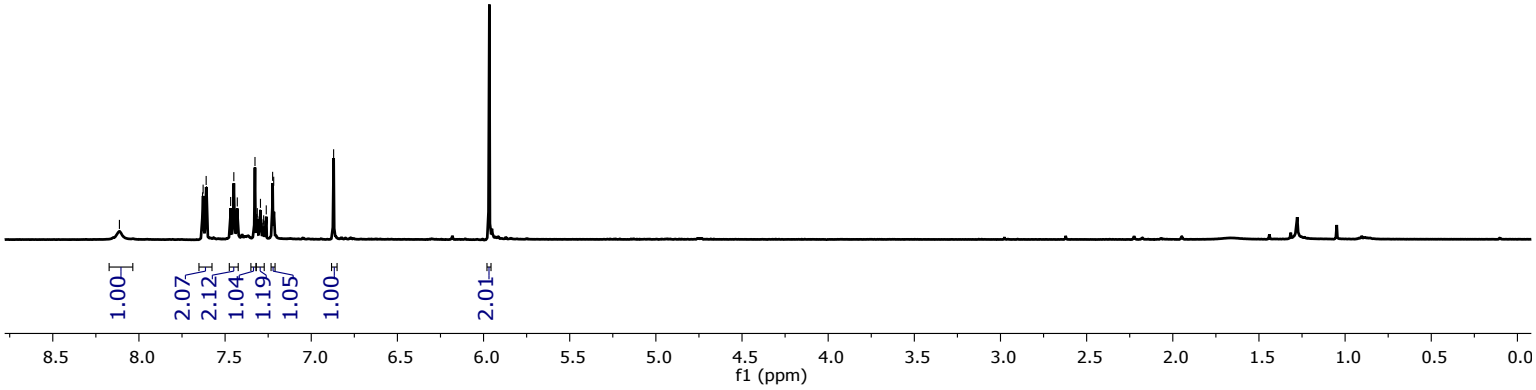


^{1}H NMR spectra of compound: 6d

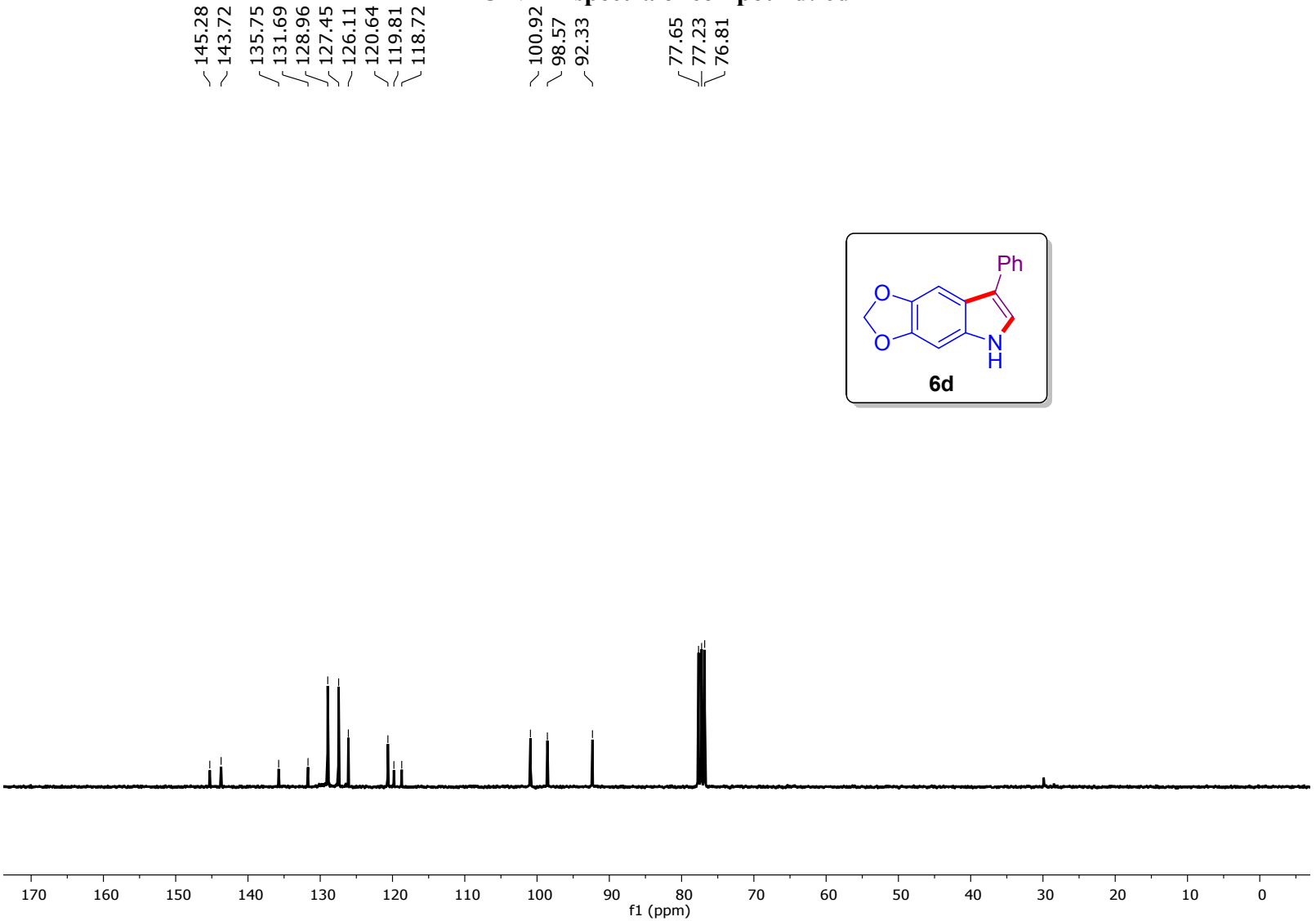






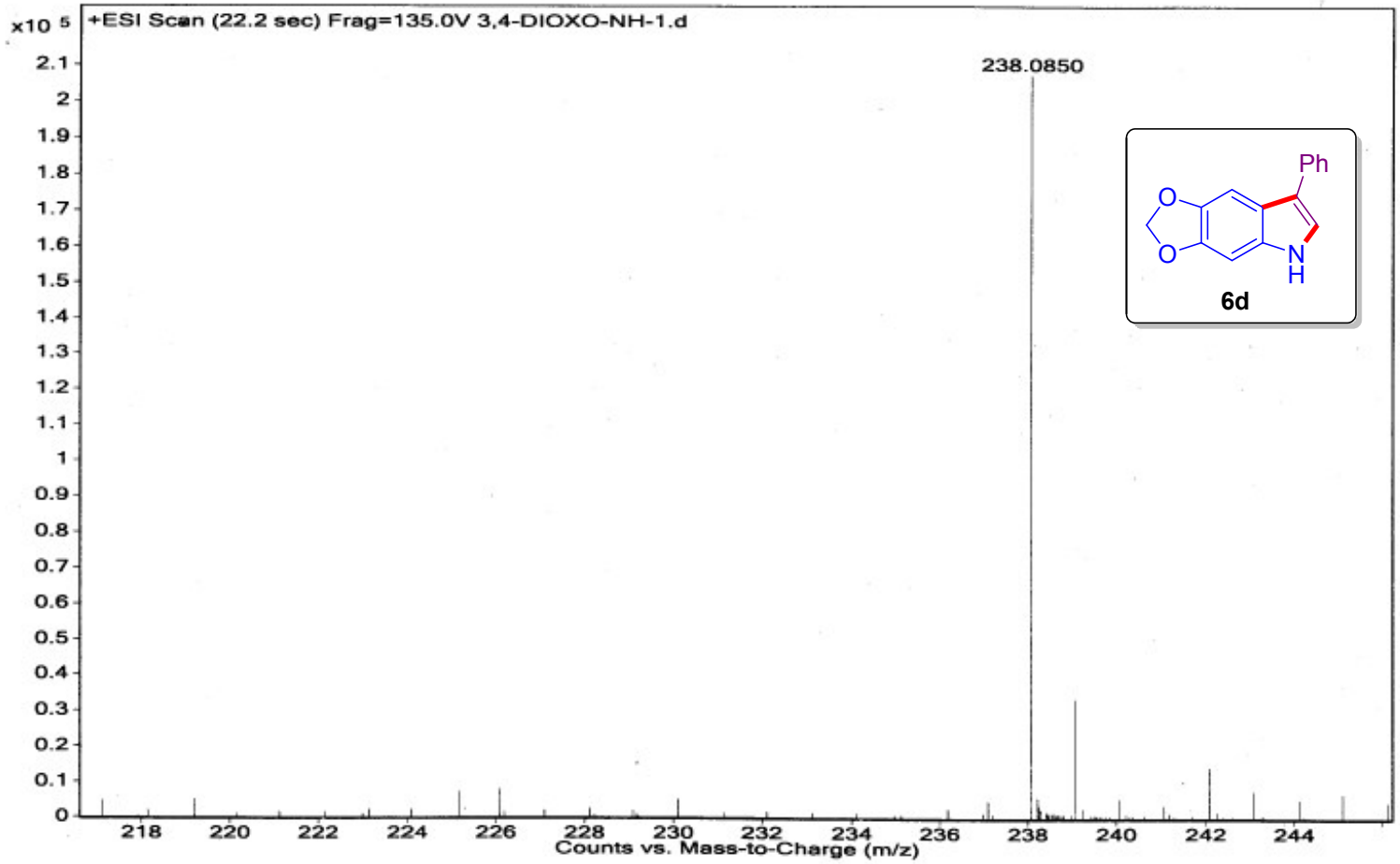


^{13}C NMR spectra of compound: 6d

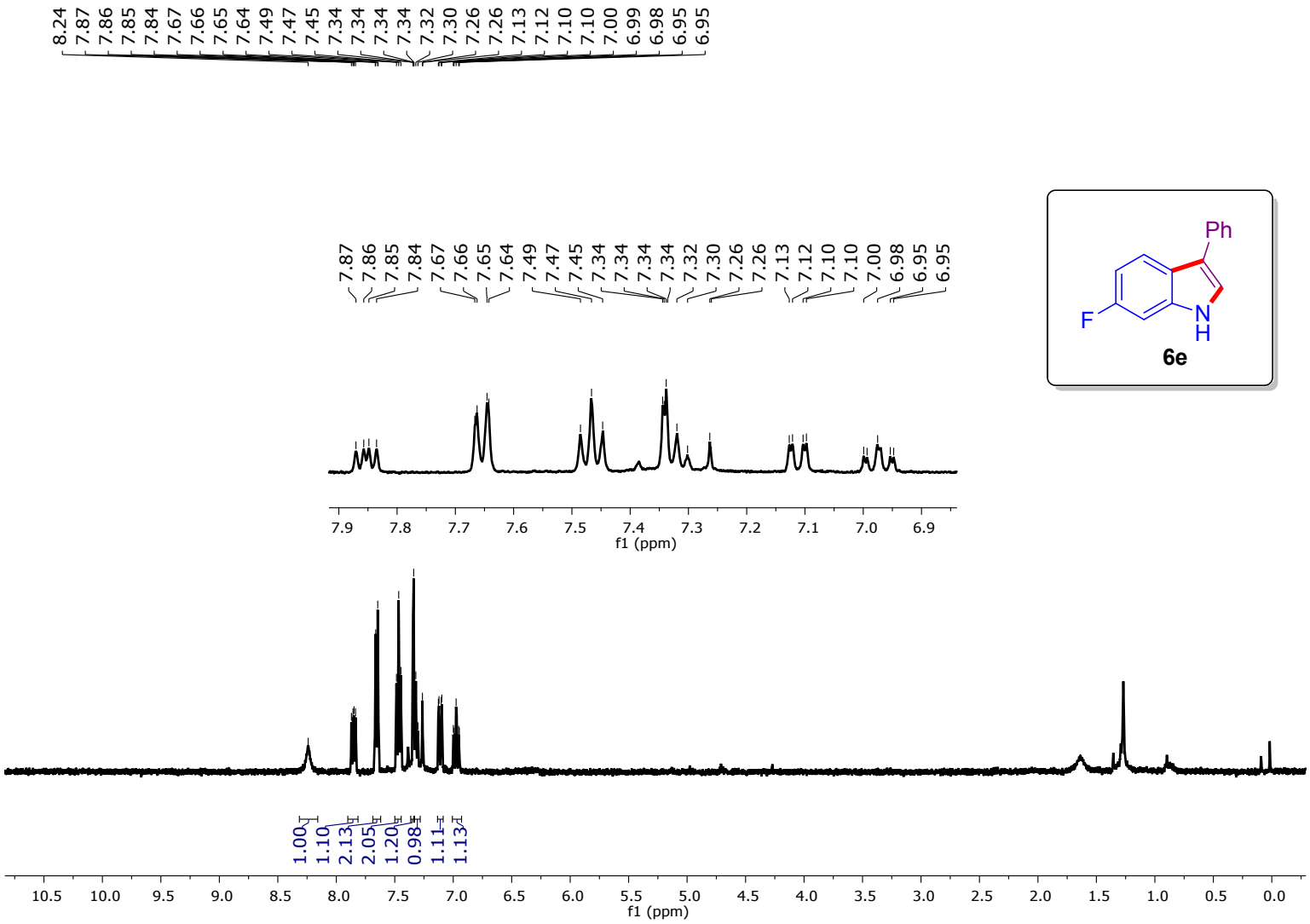


HRMS spectra of compound: 6d

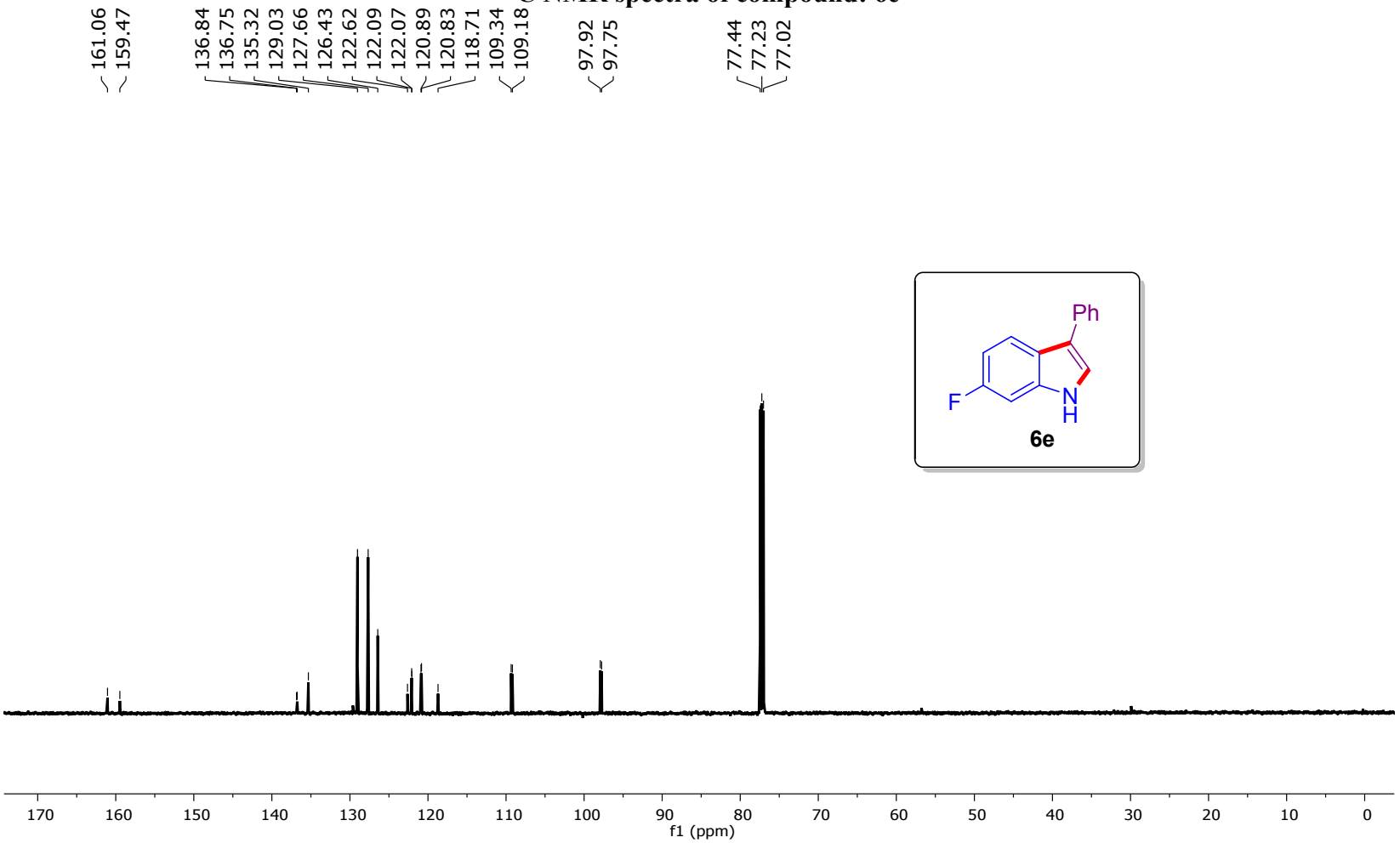
Sample Name	Unavailable	**Position**	Unavailable	**Instrument Name**	Unavailable	**User Name**	Unavailable
Inj Vol	Unavailable	**InjPosition**	Unavailable	**SampleType**	Unavailable	**IRM Calibration Status**	Some Ions Missed
Data Filename	3,4-DIOXO-NH-1.d	**ACQ Method**		**Comment**	Sample Information is unavailable	**Acquired Time**	Unavailable



^{1}H NMR spectra of compound: 6e

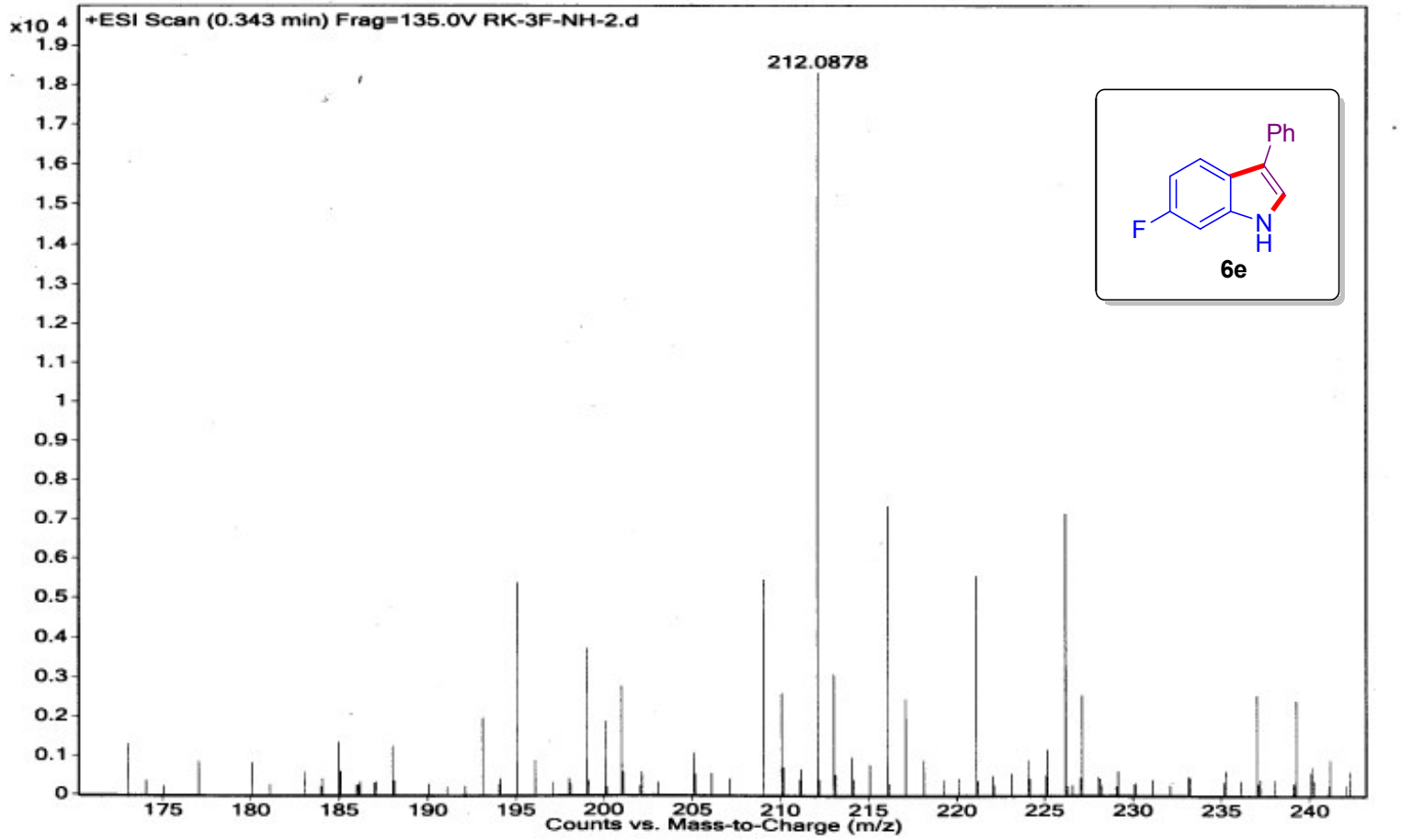


^{13}C NMR spectra of compound: 6e

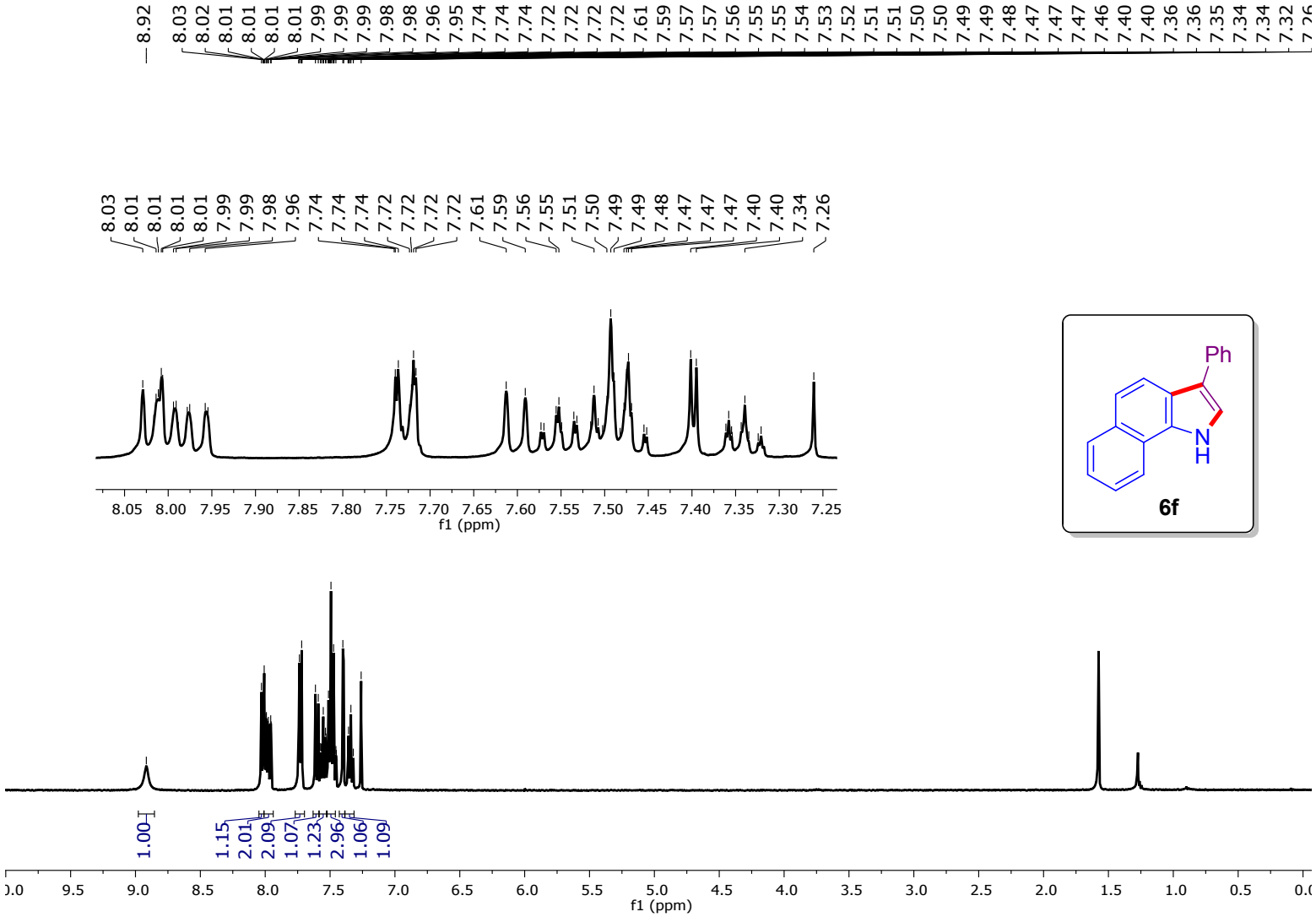


HRMS spectra of compound: 6e

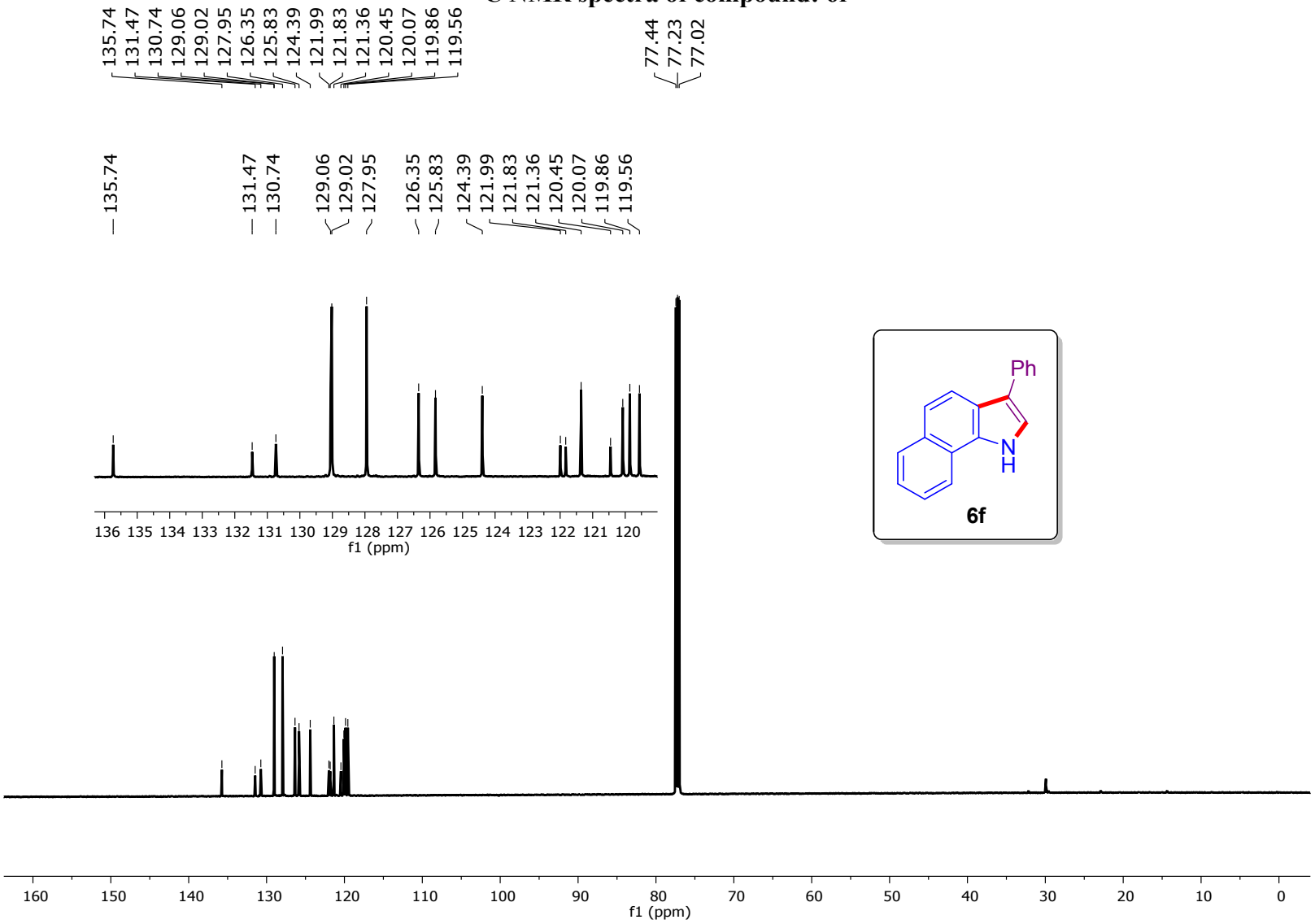
Sample Name	RK-3F-NH-2	**Position**	Vial 1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	RK-3F-NH-2.d	**ACQ Method**		**Comment**		**Acquired Time**	12/1/2017 6:20:30 PM



^{1}H NMR spectra of compound: 6f

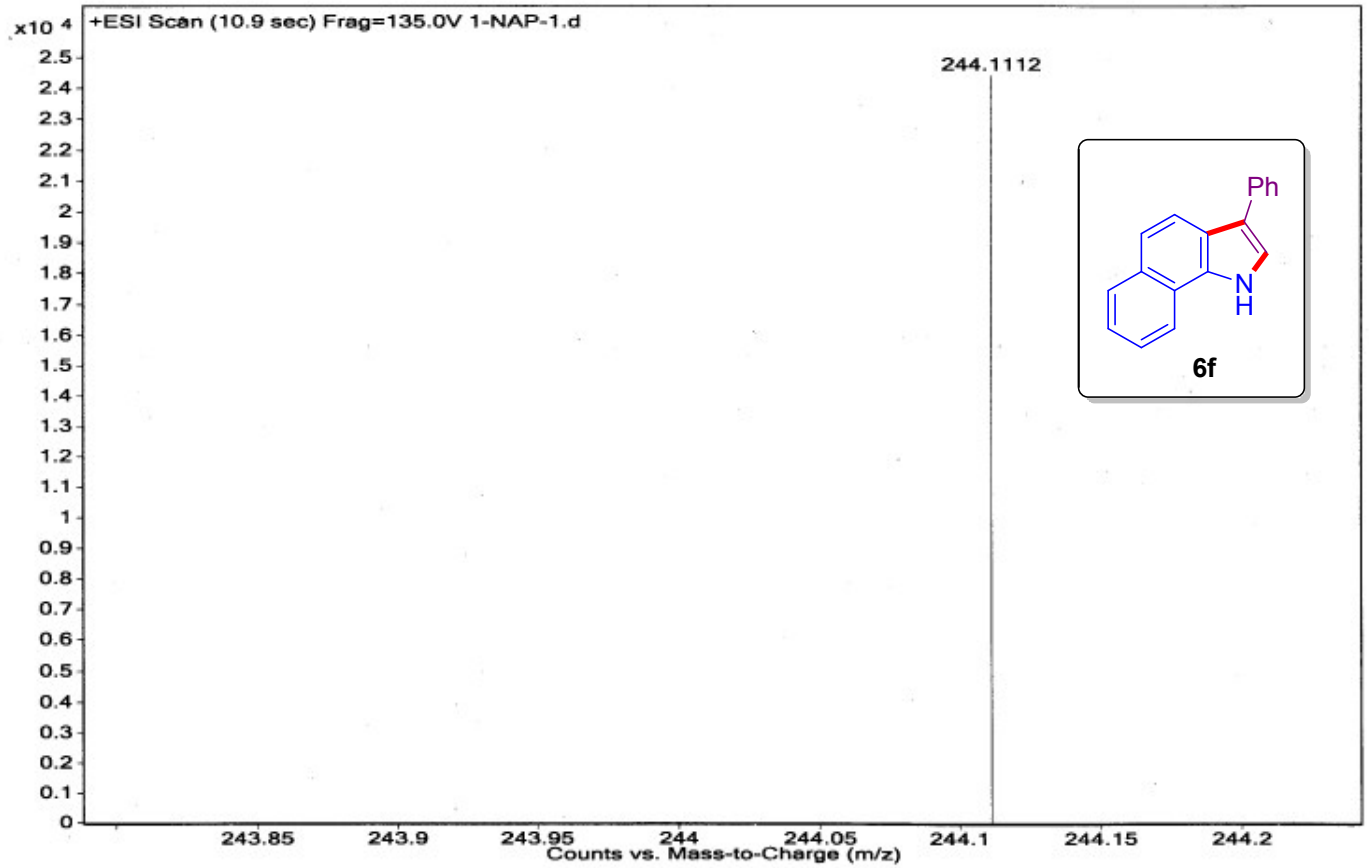


^{13}C NMR spectra of compound: 6f

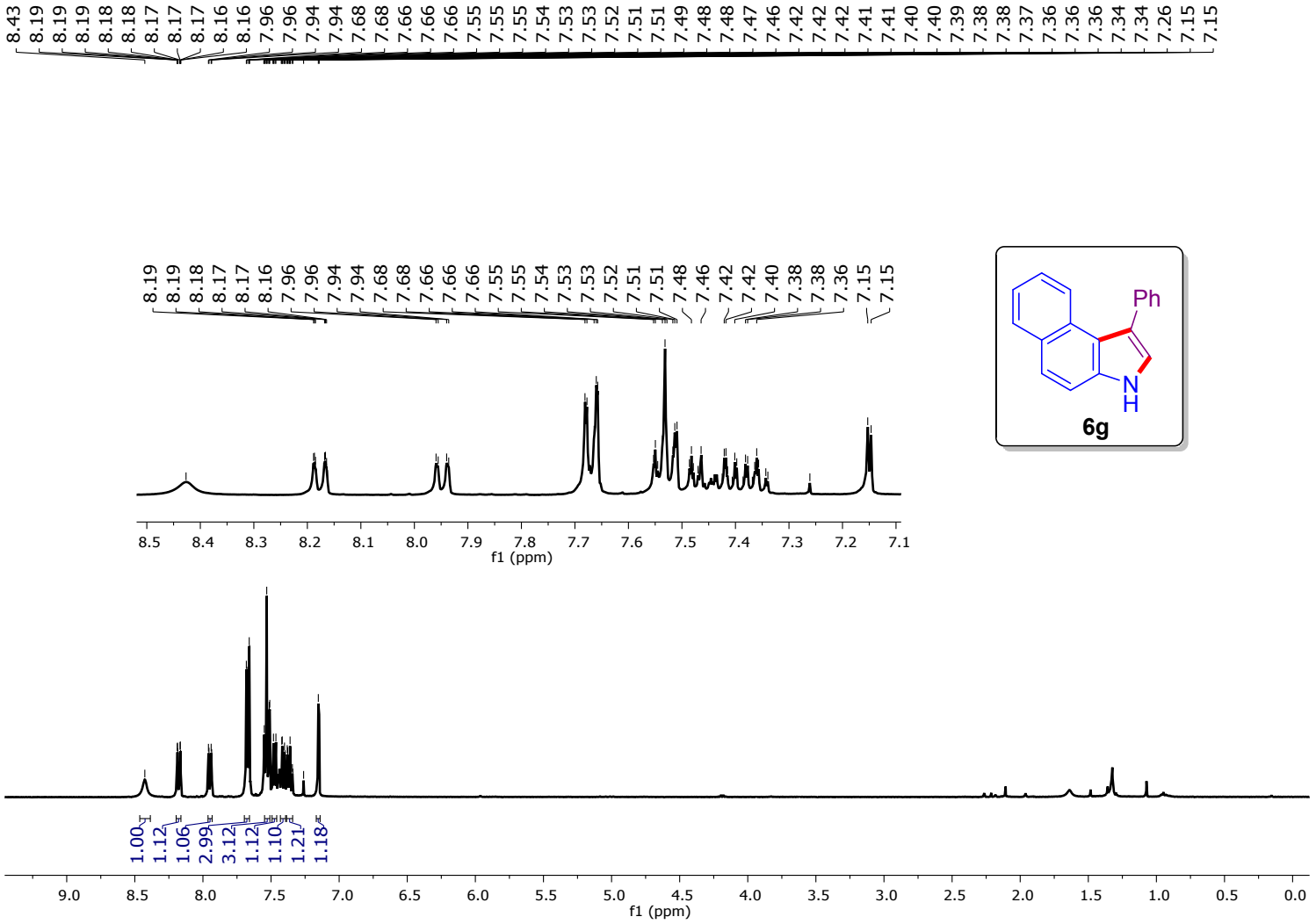


HRMS spectra of compound: 6f

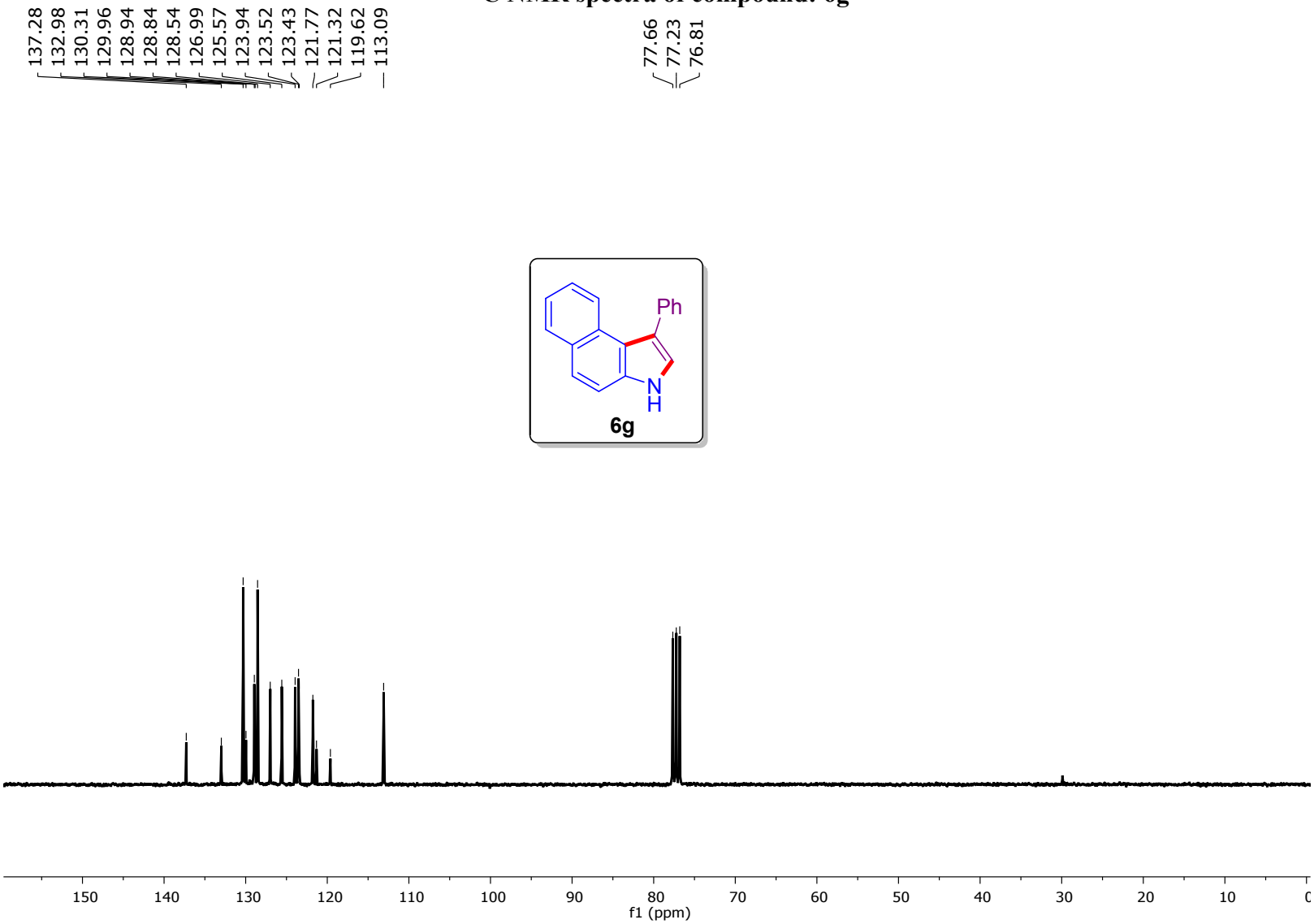
Sample Name	Unavailable	**Position**	Unavailable	**Instrument Name**	Unavailable	**User Name**	Unavailable
Inj Vol	Unavailable	**InjPosition**	Unavailable	**SampleType**	Unavailable	**IRM Calibration Status**	Some Ions Missed
Data Filename	1-NAP-1.d	**ACQ Method**		**Comment**	Sample information is unavailable	**Acquired Time**	Unavailable



^{1}H NMR spectra of compound: 6g

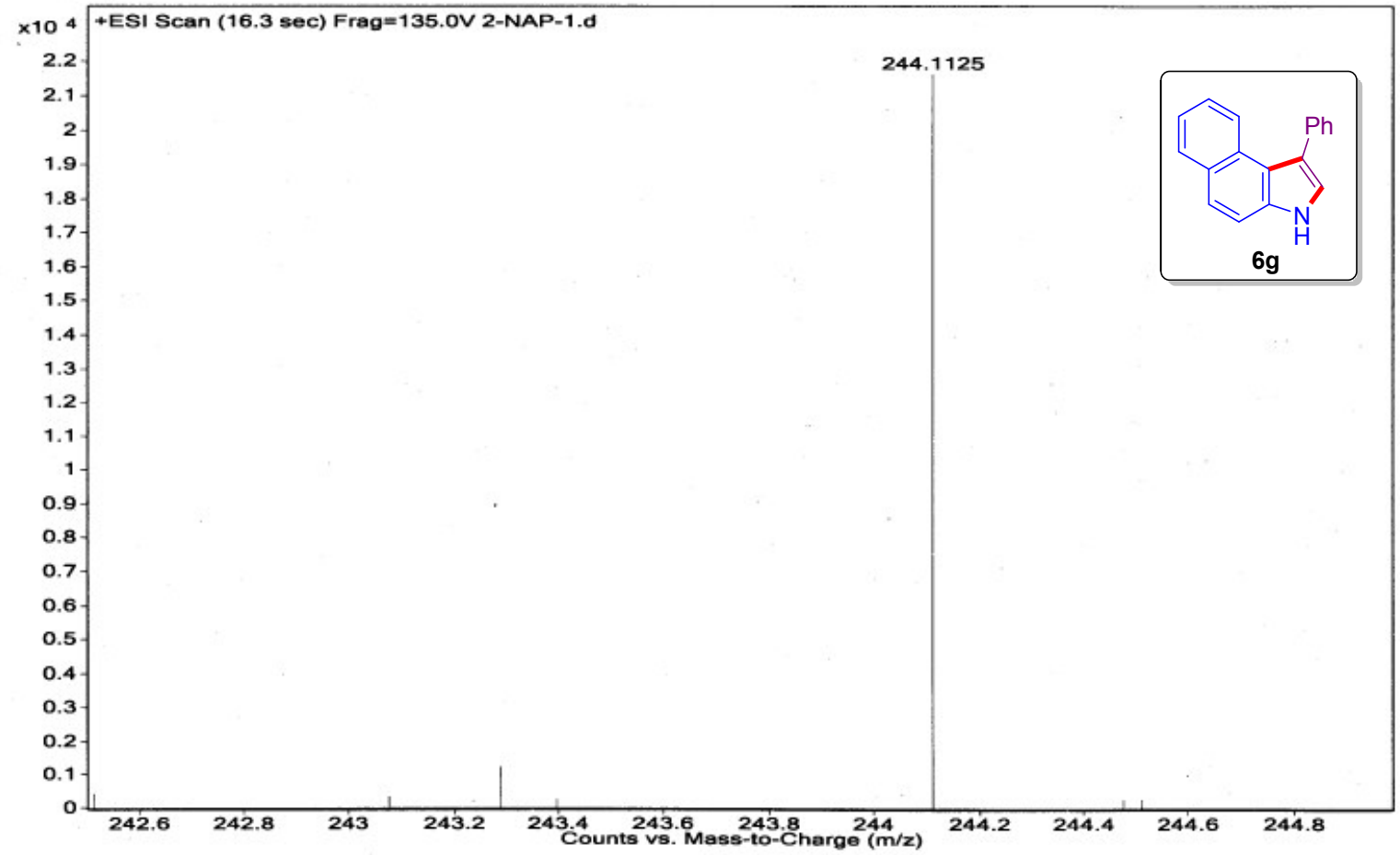


^{13}C NMR spectra of compound: 6g

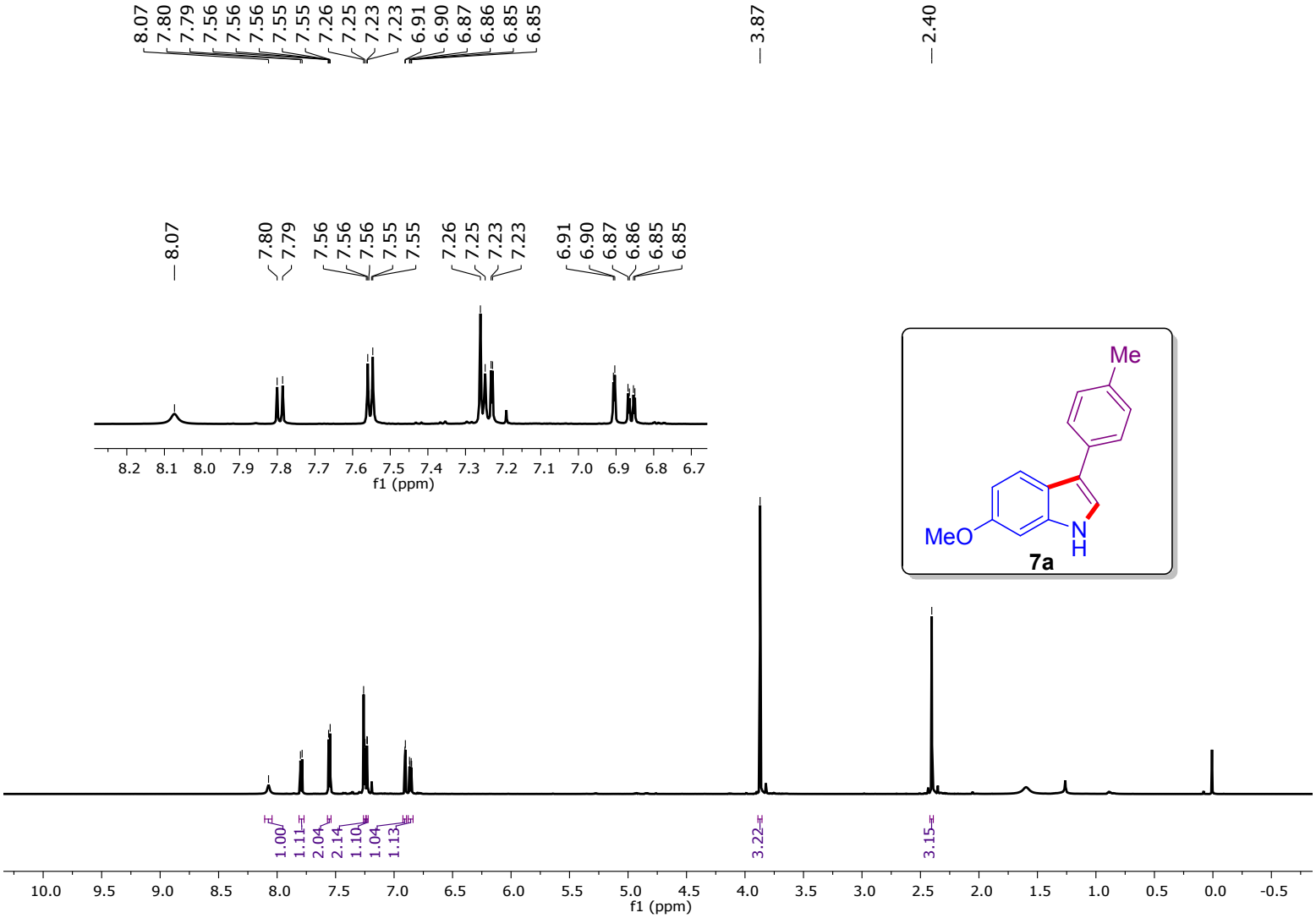


HRMS spectra of compound: 6g

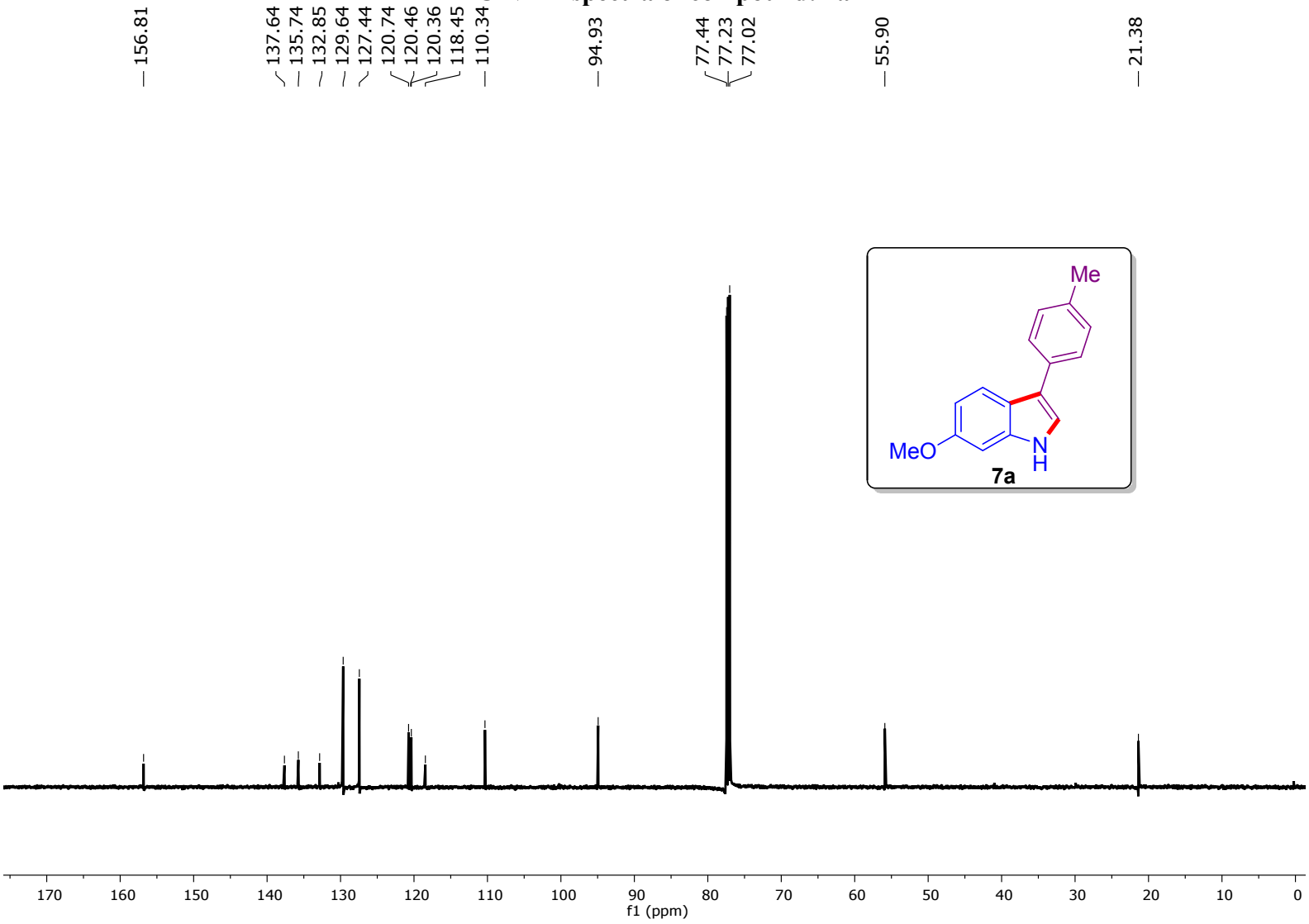
Sample Name	Unavailable	**Position**	Unavailable	**Instrument Name**	Unavailable	**User Name**	Unavailable
Inj Vol	Unavailable	**InjPosition**	Unavailable	**SampleType**	Unavailable	**IRM Calibration Status**	Some Ions Missed
Data Filename	2-NAP-1.d	**ACQ Method**		**Comment**	Sample information is unavailable	**Acquired Time**	Unavailable



^{1}H NMR spectra of compound: 7a

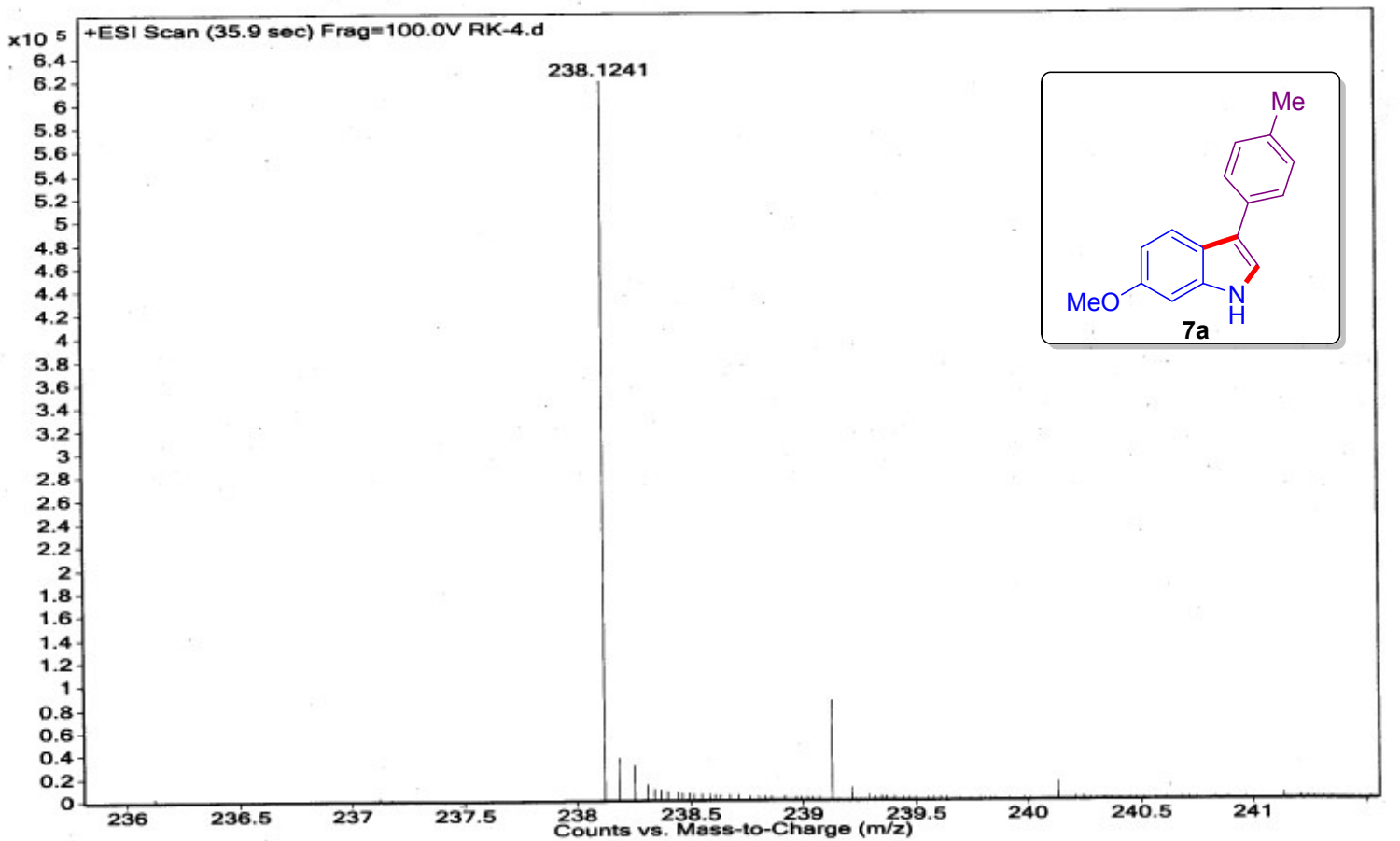


^{13}C NMR spectra of compound: 7a

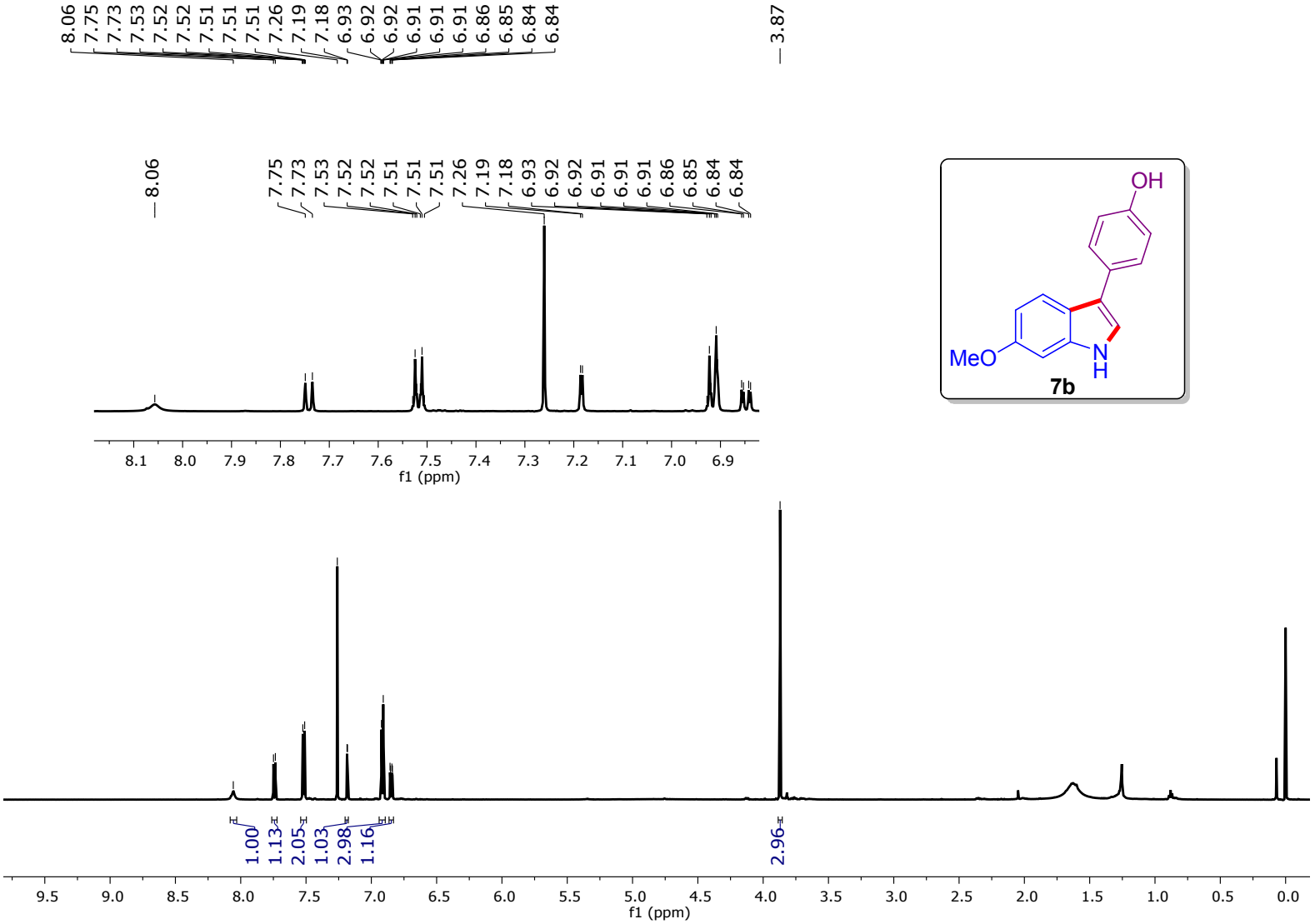


HRMS spectra of compound: 7a

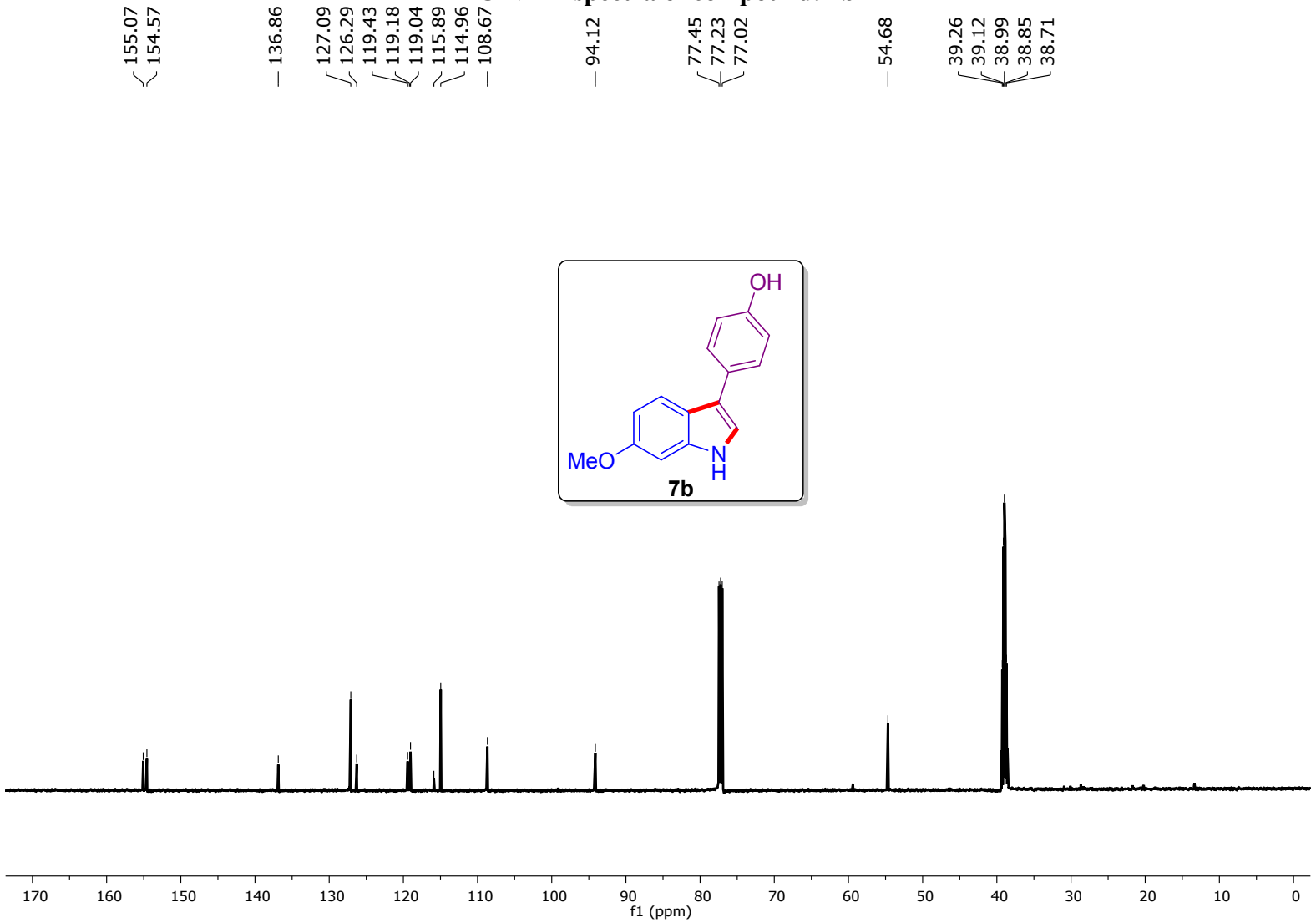
Sample Name	RK-4	**Position**	Vial 1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	0	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	All Ions Missed
Data Filename	RK-4.d	**ACQ Method**		**Comment**		**Acquired Time**	8/7/2017 1:31:13 PM



^{1}H NMR spectra of compound: 7b

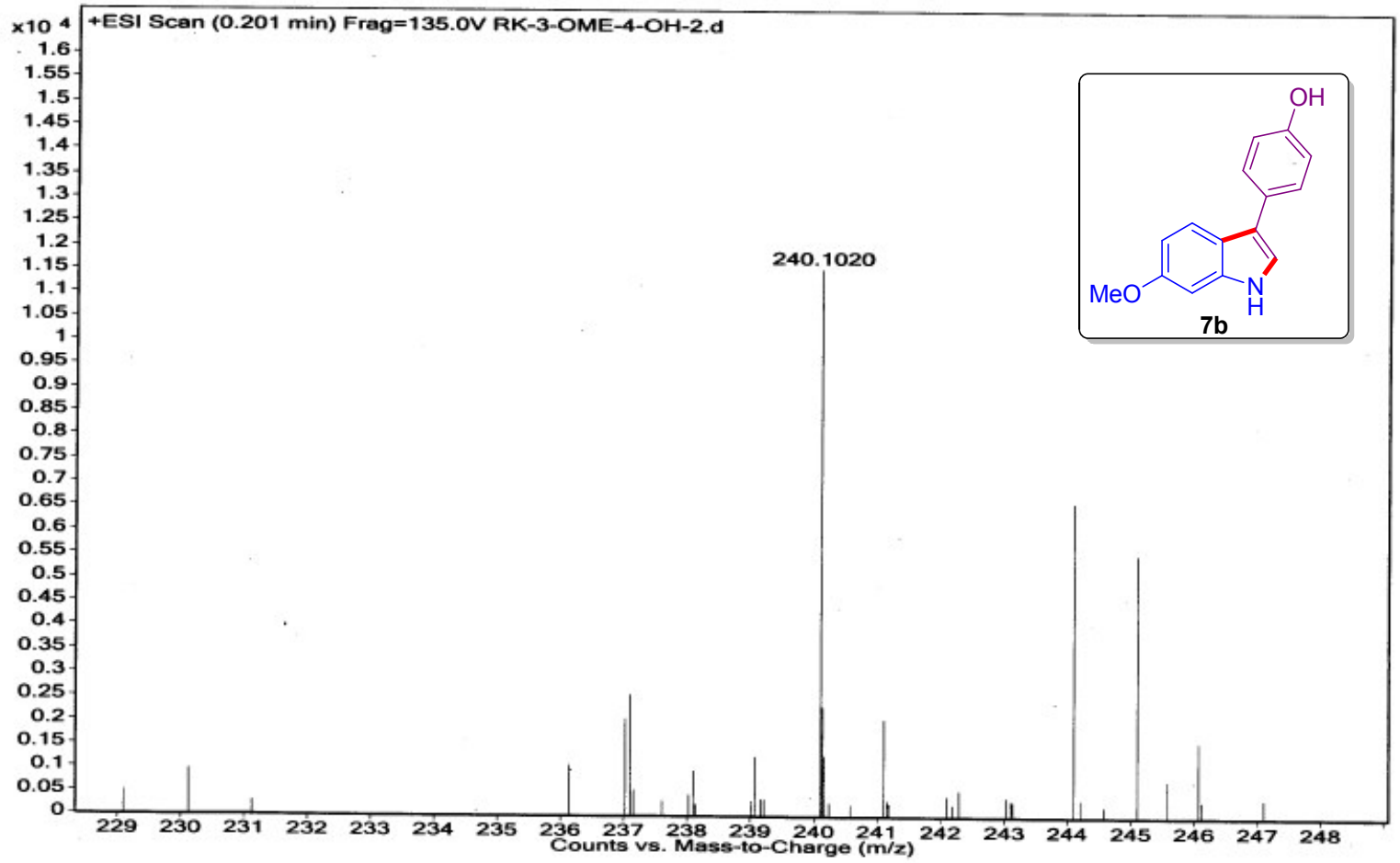


^{13}C NMR spectra of compound: 7b

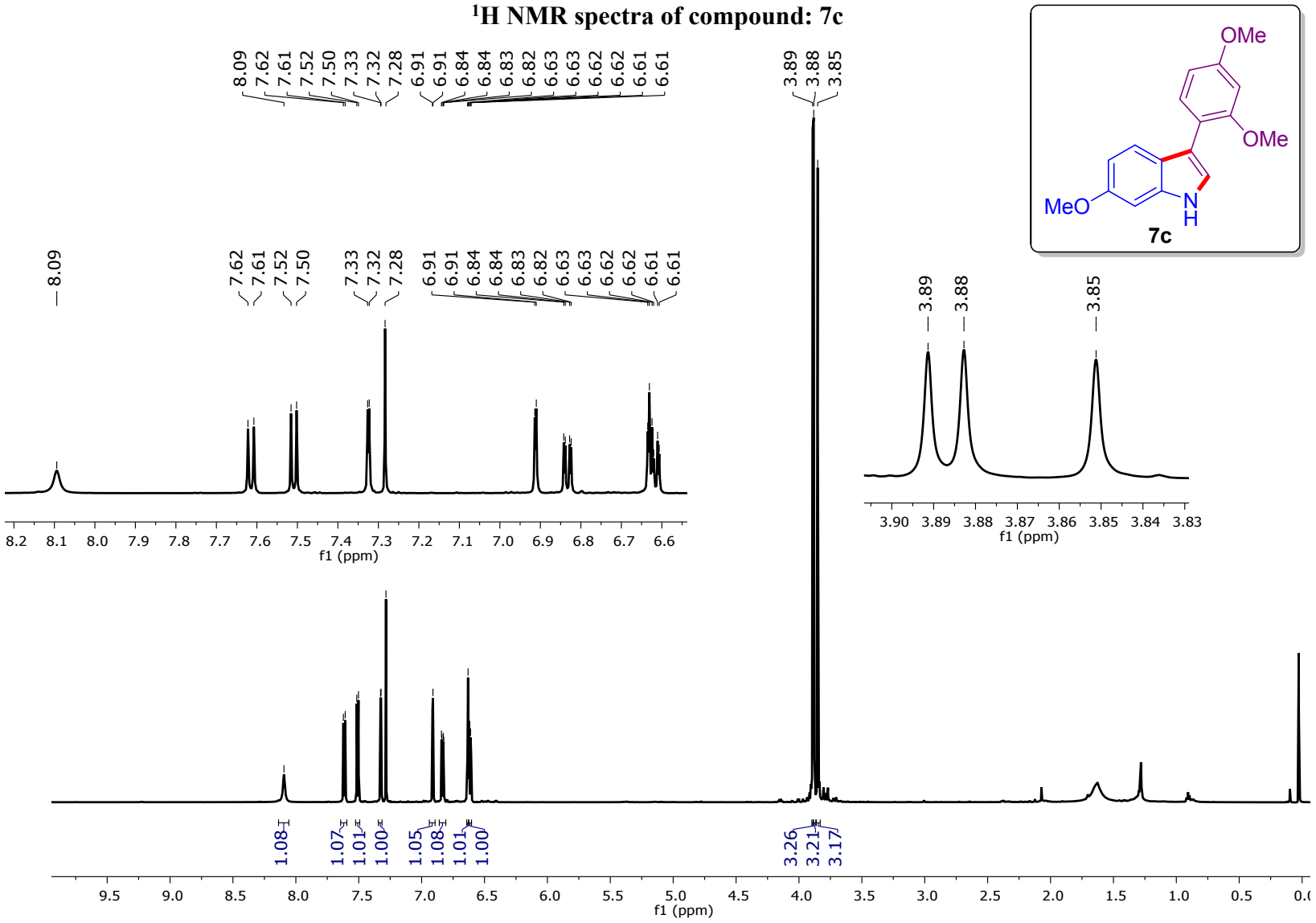


HRMS spectra of compound: 7b

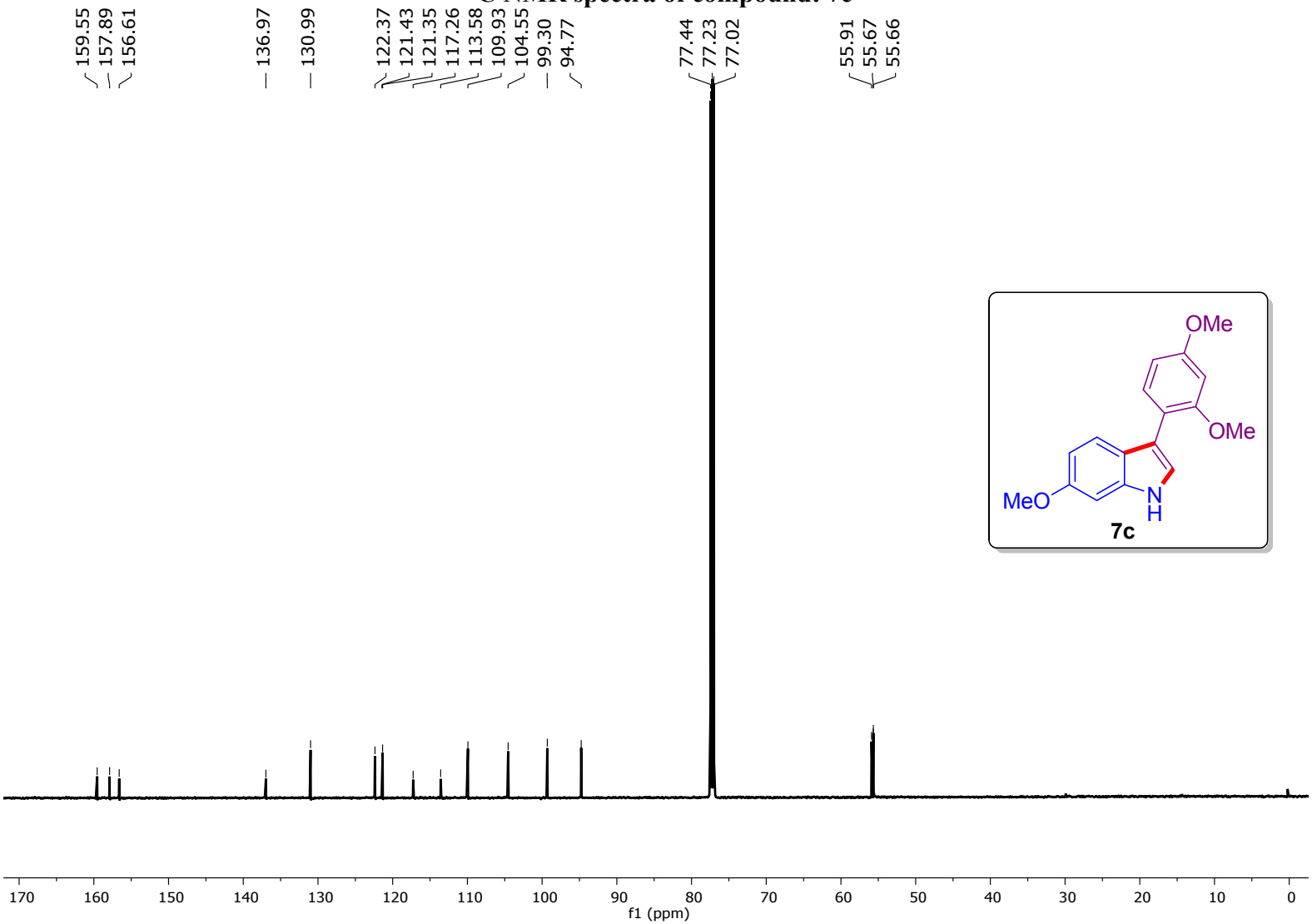
Sample Name	RK-3-OME-4-OH-2	**Position**	Vial 1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	RK-3-OME-4-OH-2.d	**ACQ Method**		**Comment**		**Acquired Time**	12/1/2017 7:24:47 PM



^{1}H NMR spectra of compound: 7c

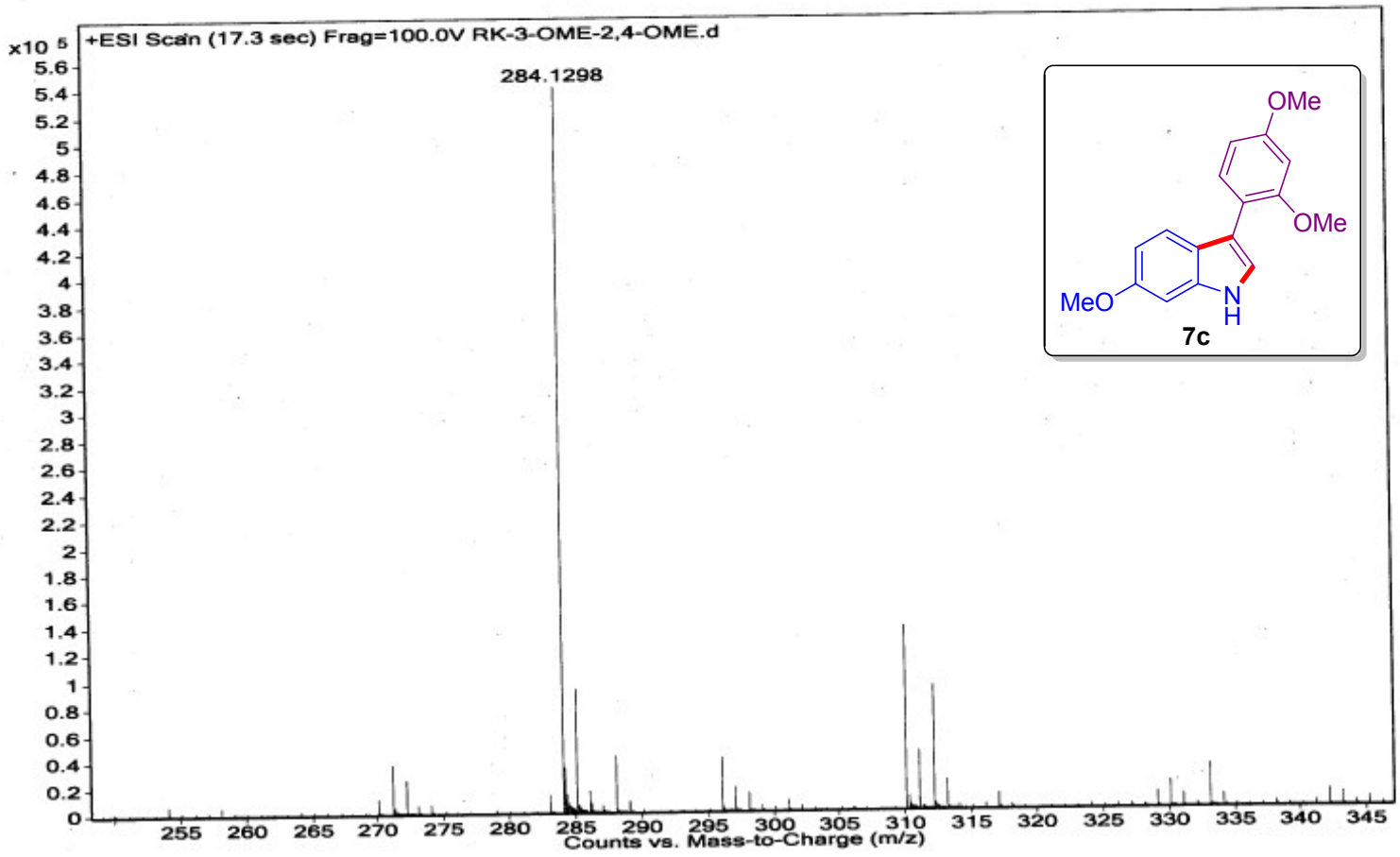


^{13}C NMR spectra of compound: 7c

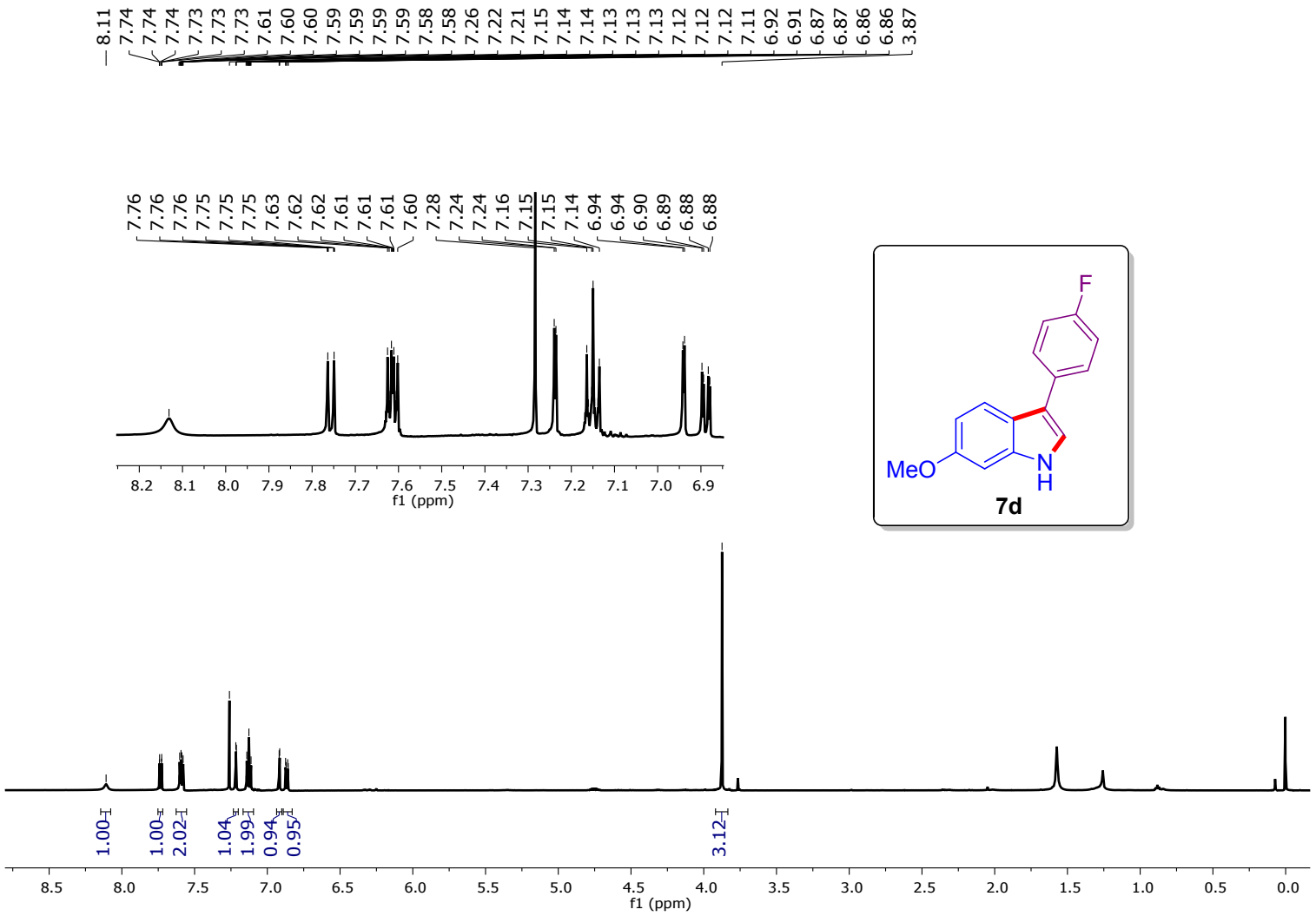


HRMS spectra of compound: 7c

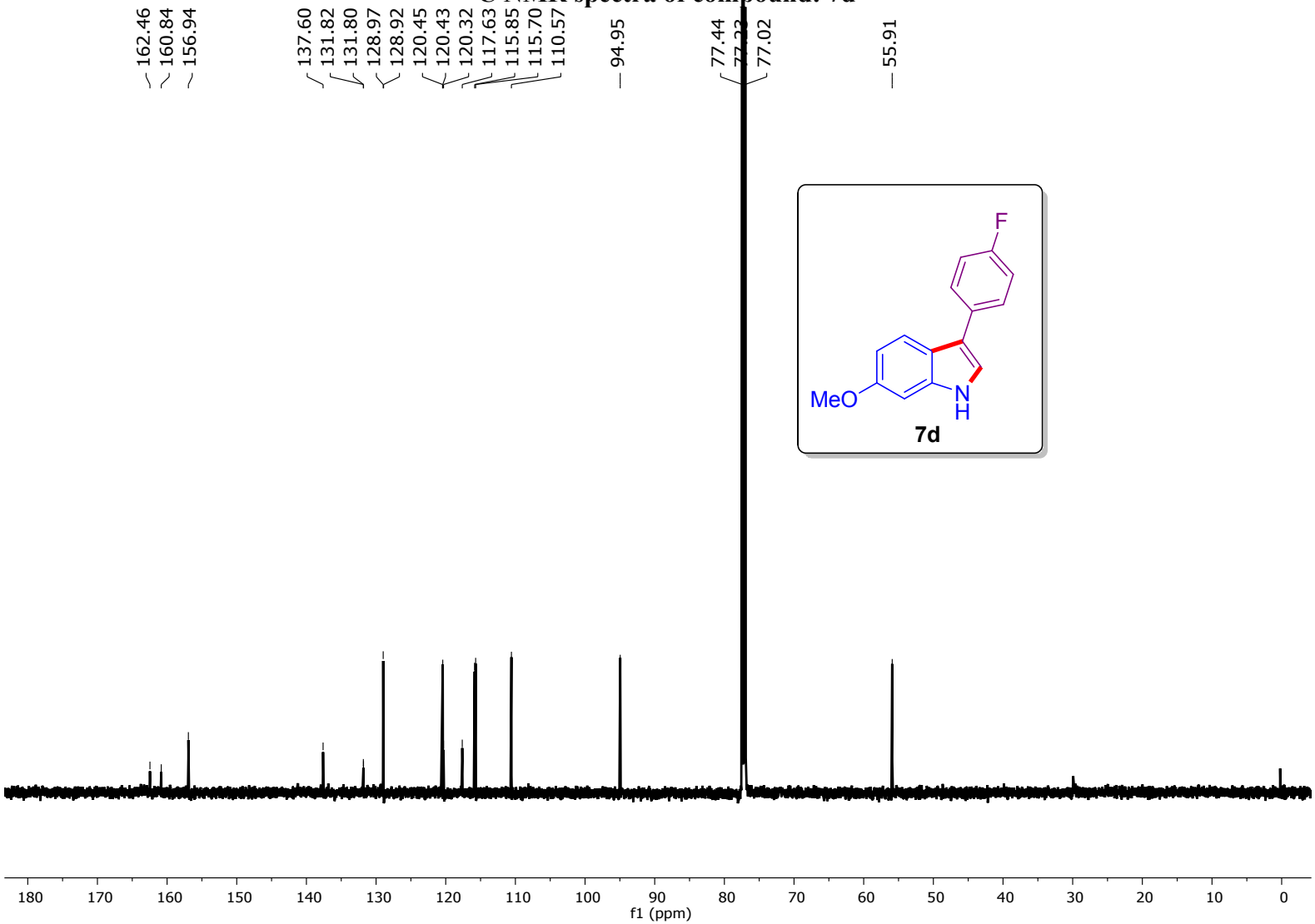
Sample Name	Unavailable	**Position**	Unavailable	**Instrument Name**	Unavailable	**User Name**	Unavailable
Inj Vol	Unavailable	**InjPosition**	Unavailable	**SampleType**	Unavailable	**IRM Calibration Status**	All Ions Missed
Data Filename	RK-3-OME-2,4-OME.d	**ACQ Method**		**Comment**	Sample information is unavailable	**Acquired Time**	Unavailable



^{1}H NMR spectra of compound: 7d

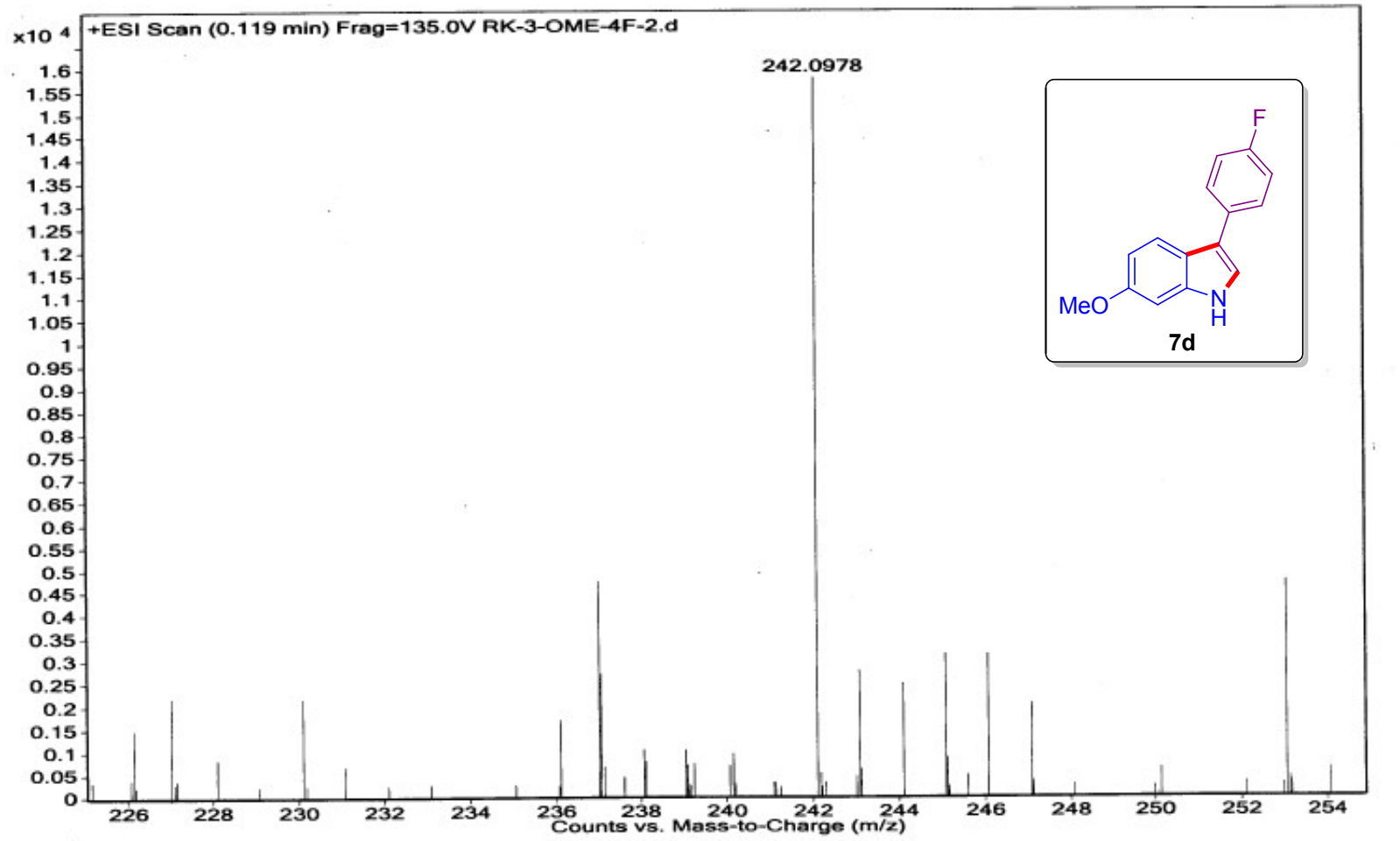


^{13}C NMR spectra of compound: 7d

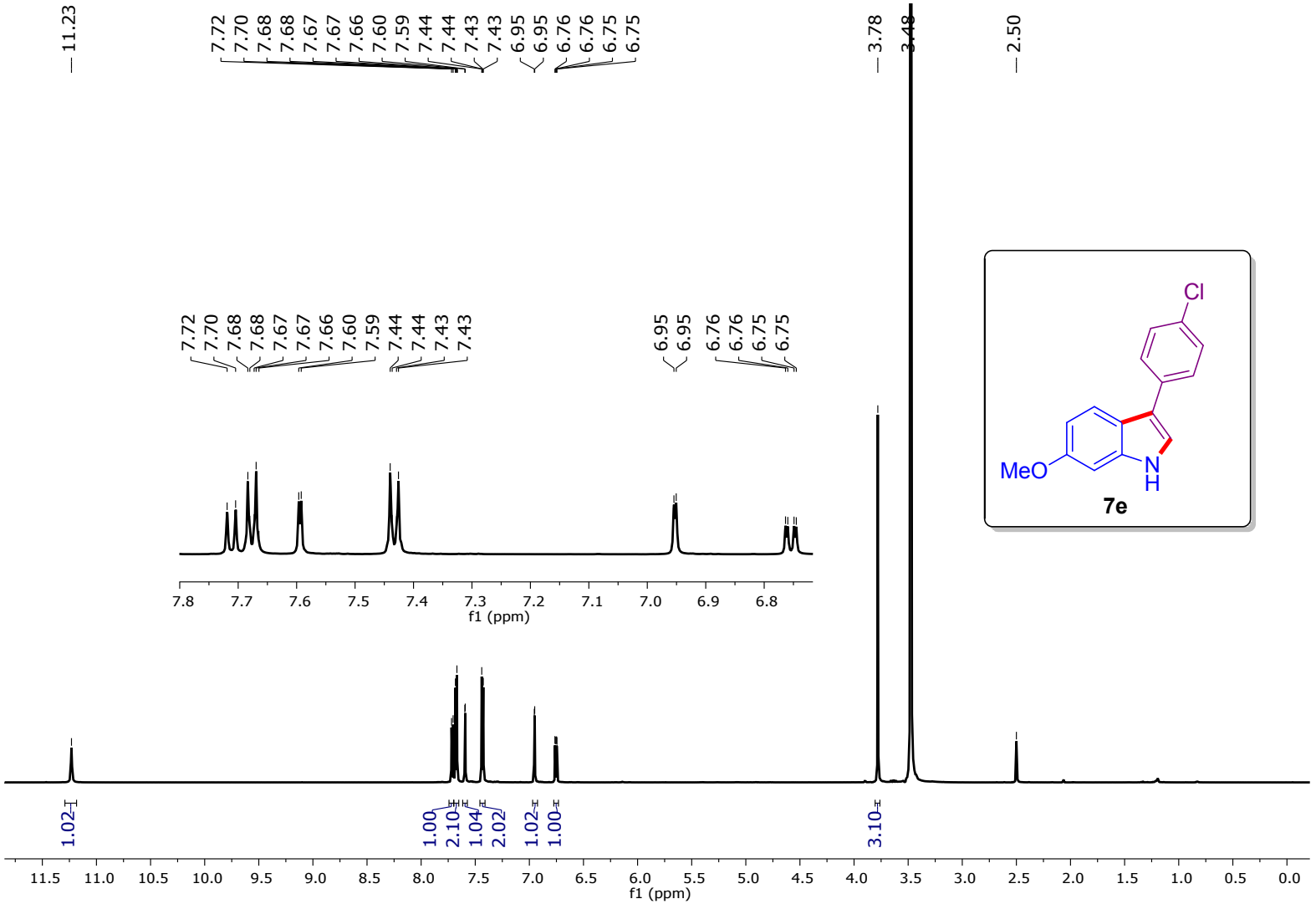


HRMS spectra of compound: 7d

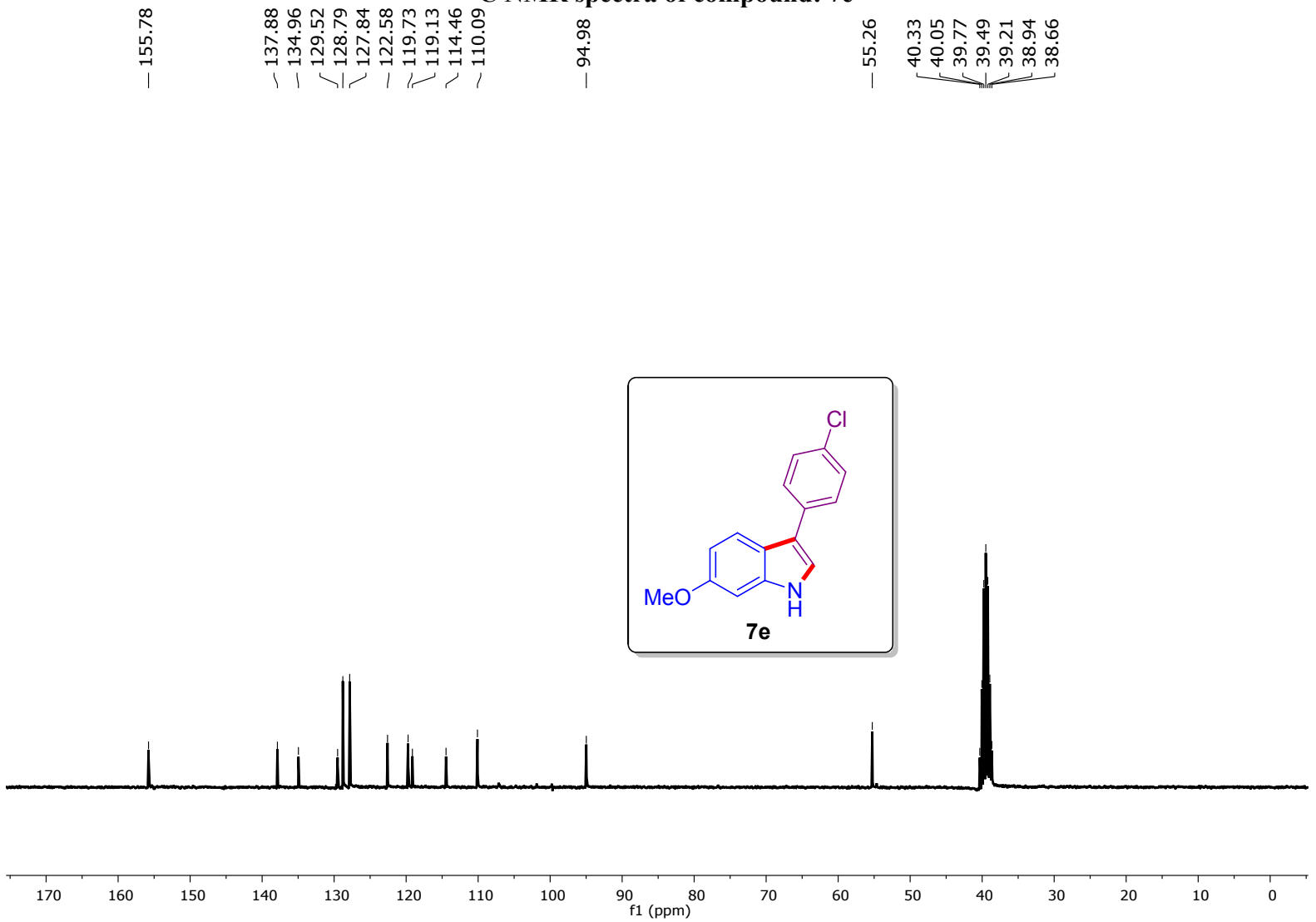
Sample Name	RK-3-OME-4F-2	**Position**	Vial 1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	RK-3-OME-4F-2.d	**ACQ Method**		**Comment**		**Acquired Time**	12/1/2017 6:29:25 PM



^{1}H NMR spectra of compound: 7e

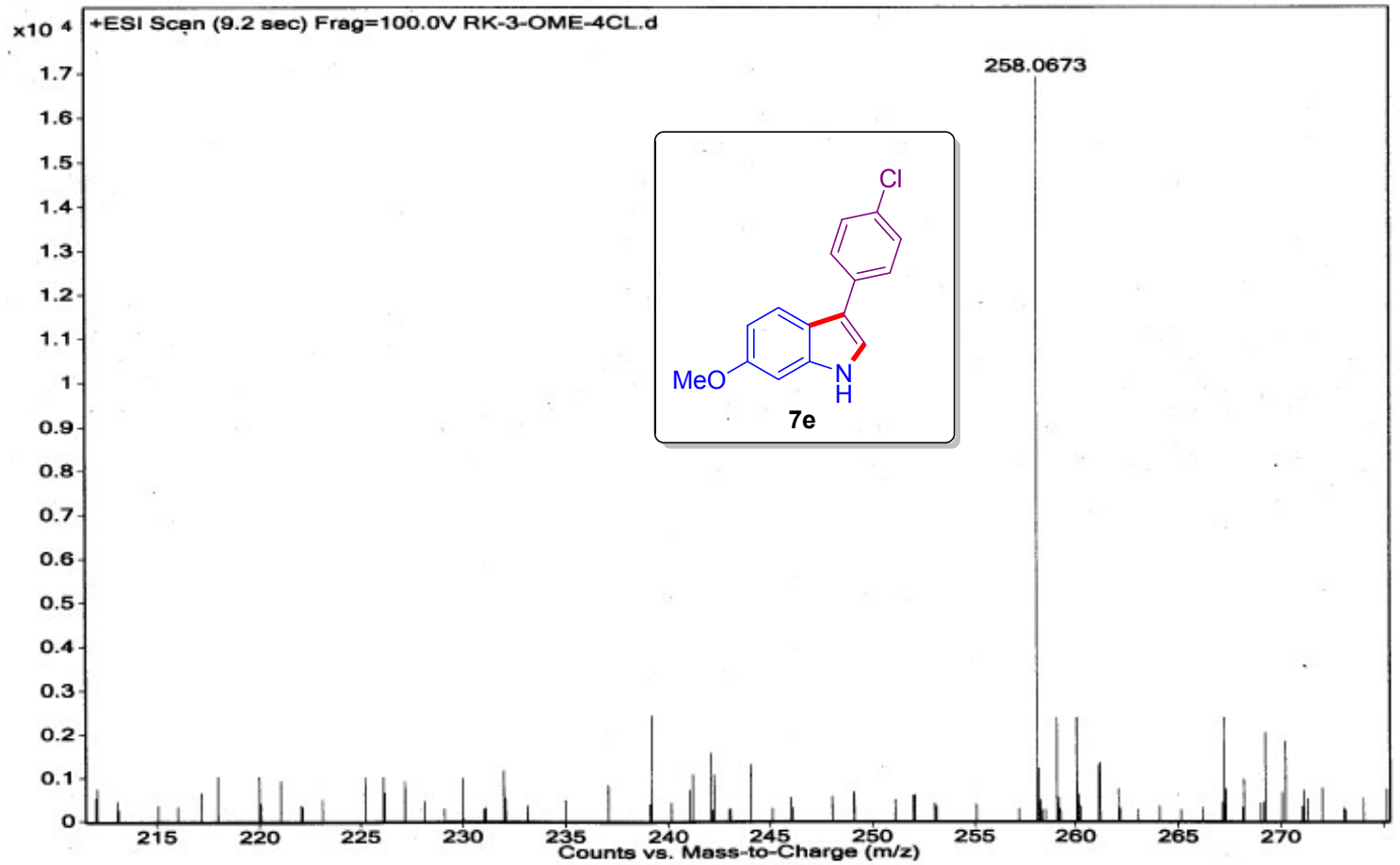


^{13}C NMR spectra of compound: 7e

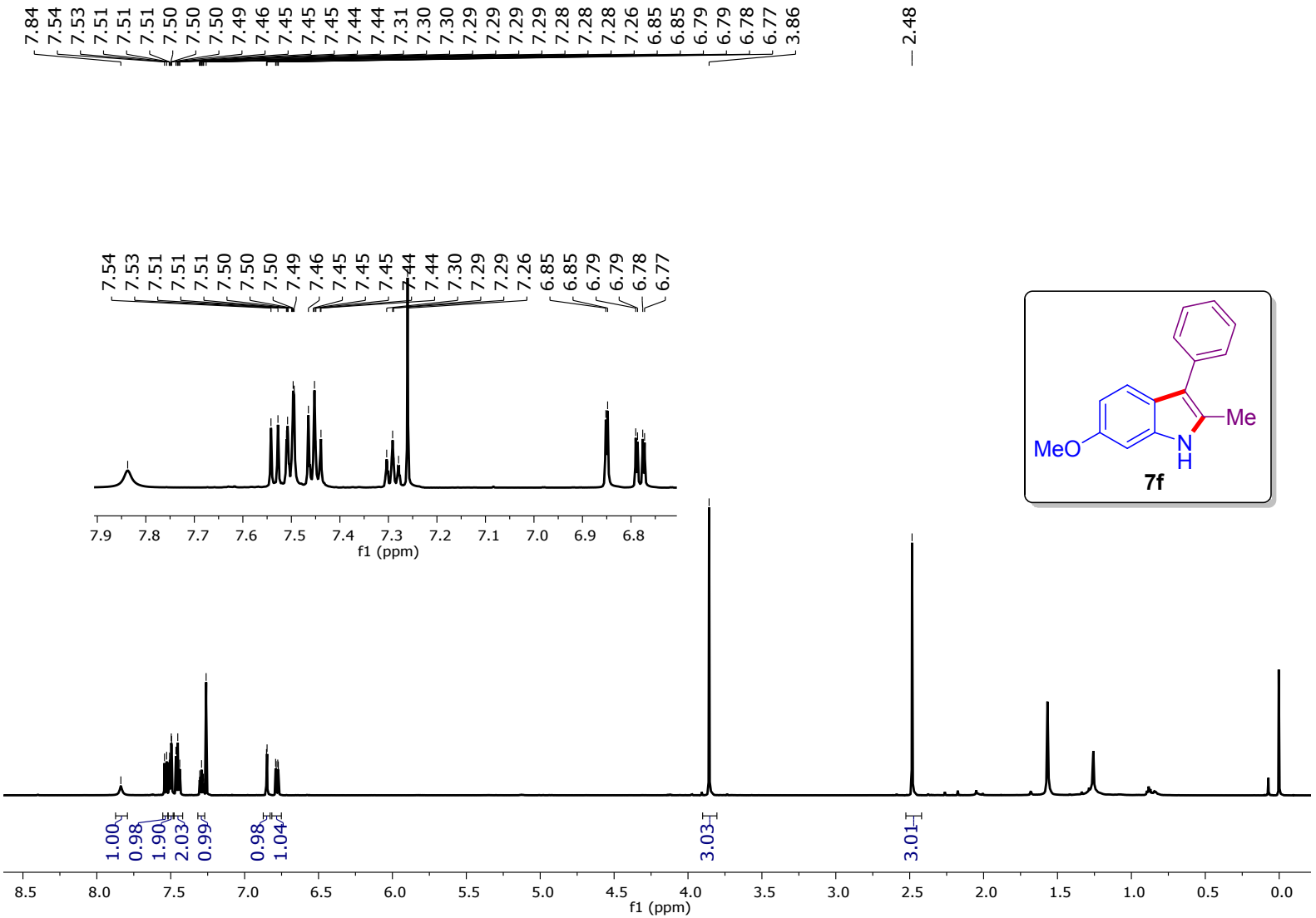


HRMS spectra of compound: 7e

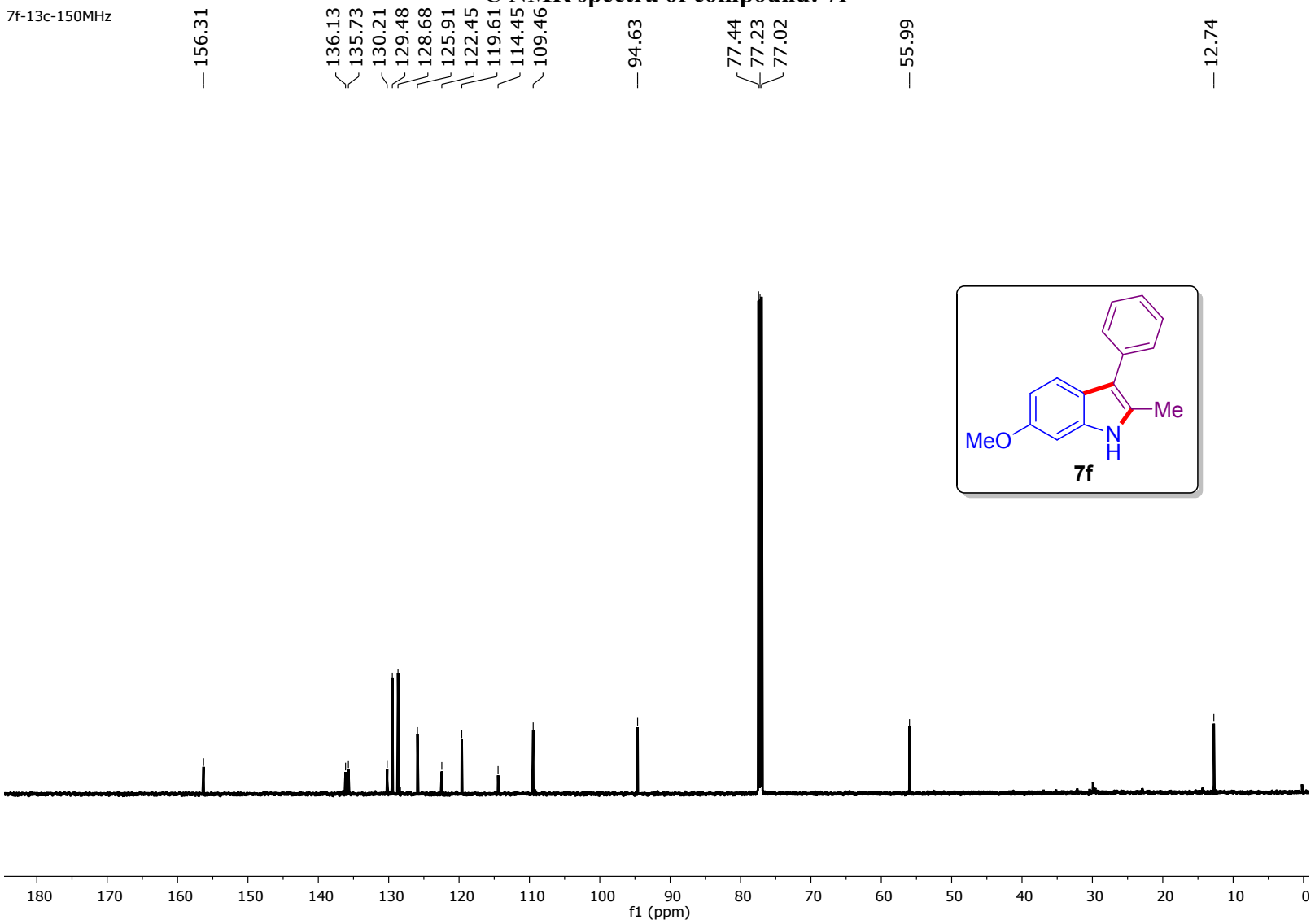
Sample Name	Unavailable	**Position**	Unavailable	**Instrument Name**	Unavailable	**User Name**	Unavailable
Inj Vol	Unavailable	**InjPosition**	Unavailable	**SampleType**	Unavailable	**IRM Calibration Status**	All Ions Missed
Data Filename	RK-3-OME-4CL.d	**ACQ Method**		**Comment**	Sample information is unavailable	**Acquired Time**	Unavailable



^{1}H NMR spectra of compound: 7f

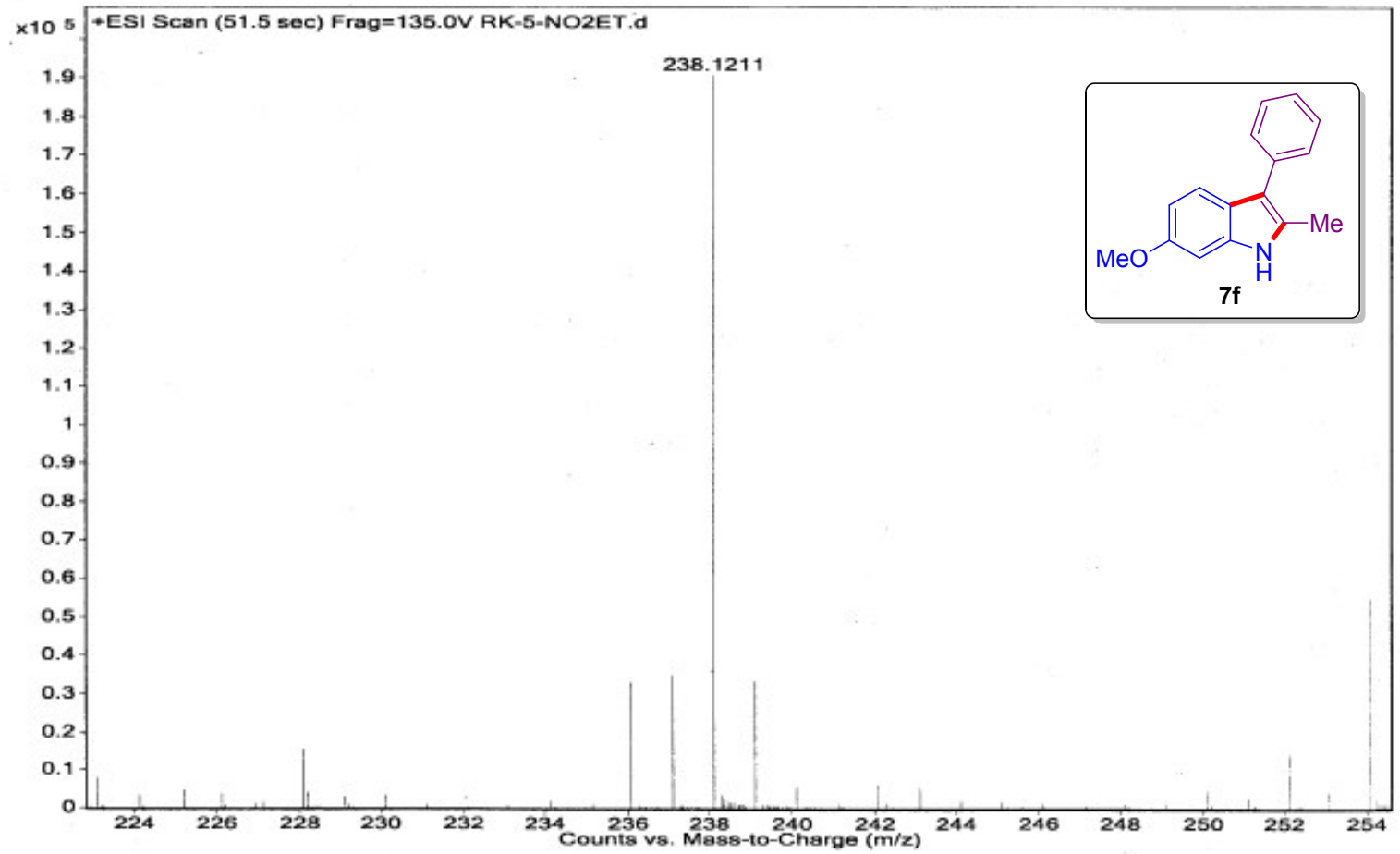


^{13}C NMR spectra of compound: 7f

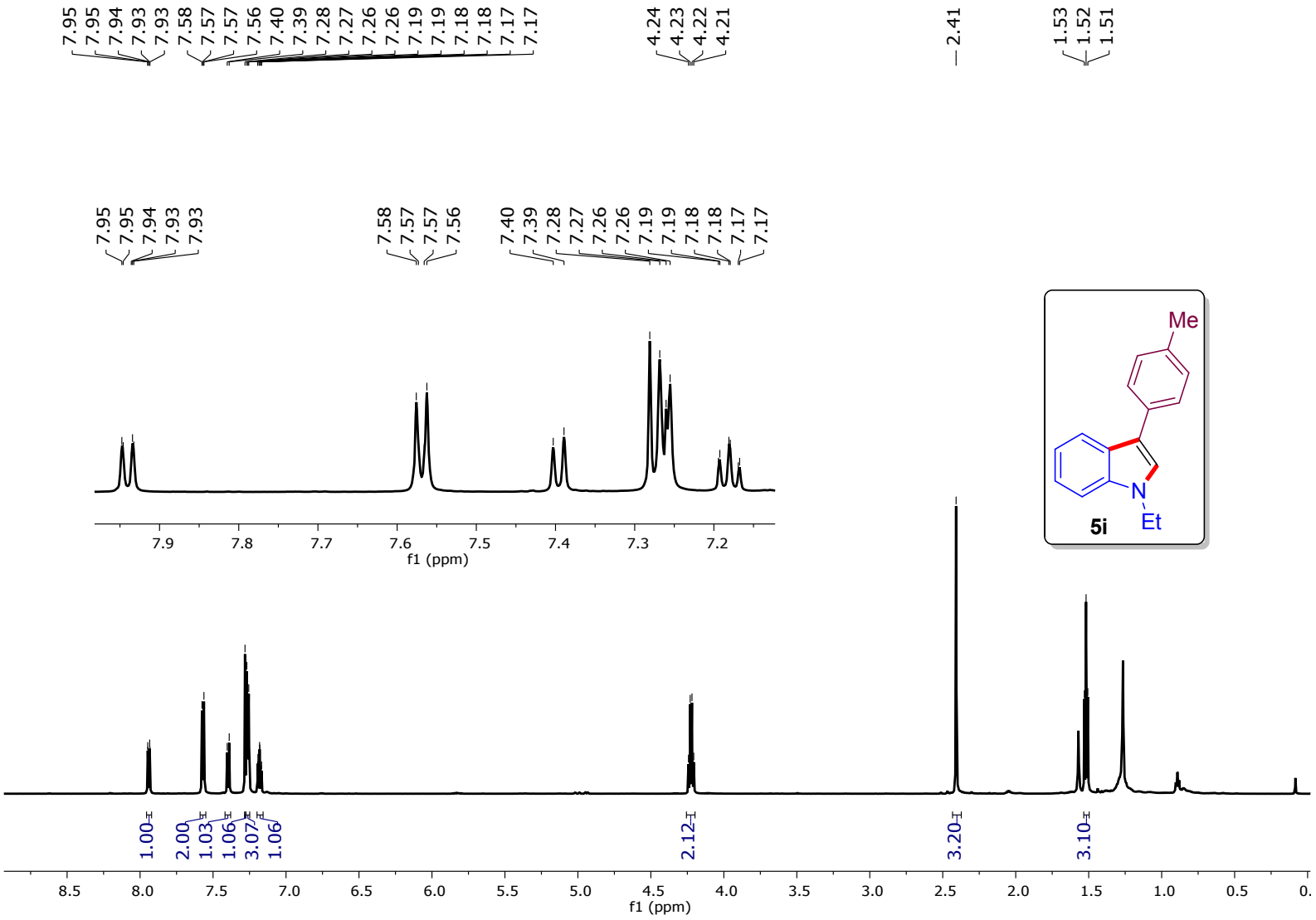


HRMS spectra of compound: 7f

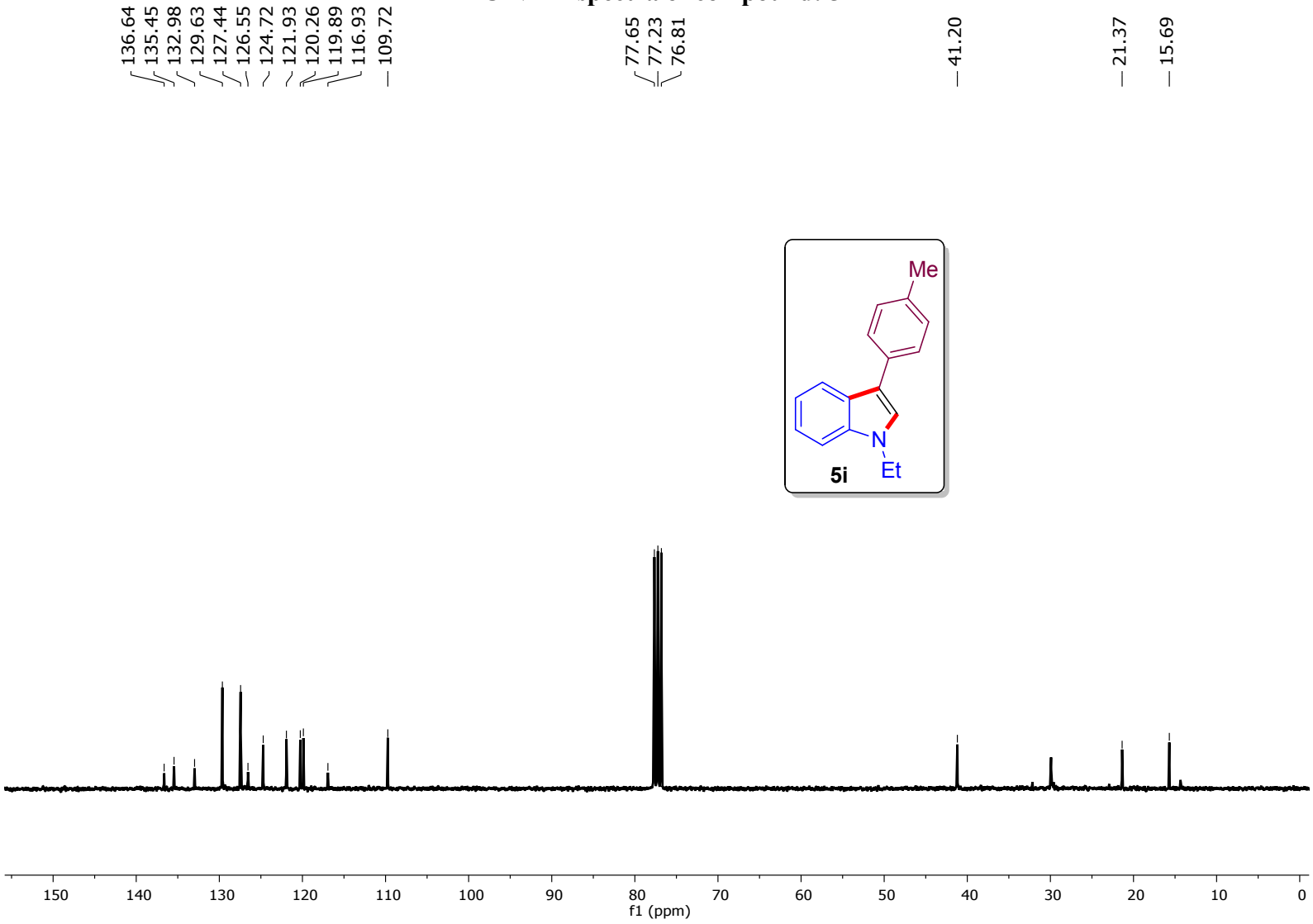
Sample Name	RK-5-NO2ET	**Position**	Vial 1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	0	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	RK-5-NO2ET.d	**ACQ Method**		**Comment**		**Acquired Time**	10/23/2017 4:47:47 PM



^{1}H NMR spectra of compound: 5i

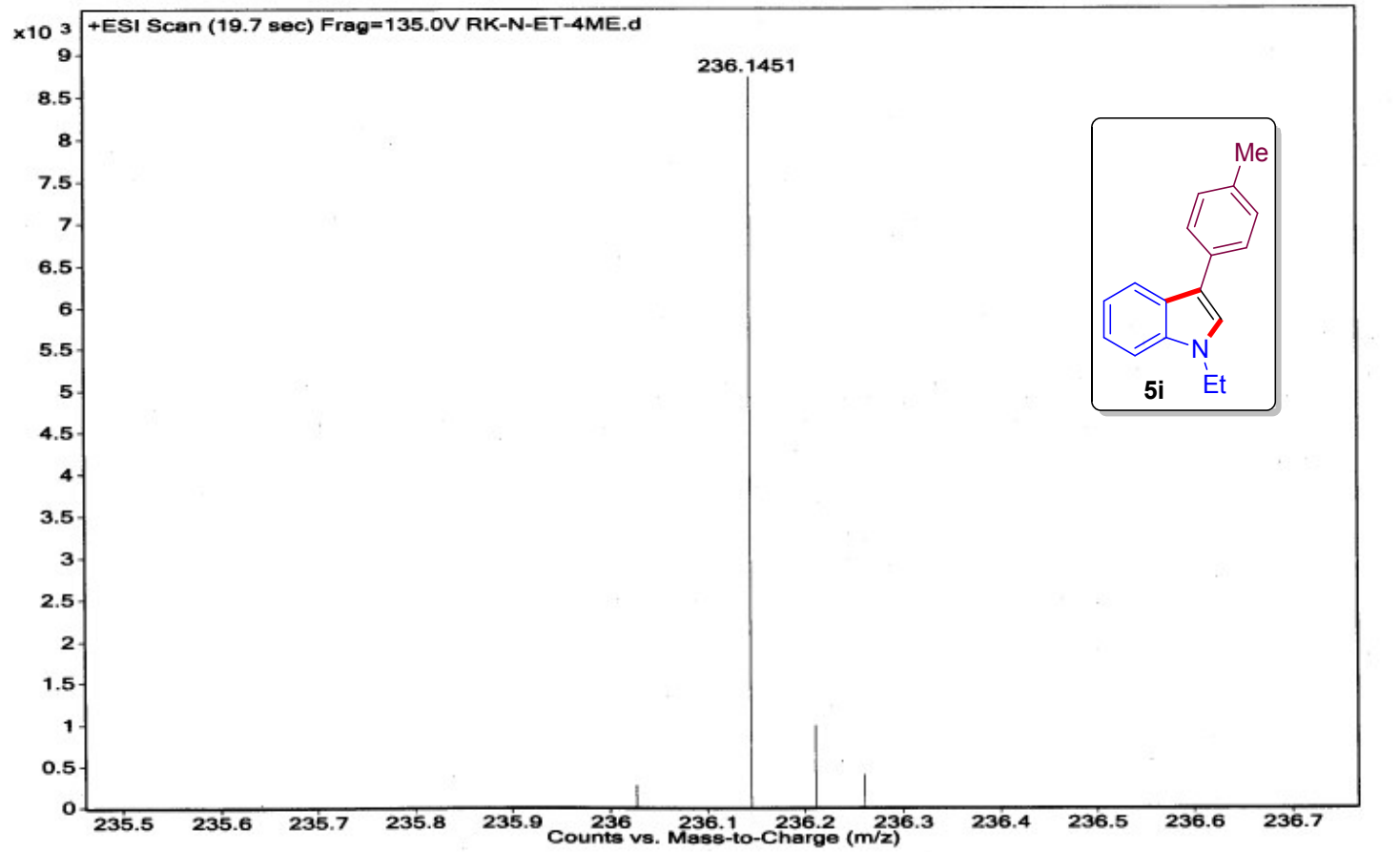


^{13}C NMR spectra of compound: 5i

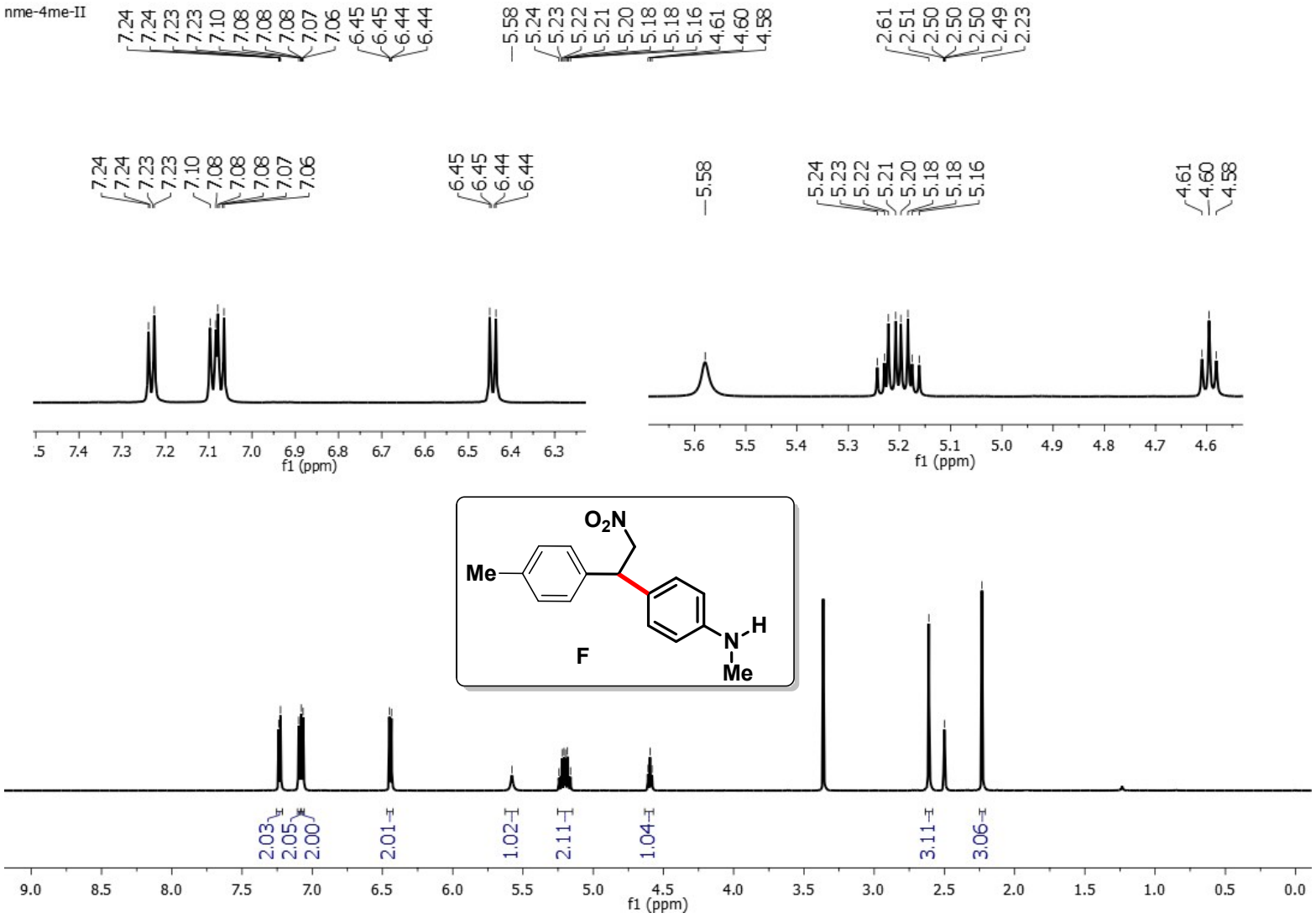


HRMS spectra of compound: 5i

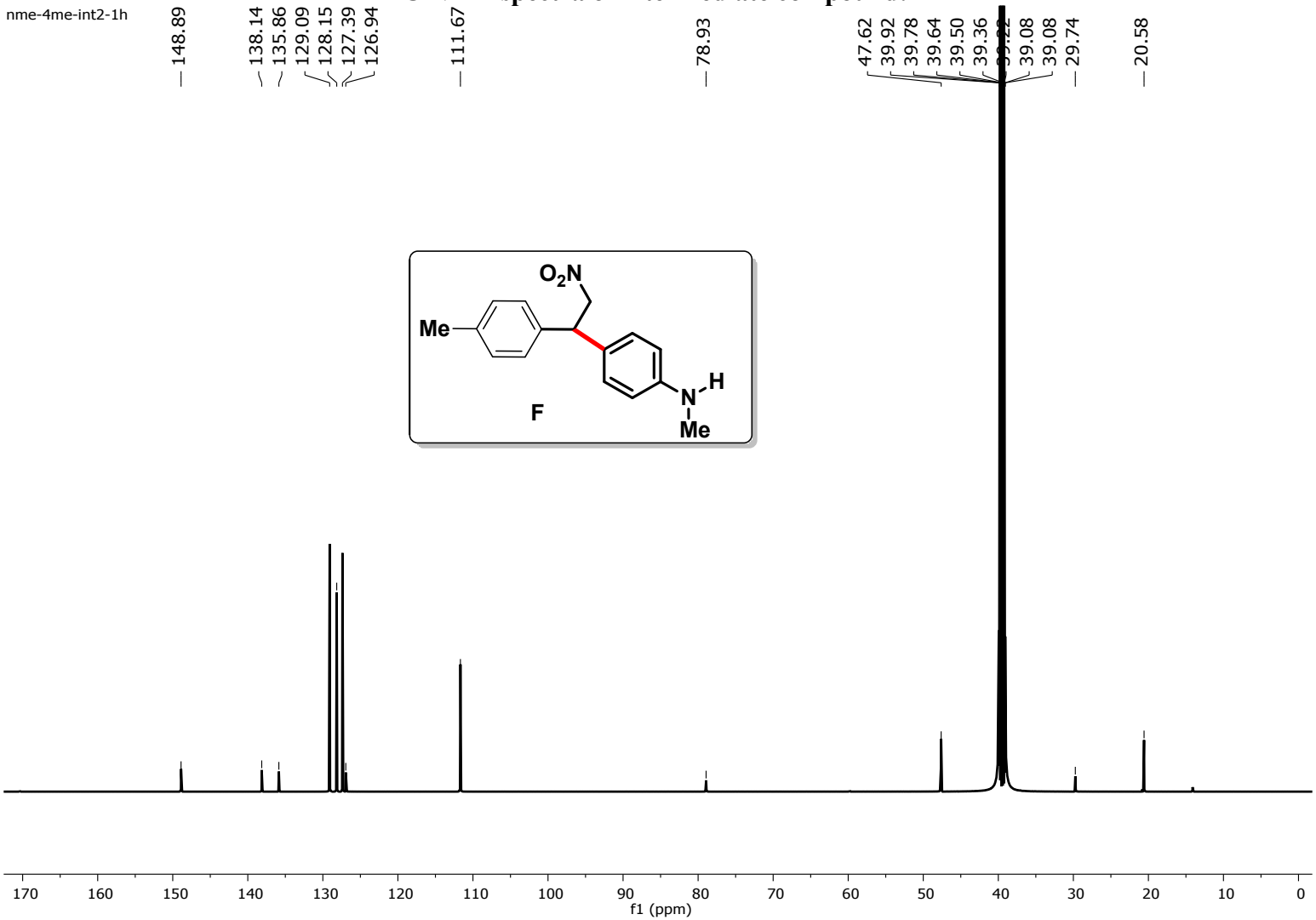
Sample Name	RK-N-ET-4ME	**Position**	Vial 1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	0	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	All Ions Missed
Data Filename	RK-N-ET-4ME.d	**ACQ Method**		**Comment**		**Acquired Time**	8/10/2017 12:15:20 PM



^{1}H NMR spectra of intermediate compound: F



^{13}C NMR spectra of intermediate compound: F



HRMS spectra of intermediate compound: F