

Copper-Mediated Radical Trifluoromethylation of Unsaturated Potassium Organotrifluoroborates

Supporting Information

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1. General considerations

All commercially available reagents, including anhydrous solvents were used without purification. In particular, Langlois' reagent (NaSO_2CF_3), TBHP, CuCl and $(\text{CH}_3\text{CN})_4\text{CuPF}_6$ were purchased. Potassium organotrifluoroborates **1a**, **1d**, **1e**, **1f**, **1j**, **3a** and **4a** are commercially available. Potassium organotrifluoroborates **1h**¹ and **1k**² were prepared according to reported procedures.

Analytical thin-layer chromatography (TLC) was performed on TLC silica gel plates (0.25 mm) precoated with a fluorescent indicator. Flash chromatography (FC) was performed on a Biotage SP4 base system using GRACE Reveleris columns (silica size 40 μm) of various sizes. Visualization was effected with ultraviolet light and ethanolic KMnO_4 .

Melting points ($^\circ\text{C}$) are uncorrected. ^1H NMR chemical shifts were referenced to the residual solvent signal; ^{13}C NMR chemical shifts were referenced to the deuterated solvent signal. Multiplicity was defined by DEPT 135 analysis. The resonance of the carbon center linked to the boron atom was not observed. ^{19}F NMR chemical shifts were referenced to external CFCl_3 (0.0 ppm). ^{11}B NMR chemical shifts were referenced to external $\text{BF}_3\cdot\text{OEt}_2$ (0.0 ppm) with a negative sign indicating an upfield shift. Data are presented as follows: chemical shift δ (ppm), multiplicity (*s* = singlet, *d* = doublet, *t* = triplet, *m* = multiplet, *br* = broad), coupling constant *J* (Hz), integration.

High-resolution mass spectra were obtained by electrospray ionization on a TOF instrument. Capillary GC-MS was carried out on a gas chromatograph, equipped with a split/splitless injection port, interfaced with an inert mass-selective detector. A DB-5MS fused silica capillary column was used; dimensions of the column were 30 m x 0.25 mm i.d., 0.25 μm film thickness. Ultra high purity helium with an in-line oxygen trap was used as carrier gas. The carrier gas-line pressure was set at a flow of 15 ml /min and column head pressure at 13 psi. Temperature of the injector was maintained at 250 $^\circ\text{C}$. The injected sample volume was 0.1 μL in the split mode with 10:1 split ratio. The interface temperature was held at 280 $^\circ\text{C}$. Oven program was: initial temperature of 50 $^\circ\text{C}$ raised to 280 $^\circ\text{C}$ at a rate of 24 $^\circ\text{C}/\text{min}$ with a final isotherm of 5 min. Mass spectrometer was used with an electron impact ionization energy of 70 eV.

2. Copies of GCMS monitoring and NMR spectra

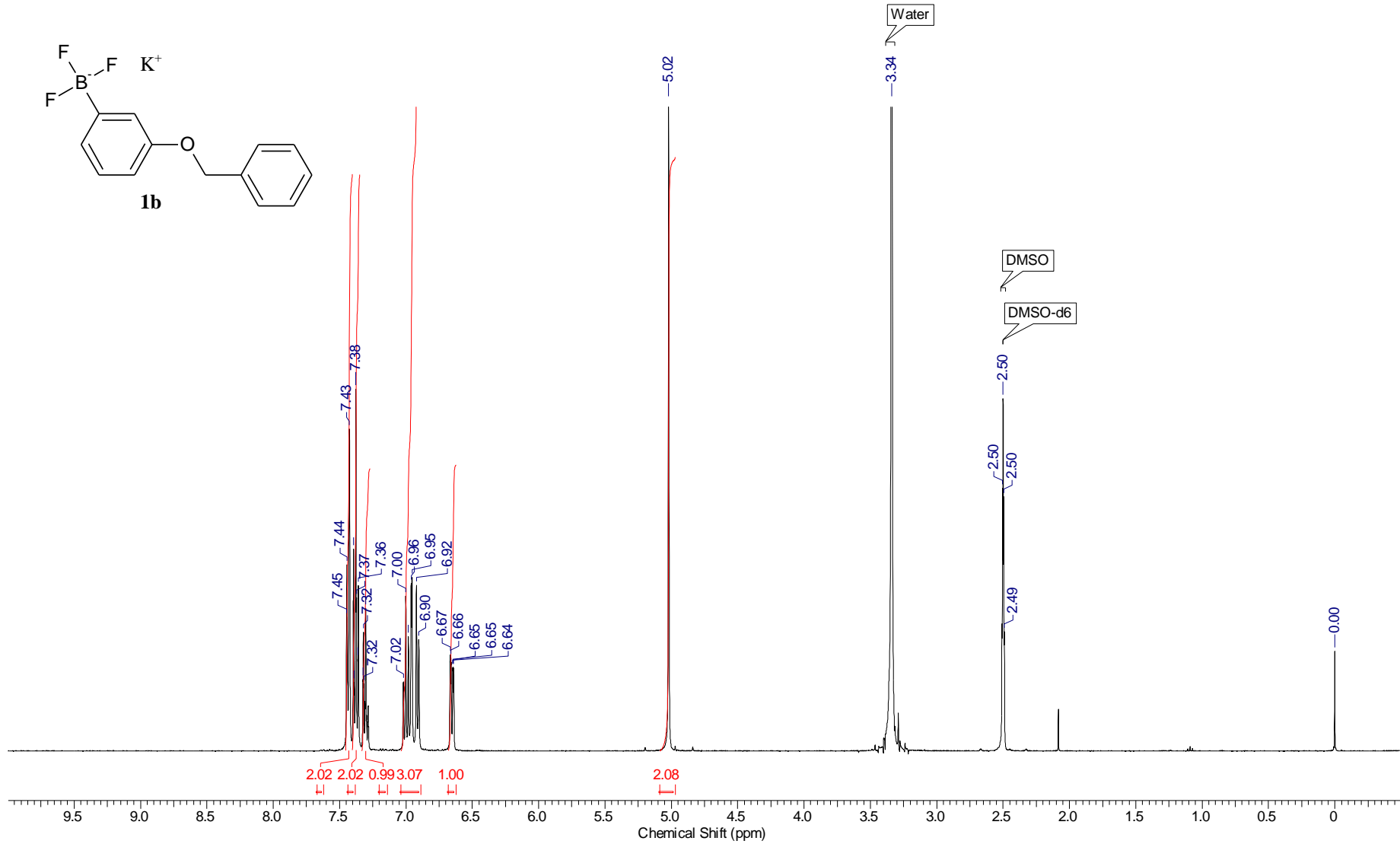
¹ Molander, G. A.; Cavalcanti, L.; Garcia-Garcia, C. *J. Org. Chem.* **2013**, 78, 6427.

² Molander, G. A.; Canturk, B.; Kennedy, L. E. *J. Org. Chem.* **2009**, 74, 973.

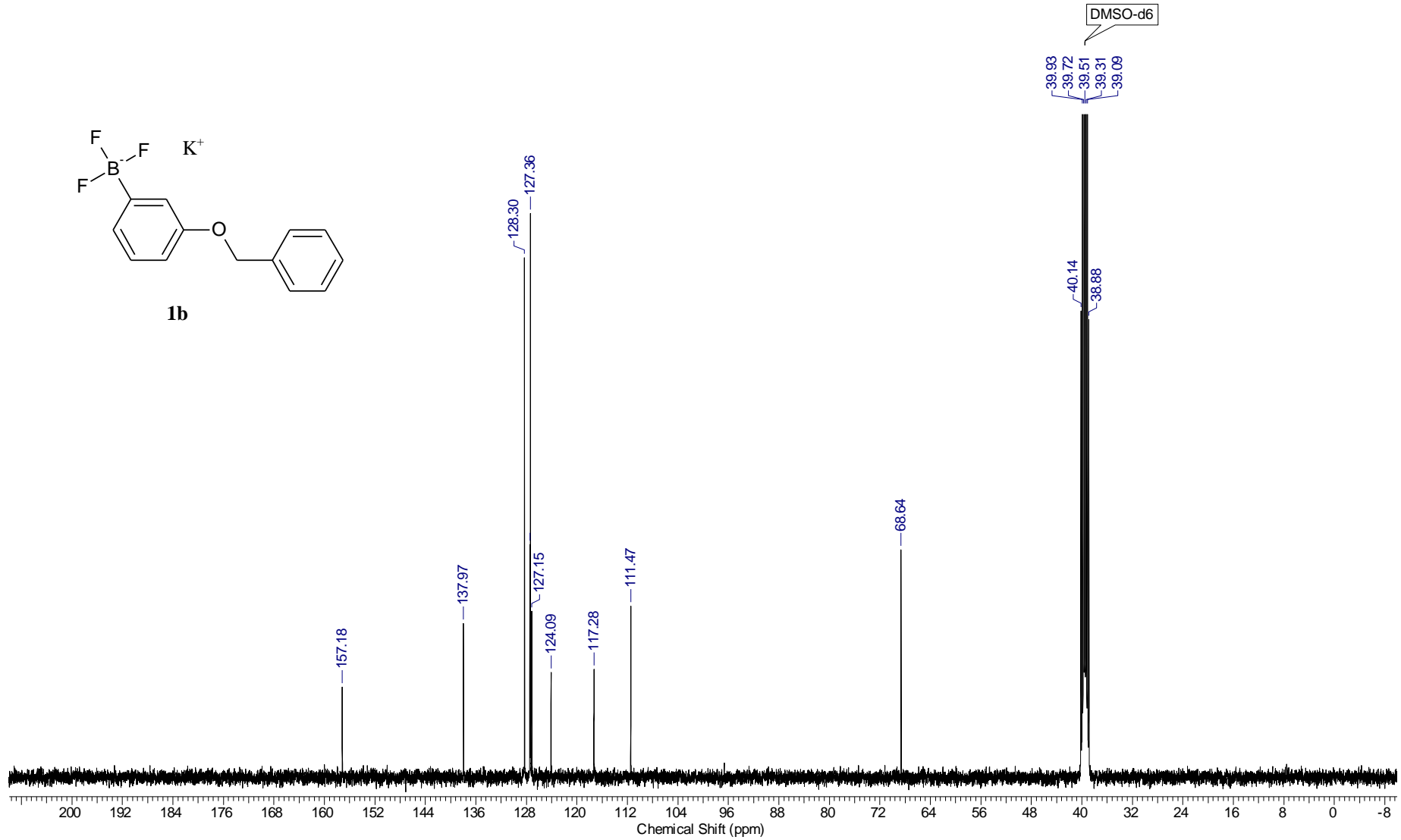
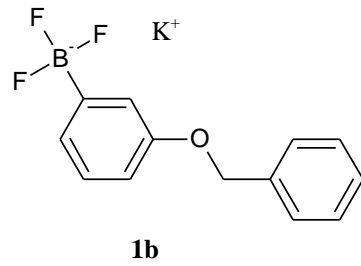
Copies of ^1H , ^{13}C , ^{11}B and ^{19}F NMR spectra for compounds **1b**, **1c**, **1g**, **1h**, **1i**, **1k**, **3b**, **4b**, **4c**, **4d**, **4e**.

Copies of ^{19}F and GCMS monitoring for all products; ^1H , ^{13}C , Dept 135, ^{11}B and ^{19}F NMR spectra for all new products.

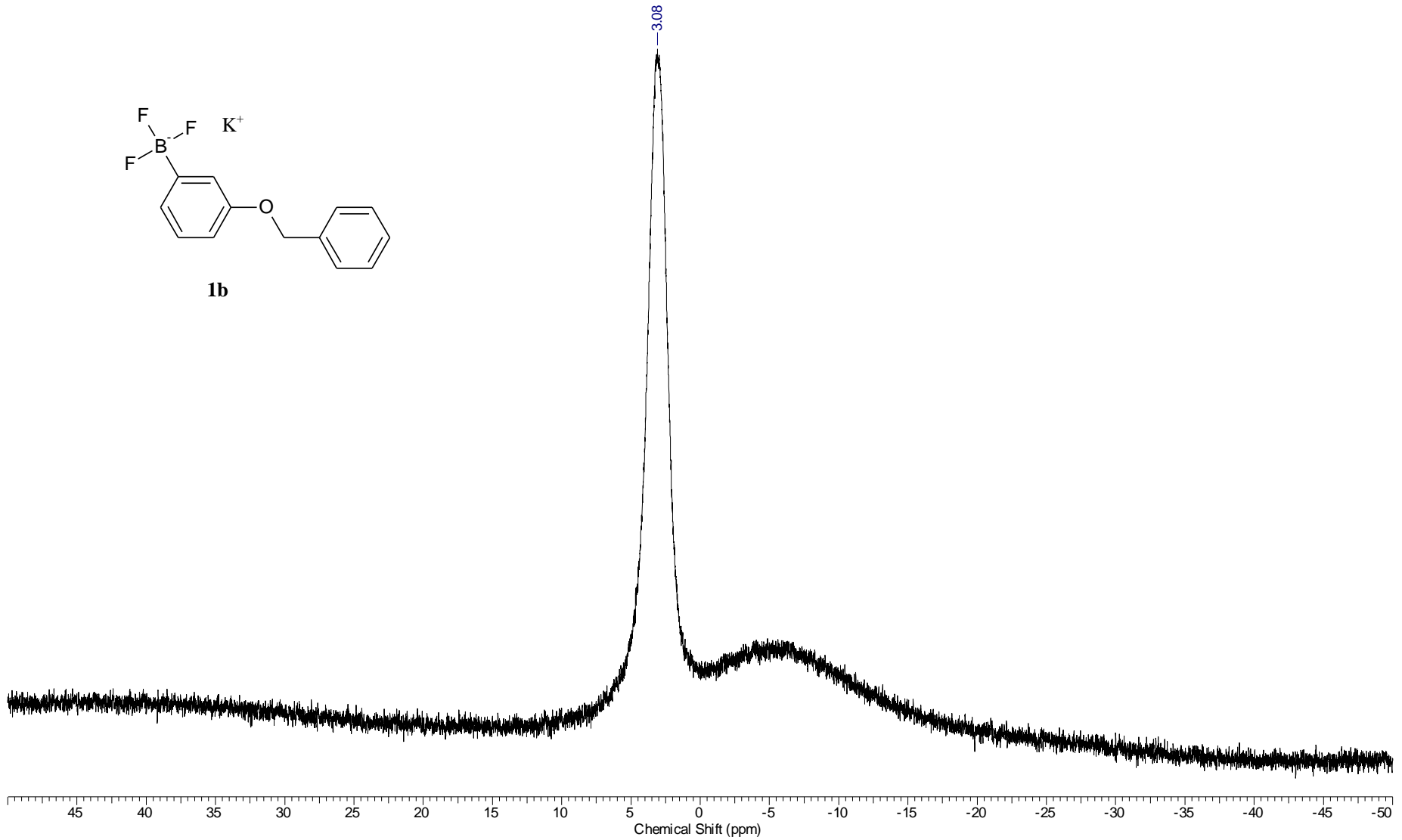
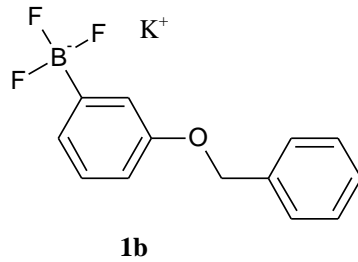
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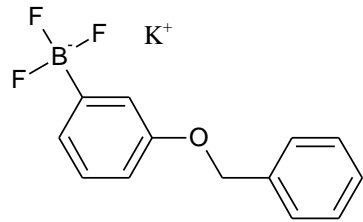
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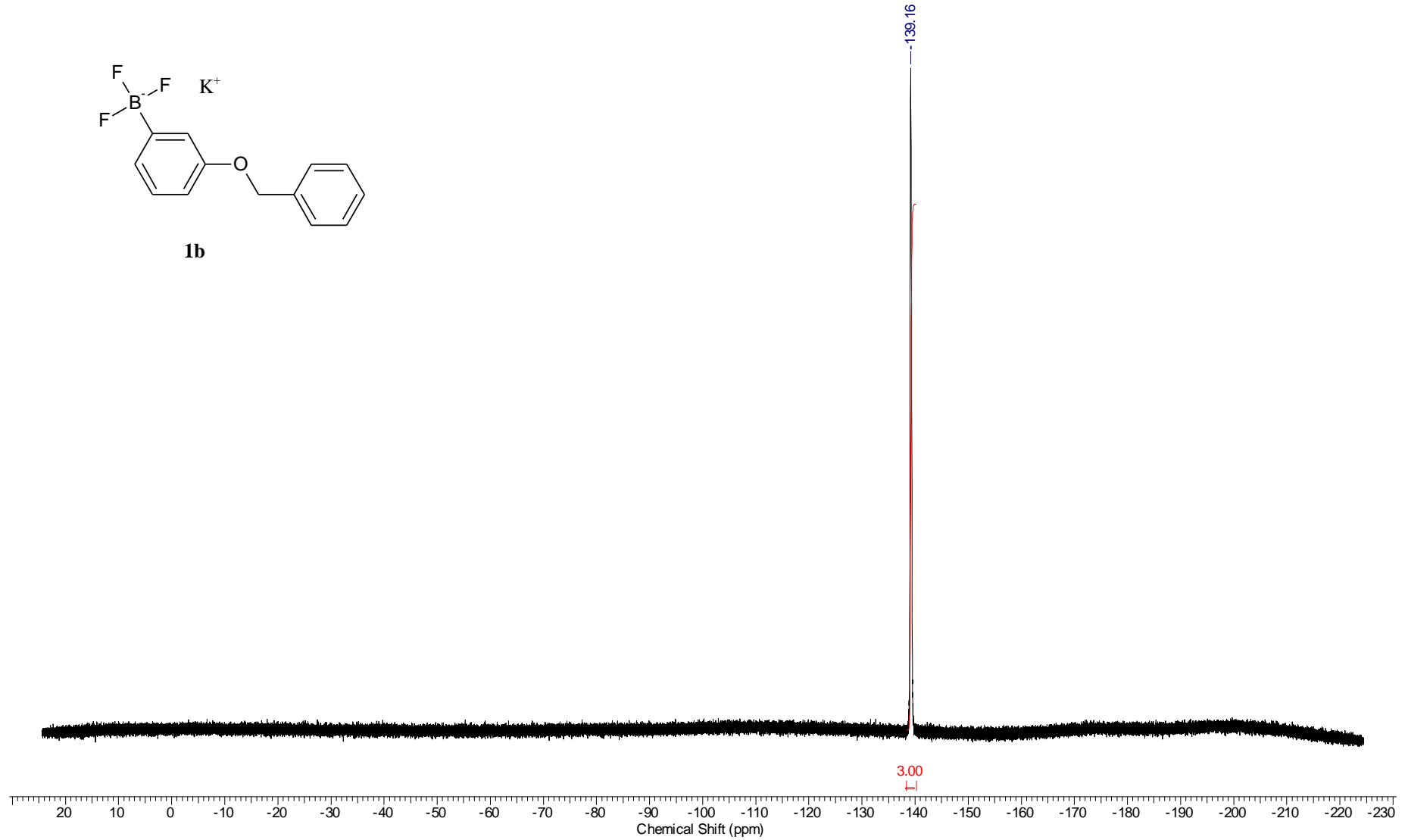
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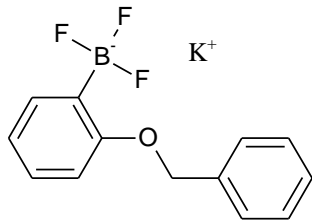
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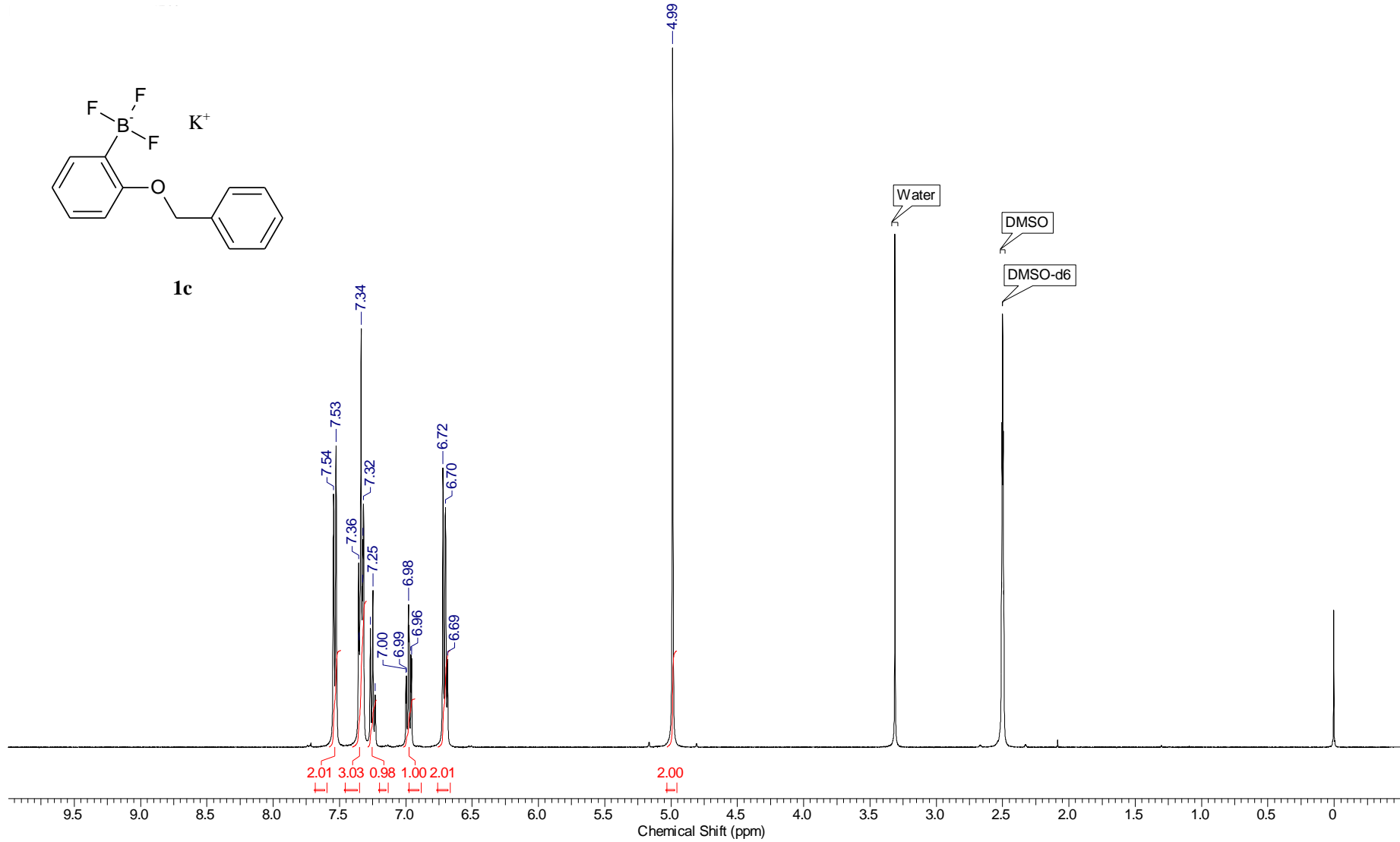
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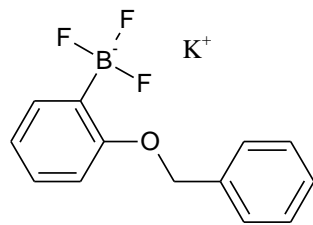
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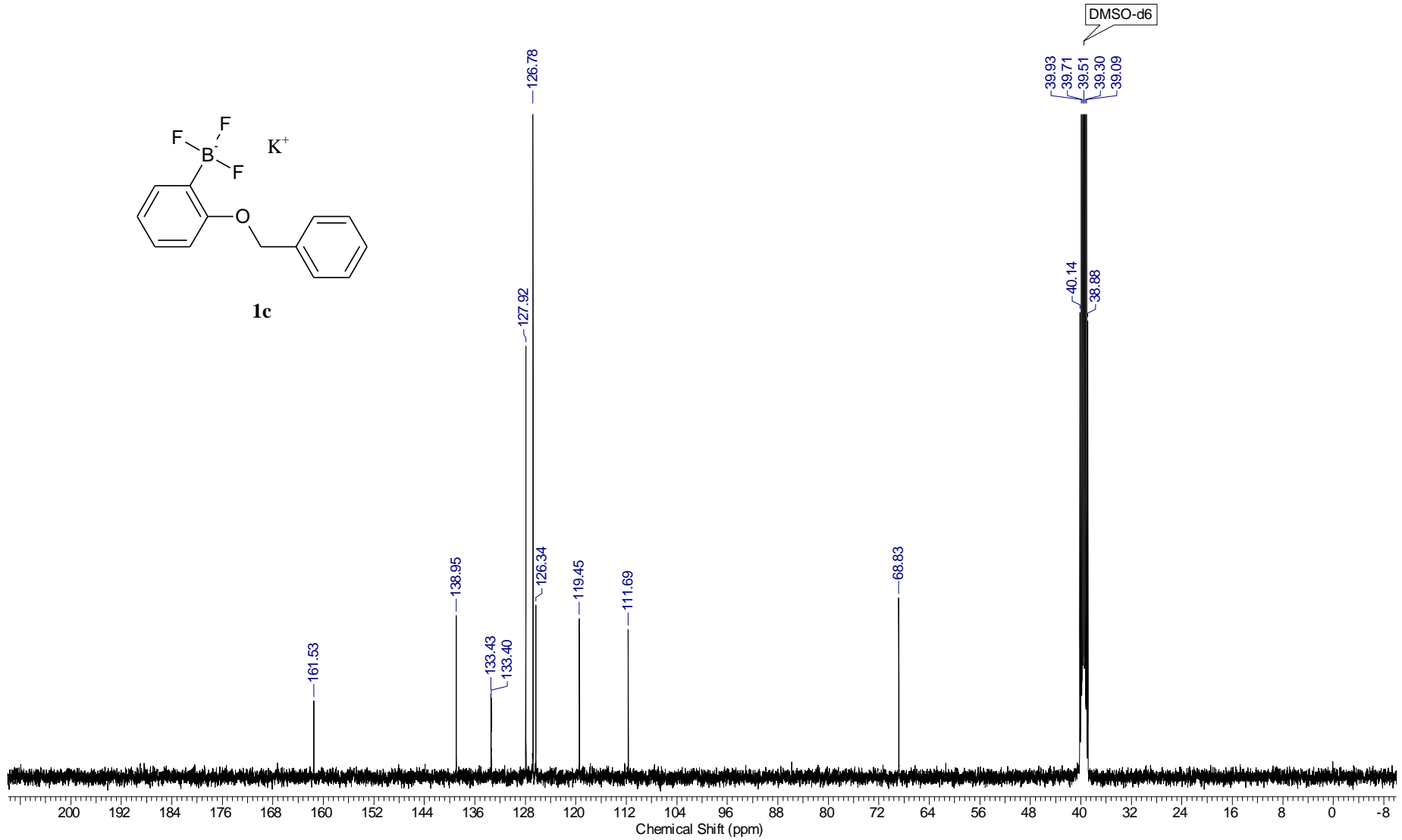
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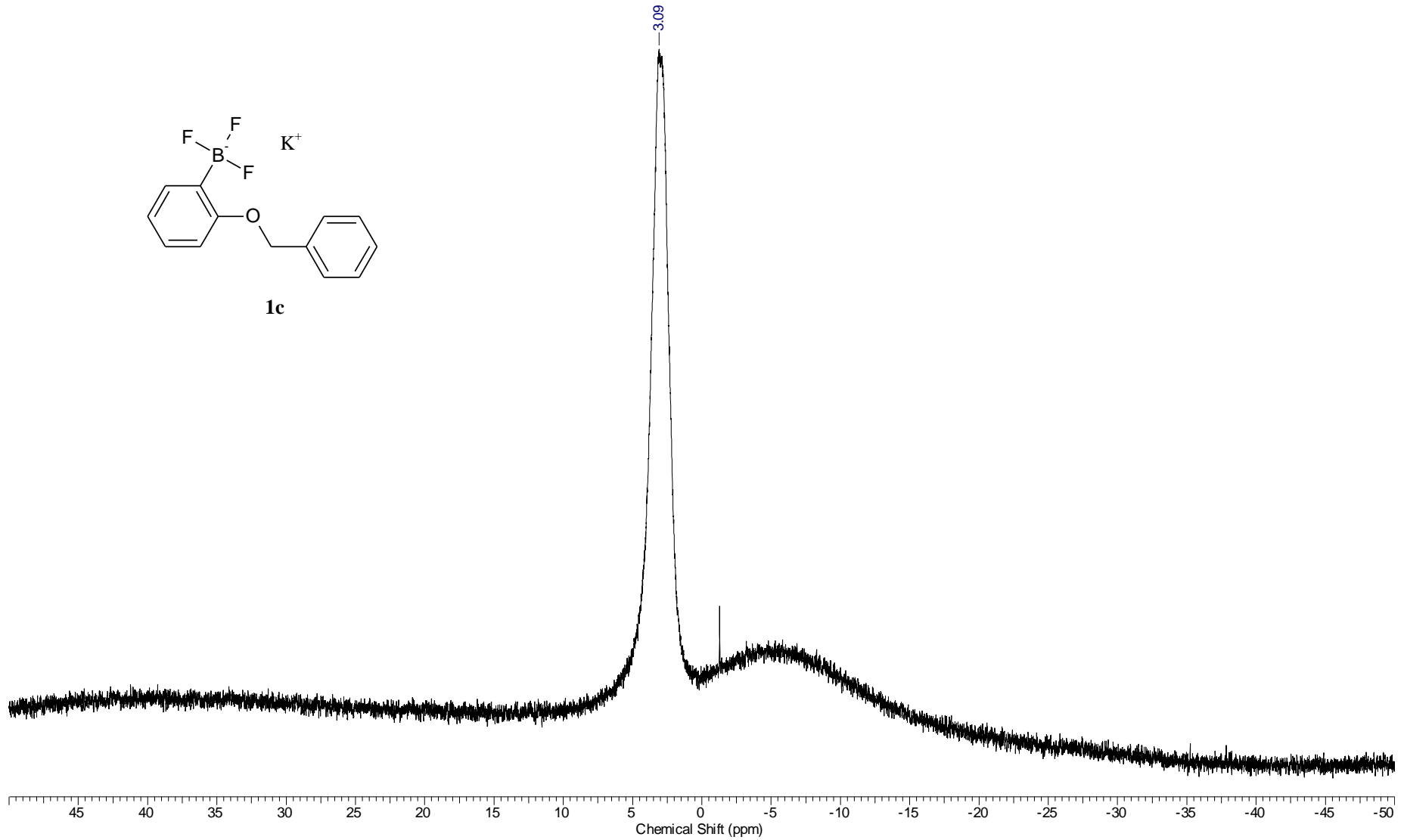
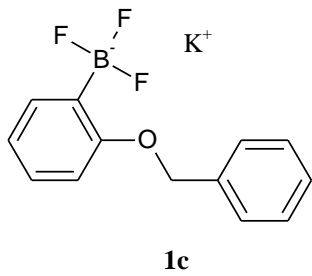
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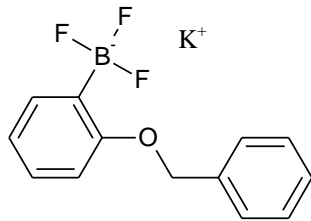
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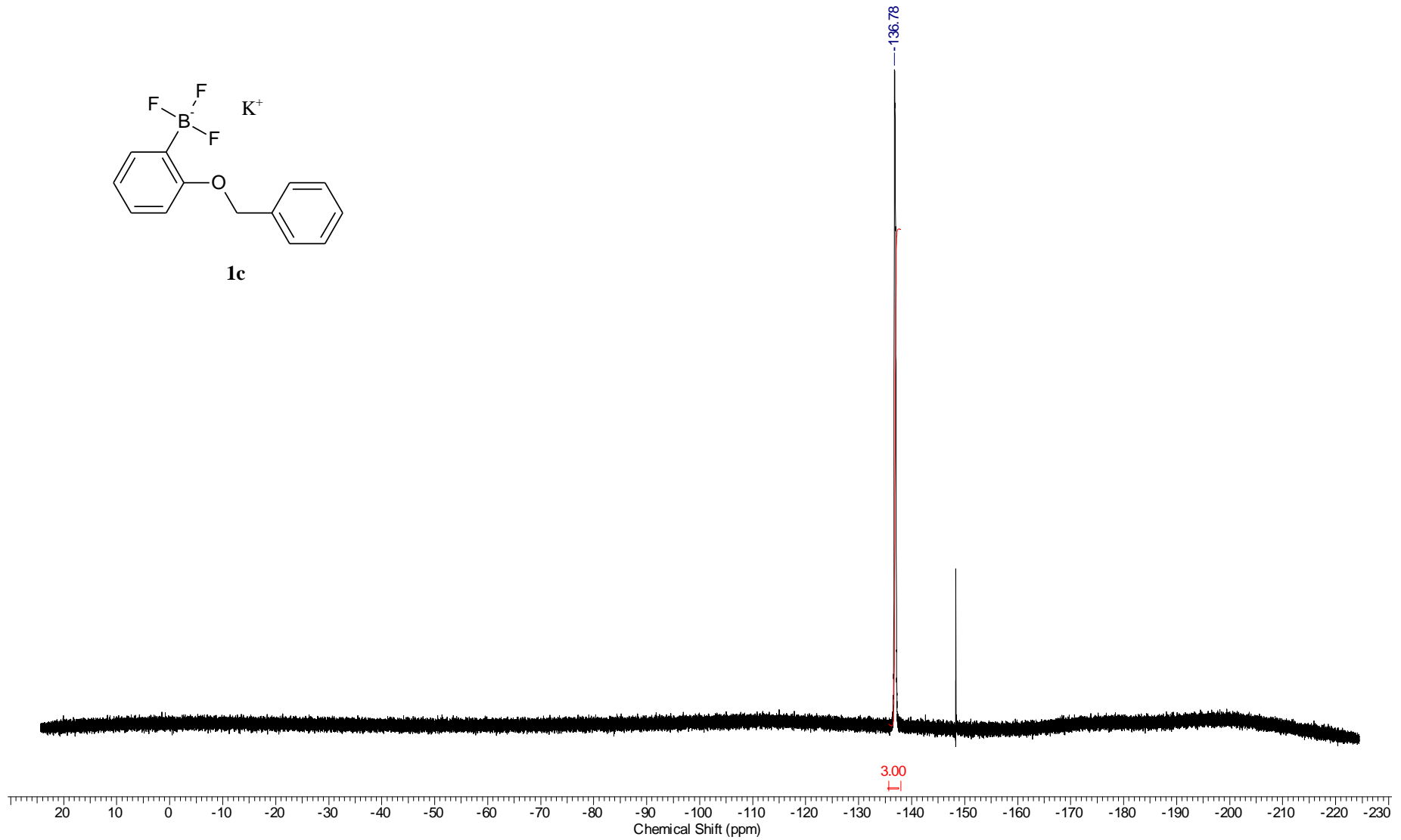
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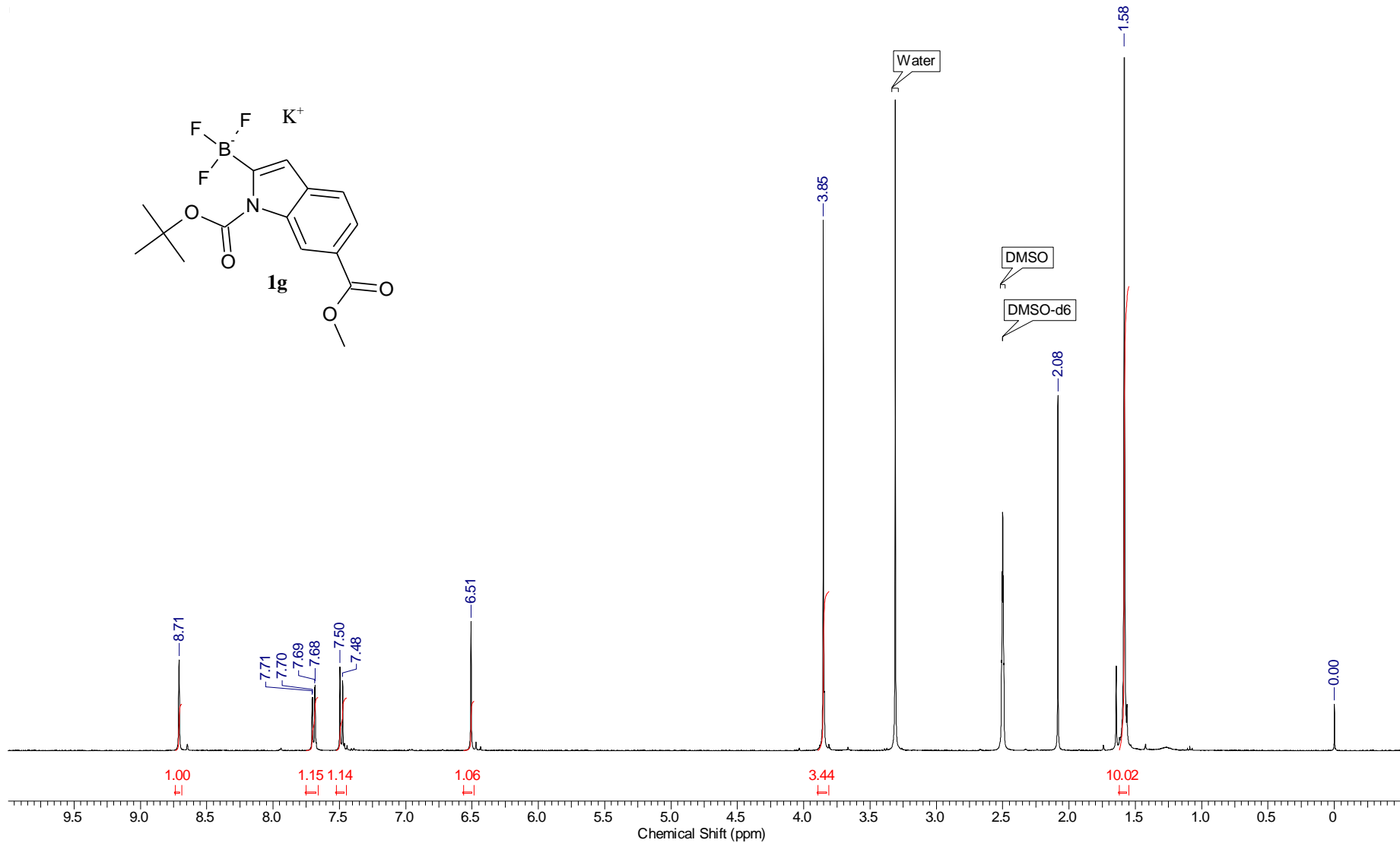
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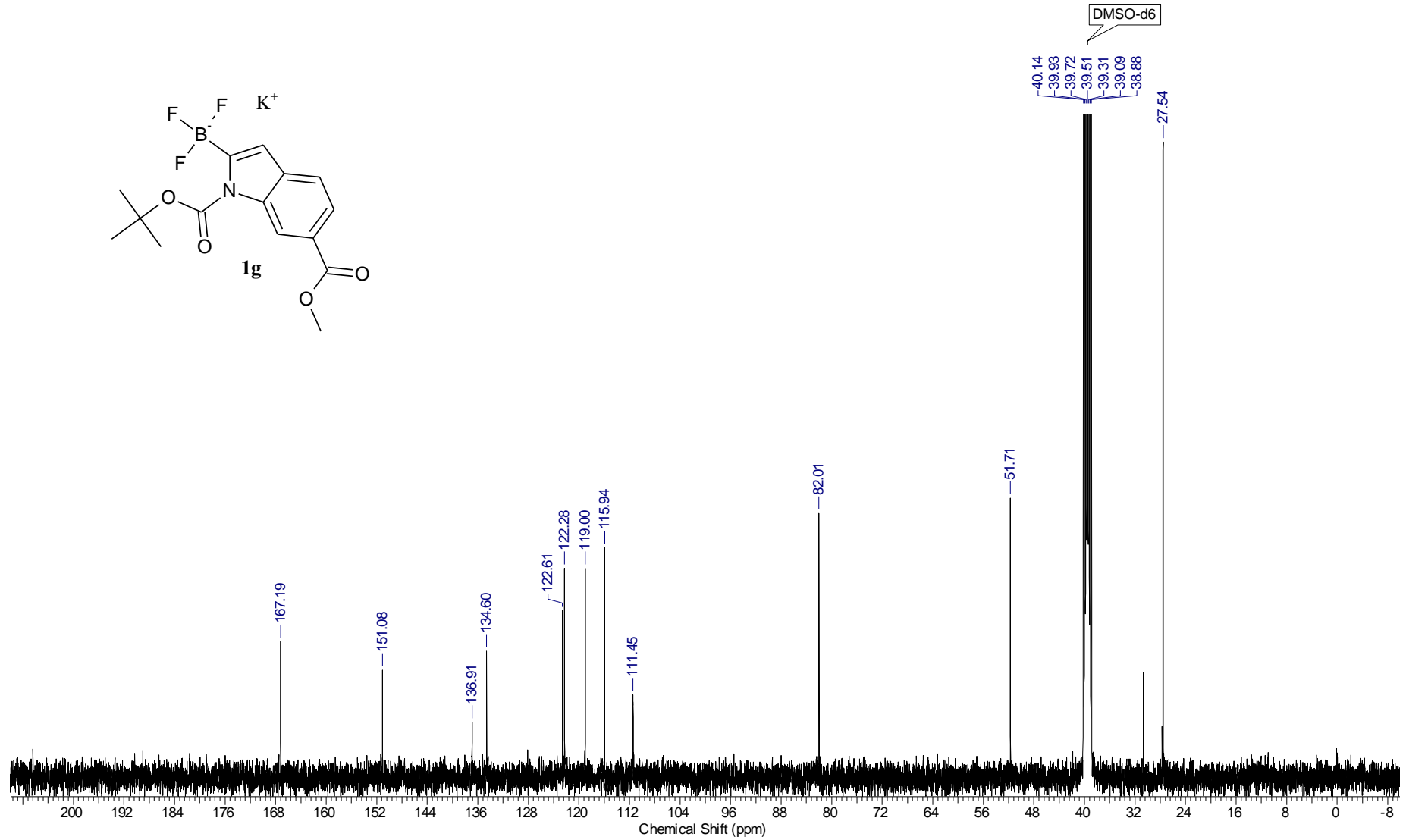
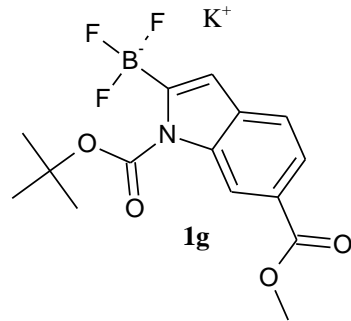
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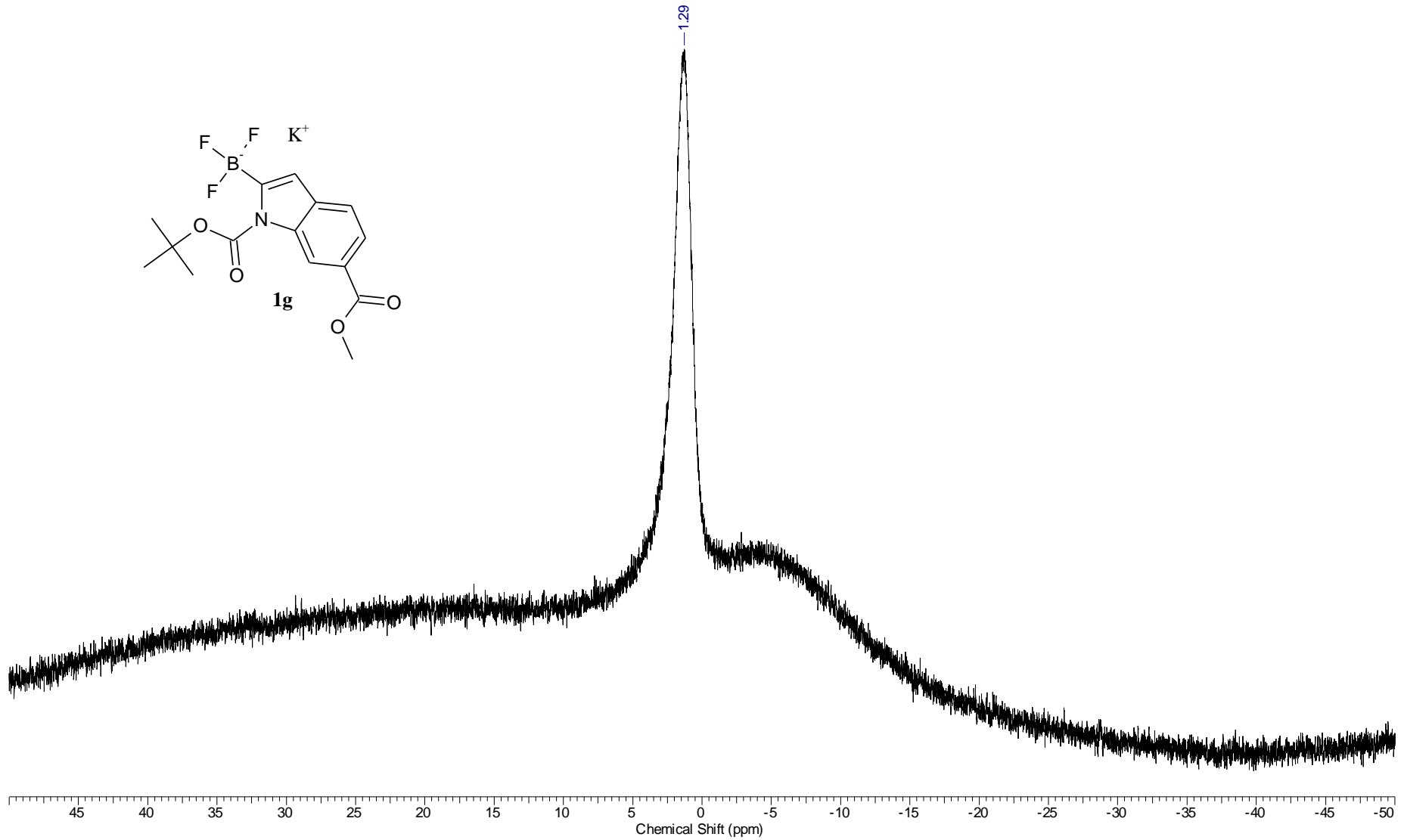
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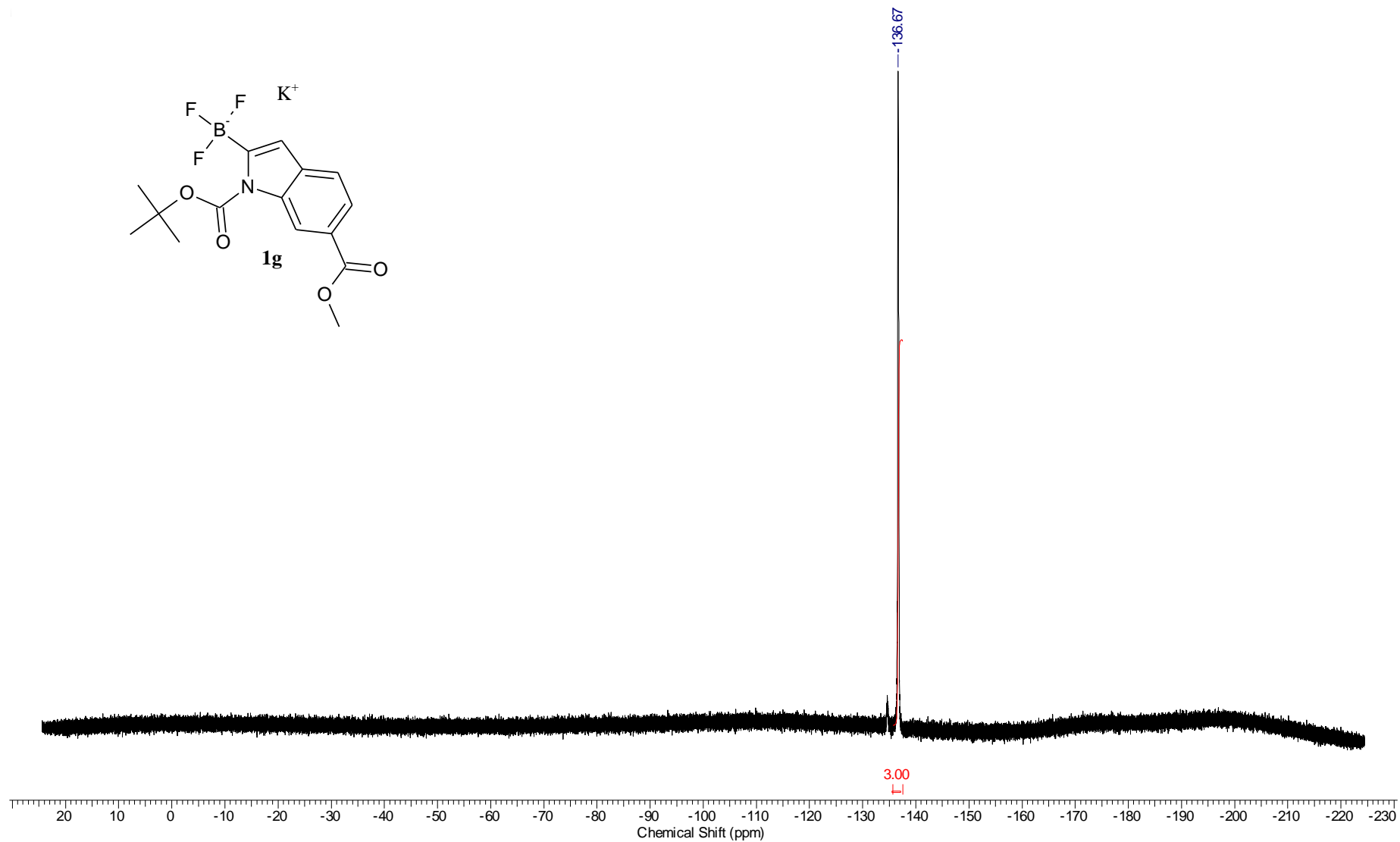
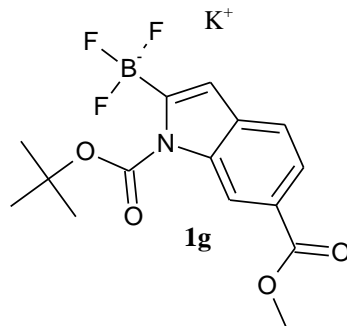
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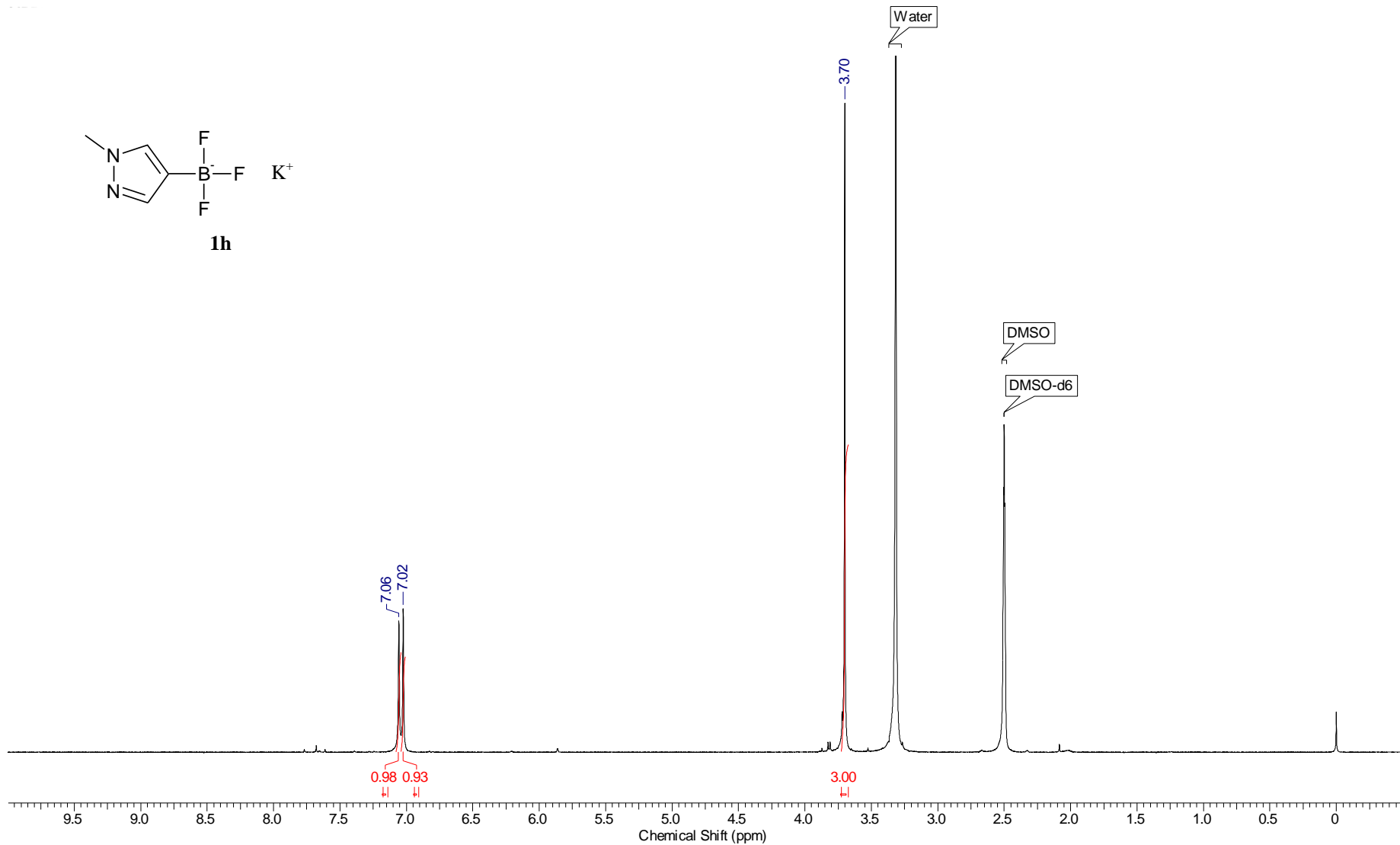
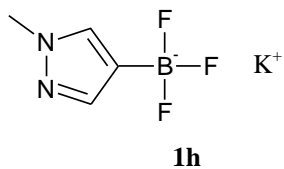
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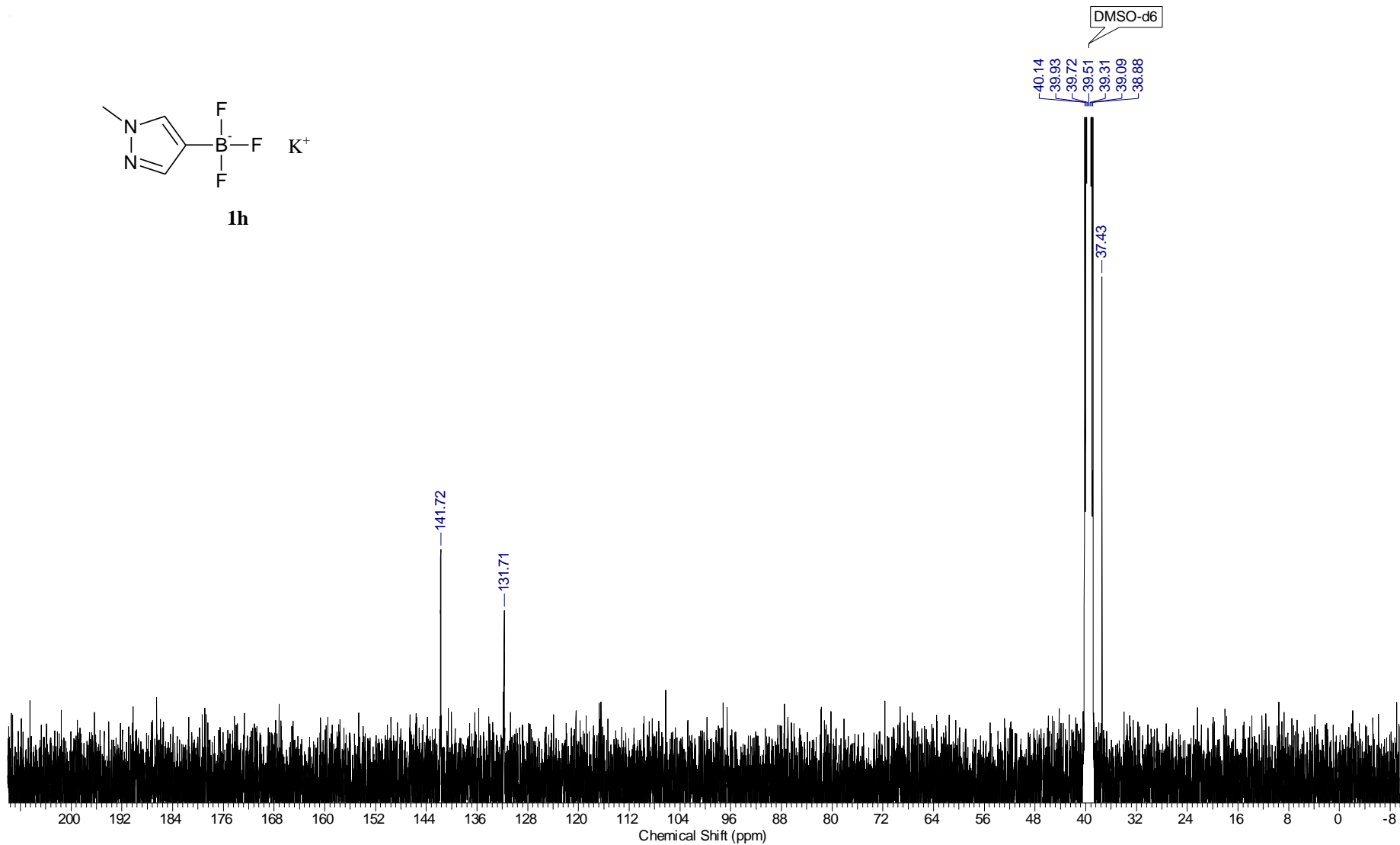
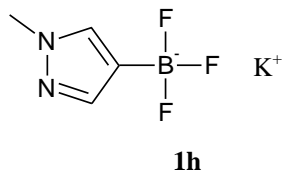
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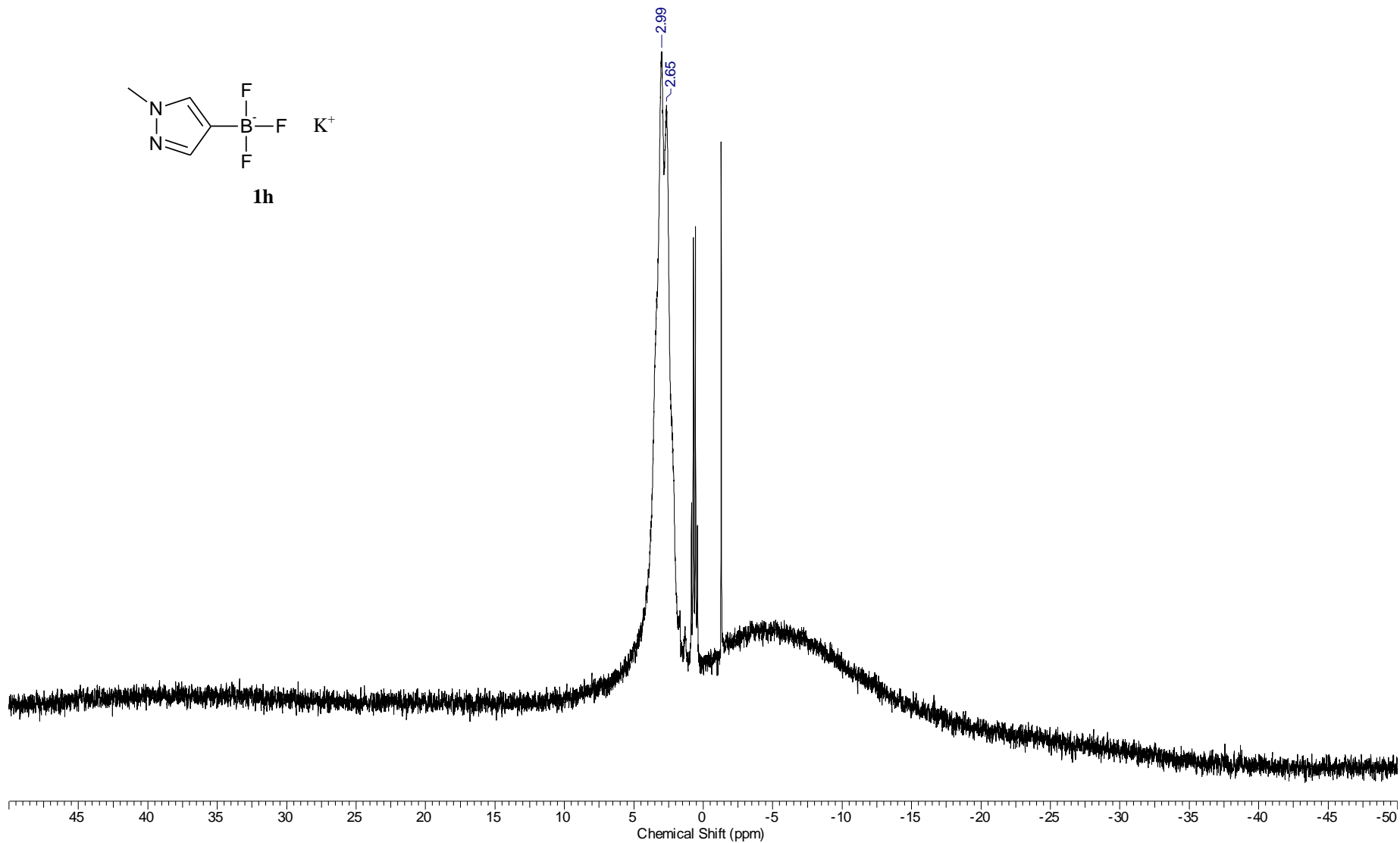
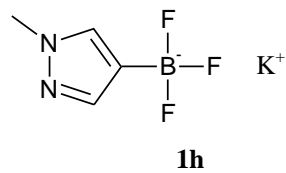
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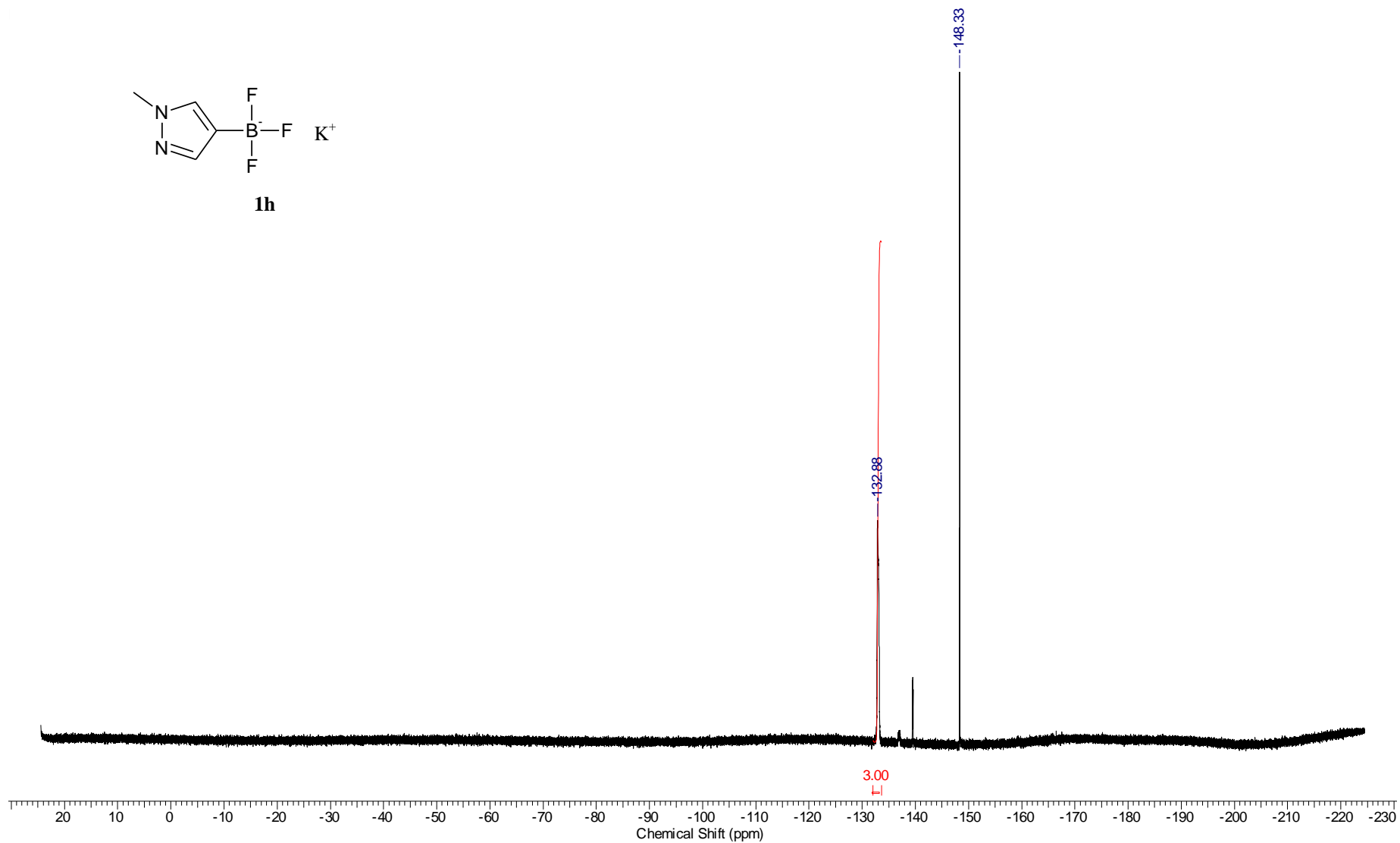
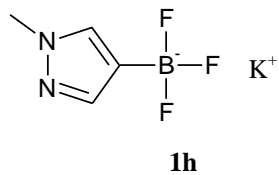
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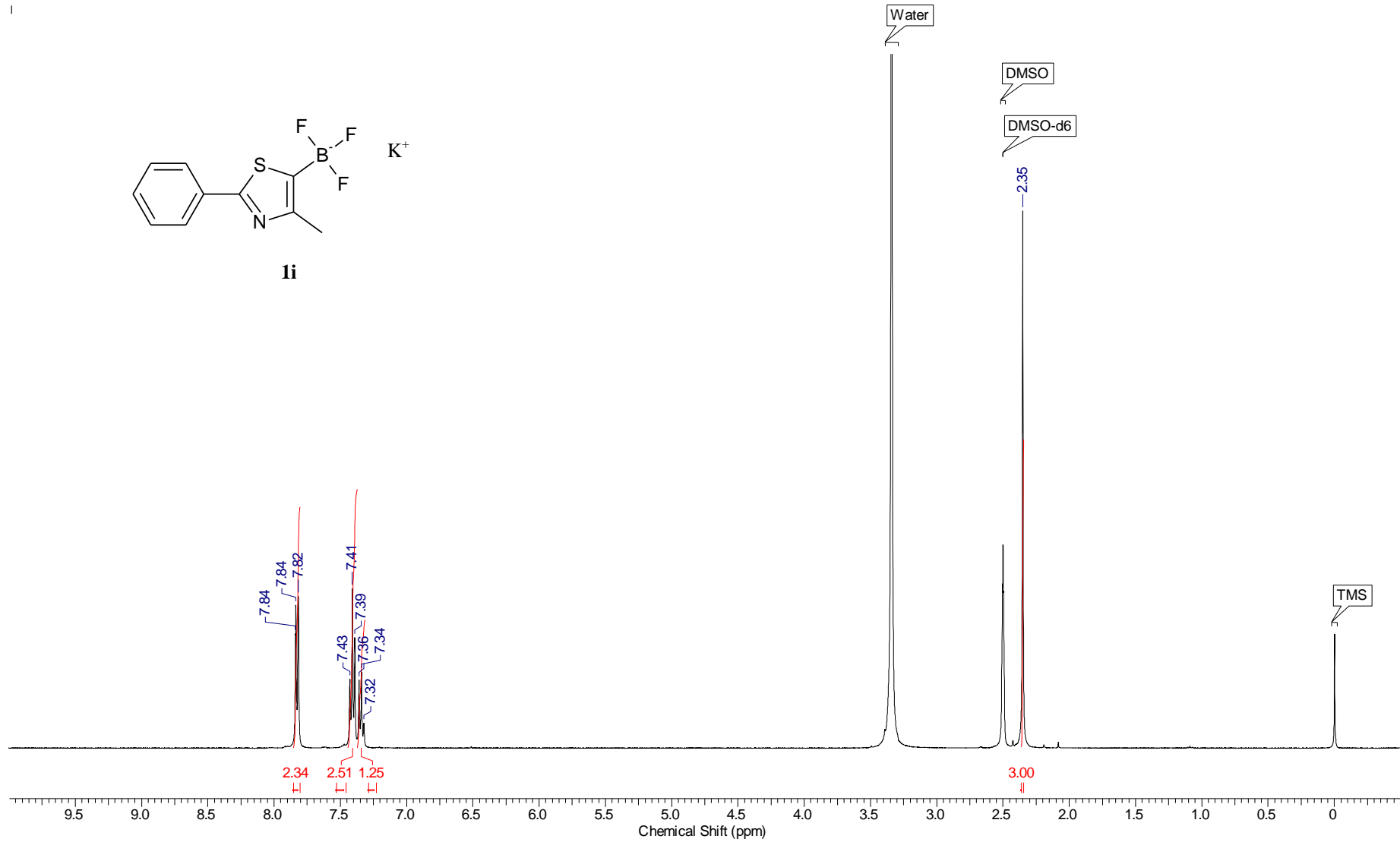
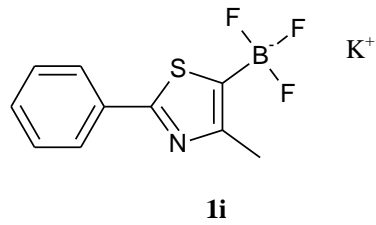
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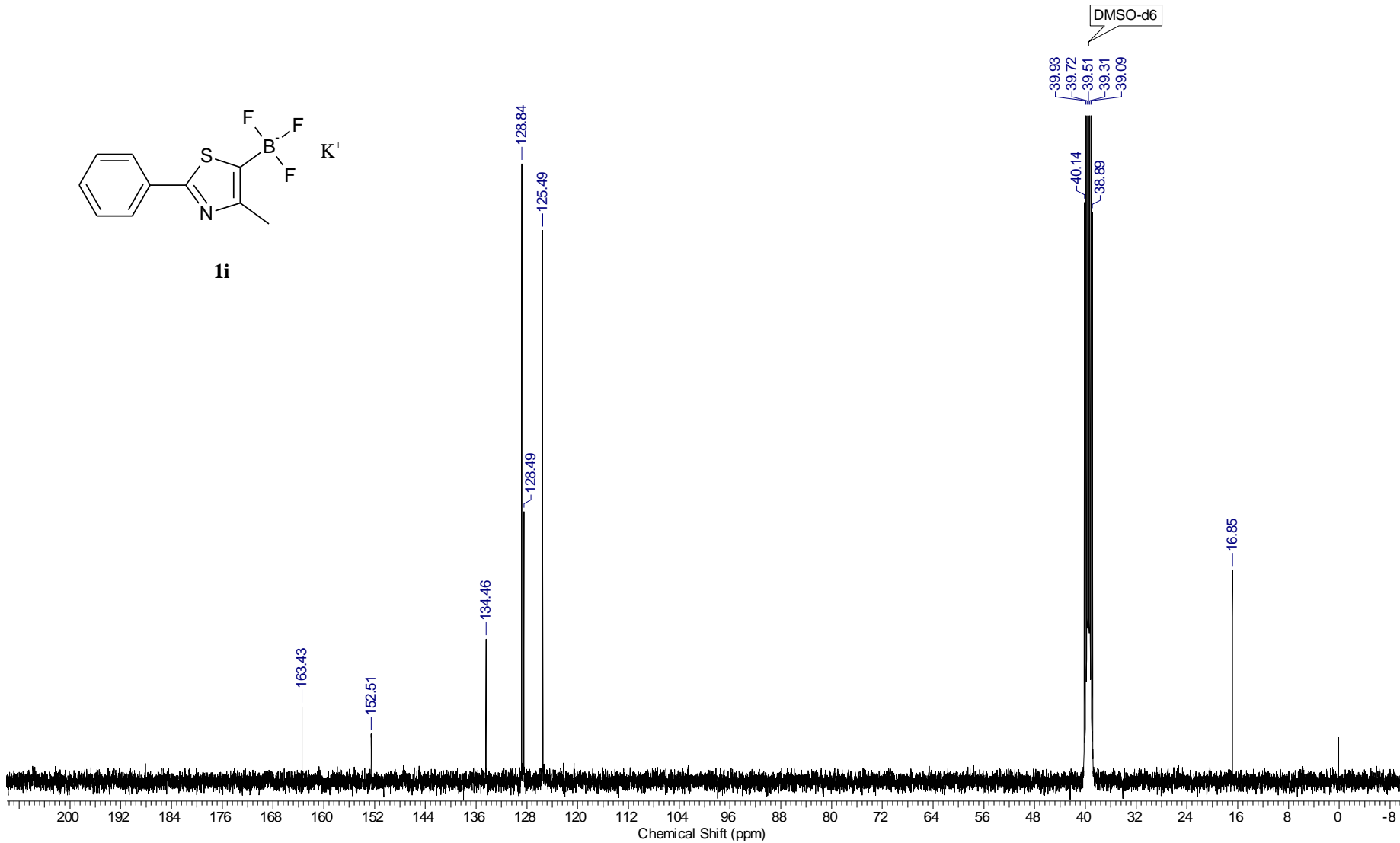
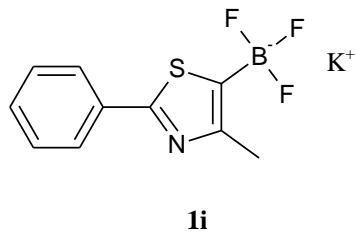
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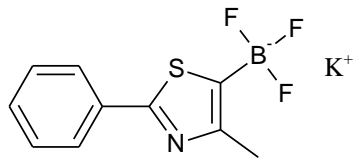
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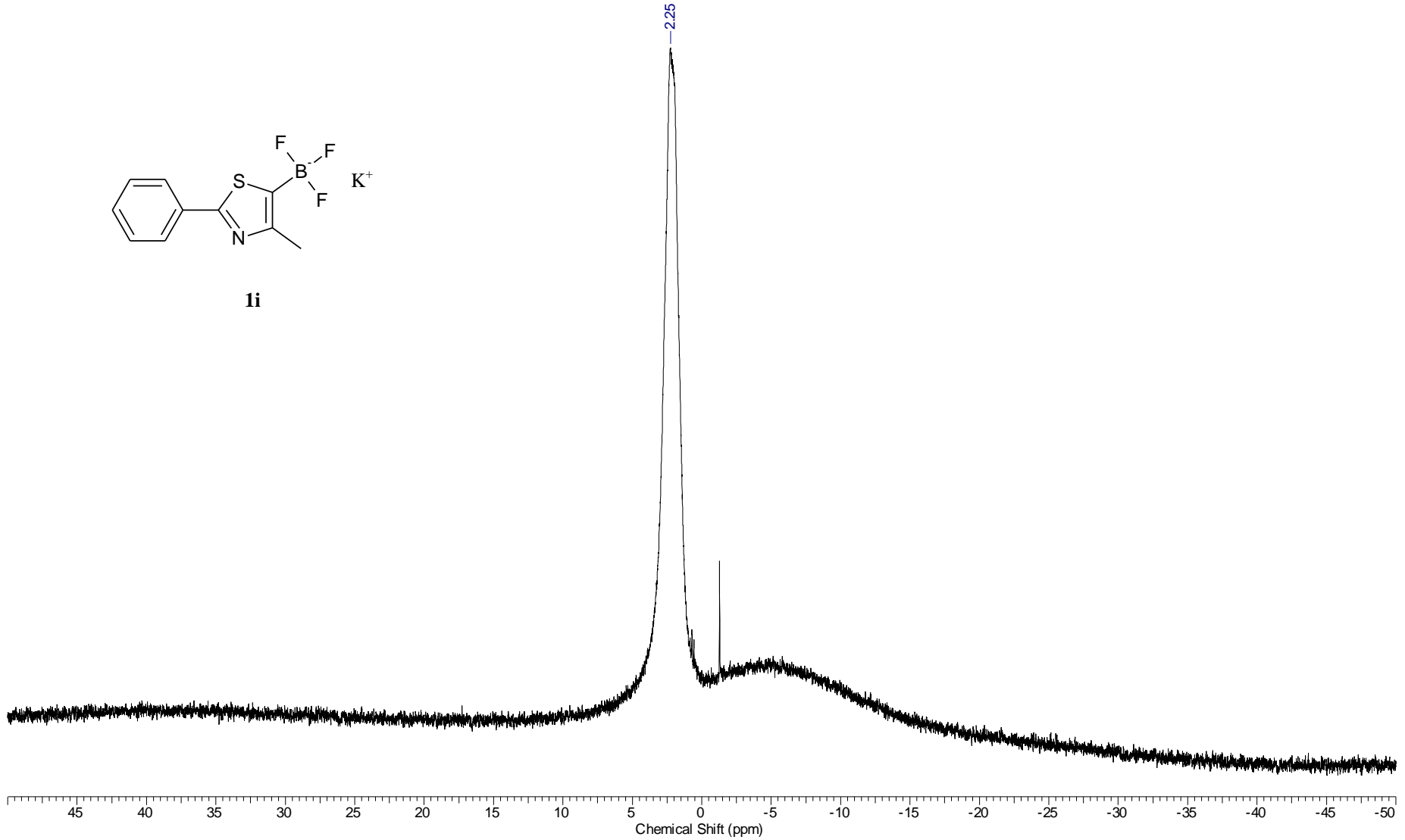
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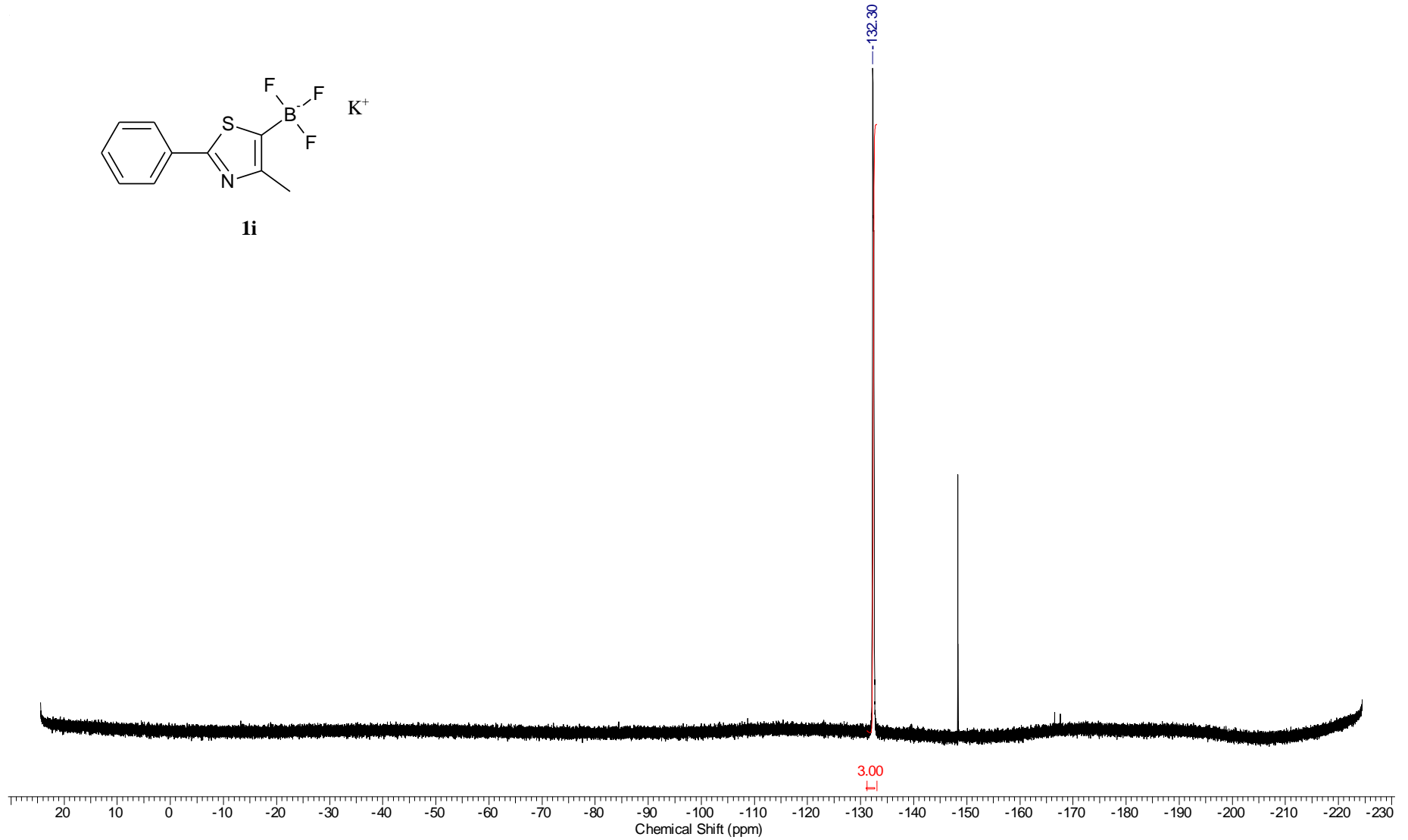
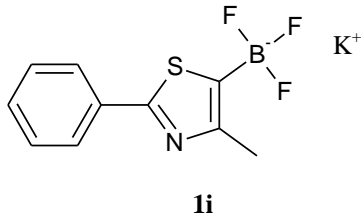
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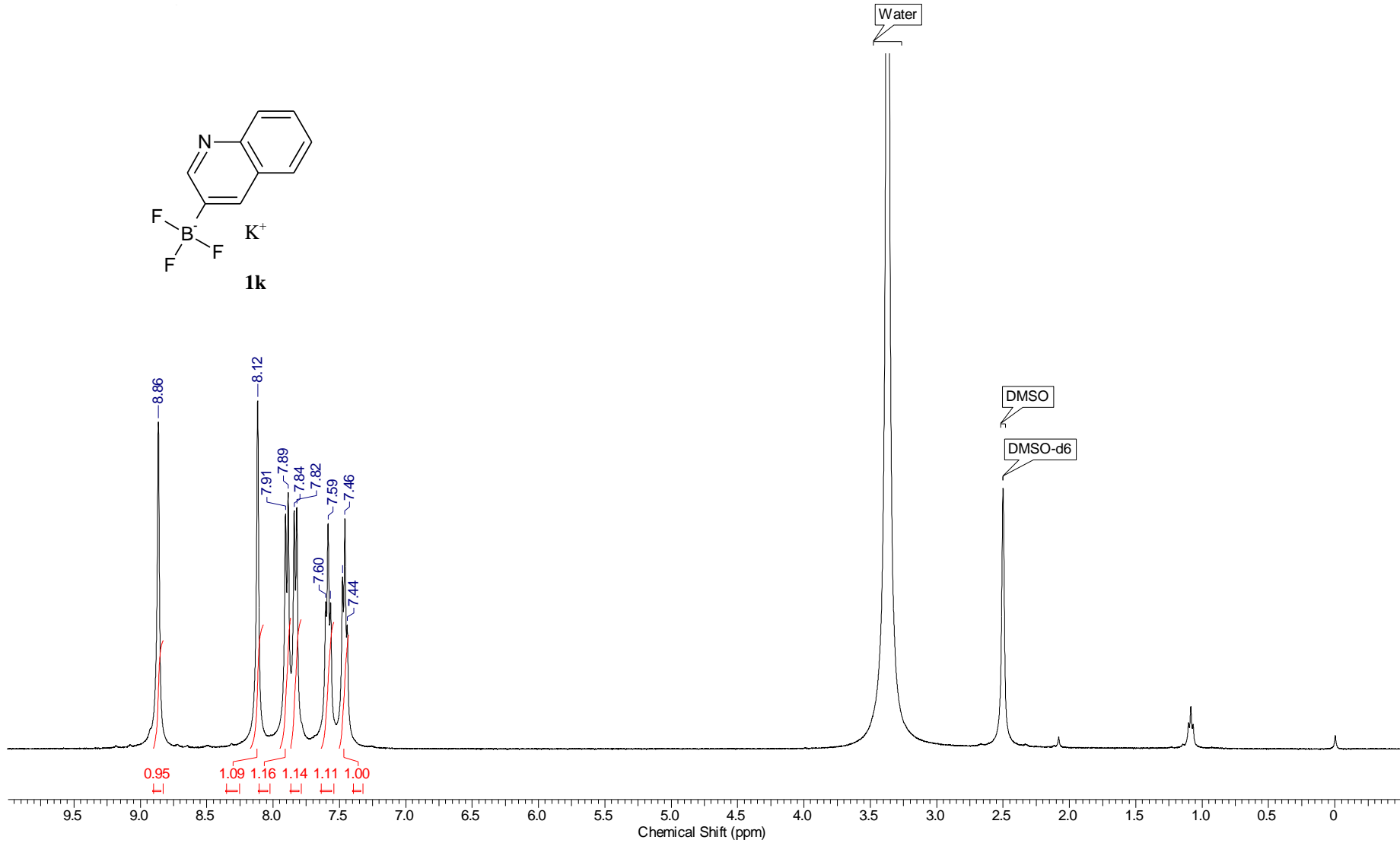
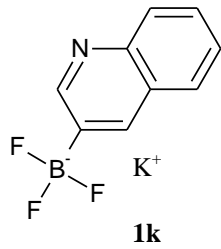
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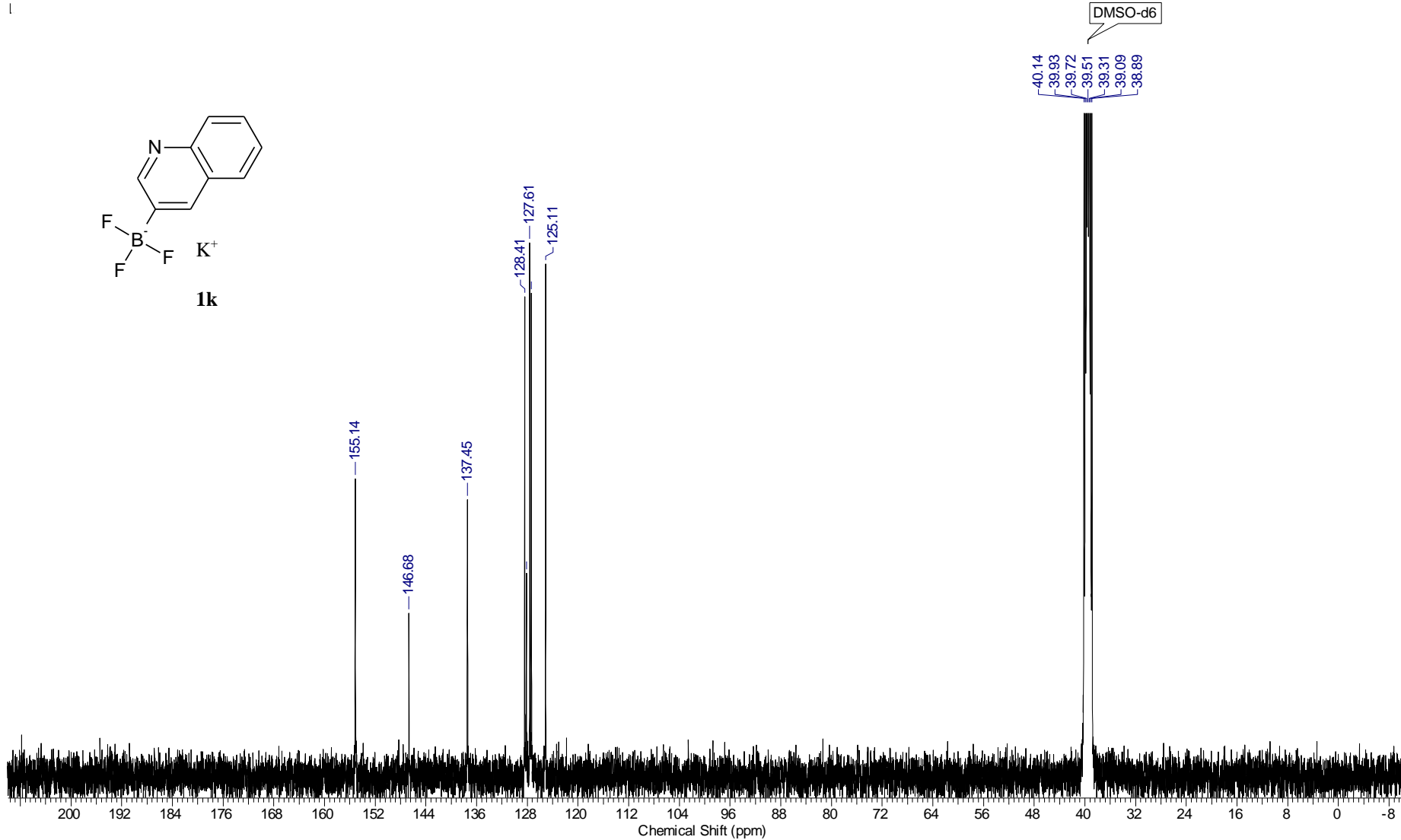
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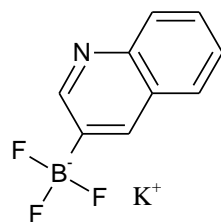
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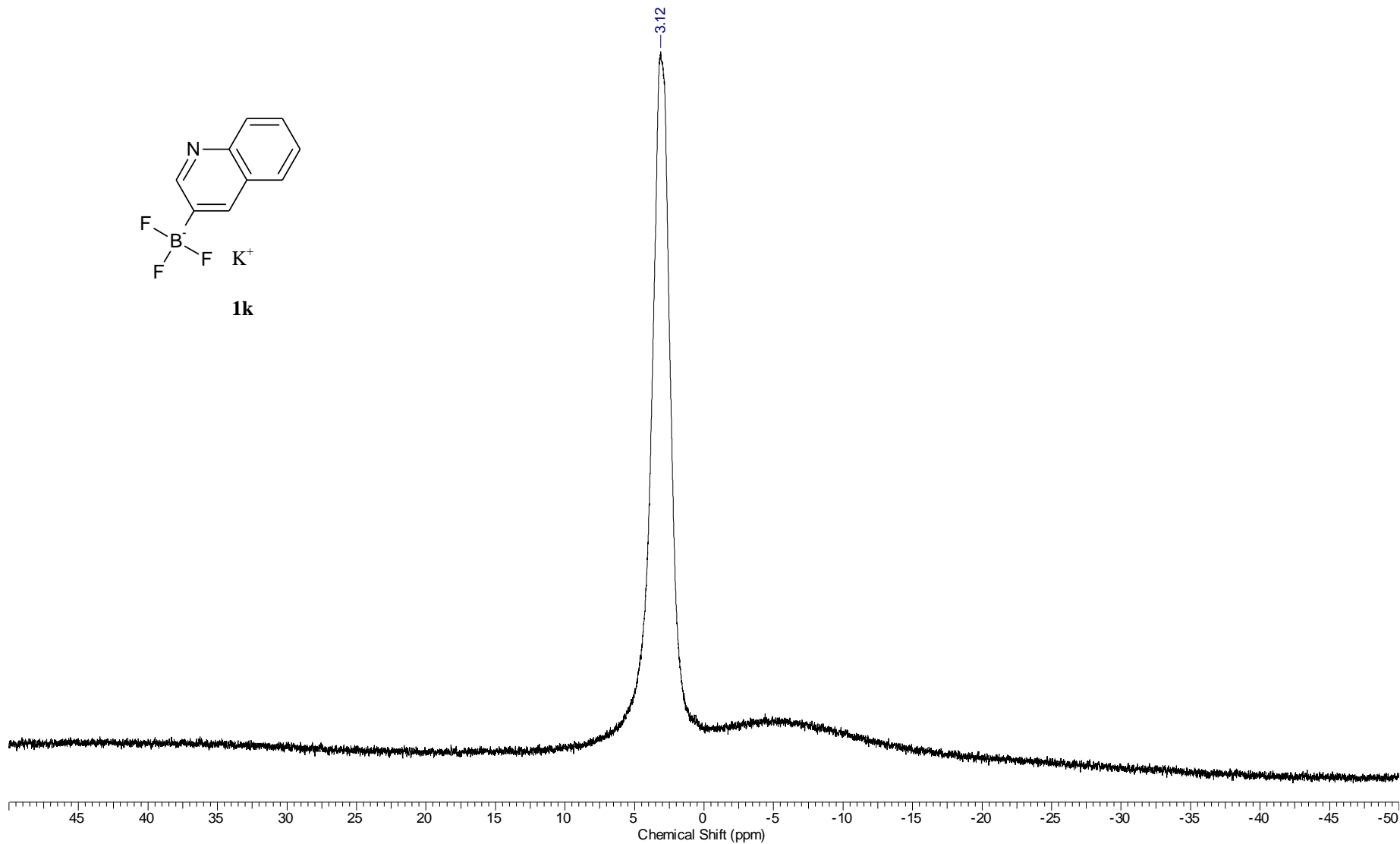
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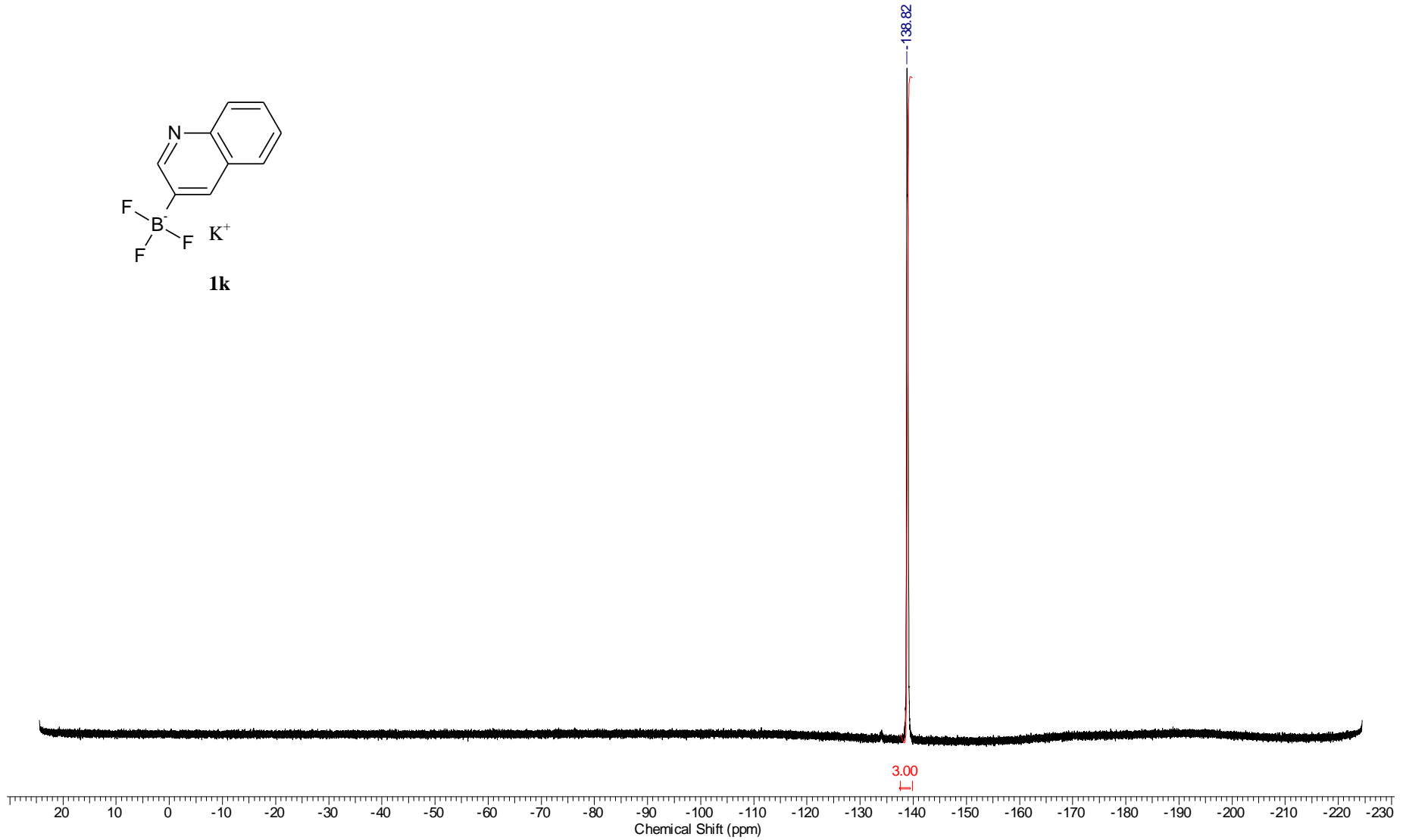
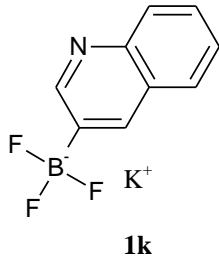
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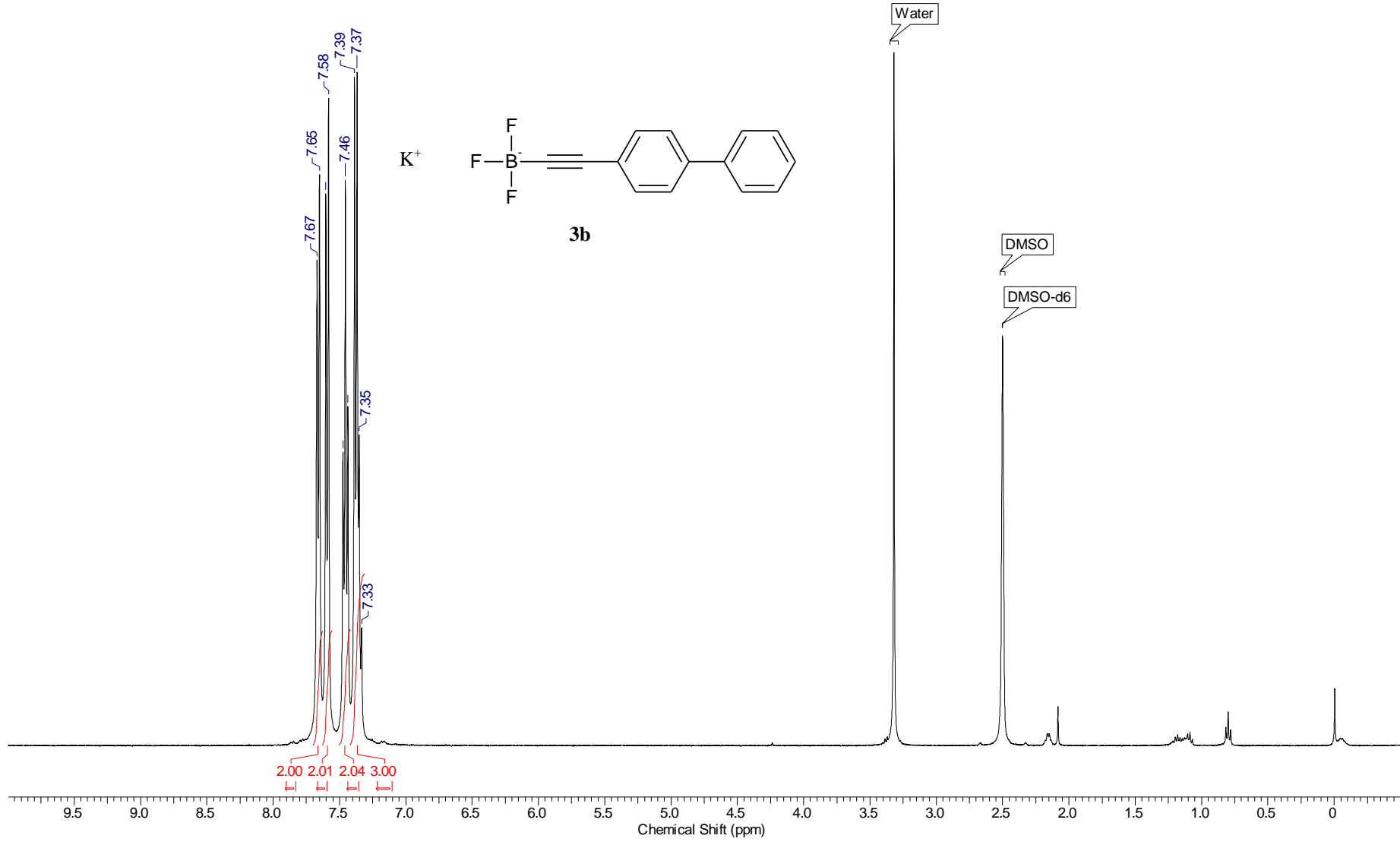
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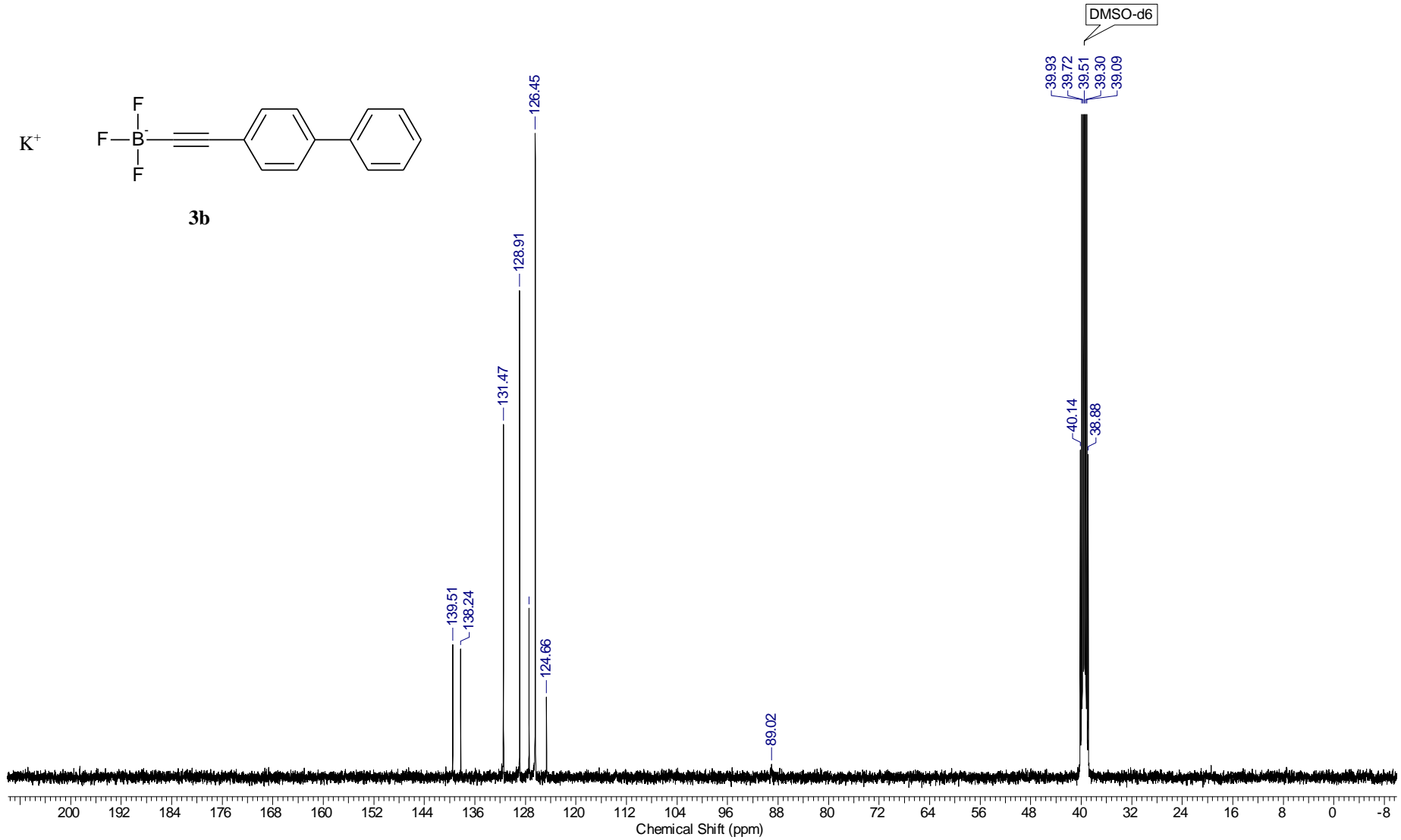
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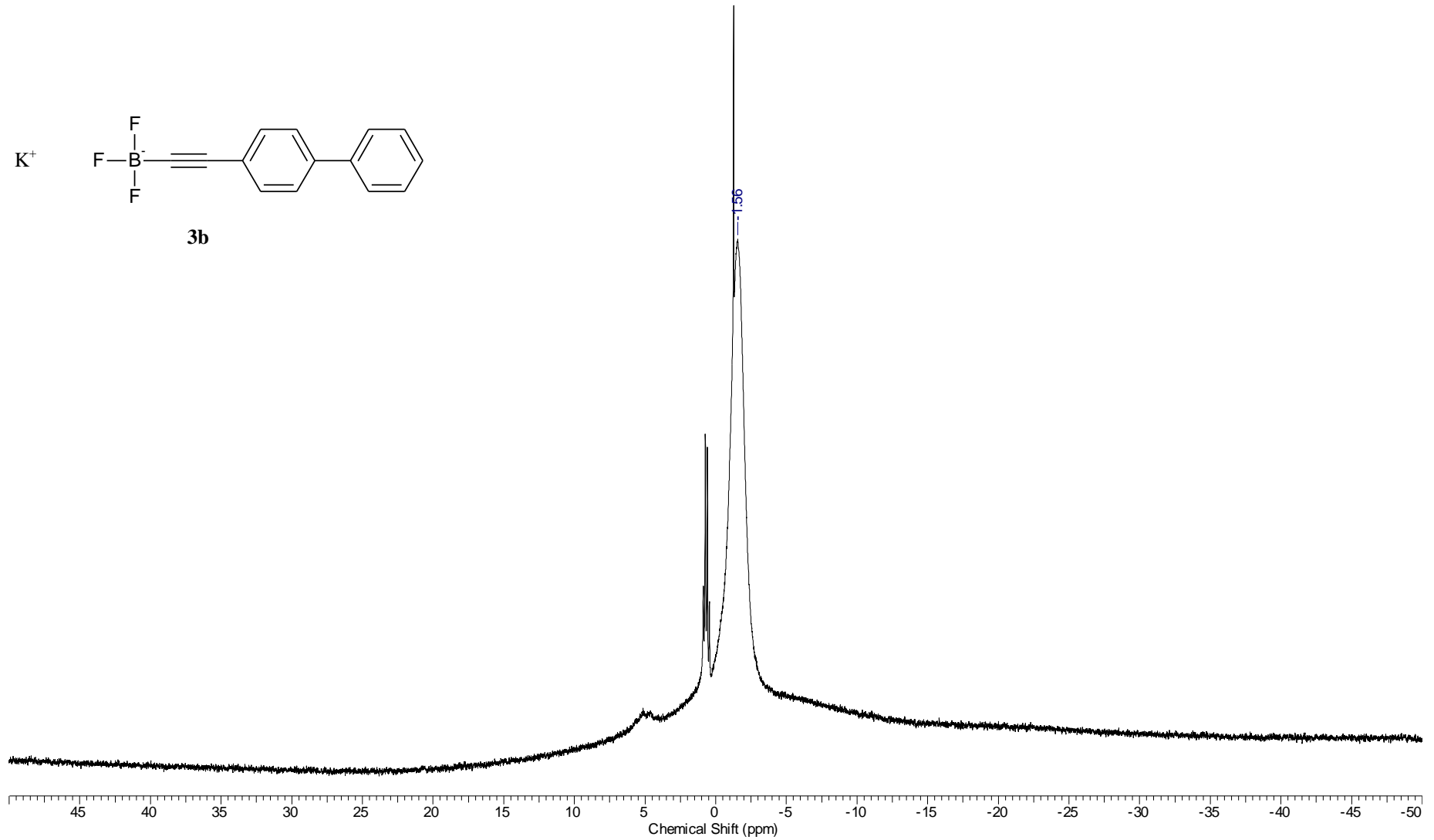
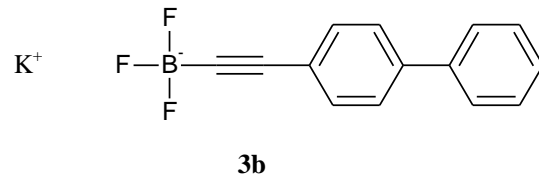
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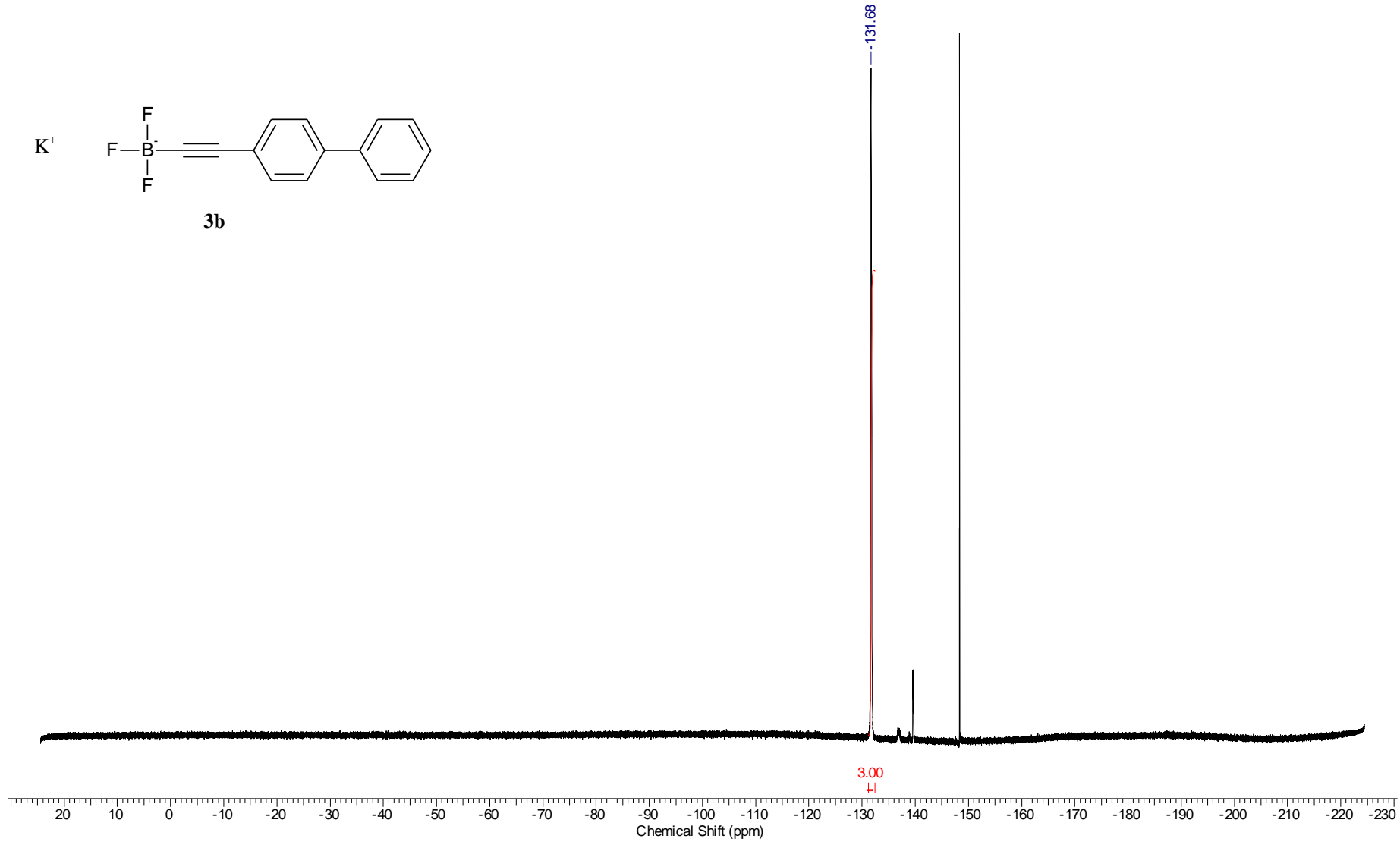
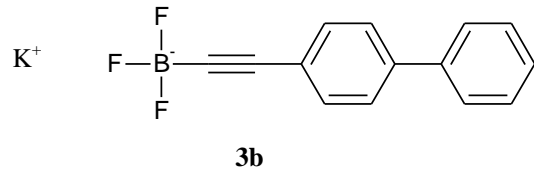
Frequency (MHz)	100.69	Nucleus	¹³ C	Number of Transients	1024	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	SW(cyclical) (Hz)	24037.73
Solvent	DMSO-d6	Spectrum Offset (Hz)	10016.6982	Sweep Width (Hz)	24036.99	Temperature (degree C)	27.000



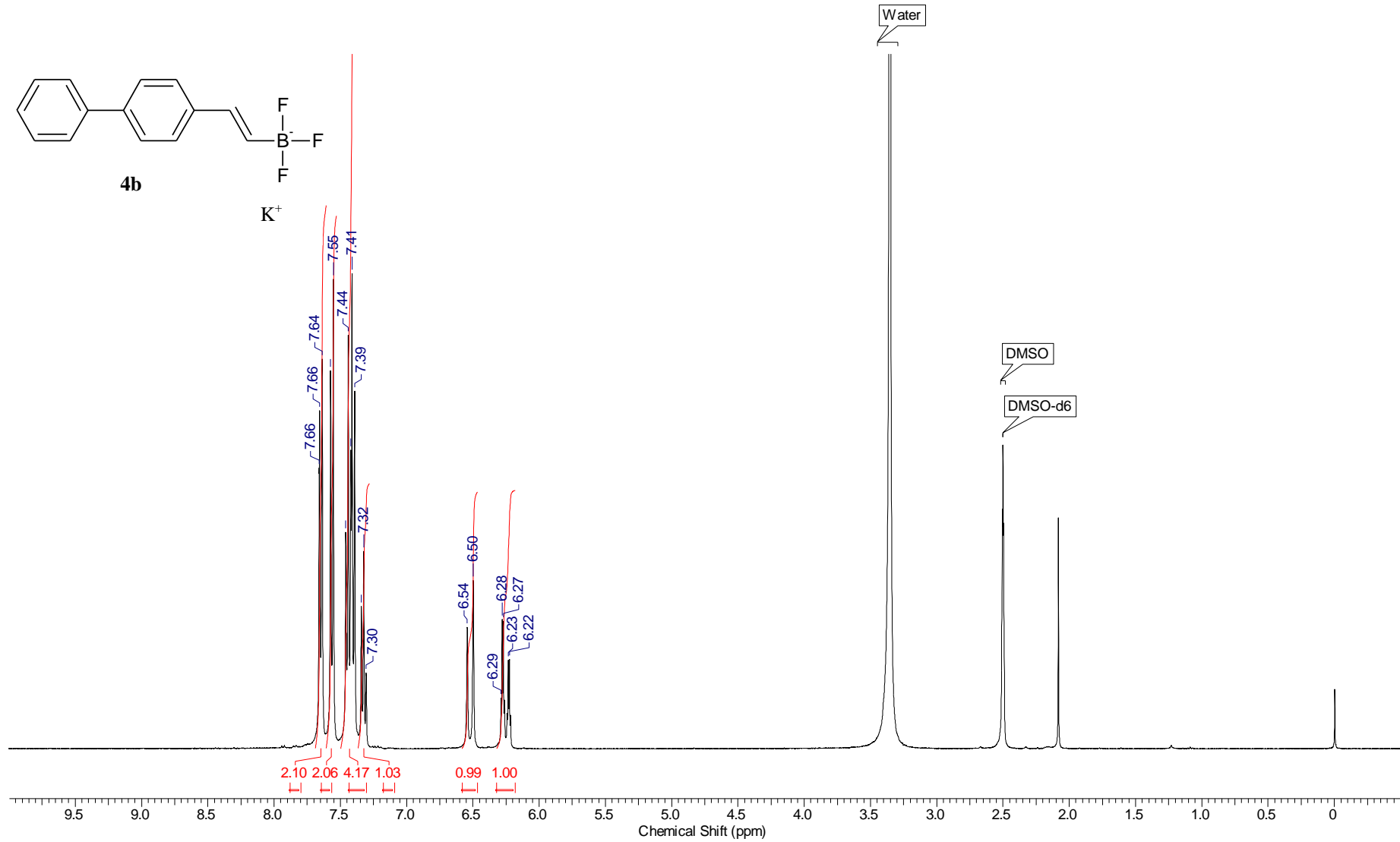
Frequency (MHz)	128.46	Nucleus	11B	Number of Transients	128	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	SW(cyclical) (Hz)	25509.43
Solvent	DMSO-d6	Spectrum Offset (Hz)	1.2842	Sweep Width (Hz)	25508.65	Temperature (degree C)	27.000



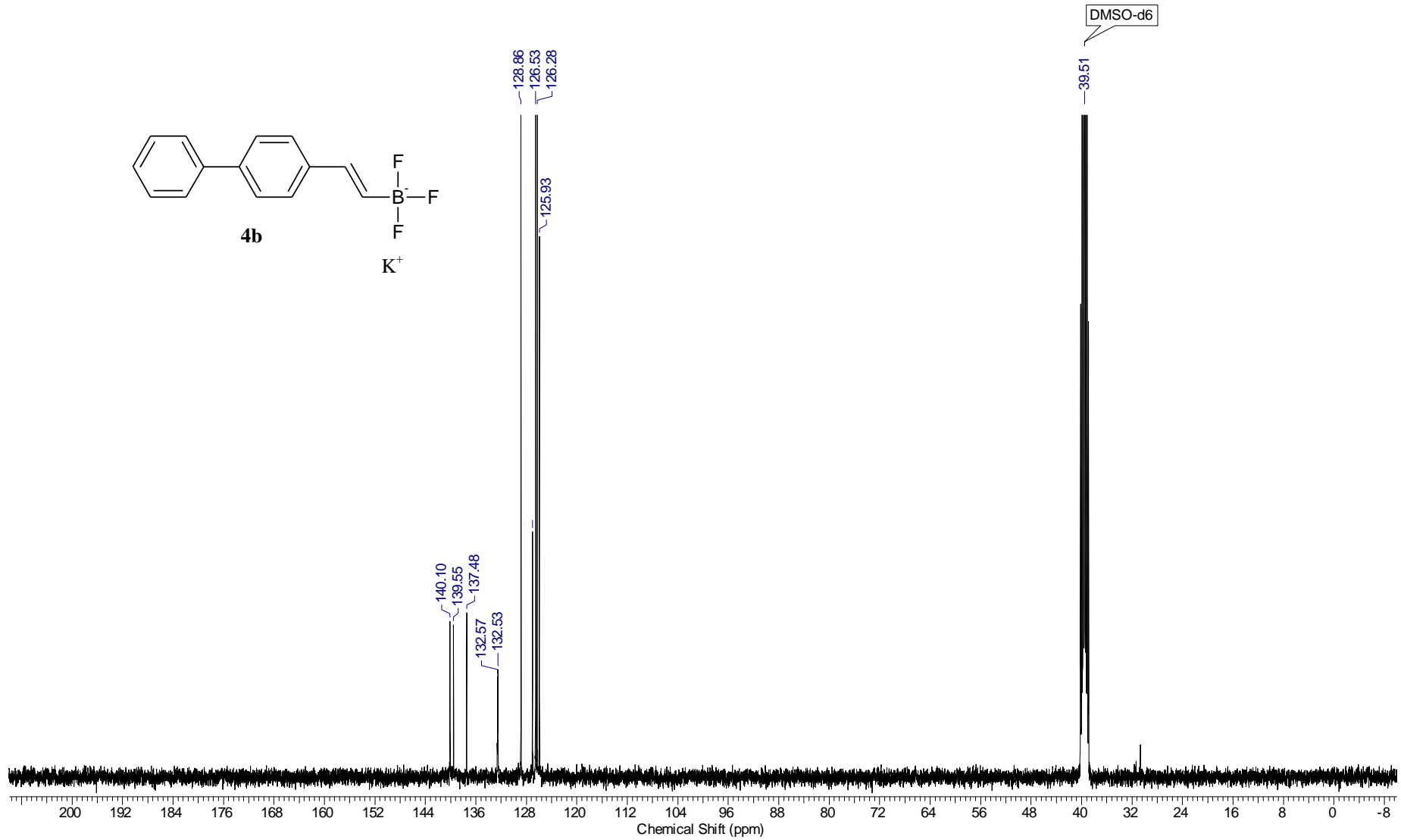
Frequency (MHz)	376.71	Nucleus	¹⁹ F	Number of Transients	64	Origin	Bruker BioSpin GmbH
Original Points Count	131072	Owner	tibbe_operator	Points Count	131072	SW(cyclical) (Hz)	93749.28
Solvent	DMSO-d6	Spectrum Offset (Hz)	-37674.7617	Sweep Width (Hz)	93748.56	Temperature (degree C)	27.000



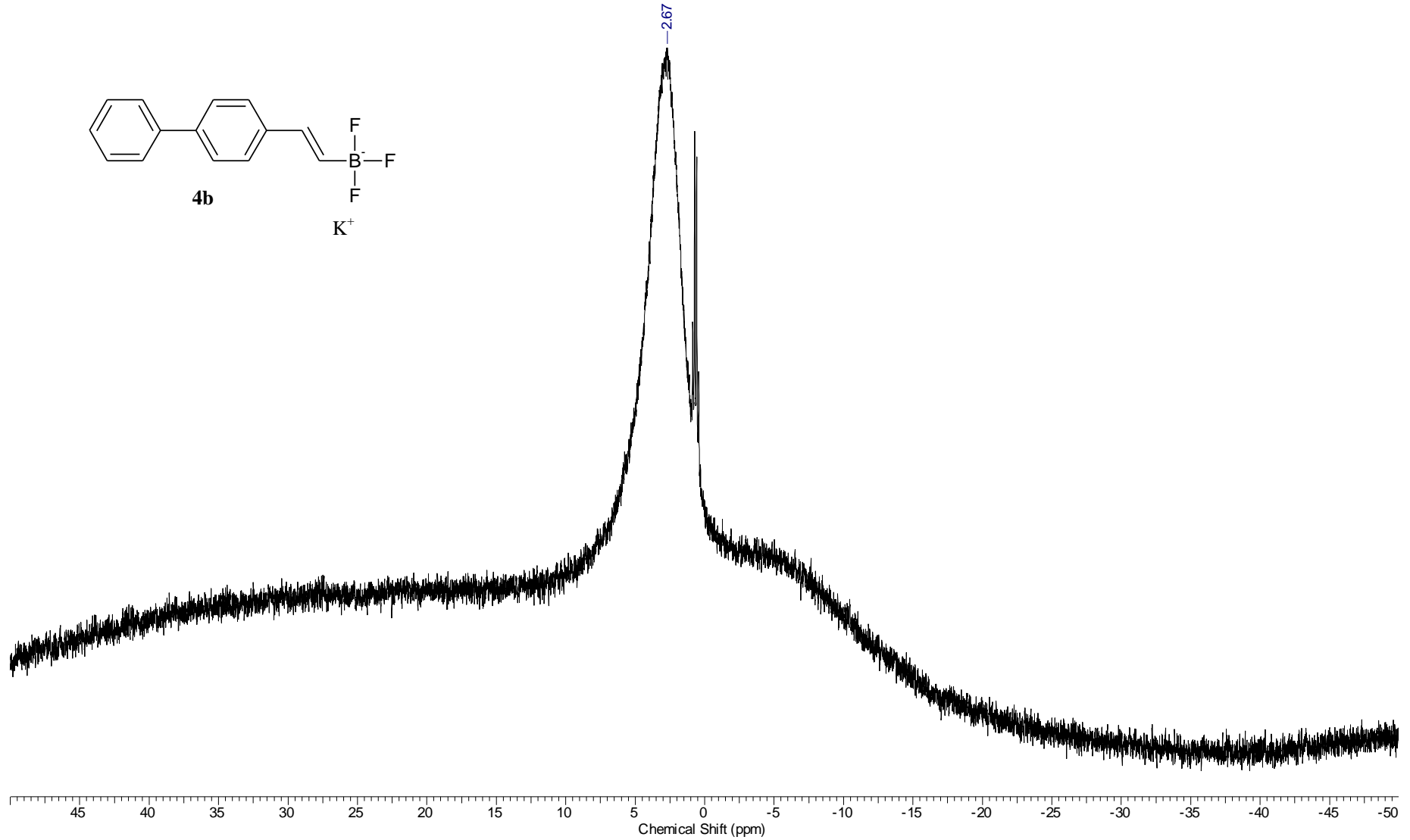
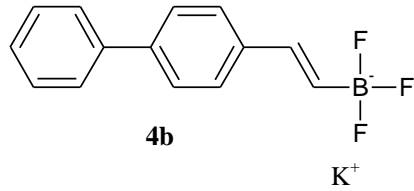
Frequency (MHz)	400.40	Nucleus	1H	Number of Transients	16	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	SW(cyclical) (Hz)	7211.32
Solvent	DMSO-d6	Spectrum Offset (Hz)	3398.5825	Sweep Width (Hz)	7211.10	Temperature (degree C)	27.000



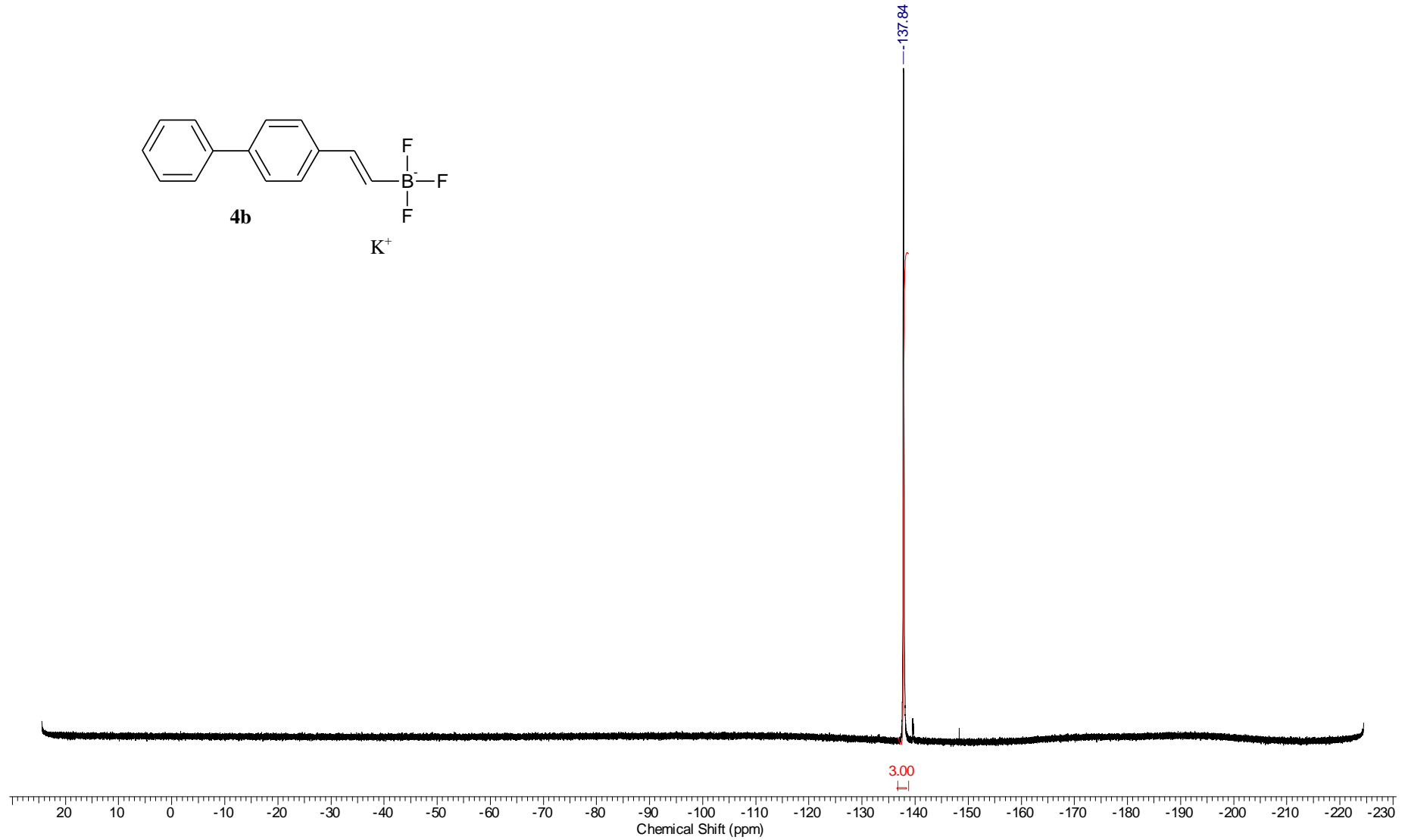
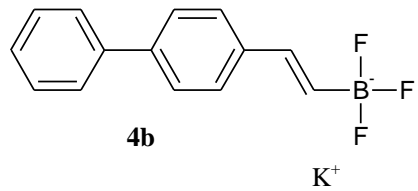
Frequency (MHz)	100.69	Nucleus	¹³ C	Number of Transients	1024	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	SW(cyclical) (Hz)	24037.73
Solvent	DMSO-d6	Spectrum Offset (Hz)	10020.3662	Sweep Width (Hz)	24036.99	Temperature (degree C)	27.000



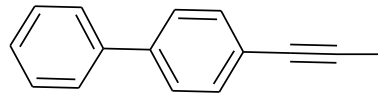
Frequency (MHz)	128.46	Nucleus	11B	Number of Transients	128	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	SW(cyclical) (Hz)	25509.43
Solvent	DMSO-d6	Spectrum Offset (Hz)	1.2842	Sweep Width (Hz)	25508.65	Temperature (degree C)	27.000



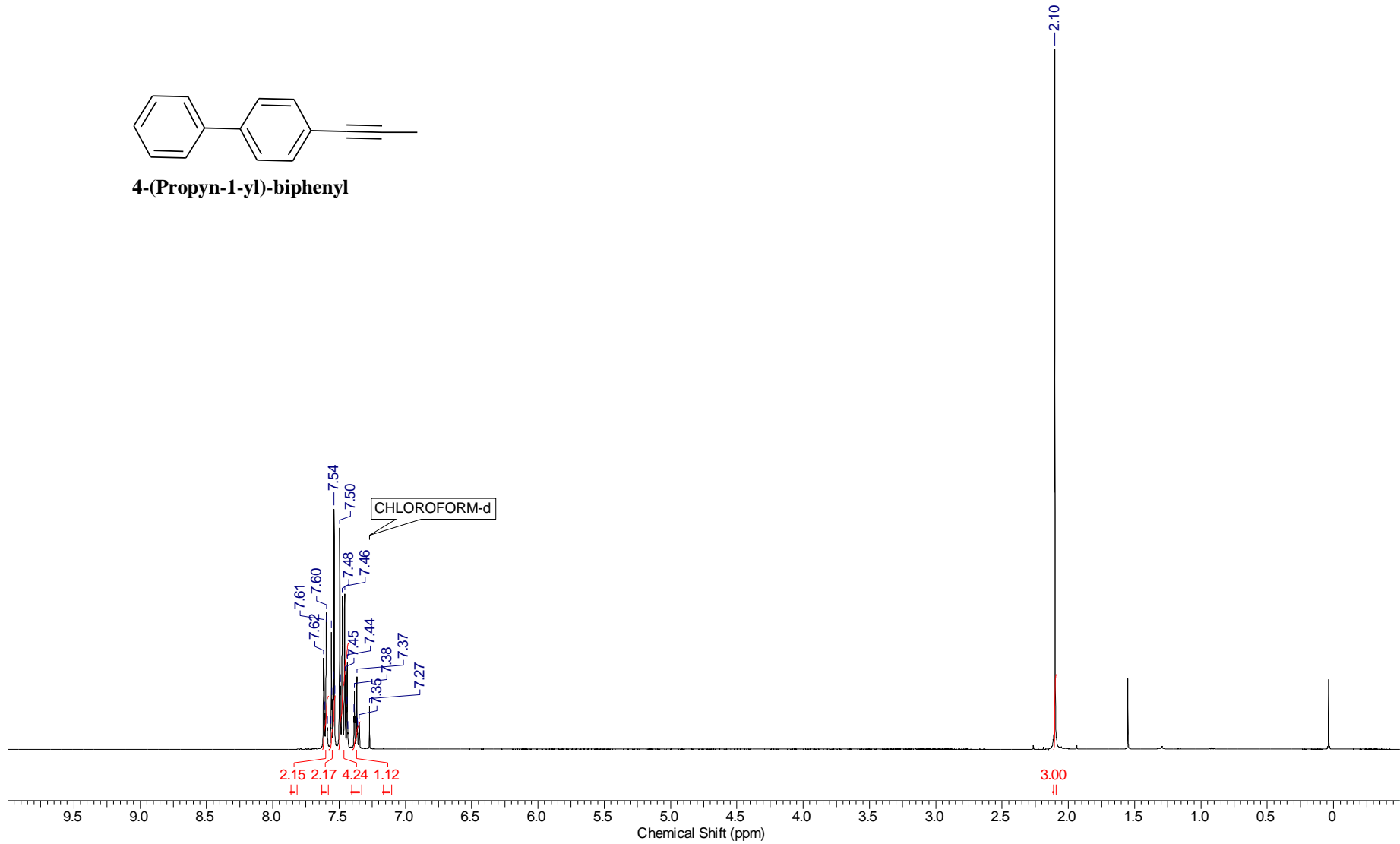
Frequency (MHz)	376.71	Nucleus	¹⁹ F	Number of Transients	64	Origin	Bruker BioSpin GmbH
Original Points Count	131072	Owner	tibbe_operator	Points Count	131072	SW(cyclical) (Hz)	93749.28
Solvent	DMSO-d6	Spectrum Offset (Hz)	-37674.7617	Sweep Width (Hz)	93748.56	Temperature (degree C)	27.000



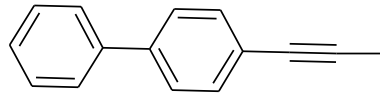
Frequency (MHz)	400.40	Nucleus	1H	Number of Transients	16	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	SW(cyclical) (Hz)	7211.32
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	3395.8613	Sweep Width (Hz)	7211.10	Temperature (degree C)	27.000



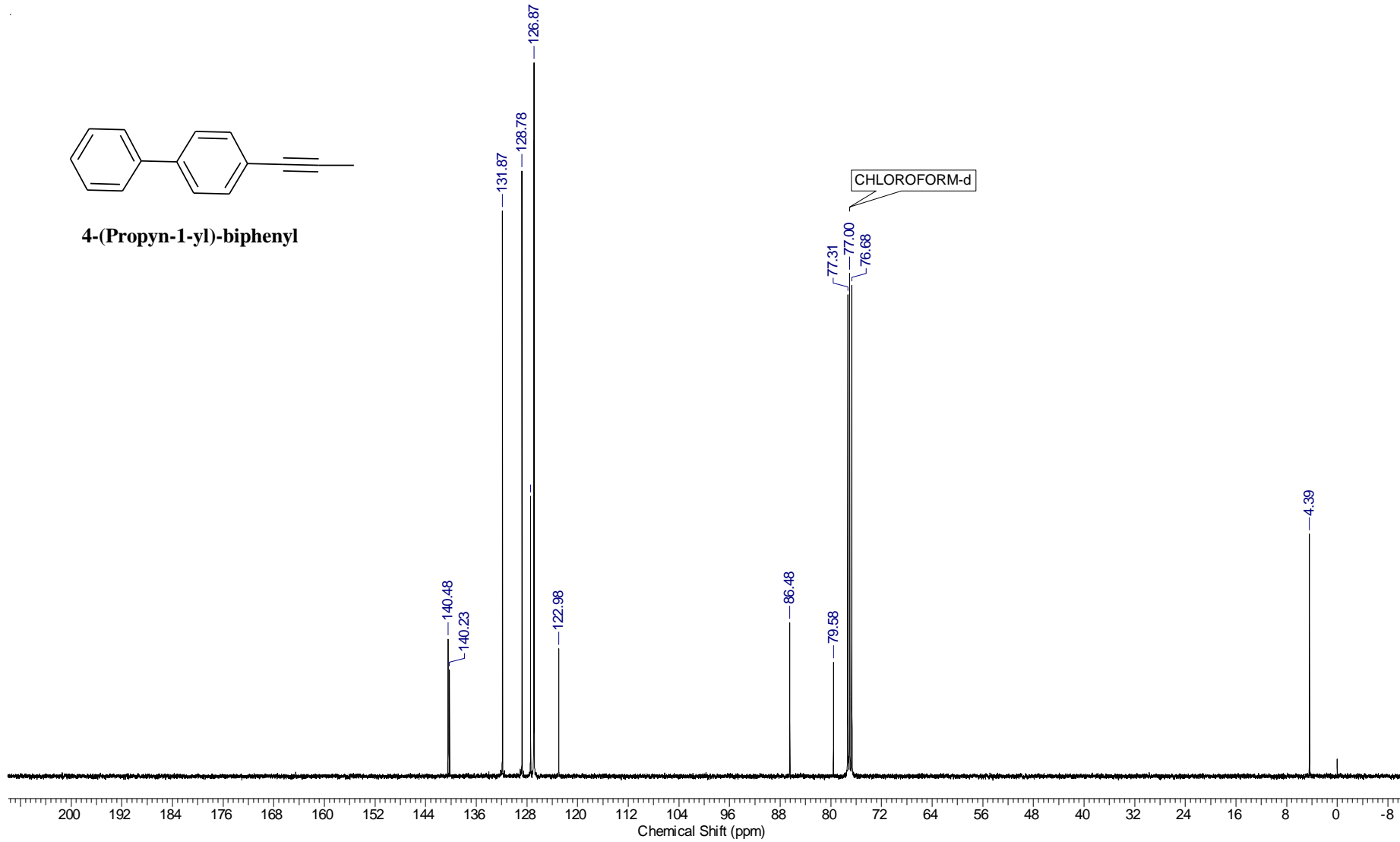
4-(Propyn-1-yl)-biphenyl



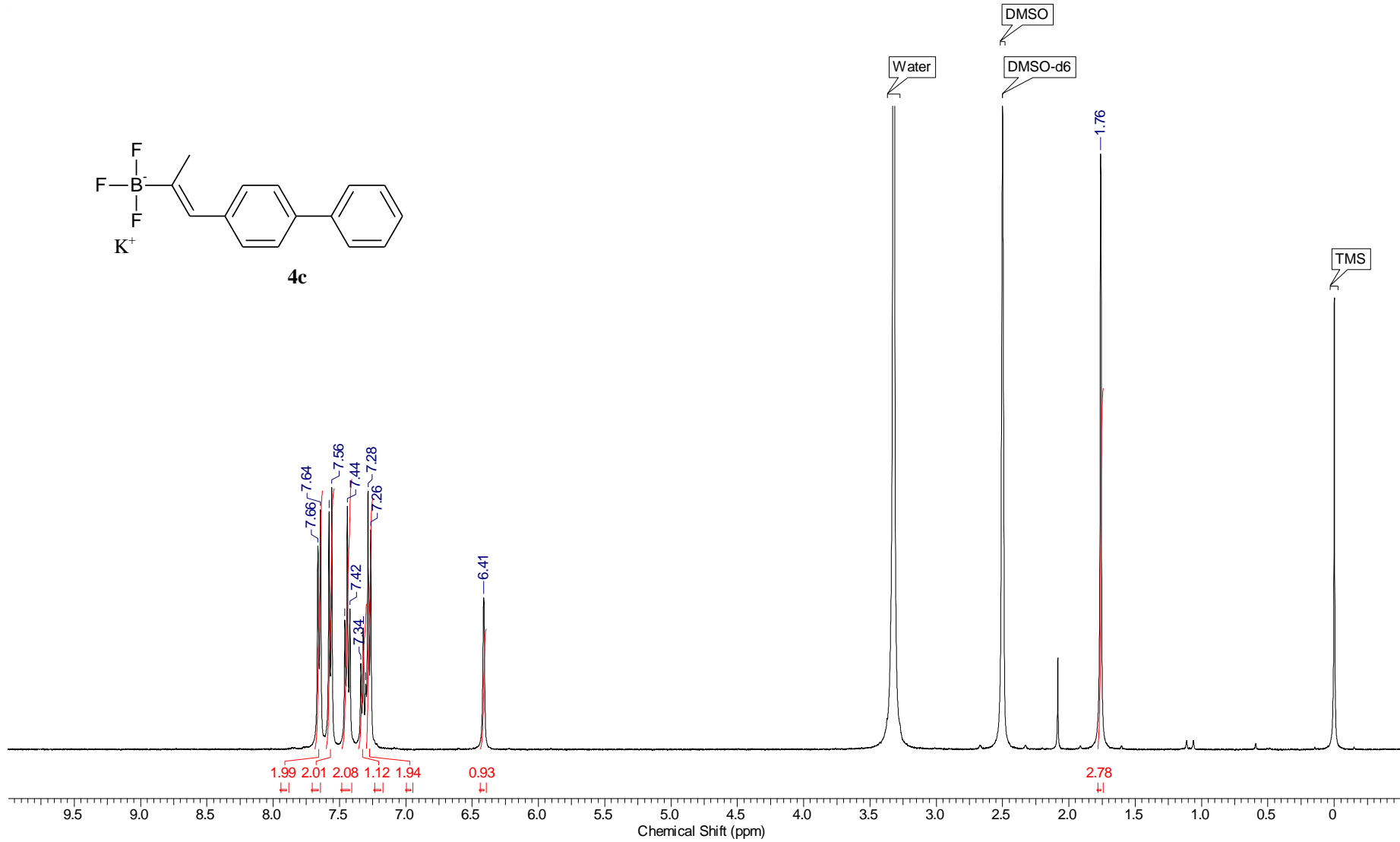
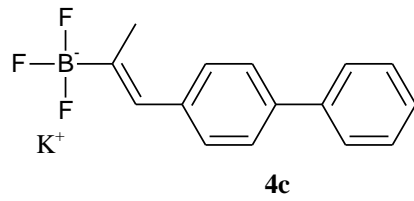
Frequency (MHz)	100.69	Nucleus	¹³ C	Number of Transients	1024	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	SW(cyclical) (Hz)	24037.73
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10063.5742	Sweep Width (Hz)	24036.99	Temperature (degree C)	27.000



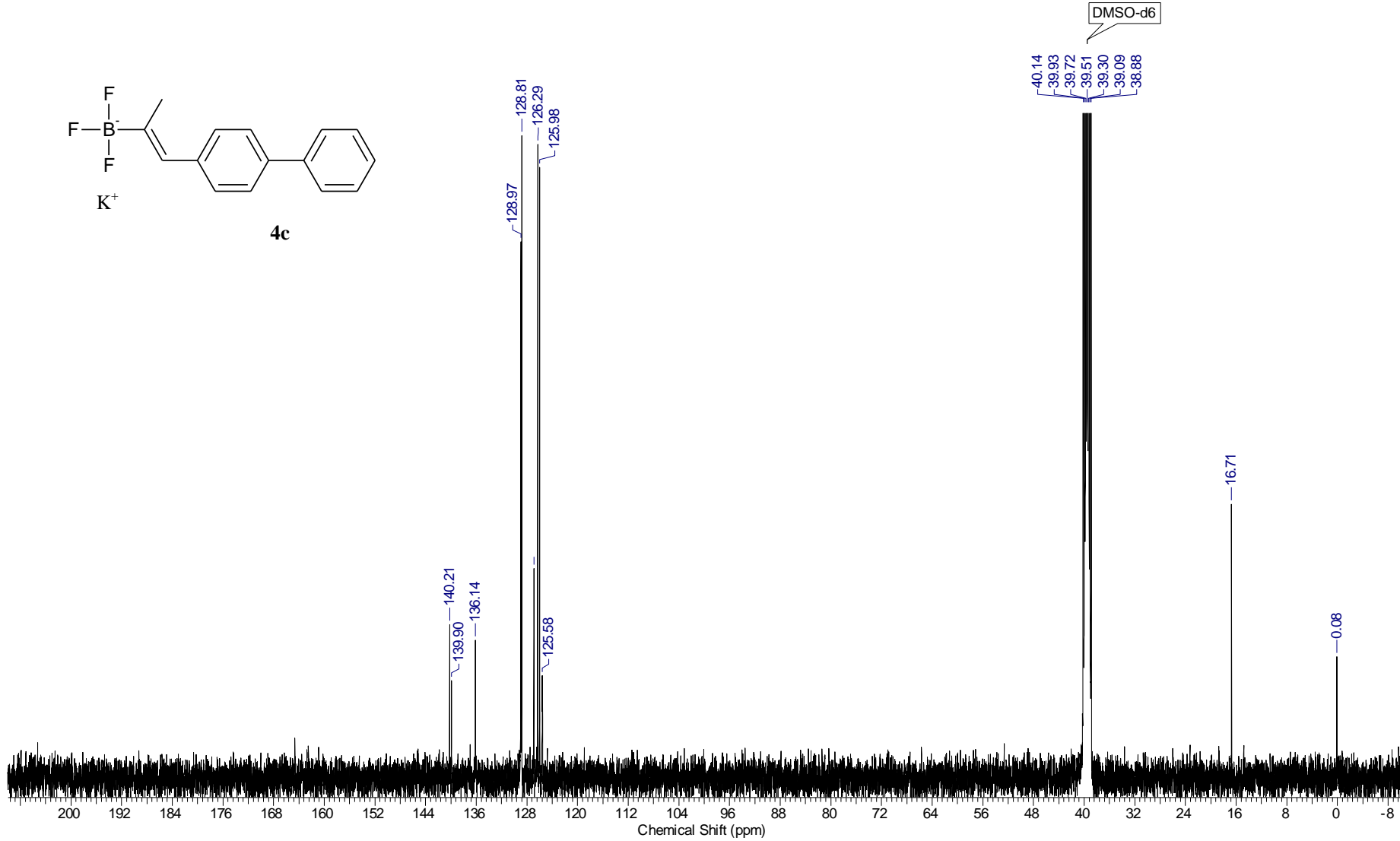
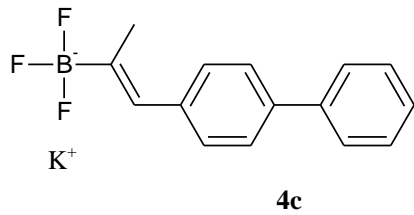
4-(Propyn-1-yl)-biphenyl



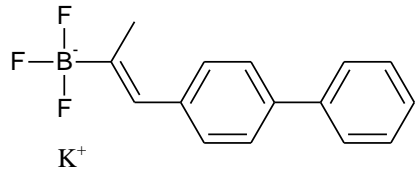
Frequency (MHz)	400.40	Nucleus	1H	Number of Transients	16	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	SW(cyclical) (Hz)	7211.32
Solvent	DMSO-d6	Spectrum Offset (Hz)	3398.8027	Sweep Width (Hz)	7211.10	Temperature (degree C)	27.000



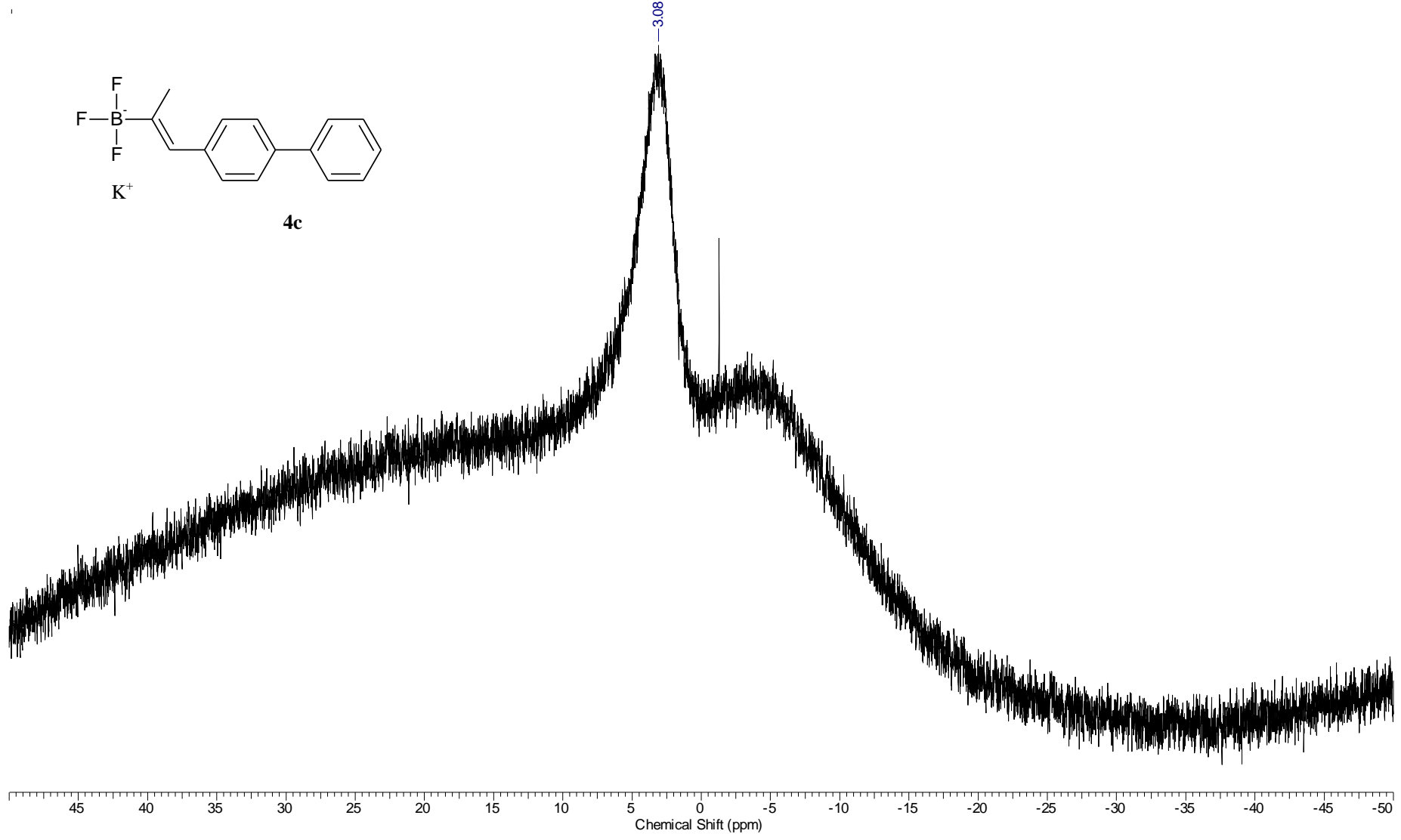
Frequency (MHz)	100.69	Nucleus	¹³ C	Number of Transients	1024	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	SW(cyclical) (Hz)	24037.73
Solvent	DMSO-d6	Spectrum Offset (Hz)	10017.4326	Sweep Width (Hz)	24036.99	Temperature (degree C)	27.000



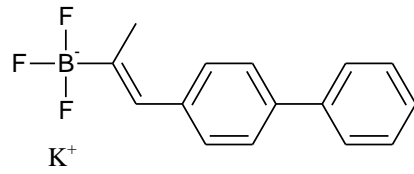
Frequency (MHz)	128.46	Nucleus	11B	Number of Transients	128	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	SW(cyclical) (Hz)	25509.43
Solvent	DMSO-d6	Spectrum Offset (Hz)	1.2842	Sweep Width (Hz)	25508.65	Temperature (degree C)	27.000



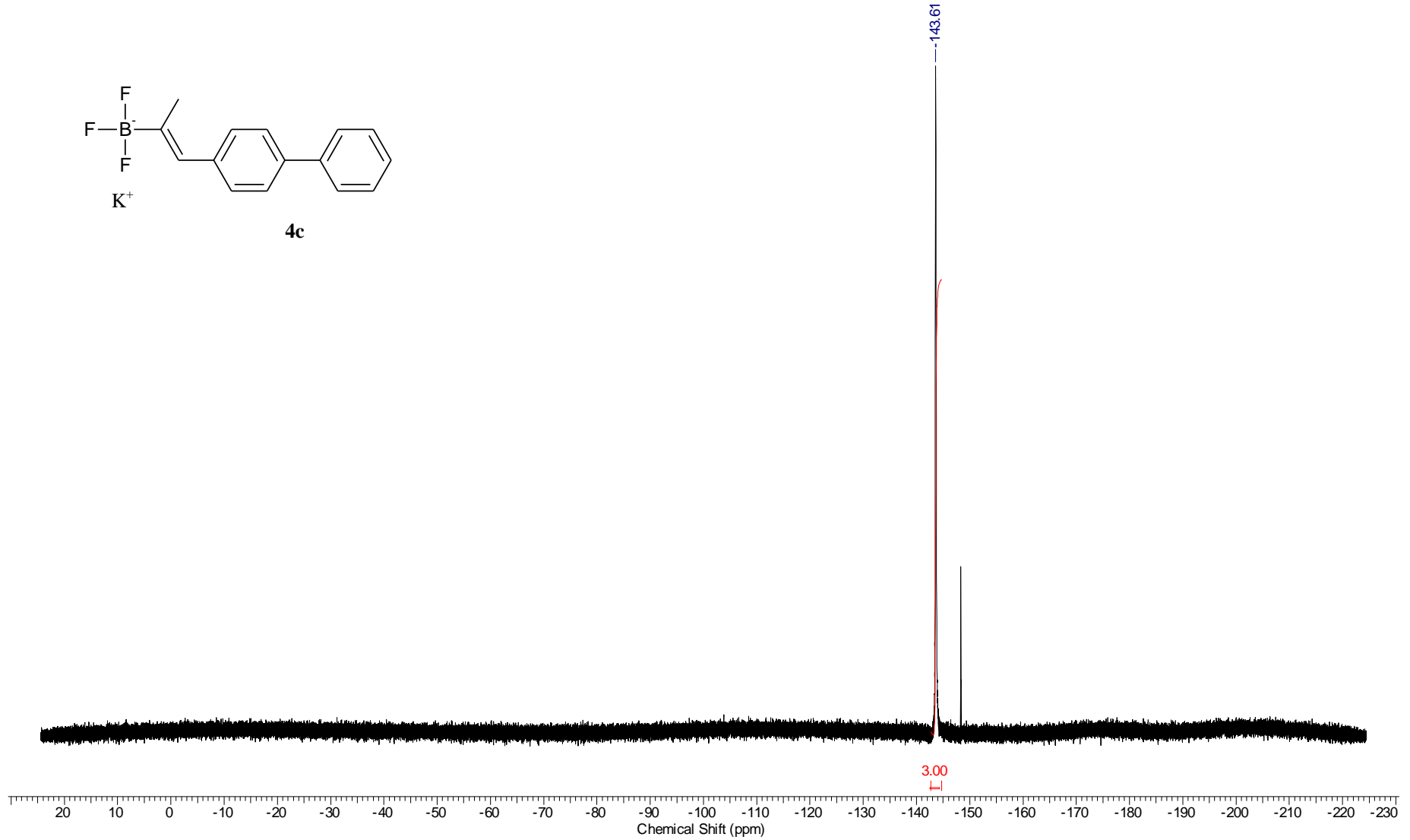
4c



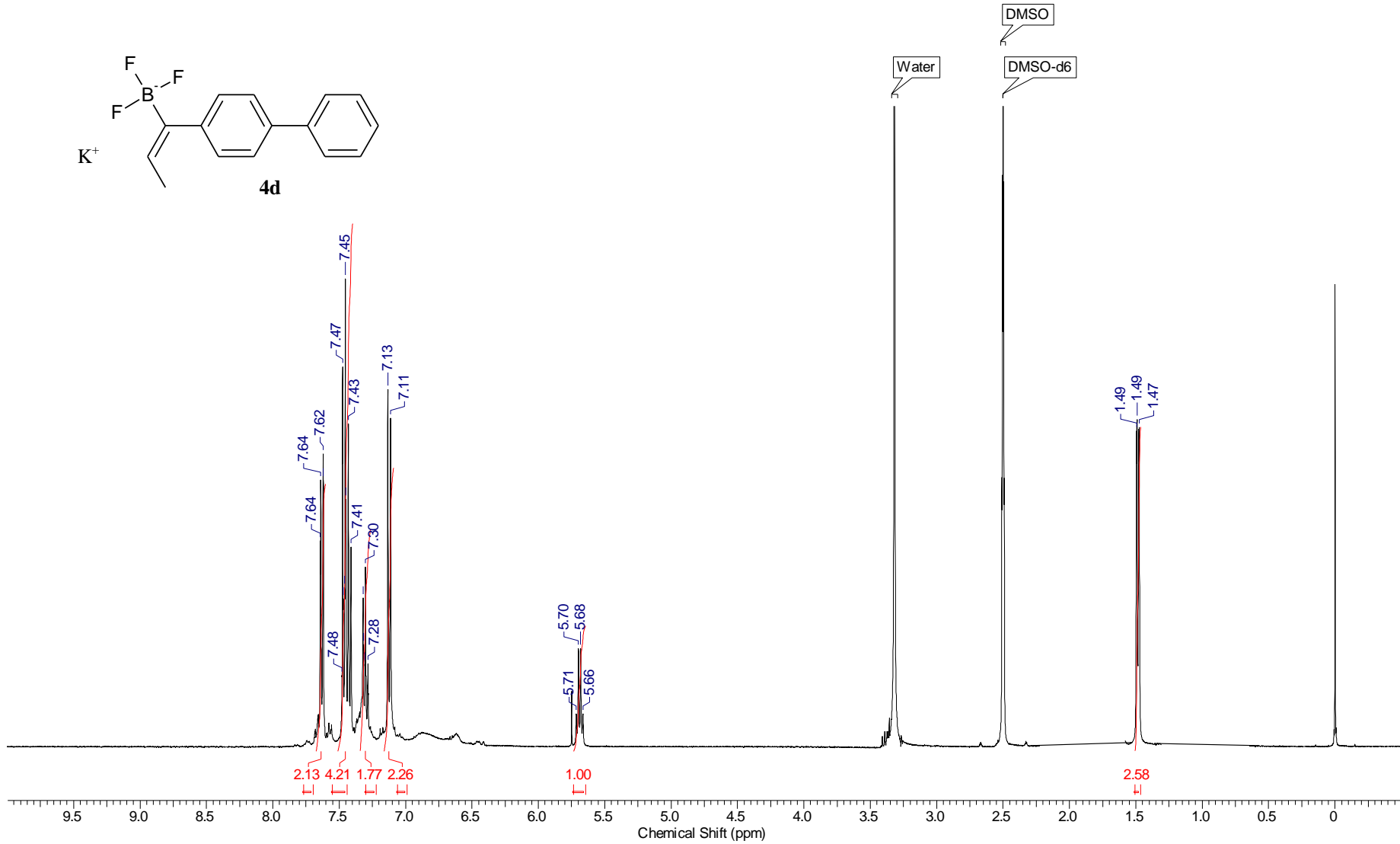
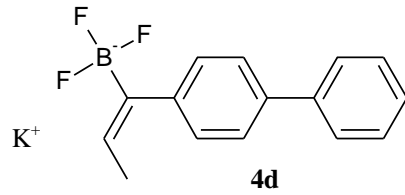
Frequency (MHz)	376.71	Nucleus	¹⁹ F	Number of Transients	64	Origin	Bruker BioSpin GmbH
Original Points Count	131072	Owner	tibbe_operator	Points Count	131072	SW(cyclical) (Hz)	93749.28
Solvent	DMSO-d6	Spectrum Offset (Hz)	-37674.7617	Sweep Width (Hz)	93748.56	Temperature (degree C)	27.000



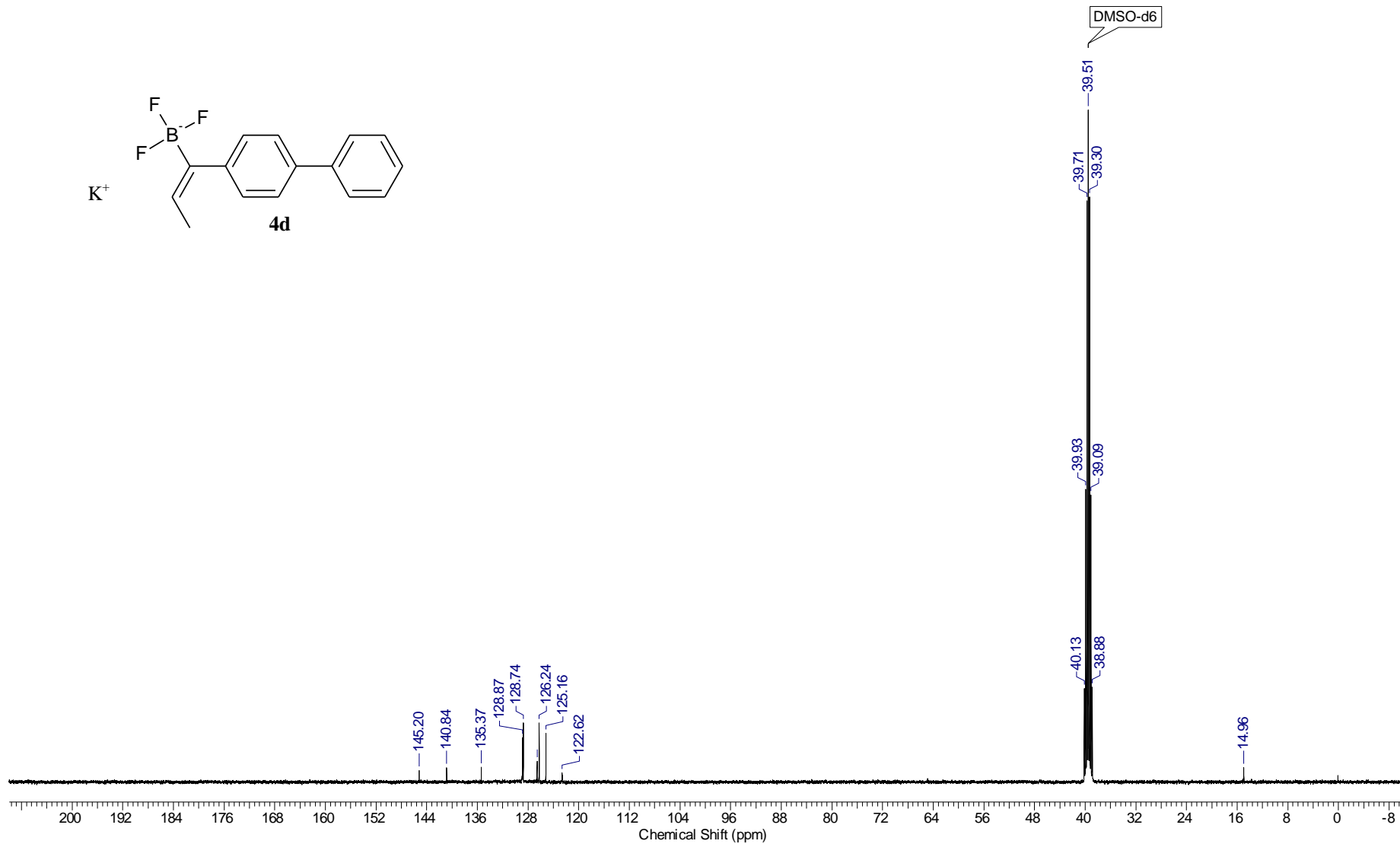
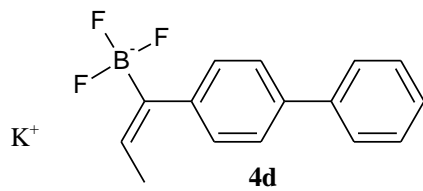
4c



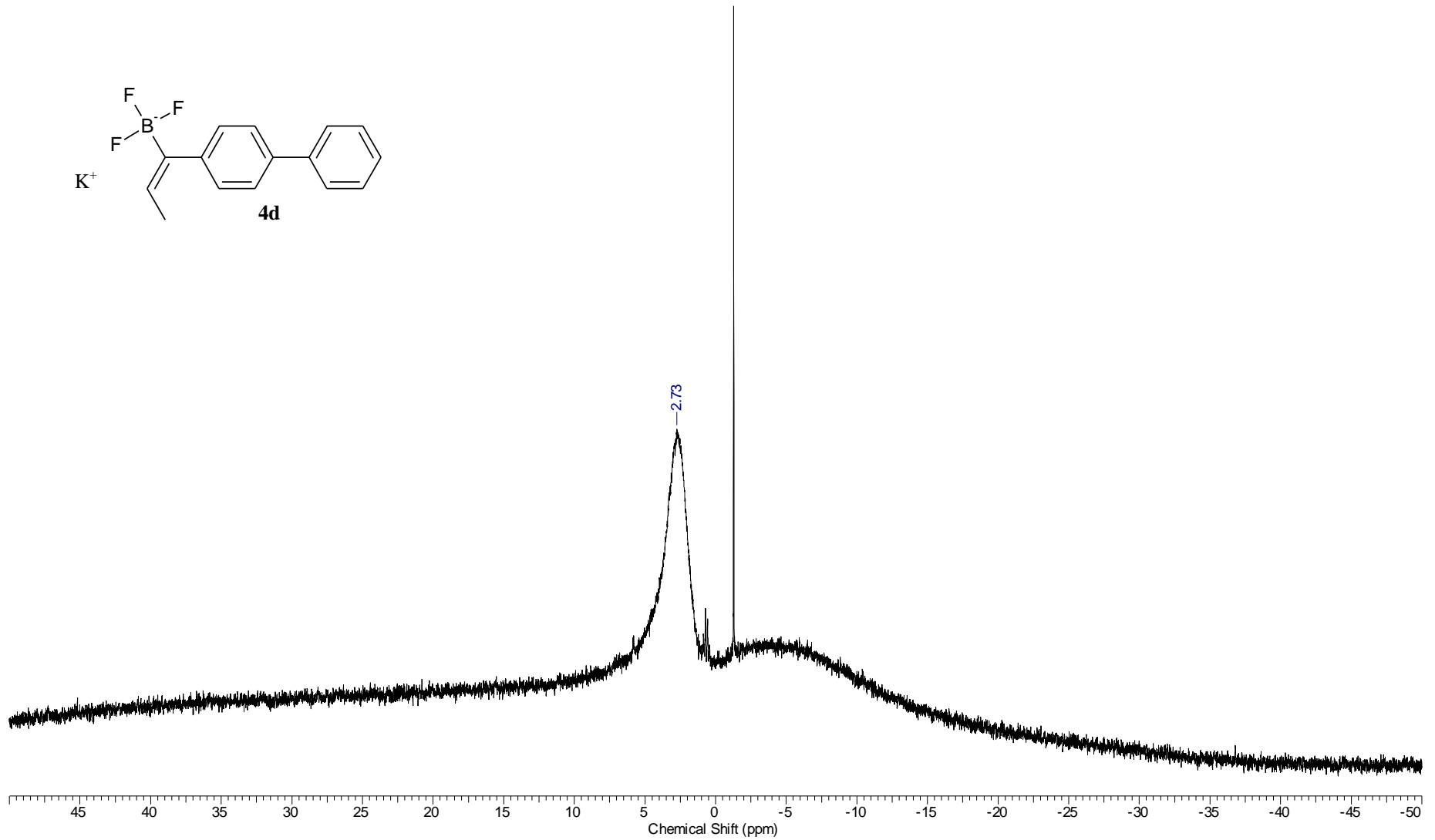
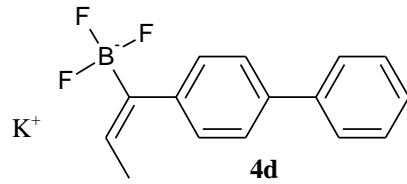
Frequency (MHz)	400.40	Nucleus	¹ H	Number of Transients	16	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	SW(cyclical) (Hz)	7211.32
Solvent	DMSO-d6	Spectrum Offset (Hz)	3398.3625	Sweep Width (Hz)	7211.10	Temperature (degree C)	27.000



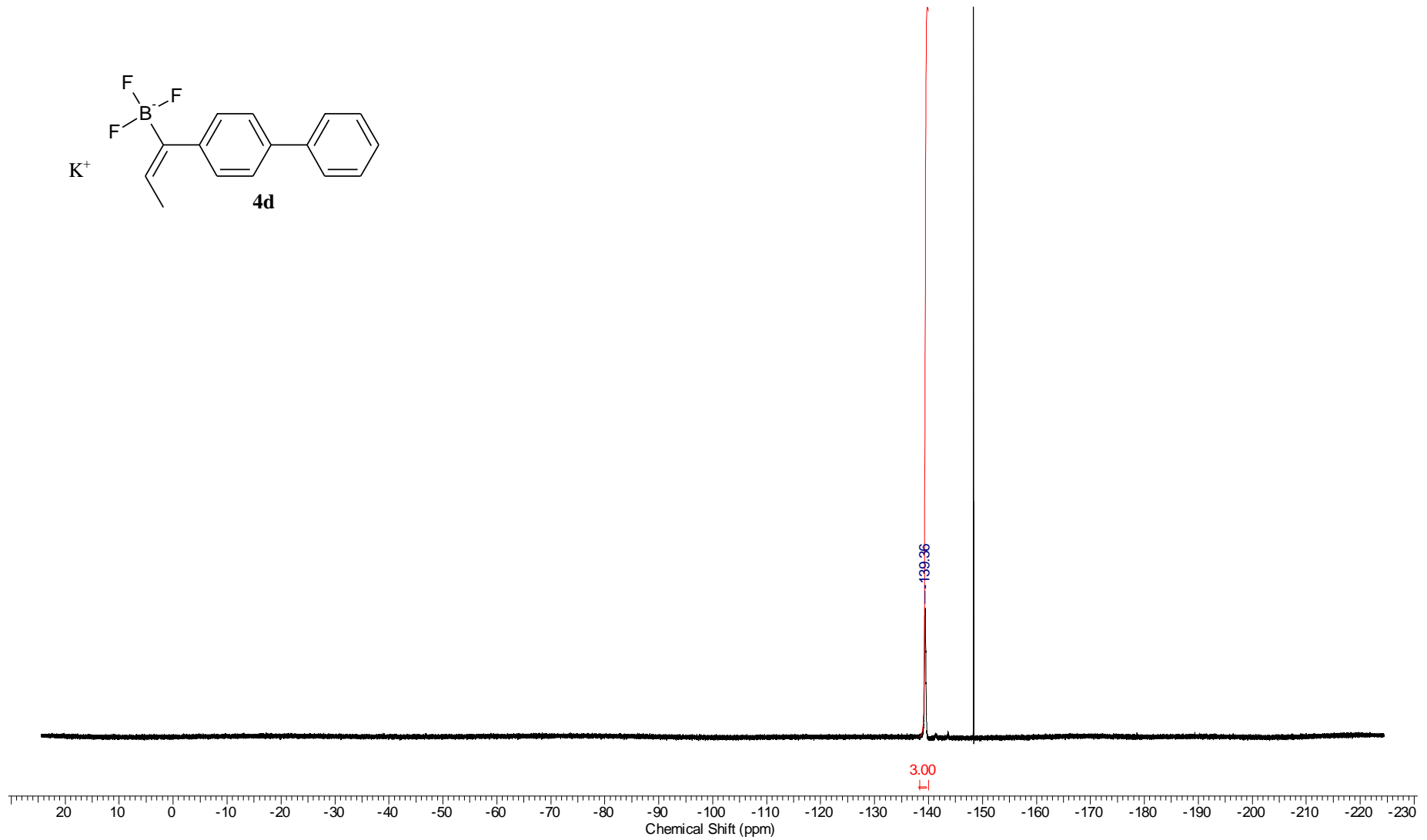
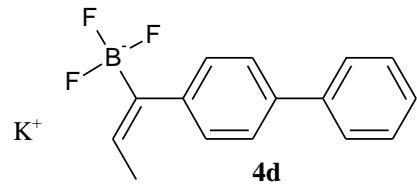
Frequency (MHz)	100.69	Nucleus	¹³ C	Number of Transients	1024	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	SW(cyclical) (Hz)	24037.73
Solvent	DMSO-d6	Spectrum Offset (Hz)	10016.6982	Sweep Width (Hz)	24036.99	Temperature (degree C)	27.000



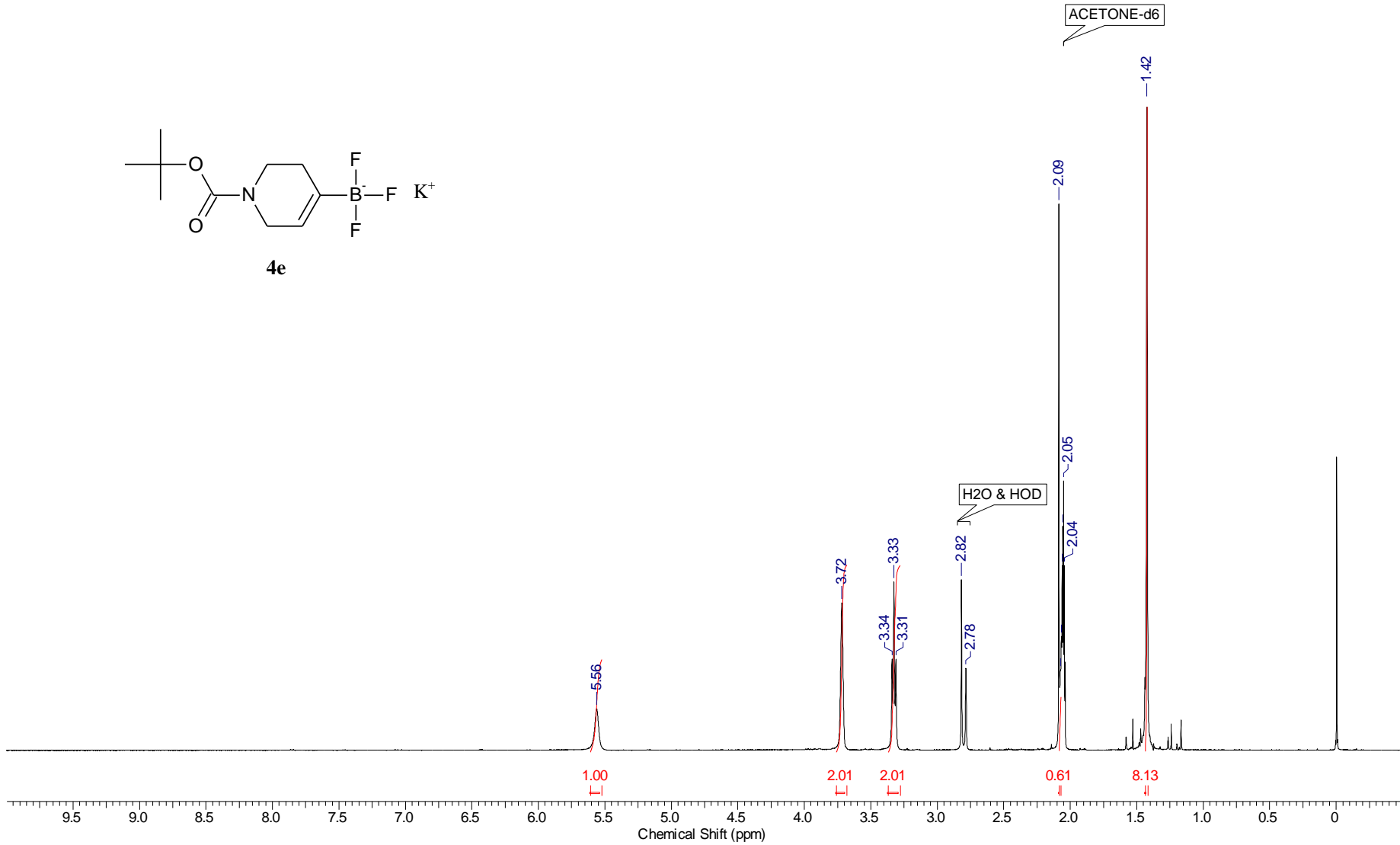
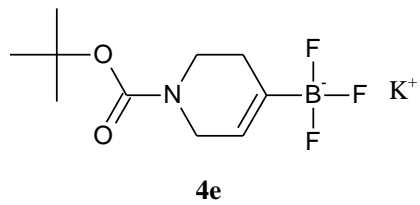
Frequency (MHz)	128.46	Nucleus	11B	Number of Transients	128	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	SW(cyclical) (Hz)	25509.43
Solvent	DMSO-d6	Spectrum Offset (Hz)	1.2842	Sweep Width (Hz)	25508.65	Temperature (degree C)	27.000



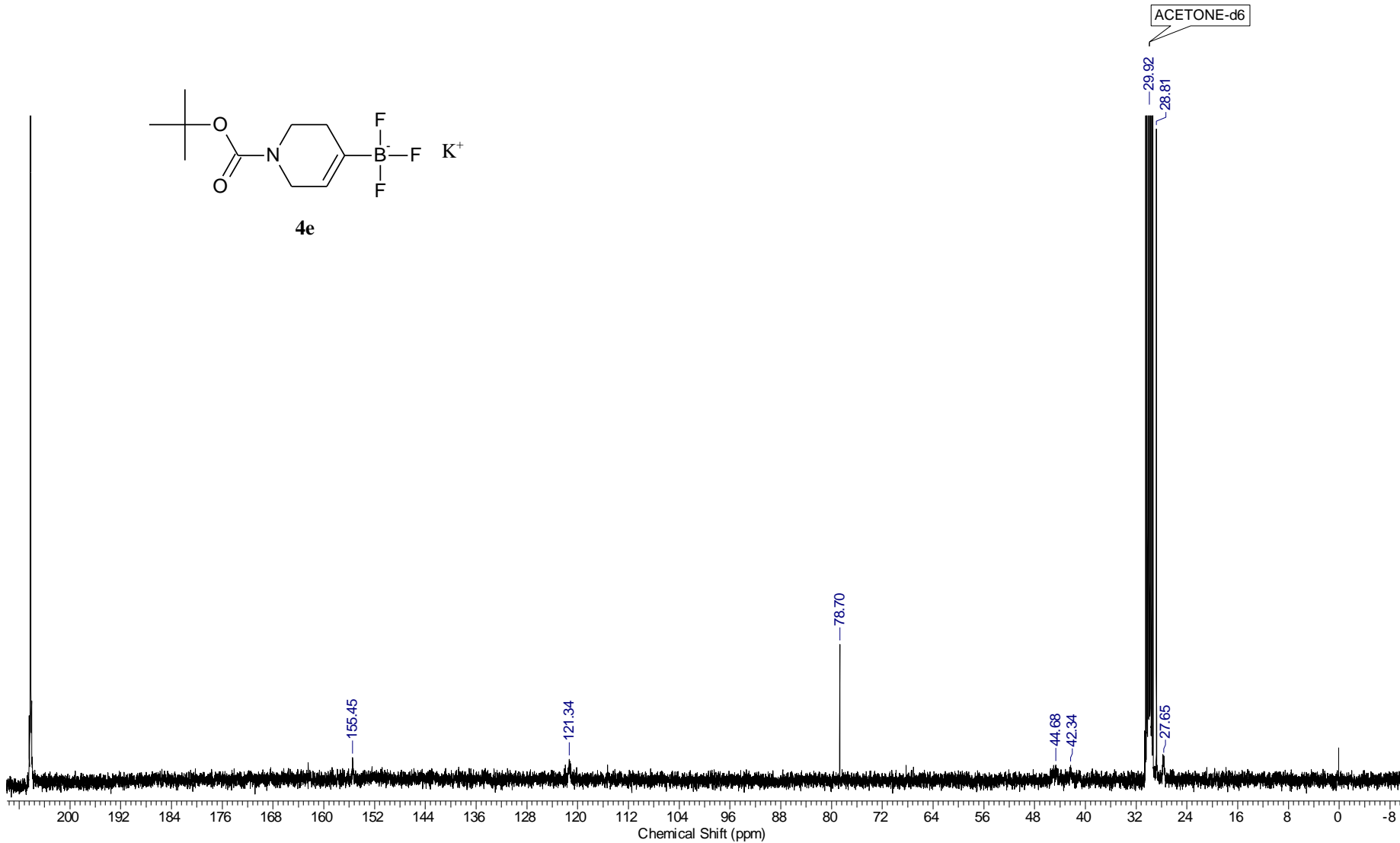
Frequency (MHz)	376.71	Nucleus	¹⁹ F	Number of Transients	64	Origin	Bruker BioSpin GmbH
Original Points Count	131072	Owner	tibbe_operator	Points Count	131072	SW(cyclical) (Hz)	93749.28
Solvent	DMSO-d6	Spectrum Offset (Hz)	-37674.7617	Sweep Width (Hz)	93748.56	Temperature (degree C)	27.000



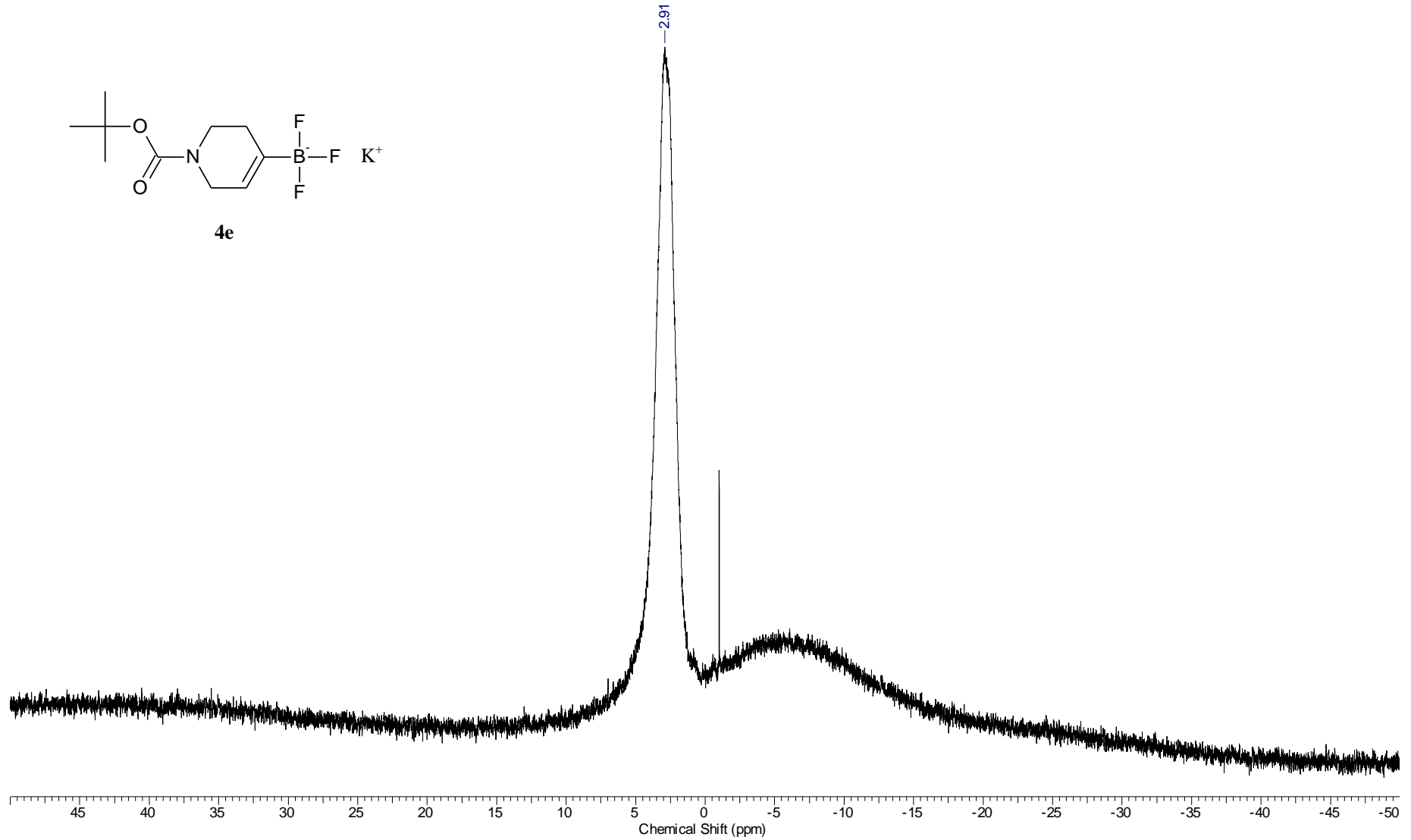
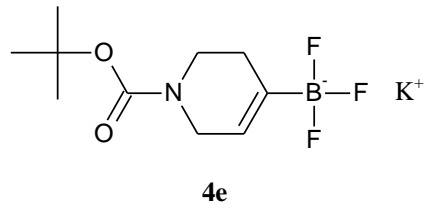
Frequency (MHz)	400.40	Nucleus	¹ H	Number of Transients	16	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	SW(cyclical) (Hz)	7211.32
Solvent	Acetone	Spectrum Offset (Hz)	3394.2385	Sweep Width (Hz)	7211.10	Temperature (degree C)	27.000



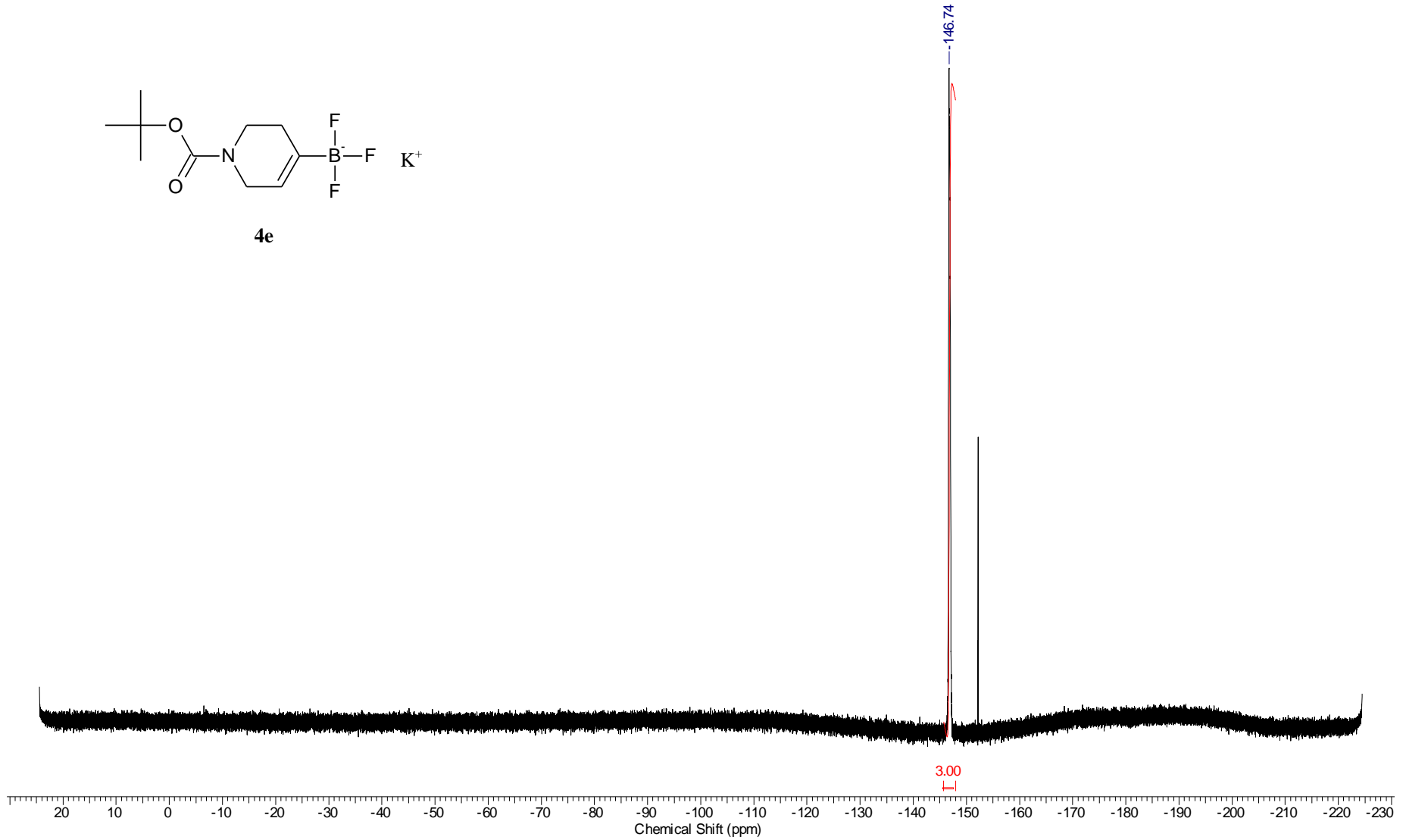
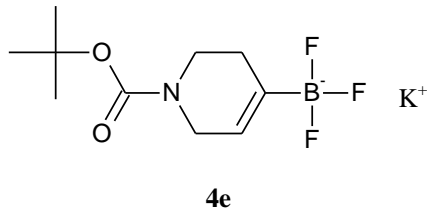
Frequency (MHz)	100.69	Nucleus	¹³ C	Number of Transients	1024	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	SW(cyclical) (Hz)	24037.73
Solvent	Acetone	Spectrum Offset (Hz)	10166.8398	Sweep Width (Hz)	24036.99	Temperature (degree C)	27.000



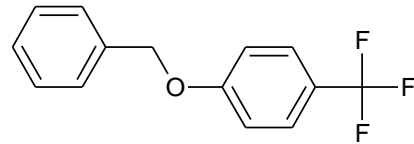
Frequency (MHz)	128.46	Nucleus	11B	Number of Transients	128	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	SW(cyclical) (Hz)	25509.43
Solvent	Acetone	Spectrum Offset (Hz)	1.2842	Sweep Width (Hz)	25508.65	Temperature (degree C)	27.000



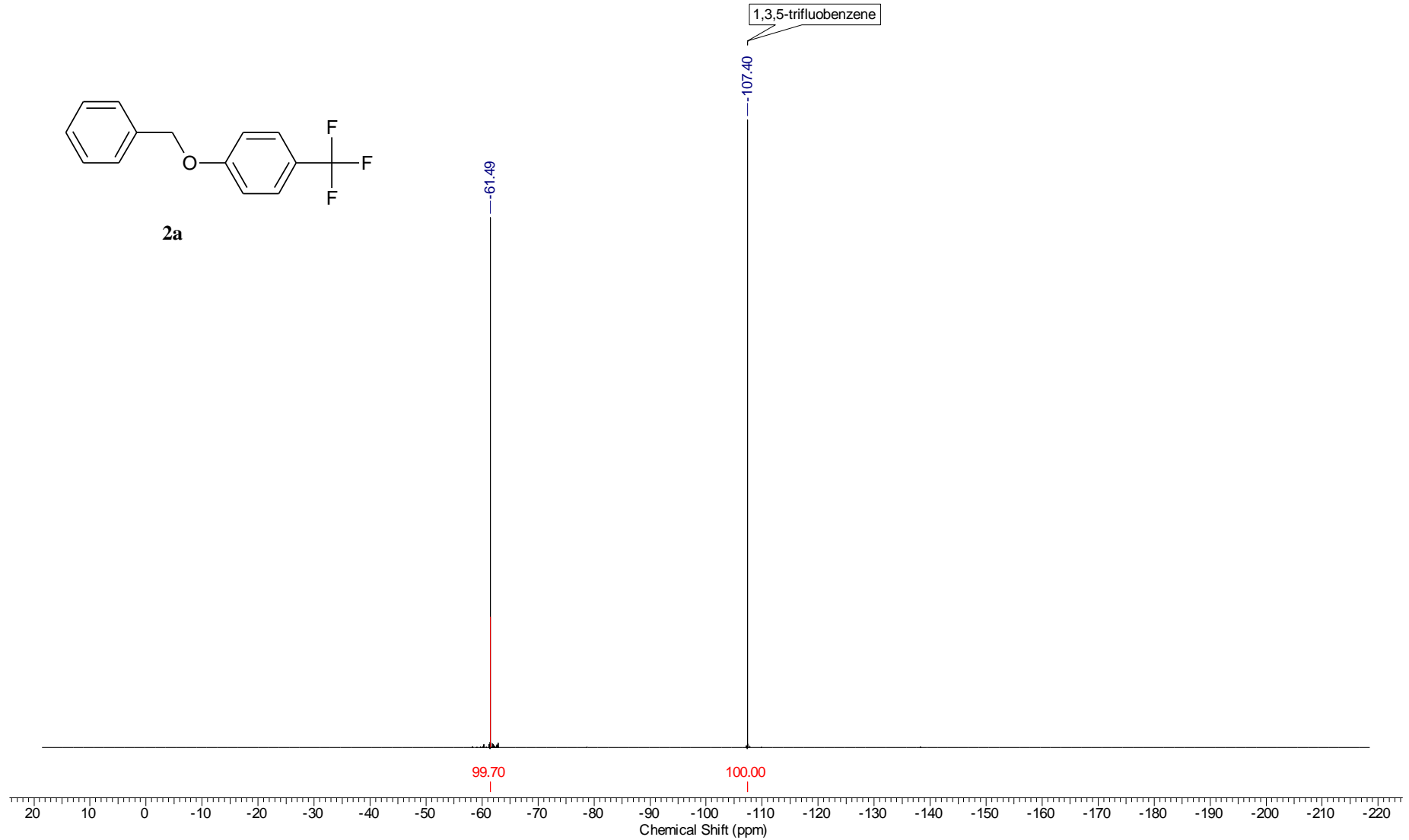
Frequency (MHz)	376.71	Nucleus	19F	Number of Transients	64	Origin	Bruker BioSpin GmbH
Original Points Count	131072	Owner	tibbe_operator	Points Count	131072	SW(cyclical) (Hz)	93749.28
Solvent	Acetone	Spectrum Offset (Hz)	-37674.7617	Sweep Width (Hz)	93748.56	Temperature (degree C)	27.000

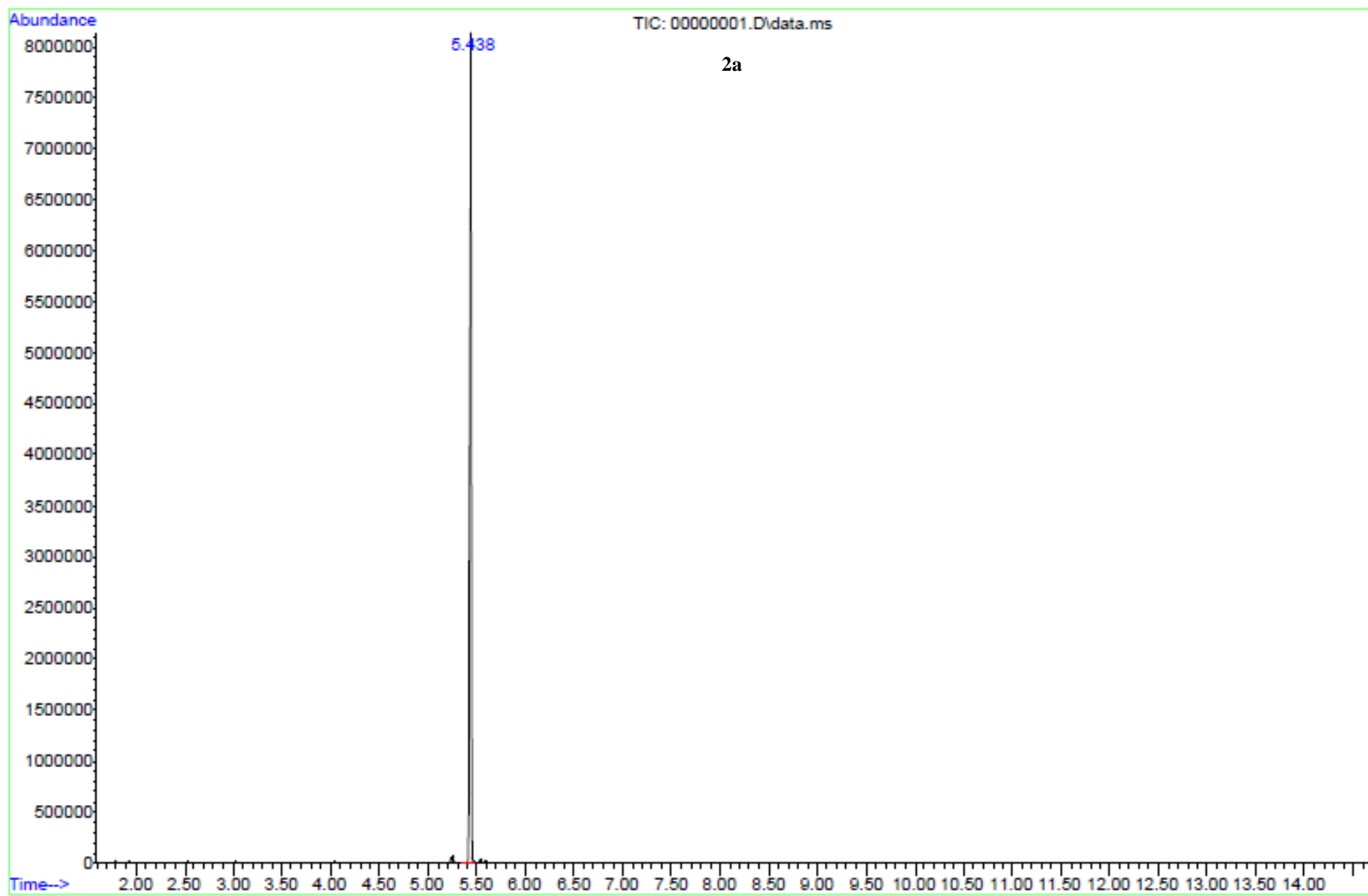


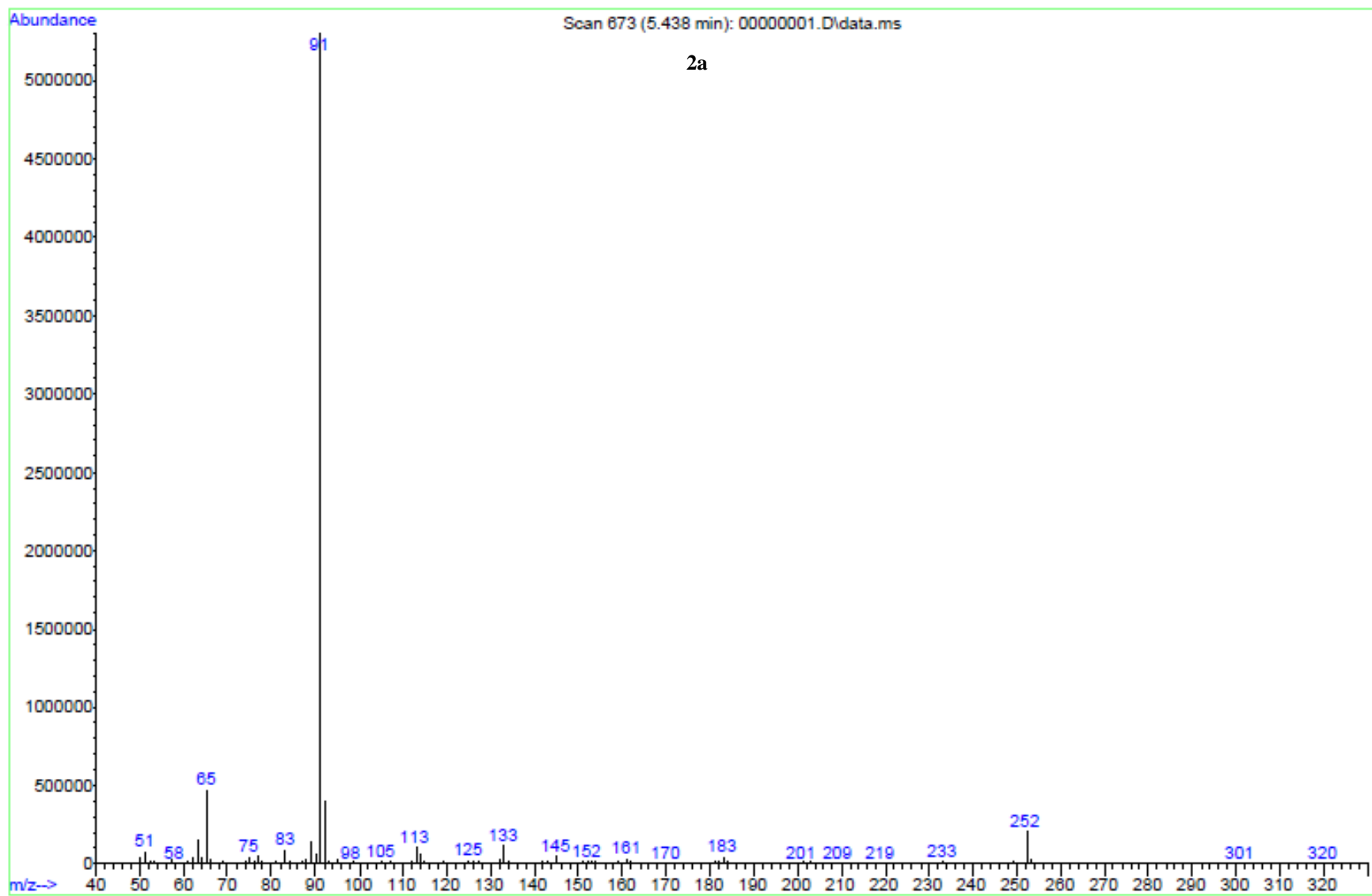
Frequency (MHz)	376.71	Nucleus	¹⁹ F	Number of Transients	64	Origin	Bruker BioSpin GmbH
Original Points Count	131072	Owner	tibbe_operator	Points Count	131072	SW(cyclical) (Hz)	89285.03
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	-37658.4492	Sweep Width (Hz)	89284.35	Temperature (degree C)	27.000



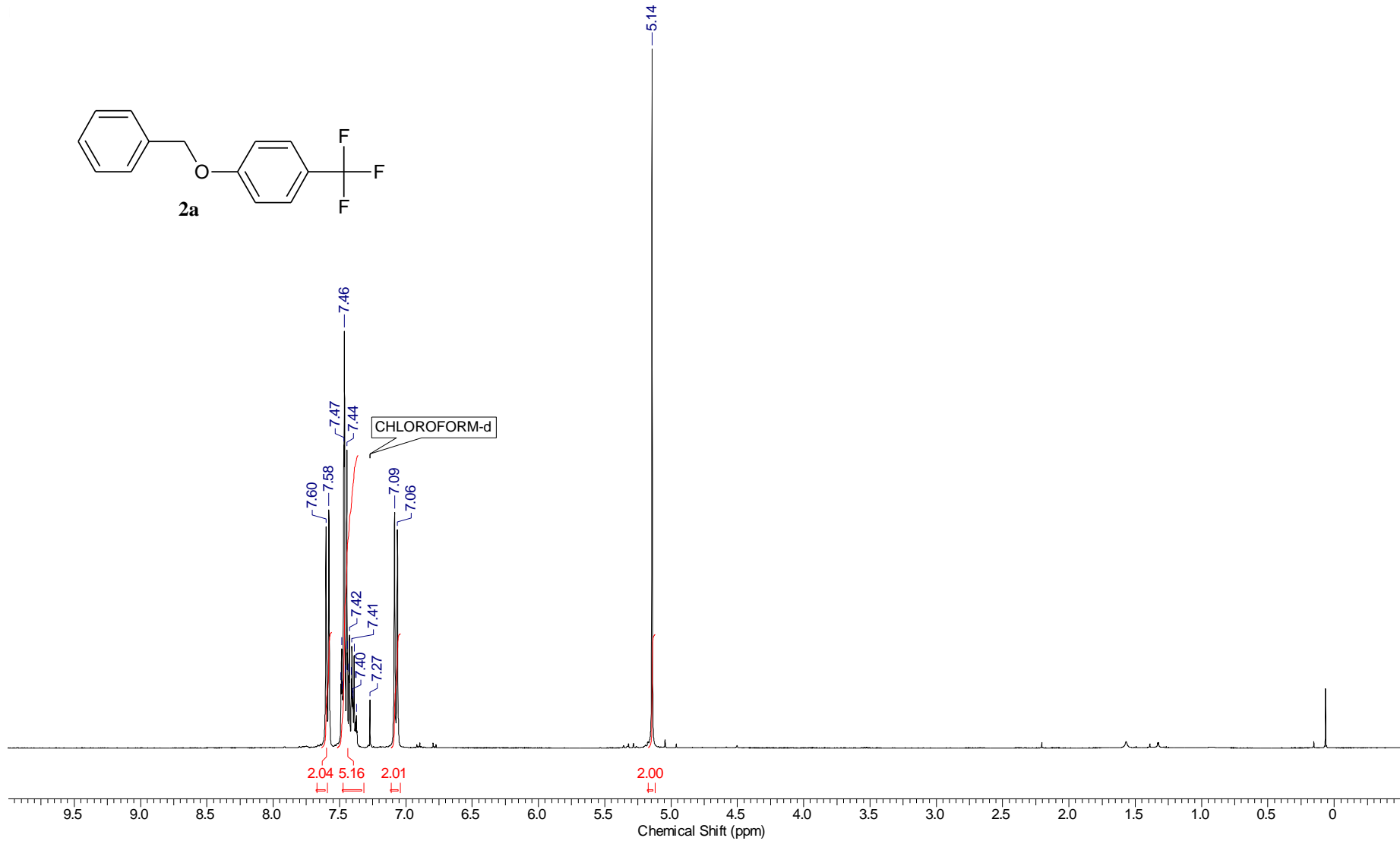
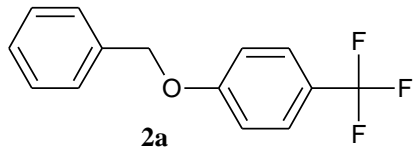
2a



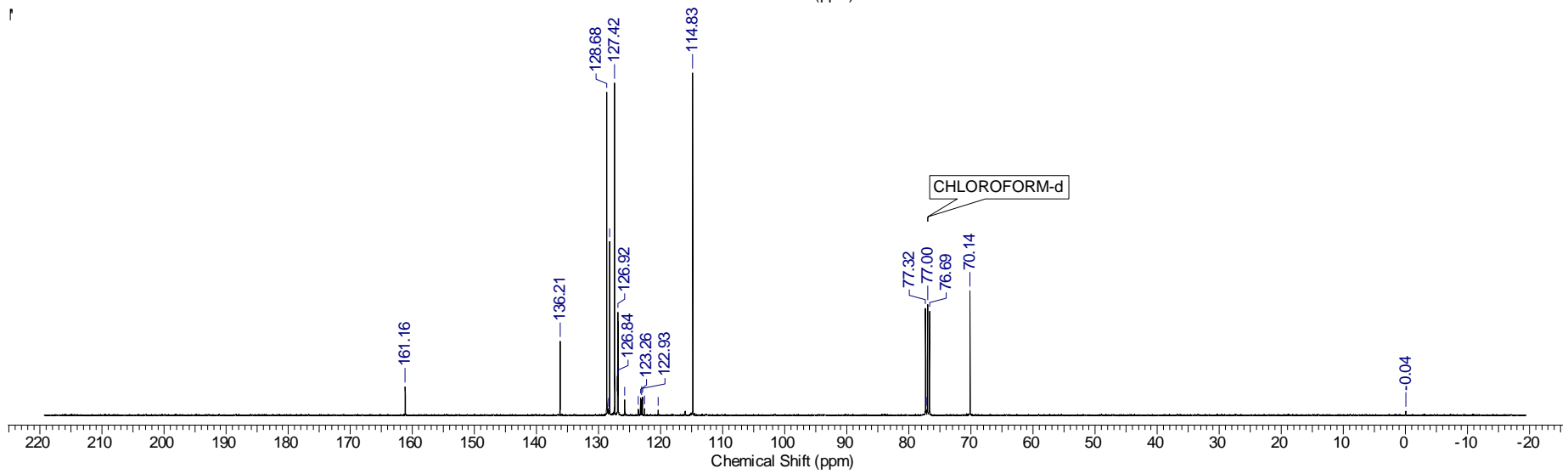
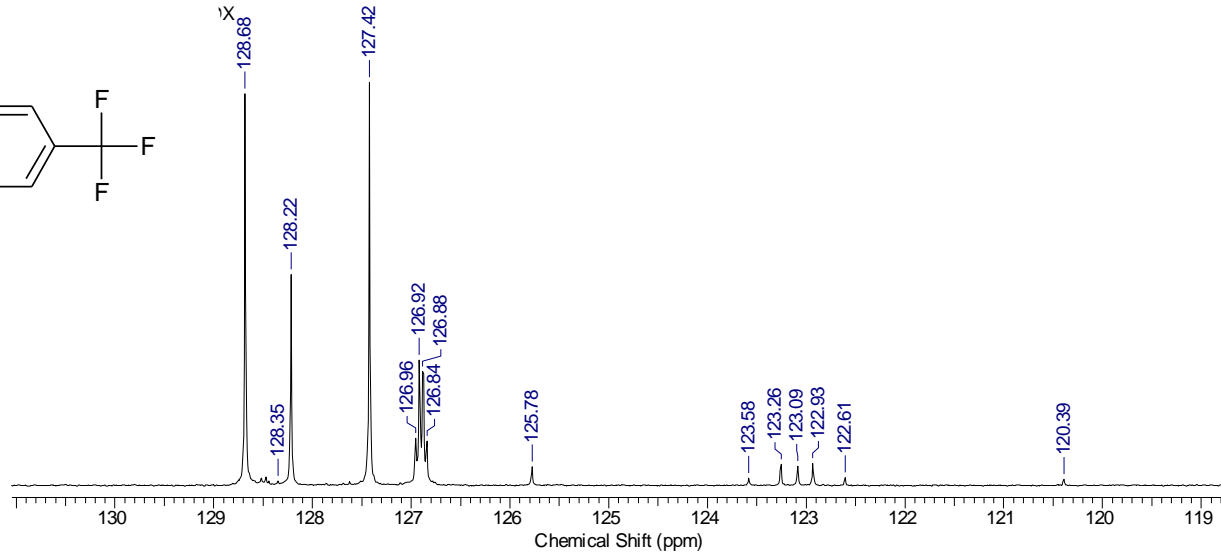
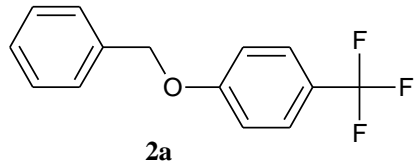




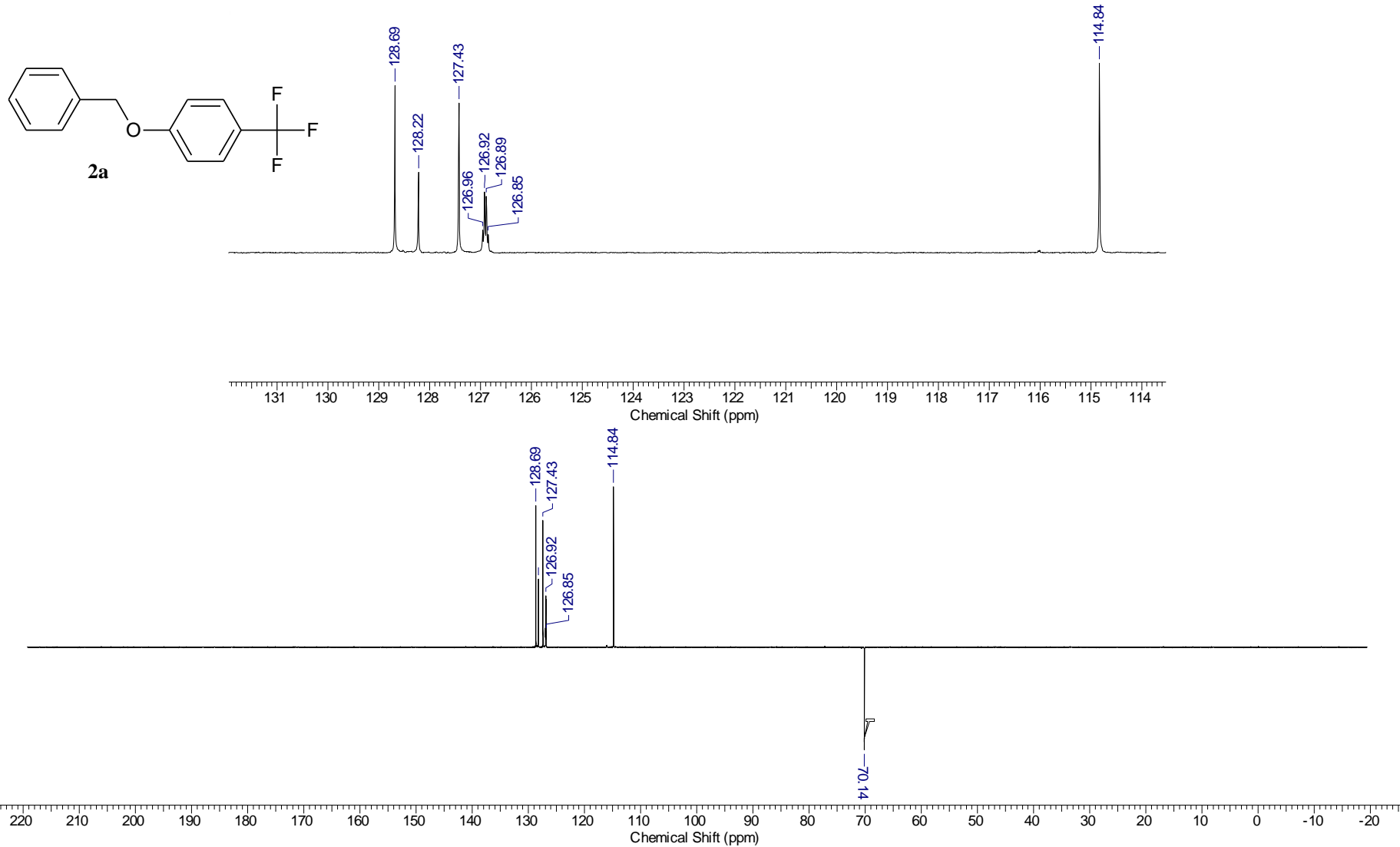
Frequency (MHz)	400.40	Nucleus	1H	Number of Transients	16	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	SW(cyclical) (Hz)	7211.32
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	3395.8613	Sweep Width (Hz)	7211.10	Temperature (degree C)	27.000



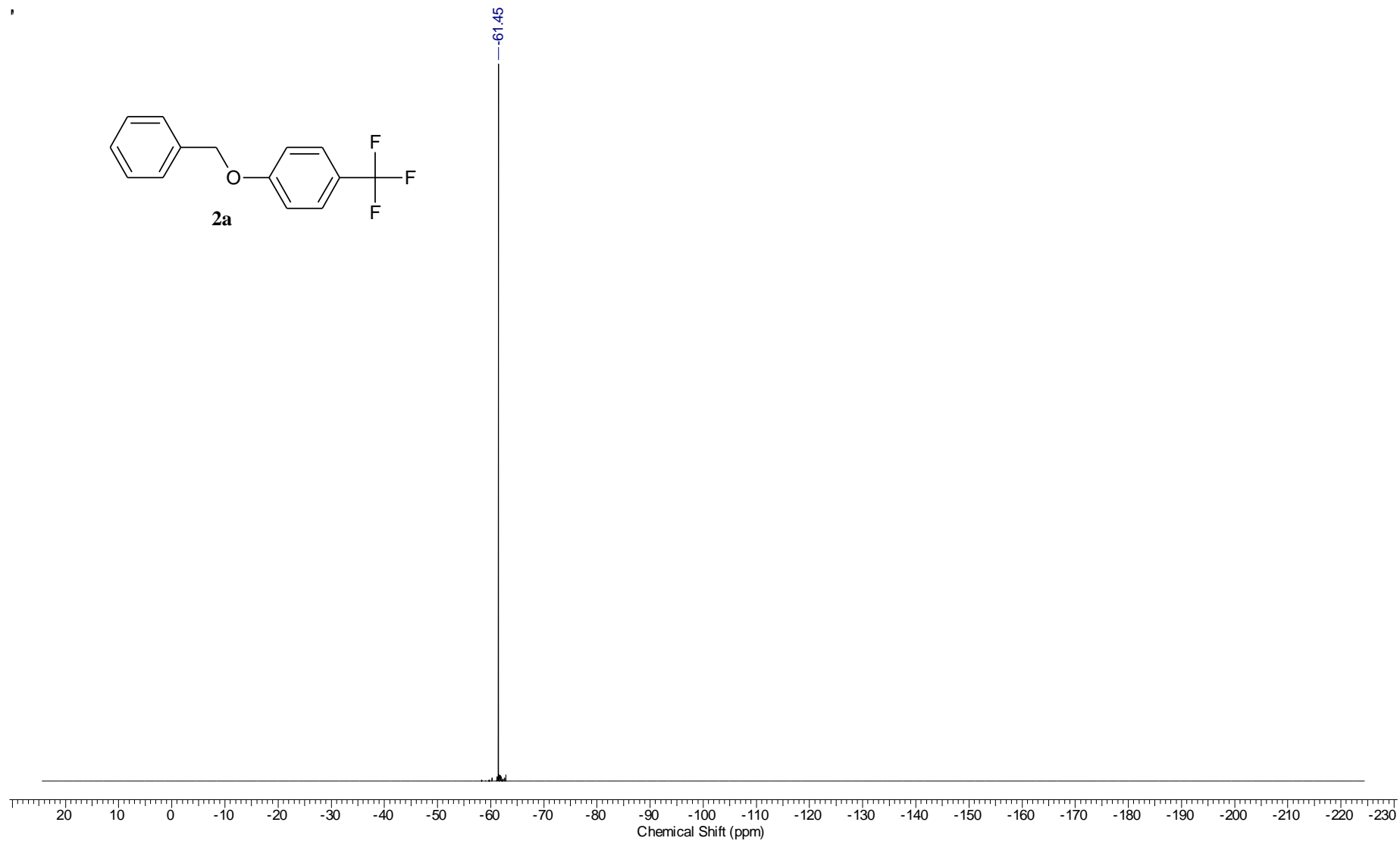
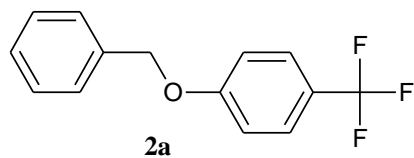
Frequency (MHz)	100.69	Nucleus	¹³ C	Number of Transients	1024	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	SW(cyclical) (Hz)	24037.73
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10062.8418	Sweep Width (Hz)	24036.99	Temperature (degree C)	27.000



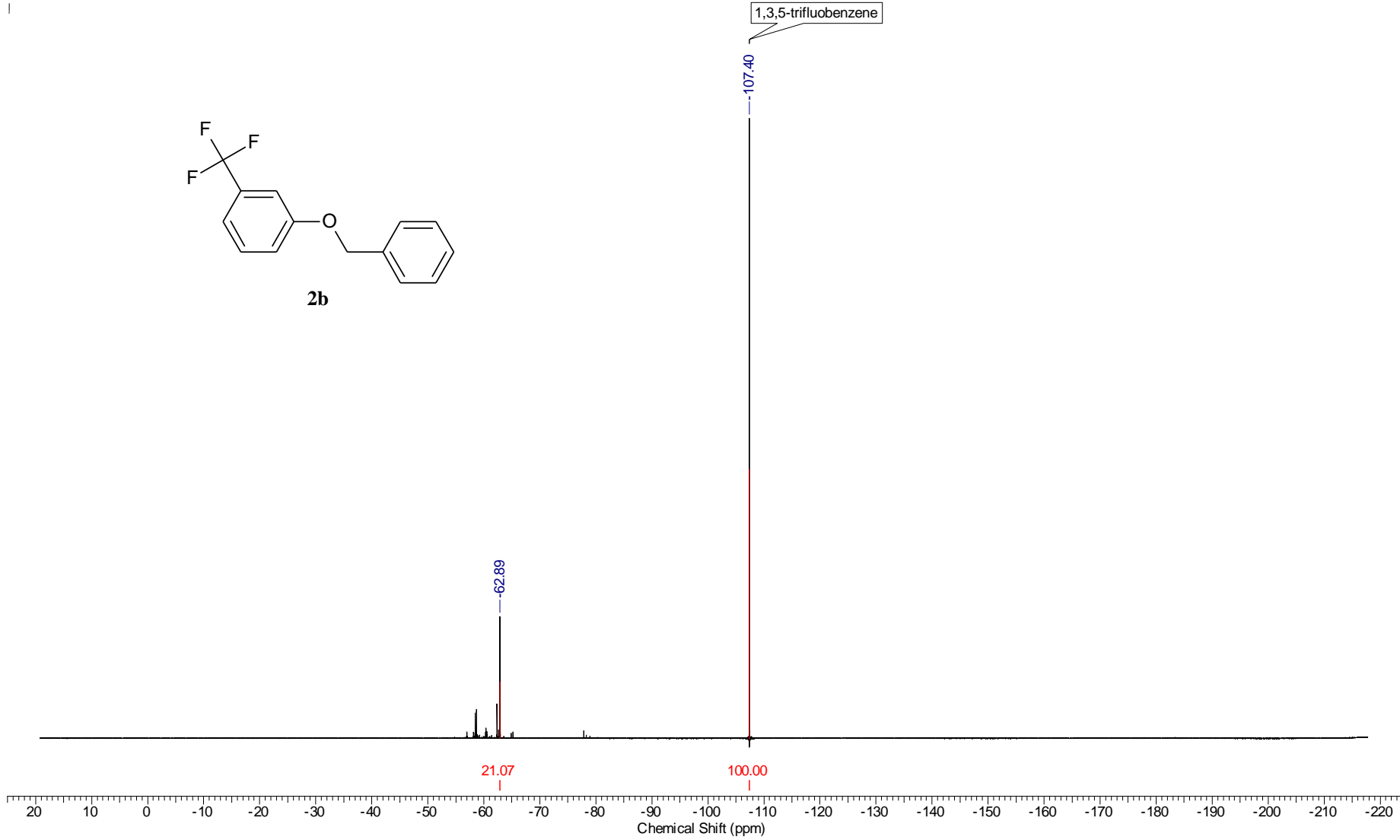
Frequency (MHz)	100.69	Nucleus	¹³ C Dept 135	Number of Transients	256	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	SW(cyclical) (Hz)	24037.73
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10063.1289	Sweep Width (Hz)	24036.99	Temperature (degree C)	28.300

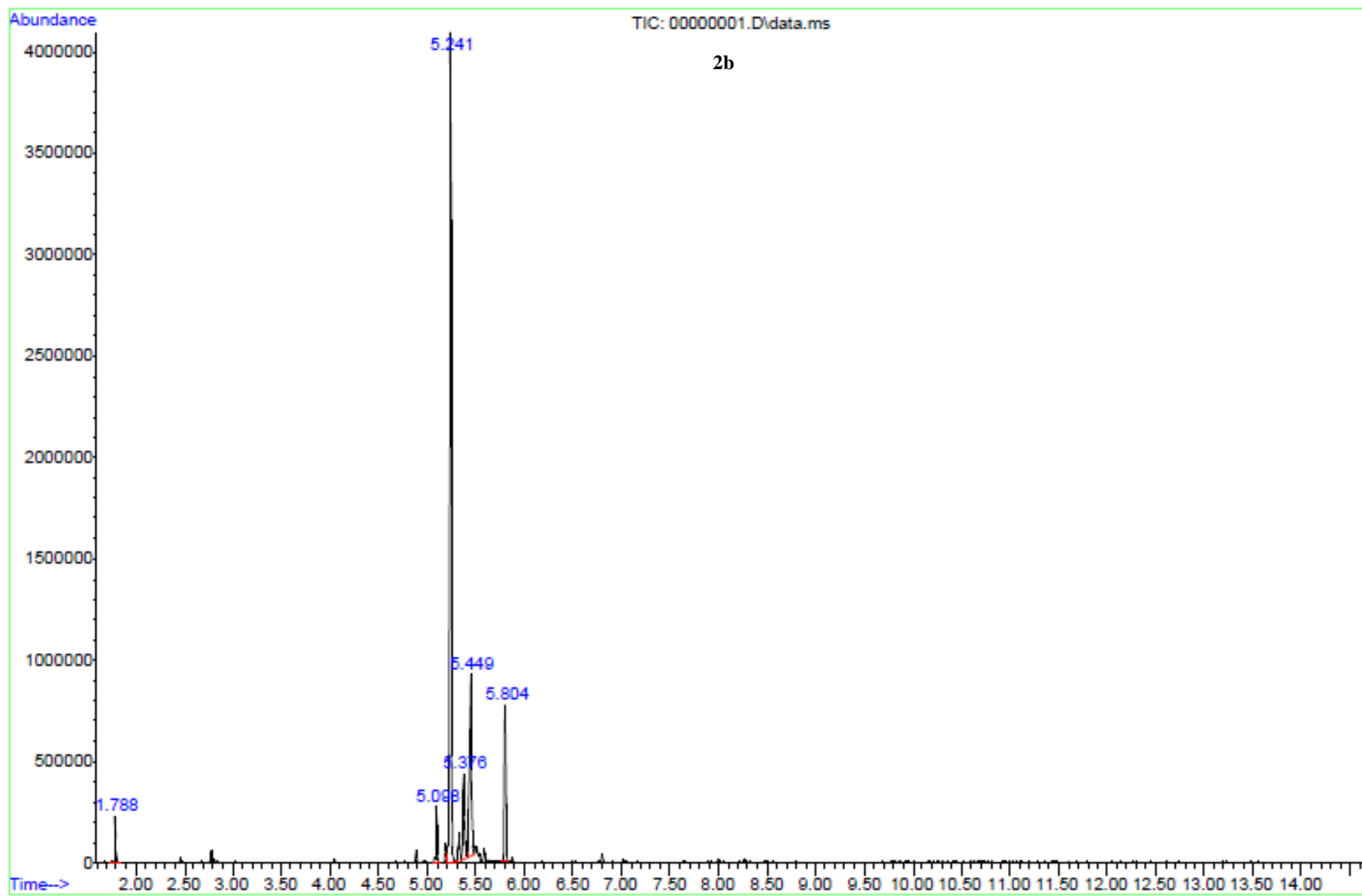


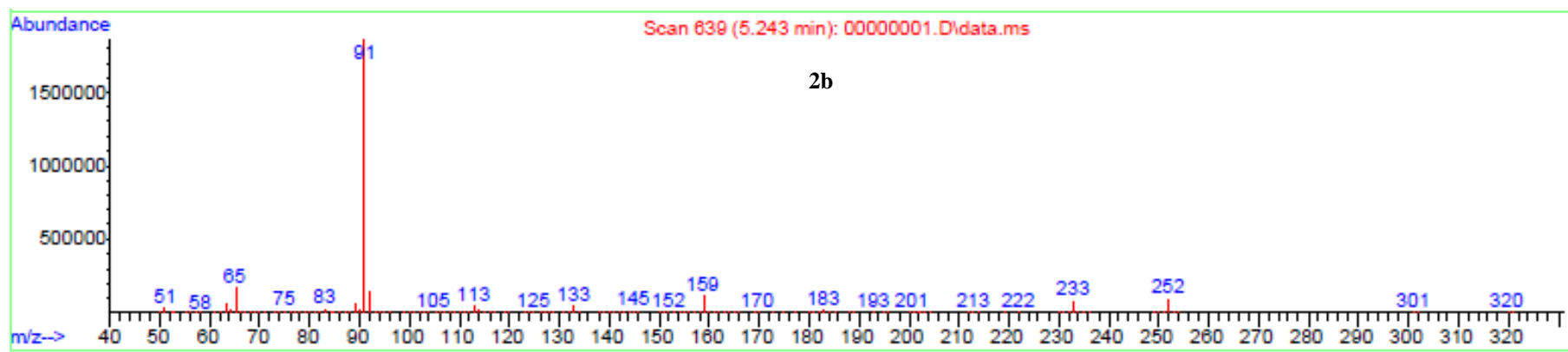
Frequency (MHz)	376.71	Nucleus	¹⁹ F	Number of Transients	64	Origin	Bruker BioSpin GmbH
Original Points Count	131072	Owner	tibbe_operator	Points Count	131072	SW(cyclical) (Hz)	93749.28
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	-37674.7617	Sweep Width (Hz)	93748.56	Temperature (degree C)	27.000



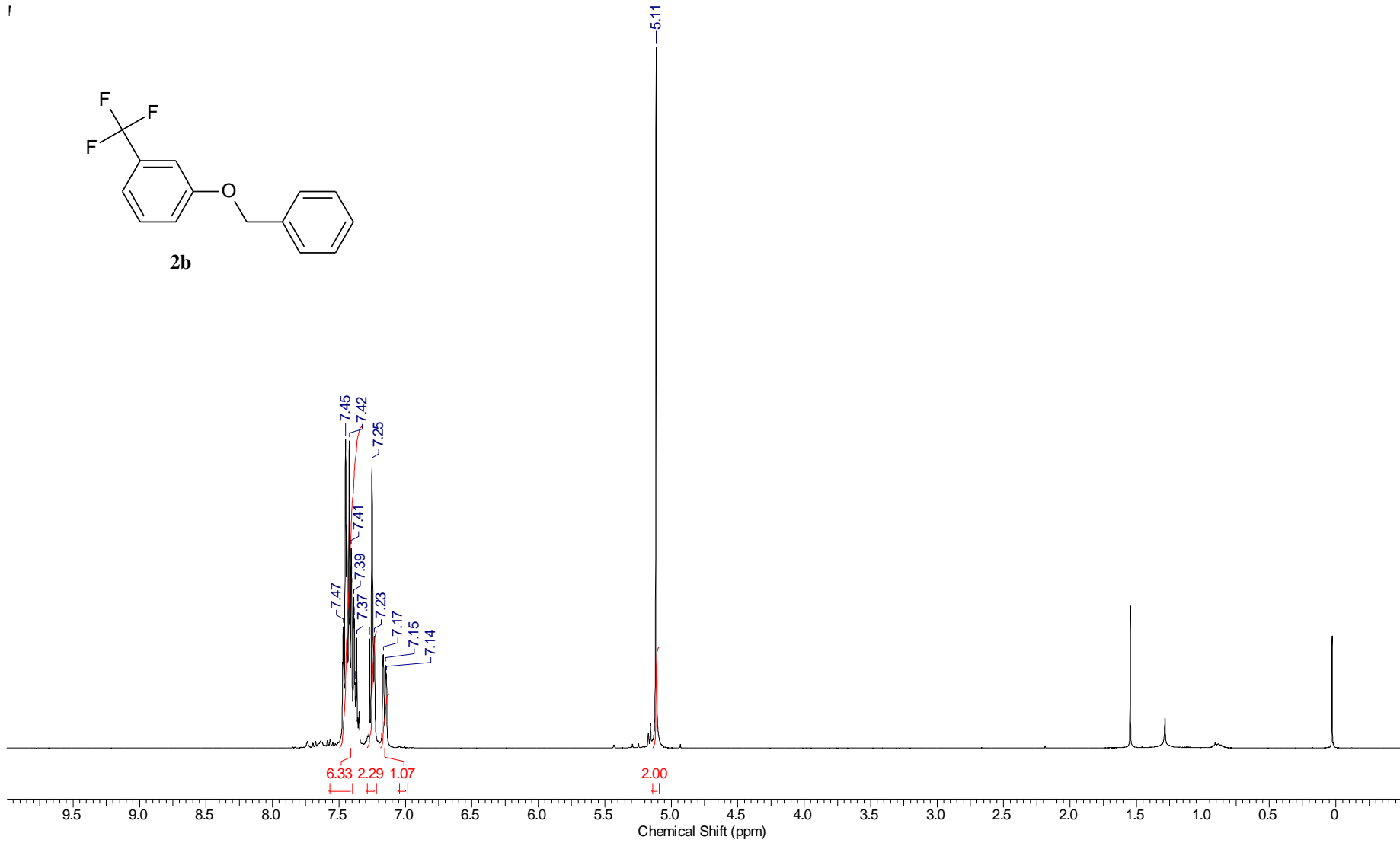
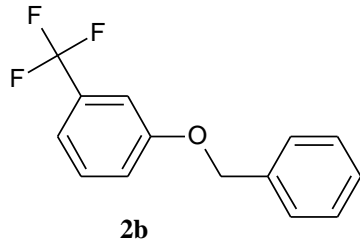
Frequency (MHz)	376.71	Nucleus	19F	Number of Transients	64	Origin	Bruker BioSpin GmbH
Original Points Count	131072	Owner	tibbe_operator	Points Count	131072	SW(cyclical) (Hz)	89285.03
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	-37389.3828	Sweep Width (Hz)	89284.35	Temperature (degree C)	27.000



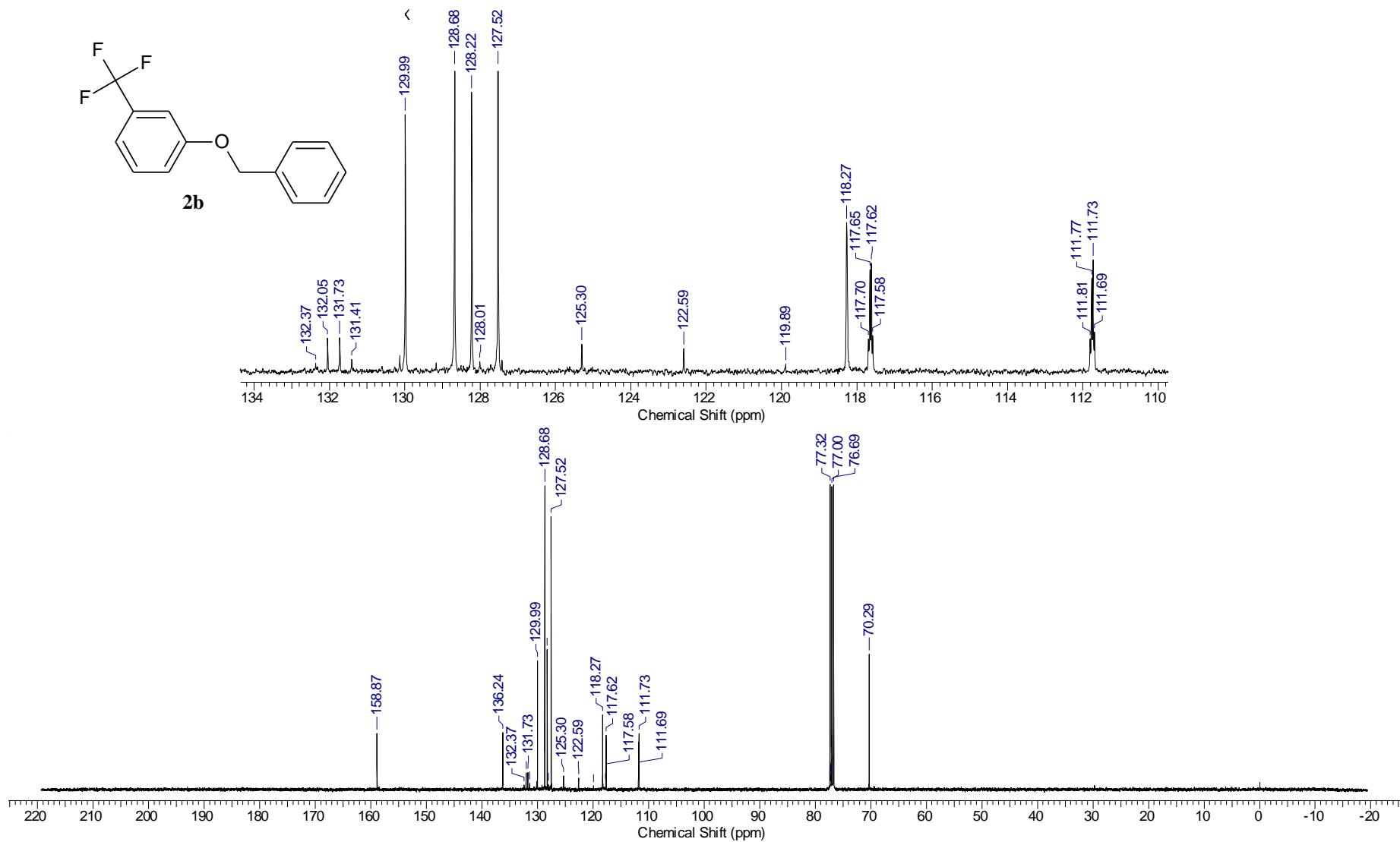




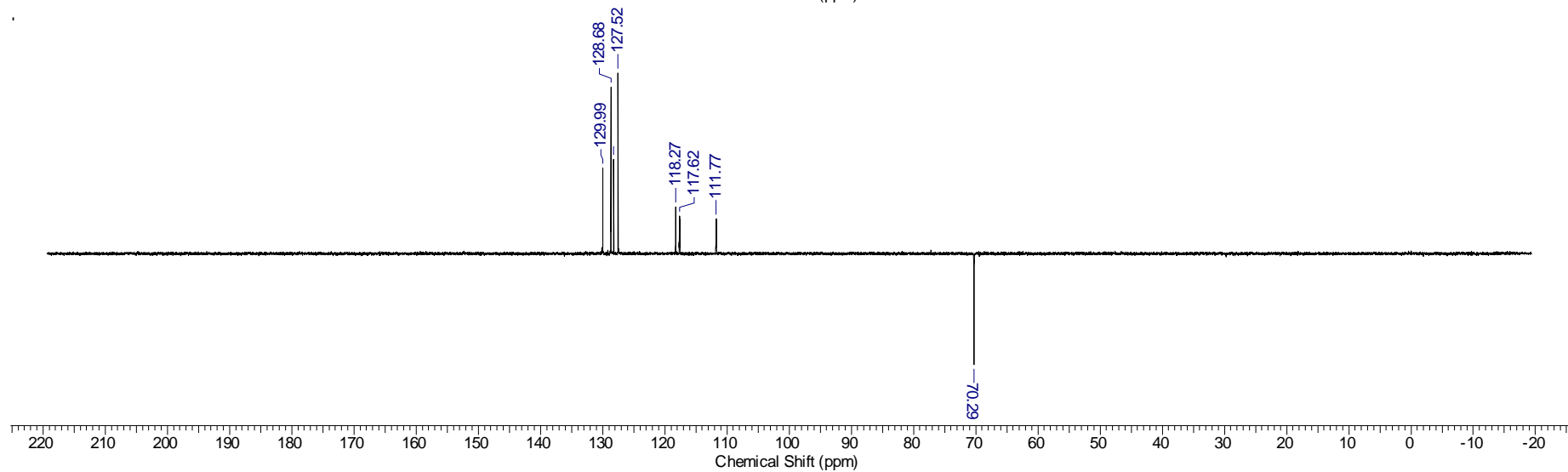
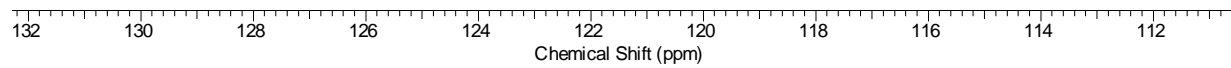
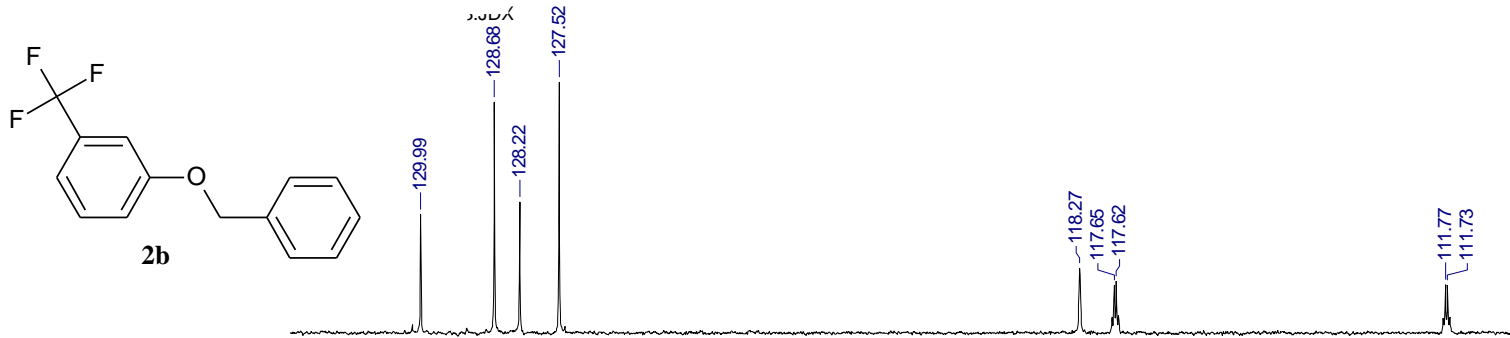
Frequency (MHz)	400.40	Nucleus	1H	Number of Transients	16	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	SW(cyclical) (Hz)	7211.32
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	3395.6414	Sweep Width (Hz)	7211.10	Temperature (degree C)	27.000



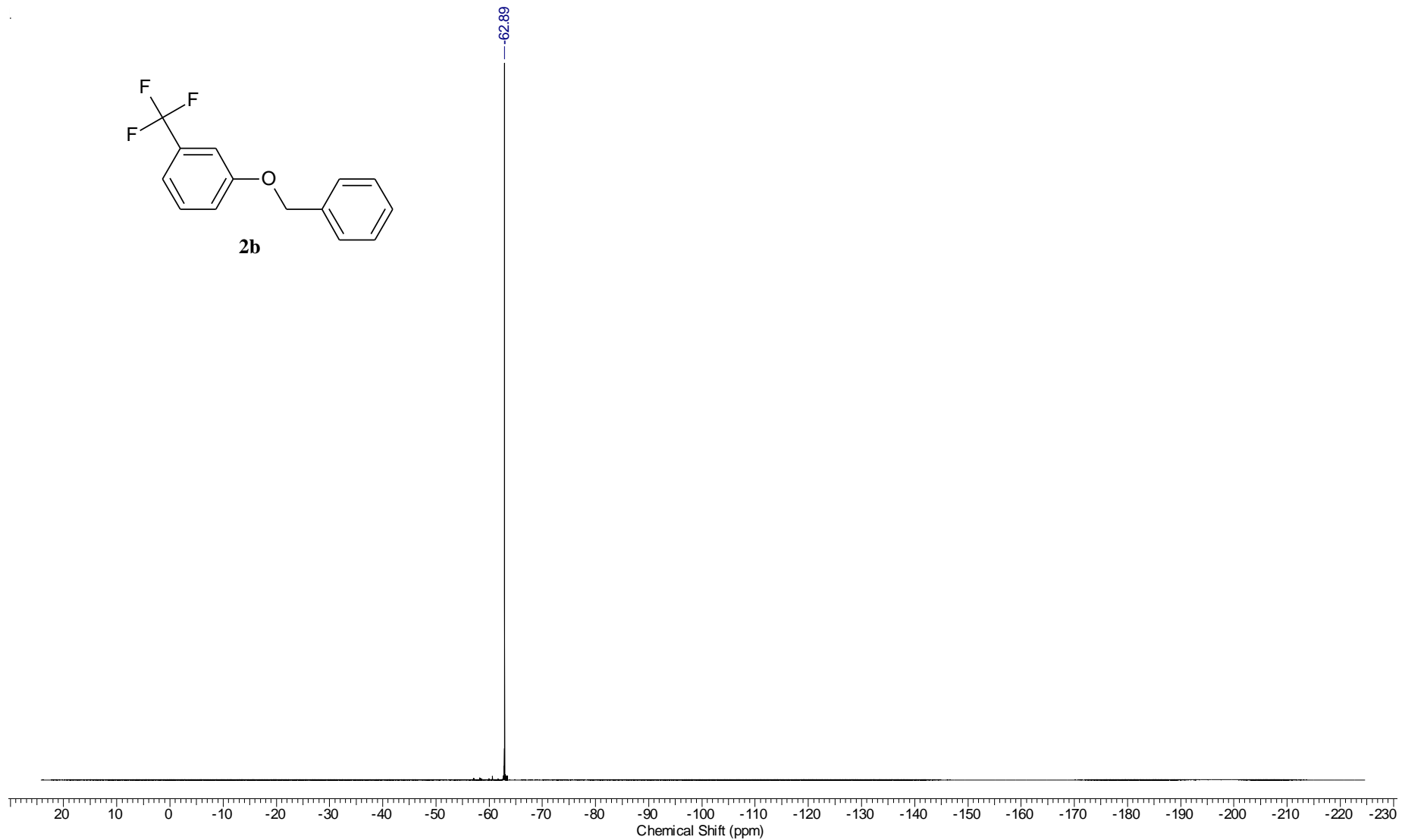
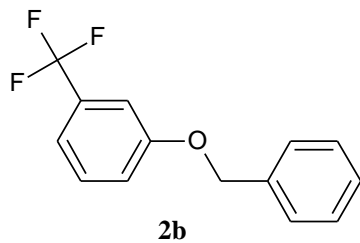
Frequency (MHz)	100.69	Nucleus	¹³ C	Number of Transients	1024	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	SW(cyclical) (Hz)	24037.73
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10066.5088	Sweep Width (Hz)	24036.99	Temperature (degree C)	27.000



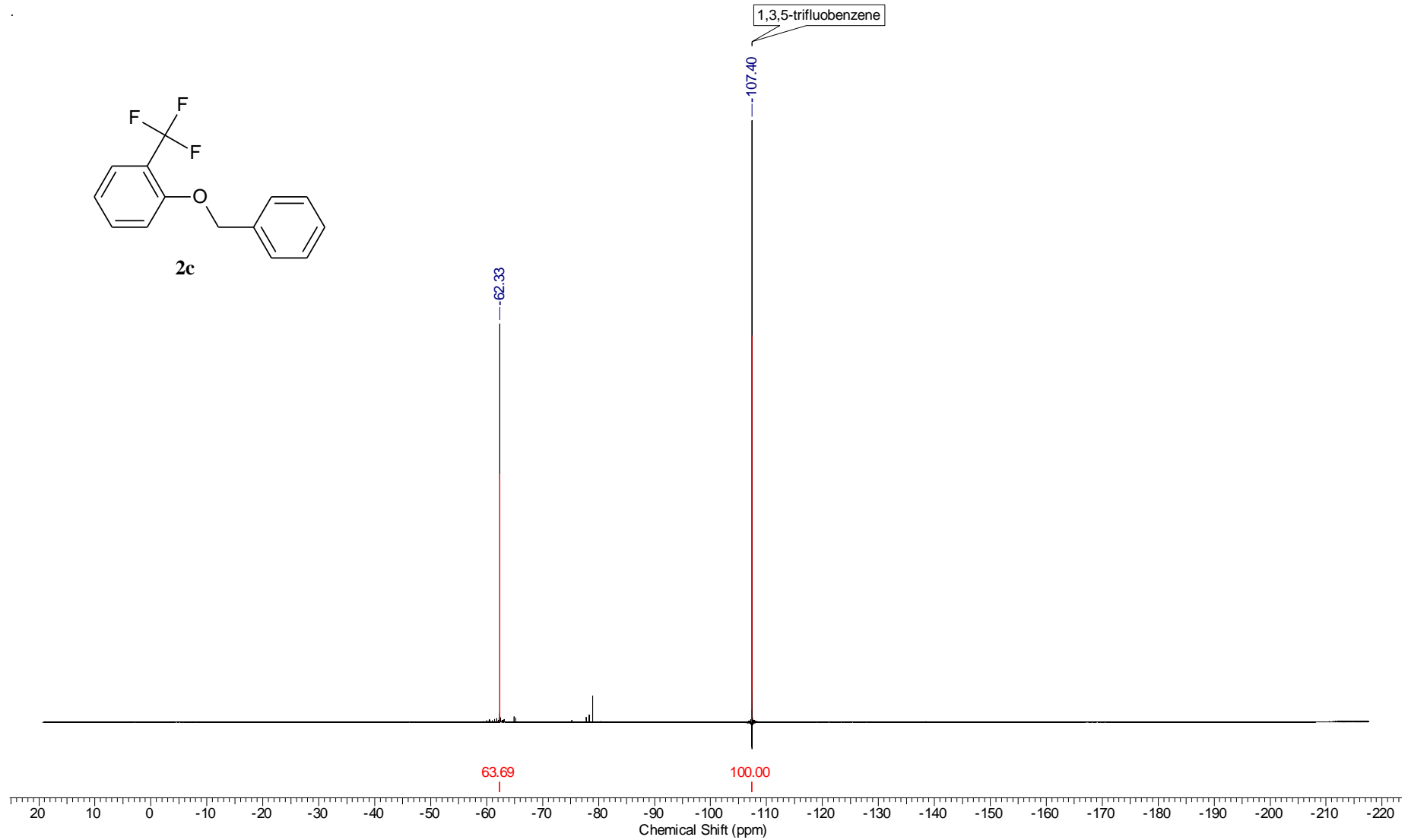
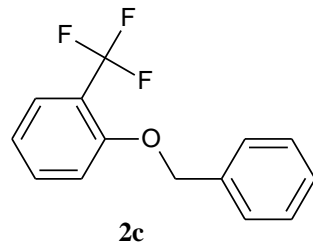
Frequency (MHz)	100.69	Nucleus	¹³ C Dept 135	Number of Transients	256	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	SW(cyclical) (Hz)	24037.73
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10066.4961	Sweep Width (Hz)	24036.99	Temperature (degree C)	27.000

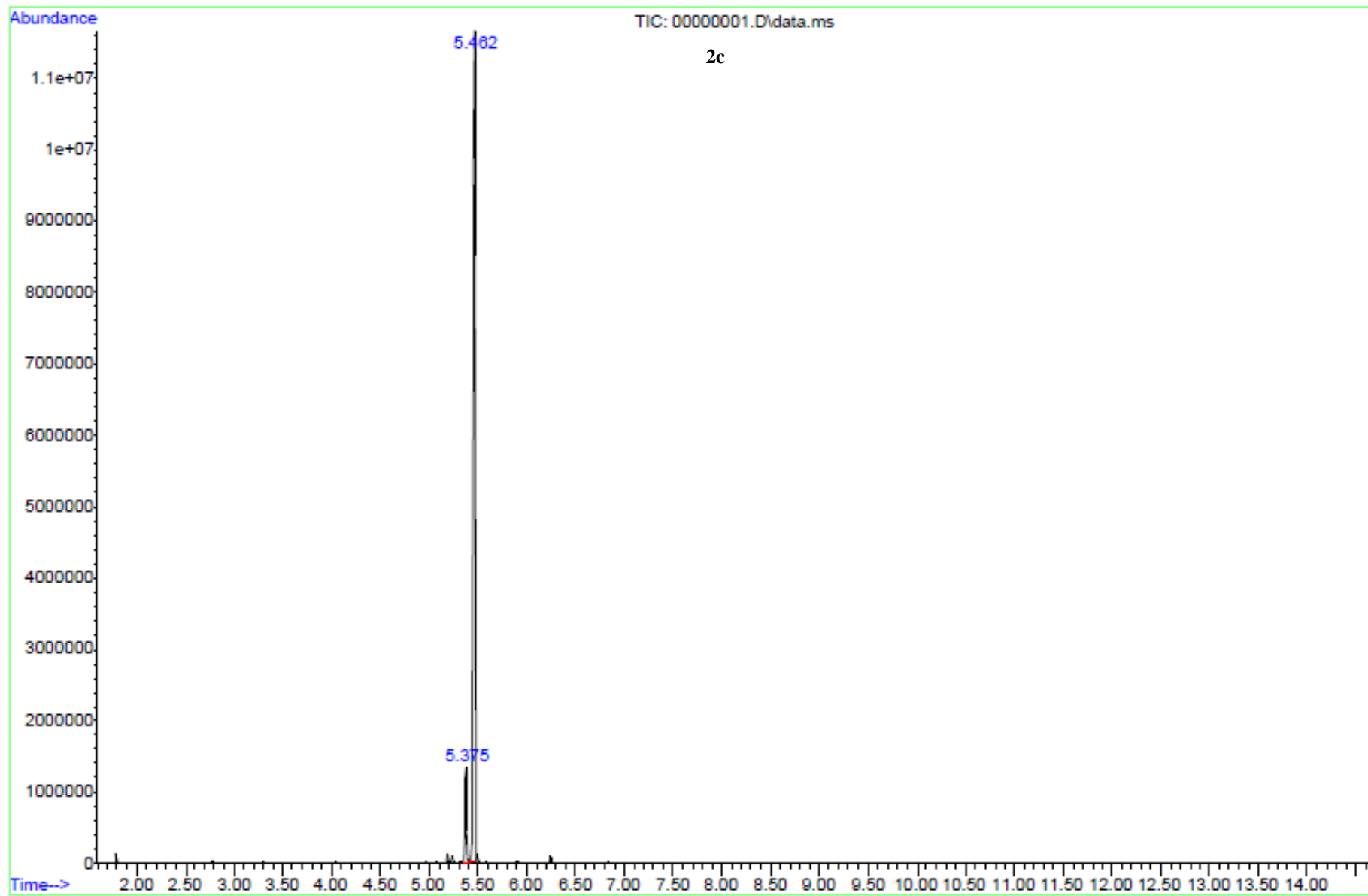


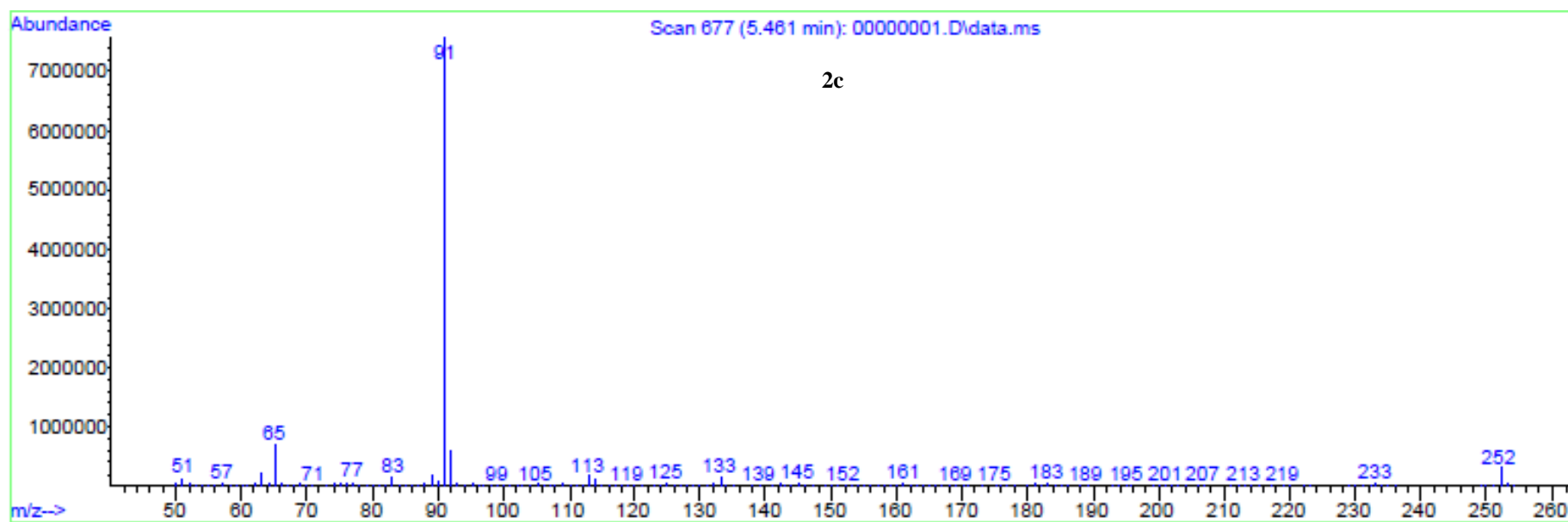
Frequency (MHz)	376.71	Nucleus	19F	Number of Transients	64	Origin	Bruker BioSpin GmbH
Original Points Count	131072	Owner	tibbe_operator	Points Count	131072	SW(cyclical) (Hz)	93749.28
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	-37741.6094	Sweep Width (Hz)	93748.56	Temperature (degree C)	27.000



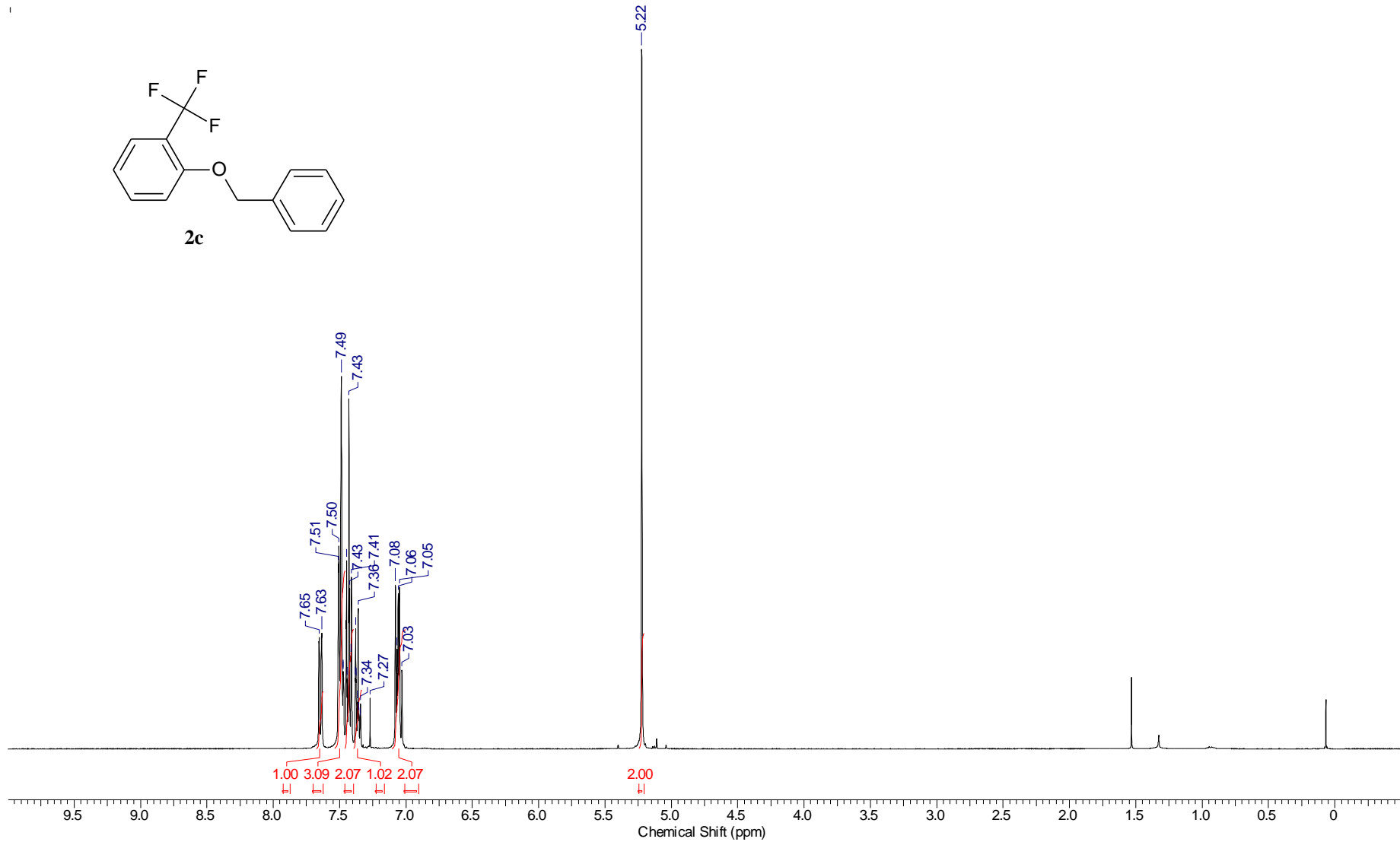
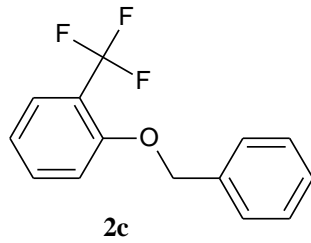
Frequency (MHz)	376.71	Nucleus	¹⁹ F	Number of Transients	64	Origin	Bruker BioSpin GmbH
Original Points Count	131072	Owner	tibbe_operator	Points Count	131072	SW(cyclical) (Hz)	89285.03
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	-37337.6094	Sweep Width (Hz)	89284.35	Temperature (degree C)	27.000



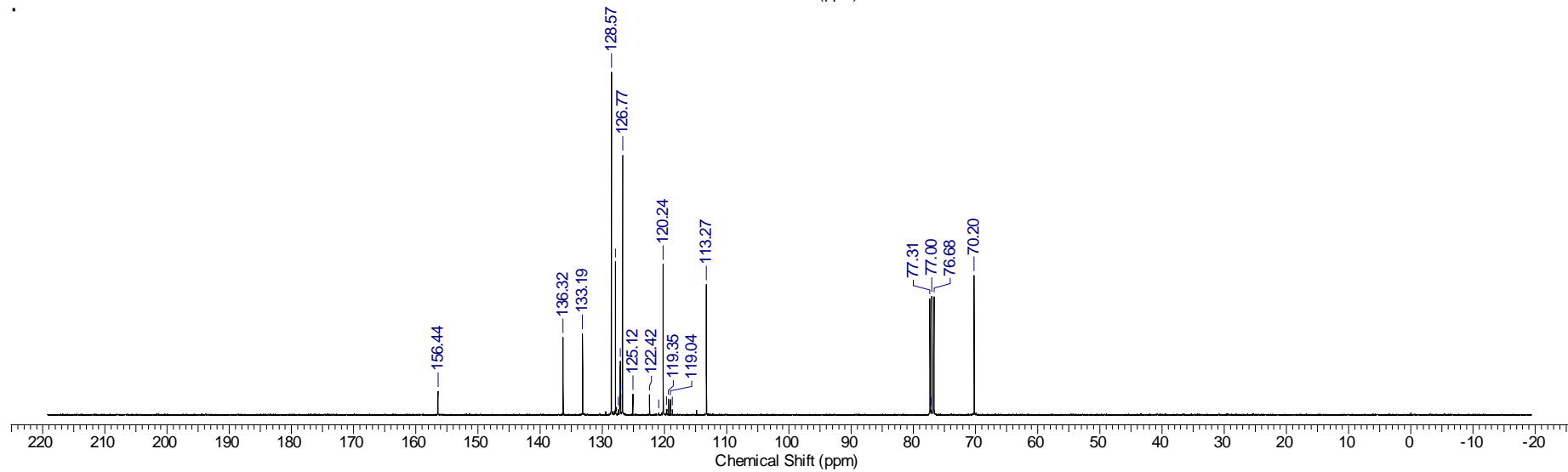
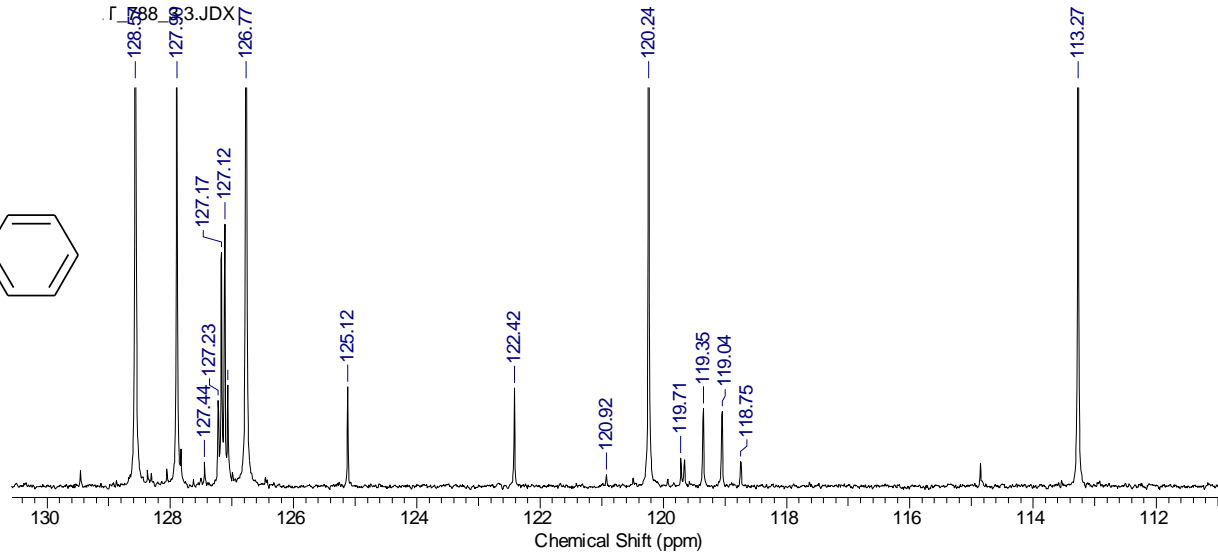
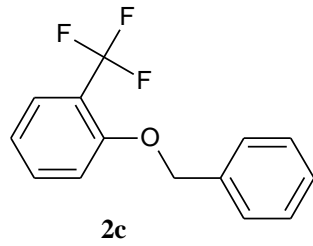




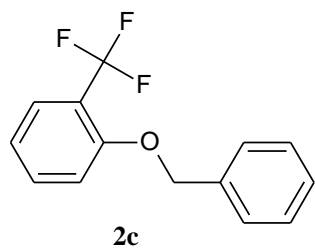
Frequency (MHz)	400.40	Nucleus	1H	Number of Transients	16	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	SW(cyclical) (Hz)	7211.32
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	3395.8613	Sweep Width (Hz)	7211.10	Temperature (degree C)	27.000



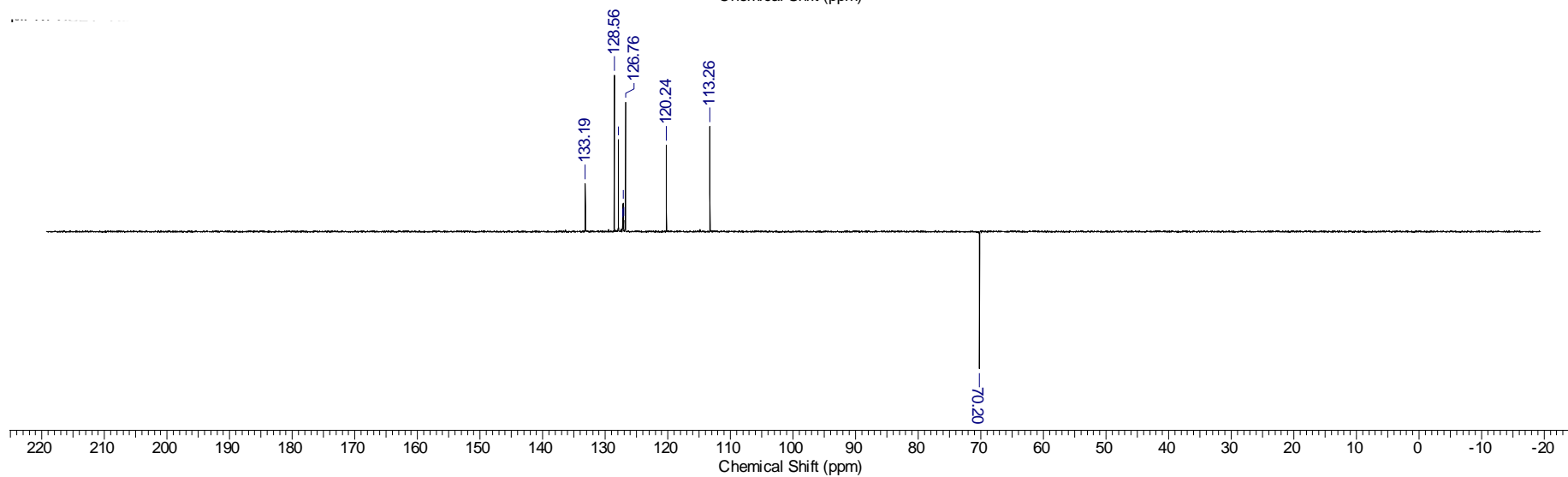
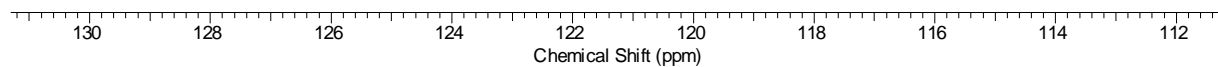
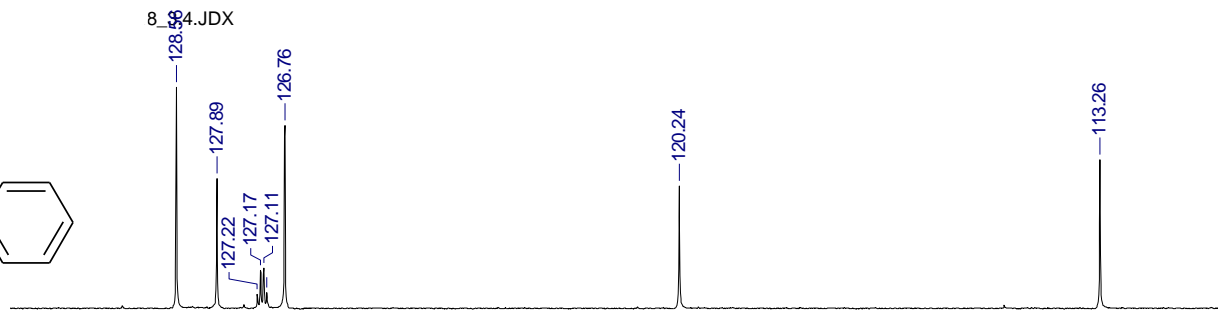
Frequency (MHz)	100.69	Nucleus	13C	Number of Transients	1024	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	SW(cyclical) (Hz)	24037.73
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10062.1084	Sweep Width (Hz)	24036.99	Temperature (degree C)	27.000



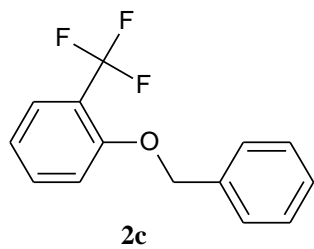
Frequency (MHz)	100.69	Nucleus	¹³ C Dent 135	Number of Transients	256	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	SW(cyclical) (Hz)	24037.73
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10061.8350	Sweep Width (Hz)	24036.99	Temperature (degree C)	27.000



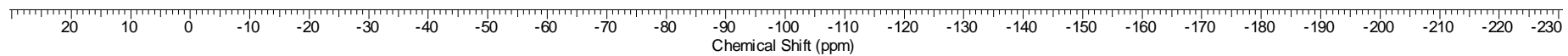
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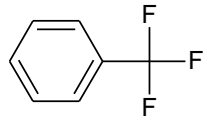
Frequency (MHz)	376.71	Nucleus	19F	Number of Transients	64	Origin	Bruker BioSpin GmbH
Original Points Count	131072	Owner	tibbe_operator	Points Count	131072	SW(cyclical) (Hz)	93749.28
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	-37730.1992	Sweep Width (Hz)	93748.56	Temperature (degree C)	27.000



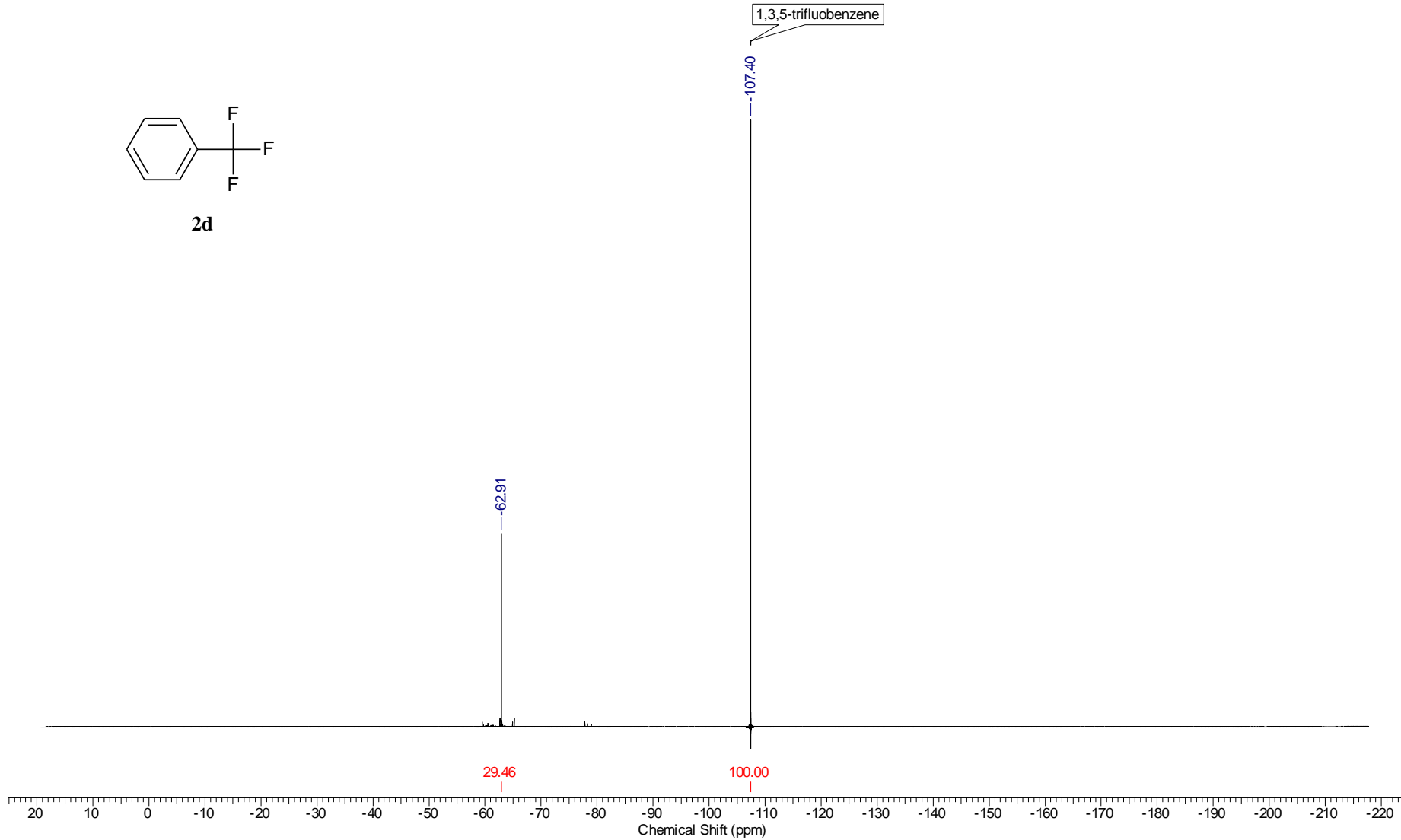
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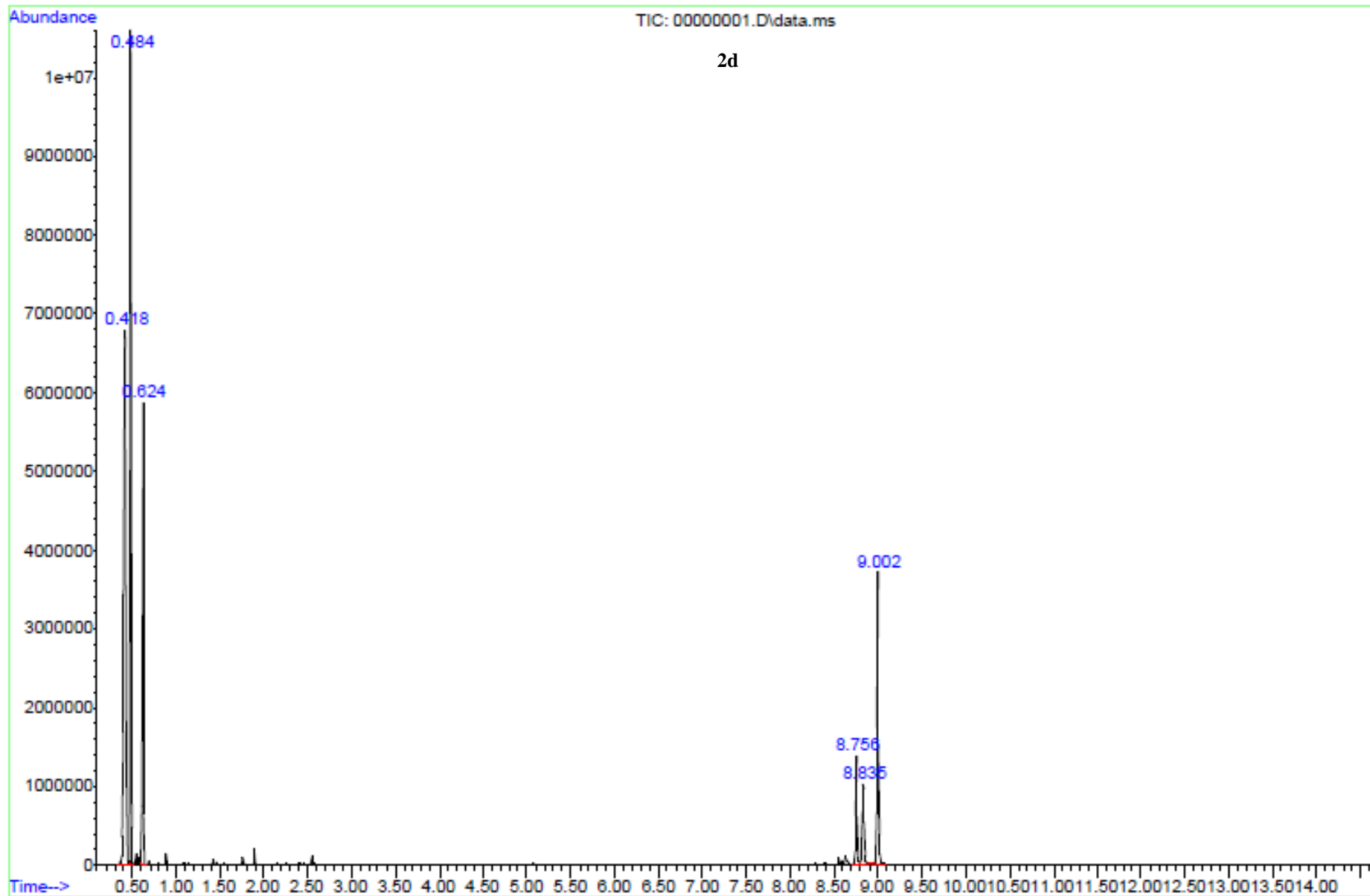


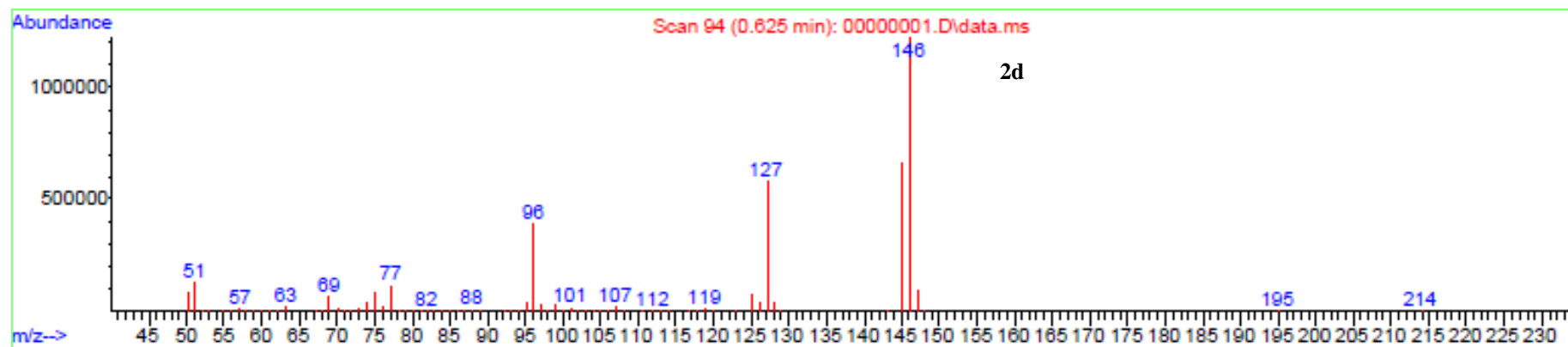
Frequency (MHz)	376.71	Nucleus	¹⁹ F	Number of Transients	64	Origin	Bruker BioSpin GmbH
Original Points Count	131072	Owner	tibbe_operator	Points Count	131072	SW(cyclical) (Hz)	89285.03
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	-37375.7539	Sweep Width (Hz)	89284.35	Temperature (degree C)	27.000



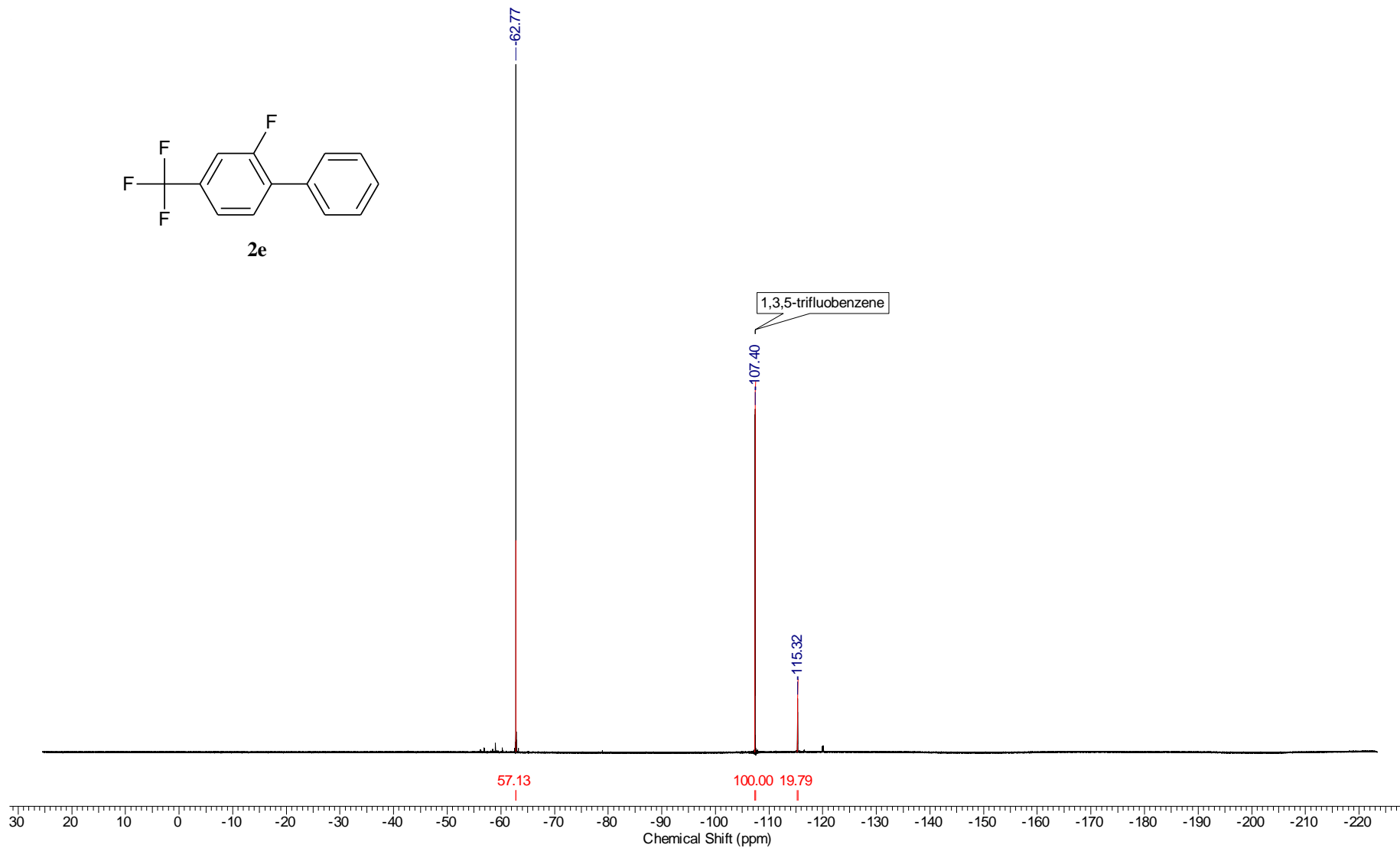
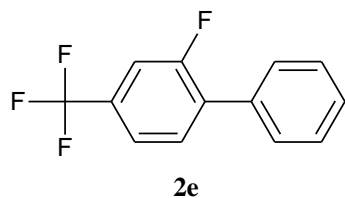
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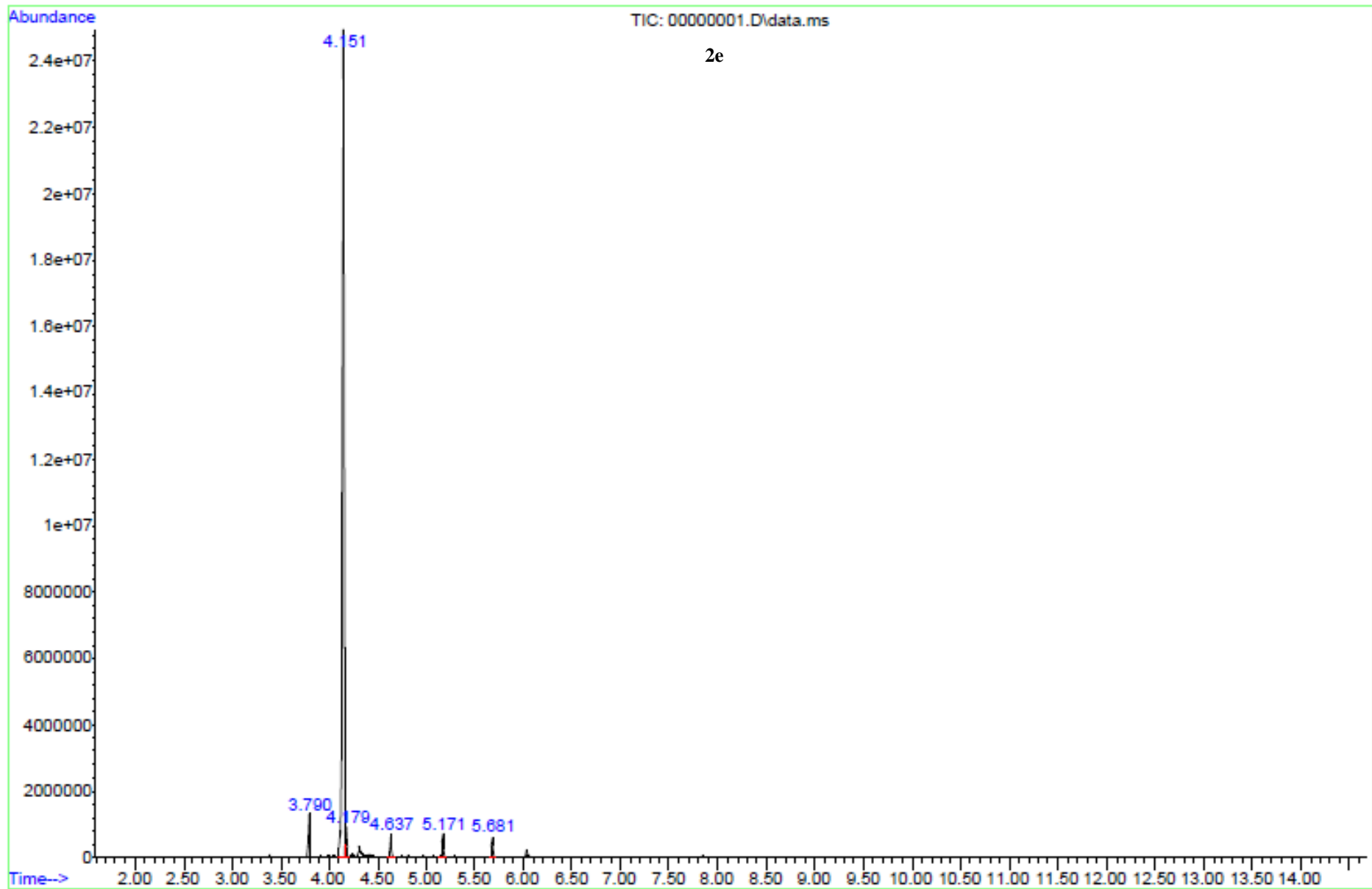


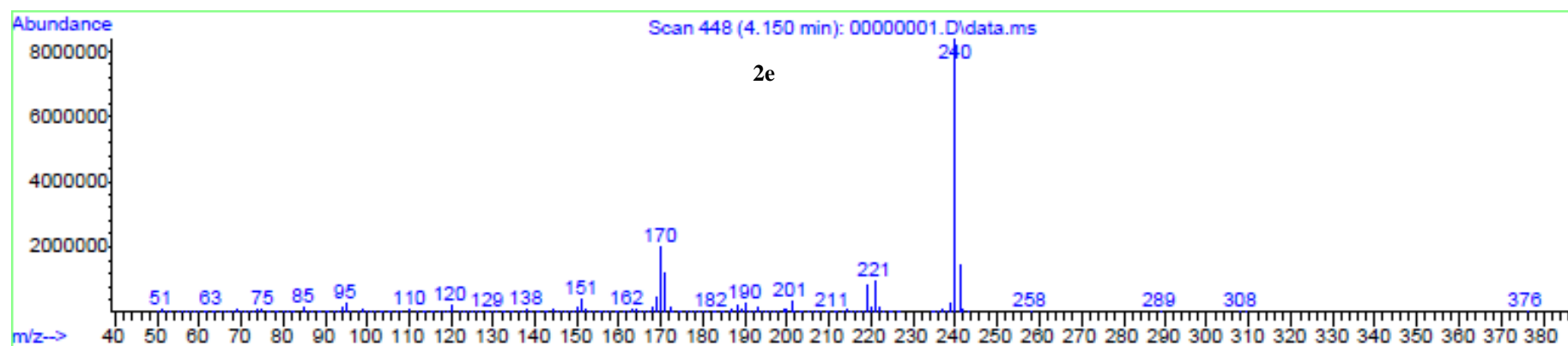




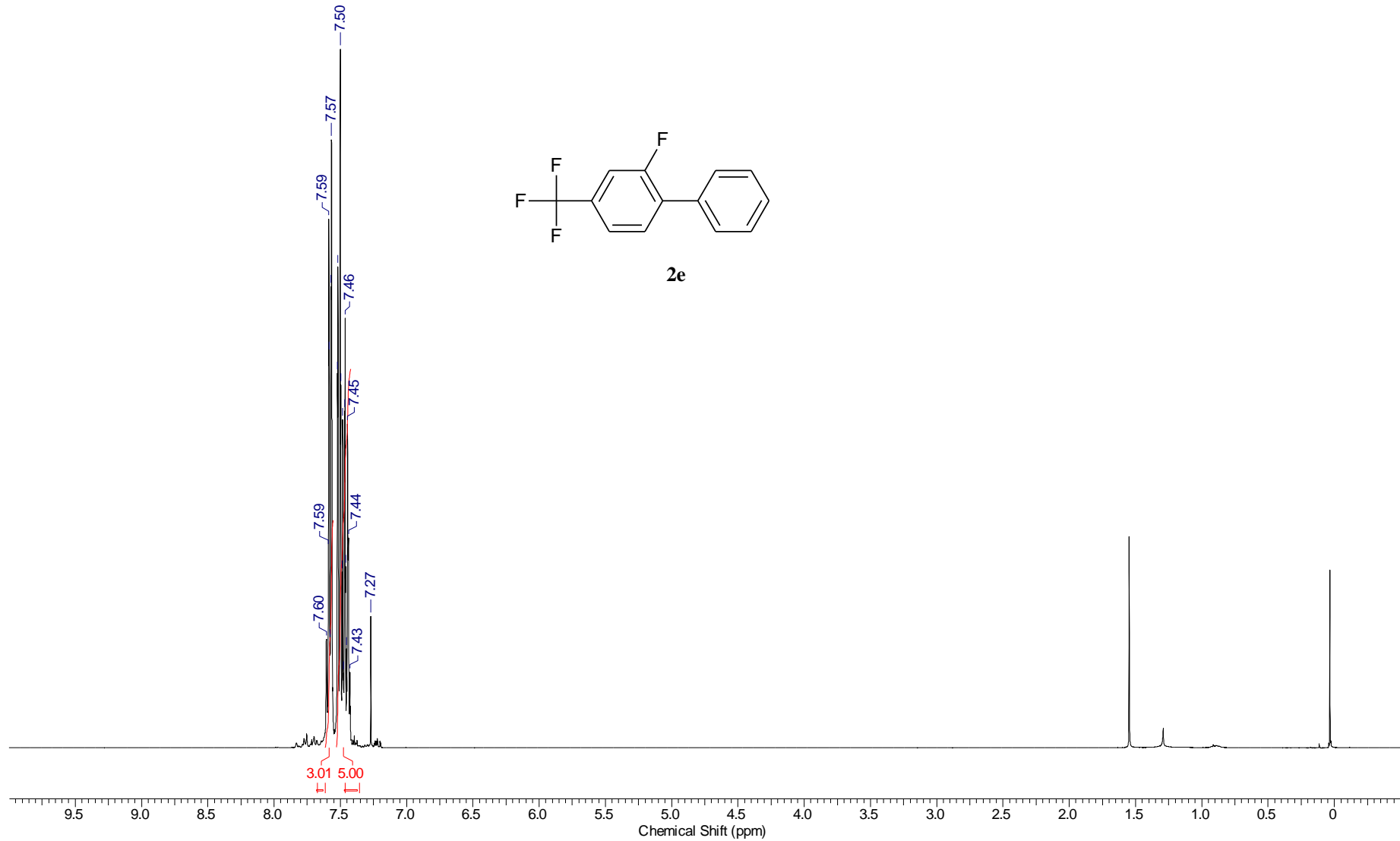
Frequency (MHz)	376.71	Nucleus	¹⁹ F	Number of Transients	64	Origin	Bruker BioSpin GmbH
Original Points Count	131072	Owner	tibbe_operator	Points Count	131072	SW(cyclical) (Hz)	93749.28
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	-37277.3711	Sweep Width (Hz)	93748.56	Temperature (degree C)	27.000



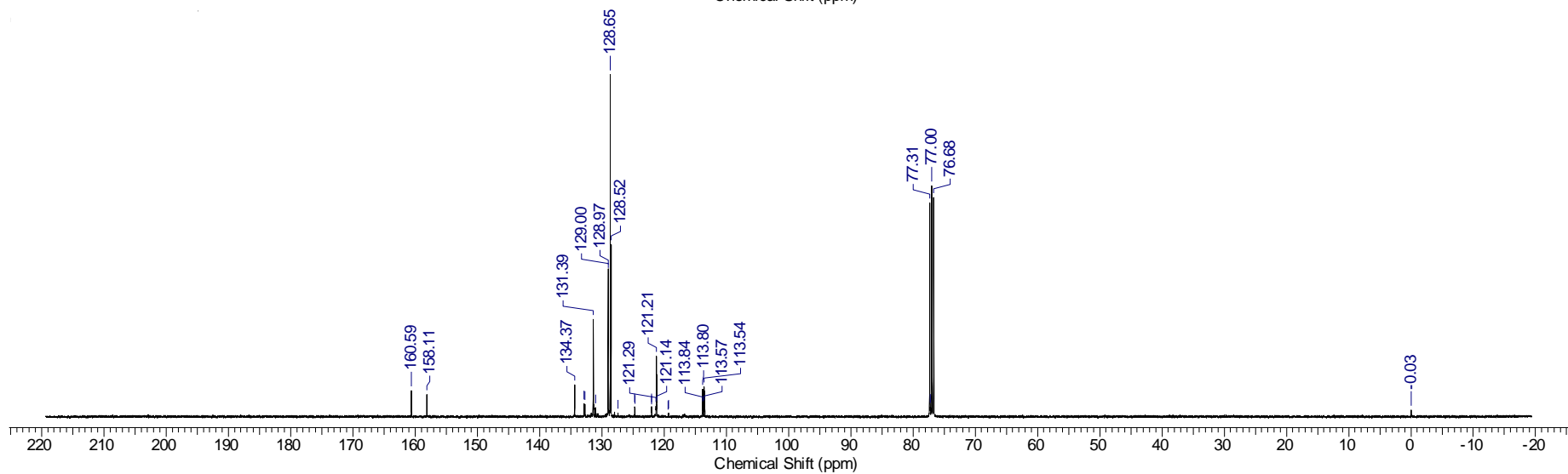
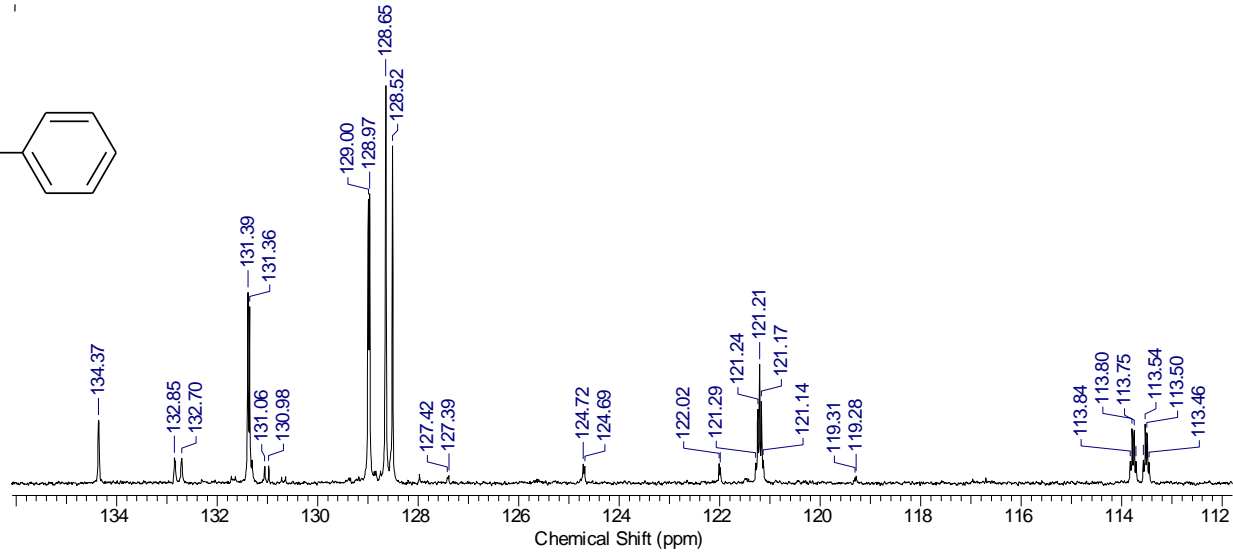
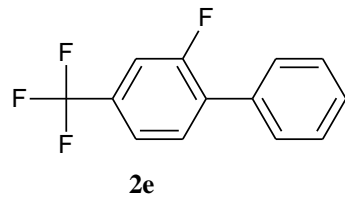




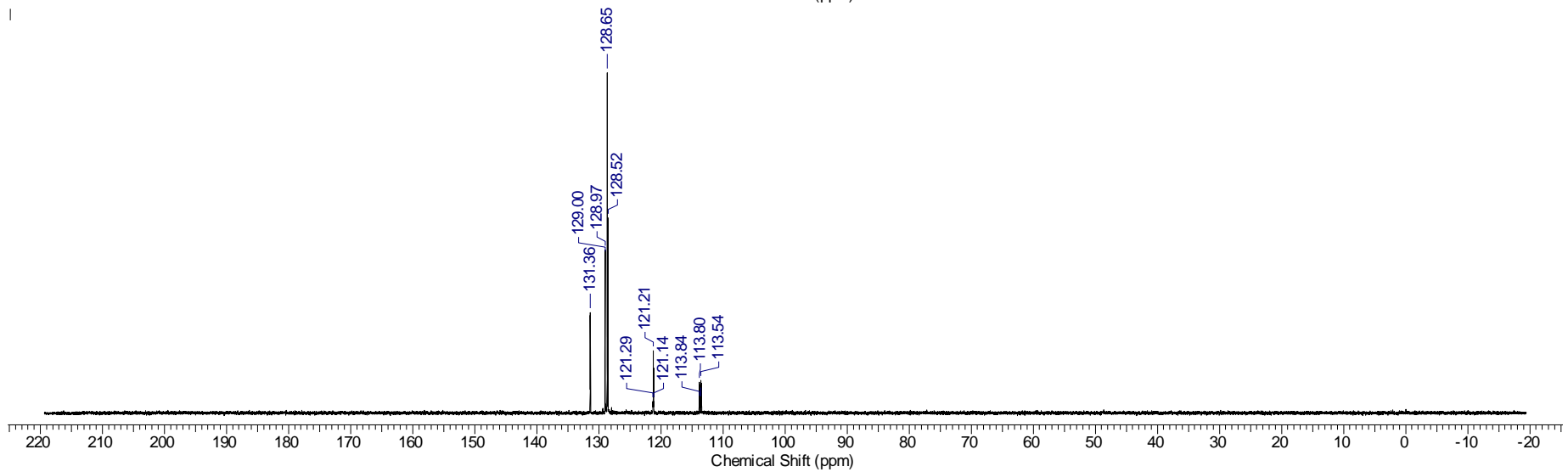
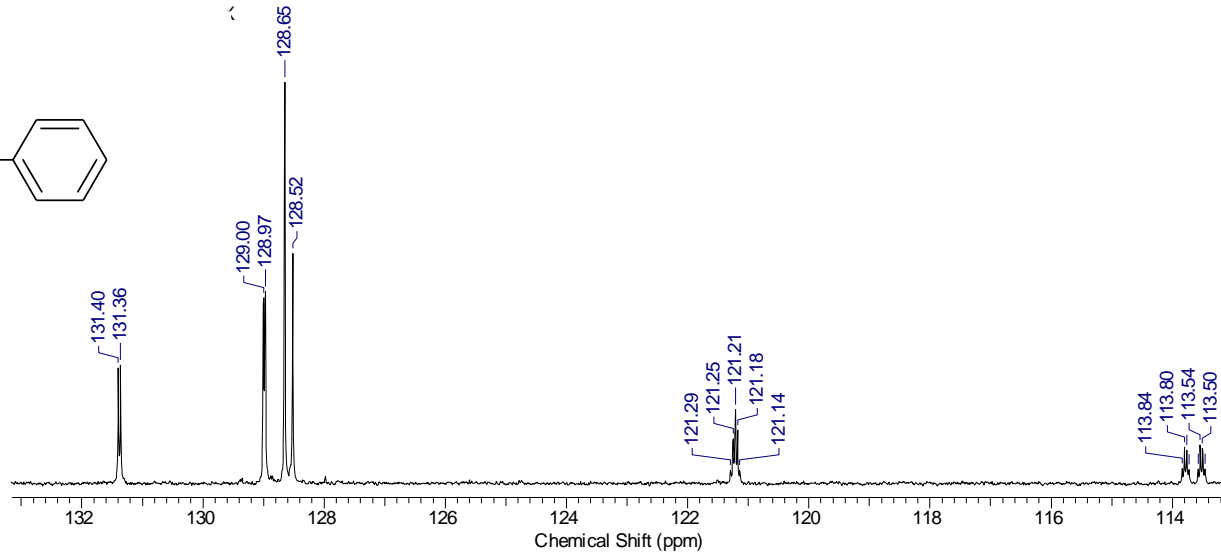
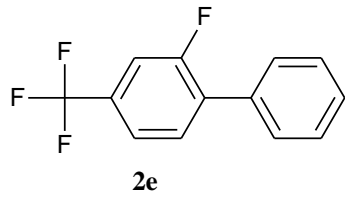
Frequency (MHz)	400.40	Nucleus	1H	Number of Transients	16	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	SW(cyclical) (Hz)	7211.32
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	3395.6414	Sweep Width (Hz)	7211.10	Temperature (degree C)	27.000



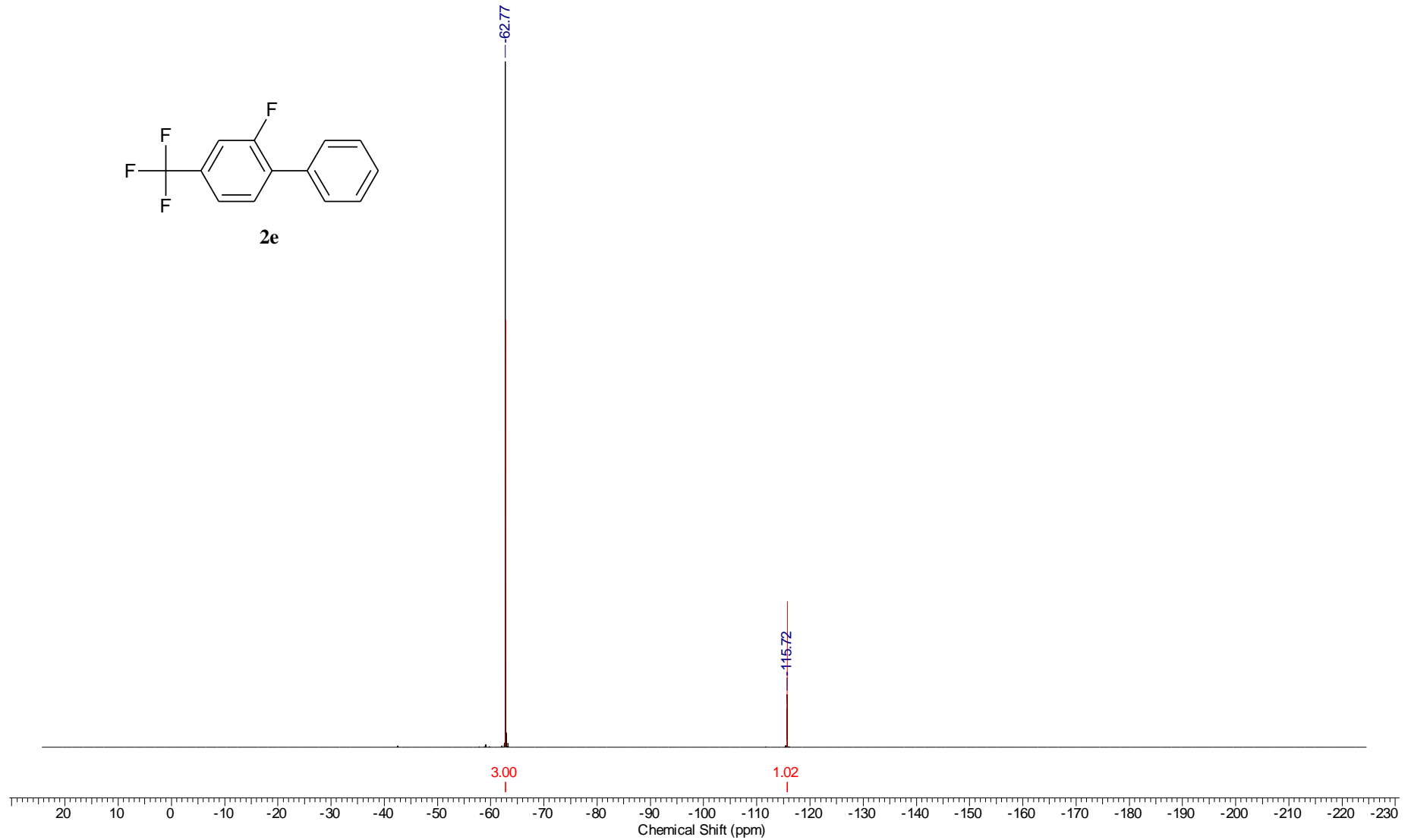
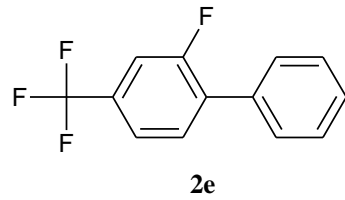
Frequency (MHz)	100.69	Nucleus	¹³ C	Number of Transients	1024	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	SW(cyclical) (Hz)	24037.73
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10066.5088	Sweep Width (Hz)	24036.99	Temperature (degree C)	27.000



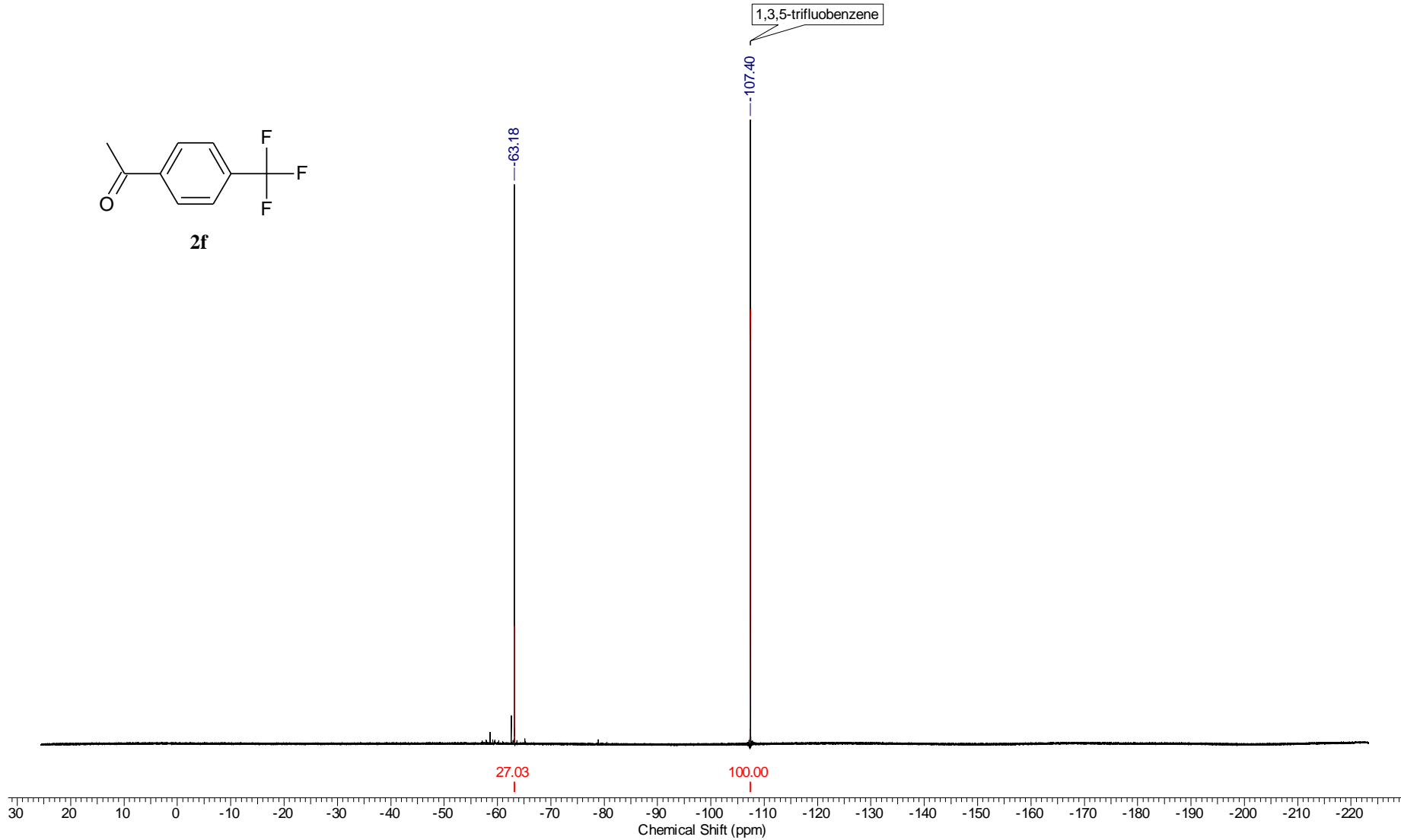
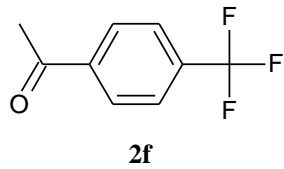
Frequency (MHz)	100.69	Nucleus	¹³ C Dept 135	Number of Transients	256	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	SW(cyclical) (Hz)	24037.73
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10066.8838	Sweep Width (Hz)	24036.99	Temperature (degree C)	27.000

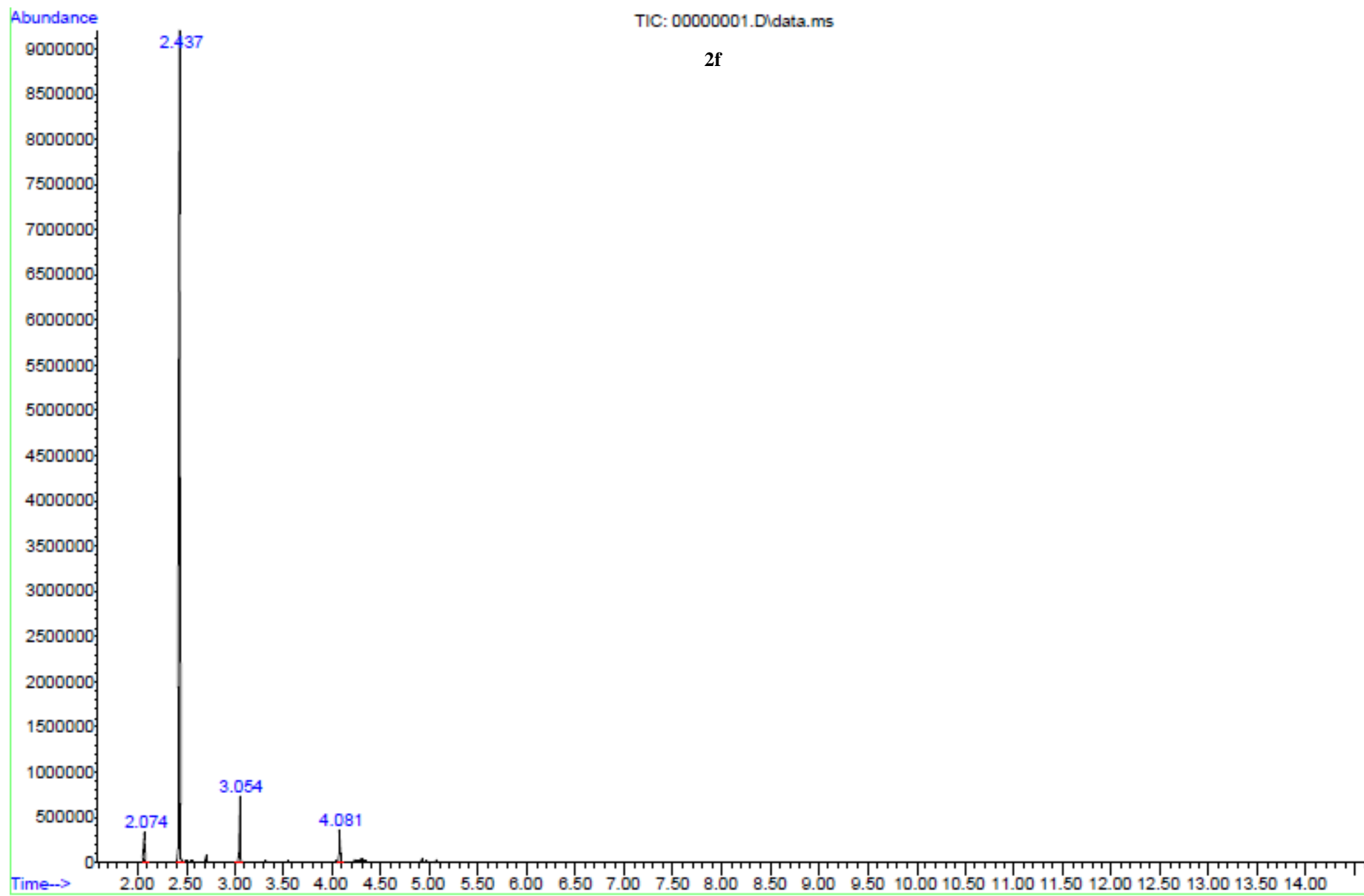


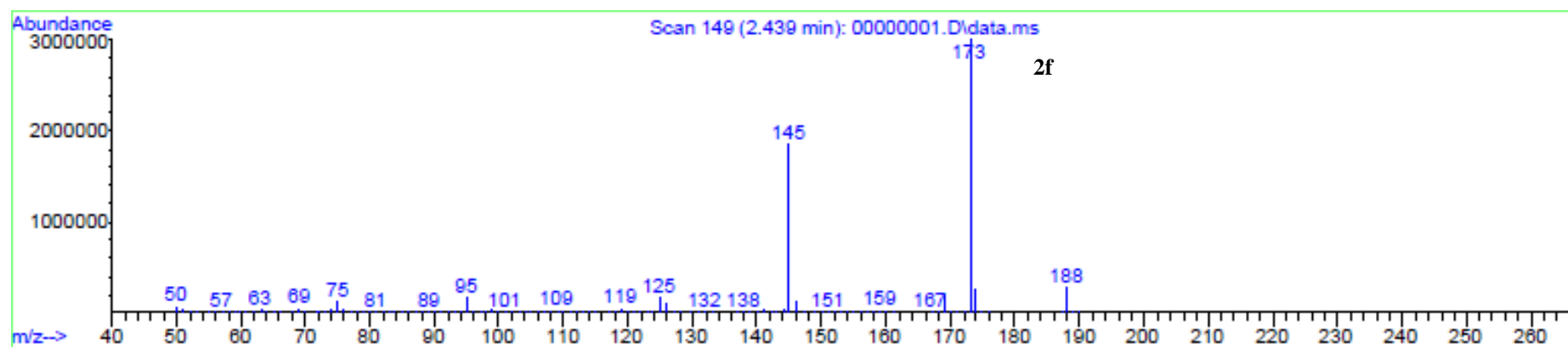
Frequency (MHz)	376.71	Nucleus	¹⁹ F	Number of Transients	64	Origin	Bruker BioSpin GmbH
Original Points Count	131072	Owner	tibbe_operator	Points Count	131072	SW(cyclical) (Hz)	93749.28
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	-37719.2891	Sweep Width (Hz)	93748.56	Temperature (degree C)	27.000



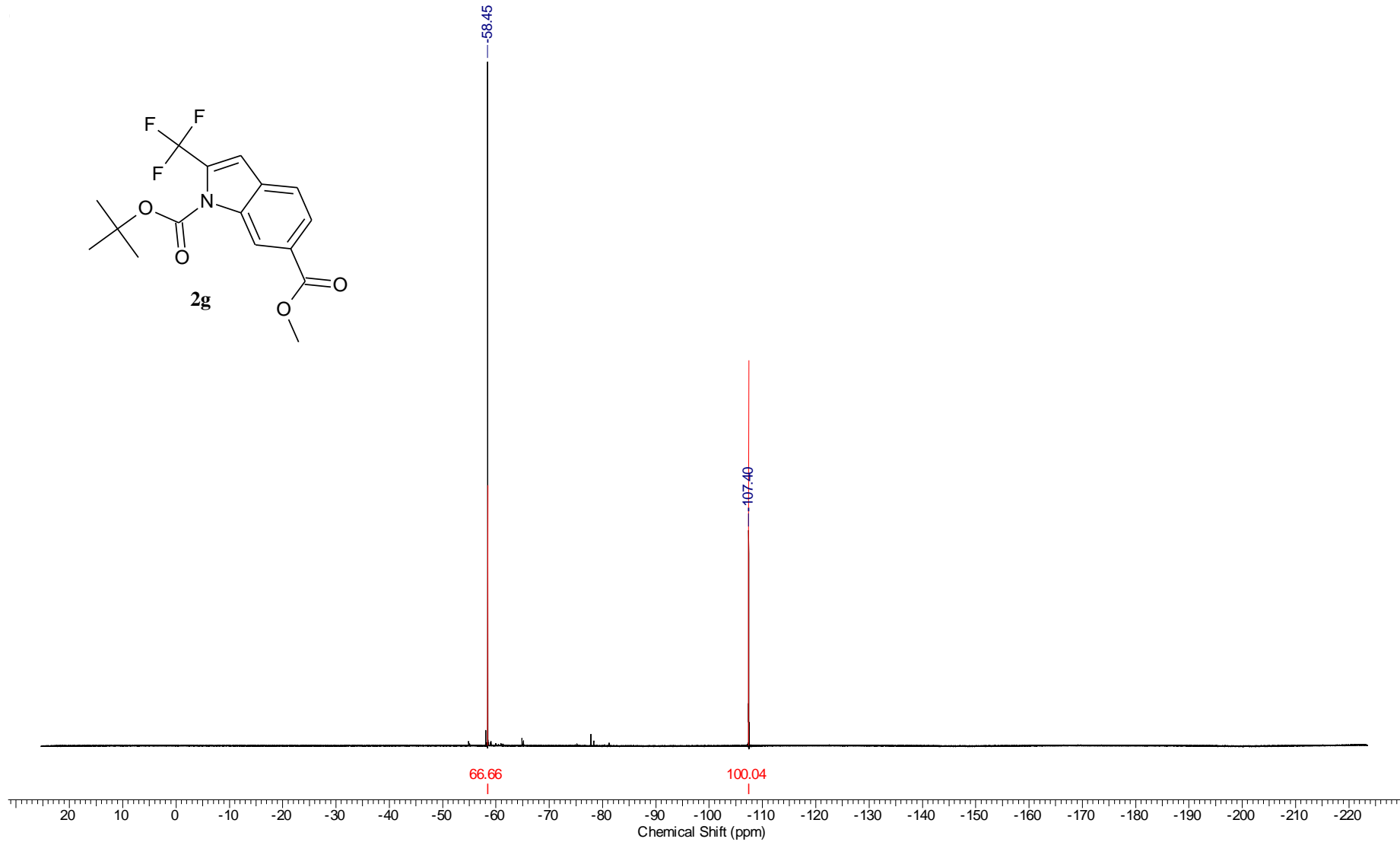
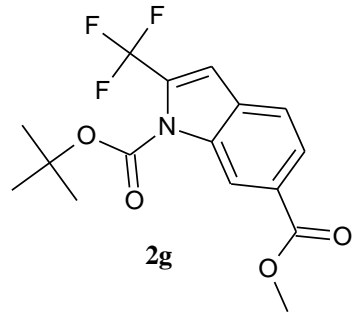
Frequency (MHz)	376.71	Nucleus	¹⁹ F	Number of Transients	64	Origin	Bruker BioSpin GmbH
Original Points Count	131072	Owner	tibbe_operator	Points Count	131072	SW(cyclical) (Hz)	93749.28
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	-37238.0313	Sweep Width (Hz)	93748.56	Temperature (degree C)	27.000

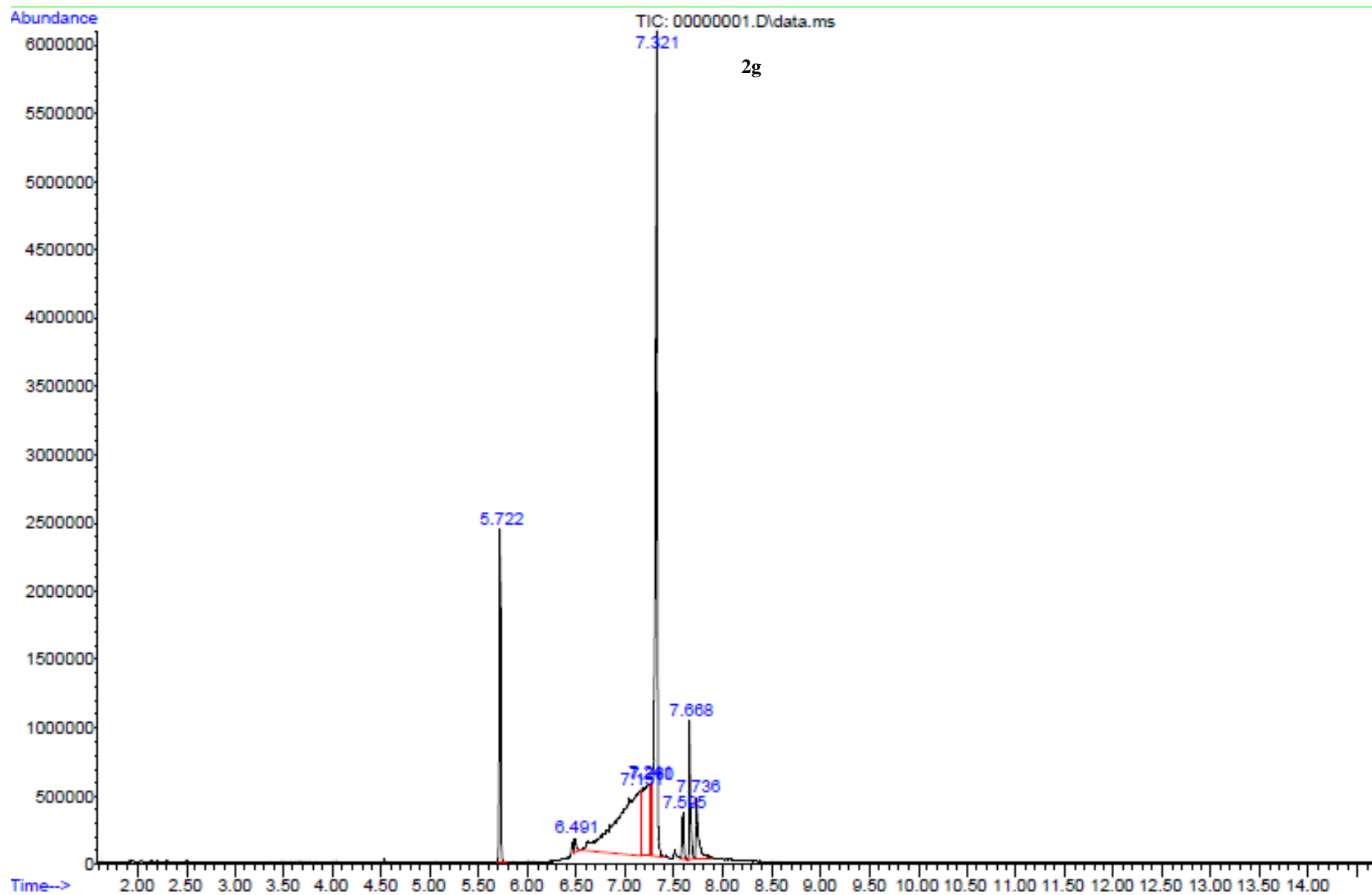


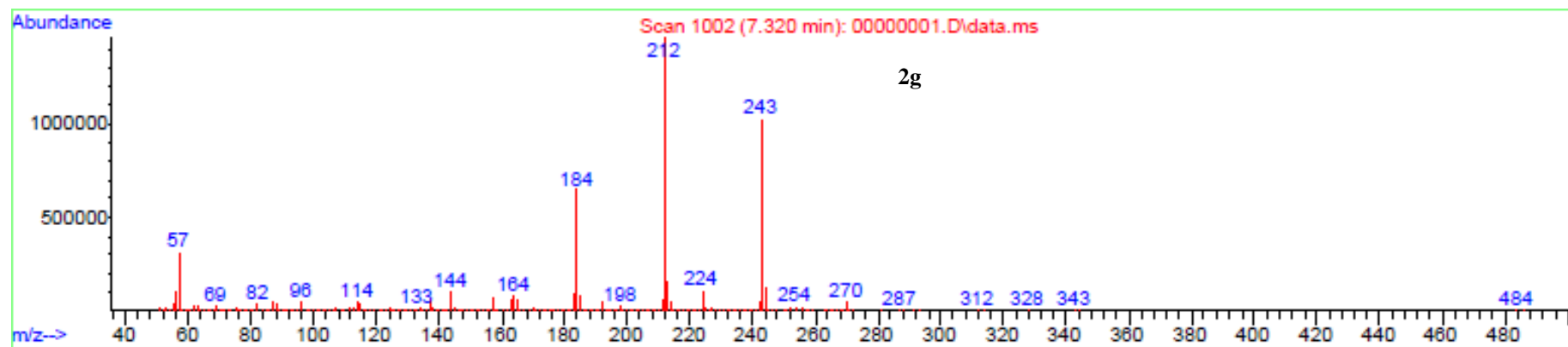




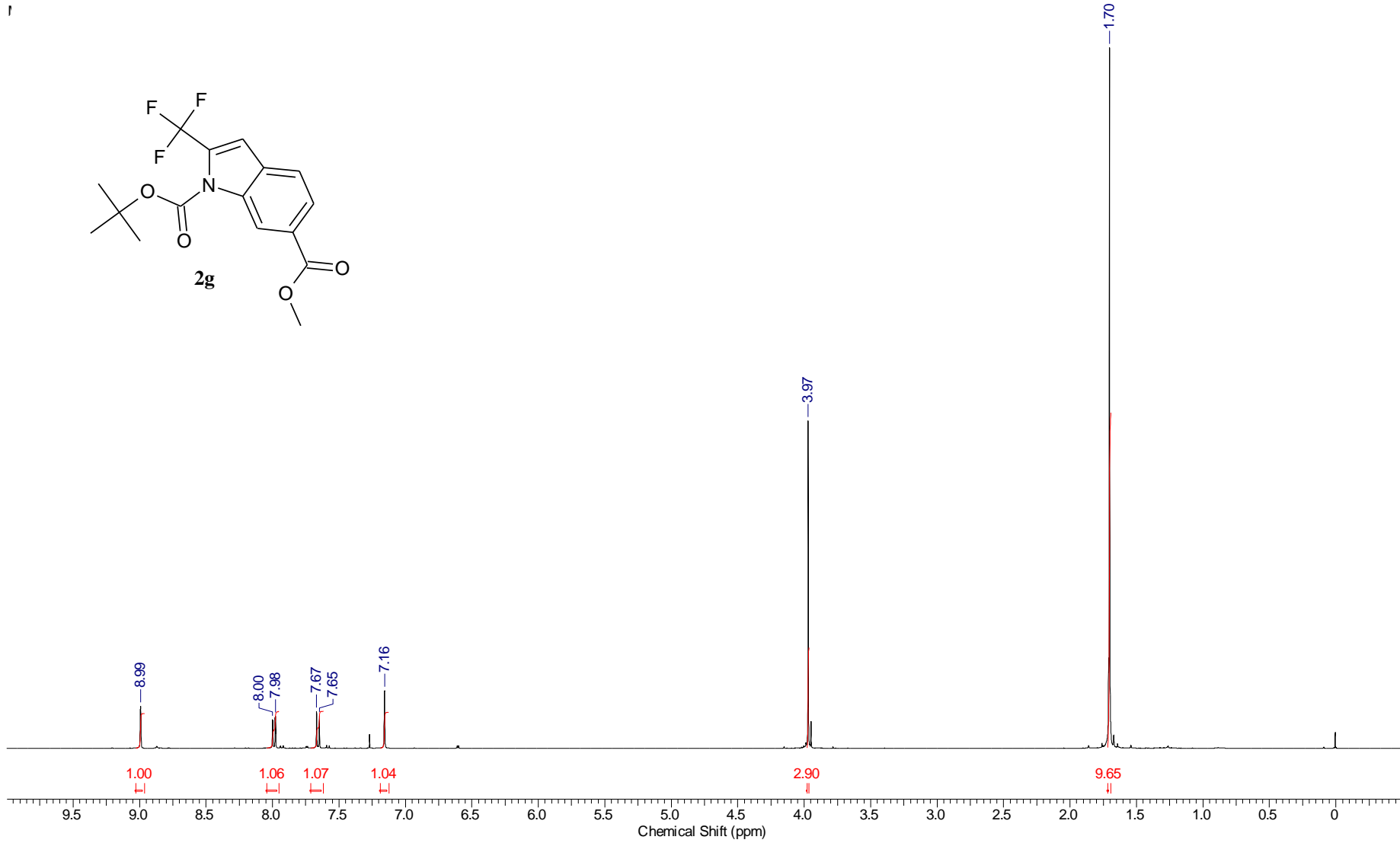
Frequency (MHz)	376.71	Nucleus	19F	Number of Transients	64	Origin	Bruker BioSpin GmbH
Original Points Count	131072	Owner	tibbe_operator	Points Count	131072	SW(cyclical) (Hz)	93749.28
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	-37318.8555	Sweep Width (Hz)	93748.56	Temperature (degree C)	27.000



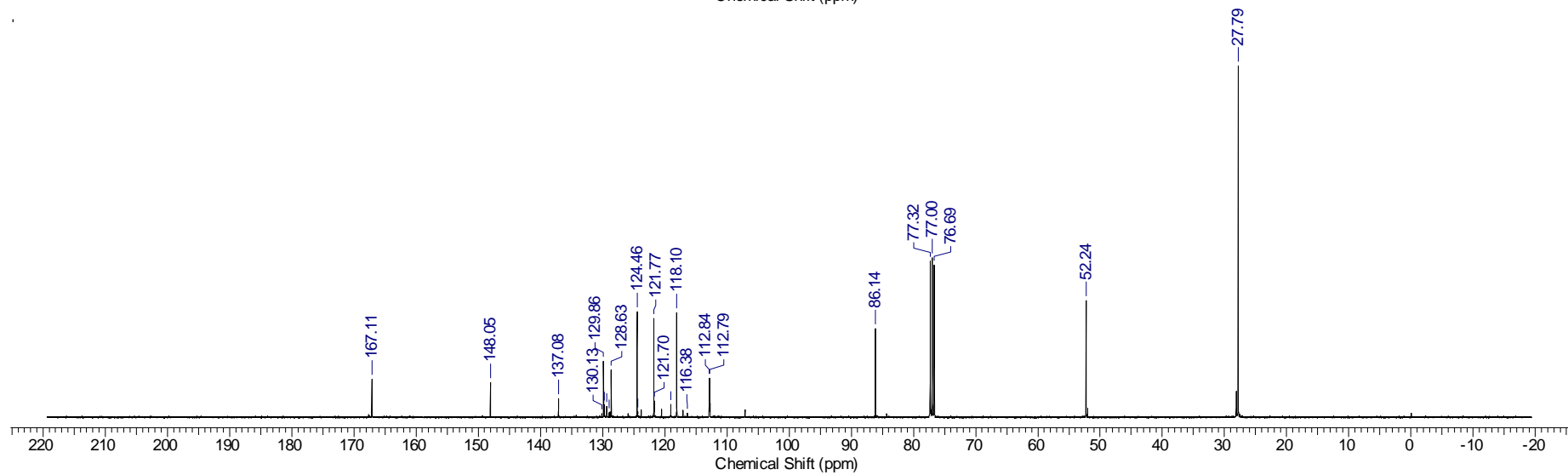
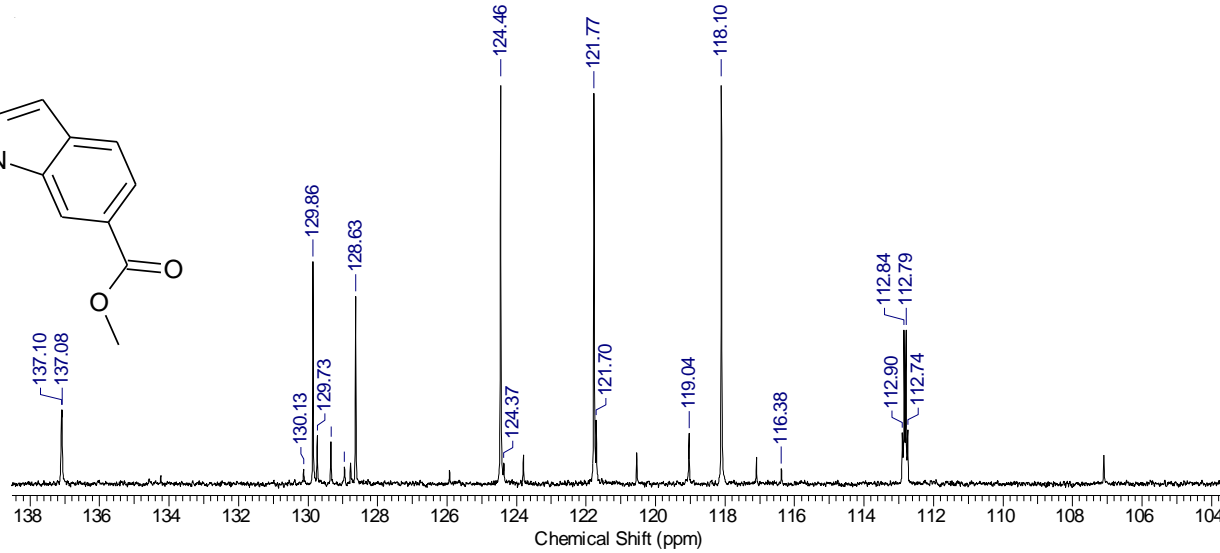
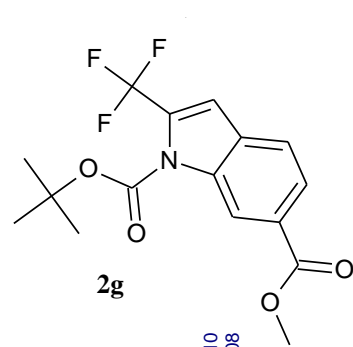




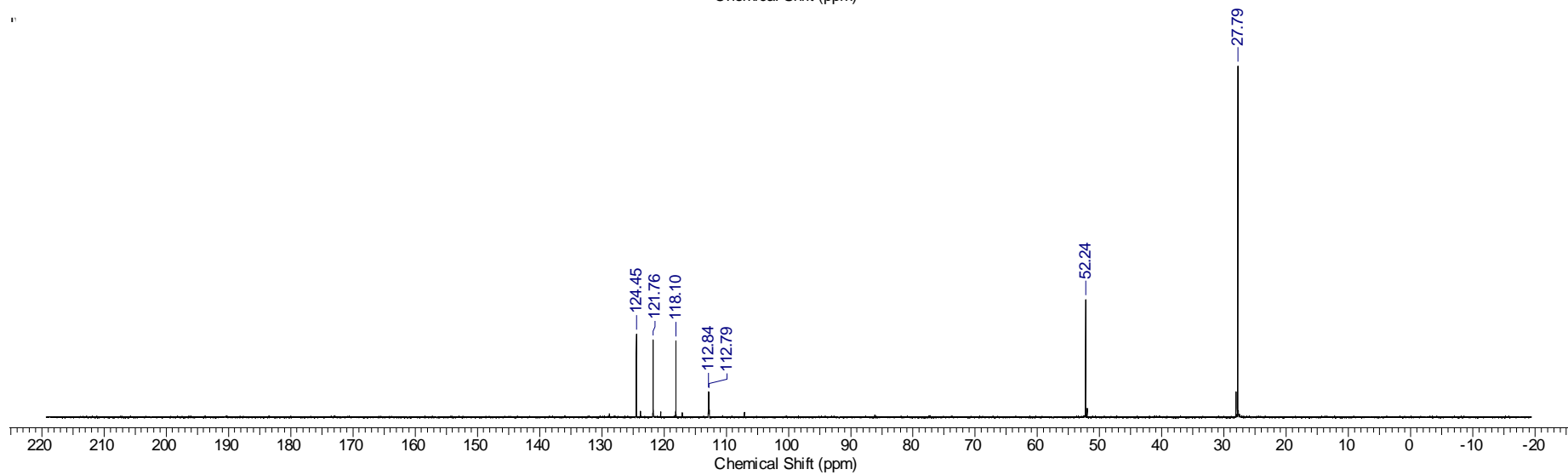
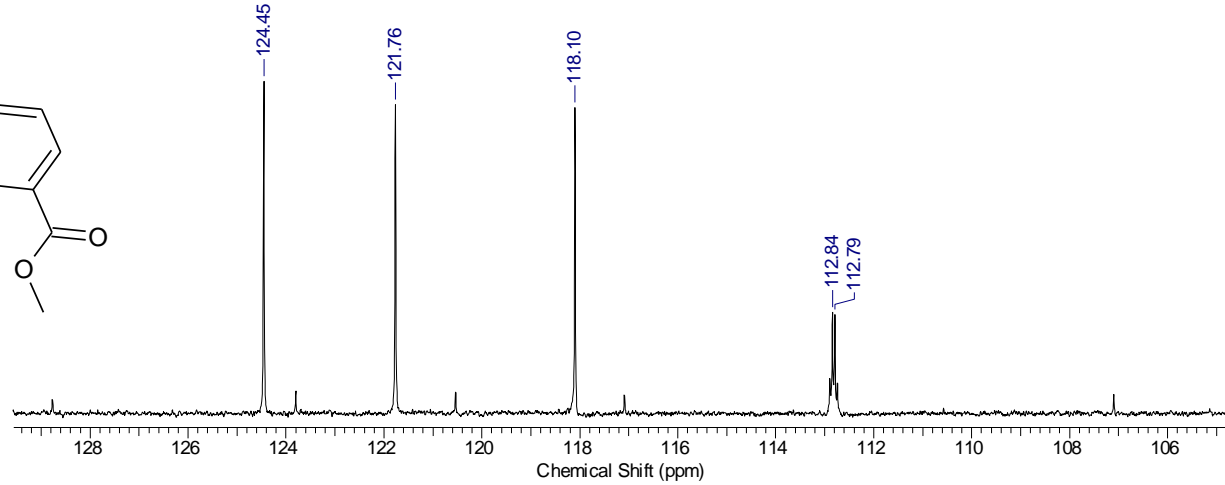
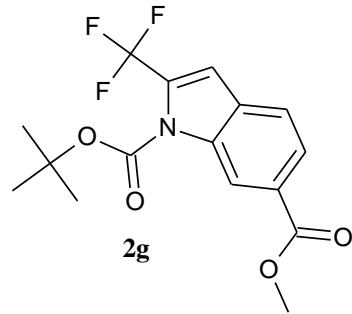
Frequency (MHz)	400.40	Nucleus	1H	Number of Transients	16	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	SW(cyclical) (Hz)	7211.32
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	3395.8613	Sweep Width (Hz)	7211.10	Temperature (degree C)	27.100



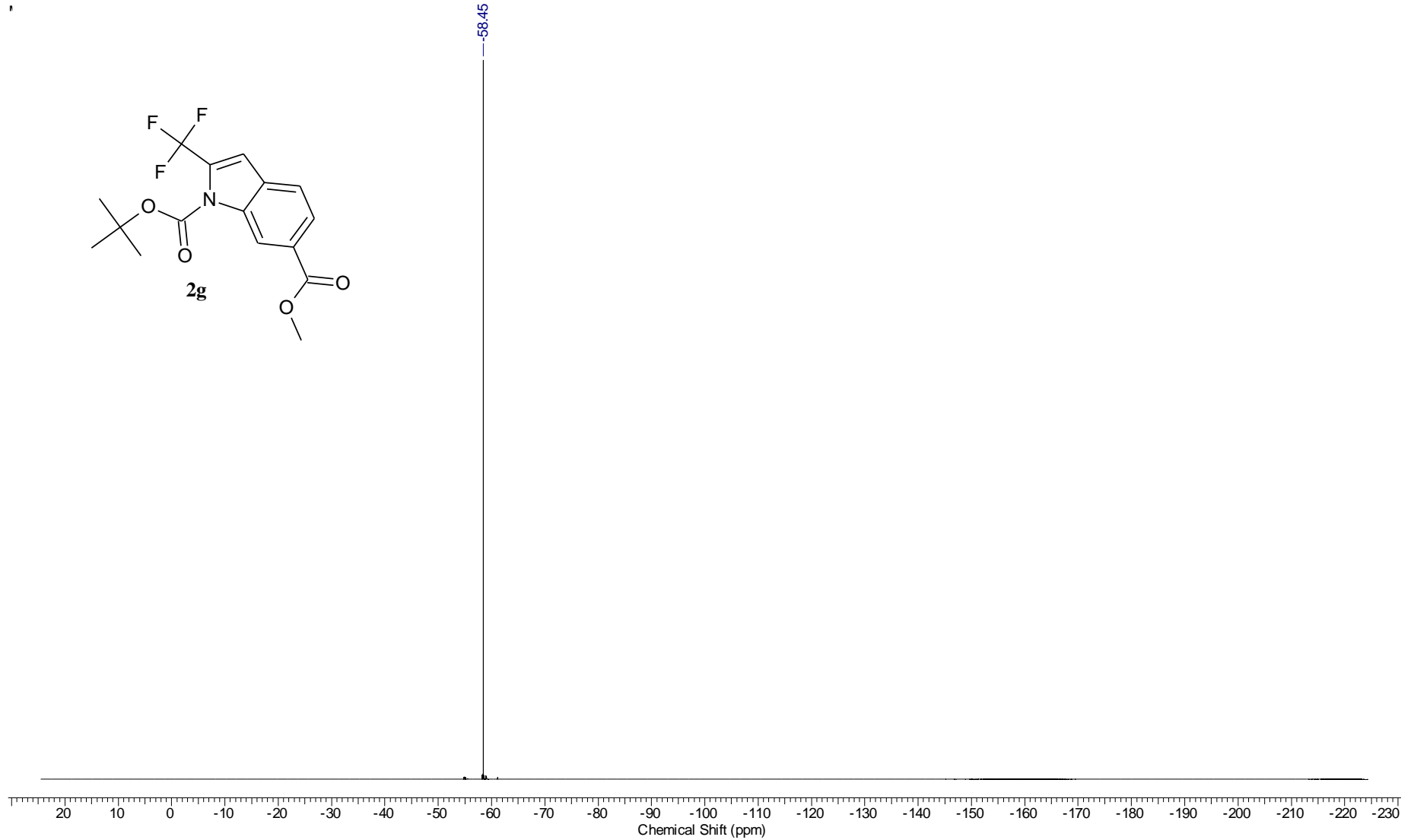
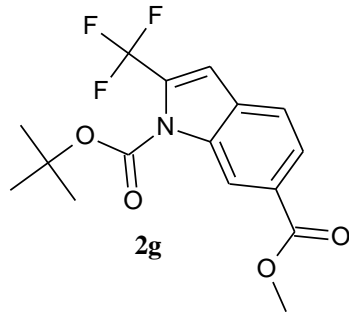
Frequency (MHz)	100.69	Nucleus	¹³ C	Number of Transients	1024	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	SW(cyclical) (Hz)	24037.73
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10065.7764	Sweep Width (Hz)	24036.99	Temperature (degree C)	27.000



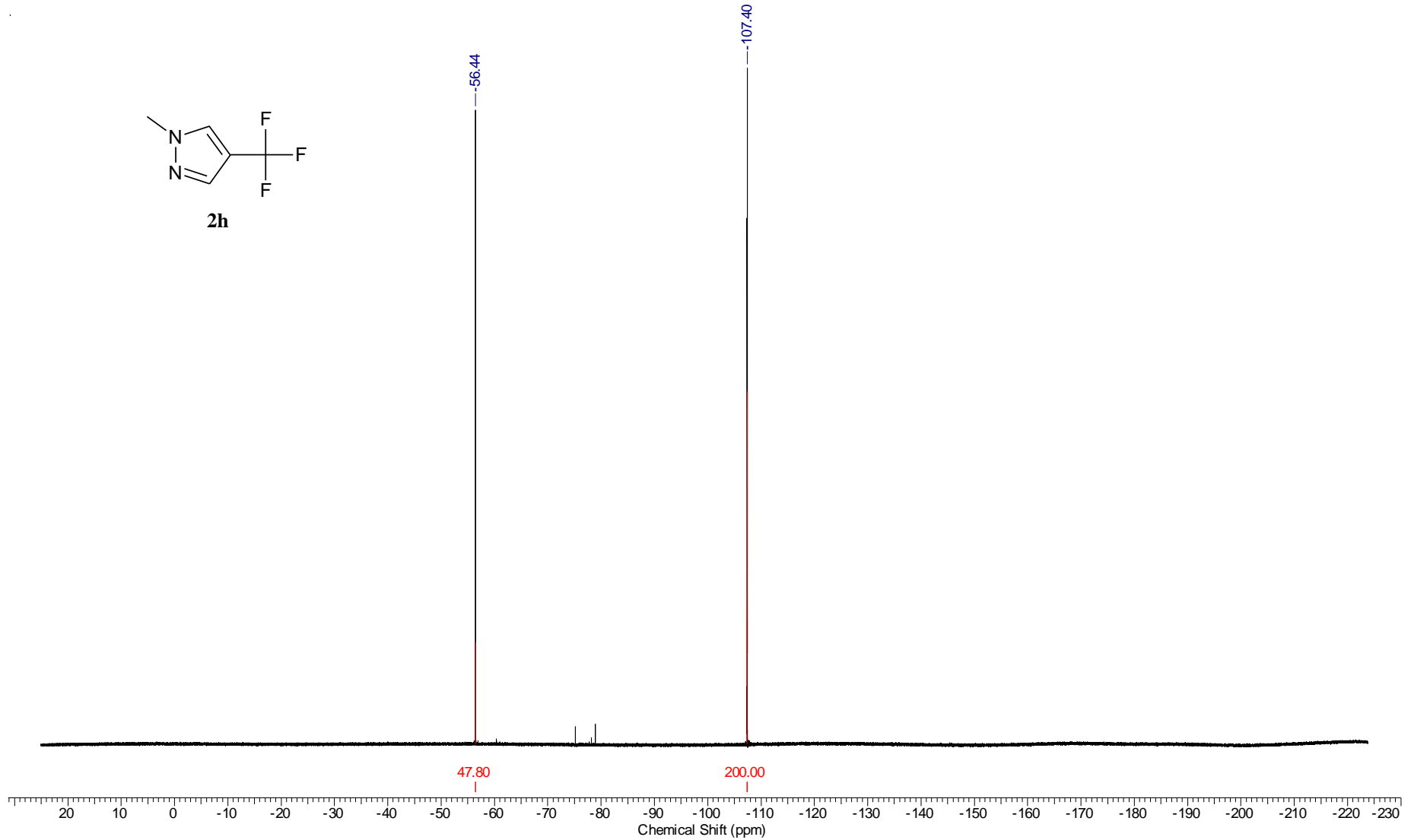
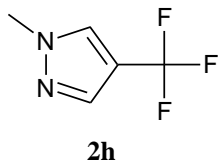
Frequency (MHz)	100.69	Nucleus	¹³ C Dent 135	Number of Transients	256	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	SW(cyclical) (Hz)	24037.73
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10065.3389	Sweep Width (Hz)	24036.99	Temperature (degree C)	27.000

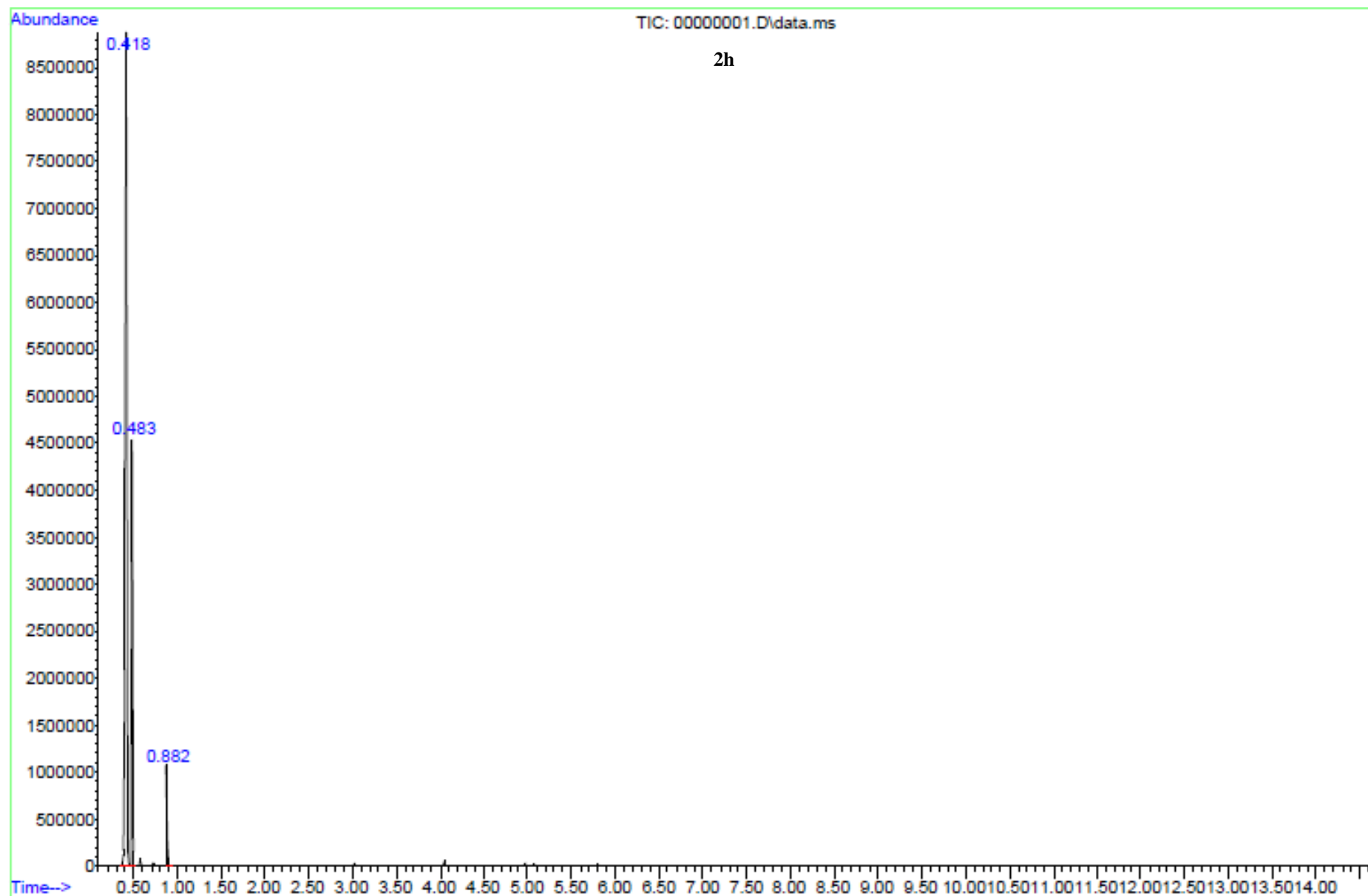


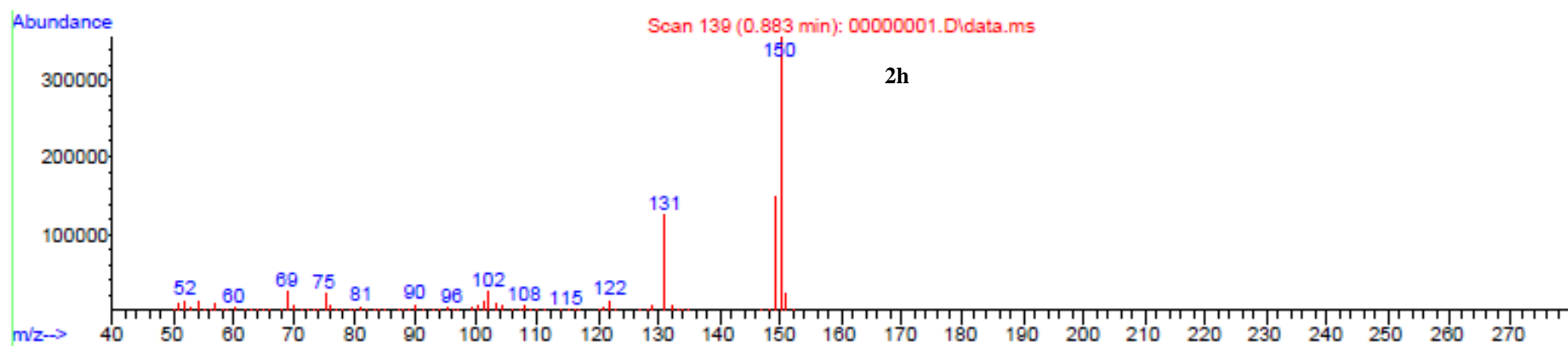
Frequency (MHz)	376.71	Nucleus	19F	Number of Transients	64	Origin	Bruker BioSpin GmbH
Original Points Count	131072	Owner	tibbe_operator	Points Count	131072	SW(cyclical) (Hz)	93749.28
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	-37637.5352	Sweep Width (Hz)	93748.56	Temperature (degree C)	27.000



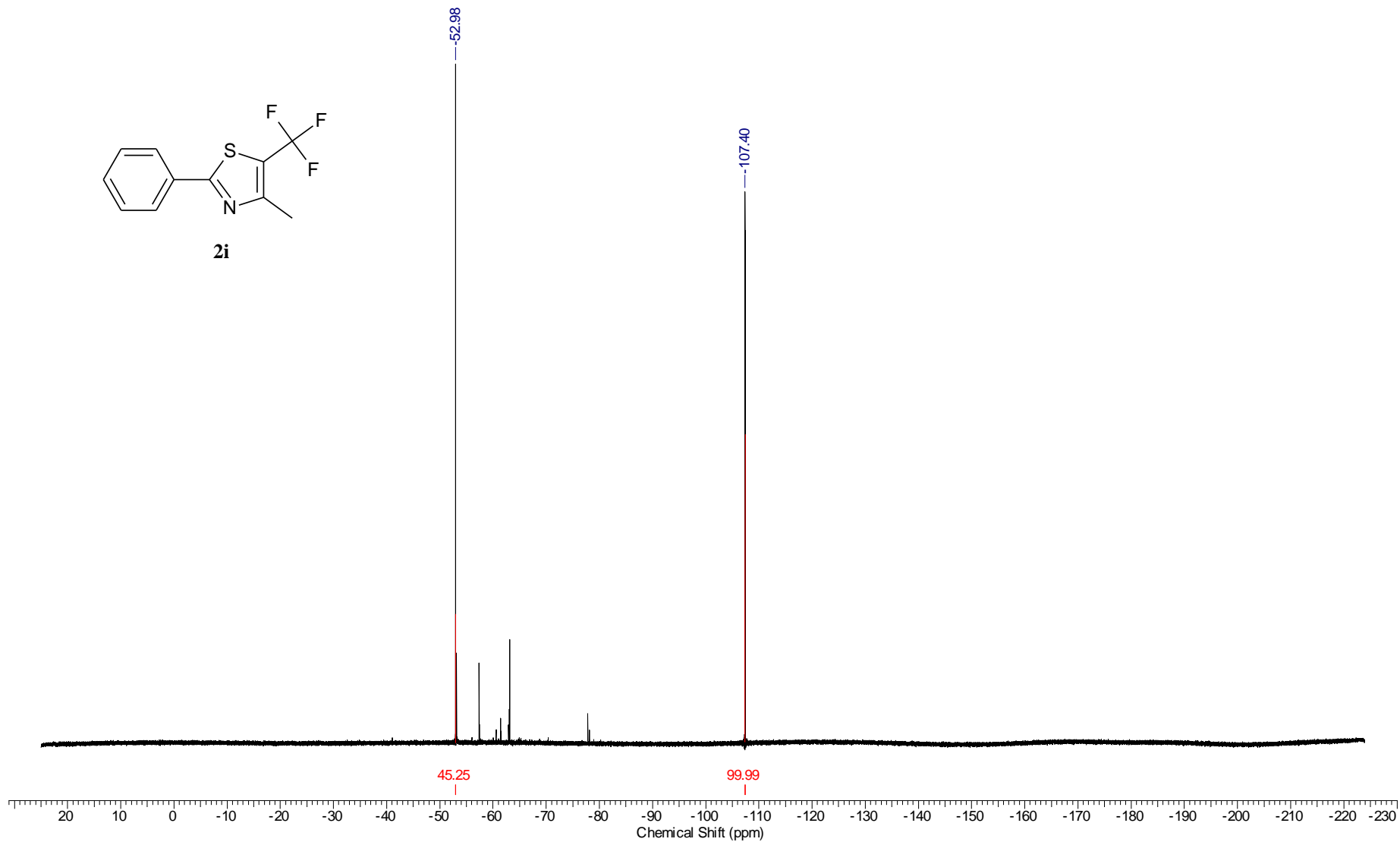
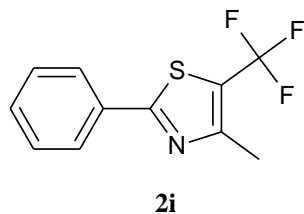
Frequency (MHz)	376.71	Nucleus	19F	Number of Transients	64	Origin	Bruker BioSpin GmbH
Original Points Count	131072	Owner	tibbe_operator	Points Count	131072	SW(cyclical) (Hz)	93749.28
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	-37433.2930	Sweep Width (Hz)	93748.56	Temperature (degree C)	27.000

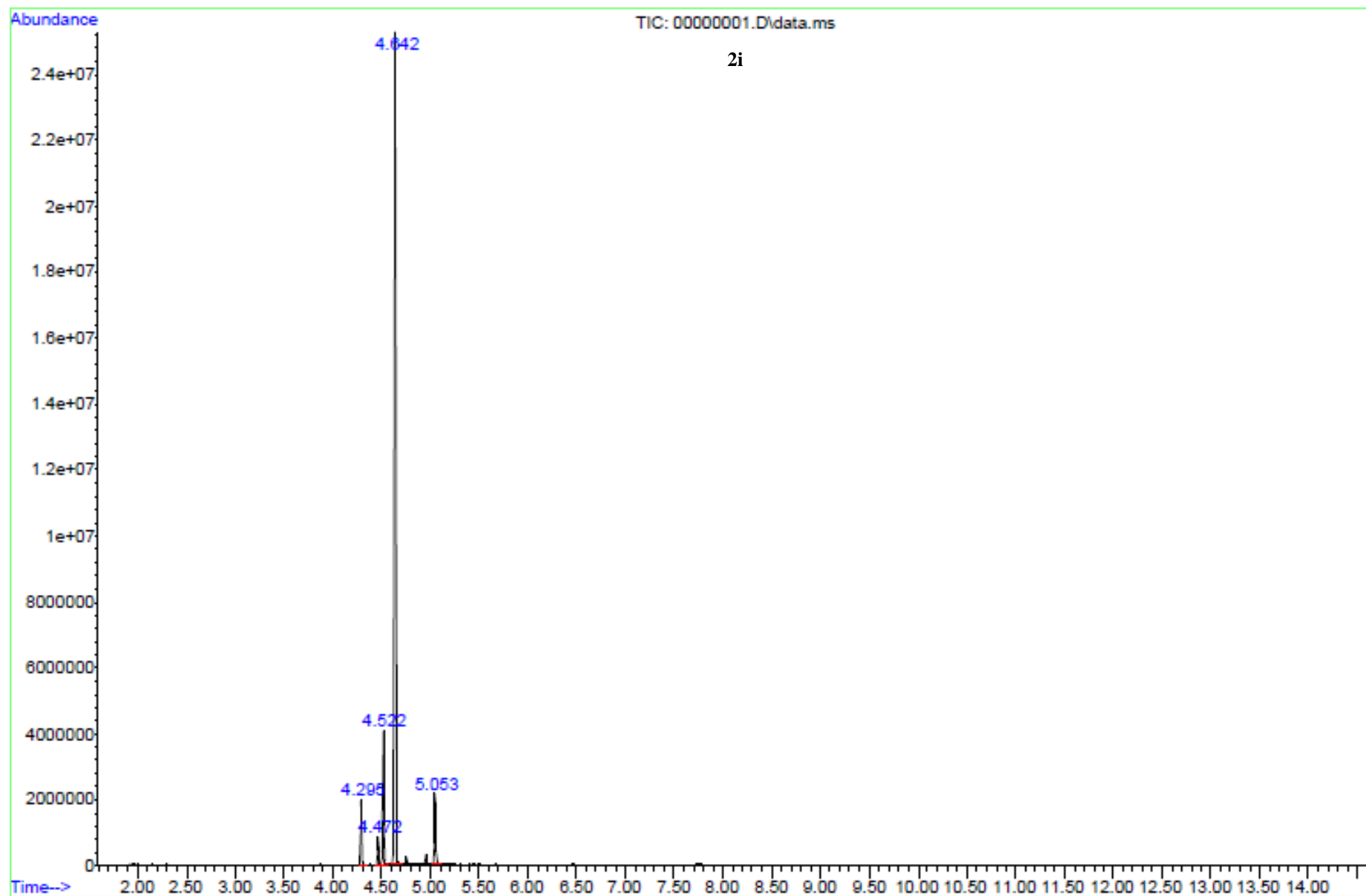


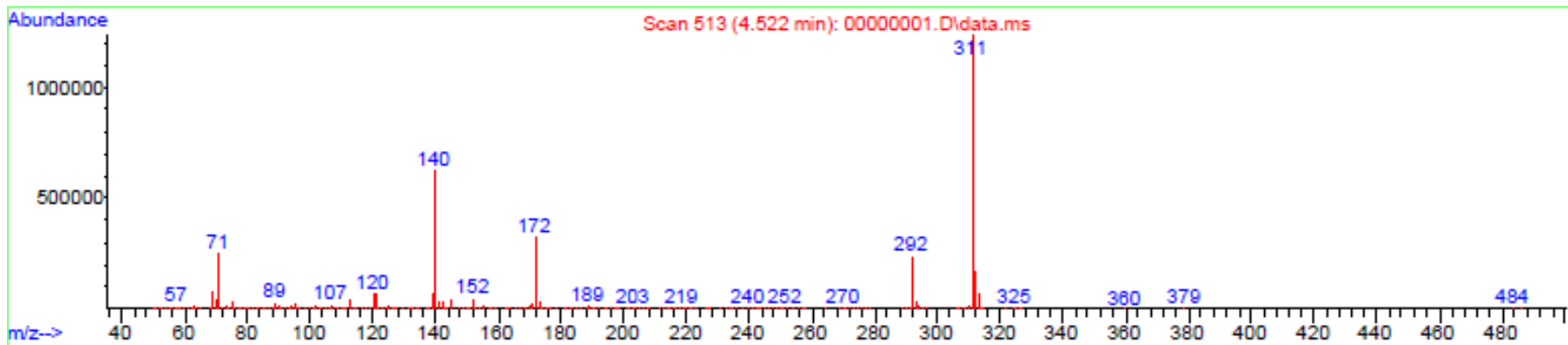
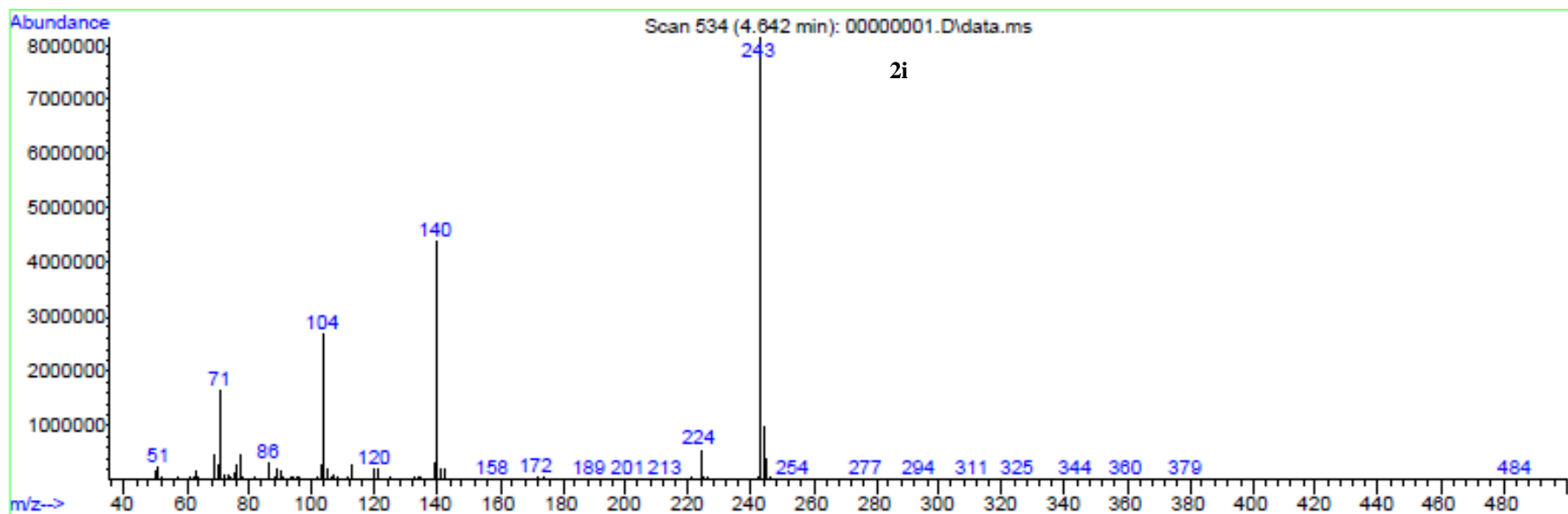




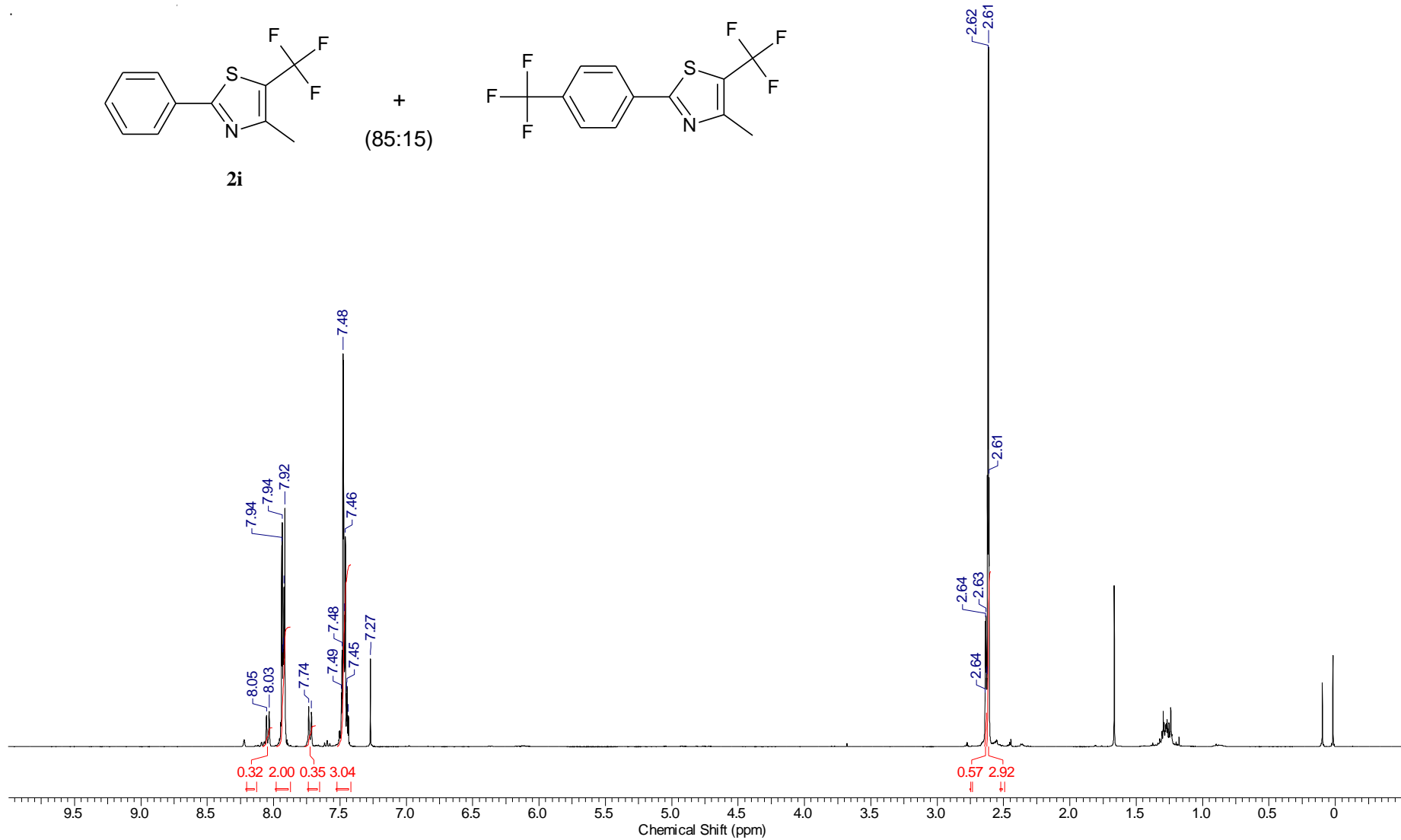
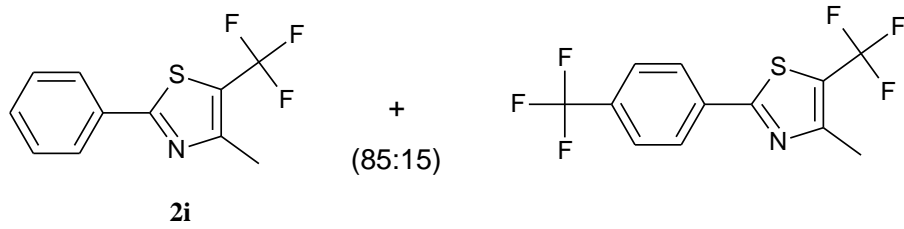
Frequency (MHz)	376.71	Nucleus	¹⁹ F	Number of Transients	64	Origin	Bruker BioSpin GmbH
Original Points Count	131072	Owner	tibbe_operator	Points Count	131072	SW(cyclical) (Hz)	93749.28
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	-37470.4922	Sweep Width (Hz)	93748.56	Temperature (degree C)	27.000



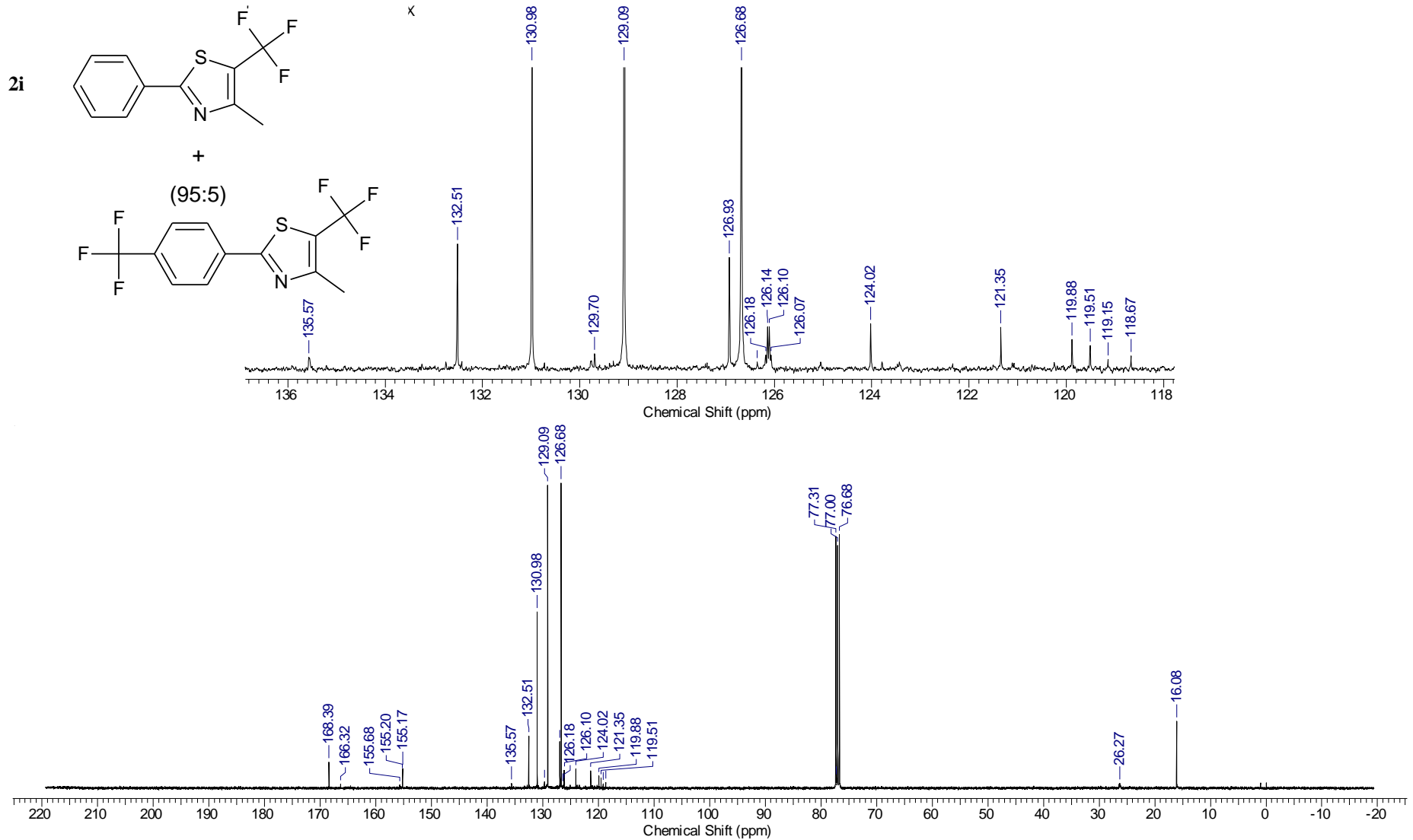




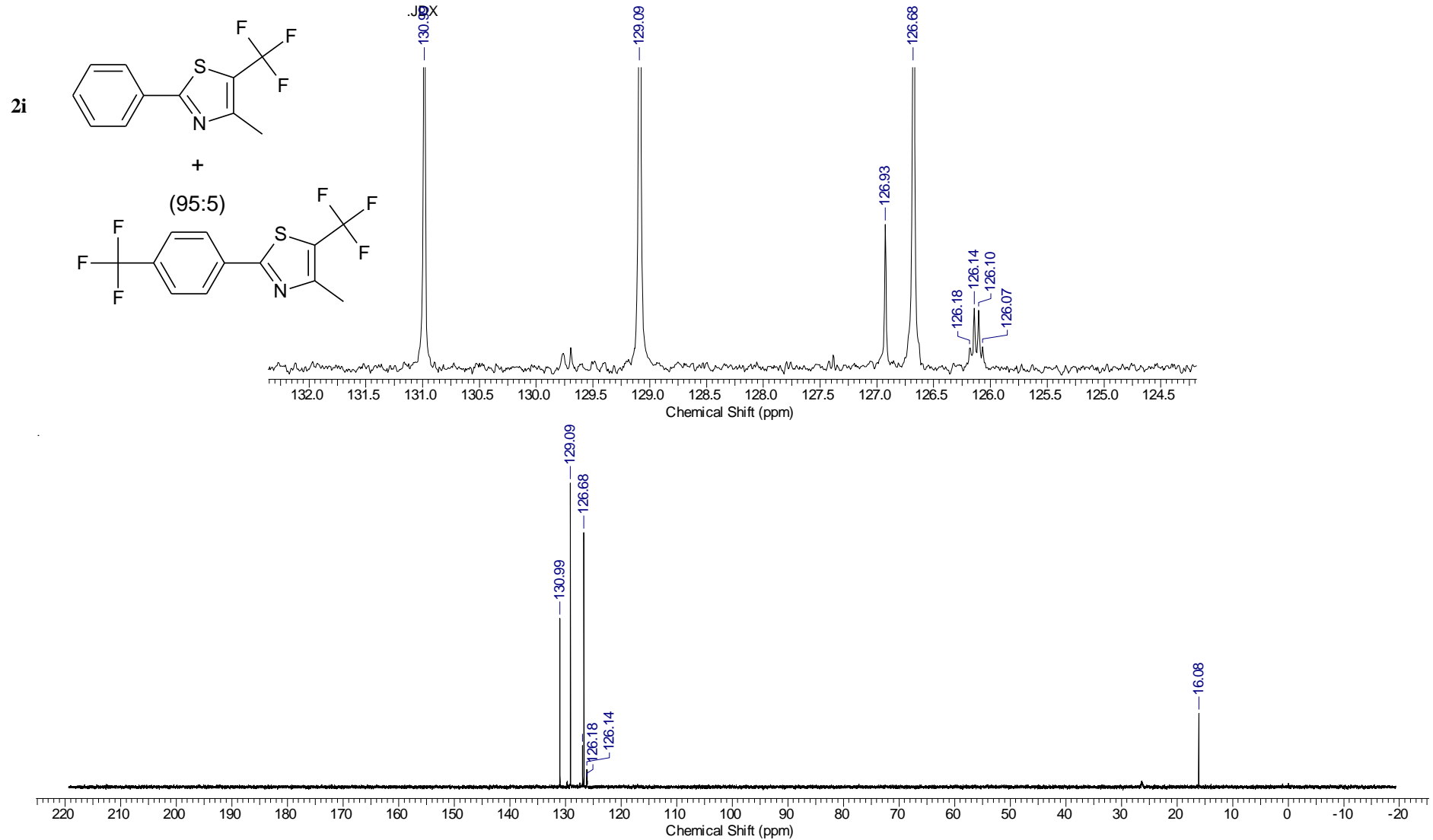
Frequency (MHz)	400.40	Nucleus	1H	Number of Transients	16	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	SW(cyclical) (Hz)	7211.32
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	3395.8611	Sweep Width (Hz)	7211.10	Temperature (degree C)	27.000



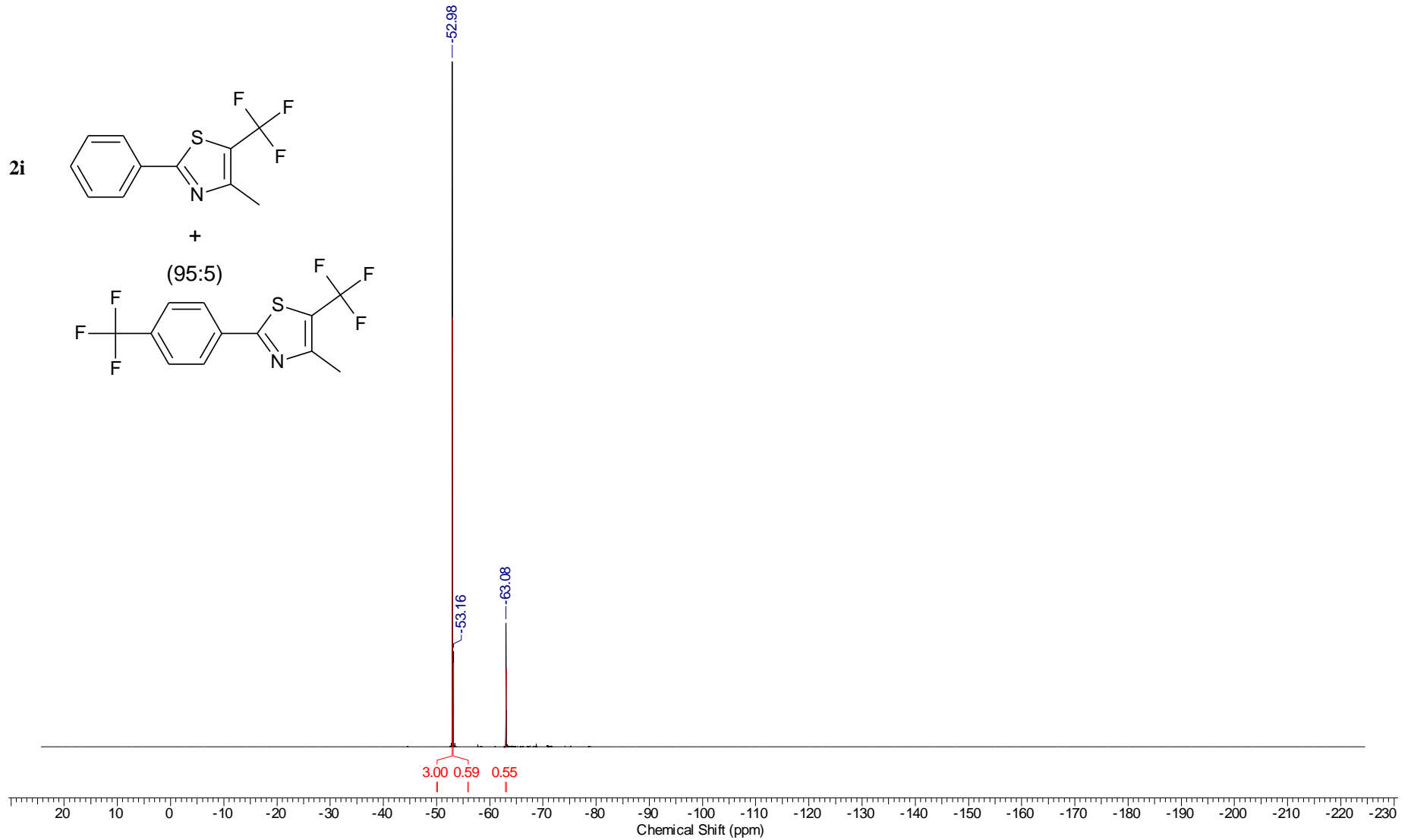
Frequency (MHz)	100.69	Nucleus	13C	Number of Transients	1024	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	SW(cyclical) (Hz)	24037.73
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10066.5088	Sweep Width (Hz)	24036.99	Temperature (degree C)	27.000



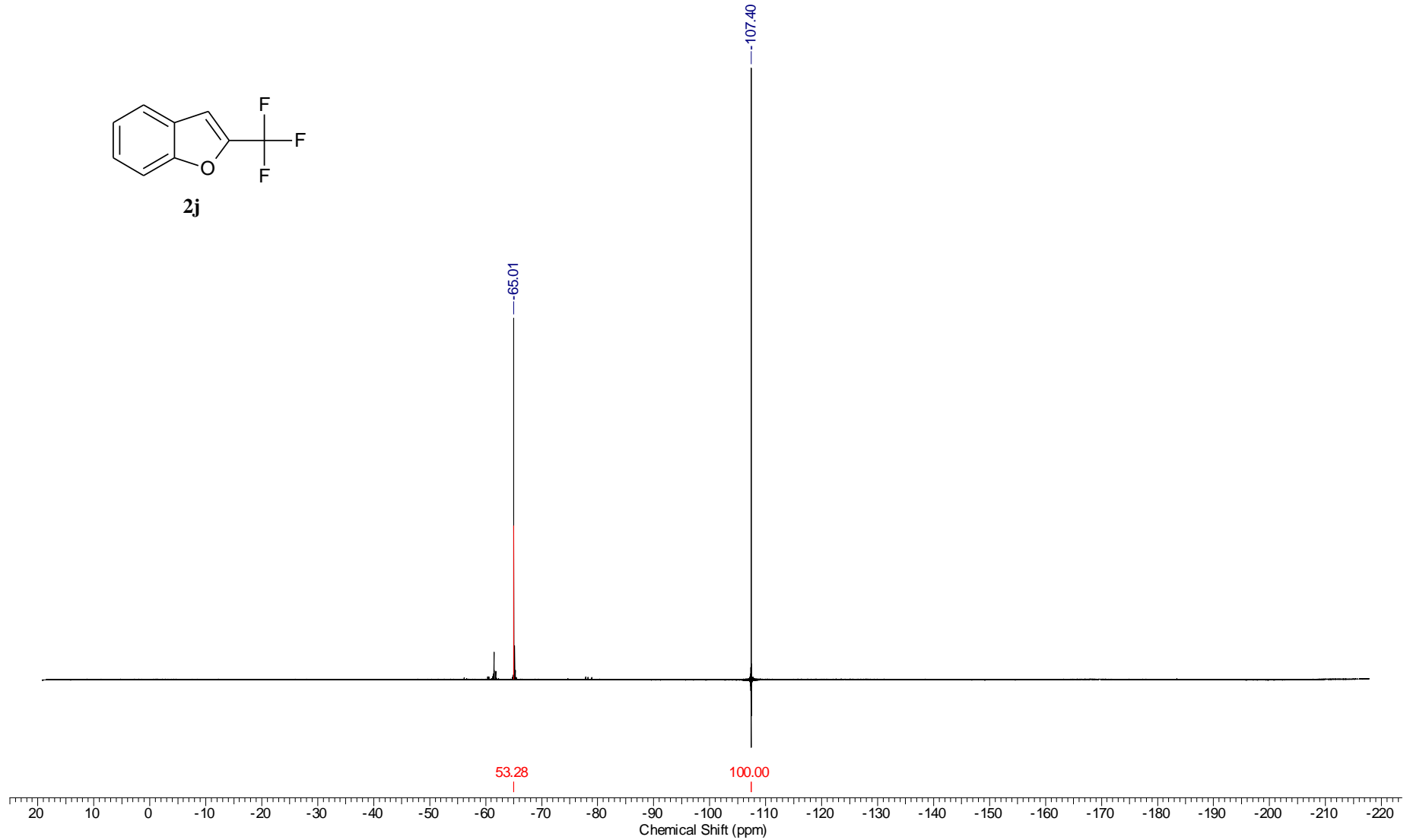
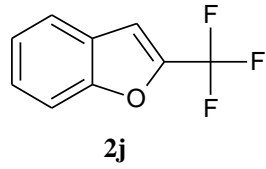
Frequency (MHz)	100.69	Nucleus	13C Dent 135	Number of Transients	256	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	SW(cyclical) (Hz)	24037.73
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10066.5693	Sweep Width (Hz)	24036.99	Temperature (degree C)	27.000

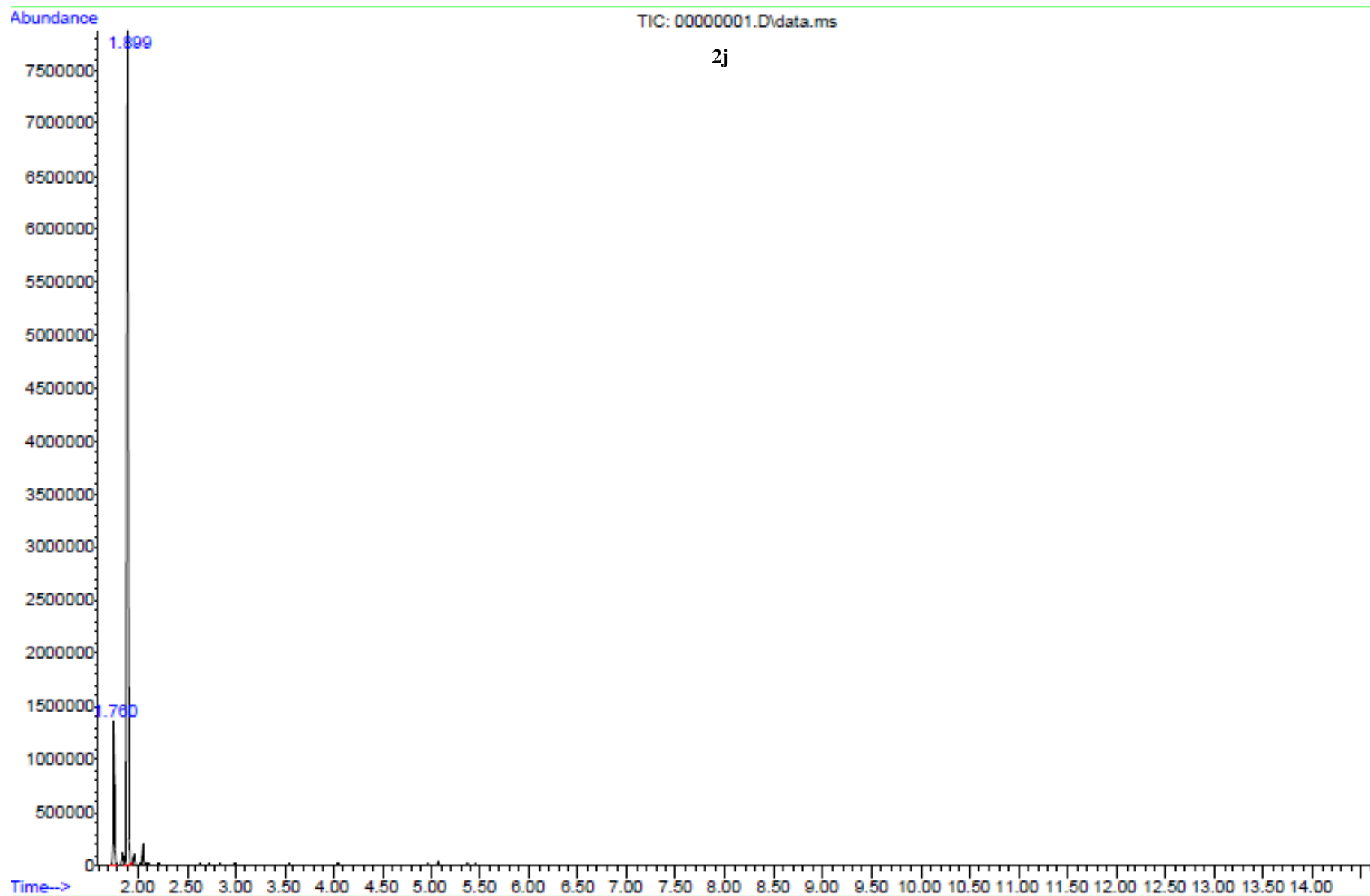


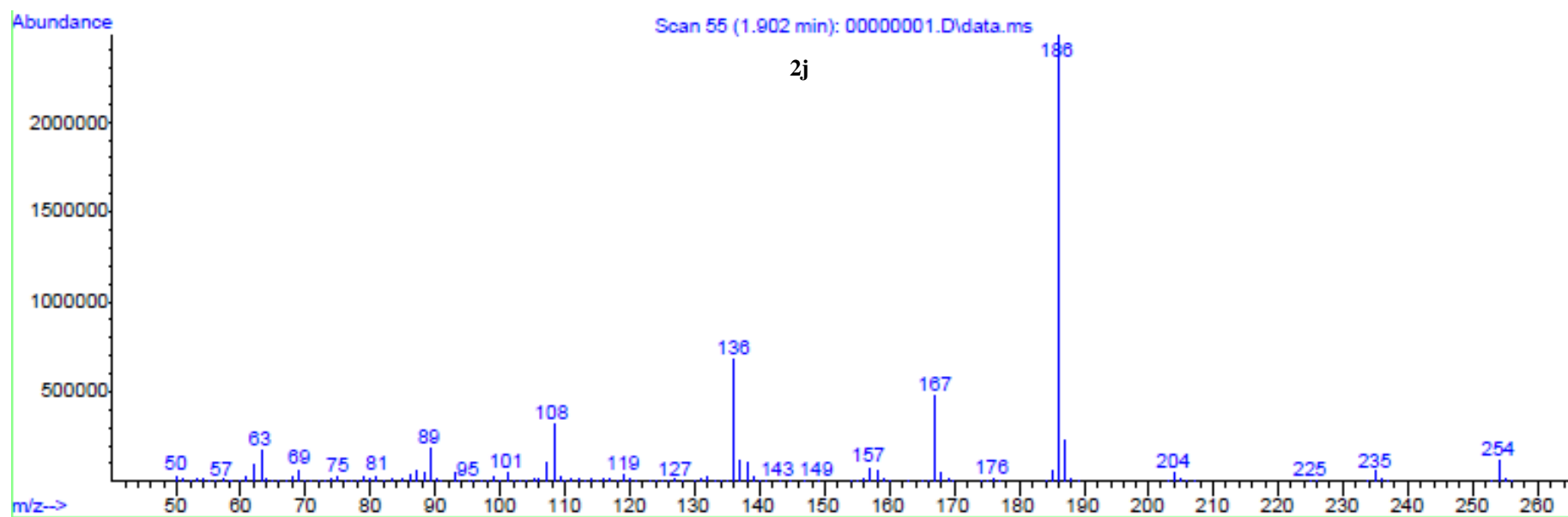
Frequency (MHz)	376.71	Nucleus	¹⁹ F	Number of Transients	64	Origin	Bruker BioSpin GmbH
Original Points Count	131072	Owner	tibbe_operator	Points Count	131072	SW(cyclical) (Hz)	93749.28
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	-37711.9258	Sweep Width (Hz)	93748.56	Temperature (degree C)	27.000



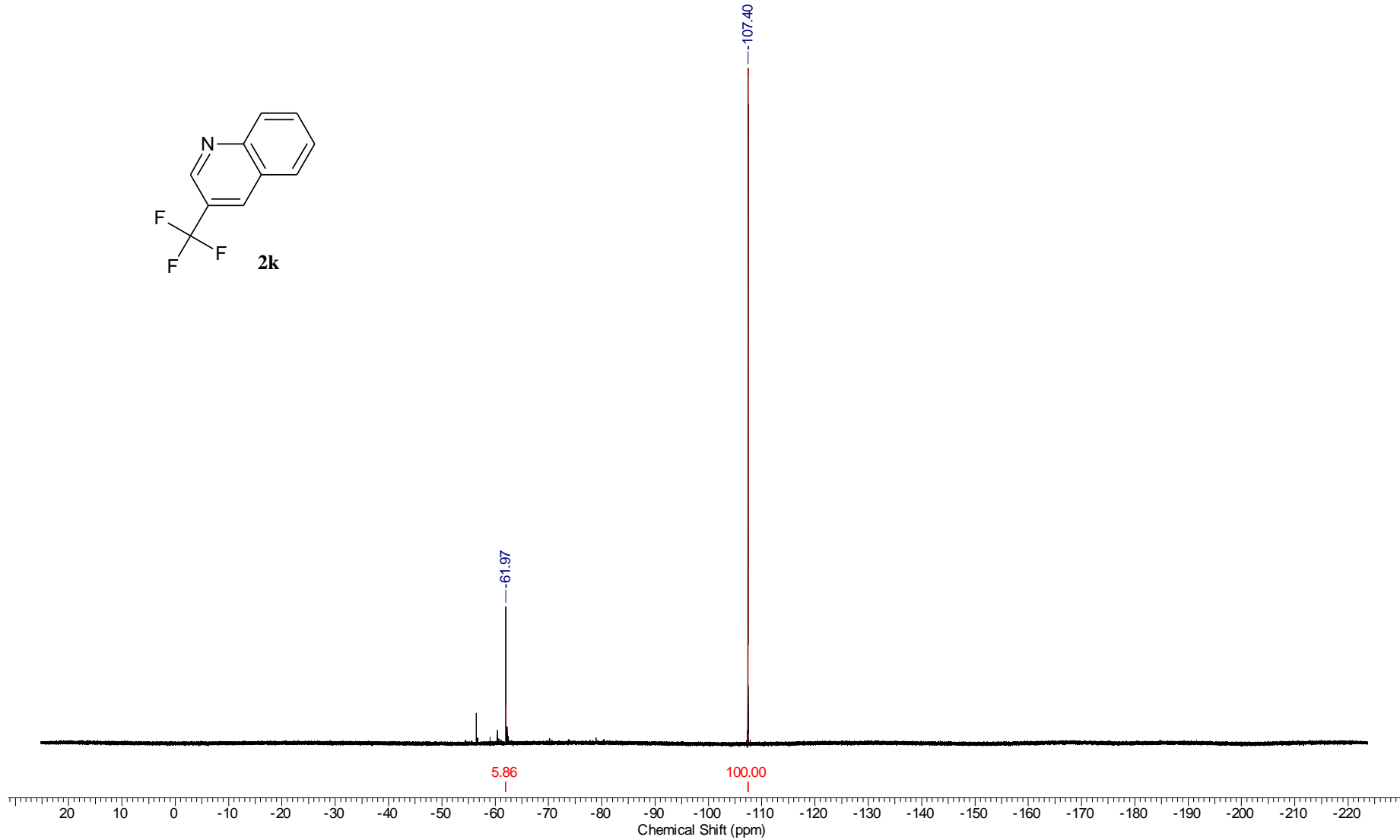
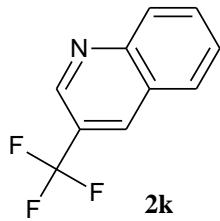
Frequency (MHz)	376.71	Nucleus	¹⁹ F	Number of Transients	64	Origin	Bruker BioSpin GmbH
Original Points Count	131072	Owner	tibbe_operator	Points Count	131072	SW(cyclical) (Hz)	89285.03
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	-37401.6406	Sweep Width (Hz)	89284.35	Temperature (degree C)	27.000

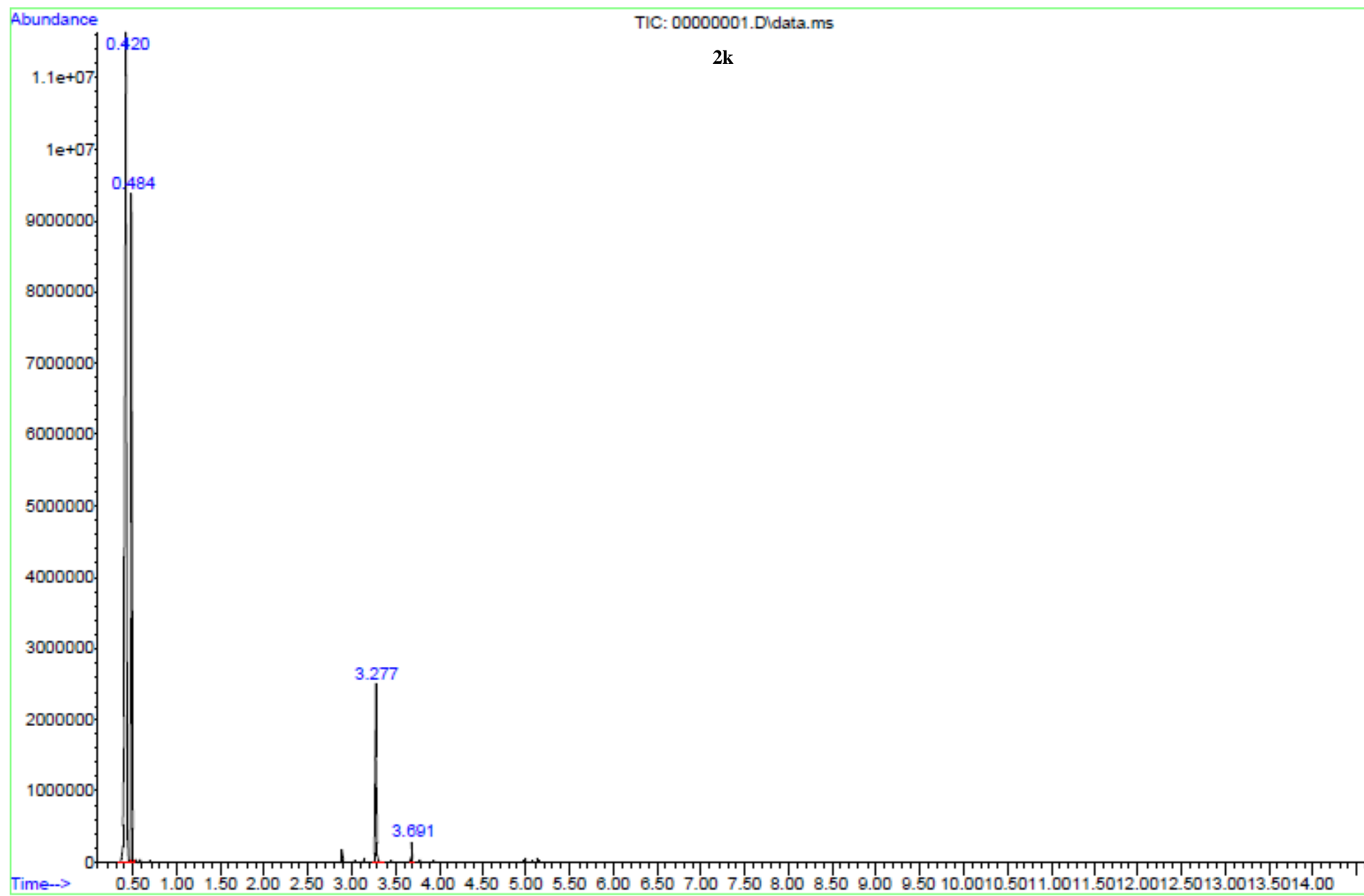


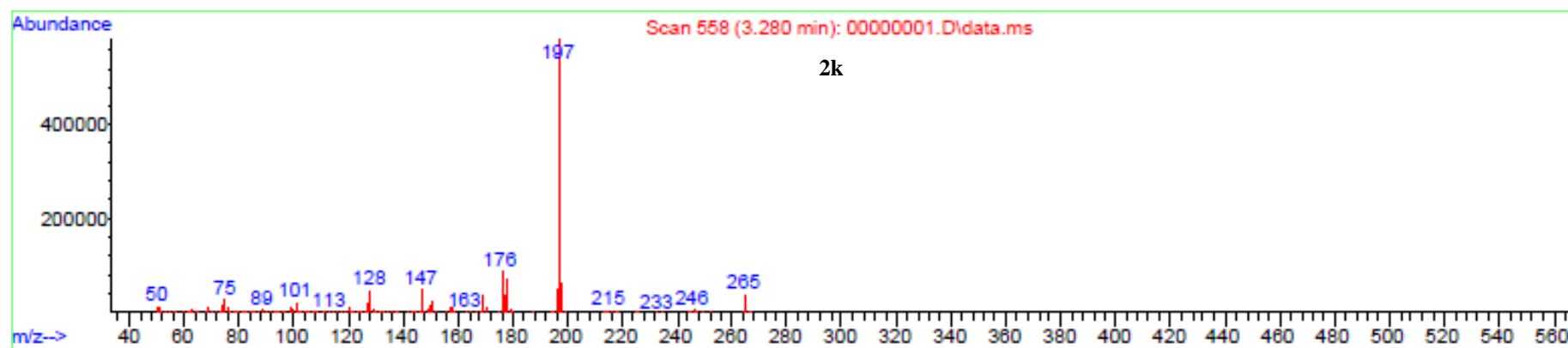




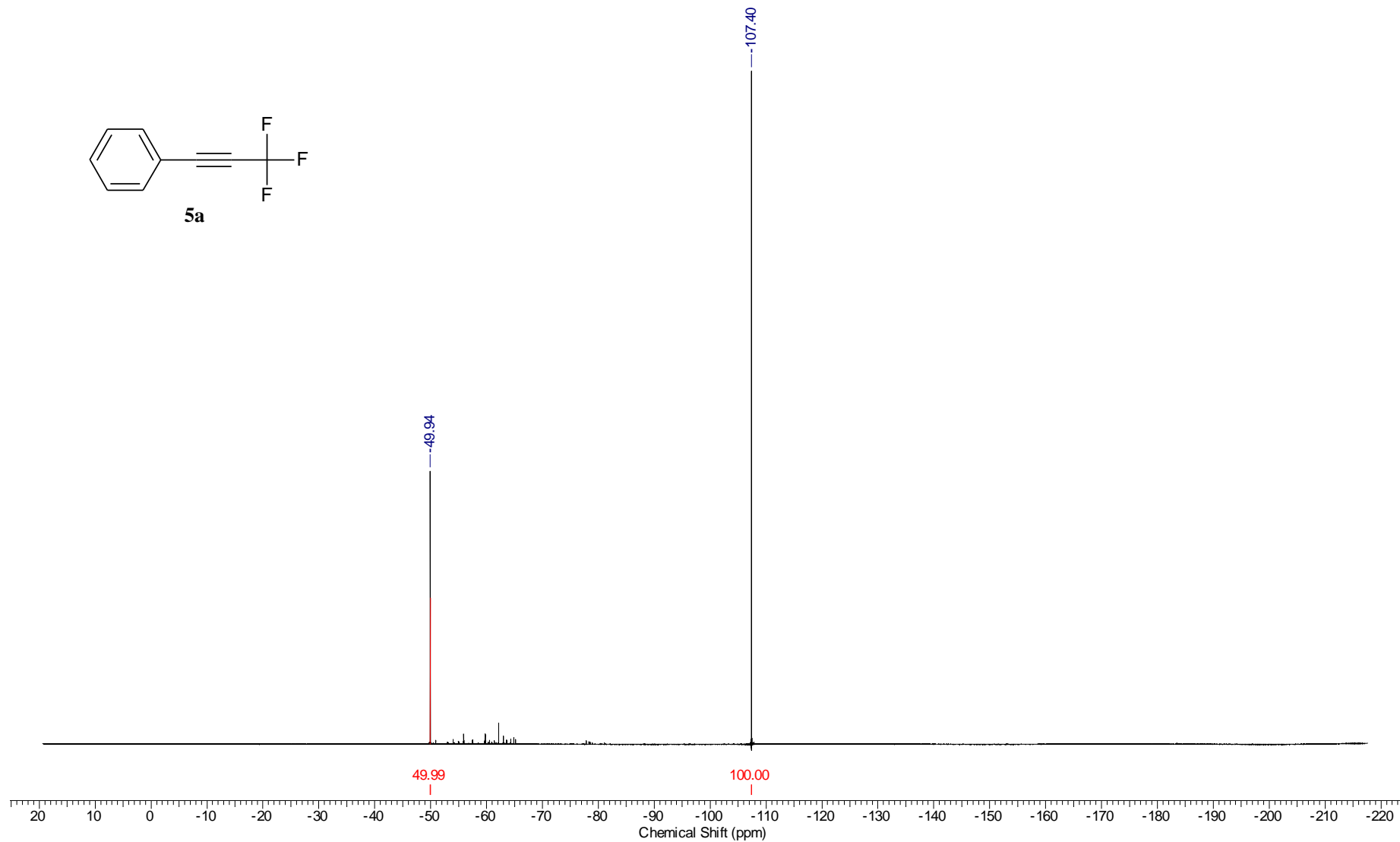
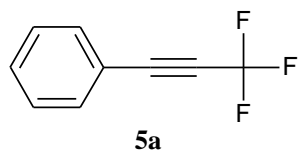
Frequency (MHz)	376.71	Nucleus	¹⁹ F	Number of Transients	64	Origin	Bruker BioSpin GmbH
Original Points Count	131072	Owner	tibbe_operator	Points Count	131072	SW(cyclical) (Hz)	93749.28
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	-37375.3594	Sweep Width (Hz)	93748.56	Temperature (degree C)	27.000

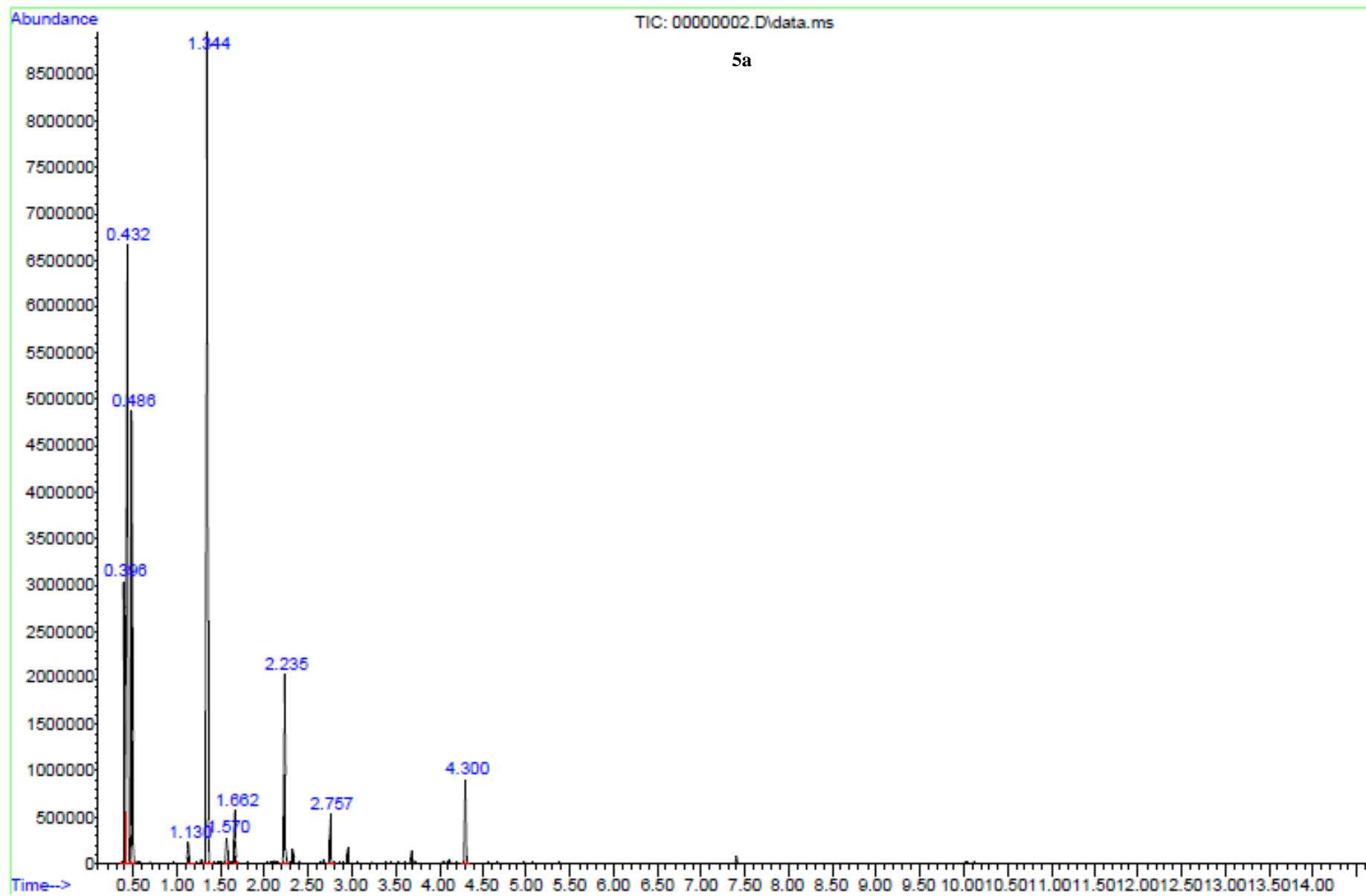


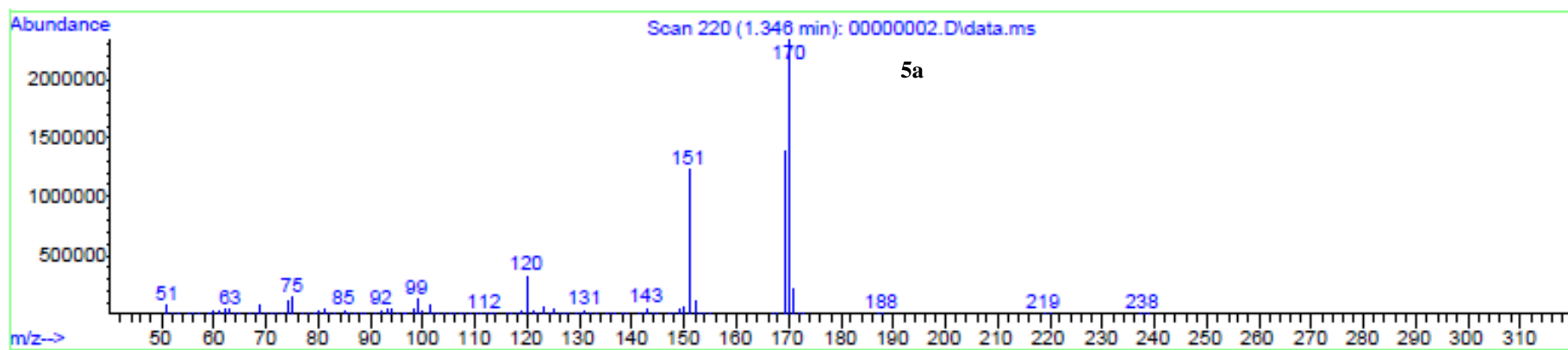




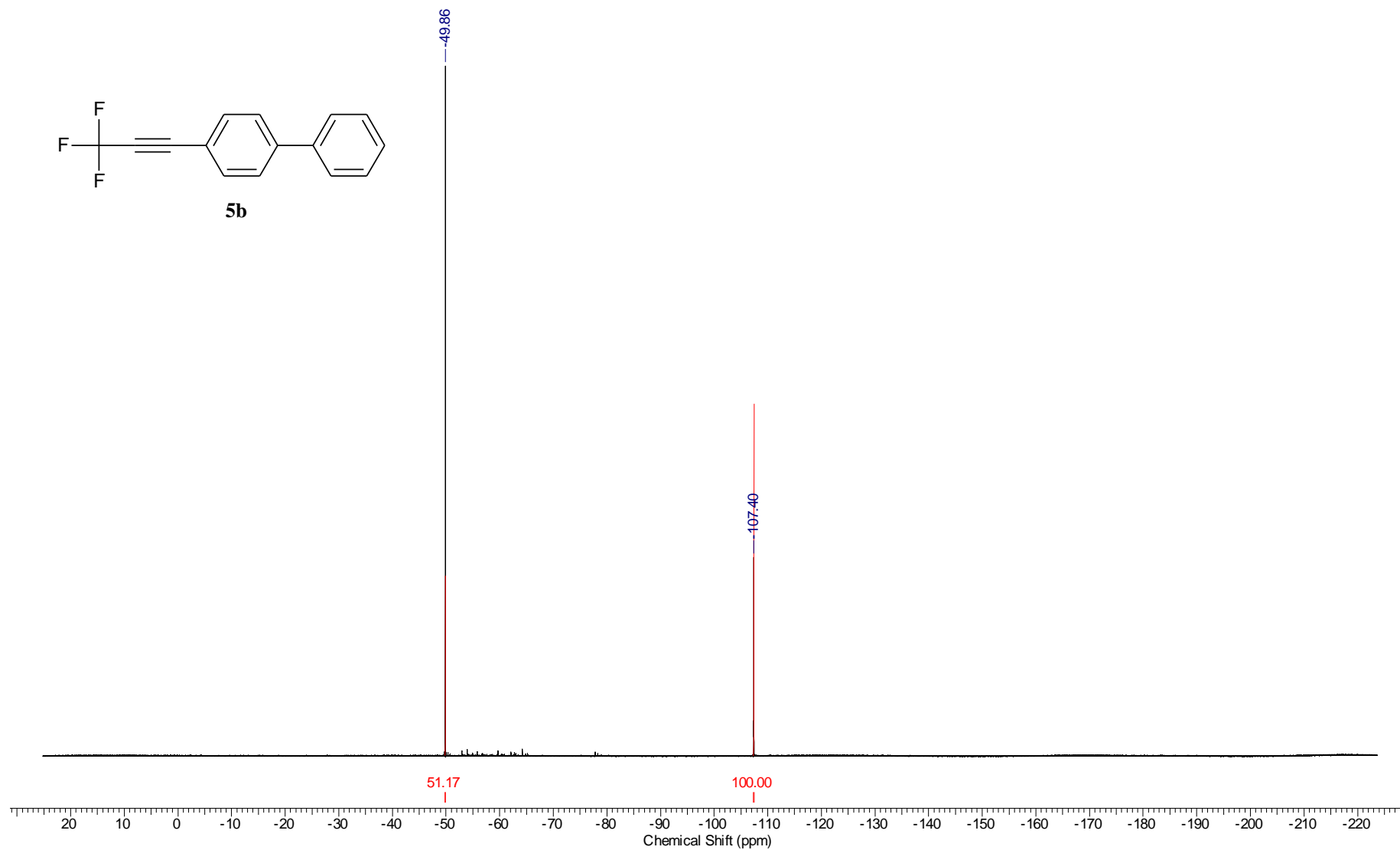
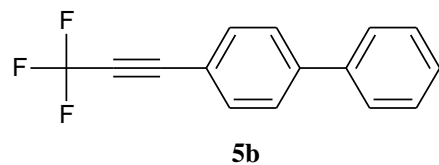
Frequency (MHz)	376.71	Nucleus	¹⁹ F	Number of Transients	64	Origin	Bruker BioSpin GmbH
Original Points Count	131072	Owner	tibbe_operator	Points Count	131072	SW(cyclical) (Hz)	89285.03
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	-37328.0703	Sweep Width (Hz)	89284.35	Temperature (degree C)	27.000

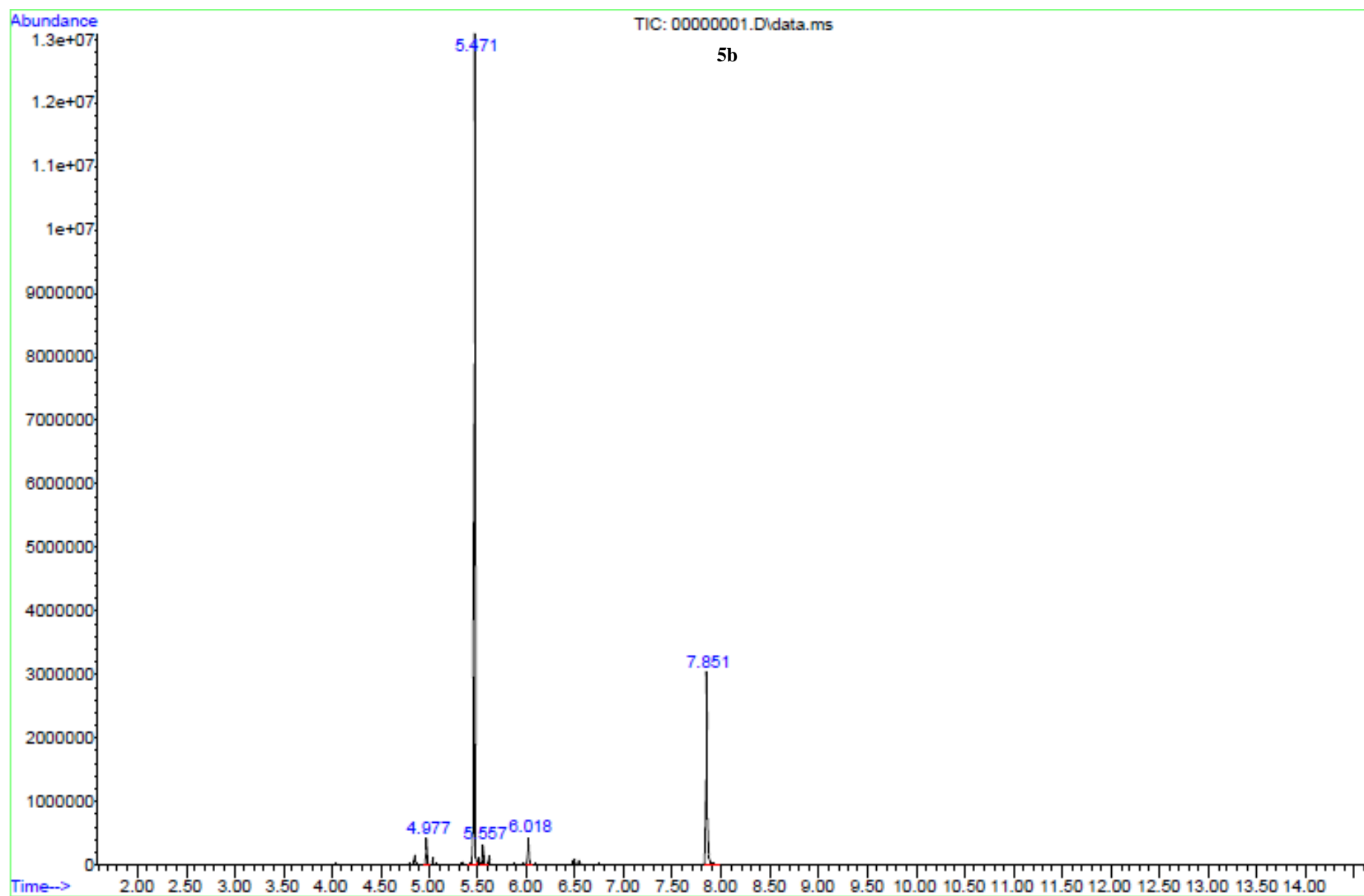


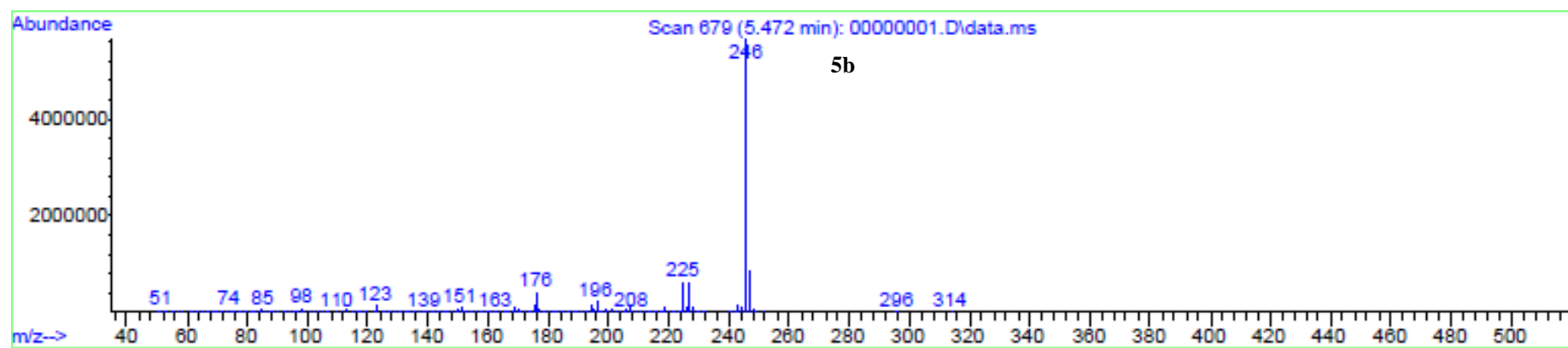




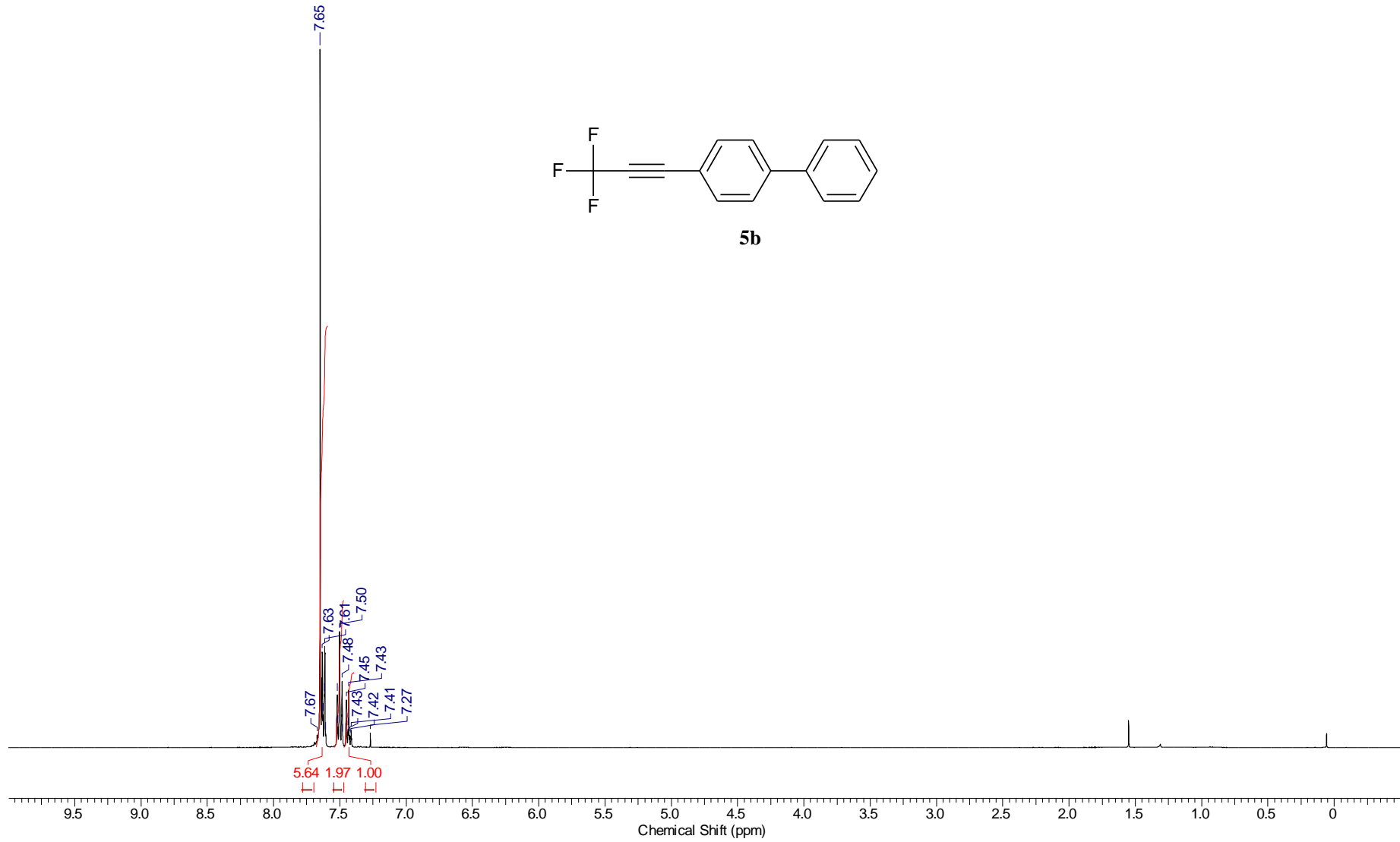
Frequency (MHz)	376.71	Nucleus	¹⁹ F	Number of Transients	64	Origin	Bruker BioSpin GmbH
Original Points Count	131072	Owner	tibbe_operator	Points Count	131072	SW(cyclical) (Hz)	93749.28
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	-37386.0859	Sweep Width (Hz)	93748.56	Temperature (degree C)	27.000



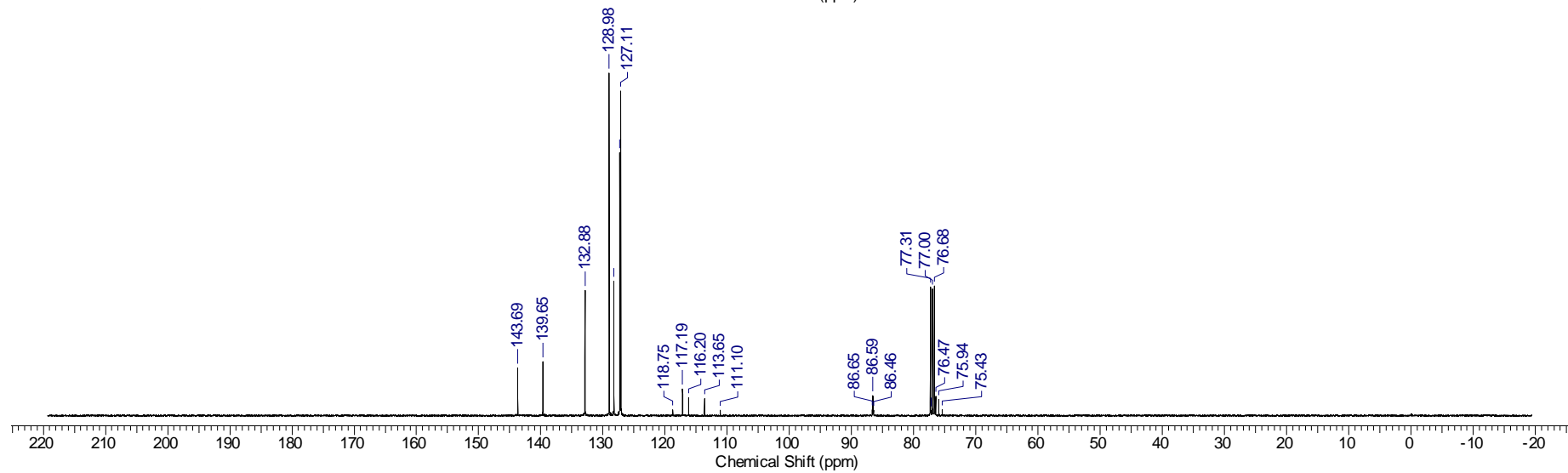
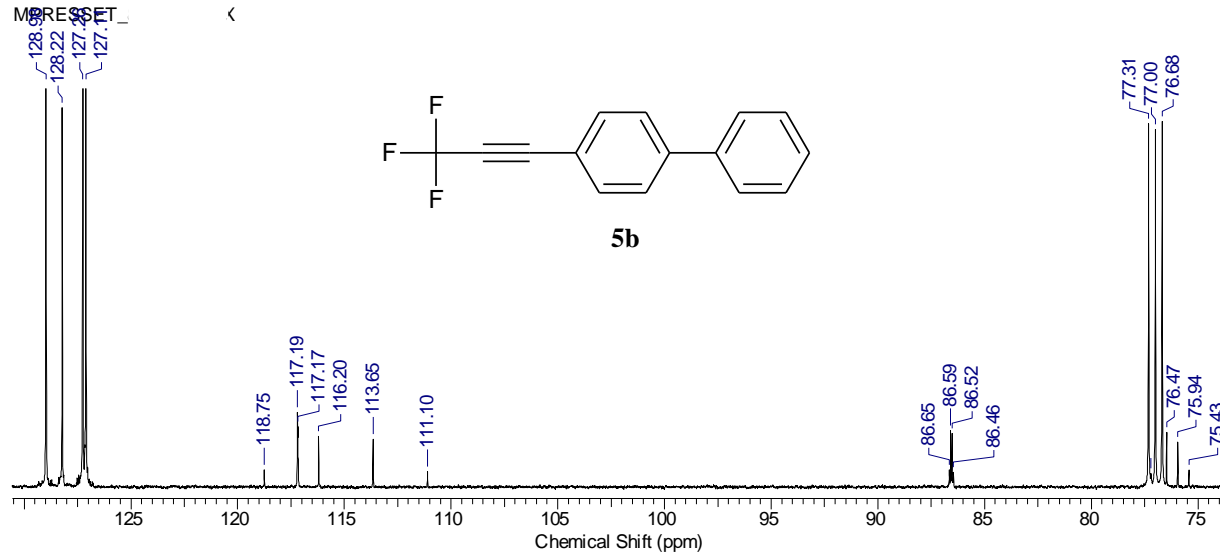




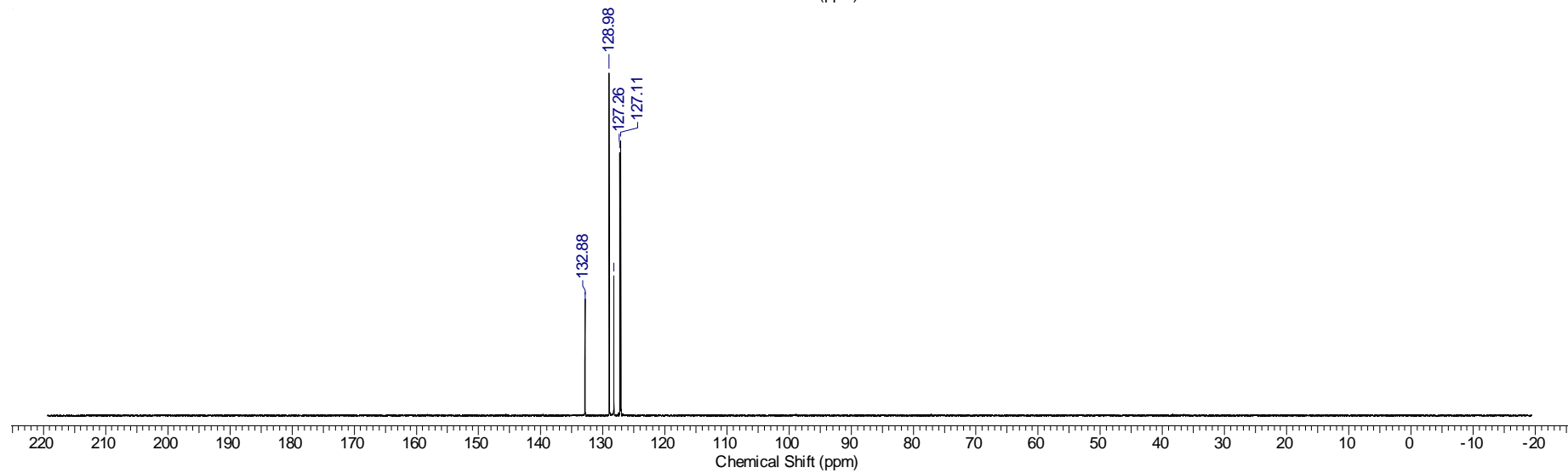
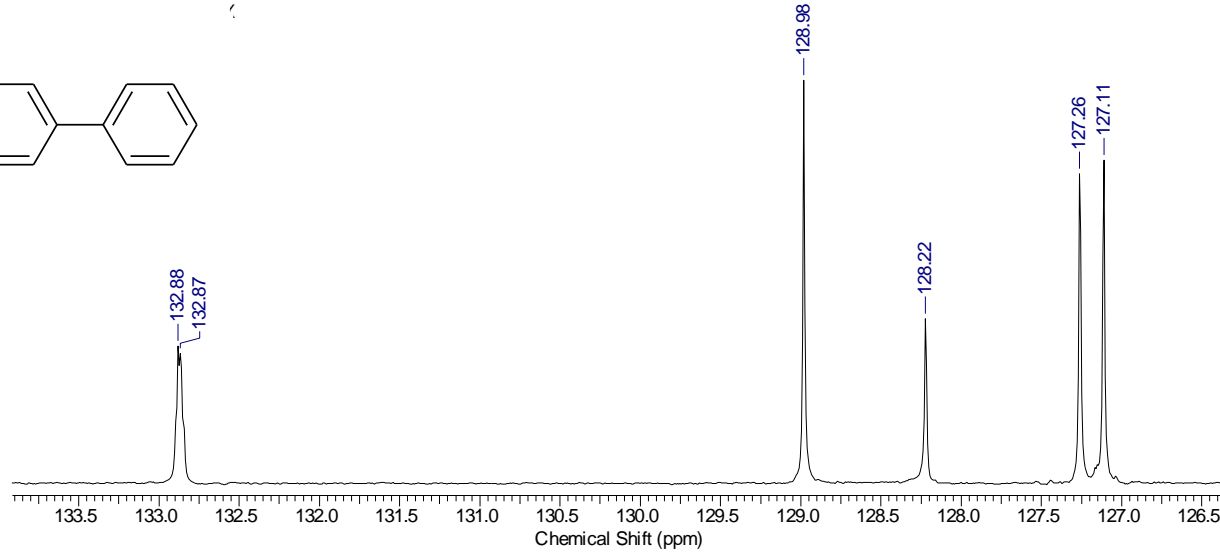
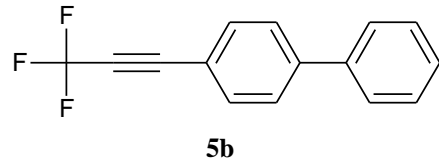
Frequency (MHz)	400.40	Nucleus	1H	Number of Transients	16	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	SW(cyclical) (Hz)	7211.32
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	3395.6414	Sweep Width (Hz)	7211.10	Temperature (degree C)	27.000



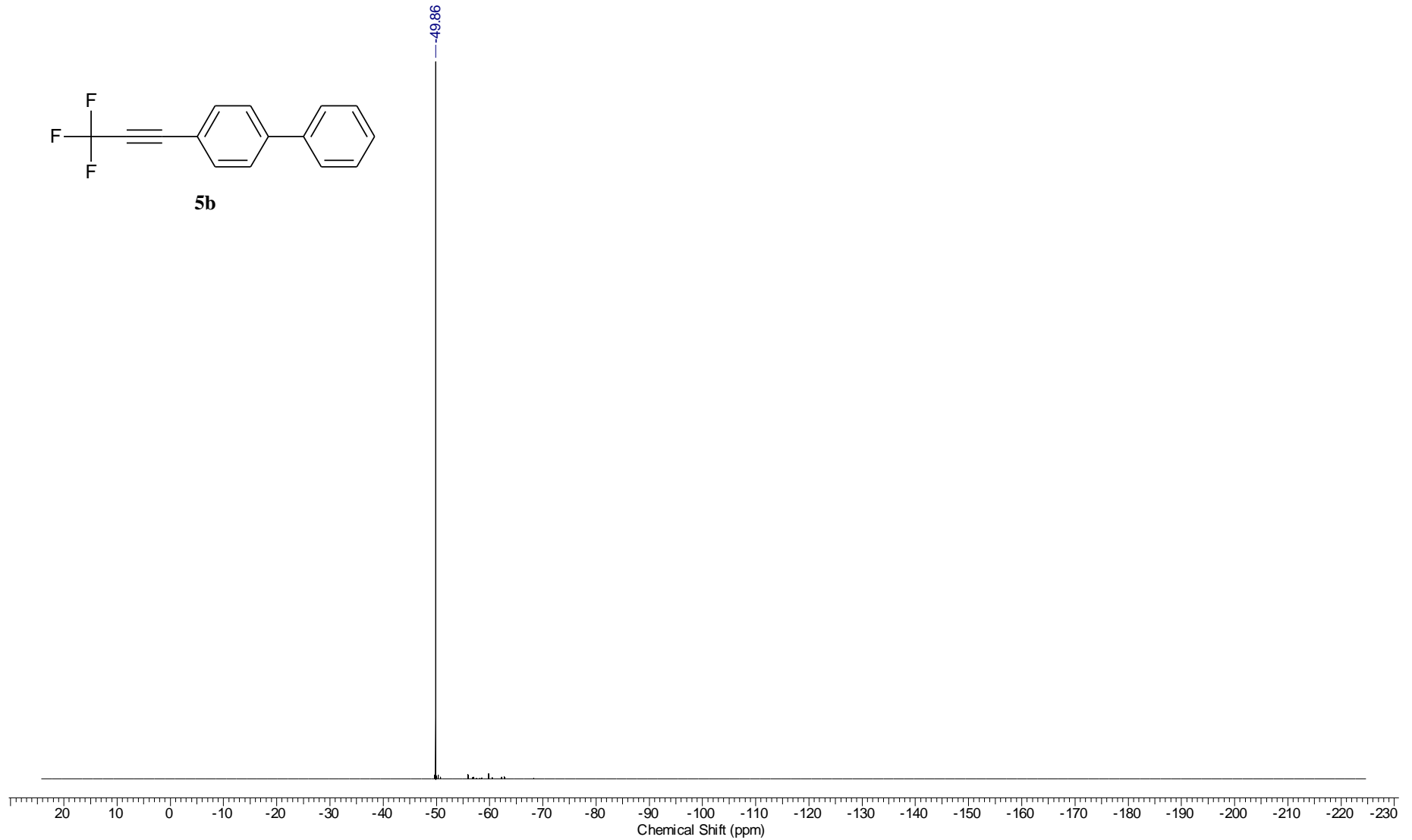
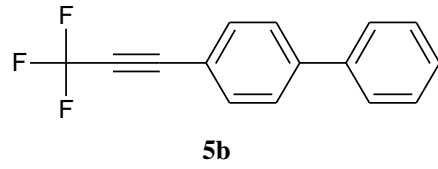
Frequency (MHz)	100.69	Nucleus	13C	Number of Transients	1024	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	SW(cyclical) (Hz)	24037.73
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10064.3086	Sweep Width (Hz)	24036.99	Temperature (degree C)	27.000



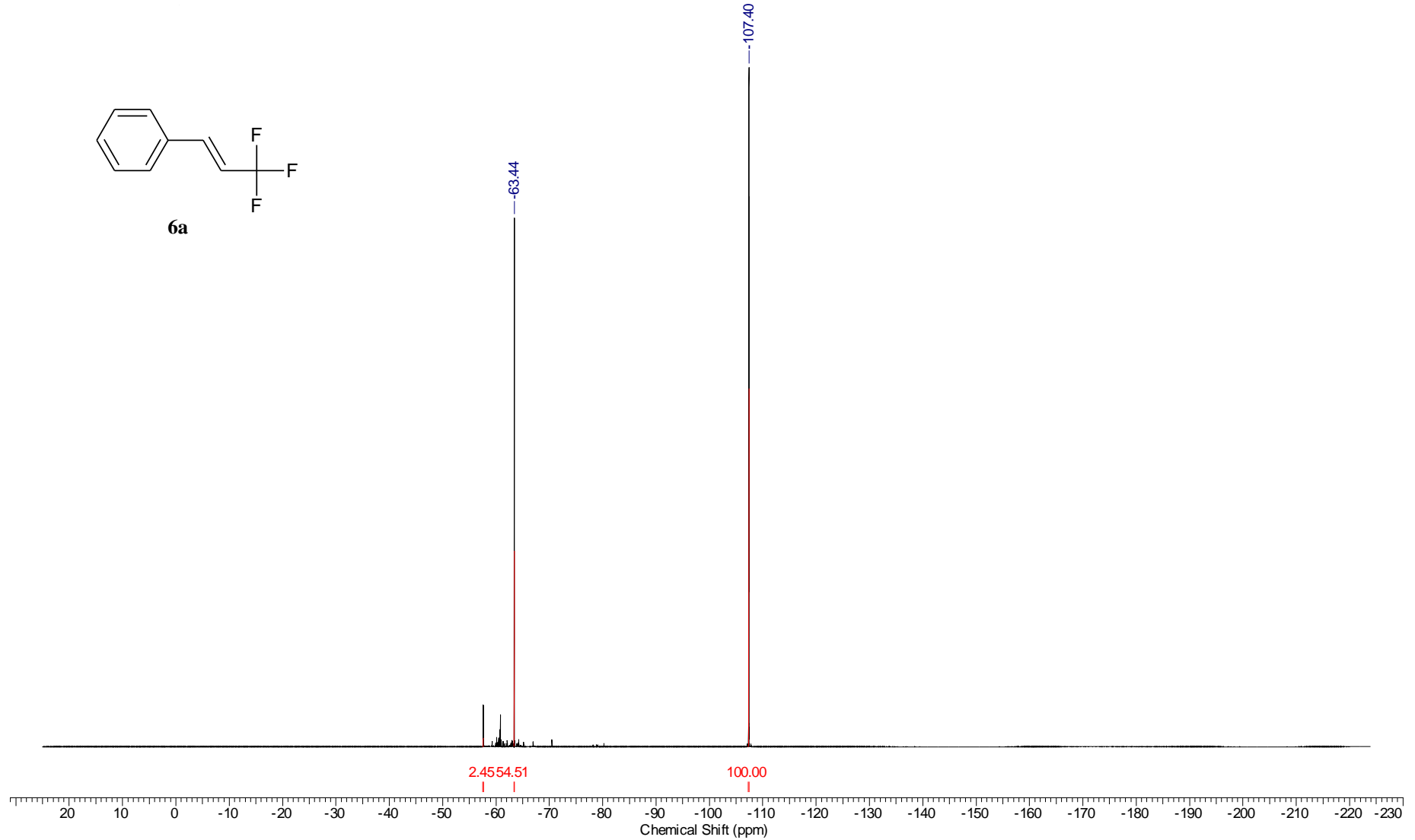
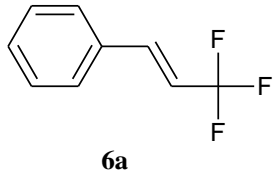
Frequency (MHz)	100.69	Nucleus	13C Dent135	Number of Transients	256	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	SW(cyclical) (Hz)	24037.73
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10064.4014	Sweep Width (Hz)	24036.99	Temperature (degree C)	27.000

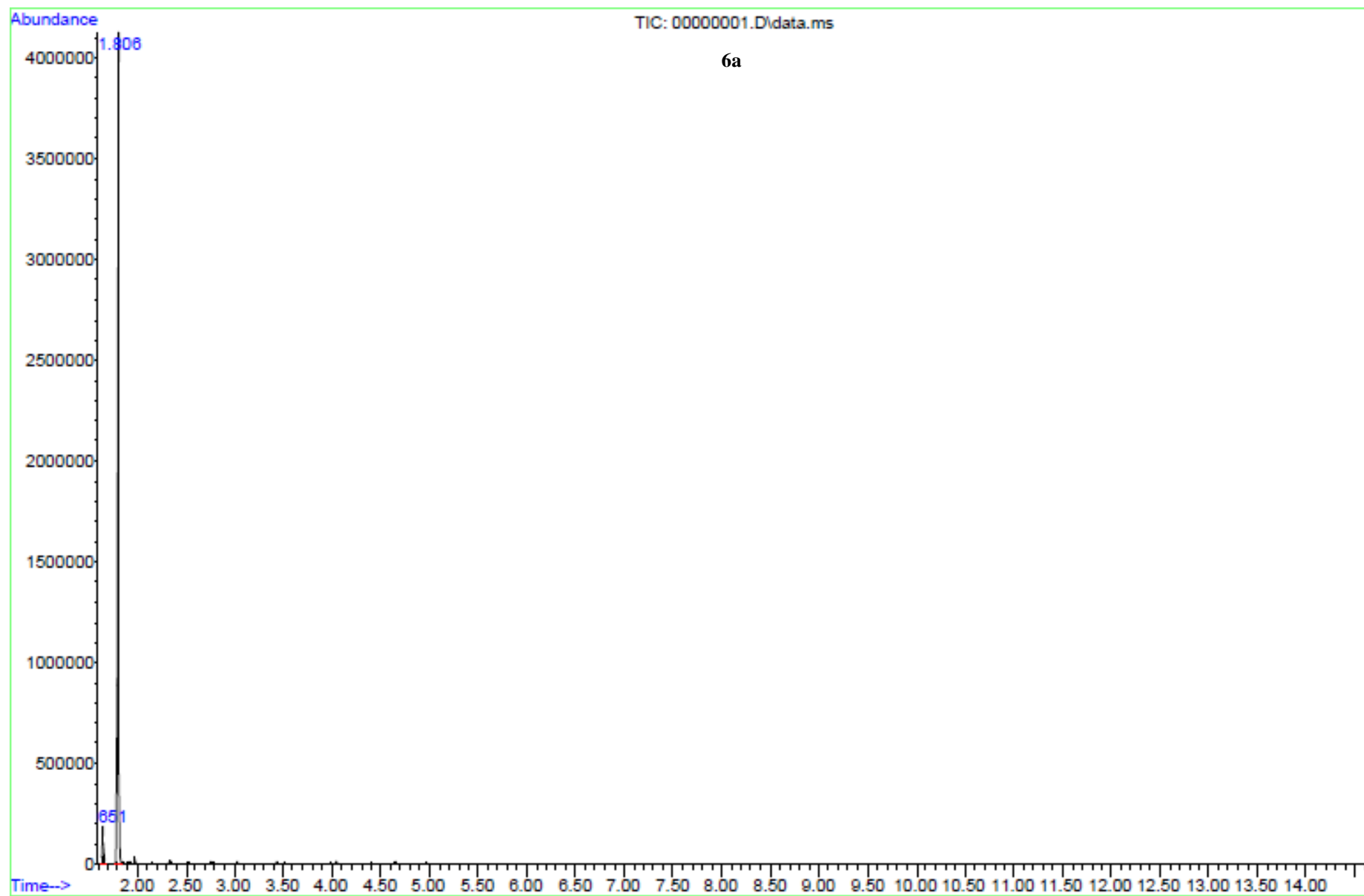


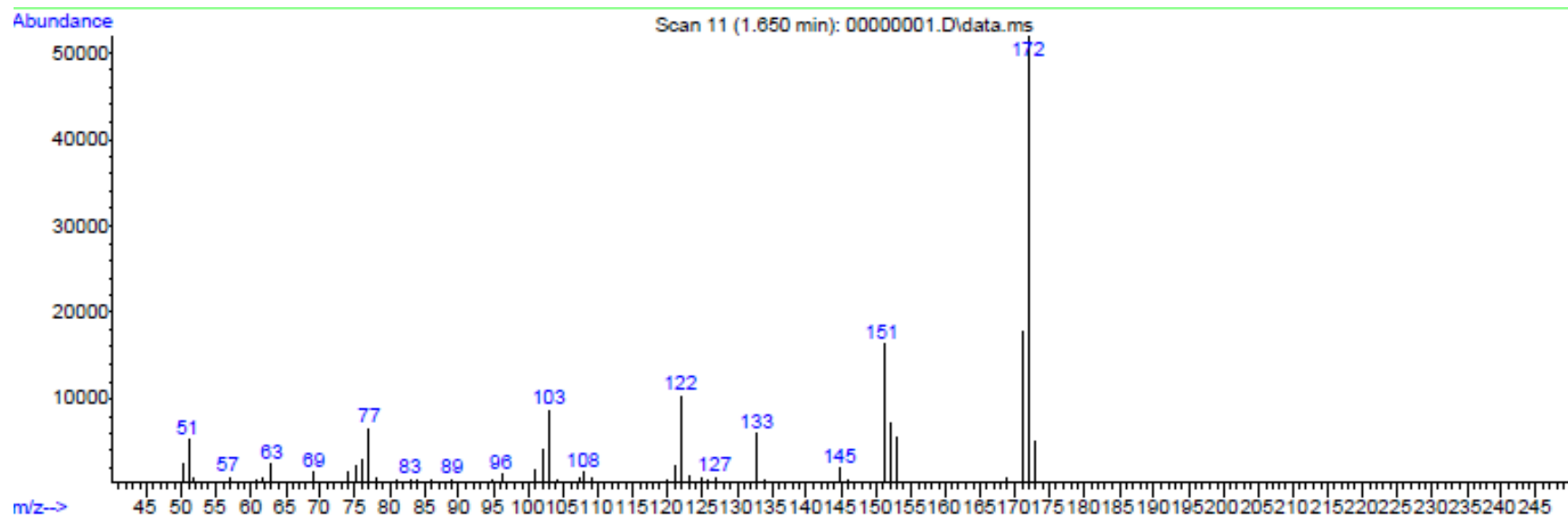
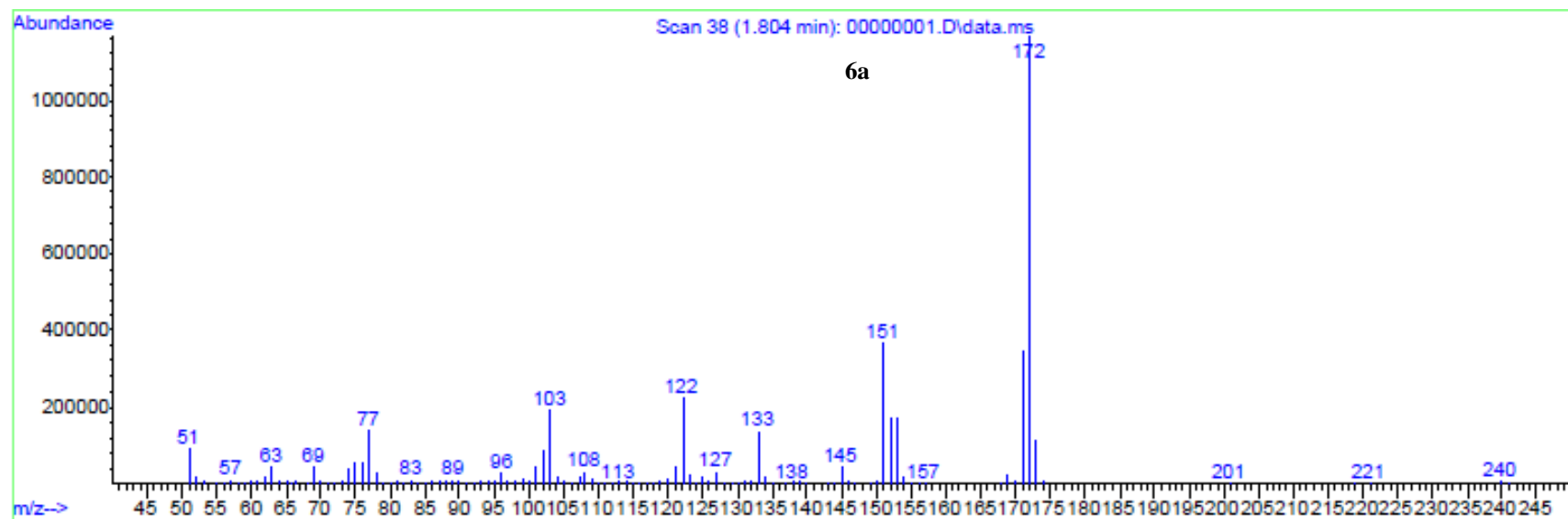
Frequency (MHz)	376.71	Nucleus	19F	Number of Transients	64	Origin	Bruker BioSpin GmbH
Original Points Count	131072	Owner	tibbe_operator	Points Count	131072	SW(cyclical) (Hz)	93749.28
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	-37752.5078	Sweep Width (Hz)	93748.56	Temperature (degree C)	27.000



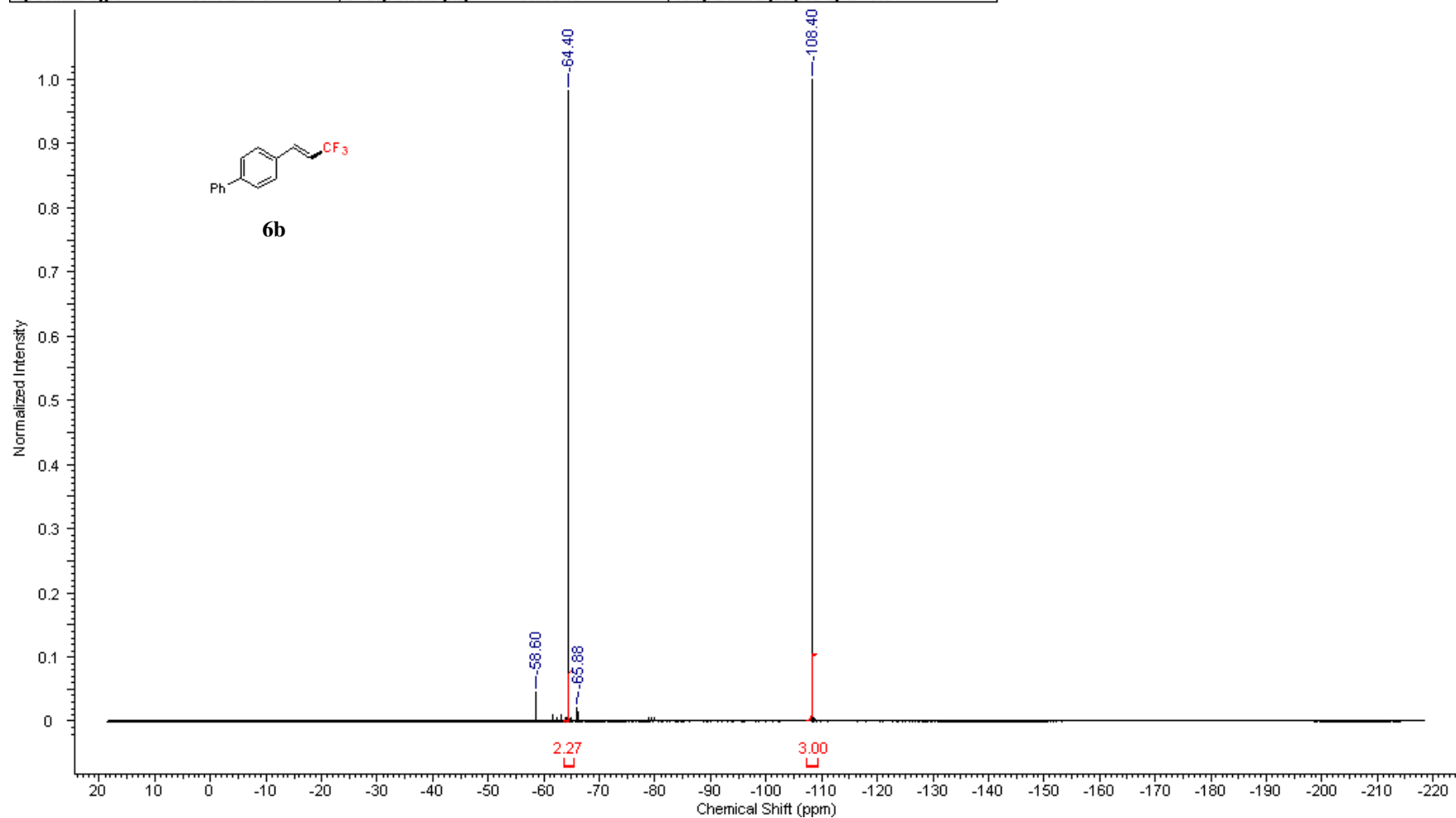
Frequency (MHz)	376.71	Nucleus	¹⁹ F	Number of Transients	64	Origin	Bruker BioSpin GmbH
Original Points Count	131072	Owner	tibbe_operator	Points Count	131072	SW(cyclical) (Hz)	93749.28
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	-37465.4805	Sweep Width (Hz)	93748.56	Temperature (degree C)	27.000

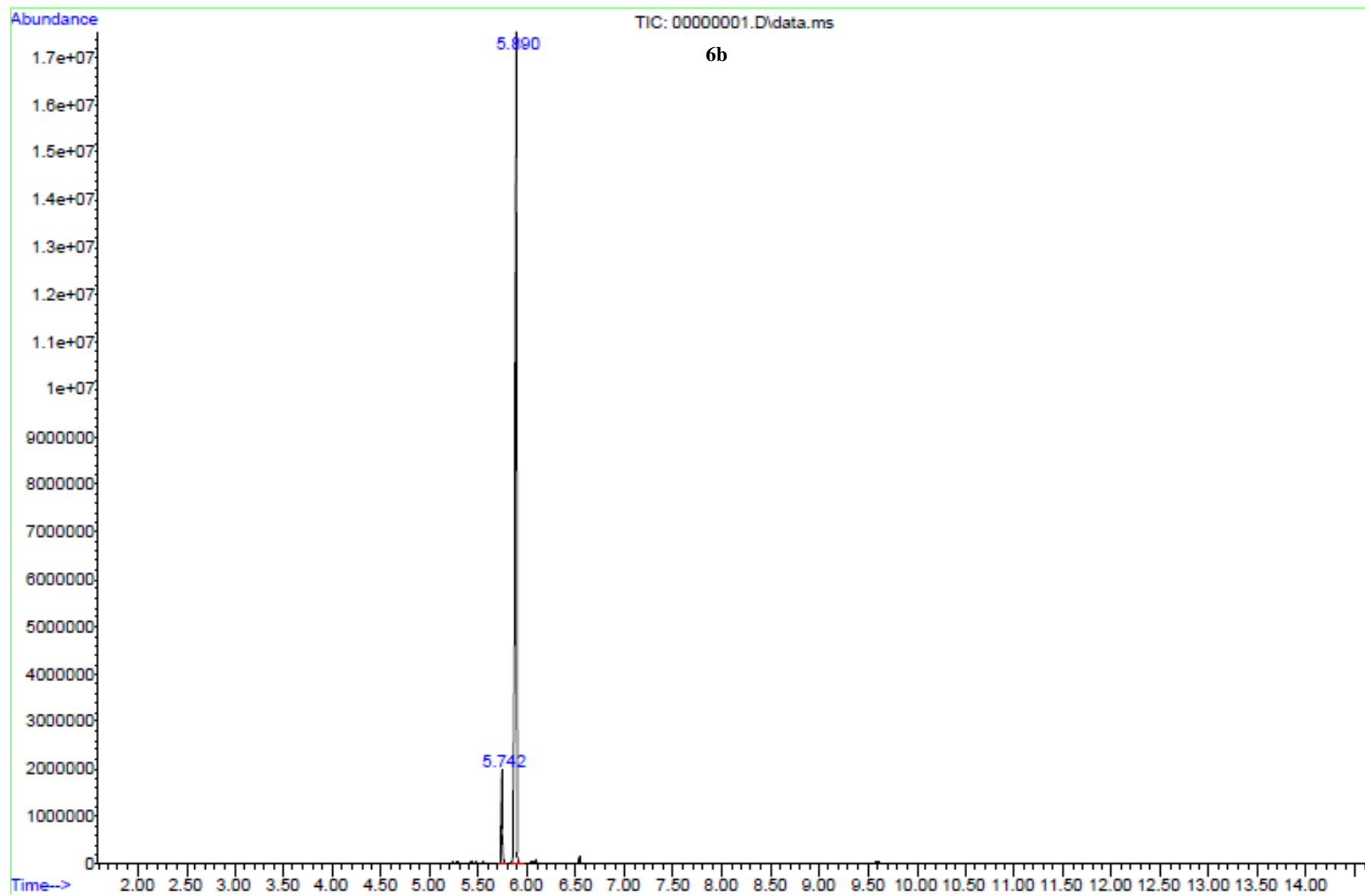


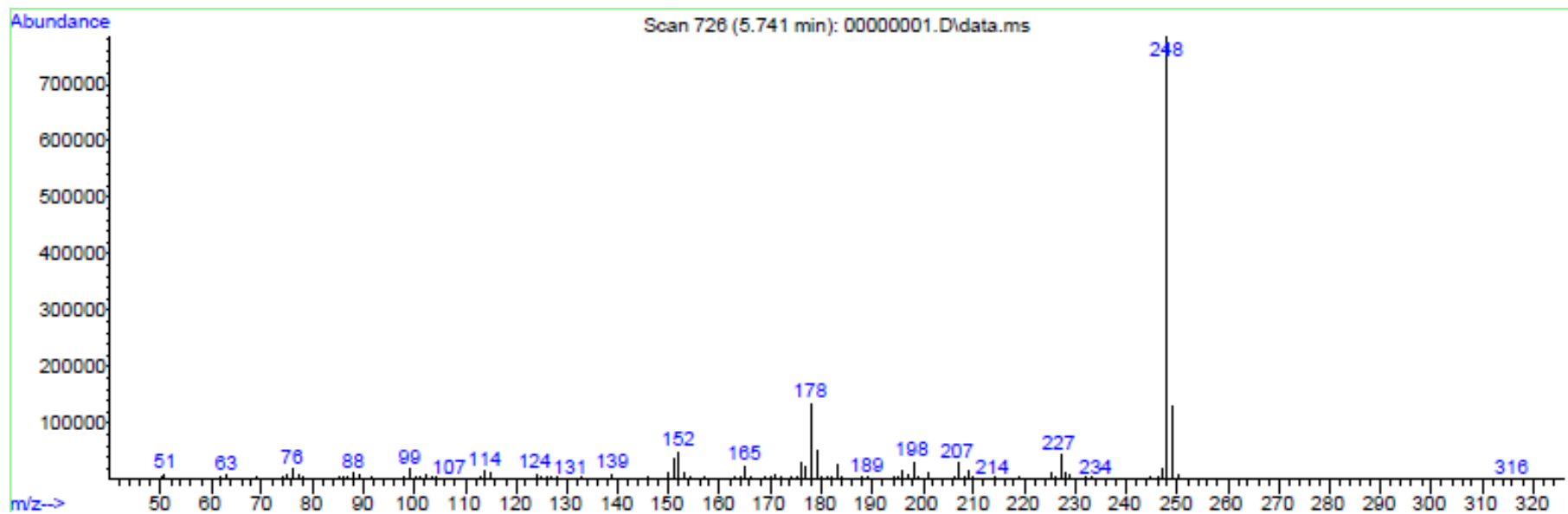
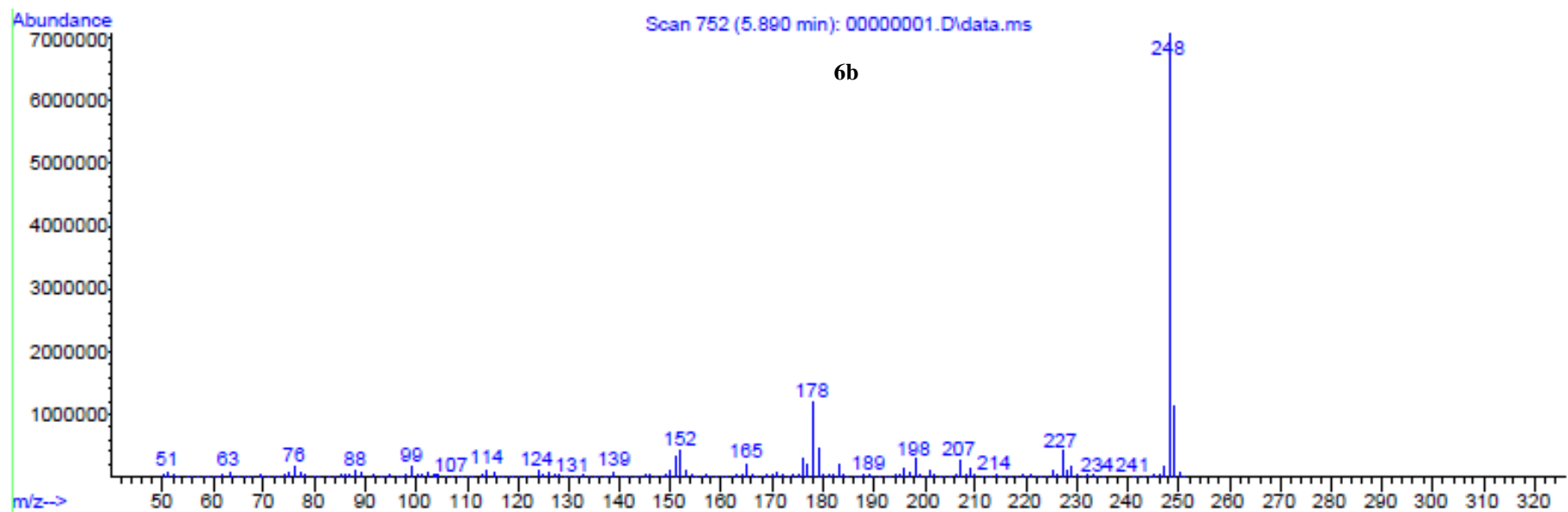




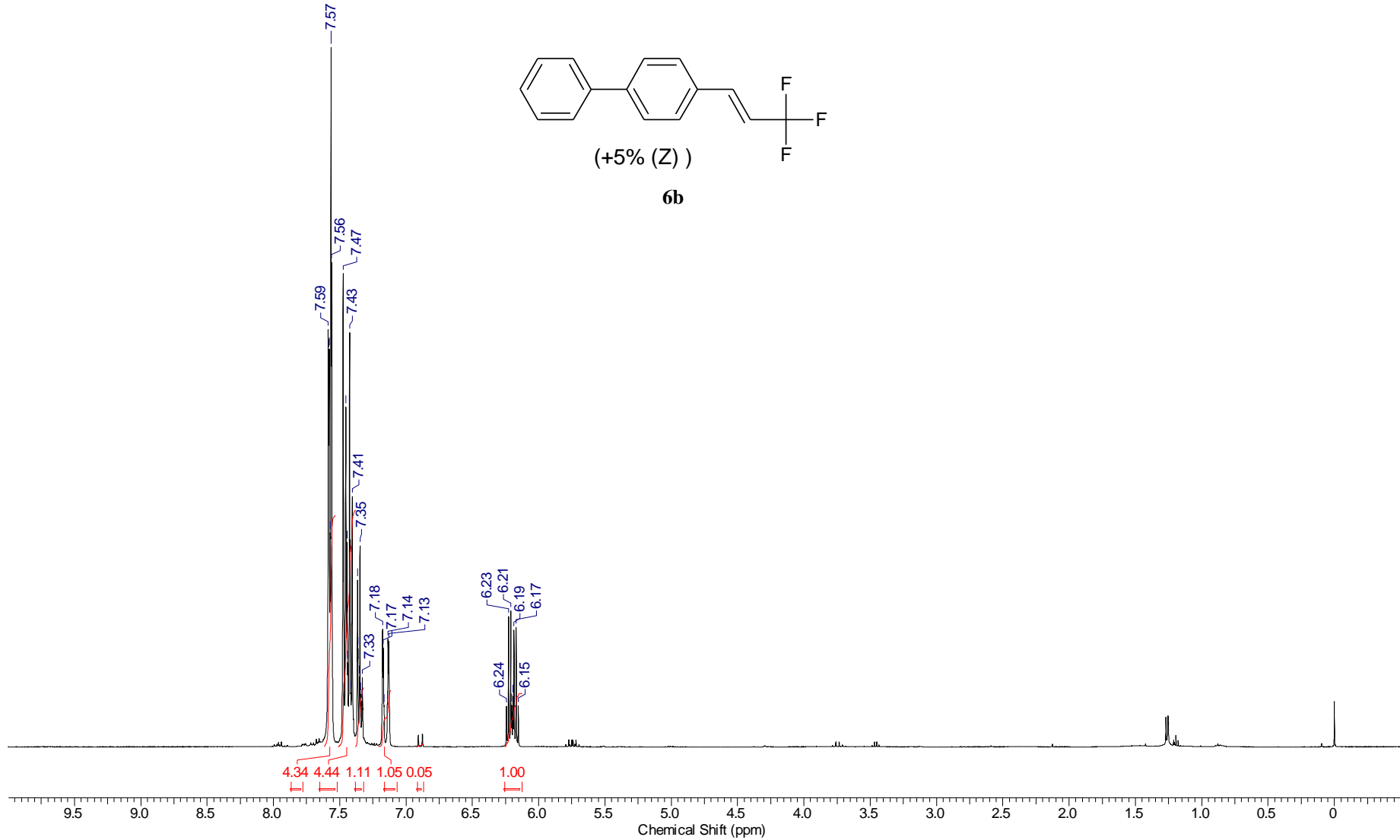
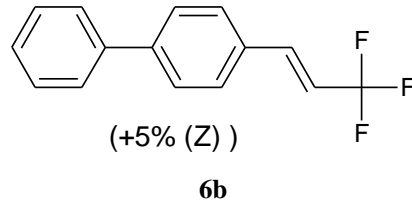
Frequency (MHz)	376.75	Nucleus	19F	Number of Transients	64	Origin	spect
Original Points Count	131072	Owner	tibbe operator	Points Count	131072	Pulse Sequence	zpg30
Receiver Gain	1620.00	SW(cyclical) (Hz)	89285.71	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	-37674.2031
Spectrum Type	STANDARD	Sweep Width (Hz)	89285.03	Temperature (degree C)	27.000		



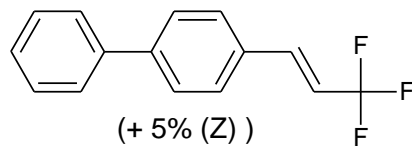




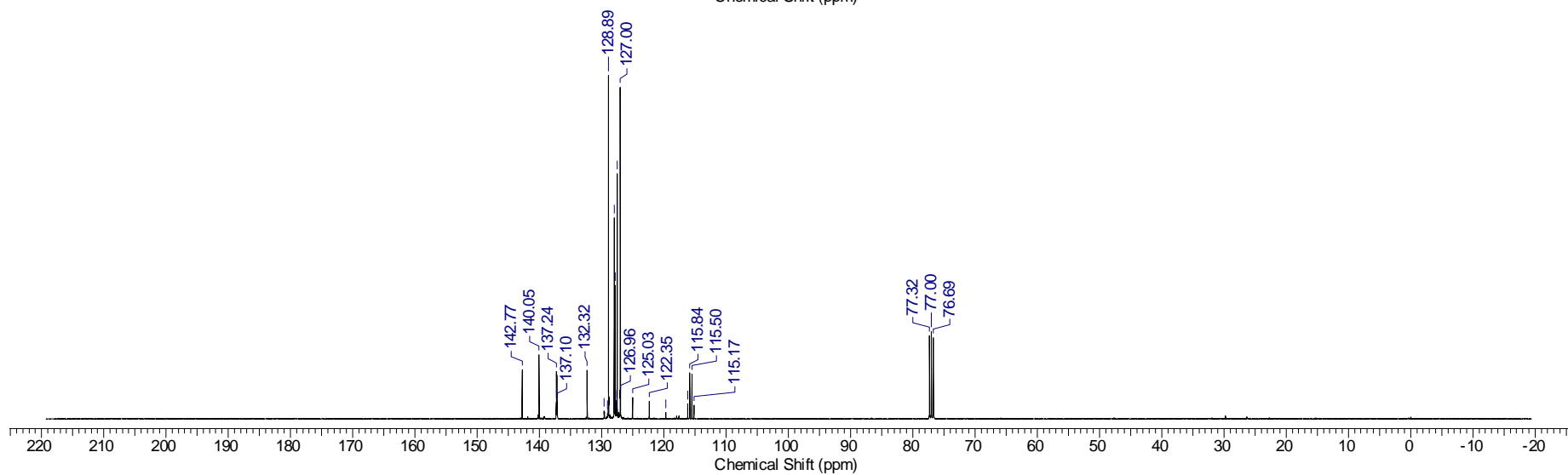
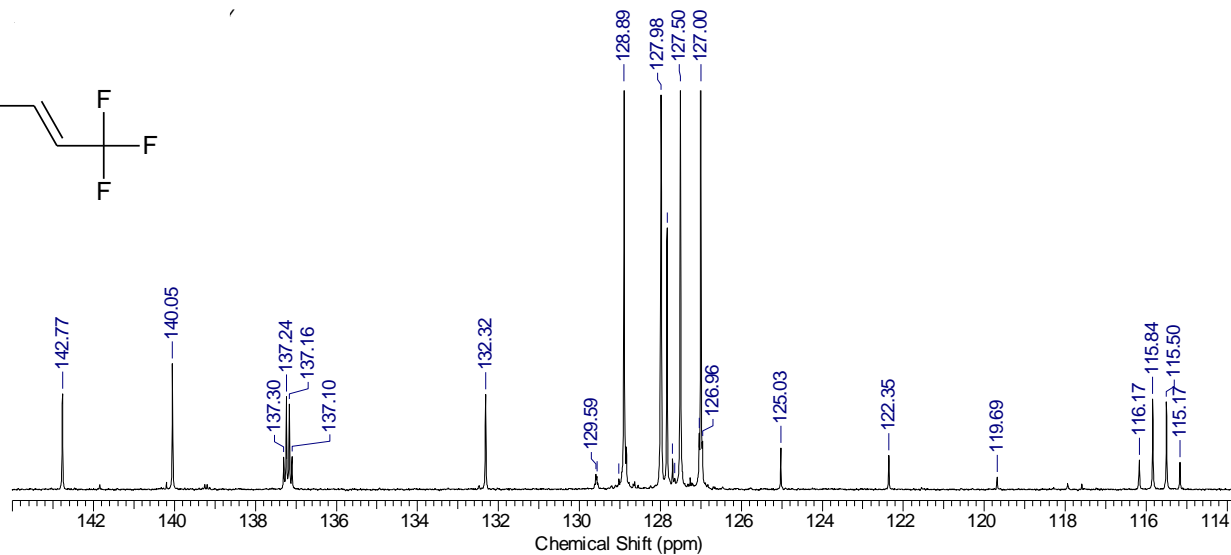
Frequency (MHz)	400.40	Nucleus	1H	Number of Transients	16	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	SW(cyclical) (Hz)	7211.32
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	3358.7139	Sweep Width (Hz)	7211.10	Temperature (degree C)	27.000



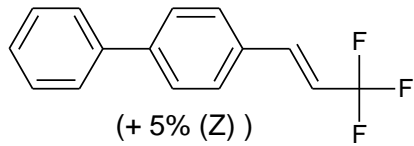
Frequency (MHz)	100.69	Nucleus	¹³ C	Number of Transients	1024	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	SW(cyclical) (Hz)	24037.73
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10060.6406	Sweep Width (Hz)	24036.99	Temperature (degree C)	27.000



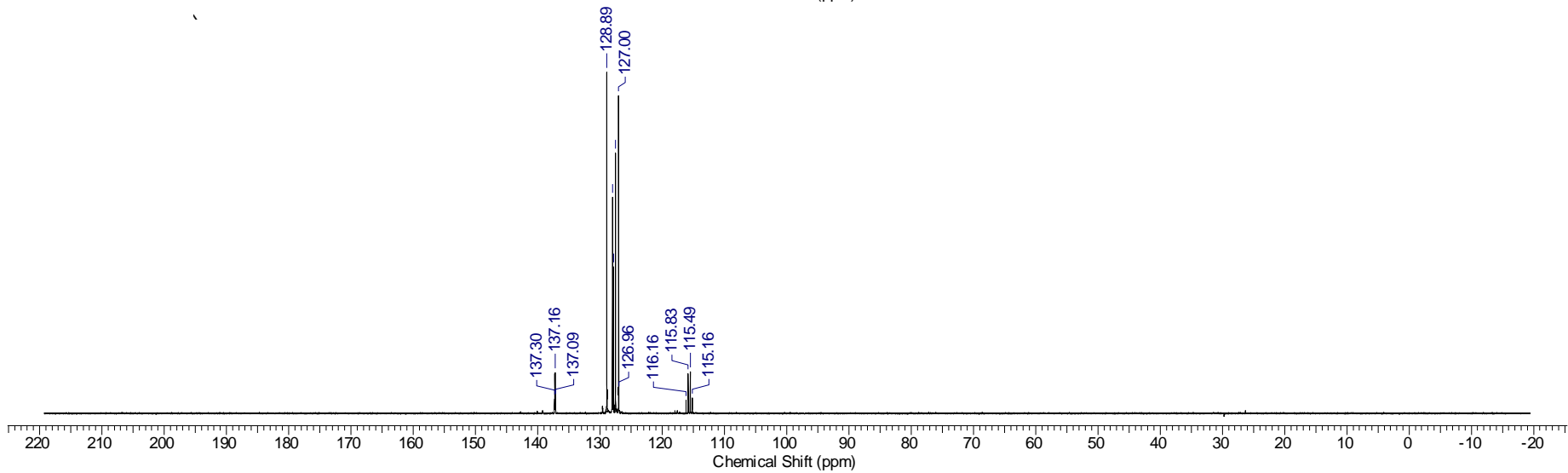
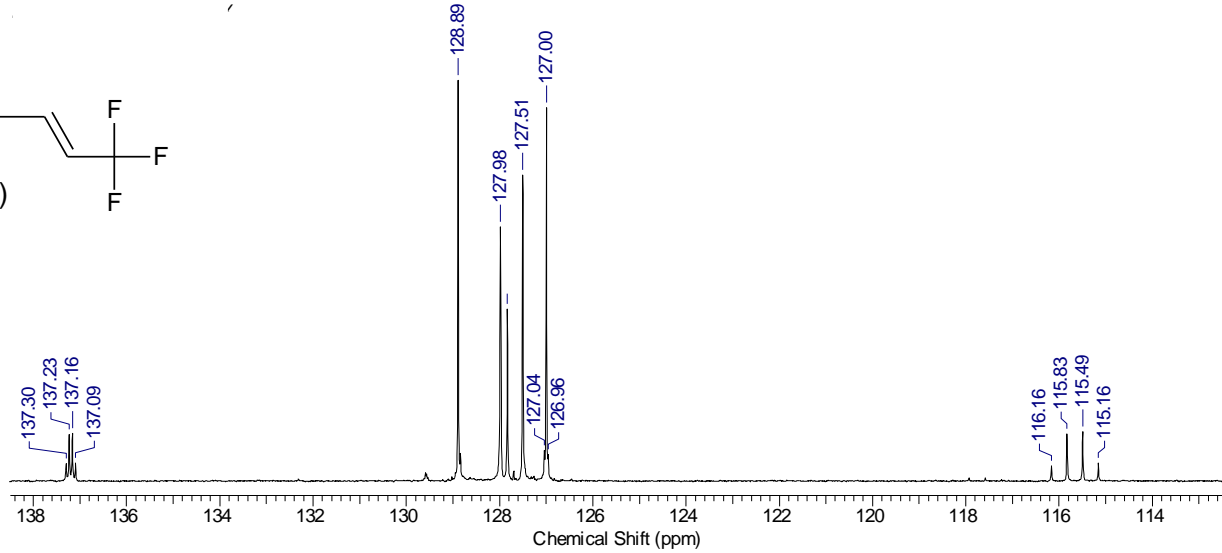
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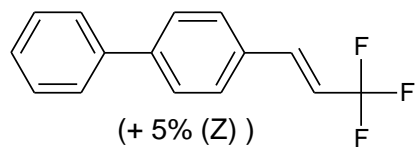
Frequency (MHz)	100.69	Nucleus	13C	Dept 135	Number of Transients	256	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator		Points Count	32768	SW(cyclical) (Hz)	24037.73
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10060.2402		Sweep Width (Hz)	24036.99	Temperature (degree C)	27.000



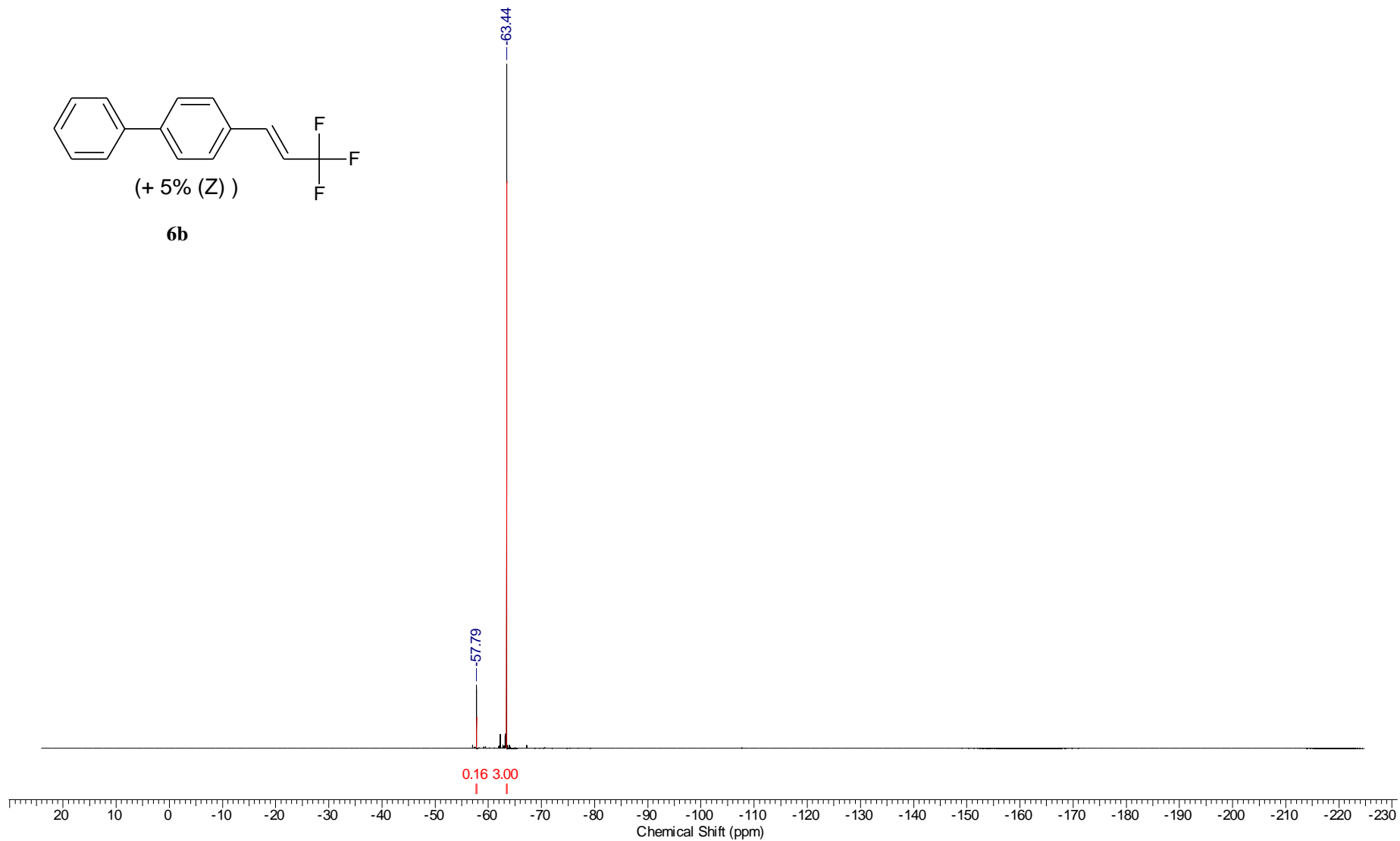
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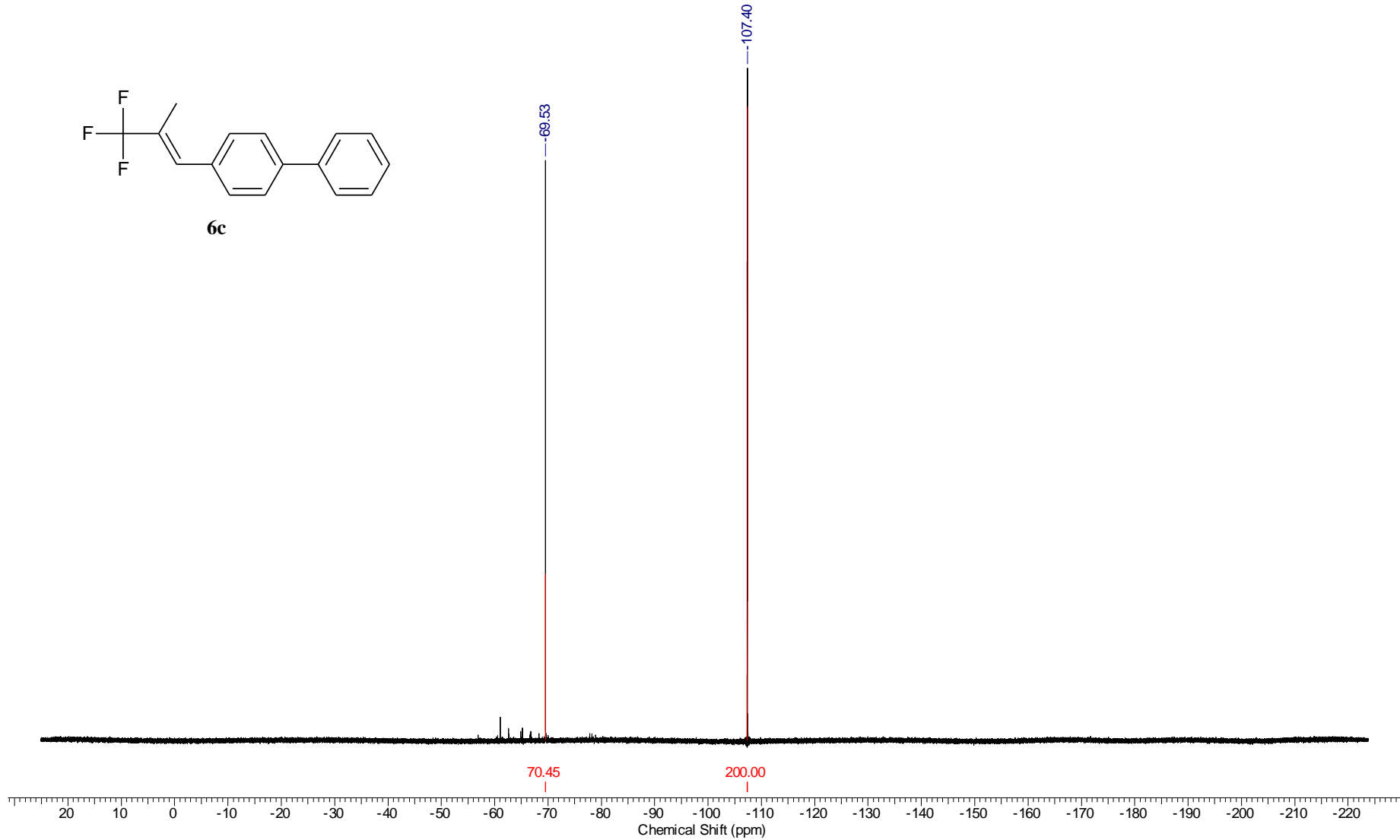
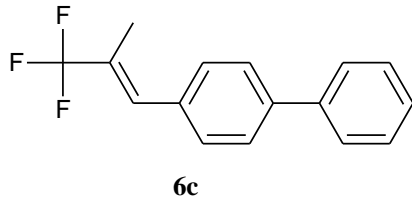
Frequency (MHz)	376.71	Nucleus	19F	Number of Transients	64	Origin	Bruker BioSpin GmbH
Original Points Count	131072	Owner	tibbe_operator	Points Count	131072	SW(cyclical) (Hz)	93749.28
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	-37810.0391	Sweep Width (Hz)	93748.56	Temperature (degree C)	27.000

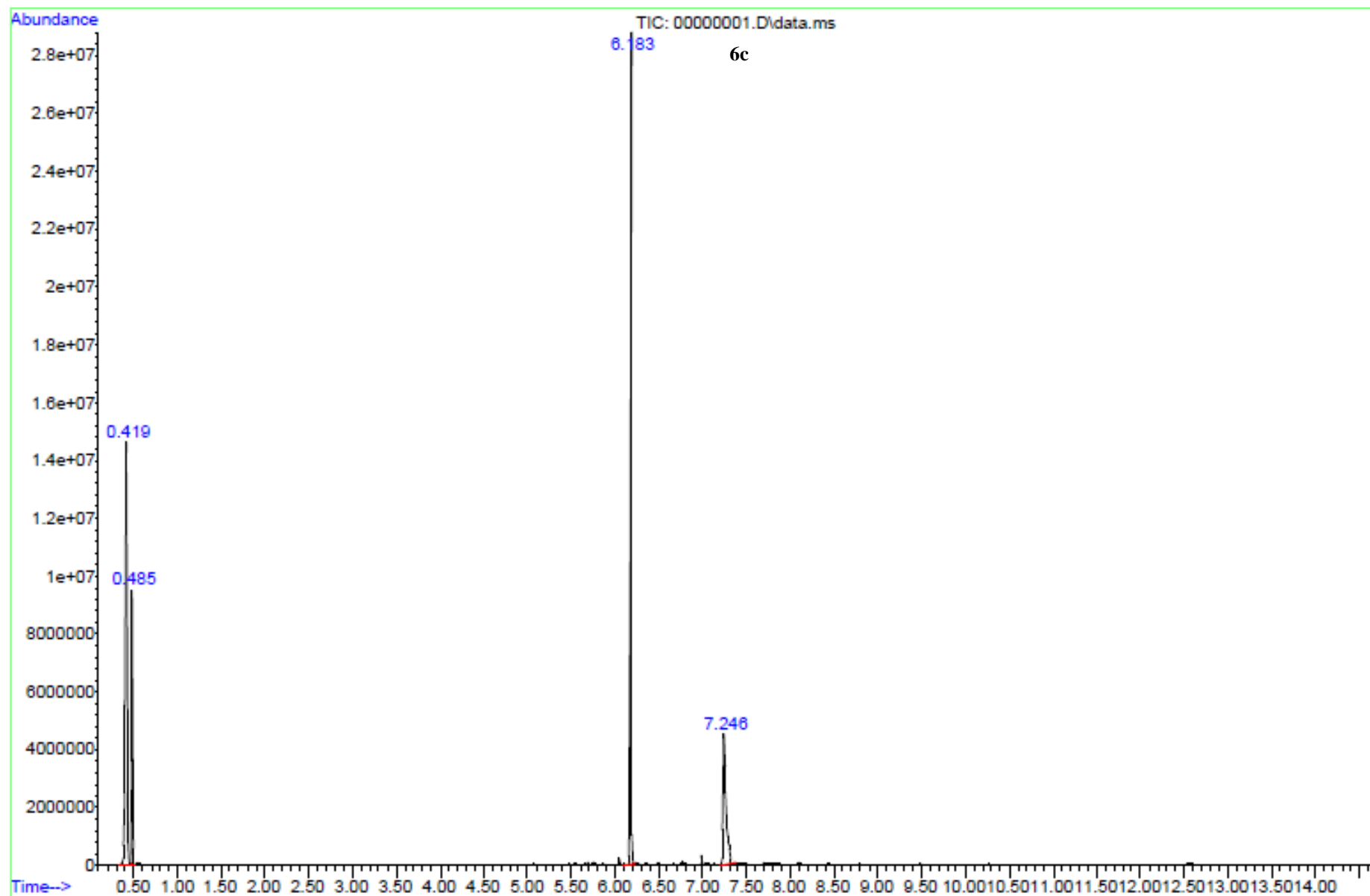


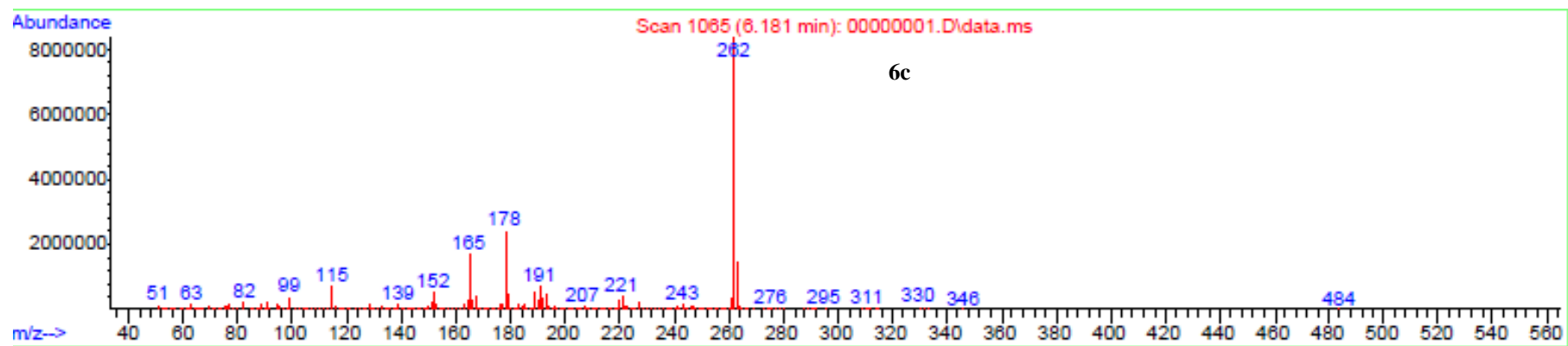
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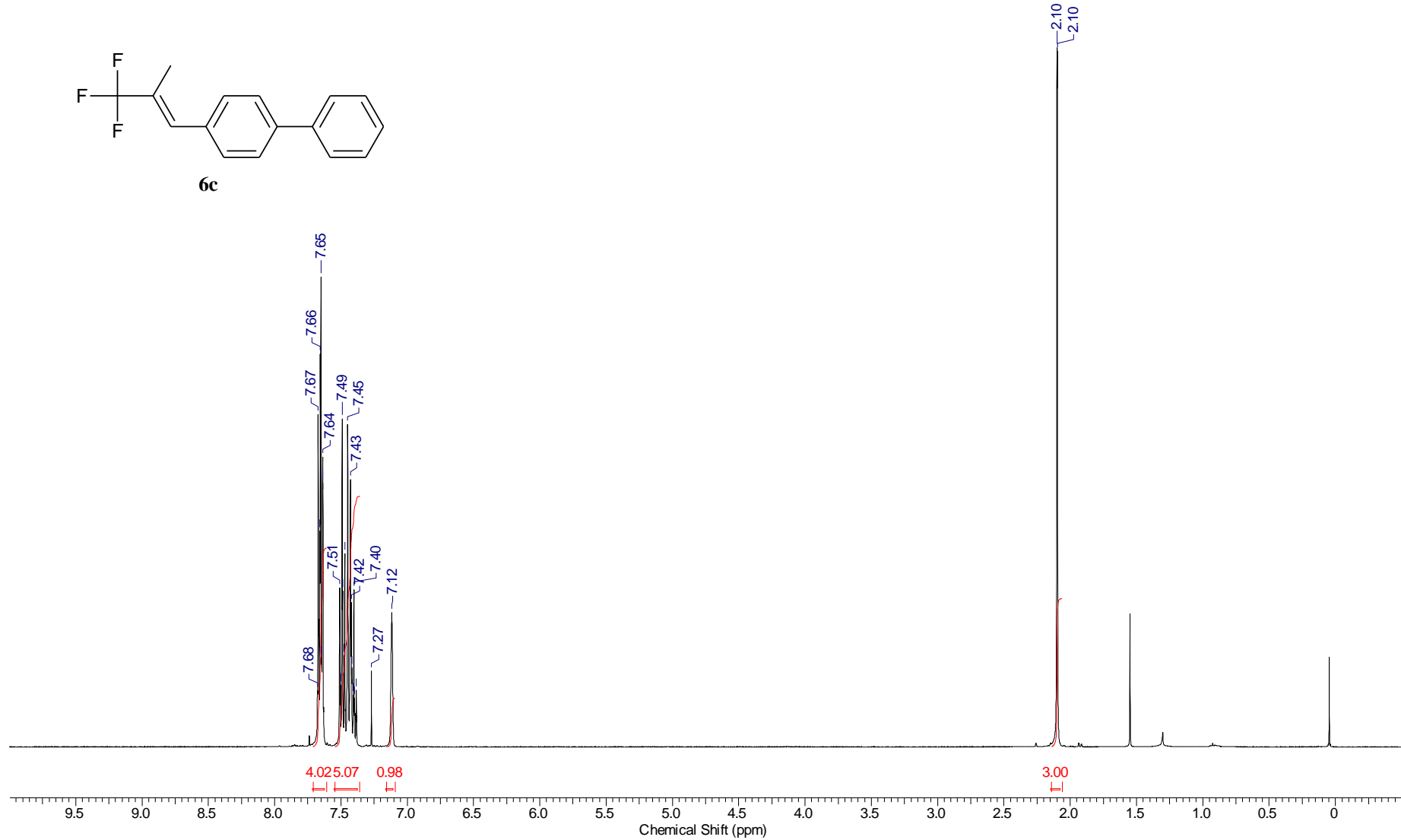
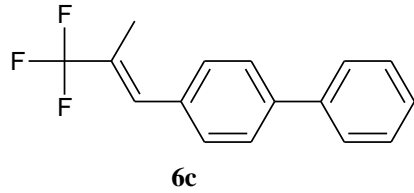
Frequency (MHz)	376.71	Nucleus	19F	Number of Transients	64	Origin	Bruker BioSpin GmbH
Original Points Count	131072	Owner	tibbe_operator	Points Count	131072	SW(cyclical) (Hz)	93749.28
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	-37420.4180	Sweep Width (Hz)	93748.56	Temperature (degree C)	27.000



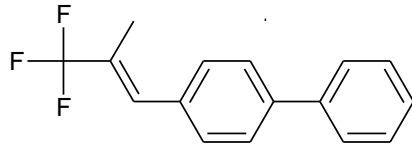




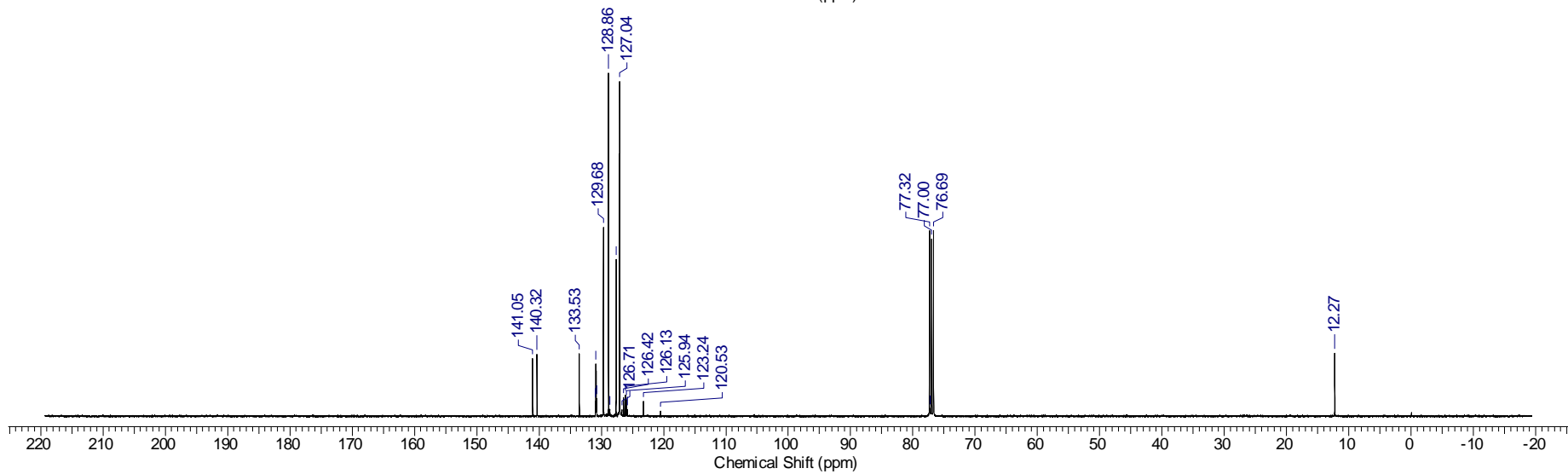
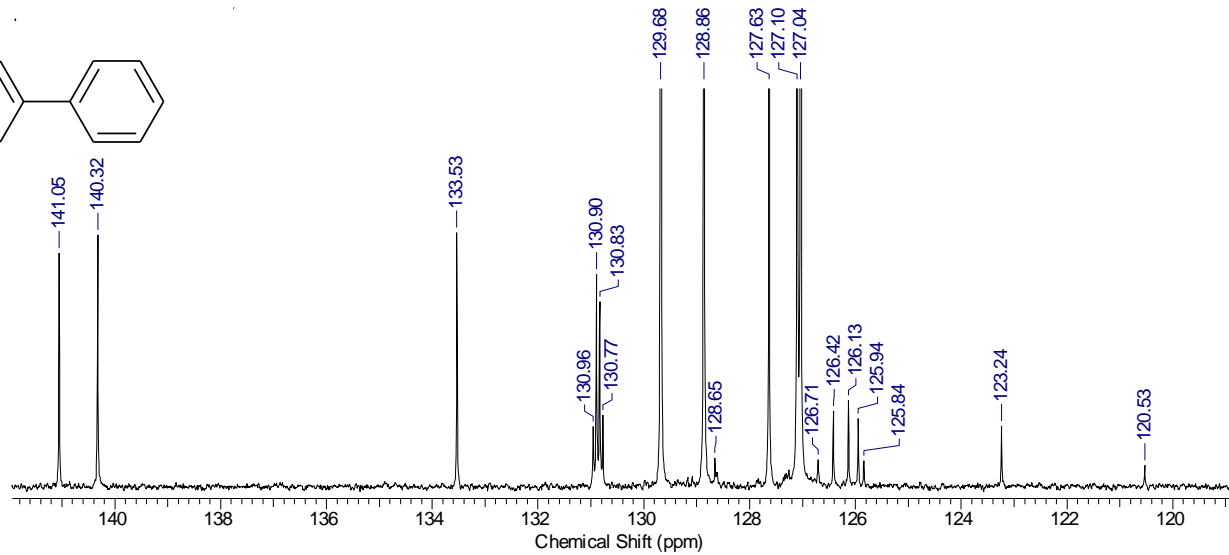
Frequency (MHz)	400.40	Nucleus	1H	Number of Transients	16	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	SW(cyclical) (Hz)	7211.32
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	3395.6414	Sweep Width (Hz)	7211.10	Temperature (degree C)	27.000



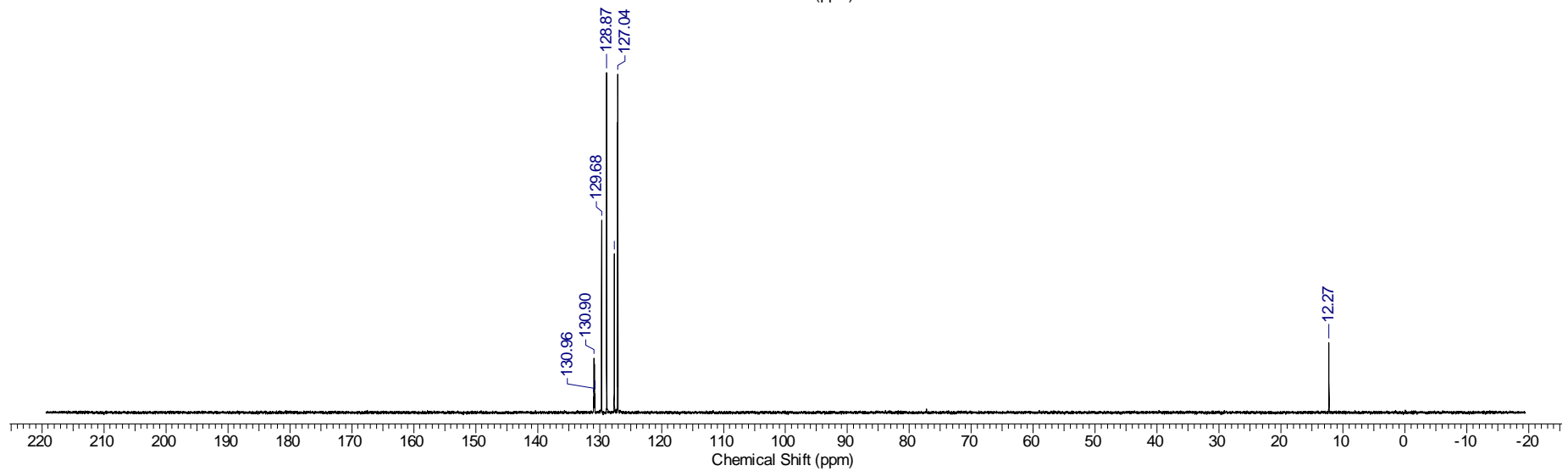
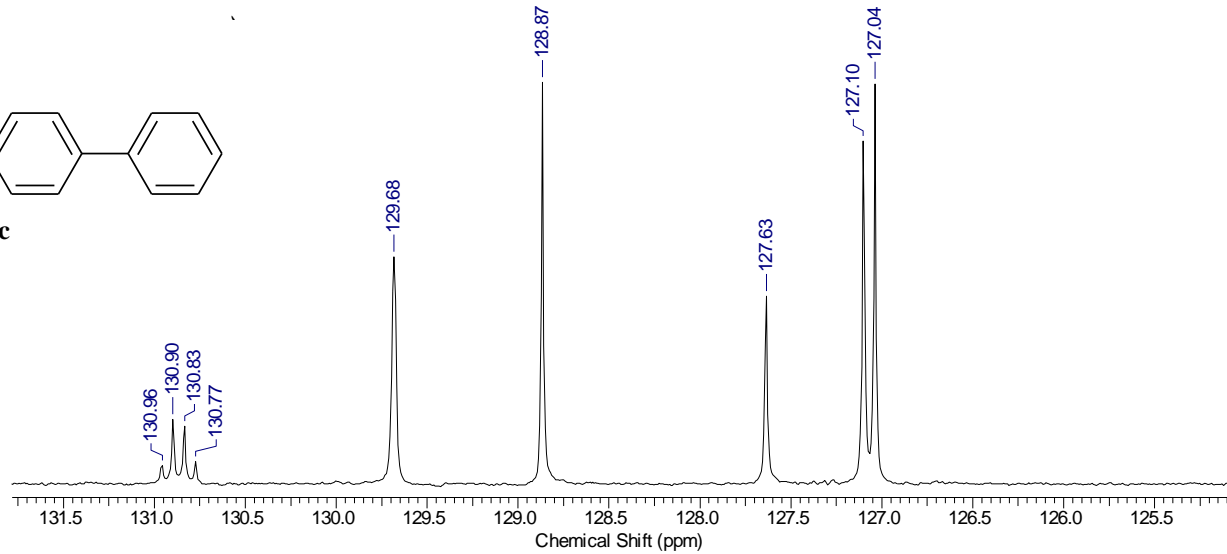
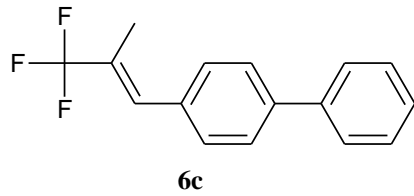
Frequency (MHz)	100.69	Nucleus	13C	Number of Transients	1024	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	SW(cyclical) (Hz)	24037.73
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10065.0420	Sweep Width (Hz)	24036.99	Temperature (degree C)	27.000



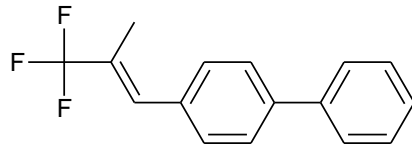
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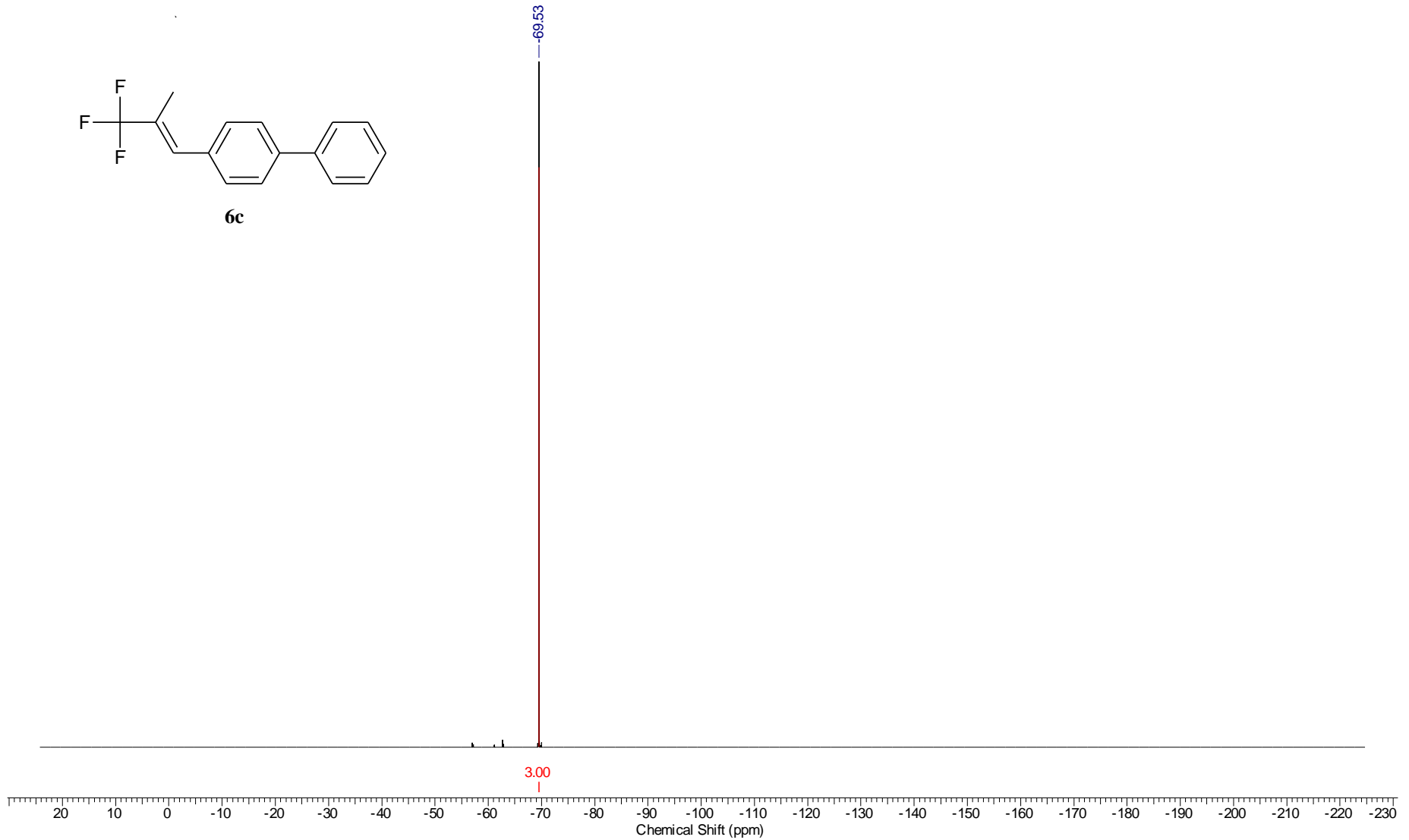
Frequency (MHz)	100.69	Nucleus	13C	Dept 135	Number of Transients	256	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator		Points Count	32768	SW(cyclical) (Hz)	24037.73
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10065.1299		Sweep Width (Hz)	24036.99	Temperature (degree C)	27.000



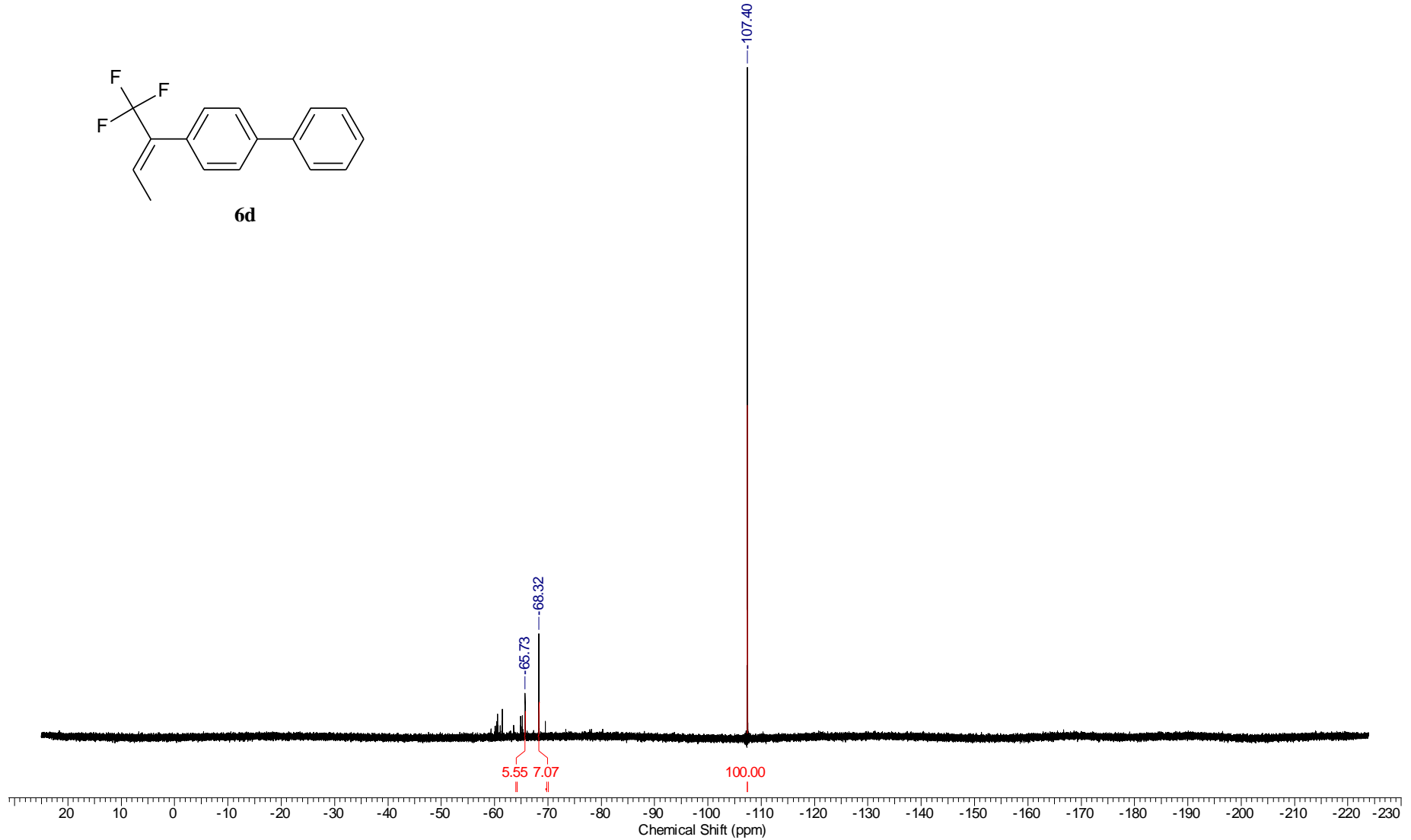
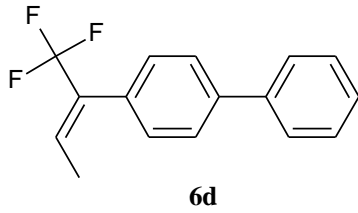
Frequency (MHz)	376.71	Nucleus	¹⁹ F	Number of Transients	64	Origin	Bruker BioSpin GmbH
Original Points Count	131072	Owner	tibbe_operator	Points Count	131072	SW(cyclical) (Hz)	93749.28
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	-37758.9258	Sweep Width (Hz)	93748.56	Temperature (degree C)	27.000

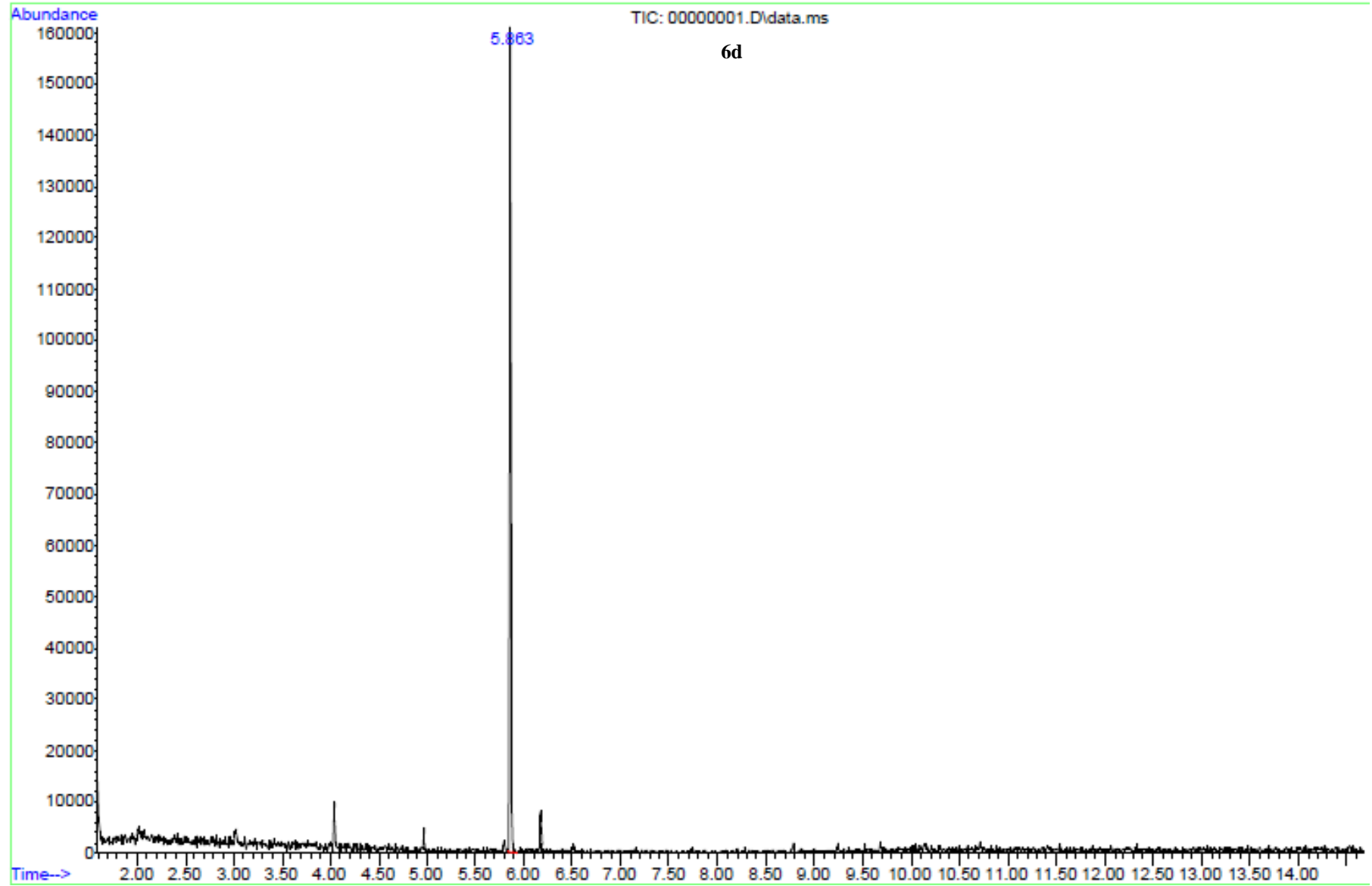


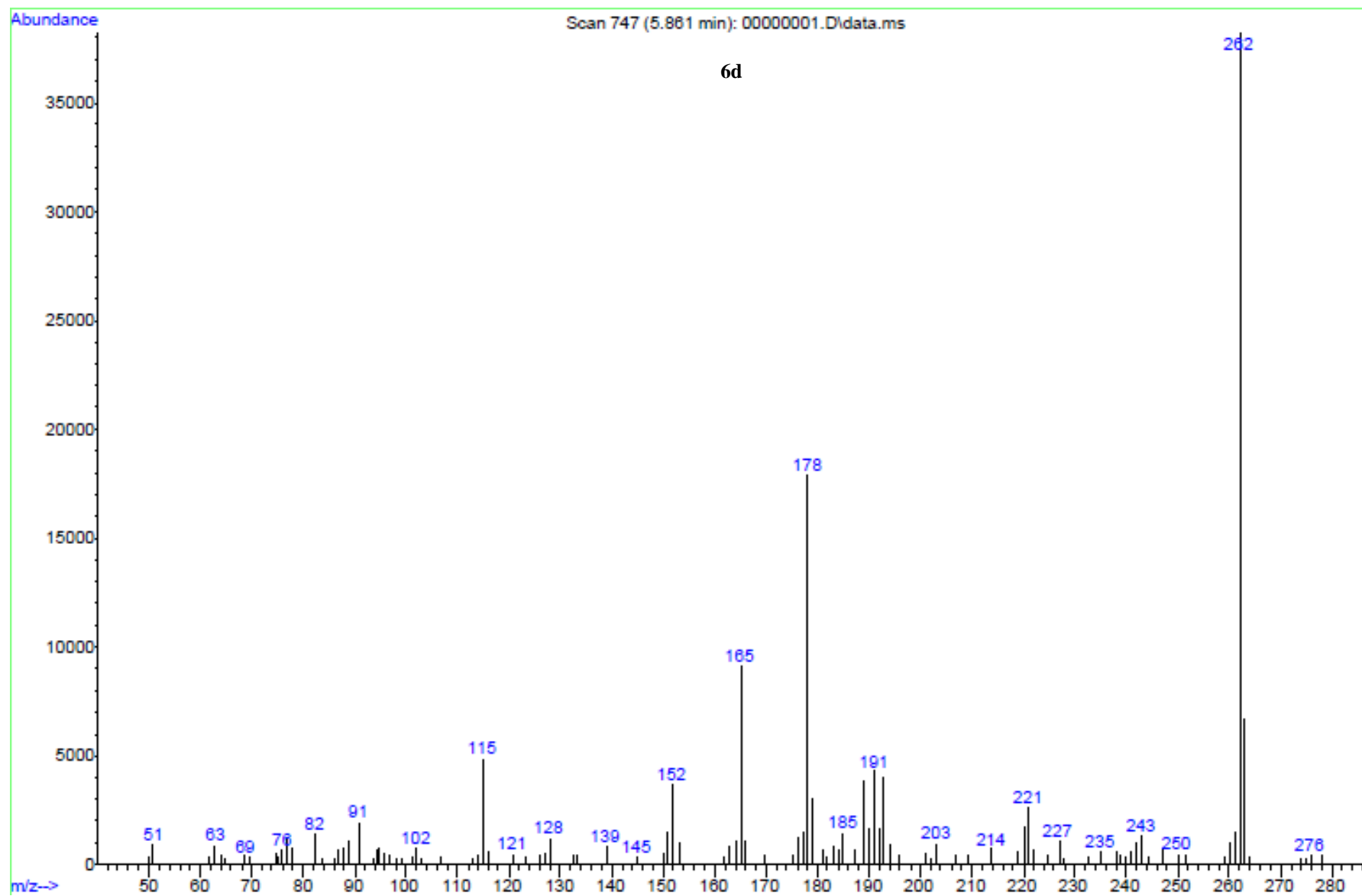
6c



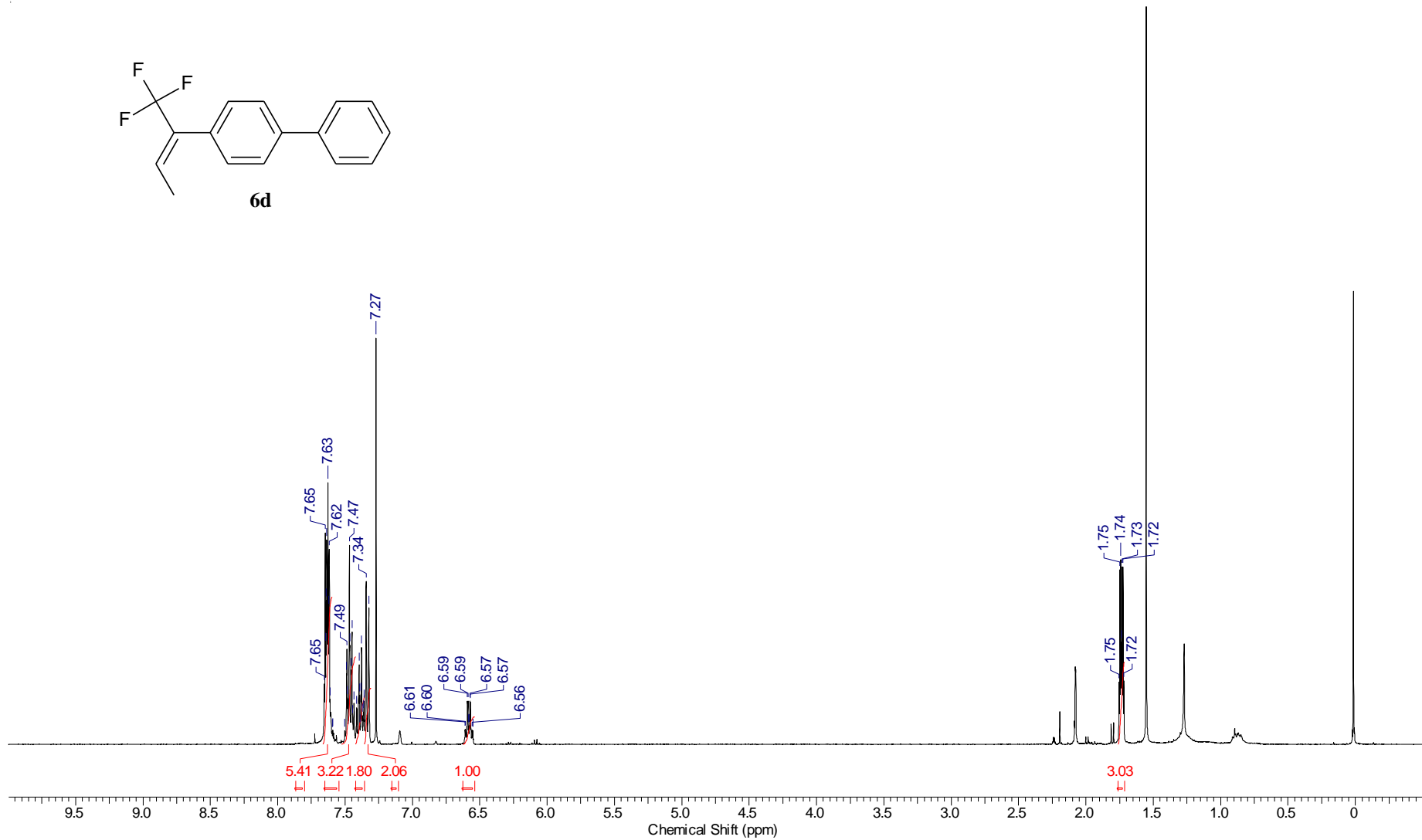
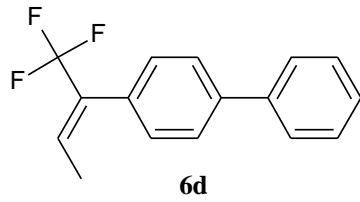
Frequency (MHz)	376.71	Nucleus	¹⁹ F	Number of Transients	64	Origin	Bruker BioSpin GmbH
Original Points Count	131072	Owner	tibbe_operator	Points Count	131072	SW(cyclical) (Hz)	93749.28
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	-37451.1758	Sweep Width (Hz)	93748.56	Temperature (degree C)	27.000



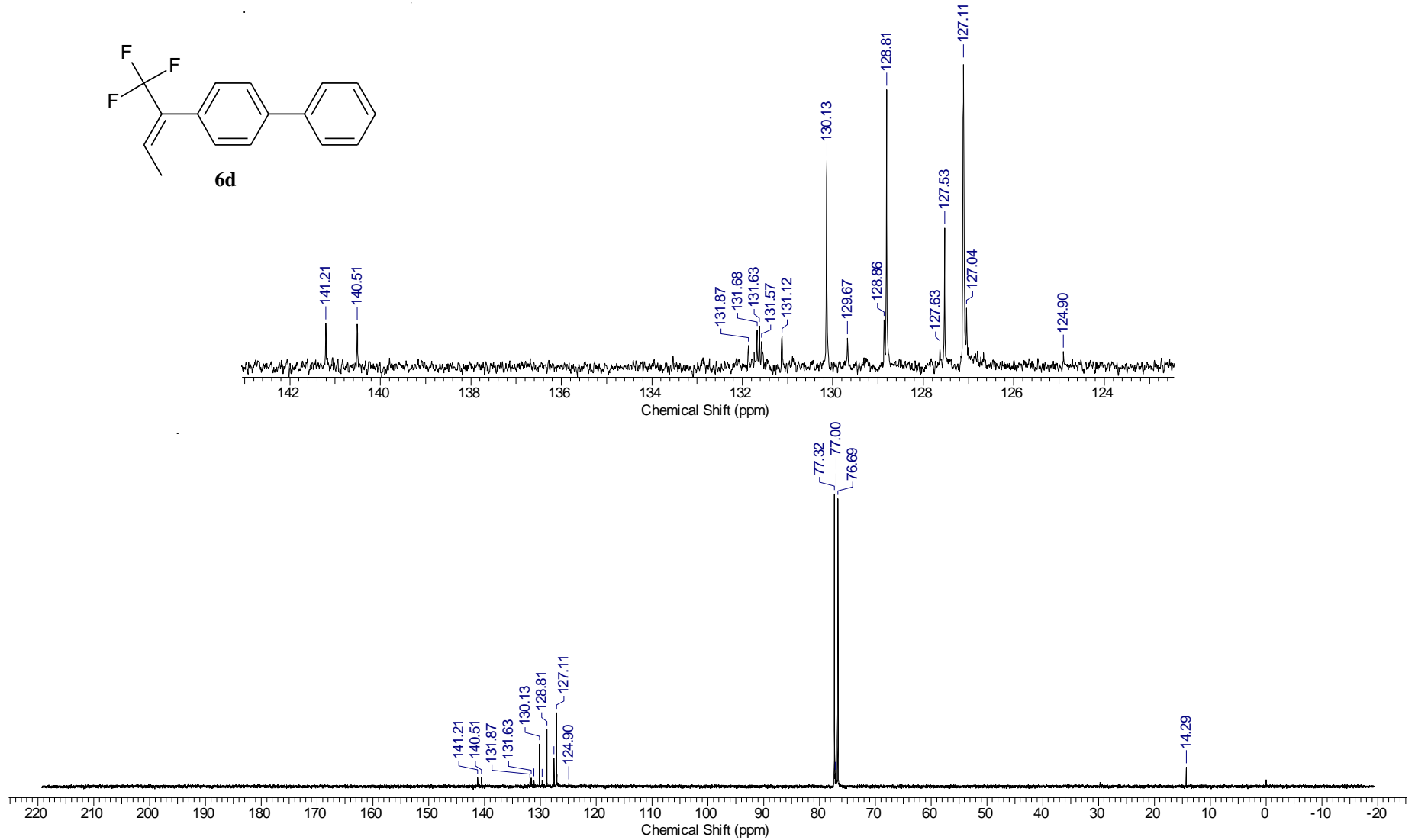
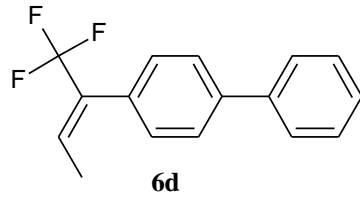




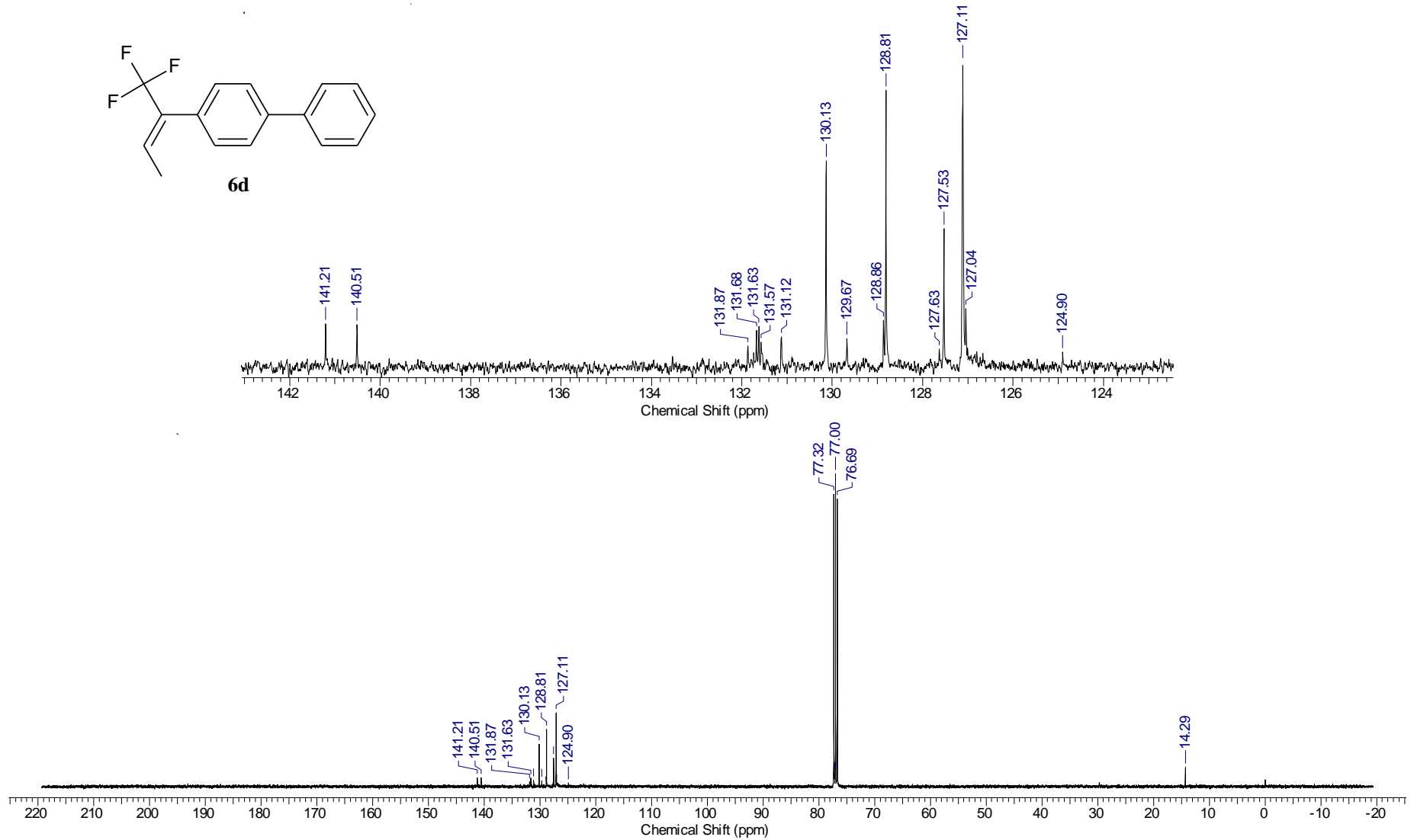
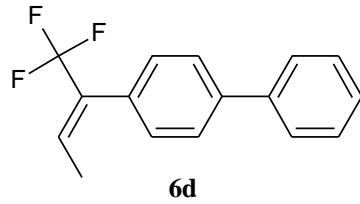
Frequency (MHz)	400.40	Nucleus	1H	Number of Transients	16	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	SW(cyclical) (Hz)	7211.32
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	3395.6411	Sweep Width (Hz)	7211.10	Temperature (degree C)	27.000



Frequency (MHz)	100.69	Nucleus	¹³ C	Number of Transients	1024	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	SW(cyclical) (Hz)	24037.73
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10067.2422	Sweep Width (Hz)	24036.99	Temperature (degree C)	27.000



Frequency (MHz)	100.69	Nucleus	¹³ C Dept 135	Number of Transients	1024	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	SW(cyclical) (Hz)	24037.73
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10067.2422	Sweep Width (Hz)	24036.99	Temperature (degree C)	27.000



Frequency (MHz)	376.71	Nucleus	¹⁹ F	Number of Transients	64	Origin	Bruker BioSpin GmbH
Original Points Count	131072	Owner	tibbe_operator	Points Count	131072	SW(cyclical) (Hz)	93749.28
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	-37760.7734	Sweep Width (Hz)	93748.56	Temperature (degree C)	27.000

