

Synthesis and Minisci Reactions of Organotrifluoroborate Building Blocks

Supporting Information

**Marc Presset,^{†,‡} Nicolas Fleury-Brégeot,[†] Daniel Oehrich,[‡] Frederik Rombouts^{*,‡} and
Gary A. Molander^{*,†}**

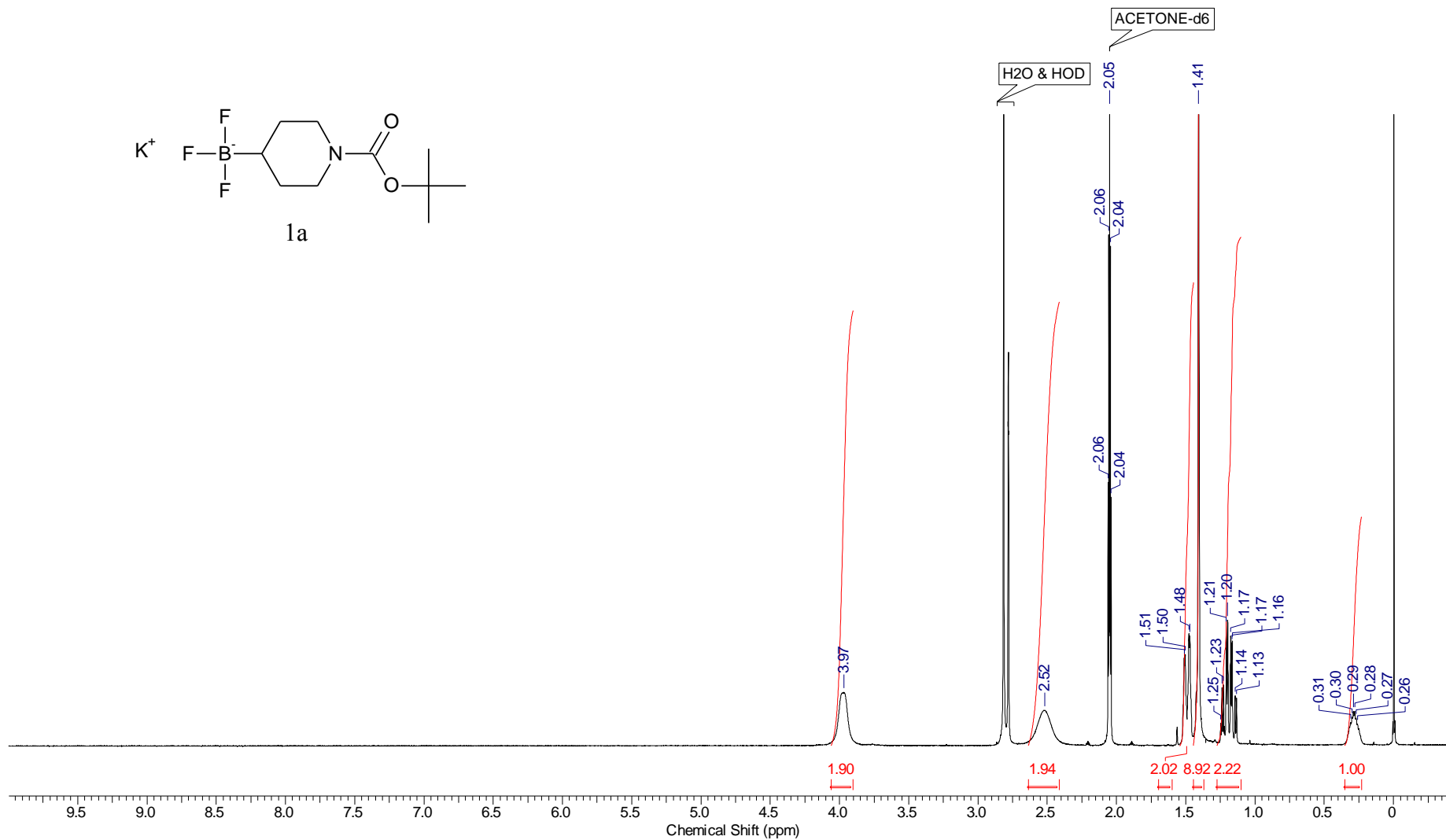
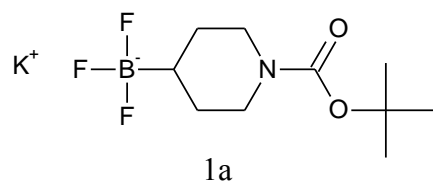
[†]Roy and Diana Vagelos Laboratories, Department of Chemistry, University of Pennsylvania, Philadelphia, Pennsylvania 19104-6323, United States, and [‡]Neuroscience Medicinal Chemistry, Research & Development, Janssen, Pharmaceutical Companies, Turnhoutseweg 30, 2340 Beerse, Belgium

frombout@its.jnj.com; gmolandr@sas.upenn.edu

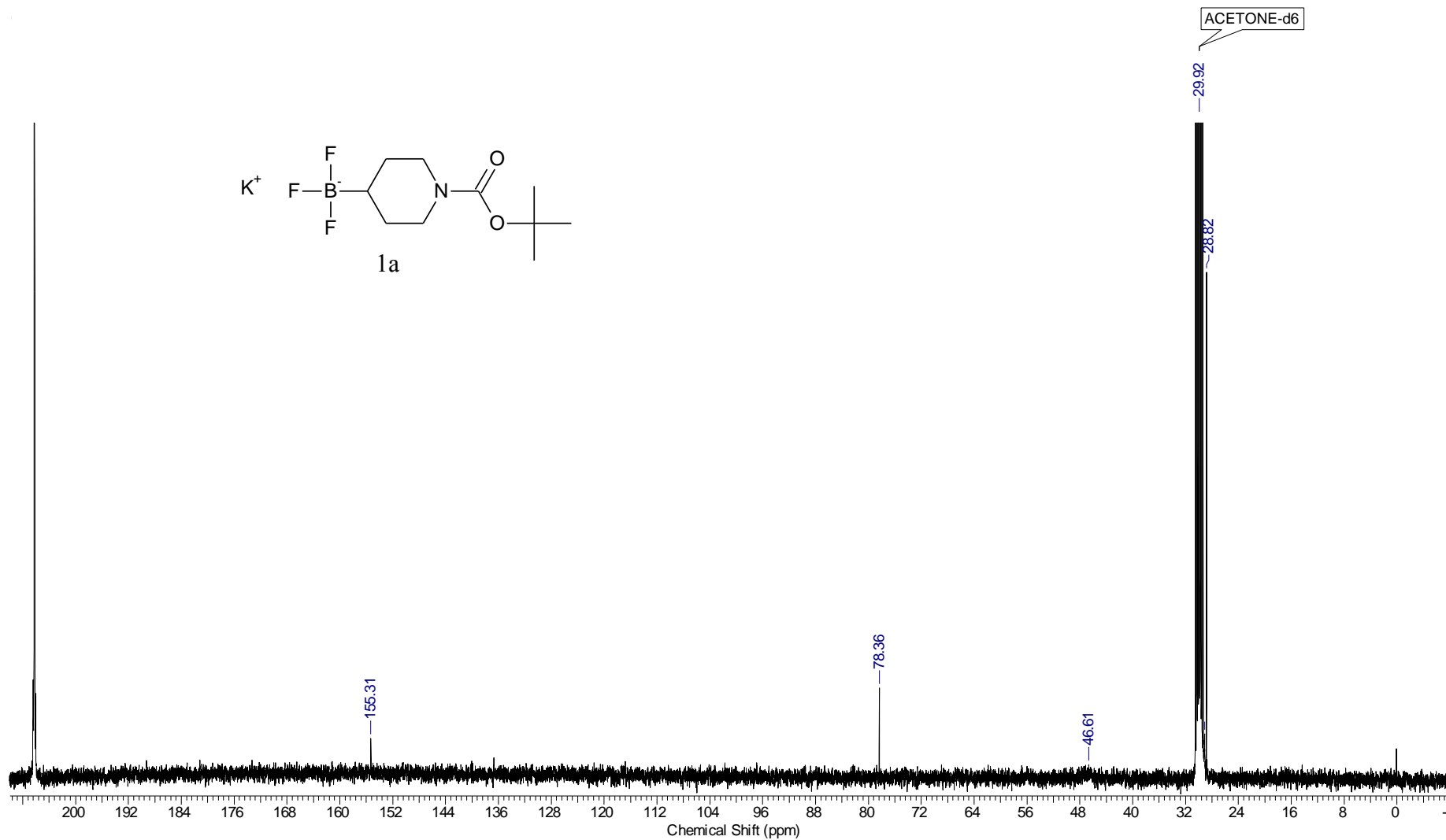
Contents:

Copies of NMR spectra: ¹H and ¹³C for all compounds; ¹¹B and ¹⁹F for organotrifluoroborates S2 – S72.

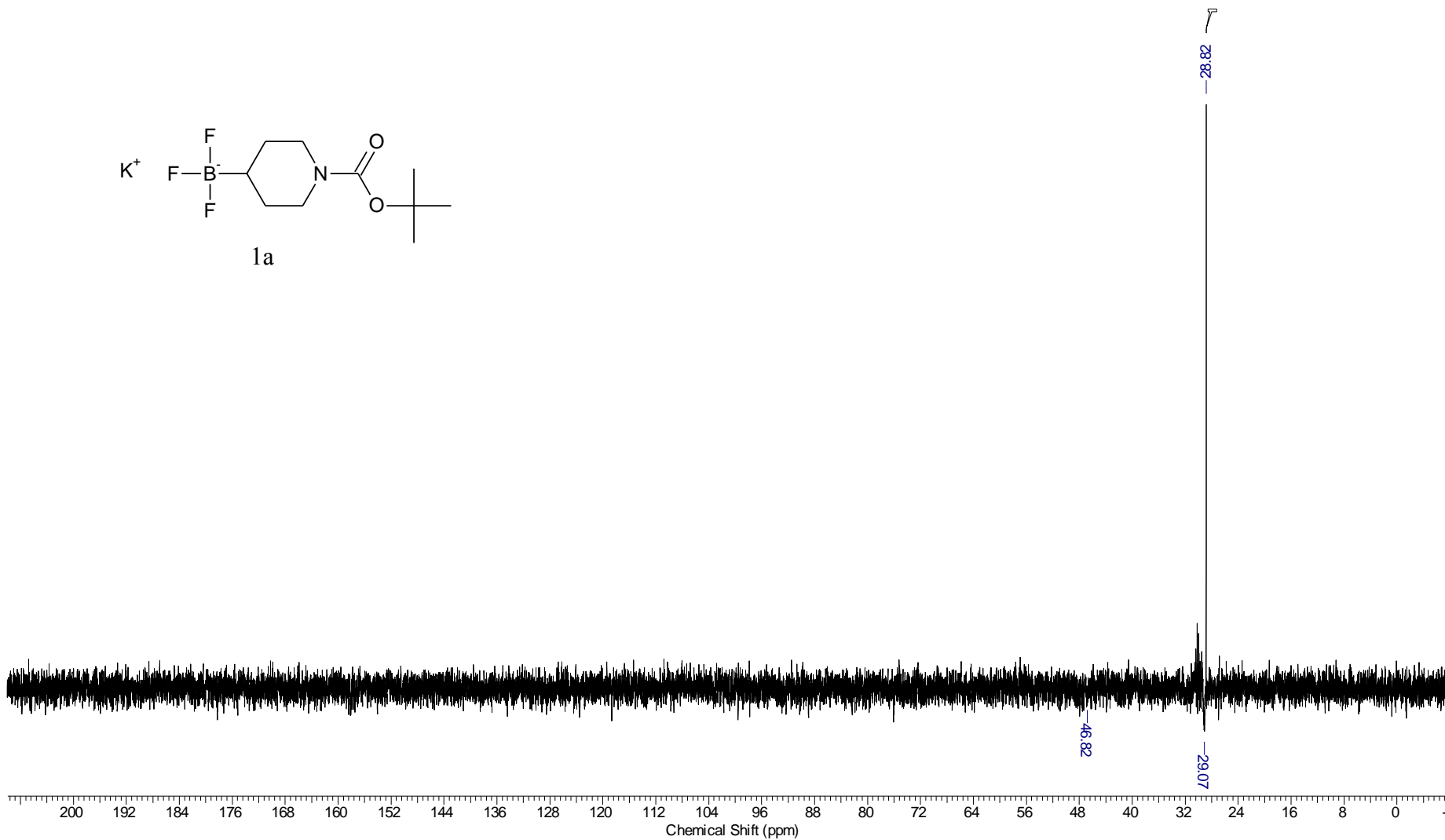
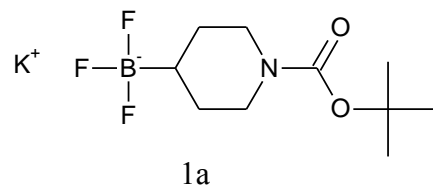
Frequency (MHz)	400.40	Nucleus	1H	Number of Transients	32	Origin	spect
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	Pulse Sequence	zg30
Receiver Gain	456.00	SW(cyclical) (Hz)	7211.54	Solvent	Acetone	Spectrum Offset (Hz)	3394.3101
Spectrum Type	STANDARD	Sweep Width (Hz)	7211.32	Temperature (degree C)	26.960		



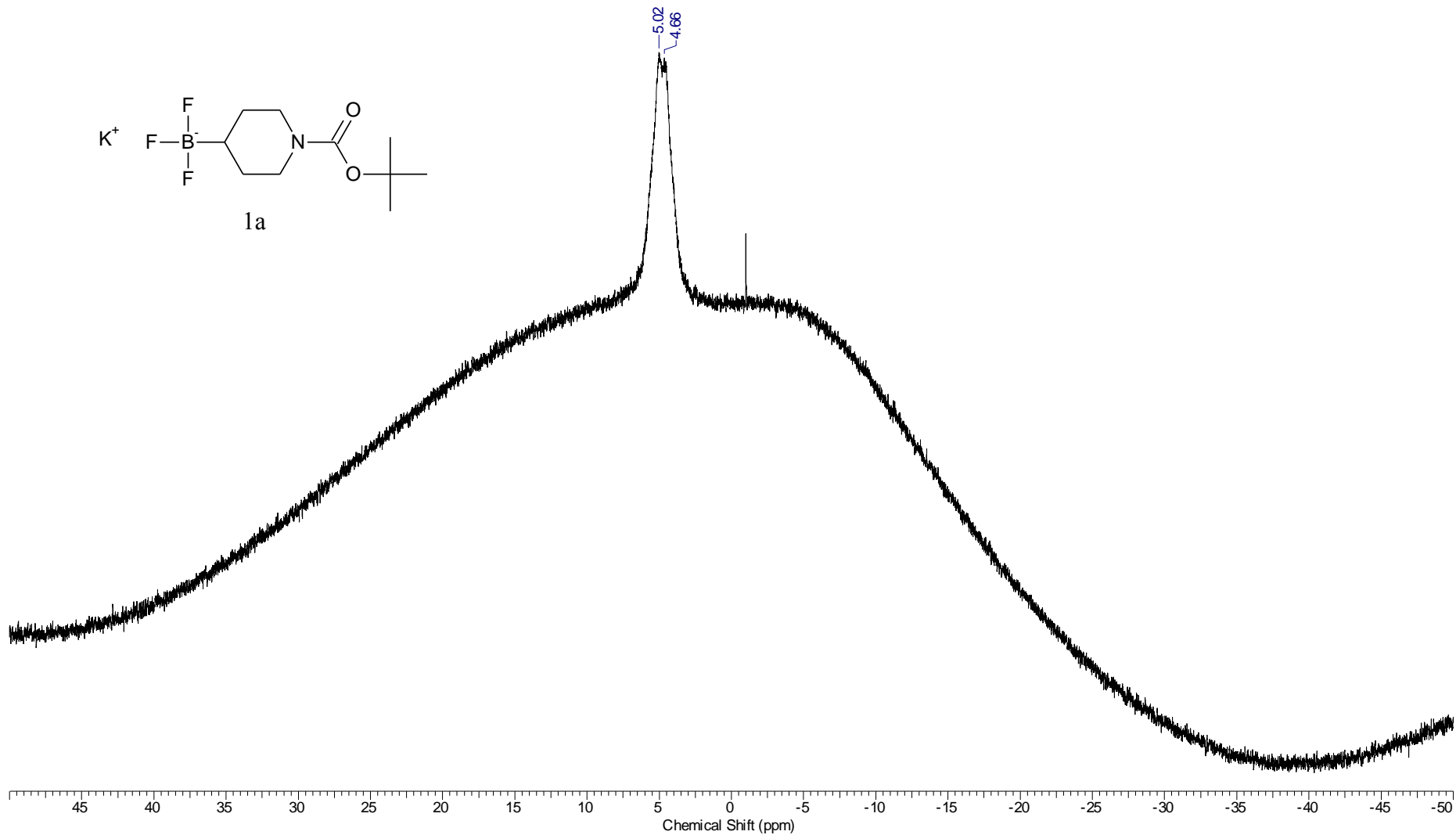
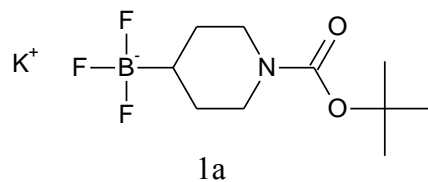
Frequency (MHz)	100.68	Nucleus	¹³ C	Number of Transients	1024	Origin	spect
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	Pulse Sequence	zgpg30
Receiver Gain	645.00	SW(cyclical) (Hz)	24038.46	Solvent	Acetone	Spectrum Offset (Hz)	10167.4873
Spectrum Type	STANDARD	Sweep Width (Hz)	24037.73	Temperature (degree C)	26.960		



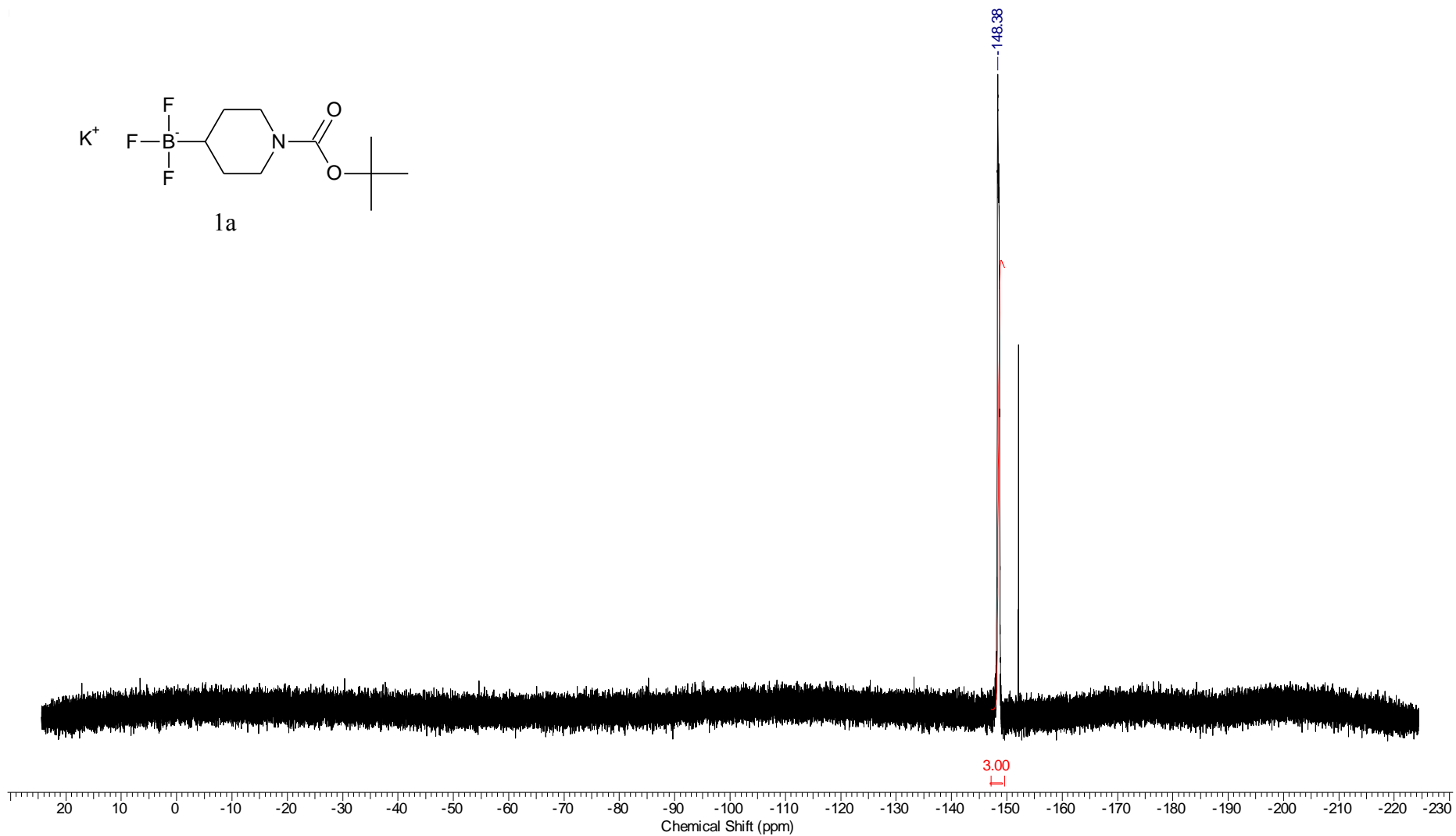
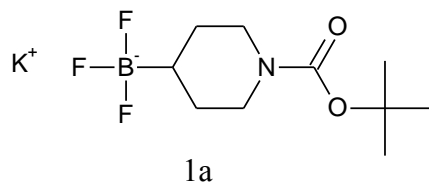
Frequency (MHz)	100.68	Nucleus	13C	Number of Transients	256	Origin	spect
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	Pulse Sequence	dept135
Receiver Gain	2050.00	SW(cyclical) (Hz)	24038.46	Solvent	Acetone	Spectrum Offset (Hz)	10167.5117
Spectrum Type	DEPT135	Sweep Width (Hz)	24037.73	Temperature (degree C)	26.960		



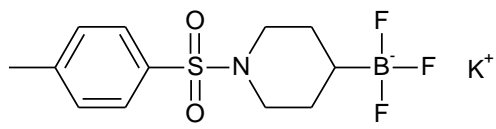
Frequency (MHz)	128.46	Nucleus	11B	Number of Transients	128	Origin	spect
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	Pulse Sequence	zg
Receiver Gain	812.00	SW(cyclical) (Hz)	25510.20	Solvent	Acetone	Spectrum Offset (Hz)	0.8954
Spectrum Type	STANDARD	Sweep Width (Hz)	25509.42	Temperature (degree C)	26.960		



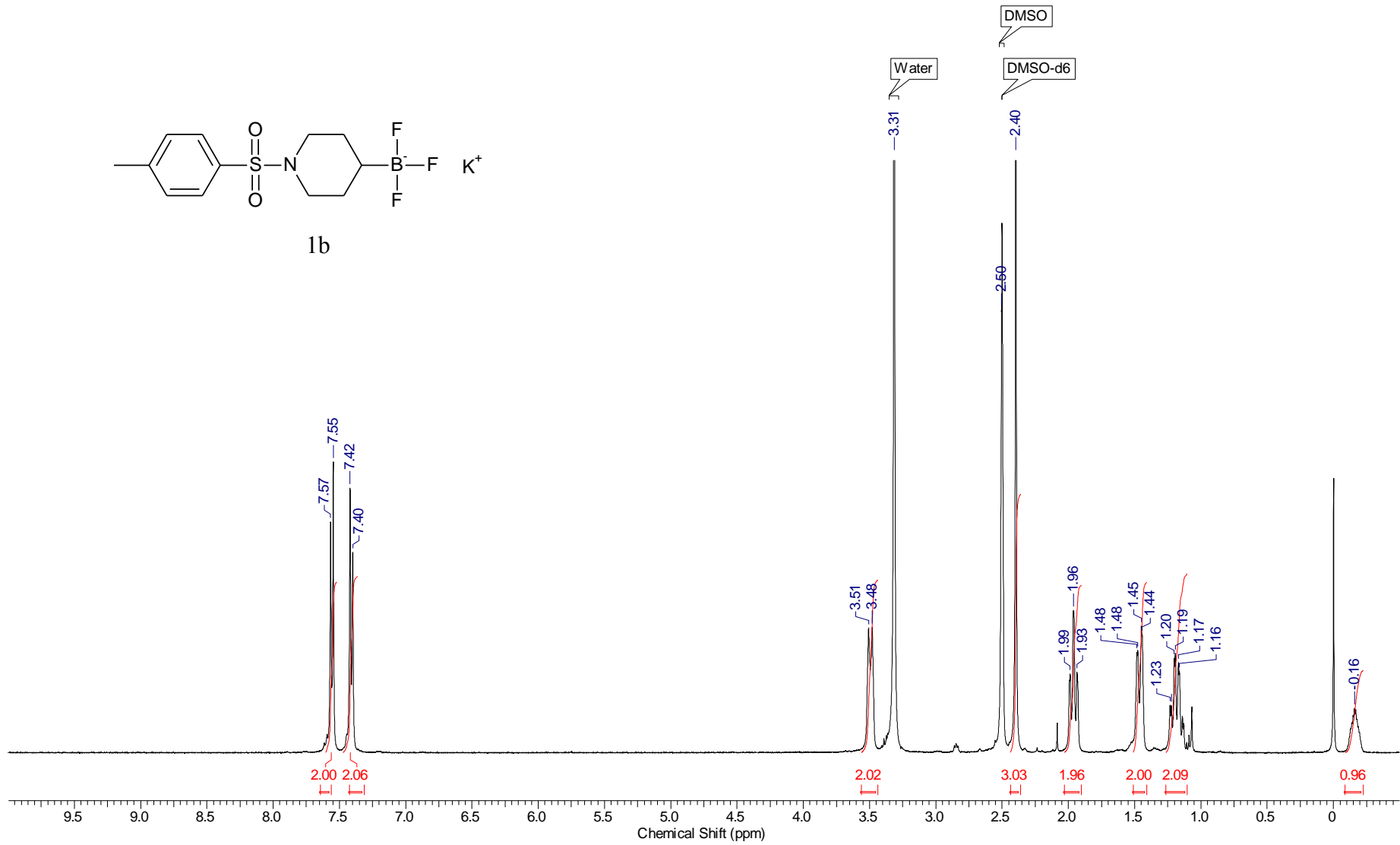
Frequency (MHz)	376.75	Nucleus	¹⁹ F	Number of Transients	64	Origin	spect
Original Points Count	133120	Owner	tibbe_operator	Points Count	131072	Pulse Sequence	zg30
Receiver Gain	2050.00	SW(cyclical) (Hz)	93750.00	Solvent	Acetone	Spectrum Offset (Hz)	-37674.1992
Spectrum Type	STANDARD	Sweep Width (Hz)	93749.28	Temperature (degree C)	26.960		



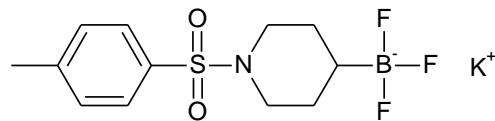
Frequency (MHz)	400.40	Nucleus	1H	Number of Transients	16	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	SW(cyclical) (Hz)	7211.32
Solvent	DMSO-d6	Spectrum Offset (Hz)	3398.3625	Sweep Width (Hz)	7211.10	Temperature (degree C)	27.000



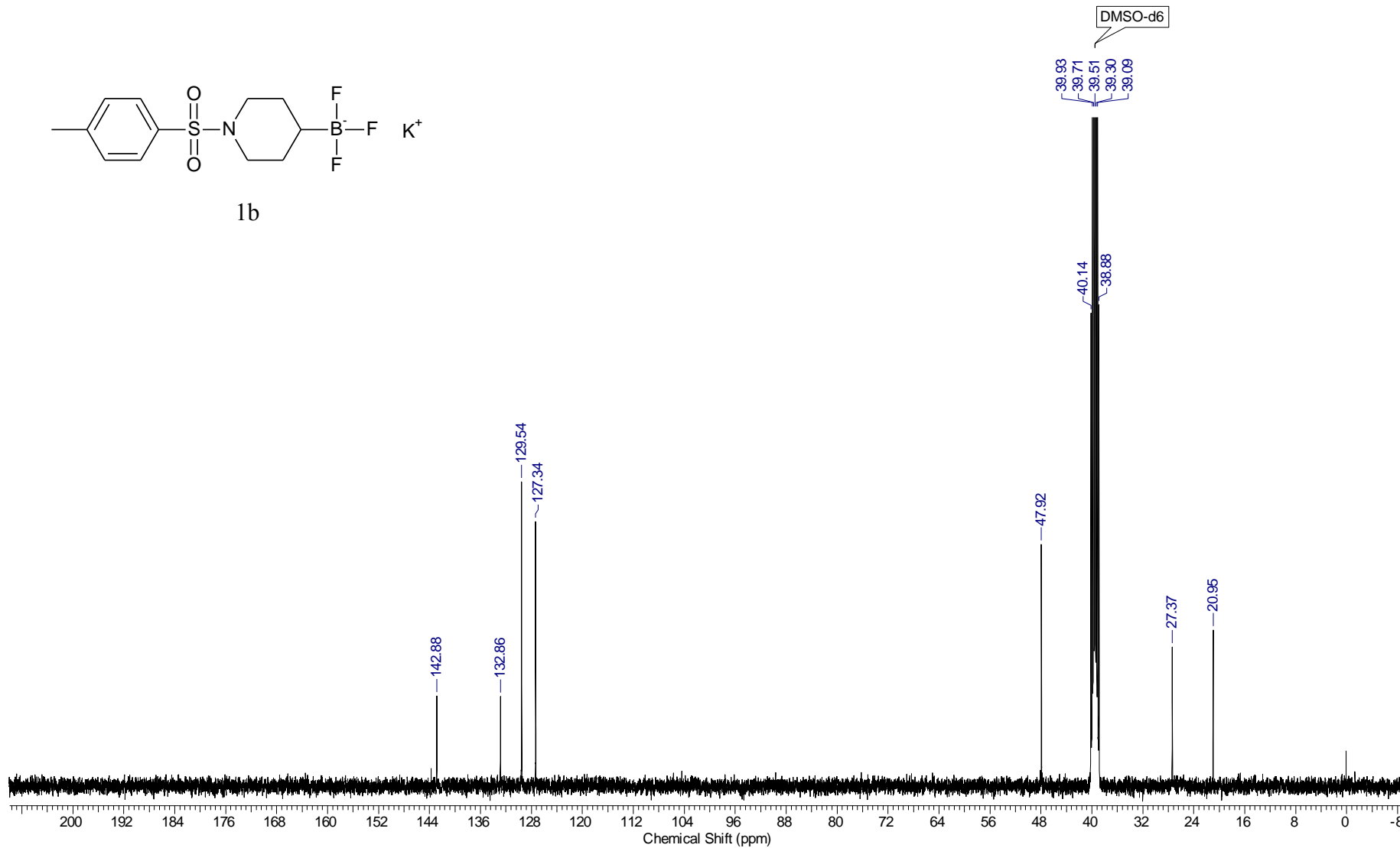
1b



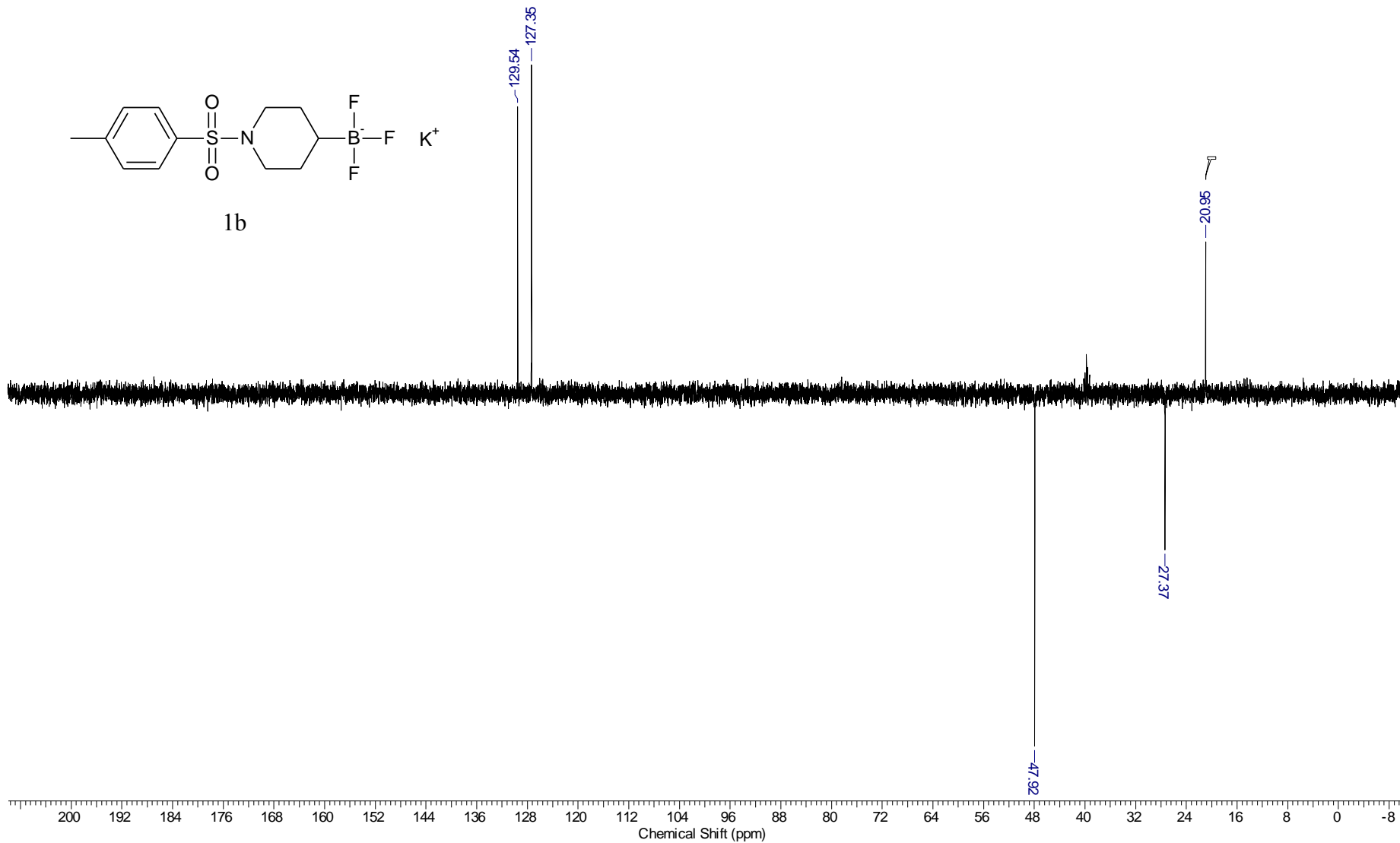
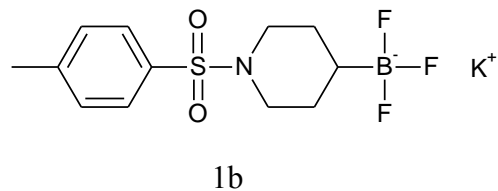
Frequency (MHz)	100.69	Nucleus	¹³ C	Number of Transients	1024	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	SW(cyclical) (Hz)	24037.73
Solvent	DMSO-d6	Spectrum Offset (Hz)	10016.6982	Sweep Width (Hz)	24036.99	Temperature (degree C)	27.000



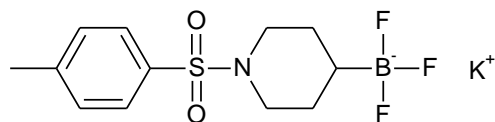
1b



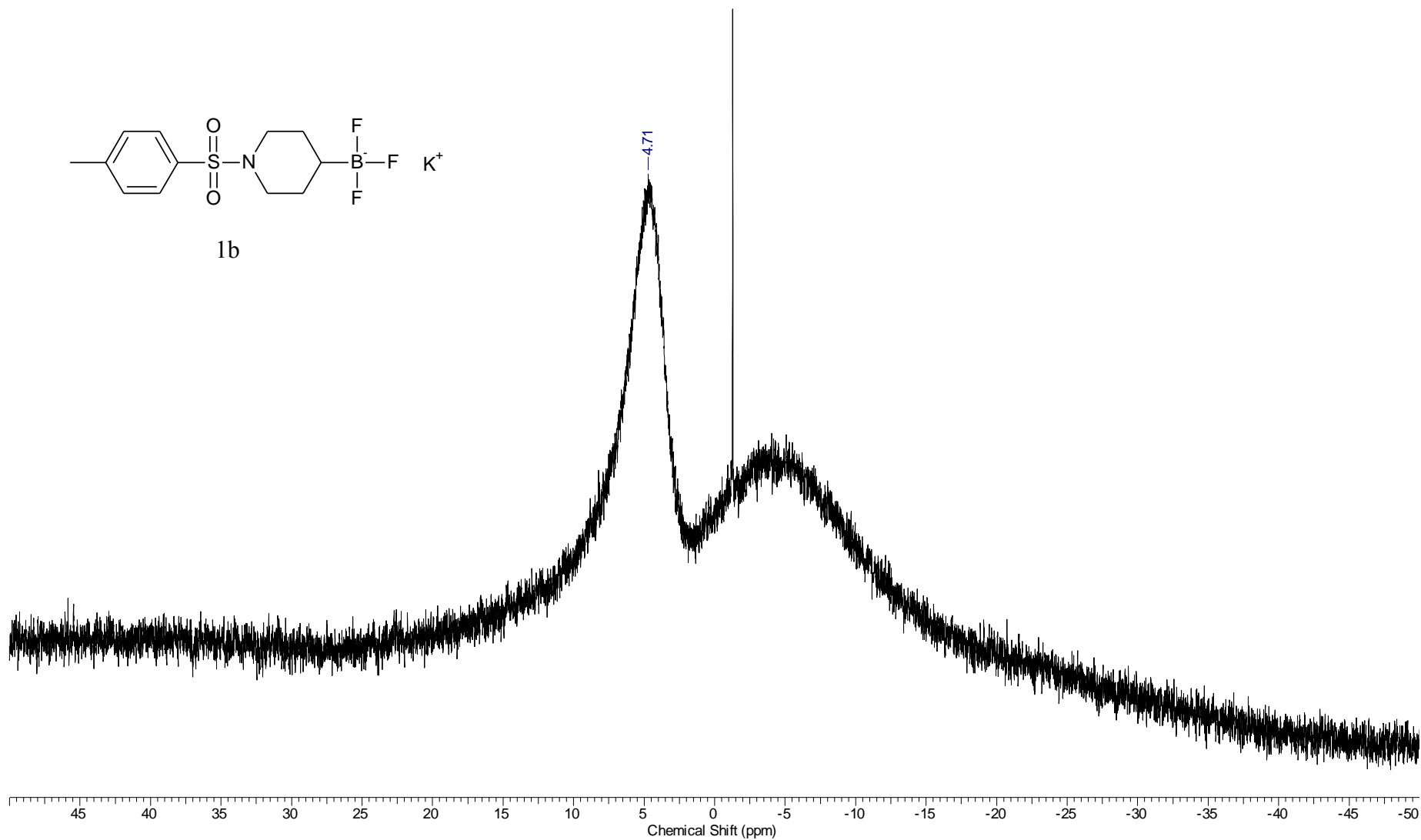
Frequency (MHz)	100.69	Nucleus	13C	Number of Transients	256	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	SW(cyclical) (Hz)	24037.73
Solvent	DMSO-d6	Spectrum Offset (Hz)	10016.2900	Sweep Width (Hz)	24036.99	Temperature (degree C)	27.000



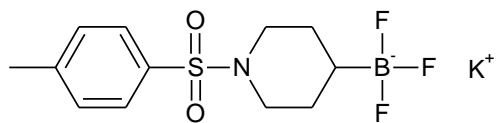
Frequency (MHz)	128.46	Nucleus	11B	Number of Transients	128	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	SW(cyclical) (Hz)	25509.43
Solvent	DMSO-d6	Spectrum Offset (Hz)	1.2842	Sweep Width (Hz)	25508.65	Temperature (degree C)	27.000



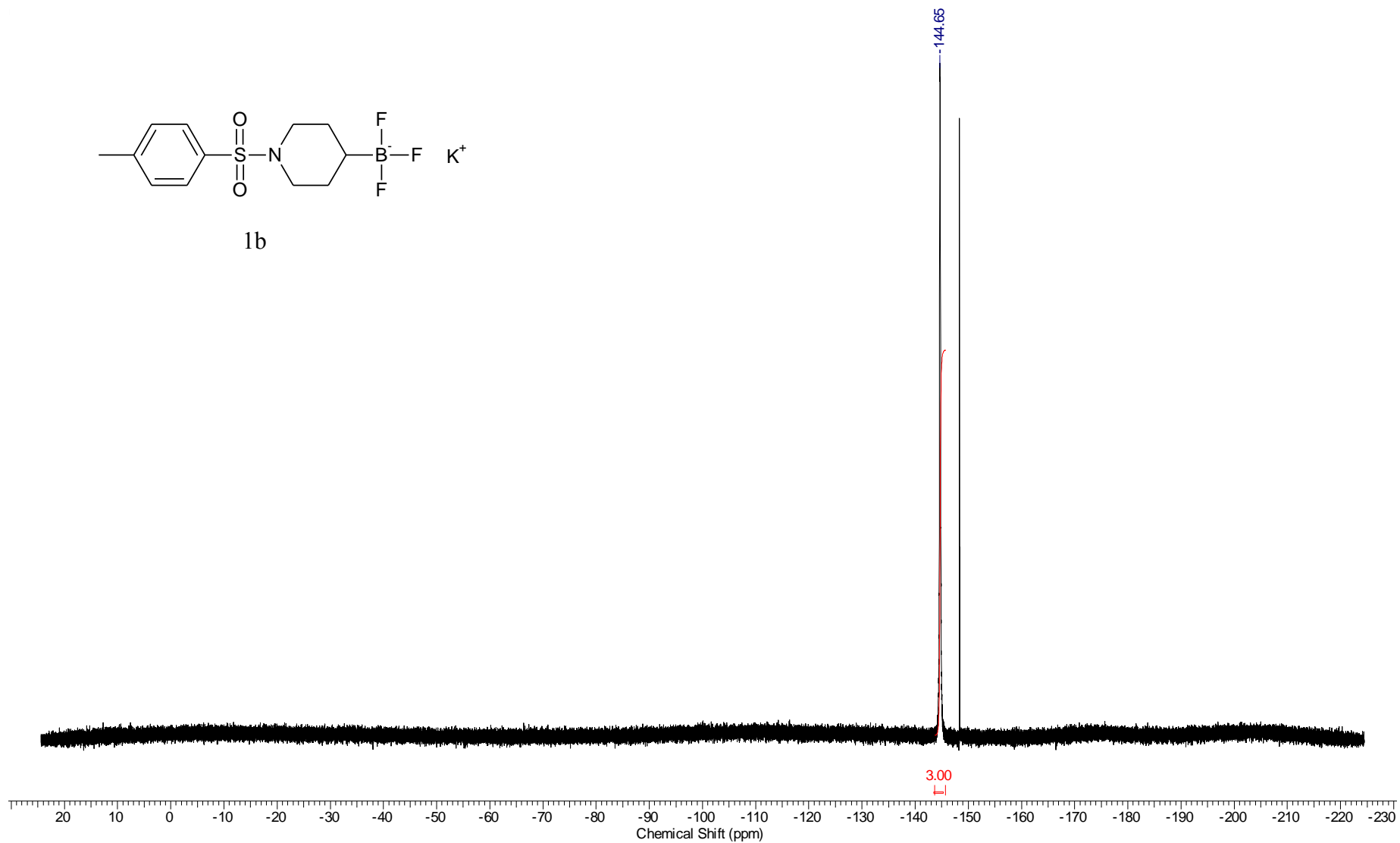
1b



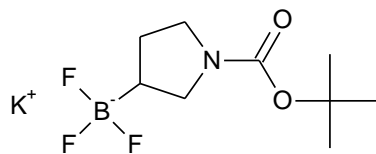
Frequency (MHz)	376.71	Nucleus	19F	Number of Transients	64	Origin	Bruker BioSpin GmbH
Original Points Count	131072	Owner	tibbe_operator	Points Count	131072	SW(cyclical) (Hz)	93749.28
Solvent	DMSO-d6	Spectrum Offset (Hz)	-37674.7617	Sweep Width (Hz)	93748.56	Temperature (degree C)	27.000



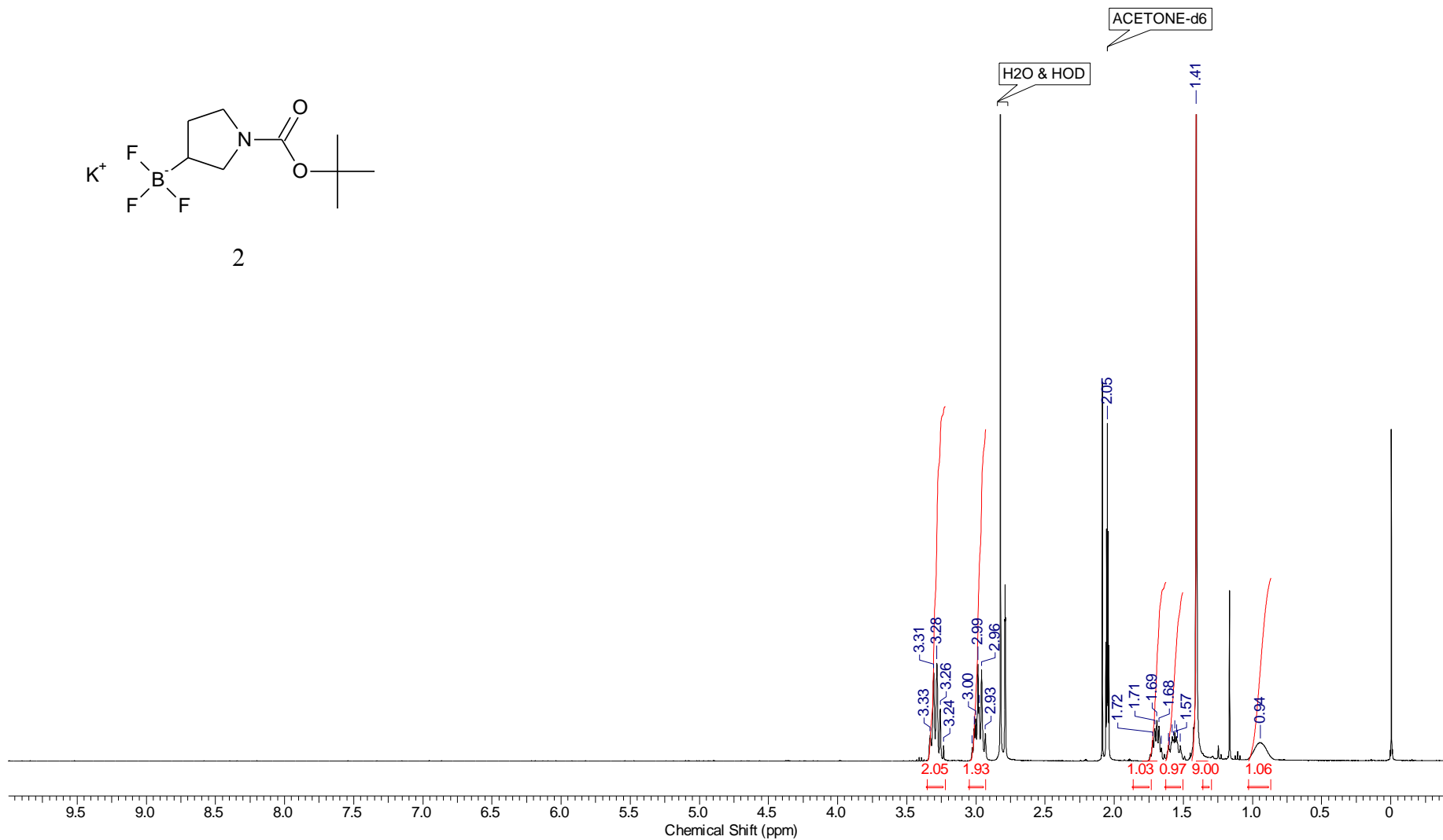
1b



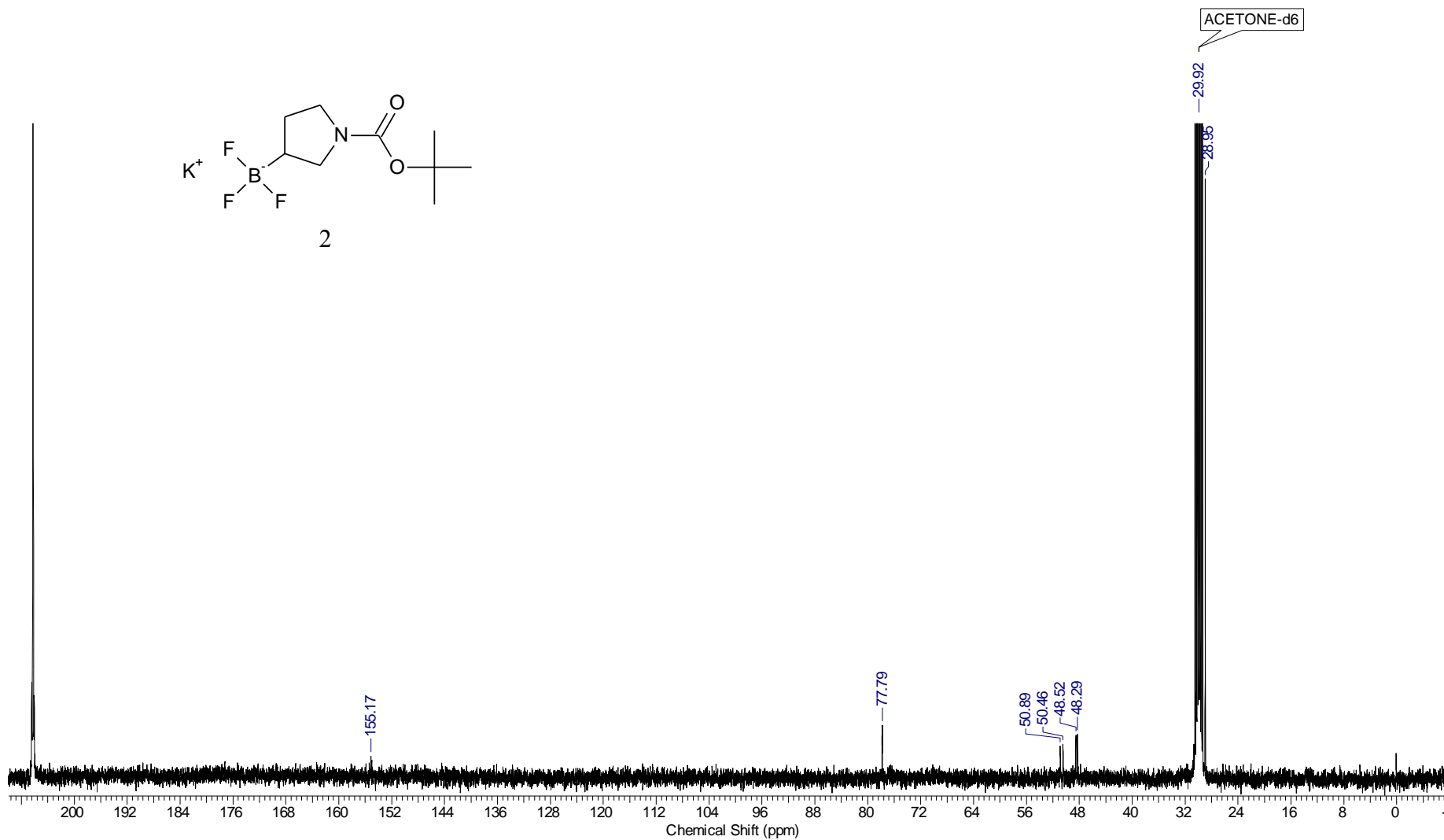
Frequency (MHz)	400.40	Nucleus	1H	Number of Transients	32	Origin	spect
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	Pulse Sequence	zg30
Receiver Gain	456.00	SW(cyclical) (Hz)	7211.54	Solvent	Acetone	Spectrum Offset (Hz)	3394.3101
Spectrum Type	STANDARD	Sweep Width (Hz)	7211.32	Temperature (degree C)	26.960		



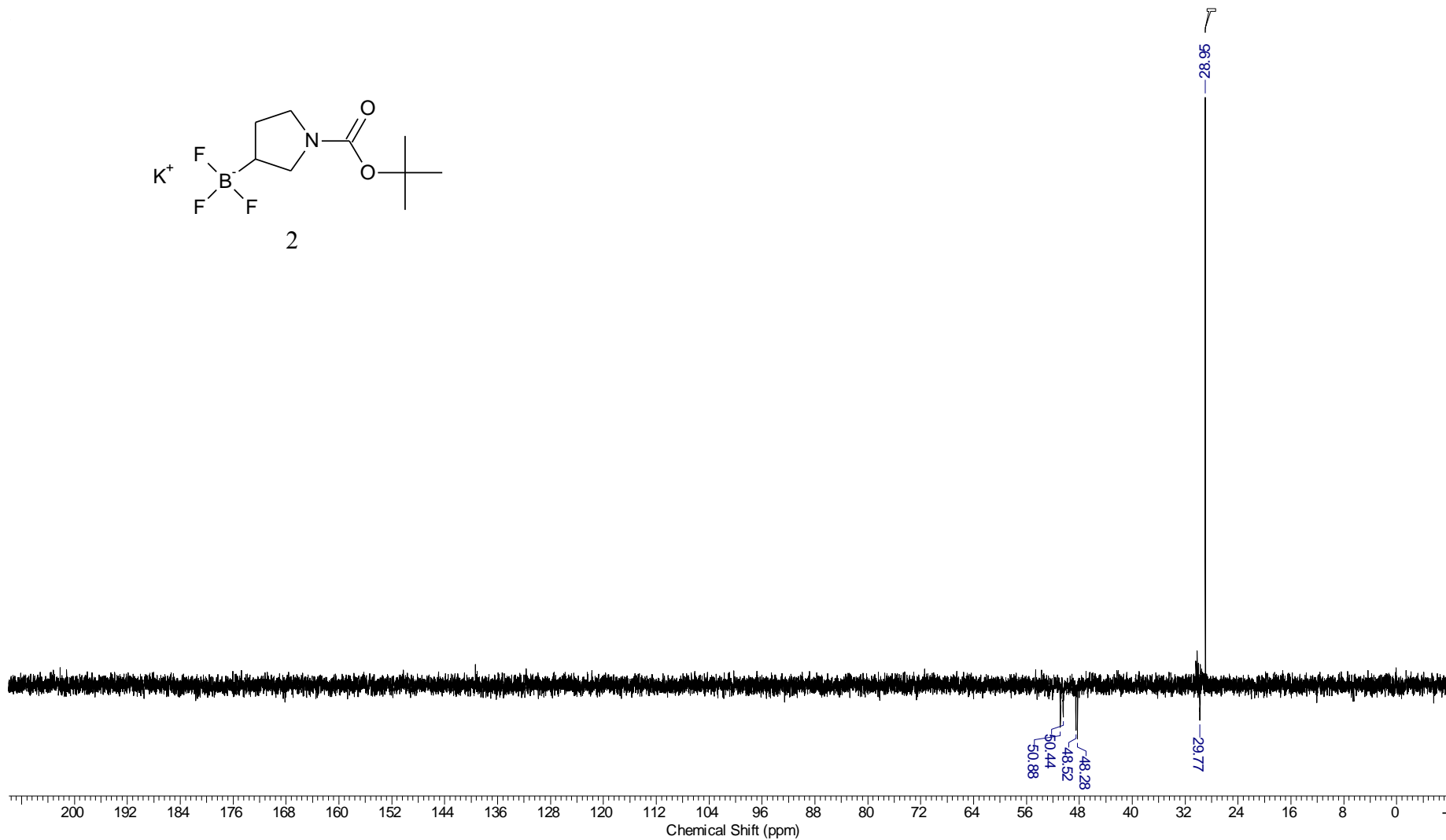
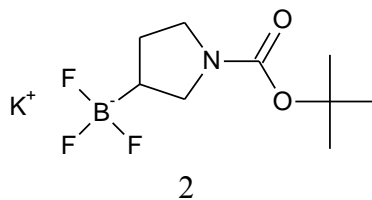
2



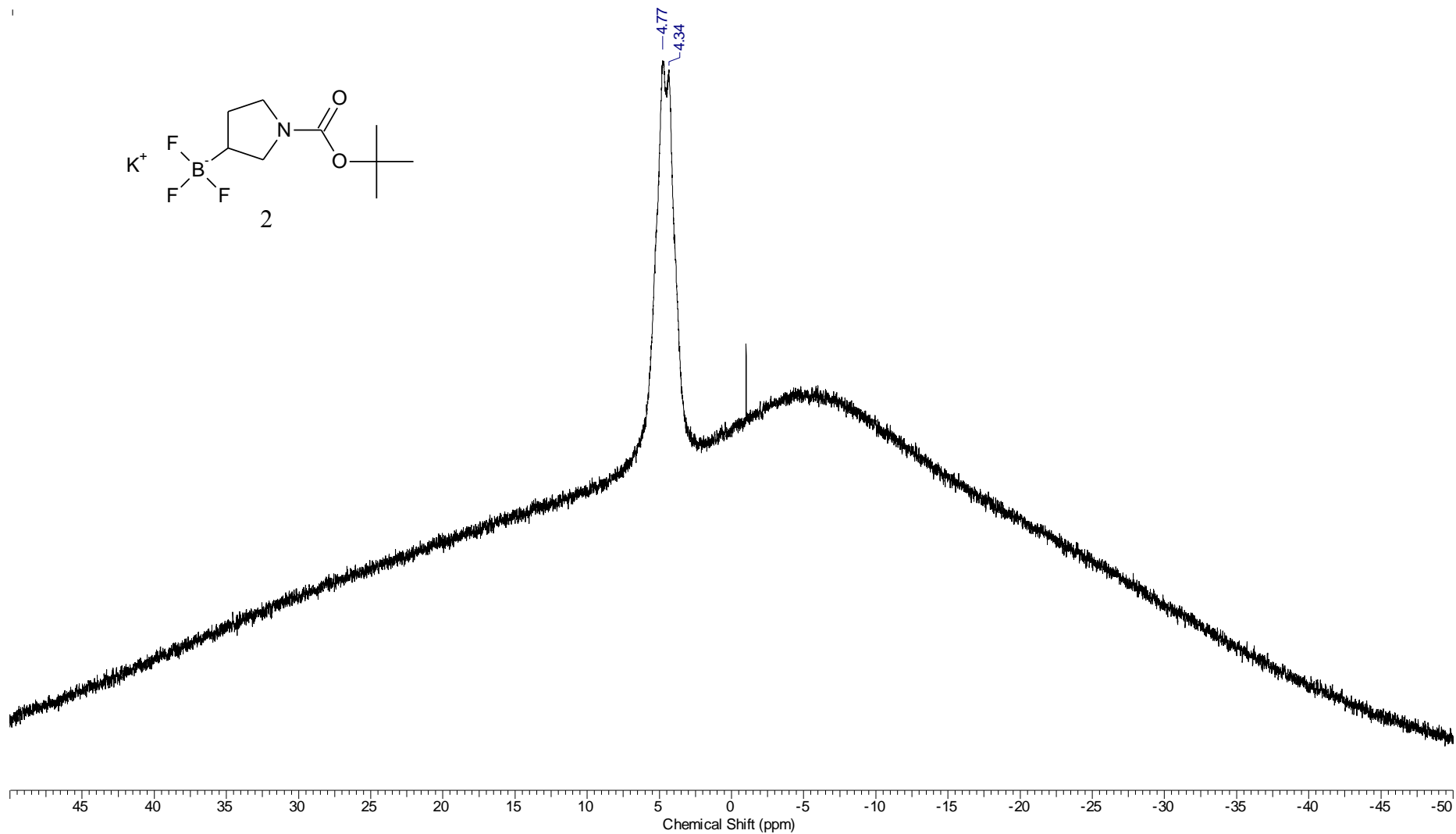
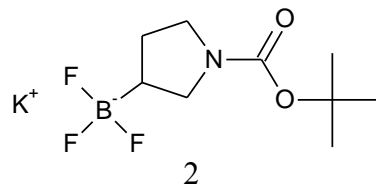
Frequency (MHz)	100.68	Nucleus	13C	Number of Transients	1024	Origin	spect
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	Pulse Sequence	zgpg30
Receiver Gain	912.00	SW(cyclical) (Hz)	24038.46	Solvent	Acetone	Spectrum Offset (Hz)	10166.7539
Spectrum Type	STANDARD	Sweep Width (Hz)	24037.73	Temperature (degree C)	26.960		



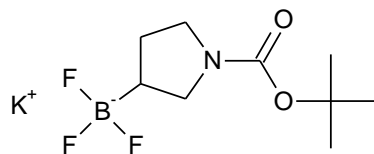
Frequency (MHz)	100.68	Nucleus	¹³ C	Number of Transients	256	Origin	spect
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	Pulse Sequence	dept135
Receiver Gain	2050.00	SW(cyclical) (Hz)	24038.46	Solvent	Acetone	Spectrum Offset (Hz)	10166.6621
Spectrum Type	DEPT135	Sweep Width (Hz)	24037.73	Temperature (degree C)	26.960		



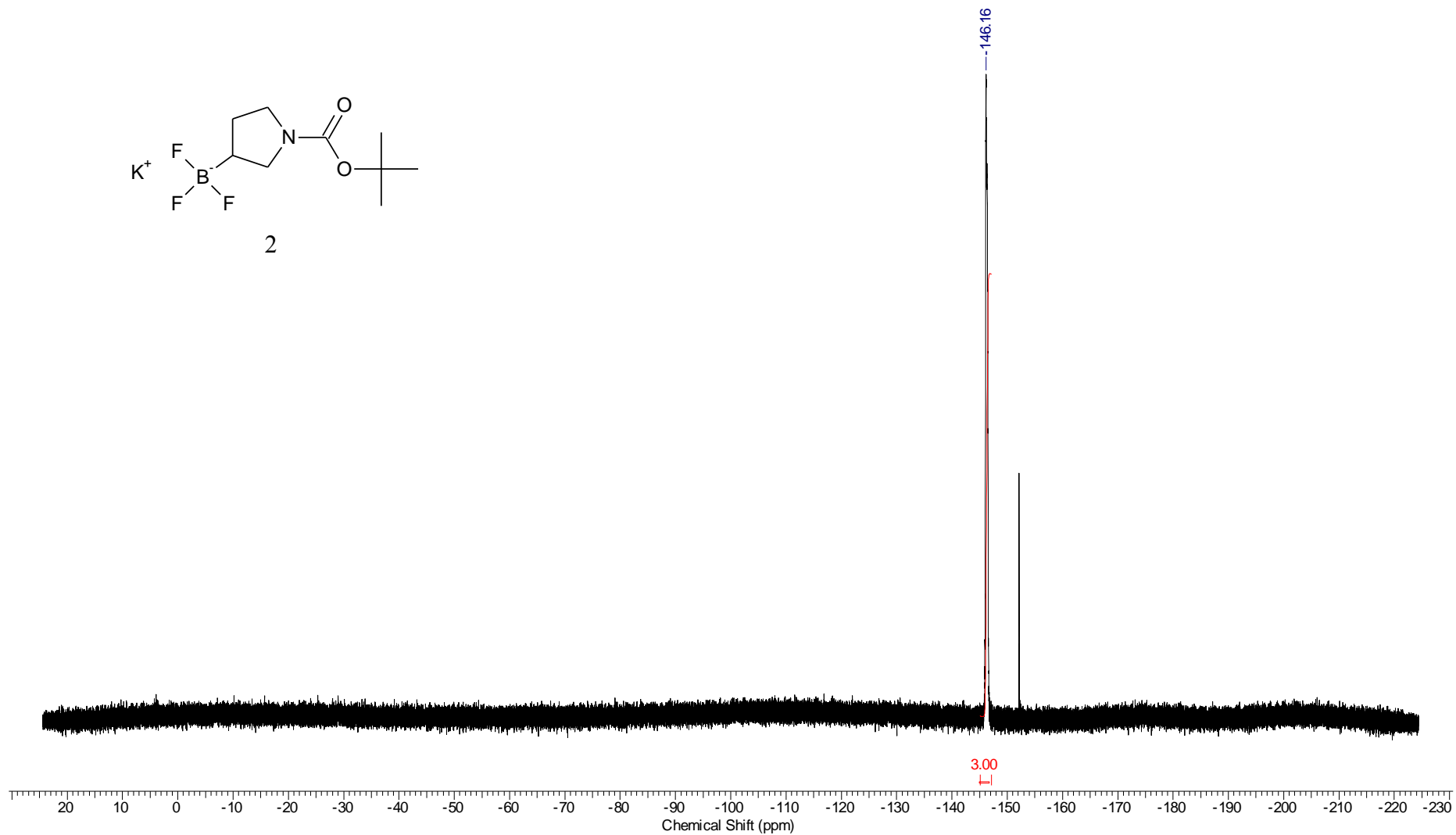
Frequency (MHz)	128.46	Nucleus	11B	Number of Transients	128	Origin	spect
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	Pulse Sequence	zg
Receiver Gain	812.00	SW(cyclical) (Hz)	25510.20	Solvent	Acetone	Spectrum Offset (Hz)	0.8954
Spectrum Type	STANDARD	Sweep Width (Hz)	25509.42	Temperature (degree C)	26.960		



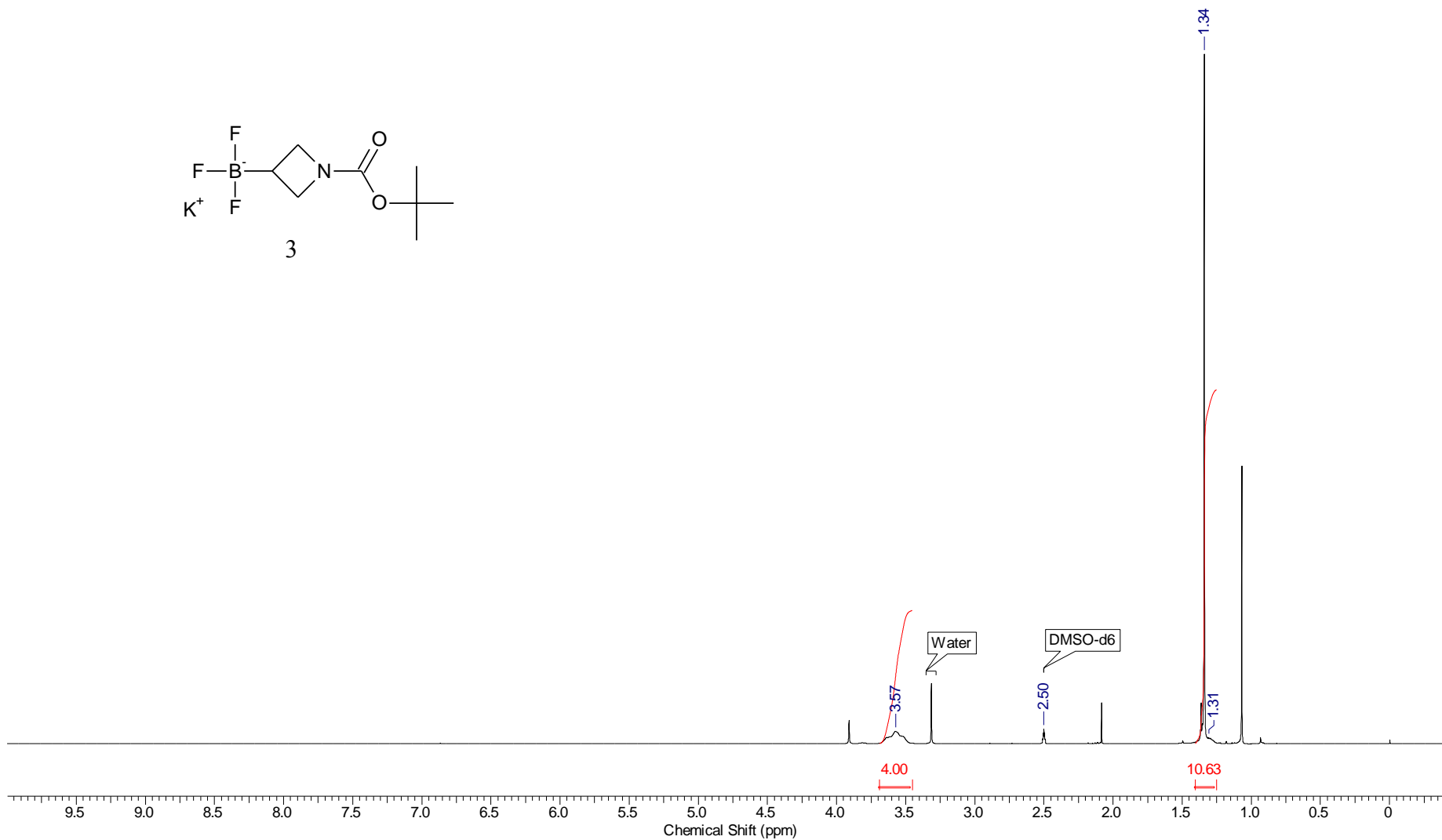
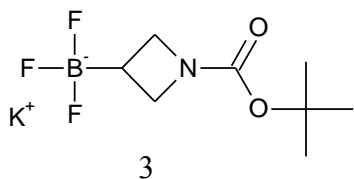
Frequency (MHz)	376.75	Nucleus	19F	Number of Transients	64	Origin	spect
Original Points Count	133120	Owner	tibbe_operator	Points Count	131072	Pulse Sequence	zg30
Receiver Gain	2050.00	SW(cyclical) (Hz)	93750.00	Solvent	Acetone	Spectrum Offset (Hz)	-37674.1992
Spectrum Type	STANDARD	Sweep Width (Hz)	93749.28	Temperature (degree C)	26.960		



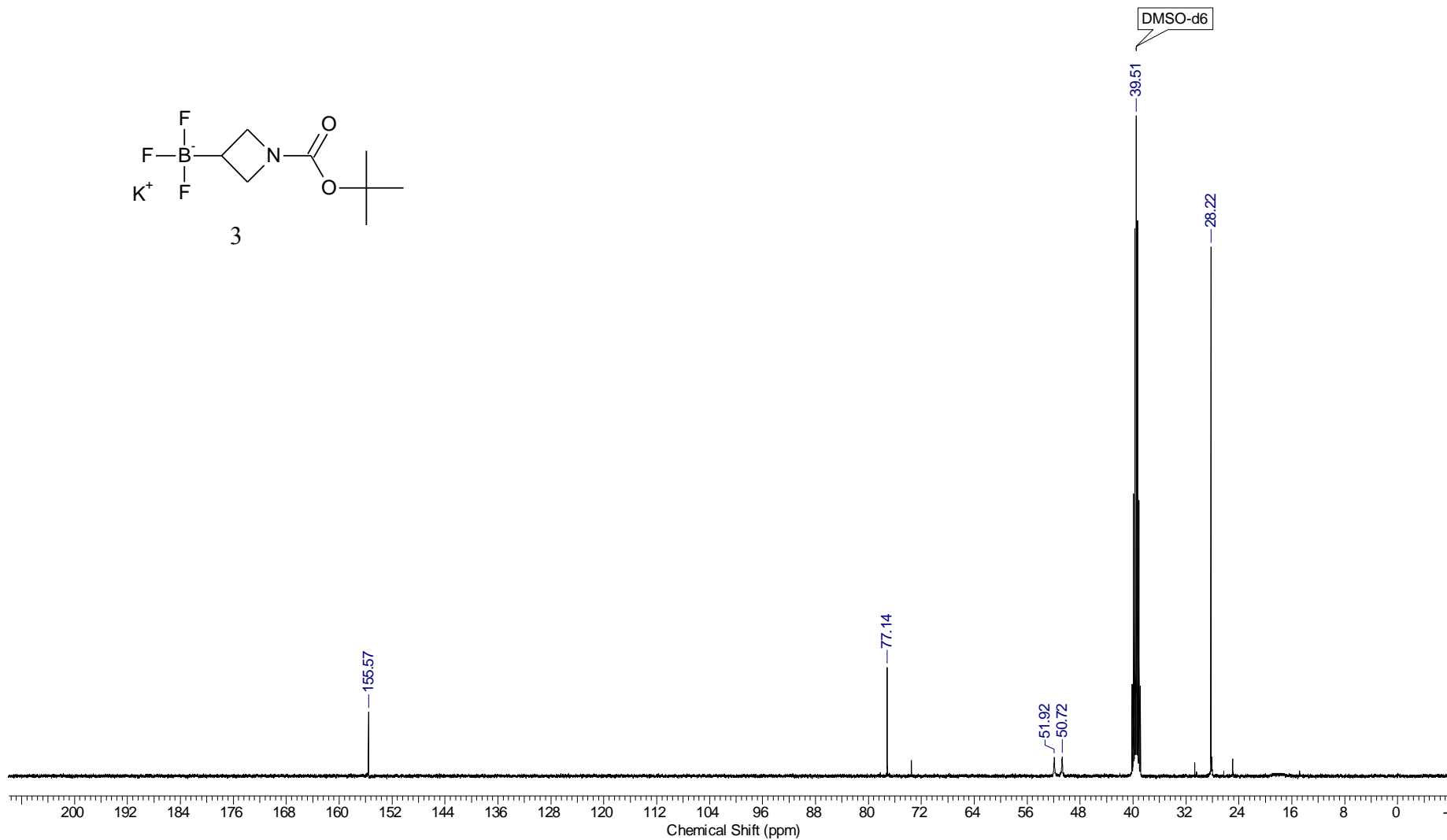
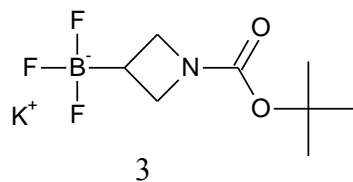
2



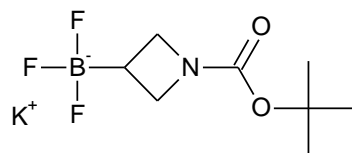
Frequency (MHz)	400.40	Nucleus	1H	Number of Transients	32	Origin	spect
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	Pulse Sequence	zg30
Receiver Gain	114.00	SW(cyclical) (Hz)	7211.54	Solvent	DMSO-d6	Spectrum Offset (Hz)	3398.2070
Spectrum Type	STANDARD	Sweep Width (Hz)	7211.32	Temperature (degree C)	27.000		



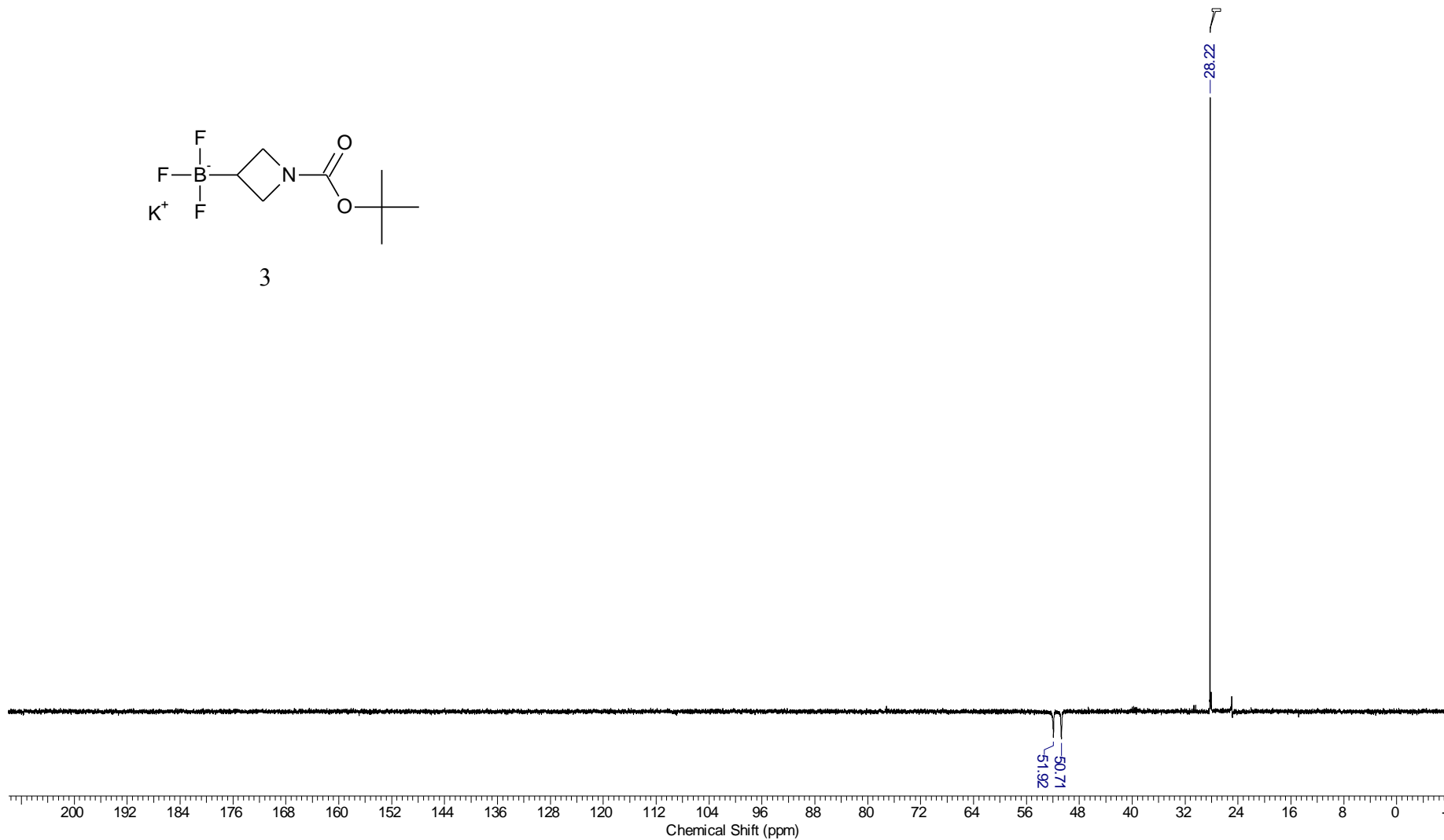
Frequency (MHz)	100.68	Nucleus	¹³ C	Number of Transients	1024	Origin	spect
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	Pulse Sequence	zgpg30
Receiver Gain	575.00	SW(cyclical) (Hz)	24038.46	Solvent	DMSO-d6	Spectrum Offset (Hz)	10018.6875
Spectrum Type	STANDARD	Sweep Width (Hz)	24037.73	Temperature (degree C)	27.000		



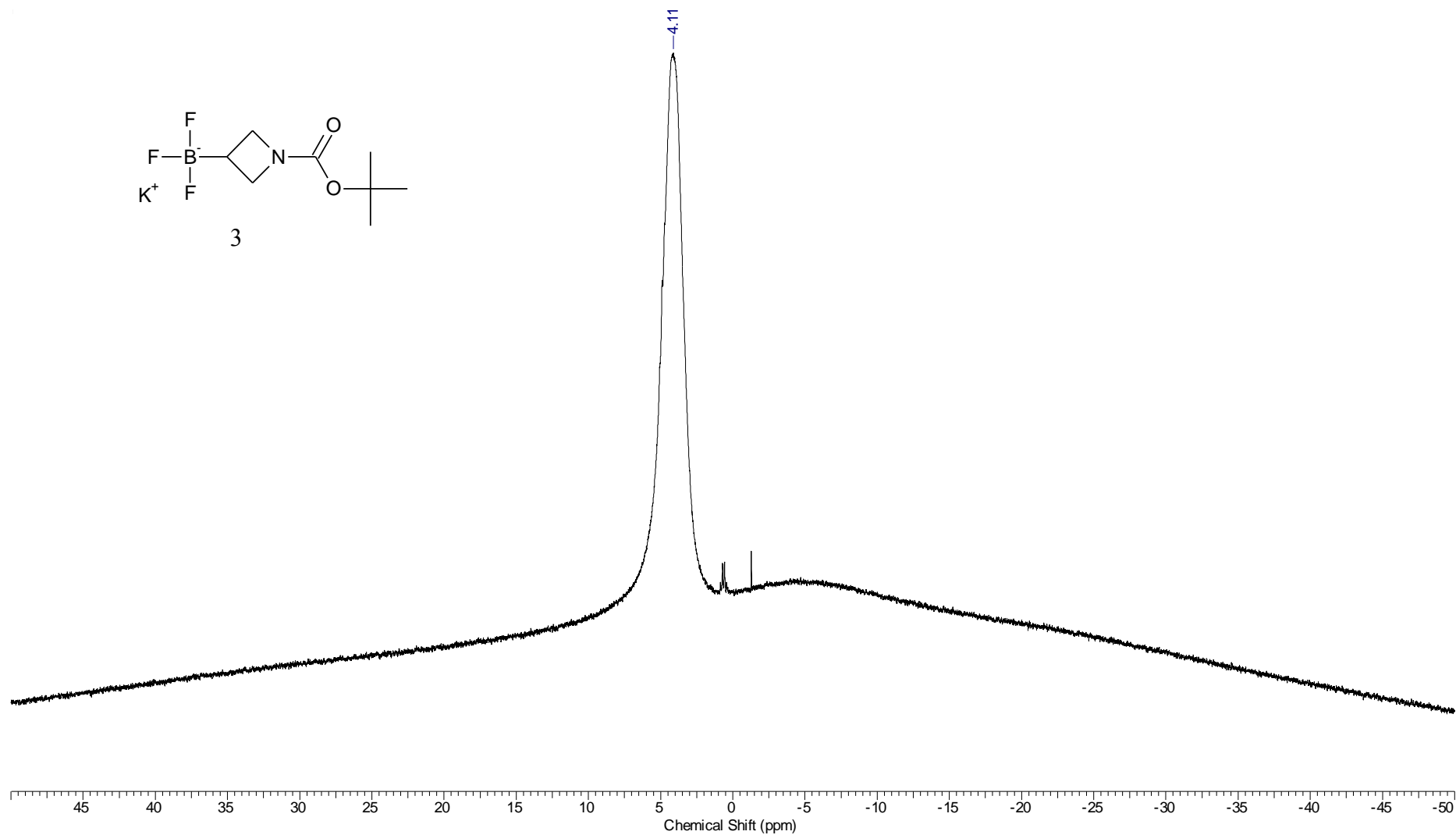
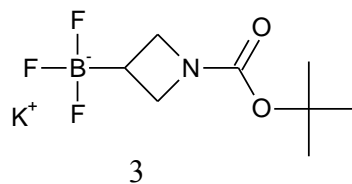
Frequency (MHz)	100.68	Nucleus	¹³ C	Number of Transients	256	Origin	spect
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	Pulse Sequence	dept135
Receiver Gain	2050.00	SW(cyclical) (Hz)	24038.46	Solvent	DMSO-d6	Spectrum Offset (Hz)	10019.0752
Spectrum Type	DEPT135	Sweep Width (Hz)	24037.73	Temperature (degree C)	27.000		



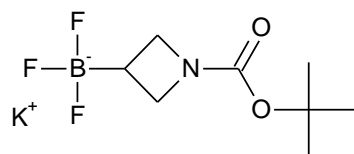
3



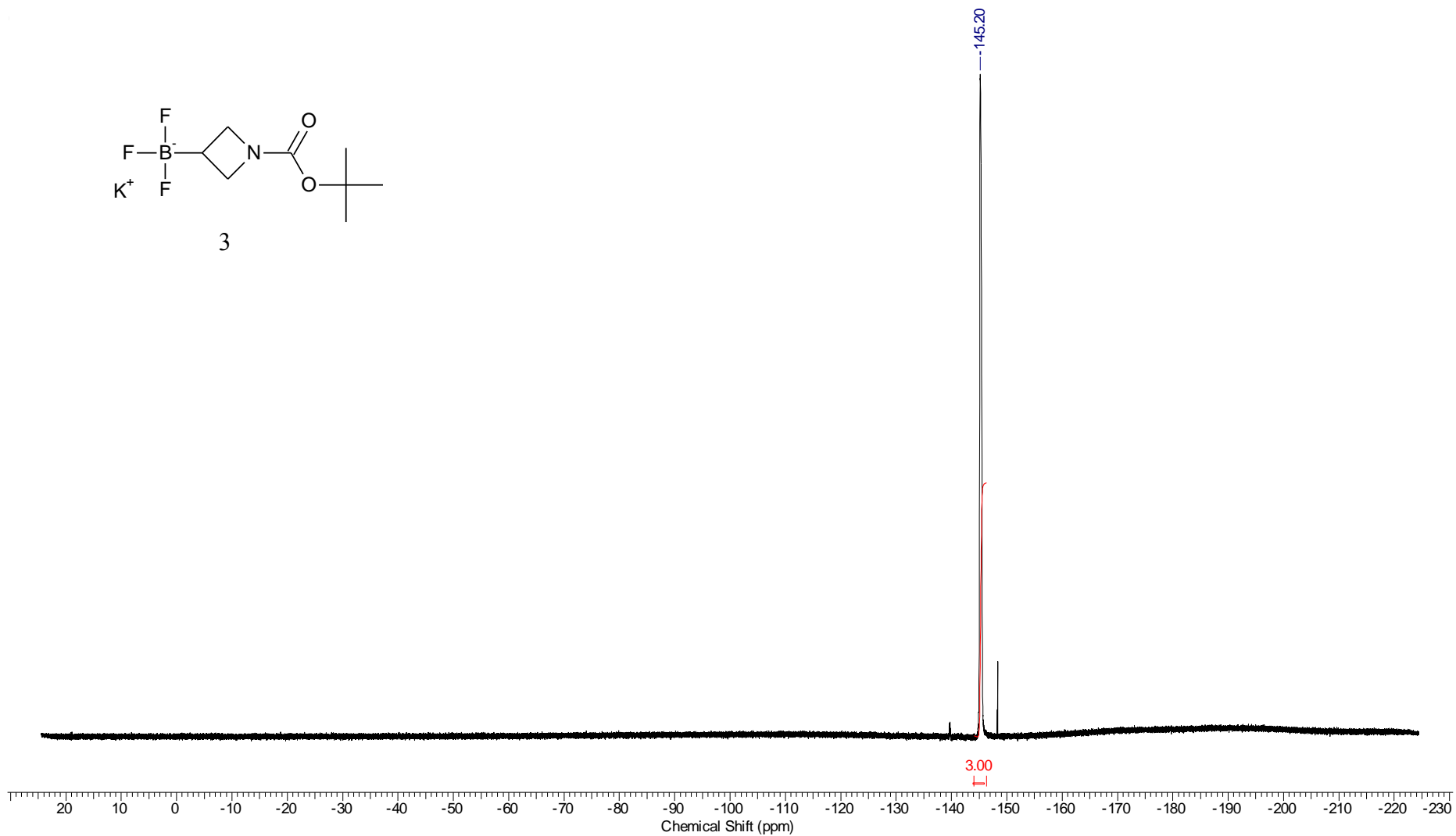
Frequency (MHz)	128.46	Nucleus	11B	Number of Transients	128	Origin	spect
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	Pulse Sequence	zg
Receiver Gain	724.00	SW(cyclical) (Hz)	25510.20	Solvent	DMSO-d6	Spectrum Offset (Hz)	0.8954
Spectrum Type	STANDARD	Sweep Width (Hz)	25509.42	Temperature (degree C)	27.000		



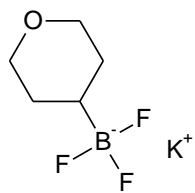
Frequency (MHz)	376.75	Nucleus	19F	Number of Transients	64	Origin	spect
Original Points Count	133120	Owner	tibbe_operator	Points Count	131072	Pulse Sequence	zg30
Receiver Gain	1820.00	SW(cyclical) (Hz)	93750.00	Solvent	DMSO-d6	Spectrum Offset (Hz)	-37674.1992
Spectrum Type	STANDARD	Sweep Width (Hz)	93749.28	Temperature (degree C)	27.000		



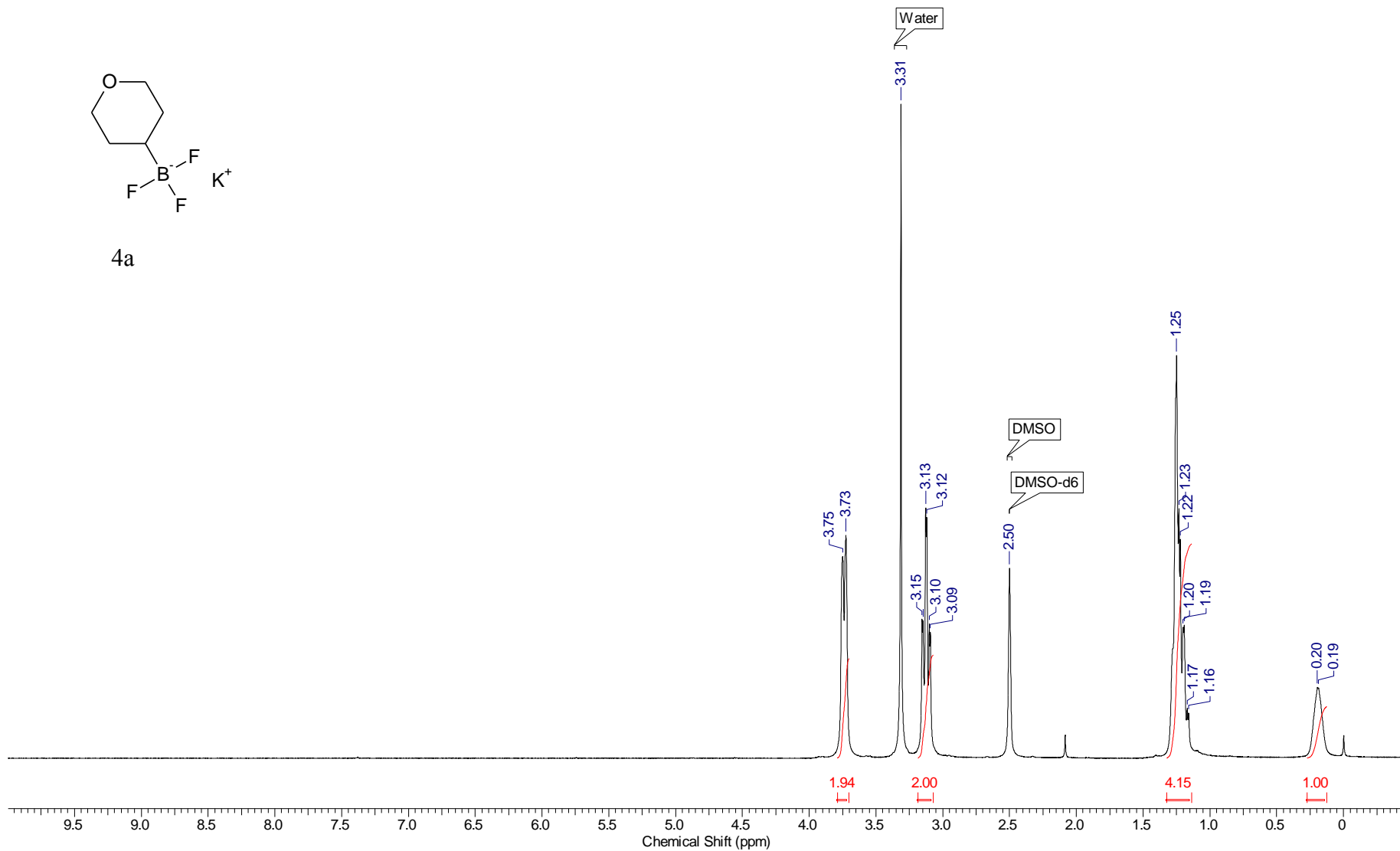
3



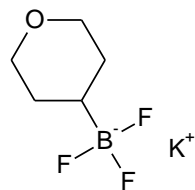
Frequency (MHz)	400.40	Nucleus	1H	Number of Transients	16	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	SW(cyclical) (Hz)	7211.32
Solvent	DMSO-d6	Spectrum Offset (Hz)	3398.5825	Sweep Width (Hz)	7211.10	Temperature (degree C)	27.000



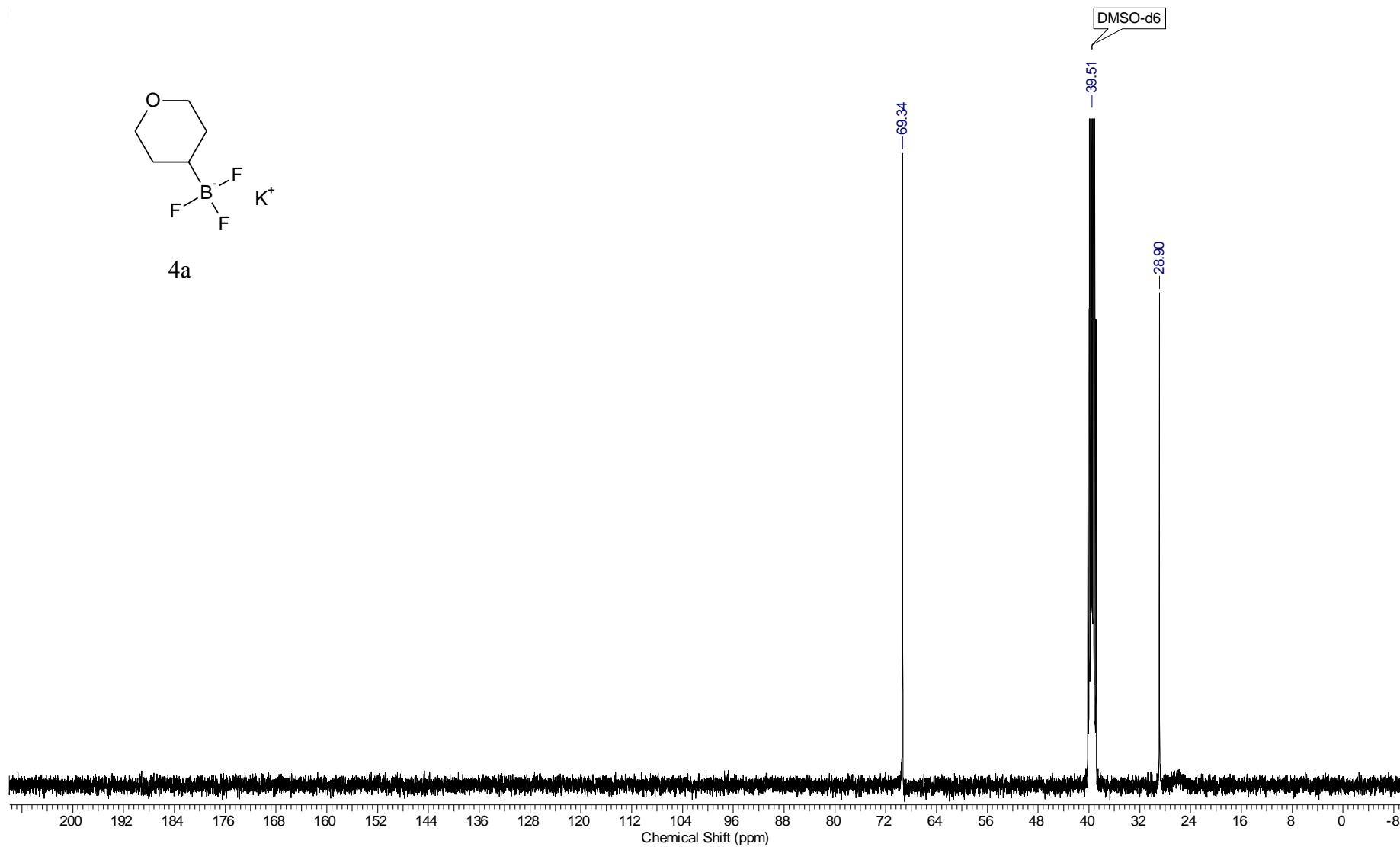
4a



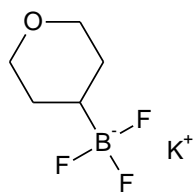
Frequency (MHz)	100.69	Nucleus	¹³ C	Number of Transients	1024	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	SW(cyclical) (Hz)	24037.73
Solvent	DMSO-d6	Spectrum Offset (Hz)	10018.1660	Sweep Width (Hz)	24036.99	Temperature (degree C)	27.000



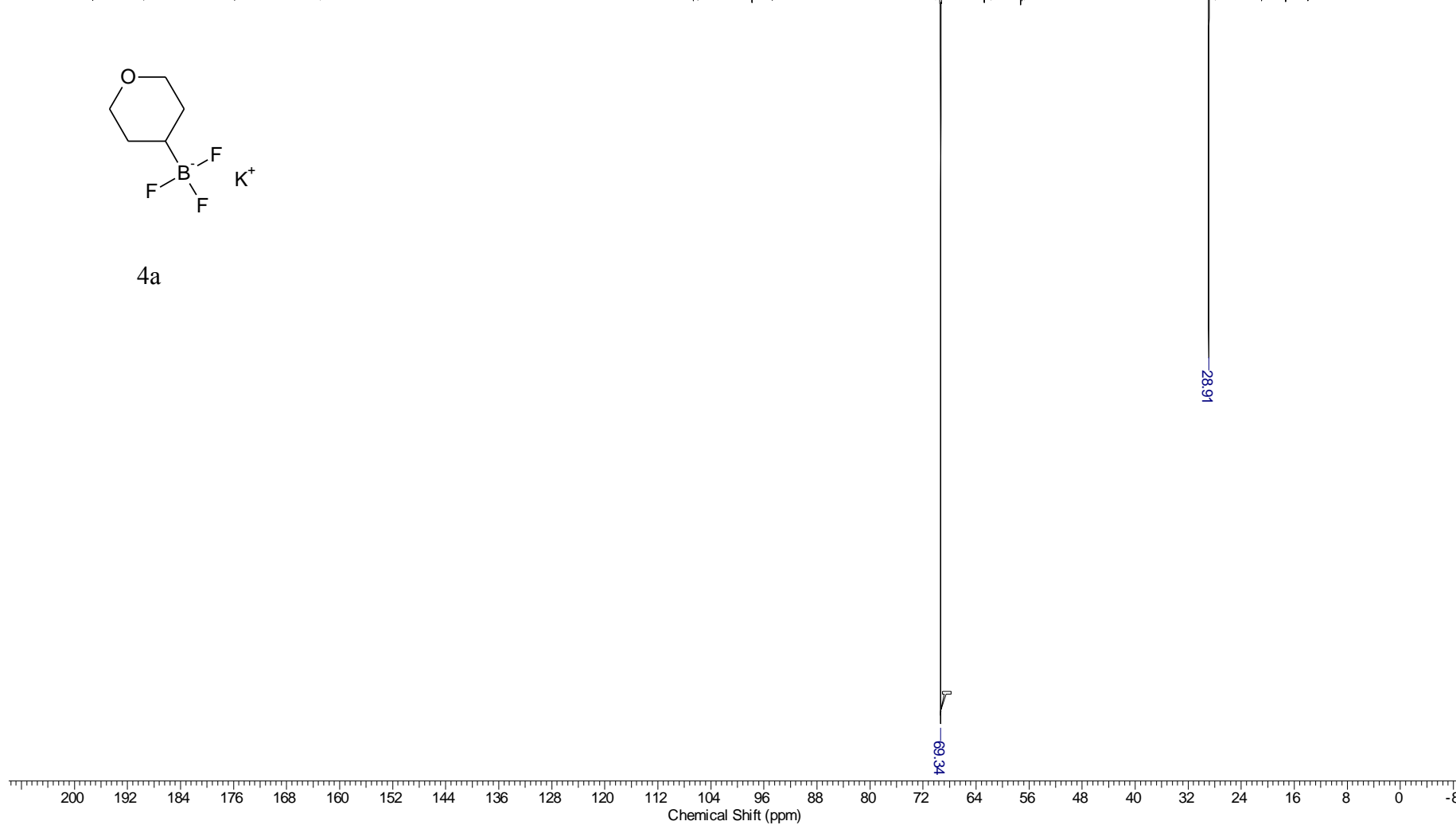
4a



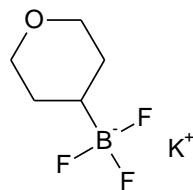
Frequency (MHz)	100.69	Nucleus	¹³ C	Number of Transients	256	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	SW(cyclical) (Hz)	24037.73
Solvent	DMSO-d6	Spectrum Offset (Hz)	10018.5215	Sweep Width (Hz)	24036.99	Temperature (degree C)	27.000



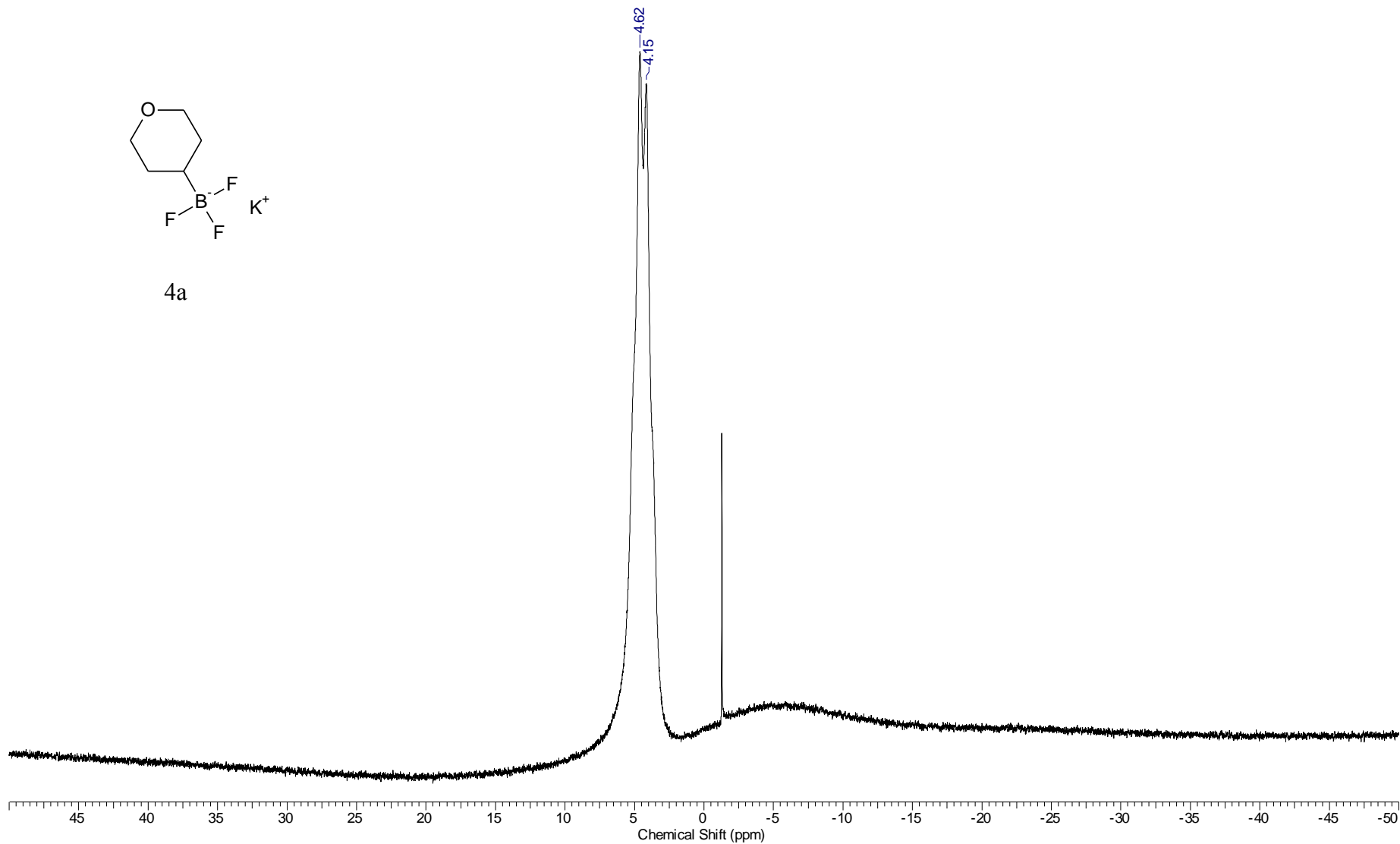
4a



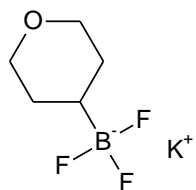
Frequency (MHz)	128.46	Nucleus	11B	Number of Transients	128	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	SW(cyclical) (Hz)	25509.43
Solvent	DMSO-d6	Spectrum Offset (Hz)	1.2842	Sweep Width (Hz)	25508.65	Temperature (degree C)	27.000



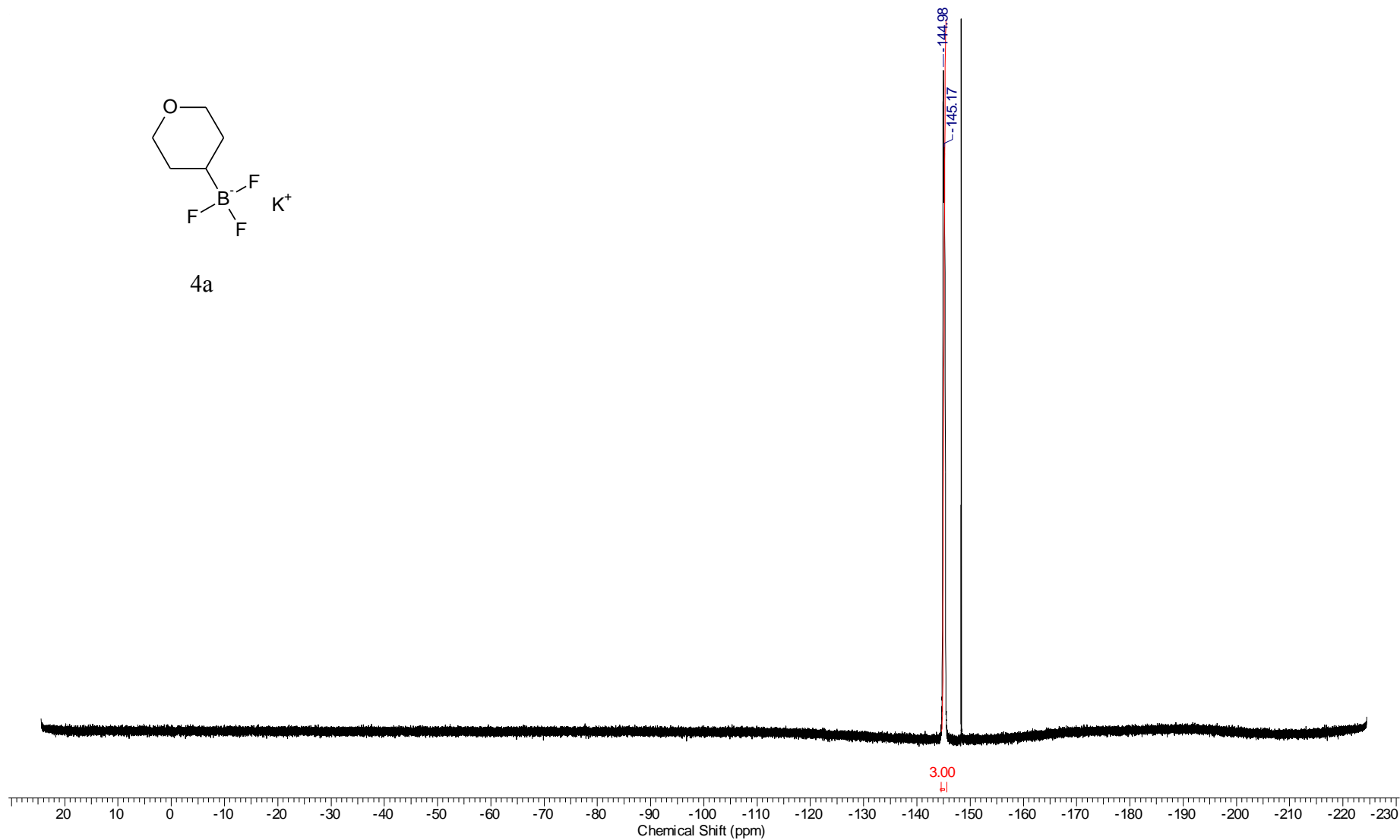
4a



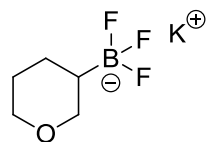
Frequency (MHz)	376.71	Nucleus	19F	Number of Transients	64	Origin	Bruker BioSpin GmbH
Original Points Count	131072	Owner	tibbe_operator	Points Count	131072	SW(cyclical) (Hz)	93749.28
Solvent	DMSO-d6	Spectrum Offset (Hz)	-37674.7617	Sweep Width (Hz)	93748.56	Temperature (degree C)	27.000



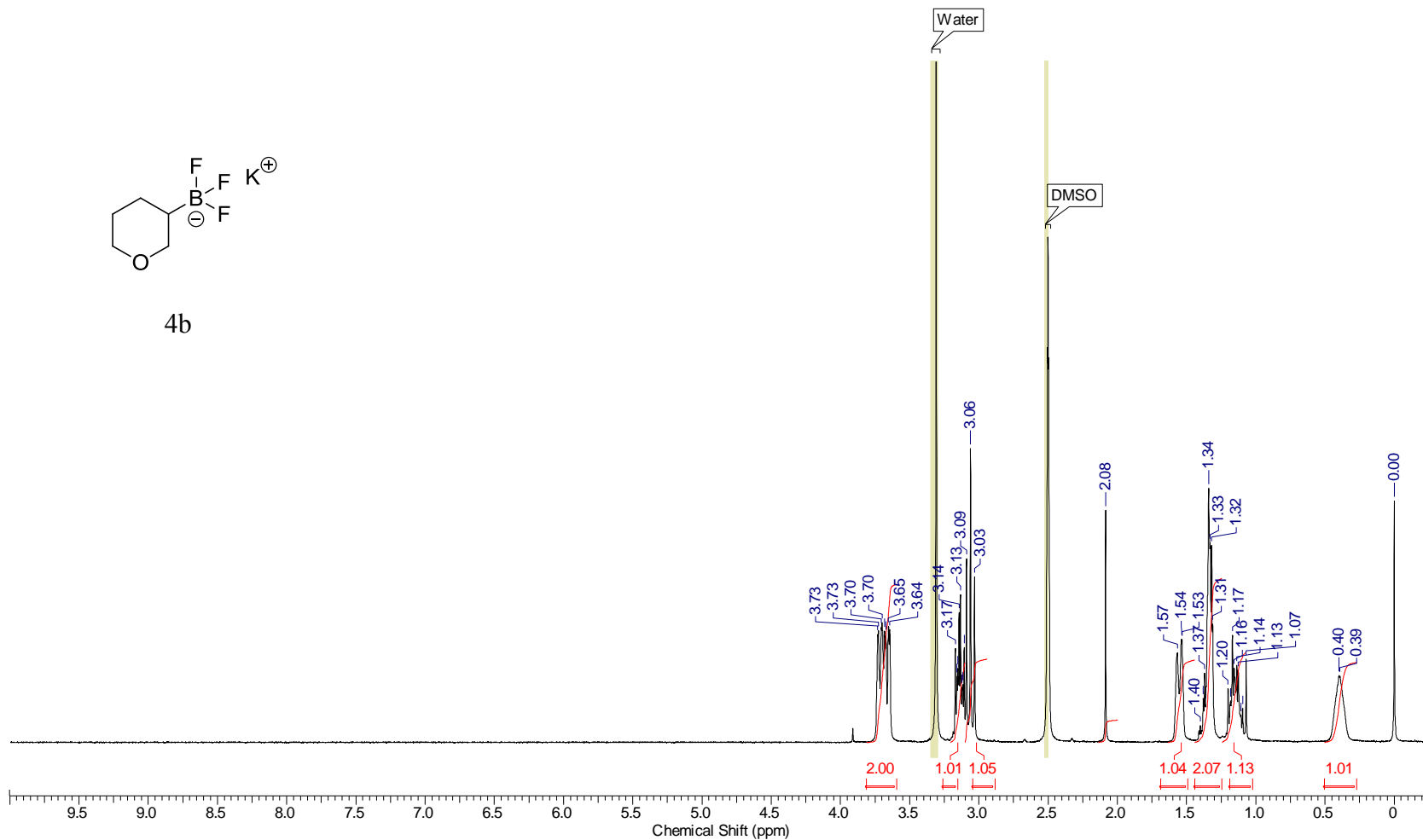
4a



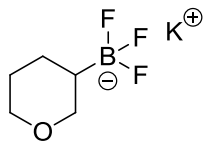
Frequency (MHz)	400.40	Nucleus	1H	Number of Transients	16	Origin	spect
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	Pulse Sequence	zg30
Receiver Gain	456.00	SW(cyclical) (Hz)	7211.54	Solvent	DMSO-d6	Spectrum Offset (Hz)	3398.8562
Spectrum Type	STANDARD	Sweep Width (Hz)	7211.32	Temperature (degree C)	27.000		



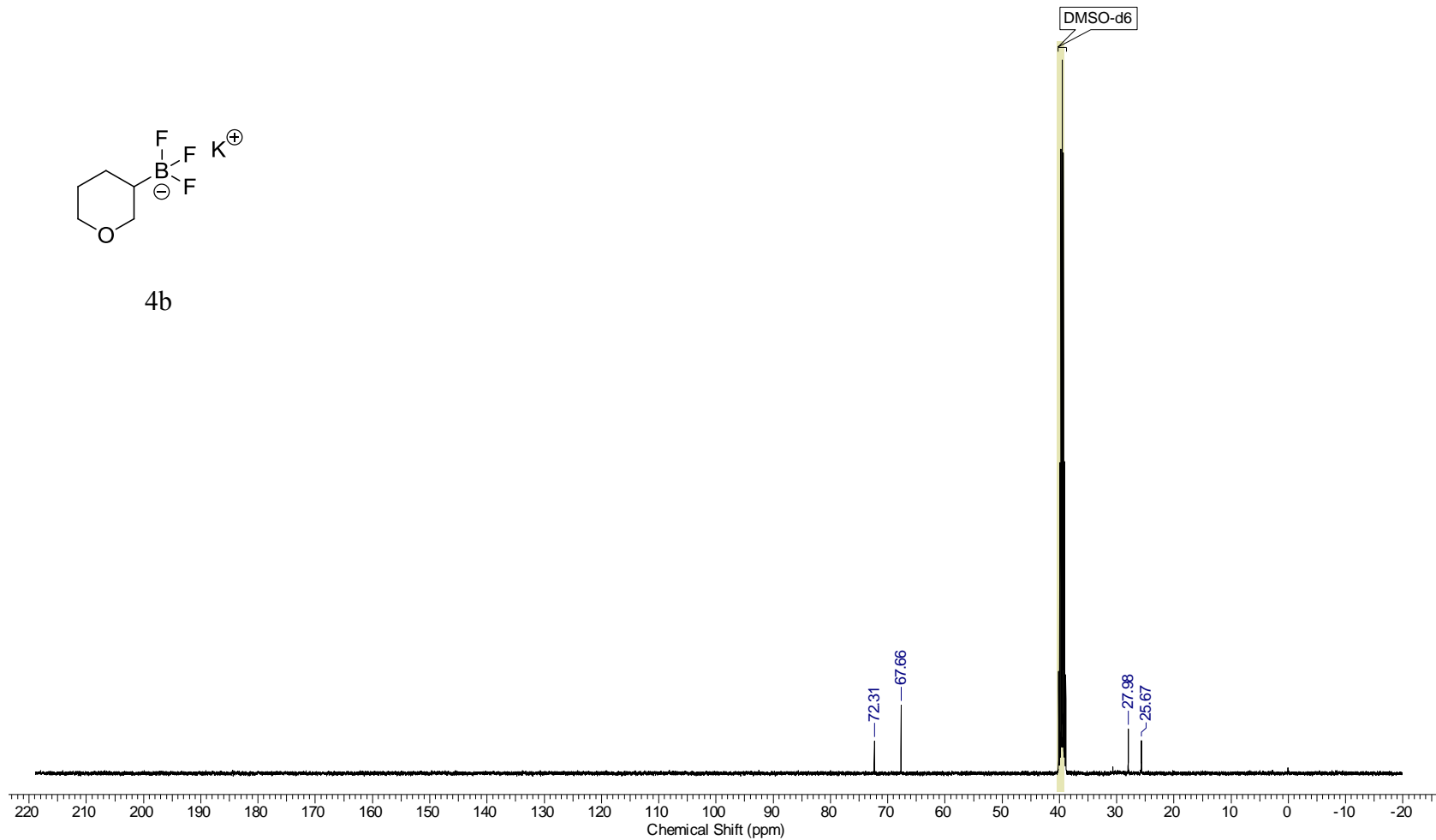
4b



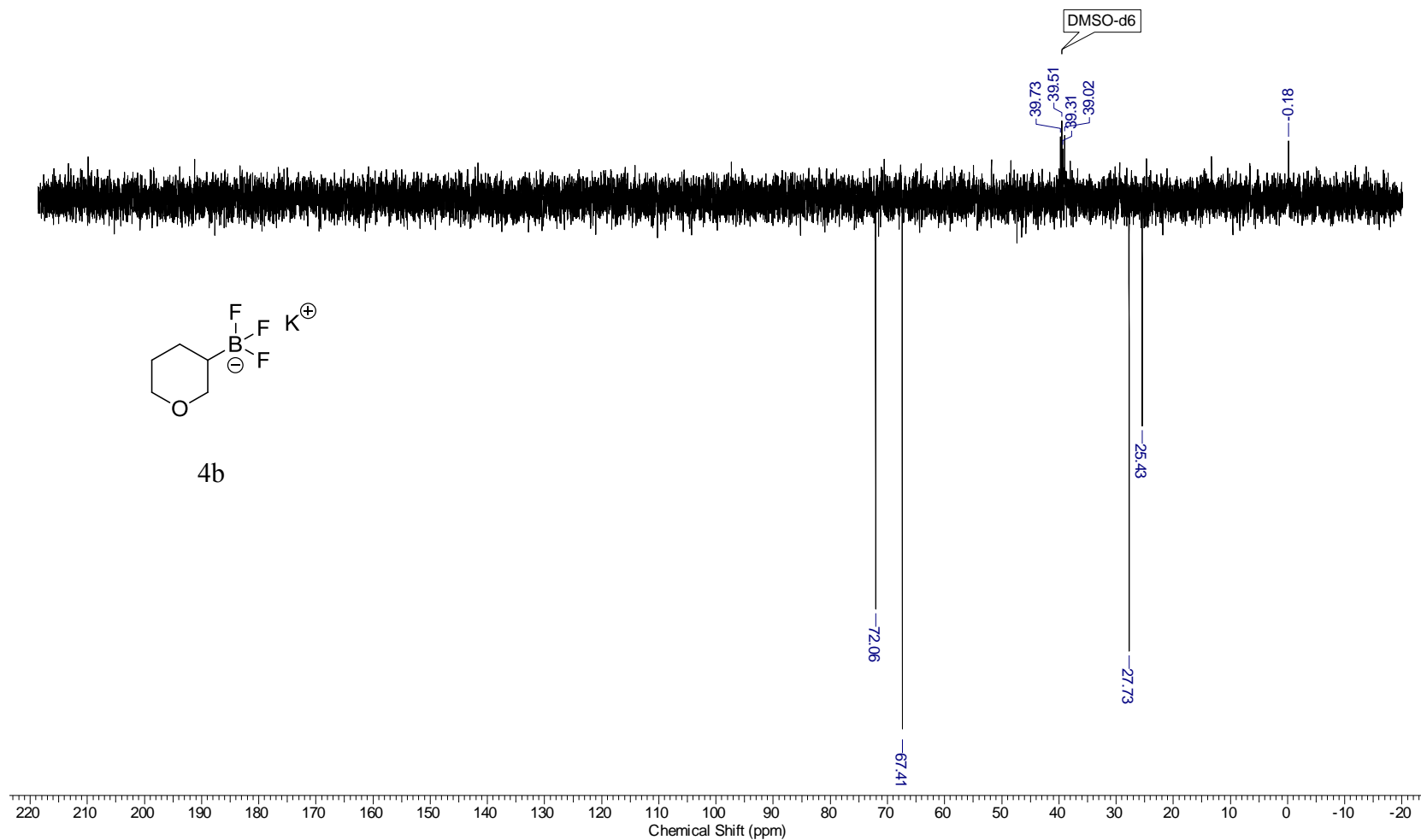
Frequency (MHz)	100.68	Nucleus	¹³ C	Number of Transients	1024	Origin	spect
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	Pulse Sequence	zgpg30
Receiver Gain	287.00	SW(cyclical) (Hz)	24038.46	Solvent	DMSO-d6	Spectrum Offset (Hz)	10017.2207
Spectrum Type	STANDARD	Sweep Width (Hz)	24037.73	Temperature (degree C)	27.000		



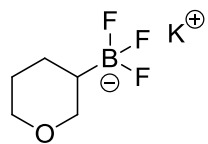
4b



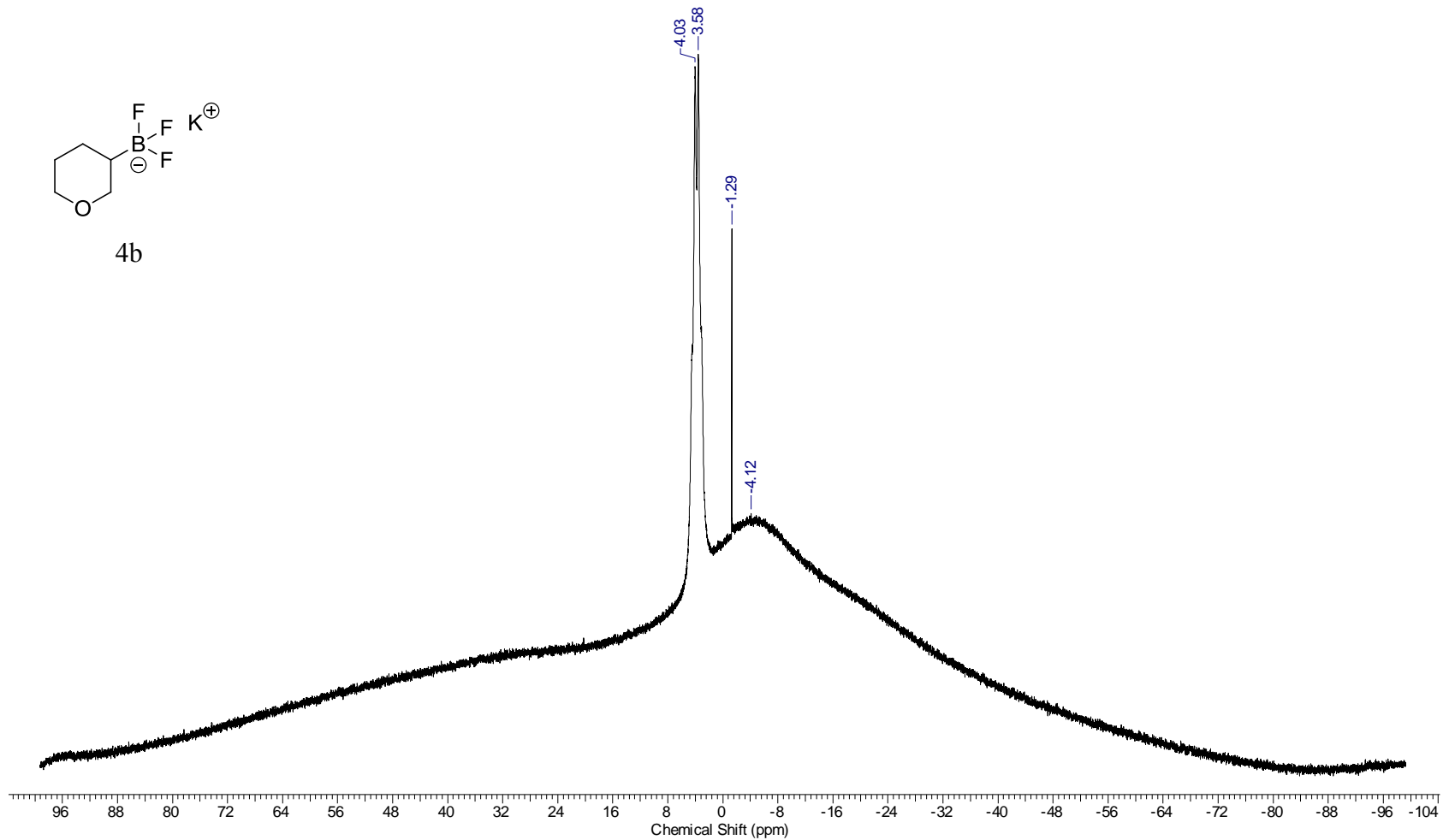
Frequency (MHz)	100.68	Nucleus	13C	Number of Transients	256	Origin	spect
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	Pulse Sequence	dept135
Receiver Gain	2050.00	SW(cyclical) (Hz)	24038.46	Solvent	DMSO-d6	Spectrum Offset (Hz)	9991.5449
Spectrum Type	DEPT135	Sweep Width (Hz)	24037.73	Temperature (degree C)	27.000		



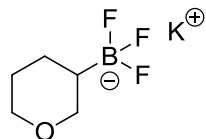
Frequency (MHz)	128.46	Nucleus	11B	Number of Transients	128	Origin	spect
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	Pulse Sequence	zg
Receiver Gain	812.00	SW(cyclical) (Hz)	25510.20	Solvent	DMSO-d6	Spectrum Offset (Hz)	0.8954
Spectrum Type	STANDARD	Sweep Width (Hz)	25509.42	Temperature (degree C)	27.000		



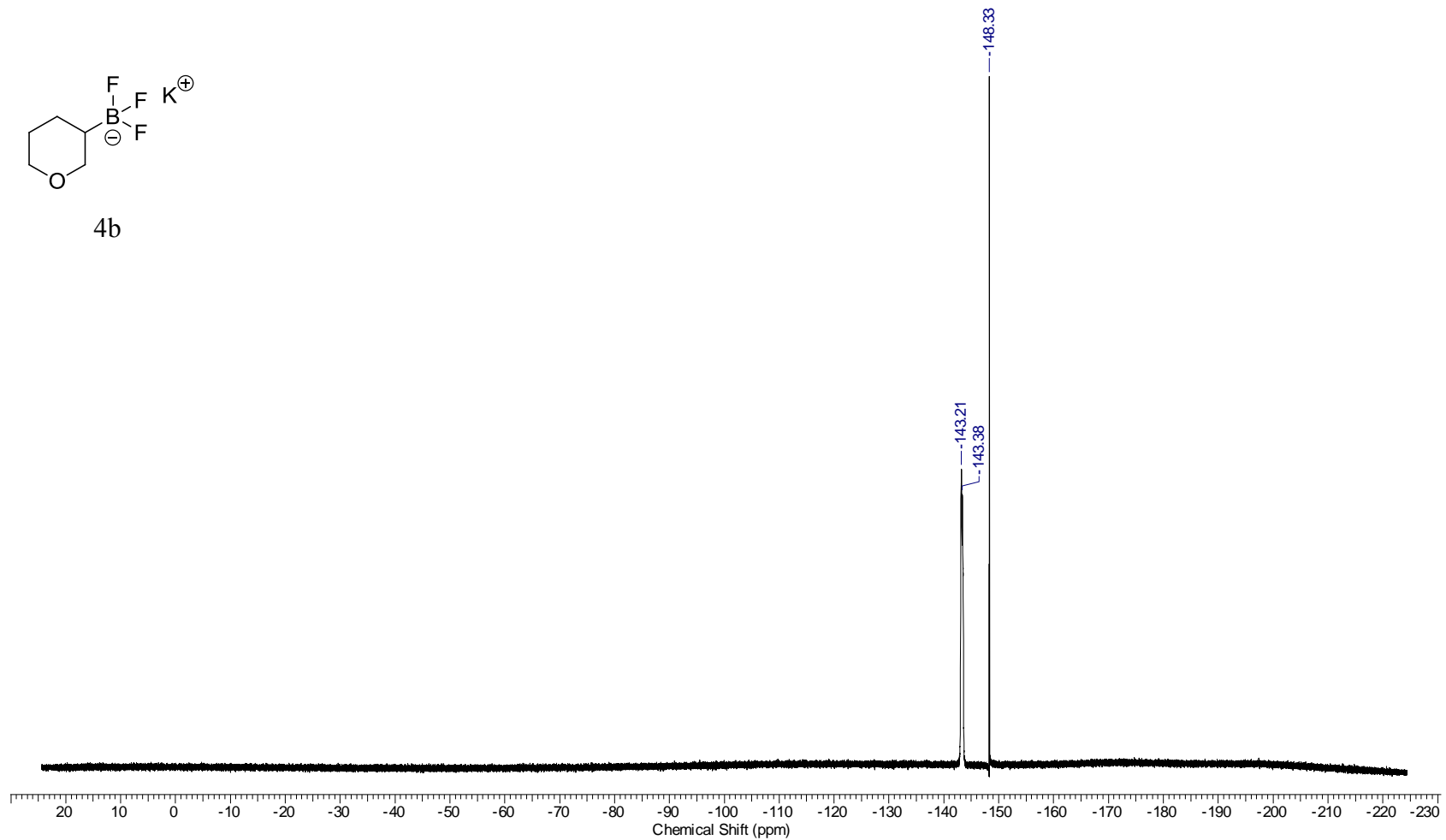
4b



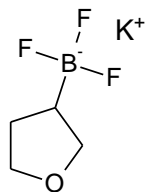
Frequency (MHz)	376.75	Nucleus	19F	Number of Transients	64	Origin	spect
Original Points Count	133120	Owner	tibbe_operator	Points Count	131072	Pulse Sequence	zg30
Receiver Gain	1820.00	SW(cyclical) (Hz)	93750.00	Solvent	DMSO-d6	Spectrum Offset (Hz)	-37674.1992
Spectrum Type	STANDARD	Sweep Width (Hz)	93749.28	Temperature (degree C)	27.000		



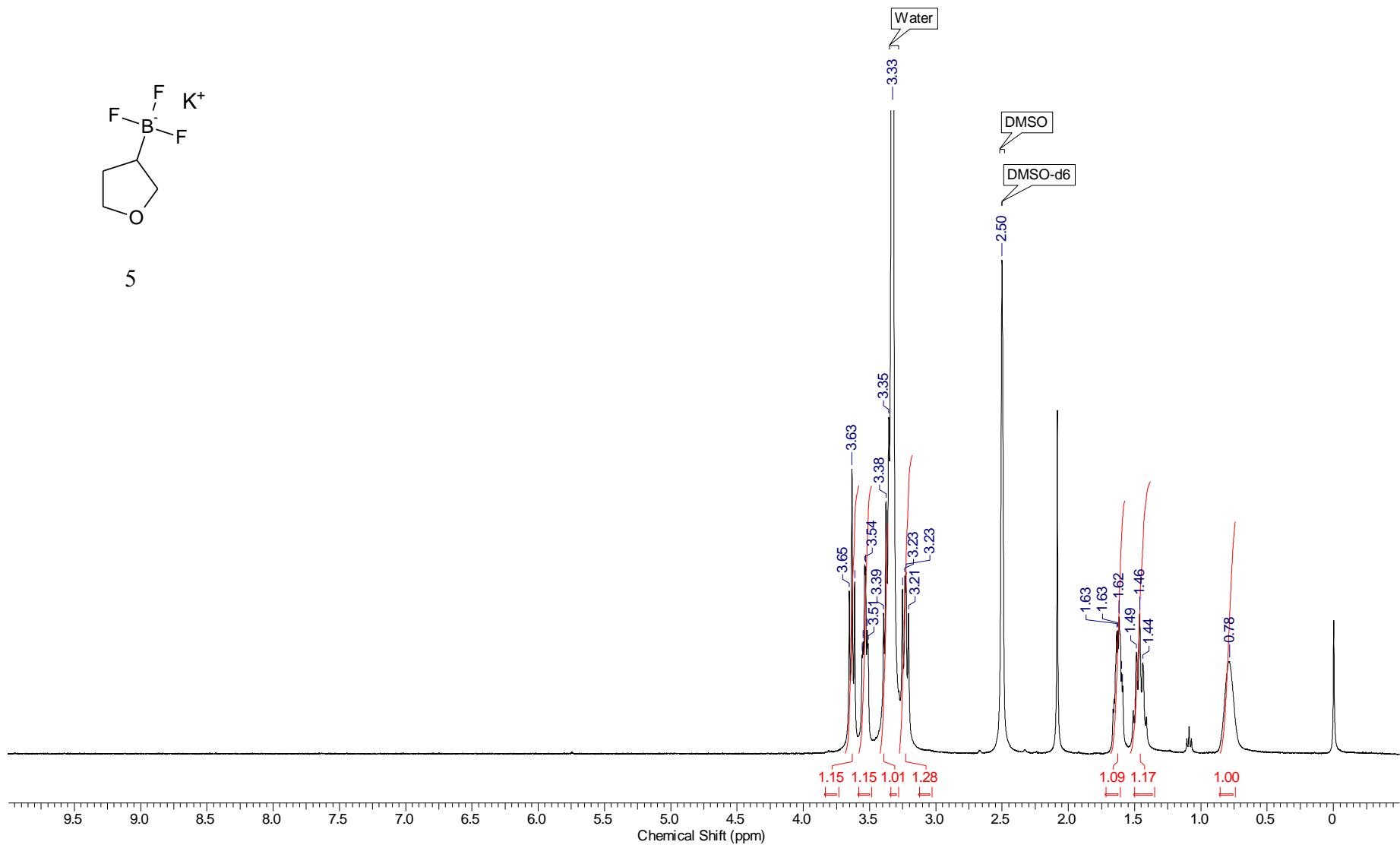
4b



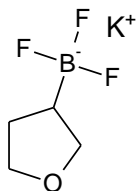
Frequency (MHz)	400.40	Nucleus	1H	Number of Transients	16	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	SW(cyclical) (Hz)	7211.32
Solvent	DMSO-d6	Spectrum Offset (Hz)	3398.8027	Sweep Width (Hz)	7211.10	Temperature (degree C)	27.000



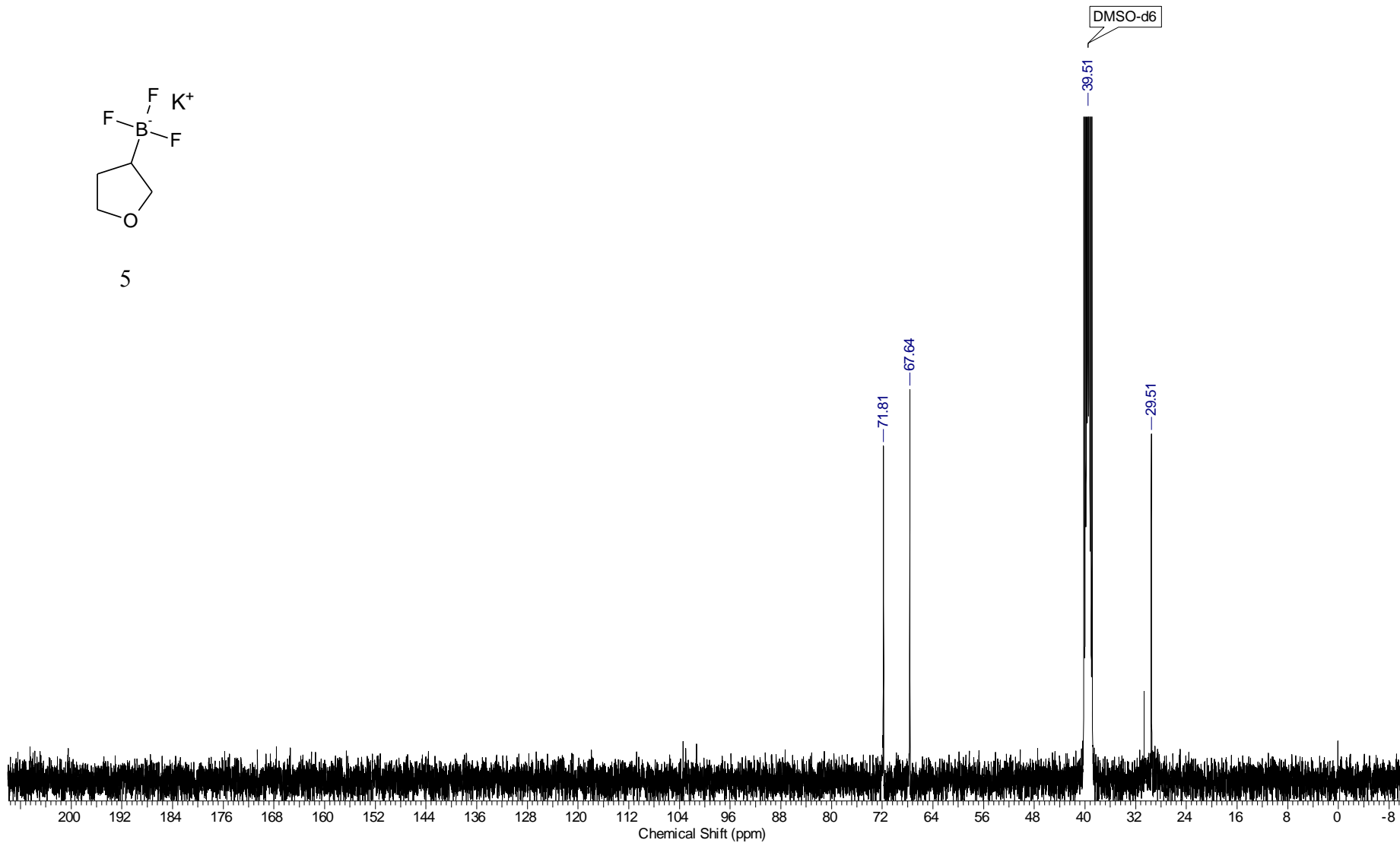
5



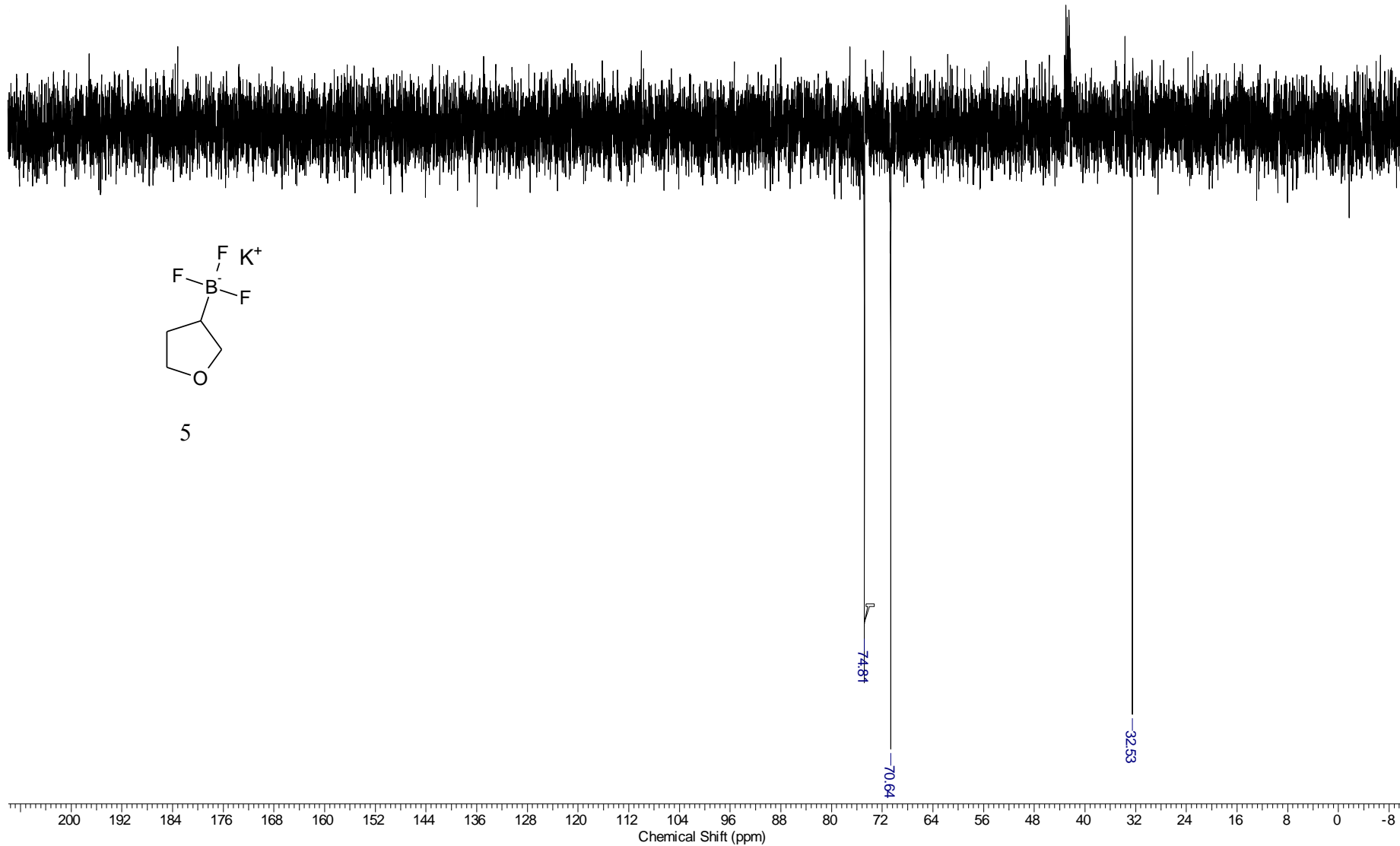
Frequency (MHz)	100.69	Nucleus	¹³ C	Number of Transients	1024	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	SW(cyclical) (Hz)	24037.73
Solvent	DMSO-d6	Spectrum Offset (Hz)	10019.6328	Sweep Width (Hz)	24036.99	Temperature (degree C)	27.000



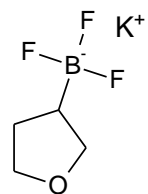
5



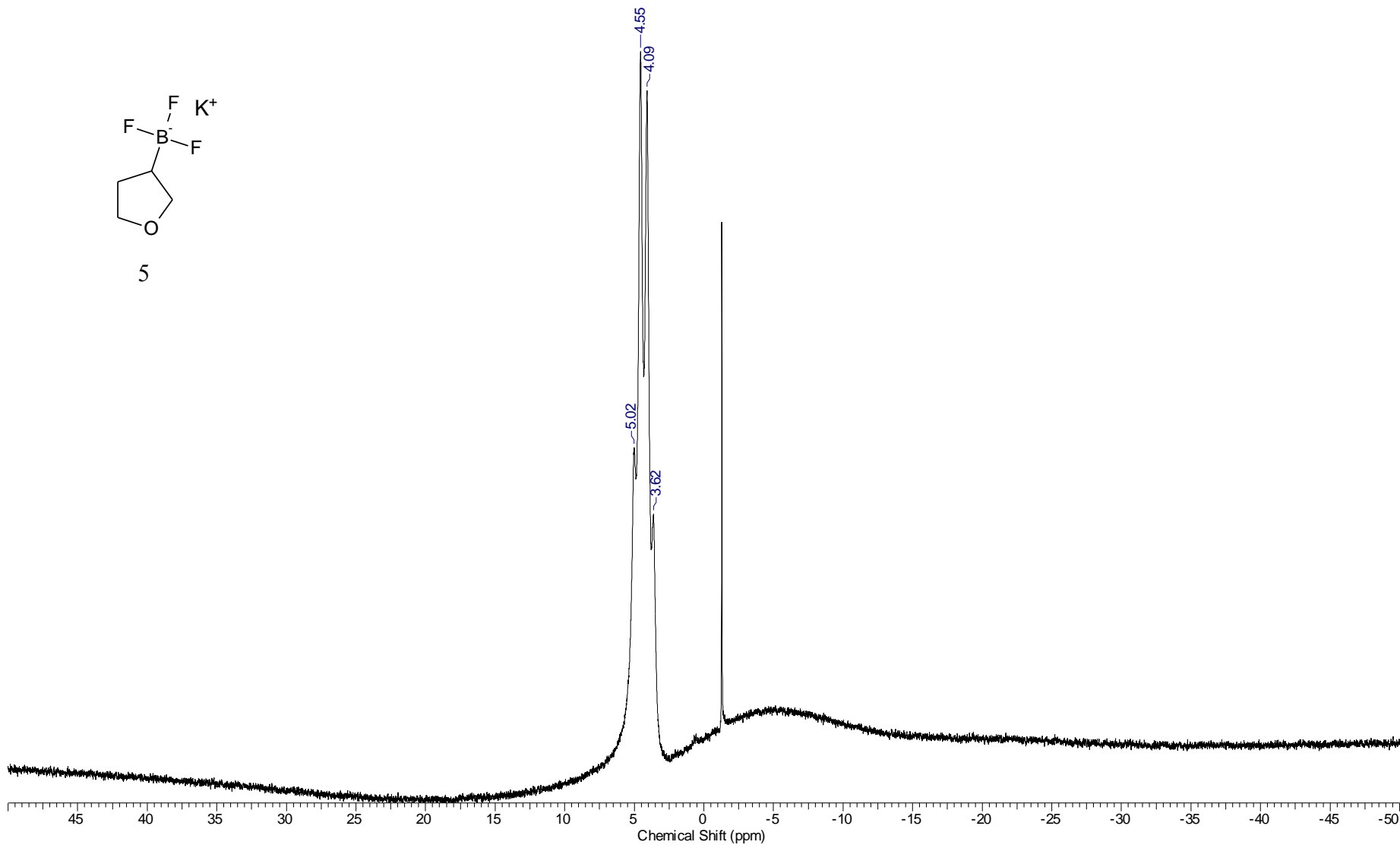
Frequency (MHz)	100.69	Nucleus	¹³ C	Number of Transients	256	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	SW(cyclical) (Hz)	24037.73
Solvent	DMSO-d6	Spectrum Offset (Hz)	10322.0850	Sweep Width (Hz)	24036.99	Temperature (degree C)	27.000



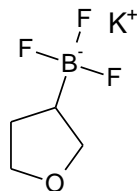
Frequency (MHz)	128.46	Nucleus	11B	Number of Transients	128	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	SW(cyclical) (Hz)	25509.43
Solvent	DMSO-d6	Spectrum Offset (Hz)	1.2842	Sweep Width (Hz)	25508.65	Temperature (degree C)	27.000



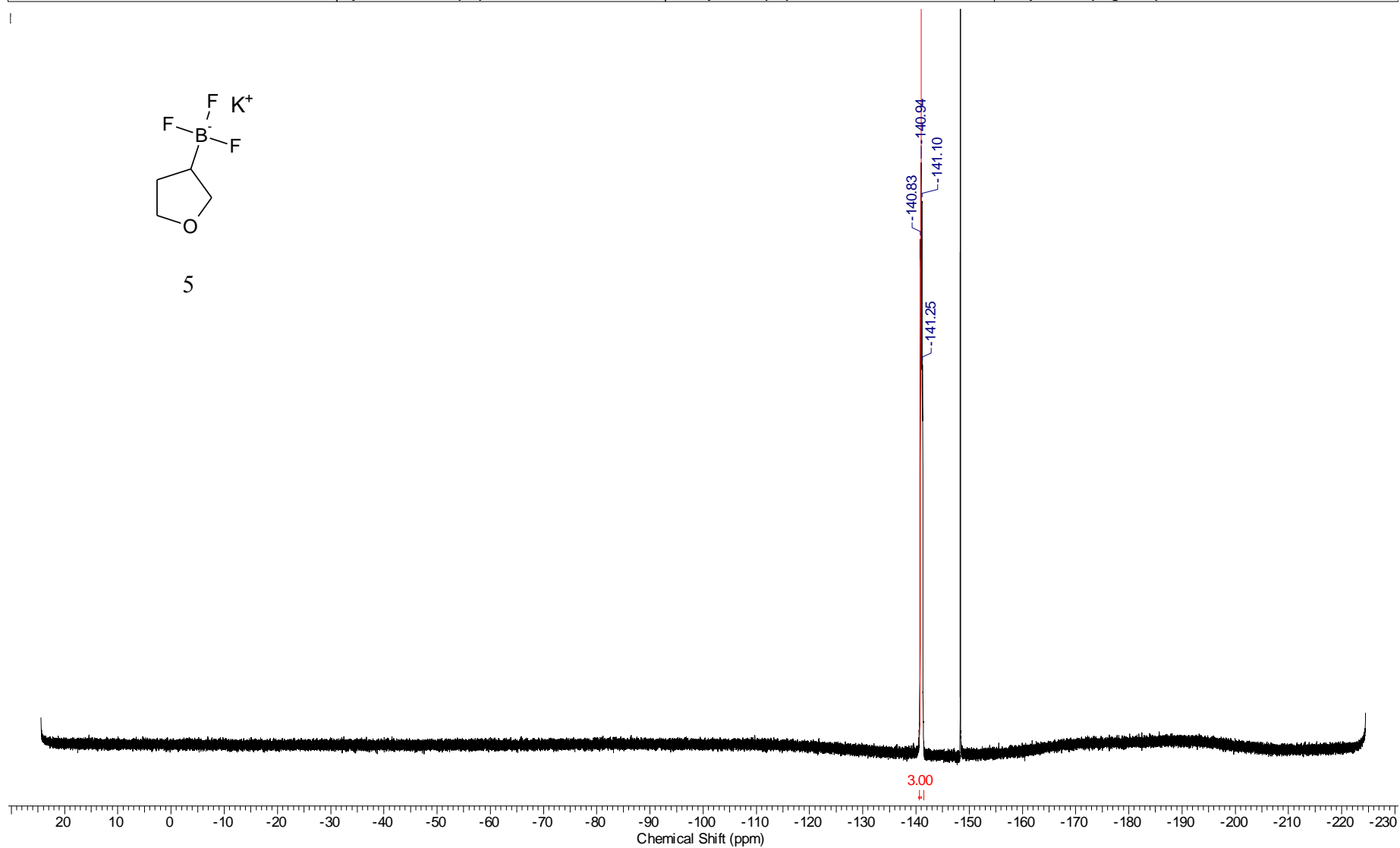
5



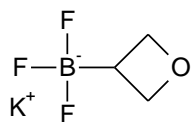
Frequency (MHz)	376.71	Nucleus	¹⁹ F	Number of Transients	64	Origin	Bruker BioSpin GmbH
Original Points Count	131072	Owner	tibbe_operator	Points Count	131072	SW(cyclical) (Hz)	93749.28
Solvent	DMSO-d6	Spectrum Offset (Hz)	-37674.7617	Sweep Width (Hz)	93748.56	Temperature (degree C)	27.000



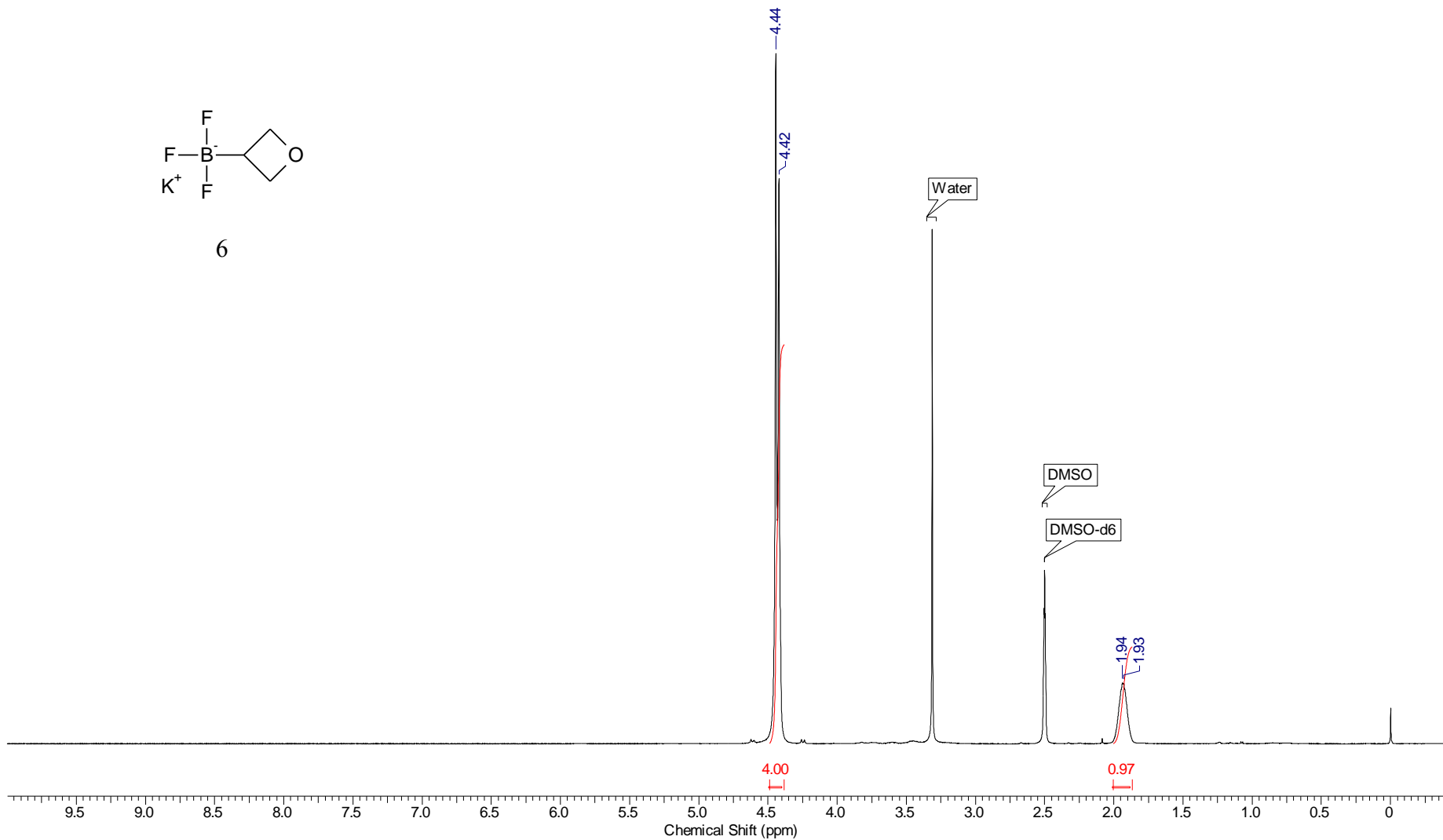
5



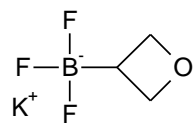
Frequency (MHz)	400.40	Nucleus	1H	Number of Transients	32	Origin	spect
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	Pulse Sequence	zg30
Receiver Gain	456.00	SW(cyclical) (Hz)	7211.54	Solvent	DMSO-d6	Spectrum Offset (Hz)	3398.4272
Spectrum Type	STANDARD	Sweep Width (Hz)	7211.32	Temperature (degree C)	27.000		



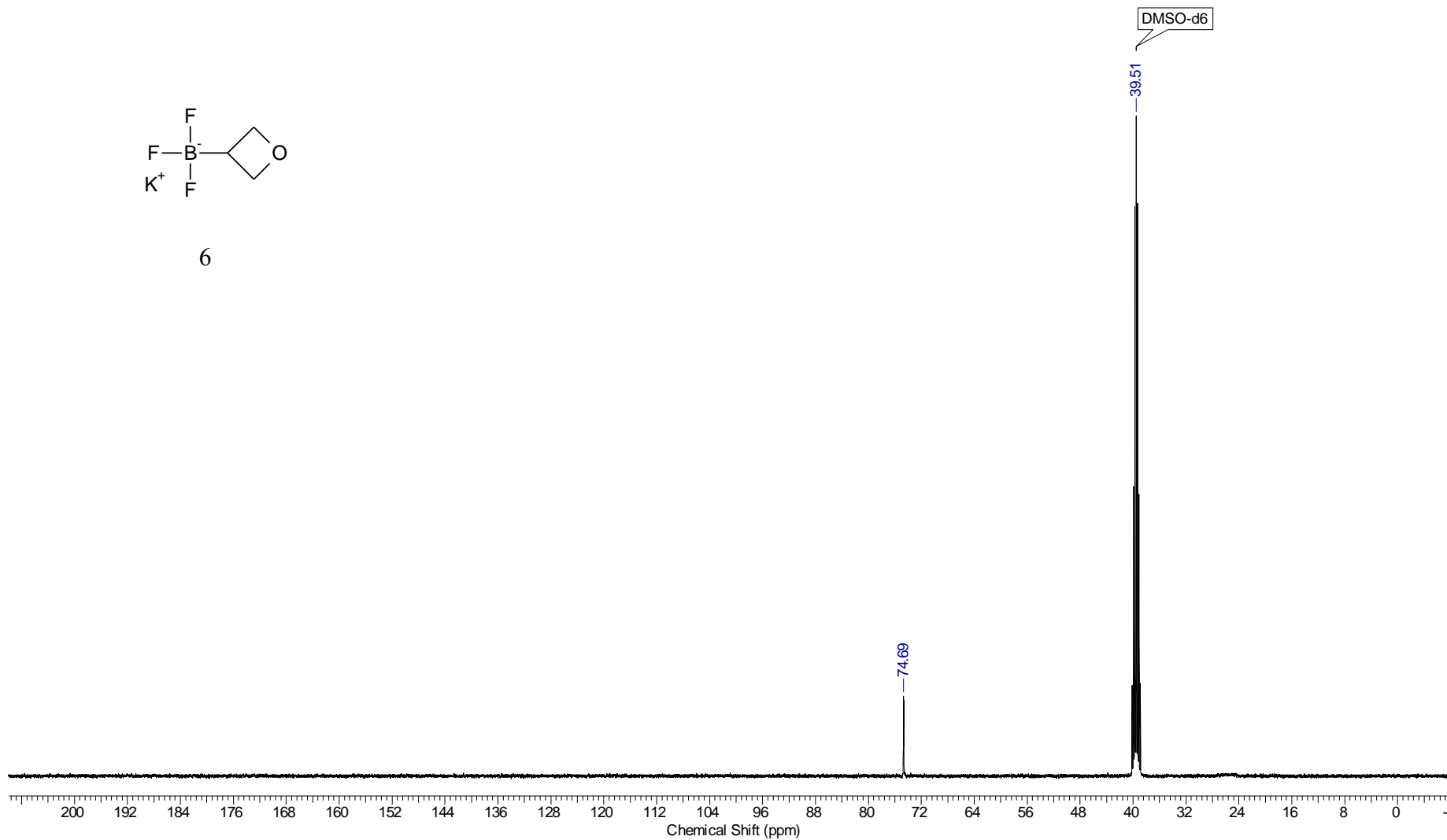
6



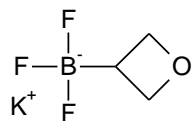
Frequency (MHz)	100.68	Nucleus	¹³ C	Number of Transients	1024	Origin	spect
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	Pulse Sequence	zgpg30
Receiver Gain	406.00	SW(cyclical) (Hz)	24038.46	Solvent	DMSO-d6	Spectrum Offset (Hz)	10018.6875
Spectrum Type	STANDARD	Sweep Width (Hz)	24037.73	Temperature (degree C)	27.000		



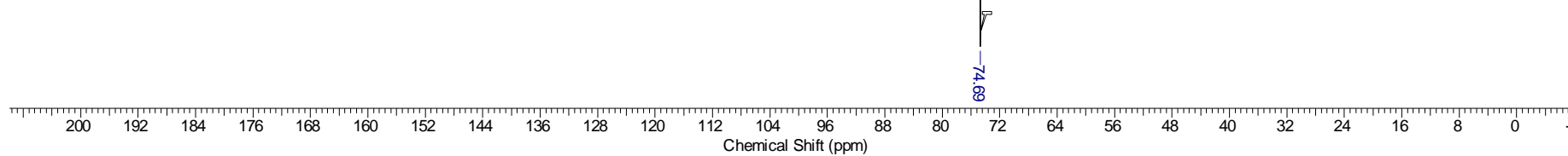
6



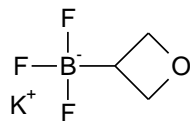
Frequency (MHz)	100.68	Nucleus	¹³ C	Number of Transients	256	Origin	spect
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	Pulse Sequence	dept135
Receiver Gain	2050.00	SW(cyclical) (Hz)	24038.46	Solvent	DMSO-d6	Spectrum Offset (Hz)	10018.8350
Spectrum Type	DEPT135	Sweep Width (Hz)	24037.73	Temperature (degree C)	27.000		



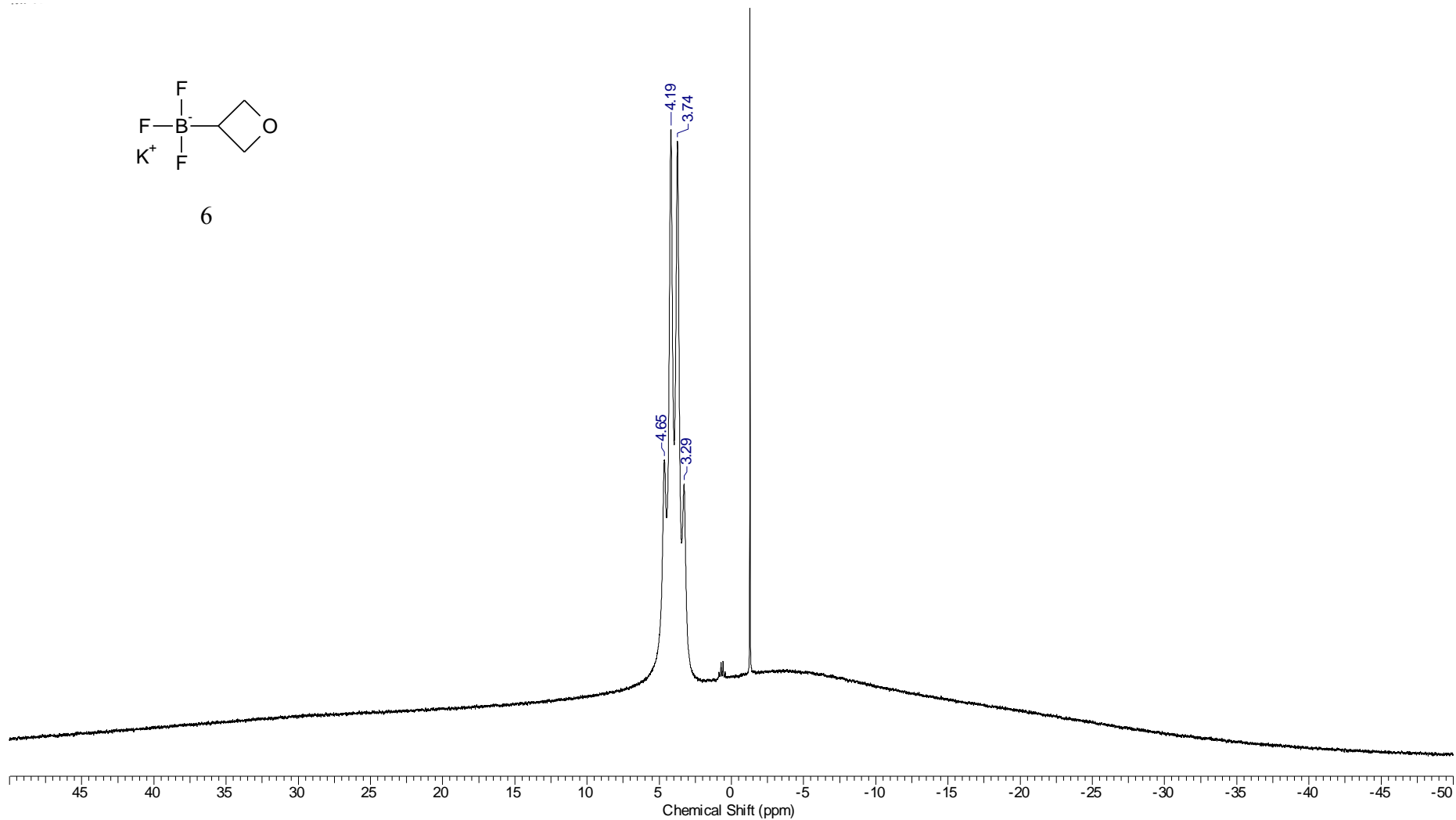
6



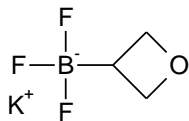
Frequency (MHz)	128.46	Nucleus	11B	Number of Transients	128	Origin	spect
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	Pulse Sequence	zg
Receiver Gain	724.00	SW(cyclical) (Hz)	25510.20	Solvent	DMSO-d6	Spectrum Offset (Hz)	0.8954
Spectrum Type	STANDARD	Sweep Width (Hz)	25509.42	Temperature (degree C)	27.000		



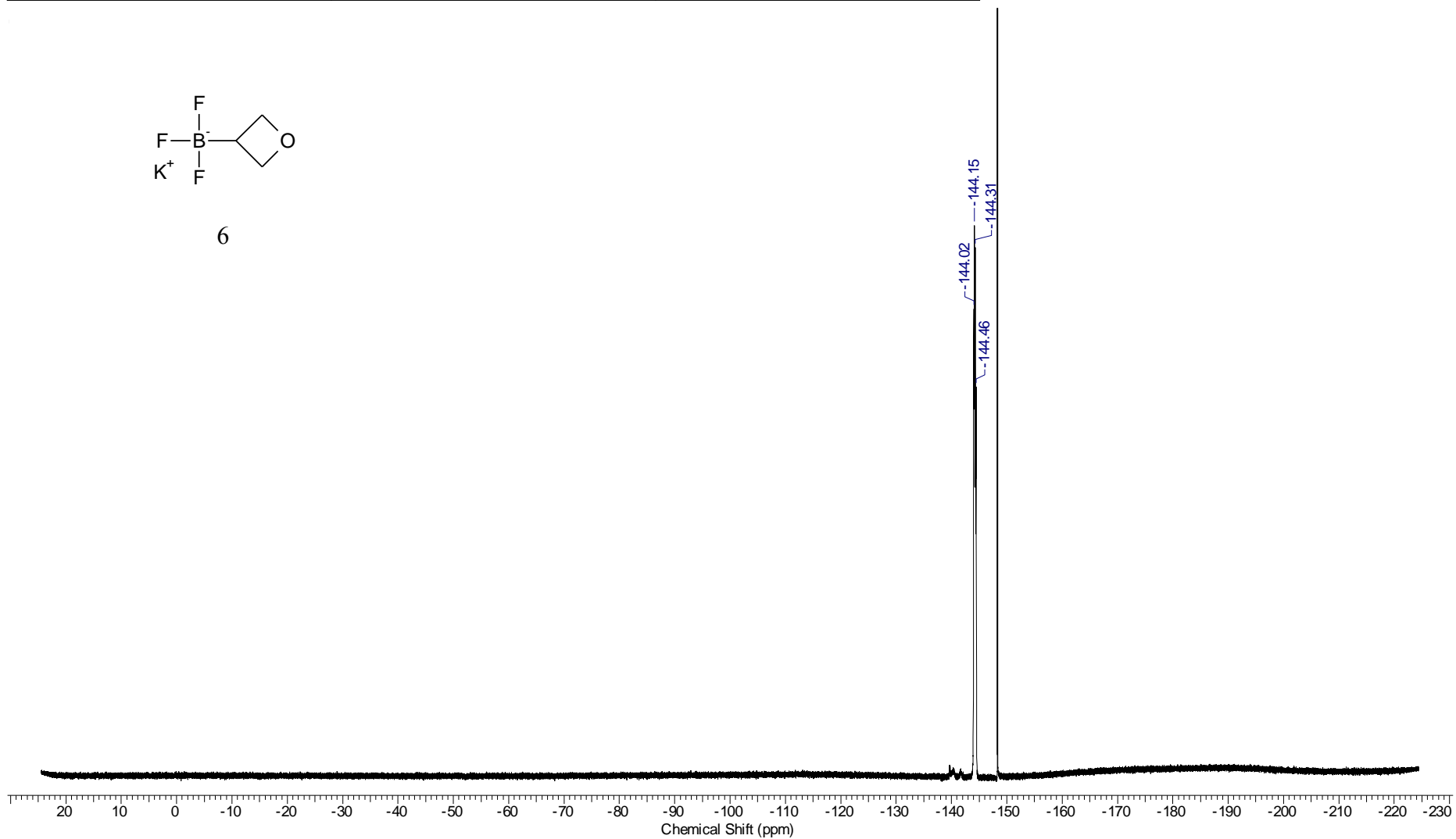
6



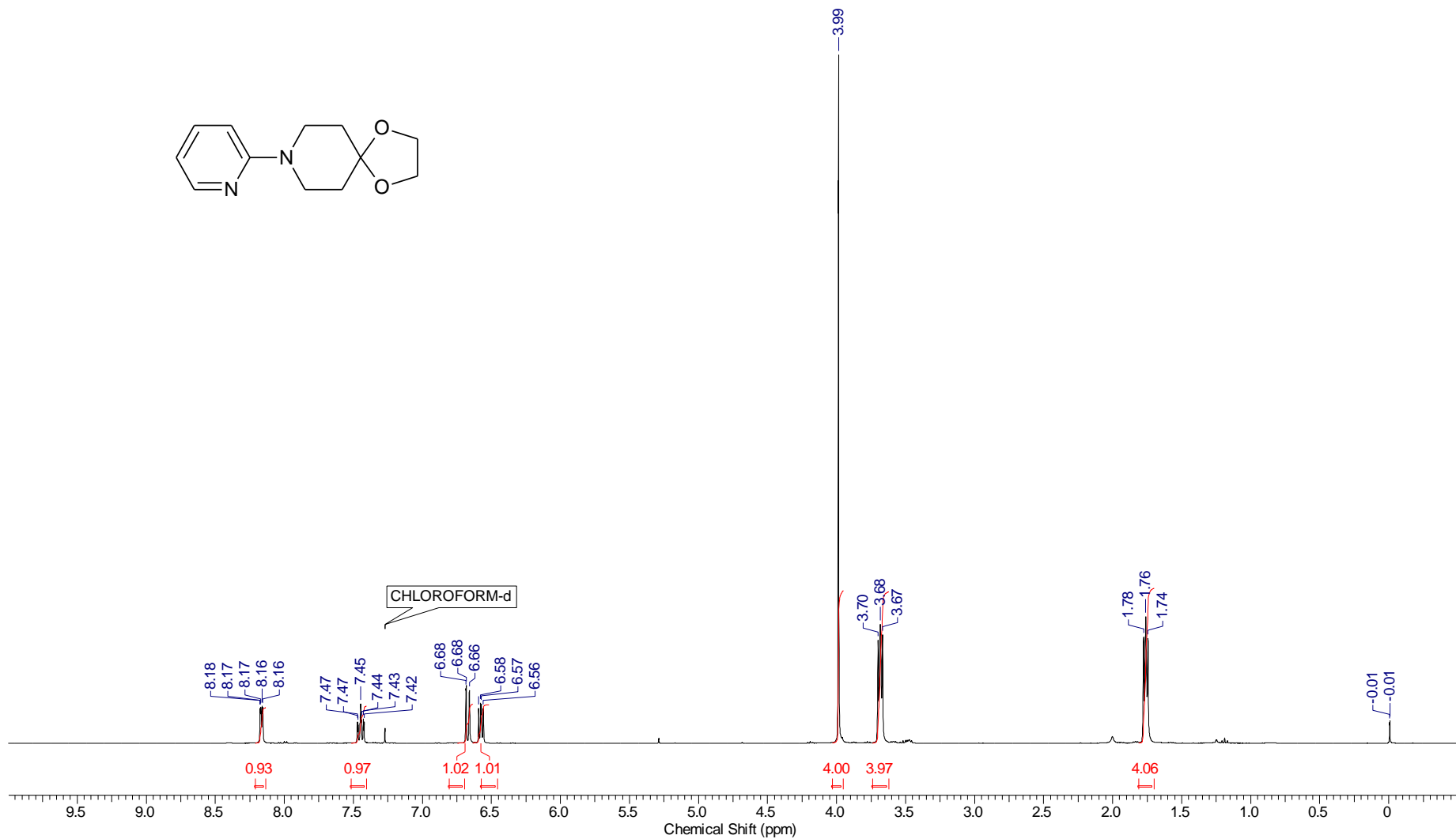
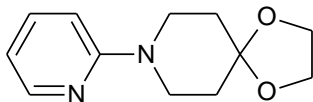
Frequency (MHz)	376.75	Nucleus	19F	Number of Transients	64	Origin	spect
Original Points Count	133120	Owner	tibbe_operator	Points Count	131072	Pulse Sequence	zg30
Receiver Gain	1620.00	SW(cyclical) (Hz)	93750.00	Solvent	DMSO-d6	Spectrum Offset (Hz)	-37674.1992
Spectrum Type	STANDARD	Sweep Width (Hz)	93749.28	Temperature (degree C)	27.000		



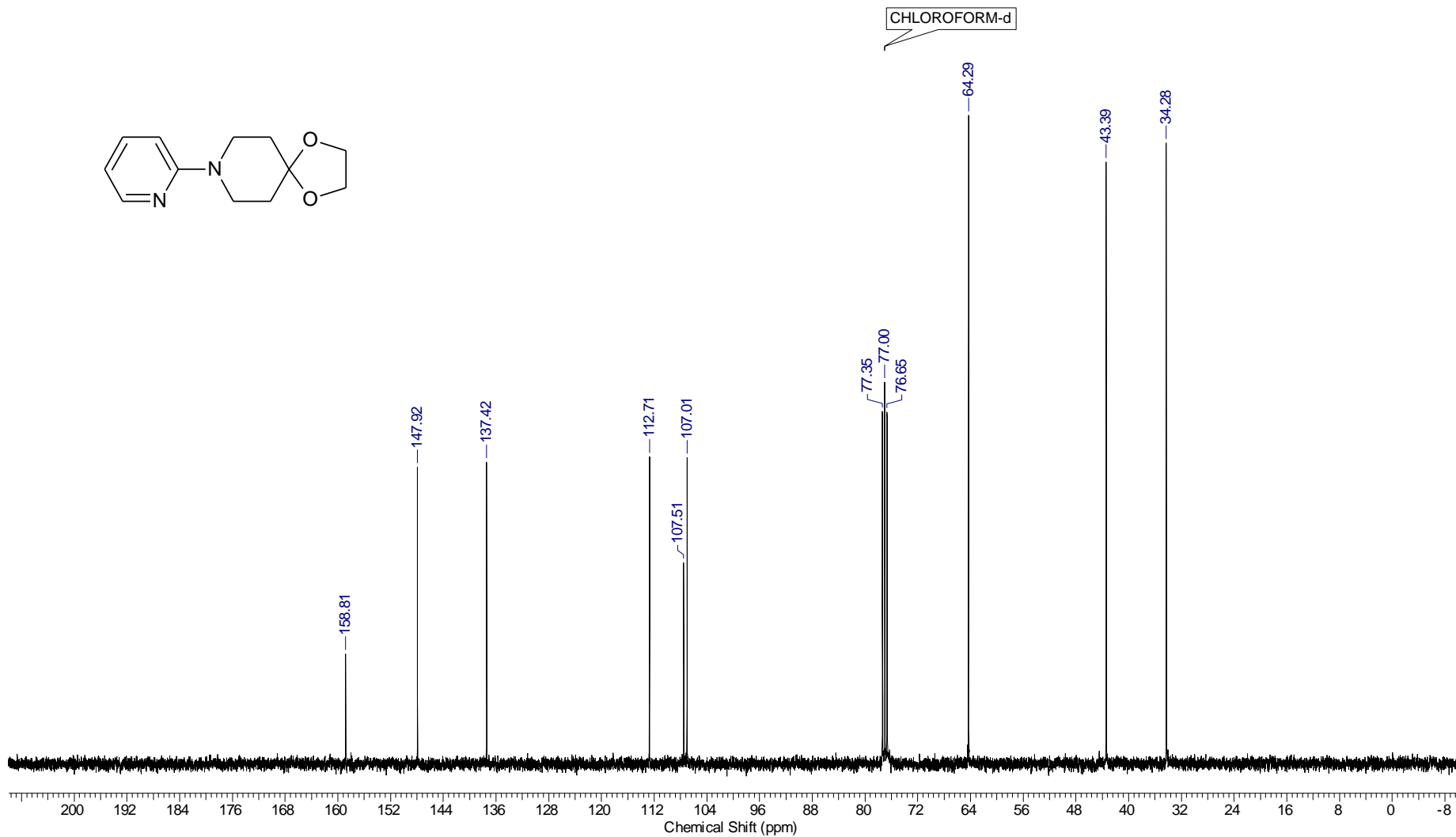
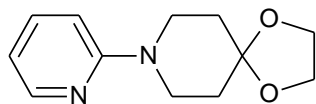
6



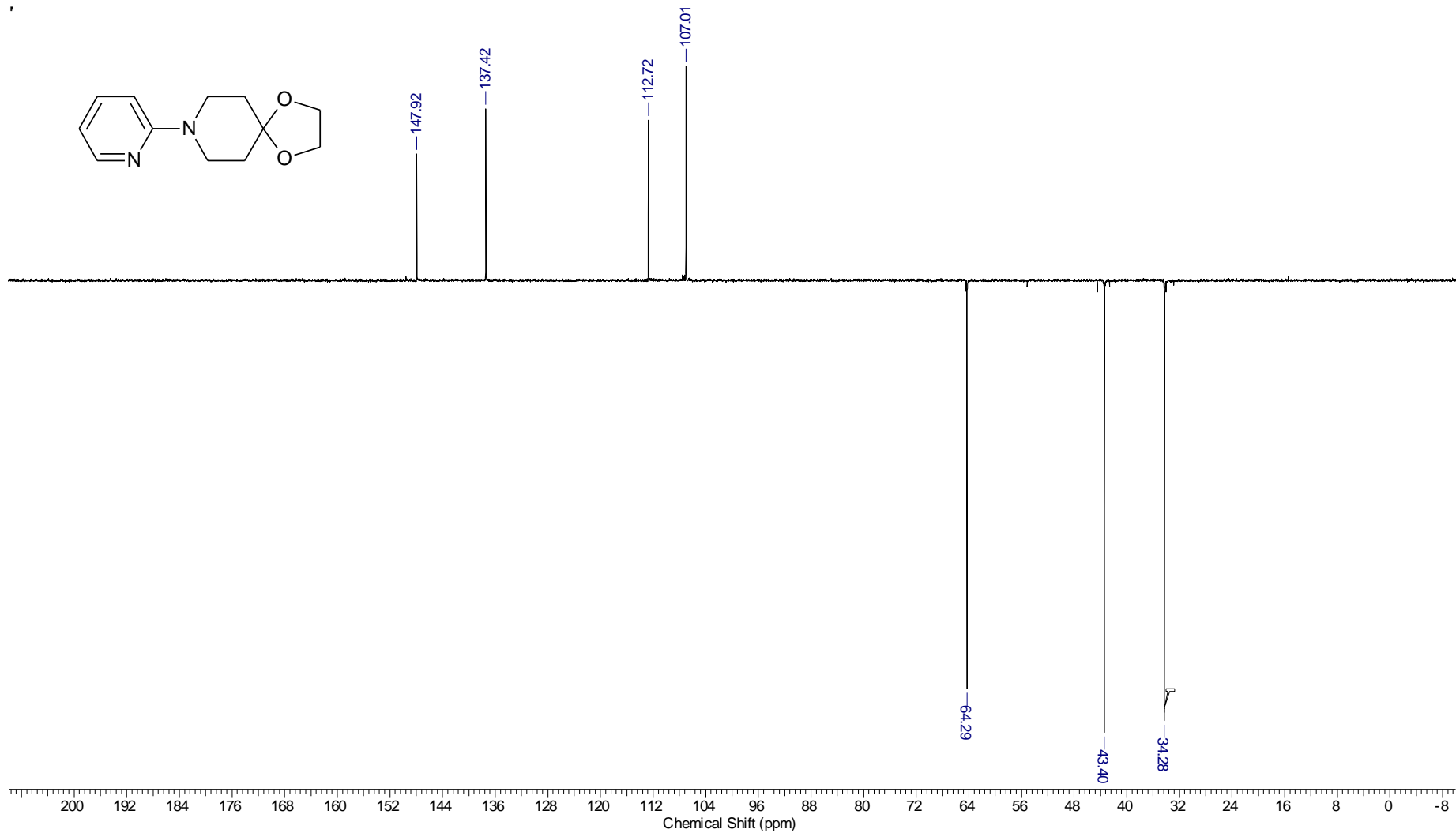
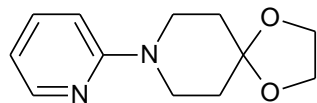
Nucleus	1H	Number of Transients	32	Origin	spect	Frequency (MHz)	360.13
Owner	SHR-NMRBDIS2	Points Count	16384	Pulse Sequence	zg30	Original Points Count	16384
SW(cyclical) (Hz)	5995.20	Solvent	CHLOROFORM-d			Receiver Gain	143.70
Spectrum Type	STANDARD	Sweep Width (Hz)	5994.84	Temperature (degree C)	27.000	Spectrum Offset (Hz)	2790.6758



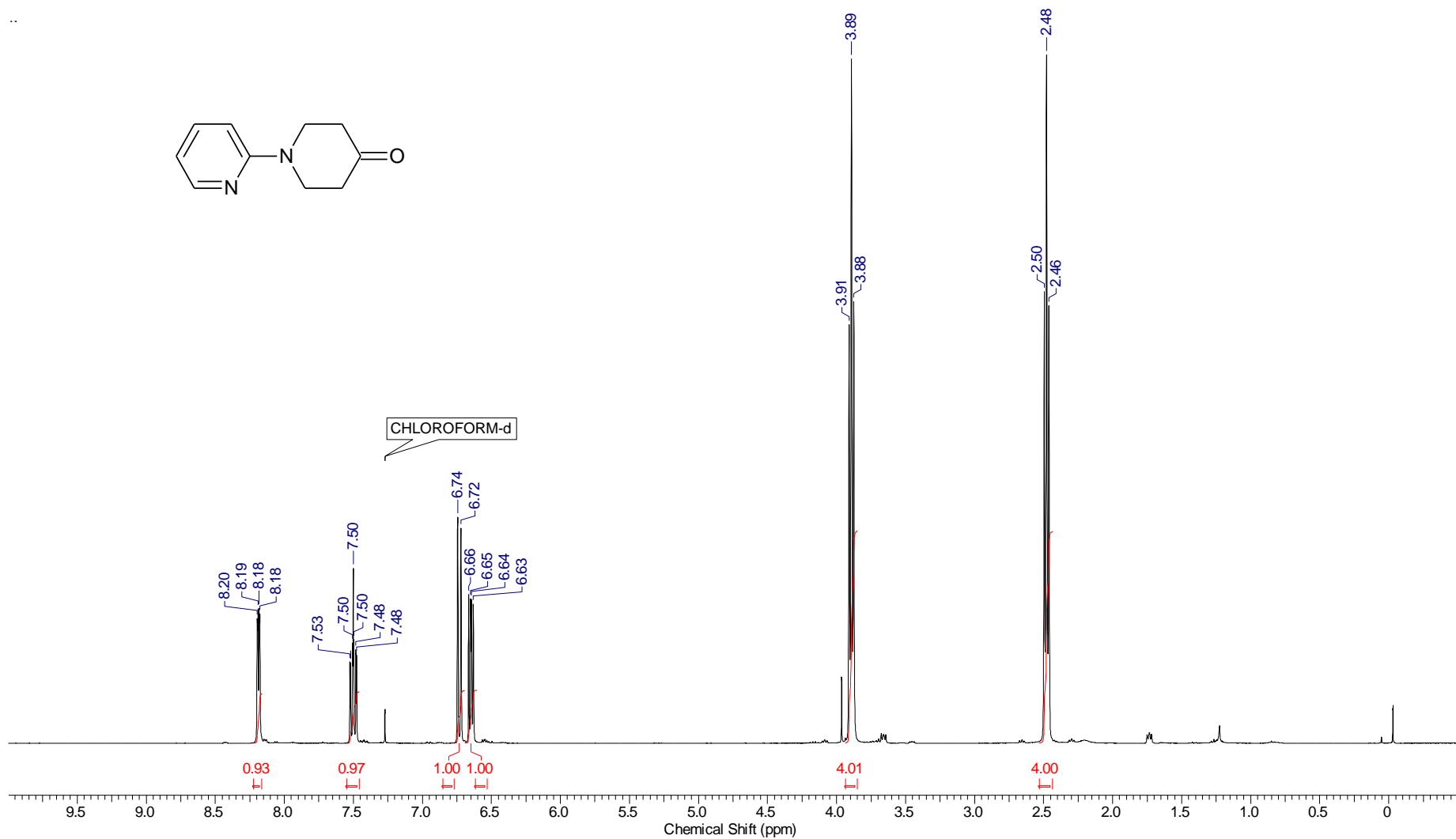
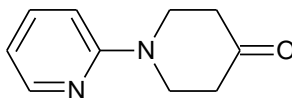
Nucleus	13C	Number of Transients	100	Origin	spect	Frequency (MHz)	90.55
Owner	SHR-NMRBDIS2	Points Count	32768	Pulse Sequence	zgpg30	Original Points Count	32768
SW(cyclical) (Hz)	21645.02	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	9045.8643	Receiver Gain	9195.20
Sweep Width (Hz)	21644.36	Temperature (degree C)	27.000			Spectrum Type	STANDARD



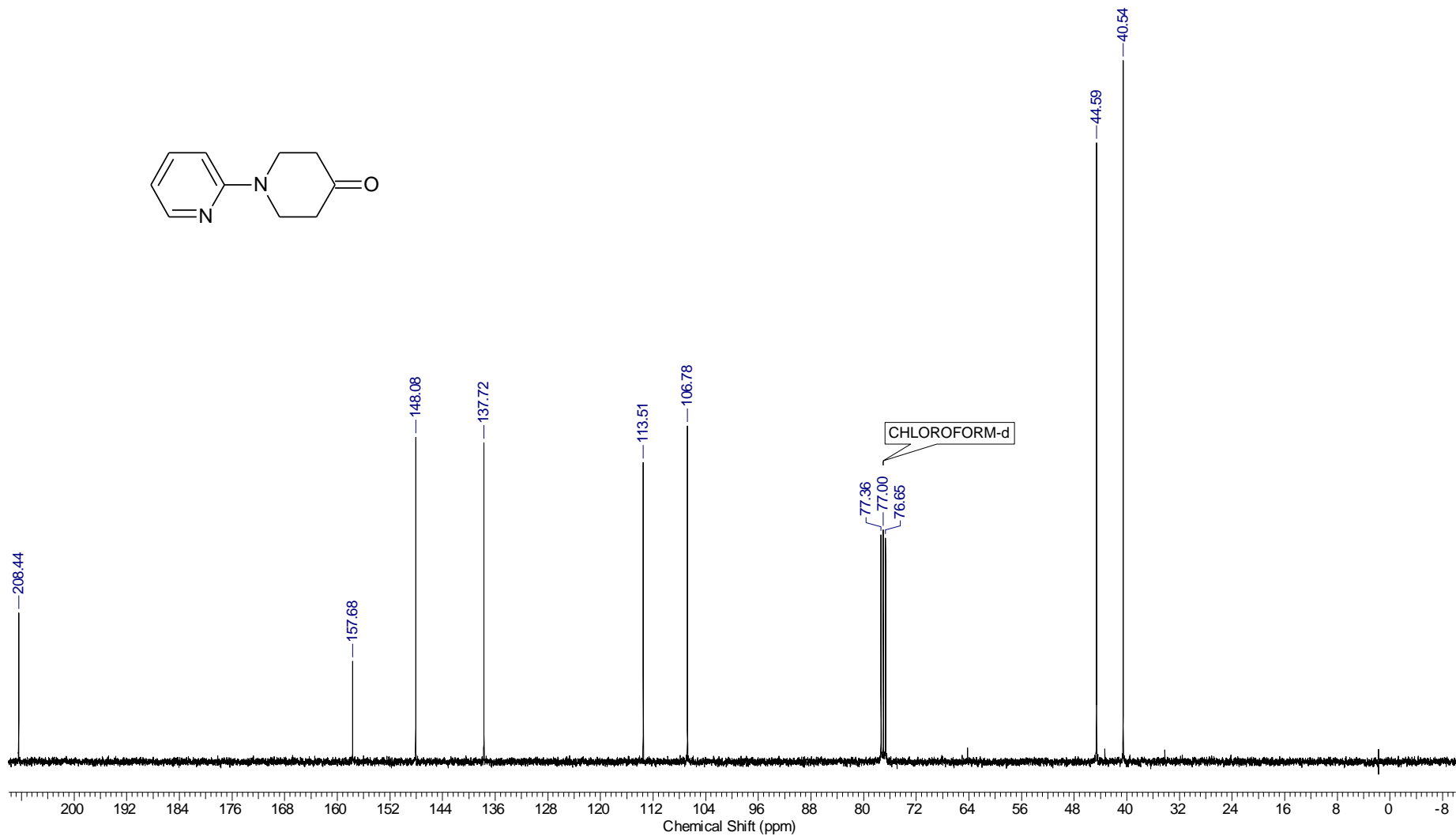
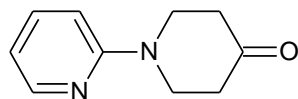
					Frequency (MHz)	90.55	
Nucleus	¹³ C	Number of Transients	512	Origin	spect	Original Points Count	32768
Owner	SHR-NMRBDIS2	Points Count	32768	Pulse Sequence	dept135	Receiver Gain	16384.00
SW(cyclical) (Hz)	21645.02	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	9046.2275	Spectrum Type	DEPT135
Sweep Width (Hz)	21644.36	Temperature (degree C)	27.000				



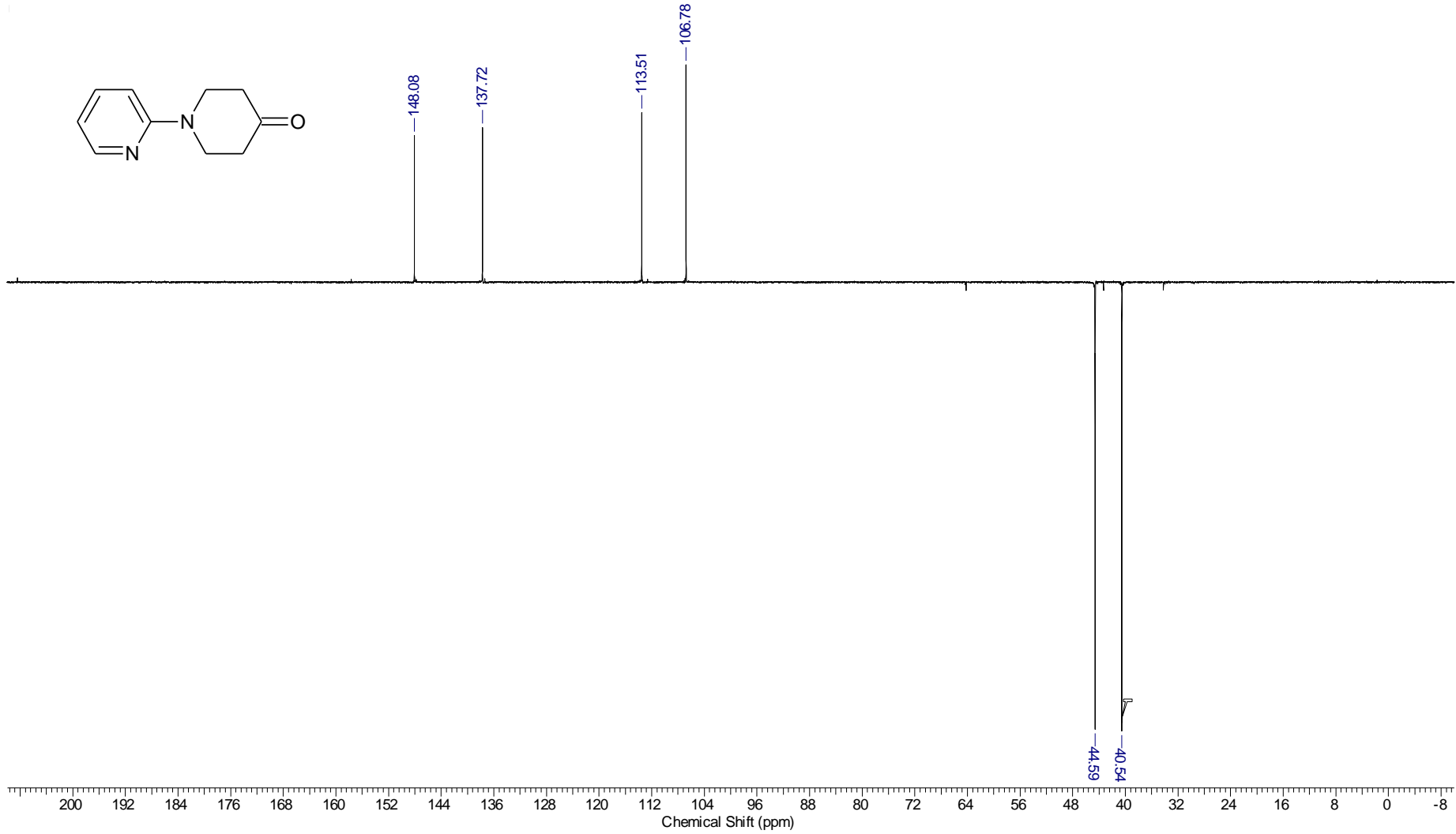
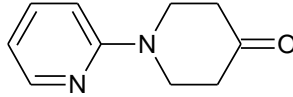
Nucleus	1H	Number of Transients	32	Origin	spect	Frequency (MHz)	360.13
Owner	SHR-NMRBDIS2	Points Count	16384	Pulse Sequence	zg30	Original Points Count	16384
SW(cyclical) (Hz)	5995.20	Solvent	CHLOROFORM-d			Receiver Gain	114.00
Spectrum Type	STANDARD	Sweep Width (Hz)	5994.84	Temperature (degree C)	27.000	Spectrum Offset (Hz)	2790.6758



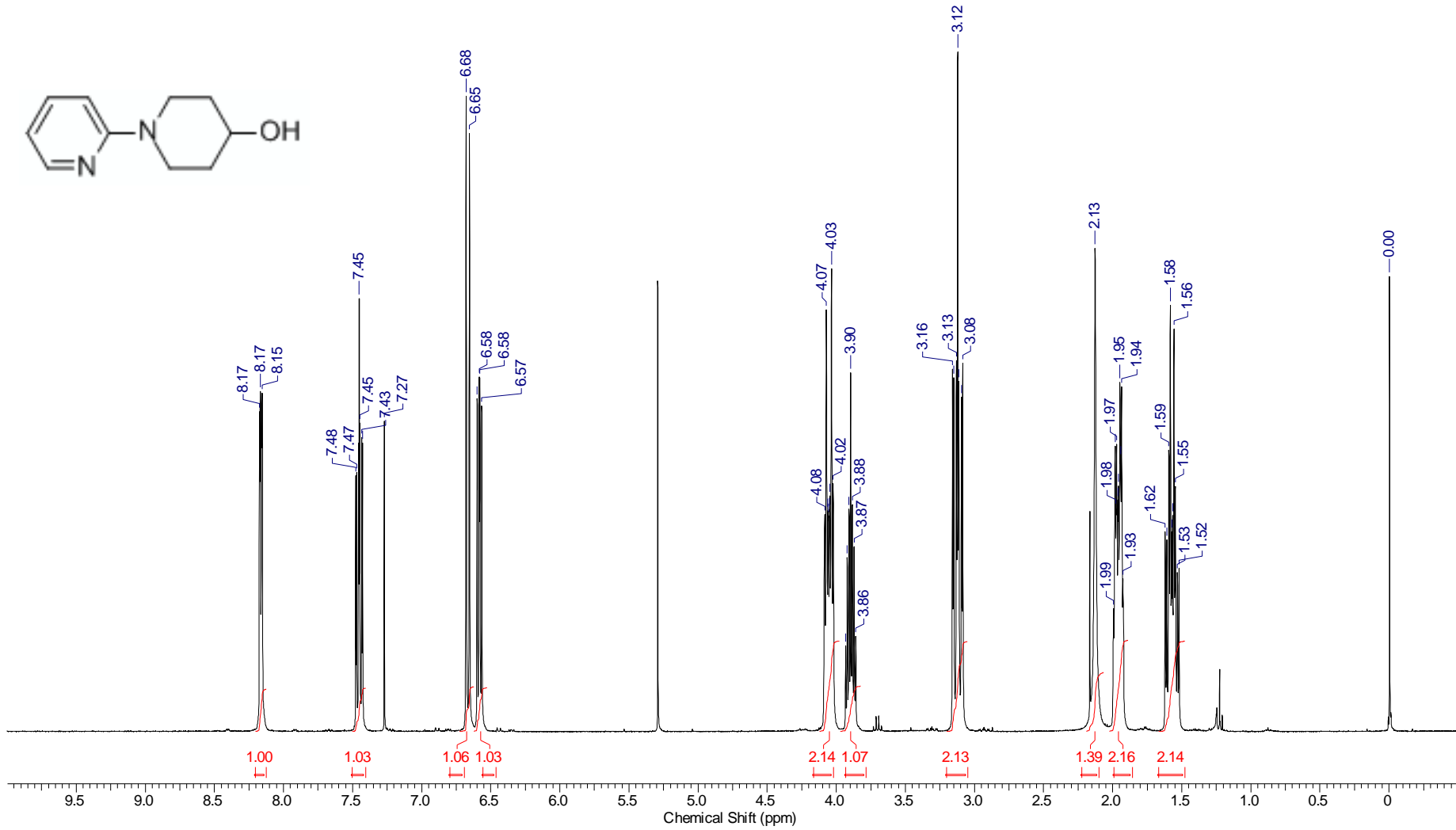
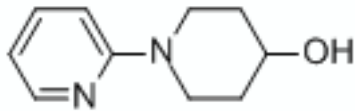
Nucleus	13C	Number of Transients	100	Origin	spect	Frequency (MHz)	90.55
Owner	SHR-NMRBDIS2	Points Count	32768	Pulse Sequence	zgpg30	Original Points Count	32768
SW(cyclical) (Hz)	21645.02	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	9041.2539	Receiver Gain	14596.50
Sweep Width (Hz)	21644.36	Temperature (degree C)	27.000			Spectrum Type	STANDARD



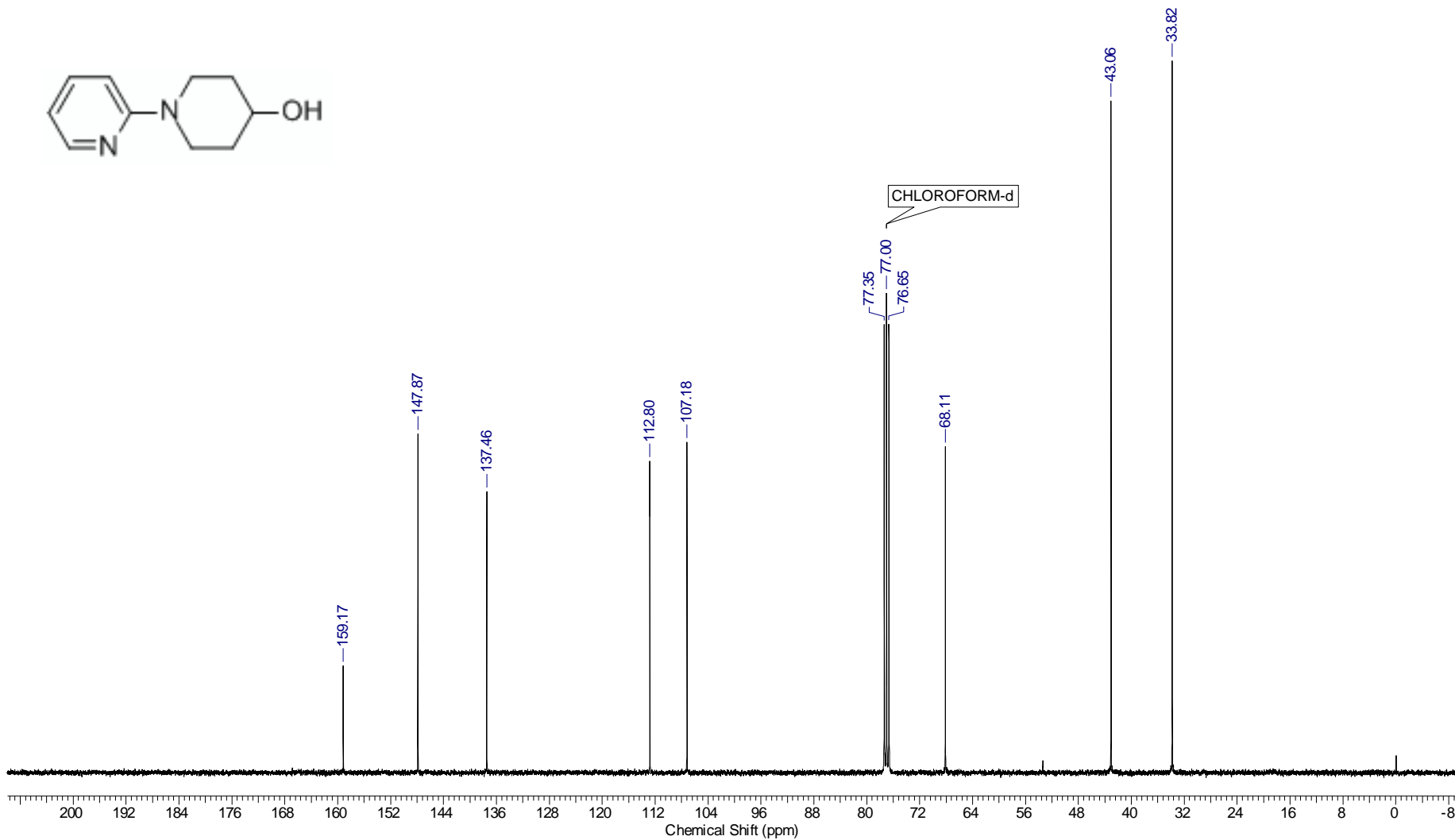
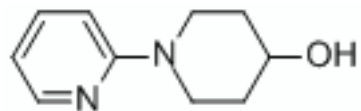
Nucleus	13C	Number of Transients	512	Origin	spect	Frequency (MHz)	90.55
Owner	SHR-NMRBDIS2	Points Count	32768	Pulse Sequence	dept135	Original Points Count	32768
SW(cyclical) (Hz)	21645.02	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	9041.0615	Receiver Gain	16384.00
Sweep Width (Hz)	21644.36	Temperature (degree C)	27.000			Spectrum Type	DEPT135



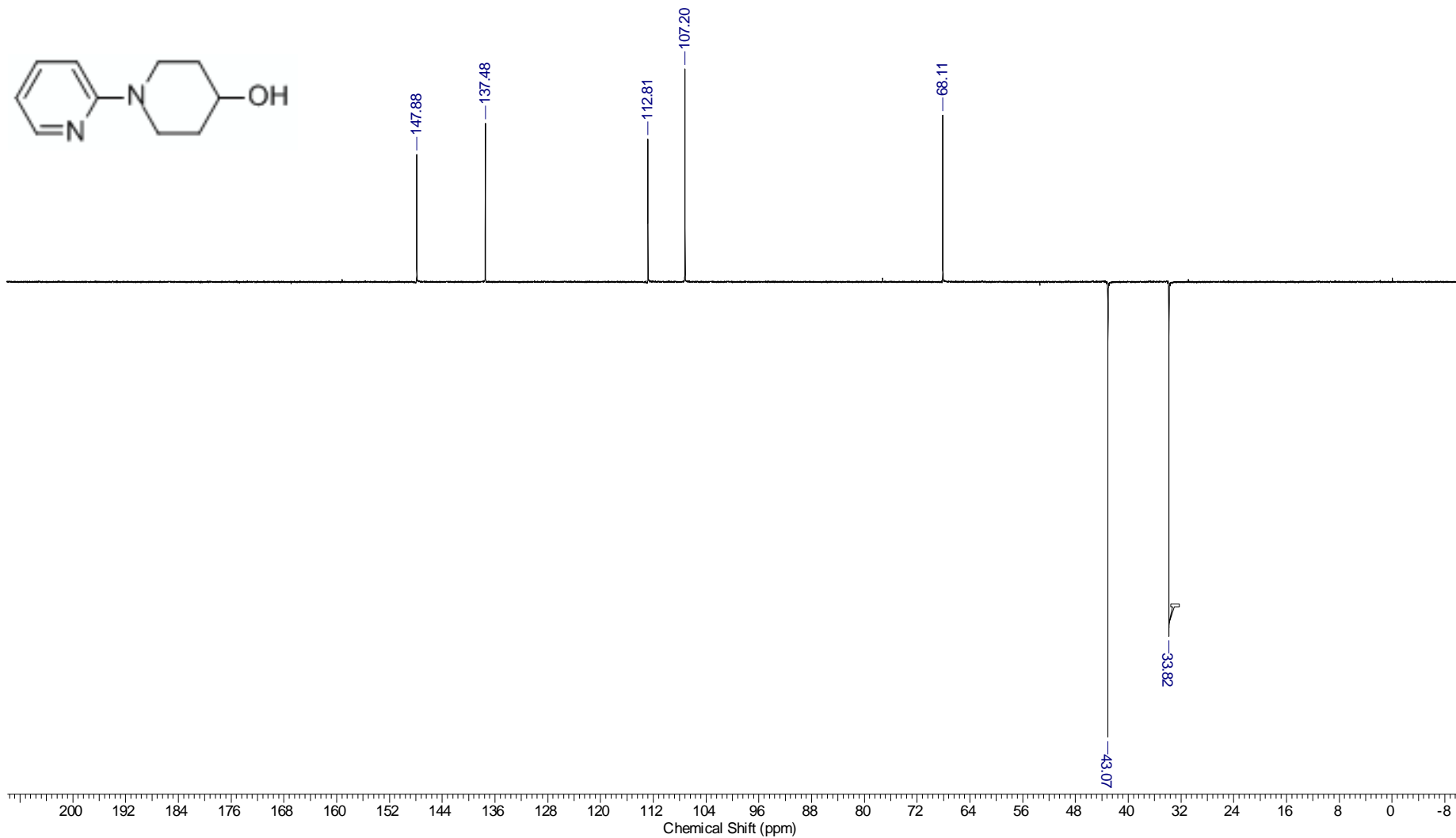
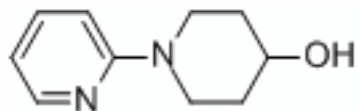
Nucleus	1H	Number of Transients	32	Origin	spect	Frequency (MHz)	360.13
Owner	SHR-NMRBDIS2	Points Count	16384	Pulse Sequence	zg30	Original Points Count	16384
SW(cyclical) (Hz)	5995.20	Solvent	CHLOROFORM-d			Receiver Gain	181.00
Spectrum Type	STANDARD	Sweep Width (Hz)	5994.84	Temperature (degree C)	27.000	Spectrum Offset (Hz)	2790.3096



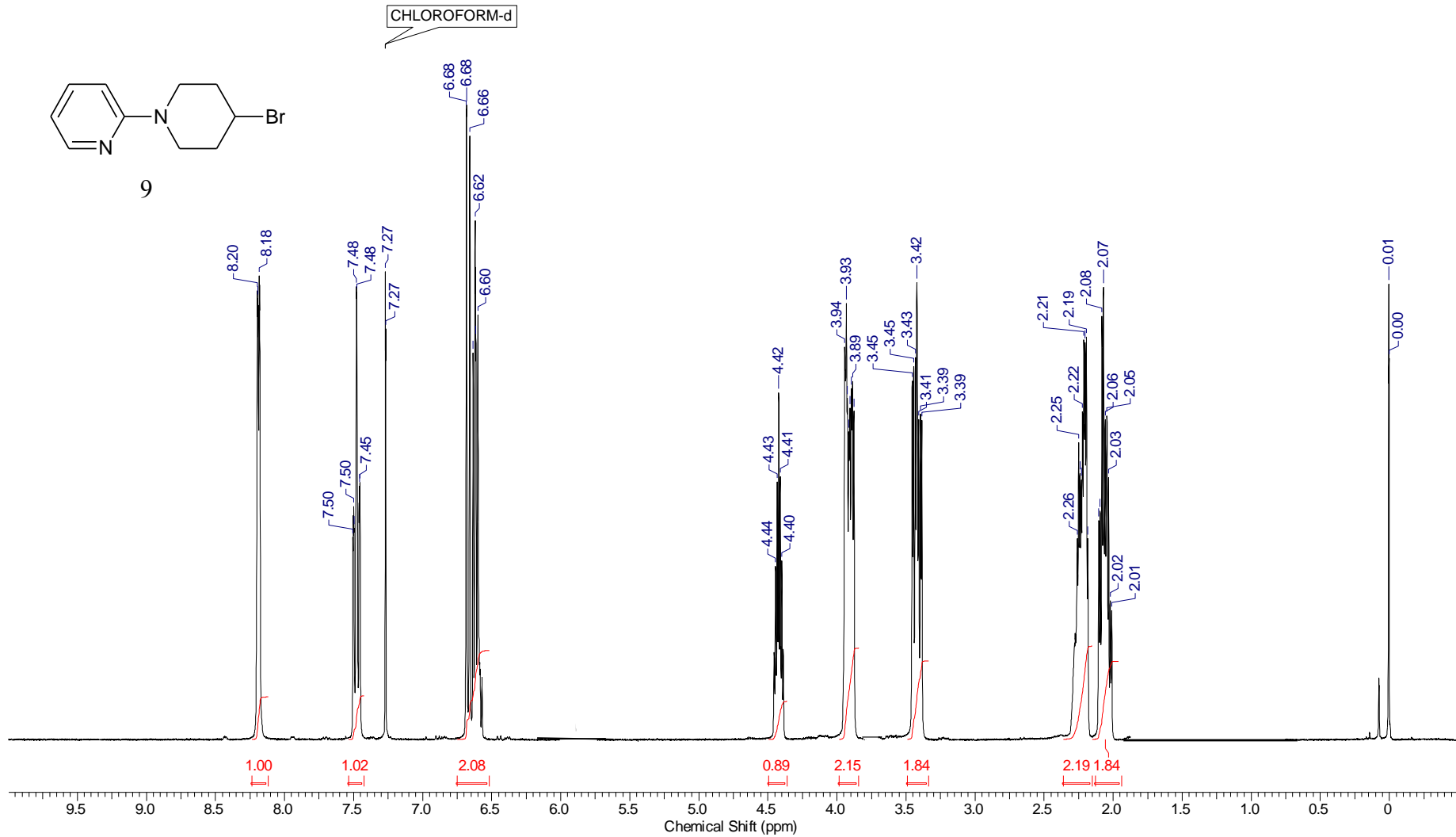
Nucleus	13C	Number of Transients	1200	Origin	spect	Frequency (MHz)	90.55
Owner	SHR-NMRBDIS2	Points Count	32768	Pulse Sequence	zgpg30	Original Points Count	32768
SW(cyclical) (Hz)	21645.02	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	9047.8457	Receiver Gain	14596.50
Sweep Width (Hz)	21644.36	Temperature (degree C)	27.000			Spectrum Type	STANDARD



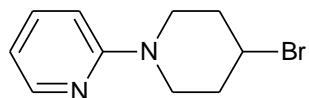
Nucleus	13C	Number of Transients	3000	Origin	spect	Frequency (MHz)	90.55
Owner	SHR-NMRBDIS2	Points Count	32768	Pulse Sequence	dept135	Original Points Count	32768
SW(cyclical) (Hz)	21645.02	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	9048.1689	Receiver Gain	16384.00
Sweep Width (Hz)	21644.36	Temperature (degree C)	27.000			Spectrum Type	DEPT135



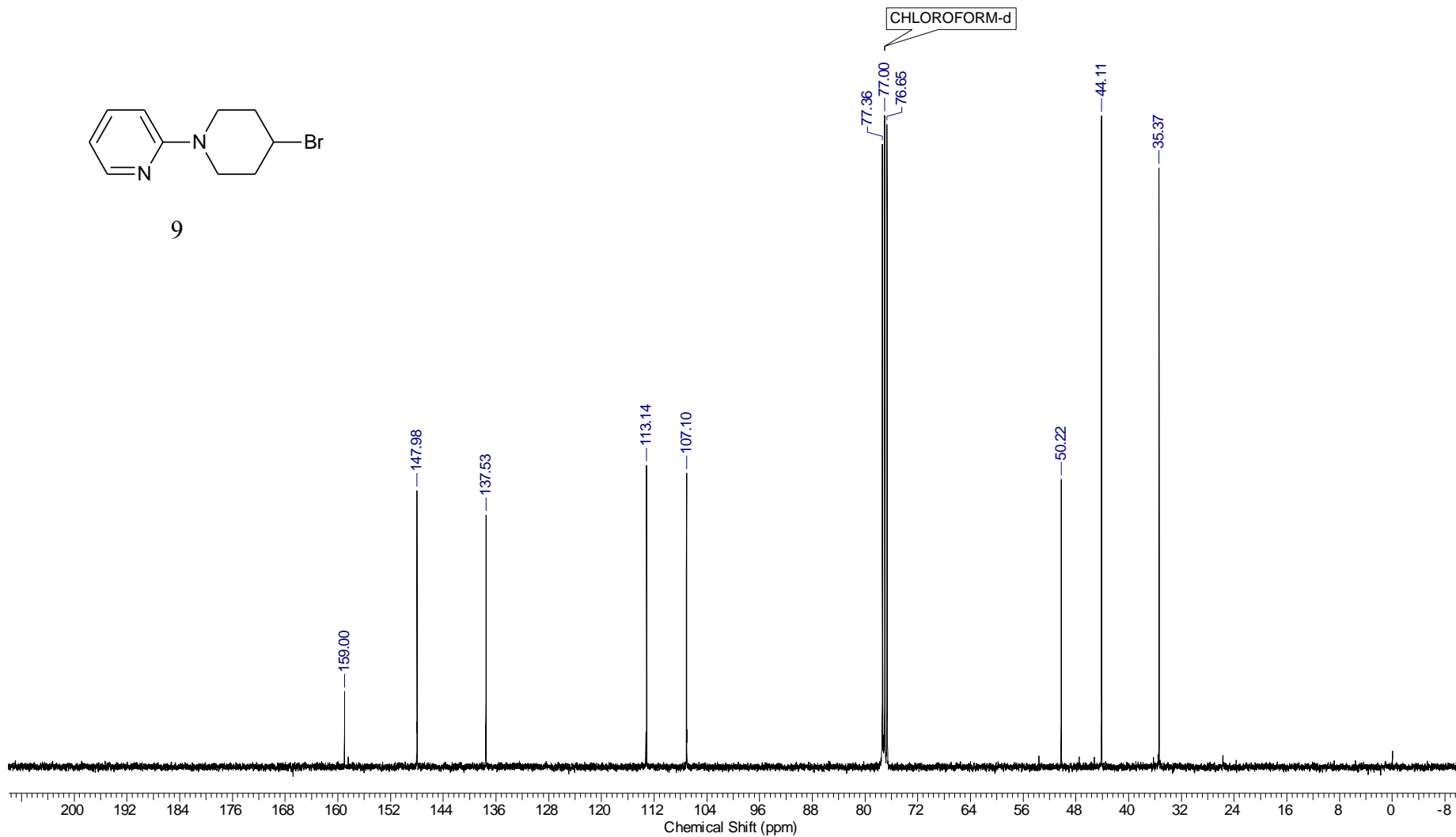
Nucleus	1H	Number of Transients	32	Origin	spect	Frequency (MHz)	360.13
Owner	SHR-NMRBDIS2	Points Count	16384	Pulse Sequence	zg30	Original Points Count	16384
SW(cyclical) (Hz)	5995.20	Solvent	CHLOROFORM-d	Spectrum Type	STANDARD	Receiver Gain	322.50
		Sweep Width (Hz)	5994.84	Temperature (degree C)	27.000	Spectrum Offset (Hz)	2789.5776



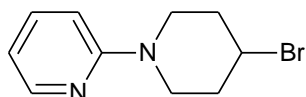
Nucleus	13C	Number of Transients	1200	Origin	spect	Frequency (MHz)	90.55
Owner	SHR-NMRBDIS2	Points Count	32768	Pulse Sequence	zgpg30	Original Points Count	32768
SW(cyclical) (Hz)	21645.02	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	9049.8271	Receiver Gain	14596.50
Sweep Width (Hz)	21644.36	Temperature (degree C)	27.000			Spectrum Type	STANDARD



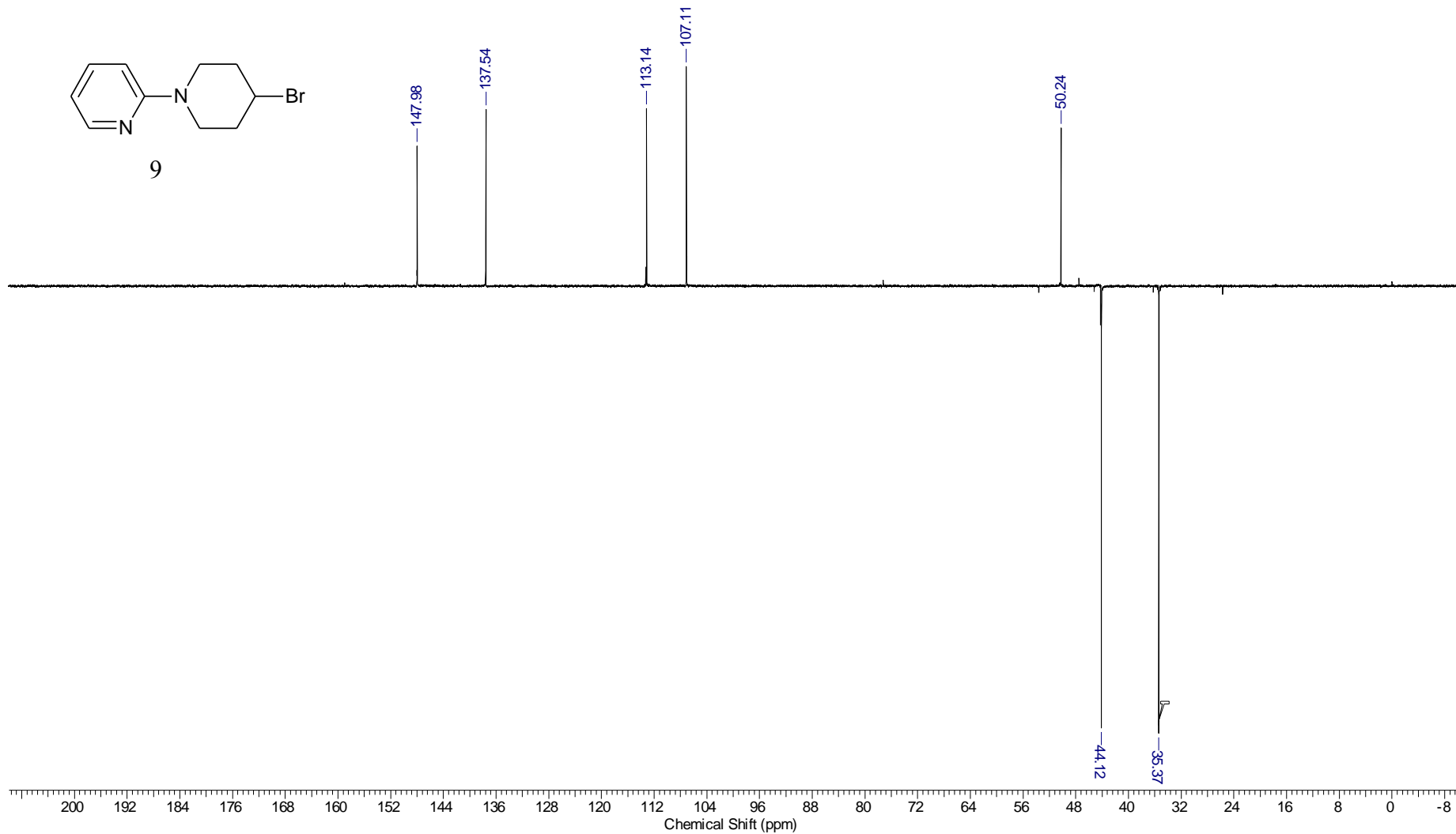
9



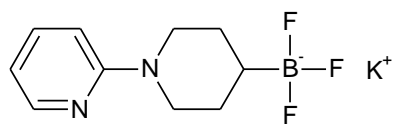
Nucleus	13C	Number of Transients	3000	Origin	spect	Frequency (MHz)	90.55
Owner	SHR-NMRBDIS2	Points Count	32768	Pulse Sequence	dept135	Original Points Count	32768
SW(cyclical) (Hz)	21645.02	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	9050.4727	Receiver Gain	16384.00
Sweep Width (Hz)	21644.36	Temperature (degree C)	27.000			Spectrum Type	DEPT135



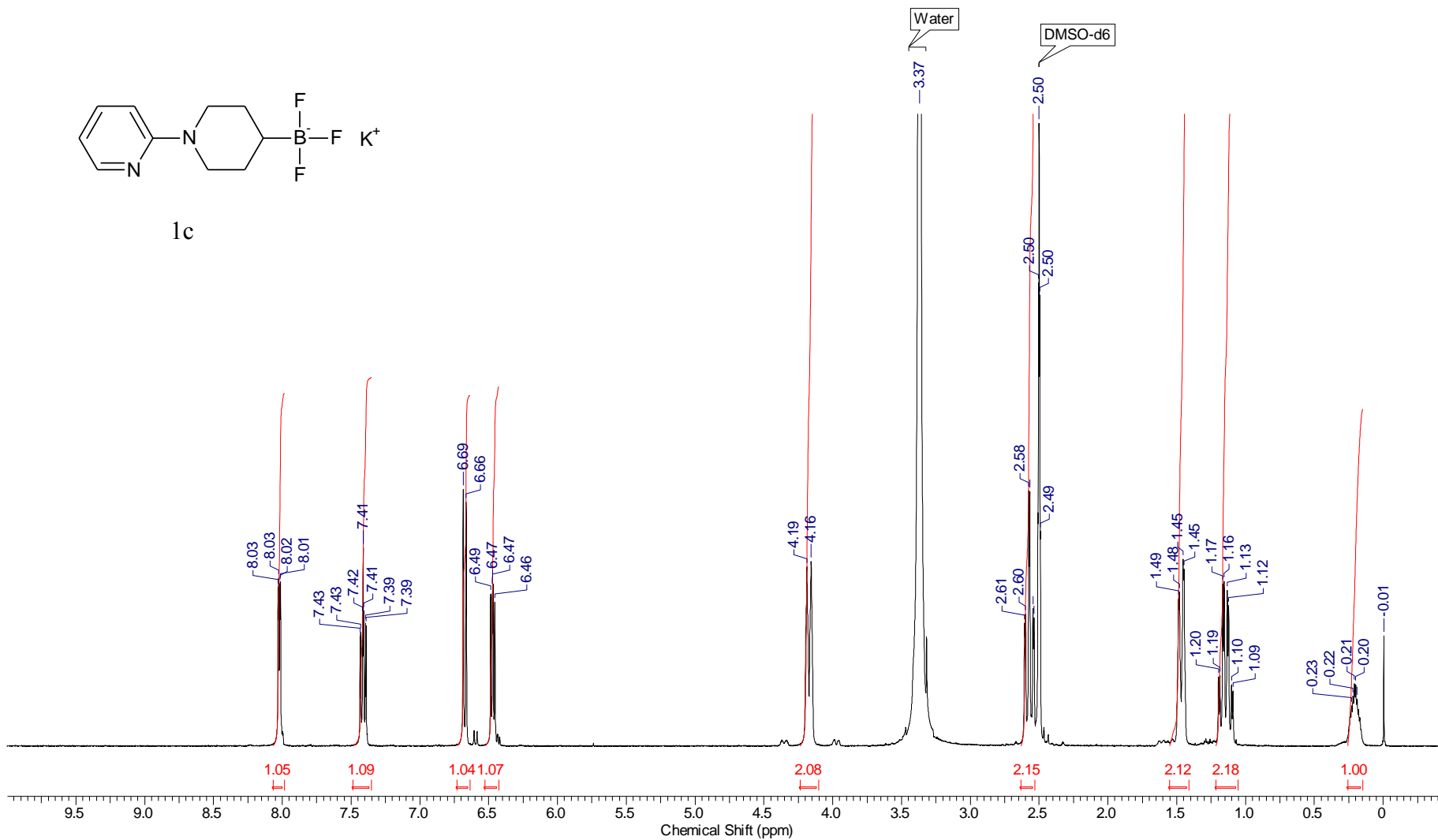
9



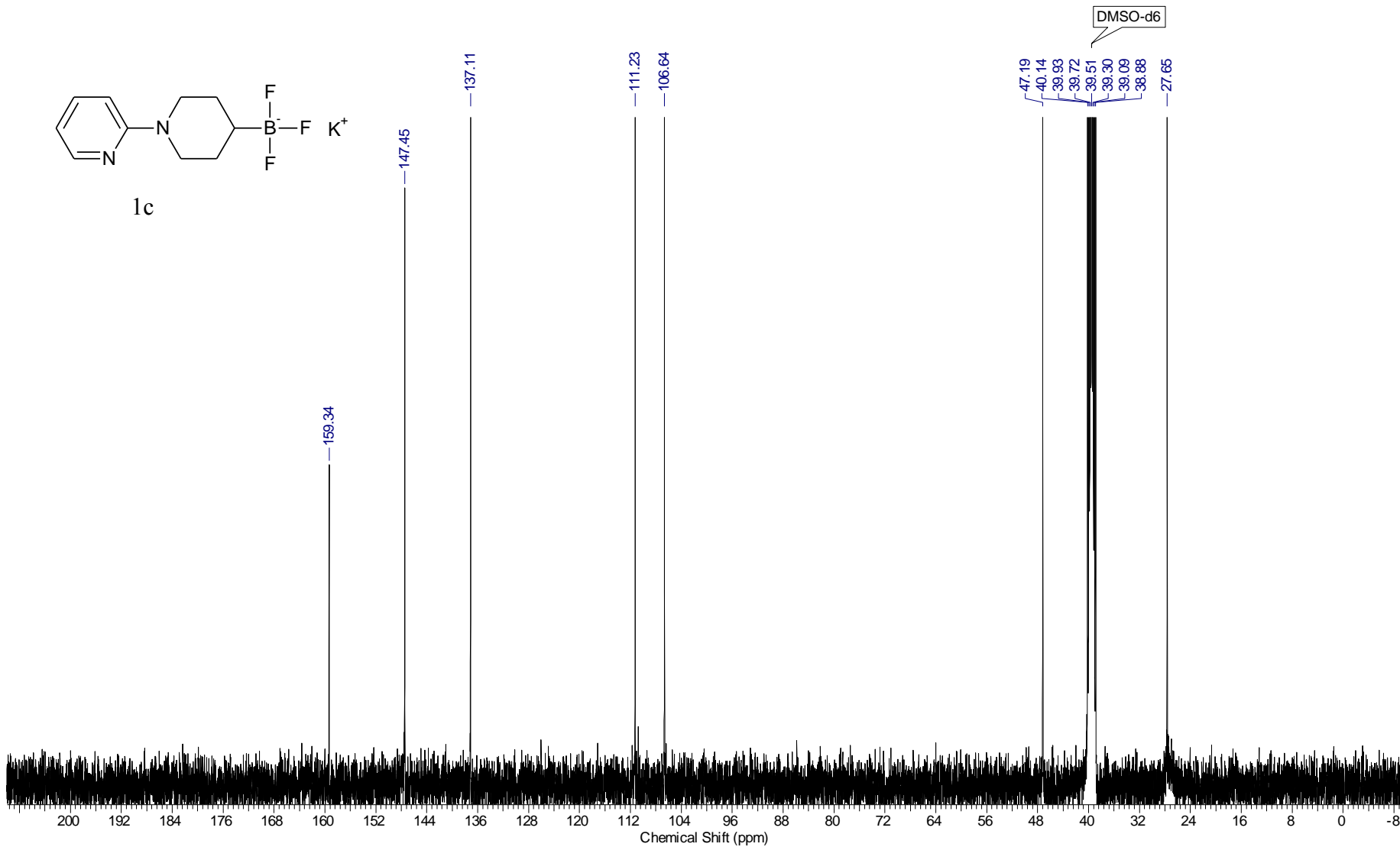
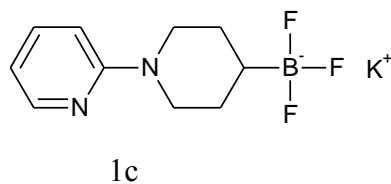
Frequency (MHz)	400.40	Nucleus	1H	Number of Transients	16	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	SW(cyclical) (Hz)	7211.32
Solvent	DMSO-d6	Spectrum Offset (Hz)	3397.9224	Sweep Width (Hz)	7211.10	Temperature (degree C)	27.000



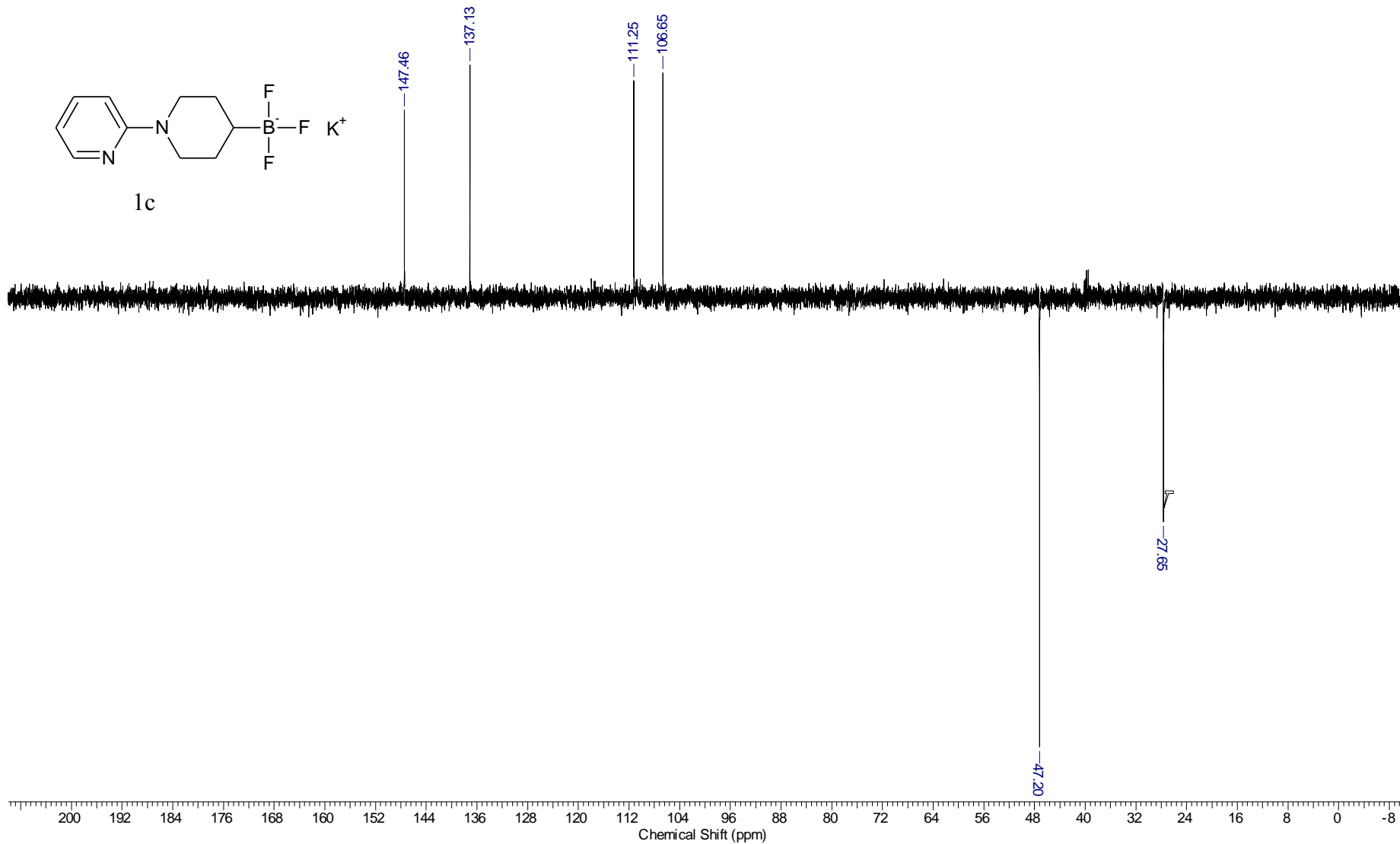
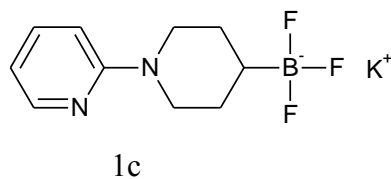
1c



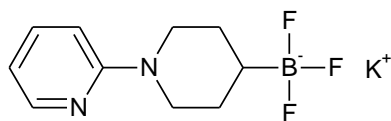
Frequency (MHz)	100.69	Nucleus	¹³ C	Number of Transients	1024	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	SW(cyclical) (Hz)	24037.73
Solvent	DMSO-d6	Spectrum Offset (Hz)	10022.5674	Sweep Width (Hz)	24036.99	Temperature (degree C)	26.100



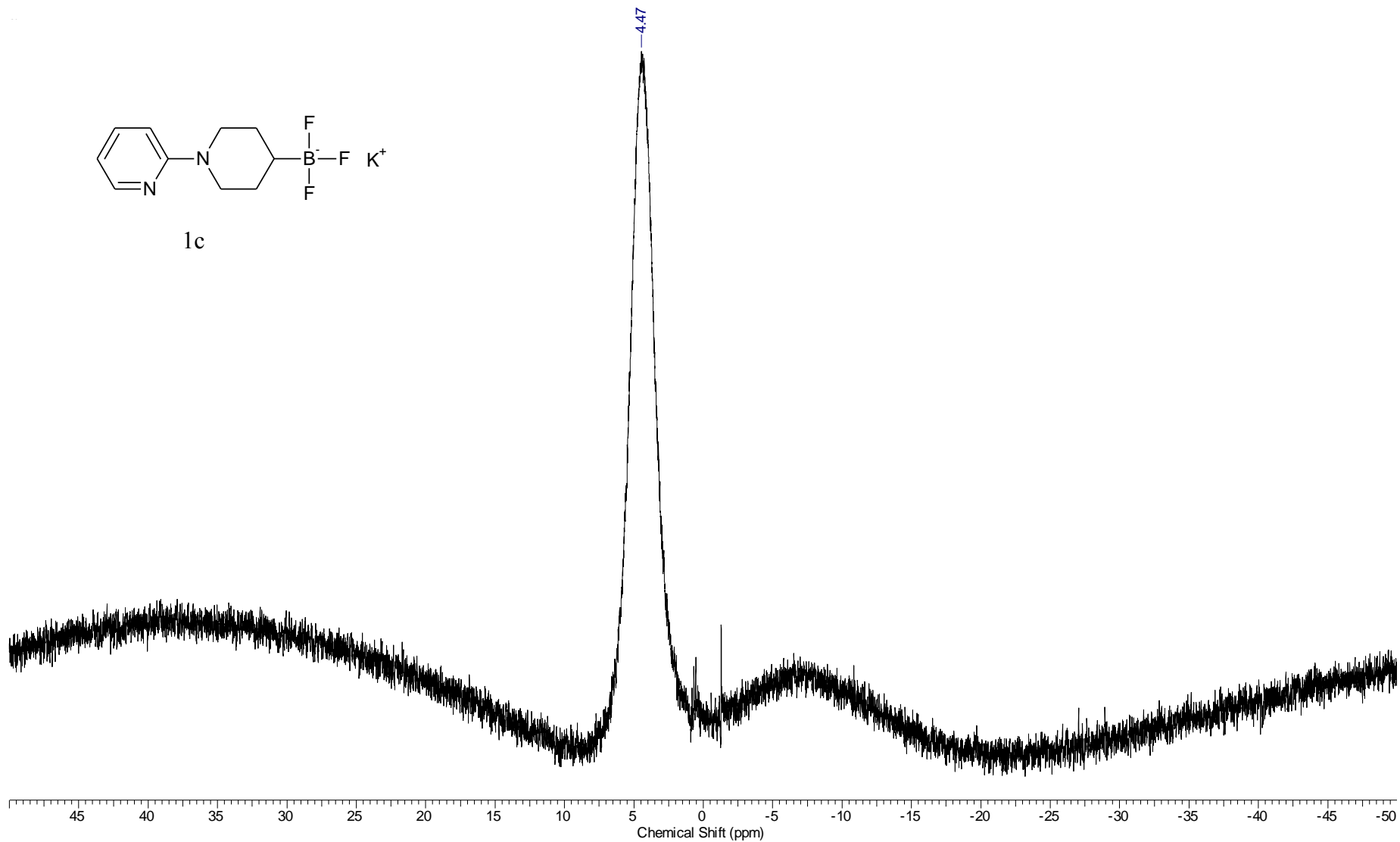
Frequency (MHz)	100.69	Nucleus	13C	Number of Transients	256	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	SW(cyclical) (Hz)	24037.73
Solvent	DMSO-d6	Spectrum Offset (Hz)	10024.0996	Sweep Width (Hz)	24036.99	Temperature (degree C)	27.000



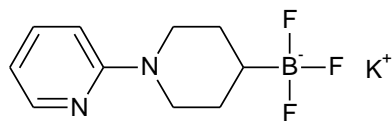
Frequency (MHz)	128.46	Nucleus	11B	Number of Transients	128	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	SW(cyclical) (Hz)	25509.43
Solvent	DMSO-d6	Spectrum Offset (Hz)	1.2842	Sweep Width (Hz)	25508.65	Temperature (degree C)	27.000



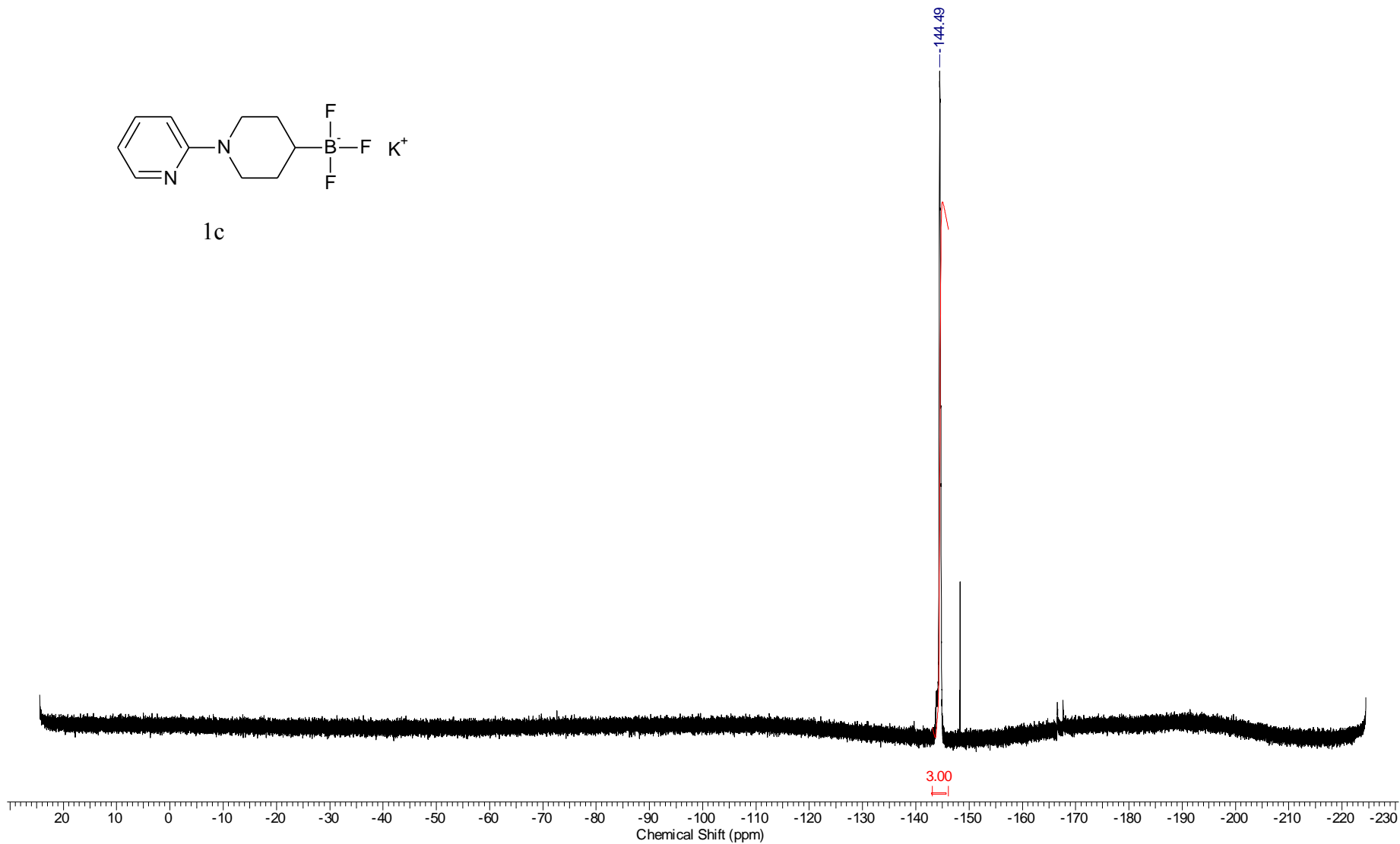
1c



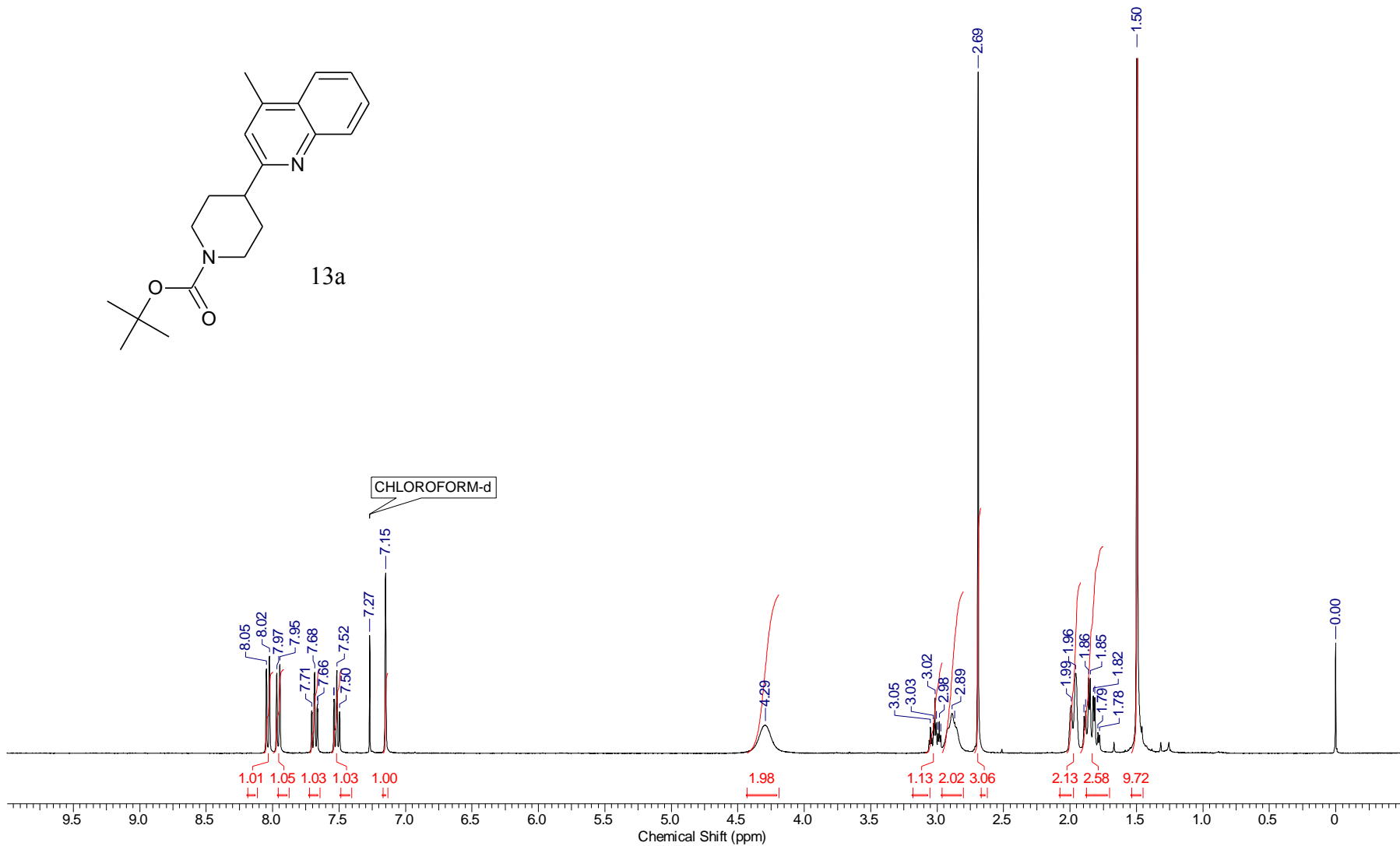
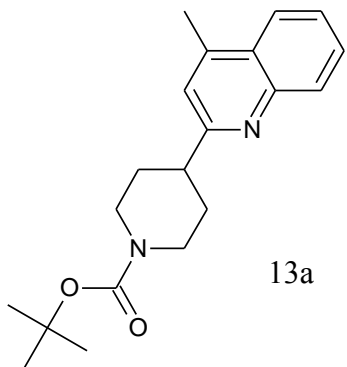
Frequency (MHz)	376.71	Nucleus	¹⁹ F	Number of Transients	64	Origin	Bruker BioSpin GmbH
Original Points Count	131072	Owner	tibbe_operator	Points Count	131072	SW(cyclical) (Hz)	93749.28
Solvent	DMSO-d6	Spectrum Offset (Hz)	-37674.7617	Sweep Width (Hz)	93748.56	Temperature (degree C)	27.000



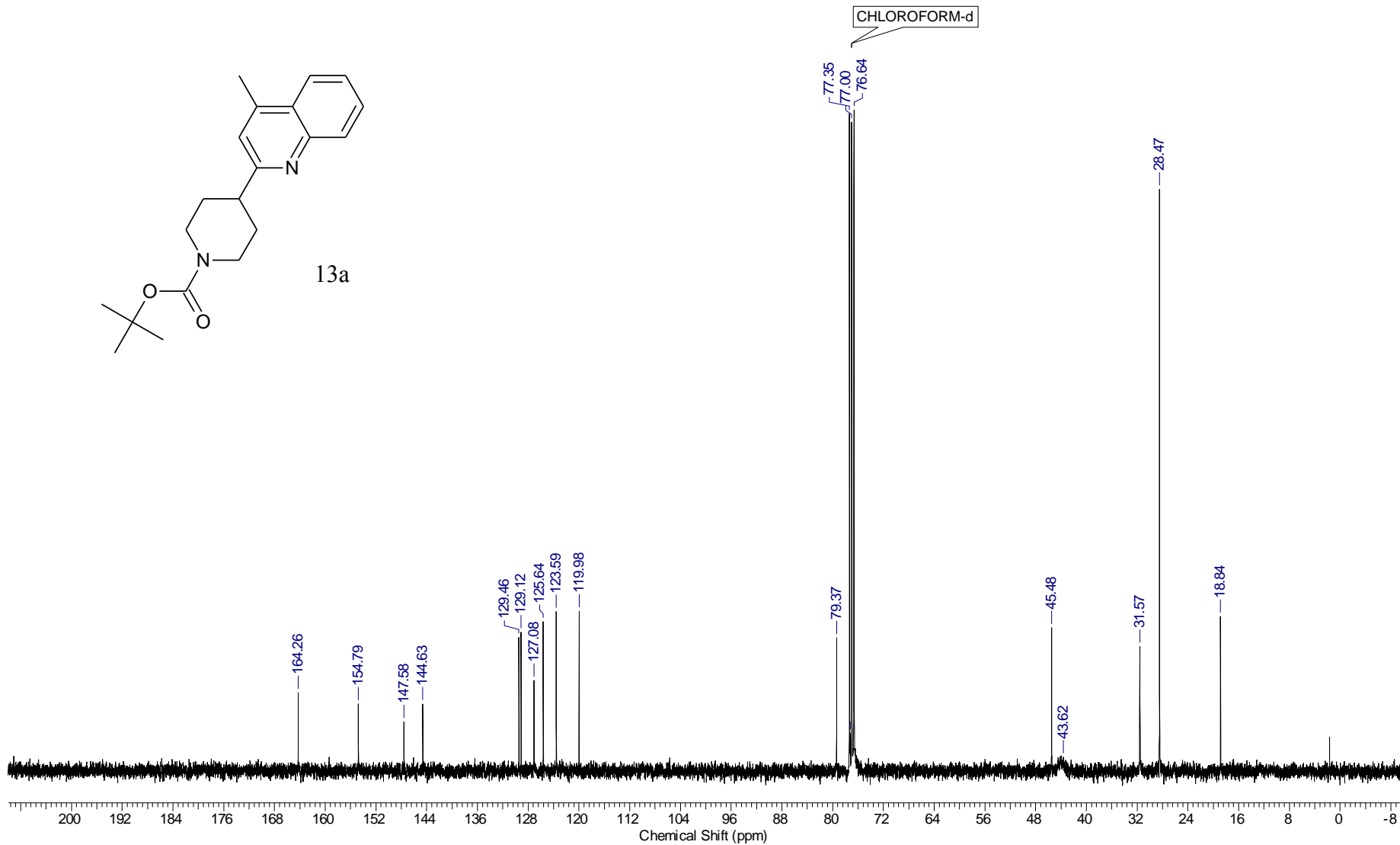
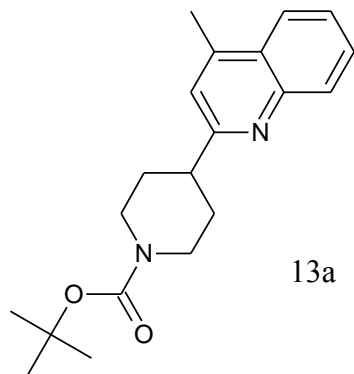
1c



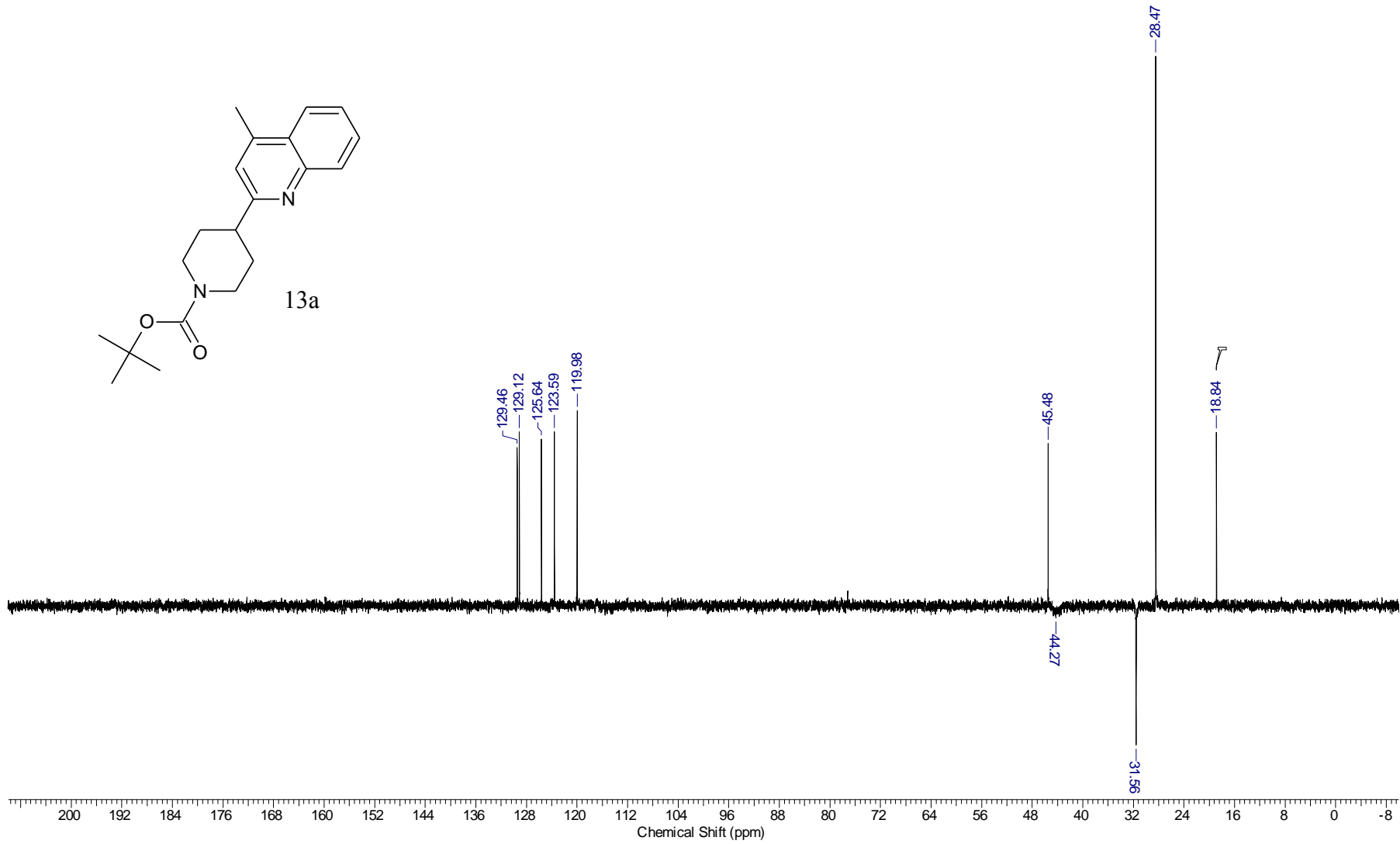
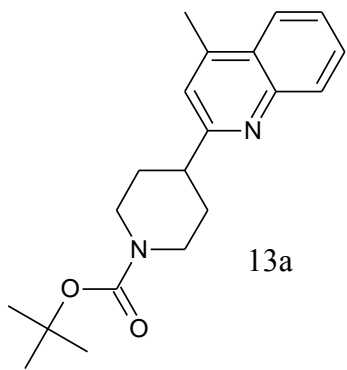
					Frequency (MHz)	360.13	
Nucleus	1H	Number of Transients	16	Origin	Bruker BioSpin GmbH		
Original Points Count	16384	Owner	SHR-NMRBDIS2	Points Count	16384	SW(cyclical) (Hz)	5995.20
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2789.9641	Sweep Width (Hz)	5994.84	Temperature (degree C)	27.000



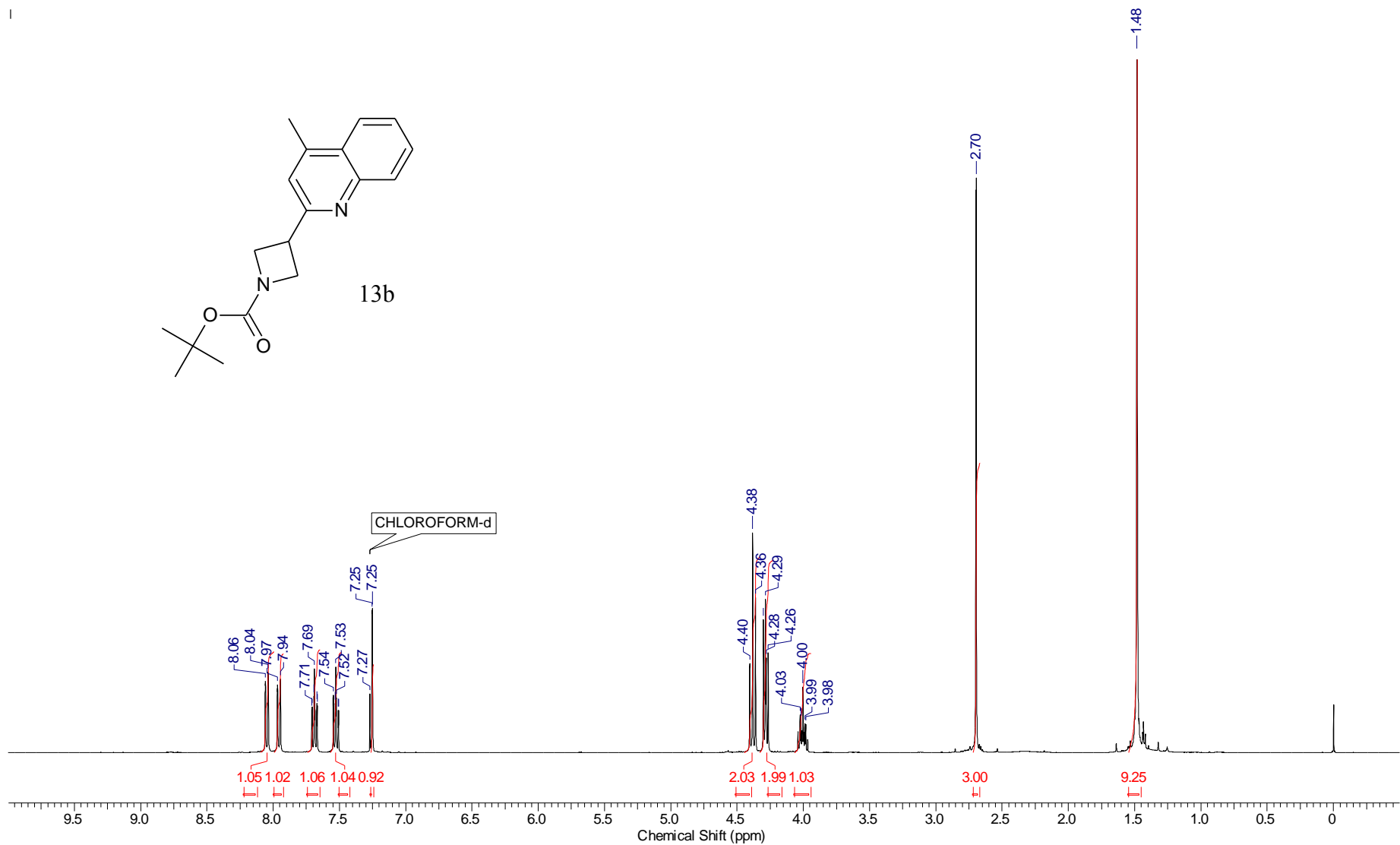
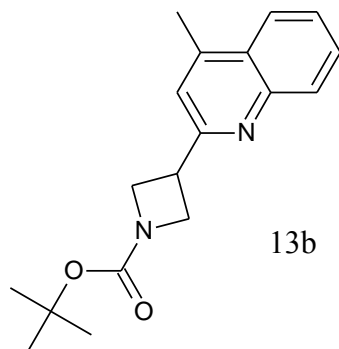
Nucleus	13C	Number of Transients	300	Origin	Bruker BioSpin GmbH	
Original Points Count	32768	Owner	SHR-NMRBDIS2	Points Count	32768	SW(cyclical) (Hz) 21645.02
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	9050.5244	Sweep Width (Hz)	21644.36	Temperature (degree C) 27.000



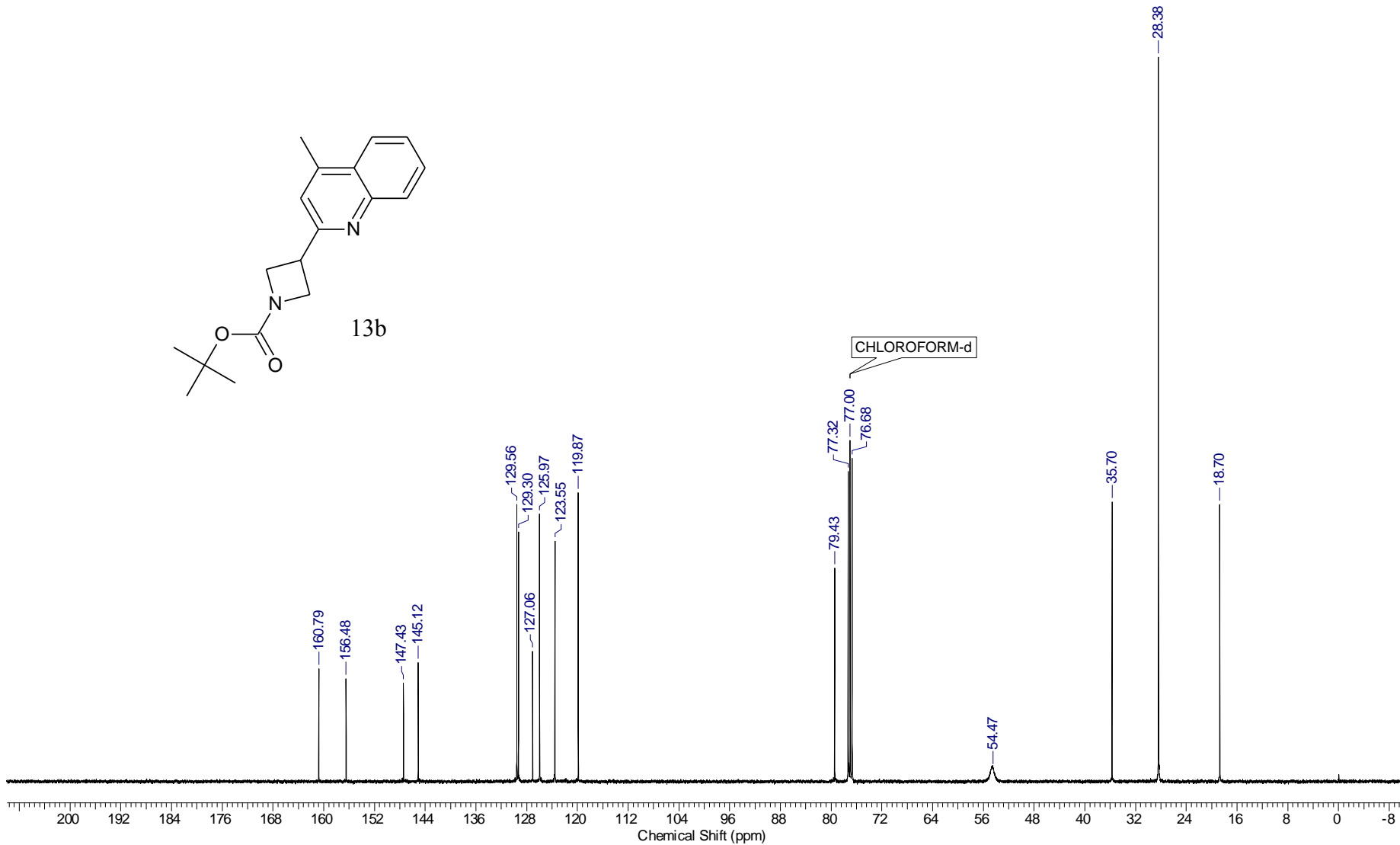
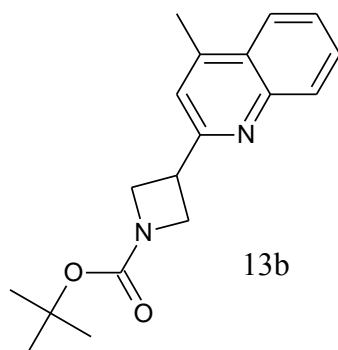
				Frequency (MHz)	
Nucleus	13C	Number of Transients	256	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	SHR-NMRBDIS2	Points Count	32768
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	9049.9277	SW(cyclical) (Hz)	21645.02
				Sweep Width (Hz)	21644.36
				Temperature (degree C)	27.000



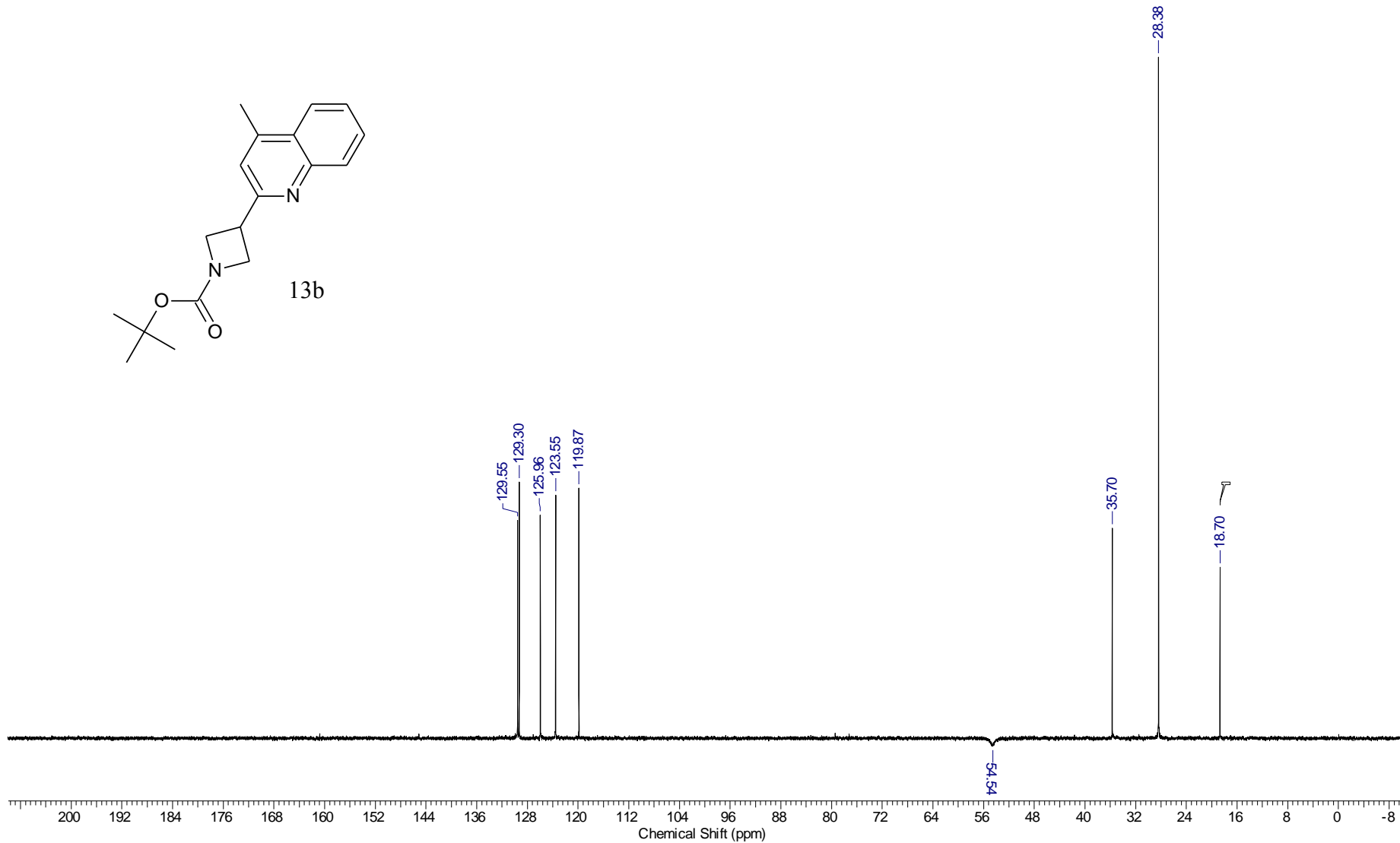
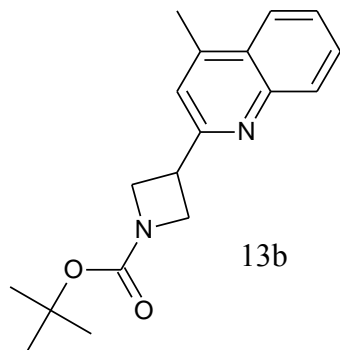
Frequency (MHz)	400.40	Nucleus	1H	Number of Transients	16	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	SW(cyclical) (Hz)	7211.32
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	3395.8613	Sweep Width (Hz)	7211.10	Temperature (degree C)	27.000



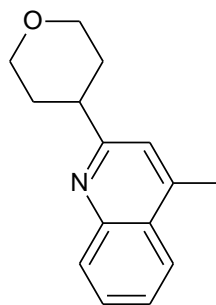
Frequency (MHz)	100.69	Nucleus	13C	Number of Transients	1024	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	SW(cyclical) (Hz)	24037.73
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10060.6406	Sweep Width (Hz)	24036.99	Temperature (degree C)	27.000



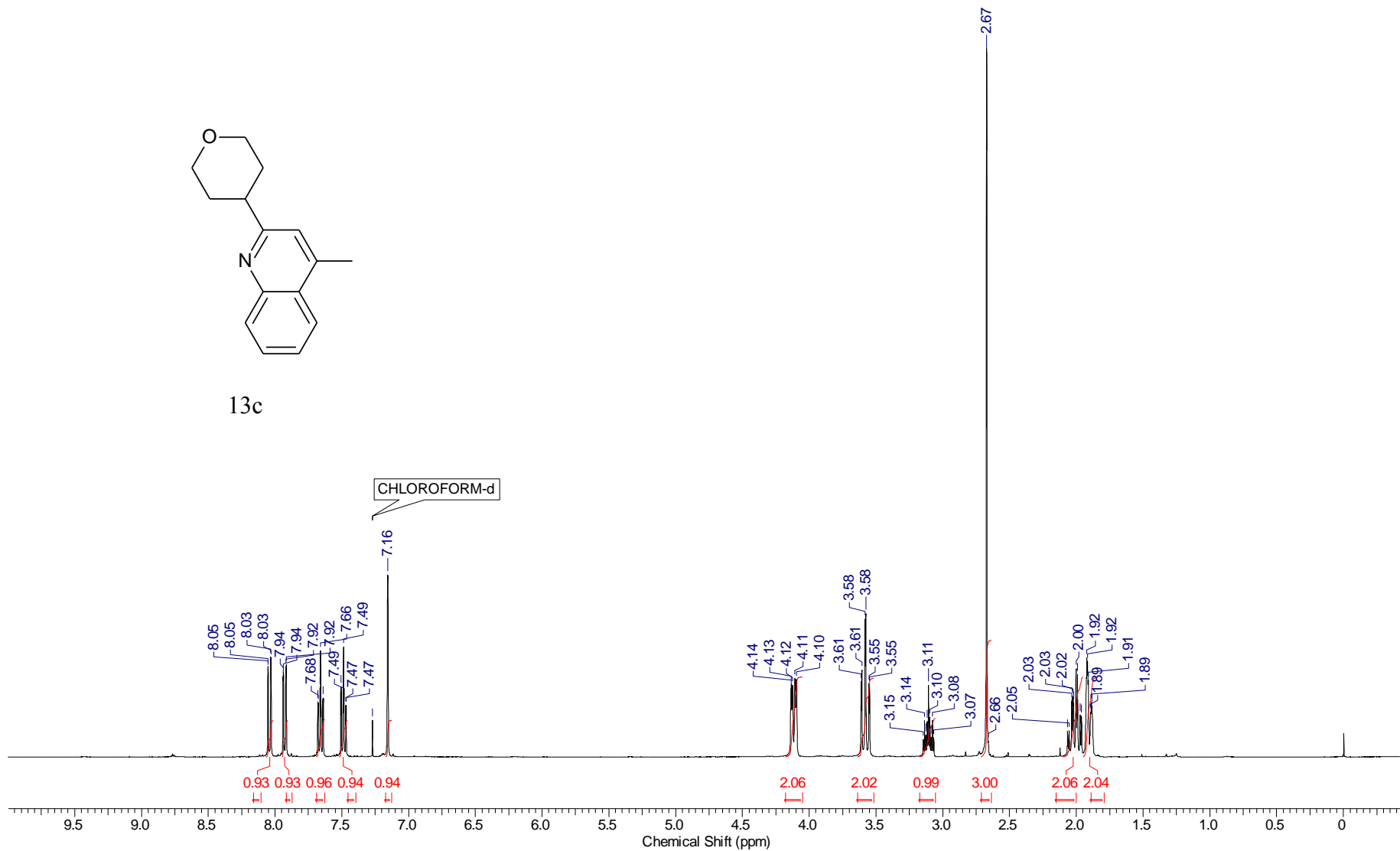
Frequency (MHz)	100.69	Nucleus	13C	Number of Transients	256	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	SW(cyclical) (Hz)	24037.73
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10060.4238	Sweep Width (Hz)	24036.99	Temperature (degree C)	27.000



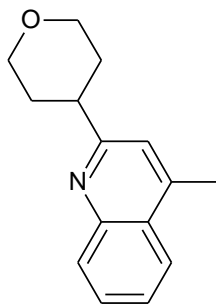
Frequency (MHz)	400.40	Nucleus	1H	Number of Transients	16	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	SW(cyclical) (Hz)	7211.32
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	3395.6414	Sweep Width (Hz)	7211.10	Temperature (degree C)	27.000



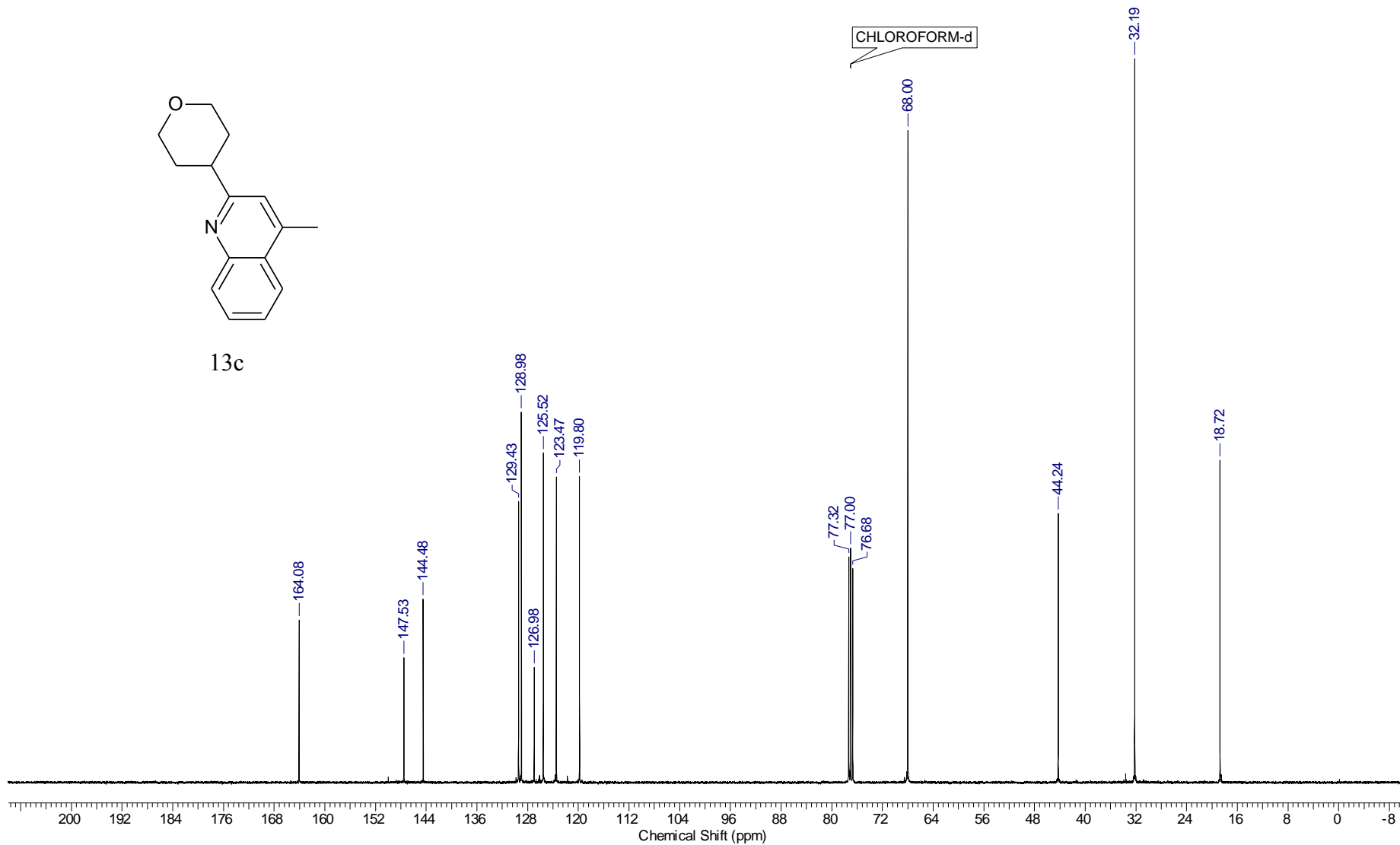
13c



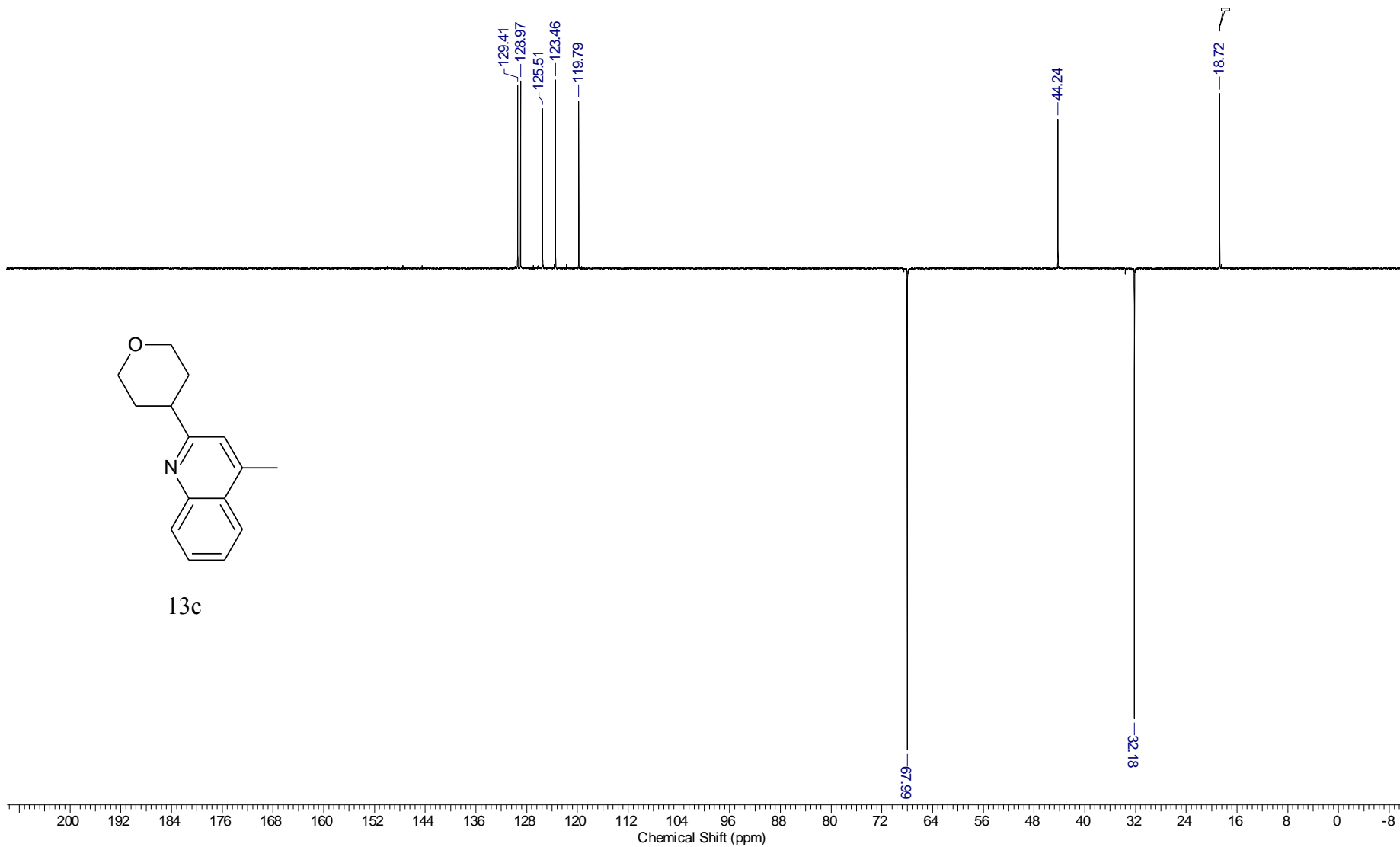
Frequency (MHz)	100.69	Nucleus	¹³ C	Number of Transients	1024	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	SW(cyclical) (Hz)	24037.73
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10055.5059	Sweep Width (Hz)	24036.99	Temperature (degree C)	27.000

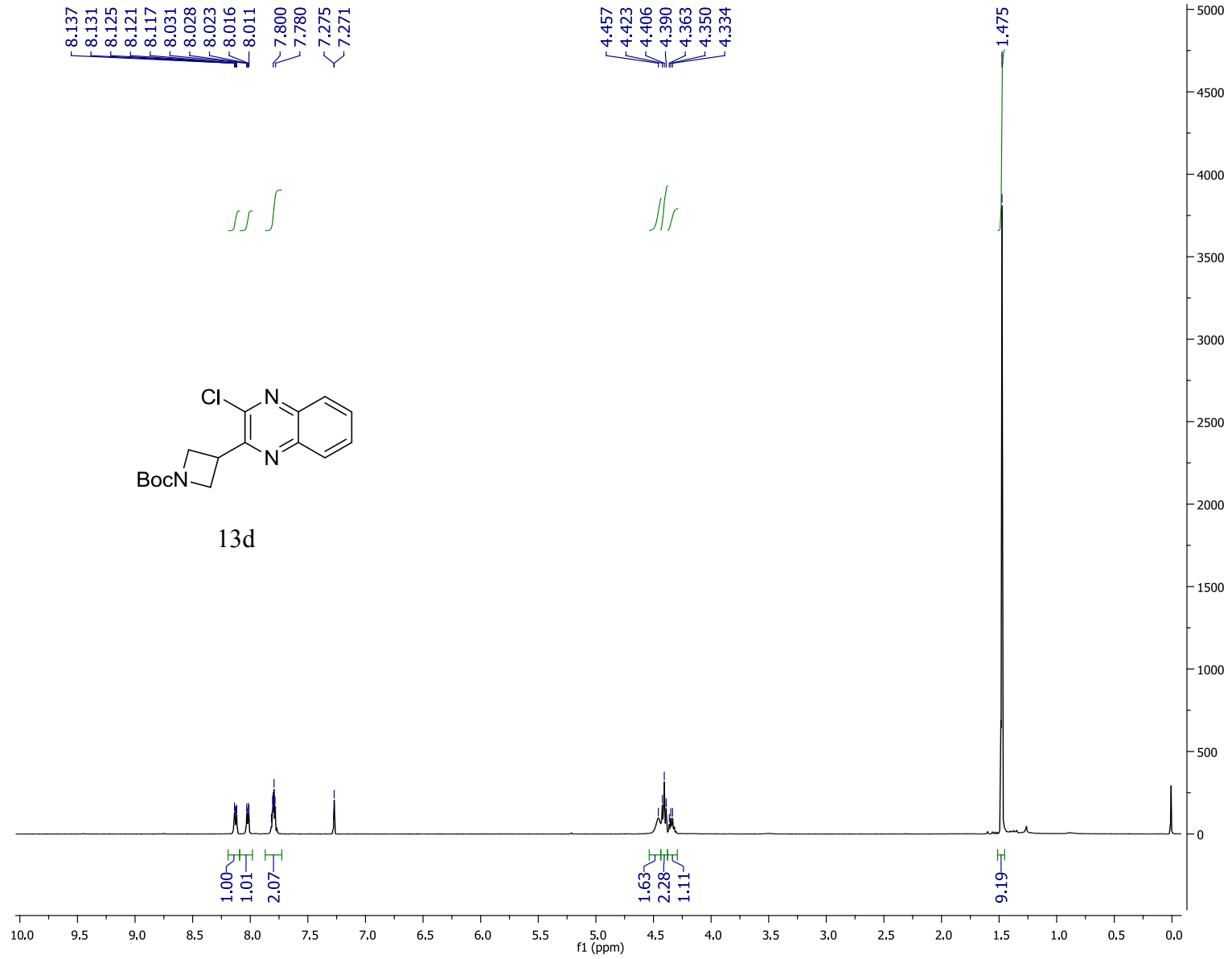


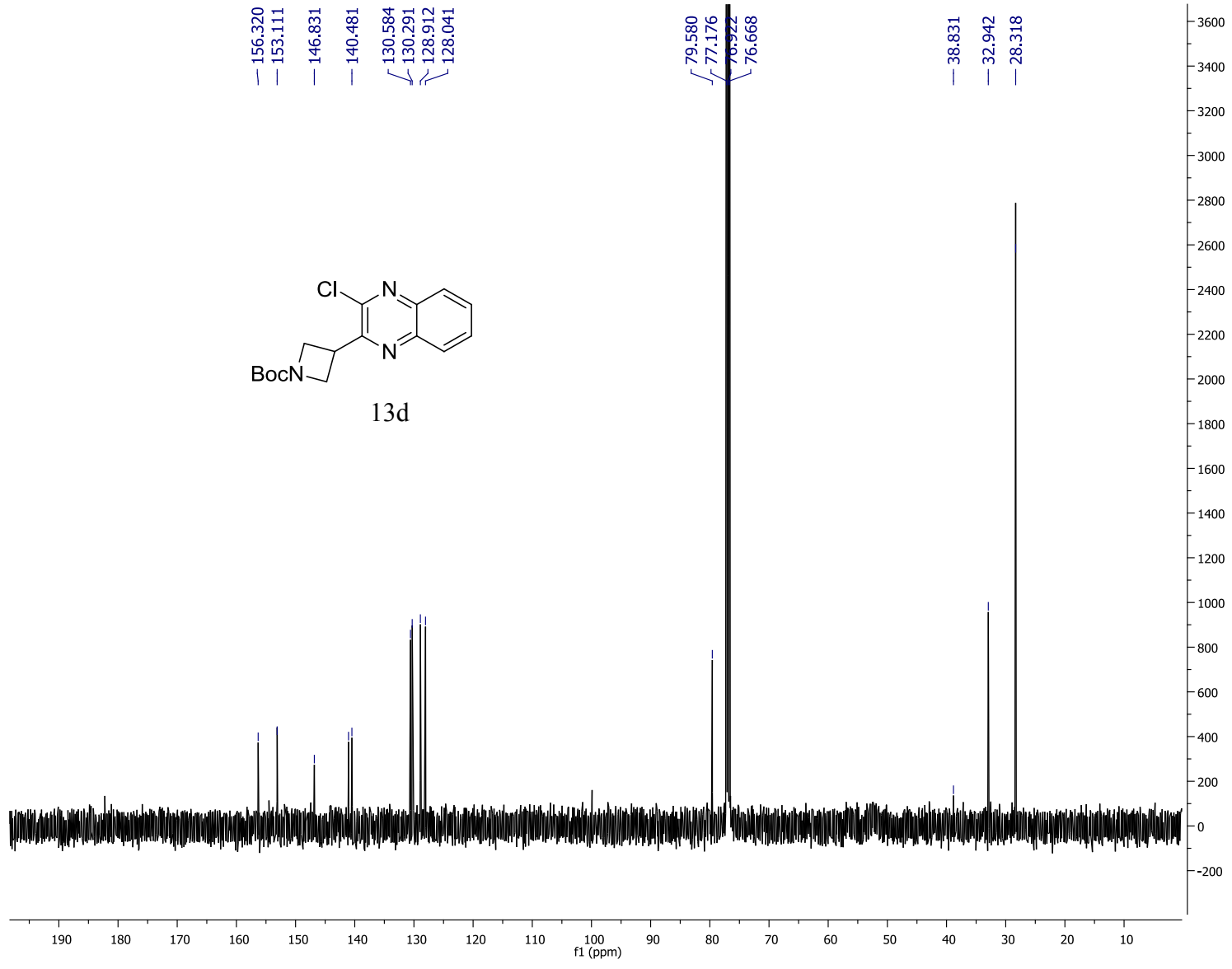
13c



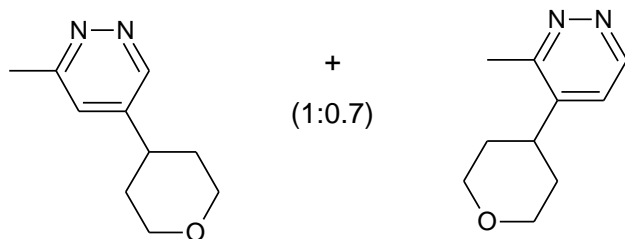
Frequency (MHz)	100.69	Nucleus	¹³ C	Number of Transients	256	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	SW(cyclical) (Hz)	24037.73
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10054.3682	Sweep Width (Hz)	24036.99	Temperature (degree C)	27.000



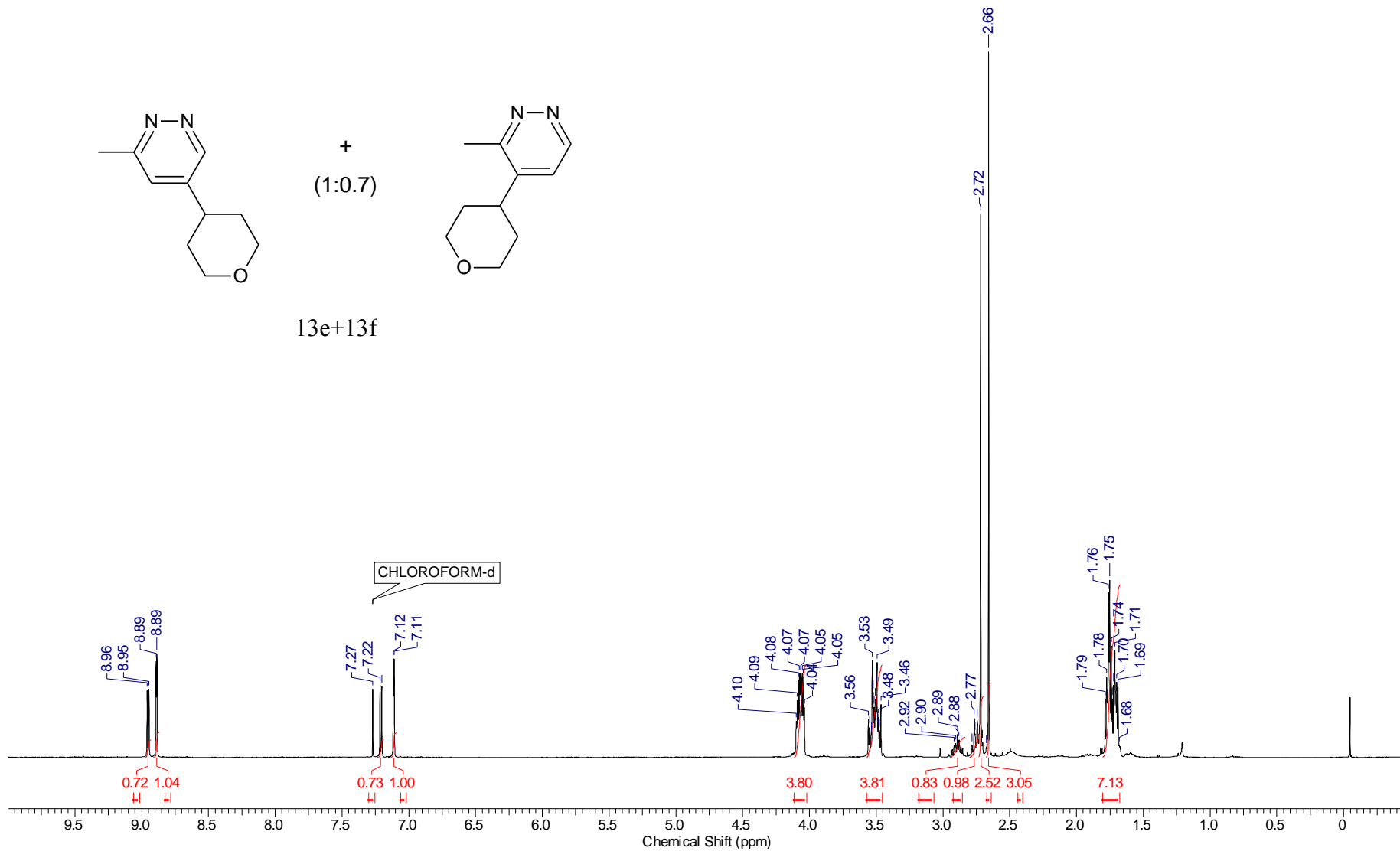




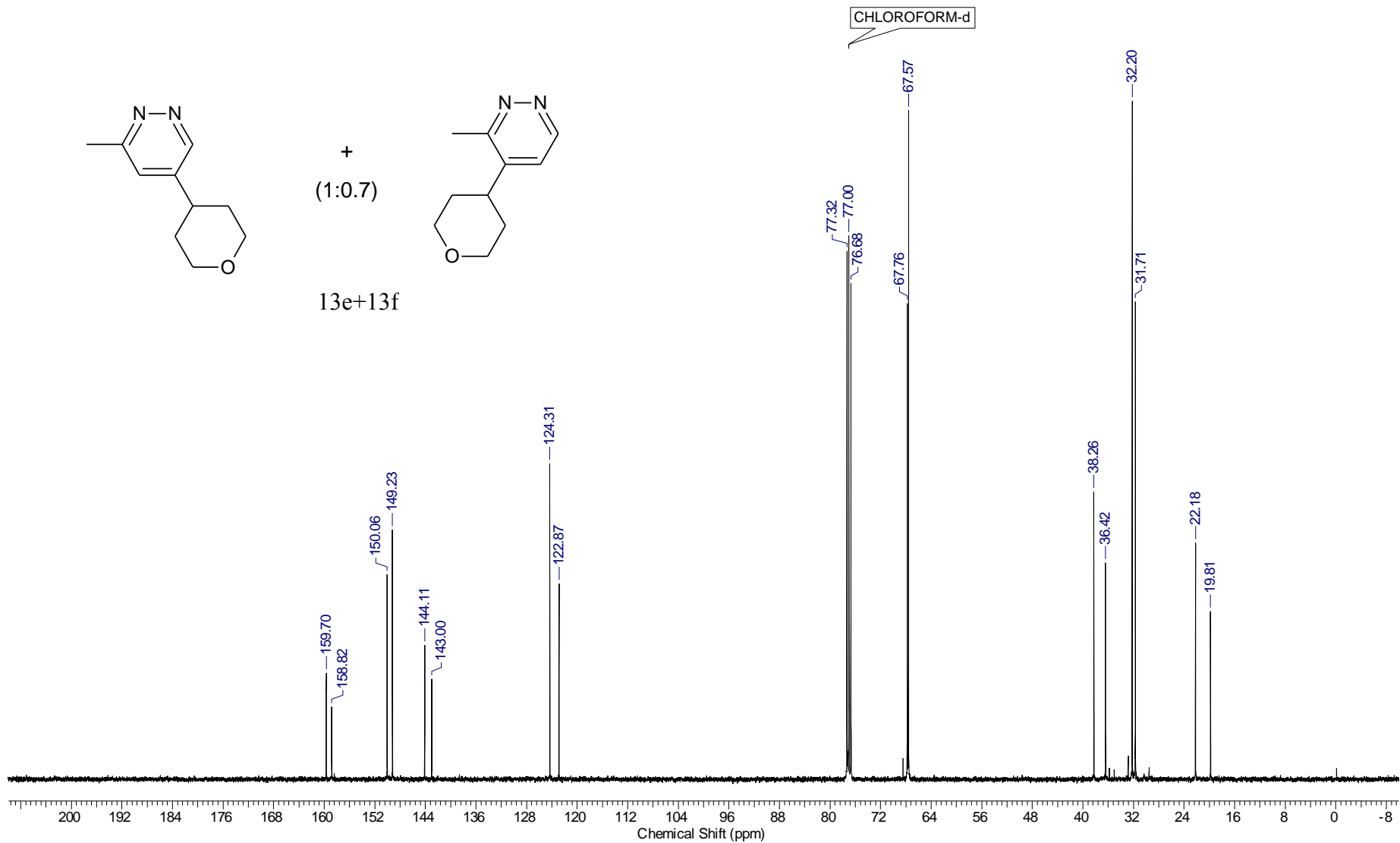
Frequency (MHz)	400.40	Nucleus	1H	Number of Transients	16	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	tibbe_operator	Points Count	32768	SW(cyclical) (Hz)	7211.32
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	3395.6414	Sweep Width (Hz)	7211.10	Temperature (degree C)	26.800



13e+13f



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)	10056.9727	Sweep Width (Hz)	24036.99	Temperature (degree C)	27.000



Frequency (MHz)	100.69	Nucleus	¹³ C	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)	10057.0195	Sweep Width (Hz)	24036.99	Temperature (degree C)	27.000

