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

Electronic Supplementary Information for:

Synthesis of *N*-[(dialkylamino)methyl)]acrylamides and *N*-[(dialkylamino)methyl]methacrylamides from Schiff base salts: Useful building blocks for smart polymers

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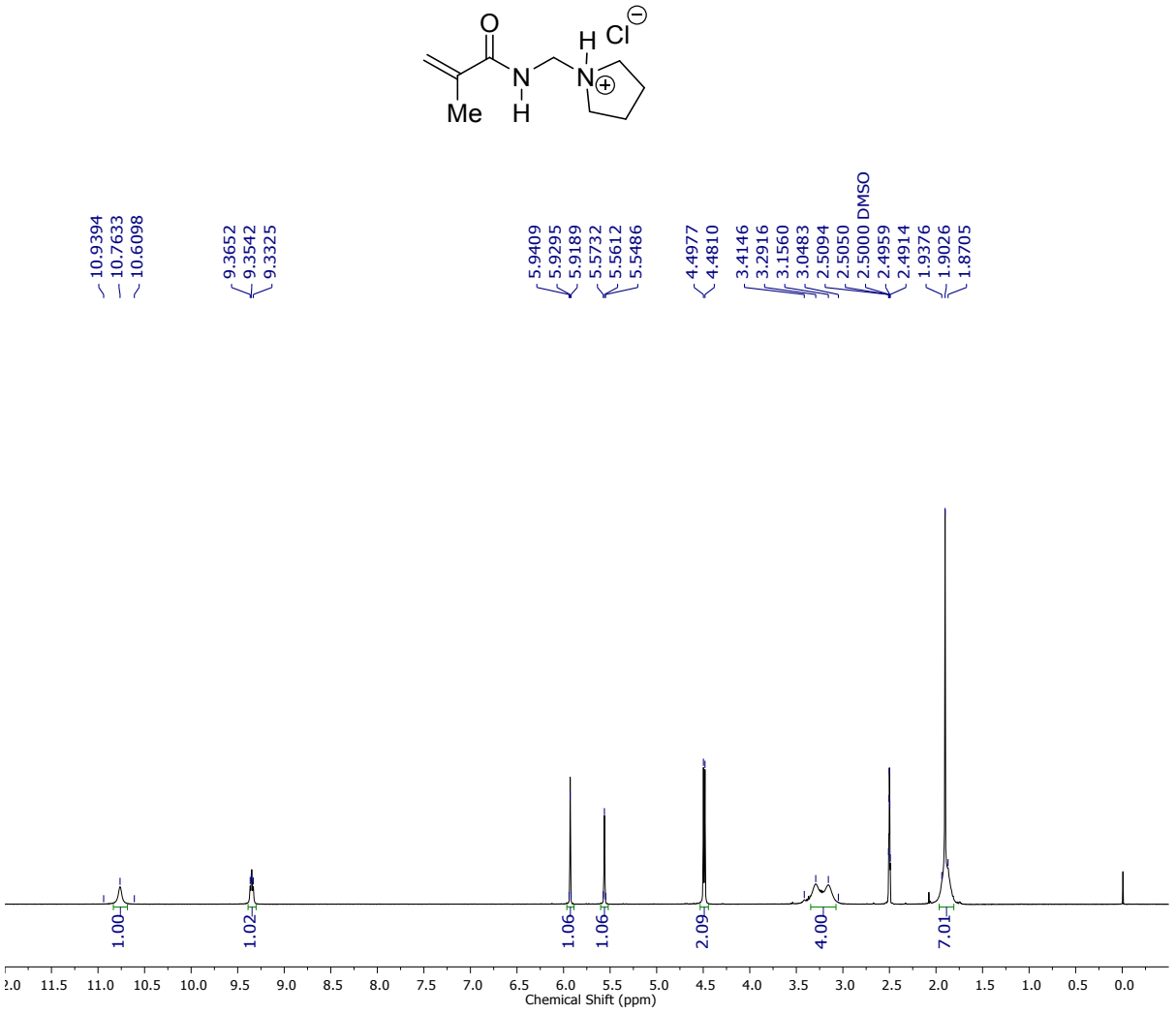
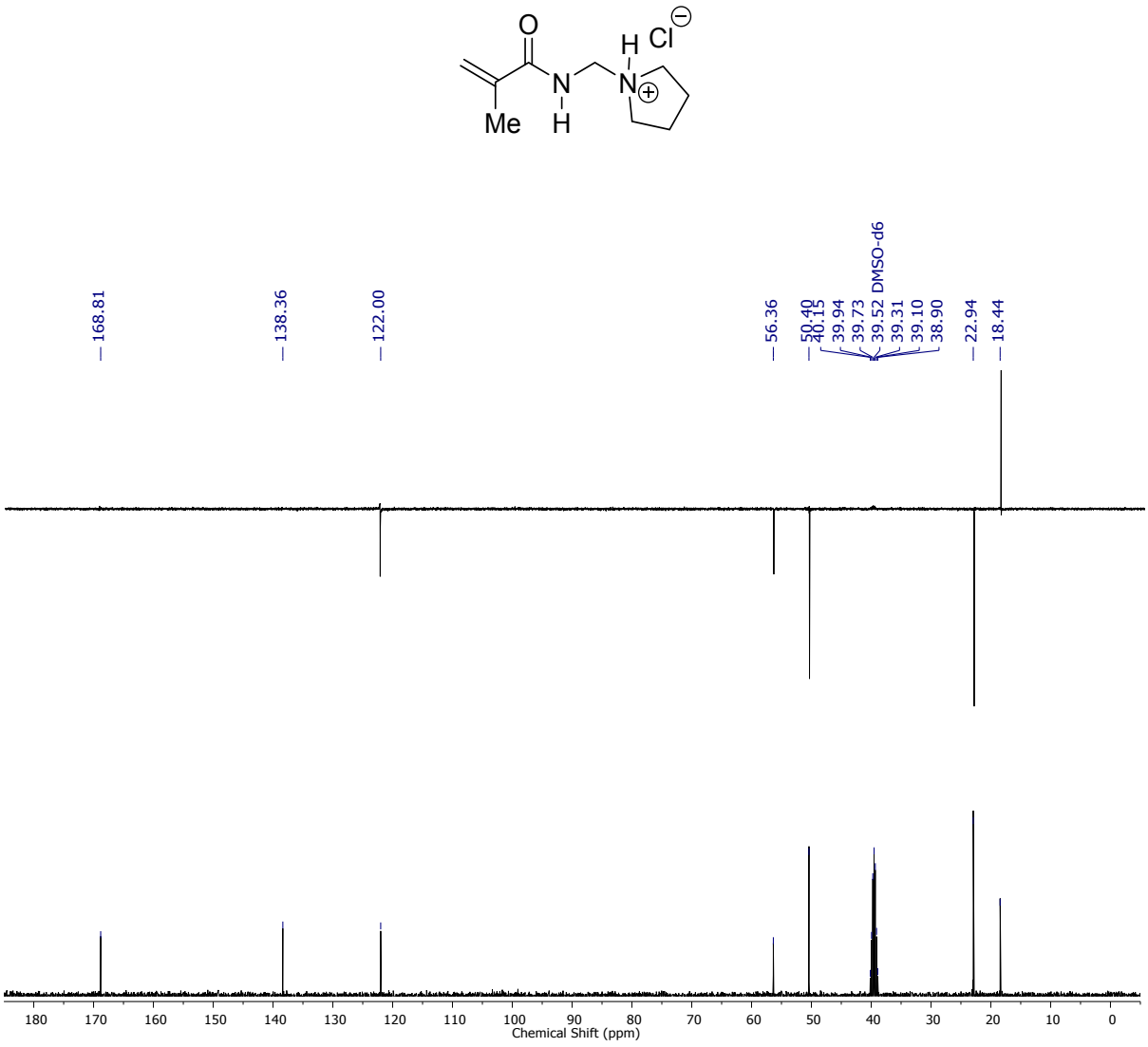
^{1}H NMR (400 MHz) of 2-methyl-*N*-[(pyrrolidin-1-yl)methyl]prop-2-enamide hydrochloride (2b.HCl) in $(CD_3)_2SO$.



^{13}C NMR (101 MHz) of 2-methyl-*N*-[(pyrrolidin-1-yl)methyl]prop-2-enamide hydrochloride (2b.HCl) in $(CD_3)_2SO$.



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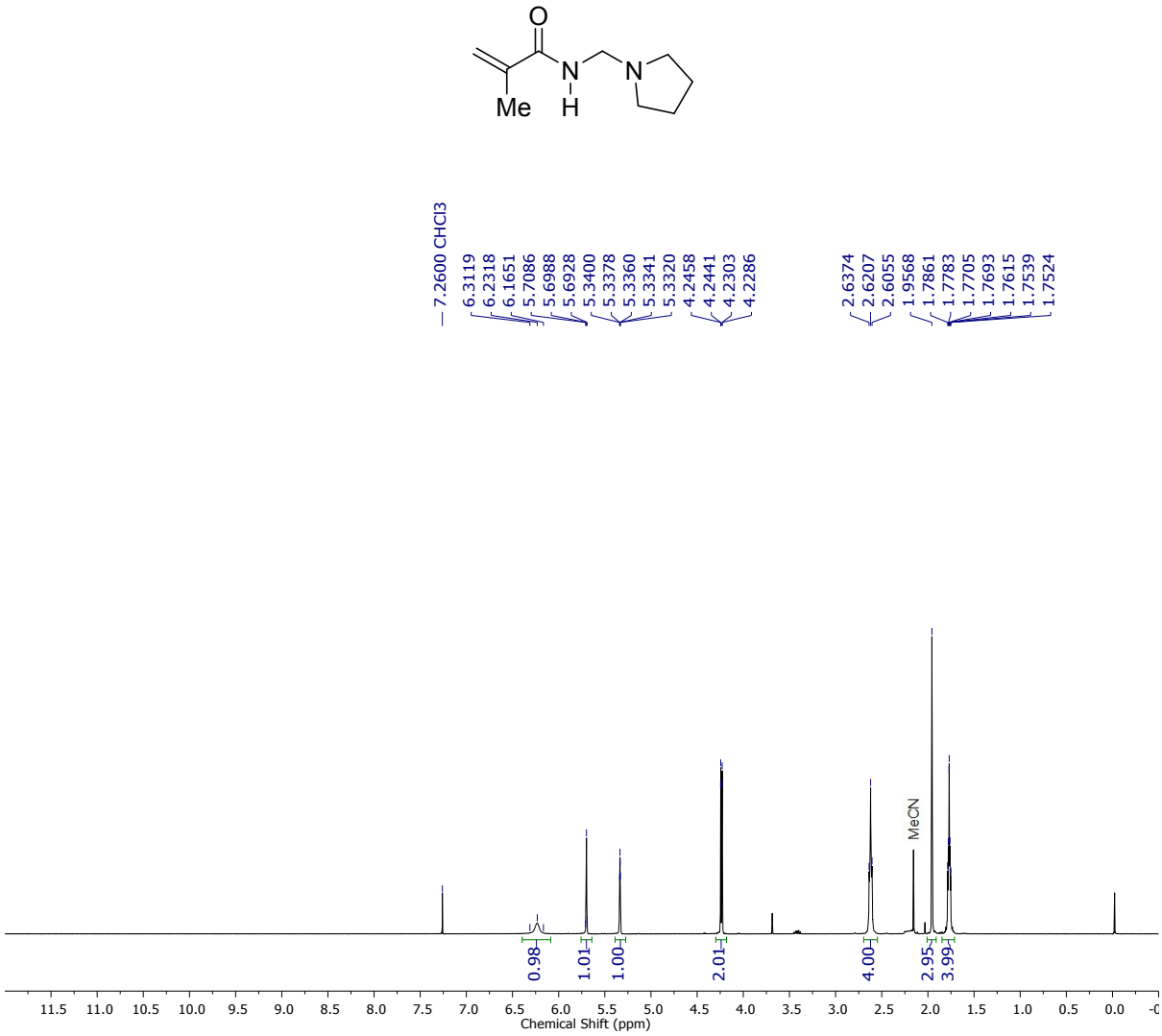

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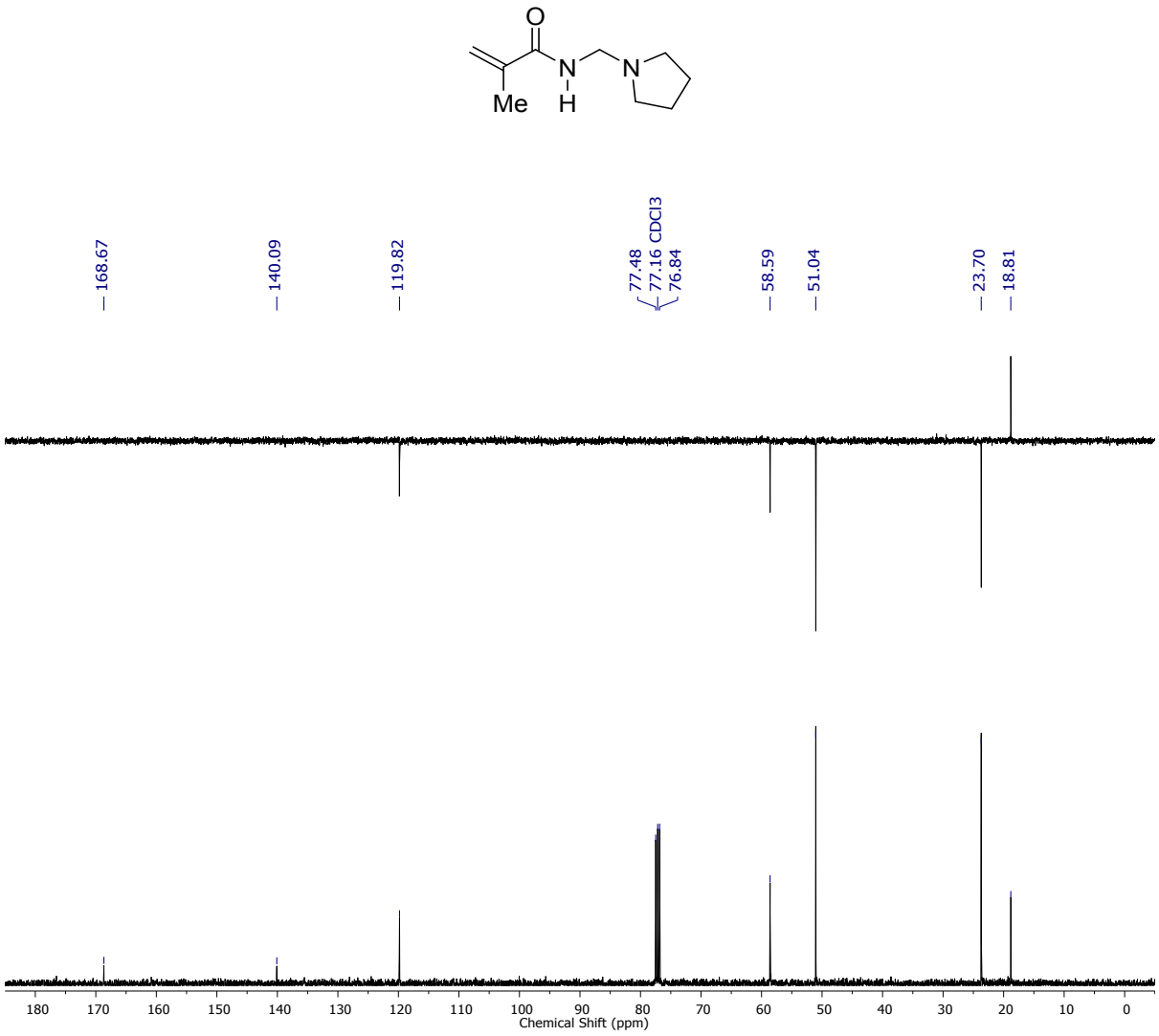
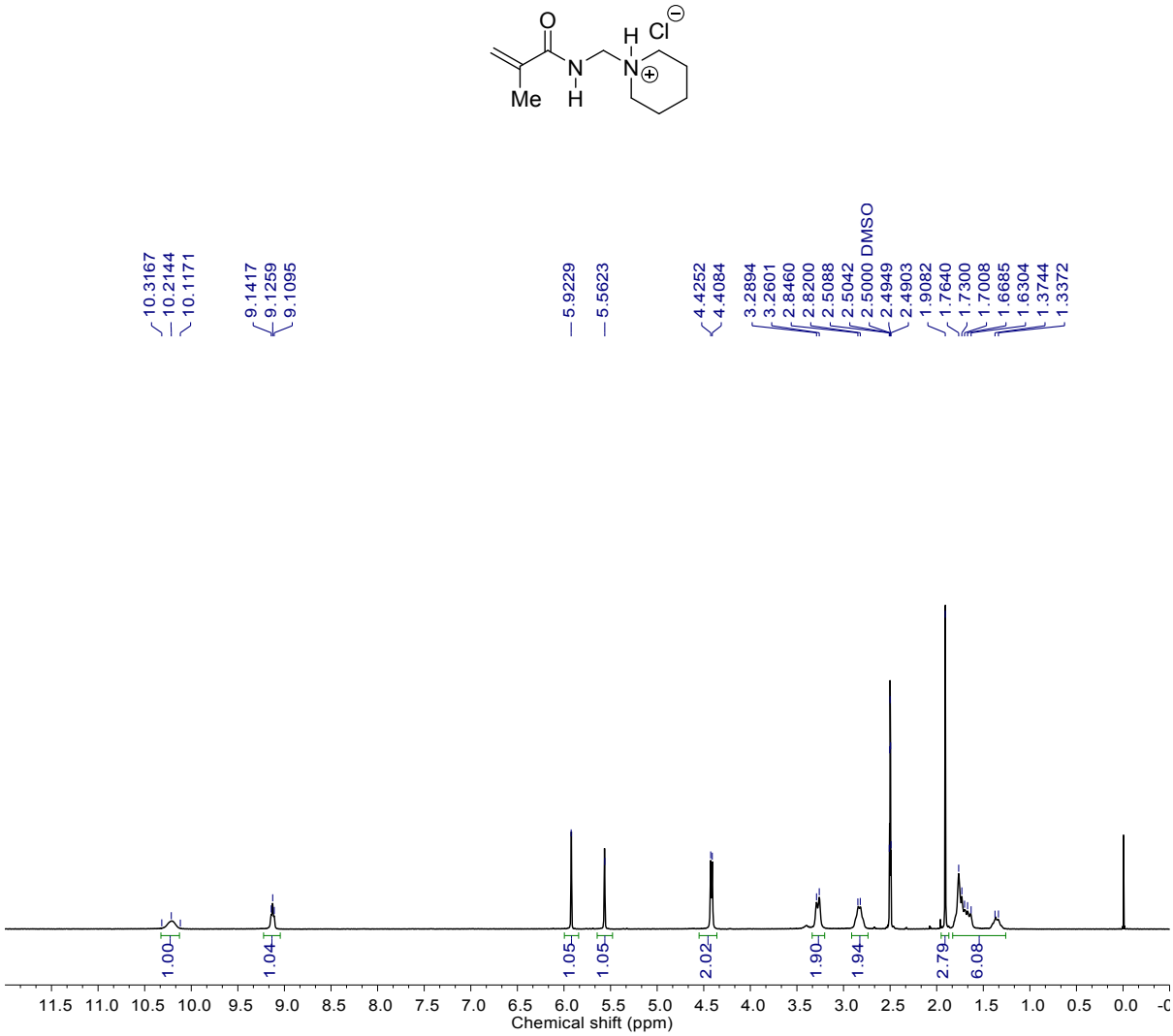
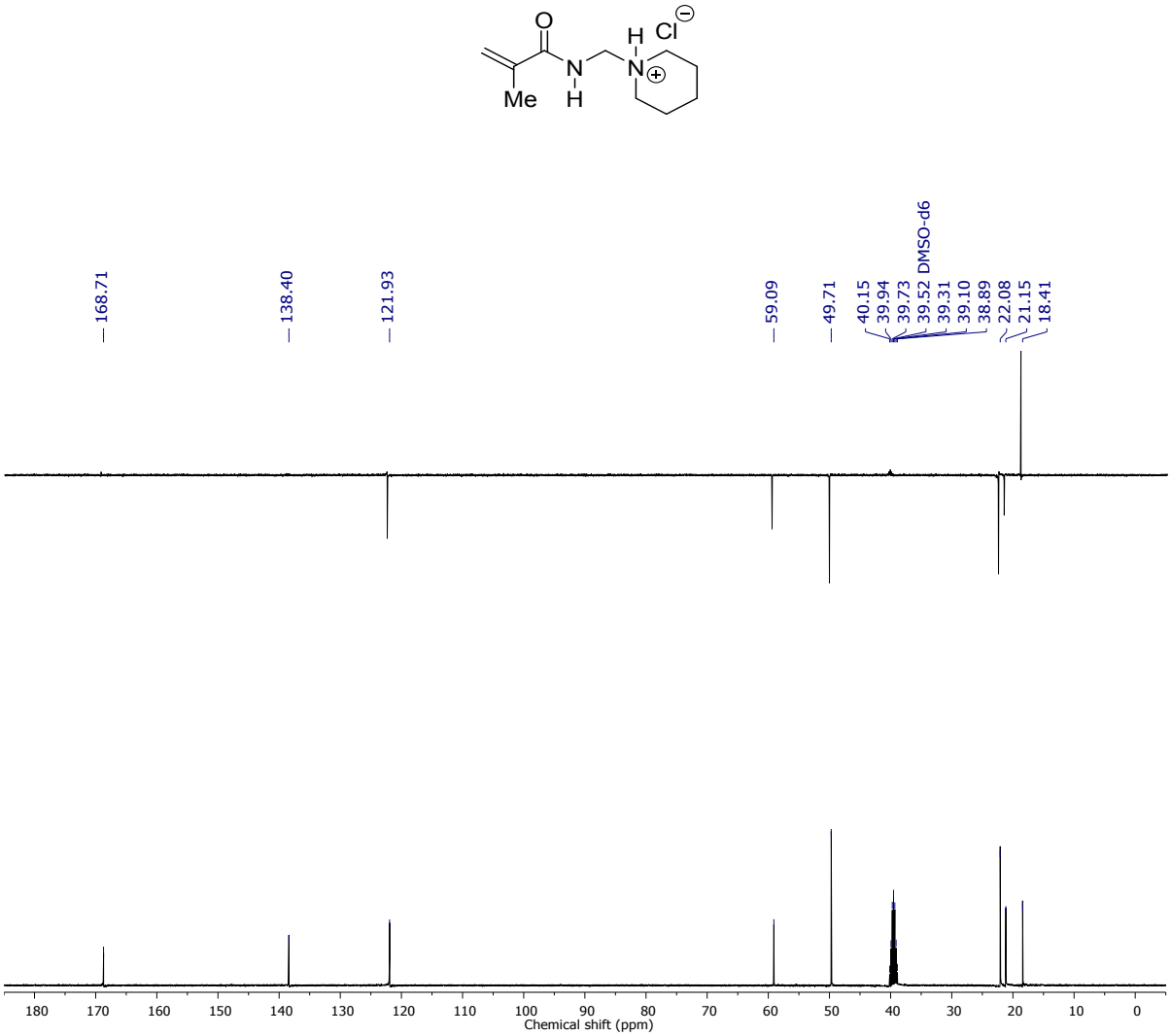


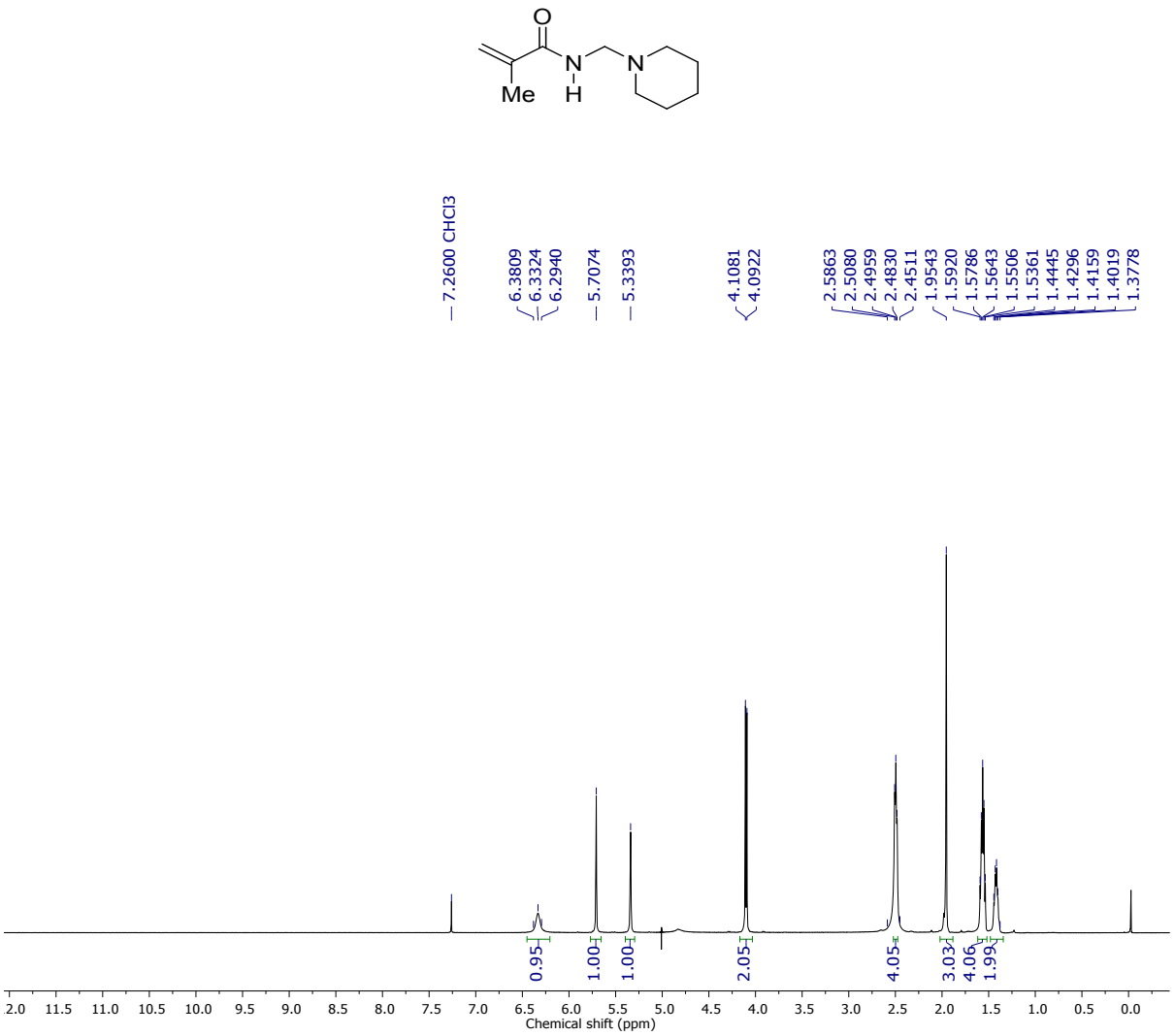
^{1}H NMR (400 MHz) of 2-methyl-*N*-[(piperidin-1-yl)methyl]prop-2-enamide hydrochloride (3b.HCl) in $(CD_3)_2SO$.



^{13}C NMR (101 MHz) of 2-methyl-*N*-[(piperidin-1-yl)methyl]prop-2-enamide hydrochloride (3b.HCl) in $(CD_3)_2SO$.



^{1}H NMR (400 MHz) of 2-methyl-*N*-[(piperidin-1-yl)methyl]prop-2-enamide (3b) in $CDCl_3$.



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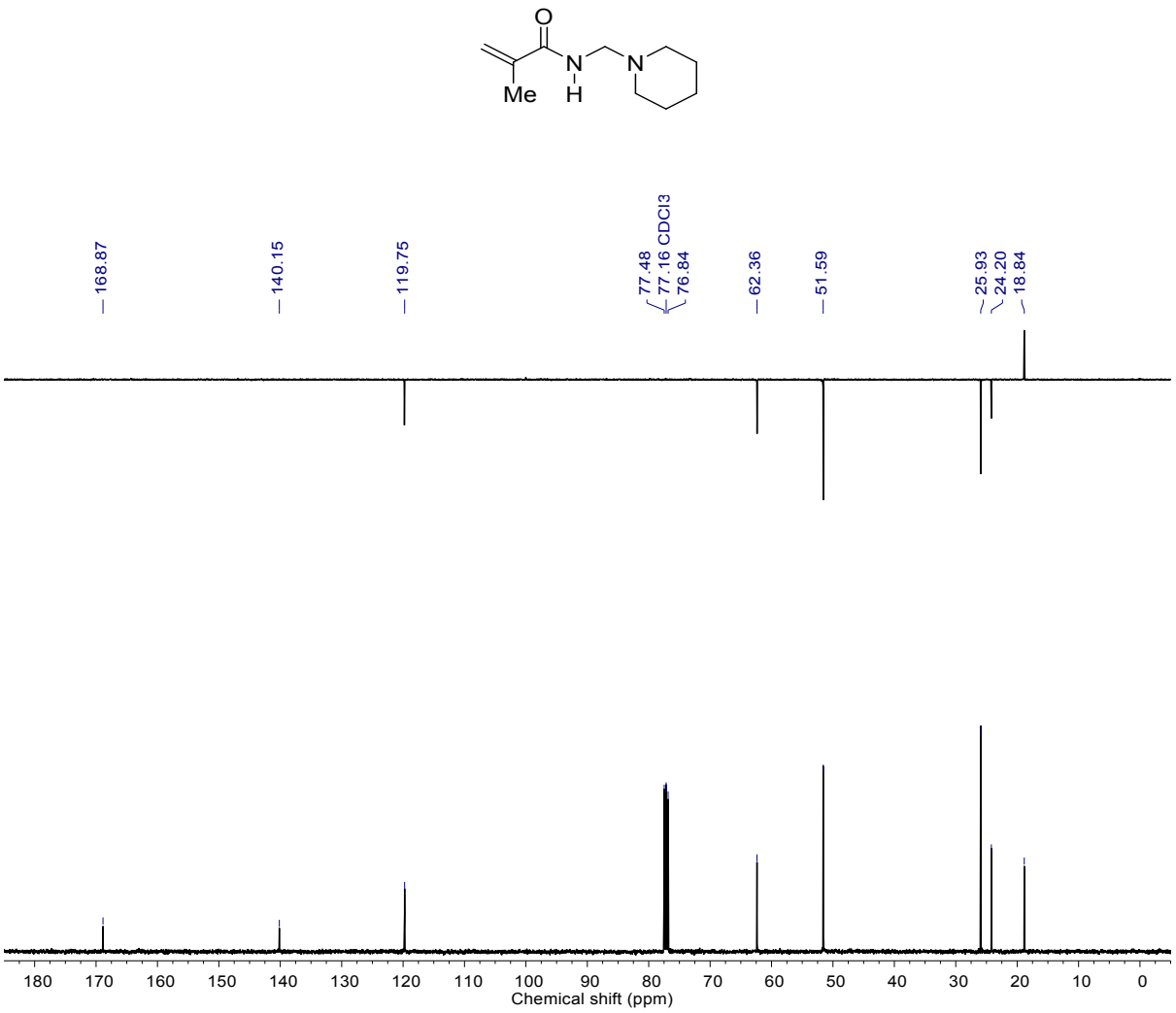
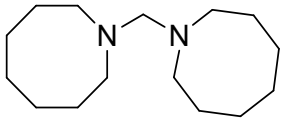
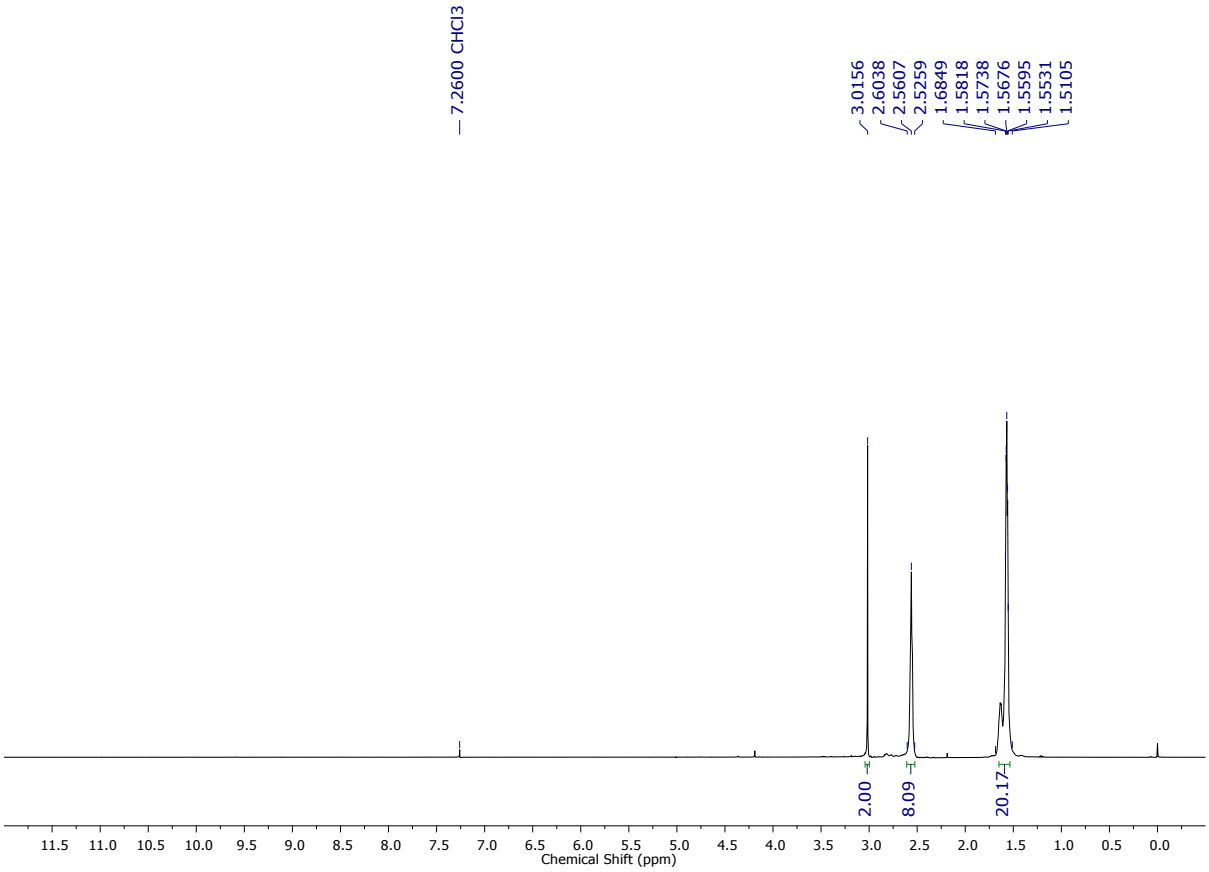


^{1}H NMR (400 MHz) of 1,1'-methylenebis(azocane) in $CDCl_3$.





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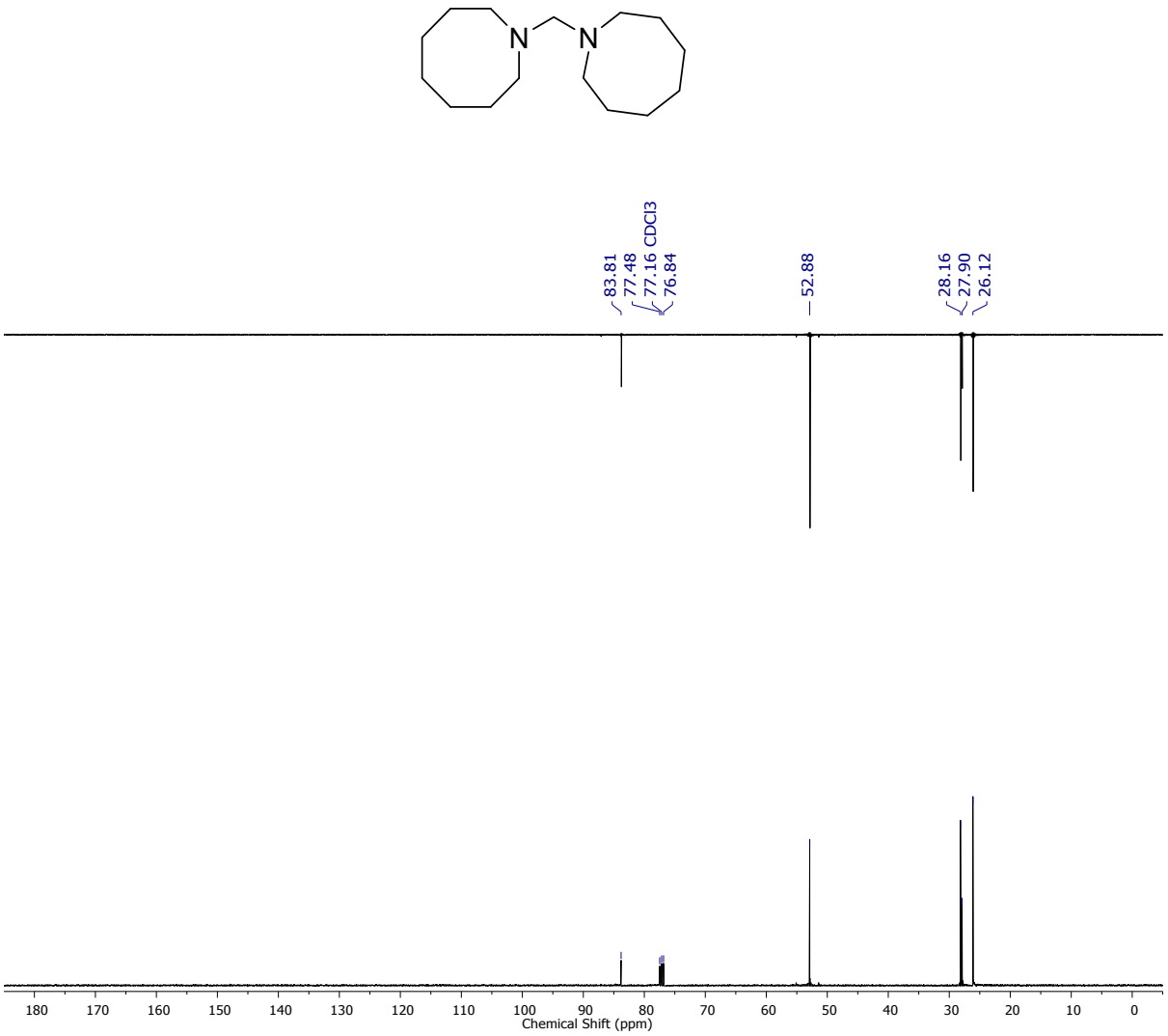
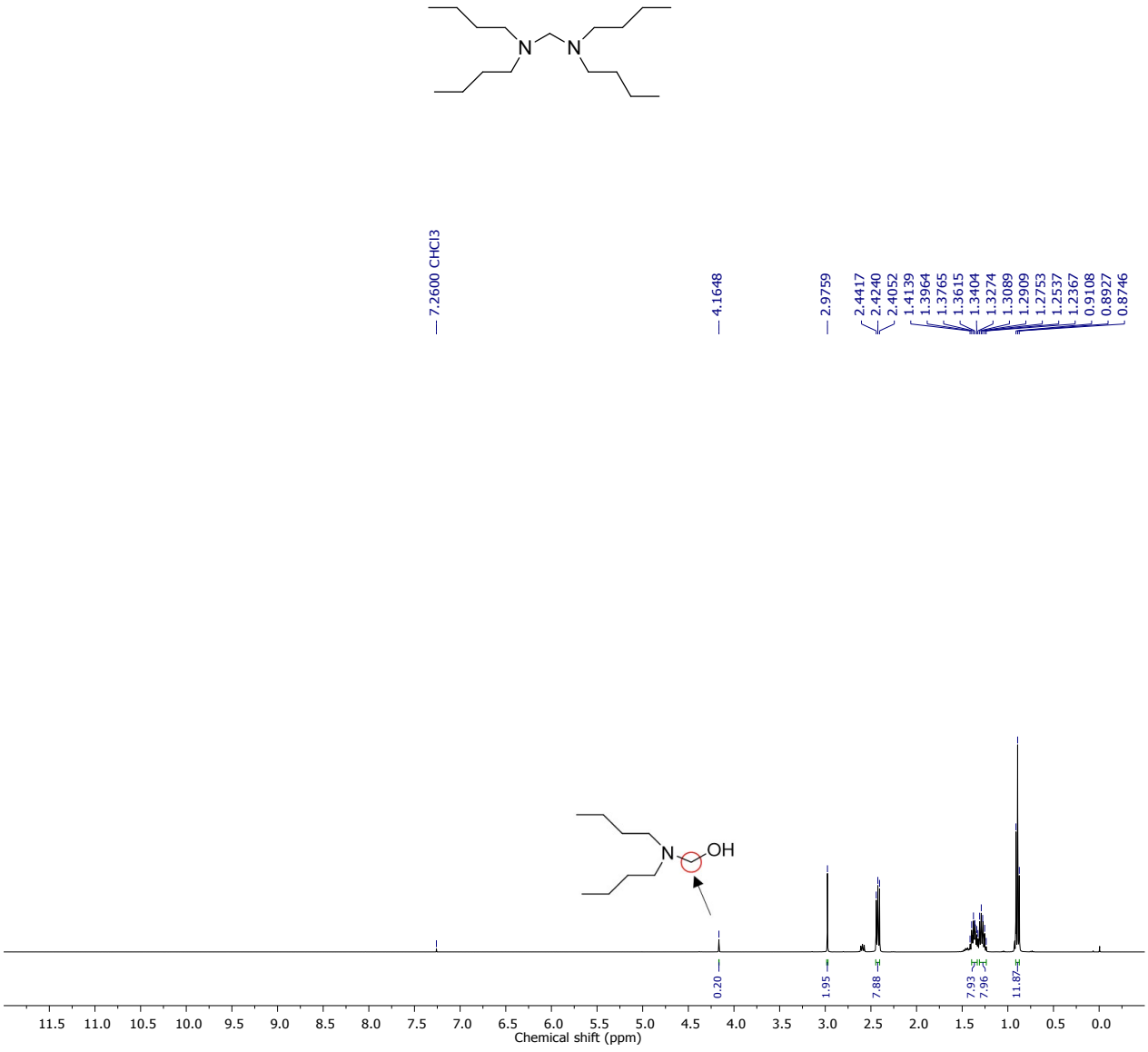
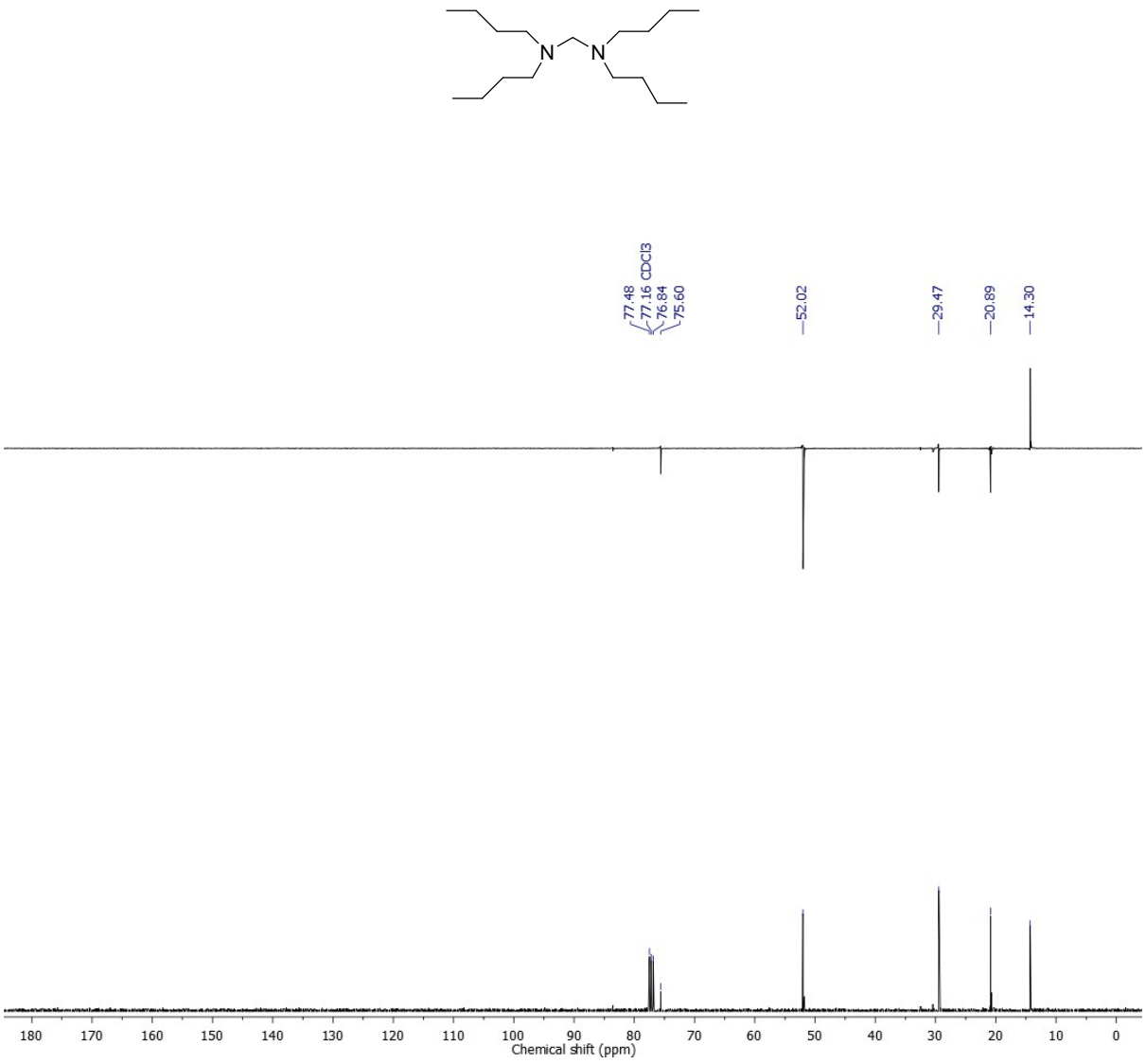


^{1}H NMR (400 MHz) of *N*,*N*,*N*′,*N*′-tetrabutylmethanediamine in $CDCl_3$.

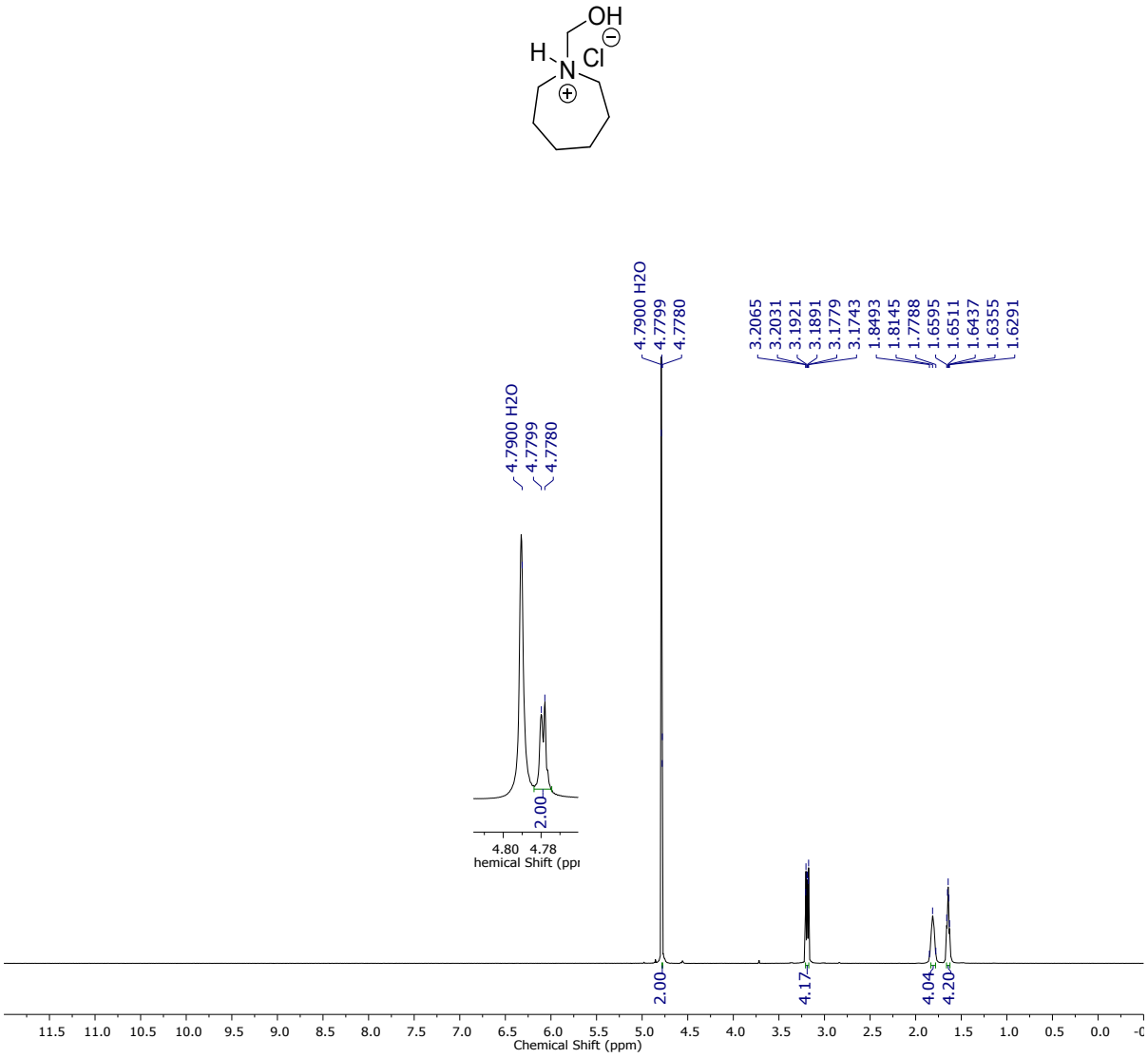


Contains the proposed hemiaminal {(dibutylamino)methanol} at about 10% estimated by comparing the integrations of the methylene peaks at 4.16 and 2.98 ppm.

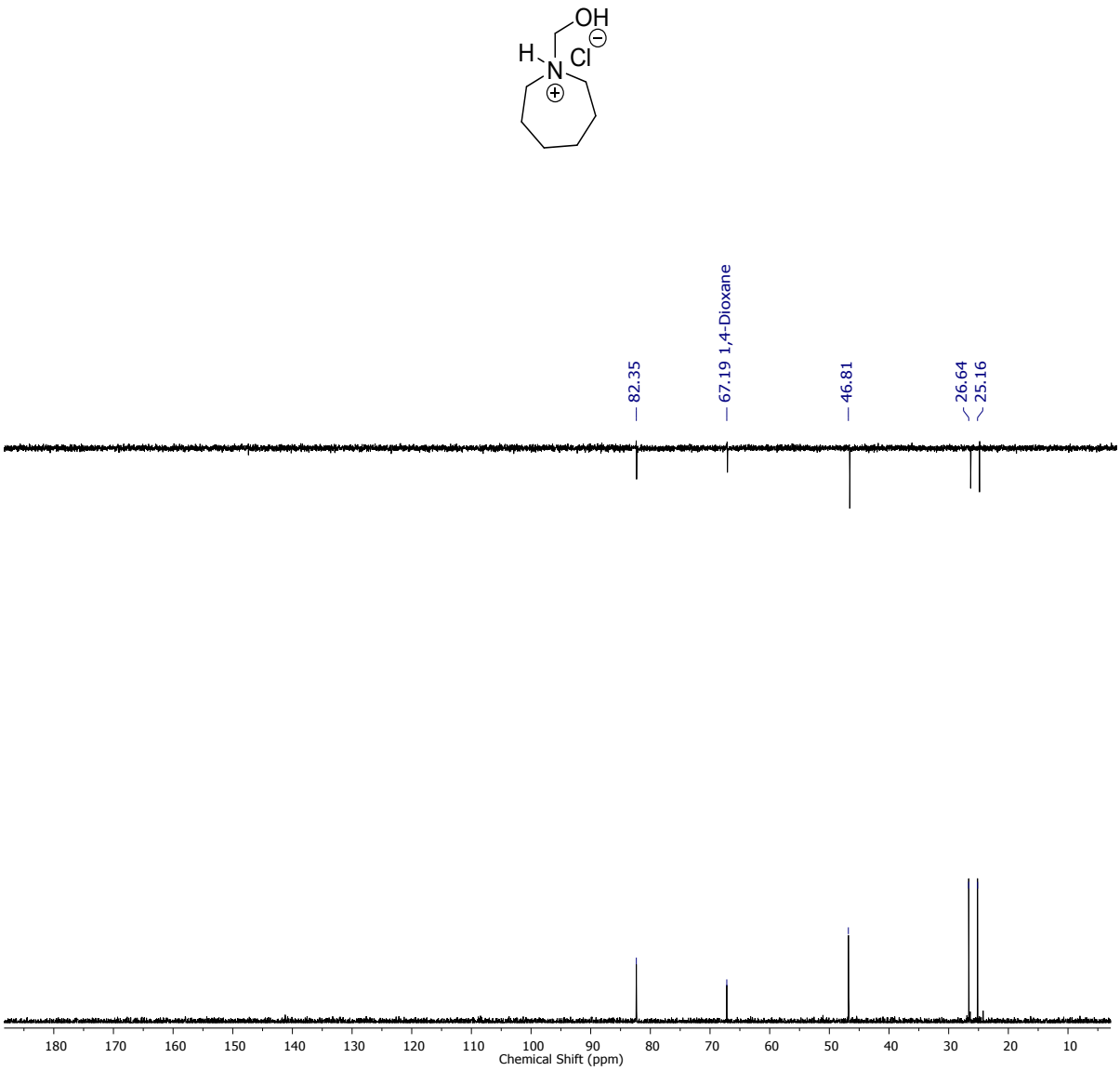
^{13}C NMR (101 MHz) of *N*,*N*,*N*′,*N*′-tetrabutylmethanediamine in $CDCl_3$.



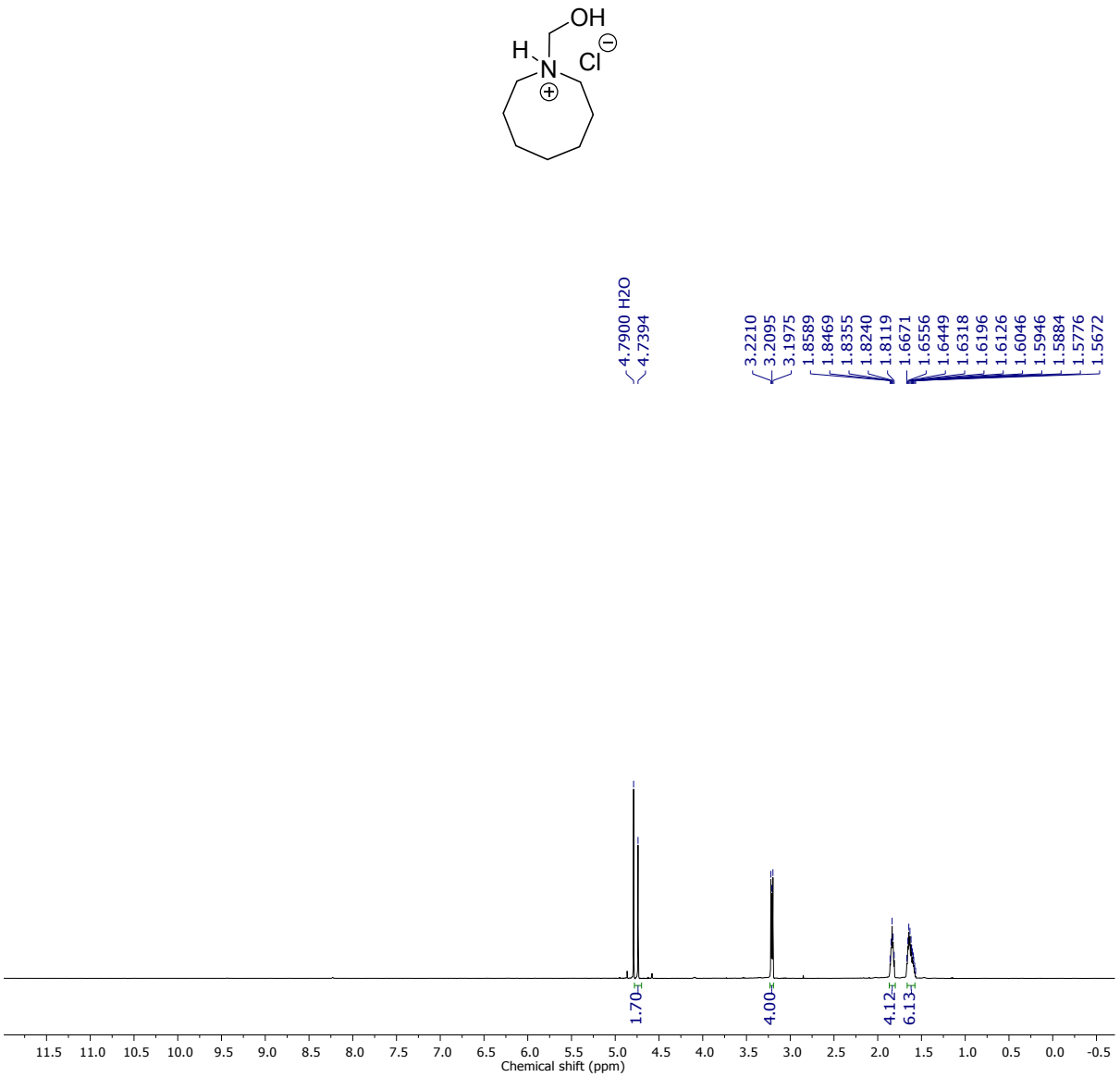
^{1}H NMR (400 MHz) of *N*-(hydroxymethyl)azepan-1-ium chloride (5a) in D_2O.



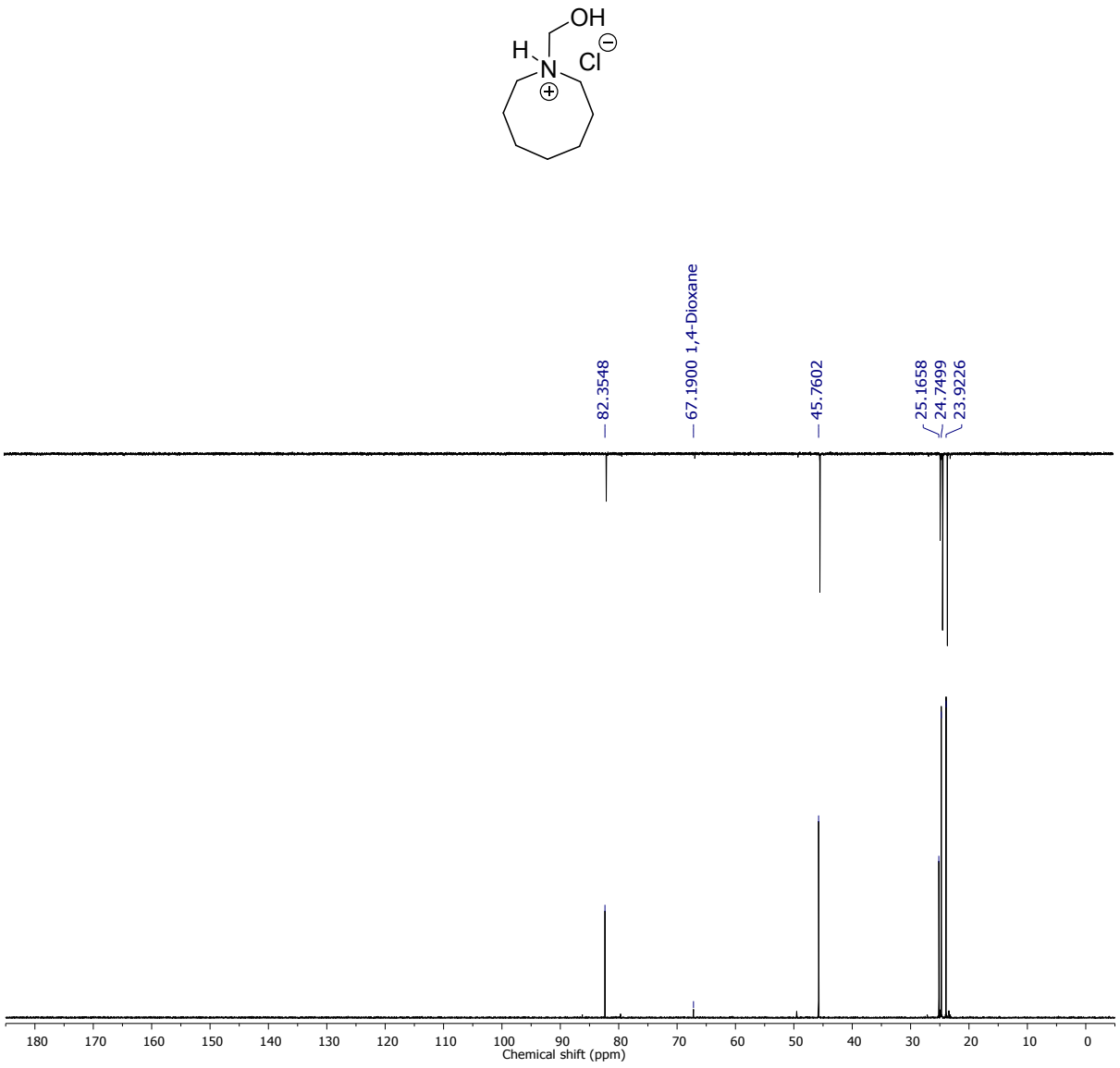
^{13}C NMR (101 MHz) of *N*-(hydroxymethyl)azepan-1-ium chloride (5a) in D_2O with 1,4-dioxane added as reference.



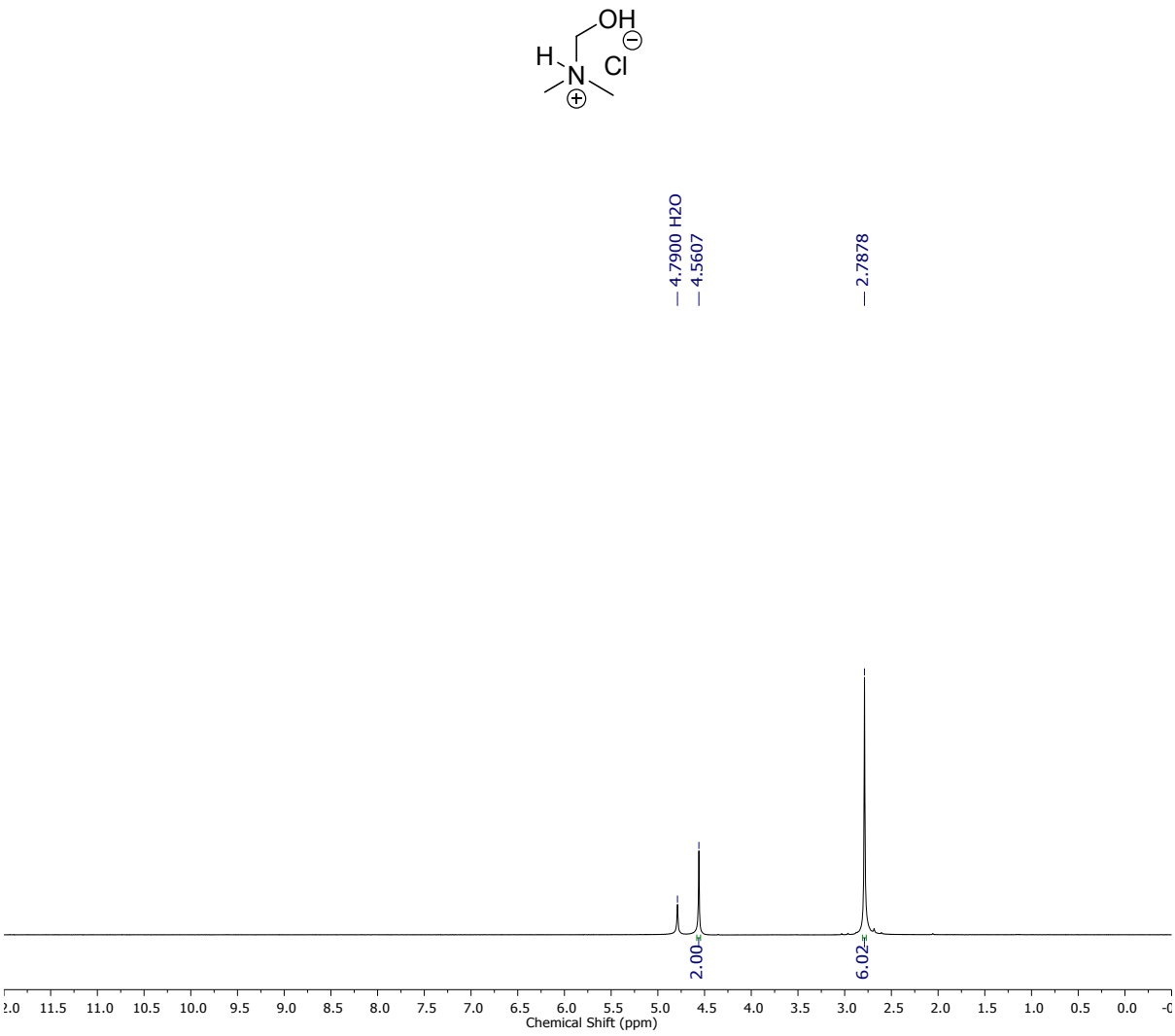
^{1}H NMR (500 MHz) of *N*-(hydroxymethyl)azocan-1-ium chloride (5b) in D_2O.



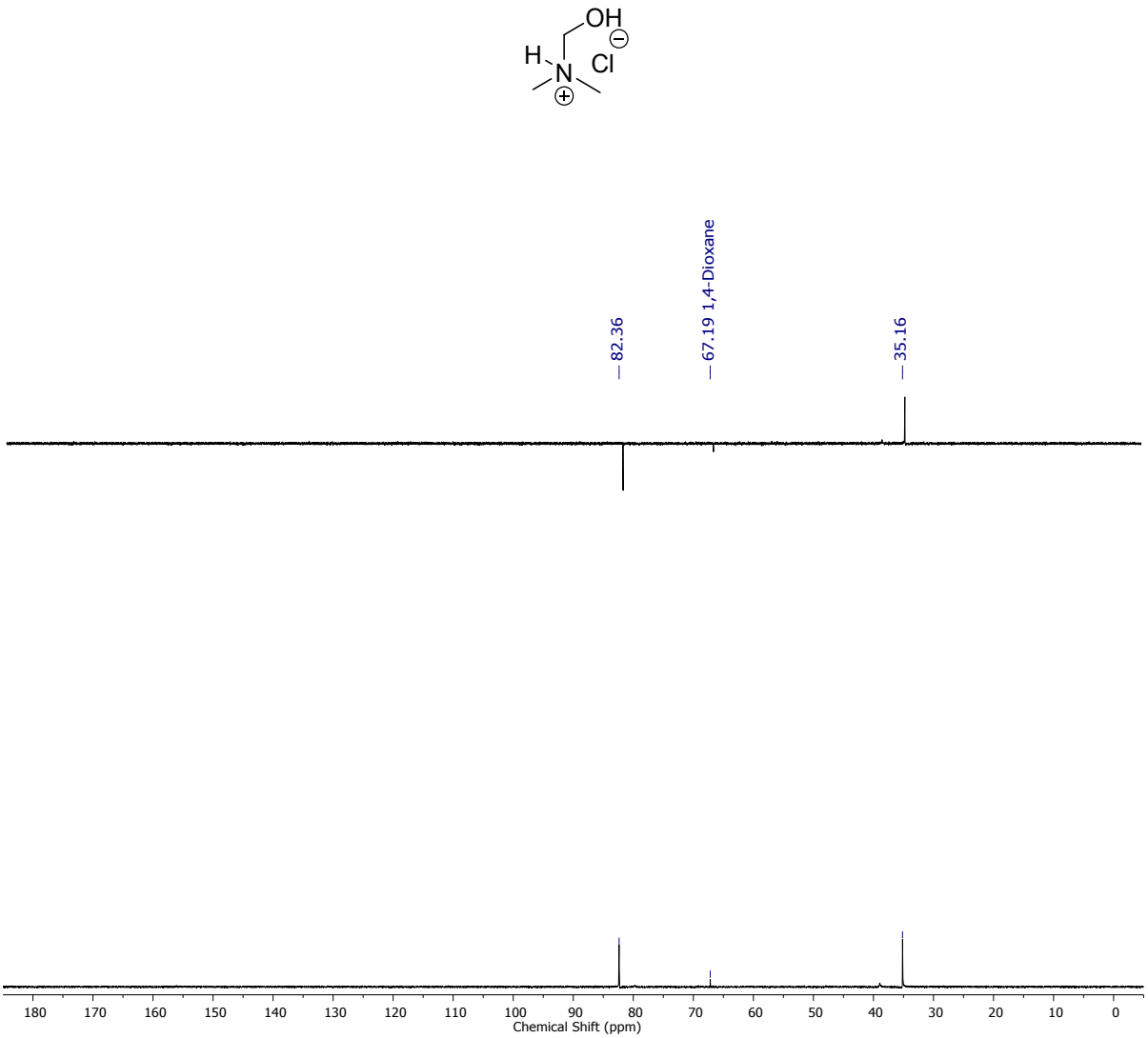
^{13}C NMR (125 MHz) of *N*-(hydroxymethyl)azocan-1-ium chloride (5b) in D_2O with 1,4-dioxane added as reference.



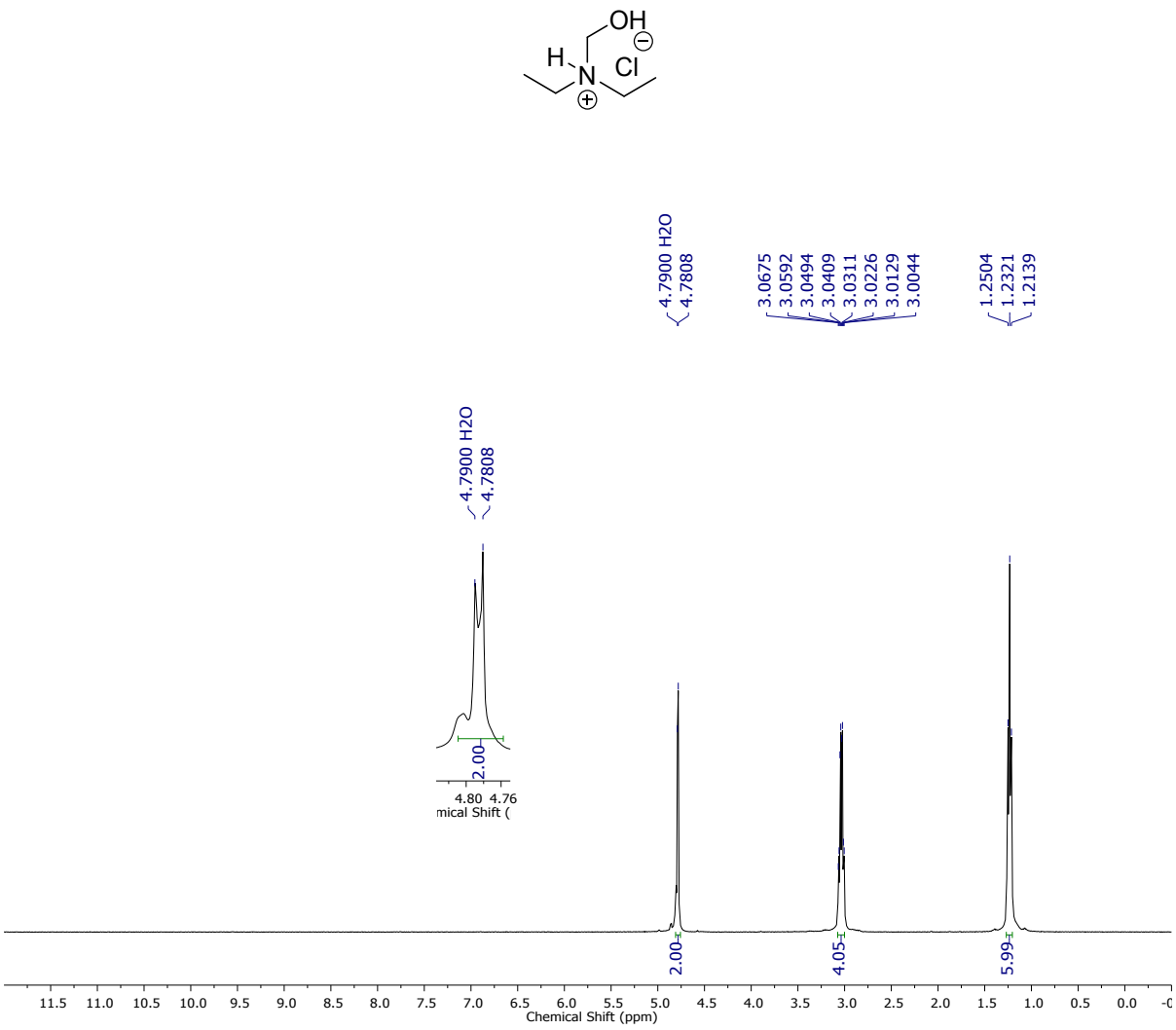
^{1}H NMR (400 MHz) of hydroxy-*N*,*N*-dimethylmethanaminium chloride (5c) in D_2O.



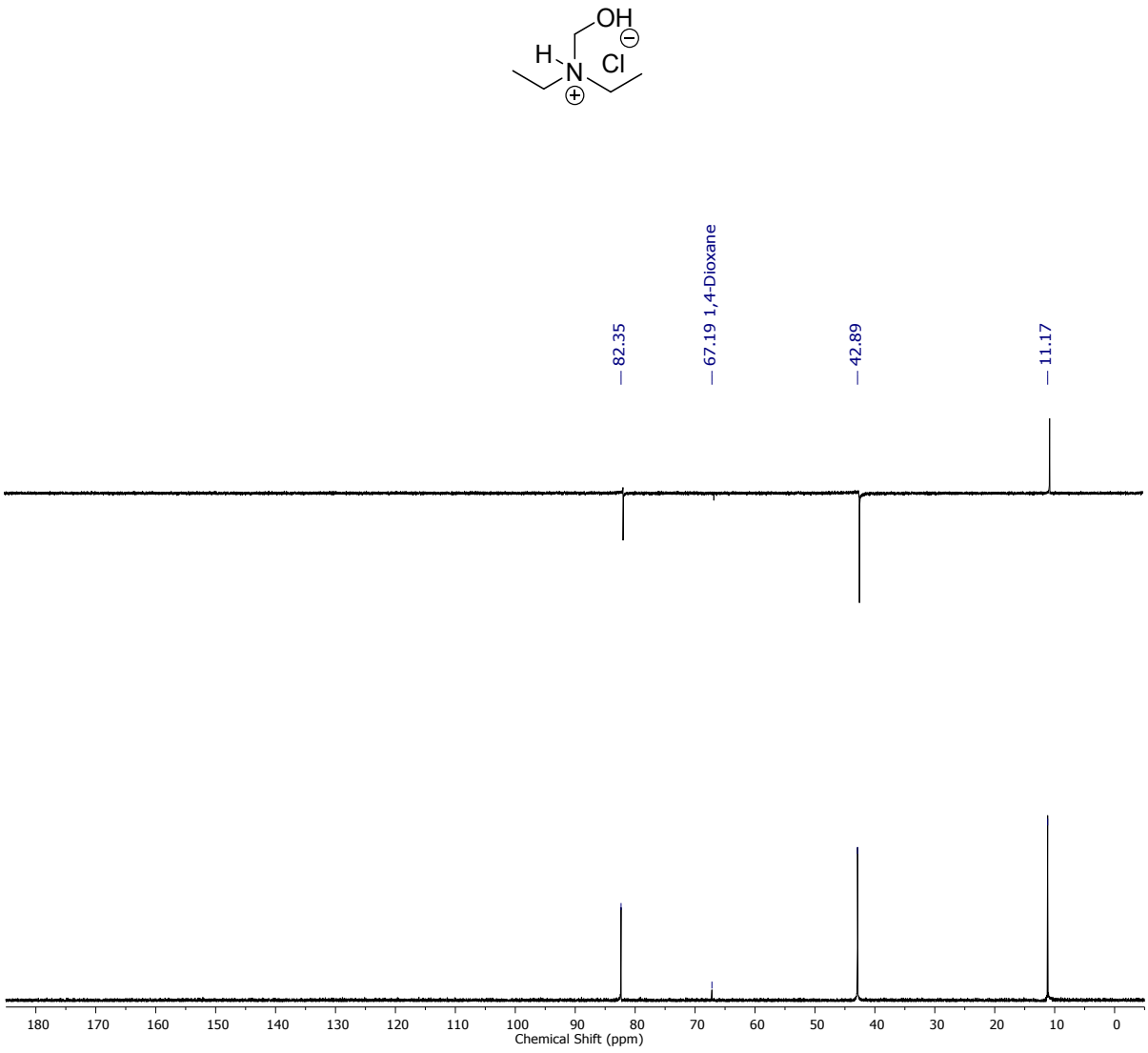
^{13}C NMR (400 MHz) of hydroxy-*N*,*N*-dimethylmethanaminium chloride (5c) in D_2O with 1,4-dioxane added as reference.



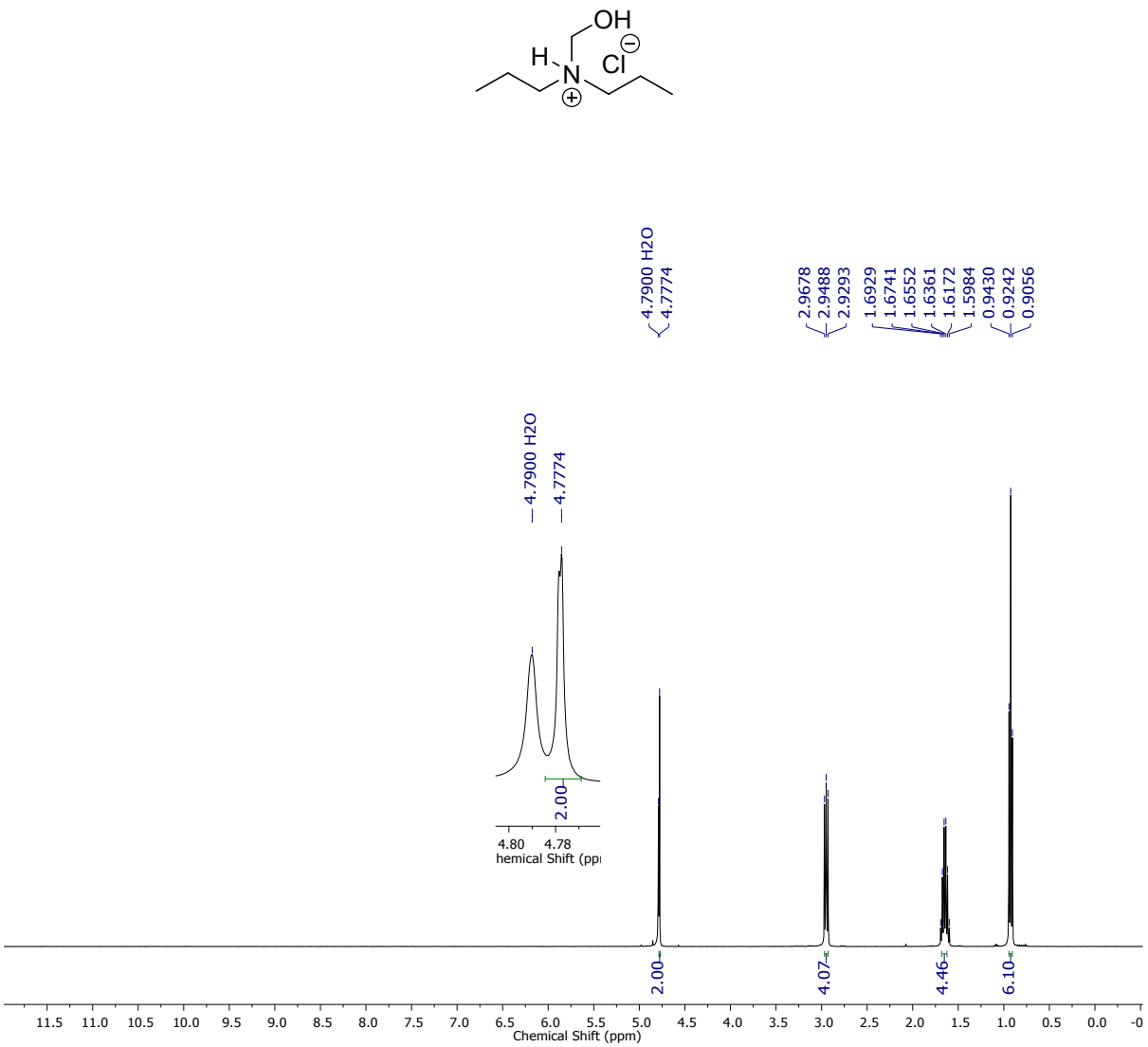
^{1}H NMR (400 MHz) of *N*-ethyl-*N*-(hydroxymethyl)ethanaminium chloride (5d) in D_2O.



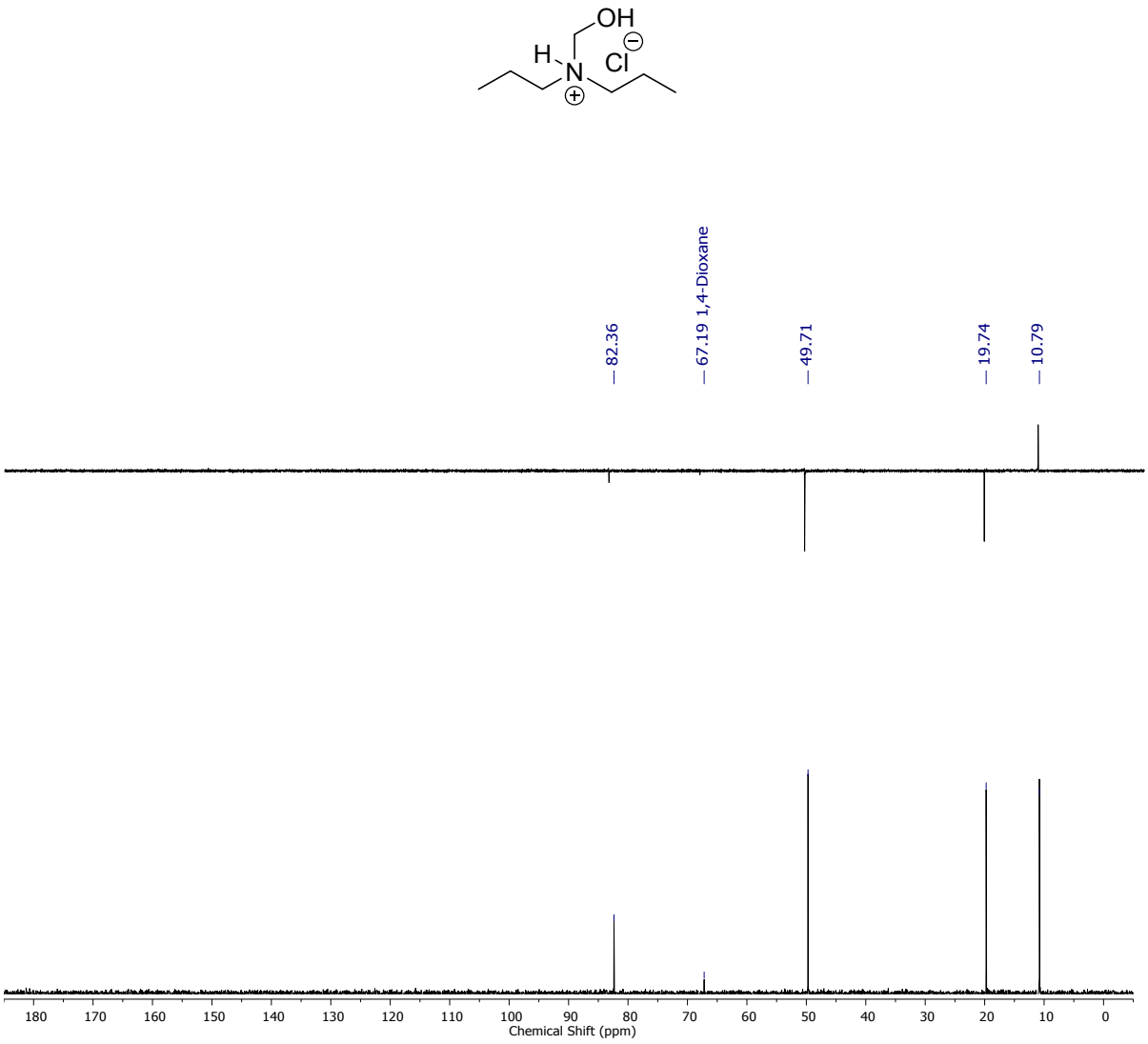
^{13}C NMR (101 MHz) of *N*-ethyl-*N*-(hydroxymethyl)ethanaminium chloride (5d) in D_2O with 1,4-dioxane added as reference.



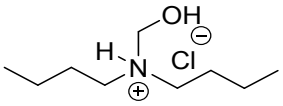
^{1}H NMR (400 MHz) of *N*-(hydroxymethyl)-*N*-propylpropanaminium chloride (5e) in D_2O.

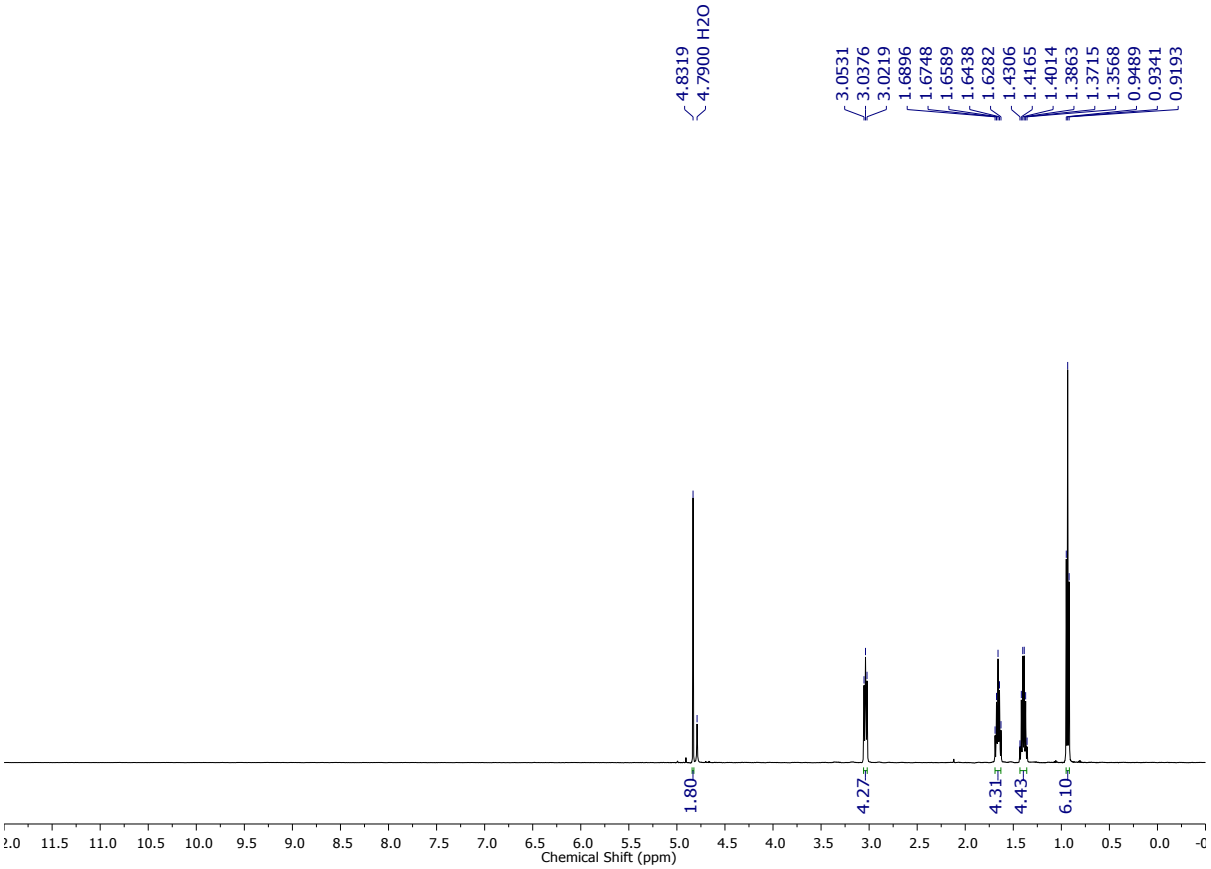


^{13}C NMR (101 MHz) of *N*-(hydroxymethyl)-*N*-propylpropanaminium chloride (5e) in D_2O with 1,4-dioxane added as reference.

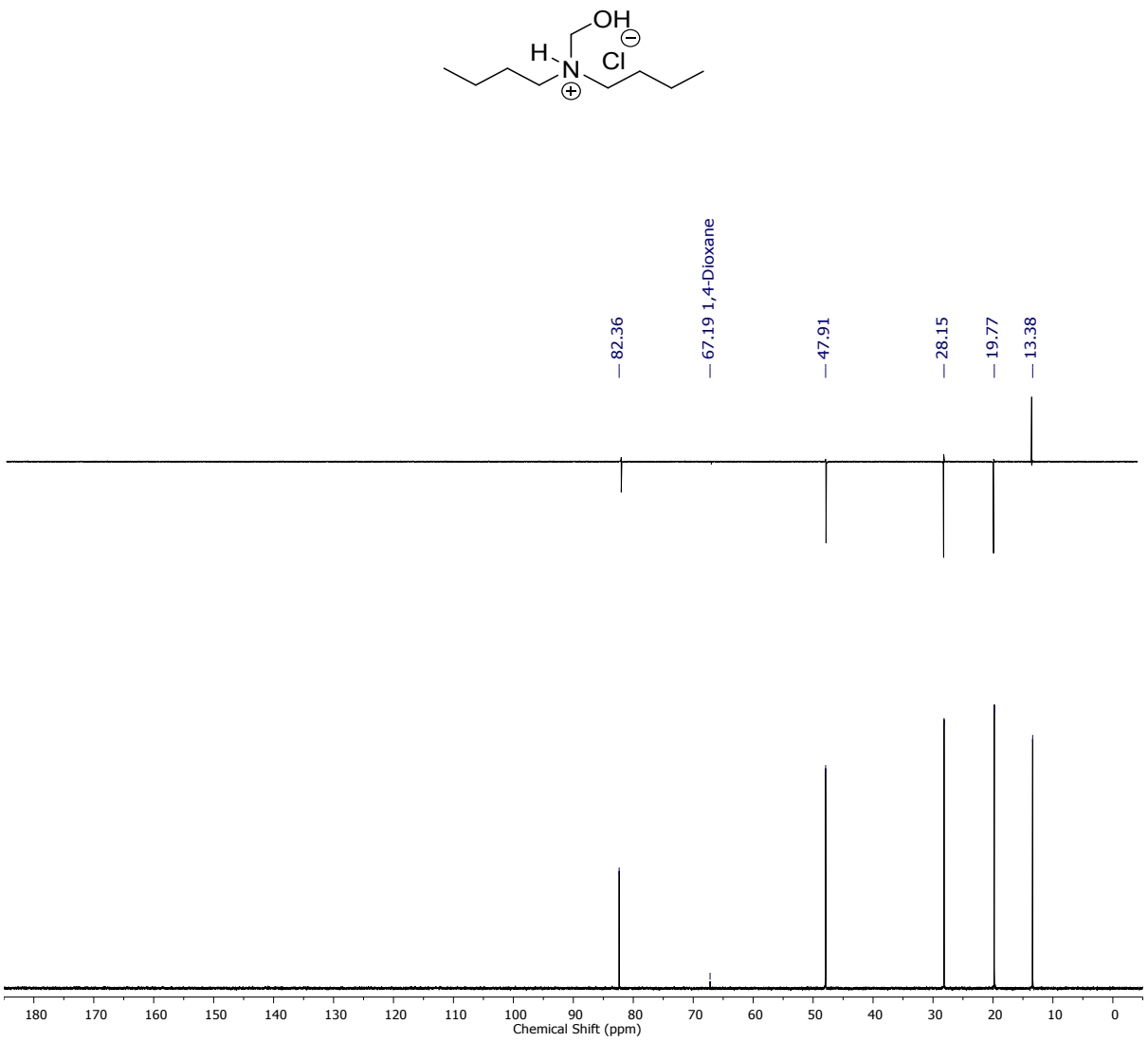


^{1}H NMR (400 MHz) of *N*-butyl-*N*-(hydroxymethyl)butanaminium chloride (5f) in D_2O.

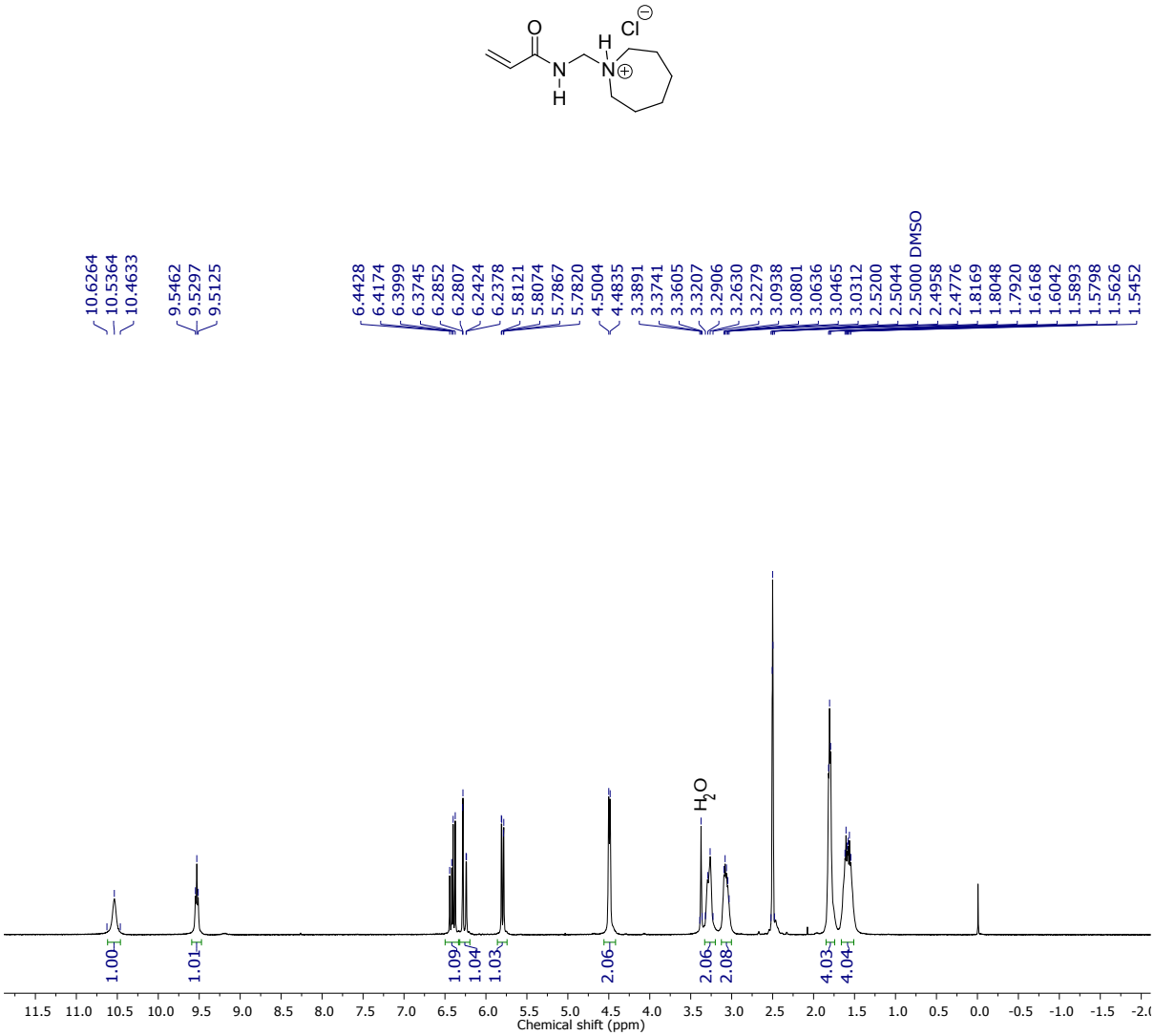




^{13}C NMR (101 MHz) of *N*-butyl-*N*-(hydroxymethyl)butanaminium chloride (5f) in D_2O with 1,4-dioxane added as reference.



^{1}H NMR (400 MHz) of *N*-[(azepan-1-yl)methyl]prop-2-enamide hydrochloride (6a.HCl) in $(CD_3)_2SO$.



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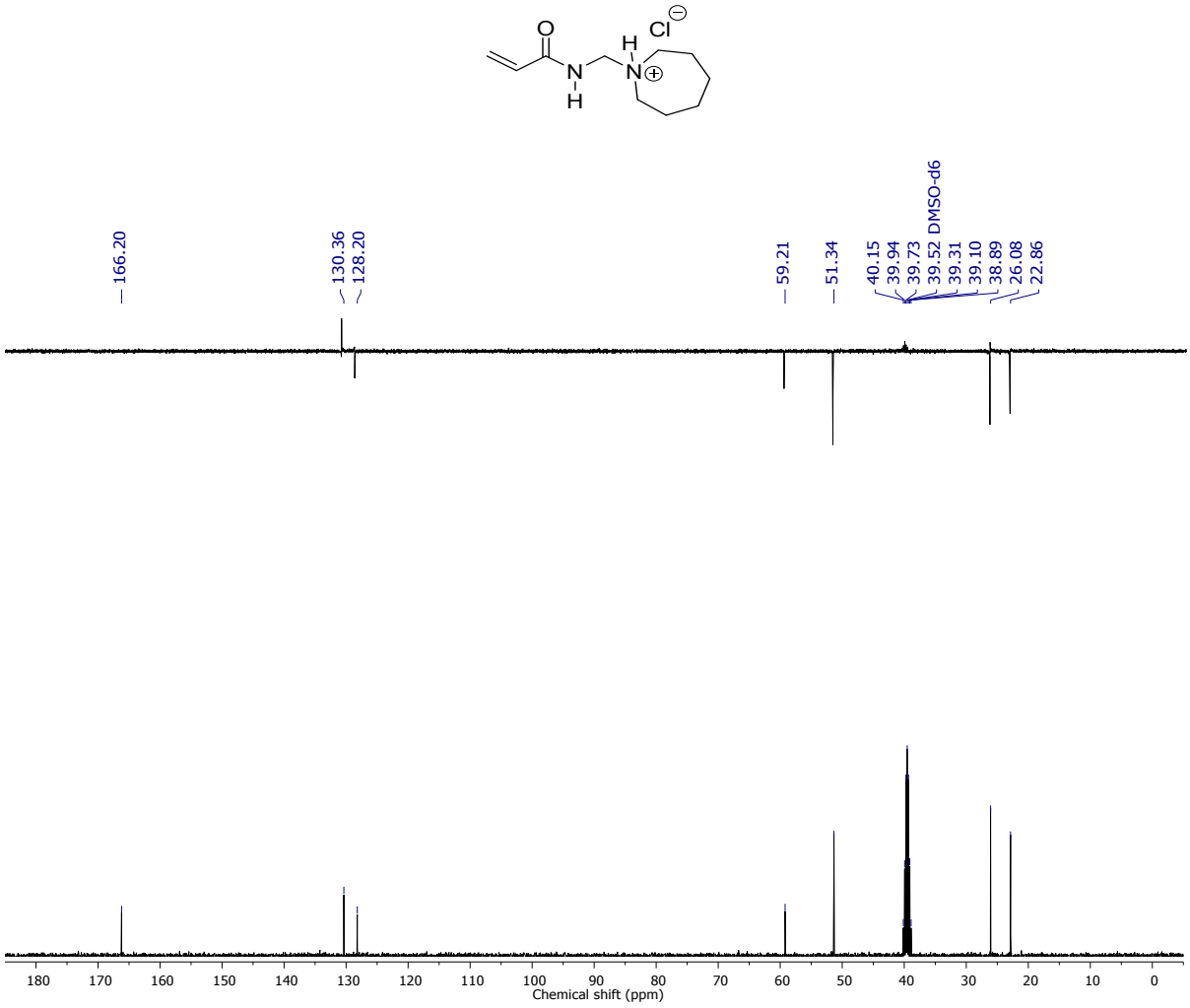
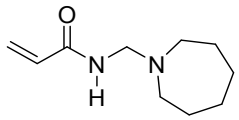
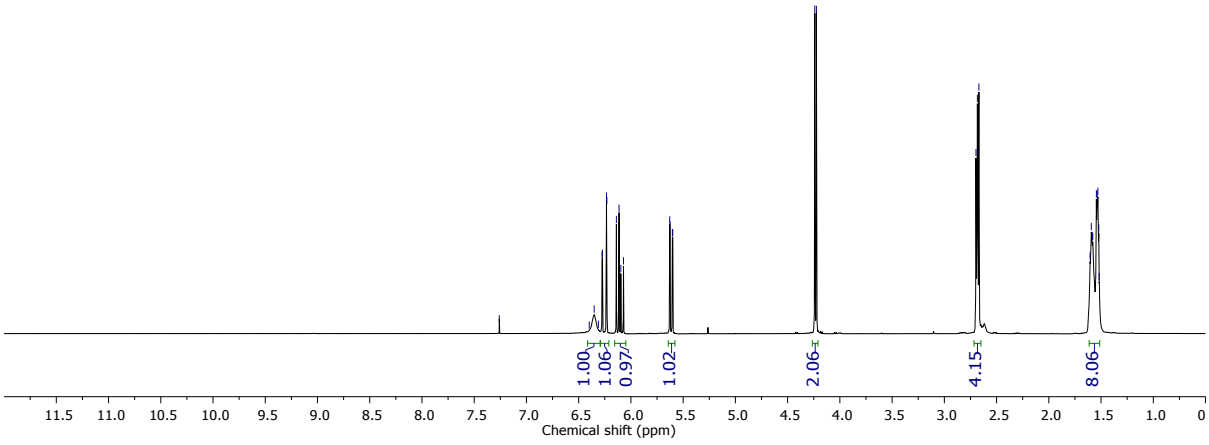


^{1}H NMR (400 MHz) of *N*-[(azepan-1-yl)methyl]prop-2-enamide (6a) in $CDCl_3$.





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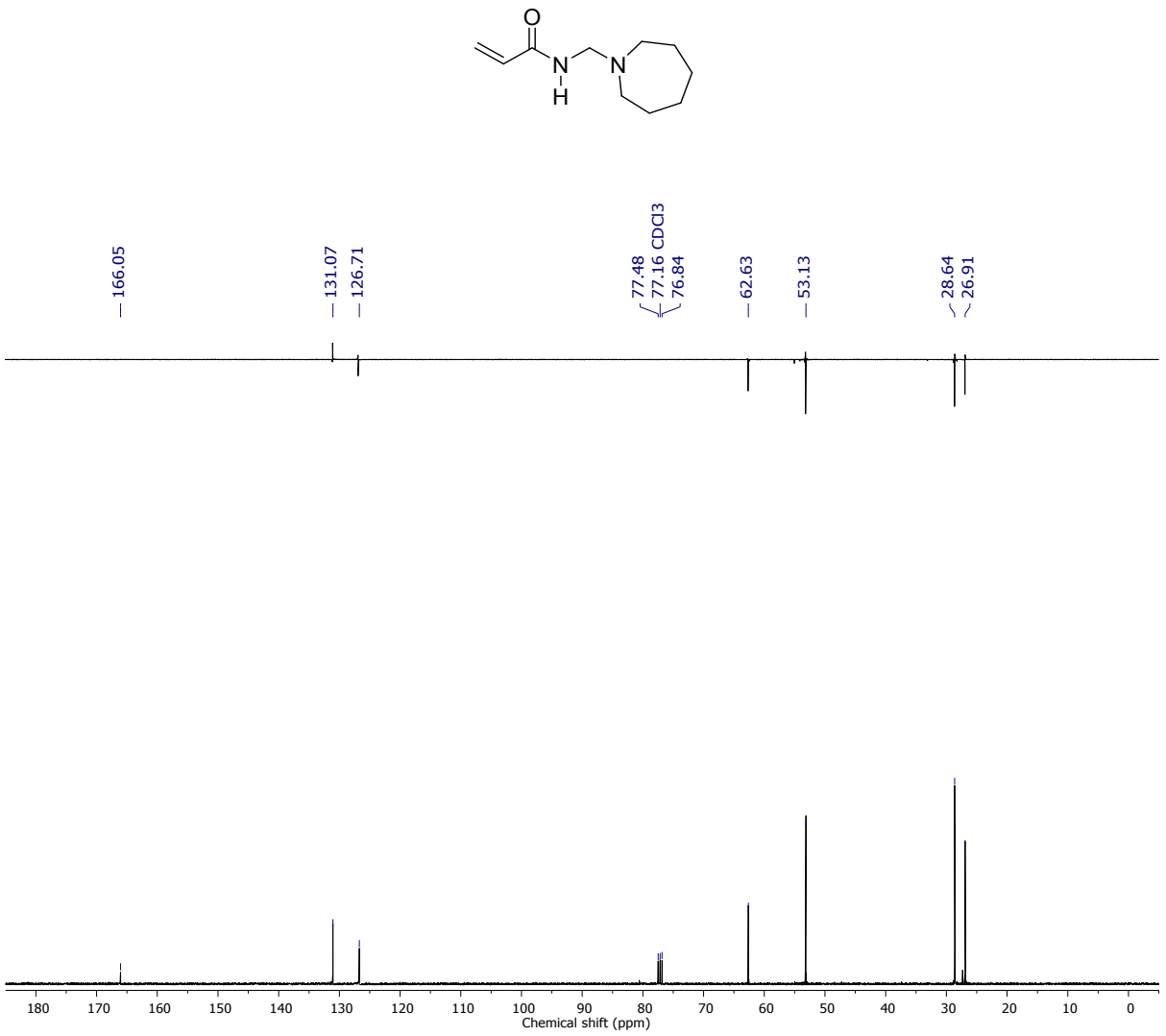
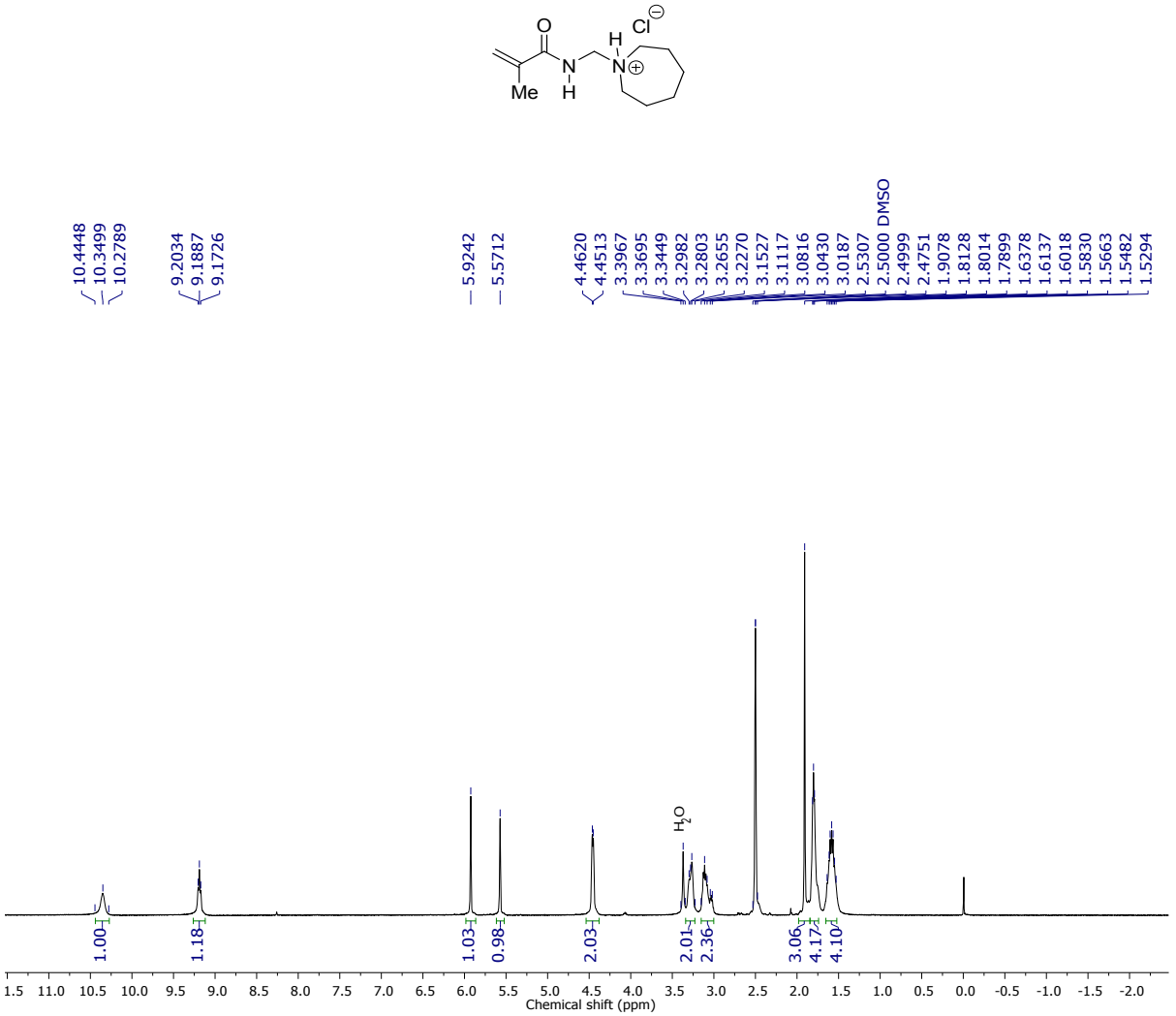
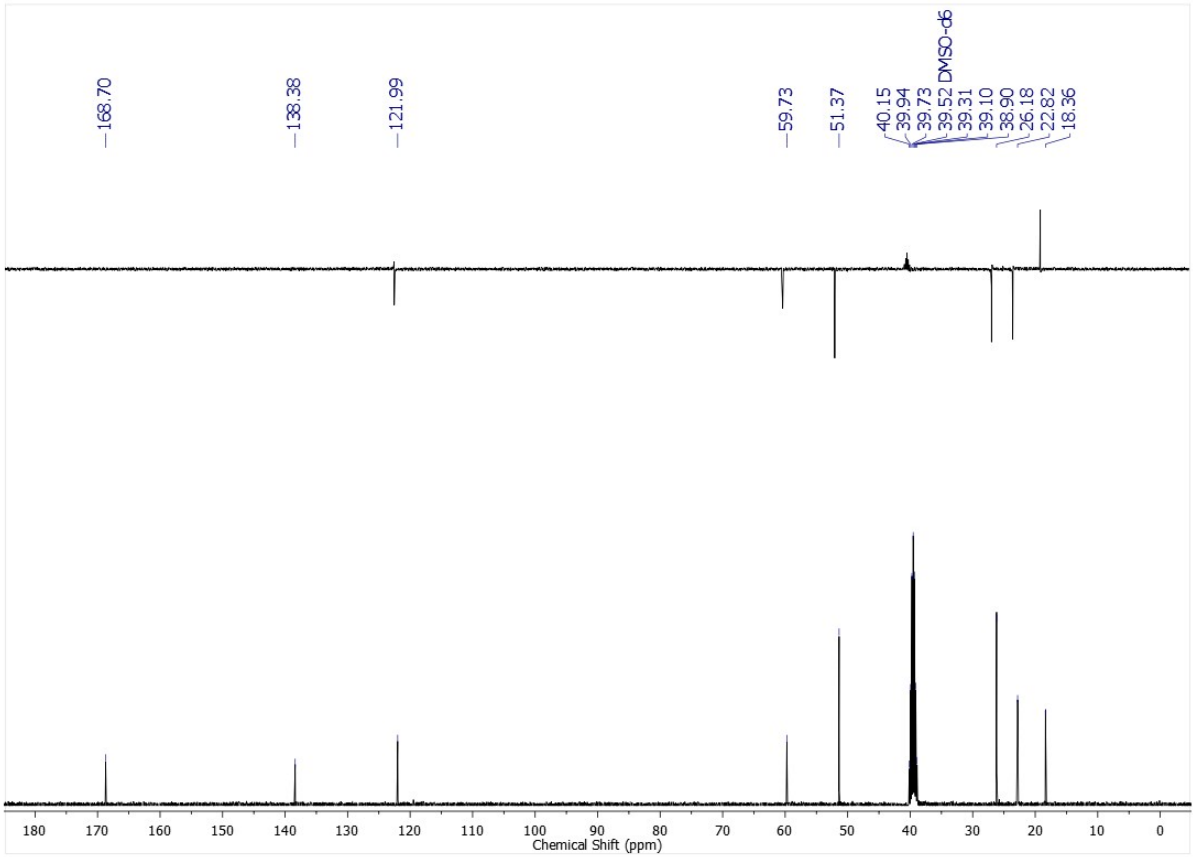


^{1}H NMR (400 MHz) of *N*-[(azepan-1-yl)methyl]-2-methylprop-2-enamide hydrochloride (6b.HCl) in $(CD_3)_2SO$.



^{13}C NMR (101 MHz) of *N*-[(azepan-1-yl)methyl]-2-methylprop-2-enamide hydrochloride (6b.HCl) in $(CD_3)_2SO$.



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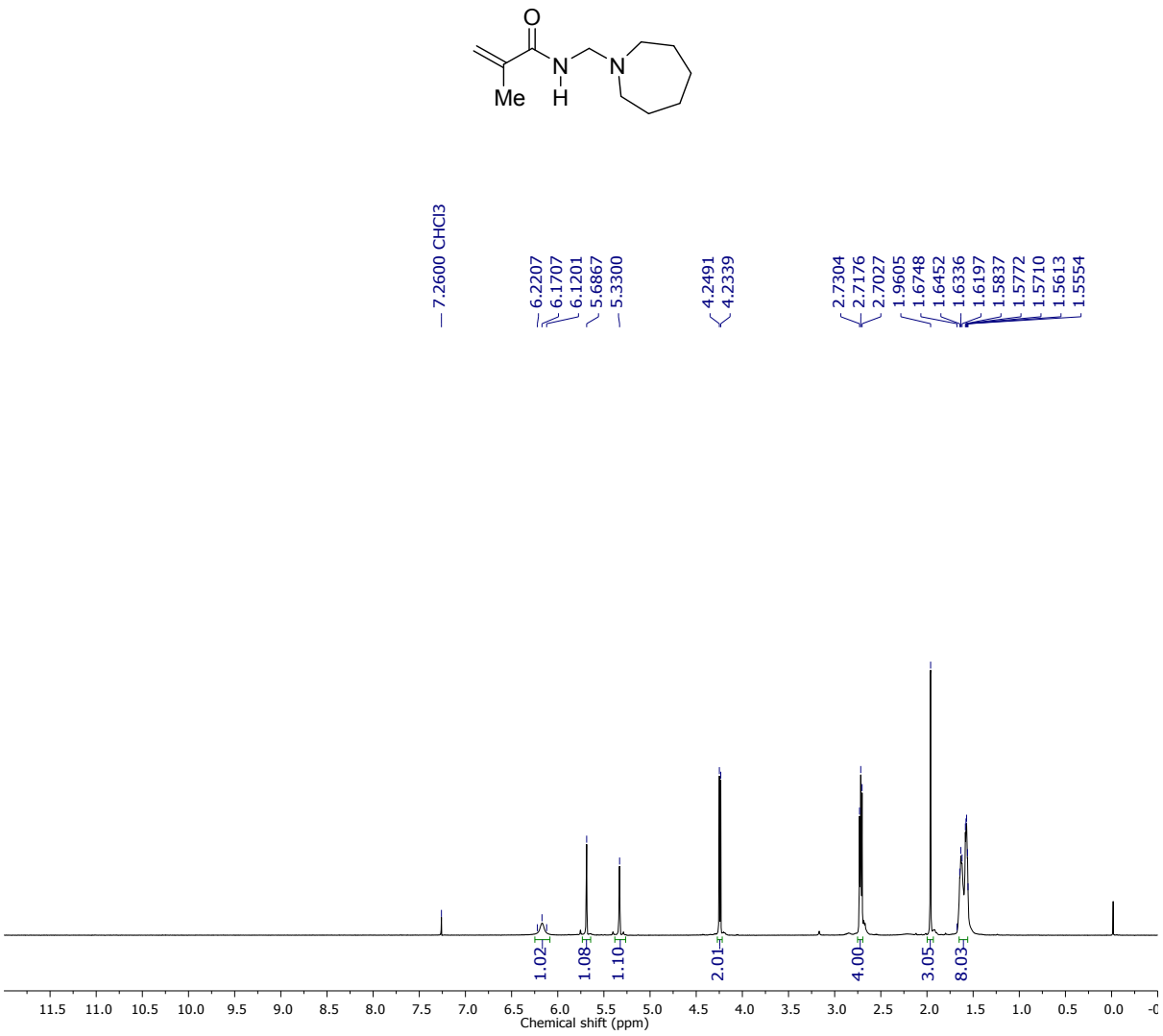

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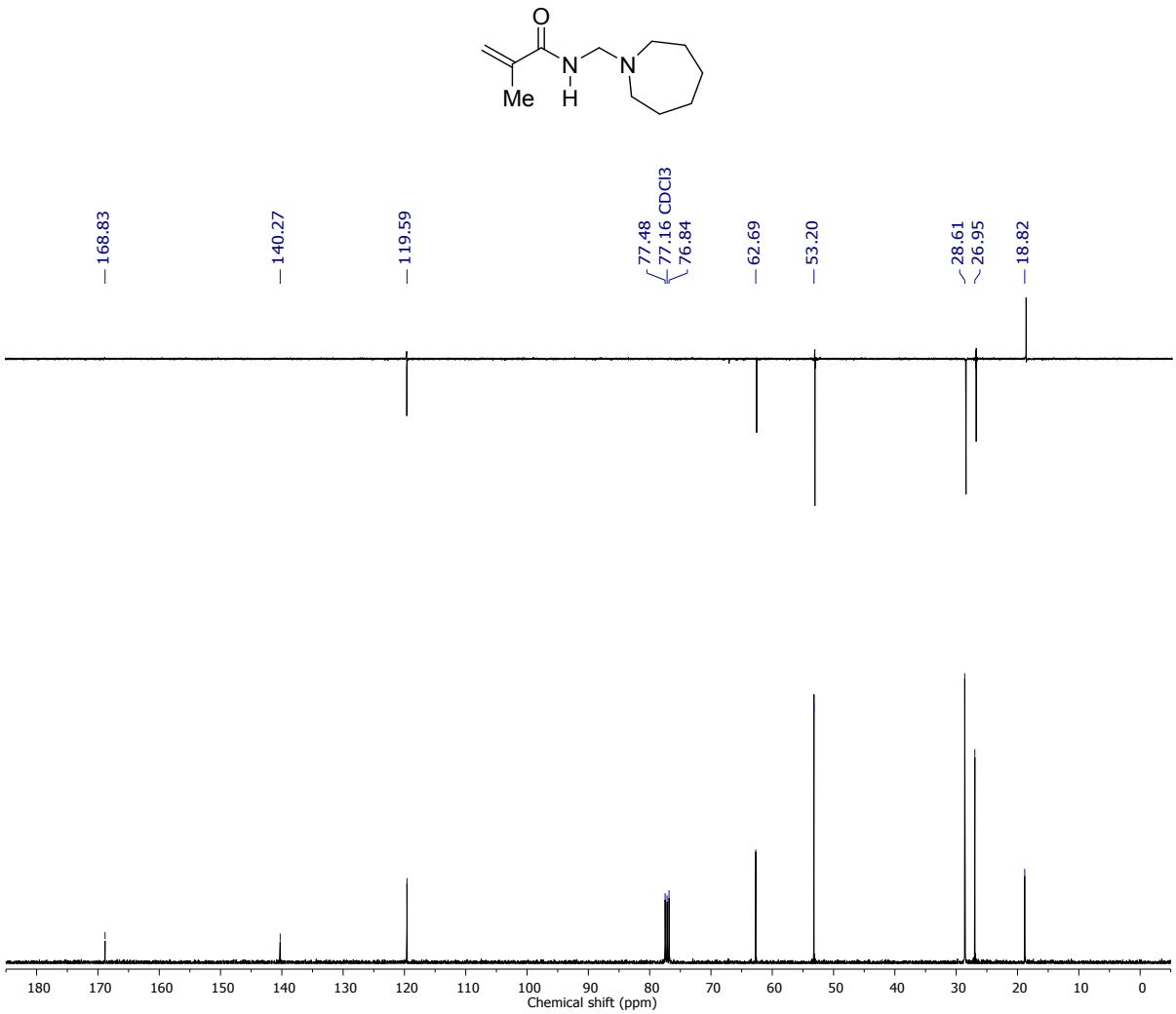
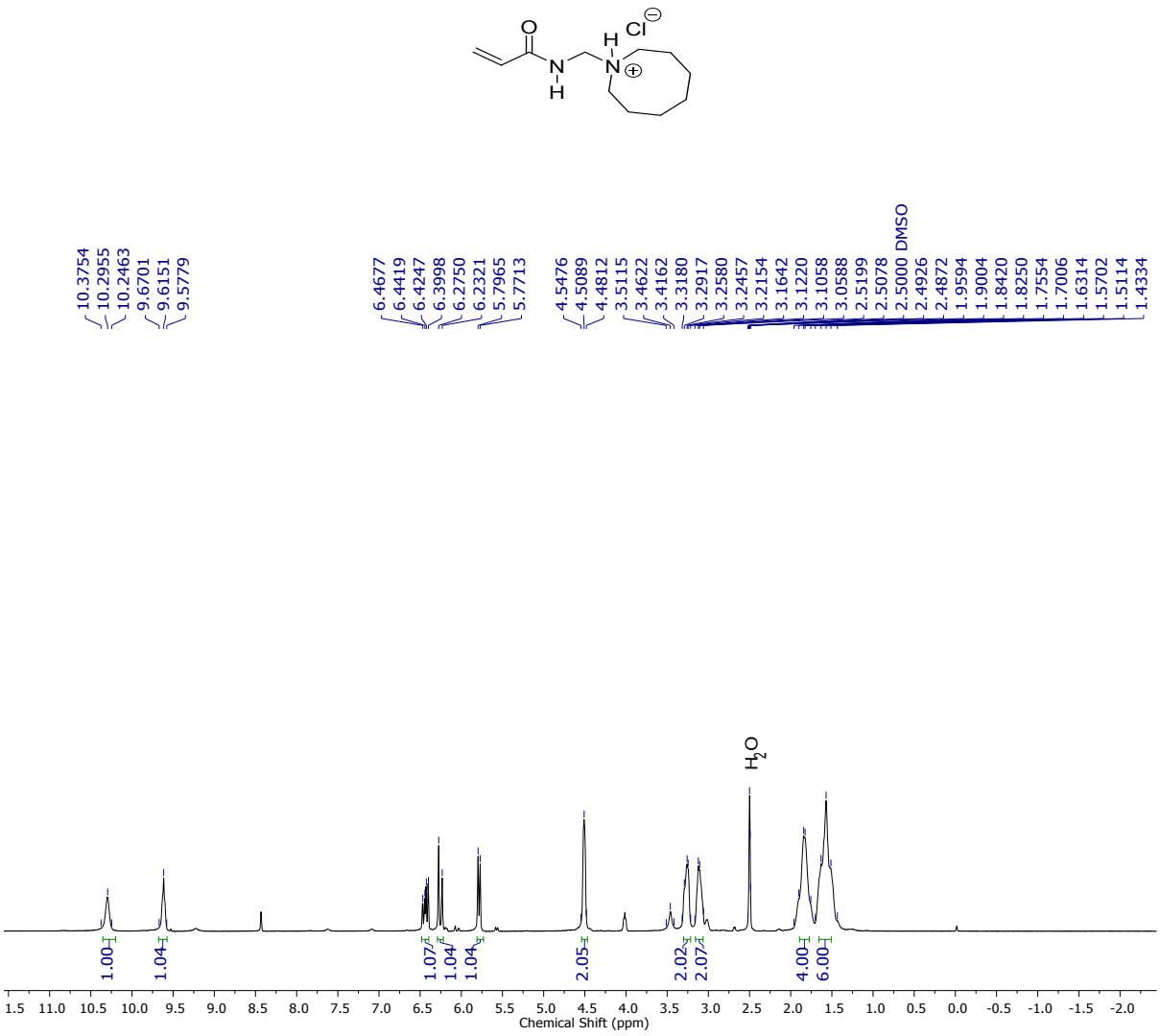
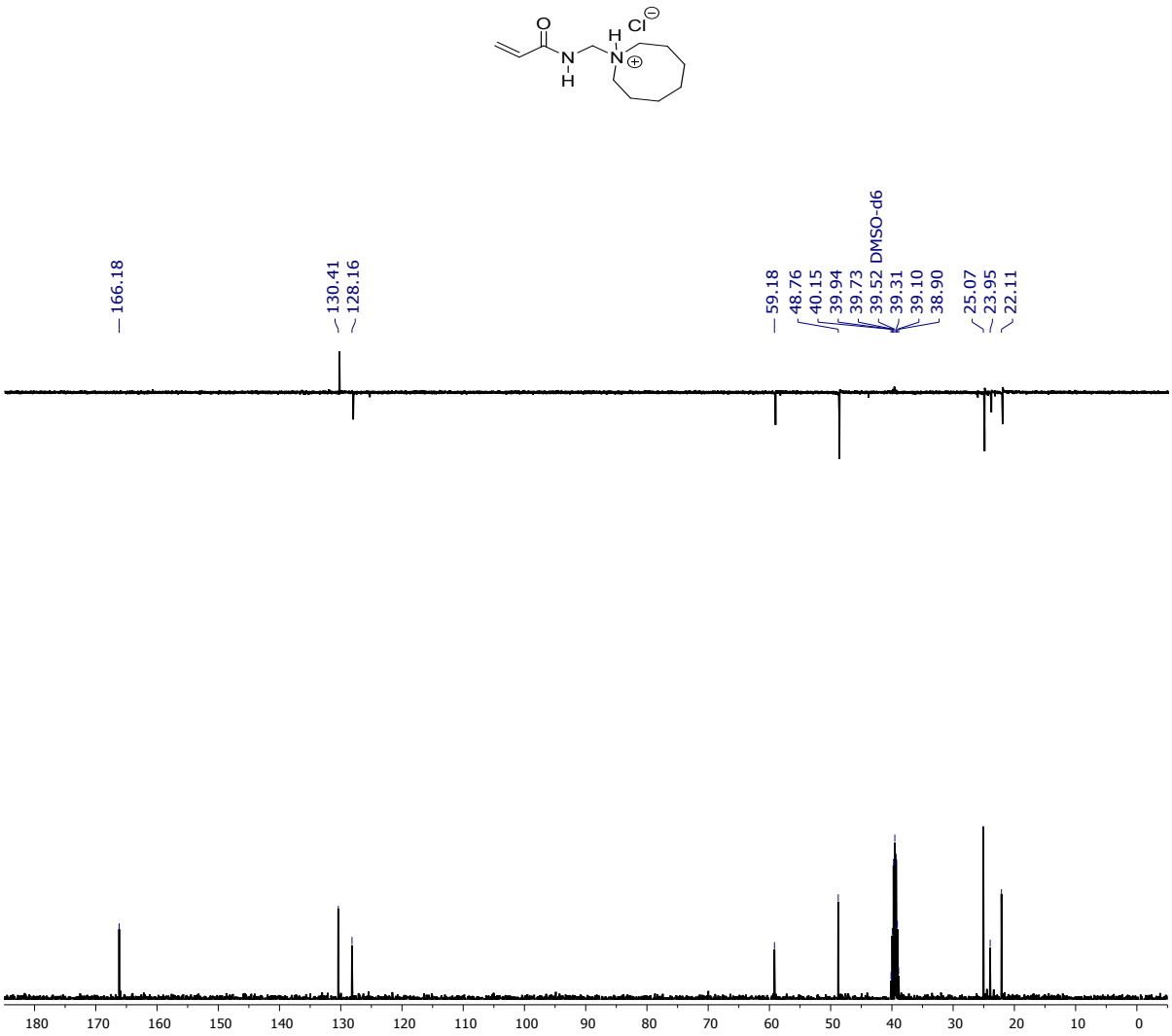


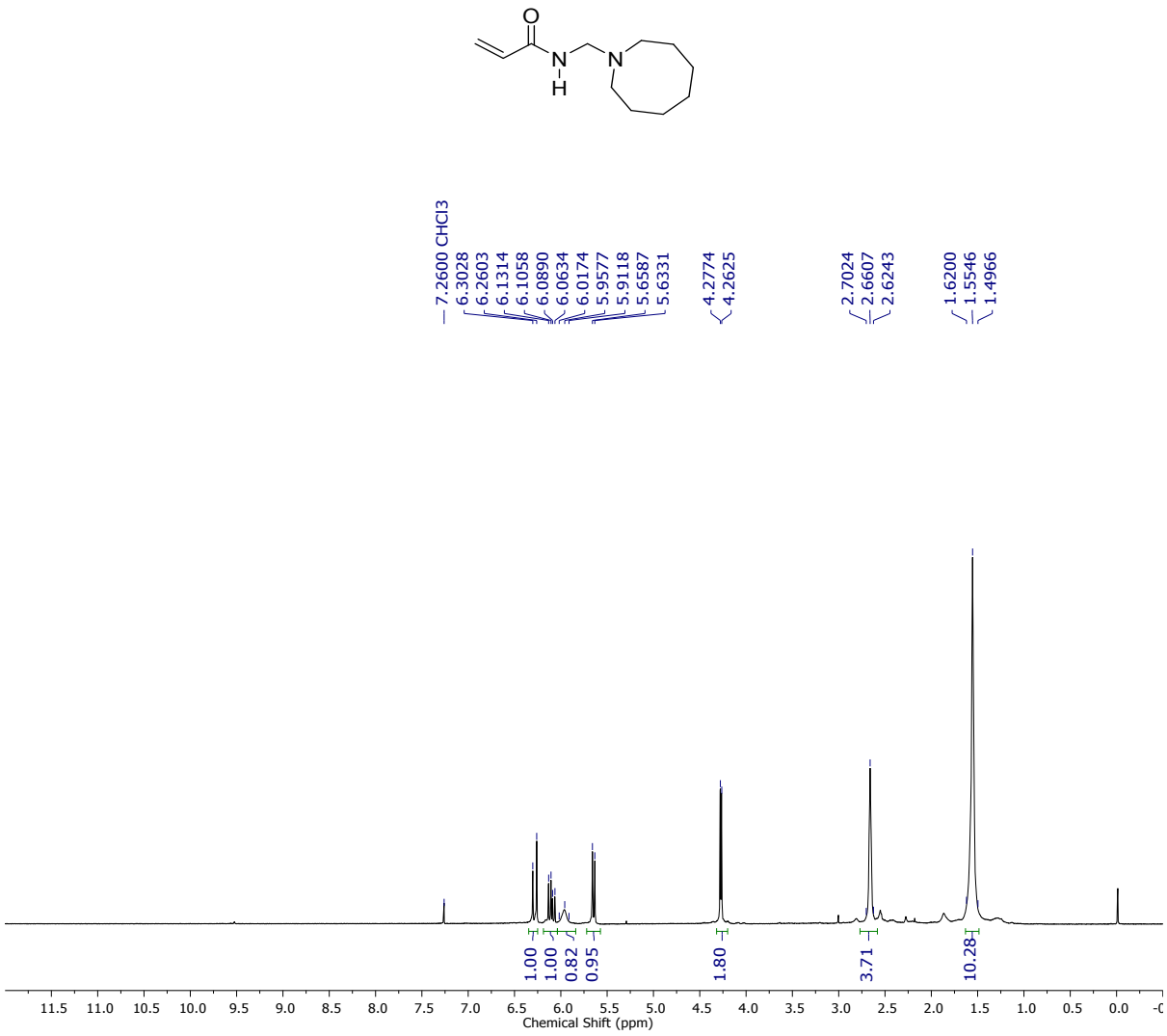
^{1}H NMR (400 MHz) of *N*-[(azocan-1-yl)methyl]prop-2-enamide hydrochloride (7a.HCl) in $(CD_3)_2SO$.



^{13}C NMR (101 MHz) of *N*-[(azocan-1-yl)methyl]-2-methylprop-2-enamide hydrochloride (7a.HCl) in $(CD_3)_2SO$.



^{1}H NMR (400 MHz) of *N*-[(azocan-1-yl)methyl]prop-2-enamide (7a) in $CDCl_3$.



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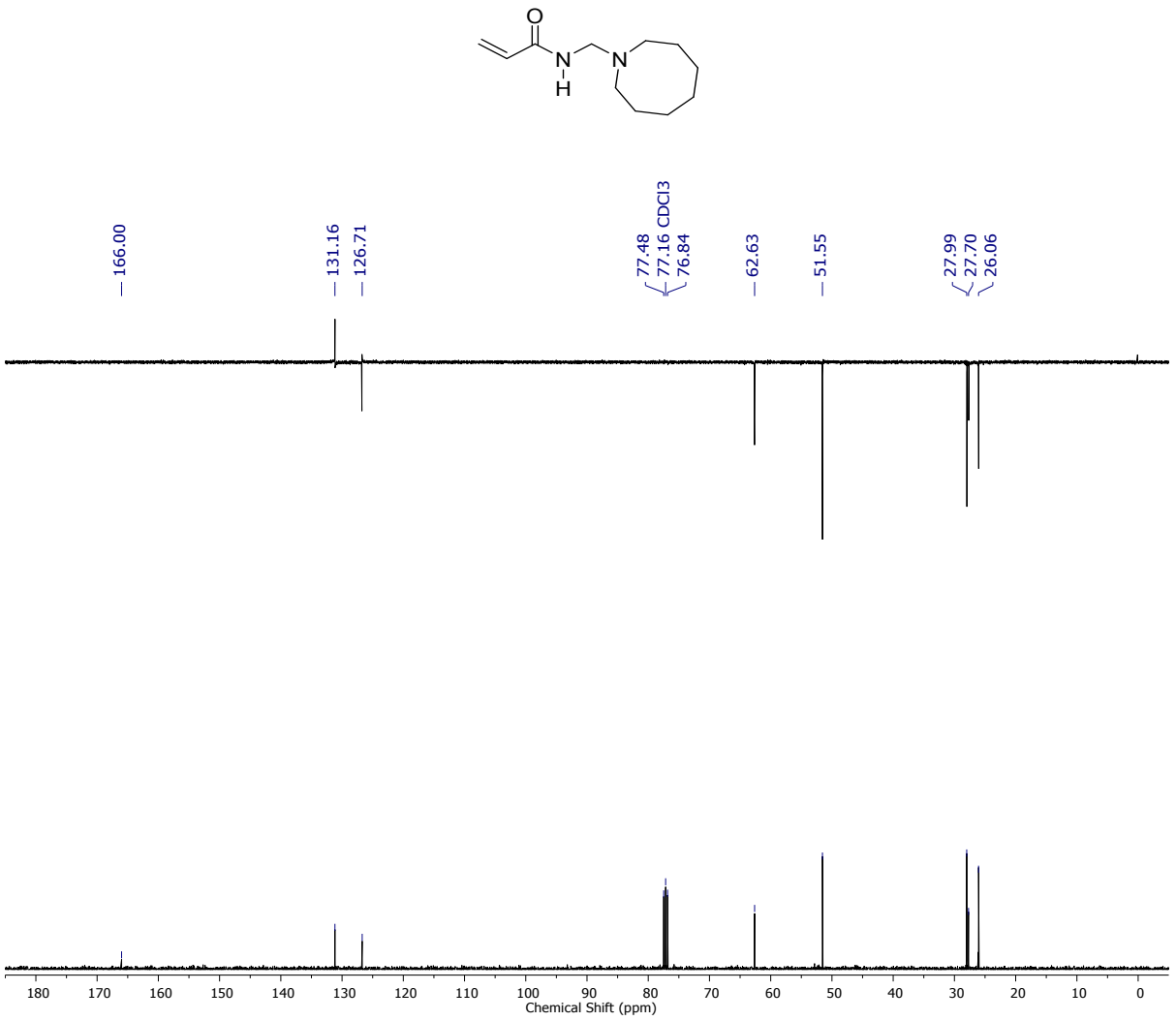
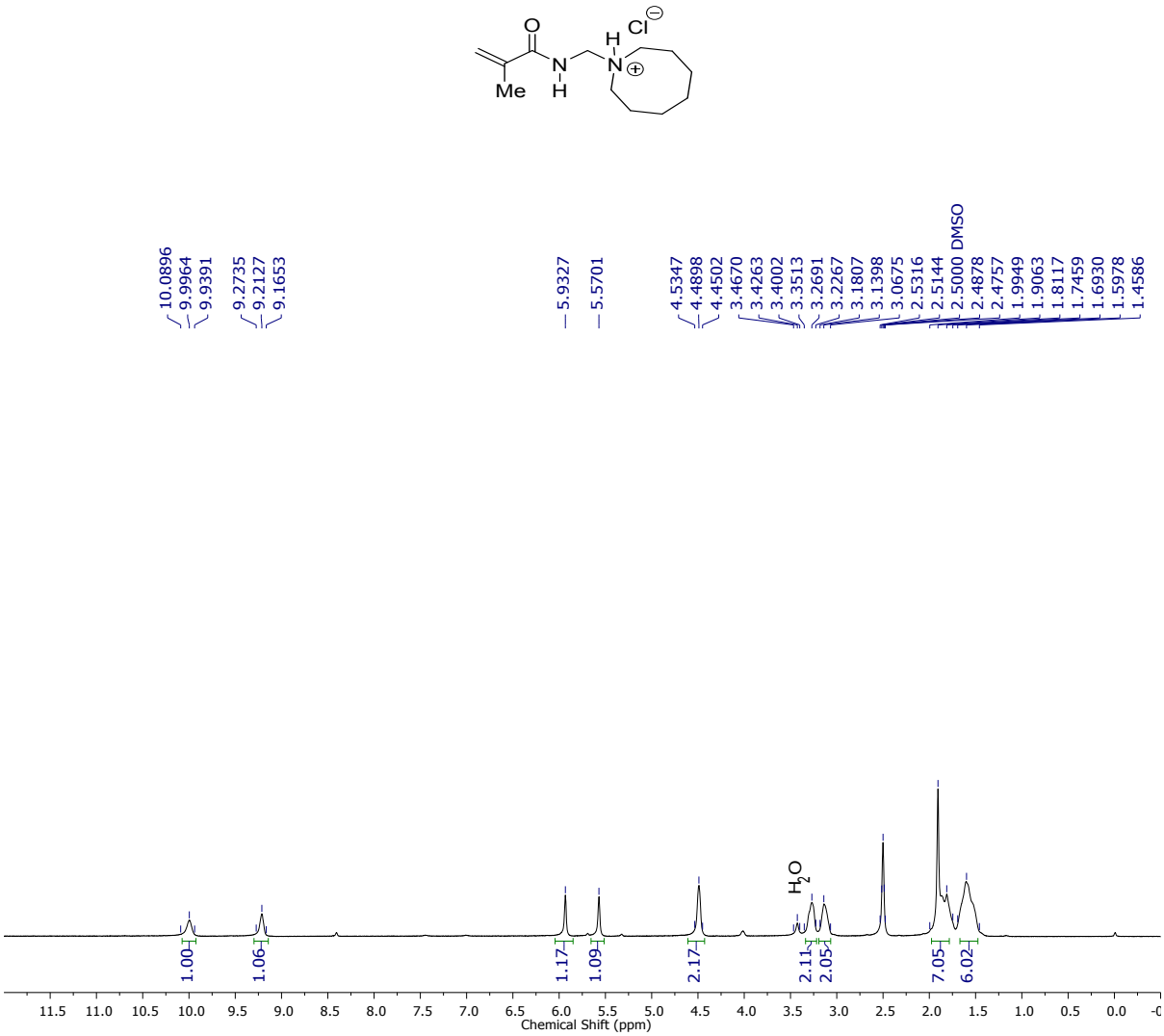
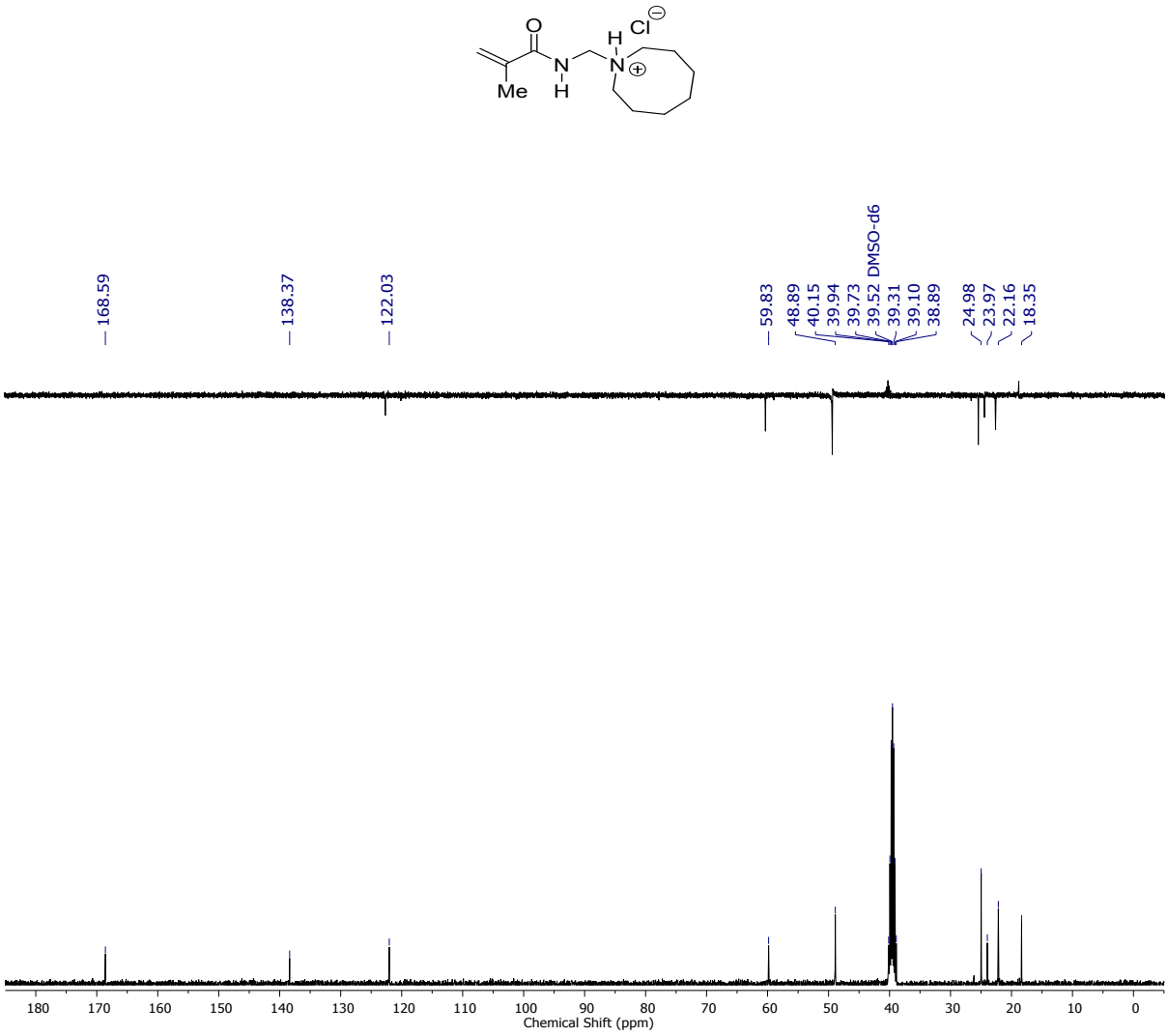


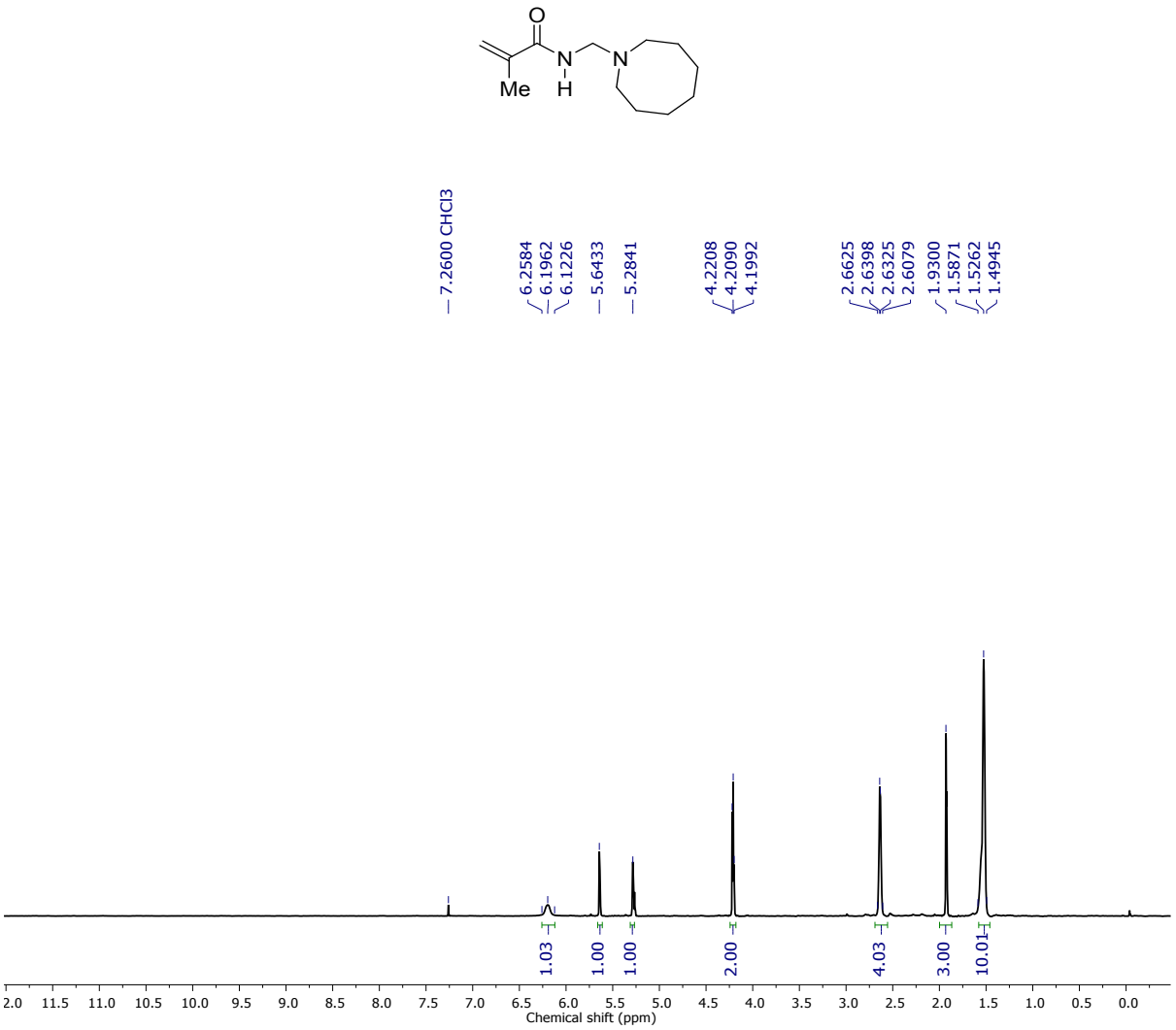
^{1}H NMR (400 MHz) of *N*-[(azocan-1-yl)methyl]-2-methylprop-2-enamide hydrochloride (7b.HCl) in $(CD_3)_2SO$.



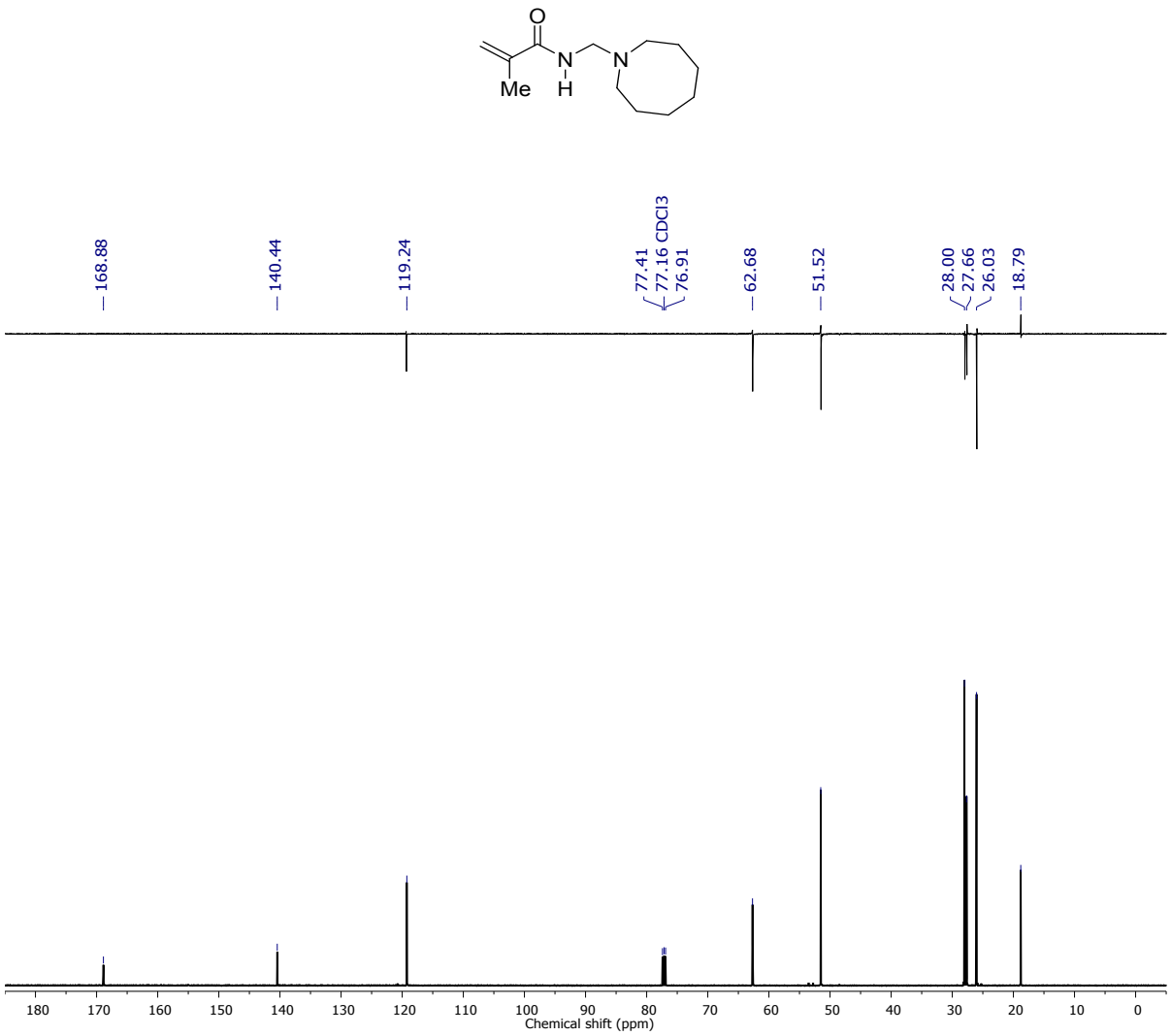
^{13}C NMR (101 MHz) of *N*-[(azocan-1-yl)methyl]-2-methylprop-2-enamide hydrochloride (7b.HCl) in $(CD_3)_2SO$.



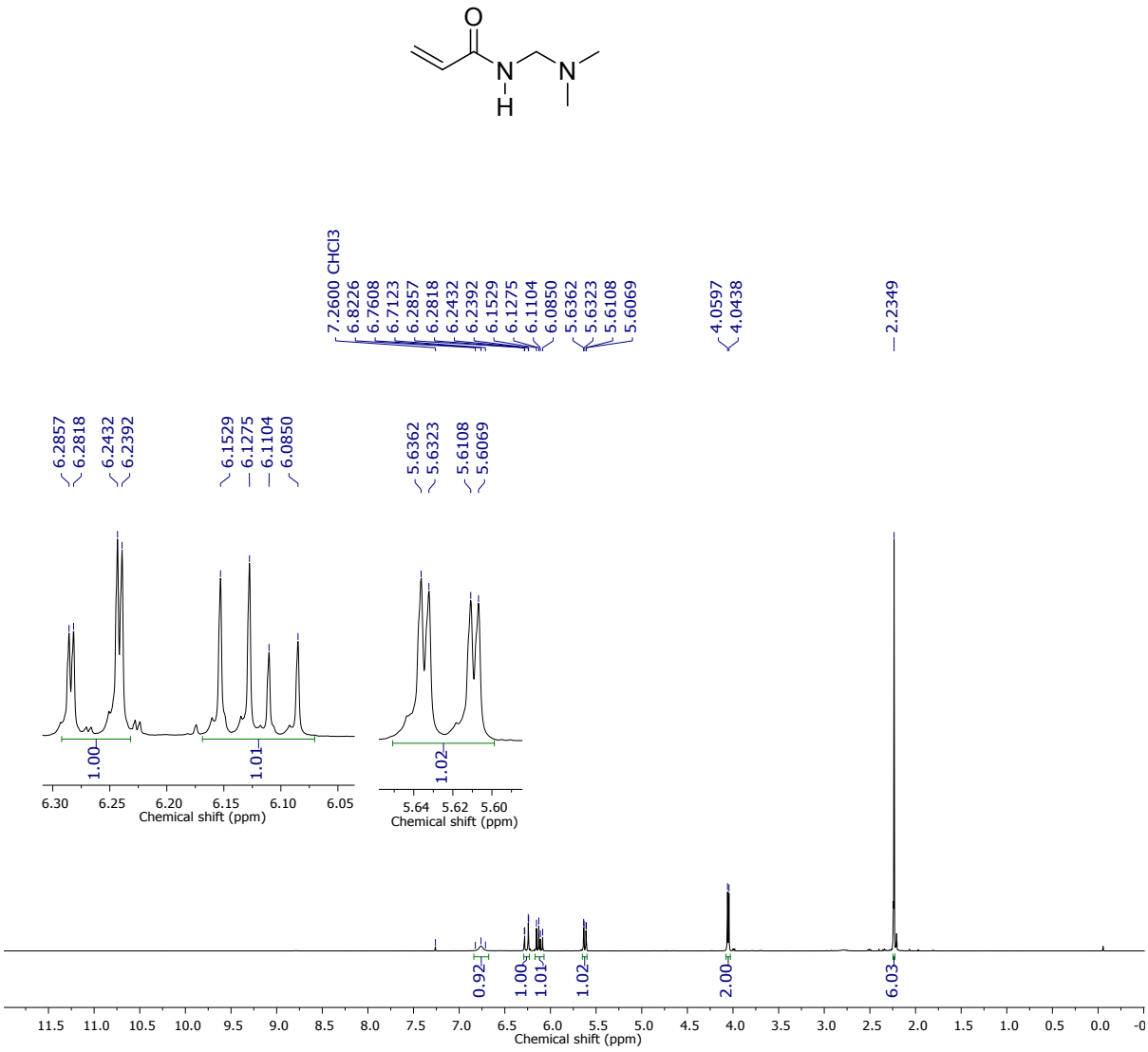
^{1}H NMR (400 MHz) of *N*-[(azocan-1-yl)methyl]-2-methylprop-2-enamide (7b) in $CDCl_3$



^{13}C NMR (101 MHz) of *N*-[(azocan-1-yl)methyl]-2-methylprop-2-enamide (7b) in $CDCl_3$.

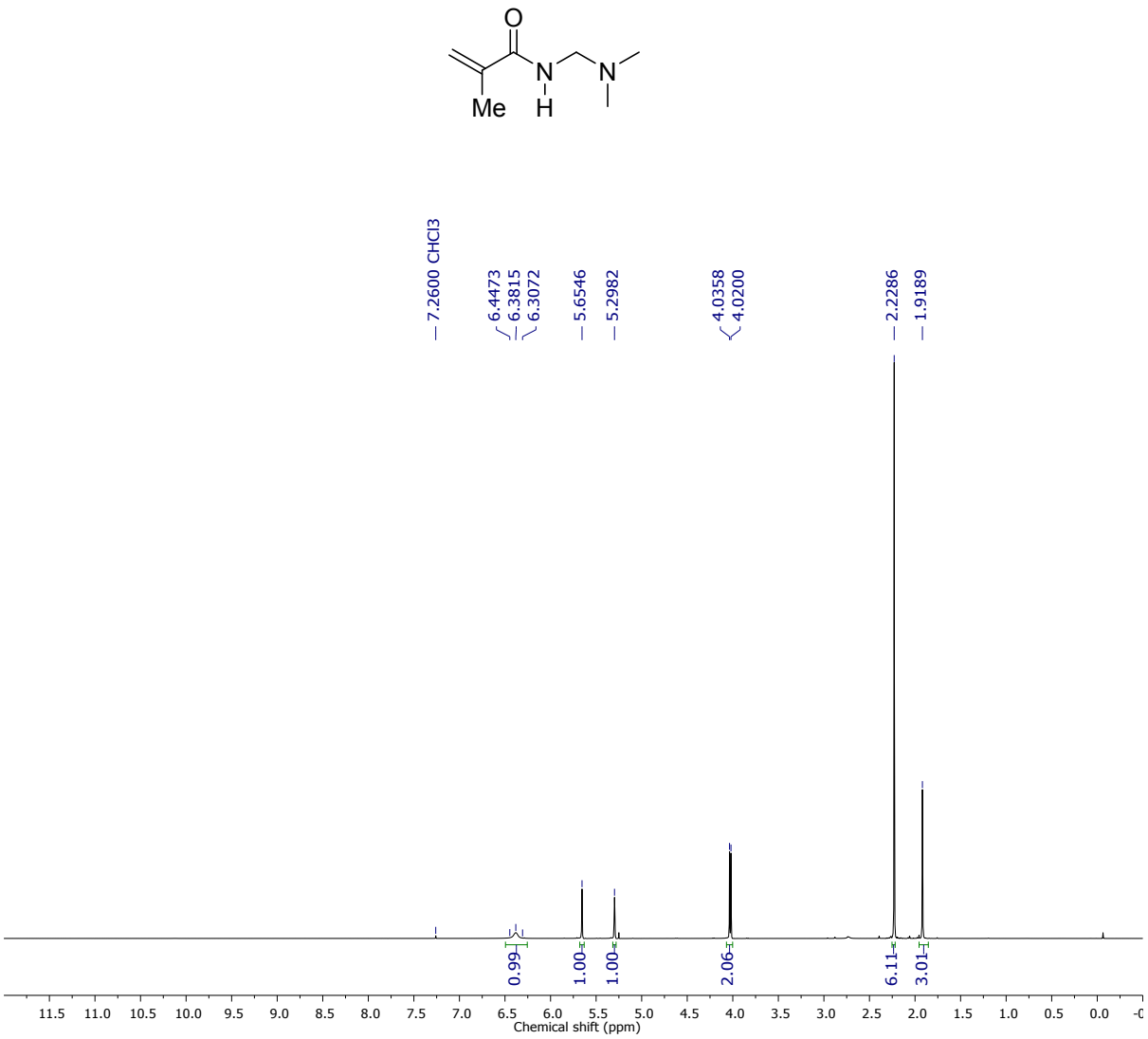


^{1}H NMR (400 MHz) of *N*-[(dimethylamino)methyl]prop-2-enamide (8a) in $CDCl_3$.

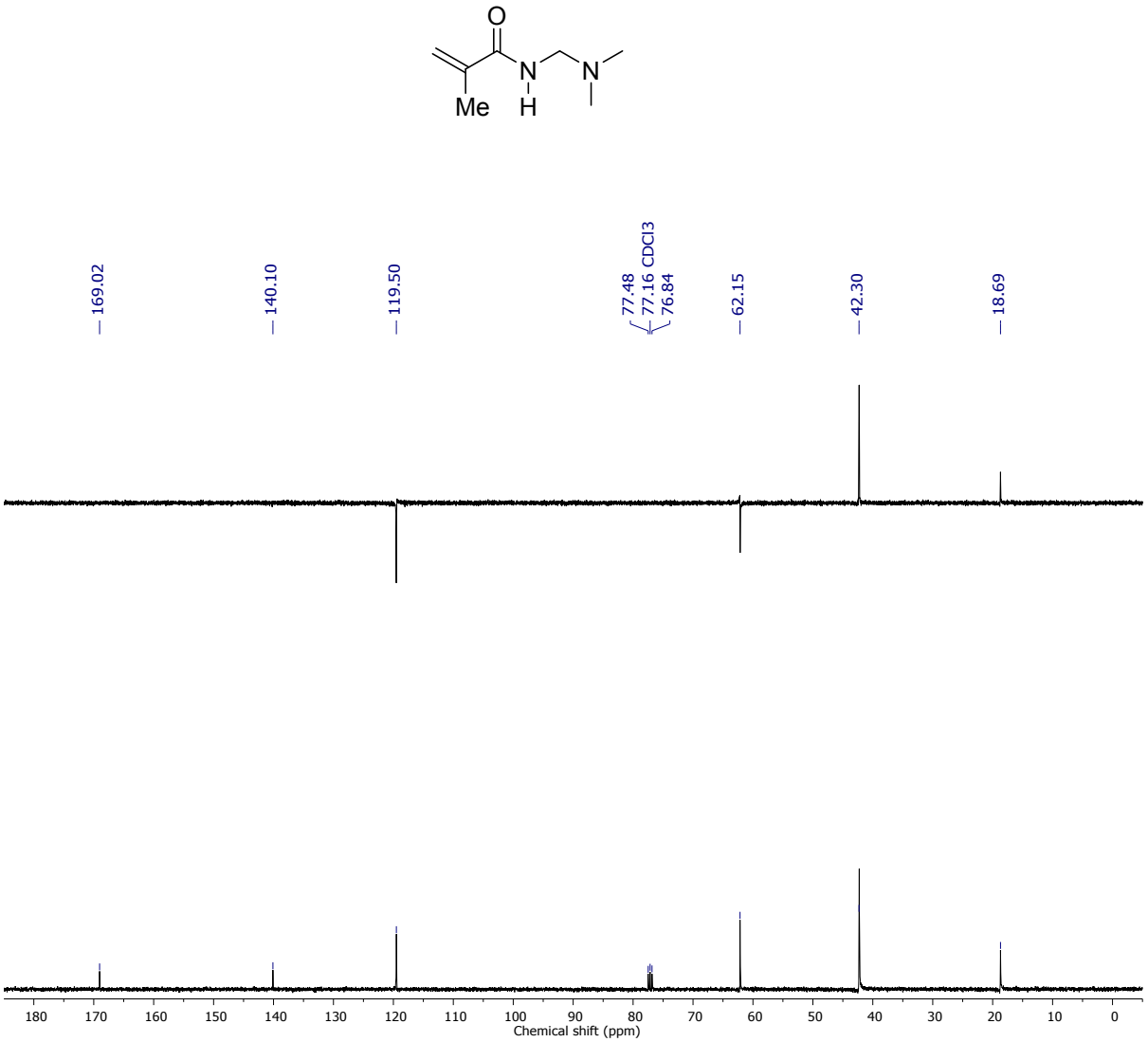


^{13}C NMR (101 MHz) of *N*-[(dimethylamino)methyl]prop-2-enamide (8a) in $CDCl_3$.

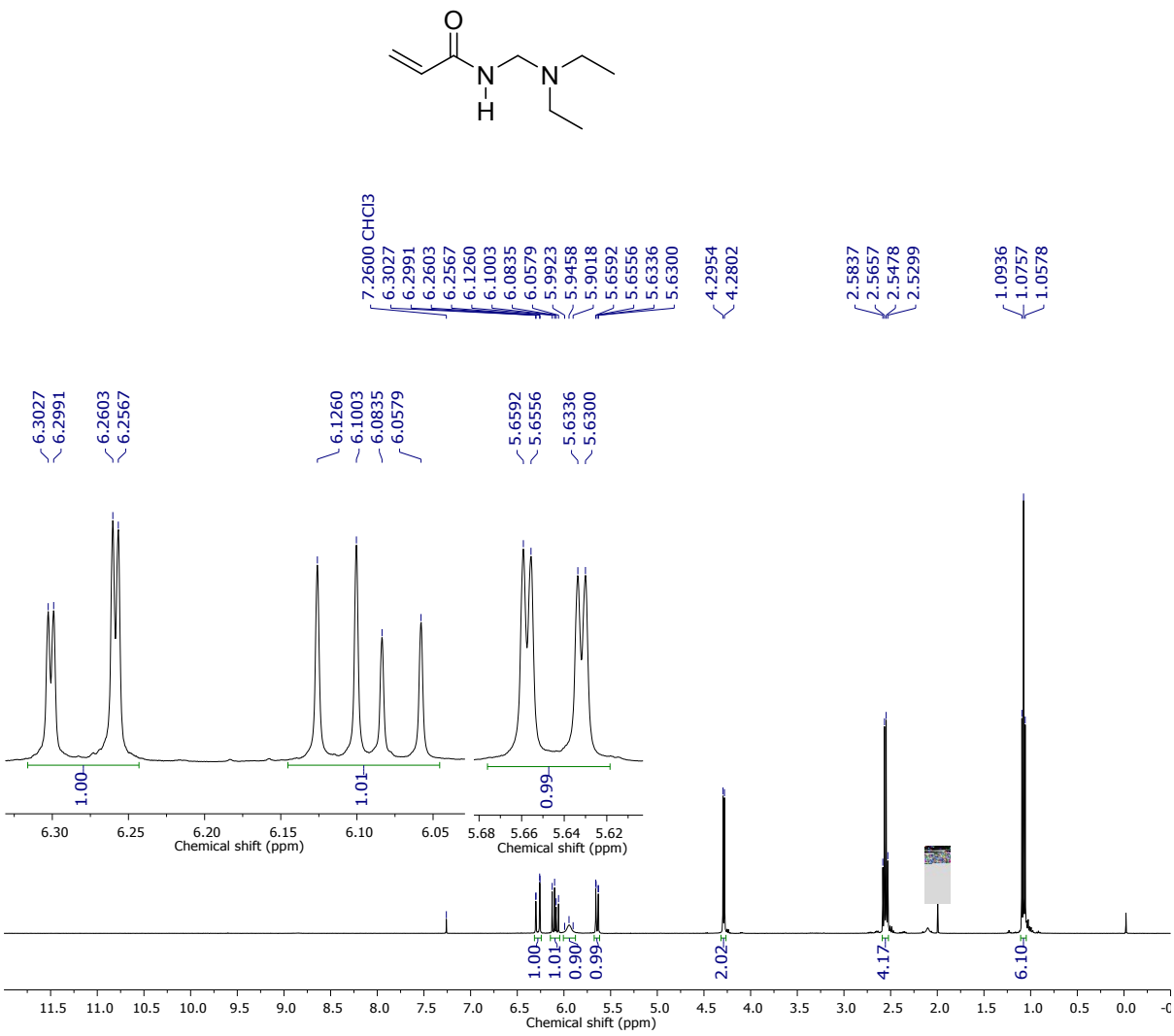
^{1}H NMR (400 MHz) of *N*-[(dimethylamino)methyl]-2-methylprop-2-enamide (8b) in $CDCl_3$.



^{13}C NMR (101 MHz) of *N*-[(dimethylamino)methyl]-2-methylprop-2-enamide (8b) in $CDCl_3$

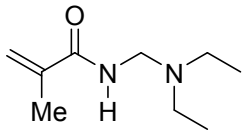


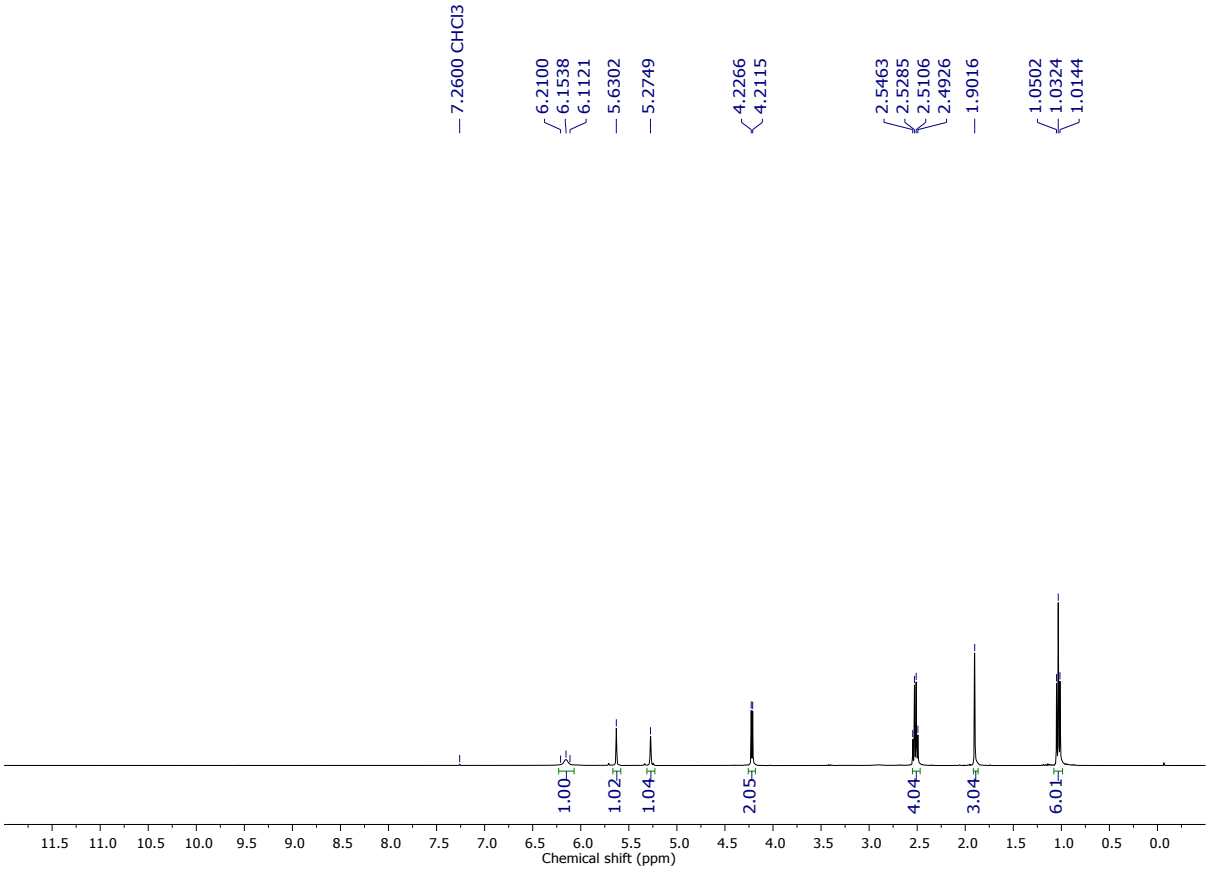
^{1}H NMR (400 MHz) of *N*-[(diethylamino)methyl]prop-2-enamide (9a) in $CDCl_3$.



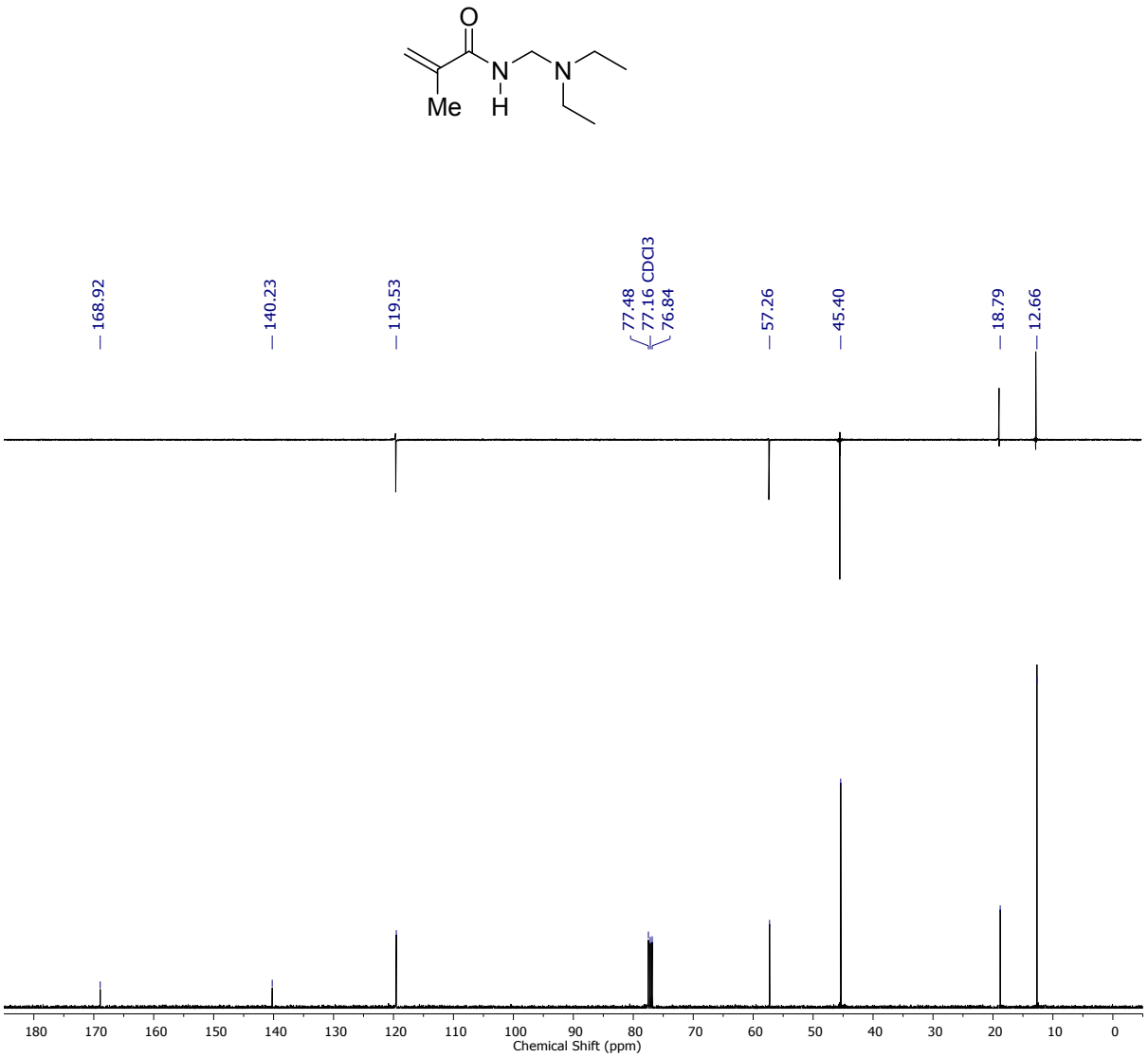
^{13}C NMR (101 MHz) of *N*-[(diethylamino)methyl]prop-2-enamide (9a) in $CDCl_3$.

^{1}H NMR (400 MHz) of *N*-[(diethylamino)methyl]-2-methylprop-2-enamide (9b) in $CDCl_3$.

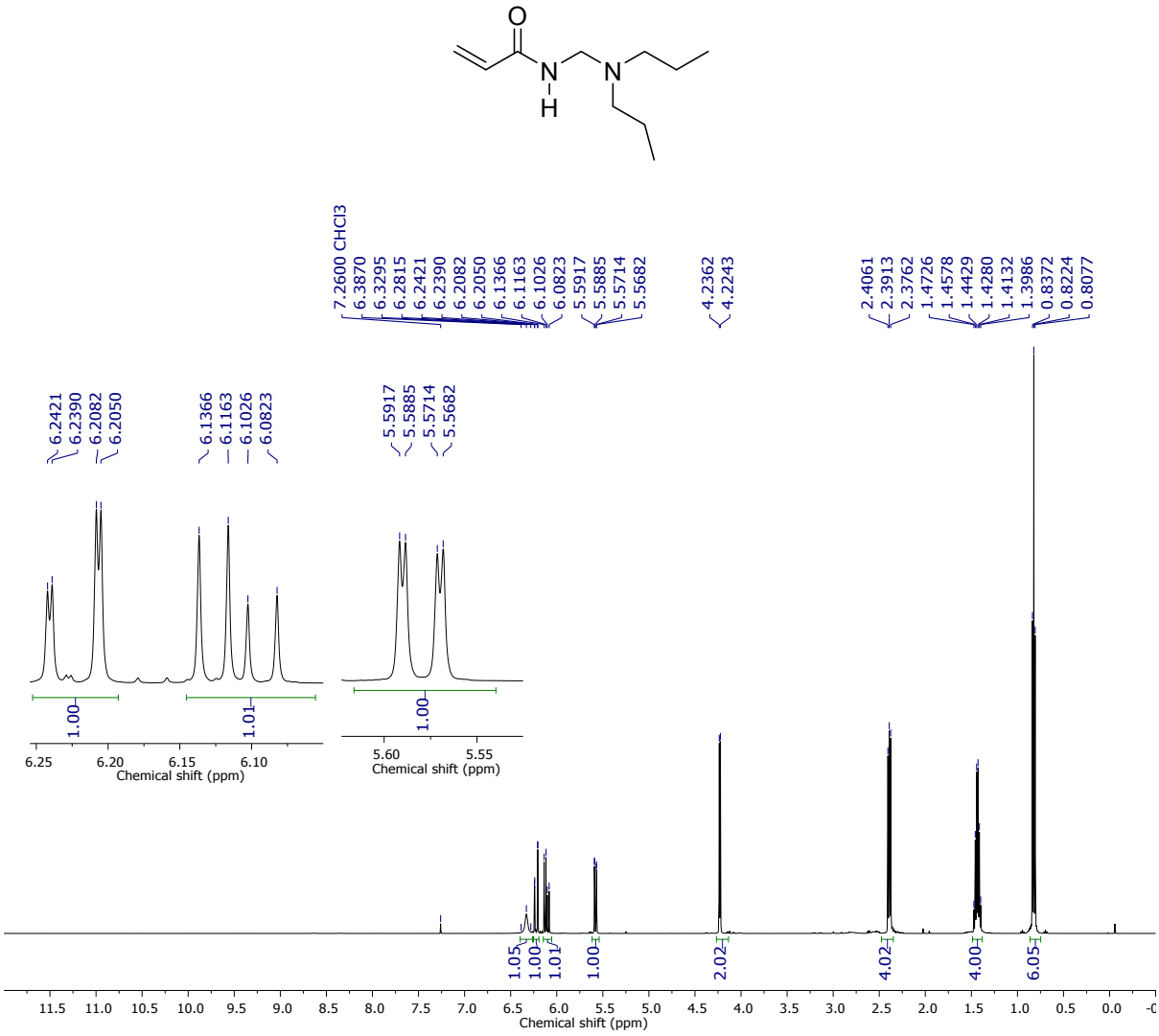




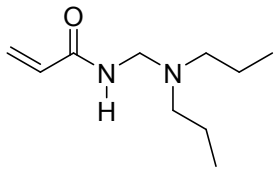
^{13}C NMR (101 MHz) of *N*-[(diethylamino)methyl]-2-methylprop-2-enamide (9b) in $CDCl_3$.

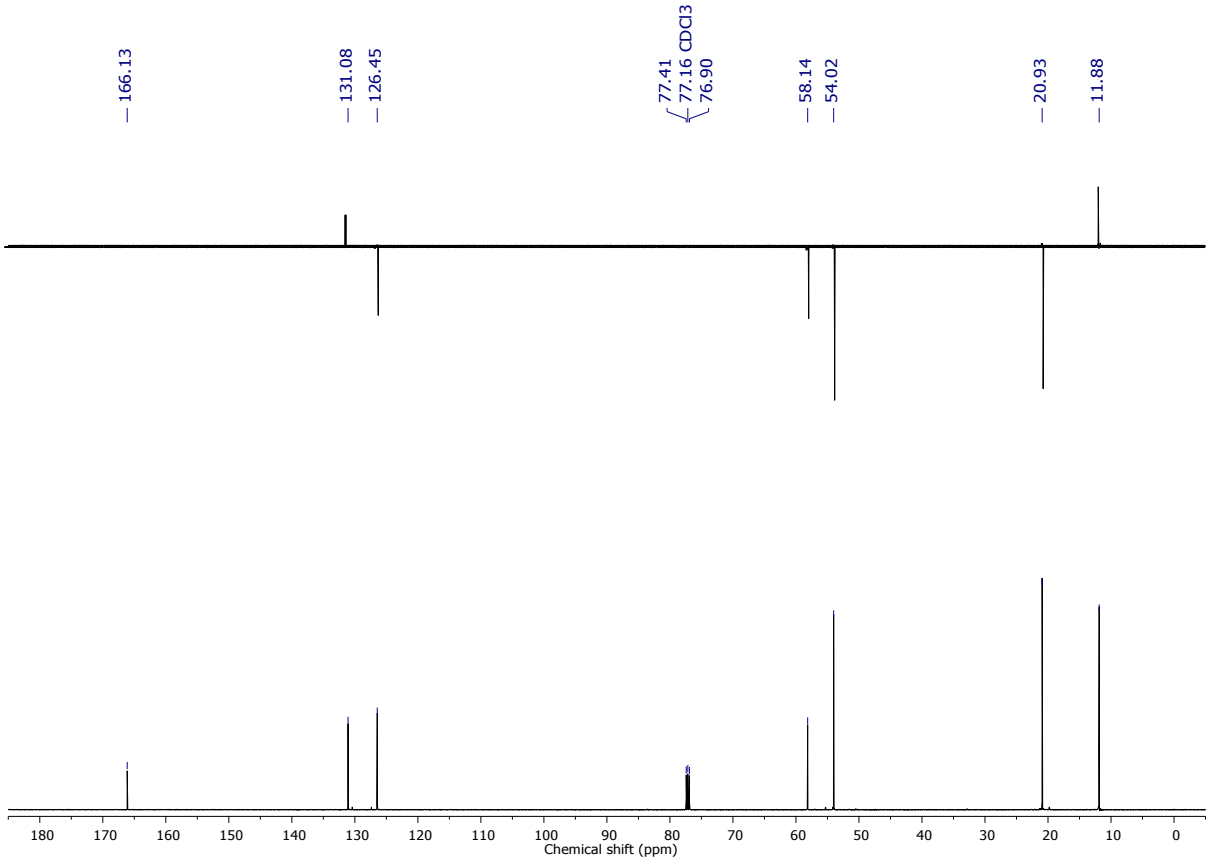


^{1}H NMR (500 MHz) of *N*-[(dipropylamino)methyl]prop-2-enamide (10a) in $CDCl_3$.

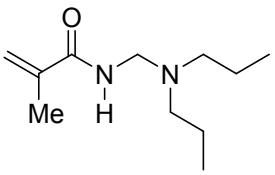


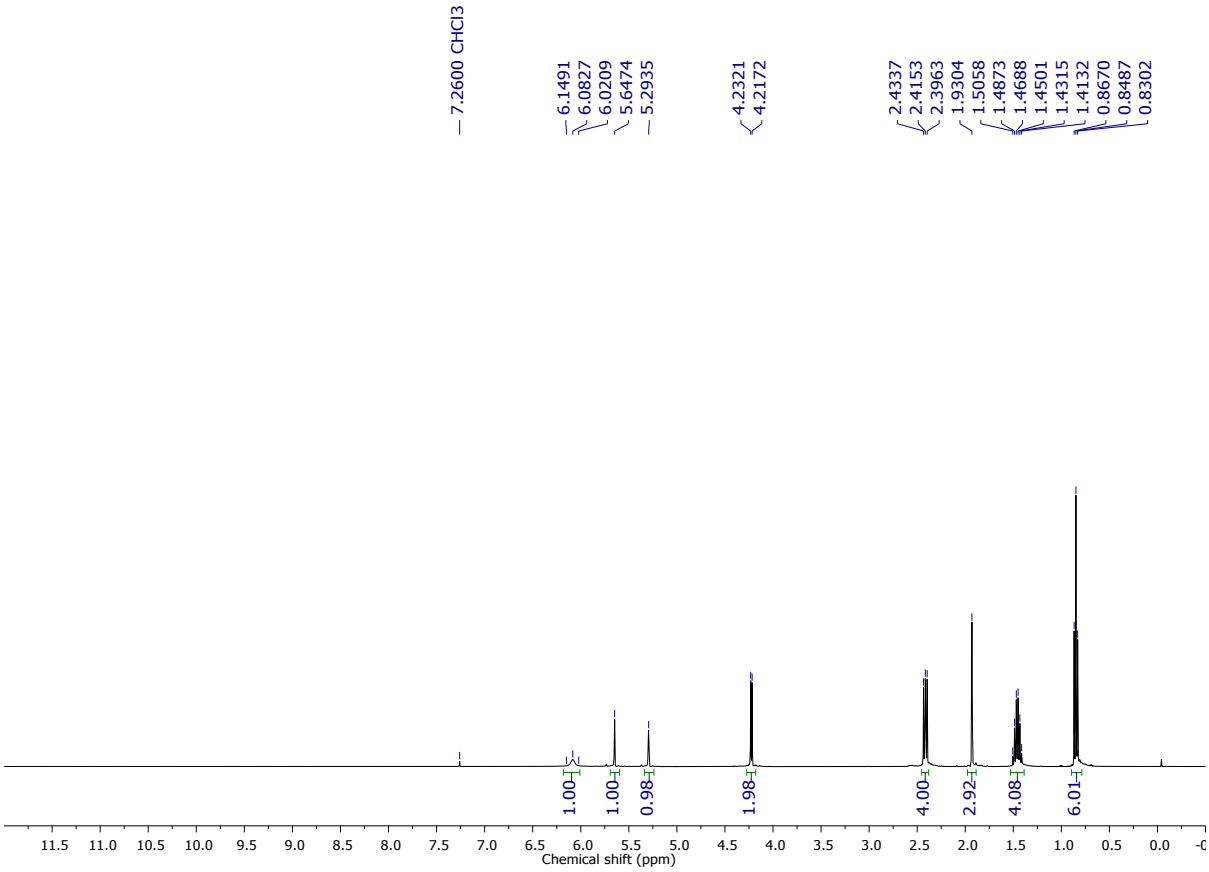
^{13}C NMR (125 MHz) of *N*-[(dipropylamino)methyl]prop-2-enamide (10a) in $CDCl_3$.



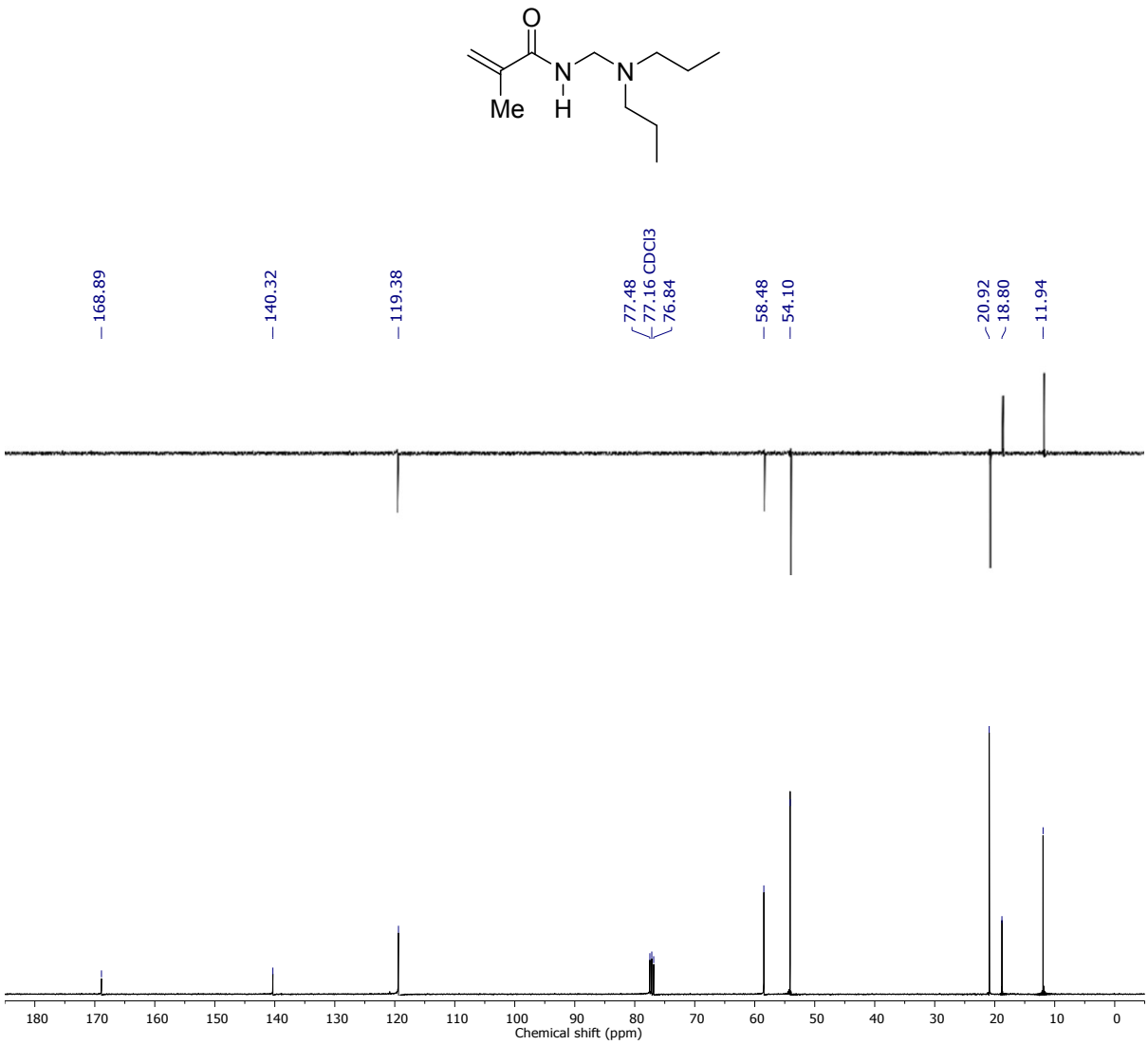


^{1}H NMR (400 MHz) of *N*-[(dipropylamino)methyl]2-methylprop-2-enamide (10b) in $CDCl_3$.

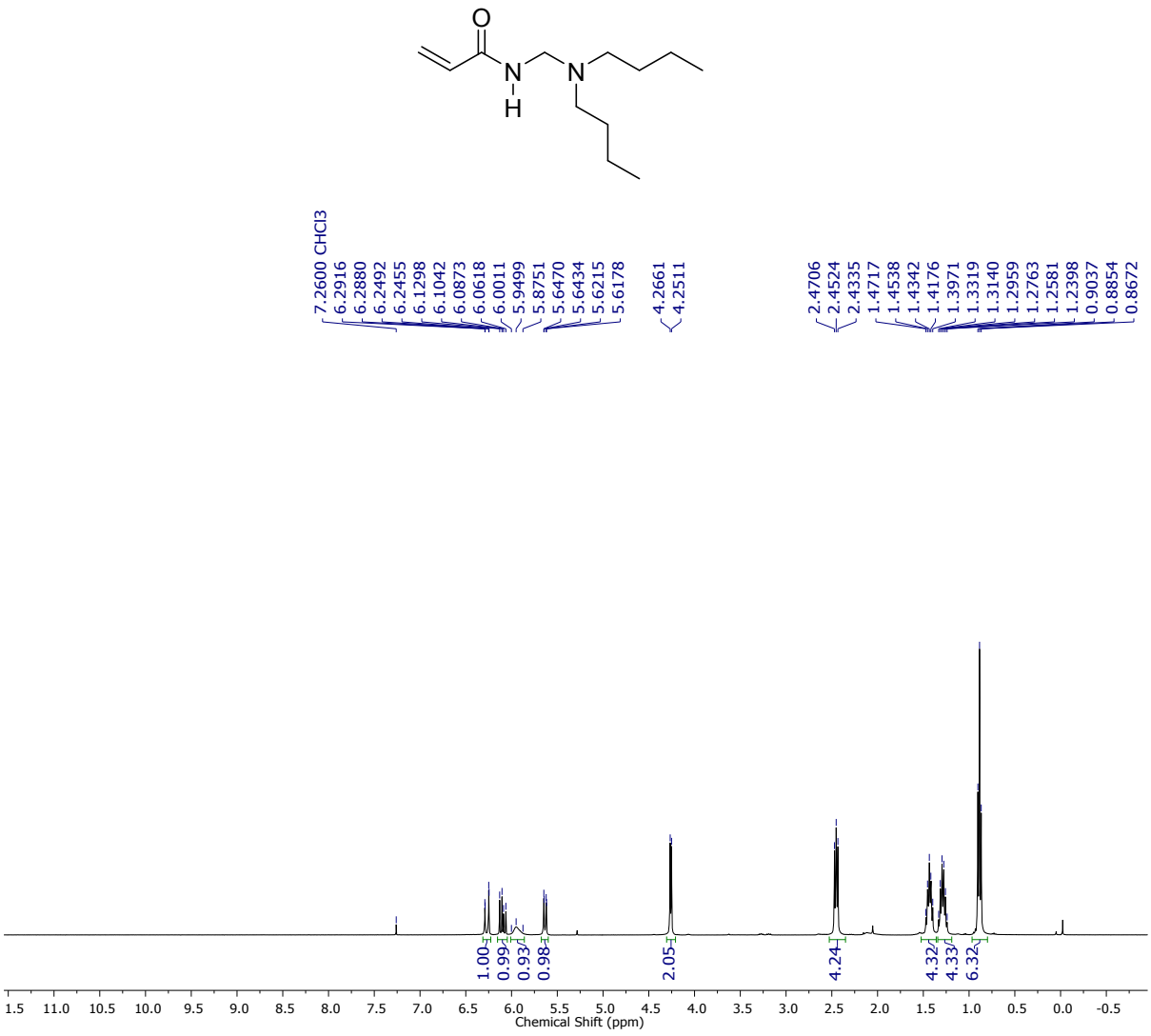




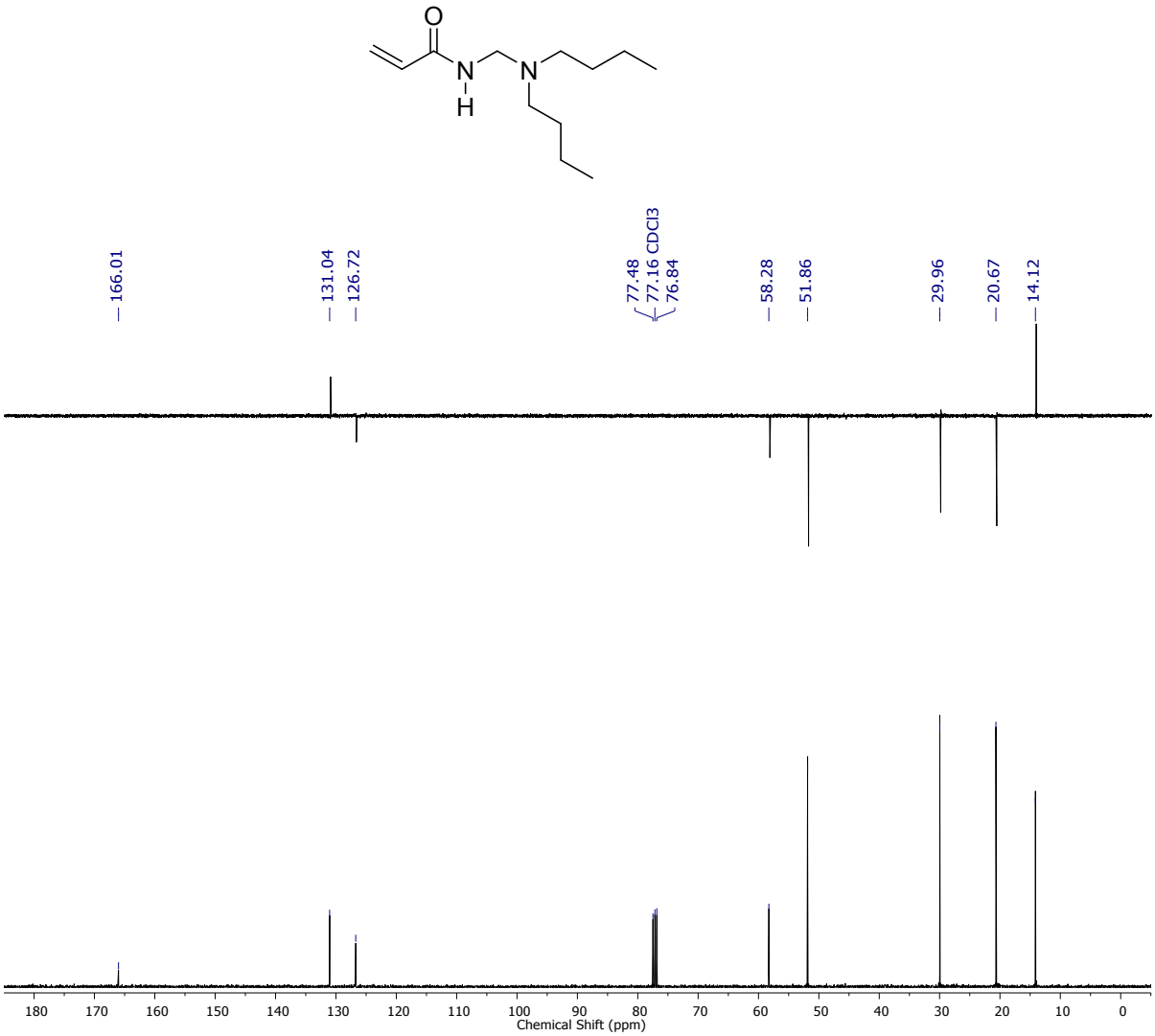
^{13}C NMR (101 MHz) of *N*-[(dipropylamino)methyl]-2-methylprop-2-enamide (10b) in $CDCl_3$.



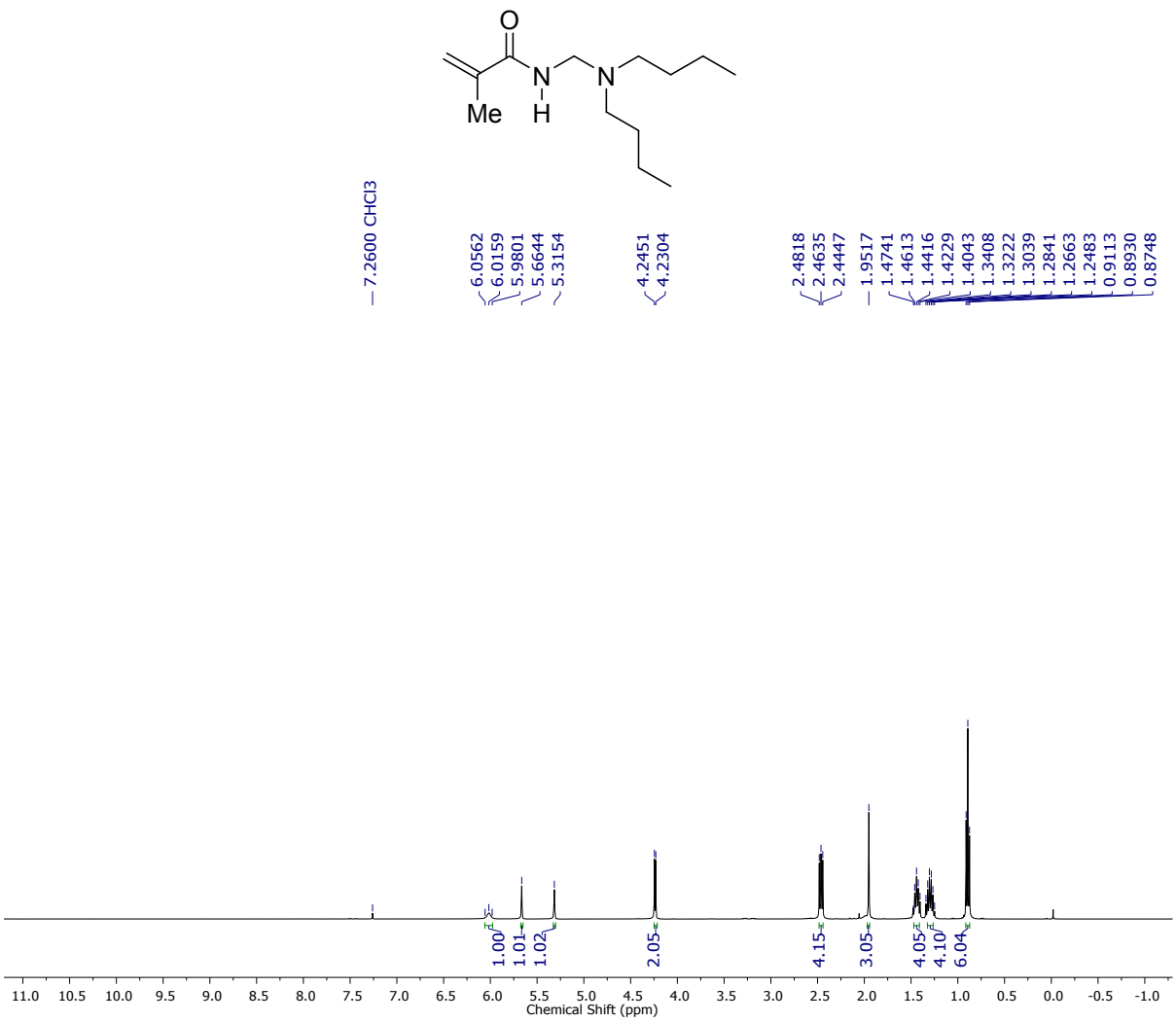
^{1}H NMR (400 MHz) of *N*-[(dibutylamino)methyl]prop-2-enamide (11a) in $CDCl_3$.



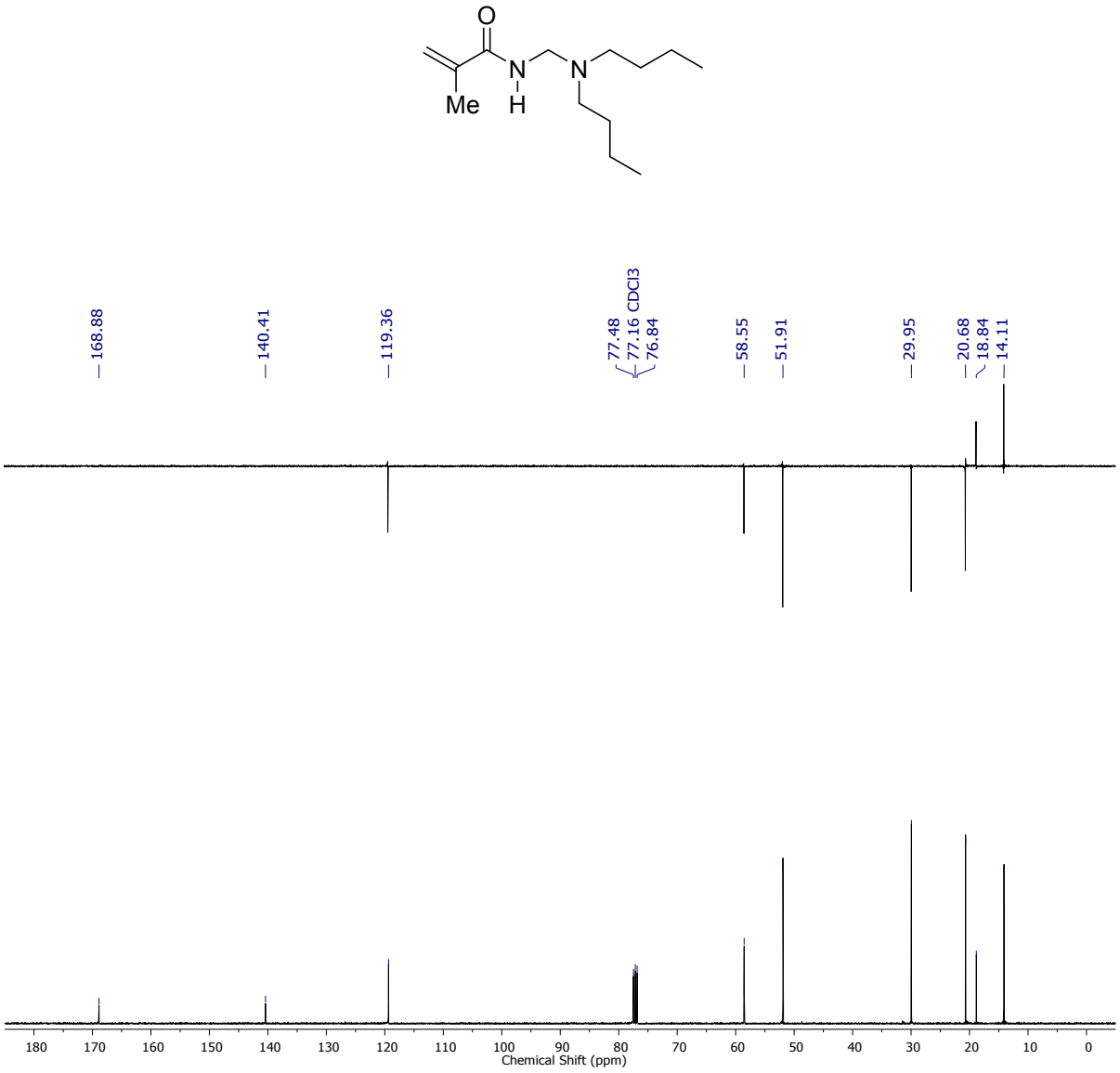
^{13}C NMR (101 MHz) of *N*-[(dibutylamino)methyl]prop-2-enamide (11a) in $CDCl_3$.



^{1}H NMR (400 MHz) of *N*-[(dibutylamino)methyl]-2-methylprop-2-enamide (11b) in $CDCl_3$.



^{13}C NMR (101 MHz) of *N*-[(dibutylamino)methyl]-2-methylprop-2-enamide (11b) in $CDCl_3$.



X-ray crystallography:

Table S1:

Hydrogen bonds for 1-(hydroxymethyl)azocan-1-ium chloride (**5b**) [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1O1)...Cl(1)	0.82	2.17	2.984(4)	174.2
N(1)-H(1)...Cl(1)#1	0.98	2.21	3.150(4)	160.3
C(7)-H(7A^a)...O(1)#2	0.97	2.35	3.247(7)	152.9
C(8)-H(8A)...O(1)#2	0.97	2.38	3.229(6)	146.3
C(8)-H(8B)...Cl(1)#3	0.97	2.78	3.667(5)	151.6

Table S2:

Hydrogen bonds for *N*-[(azocan-1-yl)methyl]prop-2-enamide hydrochloride (**7a**.**HCl**) [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(4)-H(4)...Cl(2)	0.86	2.34	3.188(3)	170.7
N(1)-H(1)...Cl(1)	0.98	2.18	3.103(3)	156.9
N(3)-H(3)...Cl(1)	0.98	2.16	3.097(3)	159.1
N(2)-H(2)...Cl(2)#1	0.86	2.35	3.199(3)	168.6
C(1)-H(1A)...O(3)	0.97	2.45	3.309(4)	147.6
C(1)-H(1B)...Cl(2)#2	0.97	2.93	3.783(4)	147.5
C(2)-H(2B)...O(3)#2	0.97	2.57	3.368(5)	139.7
C(8)-H(8A)...O(3)#2	0.97	2.45	3.311(4)	147.7
C(8)-H(8B)...O(4)#3	0.97	2.31	3.276(5)	171.9
C(10)-H(10)...Cl(2)#1	0.93	2.96	3.714(4)	138.7
C(17)-H(17A)...O(4)#3	0.97	2.63	3.385(5)	134.8
C(18)-H(18A)...Cl(2)#4	0.97	2.89	3.773(4)	151.4
C(18)-H(18B)...O(4)	0.97	2.51	3.348(5)	145.2
C(19)-H(19A)...O(4)#3	0.97	2.38	3.251(4)	148.8
C(19)-H(19B)...O(3)#2	0.97	2.34	3.307(5)	172.8

Symmetry transformations used to generate equivalent atoms:

#1 x,y-1,z #2 -x,-y+1,-z+1 #3 -x+1,-y+1,-z+1 #4 -x+1,-y+2,-z+1

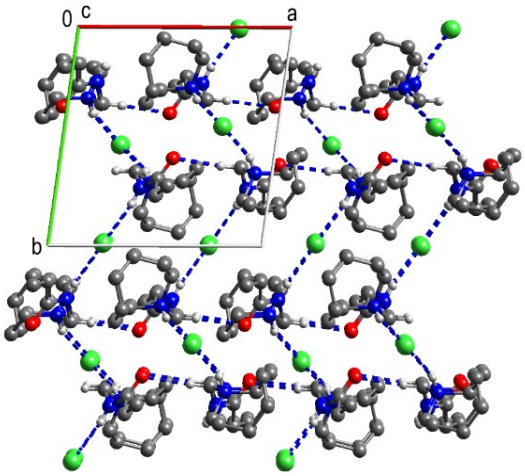


Figure S1. Crystal structure of *N*-[(azocan-1-yl)methyl]prop-2-enamide hydrochloride (**7a**.**HCl**) viewed down the *c*-axis.

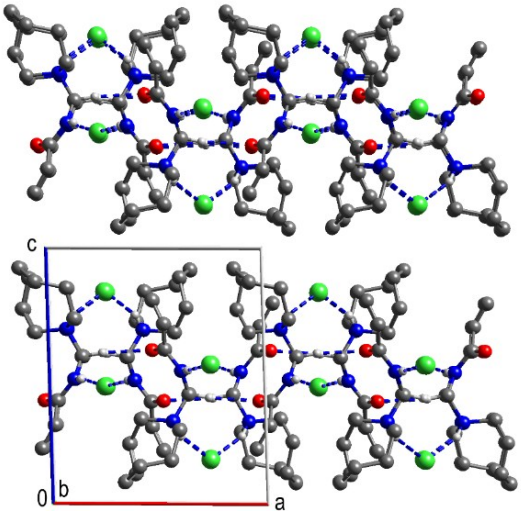


Figure S2. Crystal structure of *N*-[(azocan-1-yl)methyl]prop-2-enamide hydrochloride (**7a**.**HCl**) viewed down the *b*-axis.