Supplementary information

New cationic linear *N*-chloramines based on *N*-*t*-Butylamide: chemical synthesis and antibacterial application

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Contents

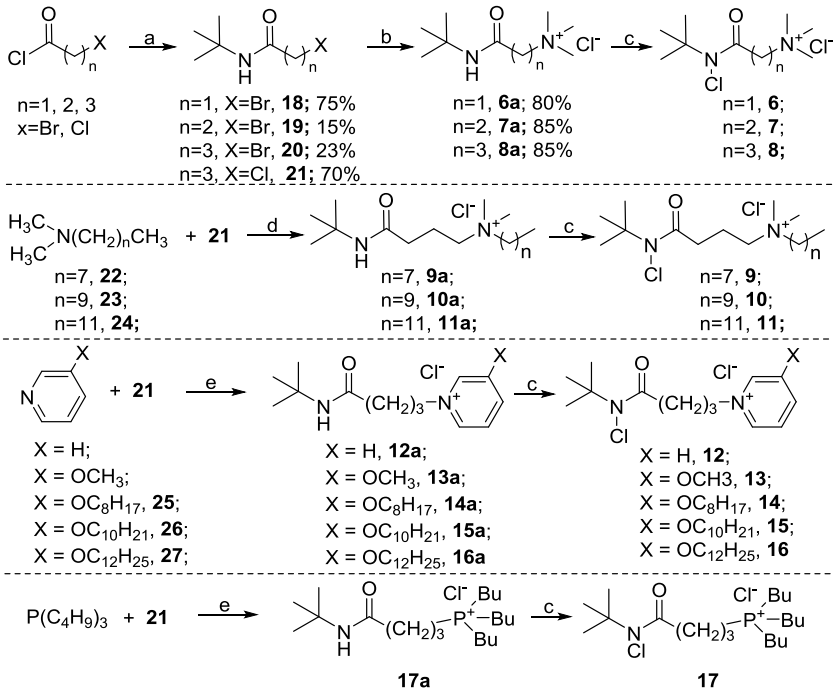
1. Reagents and materials

All reagents and solvents purchased from commercial suppliers (Aladdin Co. China) were used in this research without further purification. All products and intermediates were purified by flash column chromatography and silica gel which received from Qingdao Haiyang Chemical Plant, China. Thin layer chromatography (TLC) was carried out by means of iodine fumigation. *Escherichia coli* ATCC 25922 and *Staphylococcus aureus* ATCC 25923 were given as a gift from Dalian Medical University and were herein used as model microorganism to challenge all biocides.

QA *N*-chloramine **1-3** were prepared according to our previous procedure, respectively;[1-3] and *t*-butylamide **18-21**,[4-8] tertiary amine **22-24**[9, 10] , alkoxypyridine **25-27**[11-13] was synthesized as described. The chlorination agent used in this work, *t*-butyl hypochlorite, was also synthesized as described.[14] The obtained NMR data of all this published compounds were in accord with those found in previous literatures.

NMR spectra were recorded at room temperature using Bruker DRX 500 instrument at the condition of $CDCl_3$ or D_2O. Mass spectra were conducted on a Q-TOF Micro mass spectrometry (Manchester, UK) equipped with Z-spray ionization source.

2. Synthesis of linear *N*-chloramines



Scheme 1. Chemical synthesis of **6-17**: a) $(CH_3)_3CNH_2$, $(Et_2)_3N$ or K_2CO_3, CH_2Cl_2, 0 ℃, 2 h; b) Aqueous $N(CH_3)_3$, EtOH, reflux, overnight; Ion-exchange (Amberlite R IRA-900, Cl^-); c) *t*-BuOCl, H_2O: *t*-BuOH (1:4, v:v), rt; d) EtOH, reflux, 24 h; e) CH_3CN, reflux, 24 h.

2.1 General synthesis of *t*-butylamide **18-21**

N-*t*-Butyl-2-bromoacetamide **18.**[4-8] As described in references, to a solution of bromoacetyl chloride (30.0 mmol) in dichloromethane (20 mL) was added dropwise into the mixture of *t*-butylamine (33.0 mmol, 1.1 equiv.) and potassium carbonate (60.0 mmol, 2.0 equiv.) in dichloromethane (30 mL) at 0℃, control the drip adding time more than 30 min, which mixture

was stirred for 2 h at room temperature. Inorganic residues were filtrated off and organic mixture was concentrated under vacuum. The crude product was applied on chromatography column (ether/ethyl acetate, 1:3, v/v) to afford **18** (4.36 g, 74.9%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.23 (s, 1H), 3.72 (s, 2H), 1.31 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 164.4, 51.9, 29.9, 28.4 (The NMR data was identical with the published literature).[4]

N-*t*-Butyl-3-bromopropionamide **19.**[4-8] As described in references, to a solution of 3-bromopropionyl chloride (30.0 mmol) in dichloromethane (20 mL) was added dropwise into the mixture of *t*-butylamine (33.0 mmol, 1.1 equiv.) and triethylamine (33.0 mmol, 1.1 equiv.) in dichloromethane (30 mL) at 0℃, control the drip adding time more than 30 min, which mixture was stirred for 24 h at room temperature. Organic residue was dissolved in water (20 mL), after separating the liquid, organic layer was washed by 10% sodium bicarbonate solution (10 mL). Organic mixture was concentrated under vacuum and the crude product was applied on chromatography column (ether/ethyl acetate, 1:3, v/v) to afford **19** (0.94 g, 15.0 %). ^{1}H NMR (500 MHz, $CDCl_3$) 3.54 (t, *J* = 6.7 Hz, 2H), 2.60 (t, *J* = 6.7 Hz, 2H), 1.29 (s, 9H); ^{13}C NMR ($CDCl_3$): δ 168.2, 51.6, 40.4, 28.7, 27.9 (The NMR data was identical with the published literature).[5]

N-*t*-Butyl-4-bromobutamide **20.**[4-8] As described in references, to a solution of 4-bromobutyryl chloride (30.0 mmol) in dichloromethane (20 mL) was added dropwise into the mixture of *t*-butylamine (33.0 mmol, 1.1 equiv.) and potassium carbonate (60.0 mmol, 2.0 equiv.) in dichloromethane (30 mL) at 0℃, control the drip adding time more than 30 min, which mixture was stirred for 24 h at room temperature. Inorganic residues were filtrated off and organic mixture was concentrated under vacuum and the crude product was applied on chromatography column (ether/ethyl acetate, 1:3, v/v) to afford **20**(1.52 g, 22.9 %). ^{1}H NMR (500 MHz, $CDCl_3$) δ 5.36 (s, 1H), 3.59 (t, *J* = 6.2 Hz, 2H), 2.27 (t, *J* = 7.1 Hz, 2H), 2.10-2.04 (m, 2H), 1.34 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 170.96, 51.32, 44.62, 34.09, 28.81, 28.17 (The NMR data was identical with the published literature).[7]

N-*t*-Butyl-4-chlorobutyramide **21.**[5-8] As described in references, to a solution of 4-chloroprene chloride (30.0 mmol) in dichloromethane (20 mL) was added dropwise into the mixture of *t*-butylamine (33.0 mmol, 1.1 equiv.) and triethylamine (33.0 mmol, 1.1 equiv.) in dichloromethane (30 mL) at 0℃, control the drip adding time more than 30 min, which mixture was stirred for 6 h at room temperature. Organic residue was dissolved in water (20 mL), after separating the liquid, organic layer was washed by 10% sodium bicarbonate solution (10 mL). Organic mixture was concentrated under vacuum and the crude product was applied on chromatography column (ether/ethyl acetate, 1:3, v/v) to afford **21** (3.74 g, 70.1 %). ^{1}H NMR (500 MHz, $CDCl_3$) δ 5.31 (s, 1H), 3.54 (t, *J* = 6.2 Hz, 2H), 2.21 (t, *J* = 7.1 Hz, 2H), 2.09-1.95 (m, 2H), 1.28 (s, 9H) (The NMR data was identical with the published literature).[8]

2.2 General synthesis of tertiary amine **22-24**

As described in references, to a solution of 1-bromoalkane (15.3 mmol), dimethylamine hydrochloride (45.9 mmol, 3.0 equiv.) and NaOH (53.6 mmol, 3.5 equiv.) in 50 mL of 95% ethanol and the mixture was refluxed for 24 h under stirring conditions. Solvent was removed and the crude product was stirred in dichloromethane (50 mL) and filtered with diatomaceous earth. The residue liquid was poured in 10% the NaOH solution (50 mL) and the solution was extracted with dichloromethane (3 × 20 mL), the tertiary amine **22-24** was obtained by combining organic phases and concentrating under reduced pressure.[9, 10]

N, N-Dimethyl octylamine **22** was prepared according the general procedure from 1-bromooctane (1.98 g, 84.2%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 2.20-2.17 (m, 2H), 2.16 (s, 6H), 1.43-1.34

(m, 2H), 1.24-1.16 (m, 10H), 0.81 (t, *J* = 7.0 Hz, 3H) (The NMR data was identical with the published literature).[9]

N, N-Dimethyl decylamine **23** was prepared according the general procedure from 1-bromodecaneas (2.43 g, 86.8%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 2.20-2.17 (m, 2H), 2.16 (s, 6H), 1.43-1.34 (m, 2H), 1.24-1.16 (m, 14H), 0.81 (t, *J* = 7.0 Hz, 3H) (The NMR data was identical with the published literature).[10]

N, N-Dimethyl dodecylamine **24** was prepared according the general procedure from 1-bromododecane (2.56 g, 80.1%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 2.20-2.17 (m, 2H), 2.16 (s, 6H), 1.43-1.34 (m, 2H), 1.24-1.16 (m, 18H), 0.81 (t, *J* = 7.0 Hz, 3H) (The NMR data was identical with the published literature).[10]

2.3 General synthesis of alkoxypyridine **25-27**

As described in references, to a solution of 3-hydroxypyridine (23.0 mmol) and potassium hydroxide (46.0 mmol, 2.0 equiv.) in *N, N*-dimethylformamide (15 mL) was stirred for 0.5 h at 70℃. Then 1-bromoalkane (23.0 mmol, 1.0 equiv.) was added the mixture, which was heated for 2 h. Water (30 mL) was added to the system for dilution, the solution was extracted with ethyl acetate (3 × 15 mL) and organic mixture was concentrated under vacuum. The crude product was applied on chromatography column (ether/ethyl acetate, 1:7, v/v) to afford the alkoxypyridine **25-27**.[11-13, 15]

3-octyloxypyridine **25** was prepared according the general procedure from 1-bromooctane (3.37 g, 71.1%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.31 (s, 1H), 8.21 (s, 1H), 7.25-7.15 (m, 2H), 4.01 (t, *J* = 6.6 Hz, 2H), 1.93-1.68 (m, 2H), 1.65-1.41 (m, 2H), 1.42-1.17 (m, 8H), 0.90 (t, *J* = 6.8 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.3, 141.9, 138.0, 123.8, 121.0, 68.3, 31.8, 29.3, 29.2, 29.2, 26.0, 22.7, 14.1 (The NMR data was identical with the published literature).[11]

3-decoxypyridine **26** was prepared according the general procedure from 1-bromodecane (3.78 g, 70.1%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.31 (s, 1H), 8.20 (s, 1H), 7.27-7.20 (m, 2H), 4.00 (t, *J* = 6.5 Hz, 2H), 1.82-1.80 (m, 2H), 1.52-1.42 (m, 2H), 1.40-1.22 (m, 12H), 0.89 (t, *J* = 6.8 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.3, 141.9, 138.1, 123.8, 121.0, 68.3, 31.9, 29.6, 29.5, 29.4, 29.3, 29.2, 26.0, 22.7, 14.1 (The NMR data was identical with the published literature).[12]

3-dodecoxypyridine **27** was prepared according the general procedure from 1-bromododecane (4.23 g, 69.8%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.31 (s, 1H), 8.20 (s, 1H), 7.20 (s, 2H), 4.00 (t, *J* = 6.5 Hz, 2H), 1.80 (m, 2H), 1.52-1.43 (m, 2H), 1.39-1.23 (m, 16H), 0.89 (t, *J* = 6.9 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.2, 141.9, 138.1, 123.7, 121.0, 68.3, 31.9, 29.7, 29.6, 29.6, 29.6, 29.6, 29.4, 29.2, 26.0, 22.7, 14.1 (The NMR data was identical with the published literature).[13]

2.4 General synthesis of linear *N*-chloramine precursor **6a-8a**

As described in references, to a solution of *t*-butylamides **18**, **19** (10.0 mmol) and trimethylamine solution (30% wt in H_2O) (30.0 mmol, 3 equiv.) in ethanol (30 mL) was heated to reflux for 24 h. Organic mixture was concentrated under vacuum and the crude product was applied on chromatography column (MeOH/CH_2Cl_2, 1:3, v/v) afford the product **6a-7a** (Br^- form), which were dissolved in a minimum amount of deionization water and then passed through Cl^- anion-exchange resin (Amberlite IRA-900, Cl^-) slowly to give target **6a-7a** (Cl^- form).[1]

Precursor **6a** was prepared according the general procedure from *t*-butylamide **18** (2.13 g, 87.5%). ^{1}H NMR (500 MHz, D_2O) δ 3.91 (s, 2H), 3.22 (s, 9H), 1.28 (s, 9H); ^{13}C NMR (126 MHz, D_2O) δ 162.9, 65.9, 54.2, 52.3, 27.4; HRMS calcd. for $C_9H_{21}N_2O$ $[M\text{-}Cl]^+$: 173.1648, found: 173.1640.

Precursor **7a** was prepared according the general procedure from *t*-butylamide **19** (1.81 g, 70.5%). ^{1}H NMR (500 MHz, D_2O) δ 3.54 (t, *J* = 7.3 Hz, 2H), 3.05 (s, 9H), 2.67 (t, *J* = 7.1 Hz, 2H), 1.23 (s, 9H); ^{13}C NMR (126 MHz, D_2O) δ 169.7, 62.4, 53.1, 51.5, 30.4, 27.6; HRMS calcd. for $C_{10}H_{23}N_2O$ $[M\text{-}Cl]^+$: 187.1815, found: 187.1810.

To a solution of *t*-butylamides **21** (10.0 mmol) and trimethylamine solution (30% wt in H_2O) (30.0 mmol, 3.0 equiv.) in ethanol (30 mL) was heated to reflux for 24 h. Organic mixture was concentrated under vacuum and the crude product was applied on chromatography column ($MeOH/CH_2Cl_2$, 1:3, v/v) afford the product **8a** (Cl^- form)[9] (1.76 g, 74.8%). ^{1}H NMR (500 MHz, D_2O) δ 3.27-3.19 (m, 2H), 3.06 (s, 9H), 2.21 (t, *J* = 7.2 Hz, 2H), 2.02-1.90 (m, 2H), 1.24 (s, 9H); ^{13}C NMR (126 MHz, D_2O) δ 173.3, 65.5, 52.9, 51.2, 32.5, 27.7, 18.8; HRMS calcd. for $C_{11}H_{25}N_2O$ $[M\text{-}Cl]^+$: 201.1963, found: 201.1967.

2.5 General synthesis of linear *N*-chloramine precursor **9a-11a**

As described in references, to a solution of butylamide **21** (6.00 mmol) and tertiary amine **22-24** (6.00 mmol, 1.0 equiv.) in acetonitrile (15 mL) was heated to reflux for 18 h. Organic mixture was concentrated under vacuum and the crude product was applied on chromatography column ($MeOH/CH_2Cl_2$, 1:5, v/v) to afford **9a-11a**.[2, 3, 16-19]

Precursor **9a** was prepared according the general procedure from tertiary amine **22** (1.56 g, 78.1%). ^{1}H NMR (500 MHz, D_2O) δ 3.24-3.14 (m, 4H), 2.99 (s, 6H), 2.19 (t, *J* = 7.0 Hz, 2H), 1.98-1.85 (m, 2H), 1.71-1.60 (m, 2H), 1.30-1.18 (m, 10H), 1.24 (s, 9H), 0.79 (t, *J* = 6.9 Hz, 3H); ^{13}C NMR (126 MHz, D_2O) δ 173.3, 64.1, 62.5, 51.2, 50.7, 32.6, 30.9, 28.1, 27.8, 25.4, 22.0, 21.7, 18.5, 16.8, 13.4; HRMS calcd. for $C_{18}H_{39}N_2O$ $[M\text{-}Cl]^+$: 299.3062, found: 299.3065.

Precursor **10a** was prepared according the general procedure from tertiary amine **23** (1.64 g, 75.1%). ^{1}H NMR (500 MHz, D_2O) δ 3.25-3.15 (m, 4H), 3.02 (s, 6H), 2.20 (t, *J* = 6.7 Hz, 2H), 1.98-1.85 (m, 2H), 1.71-1.60 (m, 2H), 1.30-1.18 (m, 14H), 1.25 (s, 9H), 0.80 (t, *J* = 6.7 Hz, 3H); ^{13}C NMR (126 MHz, D_2O) δ 172.96, 63.62, 61.92, 51.14, 48.85, 32.32, 31.60, 29.21, 28.95, 28.86, 28.65, 28.00, 25.63, 22.29, 21.90, 18.49, 13.70; HRMS calcd. for $C_{20}H_{44}N_2O$ $[M\text{-}Cl]^+$: 328.3454, found: 328.3461.

Precursor **11a** was prepared according the general procedure from tertiary amine **24** (1.79 g, 76.5%). ^{1}H NMR (500 MHz, D_2O) δ 3.30-3.15 (m, 4H), 3.04 (s, 6H), 2.22 (t, *J* = 6.5 Hz, 2H), 1.97-1.86 (m, 2H), 1.70-1.55 (m, 2H), 1.35-1.20 (m, 18H), 1.26 (s, 9H), 0.80 (t, *J* = 6.8 Hz, 3H); ^{13}C NMR (126 MHz, D_2O) δ 172.73, 63.09, 61.31, 51.49, 50.82, 32.14, 31.93, 29.78, 29.74, 29.41, 29.31, 29.15, 28.23, 25.91, 22.59, 22.07, 18.53, 13.83; HRMS calcd. for $C_{22}H_{47}N_2O$ $[M\text{-}Cl]^+$: 355.3682, found: 355.3688.

2.6 General synthesis of linear *N*-chloramine precursor **12a-17a**

As described in references, to a solution of pyridine (5.00 mmol), 3-methoxypyridine (5.00 mmol, 1 equiv.), alkoxypyridine **25-27** (5.00 mmol, 1 equiv.) or tributyl phosphine (5.00 mmol, 1 equiv.) and *N*-*t*-Butyl-4-chlorobutyramide **21** (5.00 mmol, 1 equiv.) in acetonitrile (15 mL) was heated to reflux for 18 h. Organic mixture was concentrated under vacuum and the crude product was applied on chromatography column ($MeOH/CH_2Cl_2$, 1:5, v/v) to afford **12a-17a.**[2, 3, 16-19]

Precursor **12a** was prepared according the general procedure from pyridine (1.01 g, 78.1%). ^{1}H NMR (500 MHz, D_2O) δ 8.85-8.75 (m, 2H), 8.50 (t, *J* = 7.9 Hz, 1H), 8.02 (t, *J* = 7.1 Hz, 2H), 4.56 (t, *J* = 7.0 Hz, 2H), 2.30-2.15 (m, 4H), 1.19 (s, 9H); ^{13}C NMR (126 MHz, D_2O) δ 173.2, 145.8, 144.3, 128.3, 61.1, 51.2, 32.7, 27.7, 26.4; HRMS calcd. for $C_{13}H_{21}N_2O$ $[M\text{-}Cl]^+$: 221.1654, found: 221.1657.

Precursor **13a** was prepared according the general procedure from 3-methoxypyridine (1.16 g,

81.1%). ^{1}H NMR (500 MHz, D_2O) δ 8.51 (s, 1H), 8.41-8.35 (m, 1H), 8.09-8.02 (m, 1H), 7.95 -7.85 (m, 1H), 4.62-4.47 (m, 2H), 3.96 (s, 3H), 2.27-2.17 (m, 4H), 1.18 (s, 9H); ^{13}C NMR (126 MHz, D_2O) δ 173.3, 158.7, 136.6, 131.9, 130.6, 128.6, 61.4, 57.2, 51.2, 32.7, 27.7, 26.3; HRMS calcd. for $C_{14}H_{23}N_2O_2$ $[M\text{-}Cl]^+$: 251.1754, found: 251.1760.

Precursor **14a** was prepared according the general procedure from 3-octyloxypyridine **25** (1.42 g, 74.1%). ^{1}H NMR (500 MHz, D_2O) δ 8.54 (s, 1H), 8.50-8.44 (m, 1H), 8.01-7.86 (m, 2H), 4.57 (t, *J* = 6.4 Hz, 2H), 4.17 (t, *J* = 6.2 Hz, 2H), 2.26-2.18 (m, 4H), 1.78-1.69 (m, 2H), 1.45-1.34 (m, 2H), 1.27-1.16 (m, 8H), 1.12 (s, 9H), 0.78 (t, *J* = 6.8 Hz, 3H); ^{13}C NMR (126 MHz, D_2O) δ 172.8, 158.0, 137.3, 131.7, 131.2, 128.9, 70.5, 61.7, 50.8, 32.6, 31.5, 29.0, 28.9, 28.4, 27.9, 26.2, 25.5, 22.4, 13.7; HRMS calcd. for $C_{21}H_{37}N_2O_2$ $[M\text{-}Cl]^+$: 49.2854, found: 349.2855.

Precursor **15a** was prepared according the general procedure from 3-decoxypyridine **26** (1.62 g, 79.1%). ^{1}H NMR (500 MHz, D_2O) δ 8.58 (s, 1H), 8.52 (t, *J* = 2.8 Hz, 1H), 7.97-7.90 (m, 2H), 4.60 (t, *J* = 6.3 Hz, 2H), 4.17 (t, *J* = 6.1 Hz, 2H), 2.28-2.18 (m, 4H), 1.77-1.66 (m, 2H), 1.42-1.34 (m, 2H), 1.28-1.18 (m, 12H), 1.10 (s, 9H), 0.80 (t, *J* = 6.8 Hz, 3H); ^{13}C NMR (126 MHz, D_2O) δ 172.6, 157.8, 137.6, 131.5, 131.2, 129.0, 70.4, 61.8, 50.7, 32.6, 31.9, 29.7, 29.5, 29.4, 28.7, 28.1, 26.2, 25.8, 22.6, 13.8; HRMS calcd. for $C_{23}H_{41}N_2O_2$ $[M\text{-}Cl]^+$: 377.3174, found: 377.3168.

Precursor **16a** was prepared according the general procedure from 3-dodecoxypyridine **27** (1.76 g, 79.6%). ^{1}H NMR (500 MHz, D_2O) δ 8.60 (s, 1H), 8.55-8.47 (m, 1H), 7.96-7.89 (m, 2H), 4.60 (t, *J* = 6.3 Hz, 2H), 4.16 (t, *J* = 5.9 Hz, 2H), 2.26-2.18 (m, 4H), 1.77-1.66 (m, 2H), 1.42-1.34 (m, 2H), 1.26-1.18 (m, 16H), 1.10 (s, 9H), 0.81 (t, *J* = 6.6 Hz, 3H); ^{13}C NMR (126 MHz, D_2O) δ 172.5, 157.7, 137.7, 131.5, 131.2, 128.9, 70.4, 61.8, 50.6, 32.6, 31.9, 29.9, 29.8, 29.8, 29.6, 29.5, 28.7, 28.1, 26.2, 25.9, 22.6, 13.9; HRMS calcd. for $C_{25}H_{45}N_2O_2$ $[M\text{-}Cl]^+$: 405.3483, found: 405.3481.

Precursor **17a** was prepared according the general procedure from tributyl phosphine (1.53 g, 81.1%). ^{1}H NMR (500 MHz, D_2O) δ 2.24 (t, *J* = 6.8 Hz, 2H), 2.18-2.02 (m, 8H), 1.82-1.70 (m, 2H), 1.52-1.32 (m, 12H), 1.24 (s, 9H), 0.85 (t, *J* = 7.2 Hz, 9H); ^{13}C NMR (126 MHz, D_2O) δ 173.7, 51.2, 36.7, 27.8, 23.3, 23.2, 22.7, 17.7, 17.3, 12.6; HRMS calcd. for $C_{20}H_{43}NOP$ $[M\text{-}Cl]^+$: 344.3086, found: 344.3082.

2.7 General synthesis of linear *N*-chloramine **6-17**

As described in references, to a solution of linear *N*-chloramine precursor **6a-17a** (1.50 mmol) in 4.5 mL of mixed solvent (*t*-BuOH: H_2O, 4:1, v/v) were added *t*-butyl hypochlorite (4.50 mmol, 3 equiv.). The mixture was then sealed in dark for 24 h. After removing excess *t*-butyl hypochlorite and the solvent, the final liner *N*-chloramine **6-17** was obtained in quantitative amount.[2, 3, 16-19]

N-chloramine **6.** ^{1}H NMR (500 MHz, D_2O) δ 4.50 (s, 1H), 3.25 (s, 4H), 1.45 (s, 4H);^{13}C NMR (126 MHz, D_2O) δ 165.9, 66.5, 64.9, 53.8, 27.7; HRMS calcd. for $C_9H_{20}ClN_2O$ $[M\text{-}Cl]^+$: 207.1259, found: 207.1253.

N-chloramine **7.** ^{1}H NMR (500 MHz, D_2O) δ 3.54 (t, *J* = 7.3 Hz, 2H), 3.15 (t, *J* = 7.3 Hz, 2H), 3.09 (s, 9H), 1.43 (s, 9H);^{13}C NMR (126 MHz, D_2O) δ 172.7, 65.8, 62.4, 62.4, 62.4, 53.2, 53.2, 53.1, 30.5, 27.9; HRMS calcd. for $C_{10}H_{22}ClN_2O$ $[M\text{-}Cl]^+$: 221.1415, found: 221.1410.

N-chloramine **8.** ^{1}H NMR (500 MHz, D_2O) δ 3.31-3.22 (m, 2H), 3.07 (s, 9H), 2.68 (t, *J* = 6.9 Hz, 2H), 2.02-1.91 (m, 2H), 1.43 (s, 9H); ^{13}C NMR (126 MHz, D_2O) δ 176.17, 65.55, 65.47, 52.81, 32.75, 28.07, 18.31; HRMS calcd. for $C_{11}H_{24}ClN_2O$ $[M\text{-}Cl]^+$: 235.1577, found: 235.1817.

N-chloramine **9.** ^{1}H NMR (500 MHz, D_2O) δ 3.24-3.18 (m, 4H), 2.99 (s, 6H), 2.66 (t, *J* = 6.8 Hz, 2H), 1.94-1.87 (m, 2H), 1.70-1.65 (m, 2H), 1.42 (s, 9H), 1.30-1.18 (m, 10H), 0.78 (t, *J* = 6.8 Hz, 3H); ^{13}C NMR (126 MHz, D_2O) δ 176.2, 65.5, 63.9, 62.5, 50.7, 32.8, 30.9, 28.1, 28.1, 25.4, 21.9, 21.7, 18.5,

17.9, 13.4. HRMS calcd. for $C_{18}H_{38}ClN_2O$ $[M\text{-}Cl]^+$: 333.2667, found: 333.2670

N-chloramine **10.** ^{1}H NMR (500 MHz, D_2O) δ 3.26-3.14 (m, 4H), 3.05 (s, 6H), 2.68 (t, *J* = 6.3 Hz, 2H), 1.94-1.86 (m, 2H), 1.71-1.60 (m, 2H), 1.43 (s, 9H), 1.33-1.19 (m, 14H), 0.80 (t, *J* = 6.6 Hz, 3H); ^{13}C NMR (126 MHz, D_2O) δ 175.7, 64.7, 62.7, 61.2, 51.7, 32.5, 31.8, 29.6, 29.5, 29.2, 29.1, 28.4, 25.7, 22.5, 21.8, 17.9, 13.8. HRMS calcd. for $C_{20}H_{42}ClN_2O$ $[M\text{-}Cl]^+$: 361.2976, found: 361.2970.

N-chloramine **11.** ^{1}H NMR (500 MHz, D_2O) δ 3.30-3.15 (m, 4H), 3.06 (s, 6H), 2.68 (t, *J* = 6.2 Hz, 2H), 1.97-1.86 (m, 2H), 1.75-1.65 (m, 2H), 1.43 (s, 9H), 1.36-1.15 (m, 18H), 0.80 (t, *J* = 6.7 Hz, 3H); ^{13}C NMR (126 MHz, D_2O) δ 175.6, 64.4, 62.4, 61.0, 51.9, 32.4, 31.9, 29.9, 29.7, 29.5, 29.4, 29.1, 28.5, 25.9, 22.6, 21.9, 18.0, 13.8. HRMS calcd. for $C_{22}H_{46}ClN_2O$ $[M\text{-}Cl]^+$: 389.3296, found: 389.3288.

N-chloramine **12.** ^{1}H NMR (500 MHz, D_2O) δ 8.85-8.75 (m, 2H), 8.50 (t, *J* = 7.8 Hz, 1H), 8.02 (t, *J* = 7.0 Hz, 2H), 4.59 (t, *J* = 7.3 Hz, 2H), 2.71 (t, *J* = 6.9 Hz, 2H), 2.25-2.18 (m, 2H), 1.37 (s, 9H); ^{13}C NMR (126 MHz, D_2O) δ 176.2, 145.8, 144.3, 128.4, 65.4, 61.1, 32.9, 28.0, 25.9; HRMS calcd. for $C_{13}H_{20}ClN_2O$ $[M\text{-}Cl]^+$: 255.1262, found: 255.1264.

N-chloramine **13.** ^{1}H NMR (500 MHz, D_2O) δ 8.53 (s, 1H), 8.45-8.35 (m, 1H), 8.08-8.00 (m, 1H), 7.96 -7.85 (m, 1H), 4.60-4.49 (m, 2H), 3.96 (s, 3H), 2.71 (t, *J* = 6.8 Hz, 2H), 2.26-2.16 (m, 2H), 1.36 (s, 9H); ^{13}C NMR (126 MHz, D_2O) δ 176.1, 158.8, 136.7, 131.9, 130.6, 128.6, 65.4, 61.4, 57.1, 32.9, 27.9, 25.8; HRMS calcd. for $C_{14}H_{22}ClN_2O_2$ $[M\text{-}Cl]^+$: 285.1364, found: 285.1370.

N-chloramine **14.** ^{1}H NMR (500 MHz, D_2O) δ 8.58 (s, 1H), 8.56-8.53 (m, 1H), 8.04-8.00 (m, 1H), 8.00-7.95 (m, 1H), 4.64 (t, *J* = 6.4 Hz, 2H), 4.20 (t, *J* = 6.1 Hz, 2H), 2.68 (t, *J* = 6.6 Hz, 2H), 2.28-2.18 (m, 2H), 1.78-1.70 (m, 2H), 1.42-1.34 (m, 2H), 1.28 (s, 9H), 1.25-1.15 (m, 8H), 0.76 (t, *J* = 6.6 Hz, 3H); ^{13}C NMR (126 MHz, D_2O) δ 175.6, 157.9, 137.6, 131.6, 131.2, 129.0, 70.4, 64.5, 61.6, 32.8, 31.7, 29.6, 29.2, 29.0, 28.2, 25.8, 25.6, 22.5, 13.8. HRMS calcd. for $C_{21}H_{36}ClN_2O_2$ $[M\text{-}Cl]^+$: 383.2464, found: 383.2470.

N-chloramine **15.** ^{1}H NMR (500 MHz, D_2O) δ 8.64-8.53 (m, 2H), 8.08-7.89 (m, 2H), 4.65 (t, *J* = 6.3 Hz, 2H), 4.20 (t, *J* = 6.1 Hz, 2H), 2.68 (t, *J* = 6.6 Hz, 2H), 2.29-2.16 (m, 2H), 1.80-1.68 (m, 2H), 1.43-1.33 (m, 2H), 1.27 (s, 9H), 1.22-1.14 (m, 12H), 0.76 (t, *J* = 6.7 Hz, 3H); ^{13}C NMR (126 MHz, D_2O) δ 175.5, 157.8, 137.7, 131.5, 131.2, 129.1, 70.4, 64.4, 61.6, 32.8, 31.9, 29.7, 29.6, 29.5, 29.4, 28.6, 28.3, 25.9, 25.9, 22.6, 13.8. HRMS calcd. for $C_{23}H_{40}ClN_2O_2$ $[M\text{-}Cl]^+$: 411.2773, found: 411.2778.

N-chloramine **16.** ^{1}H NMR (500 MHz, D_2O) δ 8.64-8.56 (m, 2H), 8.05-7.95 (m, 2H), 4.60 (t, *J* = 6.0 Hz, 2H), 4.20 (t, *J* = 6.2 Hz, 2H), 2.28-2.17 (m, 2H), 1.81-1.66 (m, 2H), 1.42-1.33 (m, 2H), 1.27 (s, 9H), 1.22-1.15 (m, 16H), 0.78 (t, *J* = 6.6 Hz, 3H); ^{13}C NMR (126 MHz, D_2O) δ 175.5, 157.8, 137.8, 131.5, 131.2, 129.2, 70.4, 64.3, 61.5, 32.8, 31.9, 29.9, 29.9, 29.8, 29.6, 29.6, 29.5, 28.7, 28.4, 26.0, 25.9, 22.6, 13.9. HRMS calcd. for $C_{25}H_{44}ClN_2O_2$ $[M\text{-}Cl]^+$: 439.3090, found: 439.3086.

N-chloramine **17.** ^{1}H NMR (500 MHz, D_2O) δ 2.73 (t, *J* = 6.7 Hz, 2H), 2.19-2.06 (m, 8H), 1.80-1.72 (m, 2H), 1.56-1.31 (m, 12H), 1.42 (s, 9H), 0.86 (t, *J* = 7.2 Hz, 9H); ^{13}C NMR (126 MHz, D_2O) δ 176.73, 65.50, 36.67, 28.12, 23.35, 22.75, 22.72, 17.42, 16.90, 12.57. HRMS calcd. for $C_{20}H_{42}ClNOP$ $[M\text{-}Cl]^+$: 378.2687, found: 378.2680.

3. NMR spectra analysis

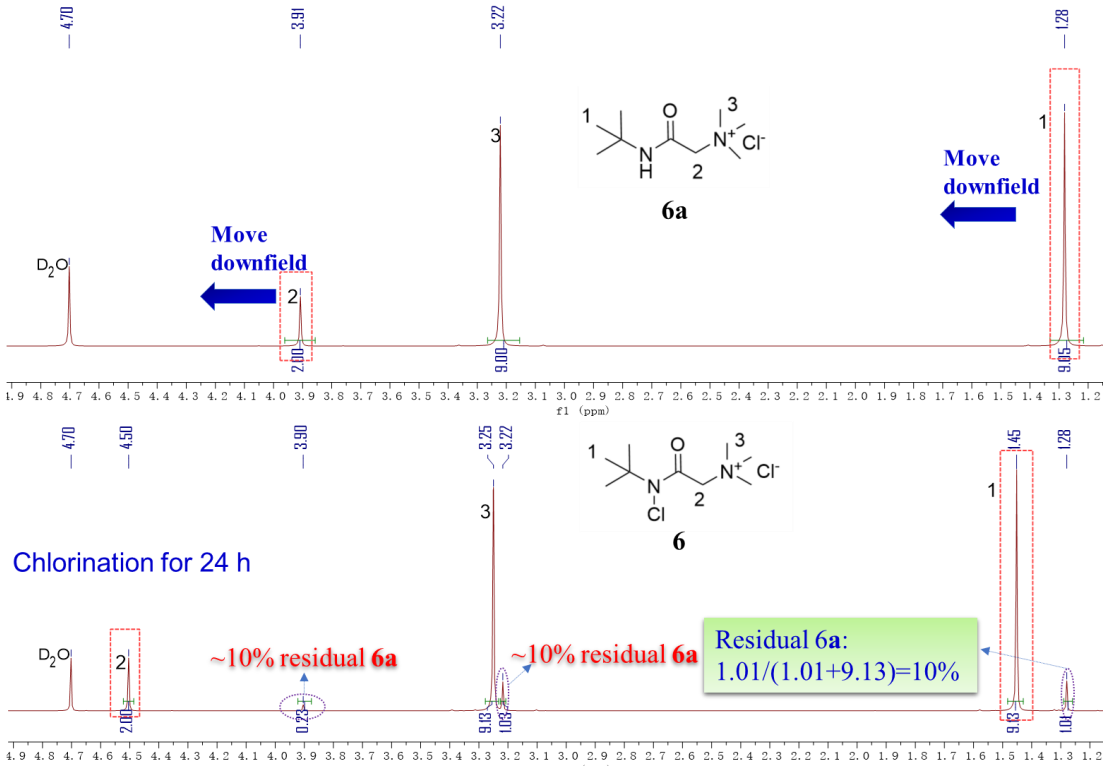


Fig. S1 ^{1}H NMR data of *N*-chloramine **6** and its precursor **6a**

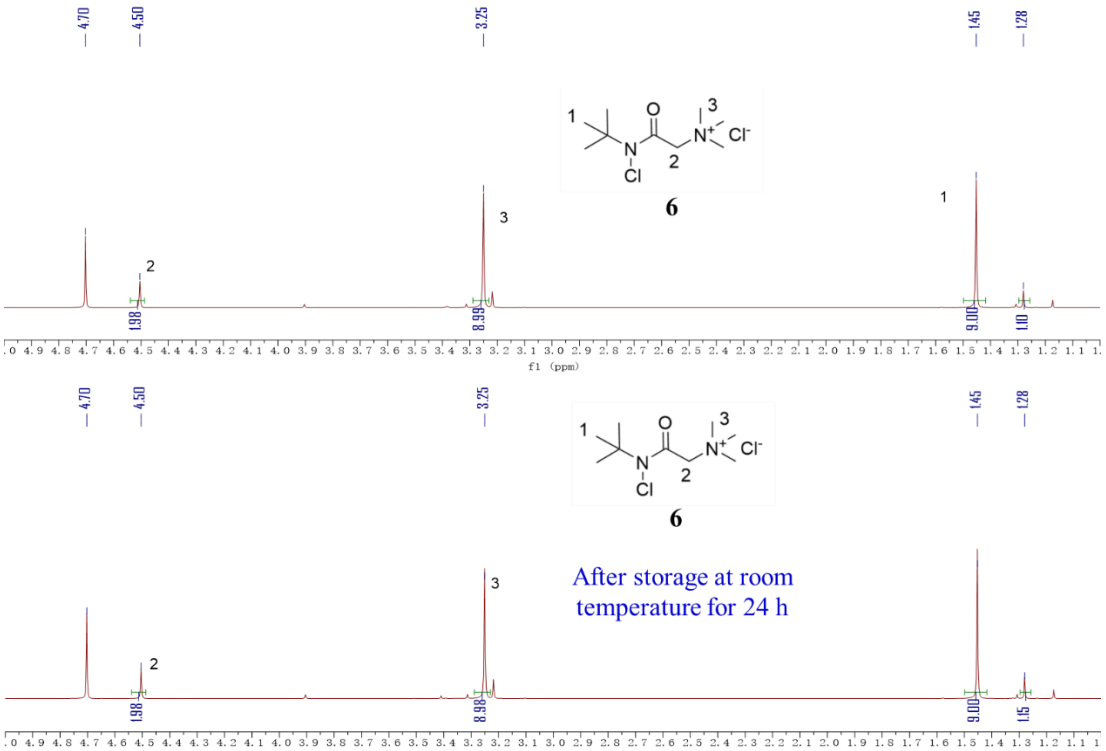


Fig. S2 ^{1}H NMR data of *N*-chloramine **6** before and after storage at room temperature for 24 h

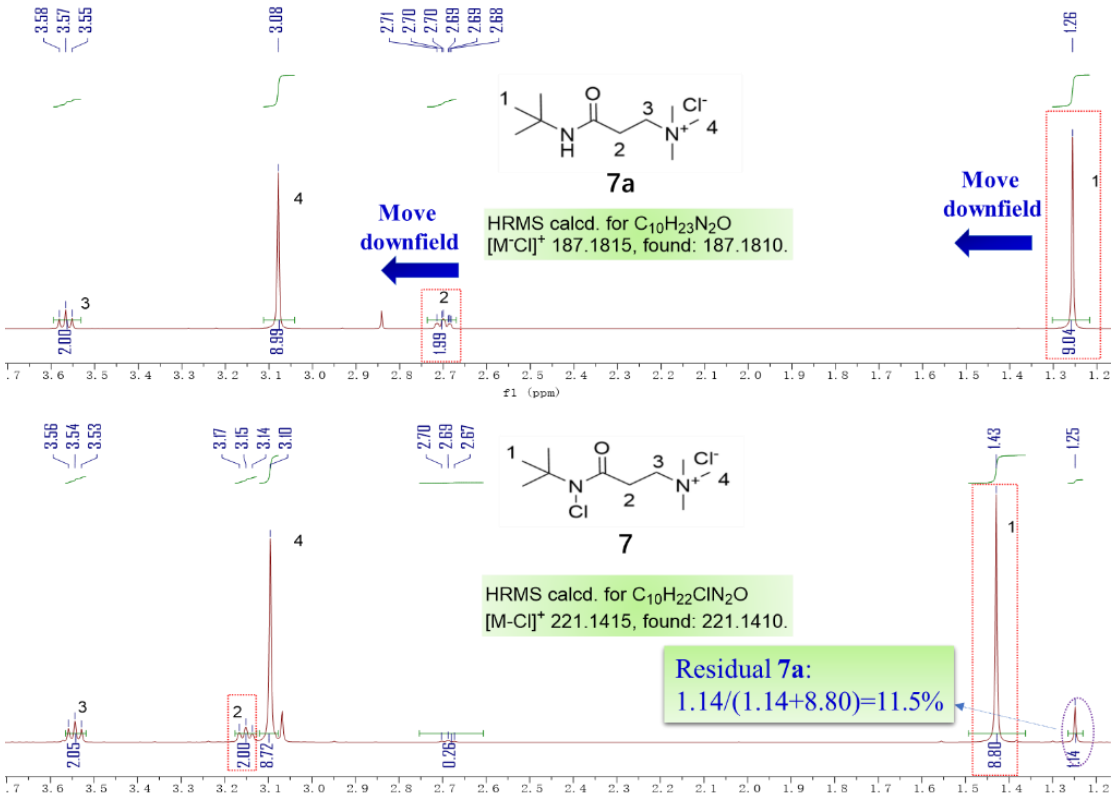


Fig. S3 ^{1}H NMR data of *N*-chloramine **7** and its precursor **7a**

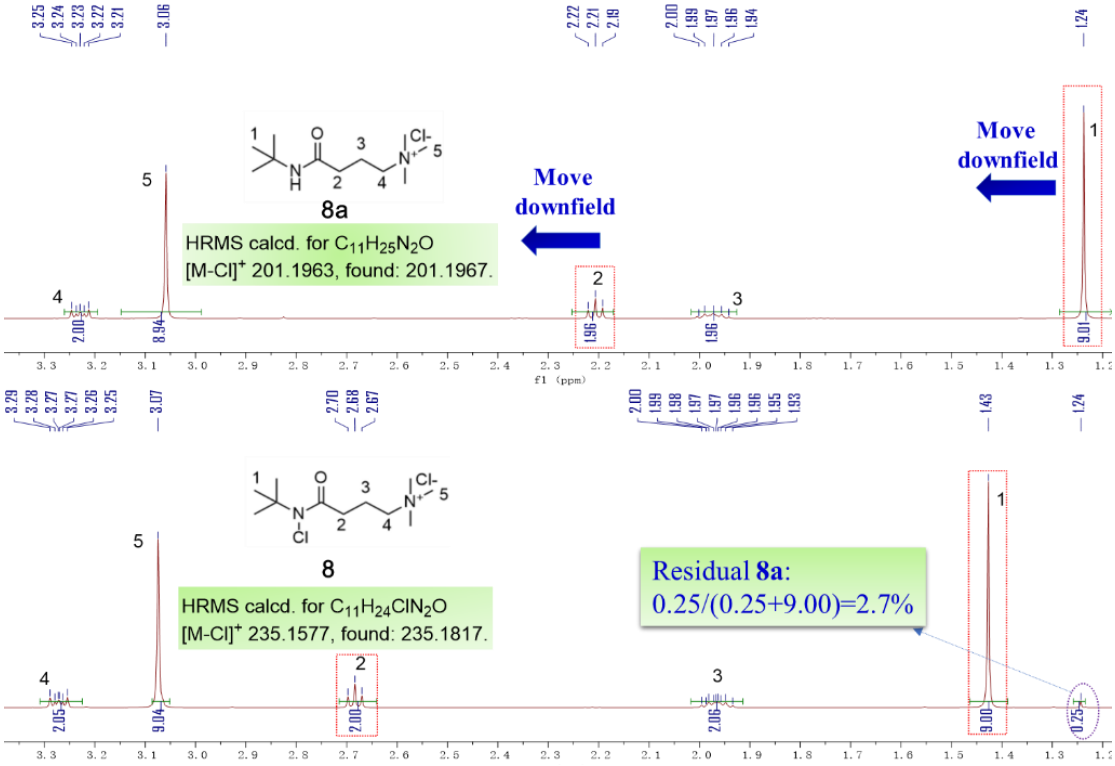


Fig. S4 ^{1}H NMR data of *N*-chloramine **8** and its precursor **8a**

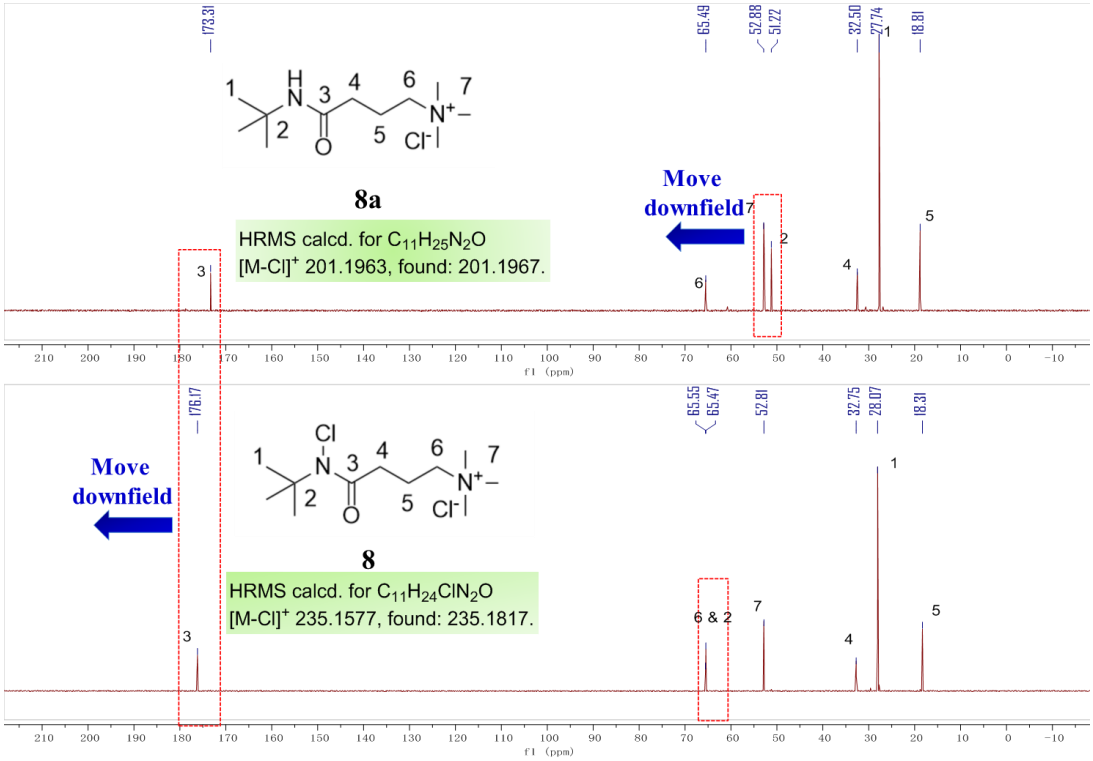


Fig. S5 ^{13}C NMR data of *N*-chloramine **8** and its precursor **8a**

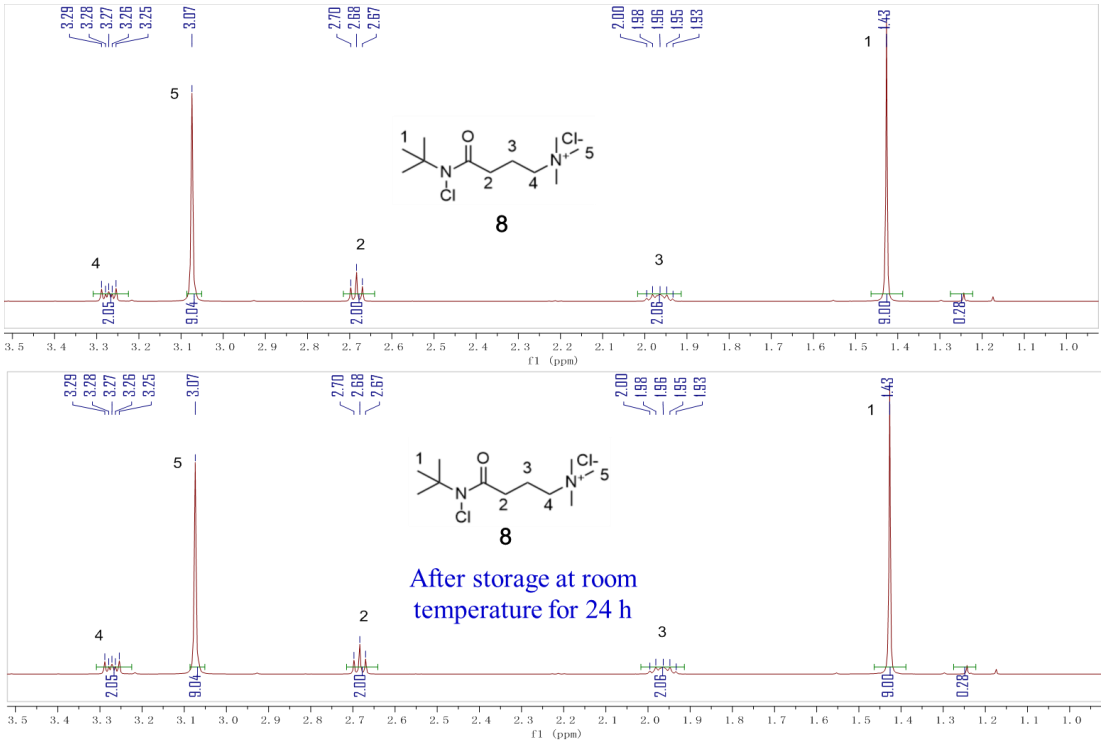


Fig. S6 ^{1}H NMR data of *N*-chloramine **8** before and after storage at room temperature for 24 h

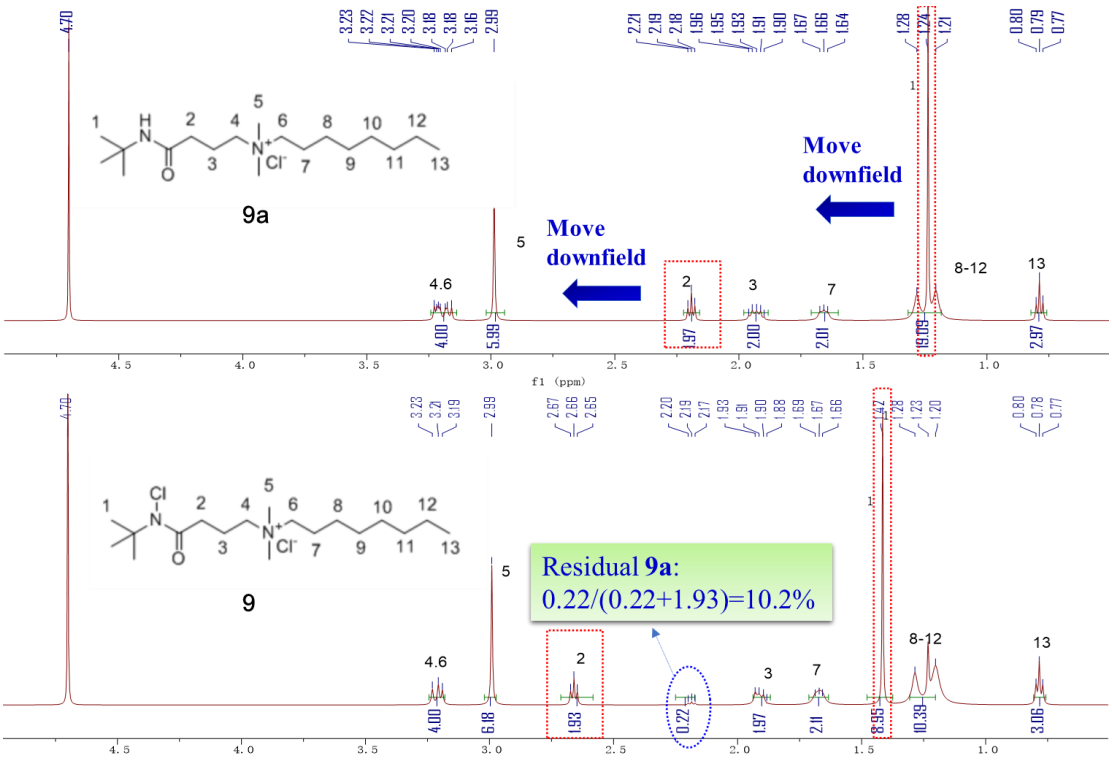


Fig. S7 ^{1}H NMR data of *N*-chloramine **9** and its precursor **9a**

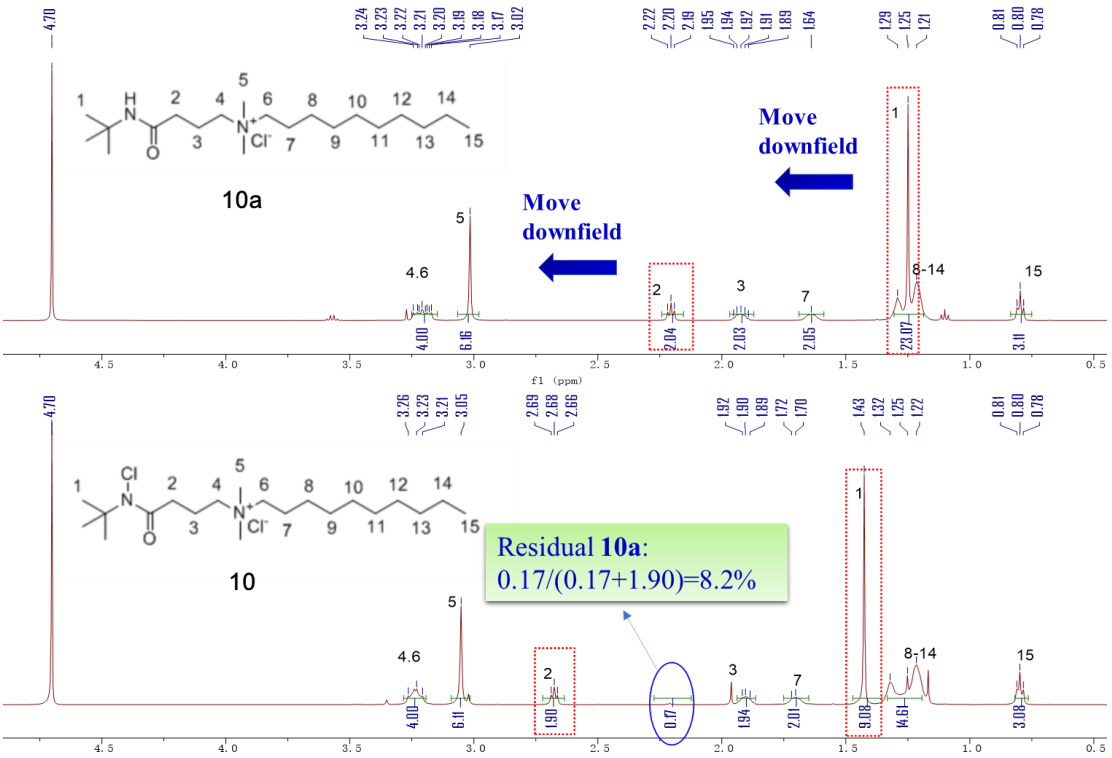


Fig. S8 ^{1}H NMR data of *N*-chloramine **10** and its precursor **10a**

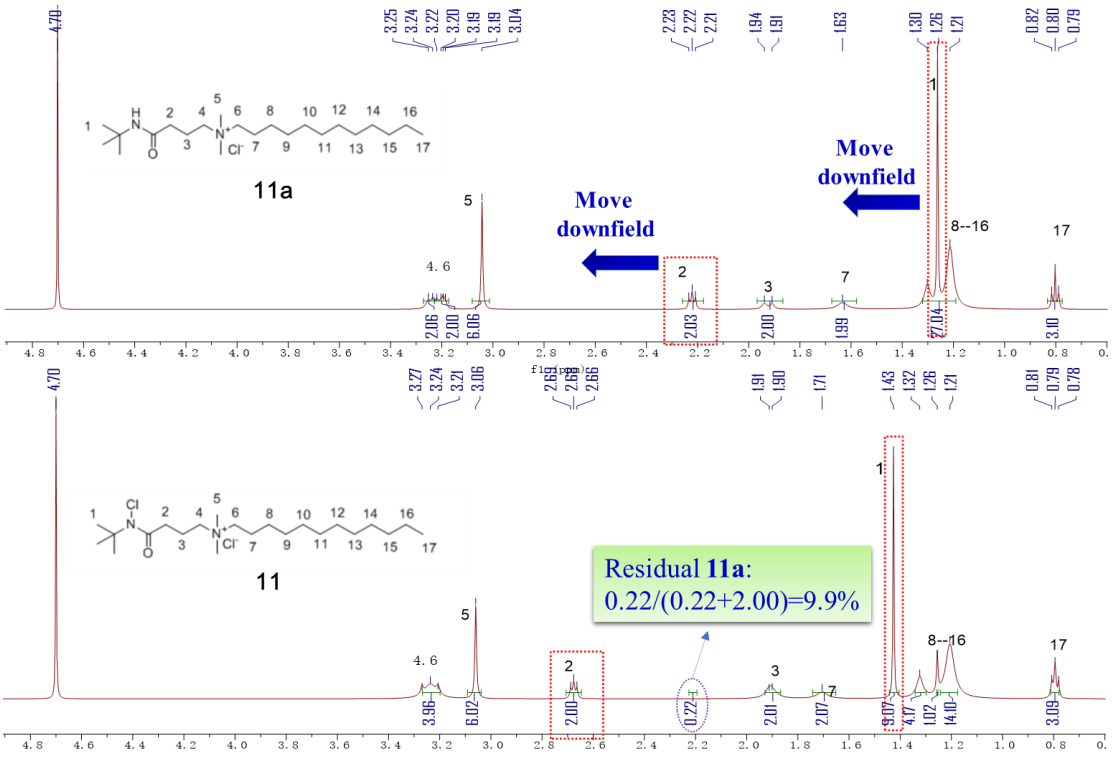


Fig. S9 ^{1}H NMR data of *N*-chloramine **11** and its precursor **11a**

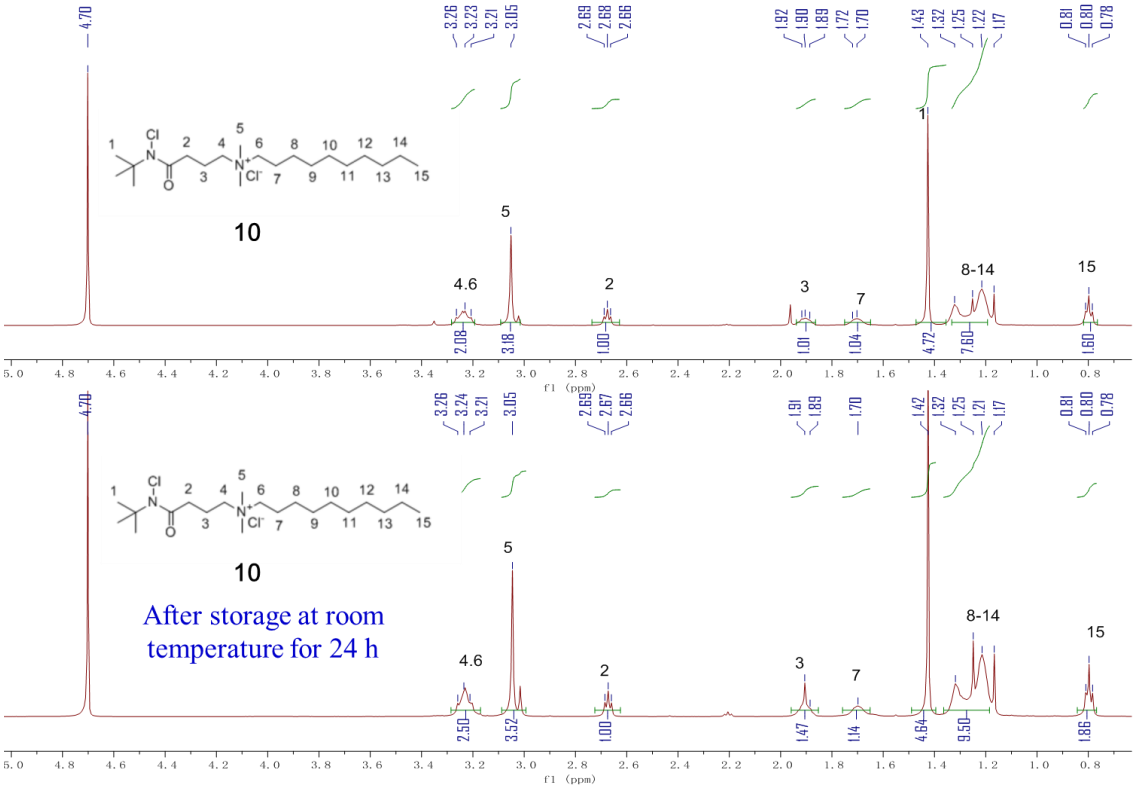


Fig. S11 ^{1}H NMR data of *N*-chloramine **10** before and after storage at room temperature for 24 h

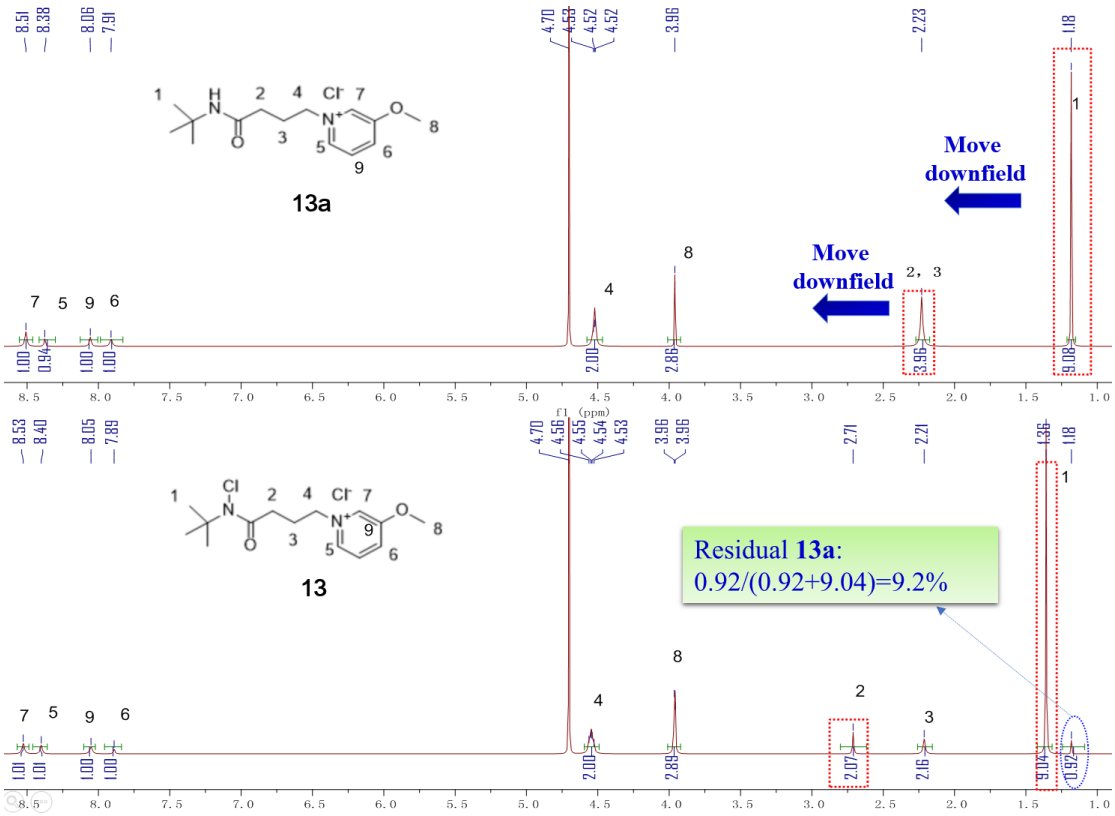


Fig. S12 ^{1}H NMR data of *N*-chloramine **13** and its precursor **13a**

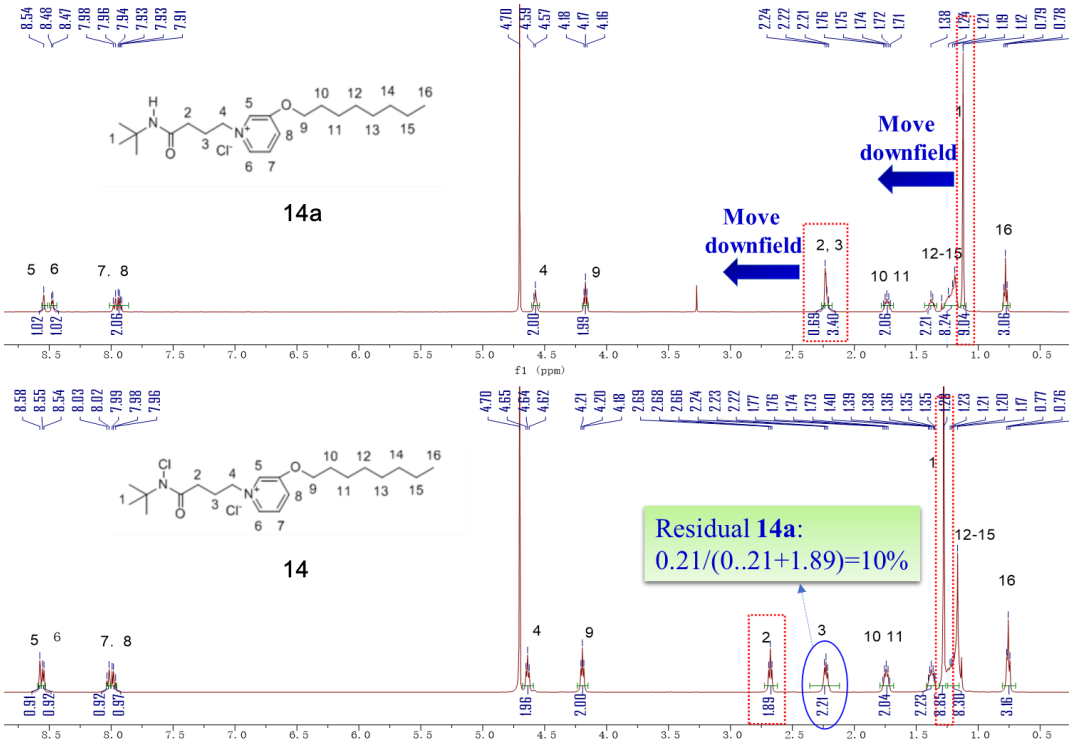


Fig. S13 ^{1}H NMR data of *N*-chloramine **14** and its precursor **14a**

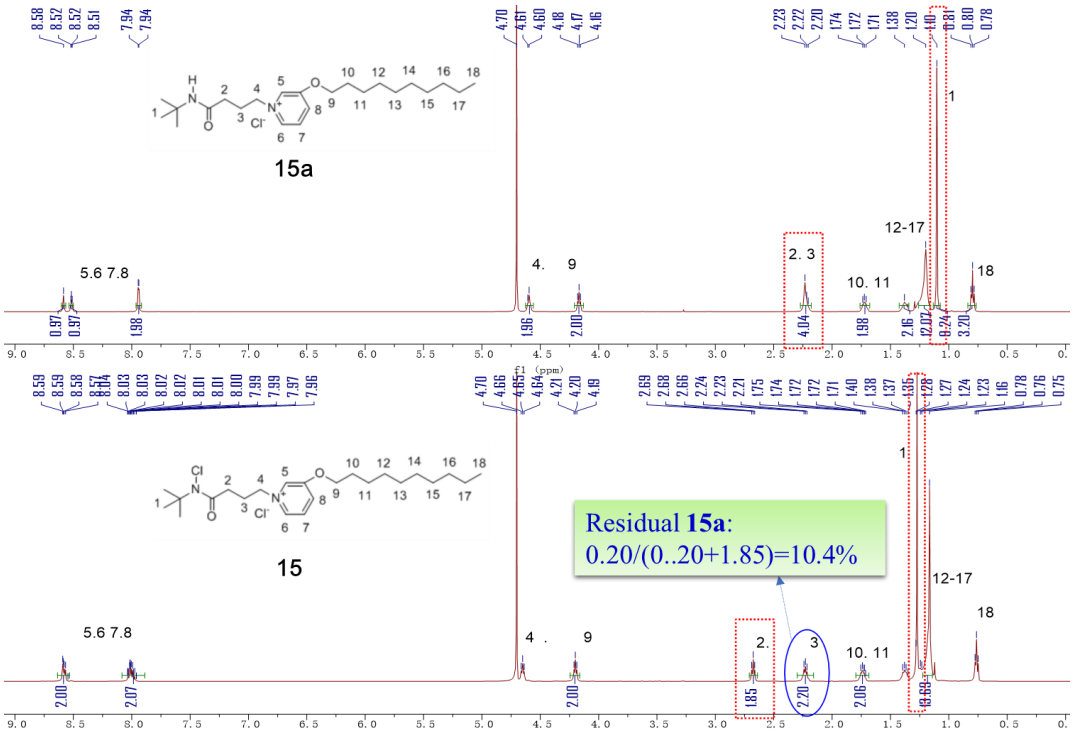


Fig. S14 ^{1}H NMR data of *N*-chloramine **15** and its precursor **15a**

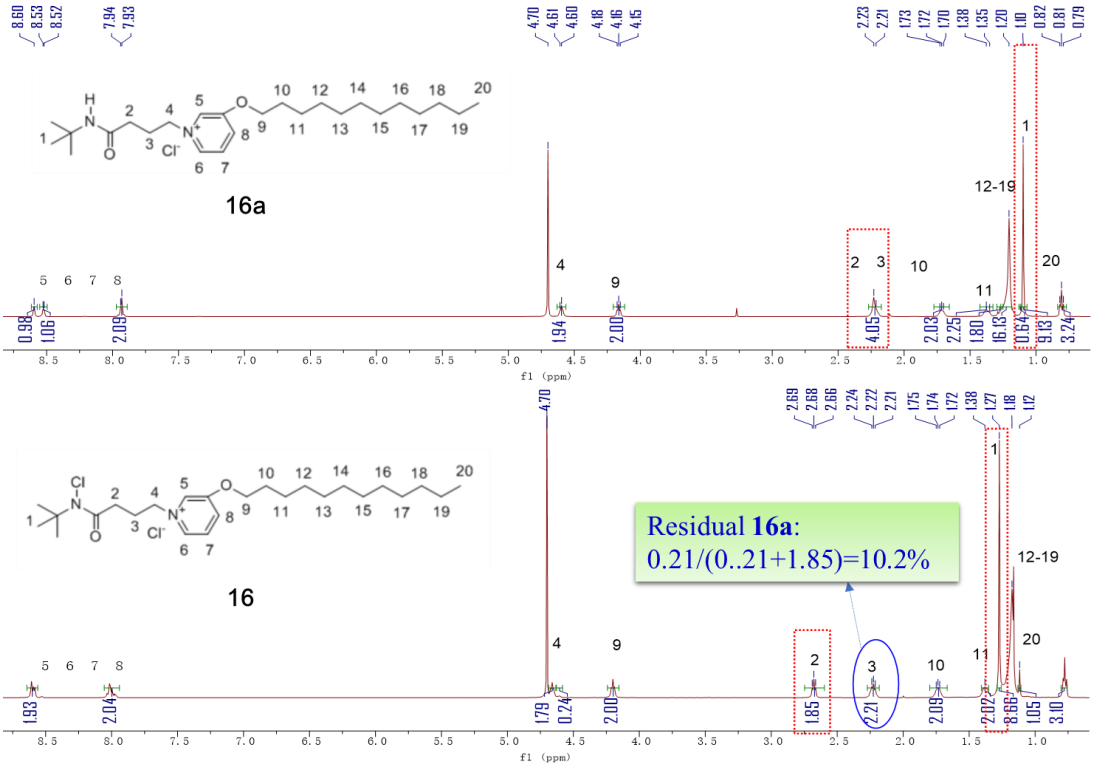


Fig. S15 ^{1}H NMR data of *N*-chloramine **16** and its precursor **16a**

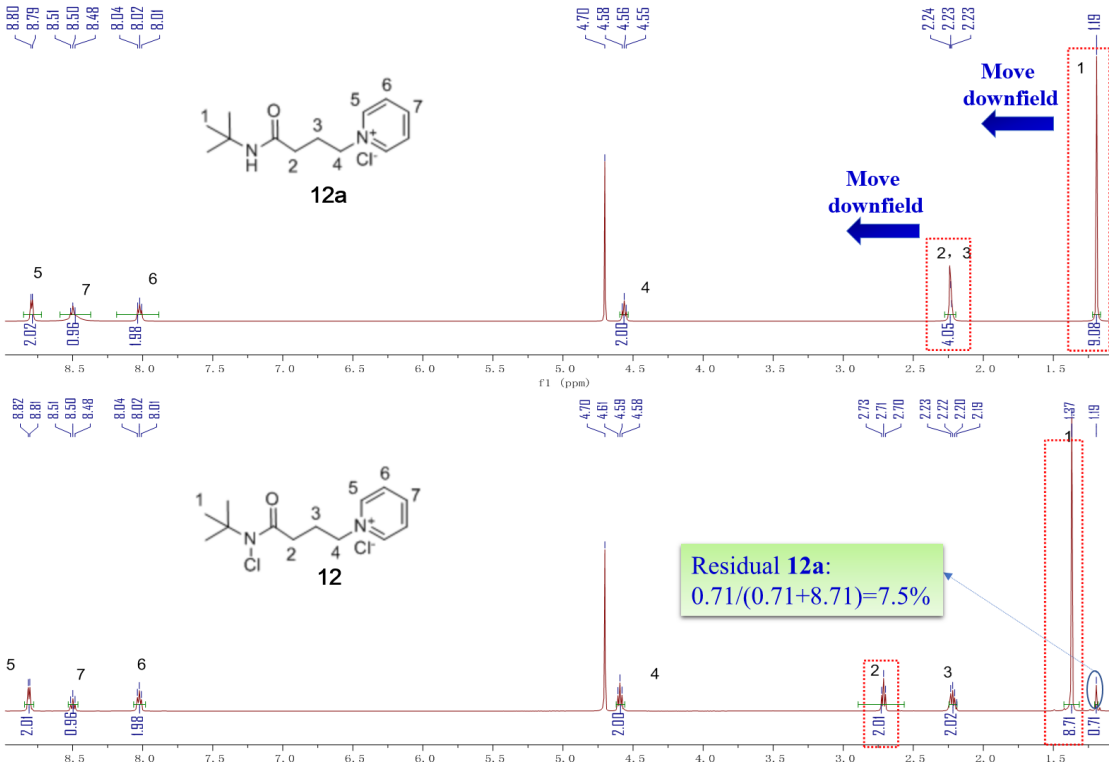


Fig. S16 ^{1}H NMR data of *N*-chloramine **12** and its precursor **12a**

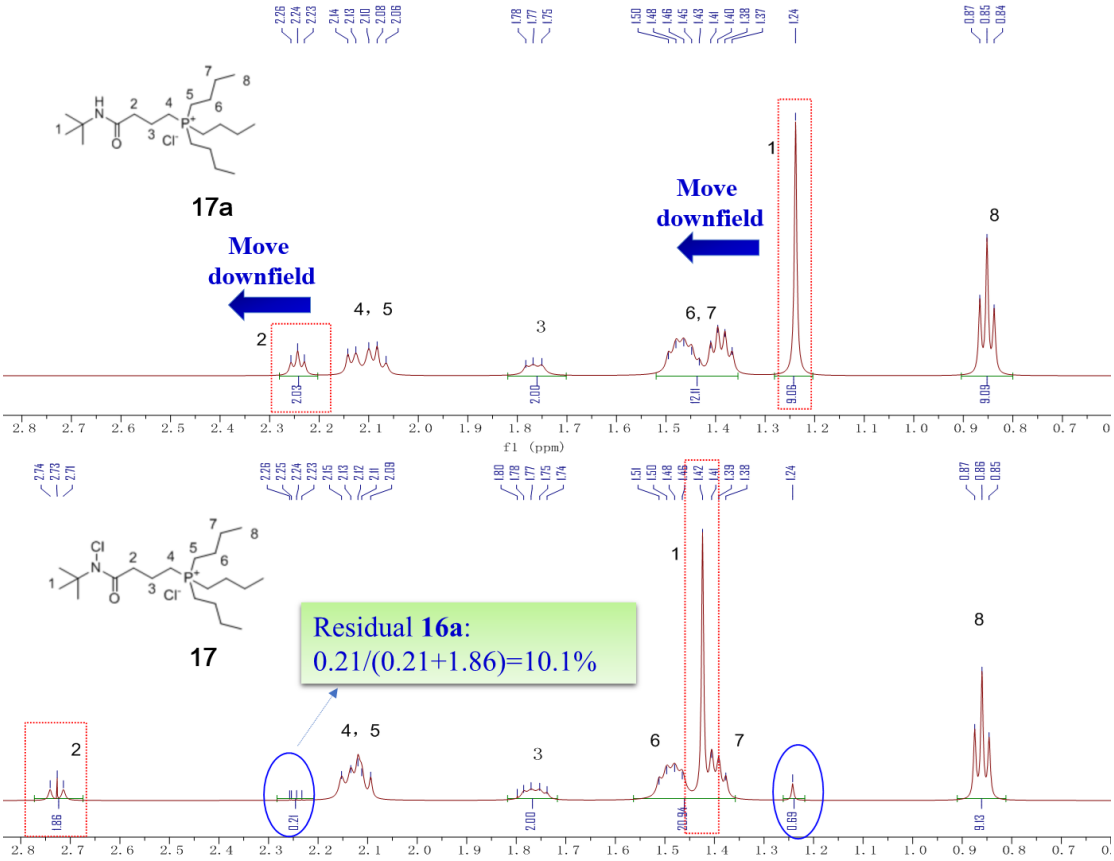


Fig. S17 ^{1}H NMR data of *N*-chloramine **17** and its precursor **17a**

4. TLC of liner N-chloramine **11** and its precursor **11a**

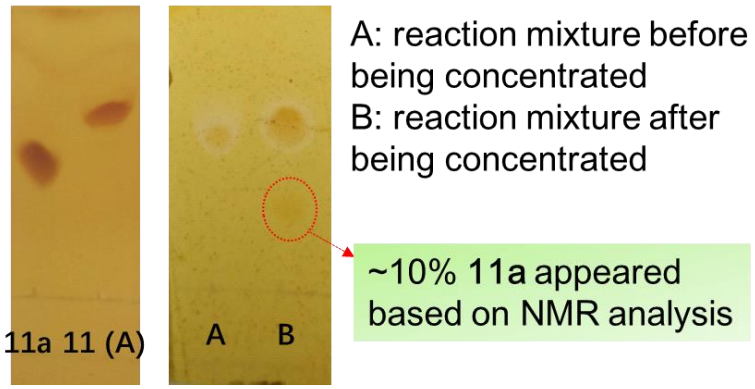


Fig. S10 TLC of *N*-chloramine **11** and its precursor **11a**

5. Antimicrobial tests

Logarithmic-phase cultures used to bacterial suspensions were obtained by culturing stock bacteria on tryptone soya agar (TSA) medium at 37°C for 18-24 h. Then a bacterial suspension (10^6~10^7 CFU mL^{-1}) was prepared in phosphate buffer solution (PBS, pH=7.0±0.1) for subsequent test of antimicrobial activity. 20 μL of liner *N*-chloramine **6-17** solution (0.28 M stock solution*, final 20 ppm [Cl^+]) was added to 10 mL of bacterial suspension in a centrifuge tube and timing of contact killing was started immediately. After an interval of 5 min and 10 min, 1 mL bacterial solution was pipetted into 1 mL of sterile 0.02 N sodium thiosulfate solution, respectively, to quench all oxidative chlorine of *N*-chloramine. After being serially diluted several times, 100 μL of each bacterial solution with gradient concentration was placed on the pre-made medium, which were cultured at 37°C for 18-24 h. The same procedure was also carried out for all *N*-chloramine precursors (**6a-17a**). The viable bacterial colonies on the plates were counted to report the reduction of bacteria by the formula as followed:

$$\text{Percentage reduction of bacteria (\%)} = (A\text{-}B)/A\times 100$$

$$\text{Log reduction} = \text{Log}\,(A/B) \text{ if } B>0;$$

$$= \text{Log}\,A \text{ if } B=0$$

where *A* is the number of bacteria retrieved from controls (CFU mL^{-1}), and *B* is the number of bacteria retrieved from *N*-chloramines or its precursors (CFU mL^{-1}).

*Real concentration was adjusted appropriately. For example, since purity of **6** is 90%, stock solution of **6** was then prepared as 0.28/0.9=0.31 M.

6. Antibacterial activity of *N*-chloramine **8, 12~17**

Table S1. Antibacterial activity of *N*-chloramines **8, 12~17**

Bacteria	Synthesis compounds	Active chloramine	5 min contact time		10min contact time	
			Percent	Log reduction	Percent	Log reduction
S. aureus [a]	**8a**[1]	0	0	0	0	0
	8[1]	20	23.9±4.5	0.12±0.03	37.8±1.1	0.21±0.02
	12a[1]	0	0	0	0	0
	12[1]	20	31.1±3.9	0.16±0.02	50.0±2.8	0.30±0.02
	17a[1]	0	0	0	0	0
	17[1]	20	44.3±0.9	0.26±0.02	60.0±1.7	0.40±0.02
	12a[2]	0	0	0	0	0
	12[2]	20	9.8±0.7	0.04±0.01	15.9±1.9	0.08±0.01
	13a[2]	0	0	0	0	0
	13[2]	20	10.9±2.2	0.05±0.01	20.1±4.1	0.10±0.02
	14a	0	80.5±0.7	0.71±0.02	90.0±1.2	1.00±0.05
	14[2]	20	99.9±0.0	4.32±0.30	100	6.88
	15a[2]	0	100	6.88	100	6.88
	15[2]	20	100	6.88	100	6.88
	16a[2]	0	100	6.88	100	6.88
	16[2]	20	100	6.88	100	6.88
E. coli [b]	**8a**[1]	0	0	0	0	0
	8[1]	20	24.4±1.9	0.12±0.01	37.7±1.5	0.21±0.02
	12a[1]	0	0	0	0	0
	12[1]	20	31.5±3.8	0.16±0.03	50.8±3.1	0.31±0.03
	17a[1]	0	0	0	0	0
	17[1]	20	45.4±6.9	0.26±0.05	67.7±2.3	0.49±0.03
	12a[2]	0	0	0	0	0
	12[2]	20	9.8±1.9	0.04±0.01	20.6±2.5	0.10±0.01
	13a[2]	0	0	0	0	0
	13[2]	20	11.4±1.6	0.05±0.01	22.7±2.2	0.11±0.01
	14a[2]	0	9.2±0.9	0.04±0.00	16.2±2.6	0.08±0.02
	14[2]	20	99.9±0.0	3.90±0.60	100	6.80
	15a[2]	0	99.9±0.0	4.50±2.30	100	6.80
	15[2]	20	100	6.80	100	6.80
	16a[2]	0	100	6.80	100	6.80
	16[2]	20	100	6.80	100	6.80

[a] Inoculum concentration was 3.60×10^6 CFU/ mL for **8**[1], **12**[1], **17**[1] and 8.40×10^6CFU mL/ for **12**[2]**-16**[2], (Colony-forming Units); [b] Inoculum concentration was 2.60×10^6 CFU/ mL for **8**[1], **12**[1], **17**[1] and 6.30×10^6CFU mL/ for **12**[2]**-16**[2]; [c] The final [Cl^+] concentration: 20 ppm for *N*-chloramines and 0 ppm for precursors

7. Bactericidal evaluation of **2**, **3**, **12** and **17**

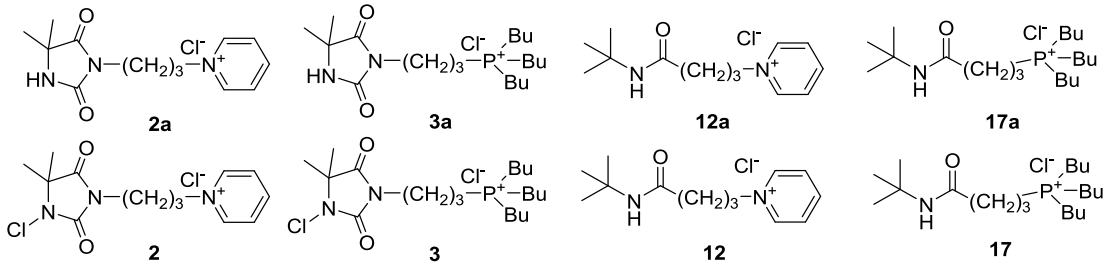


Table S2. Antibacterial activity of liner *N*-chloramine **2**, **3, 12, 17**

Bacteria	Synthesis compounds	Active chloramine [ppm][c]	5 min contact time	
			Percent reduction/%	Log reduction
S. aureus [a]	**2a**	0	0	0
	2	20	38.3±2.0	0.21±0.01
	3a	0	0	0
	3	20	76.2±1.1	0.62±0.02
	12a	0	0	0
	12	20	35.8±1.5	0.19±0.01
	17a	0	0	0
	17	20	73.6±3.2	0.58±0.02
E. coli [b]	**2a**	0	0	0
	2	20	80.3±2.0	0.58±0.03
	3a	0	0	0
	3	20	85.5±1.3	0.84±0.04
	12a	0	0	0
	12	20	29.8±2.6	0.15±0.02
	17a	0	0	0
	17	20	25.6±0.7	0.13±0.01

[a] Inoculum concentration was 6.98×10^6 CFU/ mL, (Colony-forming Units). [b] Inoculum concentration was 3.04×10^6 CFU/ mL. [c] The final [Cl^+] concentration: 20 ppm for *N*-chloramines and 0 ppm for precursors

8. References and notes

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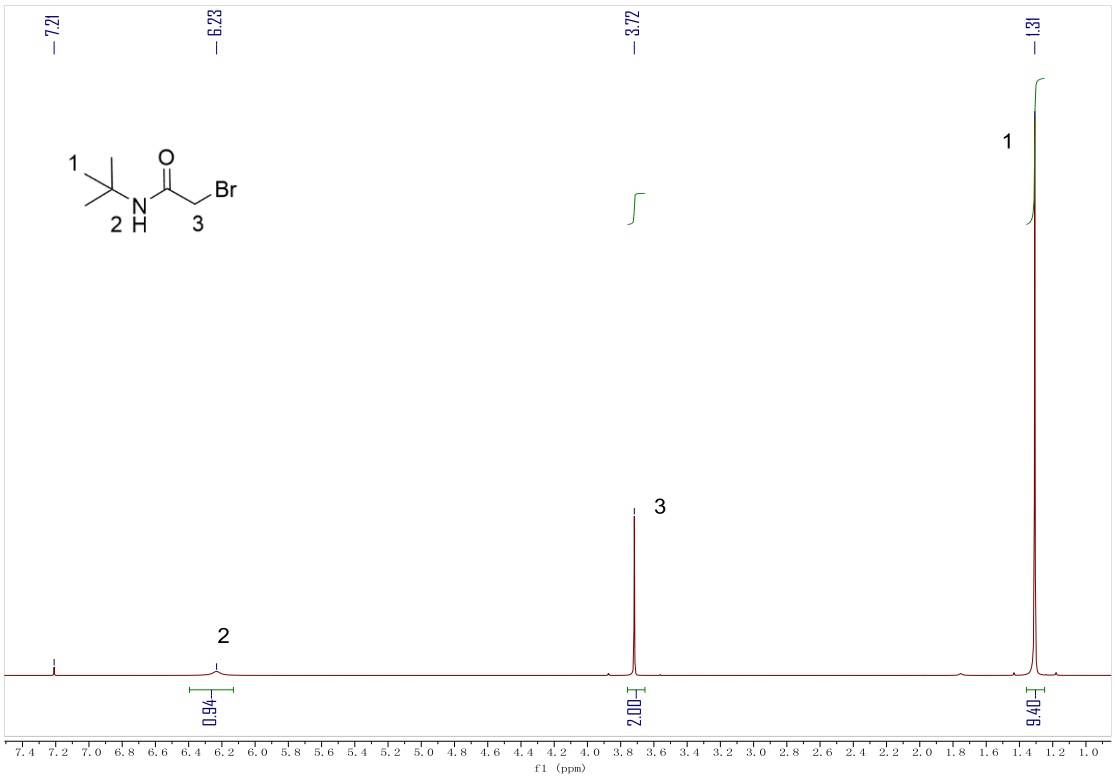
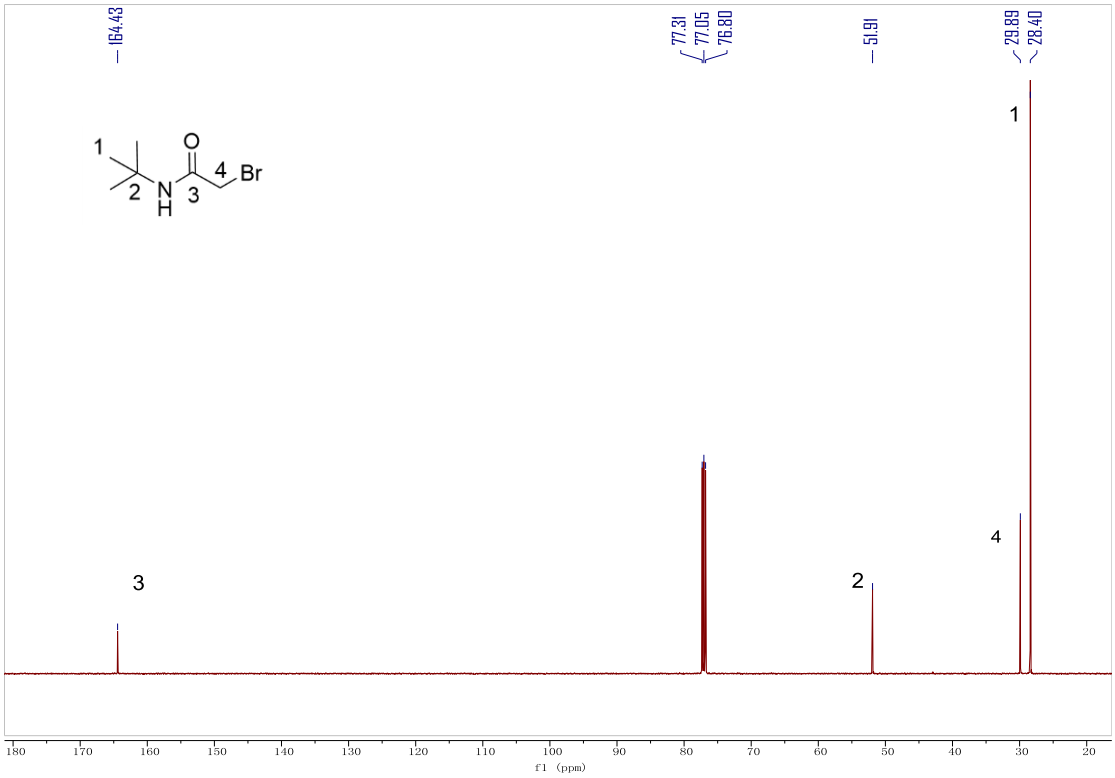
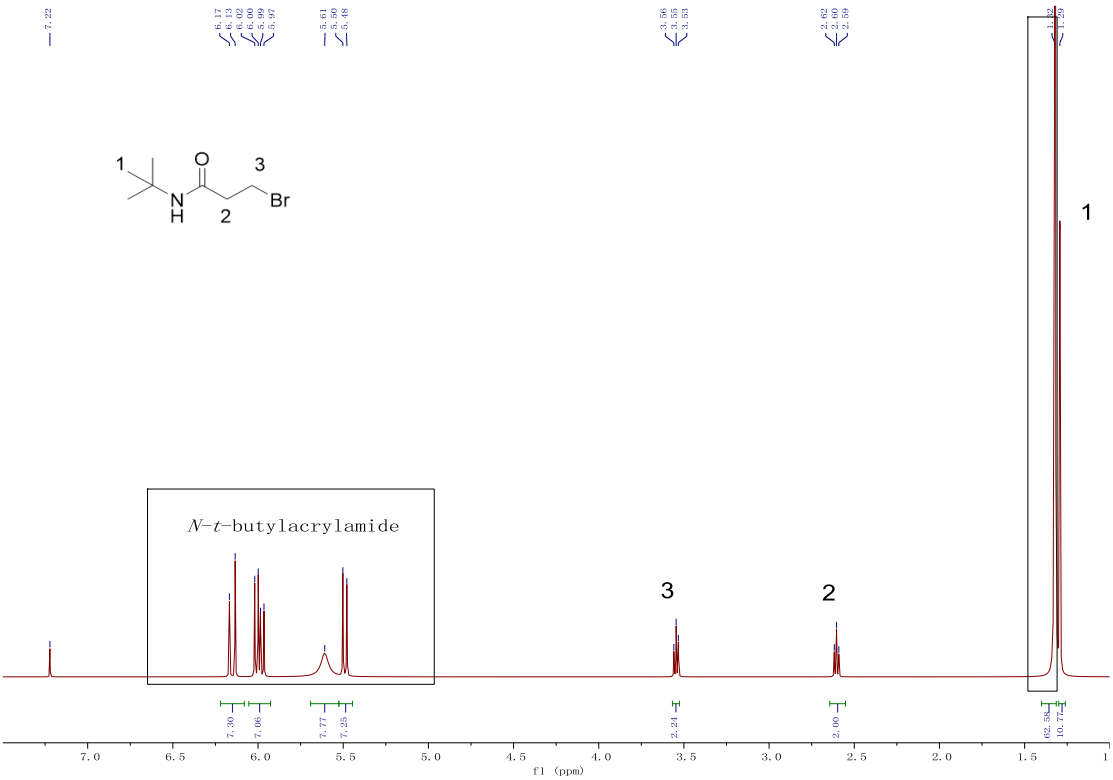
9. Original NMR spectra data



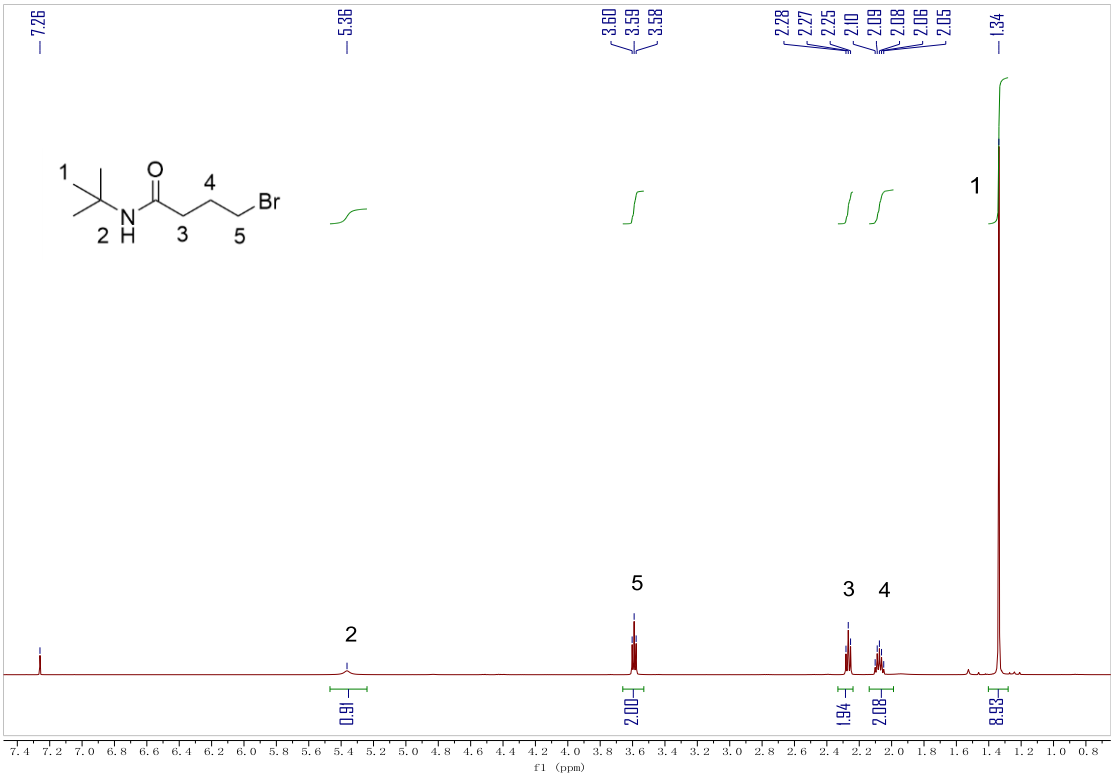
The ^{1}H NMR spectrum of compound **18**



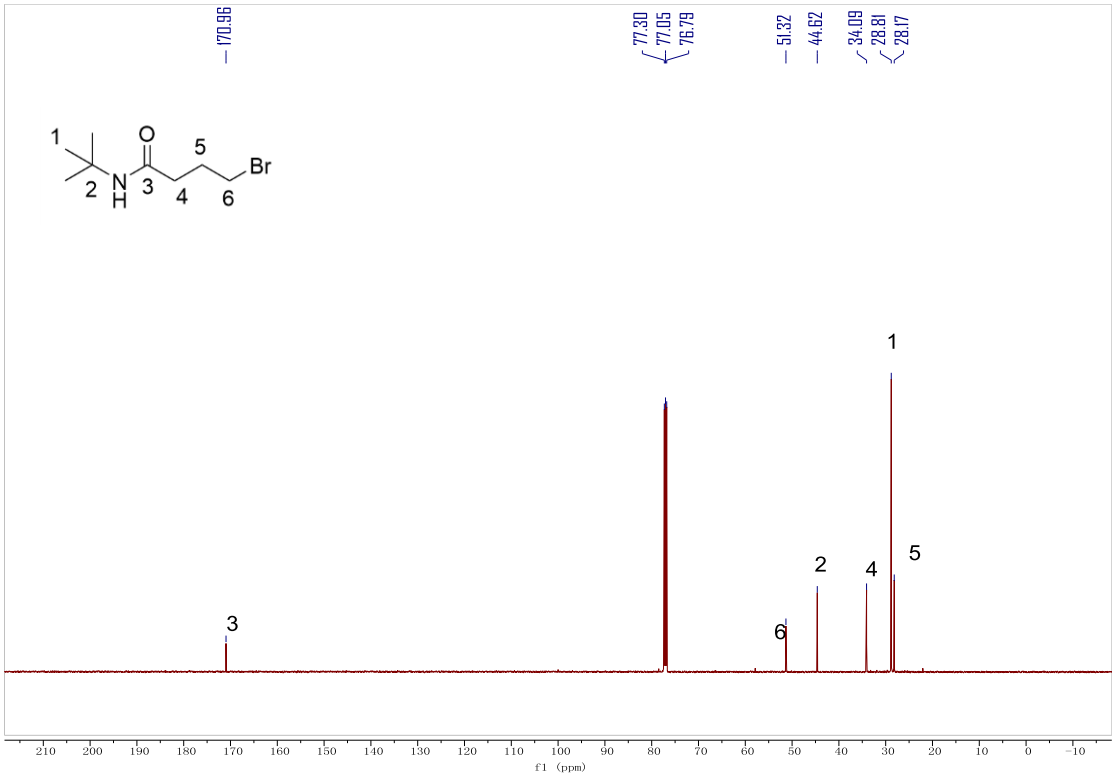
The ^{13}C NMR spectrum of compound **18**



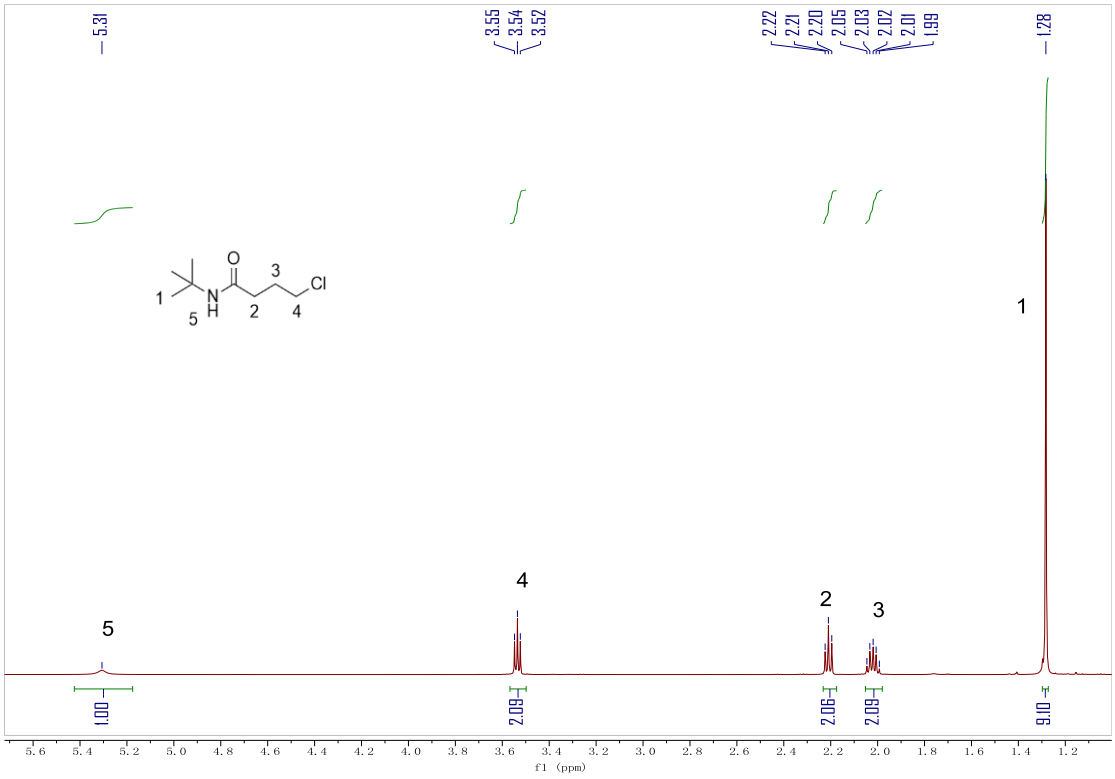
The ^{1}H NMR spectrum of compound **19** (containing *N*-*t*-butylacrylamide)



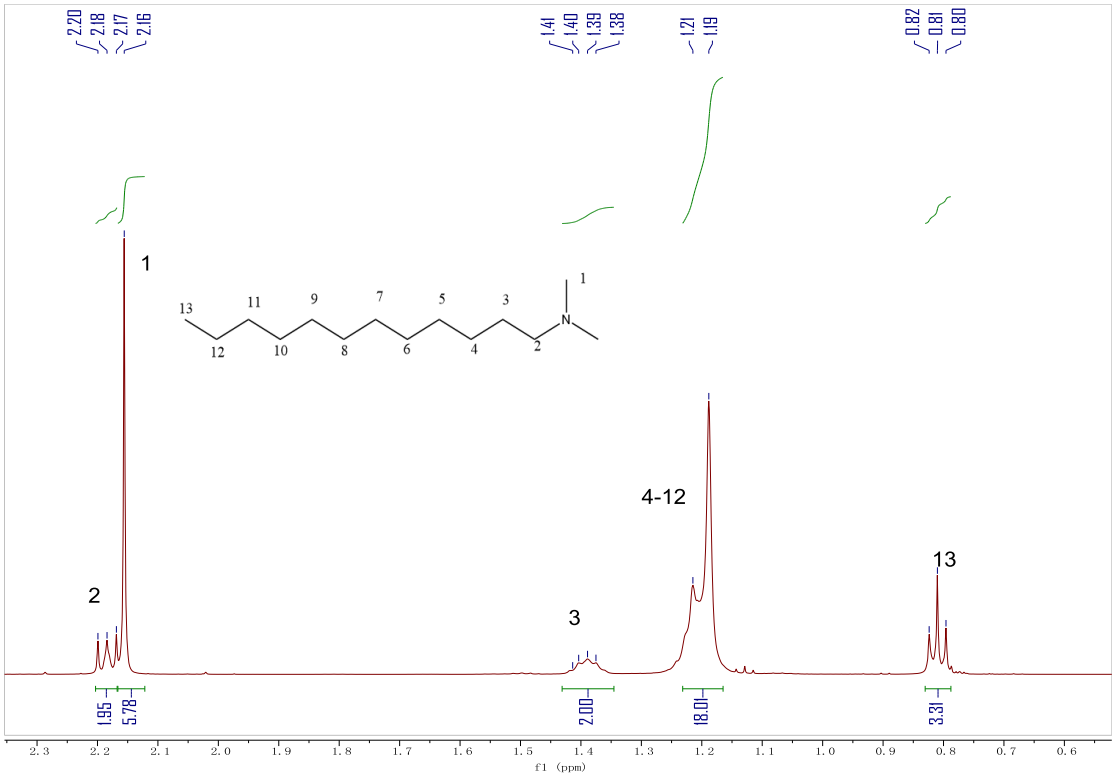
The ^{1}H NMR spectrum of compound **20**



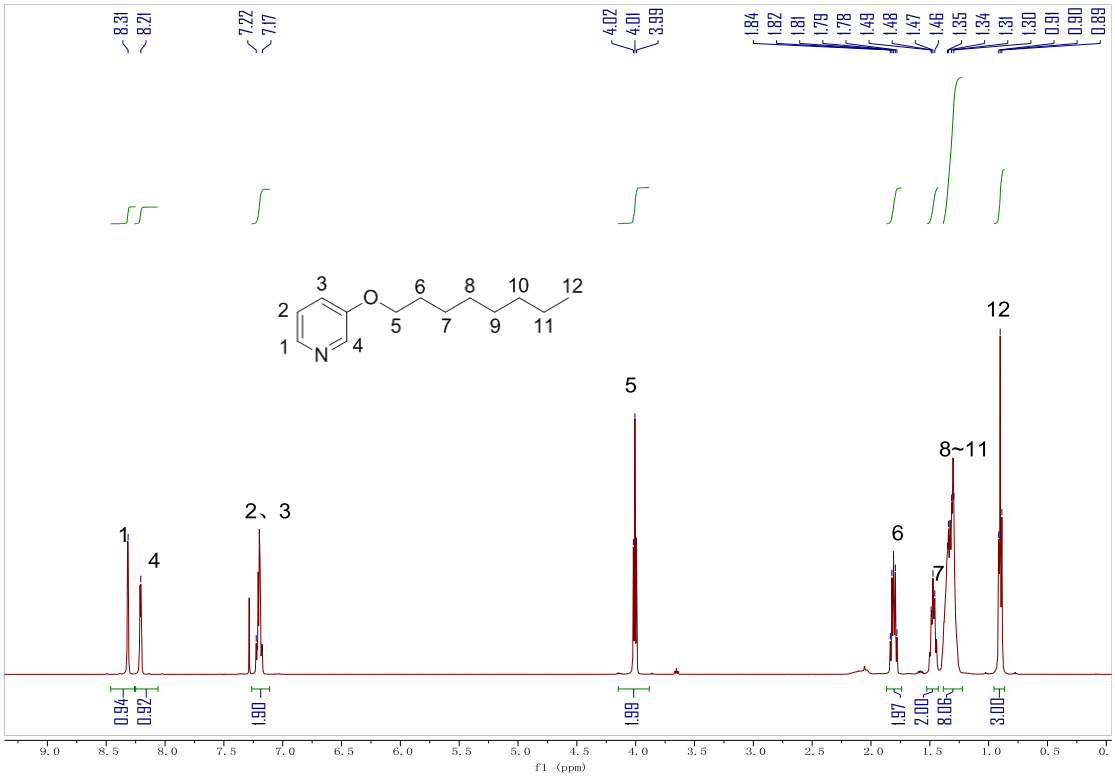
The ^{13}C NMR spectrum of compound **20**



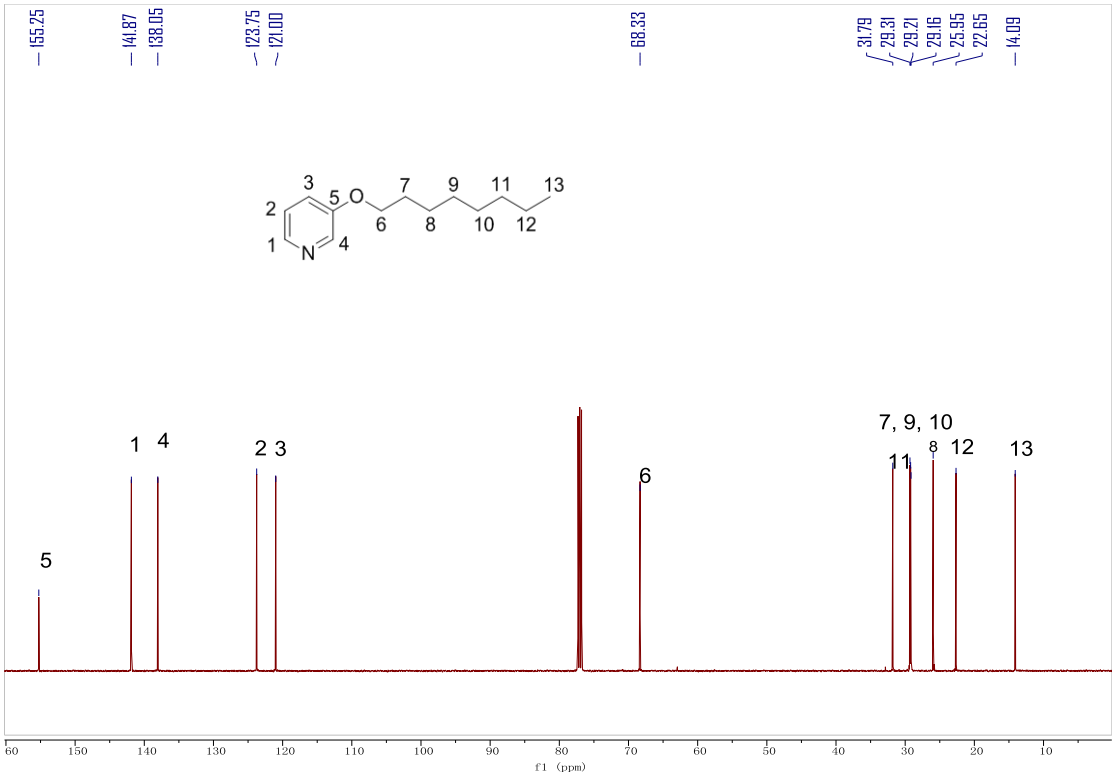
The ^{1}H NMR spectrum of compound **21**



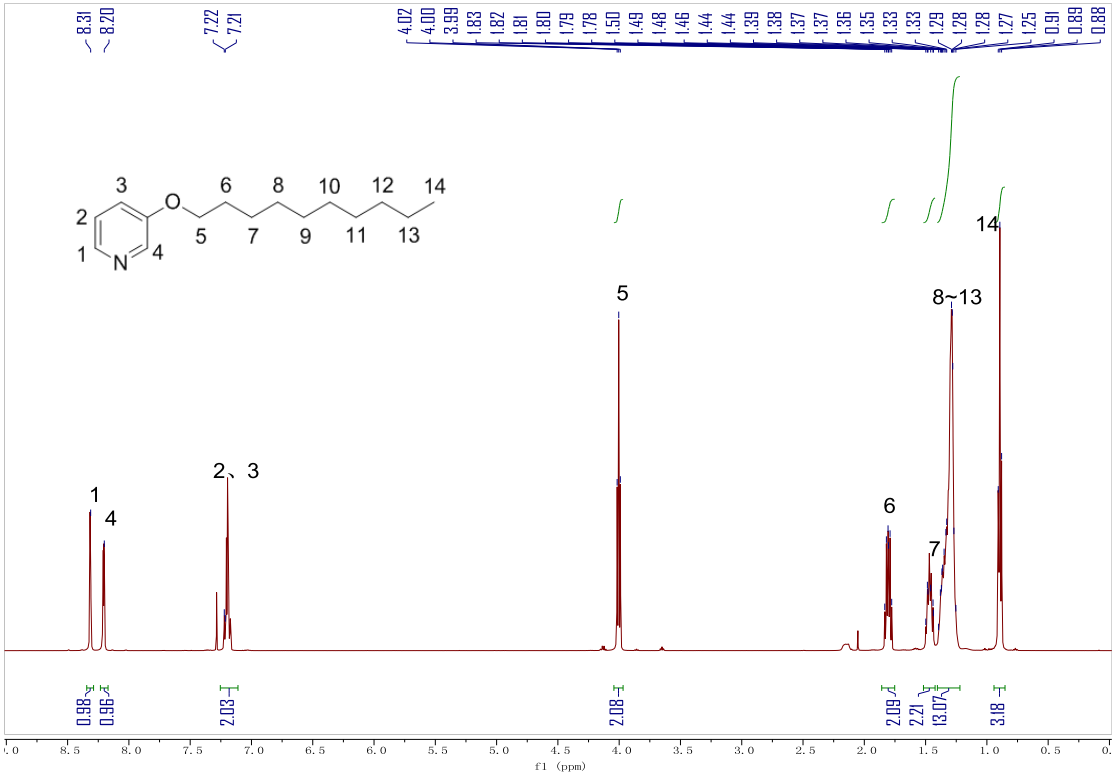
The ^{1}H NMR spectrum of compound **24**



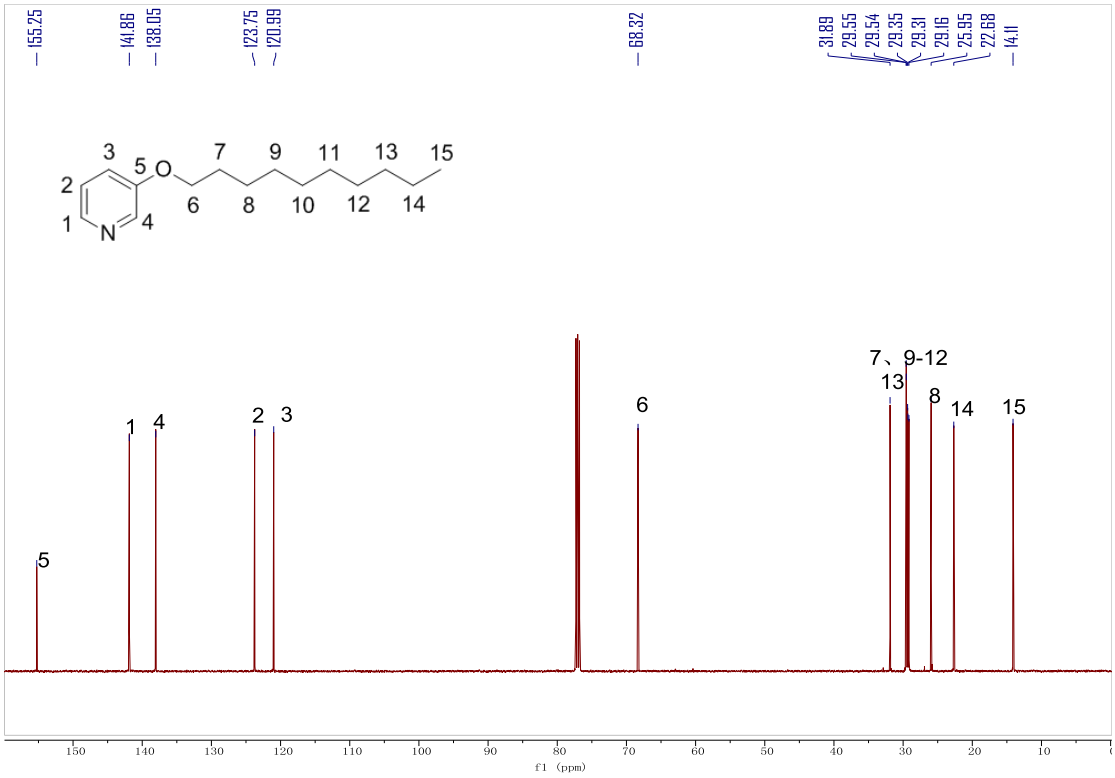
The ^{1}H NMR spectrum of compound **25**



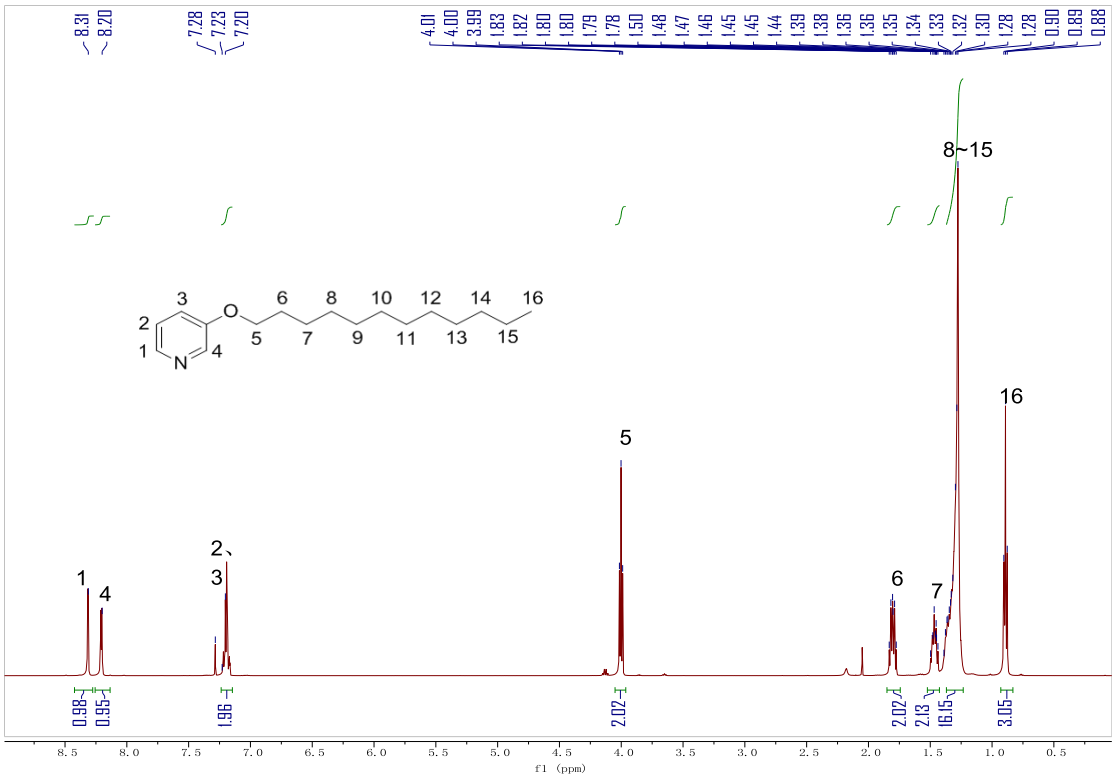
The ^{13}C NMR spectrum of compound **25**



The ^{1}H NMR spectrum of compound **26**



The ^{13}C NMR spectrum of compound **26**



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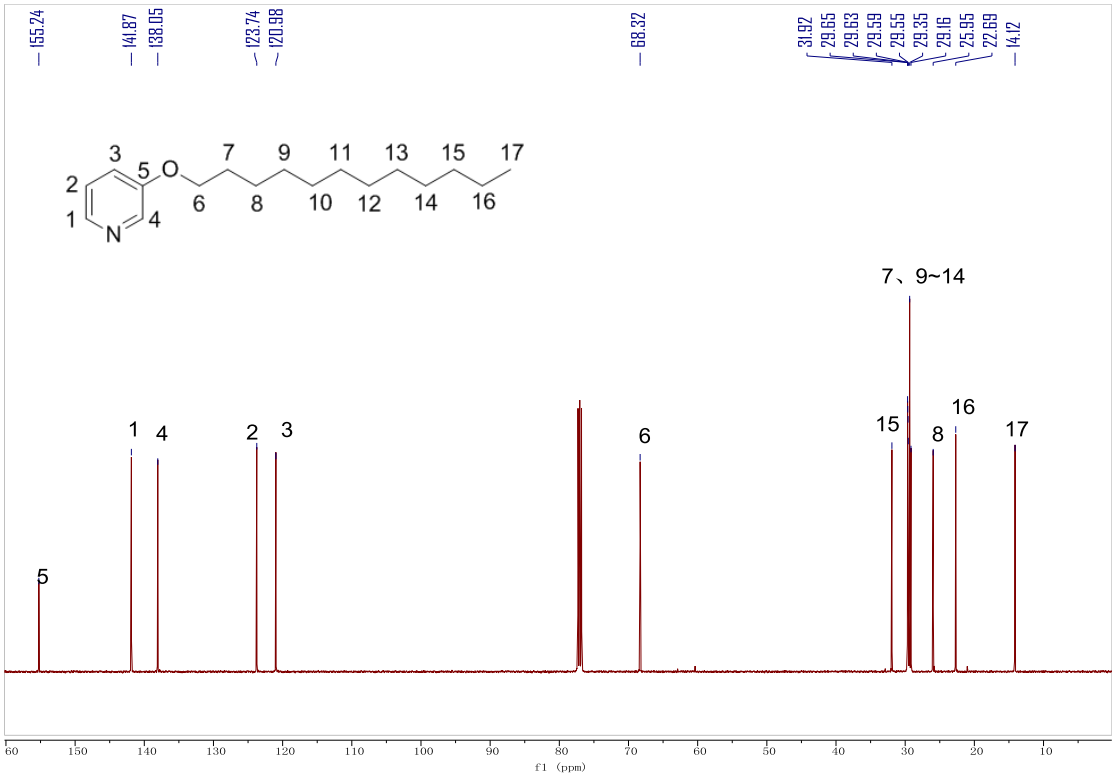

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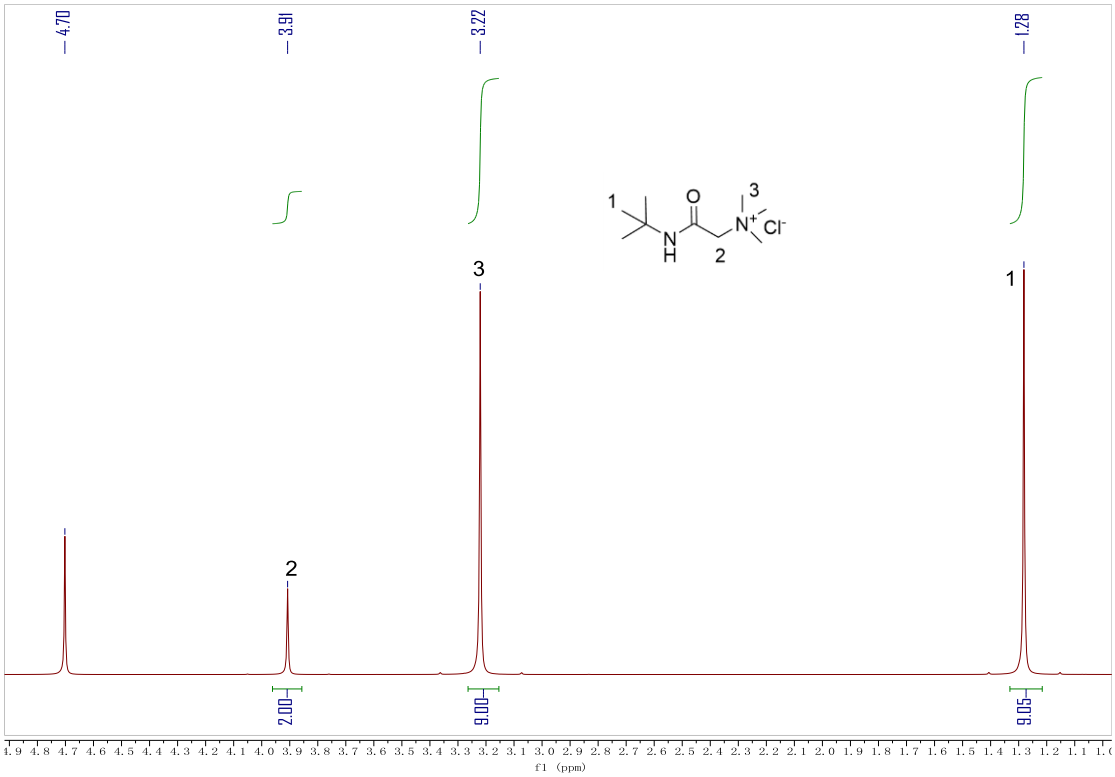
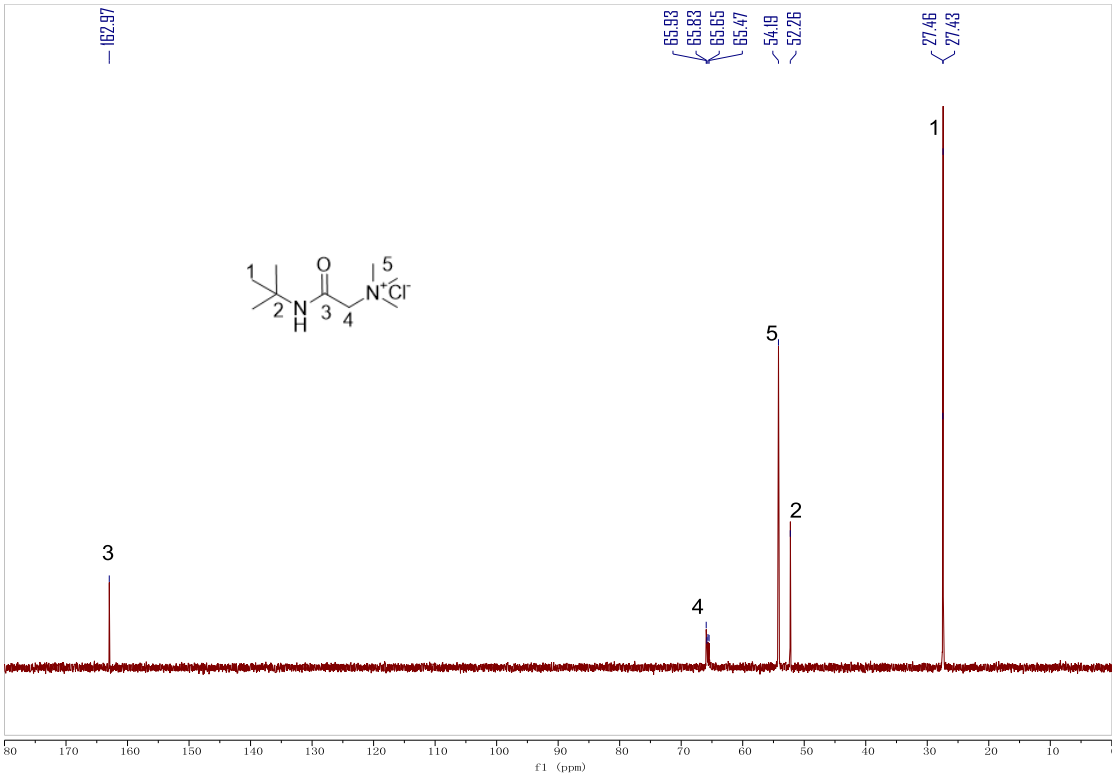
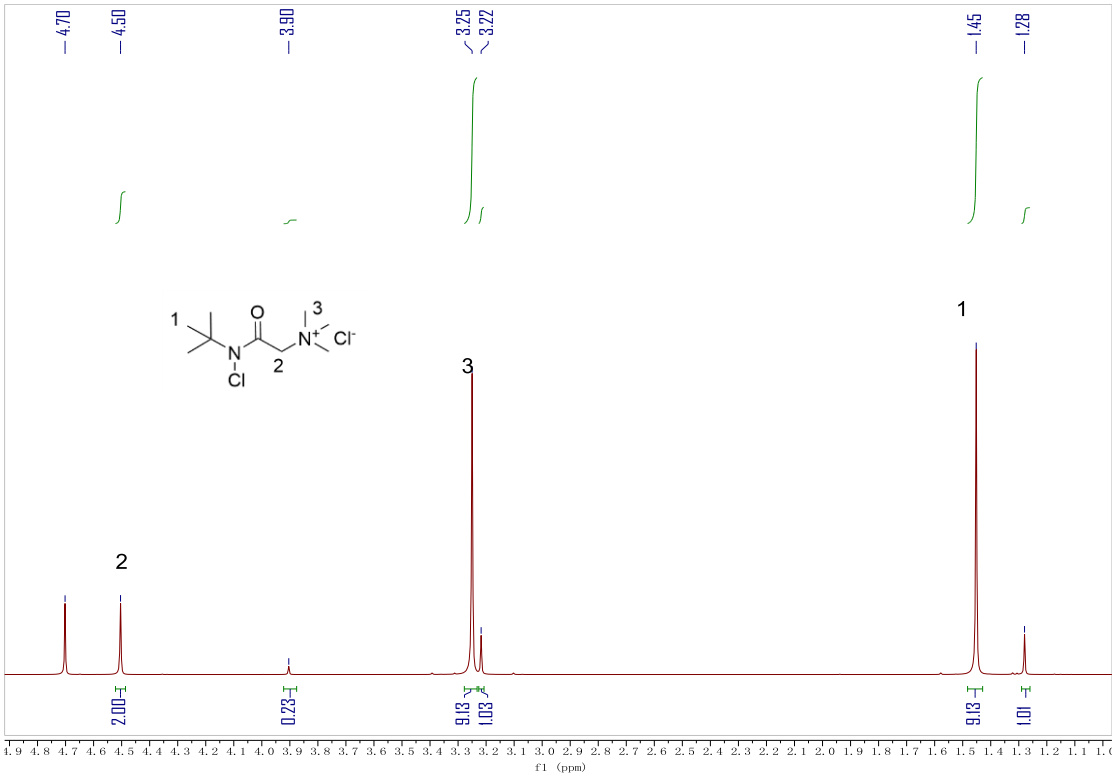


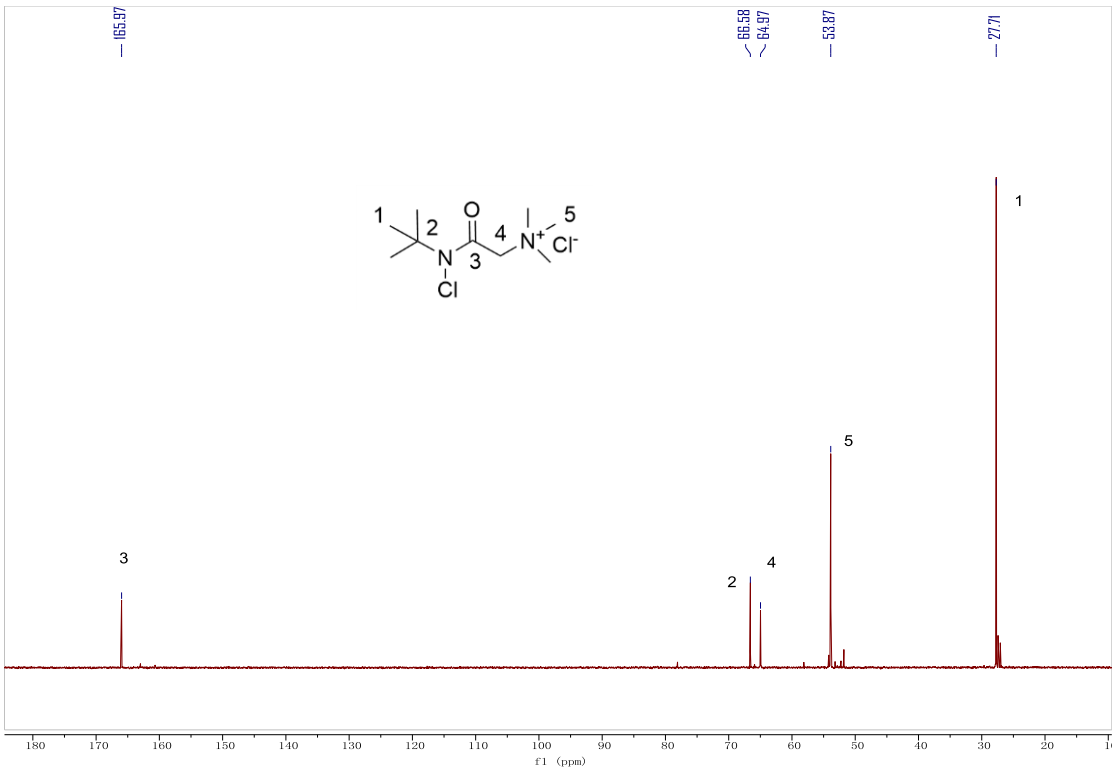
The ^{1}H NMR spectrum of compound **6a**



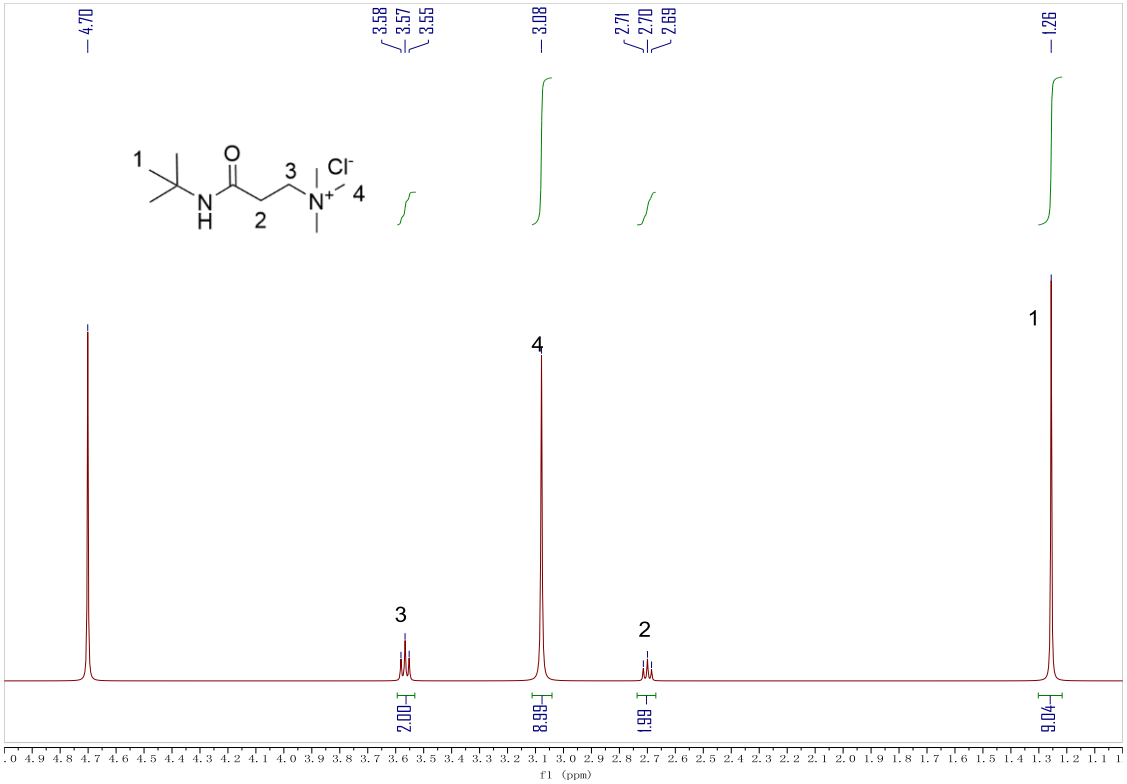
The ^{13}C NMR spectrum of compound **6a**



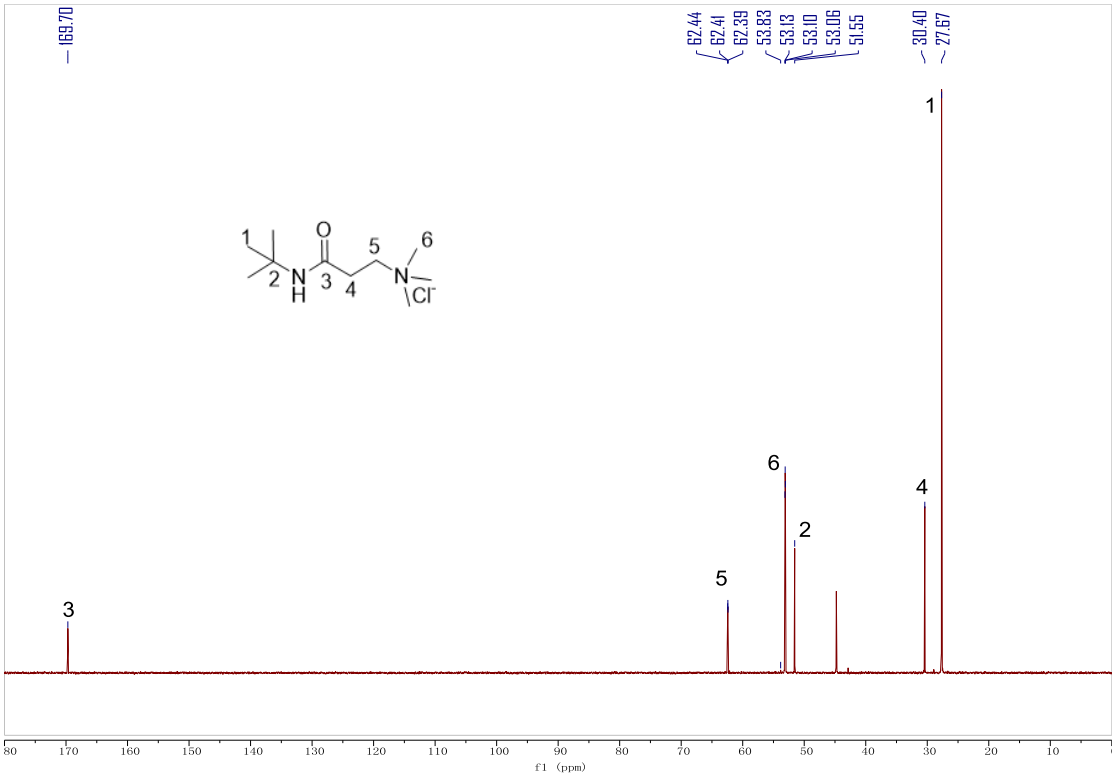
The ^{1}H NMR spectrum of compound **6**



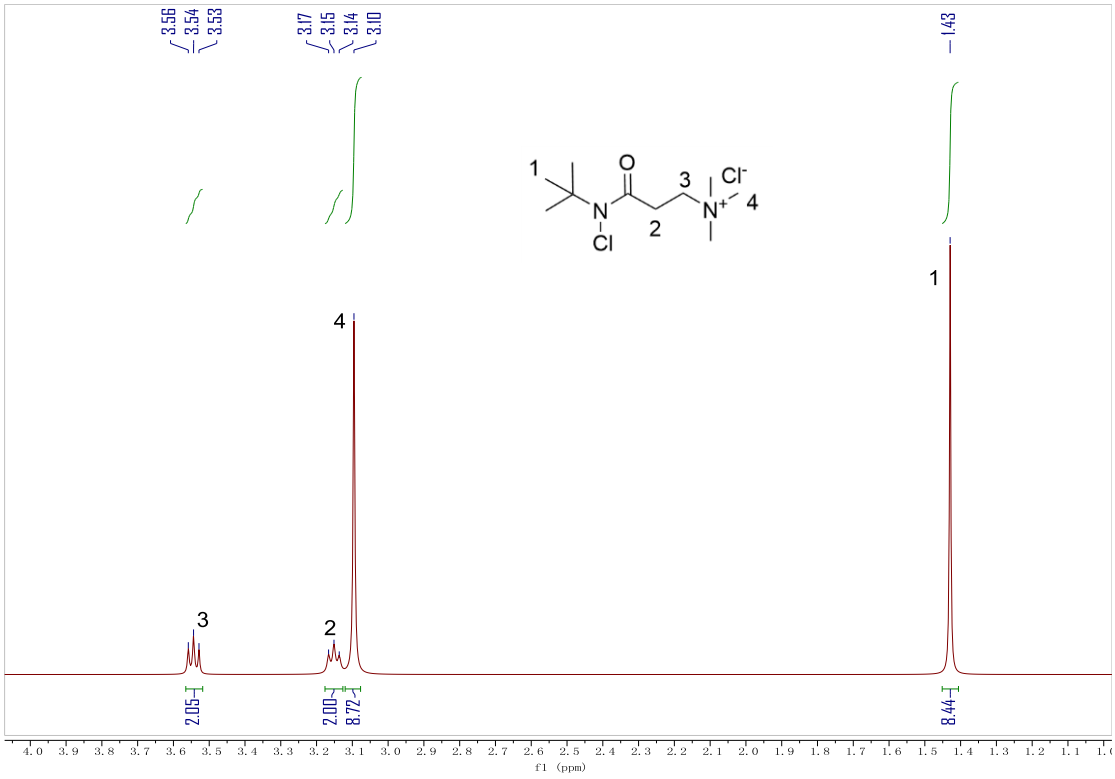
The ^{13}C NMR spectrum of compound **6**



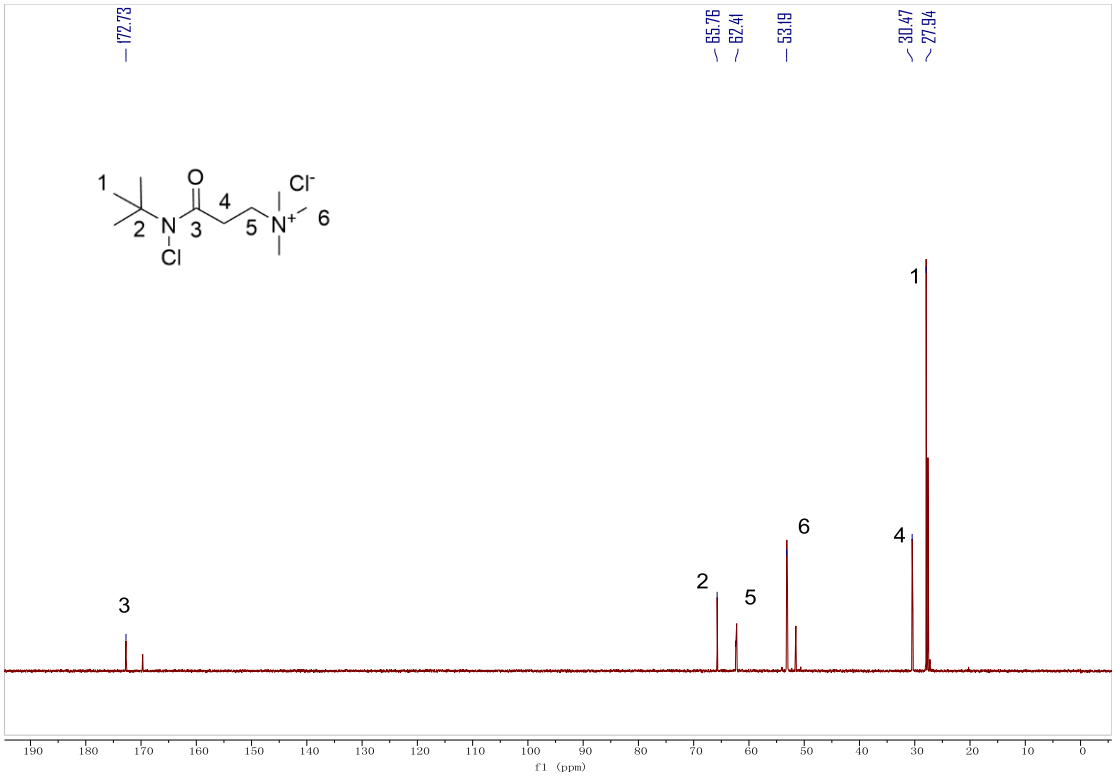
The ^{1}H NMR spectrum of compound **7a**



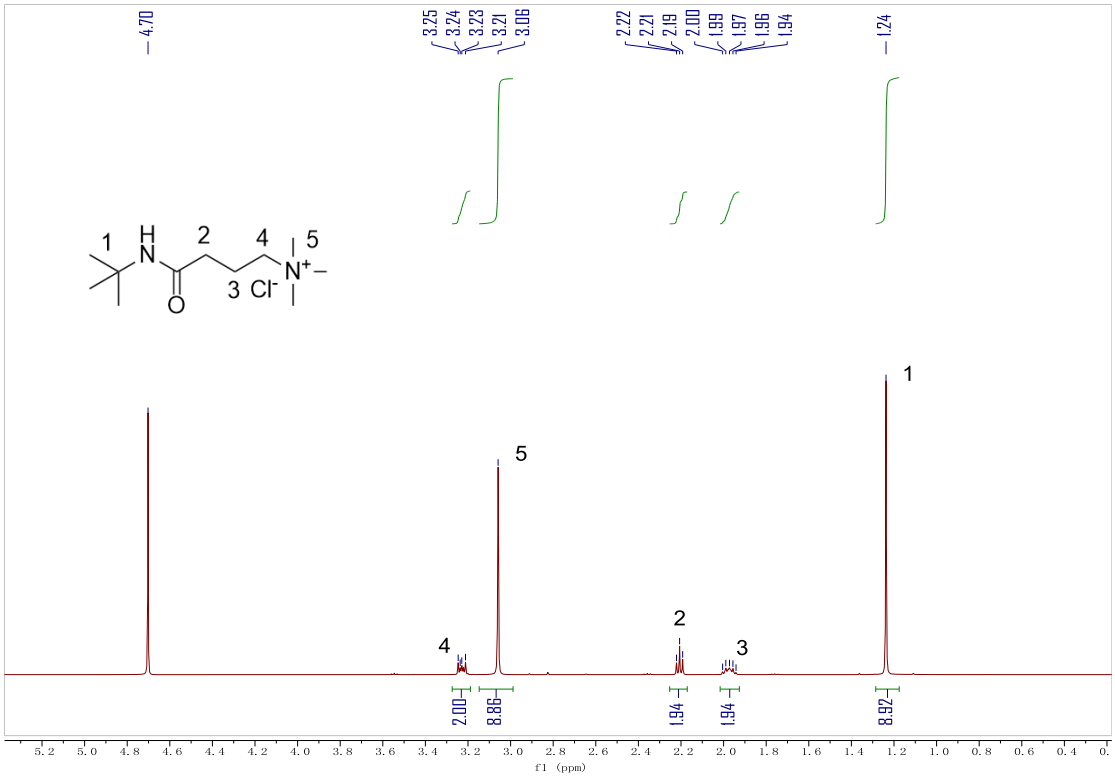
The ^{13}C NMR spectrum of compound **7a**



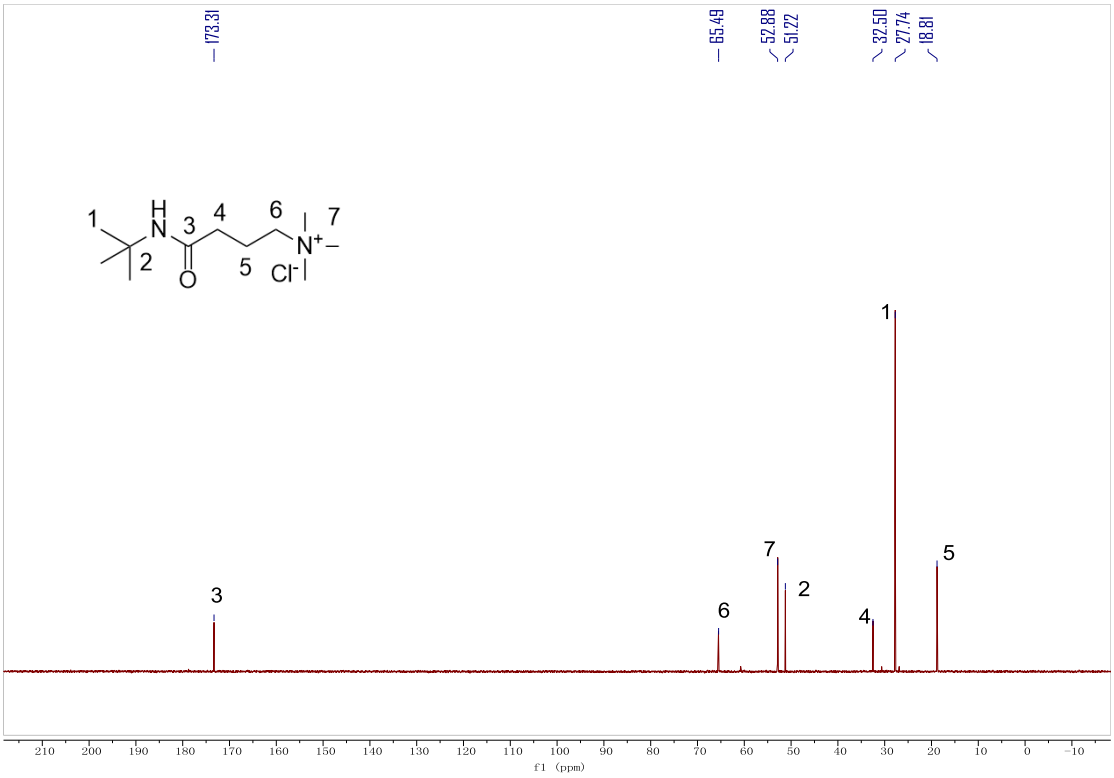
The ^{1}H NMR spectrum of compound **7**



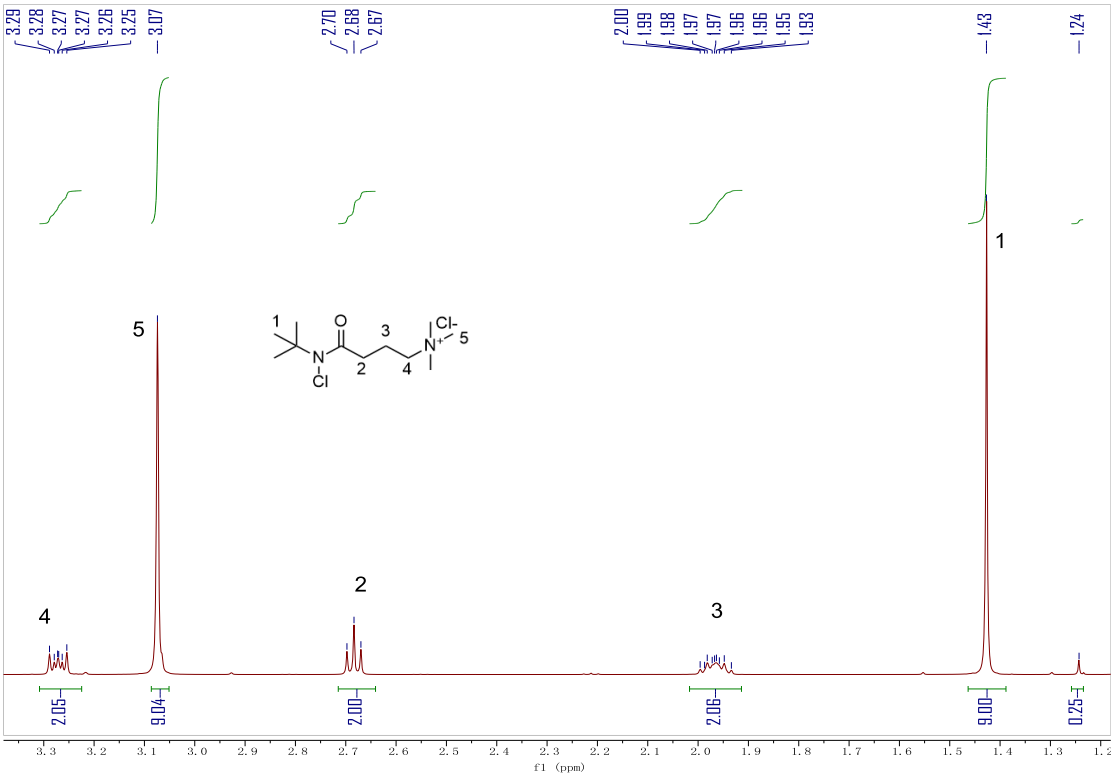
The ^{13}C NMR spectrum of compound **7**



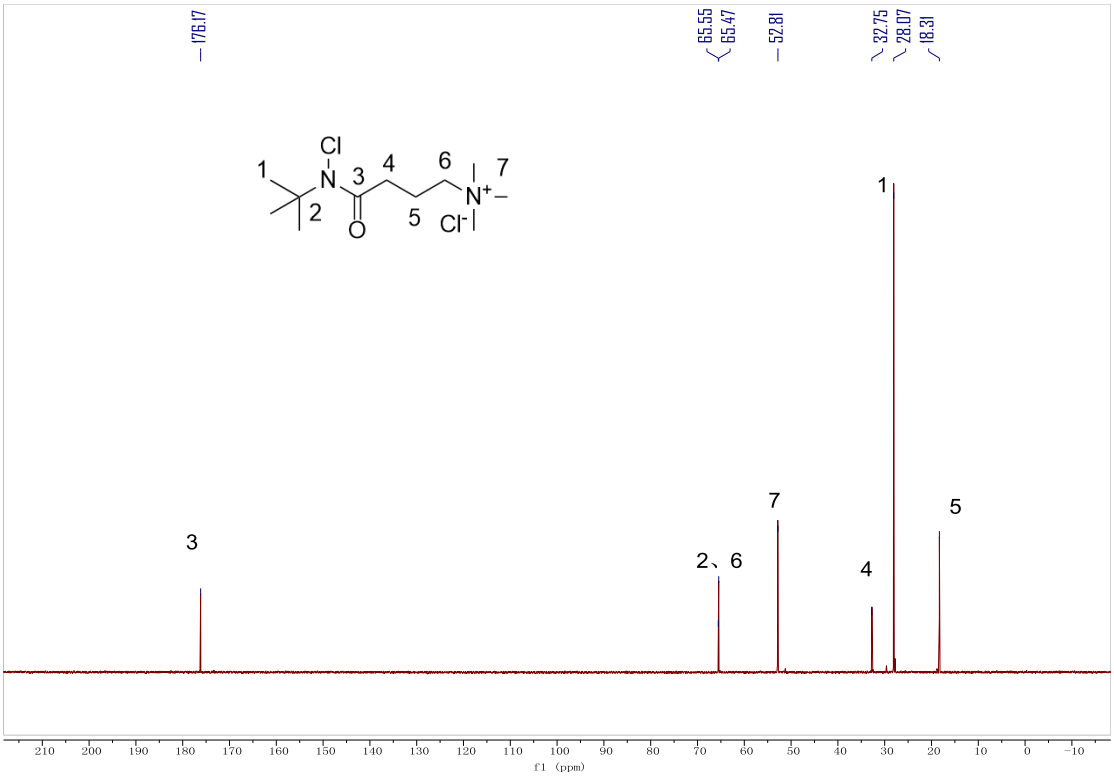
The ^{1}H NMR spectrum of compound **8a**



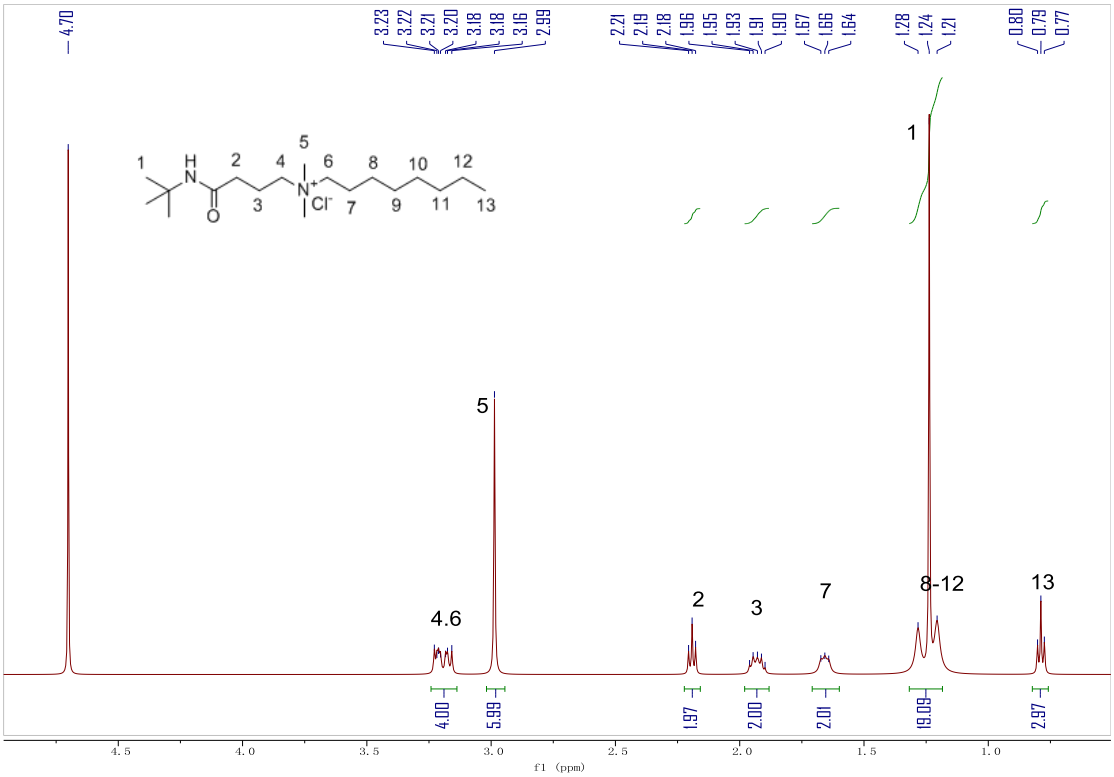
The ^{13}C NMR spectrum of compound **8a**



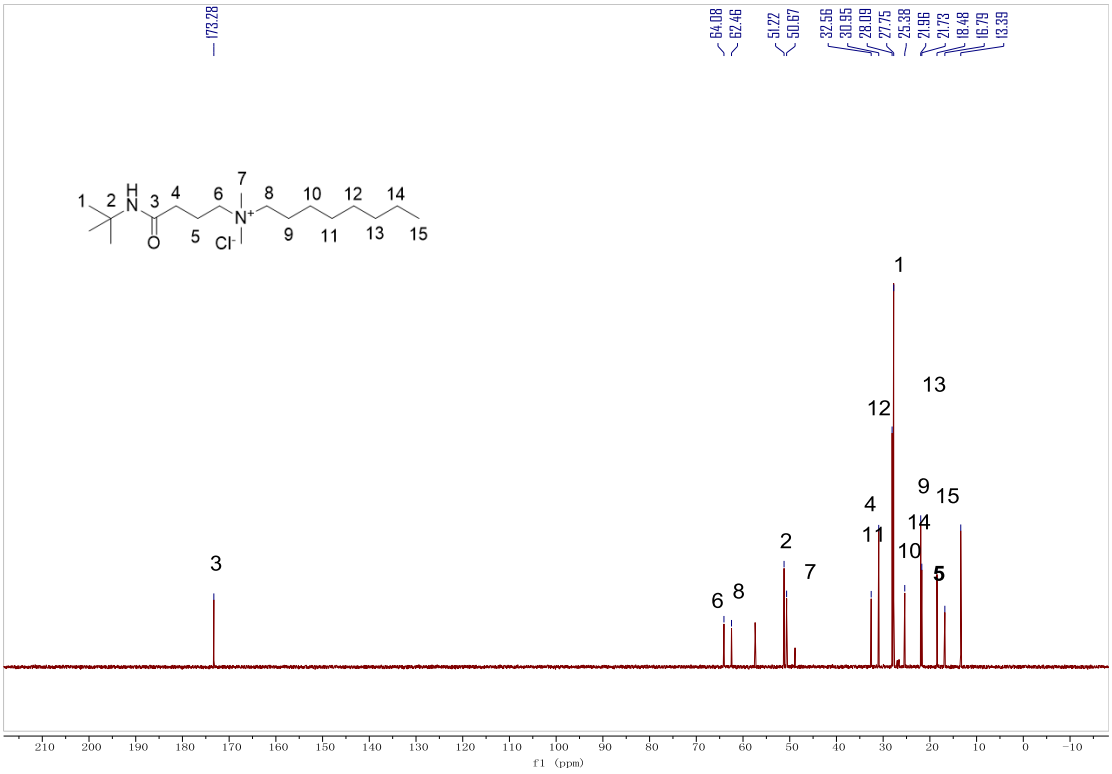
The ^{1}H NMR spectrum of compound **8**



The ^{13}C NMR spectrum of compound **8**



The ^{1}H NMR spectrum of compound **9a**



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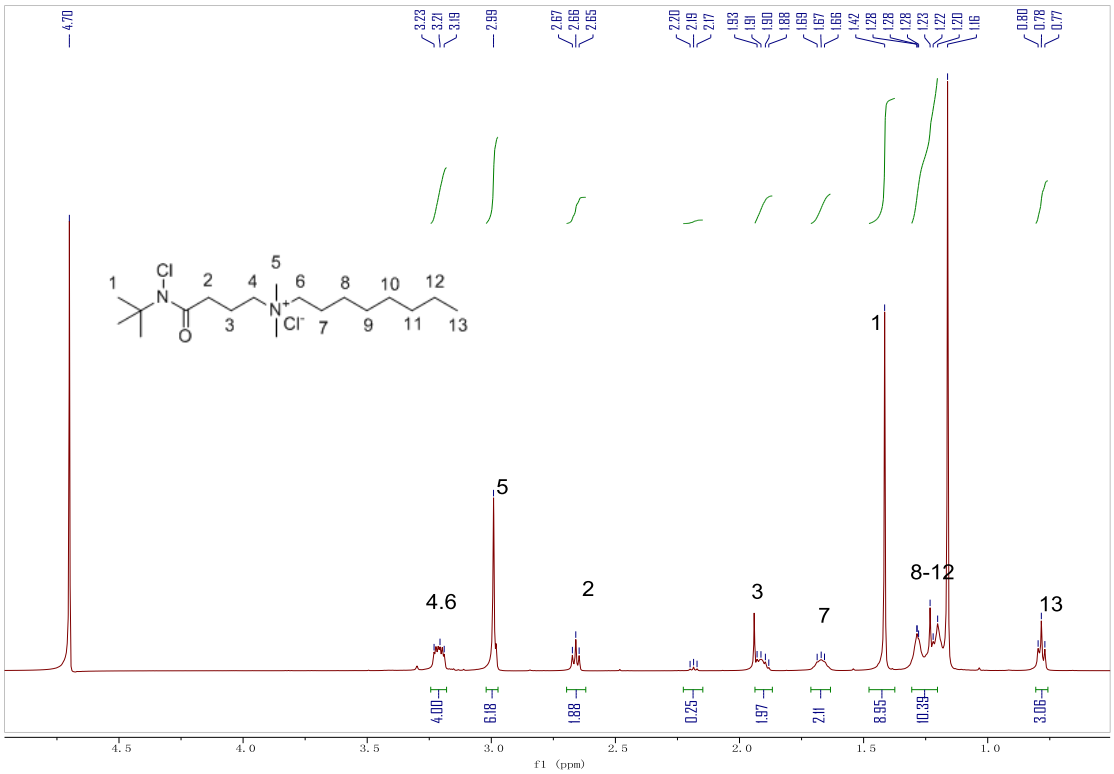

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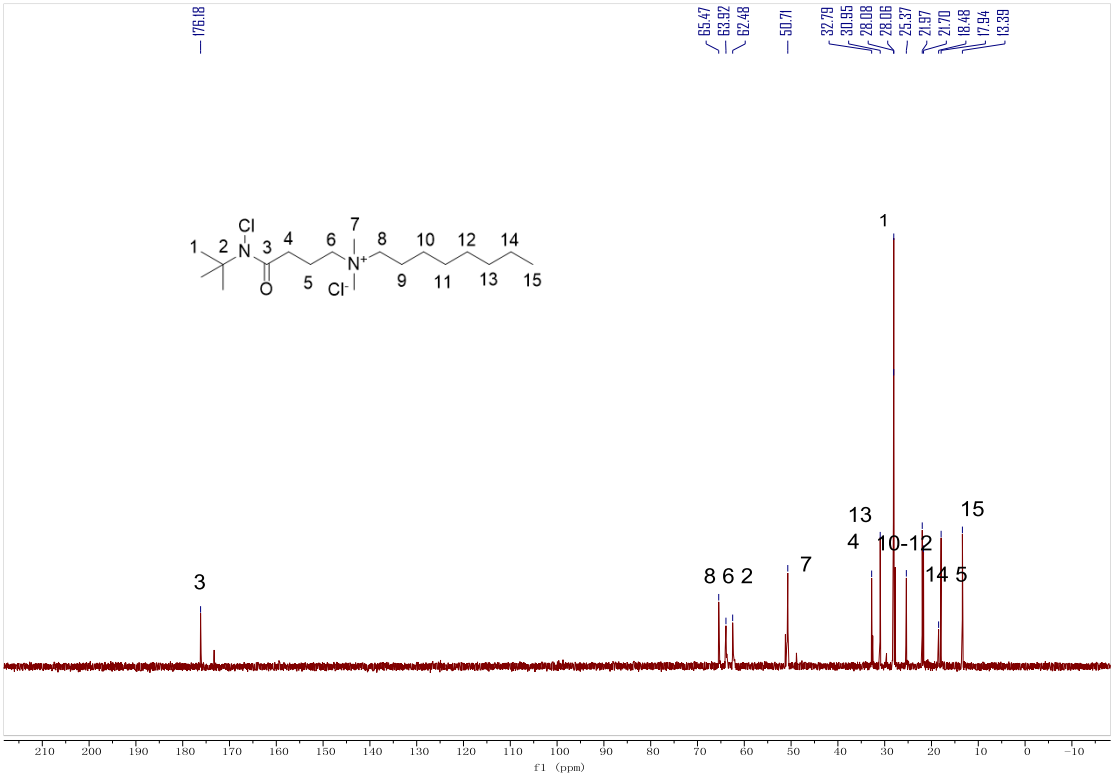
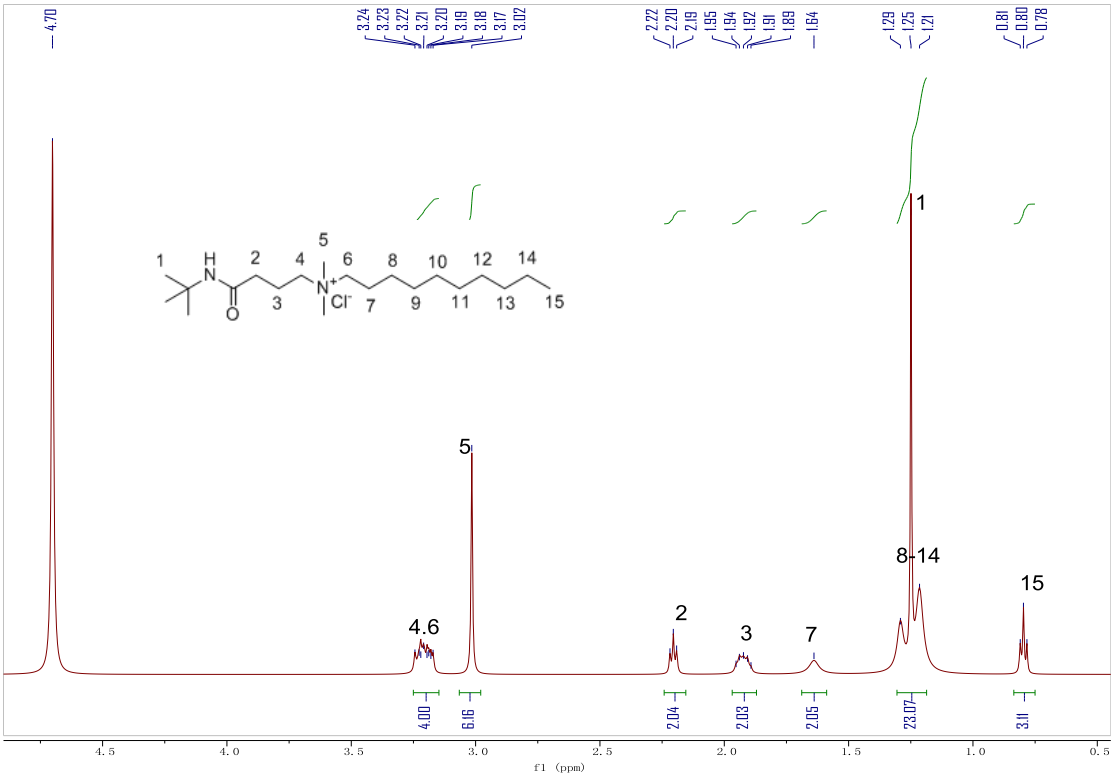


The ^{13}C NMR spectrum of compound **9**



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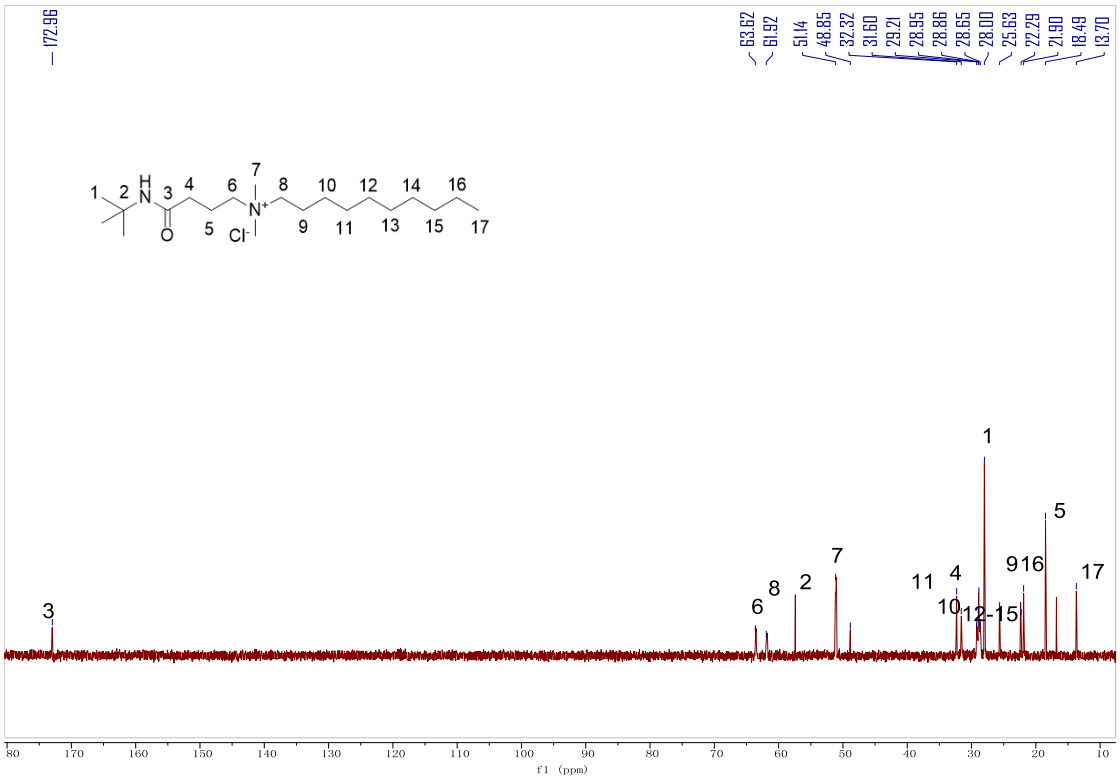
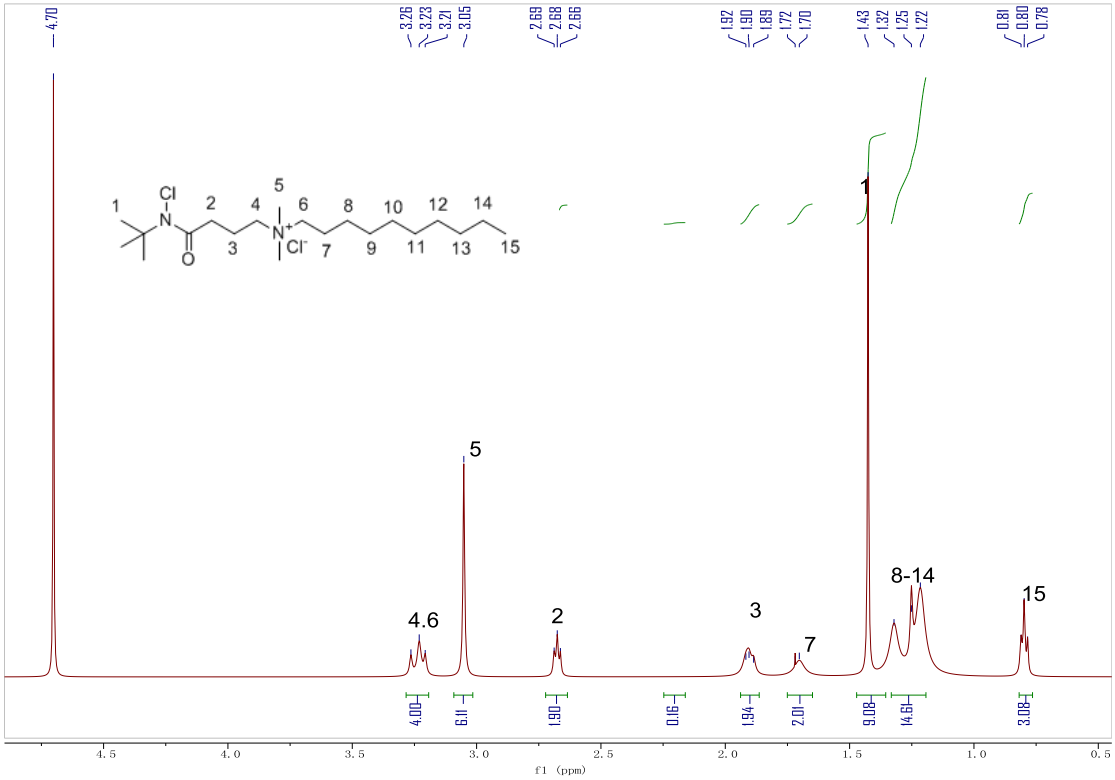


The ^{13}C NMR spectrum of compound **10a**



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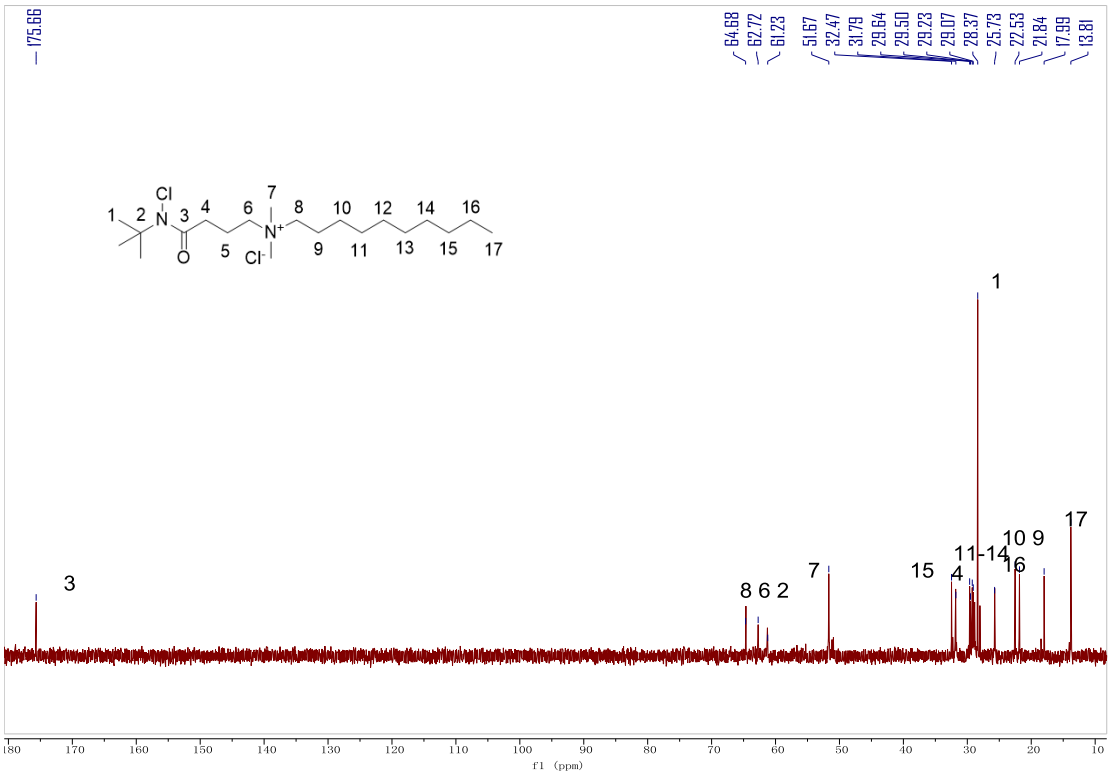

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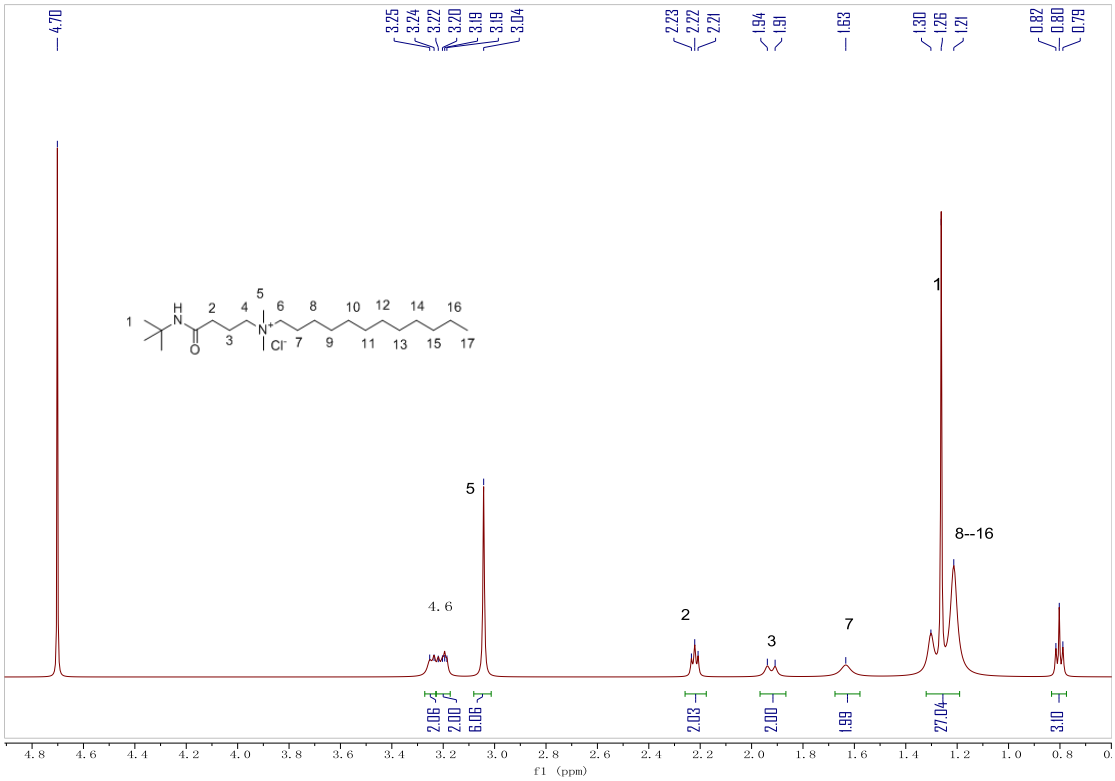
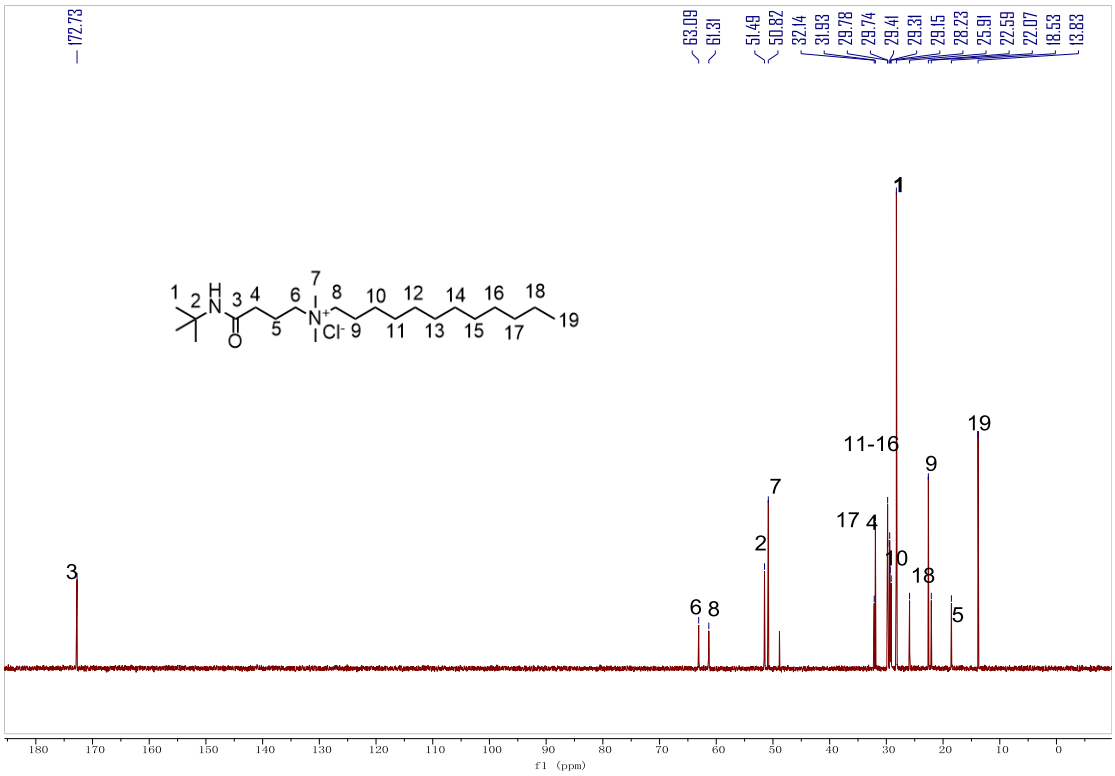
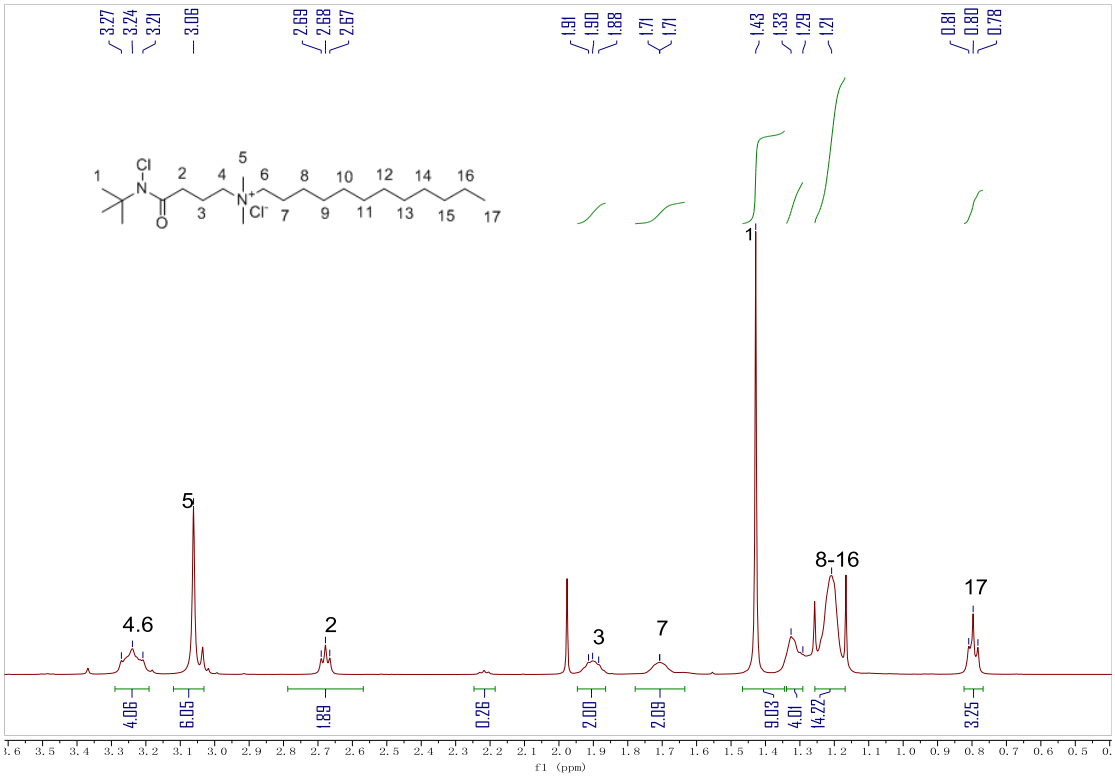


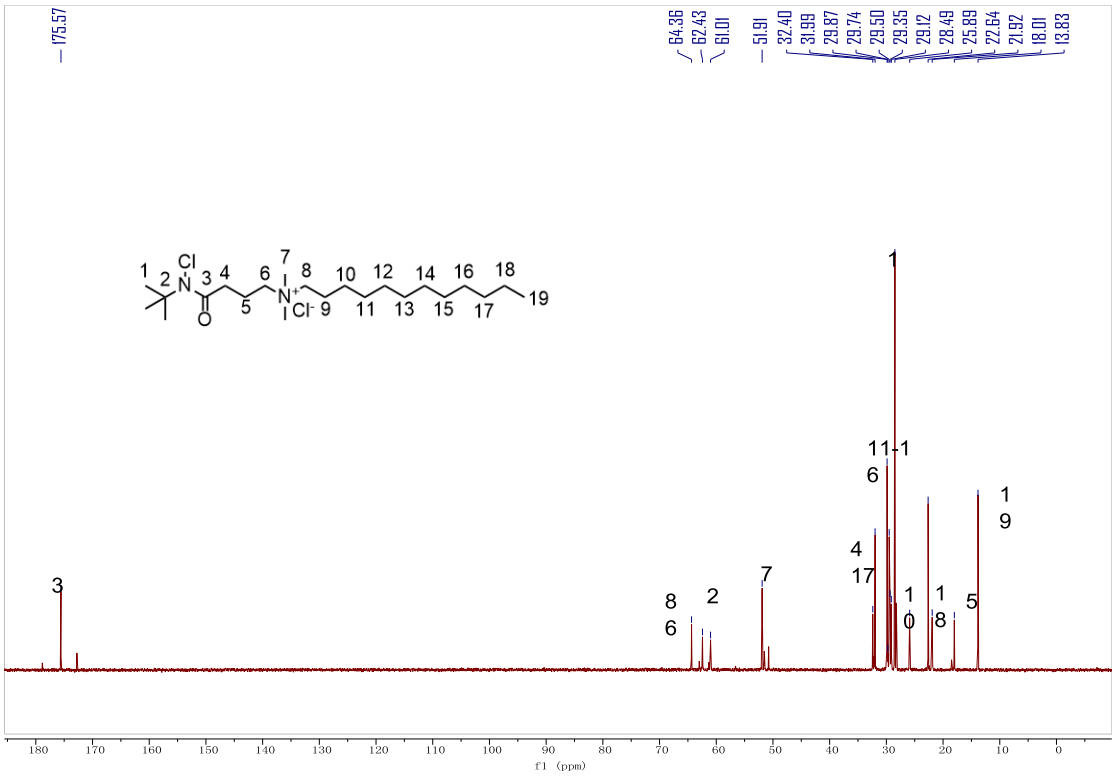
The ^{1}H NMR spectrum of compound **11a**



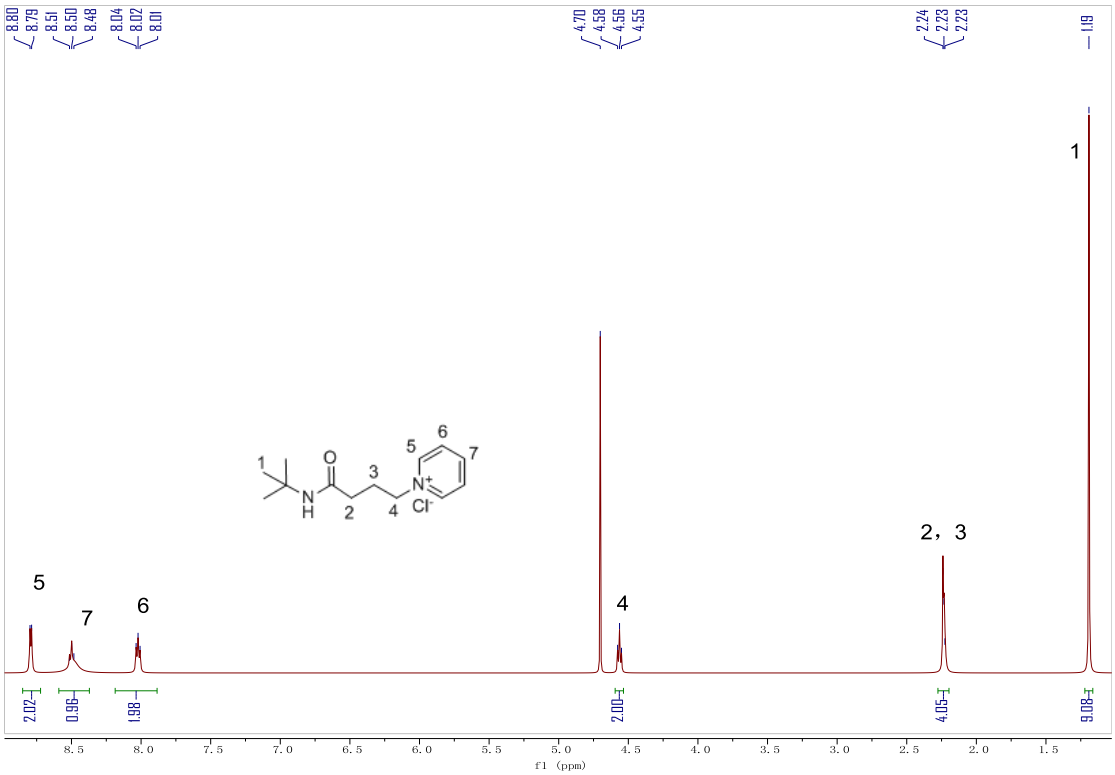
The ^{13}C NMR spectrum of compound **11a**



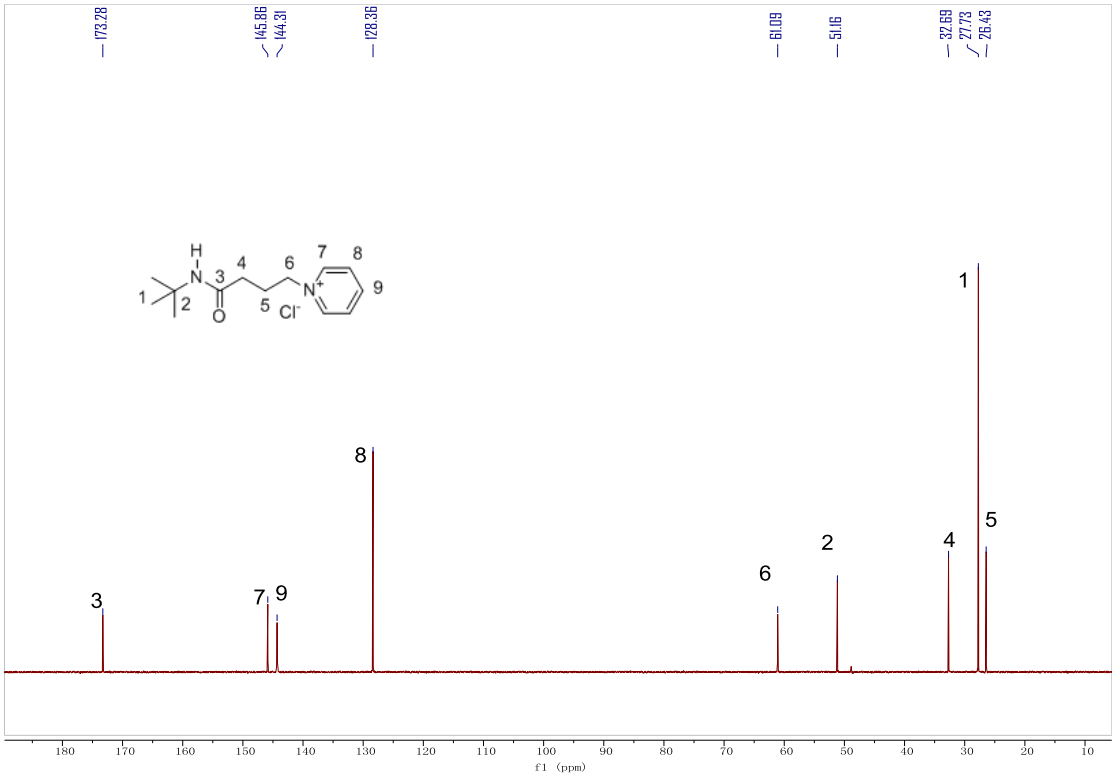
The ^{1}H NMR spectrum of compound **11**



The ^{13}C NMR spectrum of compound **11**



The ^{1}H NMR spectrum of compound **12a**



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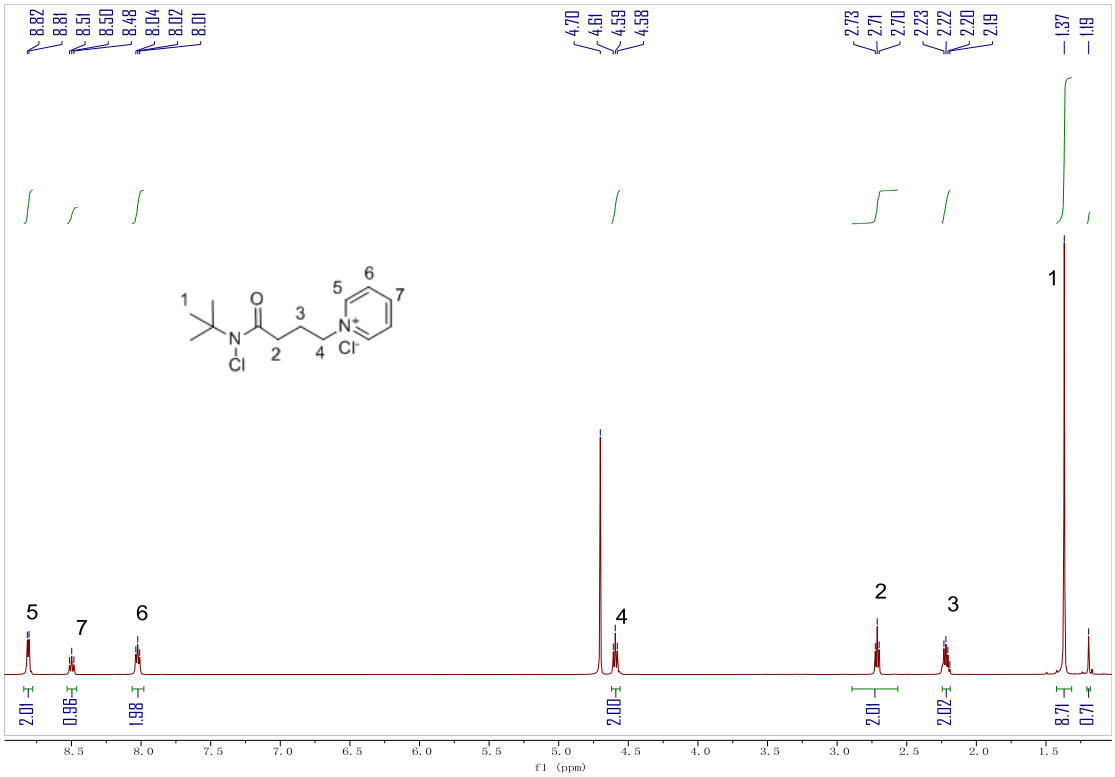
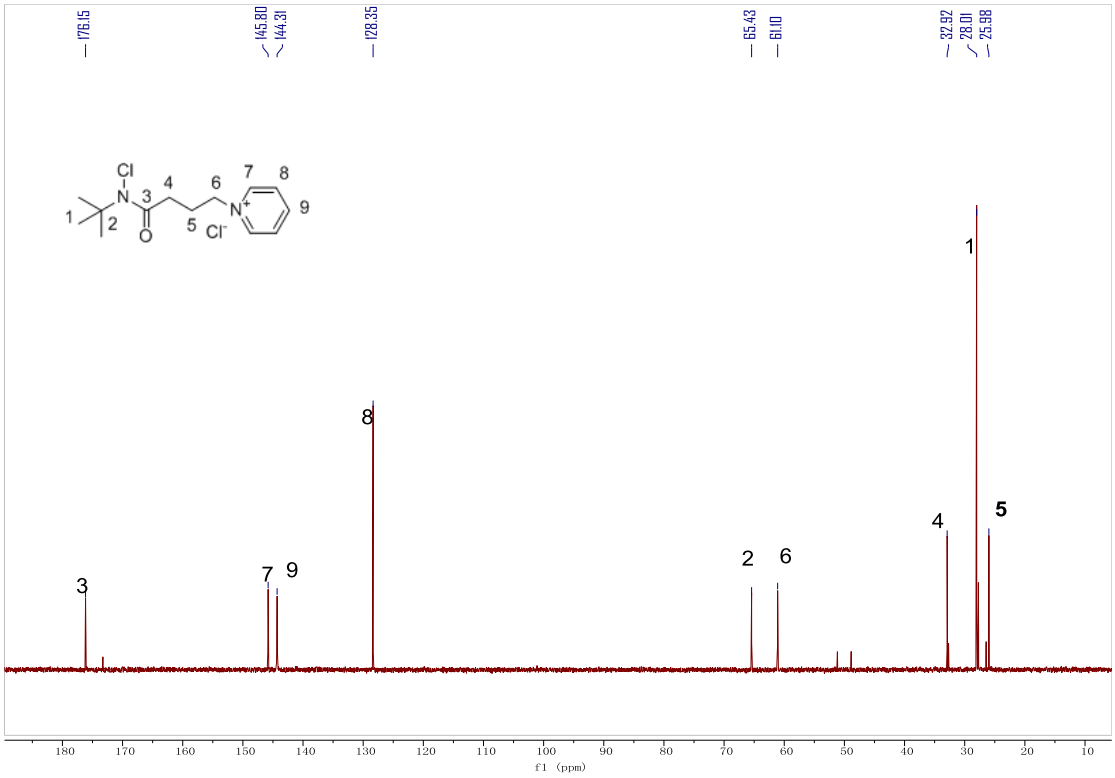


The ^{1}H NMR spectrum of compound **12**



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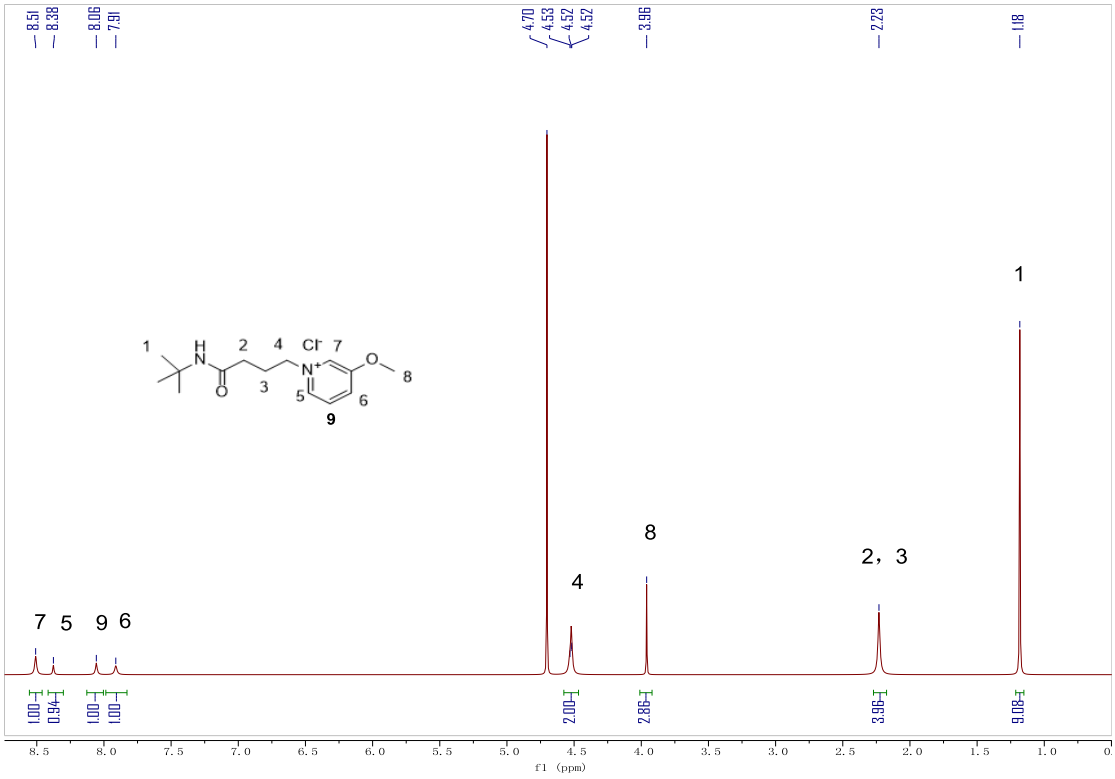
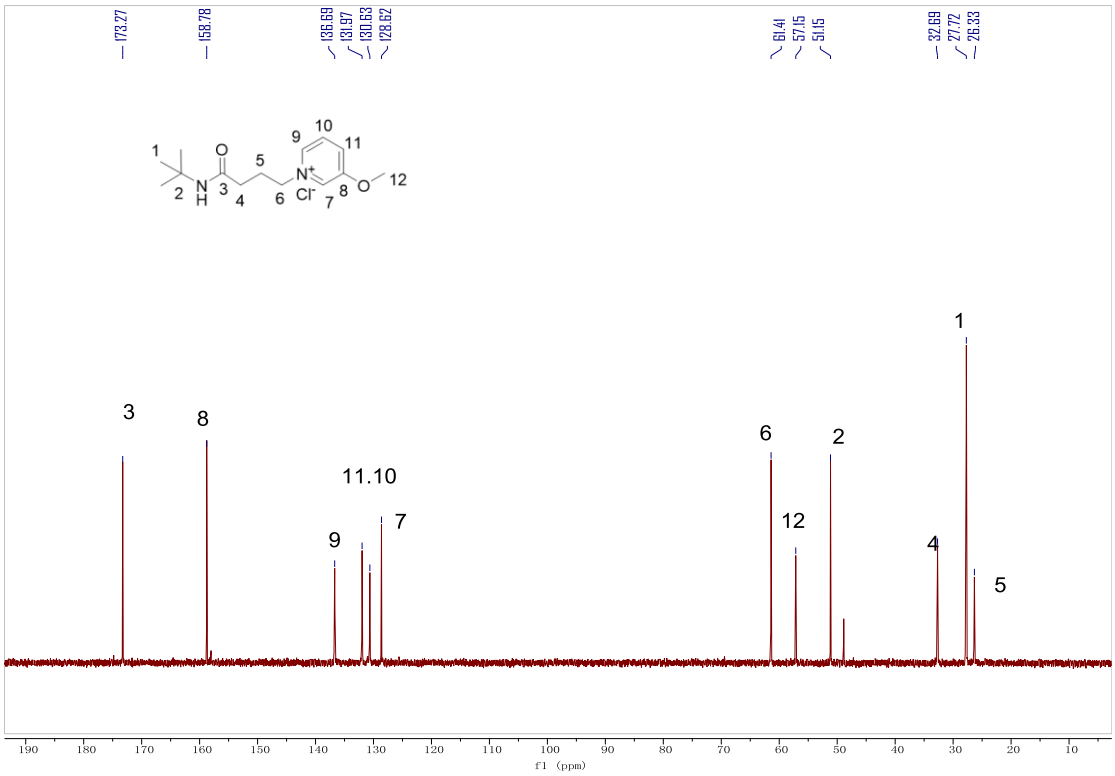


The ^{1}H NMR spectrum of compound **13a**



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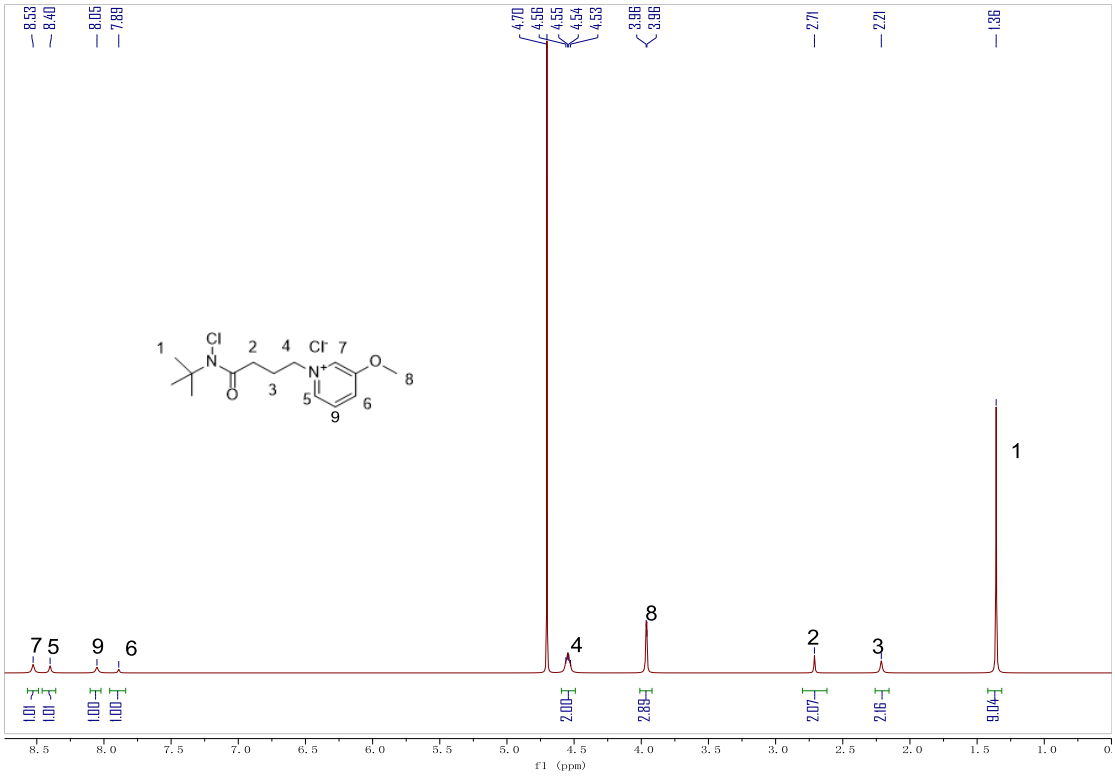

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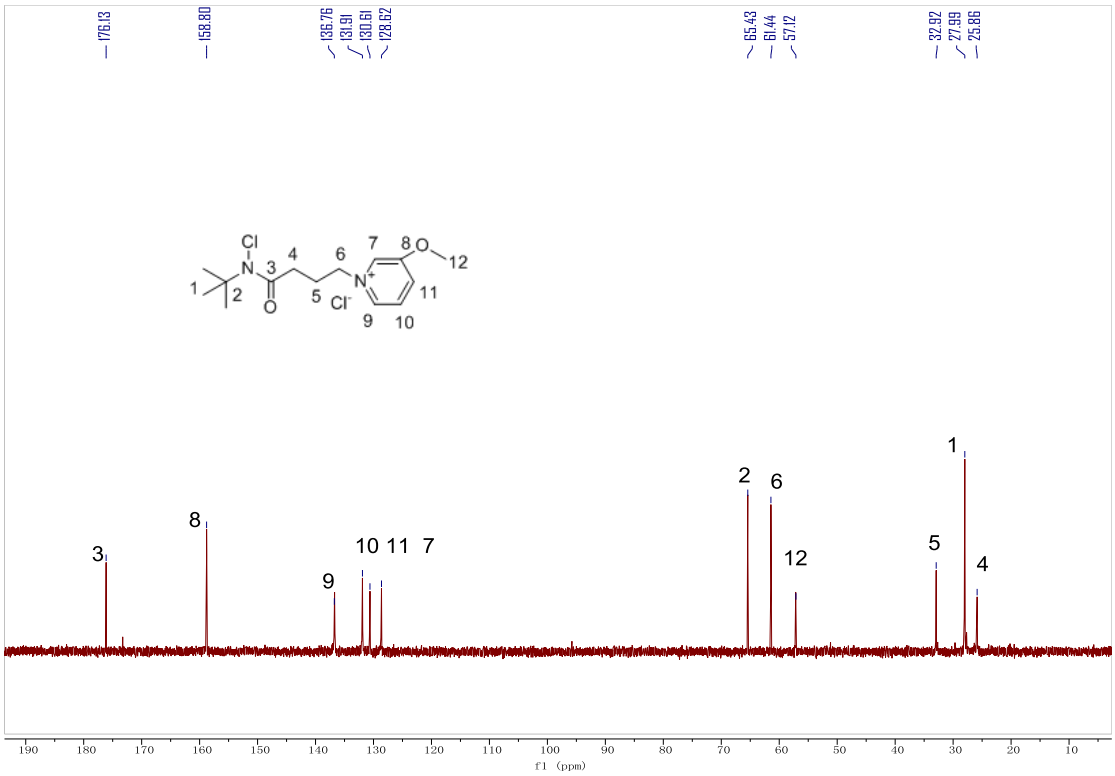

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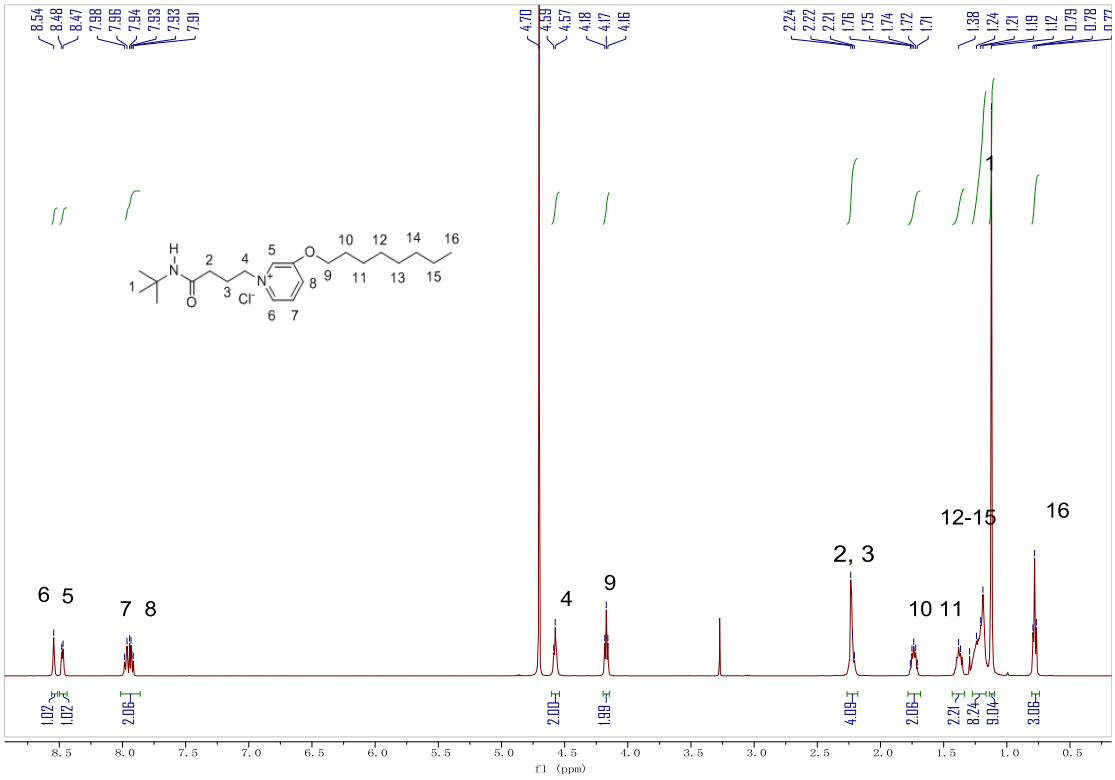
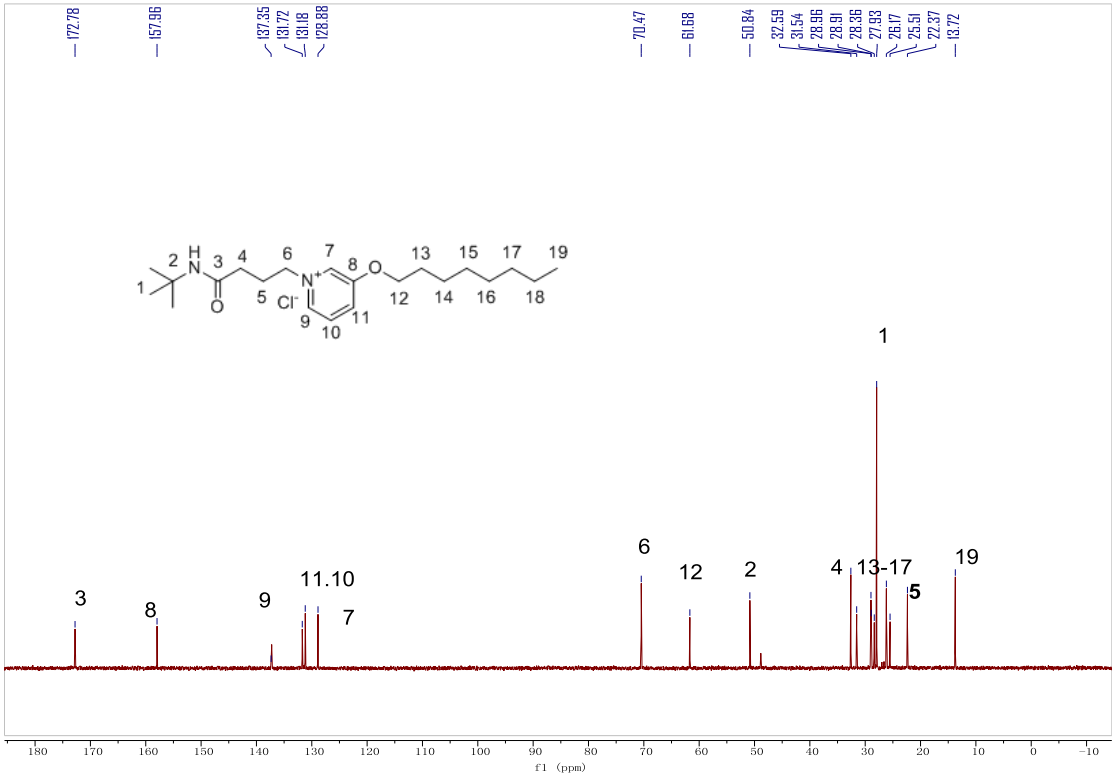


The ^{1}H NMR spectrum of compound **14a**



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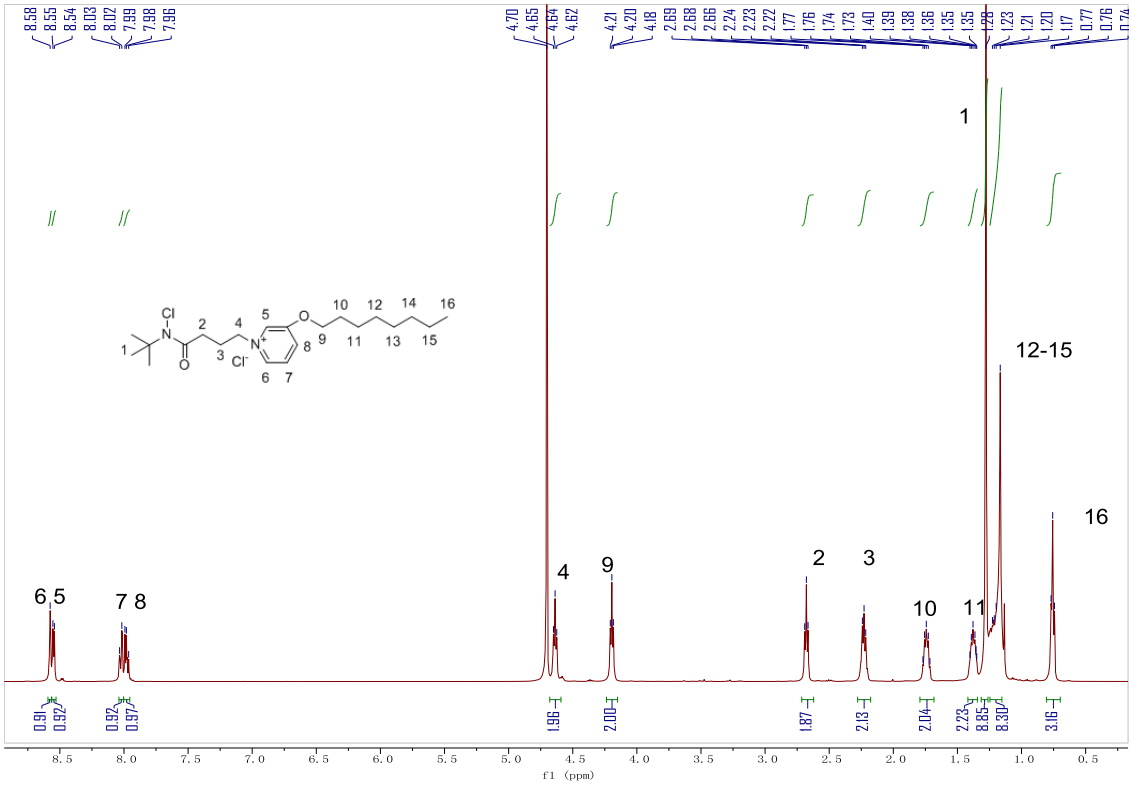

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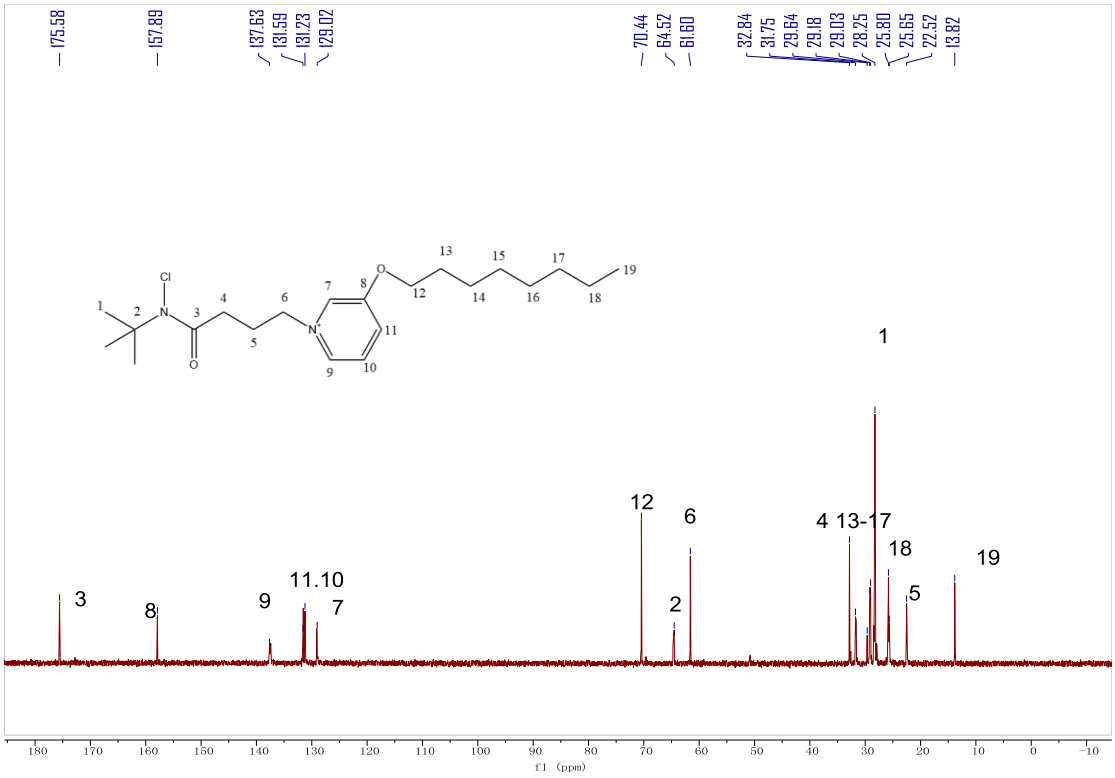

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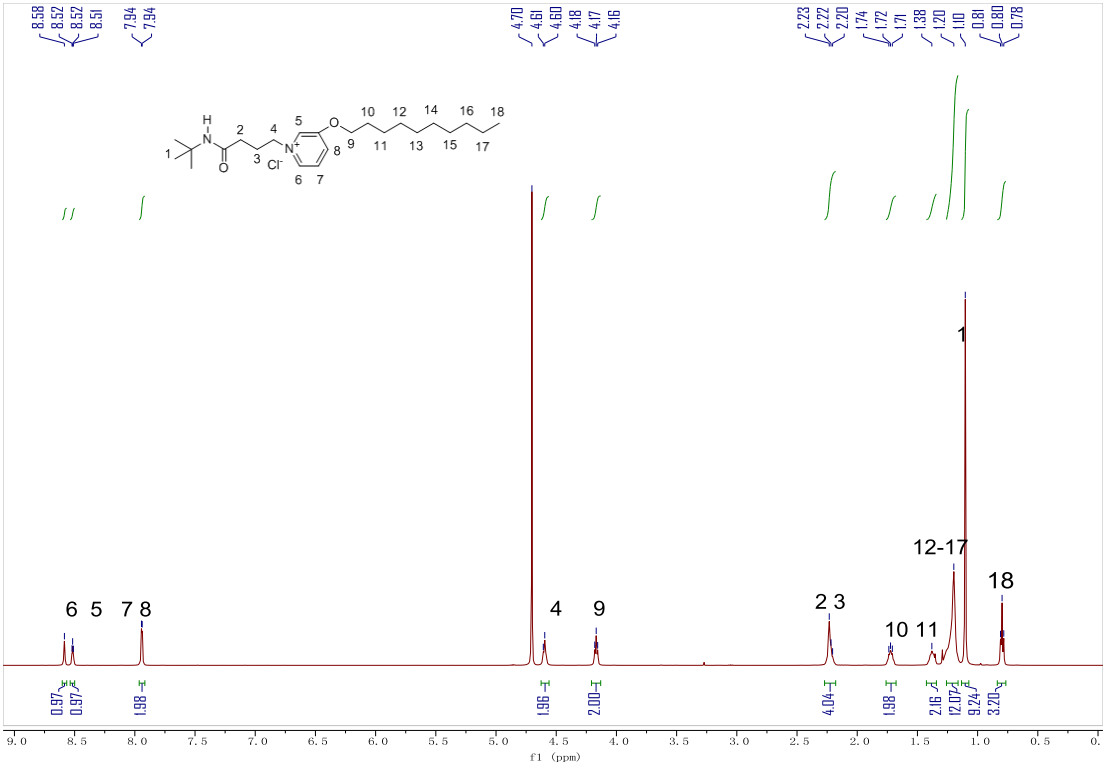
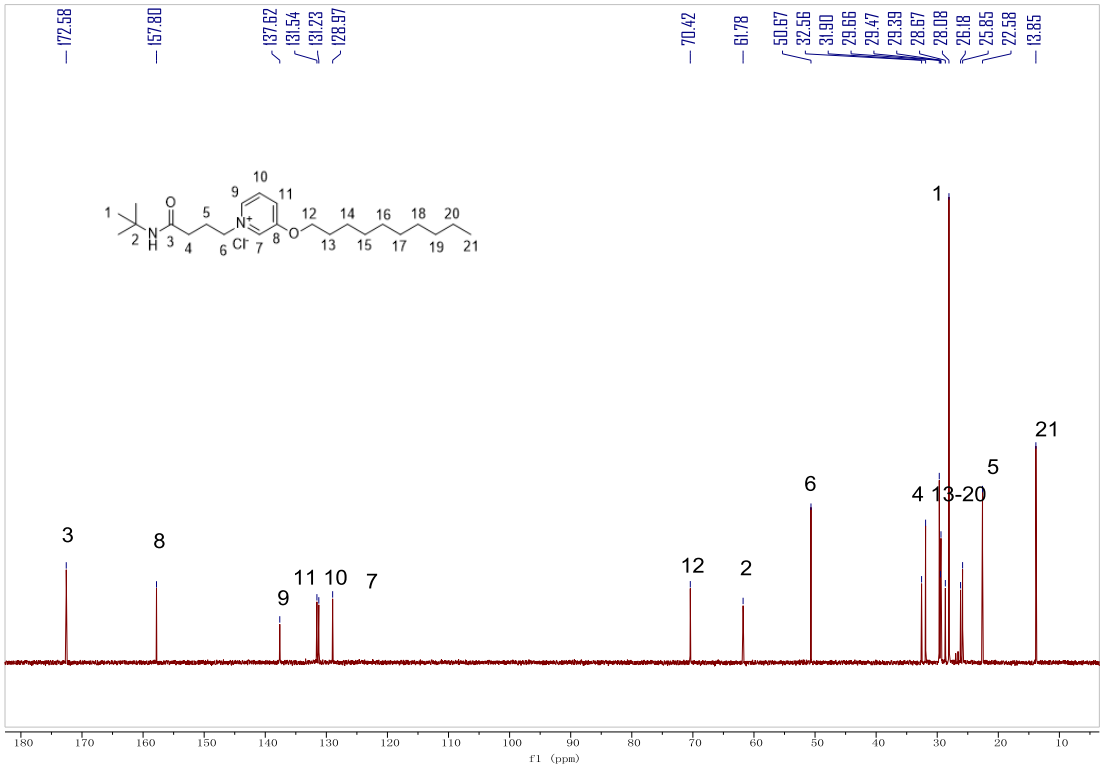
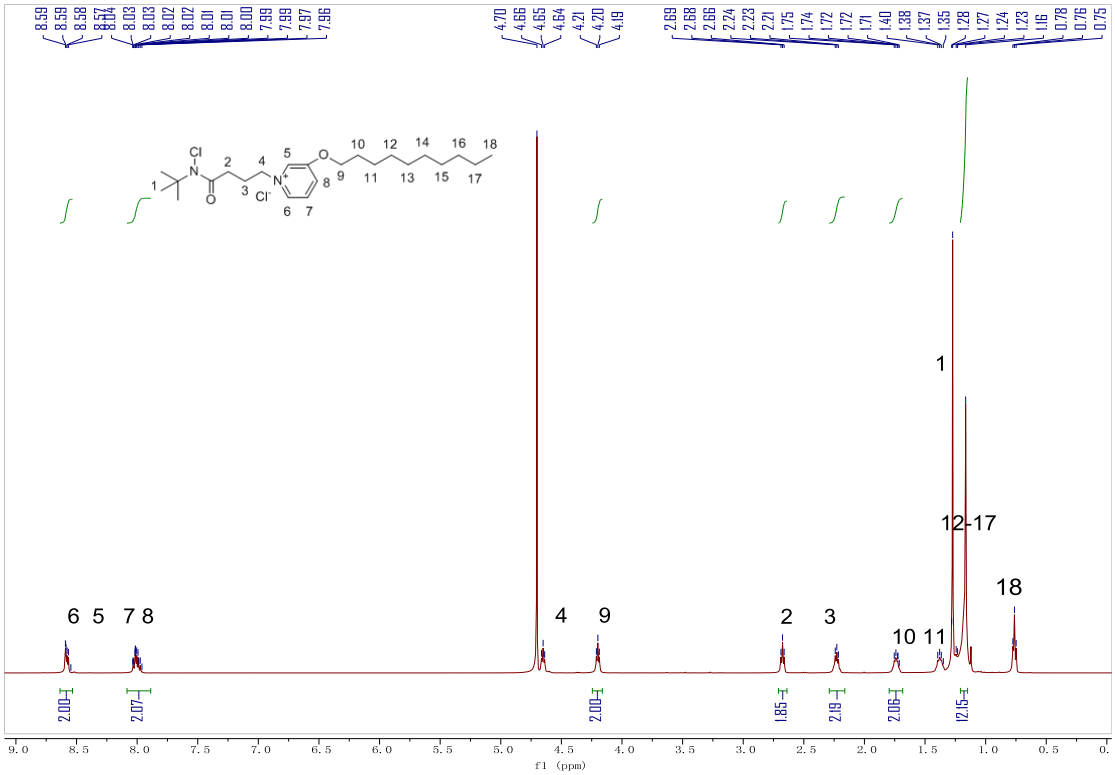


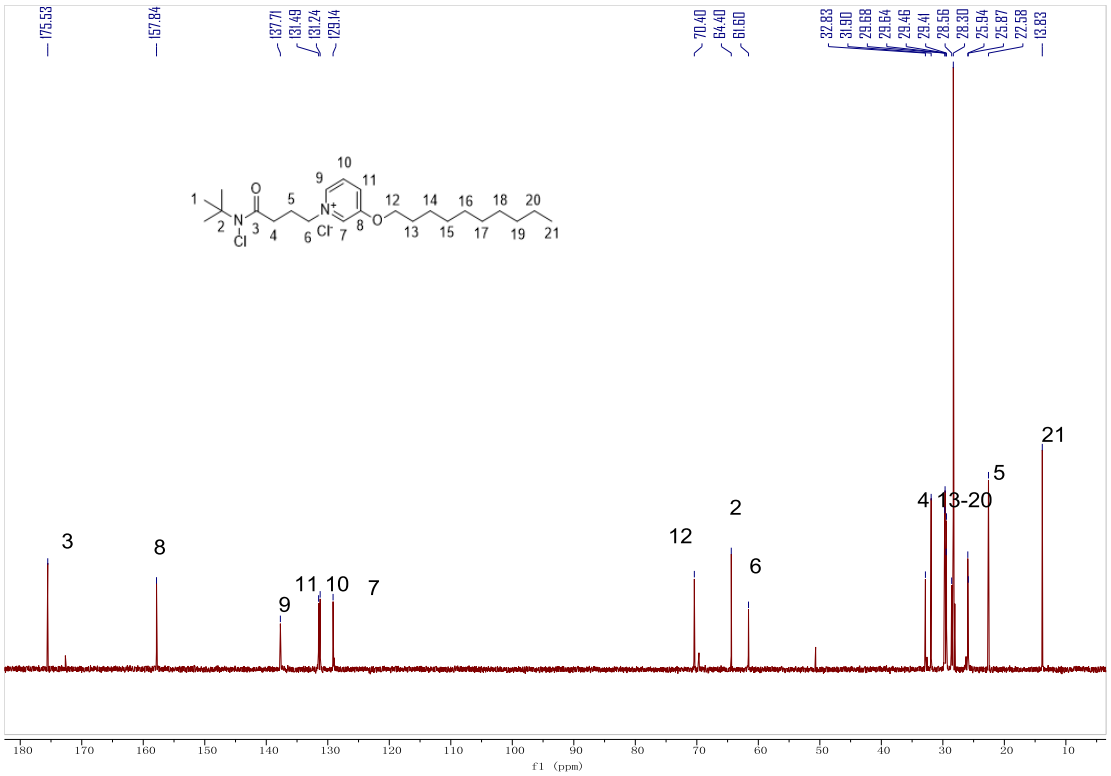
The ^{1}H NMR spectrum of compound **15a**



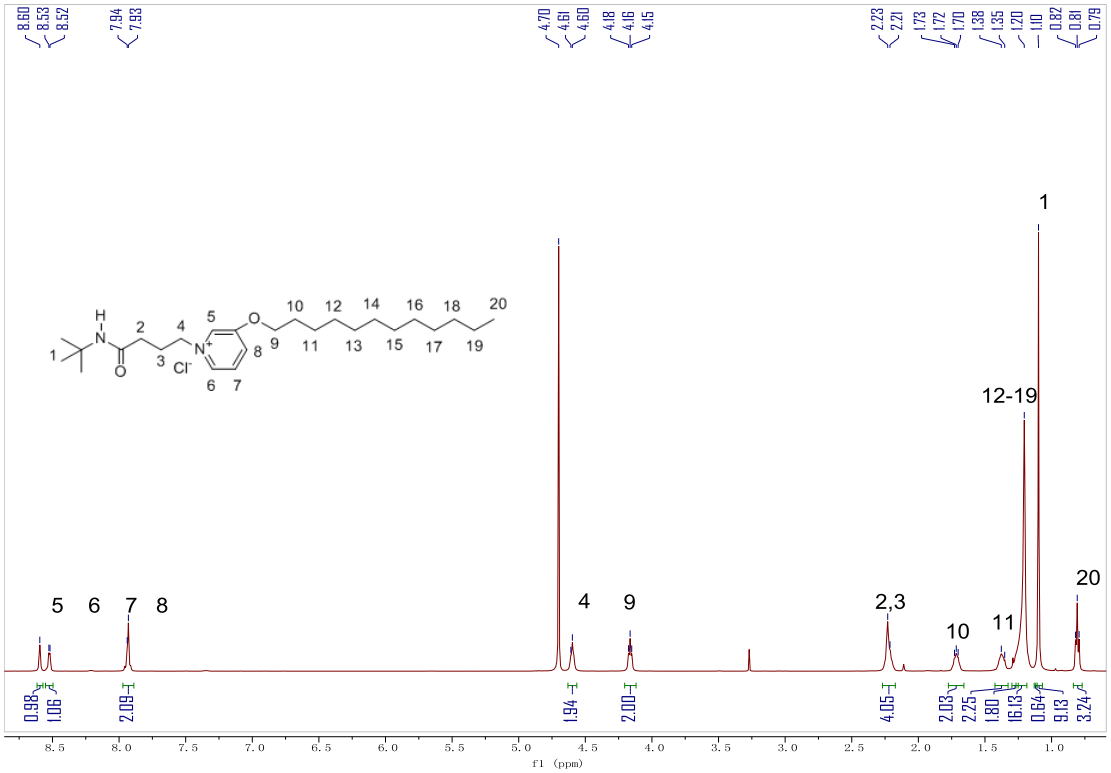
The ^{13}C NMR spectrum of compound **15a**



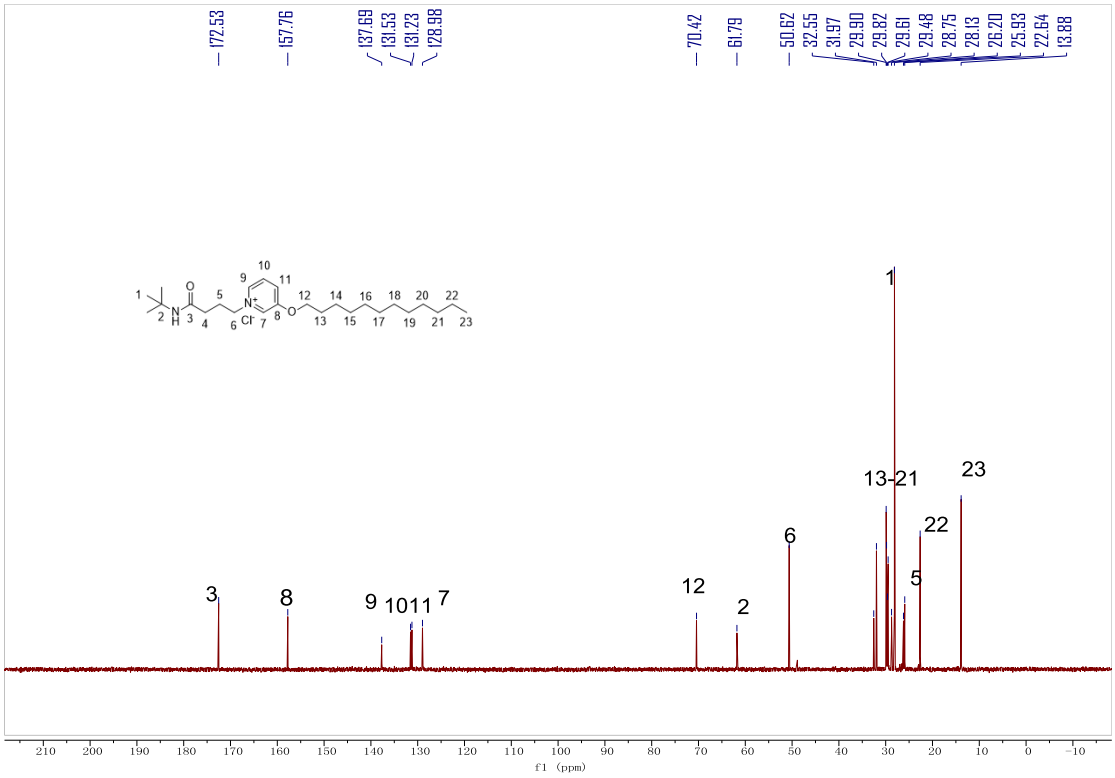
The ^{1}H NMR spectrum of compound **15**



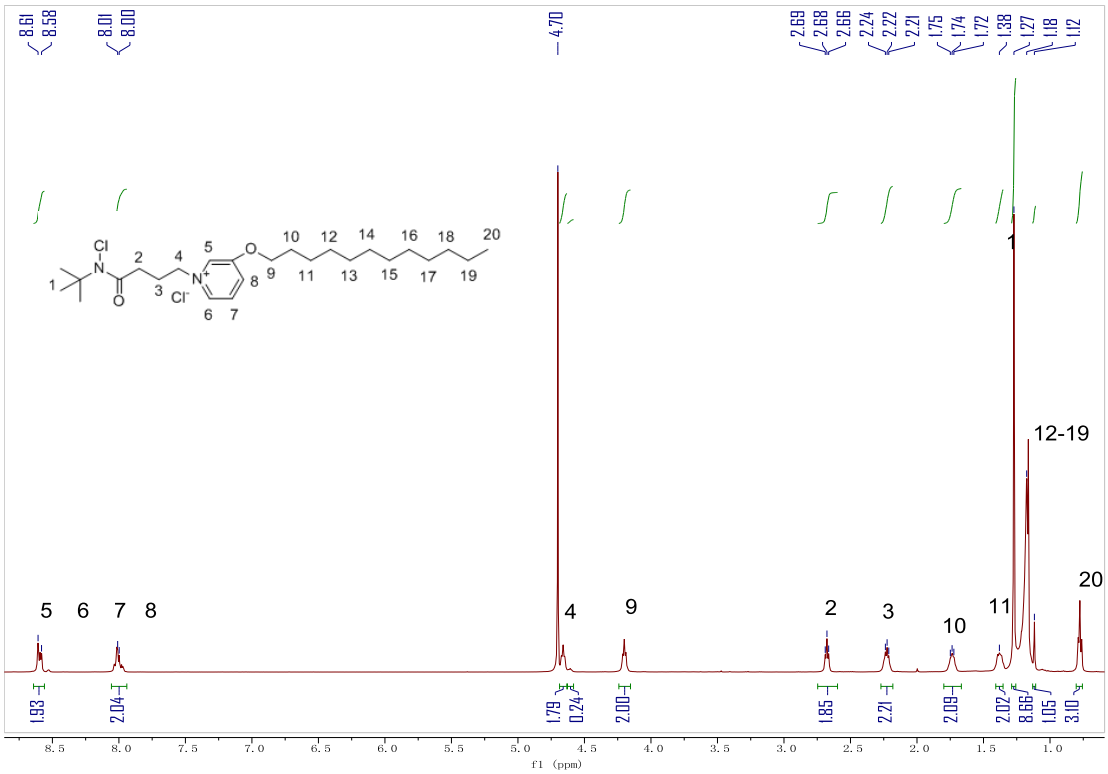
The ^{13}C NMR spectrum of compound **15**



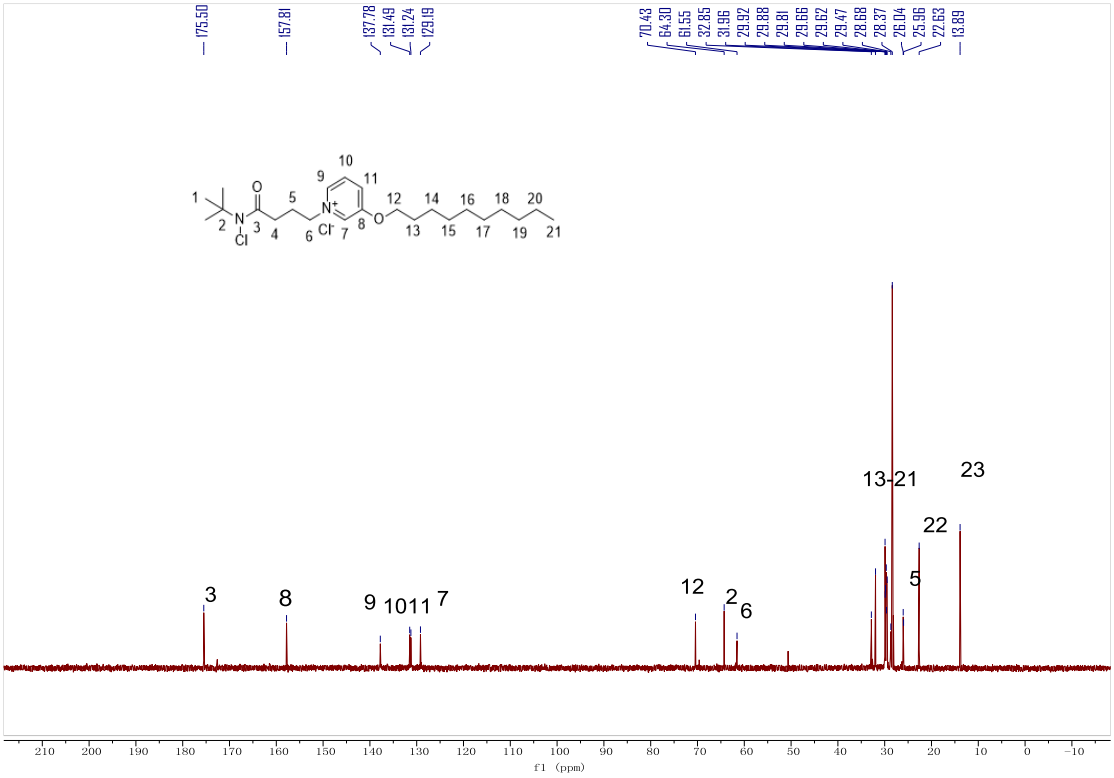
The ^{1}H NMR spectrum of compound **16a**



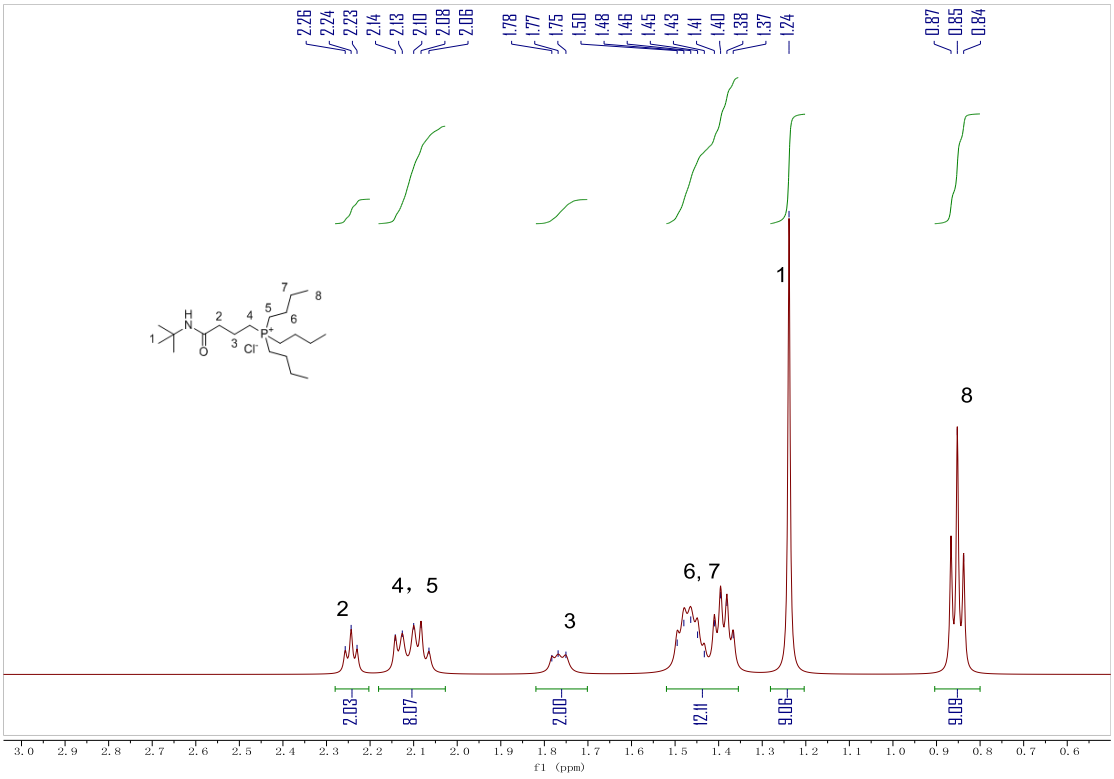
The ^{13}C NMR spectrum of compound **16a**



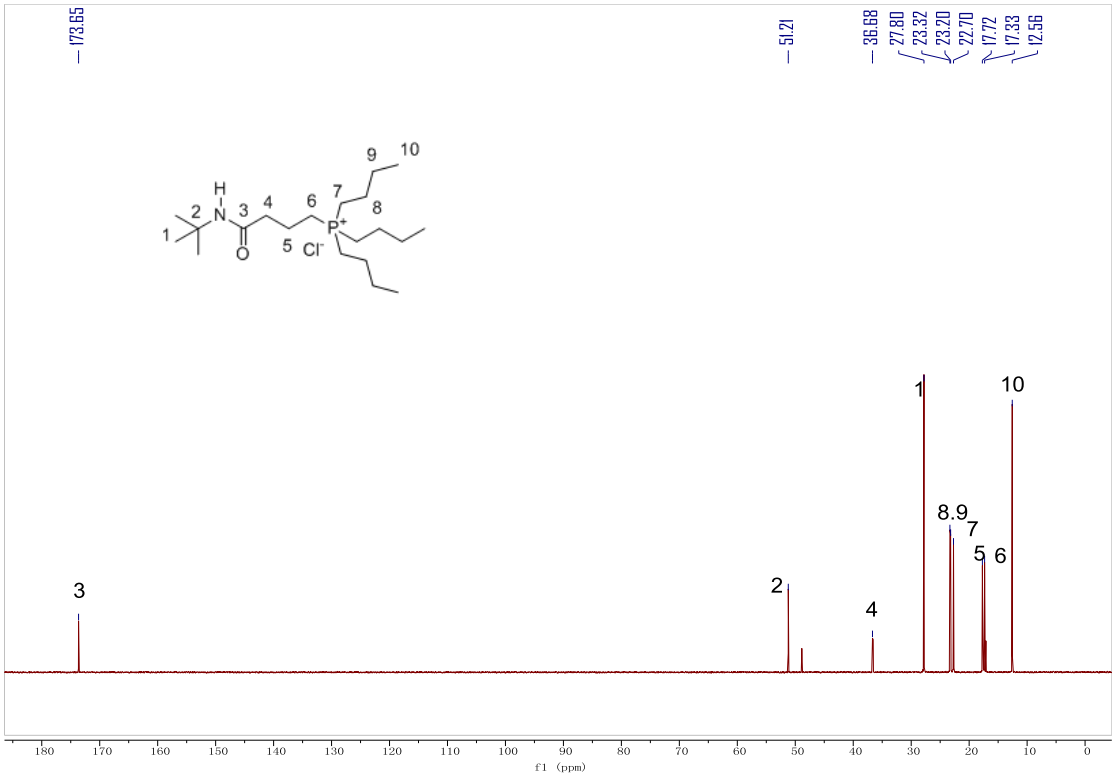
The ^{1}H NMR spectrum of compound **16**



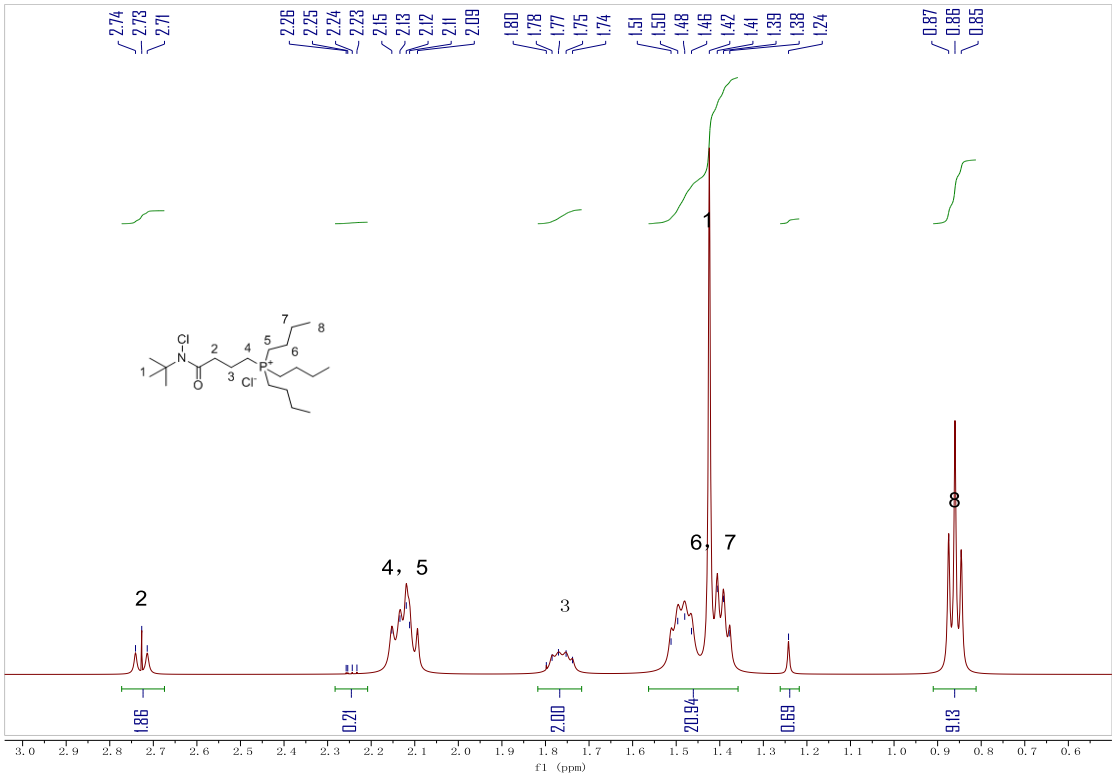
The ^{13}C NMR spectrum of compound **16**



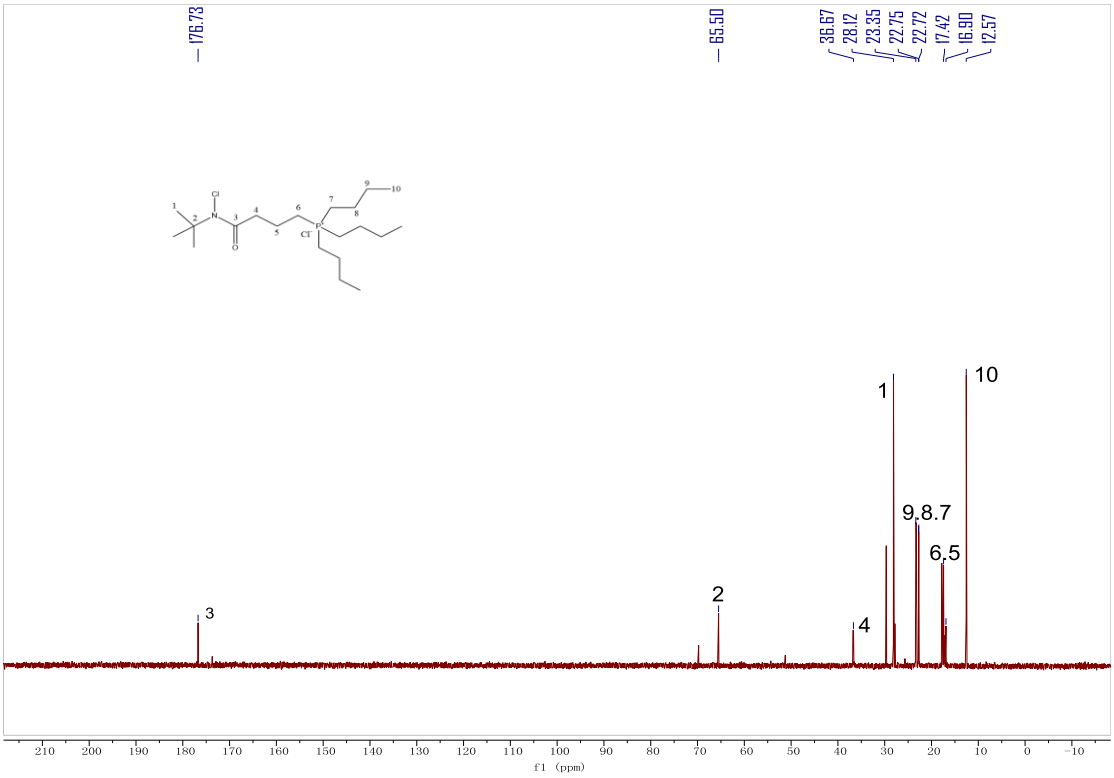
The ^{1}H NMR spectrum of compound **17a**



The ^{13}C NMR spectrum of compound **17a**



The ^{1}H NMR spectrum of compound **17**



The ^{13}C NMR spectrum of compound **17**