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Supplementary Material

Long-chained pyridinium *N*-Chloramines: synthesis and remarkable biocidal efficacies for antibacterial application

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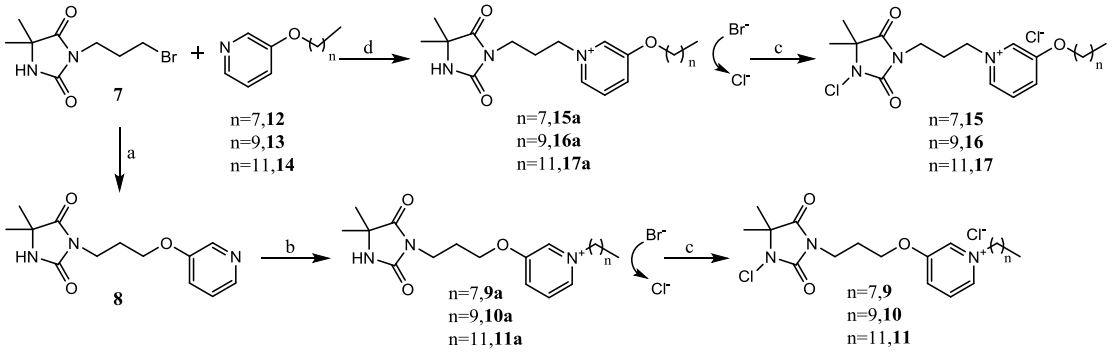
1 Reagents and materials

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

DMH-bromide **7**, pyridinium *N*-chloramine **2** and its precursor **2a** were prepared according to our previously reports, respectively.[1-5] In addition, *t*-butyl hypochlorite, the chlorination agent used in this work, was also synthesized as described in the literatures.[1] The obtained NMR data of all published compounds are identical with those found in previous literatures.

2 Synthesis of long-chained pyridinium *N*-chloramines



Scheme 1. Chemical synthesis of **9-11** and **15-17**: (a) K_2CO_3, 3-hydroxypyridine, reflux; (b) $Br(CH_2)_nCH_3$, reflux, ion-exchange (Amberlite R IRA-900, Cl^-); (c) *t*-BuOCl, H_2O/BuOH, rt; (d) reflux, ion-exchange (Amberlite R IRA-900, Cl^-).

2.1 General synthesis of 8

To a solution of 3-hydroxypridine (1.5 g, 16.0 mmol) in CH_3CN (30 mL) was added potassium carbonate (6.6 g, 48.0 mmol), and then the mixture was heated to reflux for 1 h. Afterward, DMH-bromide **7** (5.0 g, 20.0 mmol) was added to the suspension, and the mixture was refluxed for 1 h. The inorganic salts were filtered and the filtrate was concentrated under reduced pressure to provide the crude product. Further purification was performed on chromatography column with MeOH/CH_2Cl_2 (1:10, v/v) to afford **8** as white solid.

DMH-pyridine ether **8** (2.9 g, 58.6%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.23 (s, 1H), 8.14-8.13 (m, 1H), 7.14-7.13 (m, 2H), 6.27 (s, 1H), 3.99 (t, *J* = 6.0 Hz, 2H), 3.66 (t, *J* = 6.8 Hz, 2H), 2.11-2.05 (m, 2H), 1.35 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 177.1, 156.0, 154.9, 142.3, 138.1, 123.8, 121.2, 66.1, 58.7, 36.1, 27.9, 25.1; HRMS calcd. for $C_{13}H_{17}N_3O_3$ $[M+H]^+$: 264.1270, found: 264.1343.

2.2 General synthesis of 9a-11a, 18a and 19a

To a solution of **8** (1.2 g, 4.4 mmol) in 20 mL CH_3CN was added bromooctane (0.9 g, 4.6 mmol) and then the mixture was heated to reflux overnight. After the solvent was removed under reduced

pressure, the residue was purified by chromatography column with MeOH/CH_2Cl_2 (2:9, v/v) to give pyridinium salt (Br^- form) in quantitative yield. The bromo form salt was dissolved in minimum distilled water and passed through anion exchange resin (Amberlite IRA-900, Cl^-). All the corresponding fractions were collected and concentrated to afford the final pyridinium salt (Cl^- form).

Pyridinium salt **9a** (1.5 g, 74.6%). ^{1}H NMR (500 MHz, D_2O) δ 4.56-4.49 (m, 2H), 1.24-1.10 (m, 10H), 0.73-0.72 (m, 3H); ^{13}C NMR (126 MHz, D_2O) δ 180.7, 157.9, 157.4, 136.9, 131.9, 130.9, 128.6, 67.9, 59.1, 48.9, 35.6, 30.9, 30.5, 28.2, 28.0, 26.7, 25.1, 23.5, 21.9, 13.4. HRMS calcd. for $C_{21}H_{34}BrN_3O_3$ [M-Br]$^+$: 376.2597, found: 376.2600.

Pyridinium salt **10a** (2.2 g, 78.3%). ^{1}H NMR (500 MHz, D_2O) δ 8.11-8.10 (m, 2H), 4.27-4.16 (m, 2H), 1.24-1.01 (m, 14H); ^{13}C NMR (126 MHz, D_2O) δ 179.9, 157. 9, 157.1, 137.1, 132.2, 130.9, 128.9, 68.3, 62.1, 58.9, 48.9, 35.51, 31.7, 31.1, 29.4, 29.2, 29.1, 28.9, 26.9, 25. 7, 23.8, 22.4.

Pyridinium salt **11a** (2.1 g, 76.4%). ^{1}H NMR (500 MHz, D_2O) δ 8.61-8.56 (m, 2H), 8.13-8.11 (m, *2*H), 8.04-7.99 (m, 1H), 4.68-4.61 (m, 2H), 4.22 (s, 2H), 3.60 (t, *J* = 6.1 Hz, 2H), 2.10-2.04 (m, 2H), 1.94 (s, 2H), 1.30 (s, 6H), 1.30-1.02 (m, 21H), 0.64 (t, *J* = 6.4 Hz, 3H); ^{13}C NMR (126 MHz, D_2O) δ 179.7, 157.9, 157.1, 137.1, 132.3, 130.8, 129.1, 68.2, 62.1, 58.9, 35.4, 31.8, 31.1, 29.6, 29.6, 29.6, 29.4, 29.2, 29.1, 27.1, 25.8, 23.8, 22.5, 13.8.

Pyridinium salt **18a** (1.6 g, 74.8%). ^{1}H NMR (500 MHz, D_2O) δ 8.61-8.56 (m, 2H), 8.13-8.11 (m, *2*H), 8.04-7.99 (m, 1H), 4.68-4.61 (m, 2H), 4.22 (s, 2H), 3.60 (t, *J* = 6.1 Hz, 2H), 2.10-2.04 (m, 2H), 1.94 (s, 2H), 1.30 (s, 6H), 1.30-1.02 (m, 23H), 0.64 (t, *J* = 6.4 Hz, 3H).

Pyridinium salt **19a** (1.25 g, 75.7%). ^{1}H NMR (500 MHz, D_2O) δ 8.44 (s, 1H), 8.33-8.34 (m, 1H), 8.00-7.98 (m, 1H), 7.87-7.88 (m, 1H), 4.30 (s, 3H), 4.18 (t, *J* = 5.4 Hz, 2H), 3.65 (t, *J* = 5.5 Hz, 2H), 2.13-2.06 (m, 2H), 1.33 (s, 6H); ^{13}C NMR (126 MHz, D_2O) δ 180.8, 157.7, 157.5, 137.7, 132.8, 130.7, 128.3, 67.9, 59.1, 48.3, 35.7, 26.7, 23.4. HRMS calcd. for $C_{14}H_{20}ClN_3O_3$ [M-Cl]$^+$: 278.1507, found: 278.1505.

2.3 General synthesis of 9-11 and 19

To a solution of **9a-11a** (0.9 g, 2.1 mmol) in 7.7 mL H_2O/*t*-butanol (1:4) was added *t*-butyl hypochlorite (0.7 g, 6.2 mmol, 0.7 mL). The mixture was then sealed and stirred in dark for 24 h. After removing excess *t*-butyl hypochlorite and the solvent, the final pyridinium *N*-chloramines were obtained in quantitative yield.

Pyridinium *N*-chloramine **9**. ^{1}H NMR (500 MHz, D_2O) δ 8.46 (s, 1H), 8.41 (m,1H), 8.01 (m, 1H), 7.90 (m, 5.9 Hz, 1H), 4.51 (t, *J* = 7.1 Hz, 2H), 4.19 (t, *J* = 5.5 Hz, 2H), 3.73 (t, *J* = 6.3 Hz, 2H), 2.11-2.09(m, 2H), 1.93-1.91(m, 2H), 1.38 (s, 6H), 1.26-1.09 (m, 11H), 0.74 (t, *J* = 6.9 Hz, 3H); ^{13}C NMR (126 MHz, D_2O) δ 180.7, 157.9, 157.4, 136.9, 131.9, 130.9, 128.6, 67.9, 62.3, 59.1, 35.6, 30.9, 30.5, 28.2, 28.0, 26.7, 25.1, 23.5, 21.9, 13.4.

Pyridinium *N*-chloramine **10**. ^{1}H NMR (500 MHz, D_2O) δ 8.52-8.50 (m, 2H), 8.11-8.09 (m, 1H), 8.02-7.95 (m, 1H), 4.59 (t, *J* = 6.2 Hz, 3H), 4.23 (s, 1H), 3.70 (t, *J* = 6.2 Hz, 2H), 2.12-2.10 (m, 2H), 1.92 (s, 2H), 1.33 (s, 4H), 1.16 (d, *J* = 9.5 Hz, 5H), 1.09 (t, *J* = 7.1 Hz, 6H), 1.02 (s, 5H), 0.62 (t, *J* = 6.7 Hz, 2H); ^{13}C NMR (126 MHz, D_2O) δ 175.7, 157.8, 155.2, 137.1, 132.3, 130.8, 129.1, 68.3,

65.9, 62.1, 37.1, 31.7, 30.9, 29.4, 29.2, 29.1, 28.9, 26.8, 25.6, 22.4, 21.4, 13.7.

Pyridinium *N*-chloramine **11**. ^{1}H NMR (500 MHz, D_2O) δ 8.59-8.58 (m, 1H), 8.55 (s, 1H), 8.15-8.13 (m, 1H), 8.04-8.01 (m, 1H), 4.64 (t, *J* = 6.3 Hz, 2H), 4.25 (t, *J* = 4.9 Hz, 2H), 3.71 (t, *J* = 6.1 Hz, 2H), 2.12 (s, 2H), 1.94 (s, 2H), 1.34 (s, 6H), 1.21-1.02 (m, 21H), 0.63 (t, *J* = 6.5 Hz, 3H); ^{13}C NMR (126 MHz, D_2O) δ 175.4, 157.8, 155.1, 137.2, 132.4, 130.9, 129.1, 68.3, 65.9, 62.1, 37.1, 31.8, 31.00, 29.7, 29.6, 29.4,.3, 29.2, 26.8, 22.5, 21.5, 13.7.

Pyridinium *N*-chloramine **19**. ^{1}H NMR (500 MHz, D_2O) δ 8.43 (s, 1H), 8.35-8.34 (m, 1H), 8.00-7.98 (m, 1H), 7.90-7.85 (m, 1H), 4.30 (s, 4H), 4.19 (t, *J* = 5.5 Hz, 2H), 3.74 (t, *J* = 6.3 Hz, 2H), 2.15-2.09 (m, 2H), 1.40 (s, 6H);^{13}C NMR (126 MHz, D_2O) δ 177.0, 157.6, 155.8, 137.8, 132.8, 130.7, 128.3, 67.9, 66.2, 48.4, 37.0, 26.6, 20.9. HRMS calcd. for $C_{14}H_{19}Cl_2N_3O_3$ $[M\text{-}Cl]^+$ 312.1121, found: 312.1115.

2.4 General synthesis of 12-14

To a solution of 3-hydroxypridine (4.4 g, 46.0 mmol) in 15 mL *N,N'*-dimethyl formamide was added potassium hydroxide (5.1 g, 92.0 mmol), and the mixture was heated to react for 1 h. Afterward, bromooctane (7.9 mL, 46.0 mmol) was added to the suspension, and the mixture was reacted for 2.5 h. The organic phase was added 30 mL $CH_3COOC_2H_5$ and washed with saturated aqueous of NH_4Cl. After being dried with $MgSO_4$, the reaction mixture was concentrated under reduced pressure and the crude product was purified by chromatography column to give the ether in quantitative yield.

Pyridine-octyl ether **12** (4.1 g, 42.9%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.31 (s, 1H), 8.21 (s, 1H), 7.20 (d, *J* = 26.4 Hz, 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, CDCl3) 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.

Pyridine-decyl ether **13** (5.4 g, 50.1%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.31 (s, 1H), 8.20 (s, 1H), 7.22 (d, *J* = 4.3 Hz, 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, 13H), 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.

Pyridine-dodecyl ether **14** (5.4 g, 45.9%). ^{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, 17H), 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, 29.4, 29.2, 26.0, 22.7, 14.1.

2.5 General synthesis of 15a-17a

To a solution of **7** (1.2 g, 5.8 mmol) in 20 mL CH_3CN was added to **12** (1.6 g, 6.4 mmol) and then the mixture was heated to reflux overnight. After the solvent was removed under reduced pressure, the residue was purified by chromatography column with $MeOH/CH_2Cl_2$ (3:20, v/v) to give pyridinium salt (Br^- form) in quantitative yield. The bromo form salt was dissolved in minimum distilled water and passed through anion exchange resin (Amberlite IRA-900, Cl^-). All the corresponding fractions were collected and concentrated to afford the final pyridinium salt (Cl^- form).

Pyridinium salt **15a** (2.0 g, 73.7%).^{1}H NMR (500 MHz, D_2O) δ 8.69 (s, 1H), 8.00 (s, 1H), 4.61 (t, *J* = 7.5 Hz, 2H), 4.20 (t, *J* = 5.0 Hz, 2H), 3.47 (t, *J* = 6.5 Hz, 2H), 2.29 (t, J = 6.4 Hz, 2H), 1.92-1.63 (m, 2H), 1.46-1.07 (m, 16H), 0.75 (s, 3H); ^{13}C NMR (126 MHz, D_2O) δ 180.1, 158.1, 156.8,

137.3, 131.8, 129.0, 70.6, 59.4, 59.1, 59.1, 34.9, 31.6, 29.3, 29.0, 28.4, 25.5, 23.6, 22.4, 13.8; HRMS calcd. for $C_{21}H_{34}N_3O_3$[M-Cl]$^+$: 376.2609, found: 376.2600.

Pyridinium salt **16a** (2.1 g, 83.8%).^{1}H NMR (500 MHz, D2O) δ 8.57 (s, 1H), 8.01 (d, J = 3.1 Hz, 2H), 4.63 (t, J = 6.8 Hz, 2H), 4.19 (t, J = 6.4 Hz, 2H), 3.43 (t, J = 6.5 Hz, 2H), 2.28 (t, J = 6.8 Hz, 2H), 1.72 (t, J = 7.7 Hz, 2H), 1.48-1.30 (m, 8H), 1.25-1.12 (m, 10H), 0.78 (t, J = 6.7 Hz, 3H); ^{13}C NMR (126 MHz, D_2O) δ 179.9, 158.0, 156.7, 137.6, 137.6, 131.6, 129.1, 70.6, 59.4, 59.0, 31.9, 29.7, 29.6, 29.4, 29.4, 29.3, 28.7, 23.7, 22.6, 13.9; HRMS calcd. for $C_{23}H_{38}N_3O_3$[M-Cl]$^+$: 404.2927, found: 404.2913.

Pyridinium salt **17a** (2.26 g, 79.5%).^{1}H NMR (500 MHz, D_2O) δ 8.73 (d, J = 9.5 Hz, 1H), 8.56 (s, 1H), 8.15-7.84 (m, 2H), 4.63 (d, J = 6.7 Hz, 2H), 4.20 (t, J = 5.9 Hz, 2H), 3.44 (t, J = 6.4 Hz, 2H), 2.28 (m, 2H), 1.72 (m, 2H), 1.54-1.30 (m, 8H), 1.33-0.93 (m, 16H), 0.77 (t, J = 9.3 Hz, 3H); ^{13}C NMR (126 MHz, D_2O) δ 179.8, 157.9, 156.7, 137.6, 131.7, 131.6, 129.1, 70.6, 59.4, 59.0, 34.8, 31.9, 29.9, 29.8, 29.8, 29.7, 29.6, 29.4, 28.7, 25.8, 23.8, 22.6, 13.9; HRMS calcd. for $C_{25}H_{42}N_3O_3$[M-Cl]$^+$: 432.3231, found: 432.3226.

2.6 General synthesis of 15-17

To a solution of **15a-17a** (0.7 g, 1.8 mmol) in 6.2 mL H_2O/*t*-butanol (1:4) was added *t*-butyl hypochlorite (0.6 g, 5.5 mmol, 0.7 mL). The mixture was then sealed and stirred in dark for 24 h. After removing excess *t*-butyl hypochlorite and the solvent, the final pyridinium *N*-chloramines were obtained in quantitative yield.

Pyridinium *N*-chloramine **15**. ^{1}H NMR (500 MHz, D_2O) δ 8.64 (d, *J* = 27.1 Hz, 1H), 8.51 (d, *J* = 39.7 Hz, 1H), 8.06 (d, *J* = 8.1 Hz, 1H), 7.98 (q, *J* = 10.2, 9.6 Hz, 1H), 4.63 (t, *J* = 11.8 Hz, 2H), 4.20 (q, *J* = 6.5 Hz, 2H), 3.57 (t, *J* = 6.3 Hz, 2H), 2.33 (q, *J* = 7.4 Hz, 2H), 1.74 (p, *J* = 6.5 Hz, 2H), 1.44-1.30 (m, 8H), 1.29-1.03 (m, 8H), 0.76 (t, *J* = 6.9 Hz, 3H); ^{13}C NMR (126 MHz, D_2O) δ 176.1, 158.0, 155.1, 137.3, 131.9, 131.5, 129.1, 70.5, 66.2, 66.2, 59.3, 36.2, 31.6, 29.0, 28.4, 25.6, 22.4, 21.2, 21.2, 13.8; HRMS calcd. for $C_{21}H_{33}ClN_3O_3$[M-Cl]$^+$: 410.2204, found: 410.2210.

Pyridinium *N*-chloramine **16**. ^{1}H NMR (500 MHz, D_2O) δ 8.69 (s, 1H), 8.58 (s, 1H), 8.04 (d, *J* = 24.1 Hz, 2H), 4.67 (t, *J* = 6.0 Hz, 2H), 4.21 (t, *J* = 6.0 Hz, 2H), 3.55 (t, *J* = 6.4 Hz, 2H), 2.34 (p, *J* = 6.5 Hz, 2H), 1.74 (d, *J* = 7.2 Hz, 2H), 1.45-1.28 (m, 8H), 1.27-1.16 (m, 14H), 0.77 (t, *J* = 6.9 Hz, 3H); ^{13}C NMR (126 MHz, D_2O) δ 175.8, 157.9, 155.0, 137.5, 131.8, 131.5, 129.3, 70.5, 66.1, 59.3, 36.2, 31.9, 29.7, 29.5, 29.4, 29.1, 28.6, 25.8, 22.6, 21.3, 13.9; HRMS calcd. for $C_{23}H_{37}ClN_3O_3$[M-Cl]$^+$: 438.2514, found: 438.2523.

Pyridinium *N*-chloramine **17**. ^{1}H NMR (500 MHz, D2O) δ 8.70 (s, 1H), 8.58 (s, 1H), 8.03 (d, J = 21.9 Hz, 2H), 4.21 (t, J = 5.7 Hz, 2H), 3.55 (t, J = 6.4 Hz, 2H), 2.51-2.13 (m, 2H), 1.89-1.66 (m, 2H), 1.43-1.32 (m, 8H), 1.19 (m, 16H), 0.80 (t, J = 6.9 Hz, 3H); ^{13}C NMR (126 MHz, D_2O) δ 175.6, 157.9, 154.9, 137.6, 131.8, 131.5, 129.3, 70.5, 66.0, 59.3, 36.2, 32.0, 29.9, 29.8, 29.6, 29.5, 29.1, 28.7, 25.9, 22.7, 21.4, 13.9; HRMS calcd. for $C_{25}H_{41}ClN_3O_3$[M-Cl]$^+$:466.2827, found: 466.2836.

3 Antibacterial test

Bacteria from stocks were cultured in tryptone soya agar (TSA) medium at 37℃ for 18-24 h to obtain logarithmic-phase cultures. Subsequent antimicrobial activity test of *N*-chloramine was also performed as followed. 20 μL of *N*-chloramine solutions (0.28 M stock solution, final concentration of Cl^+ of 20 ppm) were added to 10 mL of bacterial suspension (10^6-10^7 CFU mL^{-1}) in a centrifuge tube and timing of exposure to biocides was started immediately. After contact duration of 5 min

and 10 min, 1 mL bacterial solution was taken out and mixed with 1mL of 0.02 N sodium thiosulfate ($Na_2S_2O_3$) solution to neutralize active chlorine. Then 100 μL of mixed solution was serially diluted and placed on Luria-Bertani plates in triplicate for incubating for 18-24 h at 37℃. The same procedure was also applied for all *N*-chloramines and precursors. The viable bacterial colonies on the plates were counted to report the reduction of bacteria by the formula as followed:

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

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

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

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

4 ^{13}C NMR spectra analysis of compound 15a and 15

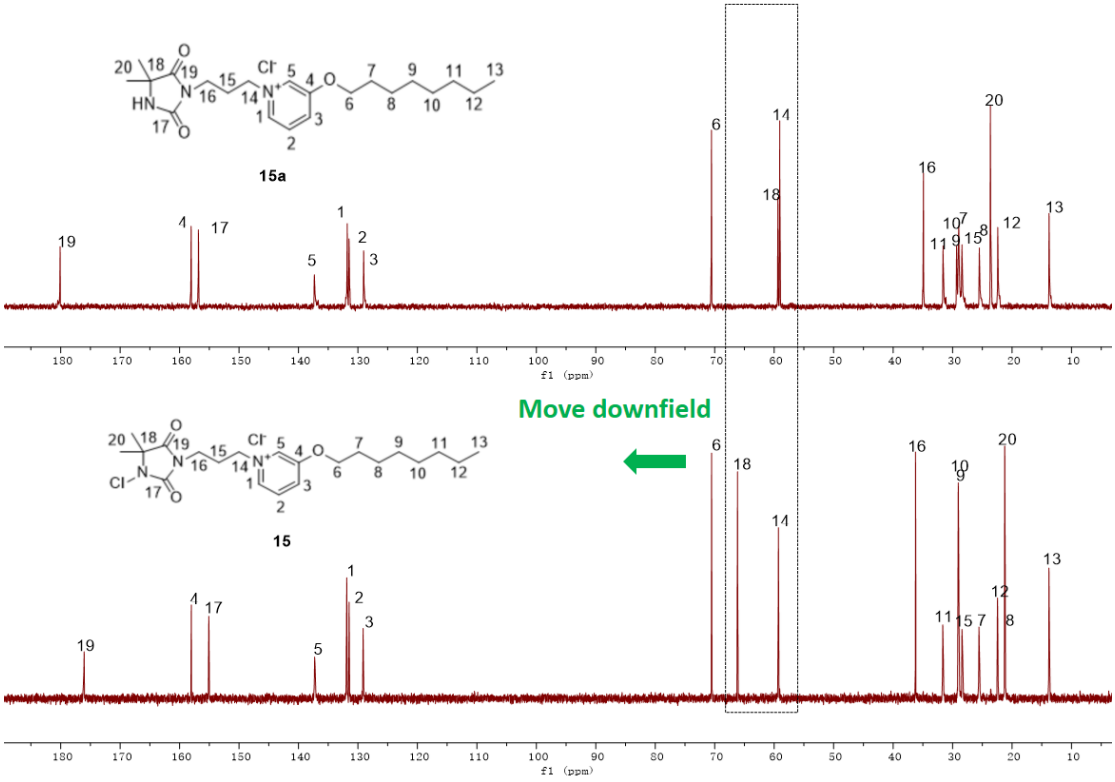


Fig. S1 ^{13}C NMR data of pyridinium *N*-chloramine **15** and its precursor **15a**

5 Bacterial results of synthetic pyridinium *N*-chloramines 2 and 19

Table S1 Bactericidal results of synthetic pyridinium *N*-chloramines **2** and **19**

Bacteria	Synthesis compounds	Active chloramine /ppm	Contact time (min)			
			5		10	
			Percent reduction/%	Log reduction	Percent reduction/%	Log reduction
S. aureus [a]	**2a**	0	0	0	0	0
	2	20	11.68±2.66	0.05±0.01	99.61±0.11	2.41±0.14
	19a	0	0	0	0	0
	19	20	15.84±2.05	0.07±0.01	28.07±2.46	0.14±0.02
E. coli [b]	**2a**	0	0	0	0	0
	2	20	62.72±1.79	0.43±0.02	100	6.75
	19a	0	0	0	0	0
	19	20	25.09±3.23	0.13±0.02	75.27±1.08	0.61±0.02

[a] Inoculum concentration was 9.76 × 10^6 CFU/mL (Colony-forming Units),[b] Inoculum concentration was 5.58 × 10^6 CFU/mL; [c] The final [Cl^+] concentration: 20 ppm for *N*-chloramines and 0 ppm for precursors.

6 NMR spectra analysis of compound 18a, 19a and 19

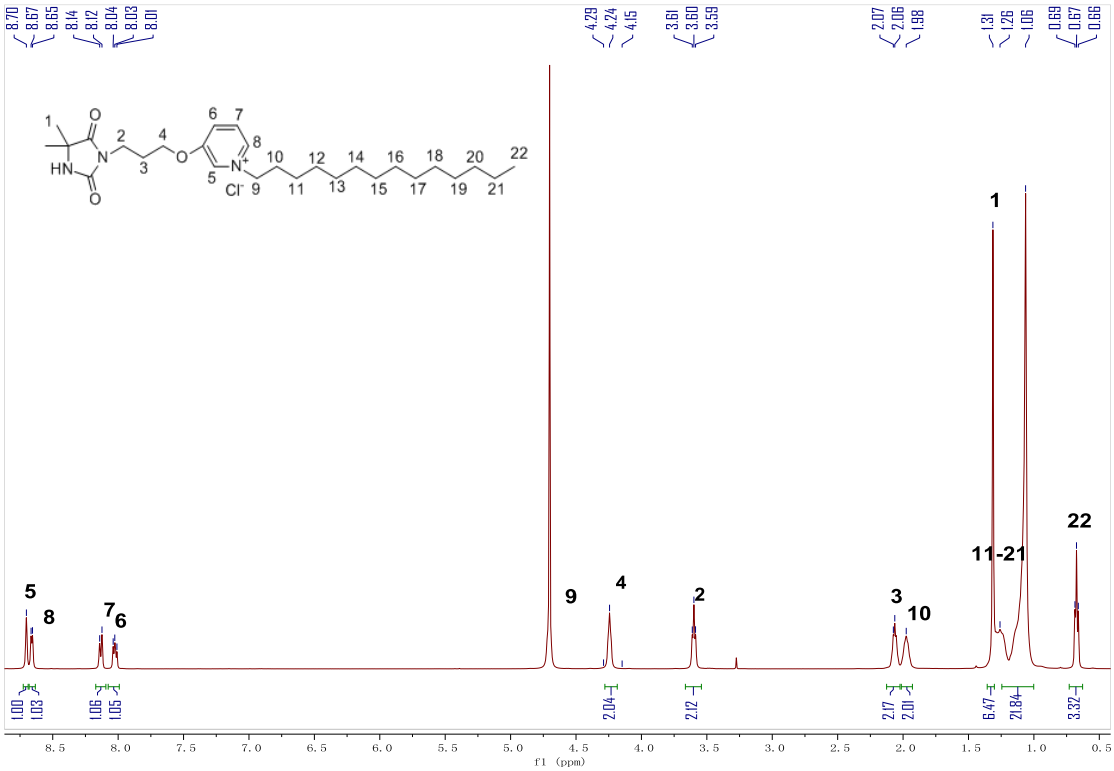


Fig. S2 ^{1}H NMR data of pyridinium *N*-chloramine **18a**

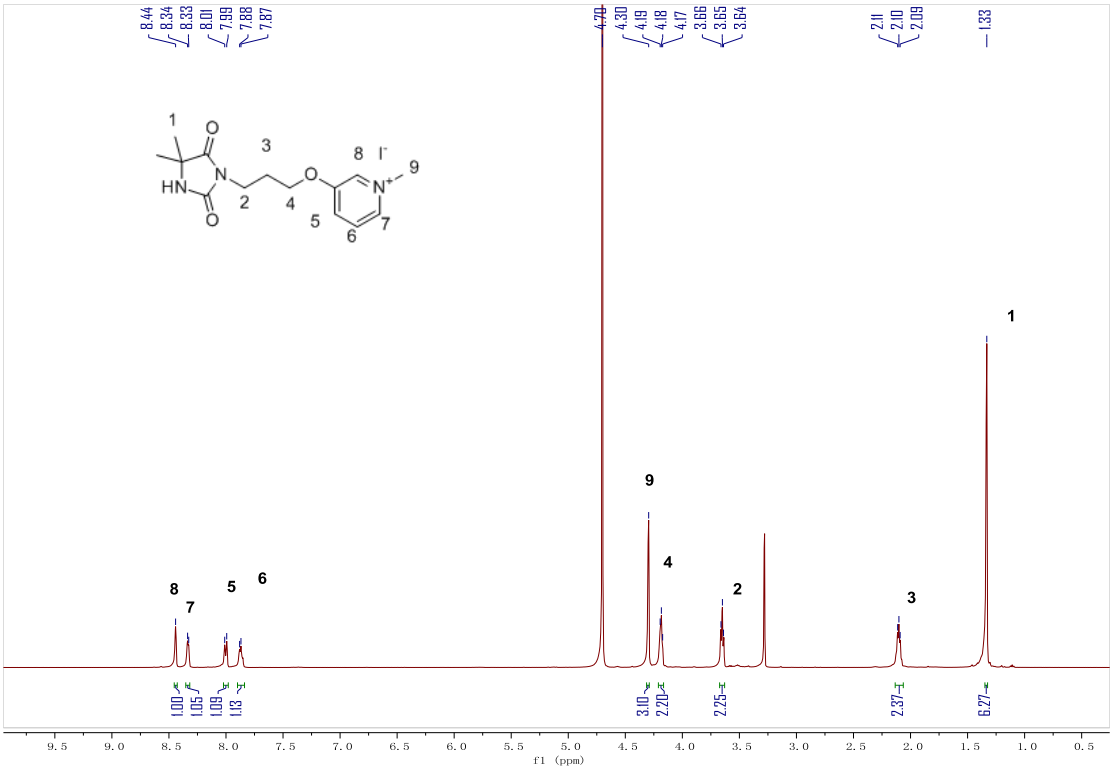


Fig. S3 ^{1}H NMR data of pyridinium *N*-chloramine **19a**

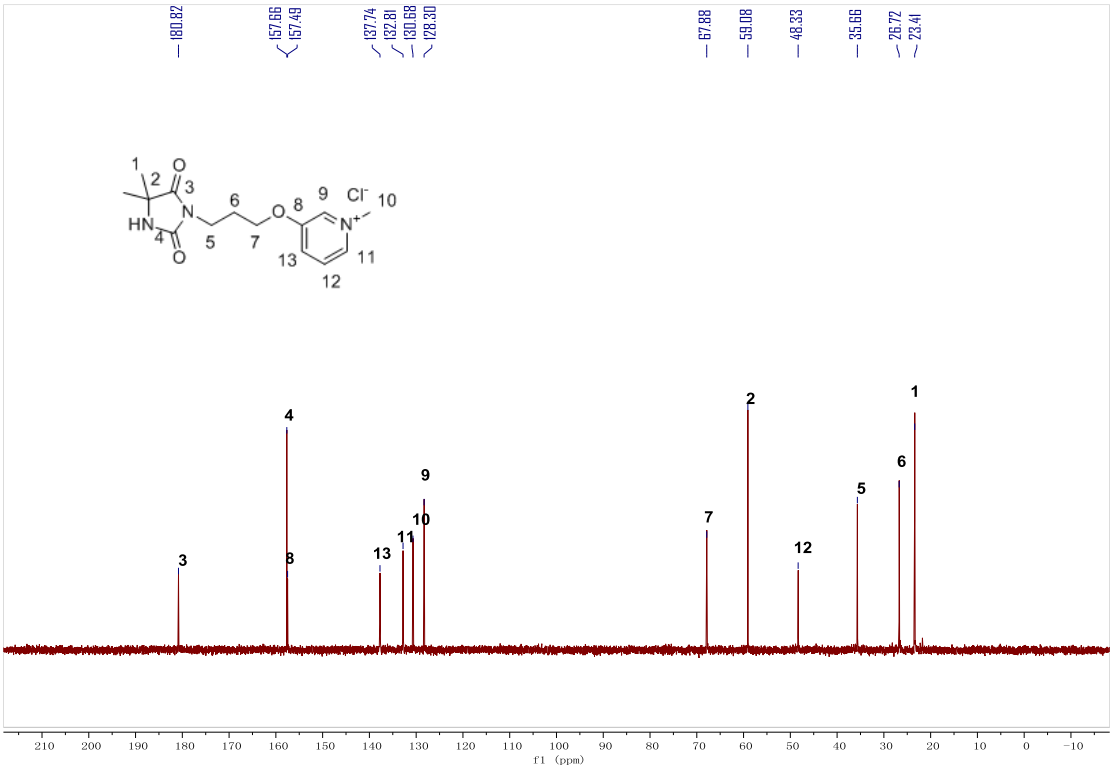


Fig. S4 ^{13}C NMR data of pyridinium *N*-chloramine **19a**

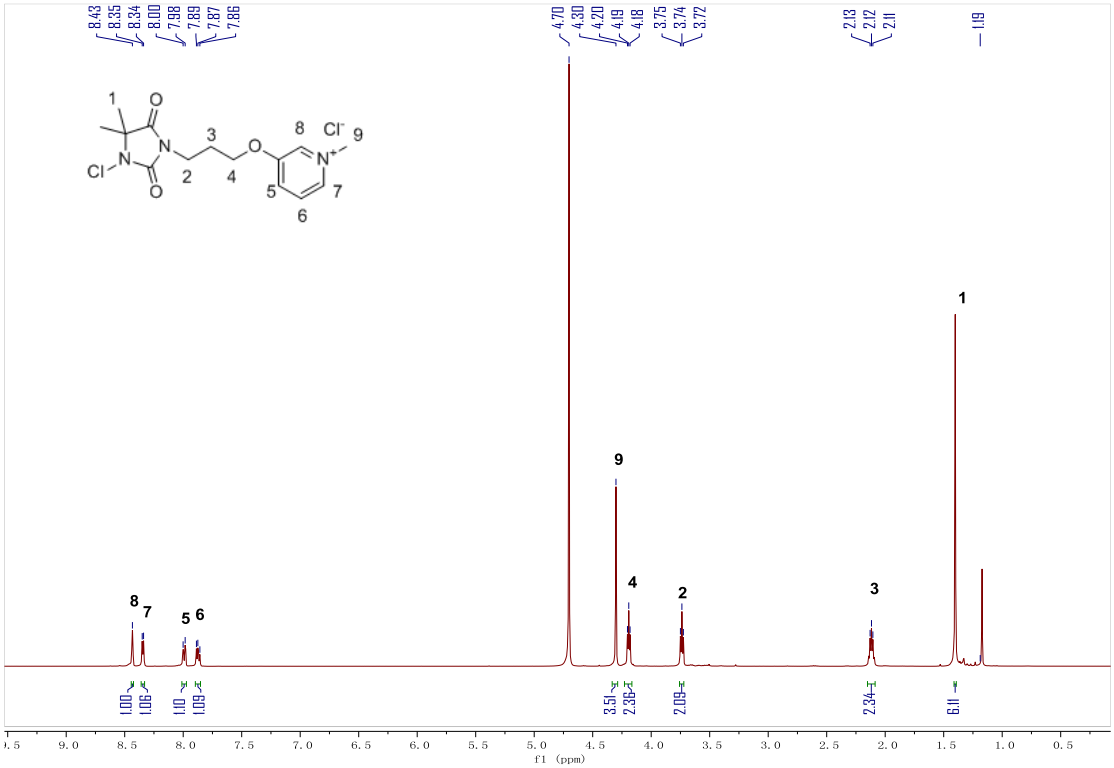


Fig. S5 ^{1}H NMR data of pyridinium *N*-chloramine **19**

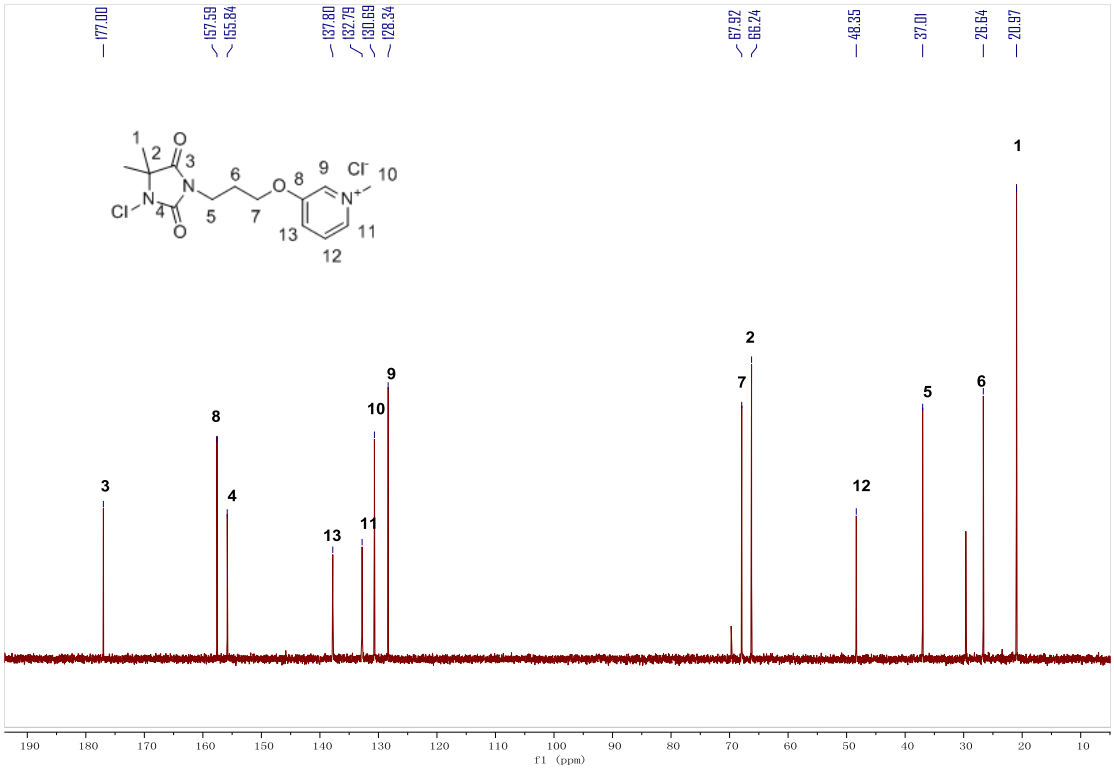


Fig. S6 ^{13}C NMR data of pyridinium *N*-chloramine **19**

7 Reference

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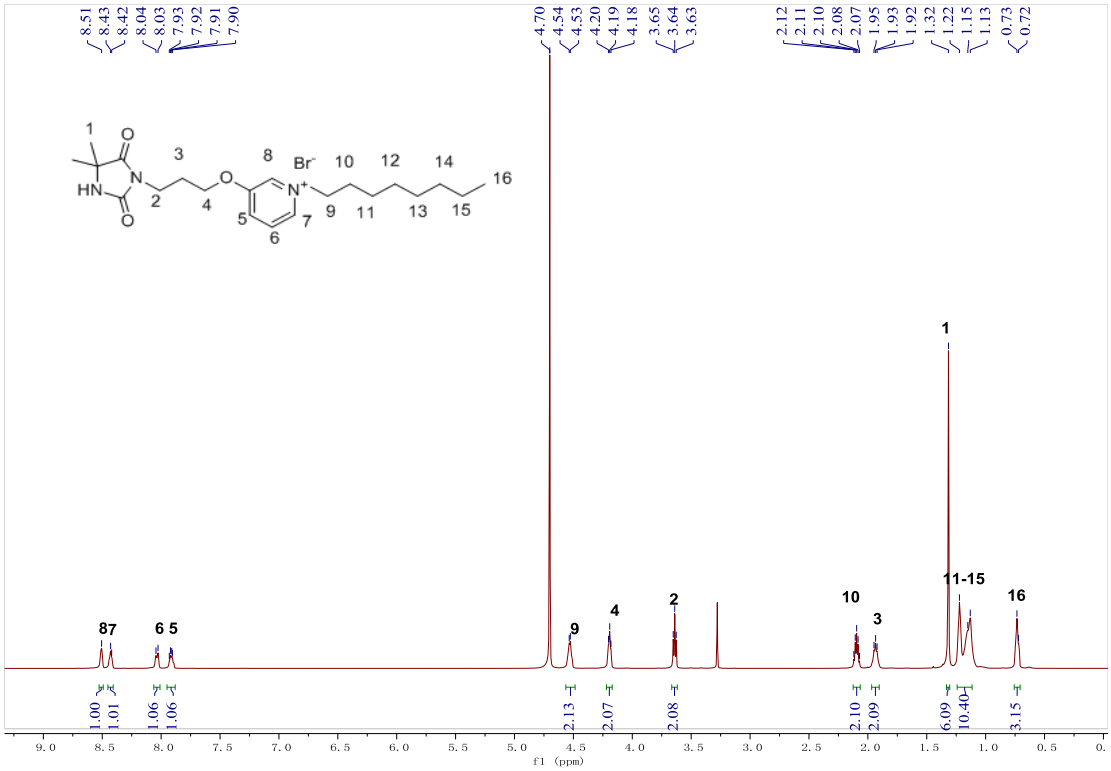
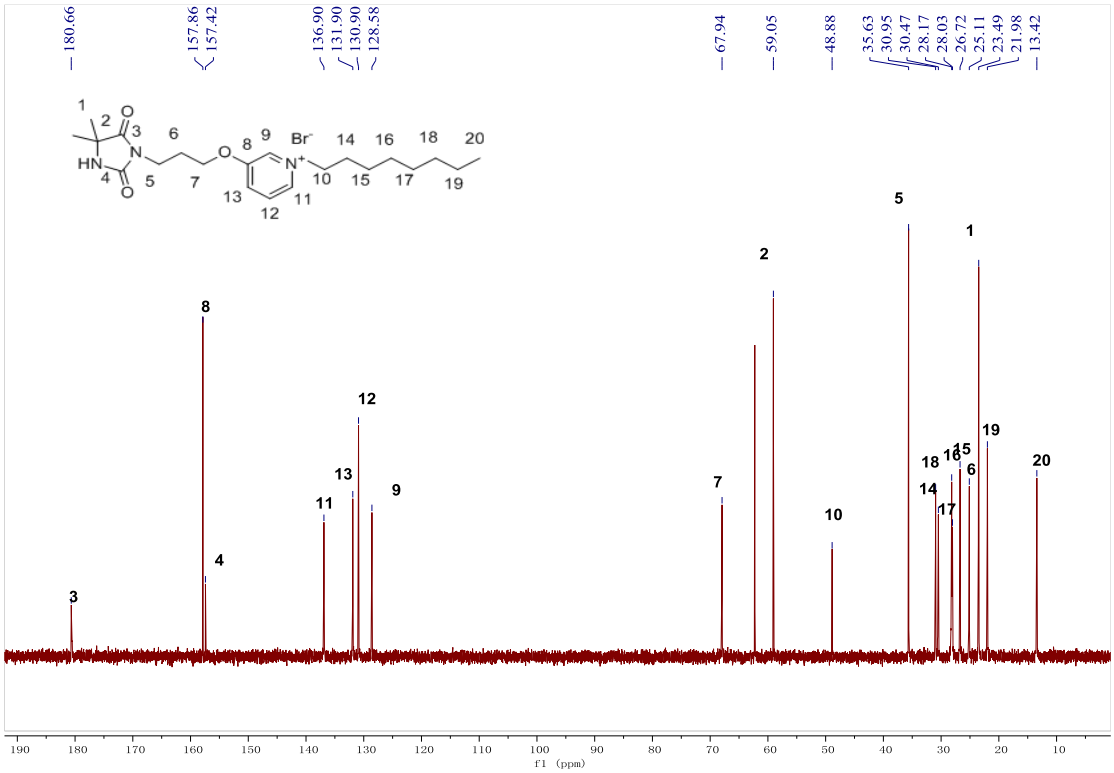
5. Li L., Wang H., Jin Y., Wang P., Jia D., *ChemistrySelect* **2019**, *4*, 11455.

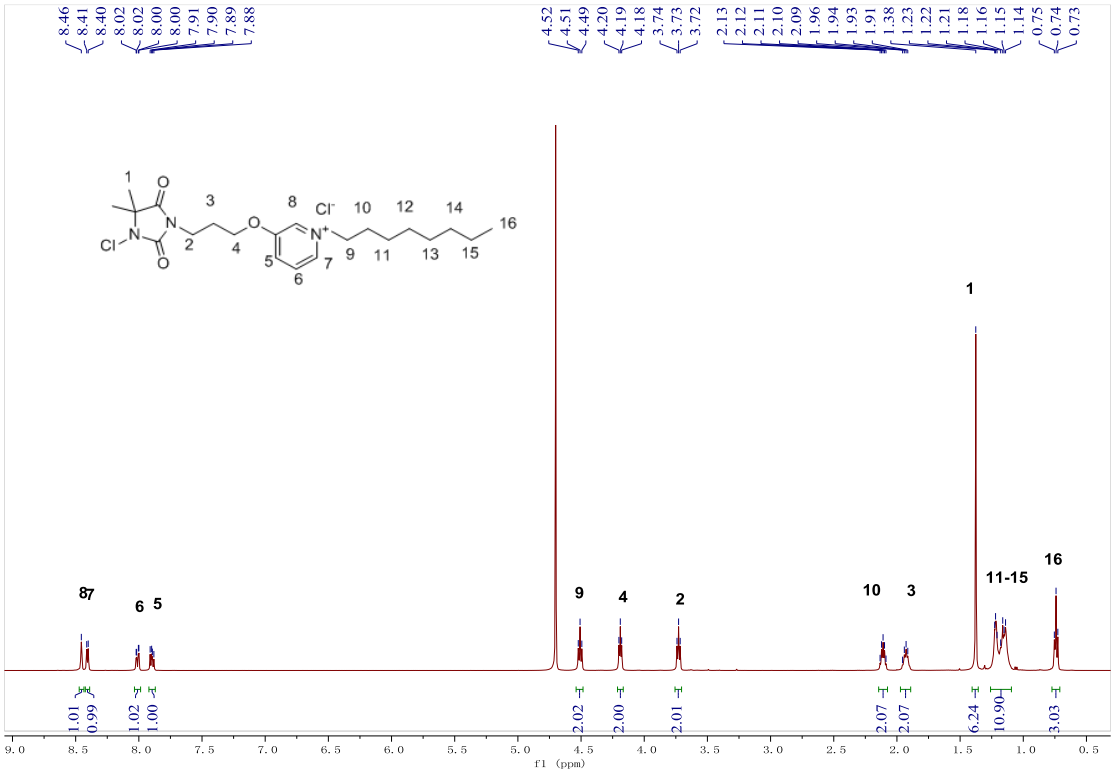
Original NMR spectra data



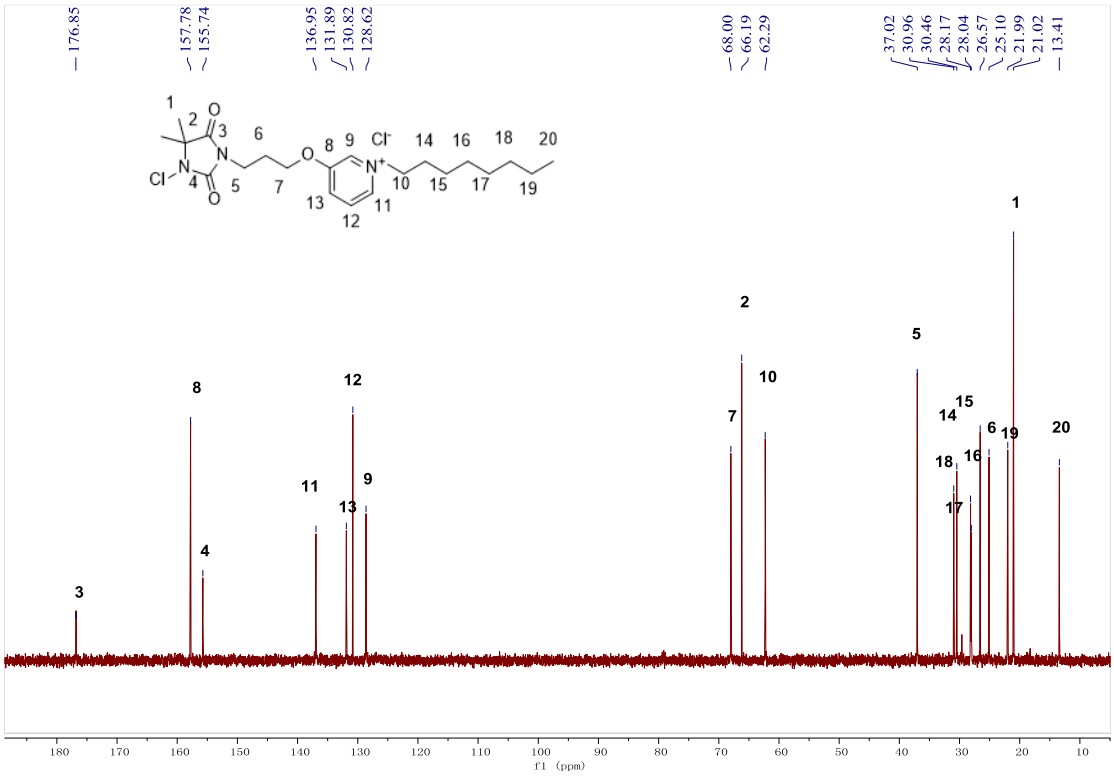
The ^{1}H NMR spectrum of compound **9a**



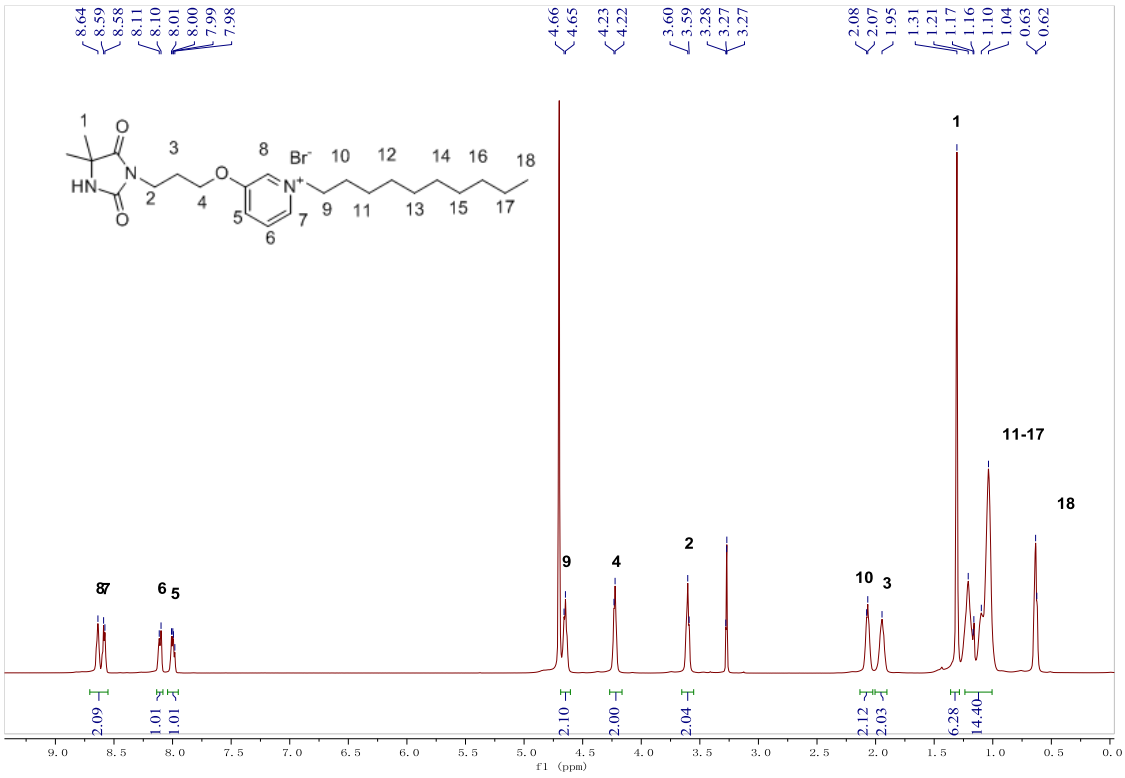
The ^{13}C NMR spectrum of compound **9a**



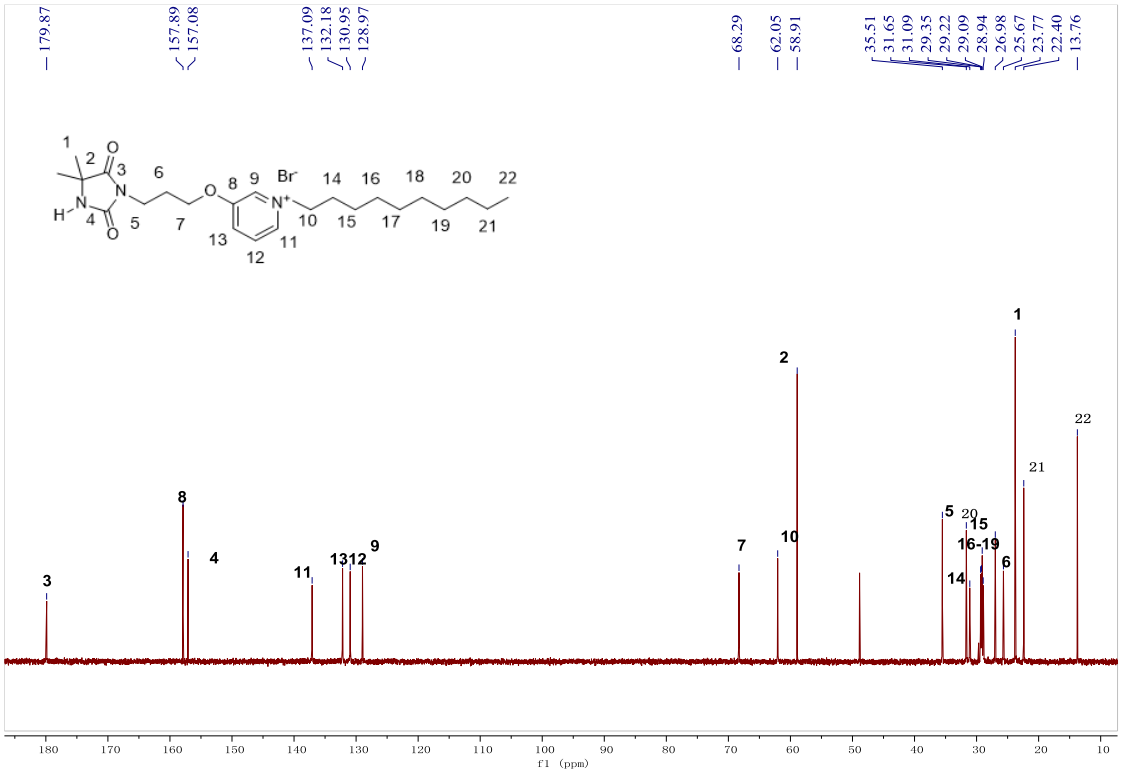
The ^{1}H NMR spectrum of compound **9**



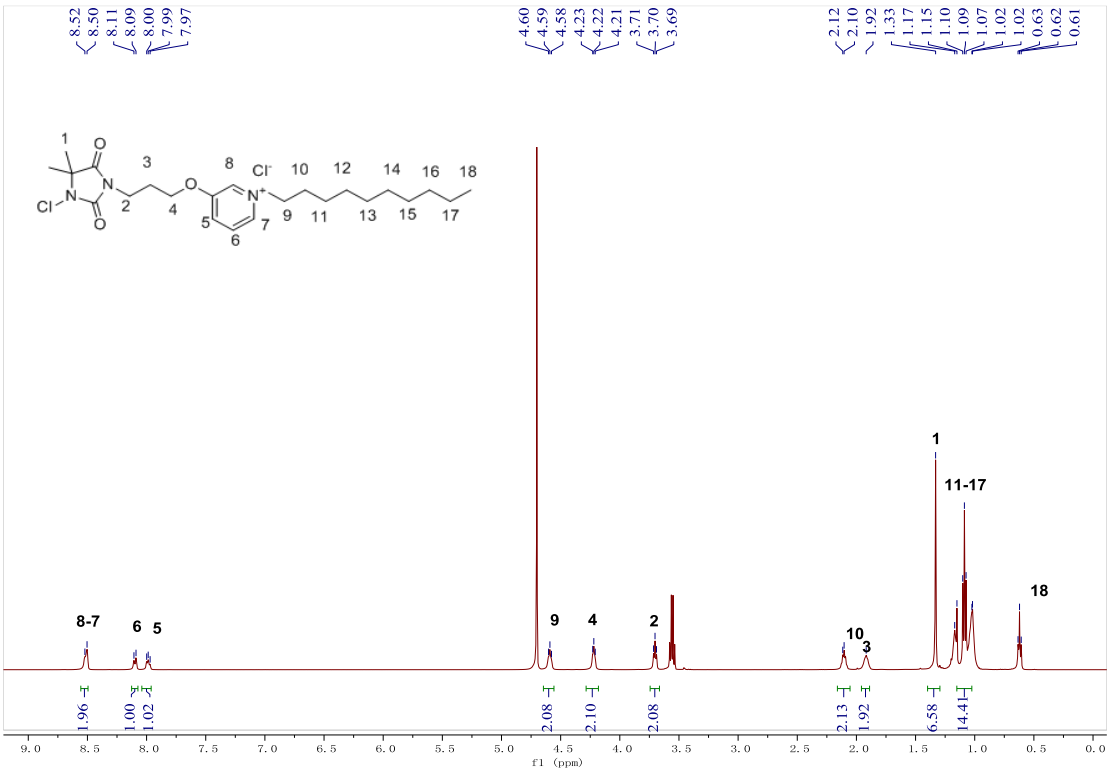
The ^{13}C NMR spectrum of compound **9**



The ^{1}H NMR spectrum of compound **10a**



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



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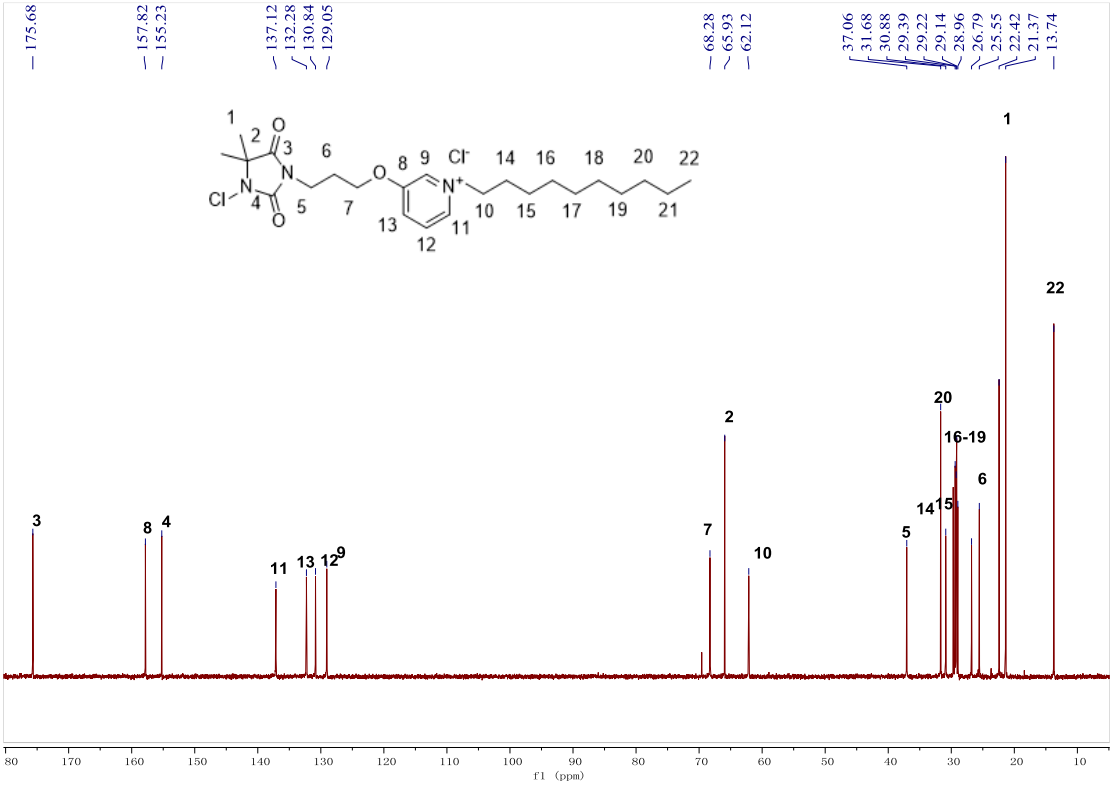

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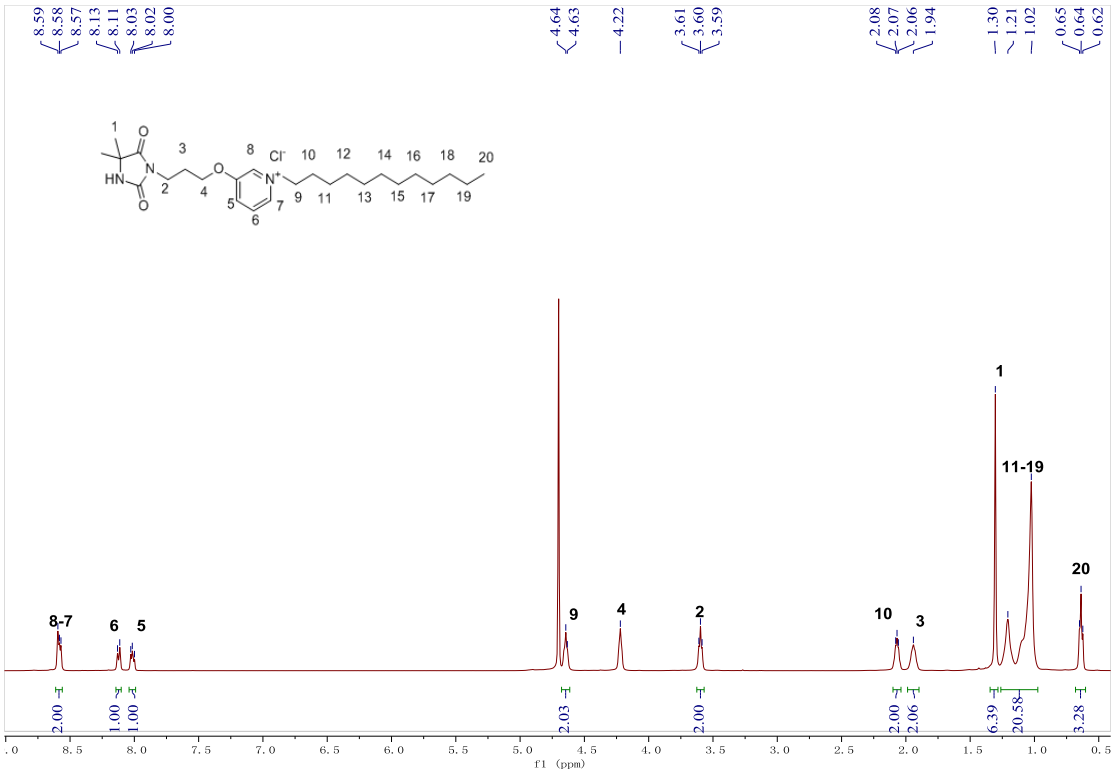
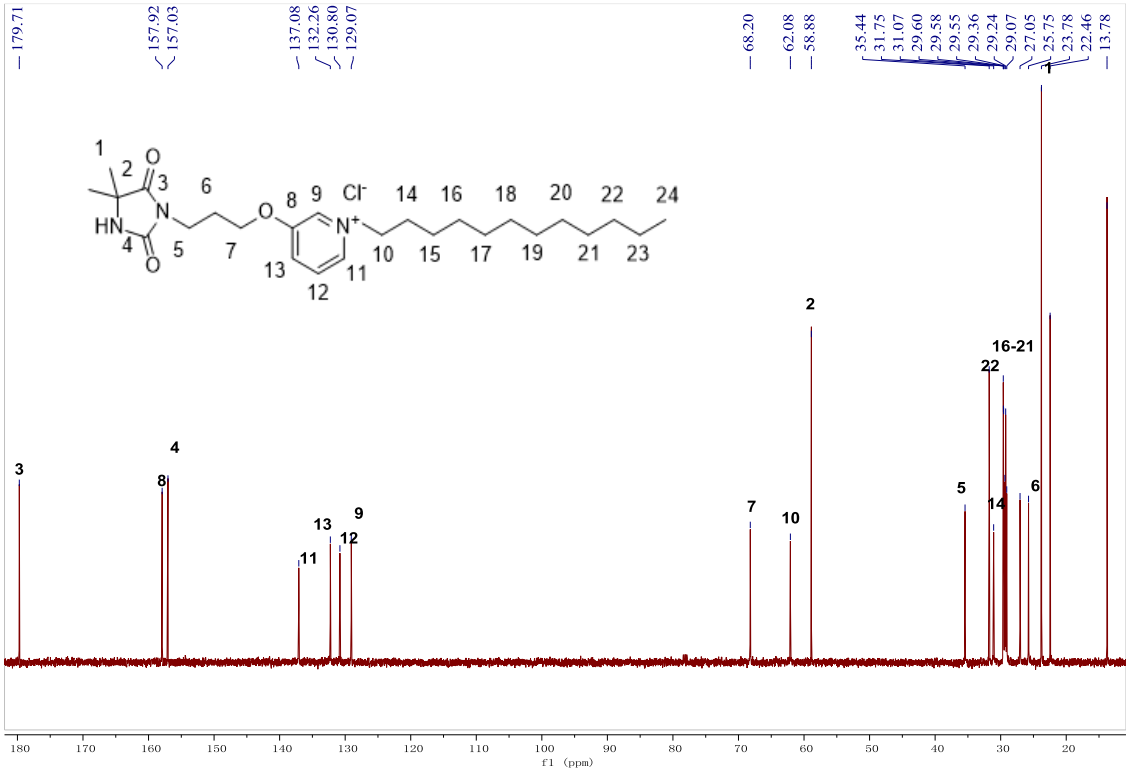
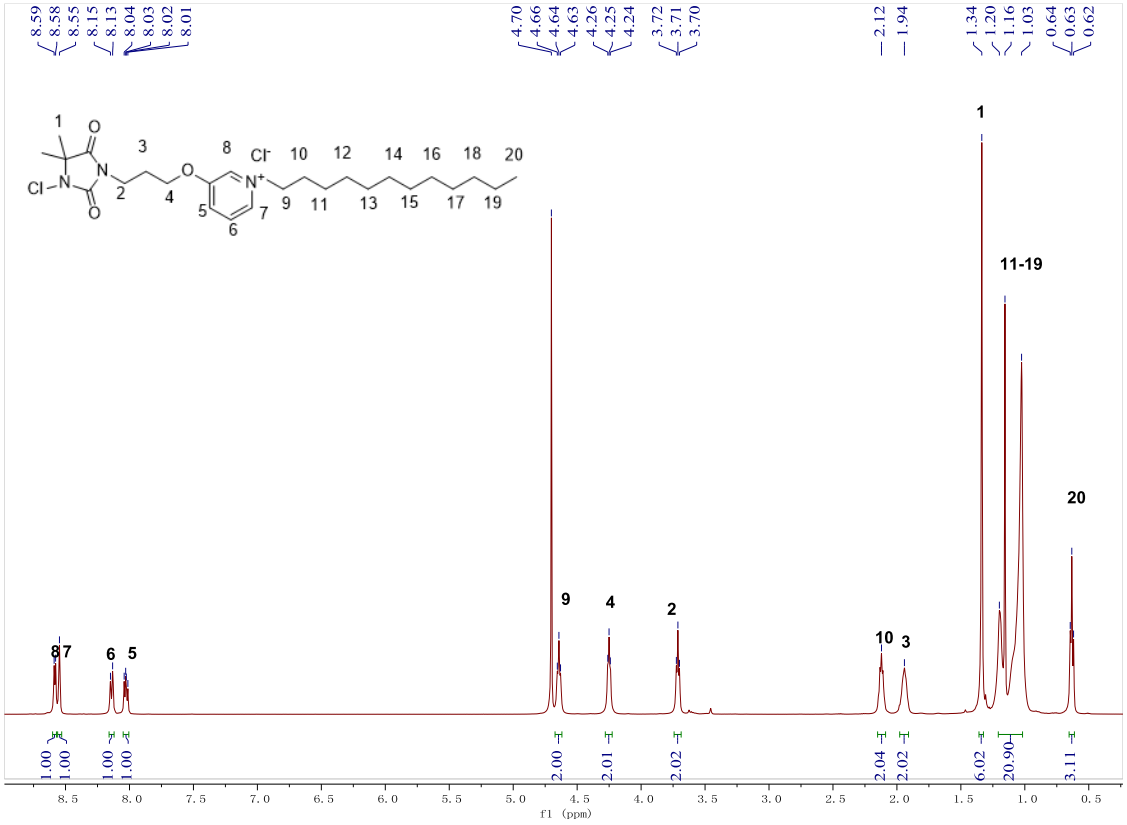


The ^{1}H NMR spectrum of compound **11a**



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



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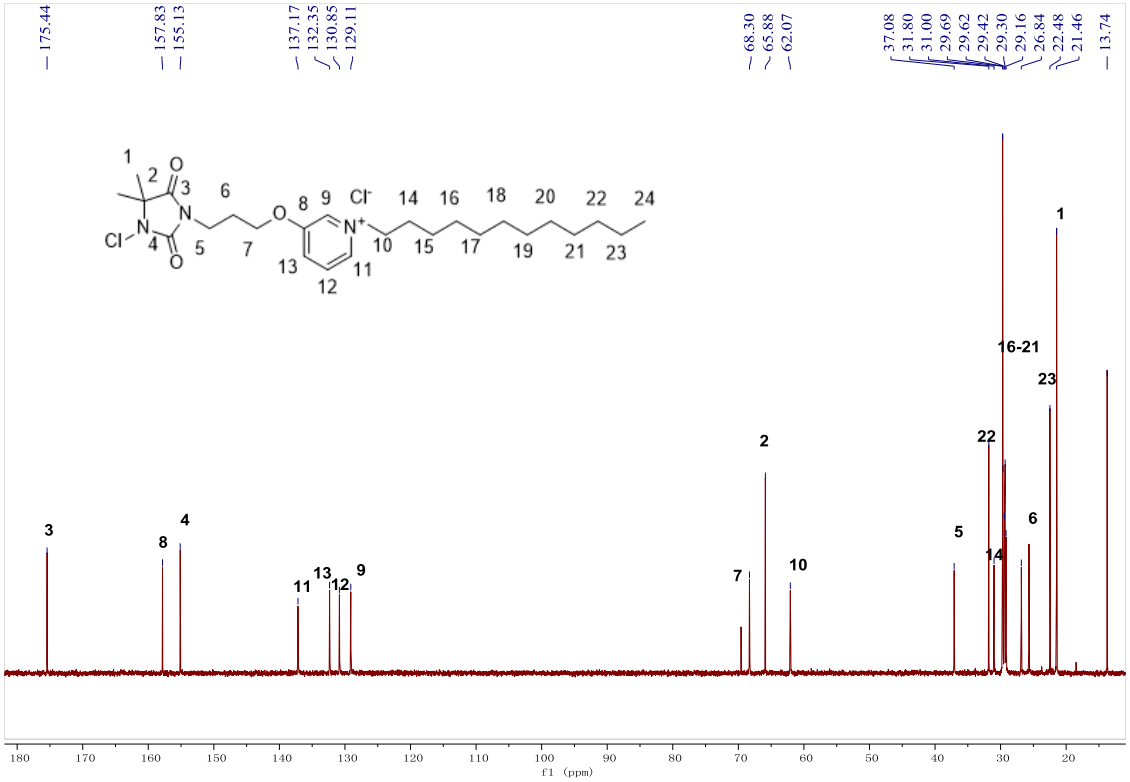

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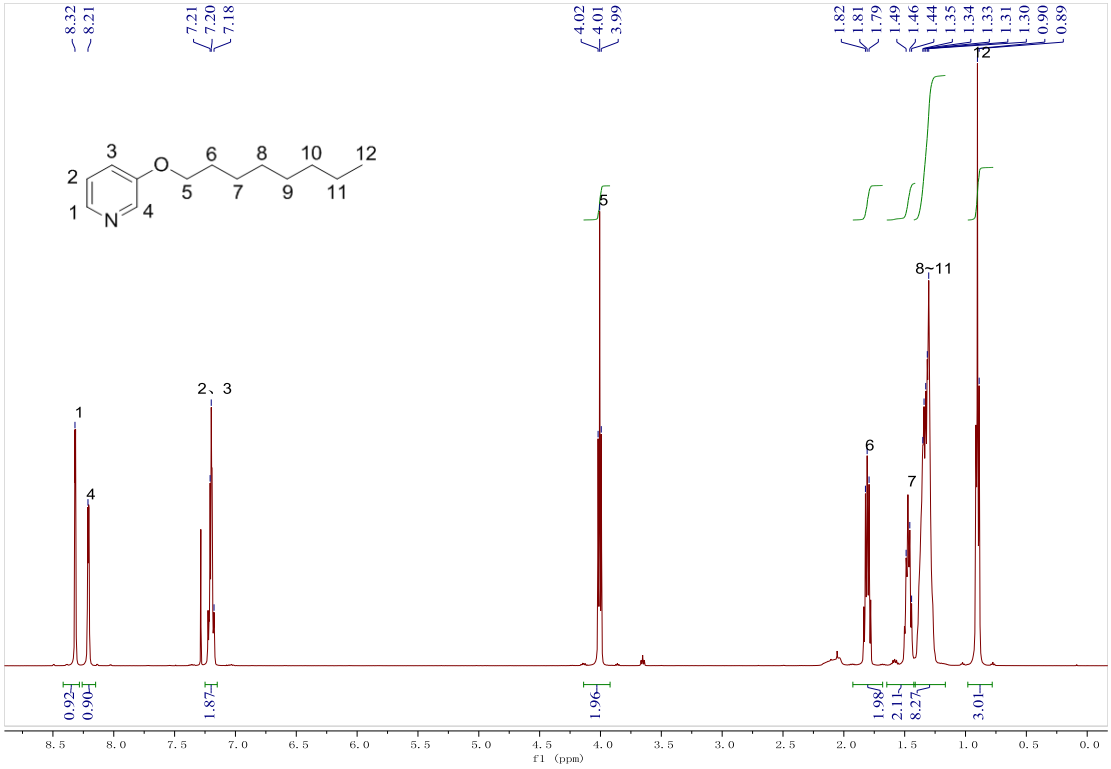
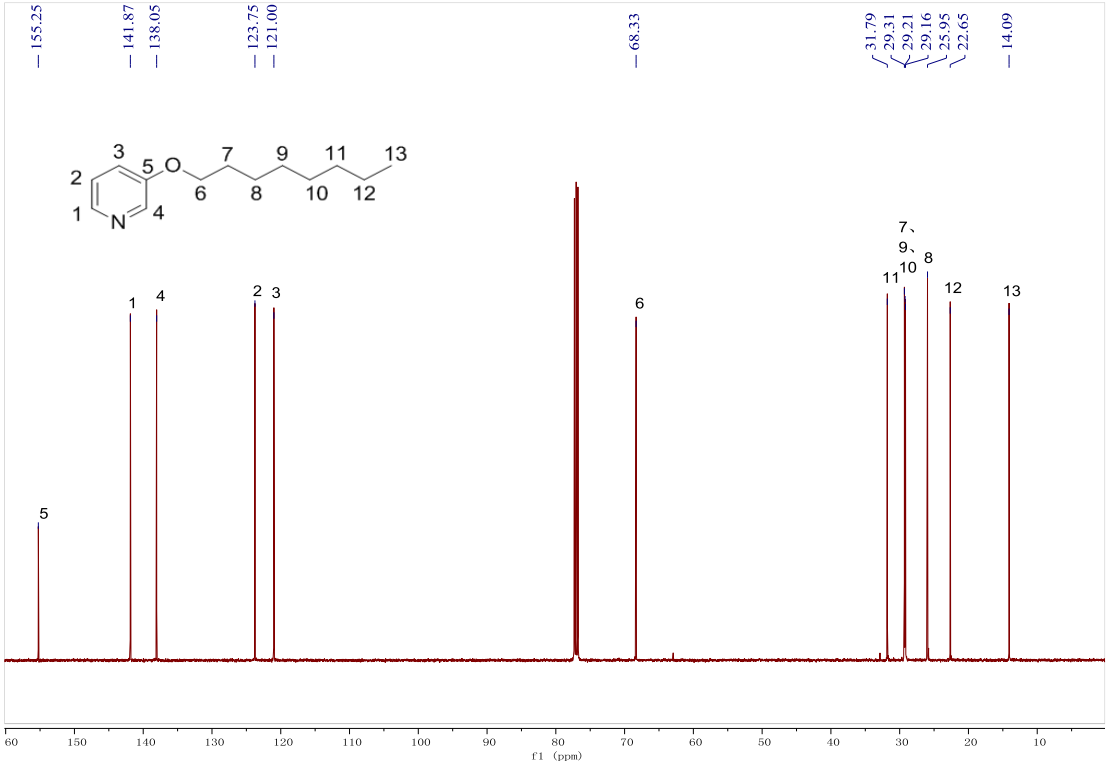


The ^{1}H NMR spectrum of compound **12**



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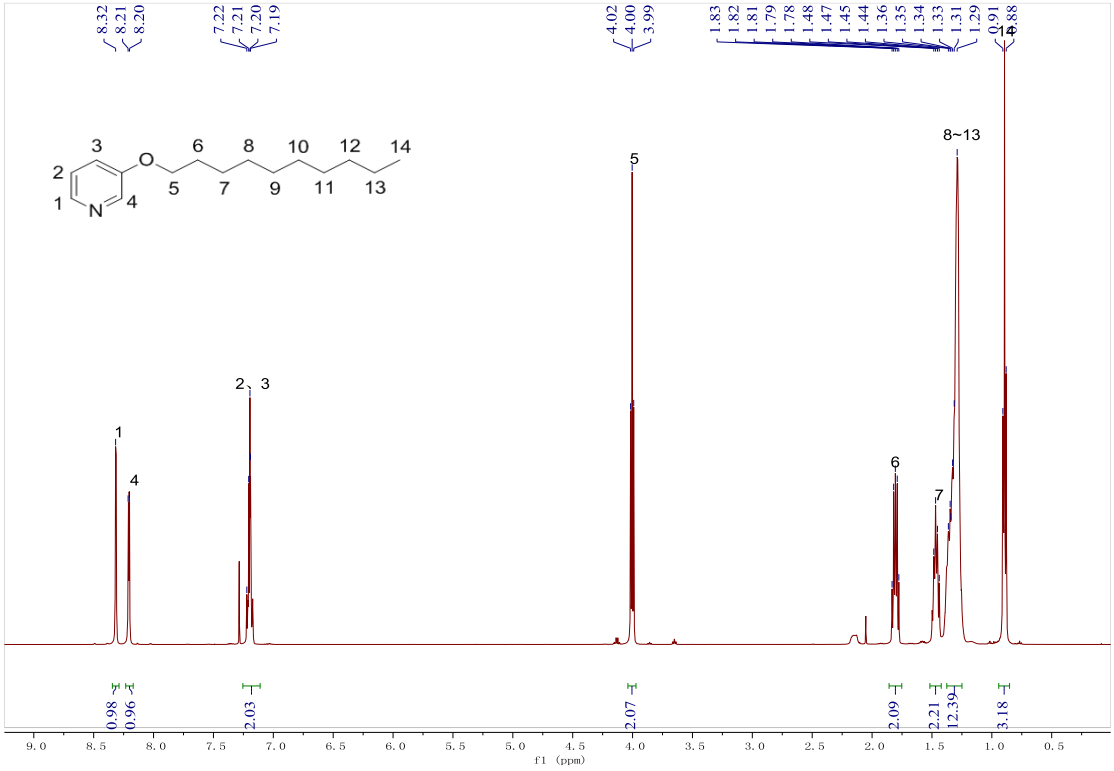

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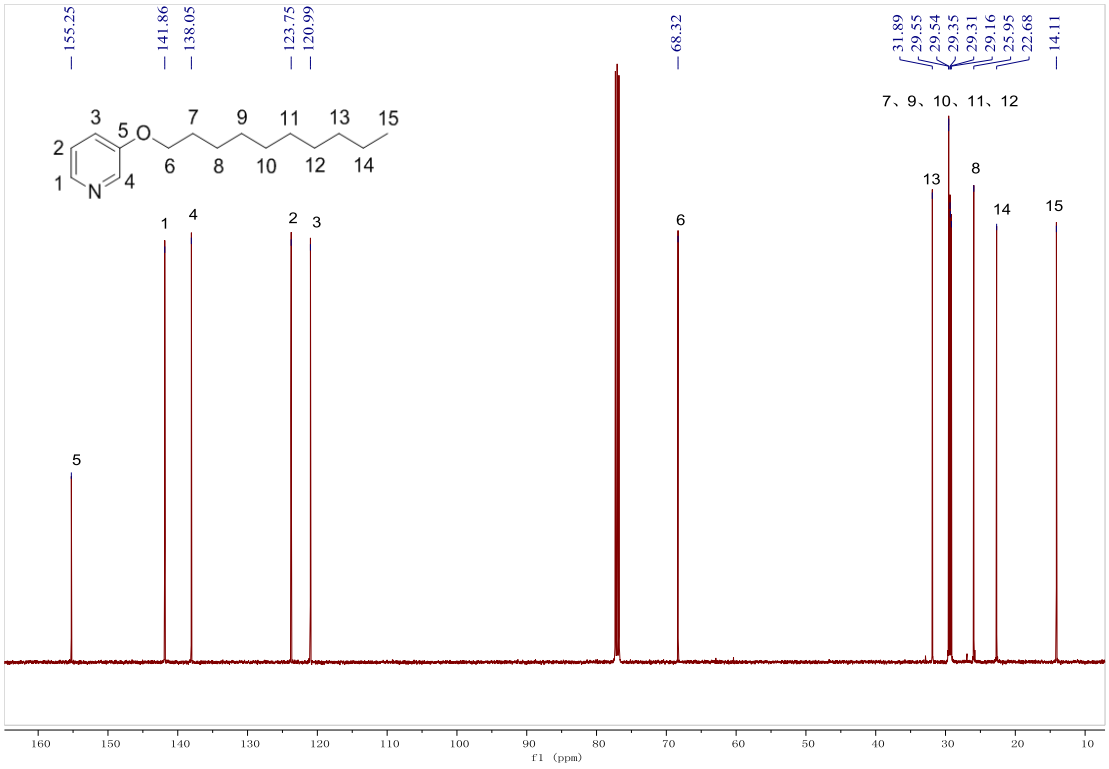

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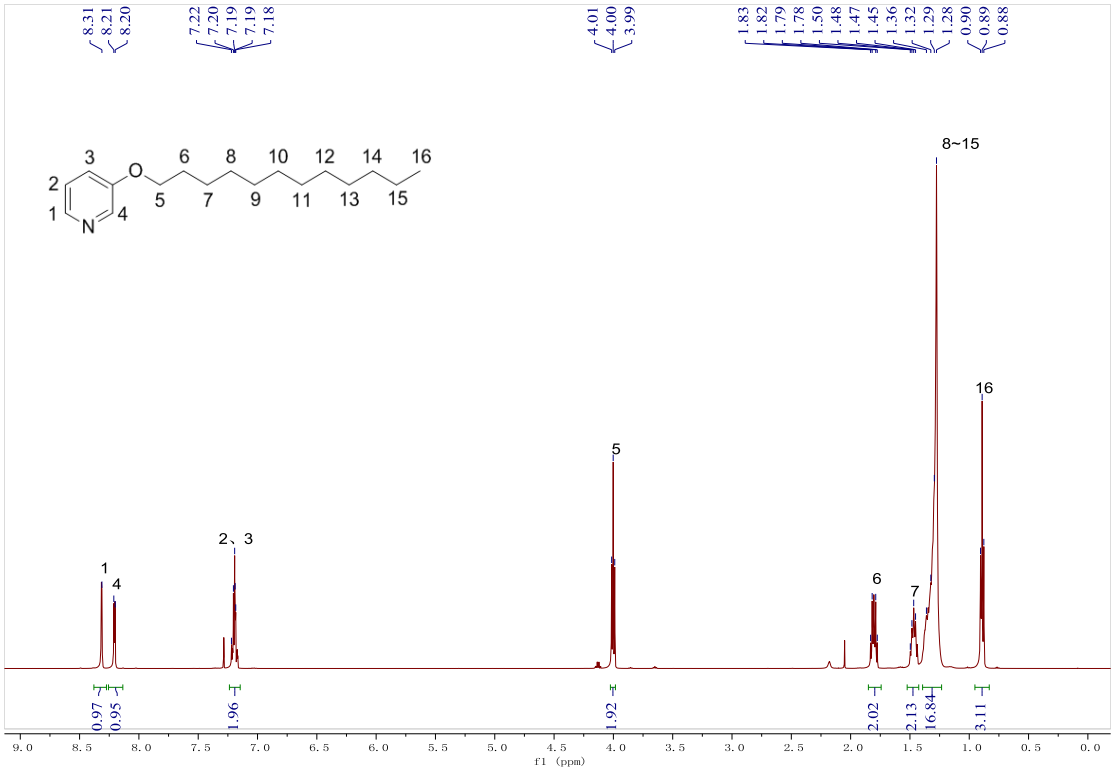

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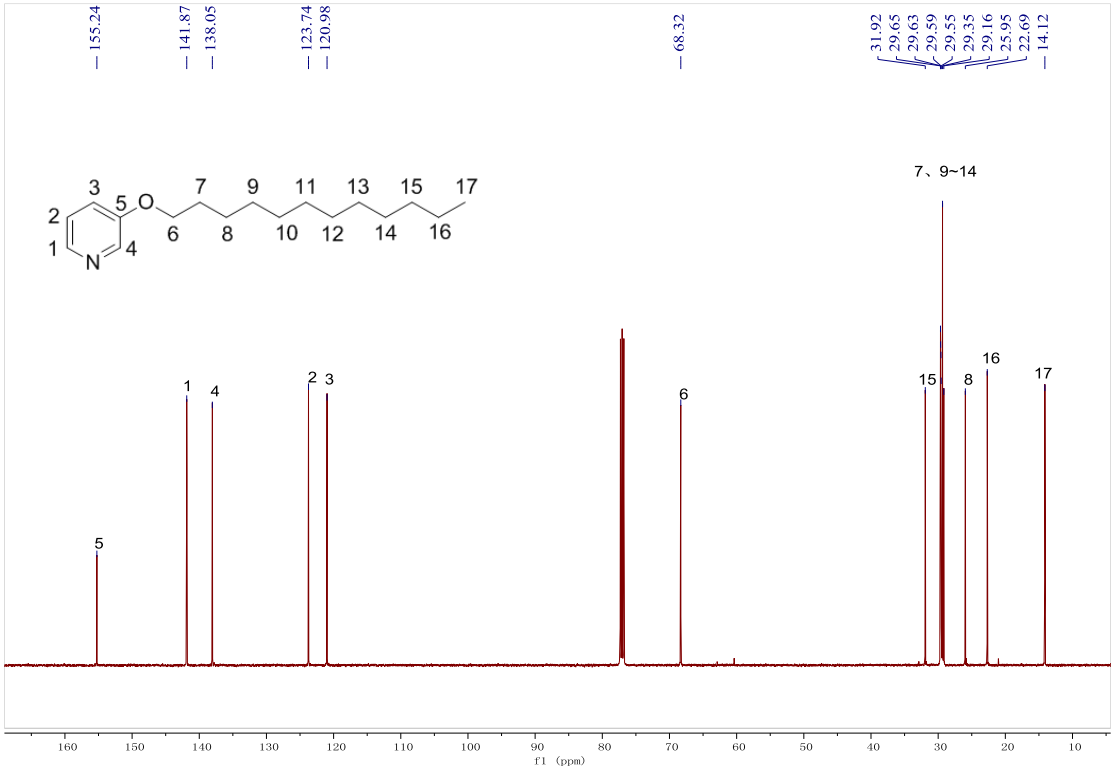

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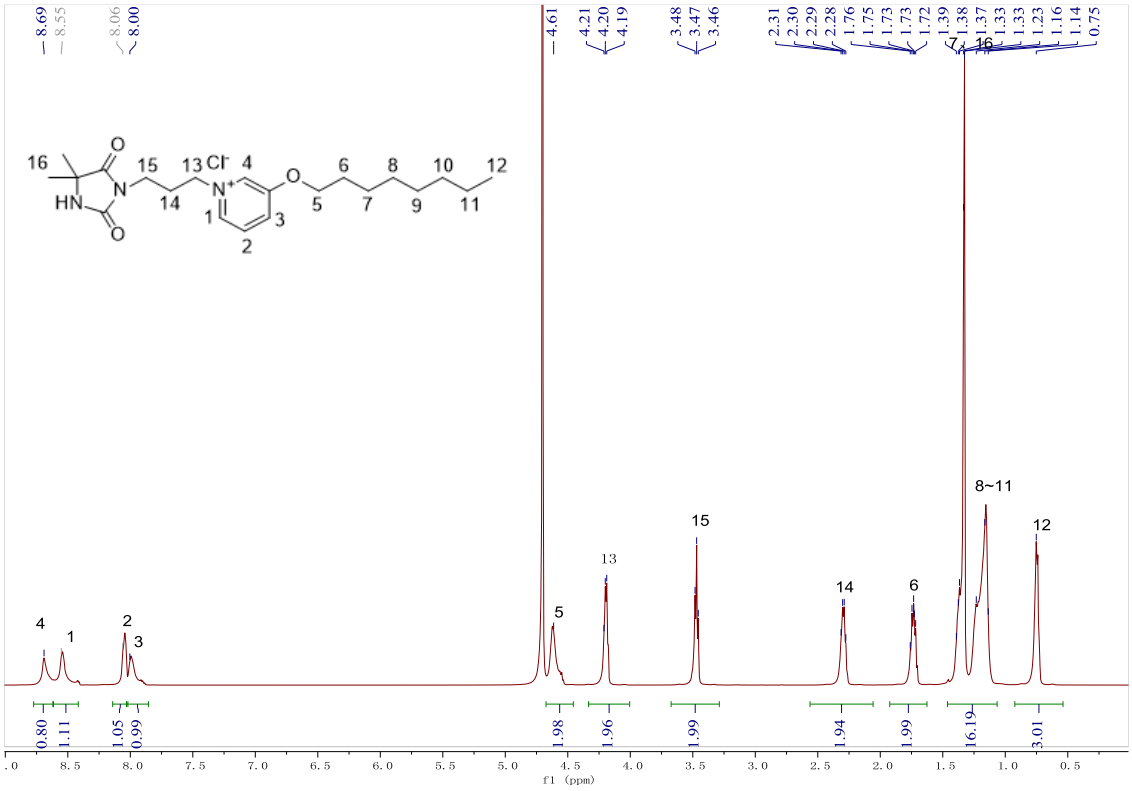

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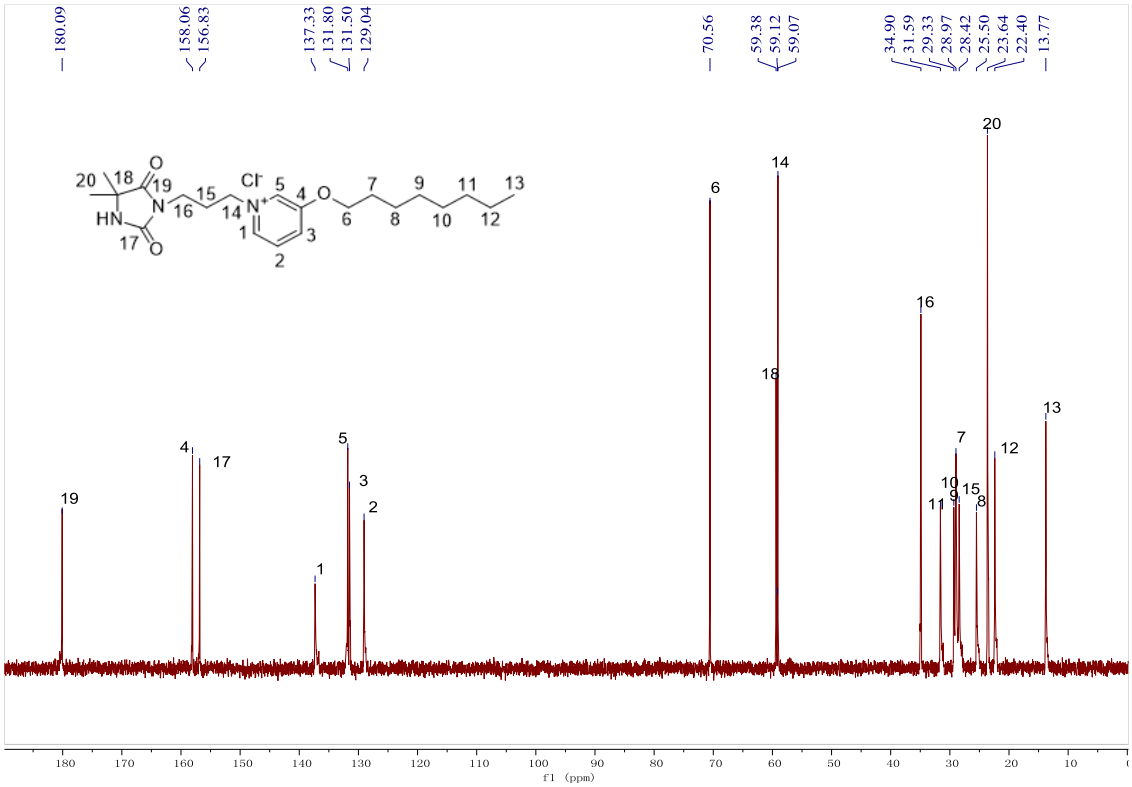

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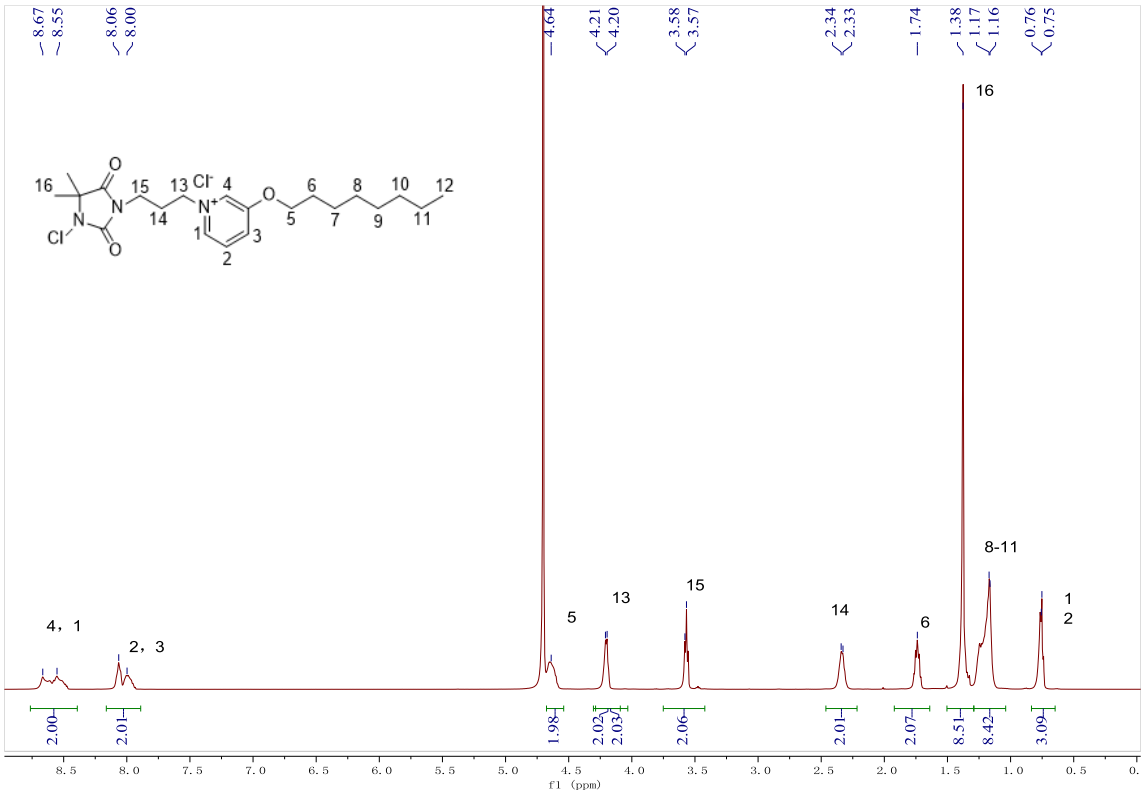

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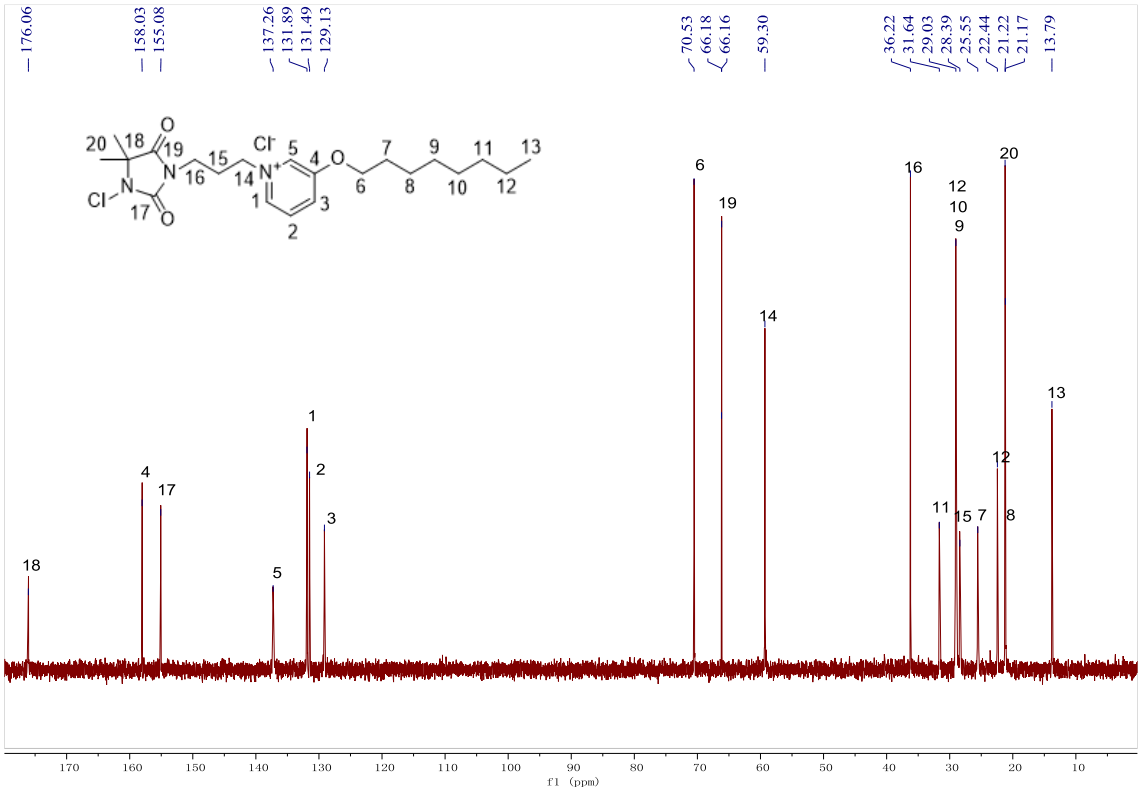

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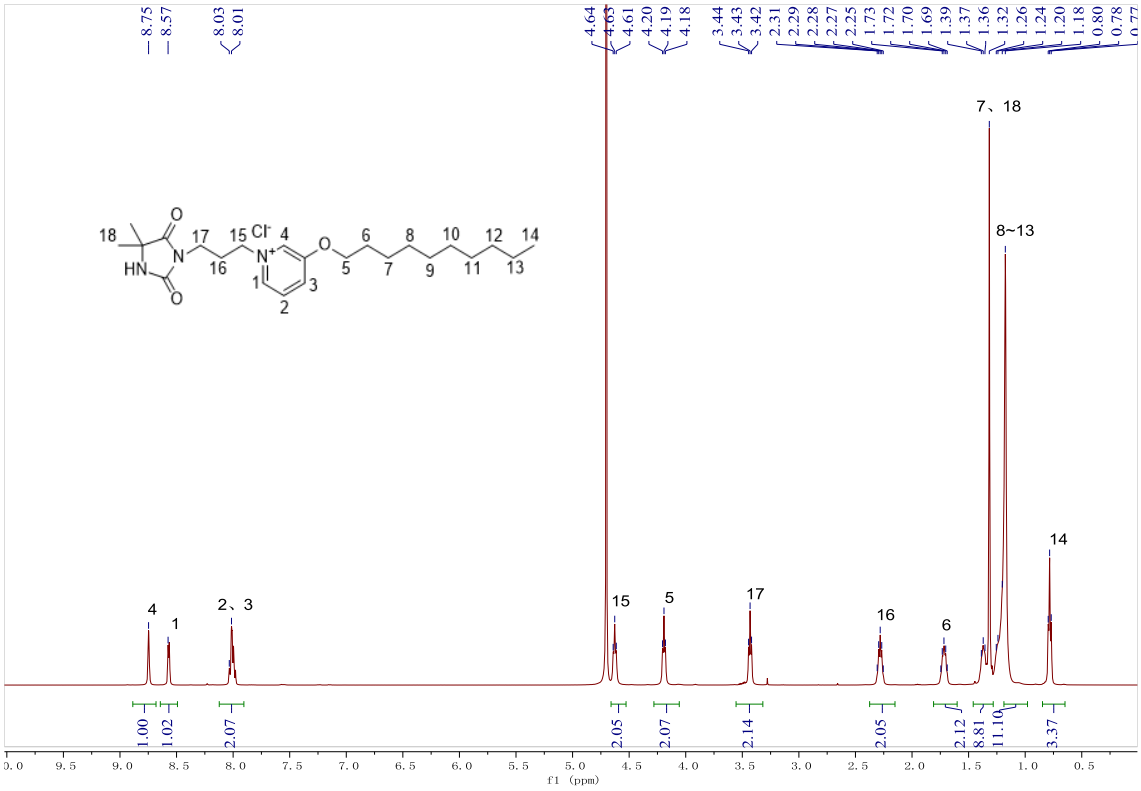

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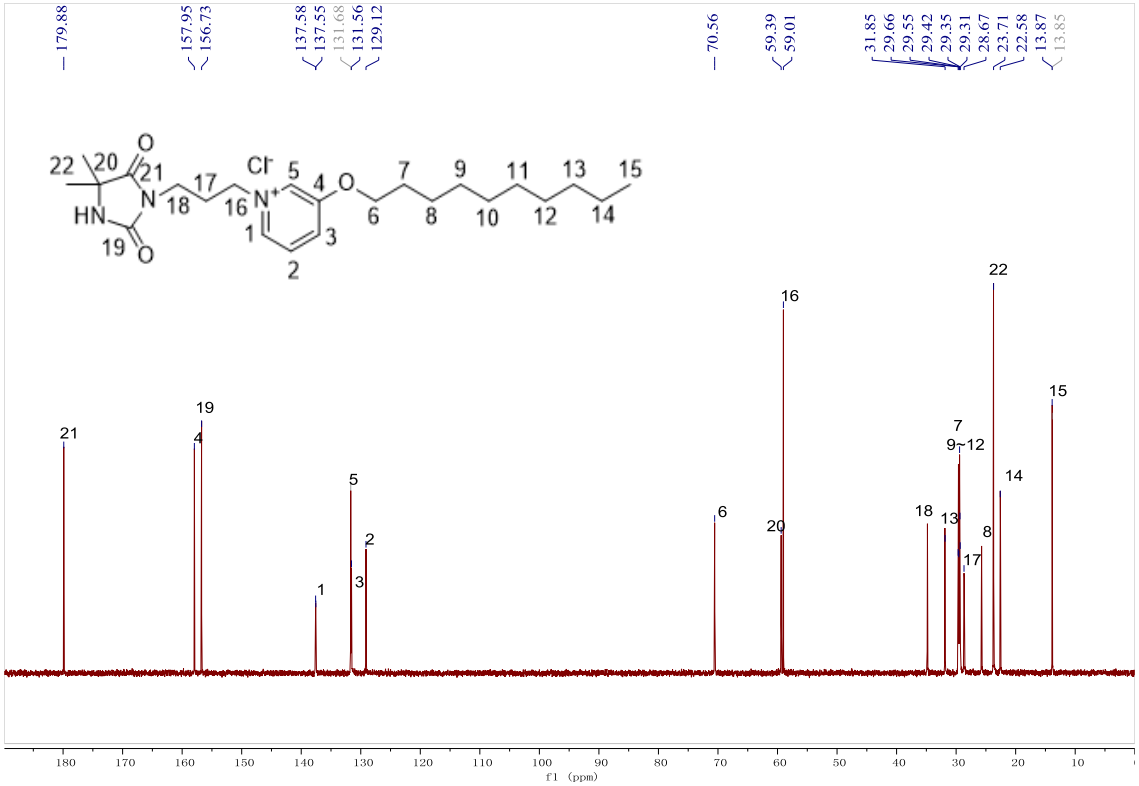

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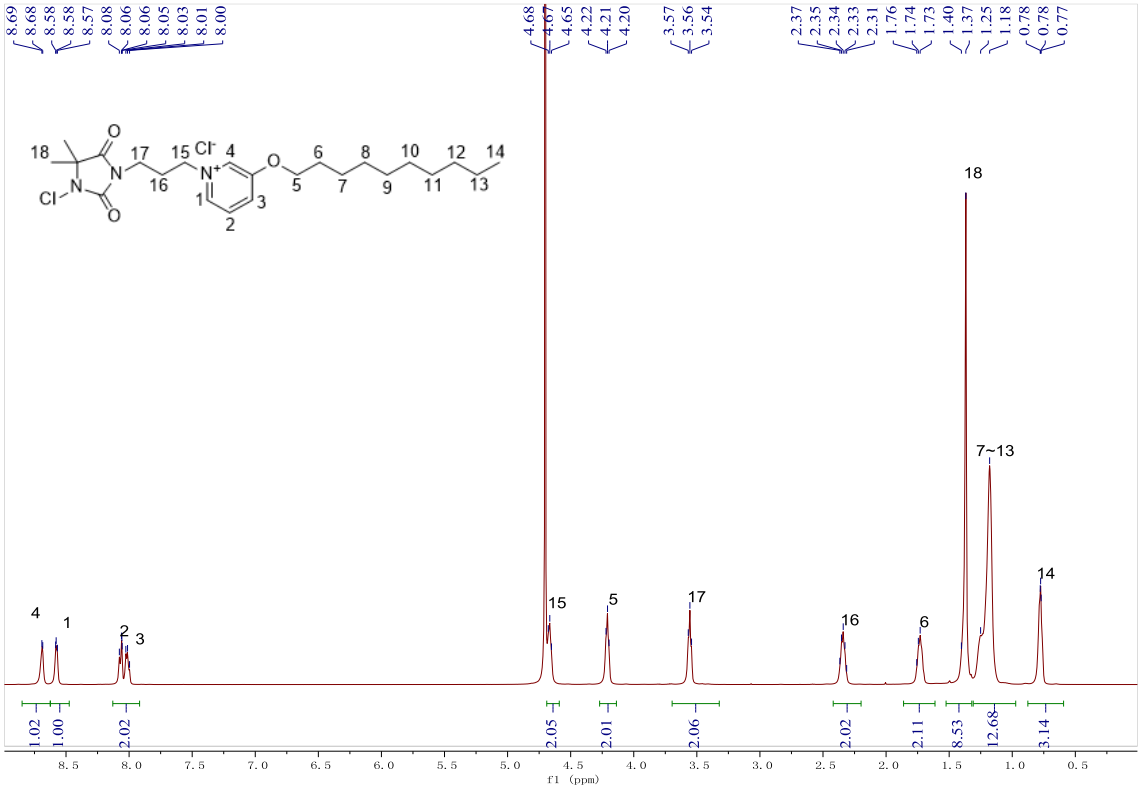

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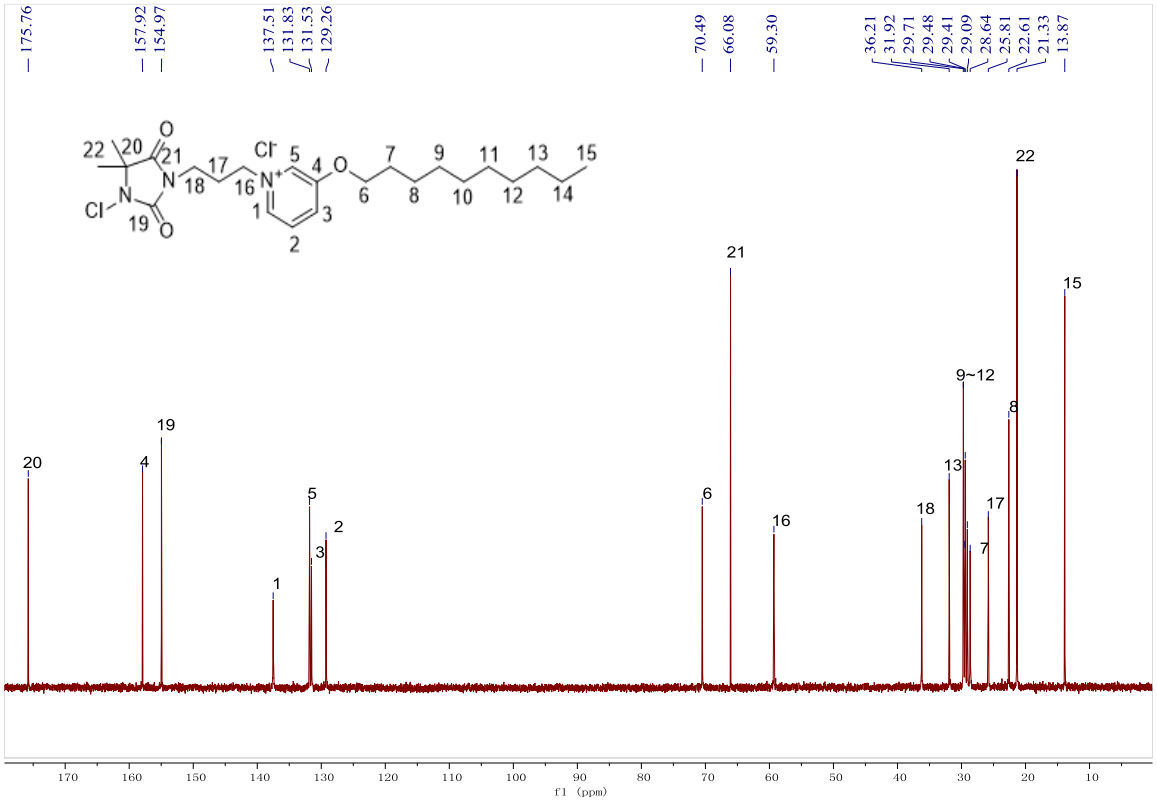

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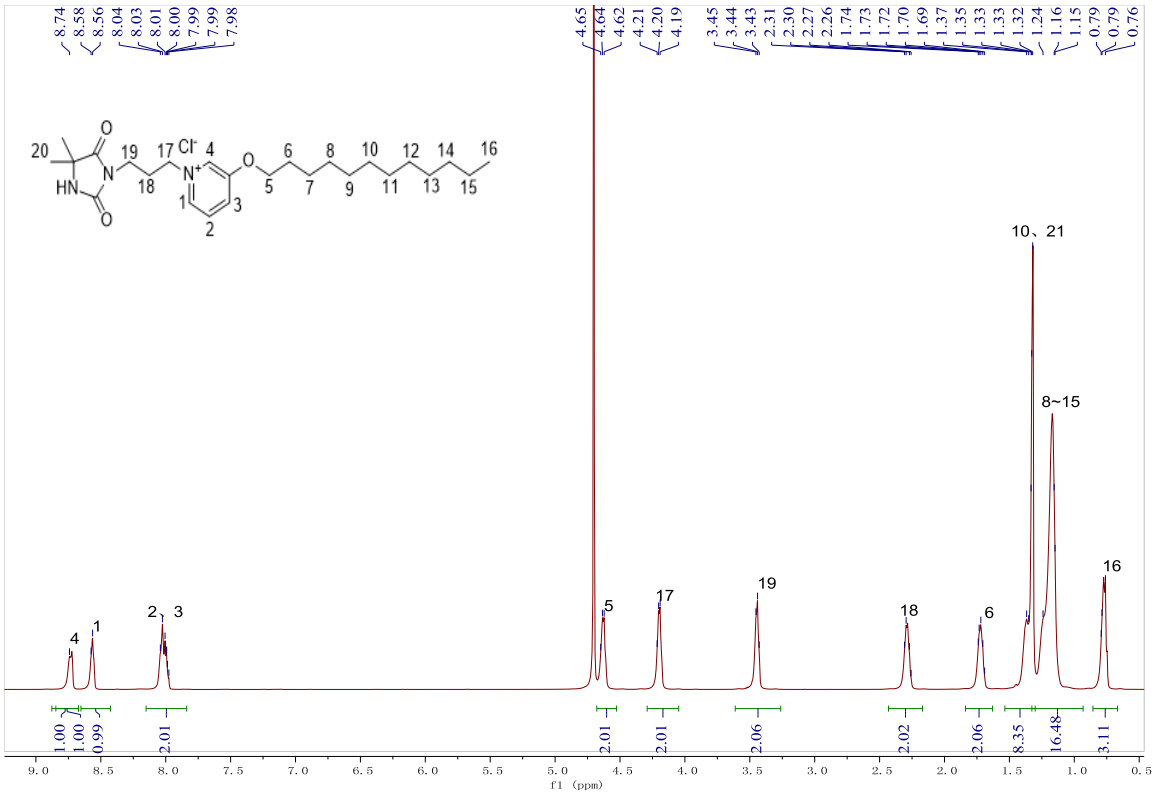

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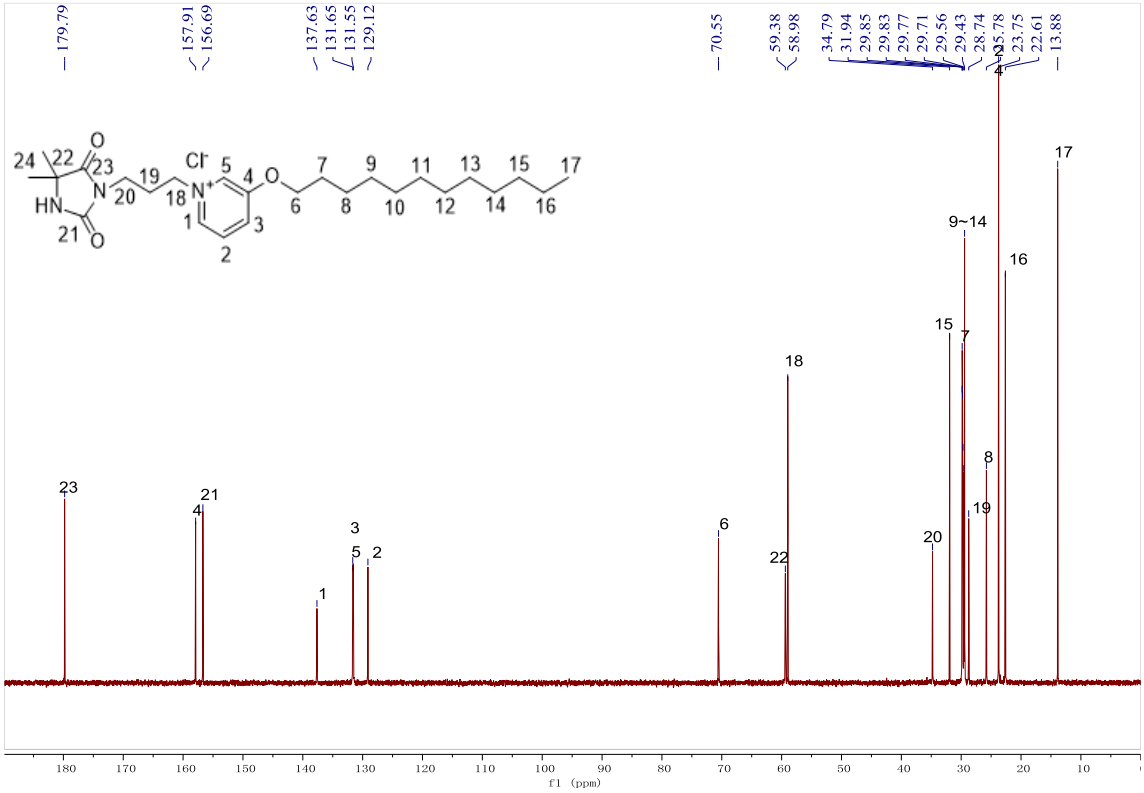

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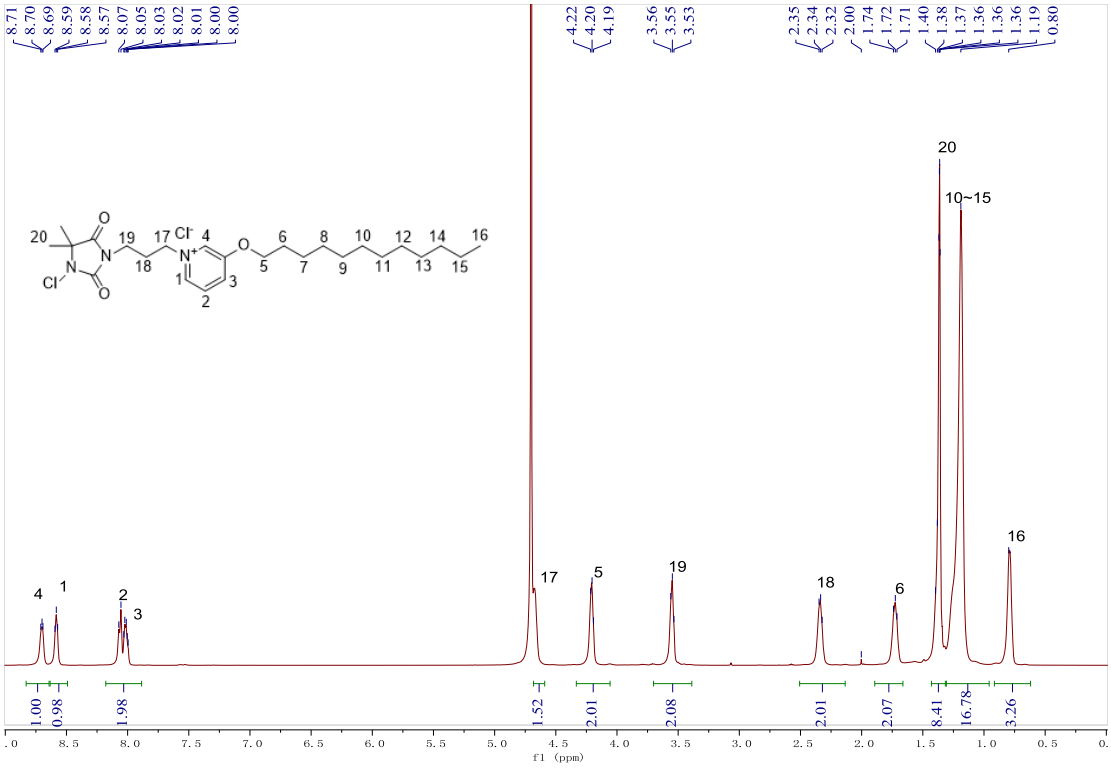

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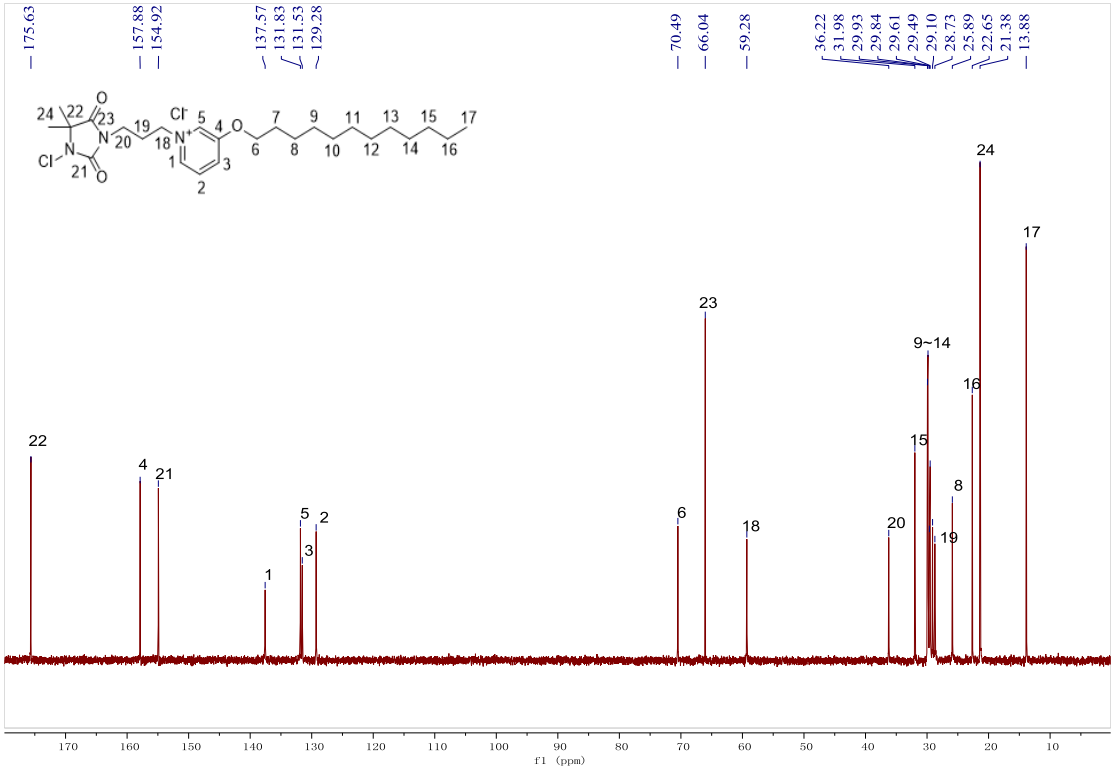

The ^{13}C NMR spectrum of compound **17**