Supplementary information

Zwitterionic pyridinium *N*-chloramine: Synthesis and Antibacterial Application

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Contents

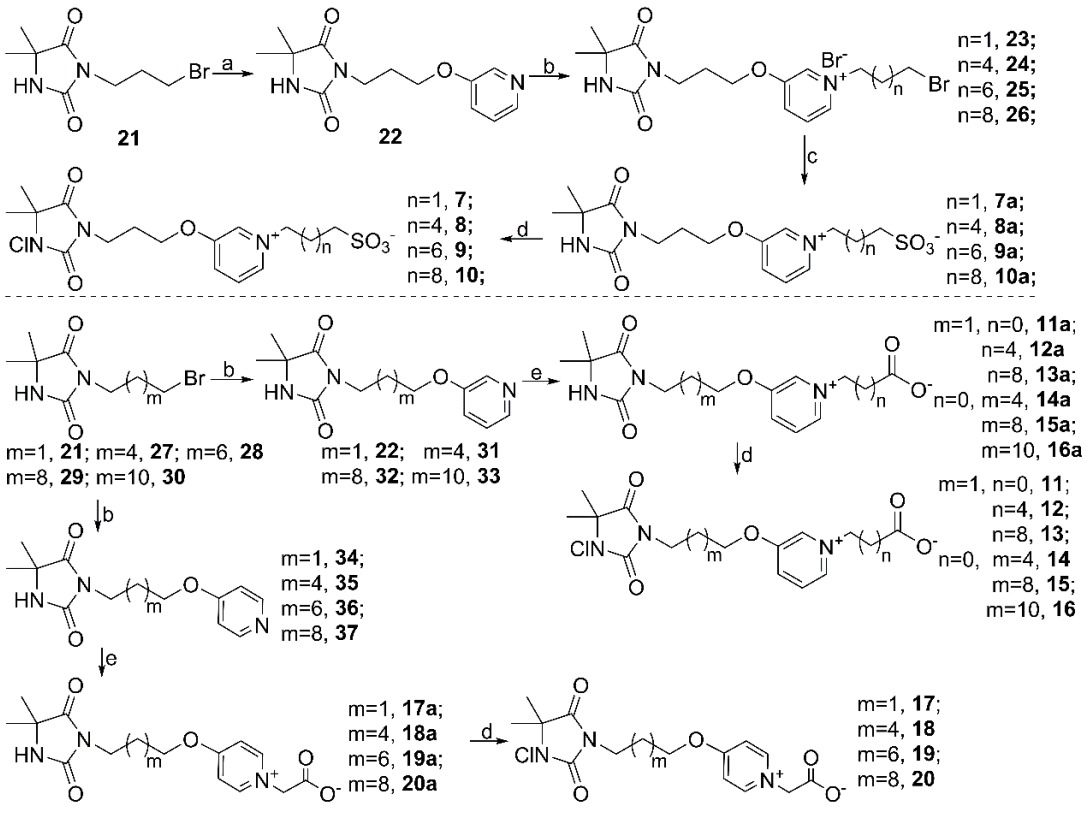
1. Reagents and materials

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. *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.

N-chloramine **2**, DMH-bromide **21** and **27**-**30**, alkoxypyridine **22** and **34** were prepared according to our previous procedure respectively,[1-3] and the chlorination agent of *t*-butyl hypochlorite was synthesized as described.[4] 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 target *N*-chloramines **7**-**20**



Scheme 1. Synthesis route of *N*-Chloramines **7**-**20**: a) CH_3CN,3-hydroxypyridine/4-hydroxypyridine, K_2CO_3, reflux; b) $Br(CH_2)_nBr$,

CH_3CN, reflux; c) Na_2SO_3, H_2O, 90℃; d) *t*-BuOH/H_2O, *t*-BuOCl, rt; e) H_2O/C_2H_5OH, NaOH/$Br(CH_2)_nCOOH$ or $NaCH_2COOCl$, 90℃.

2.1 General synthesis of **23**-**26**

Typical synthesis procedure for **23** was adopted in a similar manner according previous work[5-6]: To the solution of **22** (1.13 g, 4.30 mmol) in 18 mL acetonitrile was added 1,3-dibromopropane (1.74 g, 8.60 mmol), and the resulting mixture was heated to reflux for 24 hours. Upon completion of the reaction via TLC monitoring, the solvent was evaporated under reduced pressure. The residual mixture was applied on flash column chromatography, and washed by using methanol/dichloromethane (10:90, v/v) as the eluent. The corresponding fractions were collected and concentrated to yield compound **23** as a slight yellow viscous liquid. Pyridinium salts **24–26** were also prepared by the identical procedure.

23: (slight yellow viscous liquid, 1.35 g, 67.5%). ^{1}H NMR (500 MHz, D_2O) δ 8.53 (s, 1H), 8.45 (d, *J*=5.3 Hz, 1H), 8.04 (d, *J*=8.6 Hz, 1H), 7.91 (t, *J*=7.3 Hz, 1H), 4.18 (d, *J*=5.3 Hz, 2H), 3.65 (t, *J*=6.2 Hz, 2H), 3.42 (td, *J*=6.2, 2.3 Hz, 2H), 2.58~2.46 (m, 2H), 2.15~2.05 (m, 2H), 1.33 (s, 6H); ^{13}C NMR (126 MHz, D_2O) δ 180.6, 157.8, 157.3, 136.8, 132.0, 131.4, 128.9, 68.1, 60.1, 59.0, 37.1, 35.7, 30.6, 26.2, 23.4.

24: (slight yellow viscous liquid, 0.84 g, 51.4%). ^{1}H NMR (500 MHz, D_2O) δ 8.50~8.45 (m, 1H), 8.39 (d, *J*=5.9 Hz, 1H), 8.01 (dt, *J*=9.0, 2.3 Hz, 1H), 7.88 (d, *J*=8.5, 5.8, 1.9 Hz, 1H), 4.51 (td, *J*=7.2, 1.9 Hz, 2H), 4.18 (td, *J*=5.6, 1.8 Hz, 2H), 3.64 (td, *J*=6.4, 1.9 Hz, 2H), 3.41 (td, *J*=6.7, 1.9 Hz, 2H), 2.10 (t, *J*=6.1 Hz, 2H), 2.00~1.91 (m, 2H), 1.82 ~1.72 (m, 2H), 1.47~1.36 (m, 2H), 1.33~1.21 (m, 8H); ^{13}C NMR (126 MHz, D_2O) δ 180.7, 157.8, 157.6, 136.7, 131.8, 130.8, 128.4, 67.8, 62.2, 59.0, 55.7, 40.8, 35.7, 30.1, 27.1, 25.6, 24.6, 24.3, 23.3.

25: (slight yellow viscous liquid, 1.42 g, 60.1%). ^{1}H NMR (500 MHz, D_2O) δ 8.44 (s, 1H), 8.35 (s, 1H), 7.95 (s, 1H), 7.83 (s, 1H), 4.46 (s, 2H), 4.13 (s, 2H), 3.59 (s, 2H), 3.35 (s, 2H), 2.18~1.98 (m, 2H), 1.88 (s, 2H), 1.67 (d, *J*=6.7 Hz, 2H), 1.23 (d, *J*=35.7 Hz, 14H); ^{13}C NMR (126 MHz, D_2O) δ 180.6, 157.8, 157.6, 136.8, 131.8, 130.8, 128.5, 67.8, 62.4, 59.0, 55.7, 35.7, 30.3, 27.9, 27.7, 27.4, 26.7, 25.1, 24.7, 23.4.

26: (slight yellow viscous liquid, 0.98 g, 59.6%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.15 (s, 1H), 8.71 (d, *J* = 5.2 Hz, 1H), 7.97 (q, *J*=8.9 Hz, 2H), 4.92 (t, *J*=7.3 Hz, 2H), 4.35 (t, *J*=5.4 Hz, 2H), 3.63 (t, *J*=6.2 Hz, 2H), 3.33 (t, *J*=6.8 Hz, 2H), 2.15~2.05 (m, 2H), 2.01~1.91 (m, 2H), 1.81~1.72 (m, 2H), 1.40 (s, 6H), 1.35~1.19 (m, 14H); ^{13}C NMR (126 MHz, D_2O) δ 181.1, 156.8, 157.4, 137.1, 132.0, 131.0, 128.3, 67.9, 62.5, 59.2, 56.8, 35.5, 30.4, 28.2, 28.2, 28.1, 27.9, 27.6, 26.7, 25.0, 24.8, 23.5.

2.2 General synthesis of precursor **7a**-**10a**

Typical synthesis procedure for **7a** was adopted in a similar manner according previous work[5-6]: To the solution of **23** (1.20 g, 2.64 mmol) in 8 mL DI water was added sodium sulphite (0.41 g, 3.27 mmol), and the resulting mixture was heated to 90℃ for 24 hours. The solvent was then evaporated under reduced pressure and the residual mixture was dispersed in 10 mL MeOH. Inorganic salt was removed by filtration and the filtrate was concentrated and subsequently applied on flash column chromatography, washing with methanol/dichloromethane (30 : 70, v/v) as the eluent. The corresponding fractions were collected and concentrated to yield compound **7a** as white solid. Pyridinium **8a**-**10a** were also prepared by the identical procedure.

7a: (White Solid, 0.54 g, 54.0%). ^{1}H NMR (500 MHz, D_2O) δ 8.51 (s, 1H), 8.42 (d, *J*=6.0 Hz, 1H), 8.01 (dd, *J*=9.0, 2.1 Hz, 1H), 7.88 (dd, *J*=8.8, 6.2 Hz, 1H), 4.67 (d, *J*=25.6 Hz, 7H), 4.16 (t, *J*=5.6 Hz, 2H), 3.62 (t, *J*=6.5 Hz, 2H), 3.25 (d, *J*=1.8 Hz, 2H), 2.88 (t, *J*=7.3 Hz, 2H), 2.37 (p, *J*=7.4 Hz, 2H), 2.07 (p, *J*=6.3 Hz, 2H), 1.31~1.28 (m, 6H); ^{13}C NMR (126 MHz, D_2O) δ 180.8, 158.1, 157.5, 137.1, 132.0, 131.3, 128.8, 68.0, 60.2, 59.1, 47.0, 35.7, 26.7, 26.2, 23.4. HRMS calcd. for $C_{16}H_{23}N_3O_6S$ $[M+Na]^+$: 408.1200, found: 408.1187.

8a: (White Solid, 0.87 g, 74.4%). ^{1}H NMR (500 MHz, D_2O) δ 8.47~8.42 (m, 1H), 8.36 (d, *J*=6.0 Hz, 1H), 7.97 (dd, *J*=8.9, 2.7 Hz, 1H), 7.84 (dd, *J*=8.9, 5.8 Hz, 1H), 4.47 (t, *J*=7.2 Hz, 2H), 4.14 (t, *J*=5.6 Hz, 2H), 3.61 (t, *J*=6.3 Hz, 2H), 2.81~2.74 (m, 2H), 2.10~2.02 (m, 2H), 1.92 (p, *J*=7.3 Hz, 2H), 1.66~1.56 (m, 2H), 1.37 (p, *J*=7.2 Hz, 2H), 1.28 (s, 8H); ^{13}C NMR (126 MHz, D_2O) δ 180.8, 157.9, 157.5, 136.8, 131.9, 130.9, 128.5, 67.9, 62.1, 59.1, 50.7, 48.9, 35.6, 30.2, 27.0, 26.7, 24.7, 23.7, 23.4. HRMS calcd. for $C_{19}H_{29}N_3O_6S$ $[M+Na]^+$: 450.1669, found: 450.1654.

9a: (White Solid, 0.81 g, 68.7%). ^{1}H NMR (500 MHz, D_2O) δ 8.45 (d, *J*=2.4 Hz, 1H), 8.36 (d, *J*=6.0 Hz, 1H), 7.97 (dd, *J*=8.9, 2.7 Hz, 1H), 7.85 (dd, *J*=8.9, 5.9 Hz, 1H), 4.47 (t, *J*=7.2 Hz, 2H), 4.14 (t, *J*=5.6 Hz, 2H), 3.61 (t, *J*=6.4 Hz, 2H), 2.80~2.73 (m, 2H), 2.06 (p, *J*=6.0 Hz, 2H), 1.91 (p, *J*=7.2 Hz, 2H), 1.59 (p, *J*=7.6 Hz, 2H), 1.28 (s, 6H), 1.25~1.17 (m, 6H); ^{13}C NMR (126 MHz, D_2O) δ 180.7, 157.9, 157.5, 136.9, 131.9, 130.9, 128.6, 67.9, 62.3, 59.1, 51.0, 35.6, 30.4, 27.9, 27.7, 27.4, 26.7, 25.0, 23.9, 23.5. HRMS calcd. for $C_{21}H_{33}N_3O_6S$ $[M+Na]^+$: 478.1982, found: 478.1970.

10a: (White Solid, 0.60 g, 65.2%). ^{1}H NMR (500 MHz, D_2O) δ 8.45 (dd, *J*=2.5, 1.3 Hz, 1H), 8.37 (d, *J*=5.8 Hz, 1H), 7.99 (dd, *J*=8.5, 2.9 Hz, 1H), 7.86 (dd, *J*=8.9, 6.0 Hz, 1H), 4.47 (t, *J*=7.1 Hz, 2H), 4.15 (t, *J*=5.6 Hz, 2H), 3.62 (t, *J*=6.4 Hz, 2H), 2.81~2.74 (m, 2H), 2.10~2.04 (m, 2H), 1.94~1.87 (m, 2H), 1.60 (td, *J*=7.4, 3.3 Hz, 2H), 1.28 (s, 8H), 1.22~1.15 (m, 10H); ^{13}C NMR (126 MHz, D_2O) δ 180.7, 157.9, 157.5, 136.9, 131.9, 130.9, 128.6, 67.9, 62.3, 59.1, 51.1, 35.6, 30.4, 28.2, 28.1, 28.1, 27.9, 27.6, 26.7, 25.0, 23.9, 23.5. HRMS calcd. for $C_{23}H_{37}N_3O_6S$ $[M+Na]^+$: 506.2295, found: 506.2281.

2.3 General synthesis of *N*-chloramine **7**-**10**

Typical synthesis procedure for **7** was adopted according previous work[1-3]：To the solution of **7a** (0.30 g, 0.78 mmol) in 2.7 mL *t*-BuOH-water (4:1, V:V) was added *t*-BuOCl (0.25 g, 2.33 mmol), and the resulting mixture was stirred at room temperature in dark for 24 hours. The solvent was then evaporated under reduced pressure to give compound N-chloramine **7** as white solid in quantitively yield. *N*-chloramine **8**-**10** were also prepared by the identical procedure.

7: (White Solid, 0.40 g, 100%). ^{1}H NMR (500 MHz, D_2O) δ 8.47 (dd, *J*=2.6, 1.4 Hz, 1H), 8.40 (dt, *J*=6.0, 1.2 Hz, 1H), 7.97 (ddd, *J*=8.9, 2.7, 1.0 Hz, 1H), 7.85 (dd, *J*=8.9, 5.9 Hz, 1H), 4.62 (t, *J*=7.4 Hz, 2H), 4.14 (t, *J*=5.5 Hz, 2H), 3.68 (t, *J*=6.3 Hz, 2H), 2.86 (t, *J*=7.3 Hz, 2H), 2.38~2.31 (m, 2H), 2.10~2.03 (m, 2H), 1.34 (s, 6H); ^{13}C NMR (126 MHz, D_2O) δ 177.0, 158.0, 155.8, 137.1, 132.0 131.3, 128.8, 68.0, 66.2, 60.2, 47.0, 37.0, 26.6, 26.2, 20.9. HRMS calcd. for $C_{16}H_{22}ClN_3O_6S$ $[M+Na]^+$: 442.0810, found: 442.0801.

8: (White Solid, 0.43 g, 100%). ^{1}H NMR (500 MHz, D_2O) δ 8.43 (dd, *J*=2.5, 1.3 Hz, 1H), 8.36 (d, *J*=6.0 Hz, 1H), 7.95 (dd, *J*=8.9, 2.6 Hz, 1H), 7.84 (dd, *J*=8.9, 5.9 Hz, 1H), 4.47 (t, *J*=7.2 Hz, 2H), 4.14 (t, *J*=5.5 Hz, 2H), 3.69 (t, *J*=6.3 Hz, 2H), 2.80~2.73 (m, 2H), 2.10~2.04 (m, 2H), 1.95~1.88 (m, 2H), 1.65~1.57 (m, 2H), 1.37 (d, *J*=7.6 Hz, 2H), 1.34 (s, 6H), 1.30~1.21 (m, 2H); ^{13}C NMR (126 MHz, D_2O) δ 177.0, 157.8, 155.8, 136.9, 131.9, 130.8, 128.6, 67.9, 66.2, 62.3, 51.0, 37.0, 30.4, 27.8, 27.7, 27.4, 26.6, 25.0, 23.8, 21.0. HRMS calcd. for $C_{19}H_{28}ClN_3O_6S$ $[M+Na]^+$: 484.1280, found: 484.1268.

9: (White Solid, 0.47 g, 100%). ^{1}H NMR (500 MHz, D_2O) δ 8.44~8.39 (m, 1H), 8.35 (d, *J*=6.0 Hz, 1H), 7.95 (dd, *J*=8.8, 2.7 Hz, 1H), 7.84 (dd, *J*=8.9, 5.8 Hz, 1H), 4.72 (s, 6H), 4.46 (t, *J*=7.2 Hz, 2H), 4.14 (t, *J*=5.5 Hz, 2H), 3.69 (t, *J*=6.3 Hz, 2H), 2.79~2.72 (m, 2H), 2.11~2.03 (m, 2H), 1.90 (p, *J*=7.1 Hz, 2H), 1.63~1.53 (m, 2H), 1.34 (s, 6H), 1.27 (t, *J*=7.6 Hz, 2H), 1.25~1.16 (m, 6H); ^{13}C NMR (126 MHz, D_2O) δ 180.7, 157.9, 157.5, 136.9, 131.9, 130. 9, 128.6, 67.9, 62.3, 59.1, 51.0, 35.6, 30.4, 27.9, 27.7, 27.4, 26.7, 25.0, 23.9, 23.5. HRMS calcd. for $C_{21}H_{32}ClN_3O_6S$ $[M+Na]^+$: 512.1593, found: 512.1580.

10: (White Solid, 0.49 g, 100%). ^{1}H NMR (500 MHz, D_2O) δ 8.43 (s, 1H), 8.37 (d, *J*=5.9 Hz, 1H), 7.97 (d, *J*=7.9 Hz, 1H), 7.85 (d, *J*=14.7 Hz, 1H), 4.47 (t, *J*=7.0 Hz, 2H), 4.16 (t, *J*=5.5 Hz, 2H), 3.71 (t, *J*=6.3 Hz, 2H), 2.88~2.71 (m, 2H), 2.17~2.03 (m, 2H), 1.97~1.82 (m, 2H), 1.60 (dt, *J*=15.4, 7.6 Hz, 3H), 1.36 (s, 6H), 1.32~1.26 (m, 4H), 1.21~1.16 (m, 10H); ^{13}C NMR (126 MHz, D_2O) δ 180.7, 157.9, 157.5, 136.9, 131.9, 130.9, 128.5, 69.7, 67.9, 62.3, 59.1, 51.0, 48.9, 35.6, 30.4, 29.6, 28.2, 28.1, 28.0, 27.8, 27.6, 26.7, 25.0, 23.9, 23.4. HRMS calcd. for $C_{23}H_{36}ClN_3O_6S$ $[M+Na]^+$: 540.1906, found: 540.1894.

2.4 General synthesis of ether **31**-**37**

Typical synthesis procedure for **34** was adopted according previous work[7-8]：To the solution of

4-hydroxy pyridine (1.0 g, 10.5 mmol) in 18 mL acetonitrile was added anhydrous K_2CO_3, and the mixture was heated to reflux for 1 h. DMH-bromide 27 (3.68 g, 12.6 mmol) was then added and the reaction mixture was continued to reflux for 4 h. Afterward, cooled the system and remove inorganic salt by filtration. The filtrate was concentrated and was then applied on flash column chromatography, and washed by using ~95% methanol in dichloromethane (v/v) as the eluent. The corresponding fractions were collected and concentrated to yield compound **34** as a white solid. **35-37** were prepared by the similar procedure, and **31**-**33** were also prepared similarly using 4-hydroxy pyridine instead.

31: (White Solid, 1.53 g, 40.0%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.24-8.20 (m, 1H), 8.16-8.10 (m, 1H), 7.16-7.09 (m, 2H), 3.92 (t, *J* = 6.4 Hz, 2H), 3.43 (t, *J* = 7.3 Hz, 2H), 1.76-1.69 (m, 2H), 1.62–1.56 (m, 2H), 1.44 (s, 2H), 1.35 (s, 6H), 1.33-1.28 (m, 2H)； ^{13}C NMR (126 MHz, $CDCl_3$) δ 177.6, 156.7, 155.2, 141.7, 137.8, 123.9, 121.2, 77.3, 68.1, 58.6, 38.4, 29.0, 27.9, 26.3, 25.5, 25.0.

32: (White Solid, 1.38 g, 30.0%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.27-8.20 (m, 1H), 8.17- 8.10 (m, 1H), 7.18-7.08 (m, 2H), 3.93 (t, *J* = 6.5 Hz, 2H), 3.44-3.38 (m, 2H), 1.75-1.67 (m, 2H), 1.57-1.51 (m, 2H), 1.41-1.37(m, 2H),1.36 (s, 8H), 1.28-1.98 (m, 10H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 177.4, 156.5, 155.3, 141.7, 137.9, 123.9, 121.3, 68.4, 58.6, 38.6, 29.5, 29.4, 29.3, 29.1, 29.0, 28.0, 26.6, 25.9, 25.1.

33: (White Solid, 1.82 g, 40.0%). ^{1}H NMR (500 MHz, $CDCl_3$) δ8.26-8.21 (m, 1H), 8.15-8.10 (m, 1H), 7.15-7.09 (m, 2H), 3.93 (t, *J* = 6.5 Hz, 2H), 3.43-3.39 (m, 2H), 1.75-1.68 (m, 2H), 1.57-1.51 (m, 2H), 1.43-1.37 (m, 2H), 1.36 (s, 6H), 1.26-1.16 (m, 14H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 177.4, 156.6, 155.3, 141.7, 137.9, 123.8, 121.2, 68.4, 58.6, 38.6, 29.5, 29.4, 29.3, 29.1, 29.0, 28.04, 26.62, 25.93, 25.07.

35: (White Solid, 2.03 g, 62.3%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.30 (d, *J*=7.6 Hz, 2H), 6.43 (d, *J*=7.6 Hz, 2H), 6.22 (s, 1H), 3.77 (t, *J*=7.2 Hz, 2H), 3.49 (d, *J*=7.2 Hz, 2H), 1.78 (p, *J*=7.3 Hz, 2H), 1.64 (p, *J*=7.1 Hz, 2H), 1.44 (s, 6H), 1.40~1.30 (m, 4H).

36: (White Solid, 1.73 g, 48.5%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.23~7.20 (m, 2H), 6.36 (d, *J*=7.5 Hz, 2H), 6.25 (s, 1H), 3.69 (t, *J*=7.2 Hz, 2H), 3.41 (t, *J*=7.2 Hz, 2H), 1.69 (p, *J*=7.1 Hz, 2H), 1.54 (p, *J*=7.3 Hz, 2H), 1.36 (s, 6H), 1.28~1.17 (m, 8H).

37: (White Solid, 1.87 g, 46.8%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.21 (d, *J*=9.0 Hz, 2H), 6.35 (d, *J*=7.5 Hz, 2H), 5.81 (s, 1H), 3.69 (t, *J*=7.2 Hz, 2H), 3.41 (t, *J*=7.3 Hz, 2H), 1.71~1.63 (m, 2H), 1.54 (p, *J*=7.0 Hz, 2H), 1.36 (s, 6H), 1.21 (dd, *J*=10.2, 4.8 Hz, 12H).

2.5 General synthesis of precursor **11a**-**16a**

Typical synthesis procedure for **11a** was adopted according previous work[6]：To the solution of **22** (1.01 g, 3.80 mmol) in 10 mL water-EtOH (4:1, V:V) was added sodium chloroacetate (0.44 g, 3.80 mmol), and the resulting mixture was heated to 90℃ for 10 hours. The reaction mixture was concentrated under reduced pressure and the residual was applied on flash column chromatography, washing with methanol/dichloromethane (30 : 70, v/v) as the eluent. The corresponding fractions were collected and concentrated to yield **11a** as white solid. **12a**-**16a** were also prepared by the similar procedure: ω-bromoalkyl carboxylic acid combined with equivalent NaOH was adopted instead respectively for **12-13**, and **31**-**33** was reacted with sodium chloroacetate respectively to produce **14**-**16**.

11a: (slight brown viscous liquid, 0.62 g, 50.1%). ^{1}H NMR (500 MHz, D_2O) δ 8.41 (s, 1H), 8.31 (d, *J*=5.9 Hz, 1H), 8.03 (t, *J*=3.4 Hz, 1H), 7.90 (d, *J*=3.4 Hz, 1H), 5.11 (s, 2H), 4.18 (t, *J*=4.3 Hz, 2H), 3.64 (m, *J*=4.4 Hz, 2H), 2.09 (t, *J*=3.8 Hz, 2H), 1.12 (s, 6H); ^{13}C NMR (126 MHz, D_2O) δ 180.8, 170.6, 157.6, 157.5, 137.9, 133.0, 131.2, 128.2, 68.0, 63.6 59.1, 48.9, 35.7, 26.7, 23.4. HRMS calcd. for $C_{15}H_{19}N_3O_5$ $[M+H]^+$: 322.1397, found: 322.1391.

12a: (slight brown viscous liquid, 1.01 g, 50.1%). ^{1}H NMR (500 MHz, D_2O) δ 8.49 (s, 1H), 8.41 (d, *J*=5.8 Hz, 1H), 8.02 (d, *J*=10.3 Hz, 1H), 7.89 (dd, *J*=8.7, 6.0 Hz, 1H), 4.52 (t, *J*=7.2 Hz, 2H), 4.20 (t, *J*=5.5 Hz, 2H), 3.66 (t, *J*=6.3 Hz, 2H), 2.12 (t, *J*=7.4 Hz, 4H), 1.97 (p, *J*=7.4 Hz, 2H), 1.54 (q, *J*=7.4 Hz, 2H), 1.33 (s, 8H); ^{13}C NMR (126 MHz, D_2O) δ 183.2, 180.8, 157.9, 157.5, 131.9, 130.9, 128.6, 67.9, 62.1, 59., 37.1, 30.3, 26.7, 25.1, 23.4. HRMS calcd. for $C_{19}H_{27}N_3O_5$ $[M+H]^+$: 378.2023, found: 378.2018.

13a: (slight yellow viscous liquid, 1.74 g, 87.5%). ^{1}H NMR (500 MHz, D_2O) δ 8.44 (s, 1H), 8.39 (s, 1H), 8.00 (d, *J*=8.7 Hz, 1H), 7.88 (d, *J*=2.9 Hz, 1H), 4.49 (s, 2H), 4.22~4.12 (m, 2H), 3.78~3.63 (m, 2H), 2.30~2.22 (m, 2H), 2.16~2.06 (m, 2H), 1.92 (s, 2H), 1.47 (s, 2H), 1.37 (s, 6H), 1.20 (d, *J*=16.4 Hz, 10H); ^{13}C NMR (126 MHz, D_2O) δ 184.1, 180.8, 157.9, 157.5, 136.9, 130.9, 128.6, 67.9, 62.3, 59.1, 37.7, 35.7, 30.4, 28.6, 28.3, 27.9, 26.7, 25.9, 25.0, 23.5. HRMS calcd. for $C_{23}H_{35}N_3O_5$ $[M+H]^+$: 434.2649, found: 434.2647.

14a: (slight yellow viscous liquid, 1.53 g, 86.1%). ^{1}H NMR (500 MHz, D_2O) δ 8.40 (s, 1H), 8.29 (d, *J*=5.8 Hz, 1H), 8.04 (d, *J*=8.9 Hz, 1H), 7.89 (d, *J*=5.9 Hz, 1H), 5.11 (s, 2H), 4.17 (t, *J*=6.3 Hz, 2H), 3.42 (t, *J*=6.9 Hz, 2H), 1.77 (m, *J*=6.5 Hz, 2H), 1.56 (m, *J*=7.0 Hz, 2H), 1.43 (m, *J*=7.4 Hz, 2H), 1.32 (s, 6H), 1.27 (m, *J*=7.4 Hz, 2H); ^{13}C NMR (126 MHz, D_2O) δ 181.0, 170.7, 157.9, 137.6, 133.0, 131.1, 128.1, 70.3, 63.5, 59.0, 48.9, 43.6, 38.4, 27.7, 27.0, 25.4, 24.6, 23.4. HRMS calcd. for $C_{18}H_{25}N_3O_5$ $[M+H]^+$: 364.1867, found: 364.1860.

15a: (slight yellow viscous liquid, 2.24 g, 80.6%). ^{1}H NMR (500 MHz, D_2O) δ 8.41 (s, 1H), 8.31 (d,

J=5.8 Hz, 1H), 7.97 (d, *J*=6.7 Hz, 1H), 7.88 (d, *J*=5.9 Hz, 1H), 5.10 (s, 2H), 4.11 (t, *J*=6.3 Hz, 2H), 3.35 (t, *J*=7.0 Hz, 2H), 1.72 (p, *J*=6.4 Hz, 2H), 1.47 (p, *J*=6.7 Hz, 2H), 1.41~1.32 (m, 8H), 1.23 (d, *J*=33.8 Hz, 10H); ^{13}C NMR (126 MHz, D_2O) δ 180.2, 170.1, 157.7, 137.9, 132.7, 131.0, 128.2, 70.4, 63.5, 58.7, 48.8, 43.2, 38.3, 28.3, 27.5, 26.1, 25.4, 23.7. HRMS calcd. for $C_{22}H_{33}N_3O_5$ $[M+H]^+$: 420.2493, found: 420.2689.

16a: (slight yellow viscous liquid, 1.74 g, 87.5%). ^{1}H NMR (500 MHz, D_2O) δ 8.41 (s, 1H), 8.31 (d, *J*=5.8 Hz, 1H), 7.92 (d, *J*=9.8 Hz, 1H), 7.86 (d, *J*=5.8 Hz, 1H), 5.07 (s, 3H), 4.08 (t, *J*=6.1 Hz, 2H), 3.32 (t, *J*=6.9 Hz, 2H), 1.78~1.62 (m, 2H), 1.55~1.42 (m, 2H), 1.41~1.31 (m, 3H), 1.21 (d, *J*=6.1 Hz, 24H); ^{13}C NMR (126 MHz, D_2O) δ 174.6, 157.4, 154.7, 138.4, 132.5, 130.8, 128.3, 70.3, 65.66, 63.7, 60.4, 39.4, 29.6, 29.1, 28.8, 27.7, 26.5, 25.6, 21.7. HRMS calcd. for $C_{24}H_{37}N_3O_5$ $[M+H]^+$: 448.2806, found: 448.2801.

2.6 General synthesis of precursor **17a**-**20a**

Typical synthesis procedure for **17a** was adopted according previous work[6]：To the solution of **34** (1.01 g, 3.80 mmol) in 10 mL water-EtOH (4:1, V:V) was added sodium chloroacetate (0.44 g, 3.80 mmol), and the resulting mixture was heated to 90℃ for 10 hours. The reaction mixture was concentrated under reduced pressure and the residual was applied on flash column chromatography, washing with methanol/dichloromethane (30 : 70, v/v) as the eluent. The corresponding fractions were collected and concentrated to yield **17a** as white solid. **18a**-**20a** were also prepared by the identical procedure

17a: (slight brown viscous liquid, 1.08 g, 56.6%). ^{1}H NMR (500 MHz, D_2O) δ 8.62 (d, *J*=7.5 Hz, 2H), 7.42 (d, *J*=7.5 Hz, 2H), 4.82 (s, 2H), 4.45 (t, *J*=7.2 Hz, 2H), 3.56 (t, *J*=6.6 Hz, 2H), 2.32~2.27 (m, 2H), 1.40 (s, 6H); ^{13}C NMR (126 MHz, D_2O) δ 180.7, 173.4, 170.4, 157.2, 145.6, 114.0, 68.1, 59.2, 57.1, 35.1, 28.7, 23.4. HRMS calcd. for $C_{15}H_{19}N_3O_5$ $[M+H]^+$: 322.1397 , found: 322.1392.

18a: (slight yellow viscous liquid, 0.90 g, 41.2%). ^{1}H NMR (500 MHz, D_2O) δ 8.47 (d, *J*=7.2 Hz, 2H), 7.29 (d, *J*=7.2 Hz, 2H), 4.30 (t, *J*=7.2 Hz, 2H), 3.33 (t, *J*=6.9 Hz, 2H), 1.82 (p, *J*=7.2 Hz, 2H), 1.46 (q, *J*=7.0 Hz, 2H), 1.27 (s, 6H), 1.19 (dt, *J*=29.3, 12.1 Hz, 4H); ^{13}C NMR (126 MHz, D_2O) δ 180.9, 173.3, 170.0, 157.6, 145.4, 113.8, 67.9, 58.9, 38.2, 30.0, 26.9, 25.2, 24.7. HRMS calcd. for $C_{18}H_{25}N_3O_5$ $[M+H]^+$: 364.1867, found: 364.1860.

19a: (slight yellow viscous liquid, 0.86 g, 40.9%). ^{1}H NMR (500 MHz, D_2O) δ 8.51 (d, *J*=7.3 Hz, 2H), 7.33 (d, *J*=7.3 Hz, 2H), 4.74 (s, 2H), 4.33 (d, *J*=7.2 Hz, 2H), 3.37 (t, *J*=6.9 Hz, 2H), 1.91~1.80 (m, 2H), 1.48 (p, *J*=7.0 Hz, 2H), 1.31 (s, 6H), 1.18 (d, *J*=40.1 Hz, 8H); ^{13}C NMR (126 MHz, D_2O) δ 181.1, 173.5, 170.0, 145.5, 113.9, 68.1, 60.1, 59.0, 38.5, 27.9, 27.1, 25.6, 25.0, 23.5. HRMS calcd. for $C_{20}H_{29}N_3O_5$ $[M+H]^+$: 392.2180, found: 392.2173.

20a: (slight yellow viscous liquid, 0.92 g, 43.7%). ^{1}H NMR (500 MHz, D_2O) δ 8.52 (d, *J*=7.2 Hz, 2H), 7.34 (d, *J*=7.2 Hz, 2H), 4.74 (s, 2H), 4.32 (t, *J*=7.1 Hz, 2H), 3.29 (t, *J*=6.8 Hz, 2H), 1.80 (s, 2H), 1.43~1.35 (m, 2H), 1.25 (s, 6H), 1.10 (d, *J*=40.0 Hz, 12H); ^{13}C NMR (126 MHz, D_2O) δ 180.5, 172.8, 169.9, 157.4, 145.6, 113.9, 60.1, 58.9, 38.4, 30.4, 27.3, 25.9, 25.4, 23.7. HRMS calcd. for $C_{22}H_{33}N_3O_5$ $[M+H]^+$: 420.2493, found: 420.2688.

2.7 General synthesis of *N*-chloramine **11**-**20**

N-chloramine **11**-**20** were prepared by the similar procedure as **7**-**10**.

11: (colorless viscous liquid, 0.66 g, 100%). ^{1}H NMR (500 MHz, D_2O) δ 8.41 (s, 1H), 8.33 (d, *J*=5.0 Hz, 1H), 8.04 (d, *J*=7.7 Hz, 1H), 7.93~7.87 (m, 1H), 5.15 (s, 2H), 4.19 (t, *J*=4.9 Hz, 2H), 3.73 (t, *J*=6.3 Hz, 2H), 2.16~2.06 (m, 2H), 1.39 (s, 6H); ^{13}C NMR (126 MHz, D_2O) δ 177.0, 157.5, 138.0, 132.9, 131.2, 128.2, 63.5, 37.0, 26.6, 20.9. HRMS calcd. for $C_{15}H_{18}ClN_3O_5$ $[M+H]^+$: 356.1008, found: 356.1000.

12: (colorless viscous liquid, 0.68 g, 100%). ^{1}H NMR (500 MHz, D_2O) δ 8.42 (s, 1H), 8.31 (d, *J*=5.9 Hz, 1H), 8.06 (d, *J*=8.8 Hz, 1H), 7.91 (d, *J*=5.9 Hz, 1H), 4.17 (t, *J*=6.3 Hz, 2H), 3.50 (t, *J*=6.9 Hz, 2H), 1.76 (p, *J*=6.5 Hz, 2H), 1.57 (dt, *J*=14.4, 6.9 Hz, 2H), 1.48~1.19 (m, 10H); ^{13}C NMR (126 MHz, D_2O) δ 178.6, 176.9, 157.8, 155.8, 136.9, 130.9, 128.6, 67.9, 66.2, 61.9, 37.0, 30.1, 29.6, 26.6, 23.5, 20.9. HRMS calcd. for $C_{19}H_{26}ClN_3O_5$ $[M+H]^+$: 412.1634, found: 412.1626.

13: (colorless viscous liquid, 0.51 g, 100%). ^{1}H NMR (500 MHz, D_2O) δ 8.40 (s, 1H), 8.32 (s, 1H), 7.95 (s, 1H), 7.87 (s, 1H), 5.12 (s, 2H), 4.09 (s, 2H), 3.44 (s, 2H), 1.70 (s, 2H), 1.51 (s, 2H), 1.35 (s, 8H), 1.20 (s, 10H); ^{13}C NMR (126 MHz, D_2O) δ 184.1, 180.8, 157.9, 157.5, 136.9, 130.9, 128.6, 67.9, 62.3, 59.1, 37.7, 35.7, 30.4, 28.6, 28.3, 27.9, 26.7, 25.9, 25.0, 23.5. HRMS calcd. for $C_{23}H_{34}ClN_3O_5$ $[M+H]^+$: 468.2260, found: 468.2258.

14: (colorless viscous liquid, 0.66 g, 100%). ^{1}H NMR (500 MHz, D_2O) δ 8.41 (s, 1H), 8.32 (s, 1H), 7.97 (s, 1H), 7.87 (s, 1H), 5.12 (s, 2H), 4.12 (s, 2H), 3.40 (d, *J*=44.4 Hz, 2H), 1.71 (s, 2H), 1.34 (s, 8H), 1.20 (s, 2H); ^{13}C NMR (126 MHz, D_2O) δ 158.0, 137.7, 133.2, 131.5, 128.2, 70.3, 62.2, 58.9, 38.3, 27.7, 25.4, 24.5, 23.4. HRMS calcd. for $C_{18}H_{24}ClN_3O_5$ $[M+H]^+$: 398.1477, found: 398.1471.

15: (colorless viscous liquid, 0.66 g, 100%).。 ^{1}H NMR (500 MHz, D_2O) δ 8.42 (s, 1H), 8.32 (d, *J*=5.8 Hz, 1H), 7.94 (dd, *J*=8.8, 2.2 Hz, 1H), 7.88 (dd, *J*=8.9, 5.9 Hz, 1H), 5.10 (t, *J*=7.2 Hz, 2H), 4.09 (t, *J*=5.5 Hz, 2H), 3.40 (t, *J*=6.3 Hz, 2H), 1.70 (t, *J*=7.3 Hz, 2H), 1.53 (p, *J*=7.4, 6.6 Hz, 2H), 1.37 (s, 6H), 1.31~1.27 (m, 12H); ^{13}C NMR (126 MHz, D_2O) δ 179.6, 177.3, 157.6, 138.1, 131.0, 70.4, 65.8, 59.9, 43.1, 38.2, 29.7, 29.3, 29.0, 28.4, 26.2, 25.4, 23.9, 21.6. HRMS calcd. for $C_{22}H_{32}ClN_3O_5$ $[M+H]^+$: 454.2103, found: 454.2097.

16: (colorless viscous liquid, 0.64 g, 100%). ^{1}H NMR (500 MHz, D_2O) δ 8.38 (s, 1H), 8.29 (d, *J* = 5.5 Hz, 1H), 7.87 (d, *J* = 8.8 Hz, 1H), 7.86~7.77 (m, 1H), 5.05 (s, 2H), 4.04 (s, 2H), 3.44 (s, 2H), 1.67 (s, 2H), 1.52 (s, 2H), 1.34 (s, 8H), 1.20 (s, 14H); ^{13}C NMR (126 MHz, D_2O) δ 174.6, 157.4, 154.7, 138.4, 132.5, 130.8, 128.3, 70.3, 65.7, 63.7, 60.4, 39.4, 29.6, 29.1, 28.8, 27.7, 26.5, 25.8, 21.7. HRMS calcd. for $C_{24}H_{36}ClN_3O_5$ $[M+H]^+$: 482.2416, found: 482.2411.

17: (colorless viscous liquid, 0.56 g, 100%). ^{1}H NMR (500 MHz, D_2O) δ 8.41 (s, 1H), 8.33 (d, *J*=5.0 Hz, 1H), 8.04 (d, *J*=7.7 Hz, 1H), 7.93~7.87 (m, 1H), 5.15 (s, 2H), 4.19 (t, *J*=4.9 Hz, 2H), 3.73 (t, *J*=6.3 Hz, 2H), 2.16~2.06 (m, 2H), 1.39 (s, 6H); ^{13}C NMR (126 MHz, D_2O) δ 176.9, 172.7, 170.2, 155.5, 145.7, 114.0, 67.6, 66.3, 57.1, 36.3, 29.6, 20.9. HRMS calcd. for $C_{15}H_{18}ClN_3O_5$ $[M+H]^+$: 356.1008, found: 356.1002.

18: (colorless viscous liquid, 0.66 g, 100%). ^{1}H NMR (500 MHz, D_2O) δ 8.40 (d, *J*=6.6 Hz, 2H), 7.21 (d, *J*=6.5 Hz, 2H), 4.63 (s, 2H), 4.22 (t, *J*=6.8 Hz, 2H), 3.34 (t, *J*=6.7 Hz, 2H), 1.81~1.68 (m, 2H), 1.45~1.36 (m, 2H), 1.27 (s, 6H), 1.15 (d, *J*=24.9 Hz, 4H); ^{13}C NMR (126 MHz, D_2O) δ 177.2, 173.4, 170.0, 156.0, 113.8, 66.1, 59.8, 39.4, 26.7, 25.2, 24.6, 20.9. HRMS calcd. for $C_{18}H_{24}ClN_3O_5$ $[M+H]^+$: 398.1477, found: 398.1472.

19: (colorless viscous liquid, 0.49 g, 100%). ^{1}H NMR (500 MHz, D_2O) δ 8.50 (d, *J*=7.1 Hz, 2H), 7.31 (d, *J*=7.1 Hz, 2H), 4.72 (s, 2H), 4.32 (t, *J*=7.2 Hz, 2H), 3.44 (t, *J*=6.9 Hz, 2H), 1.84 (q, *J*=6.4 Hz, 2H), 1.48 (p, *J*=7.0 Hz, 2H), 1.36 (s, 6H), 1.19 (d, *J*=13.4 Hz, 8H); ^{13}C NMR (126 MHz, D_2O) δ 177.3, 173.5, 170.0, 156.1, 69.8, 66.2, 60.0, 39.8, 30.1, 27.9, 26.9, 25.6, 25.0, 21.1. HRMS calcd. for $C_{20}H_{28}ClN_3O_5$ $[M+H]^+$: 426.1790, found: 426.1783.

20: (colorless viscous liquid, 0.58 g, 100%). ^{1}H NMR (500 MHz, D_2O) δ 8.53 (d, *J*=7.2 Hz, 2H), 7.35 (d, *J*=7.2 Hz, 2H), 4.34 (t, *J*=7.1 Hz, 2H), 3.41 (t, *J*=6.8 Hz, 2H), 1.83 (s, 2H), 1.47~1.41 (m, 2H), 1.34 (s, 6H), 1.14 (d, *J*=40.0 Hz, 12H); ^{13}C NMR (126 MHz, D_2O) δ 176.4, 170.1, 155.6, 145.5, 113.9, 68.1, 66.0, 60.0, 39.6, 30.4, 29.7, 28.3, 27.2, 25.9, 23.6, 21.3. HRMS calcd. for $C_{22}H_{32}ClN_3O_5$ $[M+H]^+$: 454.2103, found: 454.2098.

3. Typical NMR spectra analysis

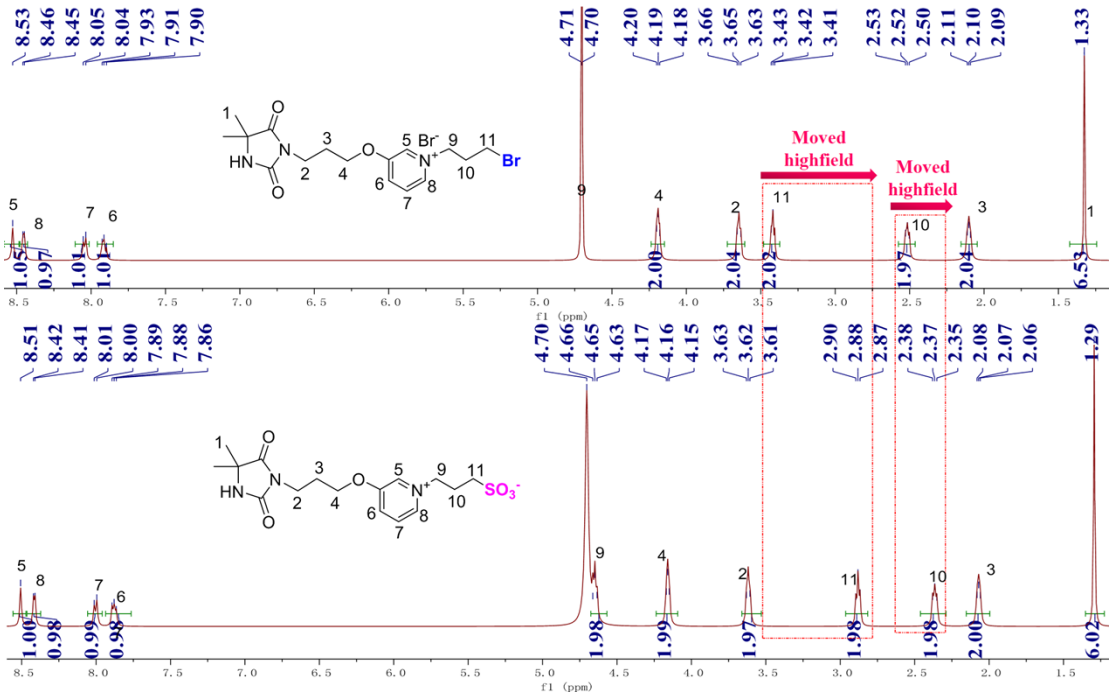


Fig. S1 ^{1}H NMR spectra of **23** and **7a** (before and after sulfonation)

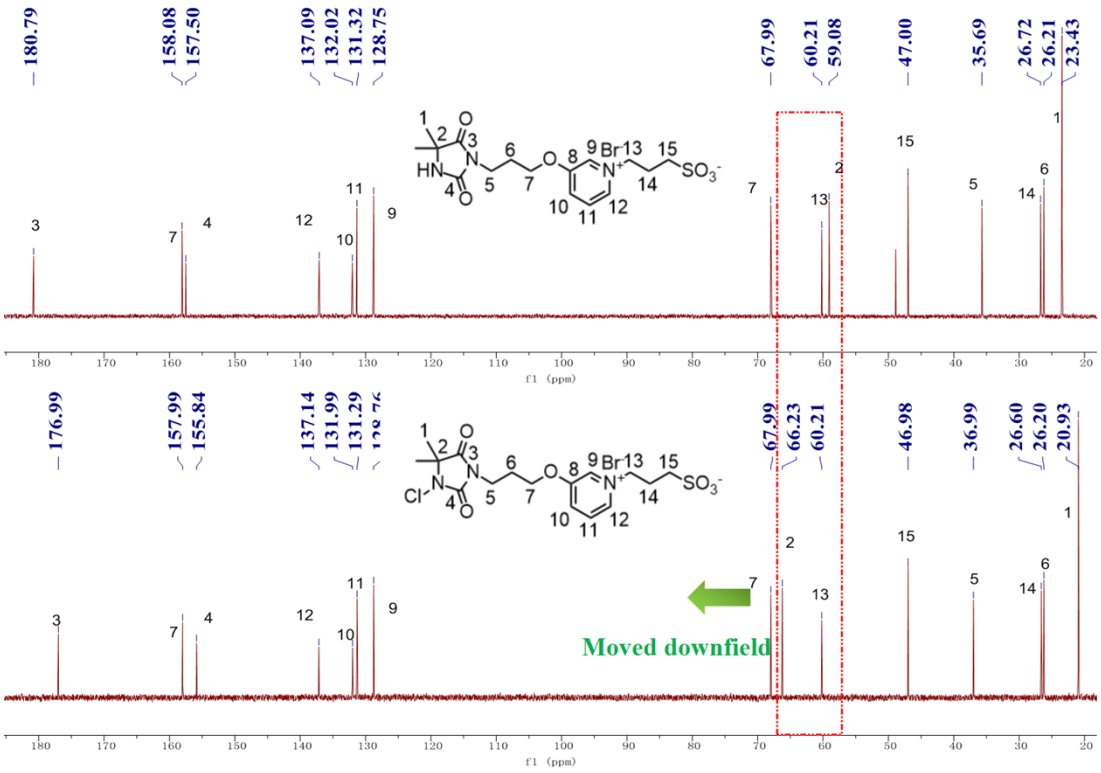


Fig. S2 ^{13}CNMR spectra of **7a** and **7** (before and after chlorination)

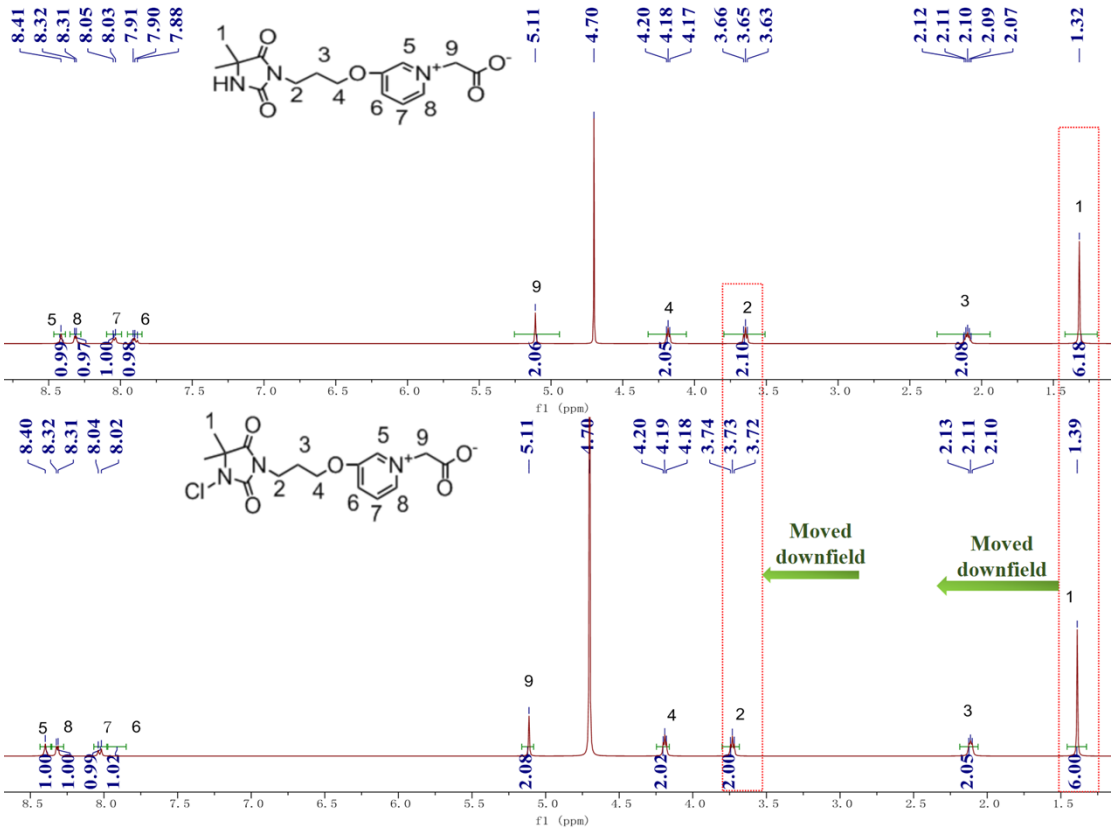


Fig. S3 ^{1}HNMR spectra of **11a** and **11** (before and after chlorination)

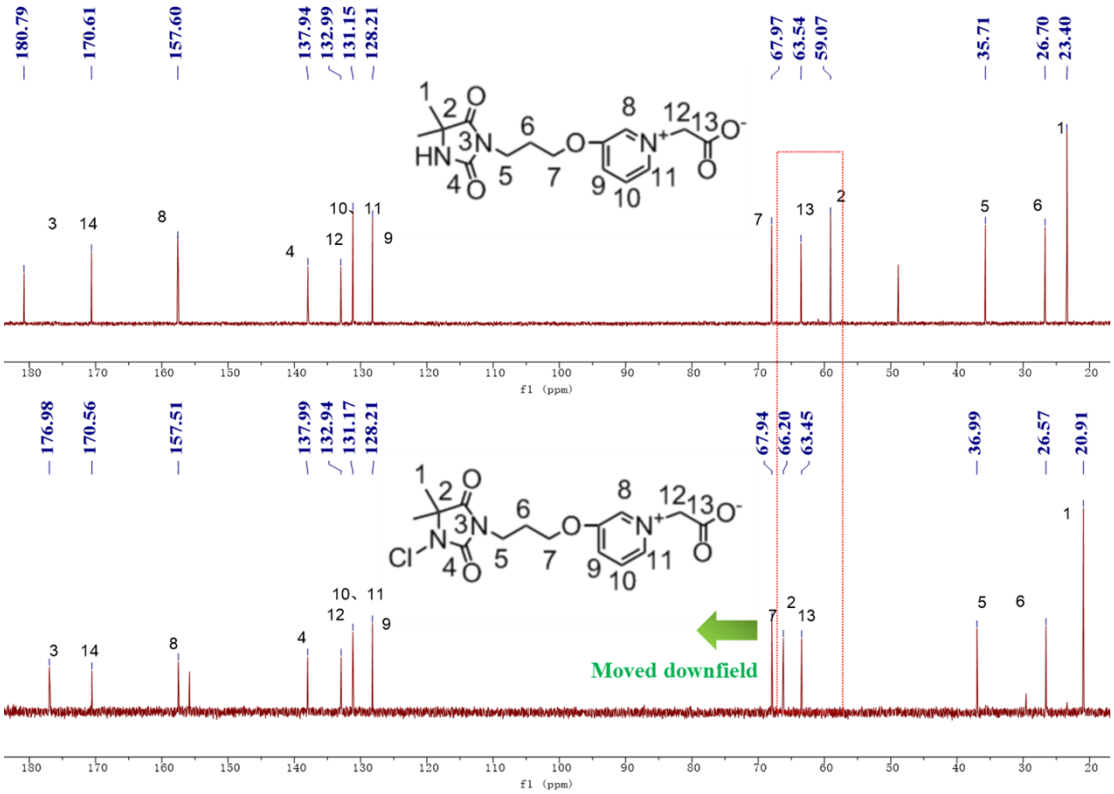


Fig. S4 ^{13}CNMR spectra of **11a** and **11** (before and after chlorination)

5. Antimicrobial test procedure

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 *N*-chloramine **7**-**20** 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}).

*It is worthwhile to mention that stock solution concentration of *N*-chloramine **10** and **16** was 0.028 M due to its comparatively poor aqueous solubility, and the antibacterial test procedure was slightly modified accordingly.

6. Antibacterial data of *N*-chloramine **7**-**10** and **11**-**13**

Table. S1 Bactericidal efficacy of *N*-chloramine **7**-**10**

Bacteria	Compouds	Active Cloramine/ppm	Contact Time (min)			
			5		10	
			KR	*KL*	*KR*	*KL*
S.aureus[a]	**2a**	0	0	0	0	0
	2	20	30.47±1.78	0.16±0.01	94.67±0.88	1.27±0.08
	7a	0	0	0	0	0
	7	20	25.74±2.96	0.13±0.02	60.65±0.30	0.41±0.01
	8a	0	0	0	0	0
	8	20	10.06±0.59	0.05±0.01	21.60±1.18	0.11±0.01
	9a	0	0	0	0	0
	9	20	14.79±1.48	0.07±0.01	32.54±2.37	0.17±0.02
	10a	0	0	0	0	0
	10	20	17.16±0.59	0.08±0.01	35.50±1.18	0.19±0.01
E.coli[b]	**2a**	0	0	0	0	0
	2	20	90.12±2.47	1.01±0.12	100	6.20
	7a	0	0	0	0	0
	7	20	74.07±3.70	0.59±0.02	99.63±0.12	2.43±0.17
	8a	0	0	0	0	0
	8	20	40.74±2.47	0.23±0.02	69.14±4.94	0.51±0.07
	9a	0	0	0	0	0
	9	20	51.85±1.23	0.32±0.01	96.30±2.47	1.43±0.17
	10a	0	0	0	0	0
	10	20	61.73±4.94	0.42±0.06	98.77±0.00	1.90±0.00

Note: [a] Inoculum concentration was 6.76×10^6 CFU/mL; [b] Inoculum concentration was 1.62×10^6 CFU/mL

Table. S2 Bactericidal efficacy of N-chloramine **11**-**13**

Bacteria	Compounds	Active Chloramine/ppm	Contact Time (min)			
			5		10	
			KR	KL	KR	KL
S.aureus[a]	2a	0	0	0	0	0
	2	20	35.71±1.78	0.19±0.01	82.14±2.14	0.75±0.03
	11a	0	0	0	0	0
	11	20	30.36±1.07	0.16±0.01	62.50±0.71	0.43±0.01
	12a	0	0	0	0	0
	12	20	21.80±2.50	0.12±0.02	26.79±1.79	0.14±0.01
	13a	0	0	0	0	0
	13	20	27.50±2.50	0.14±0.02	50.36±2.86	0.30±0.02
E.coli[b]	2a	0	0	0	0	0
	2	20	55.22±2.99	0.35±0.03	96.27±2.99	1.43±0.21
	11a	0	0	0	0	0
	11	20	51.79±1.43	0.32±0.02	92.85±2.14	1.15±0.15
	12a	0	0	0	0	0
	12	20	33.58±0.75	0.18±0.01	83.58±2.24	0.78±0.07
	13a	0	0	0	0	0
	13	20	46.27±1.49	0.27±0.01	91.04±4.48	1.05±0.30

Note: [a] Inoculum concentration was 5.60×10^6 CFU/mL; [b] Inoculum concentration was 2.68×10^6 CFU/mL

7. References and notes

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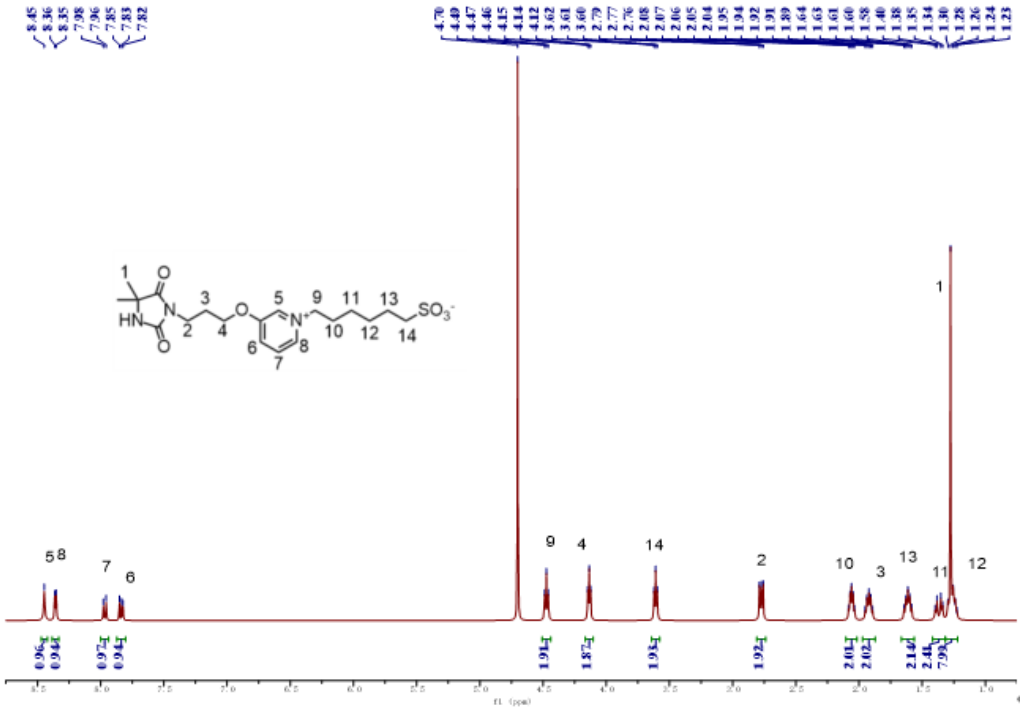
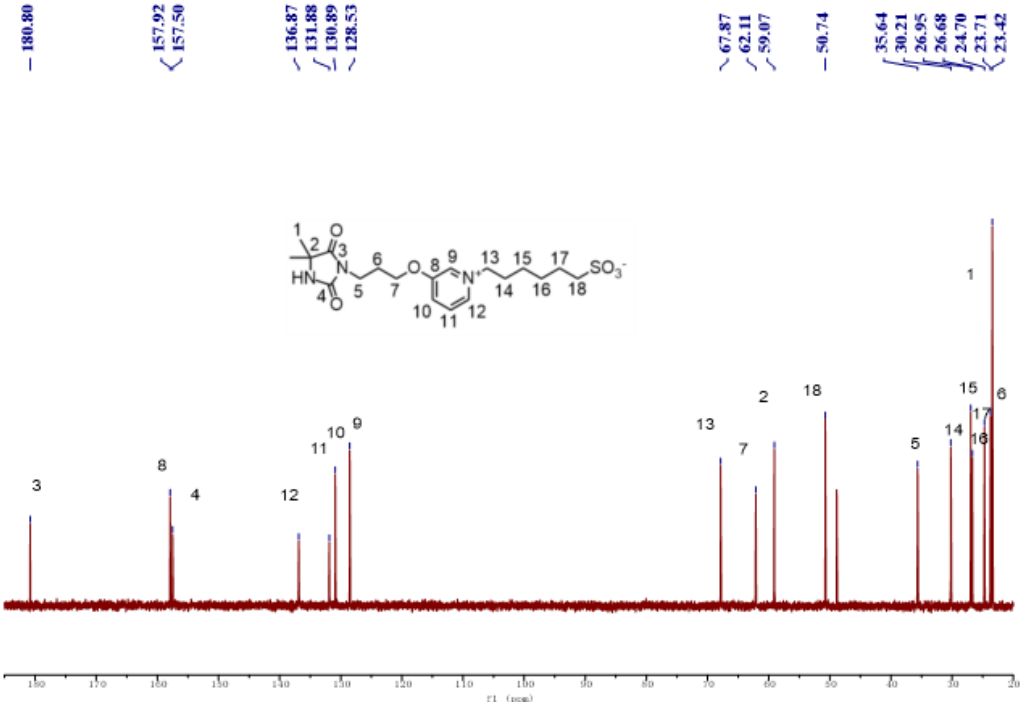
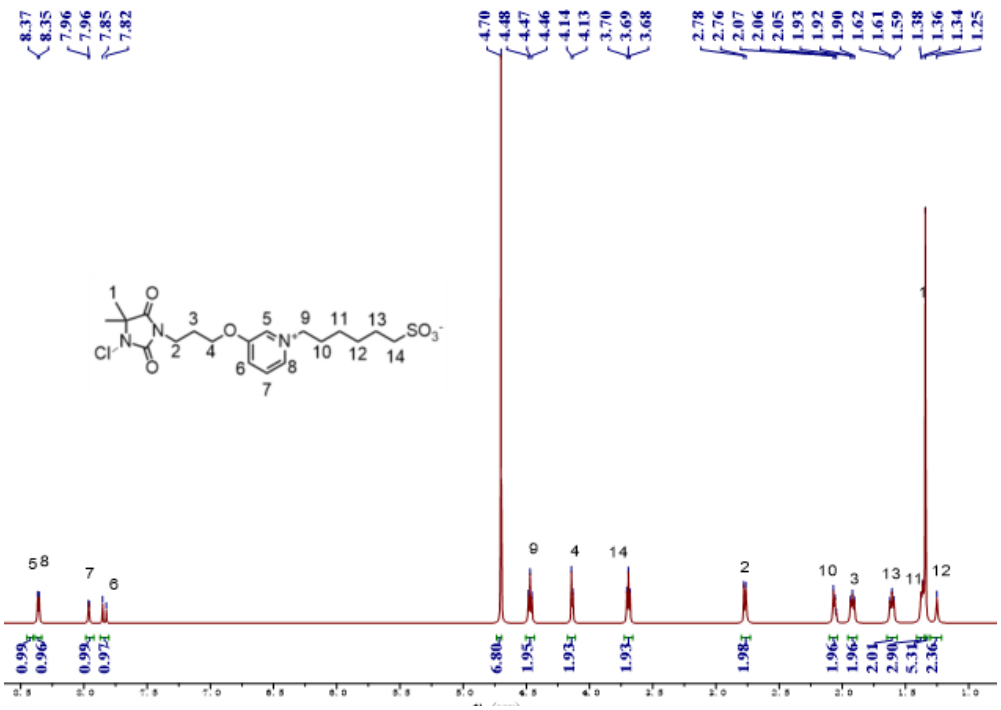
7. Original NMR spectra data



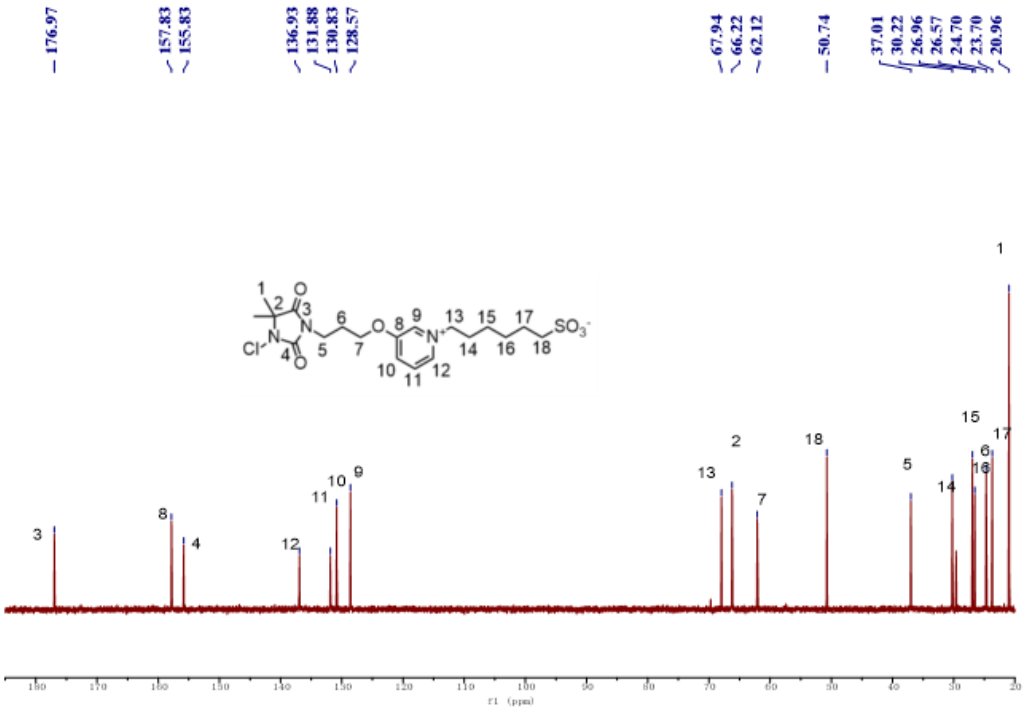
^{1}H NMR spectra of *N*-chloramine precursor **8a**



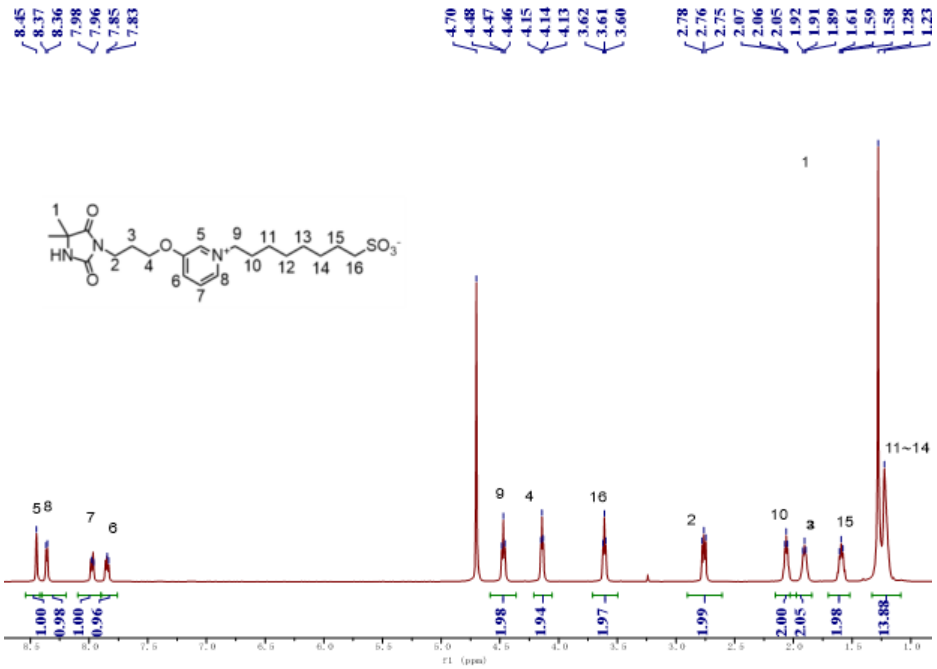
^{13}C NMR spectra of precursor **8a**



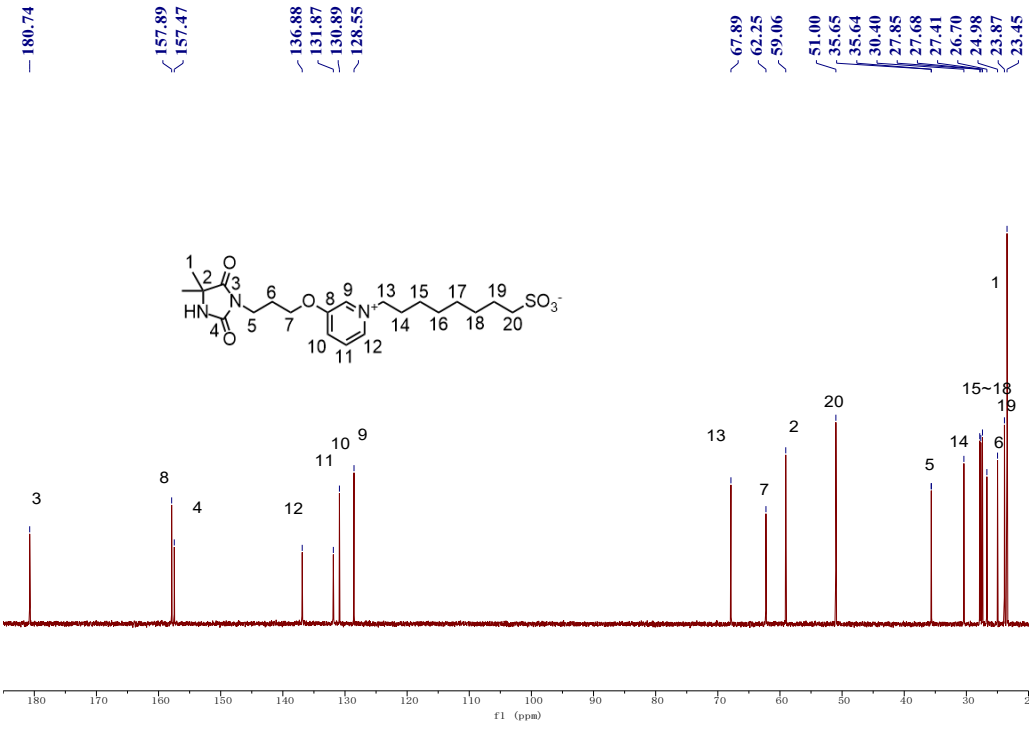
^{1}H NMR spectra of *N*-chloramine **8**



^{13}C NMR spectra of *N*-chloramine **8**



^{1}H NMR spectra of precursor **9a**



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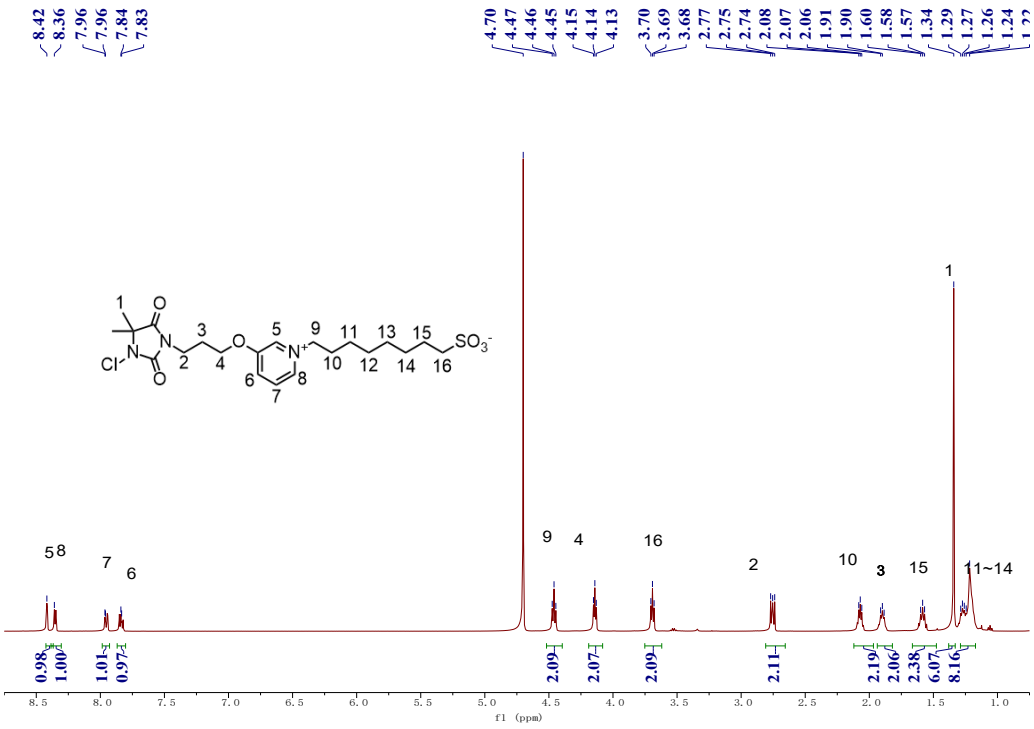
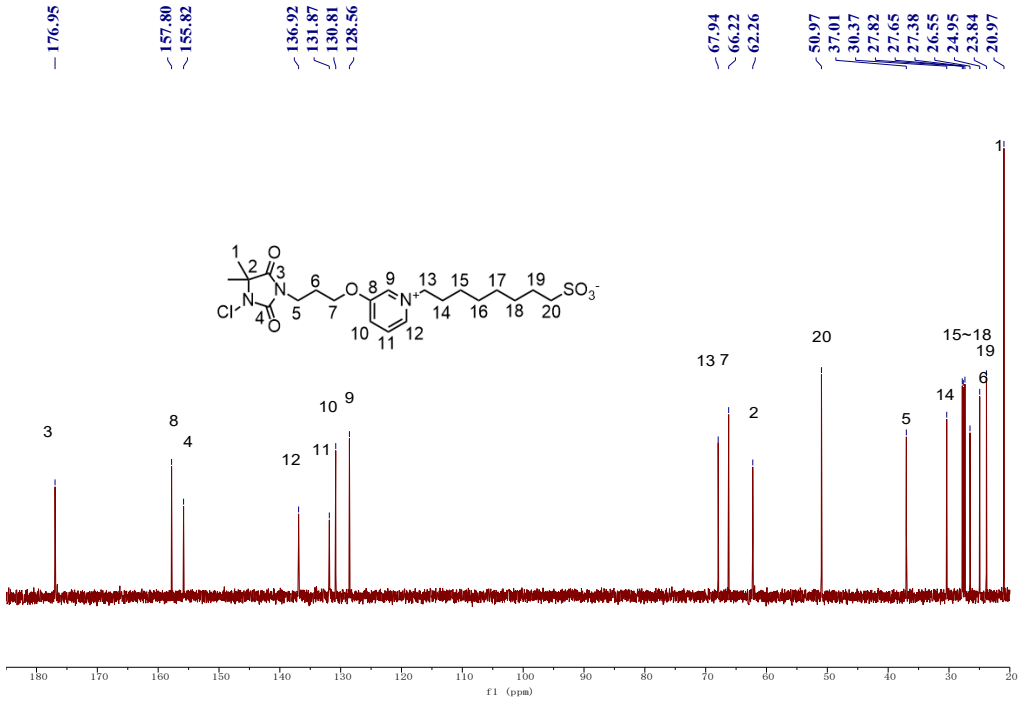
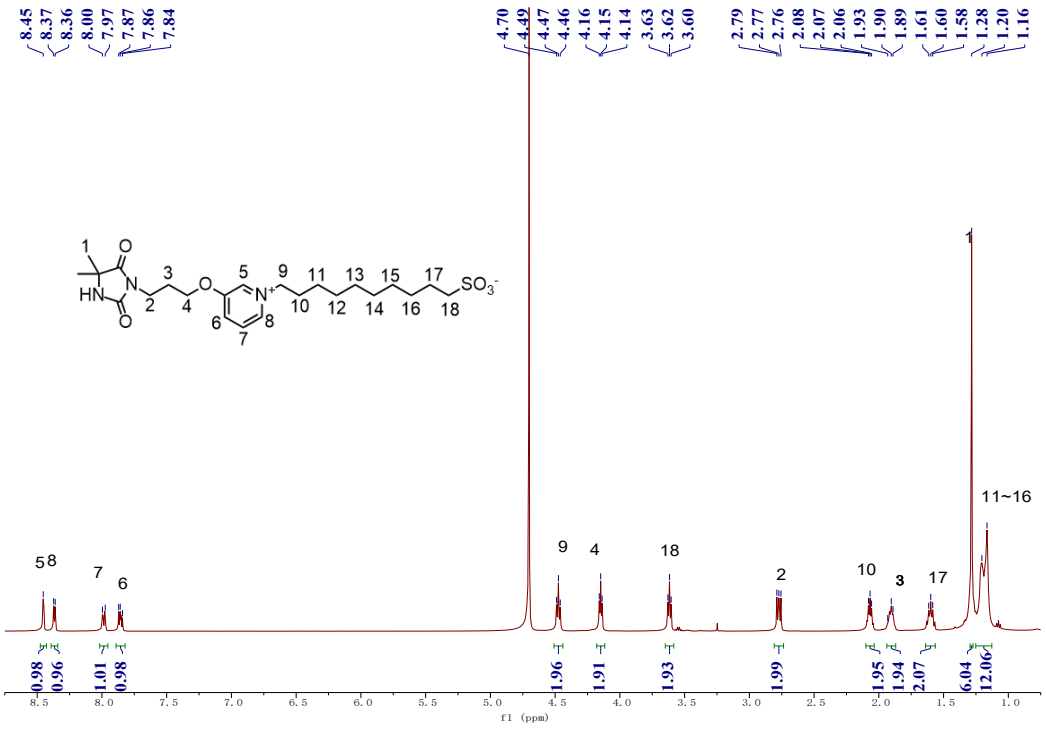


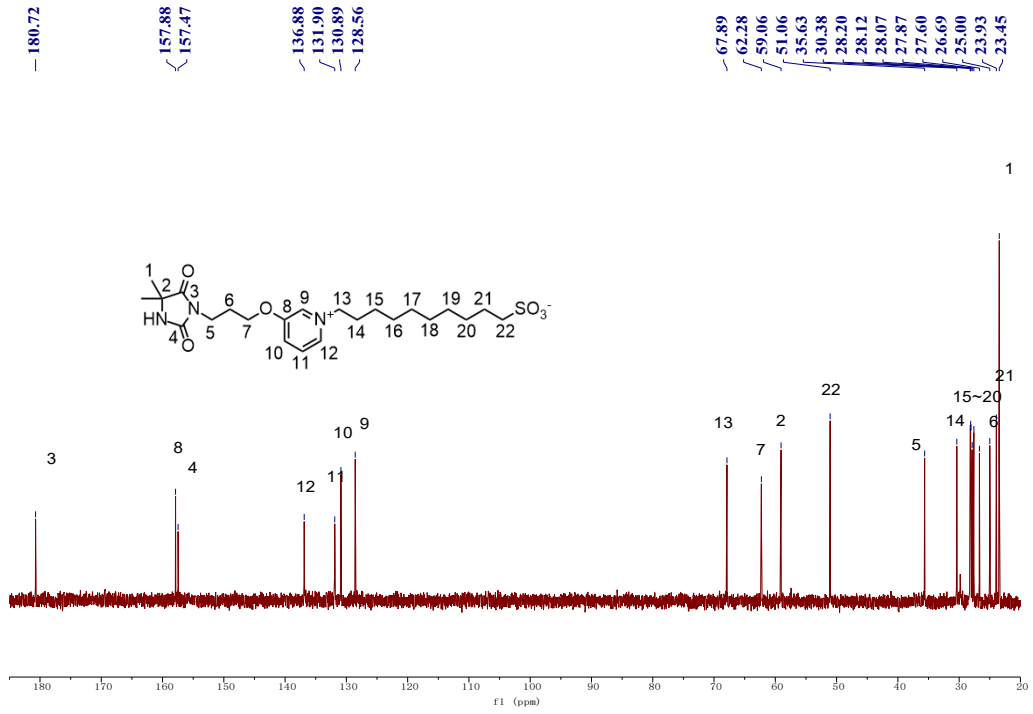
^{1}H NMR spectra of *N*-chloramine **9**



^{13}C NMR spectra of *N*-chloramine **9**



^{1}H NMR spectra of precursor **10a**



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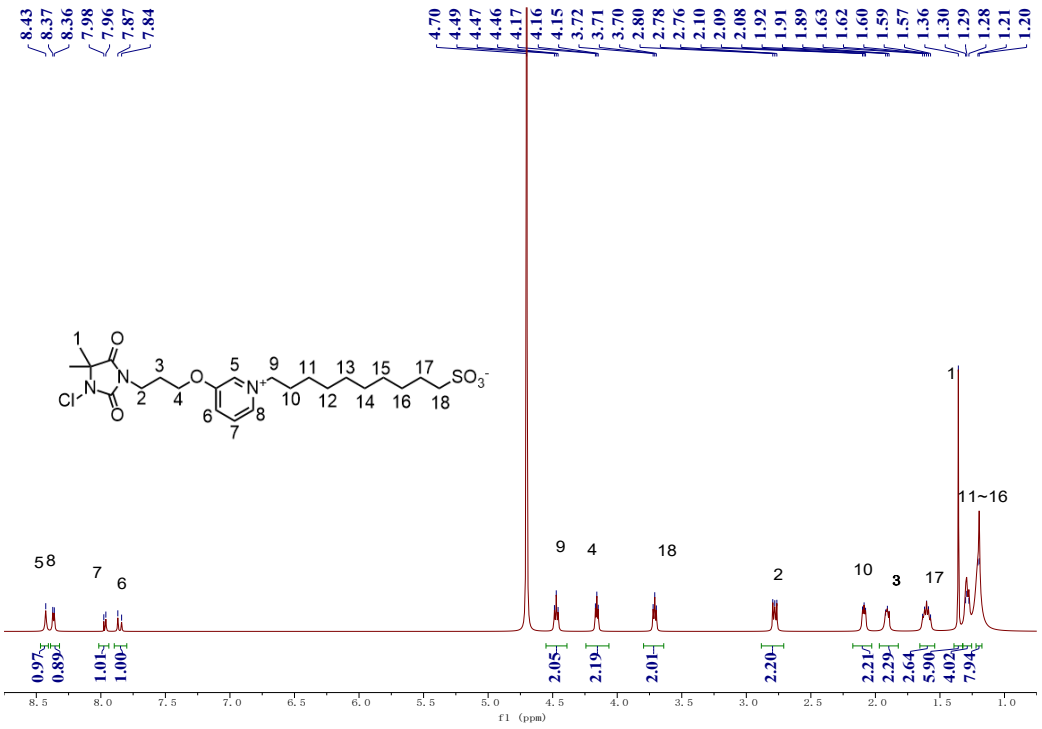
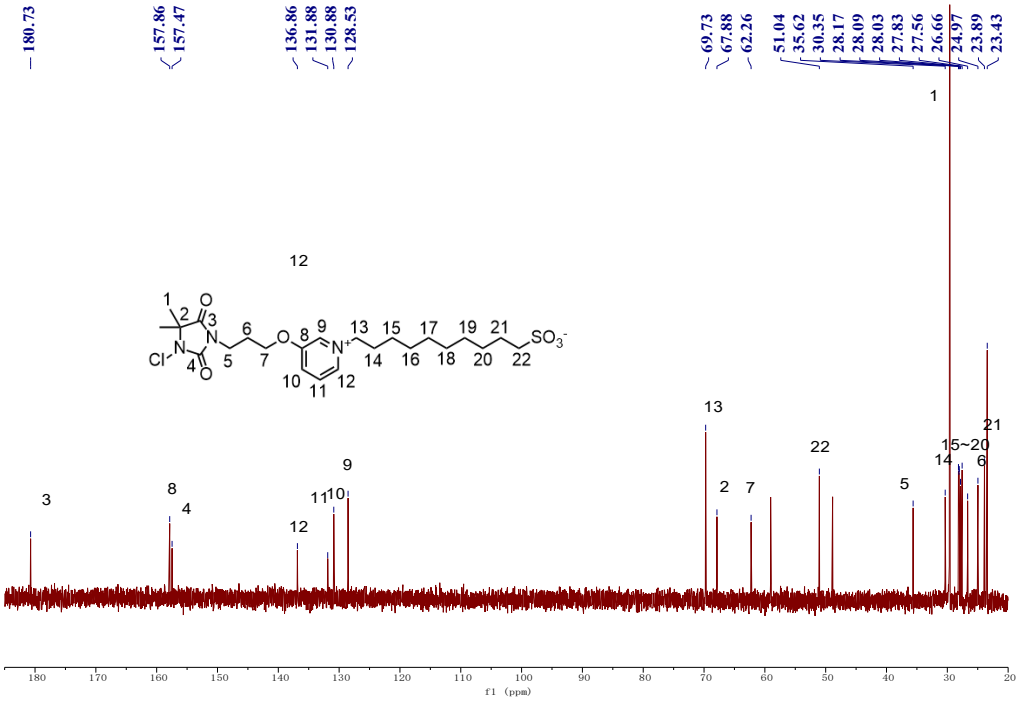
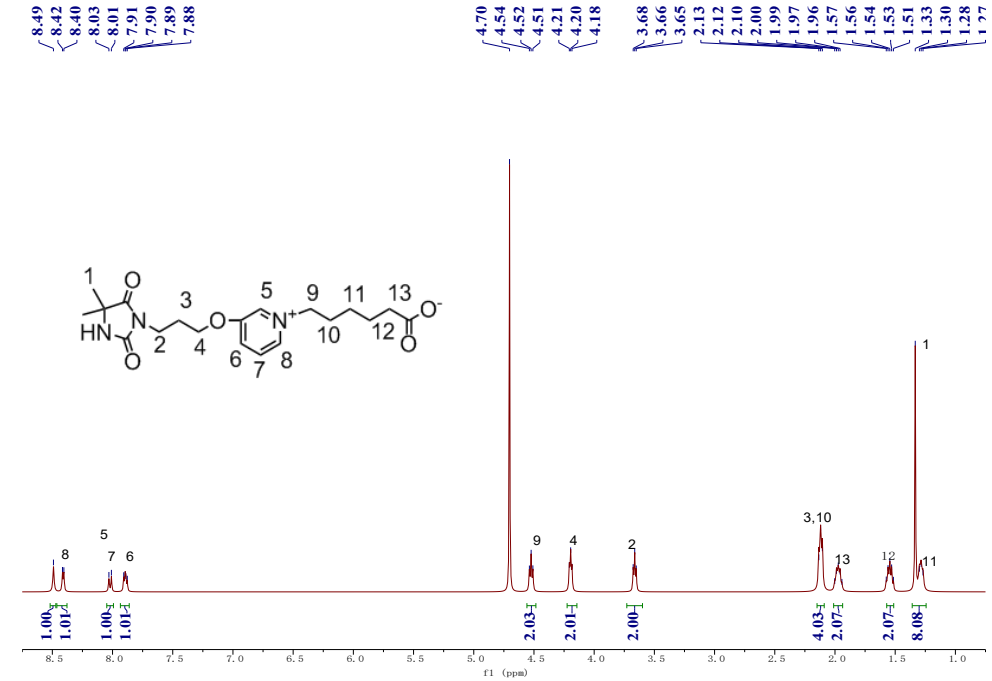


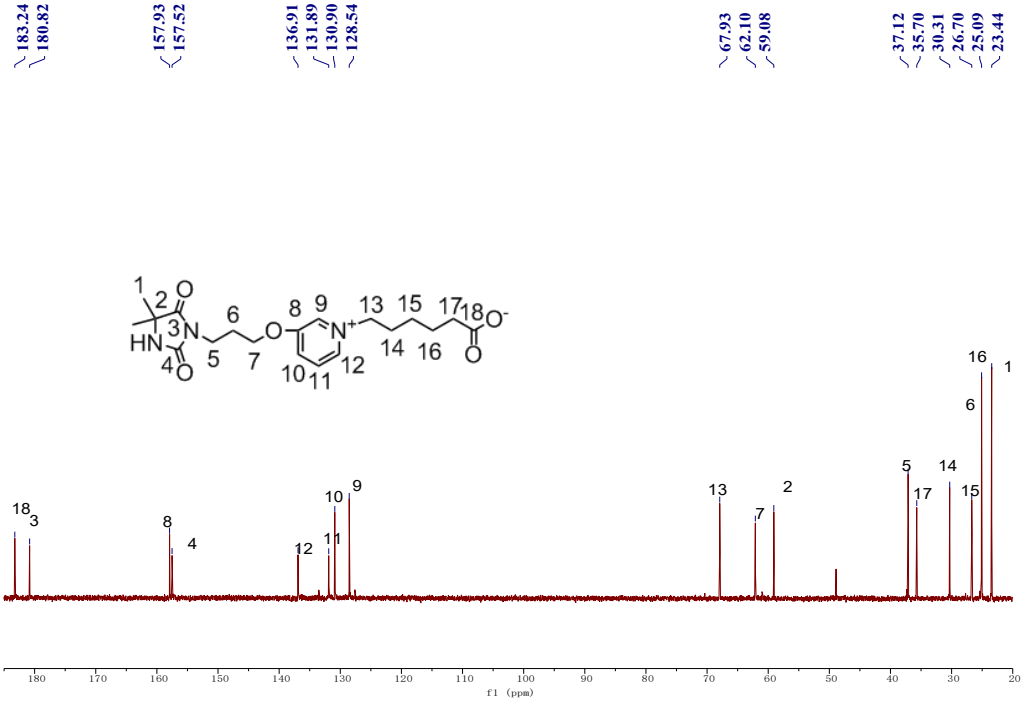
^{1}H NMR spectra of *N*-chloramine **10**



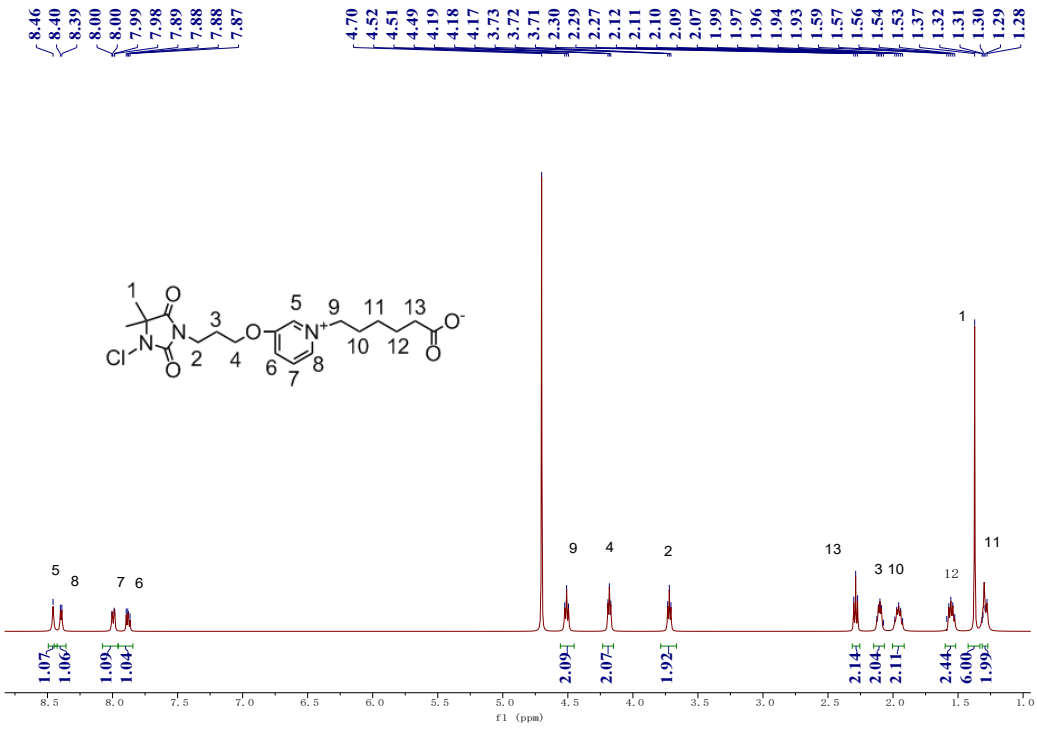
The ^{13}C NMR spectra of *N*-chloramine **10**



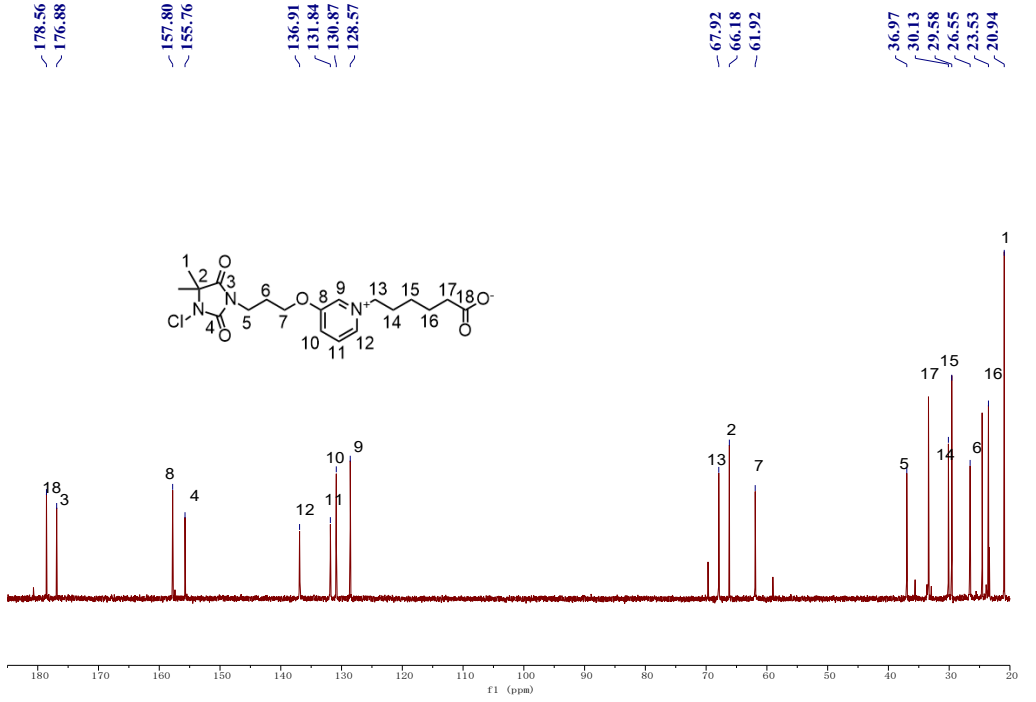
^{1}H NMR spectra of precursor **12a**



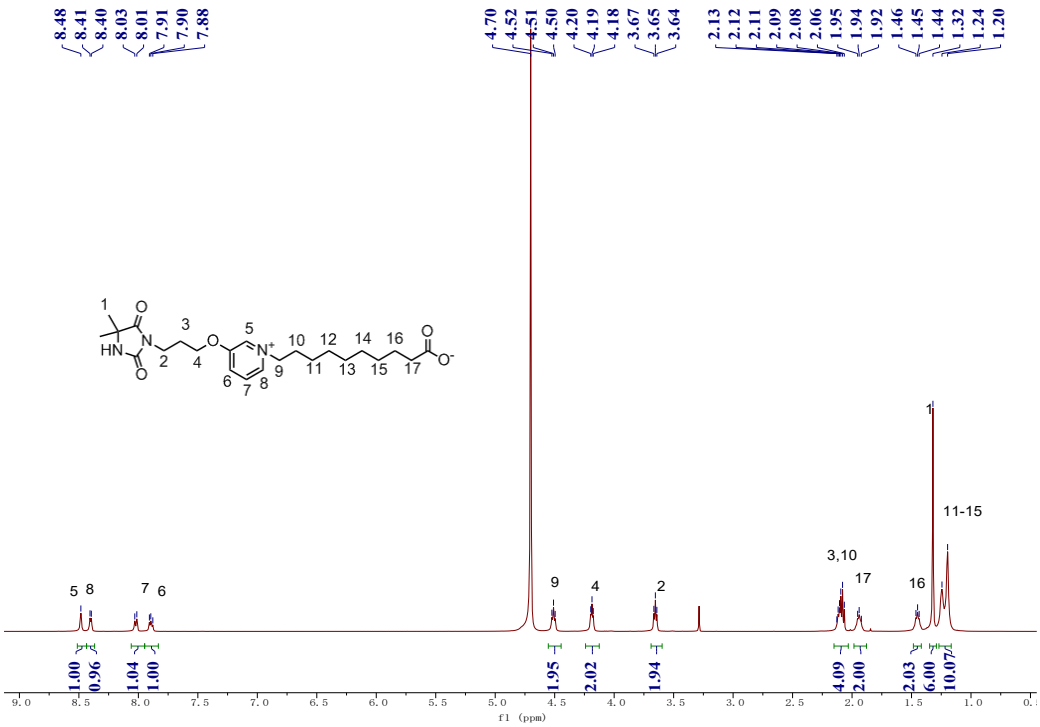
^{13}C NMR spectra of precursor **12a**



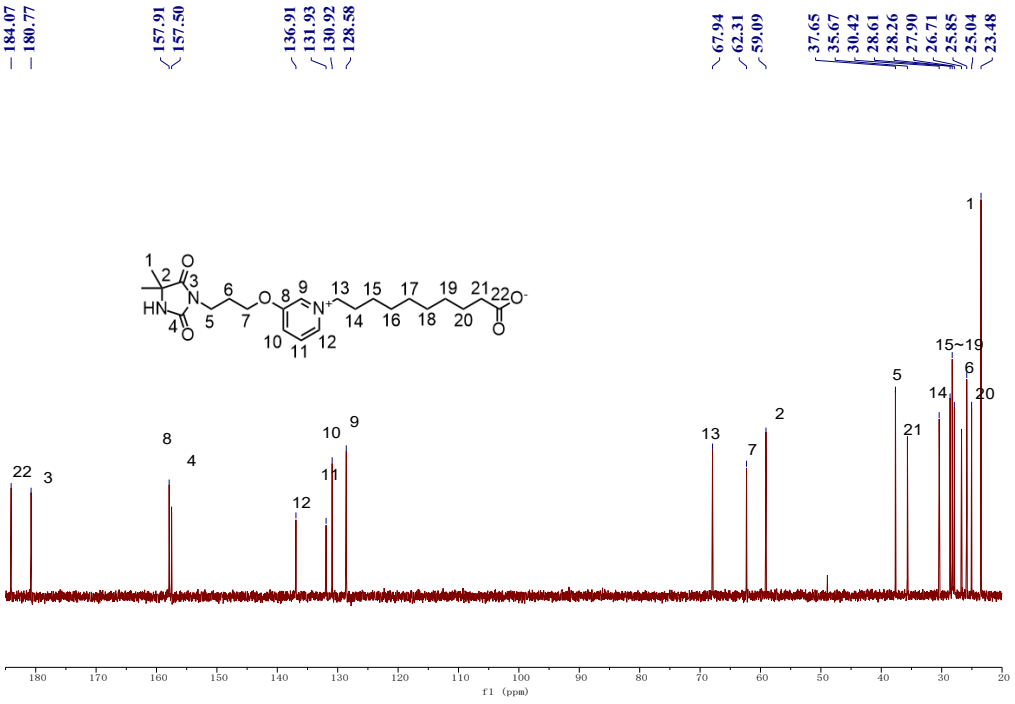
^{1}H NMR spectra of *N*-chloramine **12**



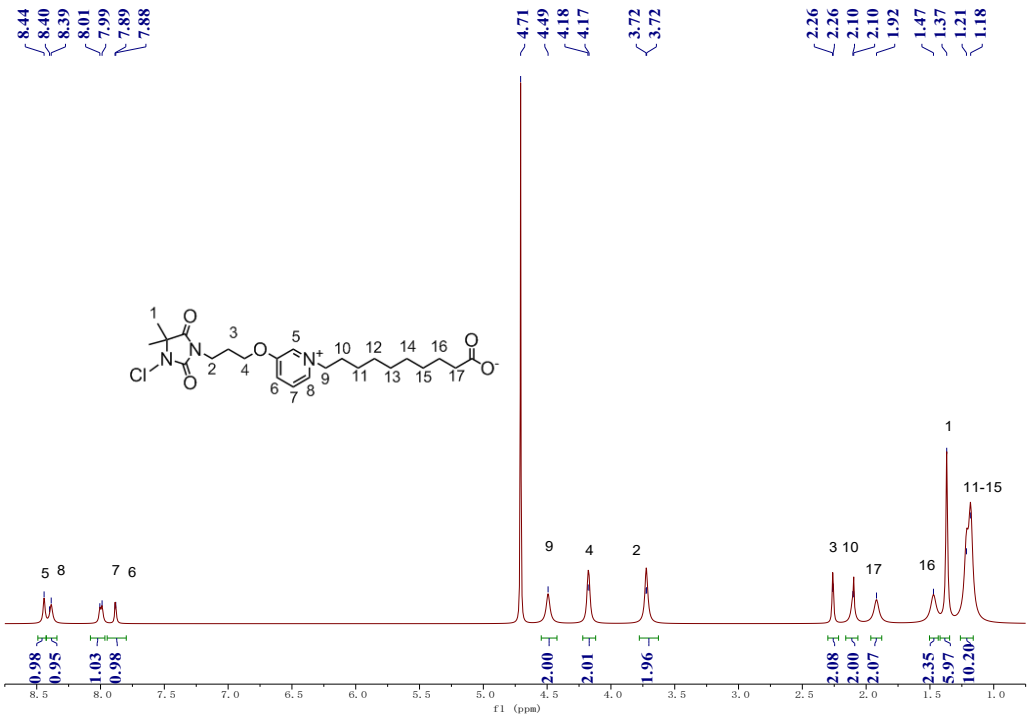
^{13}C NMR spectra of *N*-chloramine **12**



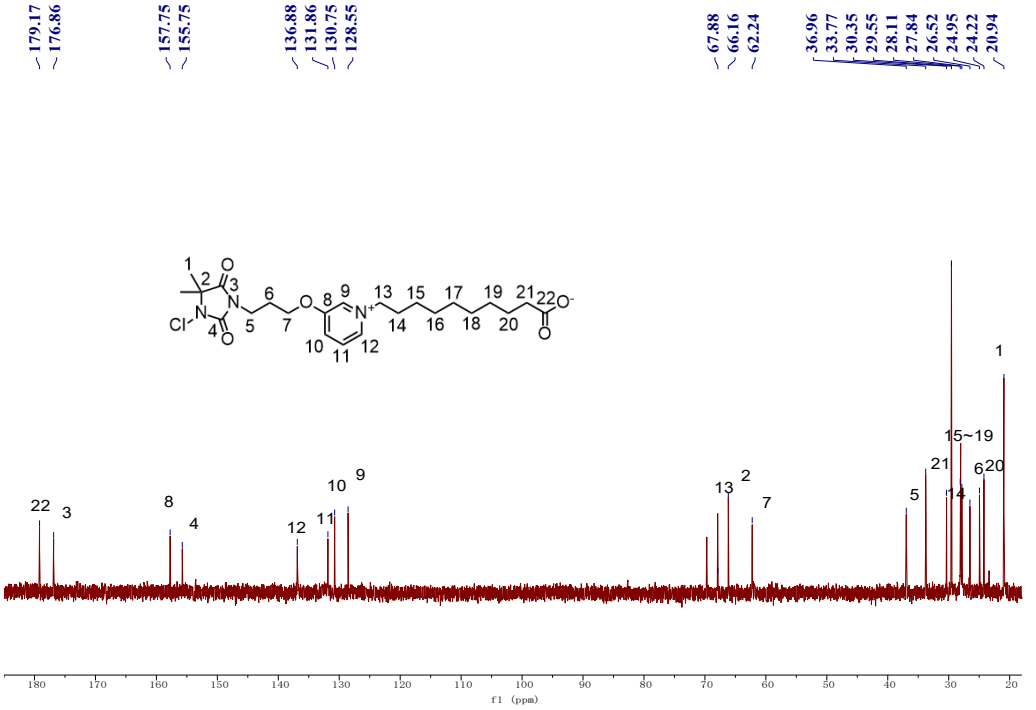
^{1}H NMR spectra of precursor **13a**



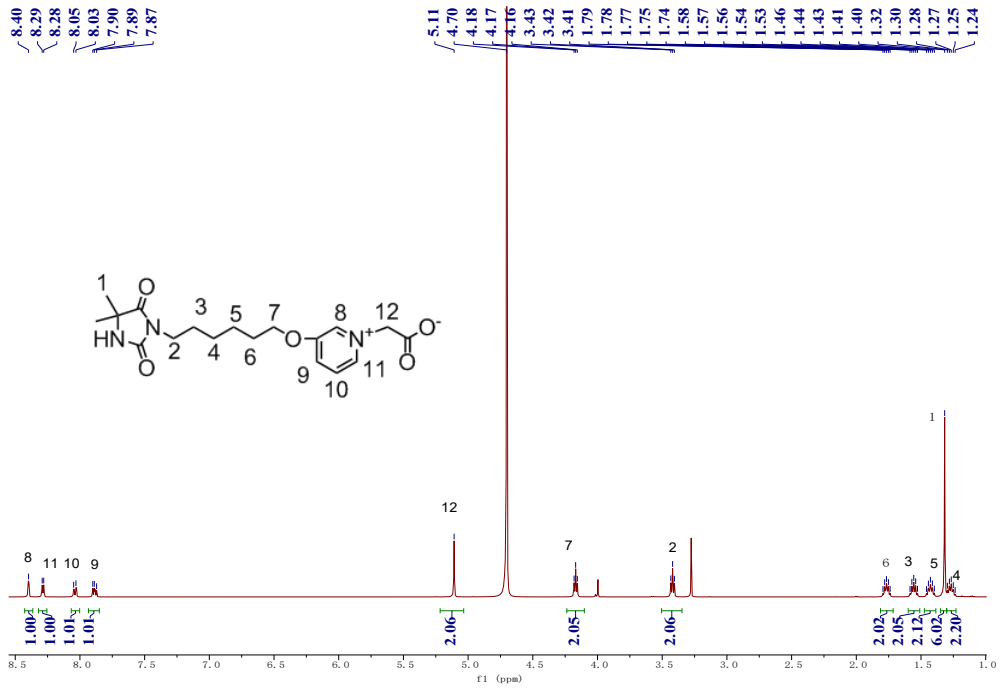
^{13}C NMR spectra of precursor **13a**



^{1}H NMR spectra of *N*-chloramine **13**



^{13}C NMR spectra of *N*-chloramine **13**



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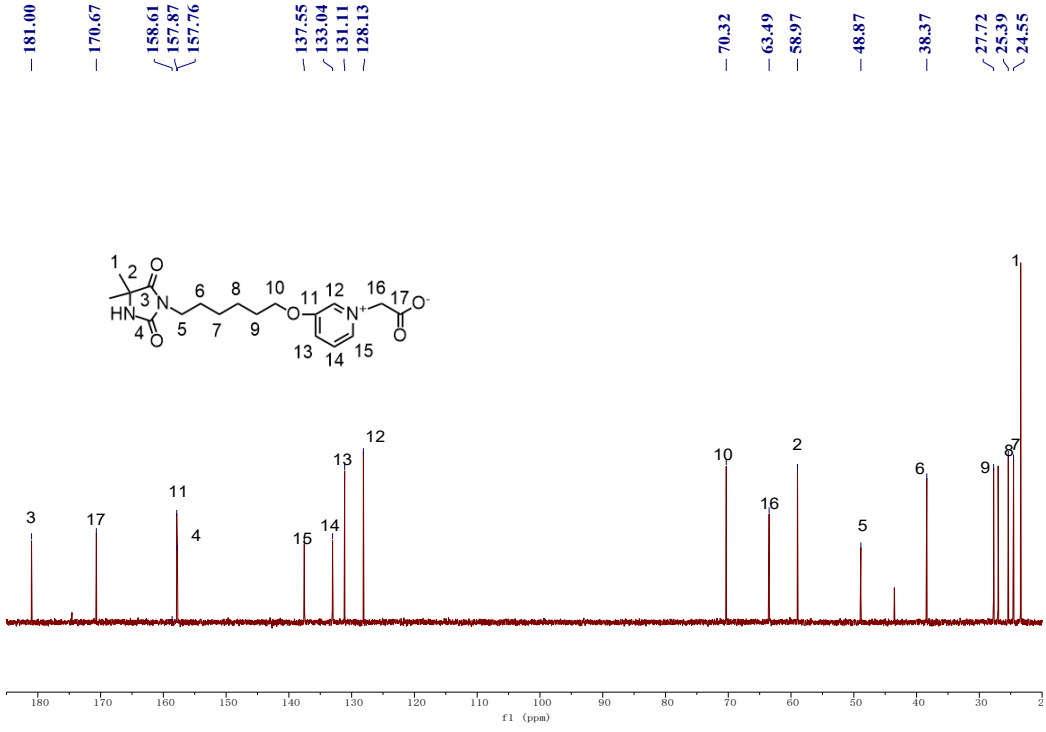

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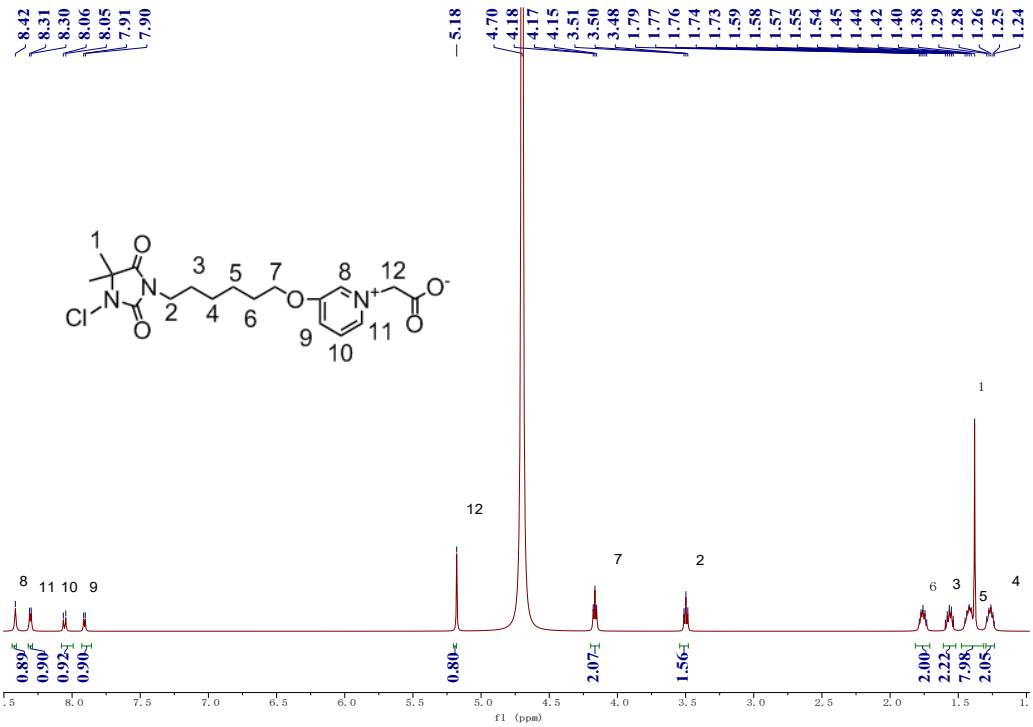
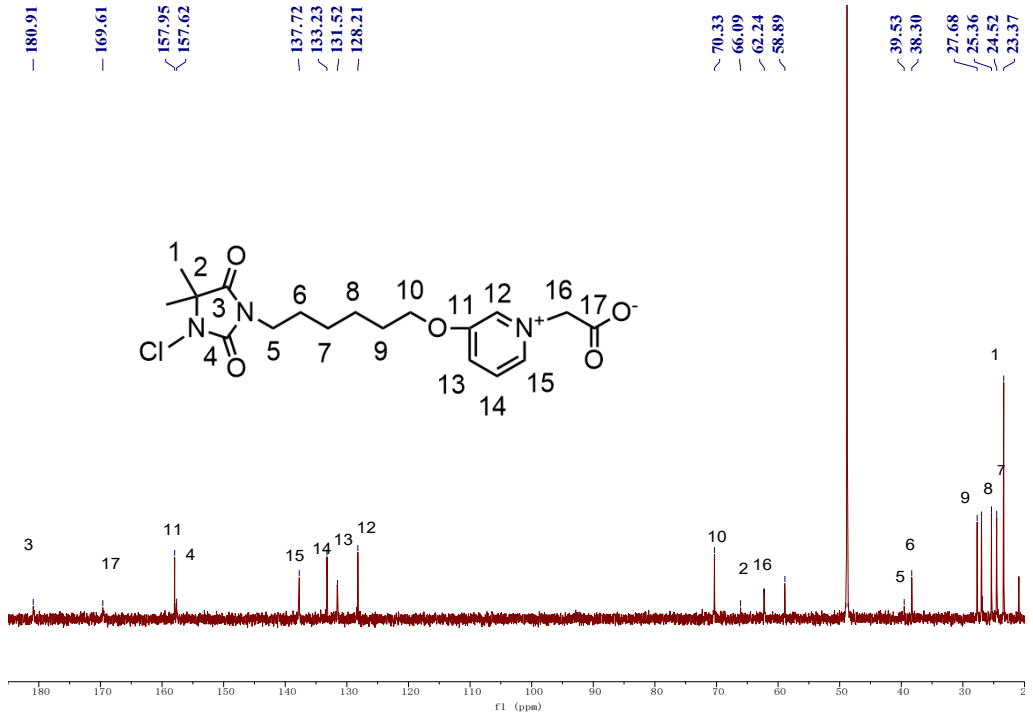
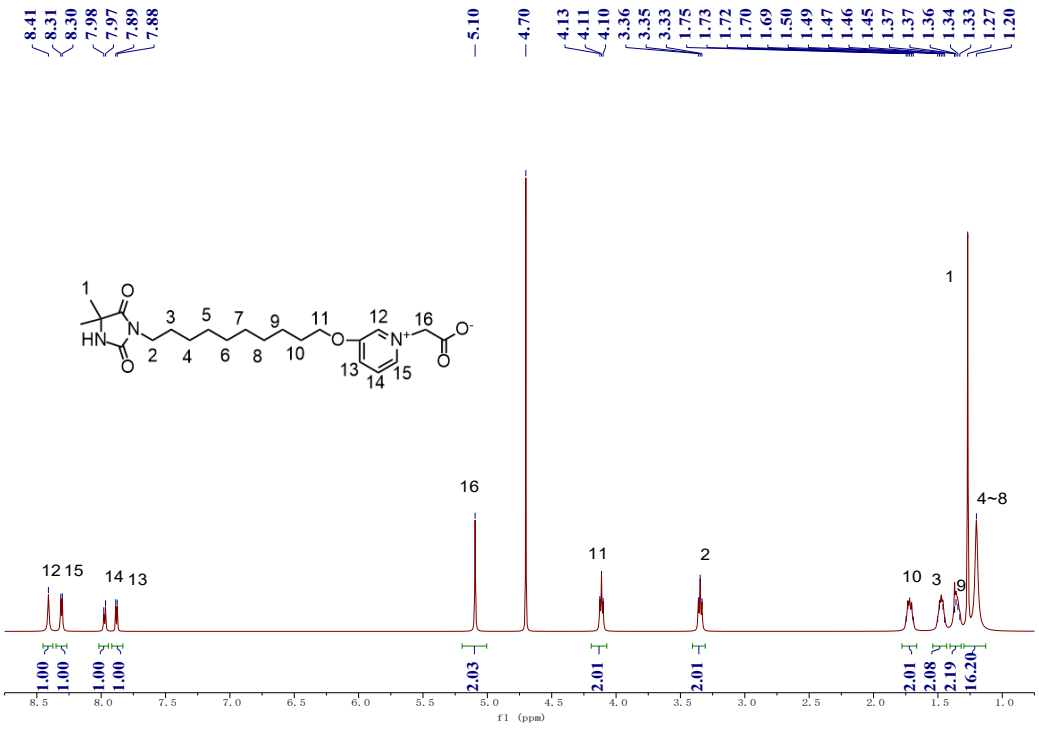


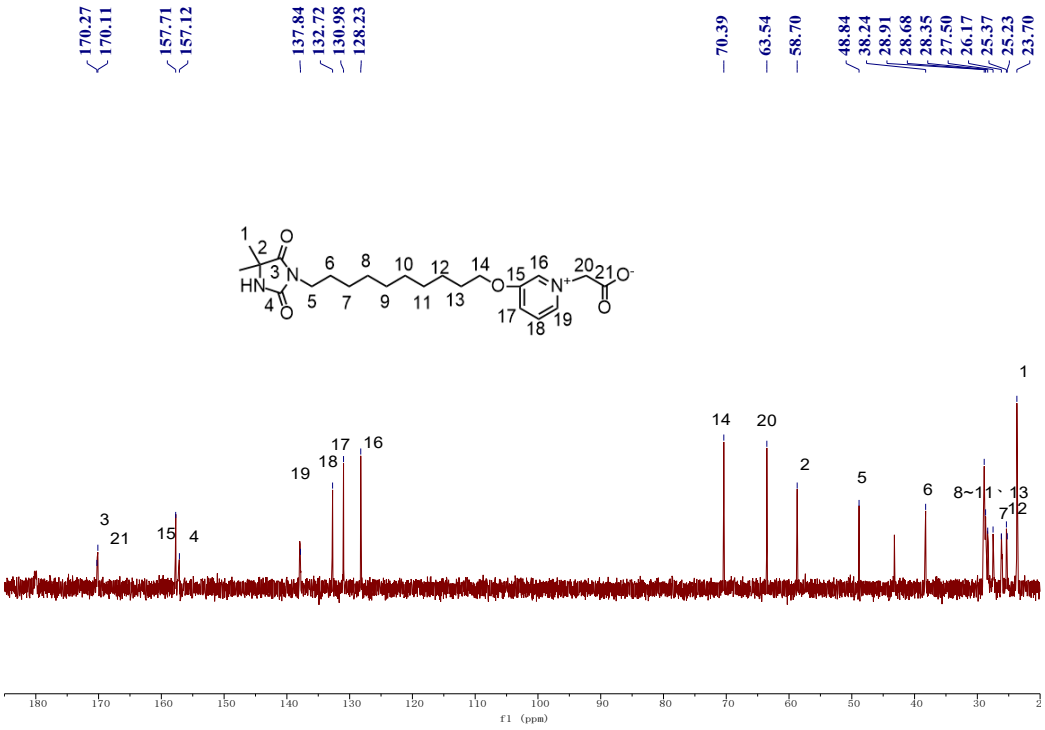
^{1}H NMR spectra of *N*-chloramine **14**



^{13}C NMR spectra of *N*-chloramine **14**



^{1}H NMR spectra of precursor **15a**



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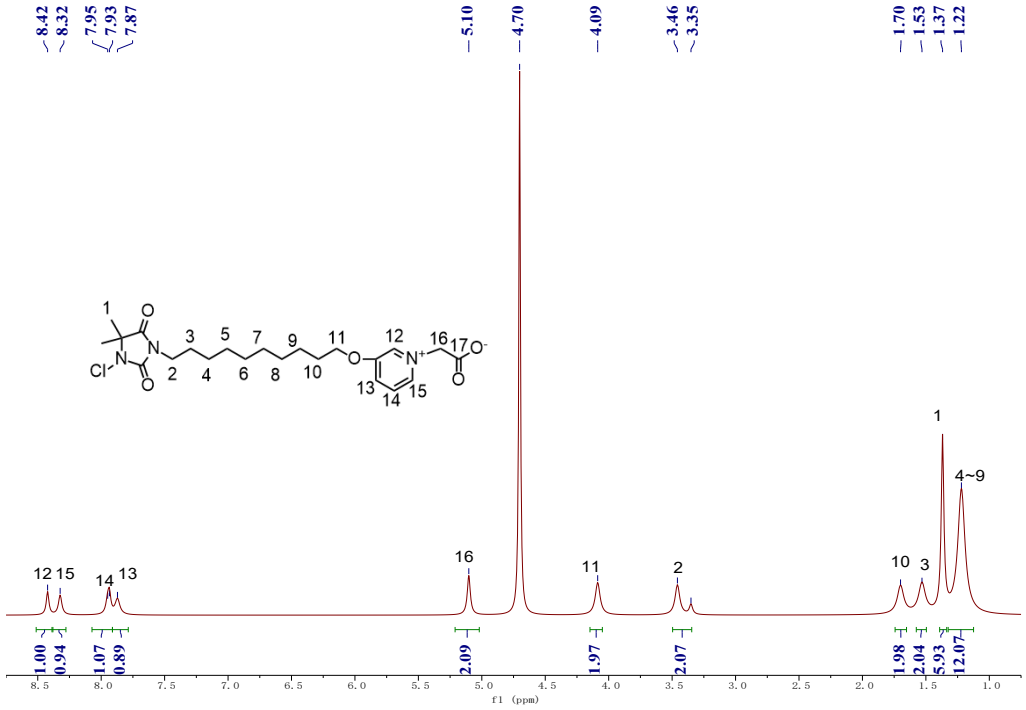
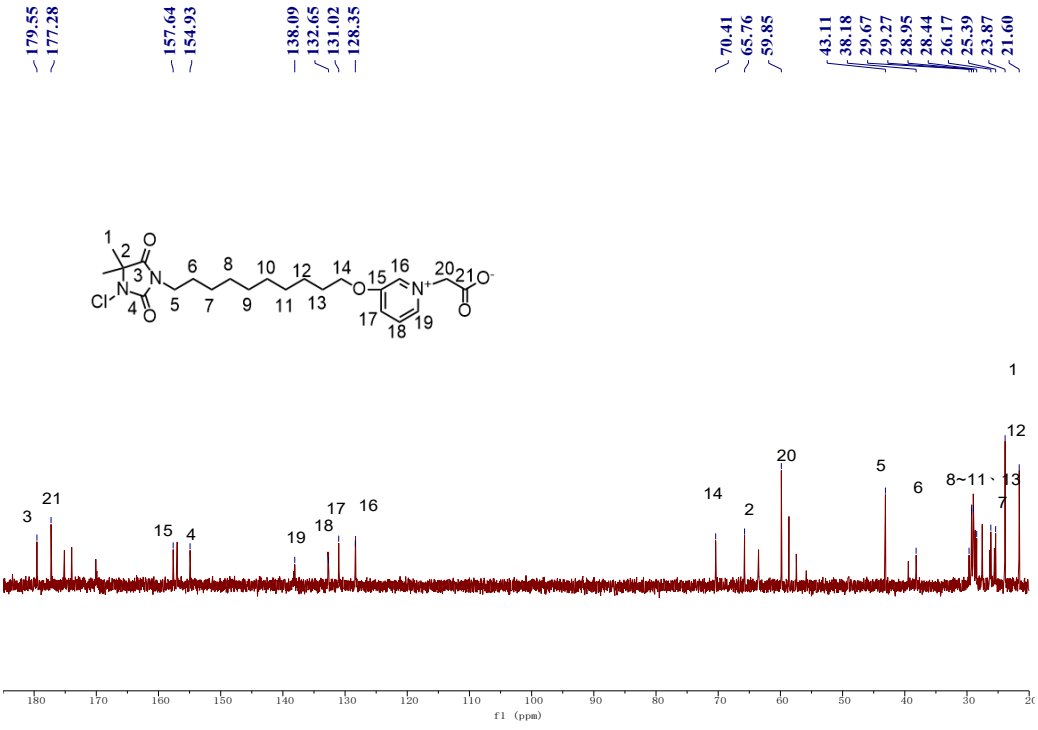
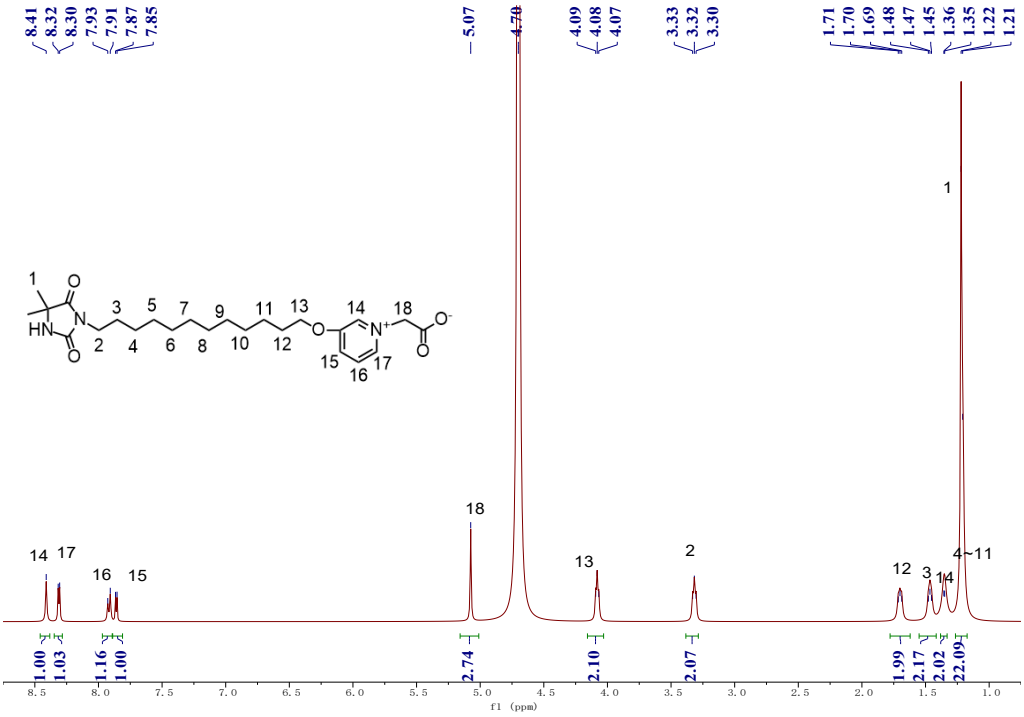


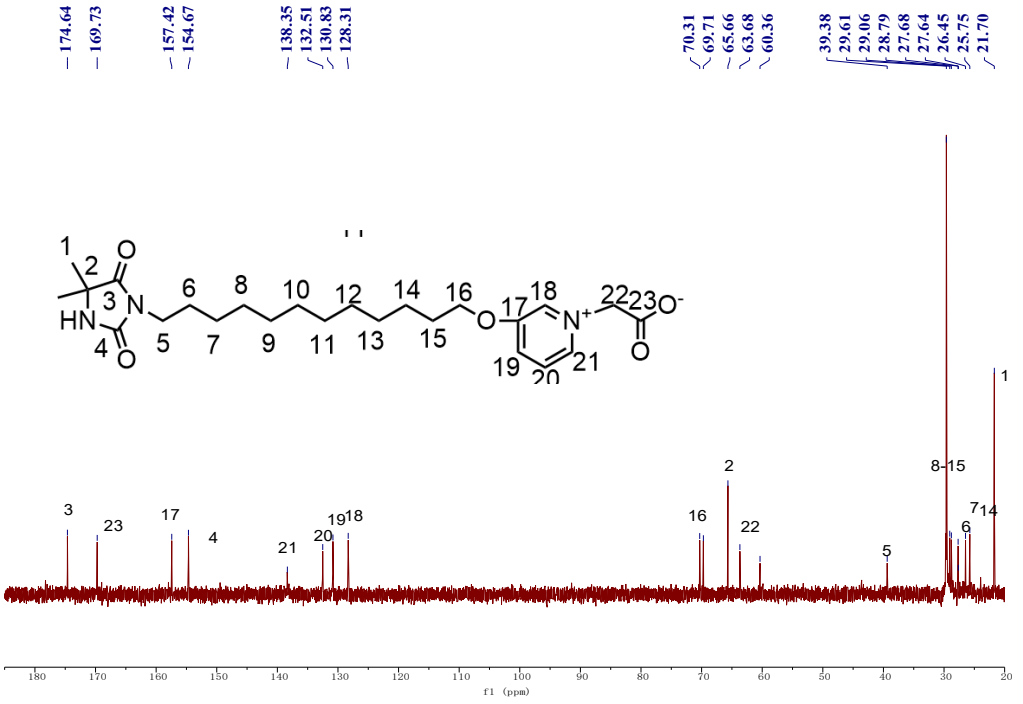
^{1}H NMR spectra of *N*-chloramine **15**



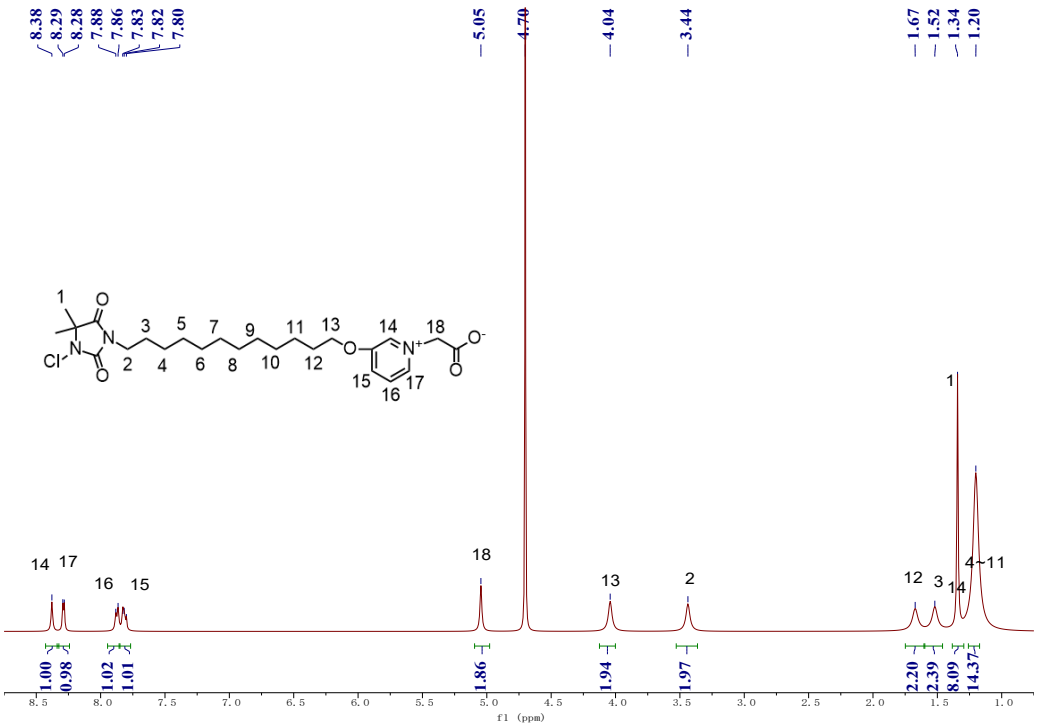
^{13}C NMR spectra of *N*-chloramine **15**



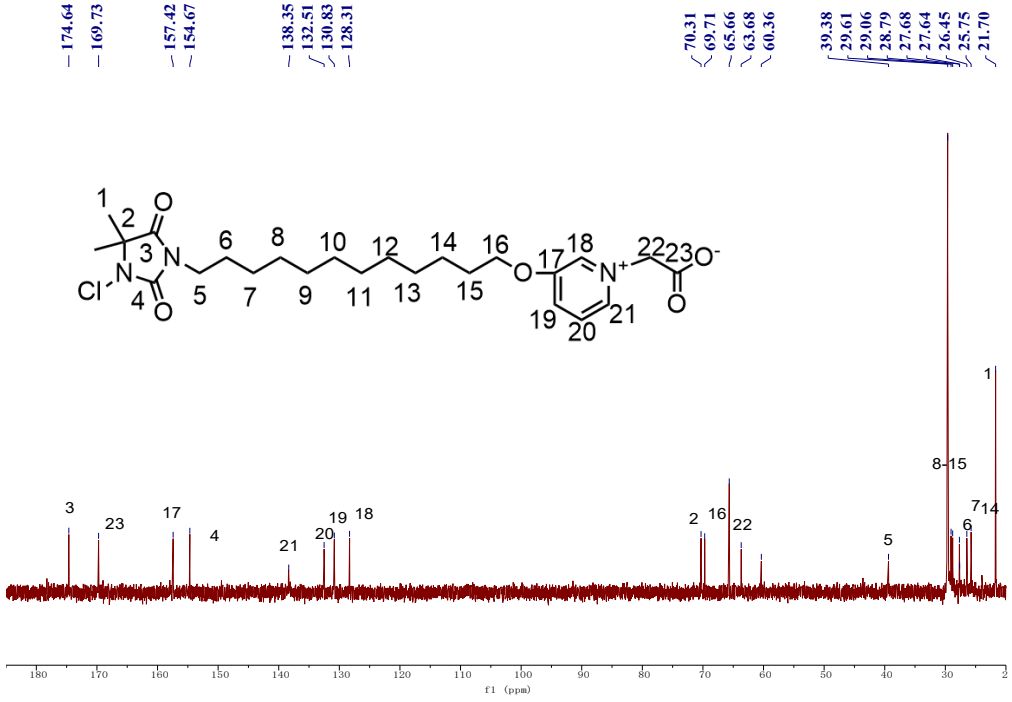
The ^{1}H NMR spectra of precursor **16a**



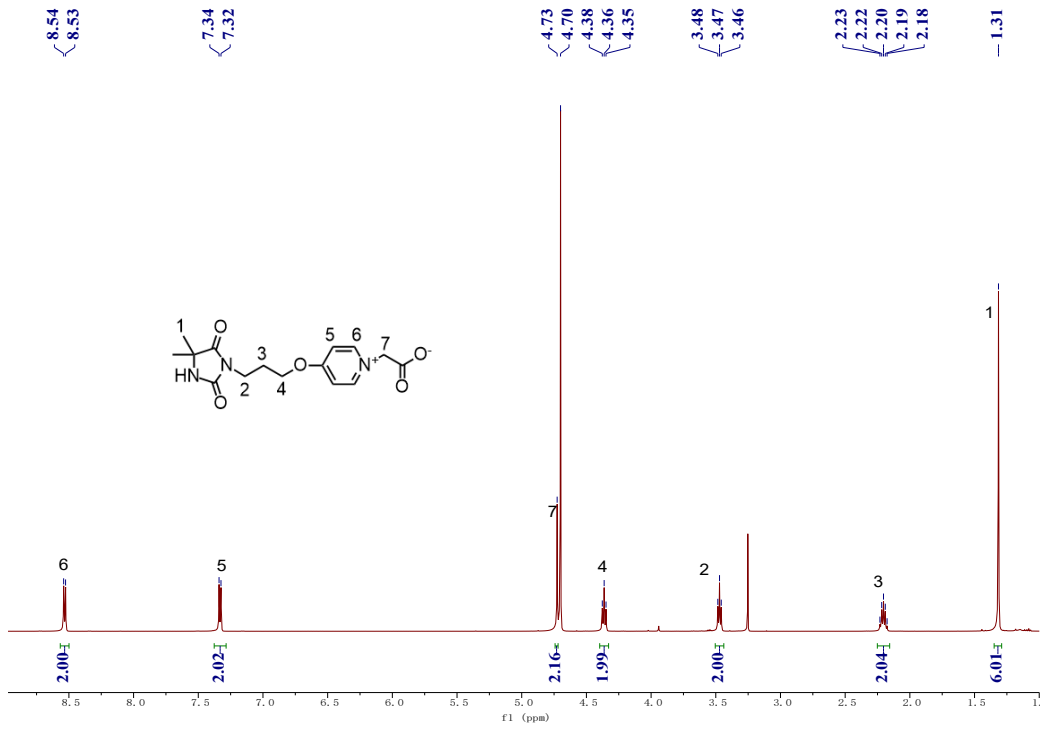
^{13}C NMR spectra of precursor **16a**



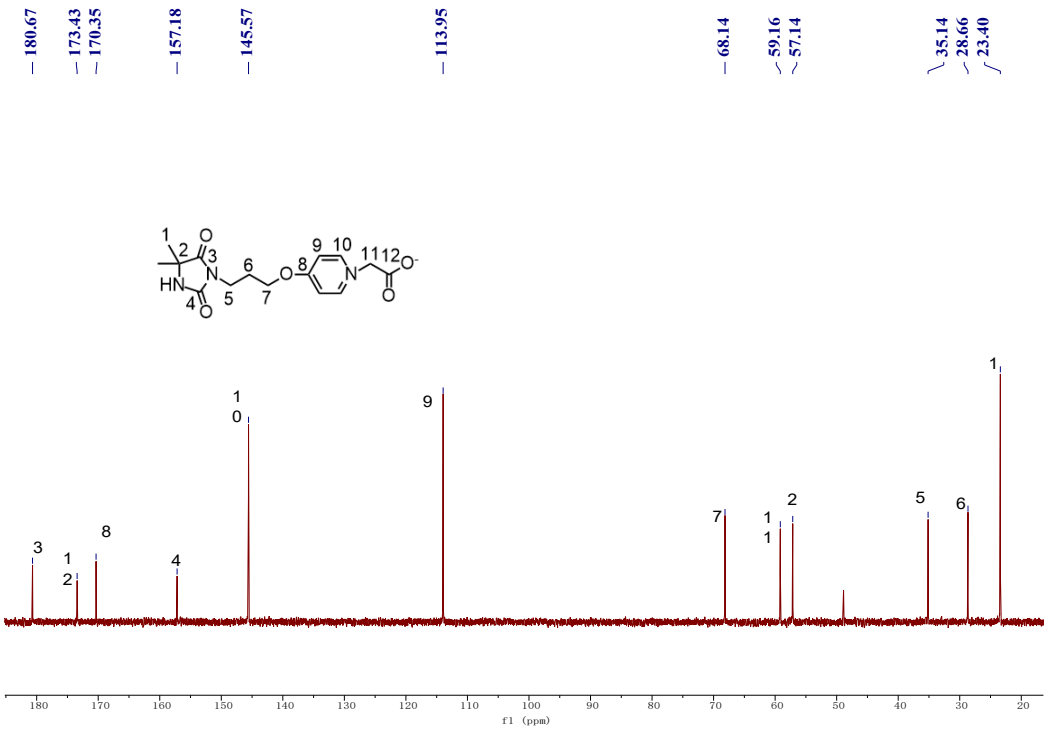
^{1}H NMR spectra of *N*-chloramine **16**



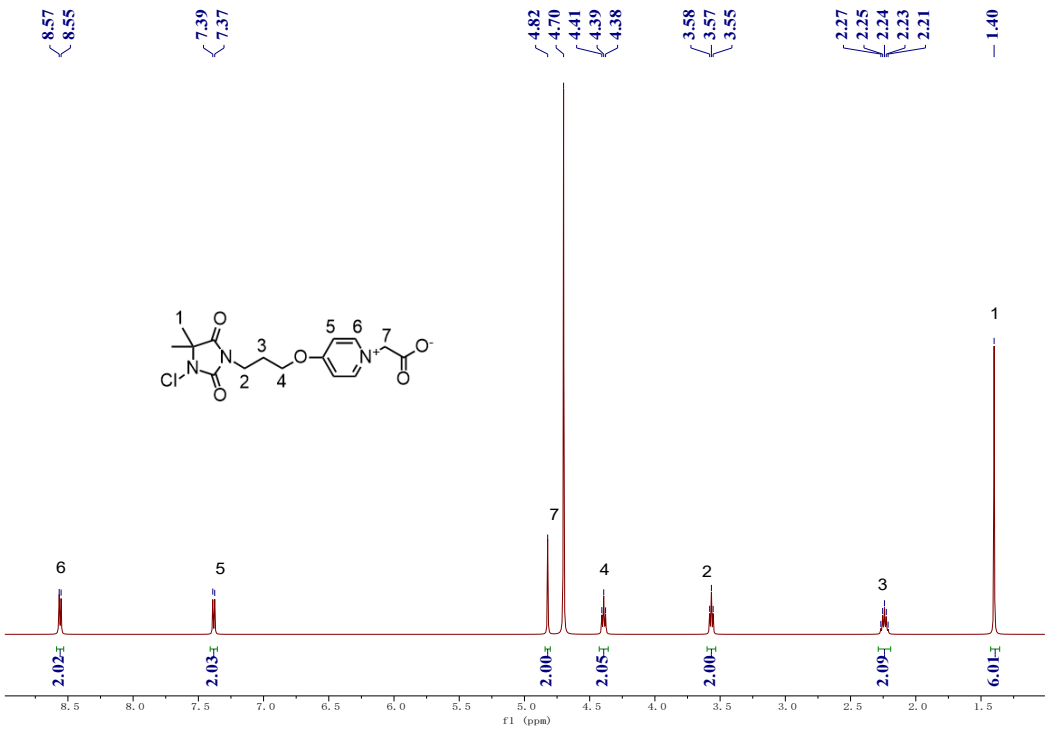
The ^{1}H NMR spectra of *N*-chloramine **16**



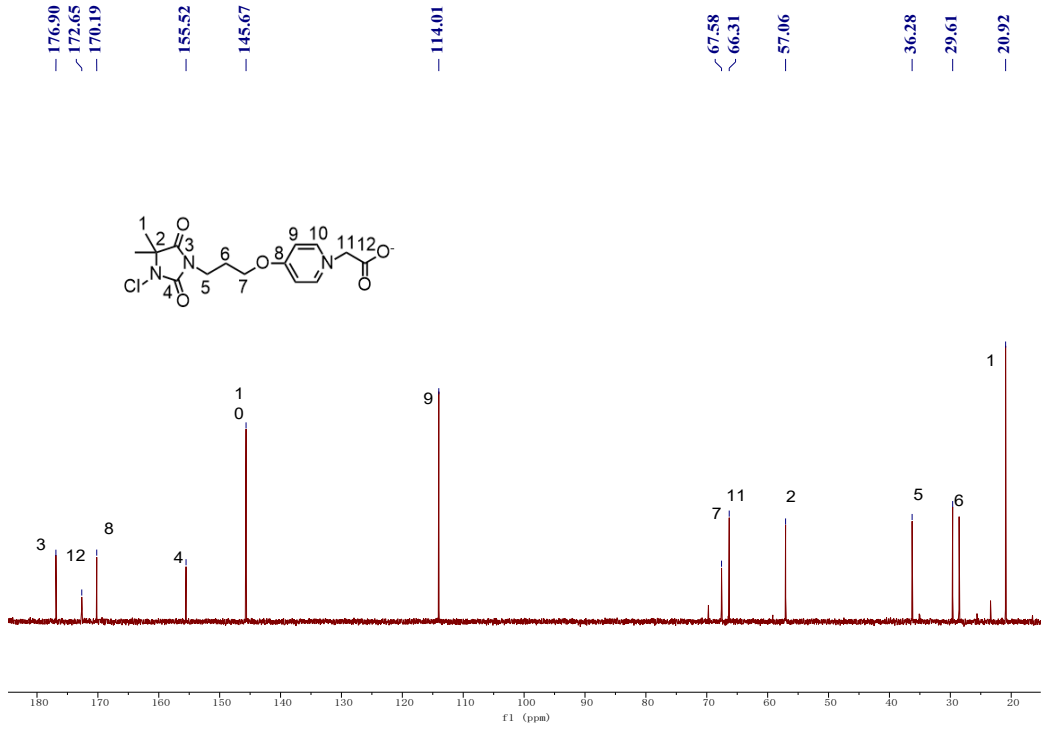
^{1}H NMR spectra of precursor **17a**



^{13}C NMR spectra of precursor **17a**

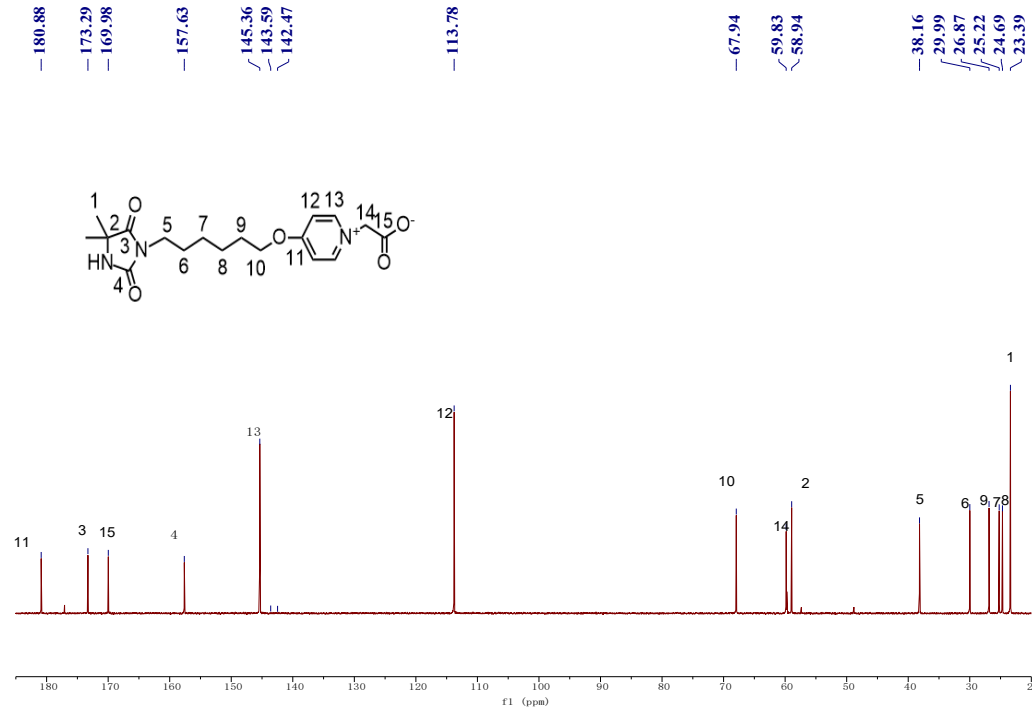


^{1}H NMR spectra of *N*-chloramine **17**



^{13}C NMR spectra of *N*-chloramine **17**

^{1}H NMR spectra of precursor **18a**



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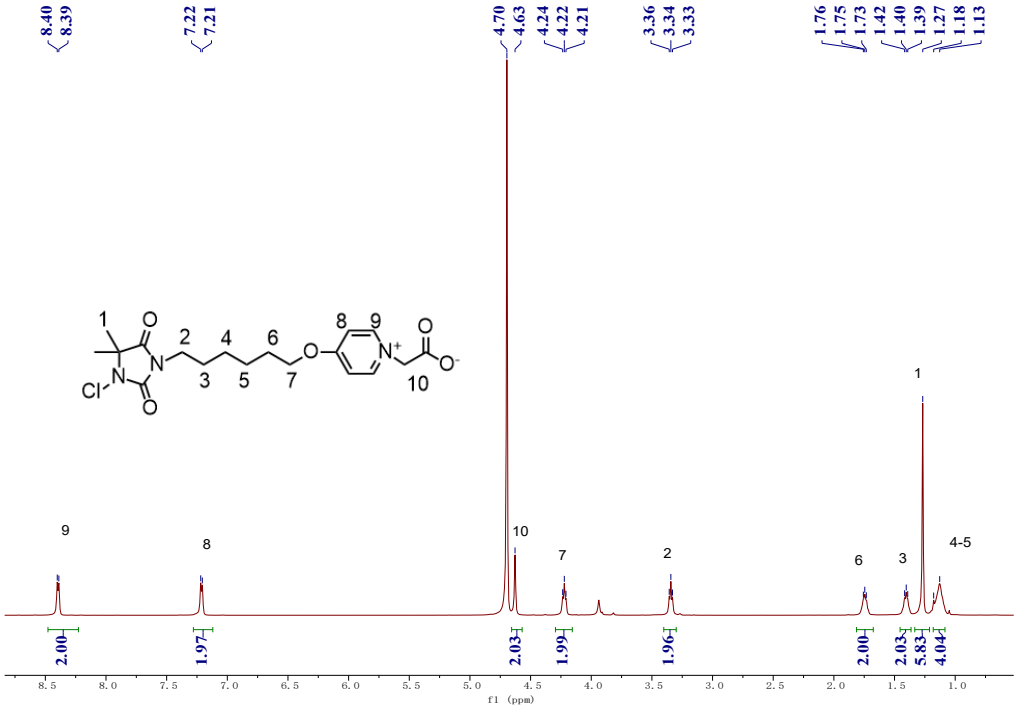
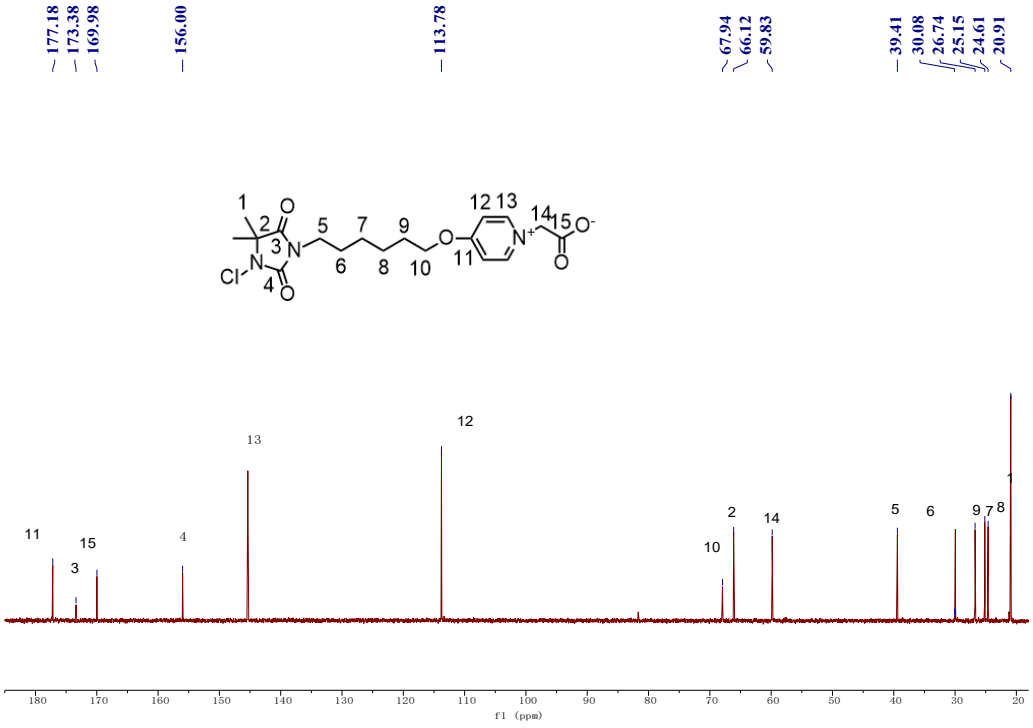
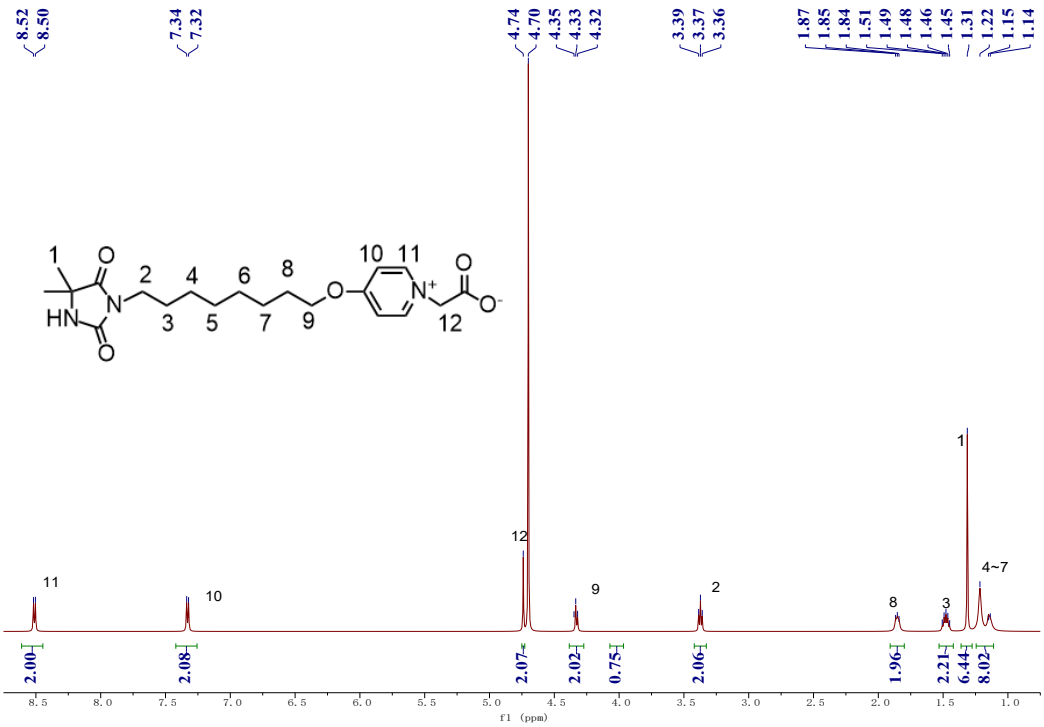


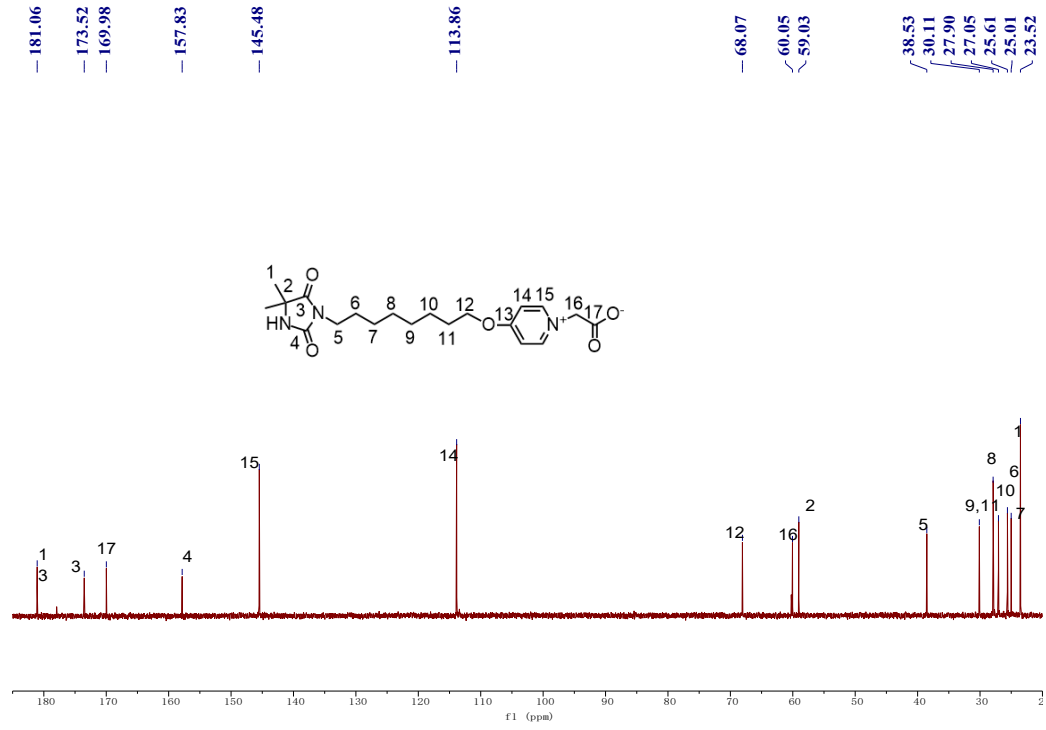
^{1}H NMR spectra of *N*-chloramine **18**



^{13}C NMR spectra of *N*-chloramine **18**

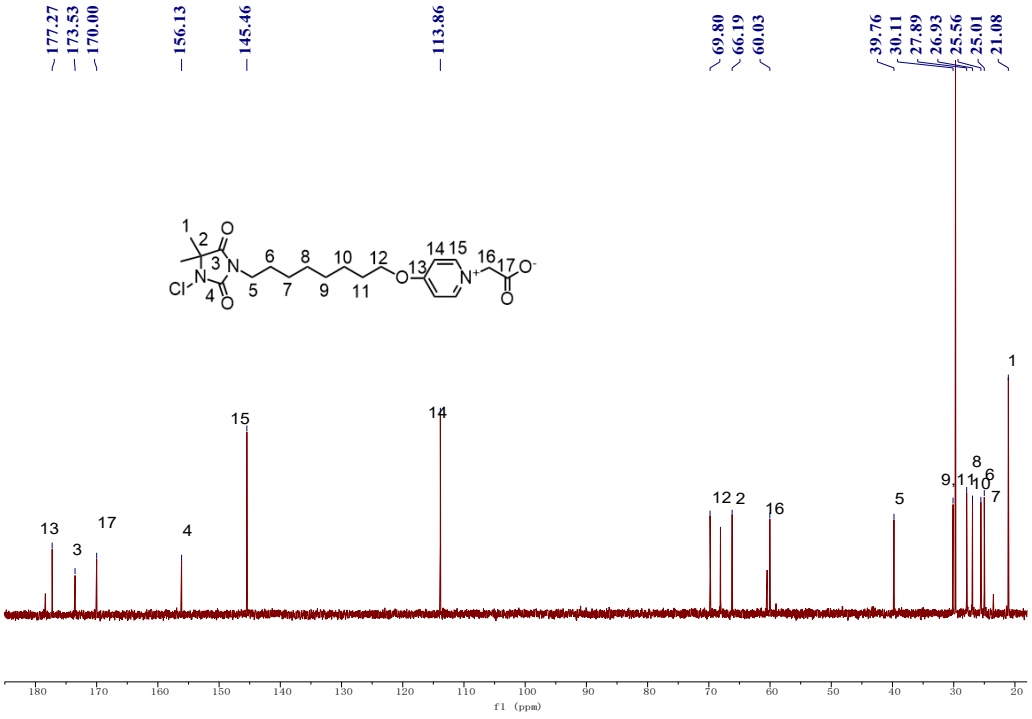


^{1}H NMR spectra of precursor **19a**

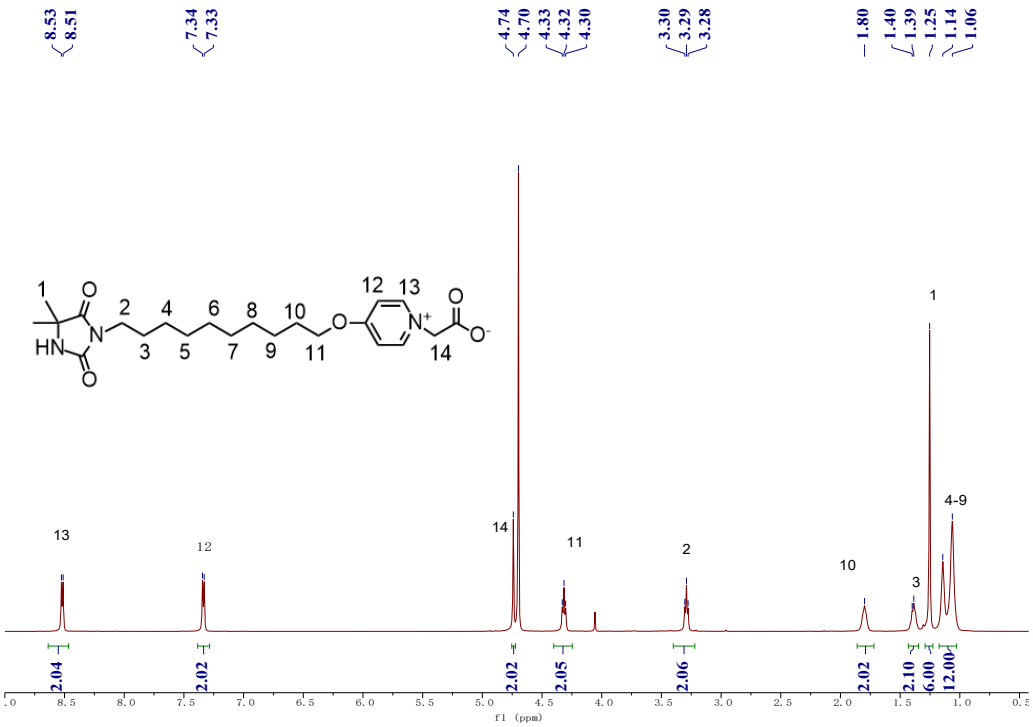


^{13}C NMR spectra of precursor **19a**

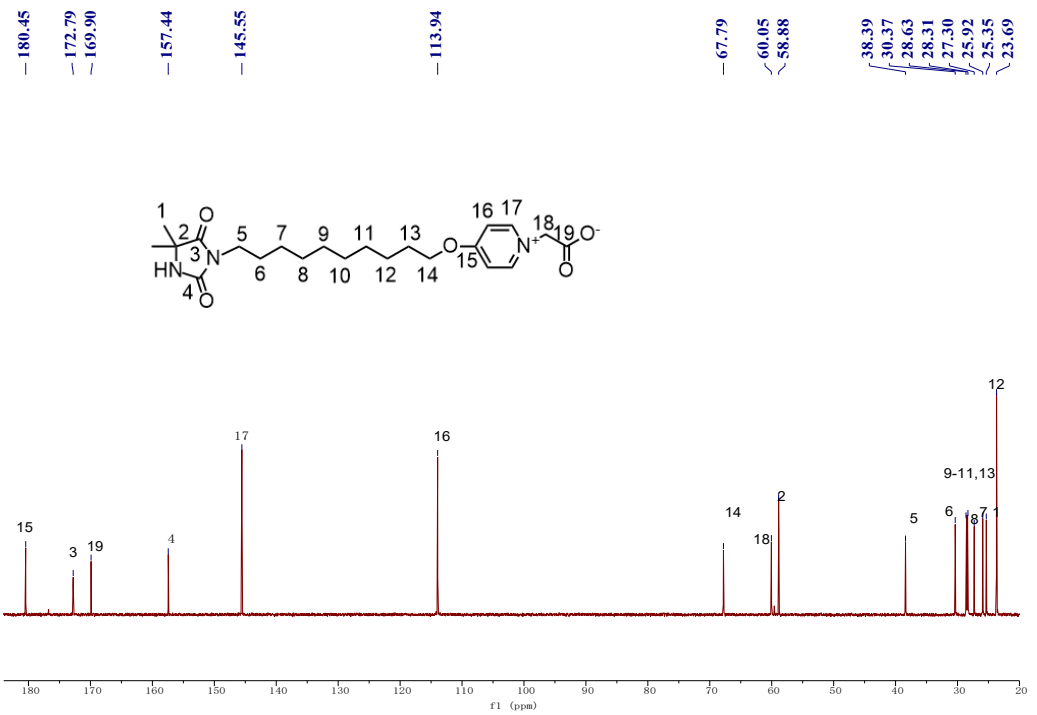
^{1}H NMR spectra of *N*-chloramine **19**



^{13}C NMR spectra of *N*-chloramine **19**

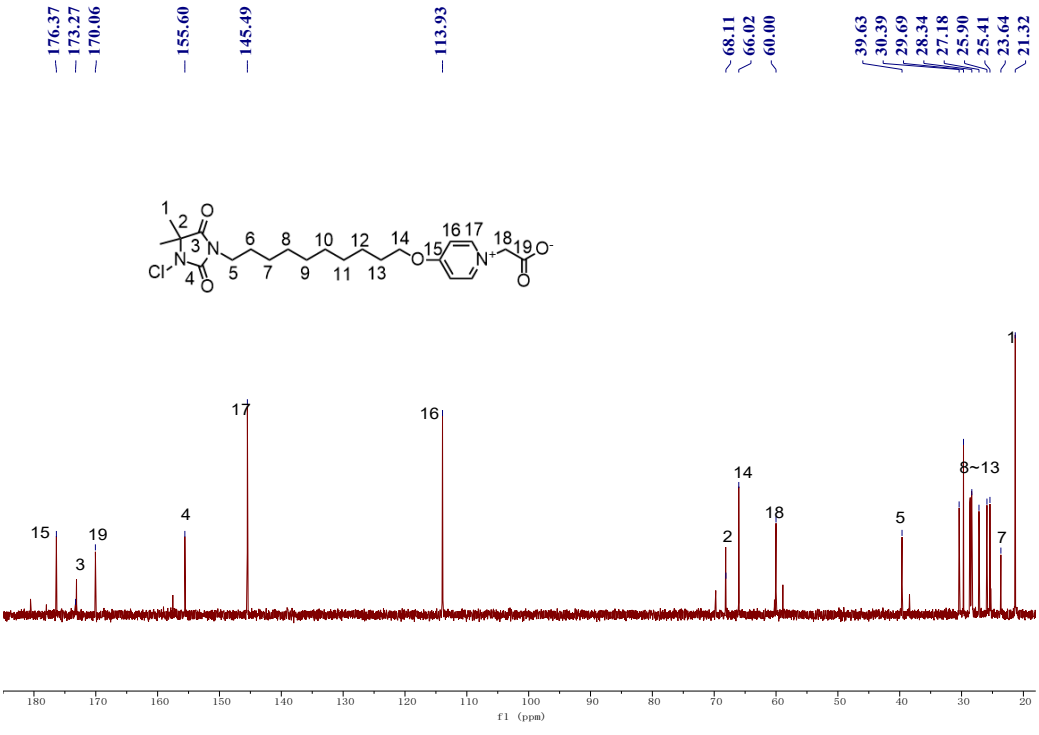


^{1}H NMR spectra of precursor **20a**

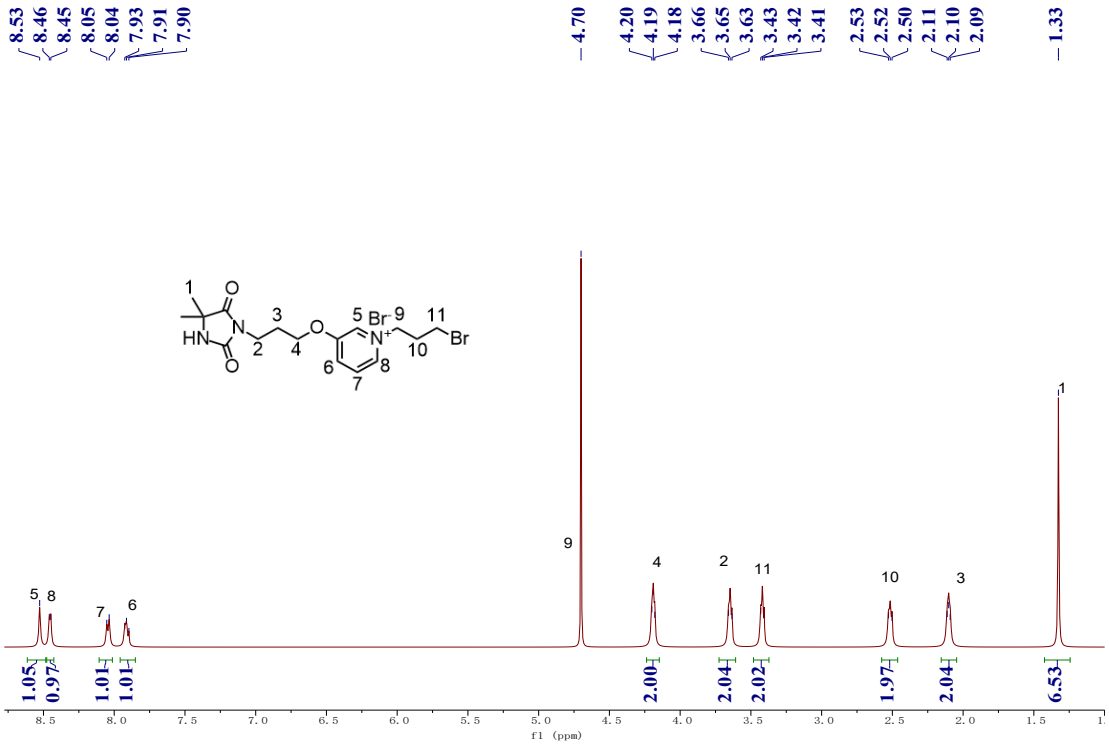


^{13}C NMR spectra of precursor **20a**

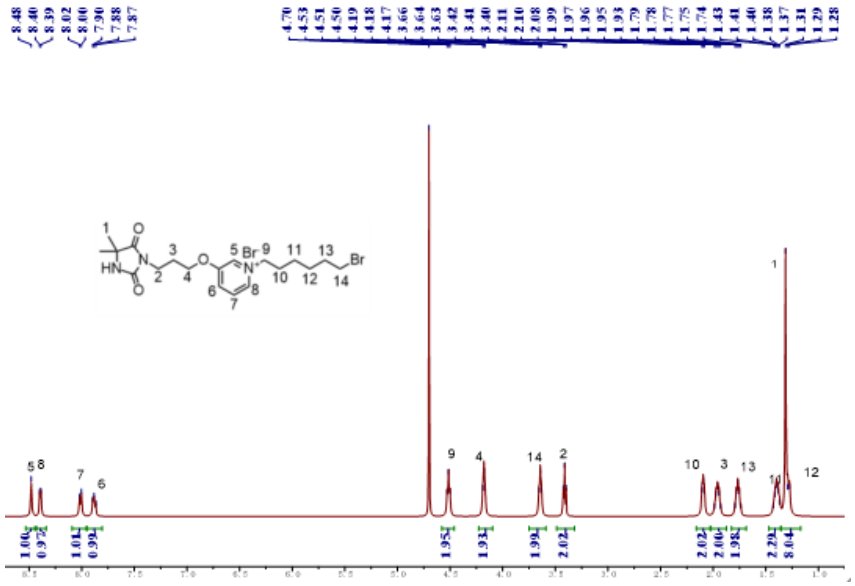
^{1}H NMR spectra of *N*-chloramine **20**



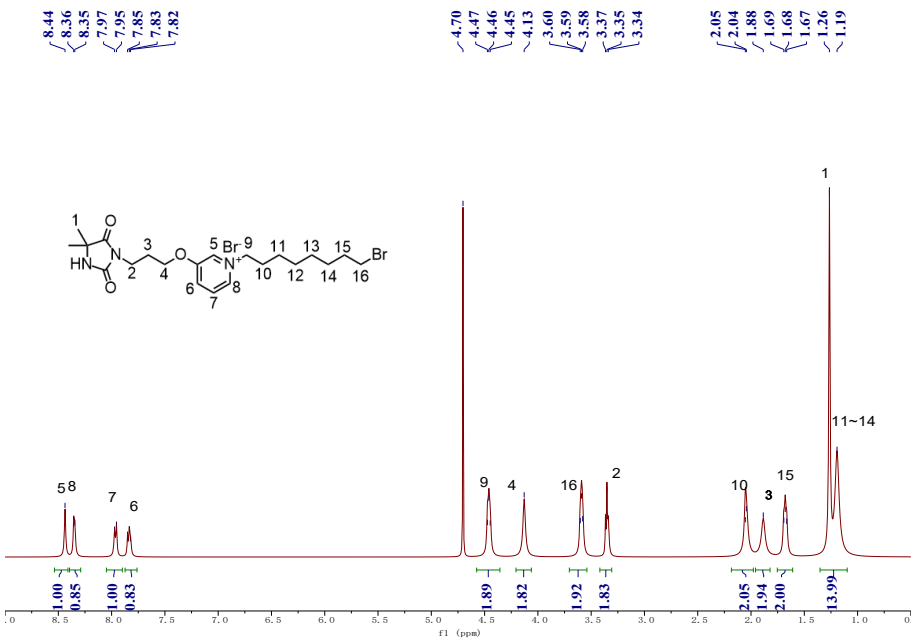
^{13}C NMR spectra of *N*-chloramine **20**



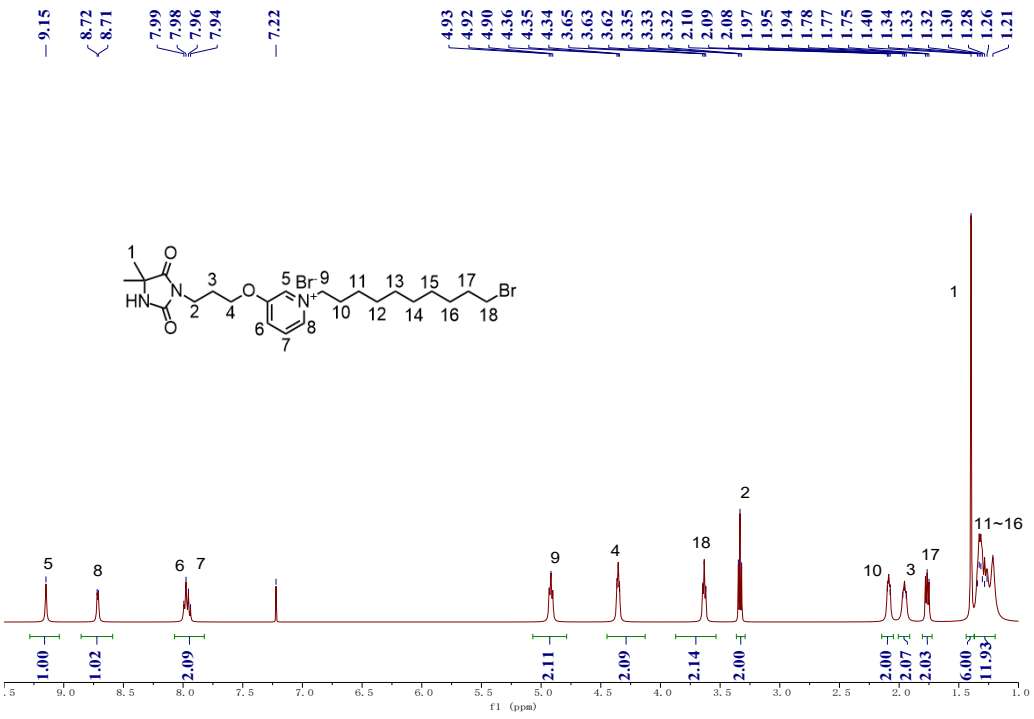
^{1}H NMR spectra of pyridinium salt **23**



^{1}H NMRspectra of pyridinium salt **24**

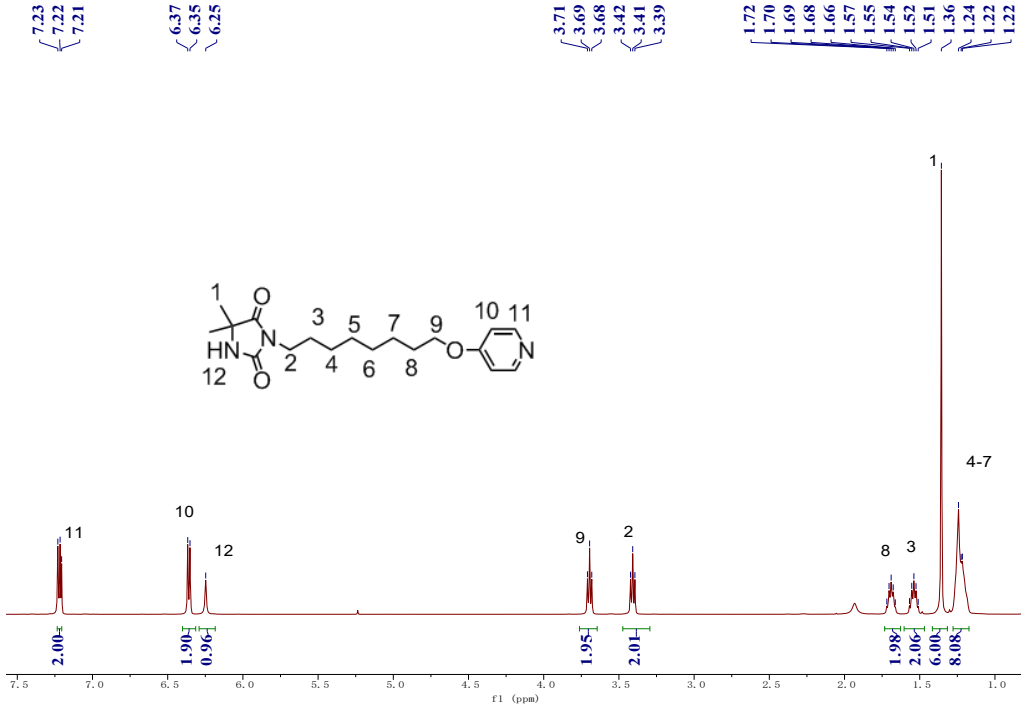


^{1}H NMR spectra of pyridinium salt **25**

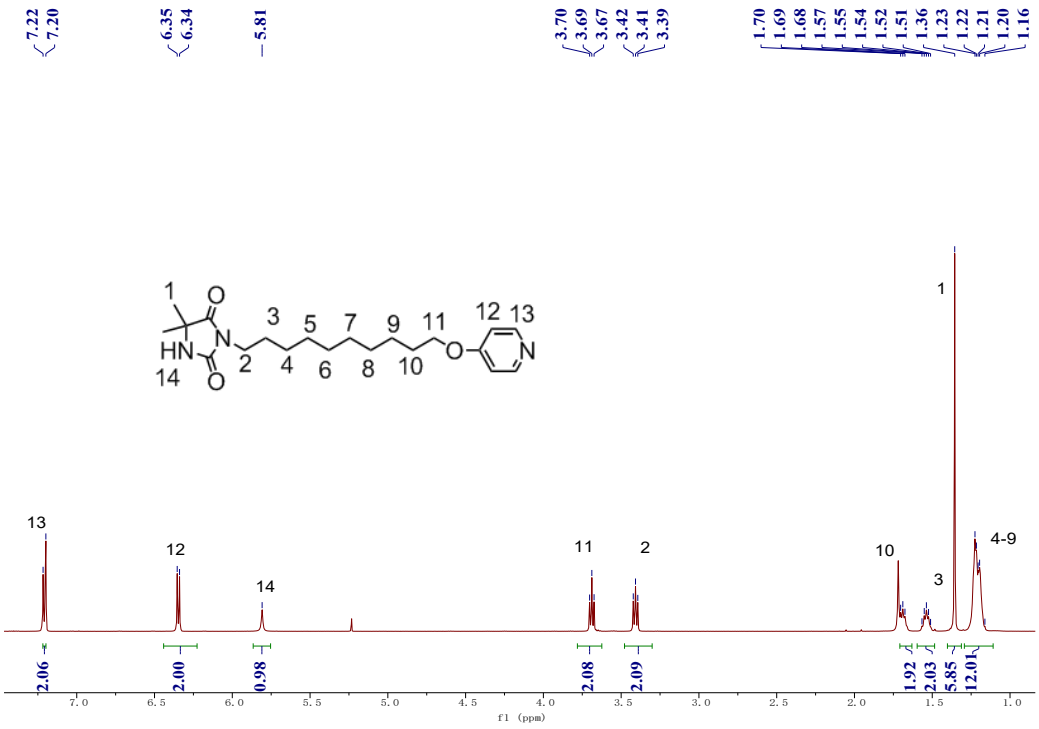


^{1}H NMR spectra of pyridinium salt **26**

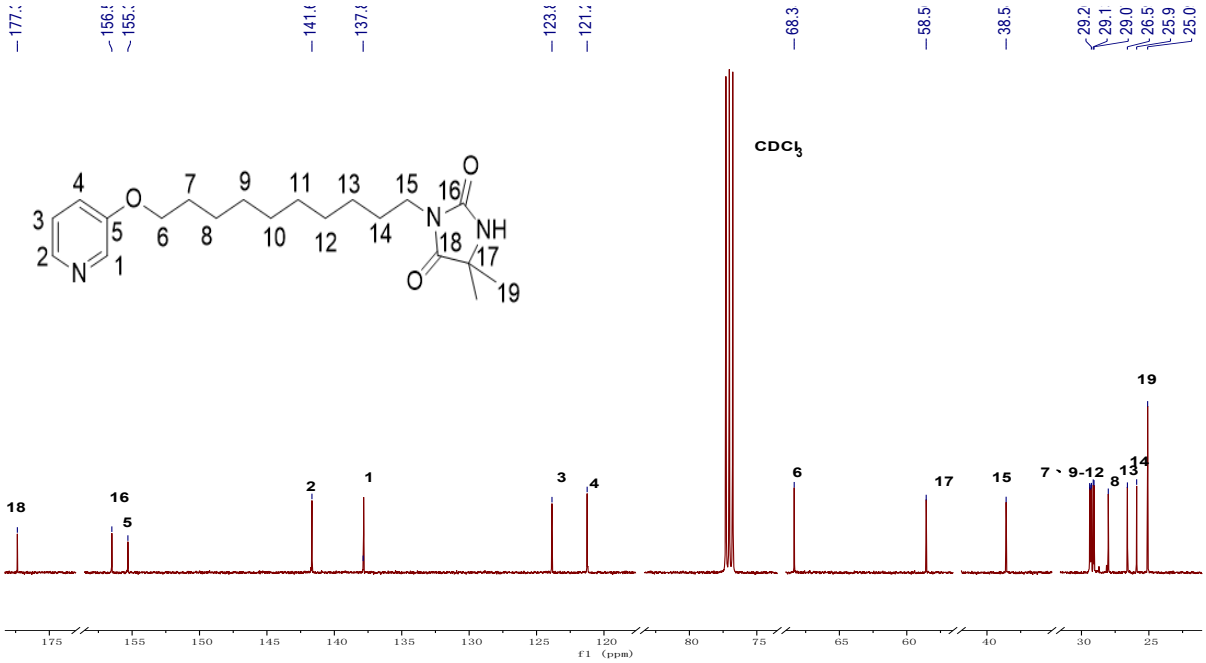
^{1}H NMR spectra of ether **35**



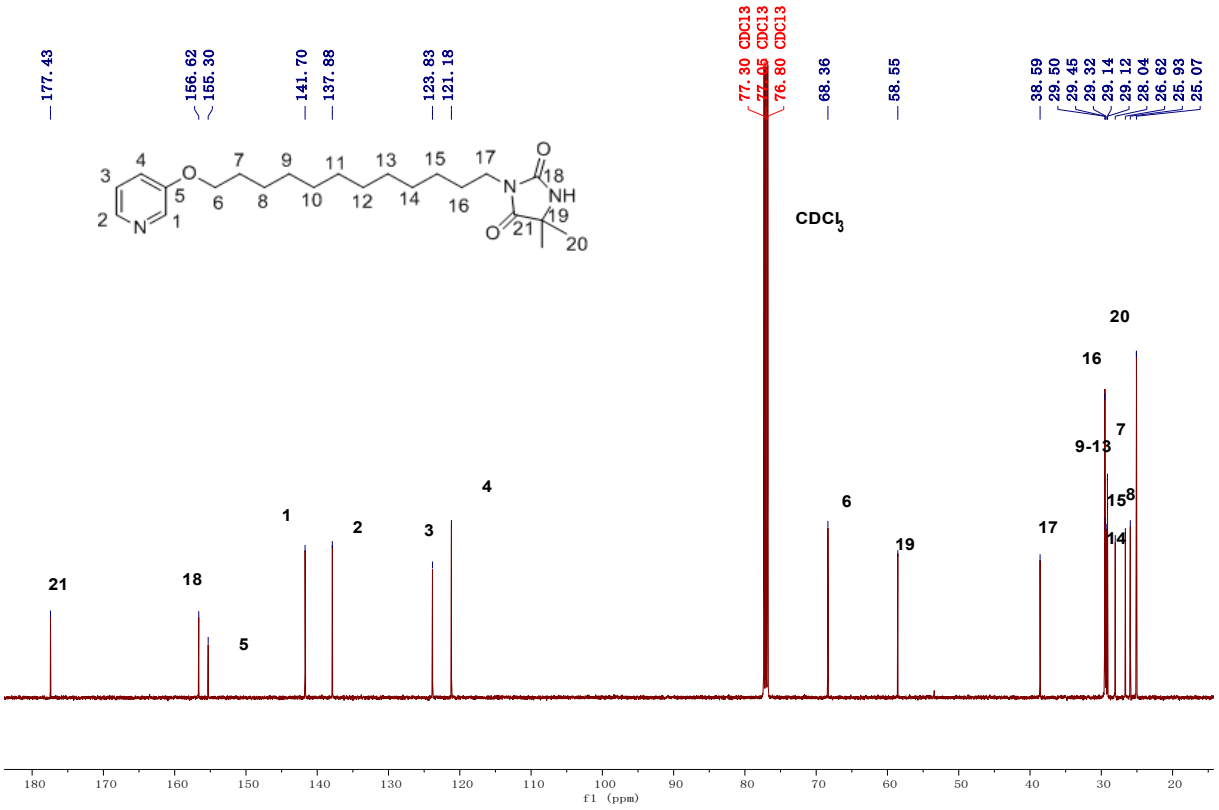
^{1}H NMR spectra of ether **36**



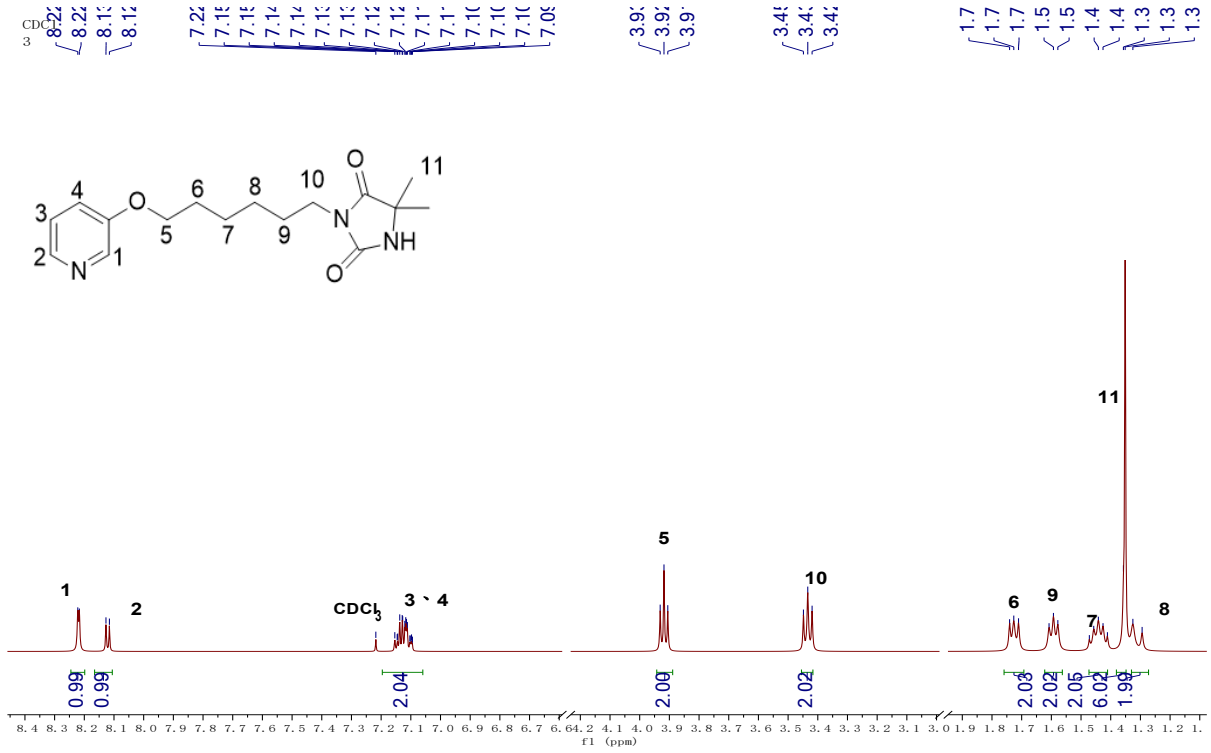
^{1}H NMR spectra of ether **37**



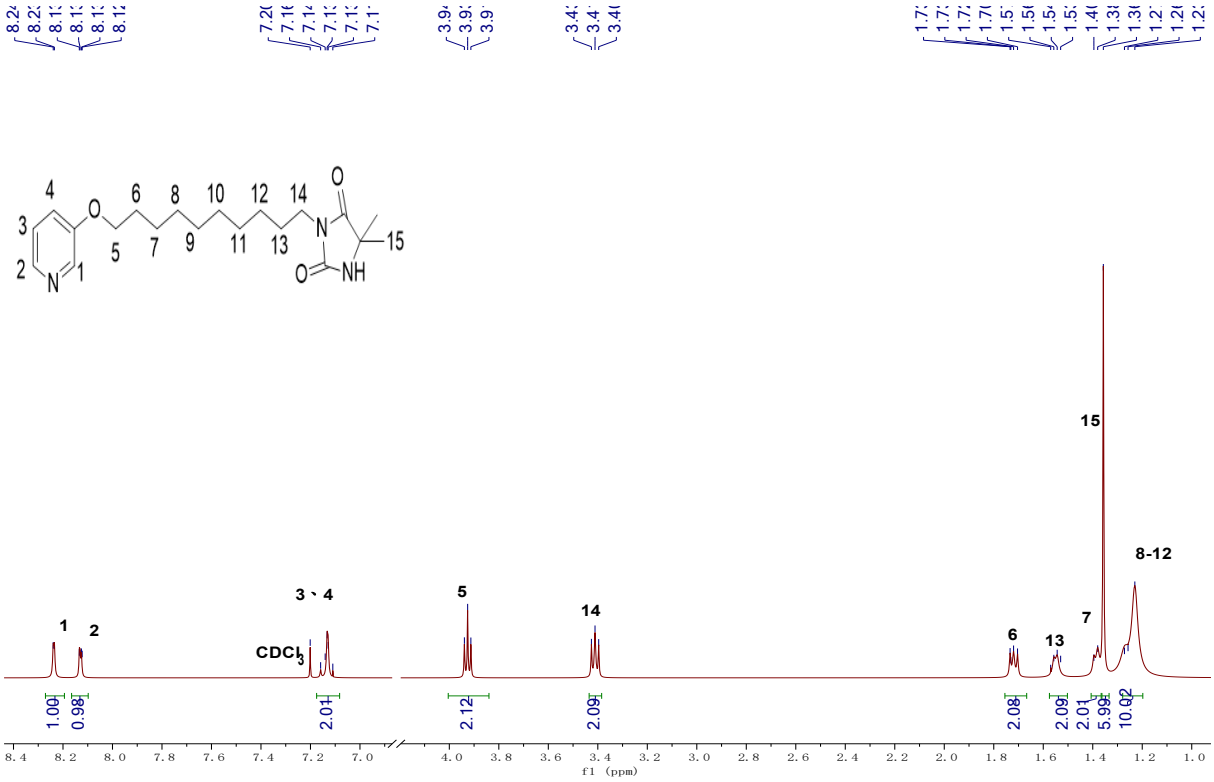
The ^{13}C NMR spectra of compound **32**



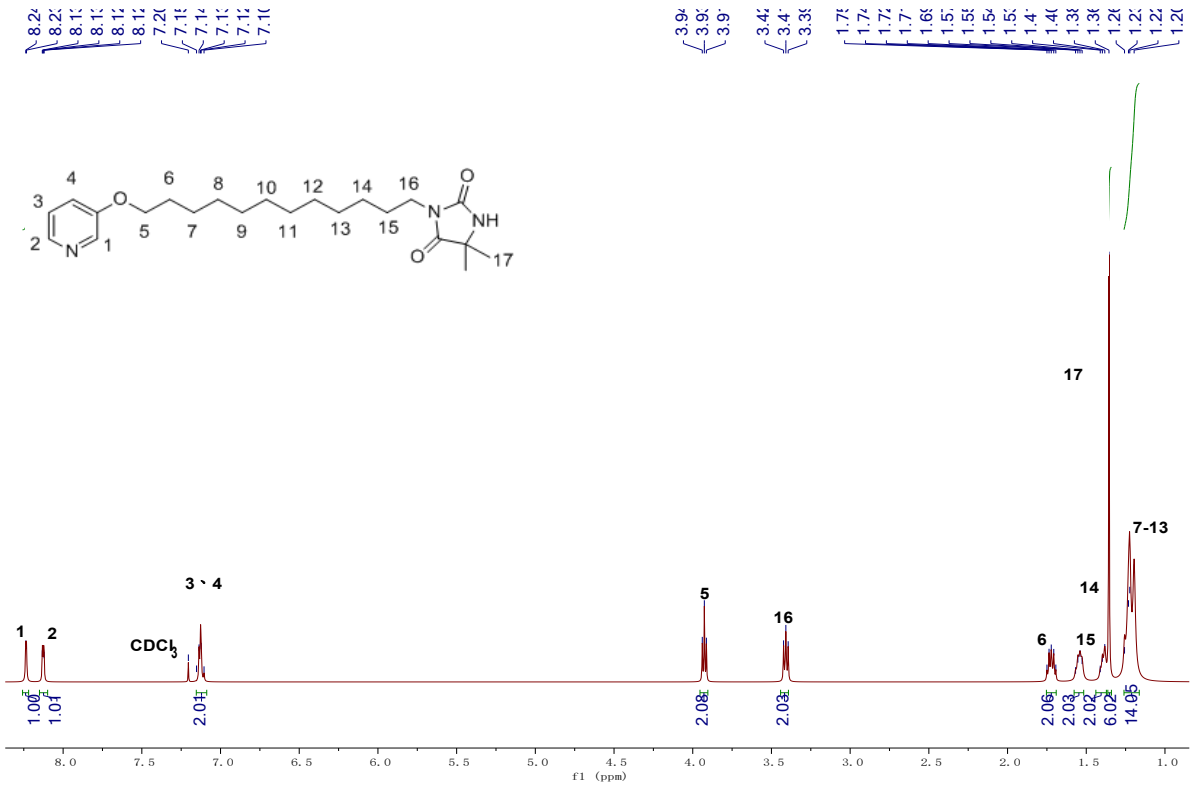
^{13}C NMR spectra of compound **33**



^{1}H NMR spectra of **31**



^{1}H NMR spectra of **32**



^{1}H NMR spectra of **33**