Supporting Information for

Antibacterial Coordination Polymer Hydrogels Consisted of Silver(I)-PEGylated Bisimidazolylbenzyl Alcohol

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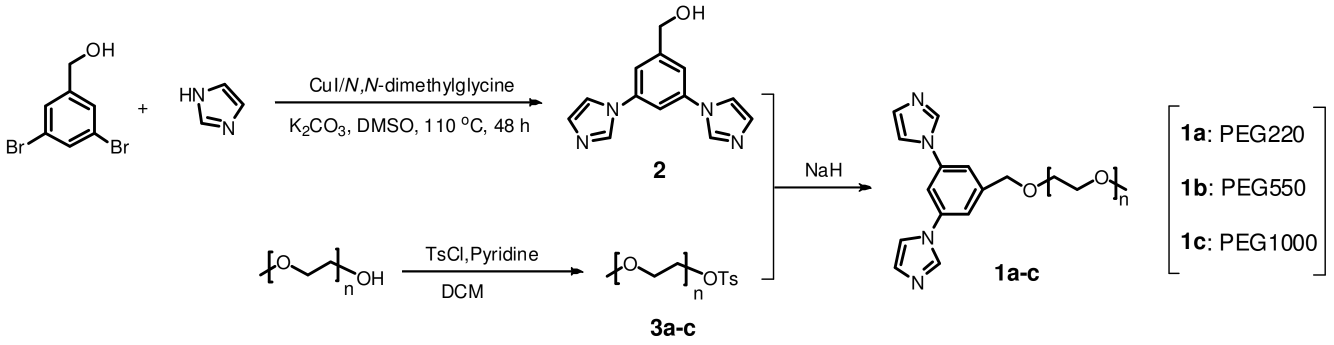
Synthesis

Scheme 1S. Synthesis of compounds **1a-c**



Compound 2.[1] A Schlenk flask was charged with (3,5-dibromophenyl) methanol (106.38 mg, 0.4 mmol), imidazole (68.08 mg, 1 mmol), CuI (15.24 mg, 0.08 mmol), *N*, *N*-dimethylglycine (16.5 mg, 0.16 mmol), and K_2CO_3(221.14 mg, 1.6 mmol). The system was then evacuated twice and back filled with N_2, followed by addition of 4 mL of DMSO. The mixture was heated at 110 ^{o}C for 48 h before it was partitioned between water and ethyl acetate. The organic layer was separated, and the aqueous layer was extracted with ethyl acetate (3 × 10 mL). The combined organic layers were washed with brine, dried over $MgSO_4$, and concentrated *in vacuo*. The residue was loaded on a silica gel column and eluted with CH_2Cl_2/CH_3OH (10/1) to give the compound **2** as a white solid with the yield of 48%.

Compound 3a-c. To a solution of poly(ethylene glycol) monomethyl ether (10 mmol) and *p*-toluenesulfonyl chloride (3.81 g, 20 mmol) in 20 mL of anhydrous CH_2Cl_2, pyridine (1.6 mL) was added. The reaction mixture was stirred at 25 ^{o}C under N_2 atmosphere for 24 h. After the addition of 5 mL aqueous solution of HCl (1 M), the mixture was extracted with CH_2Cl_2 (3 × 30 mL). The combined organic layers were washed with brine, dried over $MgSO_4$, and concentrated *in vacuo*. The residue was loaded on a silica gel column and eluted with CH_2Cl_2/CH_3OH (10/1) to give the desired product as a colorless oil.

Compound 1a.[2] NaH (9.60 mg, 0.4 mmol) was added to a solution of compound **2** (48.1 mg, 0.2 mmol) in dry *N*,*N*-dimethylformamide (DMF, 2 mL) at room temperature. After the mixture was stirred at room temperature for 1 h, compound **3a** (83.4 mg, 0.24 mmol) in an anhydrous DMF (1.5 mL) was added slowly. The reaction mixture was stirred at 100 °C under N_2 atmosphere for 20 h, cooled to room temperature, and poured over 10 mL of icy water. The mixture was extracted with CH_2Cl_2 (3 × 10 mL). The combined organic phase was washed with brine (30 mL), dried over $MgSO_4$, and concentrated *in vacuo.* The residue was loaded on a silica gel column and eluted with CH_2Cl_2/CH_3OH (10/1) to give the product as a colorless oil with the yield of 78%. ^1H NMR (400 MHz, $CDCl_3$): δ 3.32 (S, 3 H), 3.49-3.71 (m, 16H), 4.66 (S, 2H), 7.21 (S, 2H), 7.33 (S, 3H), 7.39 (S, 2H), 7.93(S, 2H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 58.93, 70.21, 70.48, 70.58, 113.20, 118.09, 118.61, 130.77, 135.52, 143.13. High resolution ESI-MS: $[M+H]^+$ calcd for $C_{22}H_{31}N_4O_5^+$ 431.2294, found 431.2287.

Compound 1b. Following the synthetic procedure of compound **1a**, compound **2** (50 mg, 0.21 mmol), NaH (9.96 mg, 0.42mmol), and compound **3b** (87.51 mg, 0.25mmol) were used. The residue was loaded on a silica gel column and eluted with CH_2Cl_2/CH_3OH (10/1) to give compound **1b** as a colorless oil with the yield of 82%. ^1H NMR (400 MHz, $CDCl_3$): δ 3.34 (S, 3H), 3.51-3.71 (m, 48H), 4.67 (S, 2H), 7.22 (S, 2H), 7.37 (S, 2H), 7.41 (S, 3H), 8.01 (S, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 58.95, 70.18, 70.59, 71.76, 113.30, 118.17, 118.63, 130.43, 135.52, 143.15. High resolution ESI-MS: $[M+H]^+$ calcd for $C_{38}H_{63}N_4O_{13}^+$ 783.4392, found 783.4383. Pairs of peaks correspond to different length oligomers (each pair containing a $[M + H]^+$).

Compound 1c. Following the synthetic procedure of compound **1a**, compound **2** (50 mg, 0.21 mmol), NaH (9.96 mg, 0.42mmol), and compound **3c** (294.7 mg, 0.25mmol) were used. The residue was loaded on a silica gel column and eluted with CH_2Cl_2/CH_3OH (10/1) to give compound **1c** as a colorless oil with the yield of 80%). ^{1}HNMR (400MHz, $CDCl_3$): δ 3.33 (S, 3H), 3.49-3.70 (m, 72H), 4.66 (S, 2H), 7.20 (S, 2H), 7.34 (S, 3H), 7.39 (S, 2H), 7.94 (S, 2H). ^{13}CNMR ($CDCl_3$, 100 MHz): δ 58.98, 70.16, 70.50, 70.61, 113.23, 118.12, 118.57, 130.71, 135.53, 143.07 High resolution ESI-MS: $[M+Na]^+$ calcd for $C_{56}H_{98}N_4NaO_{22}^+$ 1201.6570, found 1201.6539. Pairs of peaks correspond to different length oligomers (each pair containing a $[M + Na]^+$).

References

1. W. J. Guan, W. J. Zhou, C. Lu, B. Z. Tang, *Angew. Chem., Int. Ed.,* 2015, **54**, 15160-15164.
2. M. A. Azagarsamy, P. Sokkalingam, S. Thayumanavan, *J. Am. Chem. Soc.,* 2009, **131**, 14184-14185.

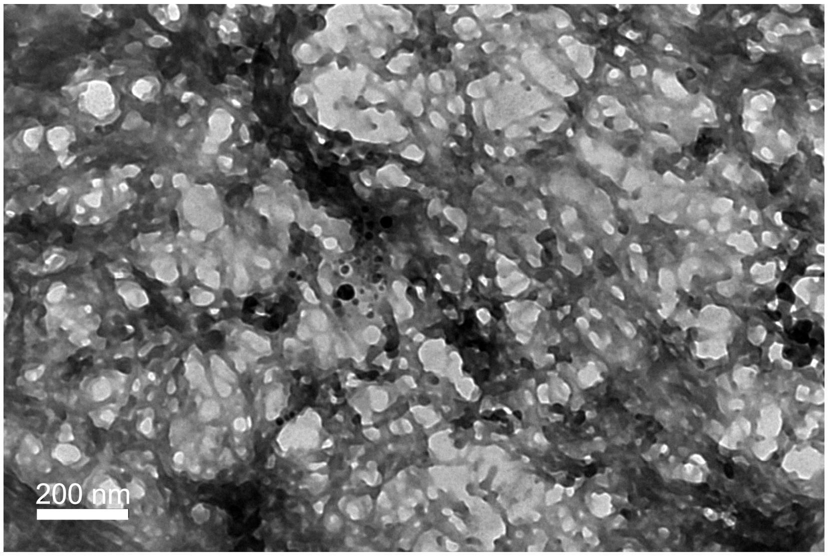


Fig. 1S. TEM micrograph of coordination polymer hydrogel of **Ag/1c**.

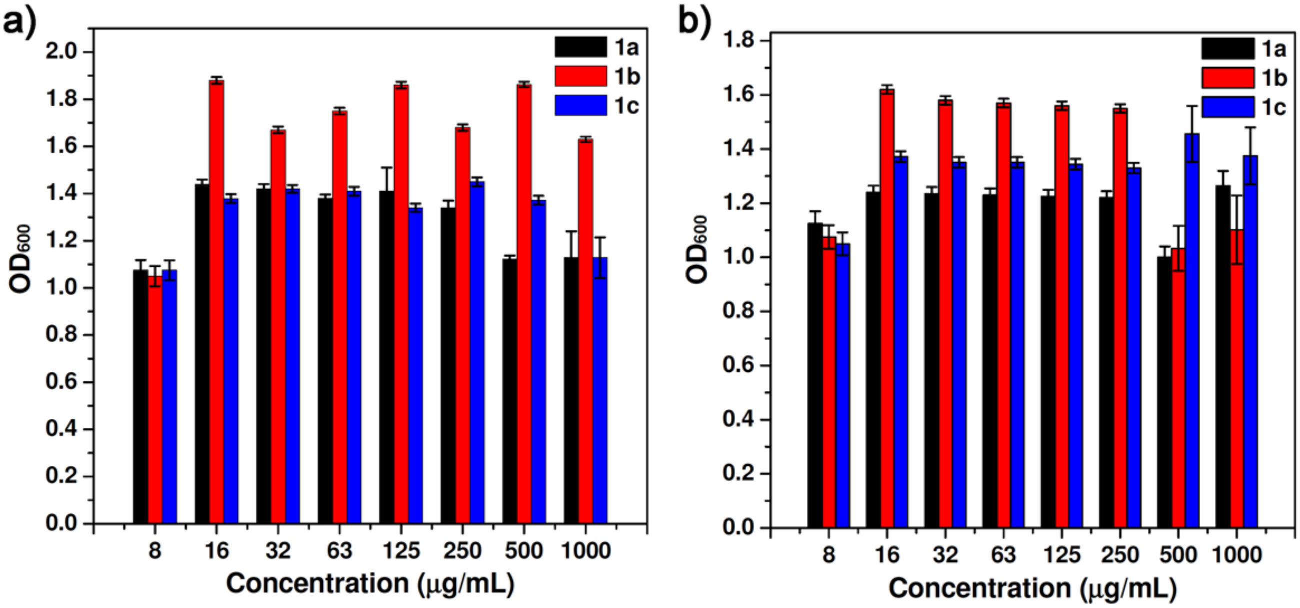


Fig. 2S. OD600 values for *S. aureus* (a) and *E. coli* (b) with different concentrations of ligands **1a-c**.

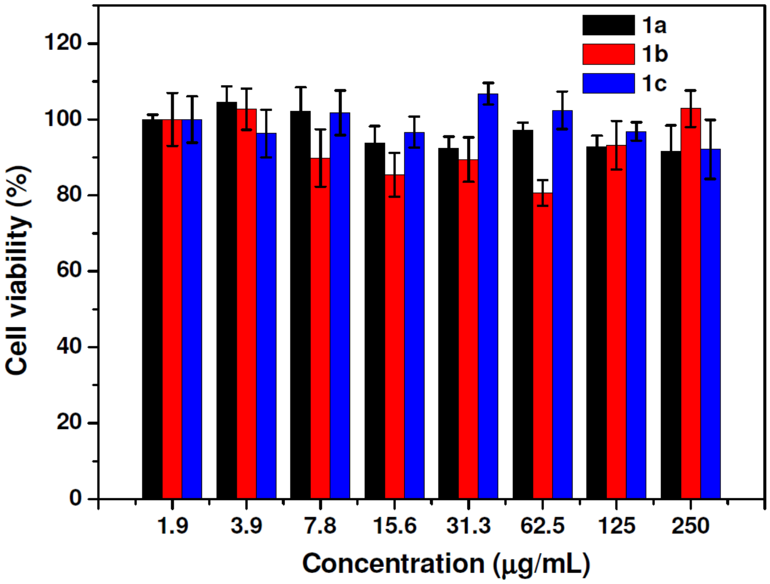
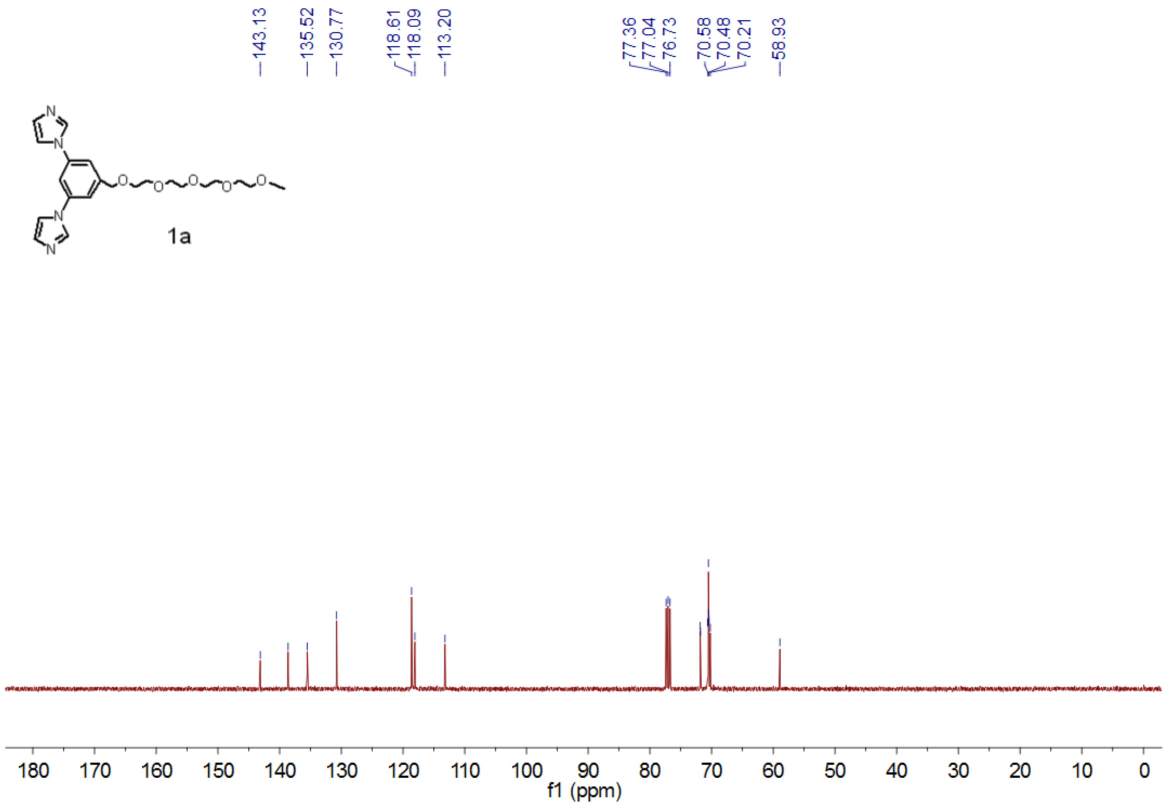
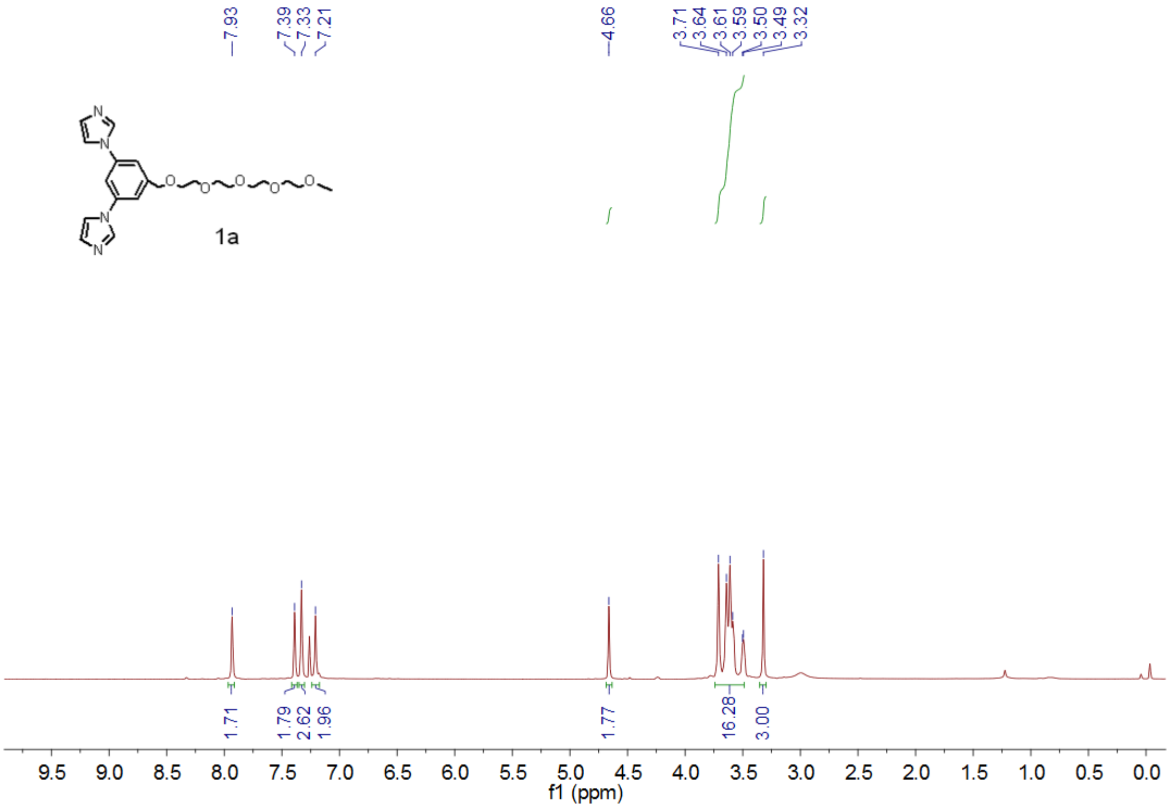
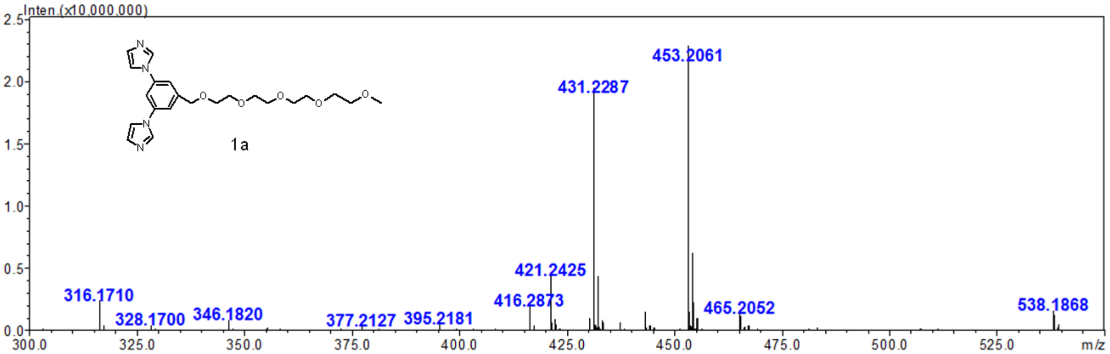


Fig. 3S. *In vitro* cytotoxicity of ligands **1a-c** against 293T cells after incubation for 24 h at 37 °C with a series of concentrations. 293T cells incubated without any materials were used as the control (mean ± SD, n = 6).

^{1}H, ^{13}C NMR, and MS Spectra of Compounds 1a-c



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416.2873
316.1710
328.1700
346.1820
377.2127
395.2181
465.2052
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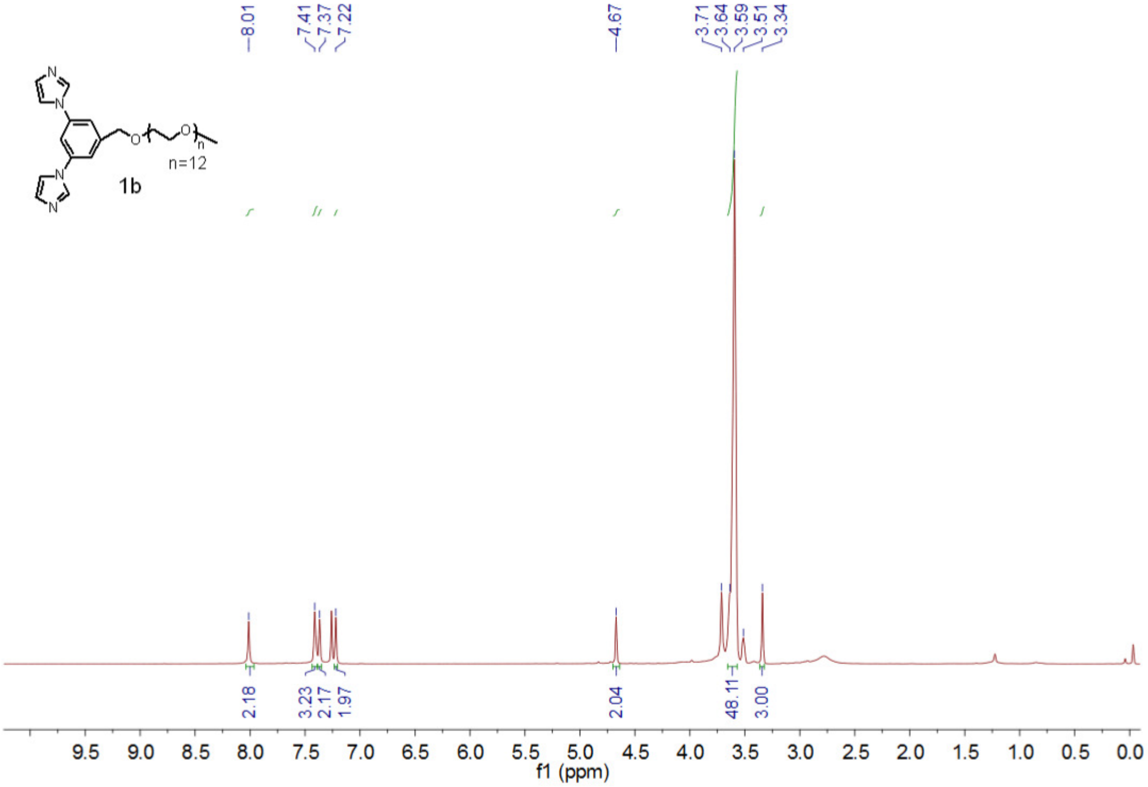
m/z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3.00
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9.0
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8.0
7.5
7.0
6.5
6.0
5.5
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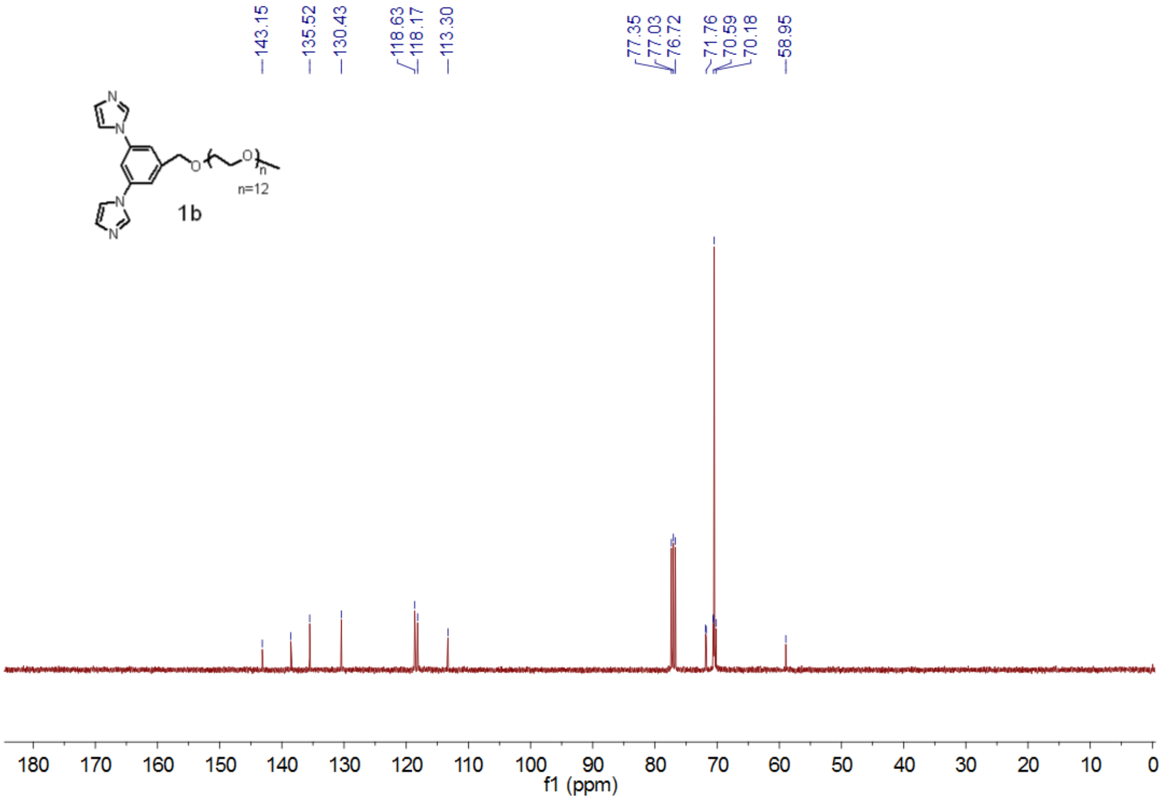
f1 (ppm)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N
N
O
O
n
n=12
1b
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70
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50
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30
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10
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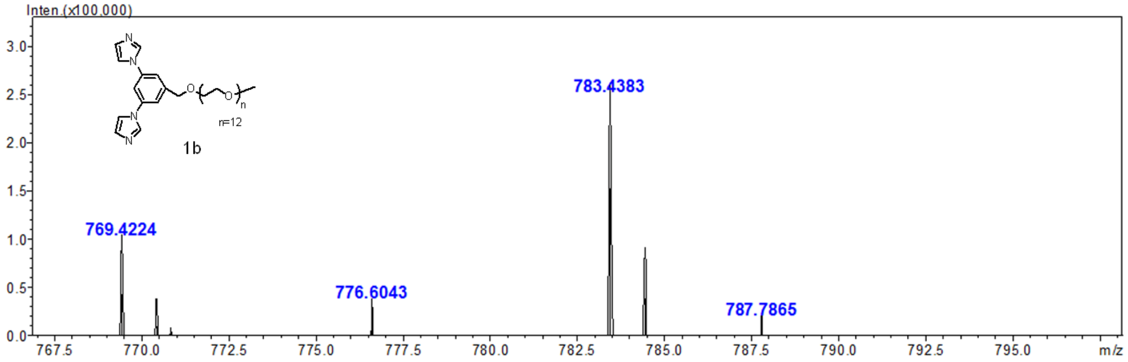
f1 (ppm)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O
n
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1b
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767.5
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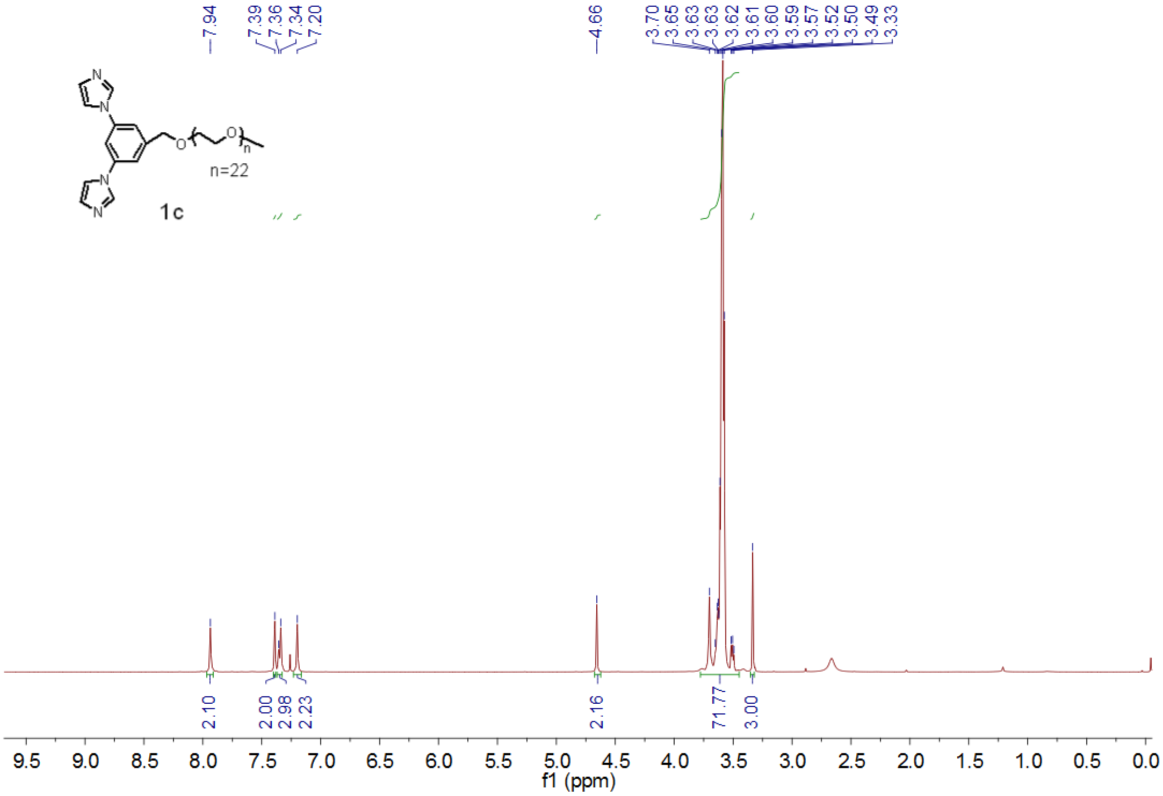
m/z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2.98
2.23
2.16
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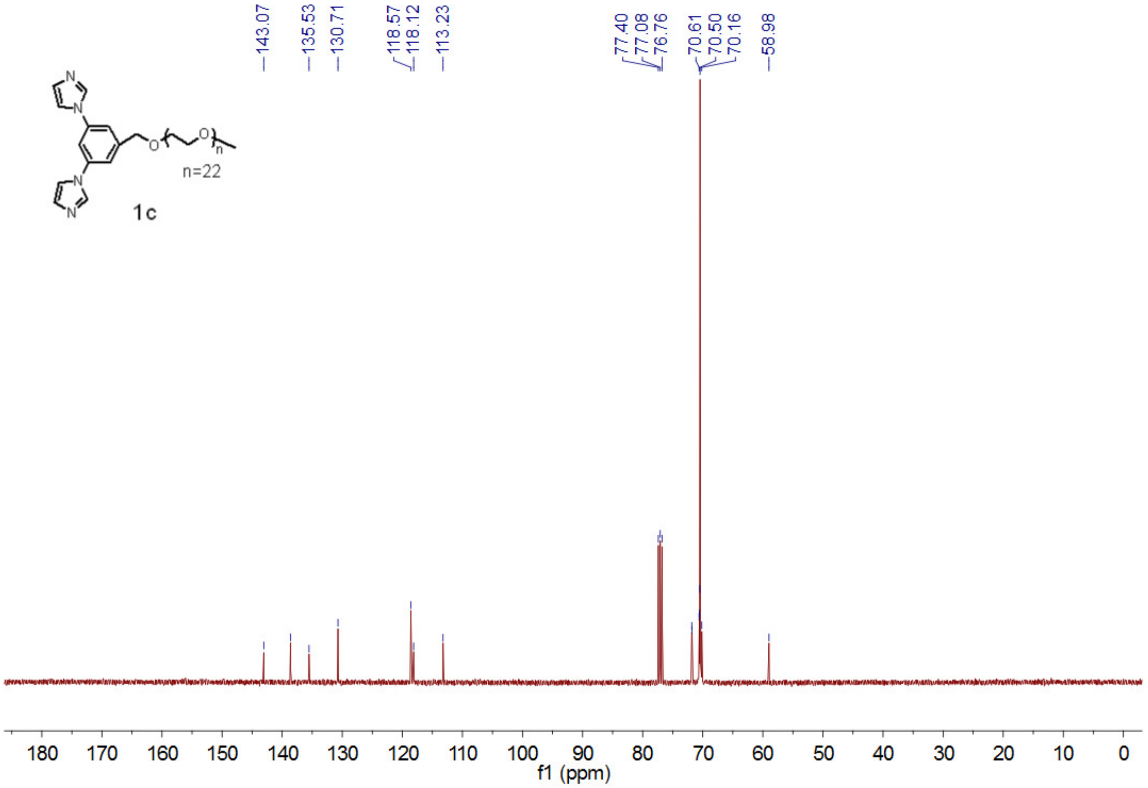
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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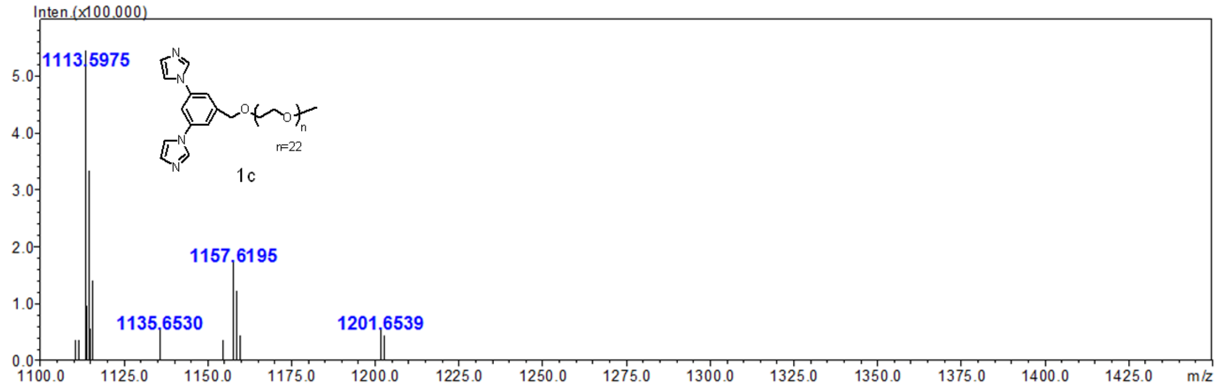
f1 (ppm)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N
N
O
O
n
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1c
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1125.0
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1200.0
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m/z