

Supporting Information

Development of electrically activable phosphonium self-assembled monolayers to efficiently kill and tackle bacterial infections on-demand.

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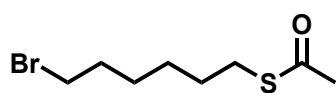
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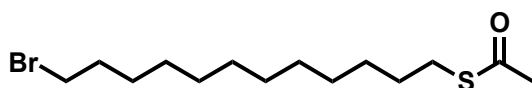
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1.1 Synthesis



S-(6-Bromohexyl) ethanethioate. (1). Dibromohexane (6 g; 24.6 mmol; 5 eq.) into acetone (125 mL) was added potassium thioacetate (561 mg; 5 mmol; 1 eq.). Then the mixture was stirred at room temperature for 16 hours. The solvent was then evaporated under high vacuum and the obtained residue was taken up into water (75 mL), the aqueous phase was extracted with DCM (3 x 50 mL). The combined organic layers were washed with brine (50 mL), dried over MgSO_4 , filtered and evaporated under vacuum. The product was purified over SiO_2 column flash chromatography (EP / AcOEt ; 95 : 5) to give a colorless oil (779 mg ; 3.26 mmol ; 65% yield). ^1H NMR (400 MHz ; CDCl_3): δ 3.39 (t, 2H, J 6.6 Hz), 2.85 (t, 2H, J 7.4 Hz), 2.31 (s, 3H), 1.84 (quint, 2H, J 7.2 Hz), 1.57 (quint, 2H, J 7.2 Hz), 1.41 (m, 4H). ^{13}C (101 MHz, CDCl_3): δ 196.6, 33.1, 32.6, 30.7, 29.4, 29, 27.9, 27.4. ESI MS : 239.1 m/z : $[\text{M}+\text{H}]^+$; 245.0 m/z : $[\text{M}+\text{Li}]^+$.



S-(6-Bromododecyl) ethanethioate (2). To a solution of 1,12-dibromododecane (5 g; 15.2 mmol; 5 eq.) into acetone (125 mL) was added potassium thioacetate (348 mg; 3 mmol; 1 eq.) under inert atmosphere. Then the mixture was let to react at room temperature for 16 hours. The solvent was then evaporated under high vacuum and the obtained residue was taken up into water (150 mL) and the aqueous phase was extracted with DCM (3 x 100 mL). The combined organic layers were washed with brine (100 mL), dried over MgSO_4 , filtered and evaporated under vacuum. The product was purified over SiO_2 column flash chromatography (EP : AcOEt ; 95 : 5) to give a colorless oil (721 mg ; 2.23 mmol; 74% yield). ^1H NMR (400 MHz ; CDCl_3): δ 3.39 (t, 2H, J 6.8 Hz), 2.85 (t, 2H, J 7.4 Hz), 2.31 (s, 3H), 1.84 (quint, 2H, J 7 Hz), 1.53 (quint, 2H, J 7.2 Hz), 1.40 (quint, 2H, J 7.2 Hz), 1.25 (br, 14H). ^{13}C NMR (101 MHz ; CDCl_3): δ 196.2, 34.2, 32.9, 30.7, 29.6, 29.2, 28.9, 28.2 ; 6 signals obscured or overlapping. ESI MS : 325 m/z : $[\text{M}+\text{H}]^+$; 342.1 m/z : $[\text{M}+\text{NH}_4]^+$; 346.9 m/z : $[\text{M}+\text{Na}]^+$.

1.2 Design of Experiments

| | Number of levels | Name /Value |
|-----------------|------------------|---------------------|
| Factor 1 | 3 | Contact time |
| Level 0 | | 30 min |
| Level 1 | | 60 min |
| Level 2 | | 120 min |
| Factor 2 | | Voltage |
| Level 0 | 4 | CA 0.2 |
| Level 1 | | CA 0.5 |
| Level 2 | | CA 0.8 |
| Level 3 | | CVM |
| Factor 3 | 7 | Ionic Liquid |
| Level 0 | | Without |
| Level 1 | | 6-12 50% |
| Level 2 | | 6-12 100% |
| Level 3 | | 8-6 50% |
| Level 4 | | 8-6 100% |
| Level 5 | | 8-12 50% |
| Level 6 | | 8-12 100% |

Figure S1. Factors and levels for DOE matrix preparation.

| Experiment | Ionic Liquid | Contact time | Voltage |
|------------|--------------|--------------|---------|
| 1 | Without | 30 | CA 0.2V |
| 12 | Without | 120 | CVM |
| 20 | 6-12 50% | 60 | CA 0.8V |
| 22 | 6-12 50% | 30 | CVM |
| 29 | 6-12 100% | 60 | CA 0.5V |
| 36 | 6-12 100% | 120 | CVM |
| 42 | 8-6 50% | 120 | CA 0.5V |
| 43 | 8-6 50% | 30 | CA 0.8V |
| 50 | 8-6 100% | 60 | CA 0.2V |
| 52 | 8-6 100% | 30 | CA 0.5V |
| 57 | 8-6 100% | 120 | CA 0.8V |
| 66 | 8-12 50% | 120 | CA 0.5V |
| 71 | 8-12 50% | 60 | CVM |
| 75 | 8-12 100% | 120 | CA 0.2V |
| 79 | 8-12 100% | 30 | CA 0.8V |
| 83 | 8-12 100% | 60 | CVM |

Figure S2. Critical factors extrapolated from the complex matrix for DOE.