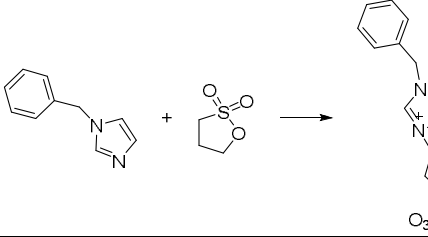
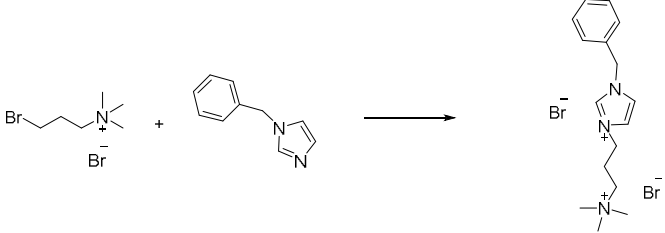
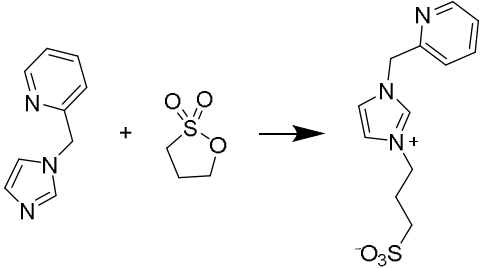
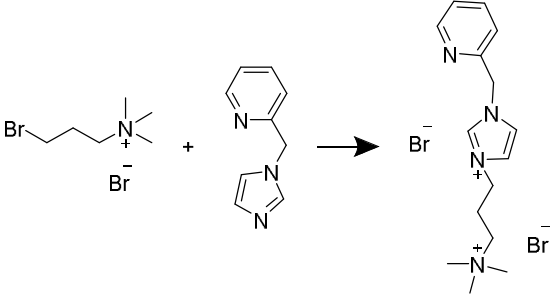
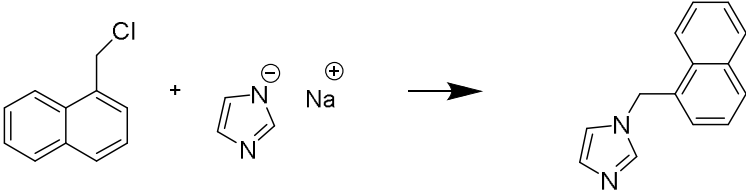
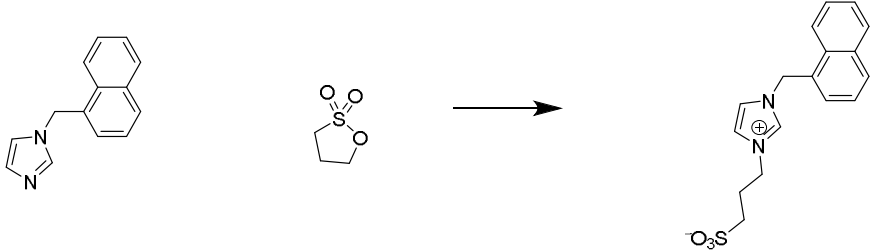
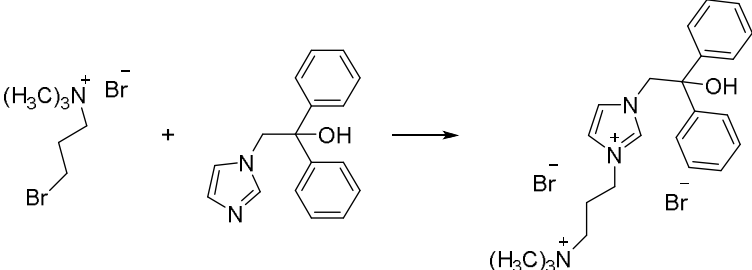
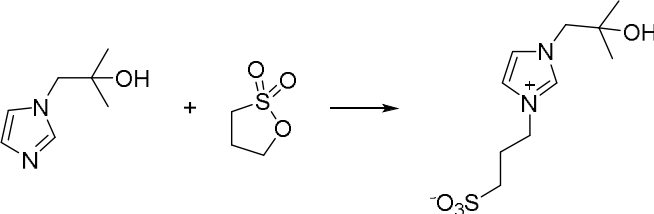
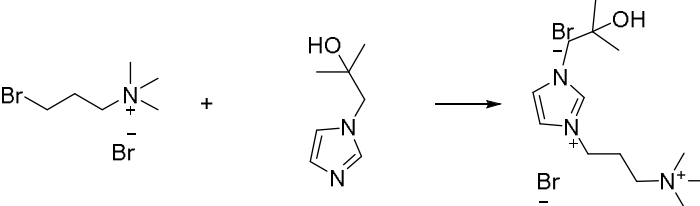
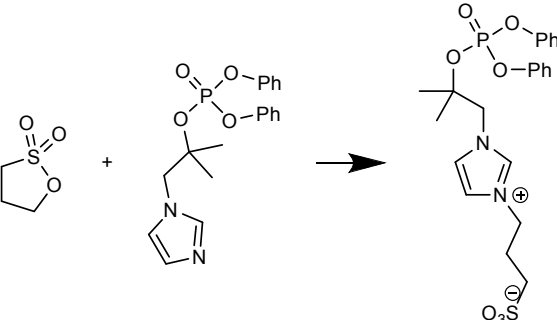
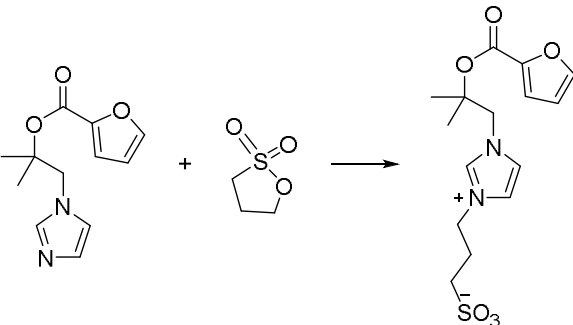
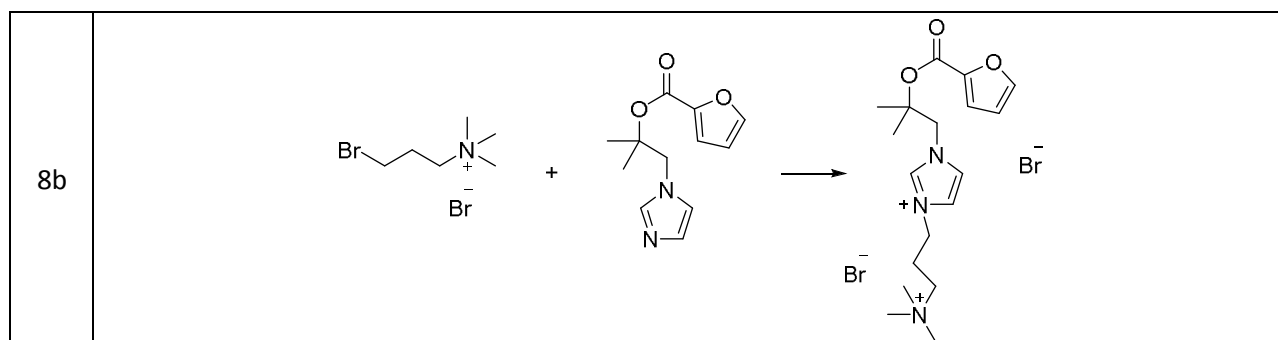


1a	
1b	
2a	
2b	
3	
3a	

3b	<p>Reaction of 1-bromo-3-(trimethylammonio)propane bromide with 1-(naphthalen-1-yl)pyrrole to form a dicationic product.</p>
4a	<p>Reaction of 1,1,1-triphenyl-2-imidazolidenylethane with ethylene sulfide to form a sulfonium salt.</p>
4b	<p>Reaction of 1,1,1-triphenyl-2-imidazolidenylethane with 1-bromo-3-(trimethylammonio)propane bromide to form a dicationic product.</p>
5i	<p>Reaction of benzophenone with a trimethylsilyl iodide salt, NaH, and <math>\text{NH}_4\text{Cl}</math> to form a cyclic acetal.</p>
5	<p>Reaction of 1,1-diphenyl-2-oxirane with imidazole to form a bicyclic product.</p>
5a	<p>Reaction of 1-(1-hydroxy-1-phenylethyl)pyrrole with ethylene sulfide to form a sulfonium salt.</p>

5b	
6a	
6b	
7a	
8a	



## Experimental

**General Procedures.** Unless otherwise noted, reactions and manipulations were performed under an inert atmosphere of Argon either in a glove box or with a standard vacuum/gas manifold using Schlenk techniques. All glassware was dried for at least 8 h at 150 °C before using. NMR spectra (1H, 13C, 31P) were taken on a Varian AS500 spectrometer (500 MHz). Chemical shifts are referenced to residual protons in the deuterated solvent and are reported in parts per million ( $\delta$ ); coupling constants are reported in hertz (Hz); and integrations are reported in number of protons (H). HRMS data was obtained on a Waters LCT Premier XE by direct injection using methanol in positive mode. Elemental analyses were performed by ALS Environmental in Tucson Arizona. Melting points were determined using an OptiMelt Automated Melting Point System with a heating rate of 1°C/min within a defined range.

## Materials.

Unless otherwise noted, all chemicals were purchased from commercial suppliers and used without further purification. Sodium hydride was washed with hexanes to remove mineral oil and dried under argon. 1-(1H-imidazol-1-yl)-2-methylpropan-2-yl furan-2-carboxylate was purchased from Broadpharm Inc. as a custom compound. Sodium imidazol-1-ide and 2-((1H-imidazol-1-yl)methyl)pyridine were synthesized using known literature procedures.<sup>1,2</sup> Acetonitrile, Tetrahydrofuran, Dimethyl sulfoxide, and diethyl ether were purchased as anhydrous solvents and stored over molecular sieves or dried using a Vacuum Atmospheres Company Closed Loop Solvent Recirculation Module.

### 3-(1-benzyl-1H-imidazol-3-ium-3-yl)propane-1-sulfonate (1a)

A 250 mL Schlenk flask was charged with 1-benzyl-1H-imidazole (12.78 g, 80 mmol), 1,2-oxathiolane 2,2-dioxide (11.97 g, 96 mmol), and acetonitrile (125 mL). The reaction flask was fitted with a reflux condenser and heated to 62°C with vigorous stirring for 48 hours. After 48 hours, the solution was found to be heterogeneous with a white precipitate. The flask was removed from the heating mantle and allowed to cool to room temperature. The product was collected via filtration, in air, and subsequently washed with 50 mL of acetonitrile and 50 mL of acetone to afford 3-(1-benzyl-1H-imidazol-3-ium-3-yl)propane-1-sulfonate (21.82 g, 78 mmol, 97 % yield). mp. 279.2-282.2°C. <sup>1</sup>H NMR (500 MHz, D<sub>2</sub>O):  $\delta$  = 2.31 (m, 2H), 2.91 (t,  $J$  = 7.3 Hz, 2H), 4.35 (t,  $J$  = 7.3 Hz, 2H), 5.38 (s, 2H), 7.41-7.50 (m, 6H), 7.55 (m, 1H), 8.86 (s, 1H). <sup>13</sup>C {<sup>1</sup>H} NMR (125 MHz, D<sub>2</sub>O):  $\delta$  = 25.0, 47.2, 47.9, 52.9, 122.58, 122.59, 128.6, 129.3, 129.3, 133.5, 135.6 ppm. Elemental Analysis: Anal. Calcd for C<sub>13</sub>H<sub>16</sub>N<sub>2</sub>O<sub>3</sub>S: C, 55.70; H, 5.75; N, 9.99. Found: C, 55.67; H, 5.85; N, 9.95. HRMS (ESI-TOF; CH<sub>3</sub>OH)  $m/z$ : [M+H]<sup>+</sup> Calcd for C<sub>13</sub>H<sub>17</sub>N<sub>2</sub>O<sub>3</sub>S 281.0960; Found 281.0958.

### 1-benzyl-3-(3-(trimethylammonio)propyl)-1H-imidazol-3-ium bromide (1b)

A 250 mL Schlenk flask was charged with 1-benzyl-1H-imidazole (12.46 g, 78 mmol), 3-bromo-N,N,N-trimethylpropan-1-aminium bromide (17.49 g, 65.0 mmol) and acetonitrile (135 mL). The reaction flask was fitted with a reflux condenser and heated to 62°C with vigorous stirring for 72 hours. After 72 hours, the solution was found to be heterogeneous with a white precipitate. The flask was removed from the heating mantle and allowed to cool to room temperature. The product was collected via filtration, in air, and subsequently washed with 50 mL of acetonitrile and 50 mL of acetone to afford 1-benzyl-3-(3-(trimethylammonio)propyl)-1H-imidazol-3-ium bromide (26.31 g, 62.8 mmol, 97 % yield). mp. 206.4-210.2°C. <sup>1</sup>H NMR (500 MHz, DMSO-d<sub>6</sub>):  $\delta$  = 2.37 (m, 2H), 3.15 (s, 9H), 3.50 (m, 2H), 4.30 (t,  $J$  = 7.1 Hz, 2H), 5.51 (s, 2H), 7.36-7.43 (m, 3H), 7.48-7.51 (m, 2H), 7.92 (m, 1H), 7.98 (m, 1H), 9.61 (s, 1H). <sup>13</sup>C {<sup>1</sup>H} NMR (125 MHz, DMSO-d<sub>6</sub>):  $\delta$  = 23.1, 46.1, 51.9, 52.3, 61.8,

<sup>1</sup> Bara, J. *Ind. Eng. Chem. Res. (Online)*, **2011**, 50, 13614–13619.

<sup>2</sup> Chiu, P. L.; Lai, C.; Chang, C.; Hu, C.; Lee, H. *Organometallics* (Online), **2005**, 24, 6169-6178.

122.6, 122.7, 128.5, 128.7, 128.9, 134.7, 136.5 ppm. Elemental Analysis: Anal. Calcd for  $C_{16}H_{25}Br_2N_3$ : C, 45.84; H, 6.01; N, 10.02. Found: C, 45.83; H, 6.11; N, 9.93. HRMS (ESI-TOF;  $CH_3OH$ )  $m/z$ :  $[M-Br]^+$  Calcd for  $C_{16}H_{25}BrN_3$  338.1232; Found 338.1225.

### 3-(1-(pyridin-2-ylmethyl)-1H-imidazol-3-ium-3-yl)propane-1-sulfonate (2a)

Synthesized on small scale using modified procedure.<sup>3</sup> A 40ml vial was charged with 1,2-oxathiolane 2,2-dioxide (0.678 g, 5.55 mmol) and 10ml acetonitrile. The solution was clear and colorless. 2-((1H-imidazol-1-yl)methyl)pyridine (0.7359 g, 4.62 mmol), dissolved in 10ml acetonitrile, was then added via pipette giving a yellowish orange, clear solution. The vial was sealed and heated to 70°C for 72 hours. After a few minutes, a precipitate could be seen forming. After 72 hours, the solution was found to be heterogeneous with white precipitate. The vial was removed from heat and allowed to cool to room temperature. The solid was filtered in air, washed with 10ml acetonitrile, followed by 10ml acetone, and dried in vacuo to afford 3-(1-(pyridin-2-ylmethyl)-1H-imidazol-3-ium-3-yl)propane-1-sulfonate (1.2363 g, 4.39 mmol, 95 % yield) as a tannish solid.  $^1H$  NMR (500 MHz,  $D_2O$ ):  $\delta$  = 2.36 (m, 2H), 2.95 (t,  $J$ = 7.5 Hz, 2H), 4.42 (t,  $J$ = 7.2 Hz, 2H), 5.56 (s, 2H), 7.46-7.48 (m, 1H), 7.52-7.56 (m, 2H), 7.64 (m, 1H), 7.92-7.96 (m, 1H), 8.53 (d,  $J$ = 4.7 Hz, 1H), 8.99 (s, 1H). Characterization matches that of the known literature.

### 1-(pyridin-2-ylmethyl)-3-(3-(trimethylammonio)propyl)-1H-imidazol-3-ium bromide (2b)

A 500ml Schlenk flask was charged with 3-bromo-N,N,N-trimethylpropan-1-aminium bromide (14 g, 53.6 mmol), 2-((1H-imidazol-1-yl)methyl)pyridine (9.46 g, 59.4 mmol), Acetonitrile (150 ml), and a stir bar. The flask was fitted with a reflux condenser and heated to 70°C with vigorous stirring for 72 hours. The reaction mixture became a homogenous clear, orange solution after reaching the reaction temperature. After 72 hours, the solution was found to be heterogeneous with white precipitate. The flask was removed from heat and allowed to cool to room temperature. The product collected via filtration, in air, washed with 50ml acetonitrile, followed by 50ml acetone, and dried in vacuo to afford 1-(pyridin-2-ylmethyl)-3-(3-(trimethylammonio)propyl)-1H-imidazol-3-ium bromide (18.4 g, 43.8 mmol, 81 % yield) as a white solid. mp. 101.1-102.1°C  $^1H$  NMR (500 MHz,  $DMSO-d_6$ )  $\delta$  = 2.39 (m, 2H), 3.16 (s, 9H), 3.49 (m, 2H), 4.35 (t,  $J$ =7.1 Hz, 2H), 5.65 (s, 2H), 7.38-7.41 (m, 1H), 7.56 (d,  $J$ =7.8, 1H), 7.87-7.91 (m, 2H), 8.01 (m, 1H), 8.54-8.56 (m, 1H), 9.56 (s, 1H).  $^{13}C$   $\{^1H\}$  NMR (125 MHz,  $DMSO-d_6$ )  $\delta$  = 23.2, 46.01, 52.3, 53.1, 61.8, 122.4, 122.7, 123.3, 123.6, 137.0, 137.5, 149.5, 153.5 ppm. Elemental Analysis: Anal. Calcd for  $C_{15}H_{24}Br_2N_4$ : C, 42.88; H, 5.76; N, 13.33. Found: C, 42.37; H, 5.89; N, 13.07. HRMS (ESI-TOF;  $CH_3OH$ )  $m/z$ :  $[M-Br]^+$  Calcd for  $C_{15}H_{24}BrN_4$  339.1184; Found 339.1179.

### 1-(naphthalen-1-ylmethyl)-1H-imidazole (3)

Known compound synthesized using new procedure.<sup>4</sup> A 250ml Schlenk flask was charged with 1-(chloromethyl)naphthalene (22 g, 112 mmol), sodium imidazol-1-ide (11.22 g, 112 mmol), Tetrahydrofuran (120 ml), and a stir bar. The naphthalene readily dissolved while imidazolidine remained. A reflux condenser was attached to the flask followed by heating to 75 °C with vigorous stirring. Solution turned yellow and remained heterogeneous once reaction temperature was reached. After 24 hours, reaction was heterogeneous with white solid in orange solution. The flask was removed from the heating mantle and allowed to cool to room temperature. The solid was filtered out in air, and washed with 50ml THF, giving yellow filtrate. Volatiles were removed from the filtrate via evaporation, leaving orange viscous oil which was dried in vacuo to afford 1-(naphthalen-1-ylmethyl)-1H-imidazole (22.4 g, 108 mmol, 96 % yield) as a dark orange viscous oil.  $^1H$  NMR (500 MHz,  $CDCl_3$ )  $\delta$  = 5.51 (s, 2H), 6.89 (s, 1H), 7.08 (s, 1H), 7.13 (d,  $J$ = 6.4, 1H), 7.41 (t,  $J$ = 7.6, 1H), 7.49-7.53 (m, 2H), 7.55 (s, 1H), 7.83-7.85 (m, 2H), 7.87-7.89 (m, 1H).  $^{13}C$   $\{^1H\}$  NMR (125 MHz,  $CDCl_3$ )  $\delta$  = 48.6, 119.46, 122.3, 125.4, 126.1, 126.2, 127.0, 129.0, 129.2, 129.5, 130.8, 131.3, 133.7, 137.5 ppm. Characterization matches that of the known literature.

### 3-(1-(naphthalen-1-ylmethyl)-1H-imidazol-3-ium-3-yl)propane-1-sulfonate (3a)

A 500ml flask was charged with 1-(naphthalen-1-ylmethyl)-1H-imidazole (10.6 g, 50.9 mmol), 1,2-oxathiolane 2,2-dioxide (7.46 g, 61.1 mmol), Acetonitrile (200 ml), and a stir bar yielding a clear, yellow solution. The flask was fitted with a reflux condenser and then heated to 75 °C with vigorous stirring. A white precipitate began to form shortly after reaching reaction temperature. After 48 hours, solution was heterogeneous with white precipitate. The flask was removed from the heating mantle and allowed

<sup>3</sup> Tomas-Mendivil, E.; Toullec, P. Y.; Diez, J.; Conejero, S.; Michelet, V.; Cadierno, V. *Org. Lett* (Online), **2012**, *14*, 2520-2523.

<sup>4</sup> Lee, H. M.; Lu, C. Y.; Chen, C. Y.; Chen, W. L.; Lin, H. C.; Chiu, P. L.; Cheng, P. Y. *Tetrahedron* (Online). **2004**, *60*, 5807-5825.

to cool to room temperature. The product collected via filtration, in air, washed with 50ml acetonitrile, followed by 50ml acetone, and dried in vacuo to afford 3-(1-(naphthalen-1-ylmethyl)-1H-imidazol-3-ium-3-yl)propane-1-sulfonate (16.0284 g, 48.5 mmol, 95 % yield) as a white solid. mp. Decomposed at 245°C. <sup>1</sup>H NMR (500 MHz, MeOH-d<sub>4</sub>) δ = 2.28 (m, 2H), 2.76 (t, *J* = 6.9 Hz, 2H), 4.39 (t, *J* = 7.1 Hz, 2H), 5.92 (s, 2H), 7.54-7.62 (m, 5H), 7.67 (m, 1H), 7.96-8.02 (m, 3H), 9.04 (s, 1H). <sup>13</sup>C {<sup>1</sup>H} NMR (125 MHz, MeOH-d<sub>4</sub>) δ = 27.1, 48.3, 52.1, 123.5, 123.93, 123.97, 124.01, 126.7, 127.6, 128.7, 129.8, 130.1, 130.3, 131.6, 132.29, 135.6, 137.8 ppm. Elemental Analysis: Anal. Calcd for C<sub>17</sub>H<sub>18</sub>N<sub>2</sub>O<sub>3</sub>S: C, 61.80; H, 5.49; N, 8.48. Found: C, 61.74; H, 5.46; N, 8.57. HRMS (ESI-TOF; CH<sub>3</sub>OH) *m/z*: [M+H]<sup>+</sup> Calcd for C<sub>17</sub>H<sub>19</sub>N<sub>2</sub>O<sub>3</sub>S 331.1116; Found 331.1105.

### 1-(naphthalen-1-ylmethyl)-3-(3-(trimethylammonio)propyl)-1H-imidazol-3-ium bromide (3b)

A 500ml flask was charged with 3-bromo-N,N,N-trimethylpropan-1-aminium bromide (11.33 g, 43.4 mmol), 1-(naphthalen-1-ylmethyl)-1H-imidazole (10.85 g, 52.1 mmol), Acetonitrile (150 ml) and a stir bar yielding a yellow solution with undissolved bromo salt. The flask was fitted with a reflux condenser and heated to 75 °C with vigorous stirring. The reaction mixture became homogenous after reaching reaction temperature and shortly after became heterogeneous with immiscible oil. After 48 hours, the solution was heterogeneous with immiscible brown oil. Transferred contents to new flask and removed volatiles via evaporation leaving brown gelatinous material. Product was washed by stirring vigorously in chloroform at 50°C, cooling in fridge, and decanting solvent. Repeated three times total (3x100ml), until chloroform was colorless. The product material was dried under high vacuum at 50°C for 72 hours to afford 1-(naphthalen-1-ylmethyl)-3-(3-(trimethylammonio)propyl)-1H-imidazol-3-ium bromide (17.6069 g, 37.5 mmol, 86 % yield) as a tan powder. mp. Decomposed at 103°C. <sup>1</sup>H NMR (500 MHz, DMSO-d<sub>6</sub>) δ = 2.36 (m, 2H), 3.15 (s, 9H), 3.50 (m, 2H), 4.30 (t, *J* = 7.1 Hz, 2H), 6.04 (s, 2H), 7.55-7.65 (m, 4H), 7.94 (m, 1H), 8.00-8.01 (m, 2H), 8.03 (s, 1H) 8.22 (d, *J* = 8.3 Hz, 1H), 9.54 (s, 1H). <sup>13</sup>C {<sup>1</sup>H} NMR (125 MHz, DMSO-d<sub>6</sub>) δ = 23.1, 46.1, 49.9, 52.3, 61.8, 122.6, 122.9, 123.1, 125.6, 126.4, 127.2, 127.9, 128.8, 129.6, 130.0, 130.4, 133.4, 136.6 ppm. Elemental Analysis: Anal. Calcd for C<sub>20</sub>H<sub>27</sub>BrN<sub>3</sub>: C, 51.19; H, 5.80; N, 8.95. Found: C, 51.02; H, 5.91; N, 8.79. HRMS (ESI-TOF; CH<sub>3</sub>OH) *m/z*: [M-Br]<sup>+</sup> Calcd for C<sub>20</sub>H<sub>27</sub>BrN<sub>3</sub> 388.1388; Found 388.1382.

### 3-(1-trityl-1H-imidazol-3-ium-3-yl)propane-1-sulfonate (4a)

A 250ml flask was charged with 1-trityl-1H-imidazole (10 g, 32.2 mmol), 1,2-oxathiolane 2,2-dioxide (4.72 g, 38.7 mmol), acetonitrile (120ml) and a stir bar. The flask was fitted with a reflux condenser and heated to 75°C. The reaction was nearly homogenous after reaching reaction temperature, with some trityl imidazole remaining. After 72 hours, the reaction was heterogeneous with white solid in a light yellow solution. The flask was removed from the heating mantle and allows to cool to room temperature. The product was collected via filtration, in air, washed with 50ml acetonitrile, followed by 50ml of acetone, and dried in vacuo to afford 3-(1-trityl-1H-imidazol-3-ium-3-yl)propane-1-sulfonate (12.4 g, 28.7 mmol, 89 % yield) as a white solid. mp. Decomposed at 245°C. <sup>1</sup>H NMR (500 MHz, DMSO-d<sub>6</sub>) δ = 2.10 (m, 2H), 2.40 (t, *J* = 7.1 Hz, 2H), 4.30 (t, *J* = 7.1 Hz, 2H), 7.20-7.22 (m, 6H), 7.42-7.48 (m, 9H), 7.53 (m, 1H), 7.93 (m, 1H), 9.10 (s, 1H). <sup>13</sup>C {<sup>1</sup>H} NMR (125 MHz, MeOH-d<sub>4</sub>) δ = ppm. Elemental Analysis: Anal. Calcd for C<sub>25</sub>H<sub>24</sub>N<sub>2</sub>O<sub>3</sub>S: C, 69.42; H, 5.59; N, 6.48. Found: C, 69.14; H, 5.75; N, 6.50. HRMS (ESI-TOF; CH<sub>3</sub>OH) *m/z*: [M+H]<sup>+</sup> Calcd for C<sub>25</sub>H<sub>25</sub>N<sub>2</sub>O<sub>3</sub>S 433.1586; Found 433.1578.

### 3-(3-(trimethylammonio)propyl)-1-trityl-1H-imidazol-3-ium bromide (4b)

A 500ml flask was charged with 3-bromo-N,N,N-trimethylpropan-1-aminium bromide (8.41 g, 32.2 mmol), 1-trityl-1H-imidazole (12 g, 38.7 mmol), Acetonitrile (250 ml), and a stir bar giving a heterogeneous solution. The flask was fitted with a reflux condenser and heated to 75 °C with vigorous stirring. Some solid material still remained after reaching reaction temperature. After 48 hours, the reaction was heterogeneous with white precipitate. The flask was removed from the heating mantle and left to sit overnight to cool to room temperature. The product was collected via filtration, in air, washed with 50ml acetonitrile, and rinsed with 50ml chloroform. The solid was transferred to a clean flask along with 150ml of chloroform and stirred vigorously for an hour. The solid was then filtered, rinsed with 50ml of chloroform, and dried in vacuo to afford 14.4117 g of crude material. NMR data shows product material as well as hydrolyzed product with trityl functional group cleaving from main imidazolium body. HRMS (ESI-TOF; CH<sub>3</sub>OH) *m/z*: [M-Br]<sup>+</sup> Calcd for C<sub>28</sub>H<sub>33</sub>BrN<sub>3</sub> 490.1858; Found 490.1855.

### 2,2-diphenyloxirane (5i)

Synthesized using modified procedure.<sup>5</sup> A 100ml schlenk flask was charged with sodium hydride (1.451 g, 60.5 mmol) and DMSO (24 ml)/THF (16 ml). After stirring for 15 minutes trimethylsulfonium iodide (12.34 g, 60.5 mmol) was added causing

<sup>5</sup> Vyas, D. J.; Larionov, E.; Besnard, C.; Guenee, L.; Mazet, C. *J. AM. Chem. Soc.*(Online), **2013**, *135*, 6177-6183

bubbling. The solution was stirred for 5 minutes and then cooled to 0°C in an ice bath while stirring. After 30 minutes, a solution of benzophenone (5.5097 g, 30.2 mmol) dissolved in 8 ml THF was added to the flask via syringe. The reaction was left in the ice bath overnight to slowly warm to room temperature. After 24 hours, 50 ml of dichloromethane was added to the flask, followed by ammonium chloride (1.62 g, 30.3 mmol), and 40 ml DI water. The solution was transferred to a separatory funnel and organic layer collected. The water layer was washed twice more with DCM (2x 50 ml). The organic fractions were collected, washed with DI water (2x 50 ml), brine (1x 50 ml), dried over Na<sub>2</sub>SO<sub>4</sub>, and filtered. Volatiles were removed via evaporation, and then under high vacuum yielding clear, colorless, viscous oil. The flask was stored in freezer overnight (-20°C) under Argon. The next day, the material had solidified giving white solid. The product 2,2-diphenyloxirane (5.42 g, 27.6 mmol, 91 % yield) was used immediately without further purification. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ = 3.29 (s, 2H), 7.26-7.37 (m, 10H). Characterization matches that of the known literature; material was not analytically pure.

### 2-(1H-imidazol-1-yl)-1,1-diphenylethanol (5)

To a 500 ml flask was added 2,2-diphenyloxirane (11.73 g, 59.8 mmol), 1H-imidazole (5 g, 73.4 mmol), and a stir bar. The flask was heated to 70°C with mild stirring. After a few minutes, all material melted giving homogenous solution. After 1 hour, the material solidified into a dark, yellow solid. Ethanol (250 ml) was added to the flask and fitted with a reflux condenser. The reaction was heated to 85°C with vigorous stirring until all material dissolved. The flask was then removed from heat and allowed to cool slowly to room temperature while still stirring. A white precipitate began to form shortly after removal from heat. Once the flask reached room temperature, it was placed in a freezer for 1 hour (-20°C). The precipitate was then collected via filtration, while still cold, washed with 35 ml of cold ethanol, rinsed with 30 ml diethyl ether, and dried in vacuo to afford 2-(1H-imidazol-1-yl)-1,1-diphenylethanol (11.998 g, 42.4 mmol, 70.9 % yield) as a white solid. mp. 204.1-205.4 °C. <sup>1</sup>H NMR (500 MHz, DMSO-*d*<sub>6</sub>): δ = 4.84 (s, 2H), 6.26 (s, 1H), 6.66 (s, 1H), 6.81 (s, 1H), 7.21 (m, 2H), 7.30 (m, 5H), 7.49 (m, 4H). <sup>13</sup>C {<sup>1</sup>H} NMR (125 MHz, DMSO-*d*<sub>6</sub>): δ = 55.3, 76.5, 120.8, 126.0, 126.76, 126.82, 127.9, 138.2, 145.4 ppm. Elemental Analysis: Anal. Calcd for C<sub>17</sub>H<sub>16</sub>N<sub>2</sub>O: C, 77.25; H, 6.10; N, 10.60. Found: C, 77.21; H, 6.44; N, 10.52. HRMS (ESI-TOF; CH<sub>3</sub>OH) *m/z*: [M+H]<sup>+</sup> Calcd for C<sub>17</sub>H<sub>17</sub>N<sub>2</sub>O 265.1341; Found 265.1333.

### 3-(1-(2-hydroxy-2,2-diphenylethyl)-1H-imidazol-3-ium-3-yl)propane-1-sulfonate (5a)

A 500 mL Schlenk flask was charged with 2-(1H-imidazol-1-yl)-1,1-diphenylethanol (10.00 g, 37.8 mmol), 1,2-oxathiolane 2,2-dioxide (5.55 g, 45.4 mmol), acetonitrile (200 mL), and a stir bar. The flask was fitted with a reflux condenser and heated to 75°C with vigorous stirring for 48 hours. The reaction mixture became homogeneous after reaching reaction temperature. After 48 hours, the solution was found to be heterogeneous with white precipitate. The flask was removed from heat and allowed to cool to room temperature. The product was collected via filtration, in air, washed with 50 mL of acetonitrile, rinsed with 50 ml acetone, and dried in vacuo to afford 3-(1-(2-hydroxy-2,2-diphenylethyl)-1H-imidazol-3-ium-3-yl)propane-1-sulfonate (14.6125 g, 37.8 mmol, 100 % yield) as a white solid. mp. Decomposed at 302°C. <sup>1</sup>H NMR (500 MHz, DMSO-*d*<sub>6</sub>): δ = 1.95 (m, 2H), 2.28 (m, 2H), 4.23 (m, 2H), 5.05 (s, 2H), 6.58 (s, 1H), 7.20 (s, 1H), 7.26 (m, 2H), 7.34 (t, *J* = 7.6 Hz, 4H), 7.43 (m, 4H), 7.57 (s, 1H), 8.78 (s, 1H). <sup>13</sup>C {<sup>1</sup>H} NMR (125 MHz, DMSO-*d*<sub>6</sub>): δ = 26.4, 47.1, 47.6, 57.7, 76.2, 121.3, 123.8, 126.0, 127.4, 128.3, 136.8, 143.9 ppm. Anal. Calcd for C<sub>20</sub>H<sub>22</sub>N<sub>2</sub>O<sub>4</sub>S: C, 62.16; H, 5.74; N, 7.25. Found: C, 62.00; H, 5.76; N, 7.24. HRMS (ESI-TOF; CH<sub>3</sub>OH) *m/z*: [M+H]<sup>+</sup> Calcd for C<sub>20</sub>H<sub>23</sub>N<sub>2</sub>O<sub>4</sub>S 387.1379; Found 387.1363.

### 1-(2-hydroxy-2,2-diphenylethyl)-3-(3-(trimethylammonio)propyl)-1H-imidazol-3-ium bromide (5b)

A 500 mL Schlenk flask was charged with 2-(1H-imidazol-1-yl)-1,1-diphenylethanol (10.67 g, 40.4 mmol), 3-bromo-N,N,N-trimethylpropan-1-aminium bromide (10.54 g, 40.4 mmol), acetonitrile (400 mL), and a stir bar. The flask was fitted with a reflux condenser and heated to 70 °C with vigorous stirring for 48 hours. The reaction mixture became homogeneous after reaching the reaction temperature. After 48 hours, the solution was found to be heterogeneous with white precipitate. The flask was removed from heat and allowed to cool to room temperature. The product was collected, in air, washed with 50 mL of acetonitrile, and dried in vacuo to afford 1-(2-hydroxy-2,2-diphenylethyl)-3-(3-(trimethylammonio)propyl)-1H-imidazol-3-ium bromide (16.4 g, 31.2 mmol, 88 % yield) as a white solid. mp. 210.7-213.5°C. <sup>1</sup>H NMR (500 MHz, DMSO-*d*<sub>6</sub>): δ = 2.21 (m, 2H), 3.11 (s, 9H), 3.35 (m, 2H), 4.24 (t, *J* = 7.0 Hz, 2H), 5.17 (s, 2H), 6.58 (s, 1H), 7.25 (t, *J* = 7.5 Hz, 2H), 7.33 (t, *J* = 7.5 Hz, 4H), 7.37 (s, 1H), 7.49 (d, *J* = 7.5 Hz, 4H), 7.75 (s, 1H), 9.03 (s, 1H). <sup>13</sup>C {<sup>1</sup>H} NMR (125 MHz, DMSO-*d*<sub>6</sub>): δ = 23.3, 45.8, 52.3, 57.4, 61.8, 76.3, 121.1, 123.9, 125.9, 127.3, 128.2, 136.9, 143.8 ppm. Anal. Calcd for C<sub>23</sub>H<sub>31</sub>BrN<sub>3</sub>O: C, 52.59; H, 5.95; N, 8.00. Found: C, 52.39; H, 6.26; N, 7.94. HRMS (ESI-TOF; CH<sub>3</sub>OH) *m/z*: [M-Br]<sup>+</sup> Calcd for C<sub>23</sub>H<sub>31</sub>BrN<sub>3</sub>O 444.1650; Found 444.1640.

### 3-(1-(2-hydroxy-2-methylpropyl)-1H-imidazol-3-ium-3-yl)propane-1-sulfonate (6a)

A 500 mL Schlenk flask was charged with 1H-imidazole (2.5 g, 36.7 mmol), 2,2-dimethyloxirane (2.65 g, 36.7 mmol), and a stir bar. The reaction flask was fitted with a reflux condenser and heated to 70 °C with vigorous stirring for 24 hours. The resulting viscous amber oil was allowed to cool to room temperature, diluted with 200 mL of acetonitrile, and stirred until homogeneous. Another solution of 1,2-oxathiolane-2,2-dioxide (5.37 g, 43.9 mmol) and 200 mL of dry acetonitrile was prepared in a separate Schlenk flask. This solution was cannulated into the reaction flask. This new reaction mixture was again fitted with a reflux condenser and heated to 70 °C with vigorous stirring for 48 hours. After approximately one hour, a fine white precipitate began to form.

After 48 hours, a large amount of precipitate was present. The reaction flask was removed from heat and allowed to cool to room temperature. The reaction mixture was filtered in air. The white solid was washed with 25 mL of acetonitrile and 25 mL of acetone and dried on a high vacuum line to afford 3-(1-(2-hydroxy-2-methylpropyl)-1H-imidazol-3-ium-3-yl)propane-1-sulfonate (9.2784 g, 35.4 mmol, 97 % yield) as a white powder. Analytically pure material was obtained from crystallization in ethanol and used for characterization. mp. 187.3-190.2 °C. <sup>1</sup>H NMR (500 MHz, DMSO-*d*<sub>6</sub>) δ = 1.08 (s, 6H), 2.10 (m, 2H), 2.44 (t, *J* = 7.5, 2H), 4.10 (s, 2H), 4.33 (t, *J* = 7.0, 2H), 5.04 (br, 1H), 7.66 (s, 1H), 7.81 (s, 1H), 9.10 (s, 1H). <sup>13</sup>C {<sup>1</sup>H} NMR (125 MHz, DMSO-*d*<sub>6</sub>) δ = 26.3, 26.6, 47.5, 47.8, 58.8, 68.1, 121.7, 124.1, 136.9 ppm. Elemental Analysis: Anal. Calcd for C<sub>10</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S: C, 45.79; H, 6.92; N, 10.68. Found: C, 45.71; H, 6.95; N, 10.58. HRMS (ESI-TOF; CH<sub>3</sub>OH) *m/z*: [M+H]<sup>+</sup> Calcd for C<sub>10</sub>H<sub>19</sub>N<sub>2</sub>O<sub>4</sub>S 263.1066; Found 263.1067.

### 1-(2-hydroxy-2-methylpropyl)-3-(3-(trimethylammonio)propyl)-1H-imidazol-3-ium bromide (6b)

A 500 mL Schlenk flask was charged with 1H-imidazole (6.10 g, 90 mmol), 2,2-dimethyloxirane (6.54 g, 91 mmol), and a stir bar. The reaction flask was fitted with a reflux condenser and heated to 70 °C with vigorous stirring for 24 hours. The resulting viscous amber oil was allowed to cool to room temperature, diluted with 200 mL of dry acetonitrile, and stirred until homogeneous. Another solution of 3-bromo-N,N,N-trimethylpropan-1-aminium bromide (20.7 g, 79 mmol) and 200 mL of dry acetonitrile was prepared in a separate Schlenk flask. This solution was cannulated into the reaction flask. This new reaction mixture was again fitted with a reflux condenser and heated to 70 °C with vigorous stirring for 48 hours. After approximately one hour, a fine white precipitate began to form.

After 48 hours, the flask was removed from heat, and the reaction mixture was filtered in air while still warm. The filtered reaction mixture was then placed in the freezer at 0 °C overnight. A white precipitate formed on the flask and was collected via filtration, washed with 25 mL of cold acetonitrile and 25 mL of cold acetone, and dried on a high vacuum line. The solid is very hygroscopic, so it is imperative that one works quickly to avoid losing product. The product 1-(2-hydroxy-2-methylpropyl)-3-(3-(trimethylammonio)propyl)-1H-imidazol-3-ium bromide (23.2 g, 58 mmol, 73 % yield) was obtained as a white solid. mp. 123.7-137.2 °C. <sup>1</sup>H NMR (500 MHz, DMSO-*d*<sub>6</sub>) δ = 1.12 (s, 6H), 2.35 (m, 2H), 3.11 (s, 9H), 3.42 (m, 2H), 4.14 (s, 2H), 4.32 (t, *J* = 7.5 Hz, 2H), 5.04 (s, 1H), 7.74 (s, 1H), 7.90 (s, 1H), 9.23 (s, 1H). <sup>13</sup>C {<sup>1</sup>H} NMR (125 MHz, DMSO-*d*<sub>6</sub>) δ = 23.2, 26.6, 45.9, 52.3, 58.8, 61.9, 68.1, 121.5, 124.1, 136.9 ppm. Elemental Analysis: Anal. Calcd for C<sub>13</sub>H<sub>27</sub>BrN<sub>3</sub>O: C, 38.92; H, 6.78; N, 10.47. Found: C, 38.19; H, 7.56; N, 10.38. HRMS (ESI-TOF; CH<sub>3</sub>OH) *m/z*: [M-Br]<sup>+</sup> Calcd for C<sub>13</sub>H<sub>27</sub>BrN<sub>3</sub>O 320.1337; Found 320.1339

### 3-(1-(2-((diphenoxyphosphoryl)oxy)-2-methylpropyl)-1H-imidazol-3-ium-3-yl)propane-1-sulfonate (7a)

A 500 mL Schlenk flask was charged with 1H-imidazole (1.02 g, 15.0 mmol), 2,2-dimethyloxirane (1.08 g, 15.0 mmol), and a stir bar. The reaction flask was fitted with a reflux condenser and heated to 70 °C with vigorous stirring for 24 hours. The resulting viscous amber oil was allowed to cool to room temperature, diluted with 200 mL of dry acetonitrile, and stirred until homogeneous. Another solution of diphenyl phosphoryl chloride (1.83 g, 15.0 mmol) and 200 mL of dry acetonitrile was prepared in a separate Schlenk flask. This solution was cannulated into the reaction flask. This new reaction mixture was again fitted with a reflux condenser and heated to 70 °C with vigorous stirring for 24 hours. After being heated and stirred again for another 24 hour period, the reaction mixture was allowed to cool to room temperature. A solution of 1,2-oxathiolane-2,2-dioxide (2.09 g, 17.1 mmol) and 50 mL of dry acetonitrile was prepared in a separate Schlenk flask. This solution was cannulated into the reaction flask. This new reaction mixture was fitted with a reflux condenser a final time and heated to 70 °C with vigorous stirring for 24 hours. After approximately one hour, a fine white precipitate began to form. A large amount of precipitate formed overnight. The reaction flask was removed from heat and allowed to cool to room temperature. The reaction mixture was filtered in air, and the white solid was washed with 50 mL of acetonitrile and 50 mL of acetone, and dried on a high vacuum line. 3-(1-(2-((diphenoxyphosphoryl)oxy)-2-methylpropyl)-1H-imidazol-3-ium-3-yl)propane-1-sulfonate (4.78 g, 9.67 mmol, 62 % yield) was obtained as a white powder. mp. 117.3-123.1 °C. <sup>1</sup>H NMR (500 MHz, DMSO-*d*<sub>6</sub>) δ = 1.50 (s, 6H), 2.09 (m, 2H), 2.42 (t, *J* = 7.5 Hz, 2H), 4.33 (t, *J* = 6.5 Hz, 2H), 4.48 (d, *J*<sub>P-H</sub> = 2.0 Hz, 2H), 7.22 (d, *J* = 9.0 Hz, 4H), 7.26 (t, *J* = 7.5 Hz, 2H), 7.43 (t, *J* = 8.0 Hz, 4H), 7.48 (s, 1H), 7.80 (s, 1H), 9.13 (s, 1H). <sup>13</sup>C {<sup>1</sup>H} NMR (125 MHz, DMSO-*d*<sub>6</sub>) δ = 24.4, 26.2, 47.2, 48.0, 57.3 (d, *J*<sub>P-C</sub> = 8.5



Hz), 83.9 (d,  $J_{P-C}$  = 6.6 Hz), 119.9 (d,  $J_{P-C}$  = 4.8 Hz), 122.3, 123.7, 125.6, 130.1, 137.2, 149.9 (d,  $J_{P-C}$  = 6.6 Hz) ppm.  $^{31}\text{P}$  { $^1\text{H}$ } NMR (202 MHz, DMSO- $d_6$ ):  $\delta$  = -16.34 ppm (s). Elemental Analysis: Anal. Calcd for  $\text{C}_{22}\text{H}_{27}\text{N}_2\text{O}_7\text{PS}$ : C, 53.44; H, 5.50; N, 5.67. Found: C, 53.07; H, 6.18; N, 5.69. HRMS (ESI-TOF;  $\text{CH}_3\text{OH}$ )  $m/z$ :  $[\text{M}+\text{H}]^+$  Calcd for  $\text{C}_{22}\text{H}_{28}\text{N}_2\text{O}_7\text{PS}$  495.1355; Found 495.1342

### **3-(1-(2-((furan-2-carbonyl)oxy)-2-methylpropyl)-1H-imidazol-3-ium-3-yl)propane-1-sulfonate (8a)**

A 100ml Schlenk flask was charged with 1-(1H-imidazol-1-yl)-2-methylpropan-2-yl furan-2-carboxylate (2.5636 g, 10.94 mmol), 1,2-oxathiolane 2,2-dioxide (1.604 g, 13.13 mmol), Acetonitrile (50 ml), and a stir bar giving an orange, homogenous solution. The flask was fitted with a reflux condenser and heated to 75°C with vigorous stirring for 48 hours. After 1 hour, a white precipitate began to form. After 48 hours, the solution was found to be heterogeneous with white precipitate. The flask was removed from heat and allowed to cool to room temperature. The product was collected via filtration, in air, washed with 50ml Acetonitrile, rinsed with 10ml acetone and dried in vacuo to afford 3-(1-(2-((furan-2-carbonyl)oxy)-2-methylpropyl)-1H-imidazol-3-ium-3-yl)propane-1-sulfonate (3.1948 g, 8.96 mmol, 82 % yield) as a white powder. mp. Decomposed at 198.8°C.  $^1\text{H}$  NMR (500 MHz, D $_2\text{O}$ ):  $\delta$  = 1.63 (s, 6H), 2.35 (m, 2H), 2.90 (t,  $J$  = 7.6 Hz, 2H), 4.44 (t,  $J$  = 7.3 Hz, 2H), 4.57 (s, 2H), 6.63-6.64 (m, 1H), 7.29 (d,  $J$  = 3.5 Hz, 1H), 7.64-7.66 (m, 2H), 7.77 (m, 1H), 9.01 (s, 1H).  $^{13}\text{C}$  { $^1\text{H}$ } NMR (125 MHz, D $_2\text{O}$ ):  $\delta$  = 22.4, 25.1, 47.1, 48.0, 57.8, 81.7, 112.4, 119.3, 122.2, 124.2, 136.7, 143.9, 147.7, 158.7 ppm. Elemental Analysis: Anal. Calcd for  $\text{C}_{15}\text{H}_{20}\text{N}_2\text{O}_6\text{S}$ : C, 50.55; H, 5.66; N, 7.86. Found: C, 50.15; H, 5.65; N, 8.00. HRMS (ESI-TOF;  $\text{CH}_3\text{OH}$ )  $m/z$ :  $[\text{M}+\text{H}]^+$  Calcd for  $\text{C}_{15}\text{H}_{21}\text{N}_2\text{O}_6\text{S}$  357.1120; Found 357.1102.

### **1-(2-((furan-2-carbonyl)oxy)-2-methylpropyl)-3-(3-(trimethylammonio)propyl)-1H-imidazol-3-ium bromide(8b)**

A 100ml Schlenk flask was charged with 3-bromo-N,N,N-trimethylpropan-1-aminium bromide (2.59 g, 9.92 mmol), 1-(1H-imidazol-1-yl)-2-methylpropan-2-yl furan-2-carboxylate (2.7875 g, 11.90 mmol), Acetonitrile (50 ml) and a stir bar giving an orange, heterogeneous solution. The flask was fitted with a reflux condenser and heated to 75°C with vigorous stirring for 48 hours. The reaction mixture became homogenous after reaching the reaction temperature. After 48 hours, the solution was found to be heterogeneous with white precipitate. The flask was removed from heat and allowed to cool to room temperature. Upon cooling, precipitate increased in amount. The product was collected via filtration, in air, washed with 50ml Acetonitrile, rinsed with 10ml acetone and dried in vacuo to afford 1-(2-((furan-2-carbonyl)oxy)-2-methylpropyl)-3-(3-(trimethylammonio)propyl)-1H-imidazol-3-ium bromide (3.7951 g, 7.66 mmol, 77 % yield) as a white solid. mp. Decomposed at 154.7°C.  $^1\text{H}$  NMR (500 MHz, DMSO- $d_6$ ):  $\delta$  = 1.57(s, 6H), 2.37 (m, 2H), 3.14 (s, 9H), 3.49 (m, 2H), 4.36 (t,  $J$  = 7.1, 2H), 4.63 (s, 2H), 6.70 (dd,  $J$  = 3.7 Hz,  $J$  = 1.7, 1H), 7.45 (m, 1H), 7.88 (s, 1H), 8.02-8.03 (m, 2H), 9.51 (s, 1H). ( $^{13}\text{C}$  { $^1\text{H}$ } NMR (125 MHz, DMSO- $d_6$ ):  $\delta$  = 22.8, 23.2, 46.1, 52.3, 57.2, 61.8, 80.7, 112.3, 118.8, 122.2, 124.1, 137.3, 143.9, 147.8, 156.7 ppm. Elemental Analysis: Anal. Calcd for  $\text{C}_{18}\text{H}_{29}\text{BrN}_3\text{O}_3$ : C, 43.65; H, 5.90; N, 8.48. Found: C, 43.09; H, 6.05; N, 8.62. HRMS (ESI-TOF;  $\text{CH}_3\text{OH}$ )  $m/z$ :  $[\text{M}]^+$  Calcd for  $\text{C}_{18}\text{H}_{29}\text{BrN}_3\text{O}_3$  414.1392; Found 414.1369. HRMS (ESI-TOF;  $\text{CH}_3\text{OH}$ )  $m/z$ :  $[\text{M}-\text{Br}]^+$  Calcd for  $\text{C}_{18}\text{H}_{29}\text{BrN}_3\text{O}_3$  414.1392; Found 414.1392.