Sulfonamide Paper ESI

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X-ray Photoelectric Spectroscopy and ToF-SIMS Data

Figure S 1. Control (untreated) CPVC XPS survey data.



Figure S 2. Treated CPVC XPS survey data.



Figure S 3. Control CPVC identification XPS data.



Figure S 4. Control CPVC Identification XPS data, continued.



Figure S 5. CPVC treated with 3a identification XPS data.





Control			Compound 3b		
Element	Concentration	Sensitivity	Element	Concentration	Sensitivity
	%	Factor		%	Factor
Br3d	0.08	2.840	Br3d	0.04	2.840
C1s	77.16	1.000	C1s	73.17	1.000
Ca2p	1.47	5.070	Ca2p	0.74	5.070
Cl2p	7.25	2.285	Cl2p	7.23	2.285
N1s	0.35	1.800	N1s	1.84	1.800
Na1s	0.17	8.520	Na1s	0.81	8.520
O1s	9.97	2.930	O1s	14.57	2.930
S2p	0.93	1.670	S2p	1.24	1.670
Si2p	2.62	0.817	Si2p	0.36	0.817

 Table S 1. Quantification XPS data for control and 3a treated CPVC samples.



Figure S 7. Positive ion ToF-SIMS survey of control CPVC material.



Figure S 8. Positive ion ToF-SIMS survey of 3a treated CPVC material.



Figure S 9. Negative ion ToF-SIMS survey of control CPVC material.



Figure S 10. Negative ion ToF-SIMS survey of 3a treated CPVC material.



Figure S 11. Composite negative ion ToF-SIMS image of $500.0 \times 500.0 \ \mu\text{m}$ section of control and **3a** treated samples. Intensity is a function of fragment quantity during analysis. Images correspond to negative ionic fragmentation products of chlorine (Cl⁻), bromine (Br⁻), ethane (C₂H⁻), tetracarbonyl ammonium (C₄N⁻), and hydroxybenzophenone (C₁₃H₉O₂⁻).

Atomic Force Microscopy and Surface Profilometry Data



Figure S 12. Contact AFM profile scan of a polycarbonate (PC) surface partially treated with 3a.



Figure S 13. Tapping AFM profile scan of a polycarbonate (PC) surface partially treated with **6a**.



Figure S 14. SP profile scan of a polycarbonate (PC) surface partially treated with 3a.



Figure S 15. SP profile scan of a polycarbonate (PC) surface partially treated with 6a.

Microbiology Data



Figure S 16. Simplified schematic representation of the large drop inoculation (LDI) method.



Figure S 17. Successive wash solutions of polystyrene coated with **3a**, exposed to 3 drops (~0.1 mL) 1000 ppm bromophenol blue dye. Samples were shaken for 30 seconds in sealed tubes containing 10 mL of distilled water. The blue colour indicates the first rinse contains the presence QAC, while the purple colour indicates the second rinse does not.



Figure S 18. Representative polystyrene samples, one left untreated (left) and treated (right) with 3a, stained with bromophenol blue.

Table S 2. Large droplet inoculation (LDI) microbiology data. Microbiological testing was performed with triplicate treated and untreated controls. The inoculum load represents the quantity of viable cells placed onto each sample material, and was determined concurrently to sample data (\pm indicates standard deviation n = 3). A value of 1.70 log(cfu) represents the lowest number of detectable cells spot plated onto 3 g L⁻¹ TSA (LOD: 50 cfu, 1 colony in 5 mL undiluted collection fluid).



2: R =	3 Hours		6.94 ± 0.05	$< 1.70 \pm 0.00$
Tol Arthrobacter sp. (IAI-3) Cotton (Fabric)	24 Hours	8.11	2.62 ± 0.05	$< 1.70 \pm 0.00$
2: R = Tol Escherichia coli (DH5a) Polystyrene	3 Hours	7.71	2.27 ± 1.11	$< 1.70 \pm 0.00$
3: R =	3 Hours		6.55 ± 0.06	$<1.70\pm0.00$
Mes Arthrobacter sp. (IAI-3) Polystyrene	24 Hours	7.01	4.96 ± 0.08	$< 1.70 \pm 0.00$
3: R =	3 Hours	7 70	2.60 ± 0.16	$< 1.70 \pm 0.00$
Mes <i>Eschericia coli</i> (DH5α) High Density Polyethylene	24 Hours	7.70	$< 1.70 \pm 0.00$	$< 1.70 \pm 0.00$
3: R =	3 Hours	5.92	3.95 ± 0.09	< 1.70 ± 0.00
Mes Staphylococcus aureus (Ryerson University) High Density Polyethylene	24 Hours		3.74 ± 0.40	$< 1.70 \pm 0.00$
	3 Hours	7.43	6.42 ± 1.32	$< 1.70 \pm 0.00$

4: R = Naph Arthrobacter sp. (IAI-3) High Density Polyethylene	24 Hours		2.73 ± 0.12	$< 1.70 \pm 0.00$
4: R = Naph Escherichia coli (DH5α) Polystyrene	3 Hours	7.71	2.27 ± 1.11	$< 1.70 \pm 0.00$
5: $R = $ CF_3 CF_3Ph <i>Arthrobacter sp.</i> (IAI-3) Polystyrene	3 Hours	7.18	6.03 ± 0.15	$< 1.70 \pm 0.00$
$F_{3}C$ $F_{3}C$ CF_{3} $(CF_{3})_{2}Ph$ $Arthrobacter sp. (IAI-3)$ $Polystyrene$	3 Hours	7.18	6.61 ± 0.01	$< 1.70 \pm 0.00$
7: R =	3 Hours	7.60	6.17 ± 0.20	6.55 ± 0.22
Et Arthrobacter sp. (IAI-3) Polystyrene	24 Hours	1.00	5.29 ± 0.47	5.97 ± 0.09
8: R =	3 Hours	7.60	6.17 ± 0.20	6.26 ± 1.04
Bu Arthrobacter sp. (IAI-3) Polystyrene	24 Hours	7.00	5.29 ± 0.47	5.89 ± 1.75



Table S 3. Tabulated large droplet inoculation (LDI) microbiology data. Microbiological testing was performed with triplicate treated and untreated controls. The inoculum load represents the quantity of viable cells placed onto each sample material, and was determined concurrently to sample data (\pm indicates standard deviation n = 3). A value of 1.70 log(cfu) represents the lowest number of detectable cells spot plated onto 3 g L⁻¹ TSA (LOD: 50 cfu, 1 colony in 5 mL undiluted collection fluid).





Table S 4. Tabulated liquid reservoir inoculation (LRI) planktonic microbiology data. Microbiological testing was performed with triplicate treated and untreated controls. Planktonic colony counts were collected prior to the collection of biofilm data. The inoculum load represents the quantity of viable cells placed onto each sample material, and was determined concurrently to sample data (± indicates standard deviation, n = 3). A value of 6.78 log(cfu ml⁻¹) represents the highest number of detectable cells spot plated onto 3 g L⁻¹ TSA (LOD: 6.00 x 10⁻⁶ cfu ml⁻¹, 600 colonies in 3 mL collection fluid, diluted by a factor of 10³). A value of 1.00 log(cfu ml⁻¹) represents the lowest number of detectable cells spot plated onto 3 g L⁻¹ TSA (LOD: 10 cfu ml⁻¹, 1 colony in 3 mL undiluted collection fluid).





Table S 5. Tabulated liquid reservoir inoculation (LRI) biofilm microbiology data. Microbiological testing was performed with triplicate treated and untreated controls. Biofilm colony counts were collected subsequently to the collection of planktonic data. The inoculum load represents the quantity of viable cells placed onto each sample material, and was determined concurrently to sample data (\pm indicates standard deviation, n = 3). A value of 1.00 log(cfu) represents the lowest number of detectable cells spot plated onto 3 g L⁻¹ TSA (LOD: 10 cfu, 1 colony in 1 mL undiluted collection fluid).





Synthetic Procedures

Precursors 4-(3-bromopropyoxy)benzophenone and diisopropyl(3-bromopropyl)phosphonate were synthesized according to published work and NMR spectra (¹H and ¹³C) corresponded well with previously published NMR data.^{23,51}

Method S1: General procedure for aromatic sulfonamide synthesis

To a flame dried, round bottom flask in an ice bath equipped with a stir bar containing an appropriate amount of anhydrous DCM, an adequate amount of respective sulfonyl chloride was added, followed by an equimolar amount of Et₃N and dropwise addition of a stoichiometric quantity of 3-(dimethylamino)propylamine. After 30 min. the reaction mixture was removed from the ice bath and allowed to stir at room temperature for the indicated time. The reaction was then transferred to a separatory funnel and extracted with an appropriate amount of distilled water. Volatiles and/or solvent were removed from the organic phase using a rotary evaporator followed by drying under high vacuum.

Method S2: General procedure for aliphatic sulfonamide synthesis

To a flame dried, round bottom flask in an ice bath equipped with a stir bar containing appropriate amount of anhydrous DCM a stoichiometric amount of 3-(dimethylamino)propylamine was added followed by the dropwise addition of the respective sulfonyl chlorides. The reaction mixture was removed from the ice bath and allowed to stir for the indicated time at room temperature. Upon completion, the reaction solvent was evaporated using a rotary evaporator. The resultant residue was then dissolved in an appropriate amount of potassium carbonate solution (0.05 M) and extracted using appropriate amount of DCM. Volatiles were removed *in vacuo*.

Method S3: General procedure for Menshutkin quaternization reaction

In an appropriately sized round bottom flask or scintillation/microwave vial, an appropriate amount of a tertiary amine-terminated sulfonamide and a trimethoxy silane, diallyl phosphonate or benzophenone alkyl halide starting material was dissolved in acetonitrile. The reaction mixture was stirred at 110 °C for the indicated time. The crude material was purified by addition of Et_2O directly into the reaction mixture followed by decanting (Et_2O wash × 3) and dried *in vacuo*.

Synthesis of N-(3-(dimethylamino)propyl)benzenesulfonamide 1

This compound was synthesized according to **Method S1** with benzenesulfonyl chloride (1.4 mL, 11.32 mmol), triethylamine (2.4 mL, 16.99 mmol, 1.5 eqv.), and 3- (dimethylamino)propylamine (2.1 mL, 16.99 mmol, 1.5 eqv.) in DCM (30 mL) stirring for 4 hours, yielding a clear solution. The solution was then washed using distilled water (40 mL), and the organic layer was removed *in vacuo* to yield a green yellow coloured oil. The product was further dried under reduced pressure, yielding the desired product as a pale yellow coloured waxy solid. Yield: 98 % (2.69 g). ¹H NMR (CDCl₃, 400 MHz, δ): 7.68 (2H, d, ³*J*_{H3-H2} = 8.3 Hz, H3), 7.35 (3H, m, H1 and H2), 2.86 (2H, t, ³*J*_{H6-H7} = 5.8 Hz, H6), 2.11 (2H, t, ³*J*_{H8-H7} = 5.9 Hz, H8), 1.98 (6H, s, H9), 1.41 (2H, m, ³*J*_{H7-H6} = 9.0 Hz, ³*J*_{H7-H8} = 3.1 Hz, H7) ppm; ¹³C {¹H} NMR (CDCl₃, 101 MHz, δ): 140.20 (C4), 132.33 (C1), 128.99 (C2), 126.96 (C3), 59.13 (C8), 45.28 (C9), 44.05 (C6), 25.12 (C7) ppm. **HRMS-ESI-TOF** (*m*/*z*): [M⁺ + H⁺] calculated for C₁₁H₁₉N₂O₂S, 243.1162, found, 243.1170.

Synthesis of N-(3-(dimethylamino)propyl)-4-methylbenzenesulfonamide 2

This compound was synthesized according to **Method S1** with *p*-toluenesulfonyl chloride (10.505 g, 55.10 mmol), triethylamine (11.5 mL, 82.65 mmol, 1.5 eqv.), and 3-(dimethylamino)propylamine (10.4 mL, 82.65 mmol, 1.5 eqv.) in DCM (100 mL) stirred for 4 hours, yielding a milky white solution. The solution was then washed using distilled water (100

mL), and the volatile organic layer removed *in vacuo* to yield a pale yellow coloured oil. The product was further dried under reduced pressure, yielding the desired product as a pale white coloured waxy solid. Yield: 98 % (13.85 g). ¹H NMR (CDCl₃, 400 MHz, δ): 7.73 (2H, d, ³*J*_{H4-H2} = 8.3 Hz, H4), 7.29 (2H, d, ³*J*_{H2-H4} = 7.9 Hz, H2), 3.03 (2H, t, ³*J*_{H7-H8} = 5.8 Hz, H7), 2.42 (3H, s, H1), 2.29 (2H, t, ³*J*_{H9-H8} = 5.8 Hz, H9), 2.16 (6H, s, H10), 1.58 (2H, tt, ³*J*_{H8-H7} = 9.2 Hz, ³*J*_{H8-H9} = 2.5 Hz, H8) ppm; ¹³C {¹H} NMR (CDCl₃, 101 MHz, δ): 142.83 (C5), 137.11 (C3), 129.44 (C2), 126.88 (C4), 58.76 (C9), 45.15 (C10), 43.65 (C7), 25.23 (C8), 21.32 (C1) ppm. HRMS-ESI-TOF (*m*/*z*): [M⁺ + H⁺] calculated for C₁₂H₂₁N₂O₂S, 257.1318, found, 257.1322.

Synthesis of N-(3-(dimethylamino)propyl)-2,4,6-trimethylbenzenesulfonamide 3

This compound was synthesized according to **Method S1** with 2,4,6-trimethylbenzene-1-sulfonyl chloride (1.99 g, 9.14 mmol), triethylamine (1.9 mL, 13.72 mmol, 1.5 eqv.), and 3-(dimethylamino)propylamine (1.7 mL, 13.72 mmol, 1.5 eqv.) in DCM (50 mL) for 3 hours yielding a clear solution. The solution was then washed using distilled water (75 mL), and the volatile organic layer removed *in vacuo* to yield a clear oil. The product was further dried under reduced pressure, yielding the desired product as a pale white coloured waxy solid. Yield 98.5 % (2.56 g). ¹**H NMR** (CDCl₃, 400 MHz, δ): 7.04 (1H, br s, H7), 6.93 (2H, s, H3), 2.94 (2H, t, ³*J*_{H8-H9} = 5.7 Hz, H8), 2.61 (6H, s, H4), 2.32 (2H, t, ³*J*_{H10-H9} = 5.6 Hz, H10), 2.27 (3H, s, H1), 2.18 (6H, s, H11), 1.62 (2H, tt, ³*J*_{H9-H8} = 9.5 Hz, ³*J*_{H9-H10} = 2.2 Hz, H9) ppm; ¹³C {¹**H**} **NMR** (CDCl₃, 101 MHz, δ): 141.74 (C6), 139.07 (C2), 133.80 (C5), 131.87 (C3), 59.66 (C10), 45.48 (C11), 60 43.72 (C8), 24.99 (C9), 22.88 (C4), 20.95 (C1) ppm. **HRMS-ESI-TOF** (*m*/*z*): [M⁺ + H⁺] calculated for C₁₄H₂₅N₂O₂S, 285.1631, found, 285.1643.

Synthesis of N-(3-(dimethylamino)propyl)naphthalene-1-sulfonamide 4

This compound was synthesized according to Method S1 with naphthalene-1-sulfonyl chloride (4 18.04 mmol), triethylamine (3.8)mL. 27.06 mmol. 1.5 g, eqv.), and 3-(dimethylamino)propylamine (3.4 mL, 27.06 mmol, 1.5 eqv.) in DCM (50 mL) for 3 hours yielding a clear solution. The solution was then washed using distilled water (50 mL), and the organic layer was evaporated to yield a greenish yellow coloured oil. The product was further dried under reduced pressure, yielding the desired product as a pale white coloured waxy solid. Yield 99.7 % (5.27 g). ¹**H** NMR (CDCl₃, 400 MHz, δ): 8.67 (1H, d, ³J_{H1-H2} = 8.5 Hz, H1), 8.25 (1H, d, ${}^{3}J_{\text{H8-H7}} = 6.2 \text{ Hz}, \text{H8}$, 8.05 (1H, d, ${}^{3}J_{\text{H6-H7}} = 8.2 \text{ Hz}, \text{H6}$), 7.95 (1H, d, ${}^{3}J_{\text{H4-H3}} = 7.8 \text{ Hz}, \text{H4}$), 7.65 (1H, m, H2), 7.59 (1H, m, H3), 7.52 (1H, m, H7), 2.95 (2H, t, ${}^{3}J_{H12-H13} = 5.6$ Hz, H12), 2.21 (2H, t, ${}^{3}J_{\text{H14-H13}} = 5.6$ Hz, H14), 2.12 (6H, s, H15), 1.55 (2H, m, H13) ppm; ${}^{13}C$ {¹H} NMR (CDCl₃, 101 MHz, δ): 134.85 (C9), 134.45 (C5), 133.96 (C4), 129.79 (C6), 129.16 (C2), 128.42 (C10), 128.21 (C3), 126.82 (C8), 124.76 (C7), 124.28 (C1), 59.80 (C14), 45.56 (C15), 44.77 (C12), 24.68 (C13) ppm. **HRMS-ESI-TOF** (m/z): [M⁺ - Br] calculated for C₁₅H₂₁N₂O₂S, 293.1318, found, 293.1319.

Synthesis of N-(3-(dimethylamino)propyl)-4-(trifluoromethyl)benzenesulfonamide 5

This compound was synthesized according to **Method S1**, with 4-(trifluoromethyl)benzenesulfonyl chloride (5.2 g, 20.44 mmol), triethylamine (3.30 mL, 22.48 mmol) and 3-(dimethylamino)-1-propylamine (2.98 mL, 22.48 mmol) in DCM (40 mL) for 21 hours, yielding a pale yellow solution. The solution was then washed with distilled water (120 mL), dried over MgSO₄ and the volatiles removed *in vacuo*, giving an off-white coloured powder. From the powder, 0.100 g was taken and recrystallized in heptanes layered over ACN, giving small, cubic crystals. Yield: 89% (5.29 g). Mp = 69-70 °C. ¹H NMR (CDCl₃, 400 MHz, δ): 8.01 (2H, d, ³*J*_{H3-H4} = 8.1 Hz, H3), 7.80 (2H, d, ³*J*_{H4-H3} = 8.2 Hz, H4), 3.11 (2H, t, ³*J*_{H9-H8} = 5.74 Hz, H9), 2.39 (2H, t, ³*J*_{H7-H8} = 5.69, H7), 2.23 (6H, s, H10), 1.69-1.63 (2H, m, H8) ppm. ¹³C {¹H} NMR (CDCl₃, 101 MHz, δ): 143.96 (s, C5), 134.01 (d, ²*J*_{C-F} = 32.9 Hz, C2), 127.48 (s, C4), 126.12 (q, ³*J*_{C-F} = 3.7 Hz, C3), 126.10 (q, *J*_{C-F} = 272.8 Hz, C1), 59.54 (s, C9), 45.22 (s, C10), 44.48 (s, C7), 24.61 (s, C8) ppm. ¹⁹F {¹H} NMR (CDCl₃, 376 MHz, δ): -63.05 ppm. HRMS-ESI-TOF (*m*/*z*): [M⁺] calculated for C₁₂H₁₇F₃N₂O₂S, 311.0996; found, 311.1035.

Synthesis of N-(3-(dimethylamino)propyl)-3,5-bis-(trifluoromethyl)benzenesulfonamide 6

This **S1**, compound synthesized according Method with 3,5was to bis(trifluoromethyl)benzenesulfonyl chloride (4.37 g, 13.98 mmol), triethylamine (3 mL, 21.50 mmol) and 3-(dimethylamino)-1-propylamine (2.72 mL, 21.50 mmol) in DCM (25 mL) for 12 hours, yielding a pale-yellow solution. The solution was then washed with distilled water (150 mL), dried over MgSO₄ and the volatiles removed in vacuo, yielding the product as yellow-tinged coloured crystals. Yield: 77% (4.03 g). Mp = 93-94 °C. ¹H NMR (CDCl₃, 400 MHz, δ): 8.30 (2H, s, H4), 8.05 (1H, s, H3), 3.12 (2H, t, ${}^{3}J_{H9-H8} = 5.66$ Hz, H9), 2.41 (2H, t, ${}^{3}J_{H7-H8} = 5.66$ H7), 2.21 (6H, s, H10), 1.69-1.63 (2H, m, H8) ppm. ¹³C {¹H} NMR (CDCl₃, 101 MHz, δ): 143.39 (C5), 132.79 (q, ${}^{2}J_{C-F}$ = 34.5 Hz, C2), 127.23 (q, ${}^{3}J_{C-F}$ = 3.1 Hz, C4), 125.77 (m, C3), 122.54 (q, J_{C-F} = 272.5 Hz, C1), 59.77 (C9), 45.13 (C10), 44.83 (C7), 24.19 (C8) ppm. ¹⁹F {¹H} NMR (376 MHz, CDCl₃, δ): -62.94 ppm. **HRMS DART** (*m*/*z*): [M⁺] calculated for C₁₃H₁₆F₆N₂O₂S, 379.0870; found, 379.0914.

Synthesis of N-(3-(dimethylamino)propyl)ethanesulfonamide 7

This compound was synthesized according to **Method S2**, with ethanesulfonyl chloride (0.7 mL, 7.78 mmol) and 3-(dimethylamino)propylamine (1.5 mL, 11.67 mmol, 1.5 eq.) in DCM (50 mL) for 4 hours. The solution was washed with K₂CO₃ (0.05 M, 50 mL), and the volatile organic layer was removed *in vacuo* yielding in clear oil. Yield: 61 % (0.92 g). ¹H NMR (CDCl₃, 400 MHz, δ): 3.19 (2H, t, ³*J*_{H4-H5} = 5.8 Hz, H4), 3.0 (2H, q, ³*J*_{H2-H1} = 7.4 Hz, H2), 2.42 (2H, t, ³*J*_{H6-H5} = 5.8 Hz, H6), 2.22 (6H, s, H7), 1.70 (2H, m, H5), 1.34 (3H, t, ³*J*_{H1-H2} = 7.4 Hz, H1) ppm; ¹³C {¹H} NMR (CDCl₃, 101 MHz, δ): 59.33 (C6), 46.05 (C2), 45.41 (C7), 44.11 (C4), 25.91 (C5), 8.35 (C1) ppm. HRMS-ESI-TOF (*m*/*z*): [M⁺ + H⁺] calculated for C₉H₂₃N₂O₂S, 223.1475, found, 223.1480.

Synthesis N-(3-(dimethylamino)propyl)butane-1-sulfonamide 8

This compound was synthesized according to **Method S2**, with butanesulfonyl chloride (1.7 mL, 12.77 mmol) and 3-(dimethylamino)propylamine (2.4 mL, 19.15 mmol, 1.5 equiv) in DCM (50 mL) for 4 hours. The solution was washed with K₂CO₃ (0.05 M, 50 mL), and the volatile organic layer was removed *in vacuo* yielding in a clear oil. Yield: 81 % (2.31 g). ¹**H NMR** (CDCl₃, 400 MHz, δ): 3.15 (2H, t, ³*J*_{H6-H7} = 5.9 Hz, H6), 2.94 (2H, t, ³*J*_{H4-H3} = 7.9 Hz, H4), 2.38 (2H, t, ³*J*_{H8-H7} = 5.9 Hz, H8), 2.18 (6H, s, H9), 1.78-1.61 (4H, m, H3 and H7), 1.48-1.34 (2H, m, H2), 0.91 (3H, t, ³*J*_{H1-H2} = 7.3 Hz, H1) ppm; ¹³C {¹H} NMR (CDCl₃, 101 MHz, δ): 59.08 (C8), 51.56 (C4), 45.38 (C9), 43.83 (C6), 26.05 (C3), 25.70 (C7), 21.54 (C2), 13.63 (C1) ppm. **HRMS ESI-TOF** (*m*/*z*): [M⁺ + H⁺] calculated for C₇H₁₀N₃O₂S, 210.1271, found, 210.1276.

Synthesis of N-(3-bromopropyl)-2,4,6-trimethylbenzenesulfonamide 9

This compound was synthesized according to Method S1 with 2,4,6-trimethylbenzene-1-sulfonyl chloride (4.89 g, 9.14 mmol), triethylamine (7.79 mL, 55.88 mmol, 2.5 eqv.), and 3bromopropylamine hydrobromide (7.34 g, 33.53 mmol, 1.5 eqv.) in DCM (50 mL) for 3 hours yielding a clear solution. The reaction mixture was then extracted using two aliquots of distilled water (25 mL), which were then discarded. The collected organic phase was then gravity filtered through magnesium sulfate to remove excess moisture and evaporated overnight to obtain 7.39 g of crude, off-white semi-crystalline product. The crude product was packed onto silica and purified by flash column chromatography ($4.5 \text{ cm} \times 5.0 \text{ cm}$ frit, 40 g silica) by eluting with DCM (120 mL) to afford 4.86 g of the desired product, as confirmed using TLC. The resulting white semicrystalline solid was recrystallized from minimal DCM to yield clear, colourless crystals. Yield: 68.0% (4.86 g). Mp = 93-94°C; ¹H NMR (CDCl₃, 400 MHz, δ) 6.97 (s, 2H, H3), 4.60 (s, 1H, H10), 3.40 (t, ${}^{3}J_{H9-H8} = 6.3$ Hz, 2H, H9), 3.08 (q, ${}^{3}J_{H7-H8} = 6.5$ Hz, 2H, H7), 2.65 (s, 6H, H5), 2.31 (s, 3H, H1), 2.01 (8, p, ${}^{3}J_{H8-H7} = 6.5$ Hz, ${}^{3}J_{H8-H9} = 6.3$ Hz, 2H, H8) ppm. ${}^{13}C$ { ${}^{1}H$ } NMR (CDCl3, 101 MHz, δ) 142.39 (C2), 139.06 (C4), 133.49 (C5), 132.07 (C3), 40.86 (C7), 32.25 (C8), 30.29 (C9), 22.96 (C3), 20.93 (C1) ppm; HRMS-DART (m/z): [M⁺] calculated for C₁₂H₁₈BrNO₂S, 320.03199; found, 320.03249.

Synthesis of N-(3-(4-benzoylphenoxy)propyl)-2,4,6-trimethylbenzenesulfonamide 10

A round bottom flask was charged with 1,3-dibromopropane, K₂CO₃ and MeCN. A solution of 4hydroxybenzophenone in MeCN was prepared and added dropwise to the previous mixture under reflux. The resultant yellow mixture was heated at reflux until a colourless solution was obtained or until thin layer chromatography showed the disappearance of starting material 4hydroxybenzophenone. Excess salt was filtered through diatomaceous earth and washed with acetone. The solution was evaporated under reduced pressure to give the crude product, which was packed onto silica and purified by dry column chromatography, first by pre-eluting with 5% ethyl acetate/hexanes then eluting acetone to retrieve the purified product. The resulting yellow oil was recrystallized from 20% ethyl acetate/hexanes to yield translucent yellow crystals. Yield: 95.9% (5.24 g). Mp = 75-76 °C. ¹H NMR (CDCl₃, 400 MHz, δ) 7.80 (d, ³J_{H12-H11} = 8.7 Hz, 2H, H12), 7.75 (d, ³J_{H16-H17} = 7.4 Hz, 2H, H16), 7.57 (t, ³J_{H18-H17} = 7.5 Hz, 1H, H18), 7.48 (t, ³J_{H17-H16} = 7.4 Hz, ³J_{H17-H18} = 7.5 Hz, 2H, H17), 6.92 (s, 2H, H3), 6.87 (d, ³J_{H11-H12} = 8.7 Hz, 2H, H11), 4.04 (t, ³J_{H9-H8} = 5.7 Hz, 2H, H9), 3.16 (t, ³J_{H7-H18} = 6.3 Hz, 2H, H7), 2.63 (s, 6H, H5), 2.27 (s, 3H, H1), 2.08 – 1.87 (m, 2H, H8). ¹³C {¹H} NMR (CDCl₃, 101 MHz) δ 195.51 (C14), 162.09 (C10), 142.24 (C6), 139.03 (C4), 138.19 (C15), 133.53 (C2), 132.51 (C12), 131.99 (C3), 131.98 (C18), 130.40 (C13), 129.72 (C16), 128.22 (C17), 113.93 (C11), 65.70 (C9), 39.97 (C7), 29.07 (C8), 22.93 (C5), 20.91 (C1). HRMS-ESI-TOF (m/z): [M⁺ - Br⁻] calculated for C₂₅H₂₈NO₄S, 438.17390; found, 438.17442.

Synthesis of 3-(4-benzoylphenoxy)-N,N-dimethyl-N-(3-(phenylsulfonamido)propyl)propan-1aminium bromide 1a

This compound was synthesized according to Method **S3**, using N-(3-(dimethylamino)propyl)phenylsulfonamide (0.921)g, 3.8 mmol) and 4-(3bromopropoxy)benzophenone (1.29 g, 4.0 mmol) in ACN (10 mL) for 48 hours; yielding in viscous pale yellow solution. The product was obtained as fluffy pale yellow-coloured powder after purification. Yield: 82% (1.74 g). ¹**H NMR** (CDCl₃, 400 MHz, δ): 7.93 (2H, m, H3), 7.82 (1H, m, H5), 7.74 - 7.62 (4H, m, H15 & H19), 7.53 (1H, m, H21), 7.49 - 7.37 (5H, m, (H1, H2, & H20)), 6.89 (2H, d, ${}^{3}J_{H14-H15} = 8.9$ Hz, H14), 4.11 (2H t, ${}^{3}J_{H12-H11} = 5.3$ Hz, H12), 3.79 - 3.56 (4H, m, H8 & H10), 3.27 (6H, s, H9), 3.01 (2H, m, H6), 2.29 (2H, m, H11), 2.10 (2H, m, H7) ppm. ¹³C {¹H} NMR (CDCl₃, 101 MHz, δ): 195.58 (C17), 161.80 (C13), 139.64 (C1), 137.99 (C4), 132.71 (C18), 132.51 (C15), 132.19 (C21), 130.60 (C16), 139.75 (C2), 129.32 (C19), 128.35 (C20), 127.22 (C3), 114.31 (C14), 64.68 (C12), 62.44 (C8), 62.06 (C10), 39.98 (C6), 23.08 (C11), 22.75 (C7) ppm. HRMS-ESI-TOF (*m*/*z*): [M⁺ - Br⁻] calculated for C₂₇H₃₃N₂O₄S, 481.2156; found 481.2155.

Synthesis of 3-(4-benzoylphenoxy)-N,N-dimethyl-N-(3-(4methylphenylsulfonamido)propyl)propan-1- aminium bromide 2a

This compound synthesized using N-(3-(dimethylamino)propyl)-4was methylphenyl)sulfonamide (1.05 g, 4.1 mmol) and 4-(3-bromopropoxy)benzophenone (1.417 g, 4.44 mmol) in ACN (10 mL) for 48 hours; yielding in viscous pale yellow solution. The product was obtained as fluffy white coloured powder after purification. Yield: 80 % (1.88 g). ¹H NMR $(CDCl_3, 400 \text{ MHz}, \delta)$: 7.80 (2H, d, ${}^{3}J_{H4-H2} = 8.2 \text{ Hz}, H4$), 7.73 – 7.65 (4H, m, H16 & H20), 7.56 – 7.59 (1H, m, H22), 7.42 (2H, t, ${}^{3}J_{H22-H21} = 7.2$ Hz, H22), 7.21 (2H, d, ${}^{3}J_{H2-H4} = 8.2$ Hz, H2), 6.89 $(2H, d, {}^{3}J_{H15-H16} = 8.8 \text{ Hz}, H15), 4.12 (2H, t, {}^{3}J_{H13-H12} = 5.4 \text{ Hz}, H13), 3.79 - 3.59 (4H, m, H9 \&$ H11), 3.29 (6H, s, H10), 3.07 – 2.90 (2H, m, H7), 2.35 – 2.23 (5H, m, H1 & H12), 2.19 – 2.03 (2H, m, H8) ppm. ¹³C {¹H} NMR (CDCl₃, 101 MHz, δ): 195.57 (C18), 161.82 (C14), 143.50 (C3), 138.05 (C5), 136.53 (C19), 132.54 (C16), 132.19 (C22), 130.69 (C17), 129.90 (C20), 129.80 (C2), 128.36 (C21), 127.34 (C4), 114.32 (C15), 64.71 (C13), 62.53 (C9), 62.11 (C11), 51.62 (C10), 40.01 (C7), 23.15 (C12), 22.75 (C8), 21.57 (C1) ppm. HRMS-ESI-TOF (m/z): [M⁺ - Br⁻] calculated for C₂₈H₃₅N₂O₄S, 495.2312; found 495.2319.

Synthesis of 3-(4-benzoylphenoxy)-N,N-dimethyl-N-(3-(2,4,6-trimethylphenylsulfonamido)propyl)propan-1-aminium bromide 3a

This compound was synthesized according to **Method S3**, using *N*-(3-(dimethylamino)propyl)-2,4,6- trimethylphenyl)sulfonamide (0.853 g, 3.0 mmol) and 4-(3-bromopropoxy)benzophenone (1.0 g, 3.13 mmol) in ACN (10 mL) for 48 hours; yielding in viscous pale yellow solution. The product was obtained as fluffy white-coloured powder after purification. Yield: 67 % (1.20 g). ¹**H NMR** (CDCl₃, 400 MHz, δ): 7.76 (2H, d, ³*J*_{H17-H16} = 8.7 Hz, H17), 7.72 (d, 2H, ³*J*_{H21-H22} = 7.2 Hz, H21), 7.56 (2H, t, ³*J*_{H23-H22} = 7.4 Hz, H23), 7.56 (2H, m, H22), 7.22 (1H, t, ³*J*_{H7-H8} = 6.2 Hz, H7), 6.94 (2H, t, ³*J*_{H16-H17} = 6.0 Hz, H16), 6.90 (2H, s, H3), 4.21 (2H, t, ³*J*_{H14-H13} = 5.4 Hz, H14), 3.85 (2H, m, H10), 3.75 (2H, m, H12), 3.37 (6H, s, H11), 3.04 (2H, m, H8), 2.63 (6H, s, H4), 2.38 (2H, m, H13), 2.25 (3H, s, H1), 2.20 (2H, m, H9) ppm. ¹³C {¹H} **NMR** (CDCl₃, 101 MHz, δ): 195.63 (C19), 161.81 (C15), 142.40 (C5), 139.24 (C2), 138.15 (20), 133.41 (C6), 132.66 (C17), 132.22 (C23), 132.18 (C3), 130.91 (C18), 129.90 (C21), 128.39 (C22), 64.72 (C14), 62.68 (C10), 62.29 (C12), 51.77 (C11), 39.36 (C8), 23.42 (C4), 23.27 (C13), 23.05 (C9), 21.03 (C1) ppm. **HRMS-ESI-TOF** (*m*/*z*): [M⁺ - Br⁻] calculated for C₃₀H₃₉N₂O4S, 523.2625; found 523.2636.

Synthesis of 3-(4-benzoylphenoxy)-N,N-dimethyl-N-(3-(naphthalene-1-sulfonamido)propyl)propan-1-aminium bromide 4a

This compound was synthesized according to Method **S3**. using N-(3-(dimethylamino)propyl)naphthalene-1-sulfonamide (0.584)g, 2.0 mmol) and 4-(3bromopropoxy)benzophenone (0.702 g, 2.2 mmol) in ACN (10 mL) for 48 hours; yielding in viscous pale yellow solution. The product was obtained as fluffy white coloured powder after purification. Yield: 82 % (1.0 g). ¹H NMR (CDCl₃, 400 MHz, δ): 8.80 (1H, d, ³J_{H1-H2} = 8.7 Hz, H1), 8.15 (1H, d, ${}^{3}J_{H8-H7} = 7.3$ Hz, H8), 7.96 (1H, s, H11), 7.91 (1H, d, ${}^{3}J_{H6-H7} = 8.3$ Hz, H6), 7.78

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(1H, d, ${}^{3}J_{H4-H3} = 8.2$ Hz, H4), 7.70 - 7.55 (4H, m, (H2, H25, & H21)), 7.51 (2H, t, ${}^{3}J_{H27-H26} = 7.4$ Hz, H27), 7.46 - 7.34 (4H, m, (H3, H26, & H7), 6.77 (2H, d, ${}^{3}J_{H20-H21} = 8.7$ Hz, H20), 3.92 (2H, m, H18), 3.59 - 3.37 (4H, m, H14 & H16), 3.19 - 2.91 (8H, m, H15 & H12), 2.04 (2H, m, H17), 1.91 (2H, m, H13) ppm. ${}^{13}C$ { ${}^{1}H$ } NMR (CDCl₃, 101 MHz, δ): 195.59 (C23), 161.77 (C19), 138.04 (C24), 134.85 (C9), 134.21 (C6), 132.50 (C25), 132.20 (C27), 130.56 (C10), 129.80 (C2), 129.36 (C8), 129.05 (C4), 128.76 (C21), 128.37 (C7), 128.00 (C22), 127.18 (C3), 125.20 (C1), 124.52 (C26), 114.25 (C20), 64.59 (C18), 62.42 (C14), 62.10 (C16), 51.42 (15), 39.83 (C12), 22.92 (C17+C13) ppm. HRMS-ESI-TOF (m/z): [M⁺ - Br⁻] calculated for C₃₁H₃₅N₂O₄S, 531.2312; found 531.2328.

Synthesis of 3-(4-benzoylphenoxy)-N-(3-((4-(trifluoromethyl)phenyl)sulfonamido) propyl)-N,N-dimethylpropan-1-aminium bromide 5a

This compound was synthesized according to **Method S3**, using *N*-(3-(dimethylamino)propyl)-4-(trifluoromethyl)benzenesulfonamide (2.40 g, 8.06 mmol) and 4-(3-bromopropoxy)benzophenone (2.52 g, 8.06 mmol) in ACN (25 mL) for 48 hours. The product was yielded as an off-white coloured powder after purification. Yield: 86% (4.38 g). Mp = 111-113°C. ¹**H NMR** (CDCl₃, 400 MHz, δ): 8.14 (2H, d, ³*J*_{H4-H3} = 7.45 Hz , H4), 7.76-7.72 (m, 6H, H3 + H16 + H20 overlap), 7.57 (t, ³*J*_{H22-H21} = 6.67 Hz, 1H, H22), 7.47 (t, ³*J*_{H21-H22} = 6.77 Hz, ³*J*_{H21-H20} = 7.29 Hz, H21), 6.96 (2H, d, ³*J*_{H15-H16} = 8.81 Hz, H15), 4.18 (2H, t, ³*J*_{H13-H12} = 5.35 Hz, H13), 3.83 (2H, t, ³*J*_{H11-H12} = 7.79 Hz, H11), 3.71 (2H, t, ³*J*_{H9-H8} = 7.85 Hz, H9), 3.35 (6H, s, H10), 3.08 (2H, m, H7), 2.36 (2H, m, H12), 2.19 (2H, m, H8) ppm. ¹³C {¹H} NMR (CDCl₃, 101 MHz, δ): 195.53 (C18), 161.59 (C14), 142.92 (C5), 137.86 (C19), 134.23 (q, ²*J*_{C-F} = 32.93 Hz, C2), 132.50 (C16), 132.20 (C22), 130.80 (C17), 129.71 (C20), 128.94 (C21), 127.79, (C4) 126.33 (q, ³*J*_{C-F} = 3.58 Hz, C3), 123.23 (q, *J*_{C-F} = 272.96
Hz, C1), 114.17 (C15), 64.48 (C13), 62.44 (C11), 62.20 (C9), 51.59 (C10), 39.91 (C7), 23.08 (C12), 22.76 (C8) ppm. ¹⁹F {¹H} NMR (CDCl₃, 376 MHz, δ): -61.32 ppm. HRMS-ESI-TOF (m/z): [M⁺] - Br⁻ calculated for C₂₈H₃₂F₃N₂O₄S, 549.2029; found, 549.203.

Synthesis of 3-(4-benzoylphenoxy)-N-(3-((3,5-bistrifluoromethyl)phenyl)sulfonamido)propyl-N,N-dimethylpropan-1-aminium bromide 6a

This compounds was synthesized according to Method S3, using N-(3-(dimethylamino)propyl)-3,5-bis-(trifluoromethyl)benzenesulfonamide (2.99)7.93 mmol), 4-(3g, bromopropoxy)benzophenone (3.28 g, 10.31 mmol), and ACN (20 mL) for 60 hours. The volatiles were removed in vacuo, giving a white coloured powder. A small portion (0.1 g) was taken from the batch, dissolved in ACN (10 mL), and passed through a 45 nm PTFE syringe filter into a 100 mL beaker which was left in the fumehood overnight, resulting in the growth of offwhite coloured crystals. The product was insoluble in MeOD, CDCl₃, and D₂O. Yield: 88% (4.84 g). Mp = 180-182 °C. ¹**H NMR** (DMSO-d₆, 400 MHz, δ): 8.55 (1H, s, H3), 8.39 (2H, s, H4), 8.26 (1H, m, H6), 7.77 (2H, d, ${}^{3}J_{\text{H16-H15}} = 8.86$ Hz, H16), 7.69-7.65 (m, 3H, H20 + H22 overlap), 7.56 $(2H, t, {}^{3}J_{H21-H22} = 7.43 \text{ Hz}, {}^{3}J_{H21-H20} = 7.52 \text{ Hz}, H21), 7.11 (2H, d, {}^{3}J_{H15-H16} = 8.87 \text{ Hz}, H15), 4.17$ $(2H, t, {}^{3}J_{H13-H12} = 5.86 \text{ Hz}, H13), 3.47 (2H, t, {}^{3}J_{H11-H12} = 7.60 \text{ Hz}, H11), 3.36 (2H, m, H9), 3.07$ (6H, s, H10), 2.90 (2H, m, H7), 2.20 (2H, quint, ${}^{3}J = 6.83$ Hz, H12), 1.89 (2H, quint, ${}^{3}J = 6.97$ Hz, H8) ppm. ¹³C {¹H} NMR (DMSO-d₆, 101 MHz, δ): 194.89 (C18), 162.33 (C14), 143.11 (C5), 138.15 (C19), 132.67 (C16), 132.63 (C22), 131.96 (q, ${}^{2}J_{C-F} = 33.84$ Hz, C2), 130.12 (C17), 129.71 (C21), 128.94 (C20), 127.79 (q, ${}^{3}J_{C-F} = 3.12$ Hz, C4), 127.25 (m, C3), 123.07 (q, $J_{C-F} = 273.27$ Hz, C1), 114.87 (C15), 65.56 (C13), 61.16 (C11), 61.04 (C9), 50.46 (C10), 22.99 (C12), 22.56 (C8) ppm. ¹⁹**F** {¹**H**} **NMR** (DMSO-d₆, 376 MHz, δ): -61.32 ppm. **HRMS-ESI-TOF** (*m/z*): [M⁺ - Br⁻] calculated for C₂₉H₃₁F₆N₂O₄S, 549.2029; found, 549.203.

Synthesis of 3-(4-benzoylphenoxy)-N-(3-(ethylsulfonamido)propyl)-N,N-dimethylpropan-1aminium bromide 7a

This compound was synthesized according to Method **S3** using N-(3-(dimethylamino)propyl)ethanesulfonamide (0.250)1.29 mmol) 4-(3g, and bromopropoxy)benzophenone (0.411 g, 1.29 mmol) in ACN (10 mL) for 48 hours; yielding in viscous pale yellow solution. The product was obtained as fluffy pale yellow coloured powder after purification. Yield: 77% (0.52 g). ¹**H NMR** (CDCl₃, 400 MHz, δ): 7.78 (2H, d, ³J_{H13-H12} = 8.7 Hz, H13), 7.72 (2H, d, ${}^{3}J_{H17-H18} = 7.4$ Hz, H17), 7.56 (2H, t, ${}^{3}J_{H19-H18} = 7.4$ Hz, H19), 7.50 - 7.40 $(2H, m, H18), 7.12 (1H, t, {}^{3}J_{H3-H4} = 6.0 \text{ Hz}, H3), 6.98 (2H, d, {}^{3}J_{H12-H13} = 8.8 \text{ Hz}, H12), 4.21 (2H, t, t)$ ${}^{3}J_{\text{H10-H9}} = 5.3 \text{ Hz}, \text{H10}, 3.80 (2\text{H}, \text{m}, \text{H6}), 3.71 (2\text{H}, \text{m}, \text{H8}), 3.35 (6\text{H}, \text{s}, \text{H7}), 3.31-3.22 (2\text{H}, \text{m}, \text{H8})$ H4), 3.07 (2H, q, ${}^{3}J_{H2-H3} = 7.3$ Hz, H2), 2.37 (2H, m, H9), 2.20 (2H, m, H5), 1.34 (3H, t, ${}^{3}J_{H1-H2} =$ 7.4 Hz, H1) ppm. ¹³C {¹H} NMR (CDCl₃, 101 MHz, δ): 195.55 (C15), 161.66 (C11), 137.94 (C16), 132.55 (C13), 132.16 (C19), 130.83 (C14), 129.78 (C17), 128.29 (C18), 114.22 (C12), 64.57 (C10), 62.46 (C6), 62.17 (C8), 51.61 (C7), 46.44 (C2), 39.95 (C4), 23.64 (C5), 23.11 (C9), 8.27 (C1) ppm. **HRMS-ESI-TOF** (m/z): [M⁺ - Br⁻] calculated for C₂₃H₃₃N₂O₄S, 433.2156; found 433.2153.

Synthesis of 3-(4-benzoylphenoxy)-N-(3-(butylsulfonamido)propyl)-N,N-dimethylpropan-1aminium bromide 8a This compound was synthesized **Method S3** using *N*-(3-(dimethylamino)propyl)butane-1-sulfonamide (0.324 g, 1.46 mmol) and 4-(3-bromopropoxy)benzophenone (0.466 g, 1.46 mmol) in ACN (10 mL) for 48 hours; yielding a viscous pale yellow solution. The product was obtained as fluffy pale yellow coloured powder after purification. Yield: 73% (0.58 g) ¹**H NMR** (CDCl₃, 400 MHz, δ): 7.74 (2H, d, ³*J*_{H15-H14} = 8.7 Hz, H15), 7.69 (2H, d, ³*J*_{H19-H20} = 7.1 Hz, H19), 7.54 (1H, t, ³*J*_{H21-H20} = 7.4 Hz, H21), 7.44 (2H, m, H20), 7.10 (1H, t, ³*J*_{H5-H6} = 5.6 Hz, H5), 6.96 (2H, d, ³*J*_{H14-H15} = 8.8 Hz, H14), 4.18 (1H, t, ³*J*_{H12-H11} = 5.2 Hz, H12), 3.79-3.61 (2H, m, H8 & H10), 3.33 (6H, s, H9), 3.24 (2H, m, H6), 3.02 (2H, m, H4), 2.33 (2H, m, H11), 2.18 (2H, m, H7), 1.73 (2H, m, H3), 1.38 (2H, m, H2), 0.87 (3H, t, ³*J*_{H1-H2} = 7.3 Hz, H1) ppm. ¹³C {¹H} **NMR** (CDCl₃, 101 MHz, δ): 195.56 (C17), 161.17 (C13), 137.89 (C18), 132.50 (C15), 132.16 (C21), 130.62 (C16), 129.71 (C19), 128.29 (C20), 114.27 (C14), 64.67 (C12), 62.30 (C8), 61.96 (C10), 51.79 (C4), 51.56 (C9), 25.37 (C3), 23.55 (C7), 23.05 (C11), 21.51 (C2), 13.64 (C1) ppm. **HRMS-ESI-TOF** (*m/z*): [M⁺ - Br⁻] calculated for C₂₅H₃₇N₂O₄S, 461.2469; found 461.2458.

Synthesis of N,N-dimethyl-3-(phenylsulfonamido)-N-(3-(trimethoxysilyl)propyl)propan-1aminium chloride 1b

This compound synthesized according Method **S3**, with N-(3was to (dimethylamino)propyl)benzenesulfonamide (1.0)4.13 mmol) (3g, and chloropropyl)trimethoxysilane (1.1 mL, 6.19 mmol, 1.5 eq.) in ACN (3 mL) for 4 hours resulting in viscous golden yellow brown solution. The product was purified using Et₂O (10 mL \times 3) and obtained as clear golden brown coloured gummy oil. Yield: 97.5 % (1.77 g). ¹H NMR (CDCl₃, 400 MHz, δ): 8.39 (1H, br s, H5), 7.96 (d, 2H, H3), 7.54 - 7.341 (3H, m, H1 & H2), 3.66 (2H, m,

H8), 3.51 (9H,s, H13), 3.34 (2H, m, H10), 3.21 (6H, s, H9), 3.00 (2H, m, H6), 2.06 (2H, m, H7), 1.75 (2H, m, H11), 0.59 (2H, t, ${}^{3}J_{H12-H11} = 7.8$ Hz, H12) ppm. 13 C { 1 H} NMR (CDCl₃, 101 MHz, δ): 139.86 (C4), 132.41 (C1), 129.14 (C2), 127.20 (C3), 65.94 (C10), 62.45 (C8), 51.10 (C9), 50.72 (C13), 39.93 (C6), 22.61 (C7), 16.45 (C11), 5.57 (C12) ppm. 29 Si { 1 H} NMR (CDCl₃, 79.4 MHz, δ): -44.41 ppm. HRMS-ESI-TOF (m/z): [M⁺ - Cl⁻] calculated for C₁₇H₃₃N₂O₅SSi, 405.1874, found, 405.8166.

Synthesis of N,N-dimethyl-3-(4-methylphenylsulfonamido)-N-(3-(trimethoxysilyl)propyl)propan-1-aminium chloride 2b

This compound was synthesized according to **Method S3**, with *N*-(3-(dimethylamino)propyl)-4methylbenzenesulfonamide (1.0 g, 3.9 mmol) and (3-chloropropyl)trimethoxysilane (1.1 mL, 5.85 mmol, 1.5 eq.) in ACN (3 mL) for 3.5 hours resulting in viscous golden yellow brown coloured solution. The product was purified using Et₂O (10 mL × 3) and obtained as clear golden brown gummy oil. Yield: 97 % (1.67 g). ¹**H NMR** (CDCl₃, 400 MHz, δ): 8.18 (1H, br s, H6), 7.85 (2H, d, ³*J*_{H4-H2} = 7.9 Hz, H4), 7.29 (2H, d, ³*J*_{H2-H4} = 7.7 Hz, H2), 3.69 (2H, m, H9), 3.55 (9H, s, H14), 3.37 (2H, m, H11), 3.25 (6H, s, H10), 3.01 (2H, m, H7), 2.40 (3H, s, H1), 2.10 (2H, m, H8), 1.79 (2H, m, H12), 0.63 (2H, t, ³*J*_{H13-H12} = 7.7 Hz, H13) ppm. ¹³C {¹H} NMR (CDCl₃, 101 MHz, δ): 143.08 (C5), 136.85 (C3), 129.70 (C2), 127.85 (C4), 65.82 (C11), 62.45 (C9), 51.10 (C14), 50.70 (C10), 39.91 (C7), 22.66 (C1), 21.46 (C8), 16.44 (C12), 5.57 (C13) ppm. ²⁹Si {¹H} NMR (CDCl₃, 79.4 MHz, δ): -44.37 ppm. **HRMS-ESI-TOF** (*m*/*z*): [M⁺ - Cl⁻] calculated for C₁₈H₃₅N₂O₅SSi, 419.2030, found, 419.2026.

Synthesis

N,N-dimethyl-3-(trimethoxysilyl)-N-(3-(2,4,6-

trimethylphenylsulfonamido)propyl)propan-1-aminium chloride 3b

This compound was synthesized according to **Method S3**, with *N*-(3-(dimethylamino)propyl)-2,4,6- trimethylbenzenesulfonamide (2.0 g, 7.03 mmol) and (3-chloropropyl)trimethoxysilane (1.9 mL, 10.55 mmol, 1.5 eq.) in ACN (3 mL) for 4.5 hours resulting in viscous golden yellow brown solution. The product was purified using Et₂O (10 mL × 3) and obtained as clear golden brown coloured gummy oil. Yield: 92.6 % (3.27 g). ¹H NMR (CDCl₃, 400 MHz, δ): 7.74 (1H, t, ³*J*_{H7-H8} = 6.0 Hz, H7), 6.90 (2H, s, H3), 3.70 (2H, m, H8), 3.53 (9H, s, H15), 3.37 (2H, m, H12), 3.25 (6H, s, H11), 2.98 (2H, m, H10), 2.62 (6H, br s, H4), 2.25 (3H, s, H1), 2.09 (2H, m, H9), 1.78 (2H, m, H13), 0.62 (2H, t, ³*J*_{H14-H13} = 7.9 Hz, H14) ppm. ¹³C {¹H} NMR (CDCl₃, 101 MHz, δ): 142.01 (C6), 139.22 (C5), 133.83 (C2), 132.01 (C3), 66.06 (C12), 62.51 (C10), 51.22 (C11), 50.81 (C15), 39.33 (C8), 23.28 (C4), 22.88 (C1), 20.95 (C9), 16.57 (C13), 5.70 (C14) ppm. ²⁹Si {¹H} NMR (CDCl₃, 79.4 MHz, δ): -44.43 ppm. HRMS-ESI-TOF (*m*/z): [M⁺ - Cl⁻] calculated for C₂₀H₃₉N₂O₅SSi, 447.2343, found, 447.2357.

Syntehsis of N,N-dimethyl-3-(naphthalene-1-sulfonamido)-N-(3-(trimethoxysilyl)propyl)propan-1-aminium chloride 4b

This synthesized according Method **S3** using compound was to N-(3-(dimethylamino)propyl)naphthalene-1-sulfonamide (0.5)g, 2.21mmol) and (3chloropropyl)trimethoxysilane (0.6 mL, 3.31 mmol, 1.5 eq.) in ACN (3 mL) for 5 hours resulting in viscous golden yellow brown solution. The product was purified using Et₂O (10 mL \times 3) and obtained as clear golden brown coloured gummy oil. Yield: 78.8 % (0.85 g). ¹H NMR (CDCl₃, 400 MHz, δ): 8.83 (1H, d, ${}^{3}J_{H8-H7}$ = 8.6 Hz, H8), 8.47 (1H, t, ${}^{3}J_{H11-H12}$ = 5.7 Hz, H11), 8.20 (1H, d, ${}^{3}J_{\text{H6-H7}} = 7.3 \text{ Hz}, \text{ H6}$), 7.99 (1H, d, ${}^{3}J_{\text{H1-H2}} = 8.1 \text{ Hz}, \text{ H1}$), 7.87 (1H, d, ${}^{3}J_{\text{H4-H3}} = 8.1 \text{ Hz}, \text{H4}$), 7.69 (1H, m, H7), 7.55 - 7.46 (2H, m, H3 & H2), 3.49 (11H, br s, H14 & H19), 3.20 (2H, m, H16),

3.06 (8H, br s, H12 & H15), 1.98 - 1.86 (2H, m, H13), 1.68 - 1.54 (2H, m, H17), 0.51 (2H, t, ${}^{3}J_{\text{H18-H17}} = 7.8$ Hz, H18) ppm. 13 C { 1 H} NMR (CDCl₃, 101 MHz, δ): 135.12 (C9), 134.16 (C5), 133.91 (C1), 129.07 (C6), 128.8 (C4), 128.56 (C7), 128.12 (C10), 127.02 (C3), 125.30 (C8), 124.31 (C2), 65.84 (C16), 62.32 (C14), 50.92 (C15), 50.69 (C19), 39.79 (C12), 22.81 (C13), 16.33 (C17), 5.48 (C18) ppm. 29 Si { 1 H} NMR (CDCl₃, 79.4 MHz, δ): -44.49 ppm. HRMS-ESI-TOF (m/z): [M⁺ - Cl⁻] calculated for C₂₁H₃₅N₂O₂SSi, 455.2030, found, 455.2018.

Synthesis of 3-(ethylsulfonamido)-N,N-dimethyl-N-(3-(trimethoxysilyl)propyl)propan-1aminium chloride 7b

This compound according Method was synthesized to **S3** with N-(3-(dimethylamino)propyl)ethanesulfonamide (1.0)g, 5.15 mmol) and (3chloropropyl)trimethoxysilane (1.4 mL, 7.72 mmol, 1.5 eq.) in ACN (3 mL) for 5 hours resulting in viscous golden yellow brown solution. The product was purified using Et₂O (10 mL \times 3) and obtained as clear golden brown coloured gummy oil. Yield: 86.0 % (1.73 g). ¹H NMR (CDCl₃, 400 MHz, δ): 7.63 (1H, s, H3), 3.66 (2H, m, H6), 3.53 (9H, m, H11), 3.36 (2H, m, H8), 3.25 -3.15 (8H, m, H7 & H4), 3.03 (2H, m, H2), 2.12 (2H, m, H5), 1.78 (2H, m, H9), 1.31 (3H, m, H1), 0.62 (2H, t, ${}^{3}J_{H10-H9} = 7.8$ Hz, H10) ppm. ${}^{13}C \{{}^{1}H\}$ NMR (CDCl₃, 101 MHz, δ): 65.89 (C8), 62.40 (C6), 51.18 (C7), 50.81 (C11), 46.37 (C2), 40.09 (C4), 23.58 (C5), 16.54 (C9), 8.28 (C1), 5.73 (C10) ppm. ²⁹Si {¹H} NMR (CDCl₃, 79.4 MHz, δ): -44.51 ppm.

Synthesis of 3-(butylsulfonamido)-N,N-dimethyl-N-(3-(trimethoxysilyl)propyl)propan-1aminium chloride 8b

This	compound	was	synthesized	according	to	Method	S 3	with	<i>N</i> -(3-
(dimethylamino)propyl)butanesulfonamide				(1.0	g,	4.50	mmol)	and	(3-

chloropropyl)trimethoxysilane (1.2 mL, 6.75 mmol, 1.5 eq.) in ACN (3 mL) for 5 hours resulting in viscous golden yellow brown solution. The product was purified using Et₂O (10 mL × 5) and obtained as clear golden brown coloured gummy oil. Yield: 60.0 % (1.13 g). ¹H NMR (CDCl₃, 400 MHz, δ): 7.62 (1H, br s, H5), 3.64 (2H, m, H8), 3.51 (9H, s, H13), 3.34 (2H, m, H4), 3.24 -3.12 (8H, m, H9 and H6), 2.98 (2H, m, H4), 2.09 (2H, m, H7), 1.83 - 1.66 (4H, m, H11 & H3), 1.38 (2H, m, H2), 0.86 (3H, m, H1), 0.60 (2H, t, ³*J*_{H12-H11} = 7.3 Hz, H12) ppm. ¹³C {¹H} NMR (CDCl₃, 101 MHz, δ): 65.82 (C10), 51.81 (C4), 51.12 (C9), 50.74 (C13), 40.04 (C6), 25.38 (C3), 23.50 (C7), 21.58 (C2), 16.50 (C11), 13.62 (C1), 5.68 (C12) ppm. ²⁹Si {¹H} NMR (CDCl₃, 79.4 MHz, δ): -44.50 ppm. HRMS-ESI-TOF (*m*/*z*): [M⁺ - Cl⁻] calculated for C₁₅H₃₇N₂O₅SSi, 385.2187, found, 385.2185. NMR Spectra of Synthesized Compounds



Figure S 19. ¹H NMR (400 MHz, CDCl₃) spectrum of 1.



Figure S 20. ¹³C NMR (101 MHz, CDCl₃) spectrum of 1.



Figure S 21. COSY 2D NMR (CDCl₃) spectrum of 1.



Figure S 22. HSQC 2D NMR (CDCl₃) spectrum of 1.



Figure S 23. ¹H NMR (400 MHz, CDCl₃) spectrum of 2.



Figure S 24. ¹³C NMR (101 MHz, CDCl₃) spectrum of 2.



Figure S 25. COSY 2D NMR (CDCl₃) spectrum of 2.



Figure S 26. HSQC 2D NMR (CDCl₃) spectrum of 2.



Figure S 27. ¹H NMR (400 MHz, CDCl₃) spectrum of 3.



Figure S 28. ¹³C NMR (101 MHz, CDCl₃) spectrum of 3.



Figure S 29. COSY 2D NMR (CDCl₃) spectrum of 3.



Figure S 30. HSQC 2D NMR (CDCl₃) spectrum of 3.



Figure S 31. ¹H NMR (400 MHz, CDCl₃) spectrum of 4.



Figure S 32. ¹³C NMR (101 MHz, CDCl₃) spectrum of 4.



Figure S 33. COSY 2D NMR (CDCl₃) spectrum of 4.



Figure S 34. HSQC 2D NMR (CDCl₃) spectrum of 4.



Figure S 35. ¹H NMR (400 MHz, CDCl₃) spectrum of 5.



Figure S 36. ¹³C NMR (101 MHz, CDCl₃) spectrum of 5.



Figure S 37. ¹⁹F NMR (376 MHz, CDCl₃) spectrum of 5.



Figure S 38. COSY 2D NMR (CDCl₃) spectrum of 5.



Figure S 39. HSQC 2D NMR (CDCl₃) spectrum of 5.



Figure S 40. ¹H NMR (400 MHz, CDCl₃) spectrum of 6.



Figure S 41. ¹³C NMR (101 MHz, CDCl₃) spectrum of 6.



Figure S 42. ¹⁹F NMR (376 MHz, CDCl₃) spectrum of 6.



Figure S 43. COSY 2D NMR (CDCl₃) spectrum of 6.



Figure S 44. HSQC 2D NMR (CDCl₃) spectrum of 6.



Figure S 45. ¹H NMR (400 MHz, CDCl₃) spectrum of 7.



Figure S 46. ¹³C NMR (101 MHz, CDCl₃) spectrum of 7.



Figure S 47. COSY 2D NMR (CDCl₃) spectrum of 7.


Figure S 48. HSQC 2D NMR (CDCl₃) spectrum of 7.



Figure S 49. ¹H NMR (400 MHz, CDCl₃) spectrum of 8.



Figure S 50. ¹³C NMR (101 MHz, CDCl₃) spectrum of 8.



Figure S 51. COSY 2D NMR (CDCl₃) spectrum of 8.



Figure S 52. HSQC 2D NMR (CDCl₃) spectrum of 8.



Figure S 53. ¹H NMR (400 MHz, CDCl₃) spectrum of 9.



Figure S 54. ¹³C NMR (101 MHz, CDCl₃) spectrum of 9.



Figure S 55. COSY 2D NMR (CDCl₃) spectrum of 9.



Figure S 56. HSQC 2D NMR (CDCl₃) spectrum of 9.



Figure S 57. ¹H NMR (400 MHz, CDCl₃) spectrum of 10.



Figure S 58. ¹³C NMR (101 MHz, CDCl₃) spectrum of 10.



Figure S 59. COSY 2D NMR (CDCl₃) spectrum of 10.



Figure S 60. HSQC 2D NMR (CDCl₃) spectrum of 10.



Figure S 61. ¹H NMR (400 MHz, CDCl₃) spectrum of 1a.



Figure S 62. ¹³C NMR (101 MHz, CDCl₃) spectrum of 1a.



Figure S 63. COSY 2D NMR (CDCl₃) spectrum of 1a.



Figure S 64. HSQC 2D NMR (CDCl₃) spectrum of 1a.



Figure S 65. ¹H NMR (400 MHz, CDCl₃) spectrum of 2a.



Figure S 66. ¹³C NMR (101 MHz, CDCl₃) spectrum of 2a.



Figure S 67. COSY 2D NMR (CDCl₃) spectrum of 2a.



Figure S 68. HSQC 2D NMR (CDCl₃) spectrum of 2a.



Figure S 69. ¹H NMR (400 MHz, CDCl₃) spectrum of 3a.



Figure S 70. ¹³C NMR (101 MHz, CDCl₃) spectrum of 3a.



Figure S 71. COSY 2D NMR (CDCl₃) spectrum of 3a.



Figure S 72. HSQC 2D NMR (CDCl₃) spectrum of 3a.



Figure S 73. ¹H NMR (400 MHz, CDCl₃) spectrum of 4a.



Figure S 74. ¹³C NMR (101 MHz, CDCl₃) spectrum of 4a.



Figure S 75. COSY 2D NMR (CDCl₃) spectrum of 4a.



Figure S 76. HSQC 2D NMR (CDCl₃) spectrum of 4a.



Figure S 77. ¹H NMR (400 MHz, CDCl₃) spectrum of 5a.



Figure S 78. ¹³C NMR (101 MHz, CDCl₃) spectrum of 5a.



Figure S 79. ¹⁹F NMR (376 MHz, CDCl₃) spectrum of 5a.



Figure S 80. COSY 2D NMR (CDCl₃) spectrum of 5a.



Figure S 81. HSQC 2D NMR (CDCl₃) spectrum of 5a.



Figure S 82. ¹H NMR (400 MHz, DMSO-d₆) spectrum of 6a.



Figure S 83. ¹³C NMR (101 MHz, DMSO-d₆) spectrum of 6a.


Figure S 84. ¹⁹F NMR (376 MHz, DMSO-d₆) spectrum of 6a.



Figure S 85. COSY 2D NMR (DMSO-d₆) spectrum of 6a.



Figure S 86. HSQC 2D NMR (DMSO-d₆) spectrum of 6a.



Figure S 87. ¹H NMR (400 MHz, CDCl₃) spectrum of 7a.



Figure S 88. ¹³C NMR (101 MHz, CDCl₃) spectrum of 7a.



Figure S 89. COSY 2D NMR (CDCl₃) spectrum of 7a.



Figure S 90. HSQC 2D NMR (CDCl₃) spectrum of 7a.



Figure S 91. ¹H NMR (400 MHz, CDCl₃) spectrum of 8a.



Figure S 92. ¹³C NMR (101 MHz, CDCl₃) spectrum of 8a.



Figure S 93. COSY 2D NMR (CDCl₃) spectrum of 8a.



Figure S 94. HSQC 2D NMR (CDCl₃) spectrum of 8a.



Figure S 95. ¹H NMR (400 MHz, CDCl₃) spectrum of 1b.



Figure S 96. ¹³C NMR (101 MHz, CDCl₃) spectrum of 1b.



Figure S 97. ²⁹Si NMR (79 MHz, CDCl₃) spectrum of 1b.



Figure S 98. COSY 2D NMR (CDCl₃) spectrum of 1b.



Figure S 99. HSQC 2D NMR (CDCl₃) spectrum of 1b.



Figure S 100. ¹H NMR (400 MHz, CDCl₃) spectrum of 2b.



Figure S 101. ¹³C NMR (101 MHz, CDCl₃) spectrum of 2b.



Figure S 102. ²⁹Si NMR (79 MHz, CDCl₃) spectrum of 2b.



Figure S 103. COSY 2D NMR (CDCl₃) spectrum of 2b.



Figure S 104. HSQC 2D NMR (CDCl₃) spectrum of 2b.



Figure S 105. ¹H NMR (400 MHz, CDCl₃) spectrum of 3b.



Figure S 106. ¹³C NMR (101 MHz, CDCl₃) spectrum of **3b**.



Figure S 107. ²⁹Si NMR (79 MHz, CDCl₃) spectrum of 3b.



Figure S 108. COSY 2D NMR (CDCl₃) spectrum of 3b.



Figure S 109. HSQC 2D NMR (CDCl₃) spectrum of 3b.



Figure S 110. ¹H NMR (400 MHz, CDCl₃) spectrum of 4b.



Figure S 111. ¹³C NMR (101 MHz, CDCl₃) spectrum of 4b.



Figure S 112. ²⁹Si NMR (79 MHz, CDCl₃) spectrum of 4b.



Figure S 113. COSY 2D NMR (CDCl₃) spectrum of 4b.



Figure S 114. HSQC 2D NMR (CDCl₃) spectrum of 4b.



Figure S 115. ¹H NMR (400 MHz, CDCl₃) spectrum of 7b.



Figure S 116. ¹³C NMR (101 MHz, CDCl₃) spectrum of 7b.



Figure S 117. ²⁹Si NMR (79 MHz, CDCl₃) spectrum of 7b.



Figure S 118. COSY 2D NMR (CDCl₃) spectrum of 7b.



Figure S 119. HSQC 2D NMR (CDCl₃) spectrum of 7b.


Figure S 120. ¹H NMR (400 MHz, CDCl₃) spectrum of 8b.



Figure S 121. ¹³C NMR (101 MHz, CDCl₃) spectrum of 8b.



Figure S 122. ²⁹Si NMR (79 MHz, CDCl₃) spectrum of 8b.



Figure S 123. COSY 2D NMR (CDCl₃) spectrum of 8b.



Figure S 124. HSQC 2D NMR (CDCl₃) spectrum of 8b.

References

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