

Supporting information
Design and Production of Environmentally Degradable Quaternary Ammonium Salt

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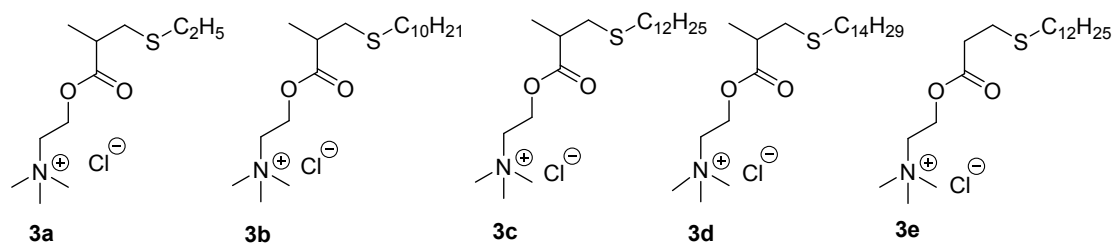
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1. Detailed synthetic procedures for 3a, 3b, 3c, 3d and 3e.



The α -substituted acrylate ester **1** (25 mmol, 1.0 eq) and the respective thiol **2** (25 mmol, 1.0 eq) were added into to a 100 mL round bottle with acetonitrile, then trimethylamine (1.25 mmol, 0.05 eq) was added *via* syringe. The reaction mixture was stirred at 300 K for 3 days. The volatiles were removed under vacuum to afford the target product **3** without further purification in quantitative yield.

3a. ¹H NMR (400 MHz, H₂O-*d*₂) 4.59 (m, 2H), 3.75 (t, ³J_{H,H} = 4 Hz, 2H), 3.21 (s, 9H), 2.90 (m, 1H), 2.79 (d, ³J_{H,H} = 8 Hz, 1H), 2.78 (d, ³J_{H,H} = 8 Hz, 1H), 2.57 (q, ³J_{H,H} = 7

Hz, 2H), 1.24-1.22 (d, $^3J_{\text{H,H}} = 8$ Hz, 3H), 1.22-1.18 (t, $^3J_{\text{H,H}} = 7$ Hz, 3H). ^{13}C NMR (101 MHz, $\text{H}_2\text{O}-d_2$) 176.61, 64.6, 58.6, 53.8, 39.9, 33.8, 25.8, 16.0, 14.0. HRMS (ESI+): calculated: 234.1522; found: 234.1516.

3b. ^1H NMR (400 MHz, $\text{H}_2\text{O}-d_2$) 4.60 (br, 2H), 3.81 (t, $^3J_{\text{H,H}} = 4$ Hz, 2H), 3.27 (s, 9H), 2.84 (m, 2H), 2.62 (m, 1H), 2.60 (t, $^3J_{\text{H,H}} = 8$ Hz, 2H), 1.6-1.2 (m, 19H), 0.88 (t, $^3J_{\text{H,H}} = 7$ Hz, 3H). ^{13}C NMR (101 MHz, $\text{H}_2\text{O}-d_2$) 175.1, 64.6, 58.7, 53.8, 39.8, 34.9, 32.4, 32.0, 29.8, 29.6, 29.5, 29.0, 22.7, 16.1, 14.0.

HRMS (ESI+): calculated: 346.2774; found: 346.2769.

3c. ^1H NMR (400 MHz, $\text{H}_2\text{O}-d_2$) 4.59 (br, 2H), 3.79 (t, $^3J_{\text{H,H}} = 4$ Hz, 2H), 3.25 (s, 9H), 2.82 (m, 2H), 2.56 (m, 1H), 2.54 (t, $^3J_{\text{H,H}} = 8$ Hz, 2H), 1.6-1.2 (m, 23H), 0.87 (t, $^3J_{\text{H,H}} = 7$ Hz, 3H). ^{13}C NMR (101 MHz, $\text{H}_2\text{O}-d_2$) 175.0, 64.6, 58.7, 53.9, 39.8, 35.0, 32.5, 32.1, 30.1, 30.0, 29.7, 29.6, 29.1, 22.7, 16.1, 14.0. HRMS (ESI+): calculated: 374.3087; found: 374.3087.

3d. ^1H NMR (400 MHz, $\text{H}_2\text{O}-d_2$) 4.60 (br, 2H), 3.83 (t, $^3J_{\text{H,H}} = 4$ Hz, 2H), 3.27 (s, 9H), 2.84 (m, 2H), 2.62 (m, 1H), 2.60 (t, $^3J_{\text{H,H}} = 8$ Hz, 2H), 1.6-1.2 (m, 27H), 0.88 (t, $^3J_{\text{H,H}} = 4$ Hz, 3H). ^{13}C NMR (101 MHz, CHCl_3-d_1) 174.6, 65.0, 58.7, 54.4, 40.2, 35.4, 33.0, 32.0, 29.8(1), 29.7(18), 29.7(6), 29.7(0), 29.5, 29.4, 29.0, 22.8, 17.0, 14.2. HRMS (ESI+): calculated: 402.3400; found: 402.3394.

3e. ^1H NMR (400 MHz, $\text{H}_2\text{O}-d_2$) 4.60 (br, 2H), 3.80 (t, $^3J_{\text{H,H}} = 4$ Hz, 2H), 3.26 (s, 9H), 2.78 (m, 4H), 2.57 (t, $^3J_{\text{H,H}} = 8\text{Hz}$, 2H), 1.58 (m, 2H), 1.18-1.47 (m, 18H), 0.87 (t, $^3J_{\text{H,H}} = 8\text{Hz}$, 3H). ^{13}C NMR (101 MHz, $\text{H}_2\text{O}-d_2$) 172.3, 64.5, 58.5, 57.4, 53.9, 34.4, 32.1, 31.8, 30.1, 30.0, 29.9, 29.7, 29.6, 29.5, 29.1, 26.4, 22.7, 16.8, 13.9. HRMS (ESI+): calculated: 360.2931; found: 360.2925.

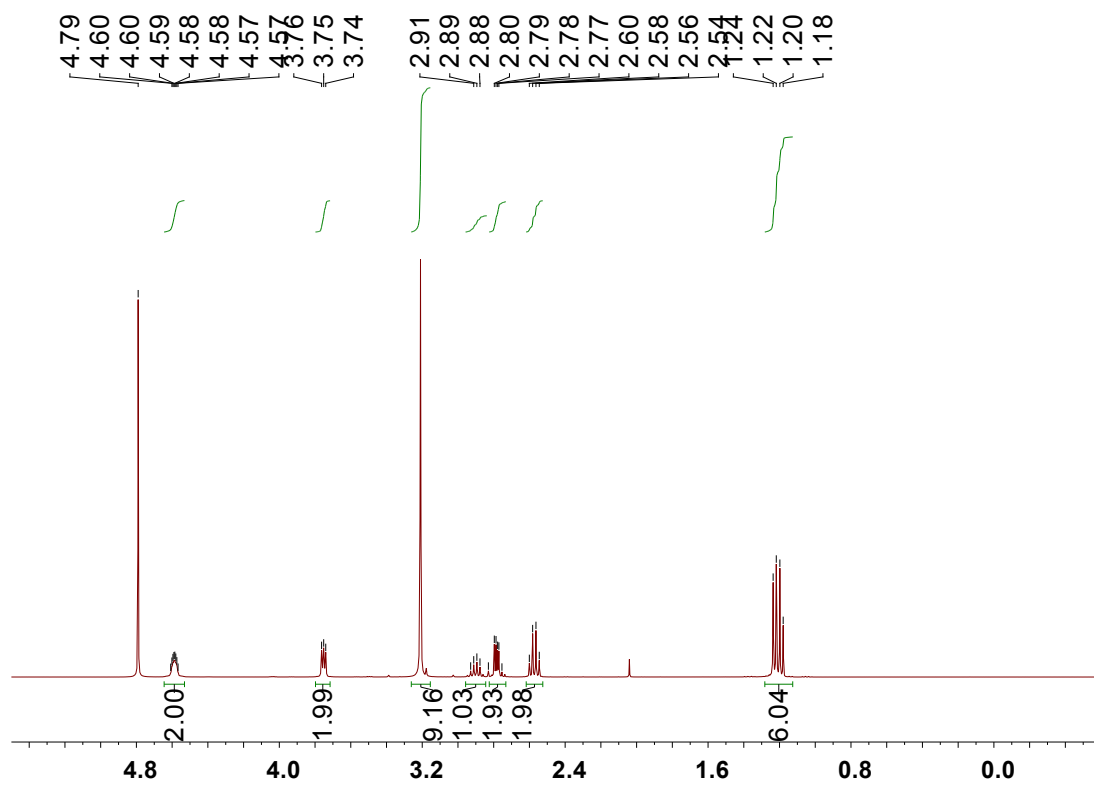


Fig S1. ^1H NMR spectrum of **3a** in D_2O .

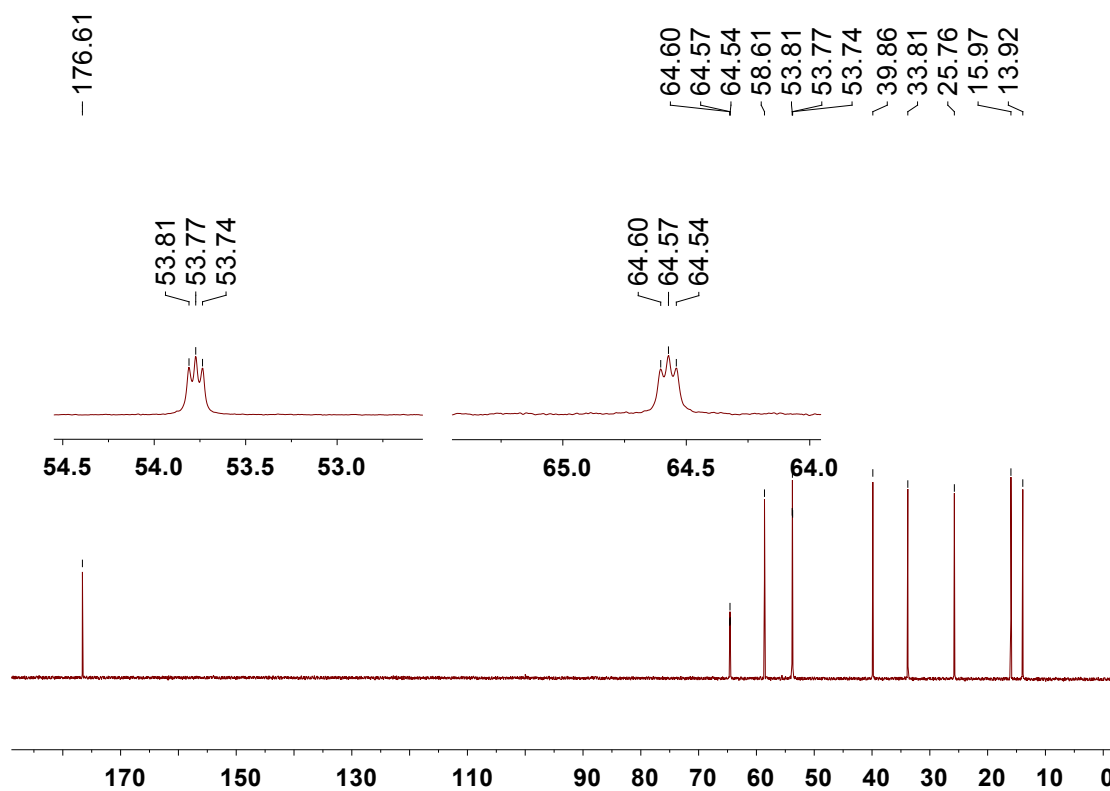


Fig S2. ^{13}C NMR spectrum of **3a** in D_2O .

T: FTMS + c ESI Full ms [50.00-600.00]

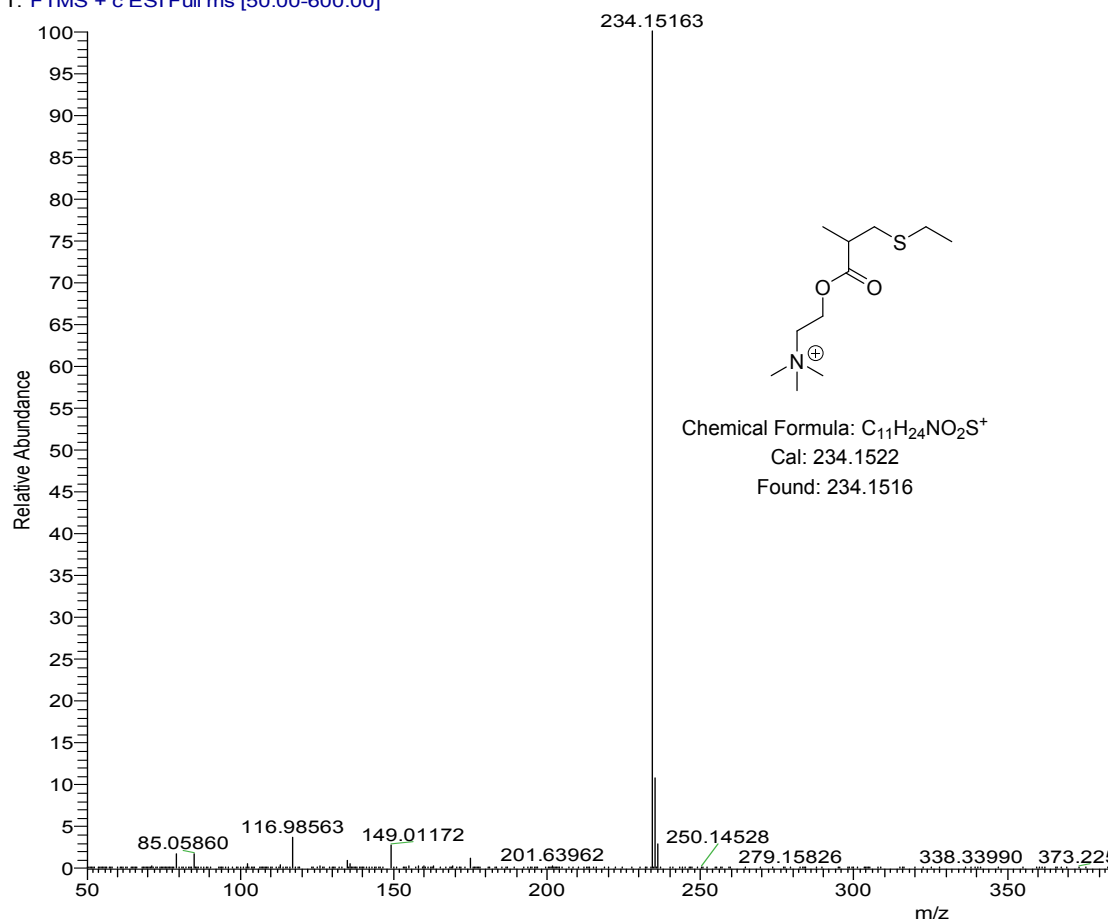


Fig S3. ESI mass spectrum of compound 3a.

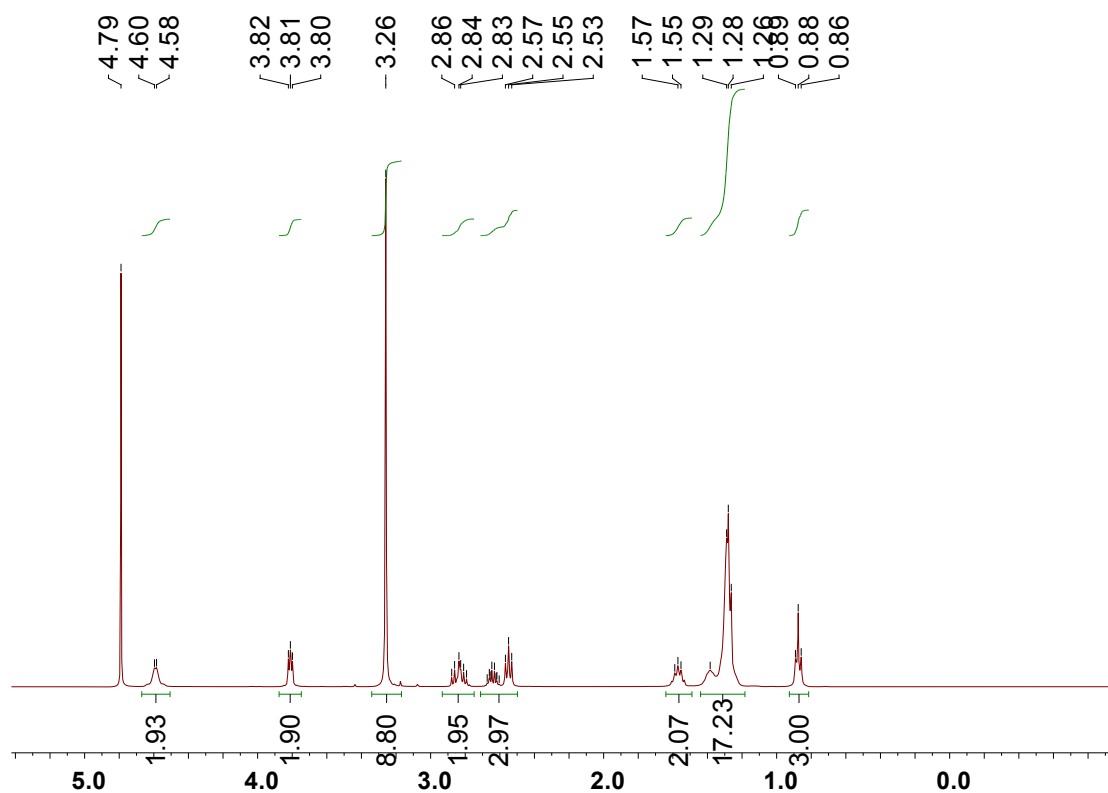


Fig S4. ¹H NMR spectrum of **3b** in D₂O.

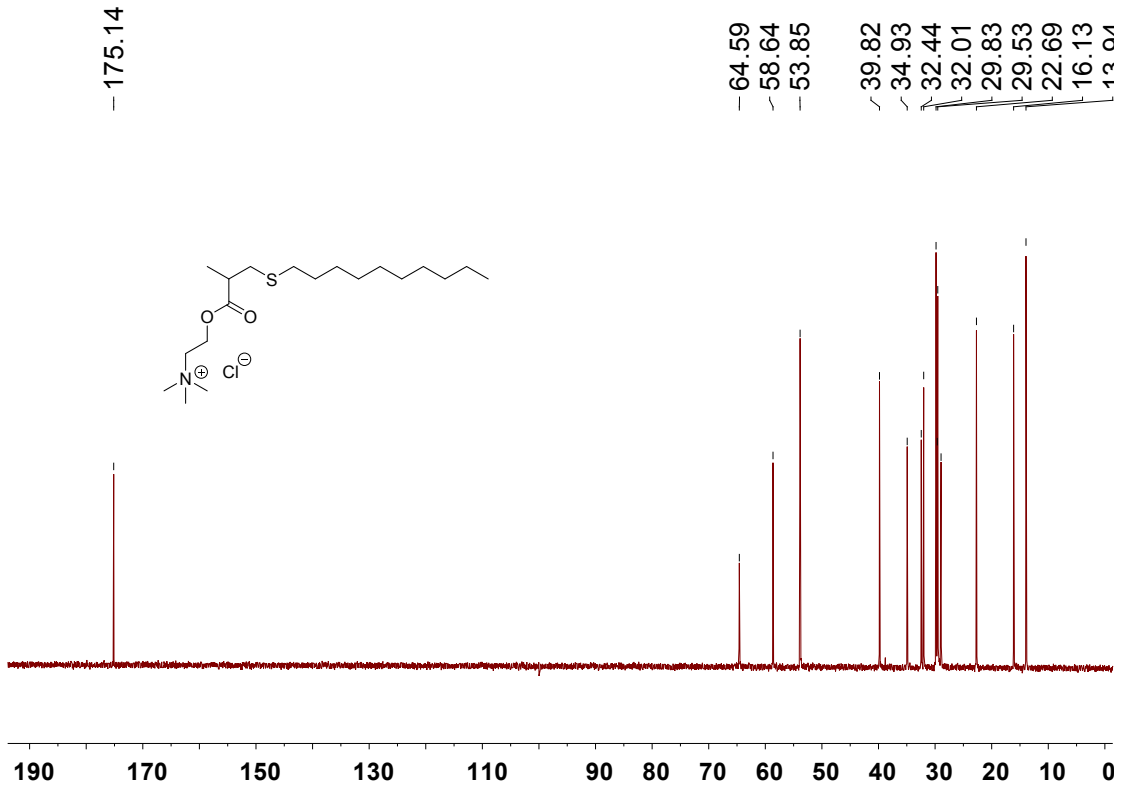


Fig S5. ¹³C NMR spectrum of **3b** in D₂O.

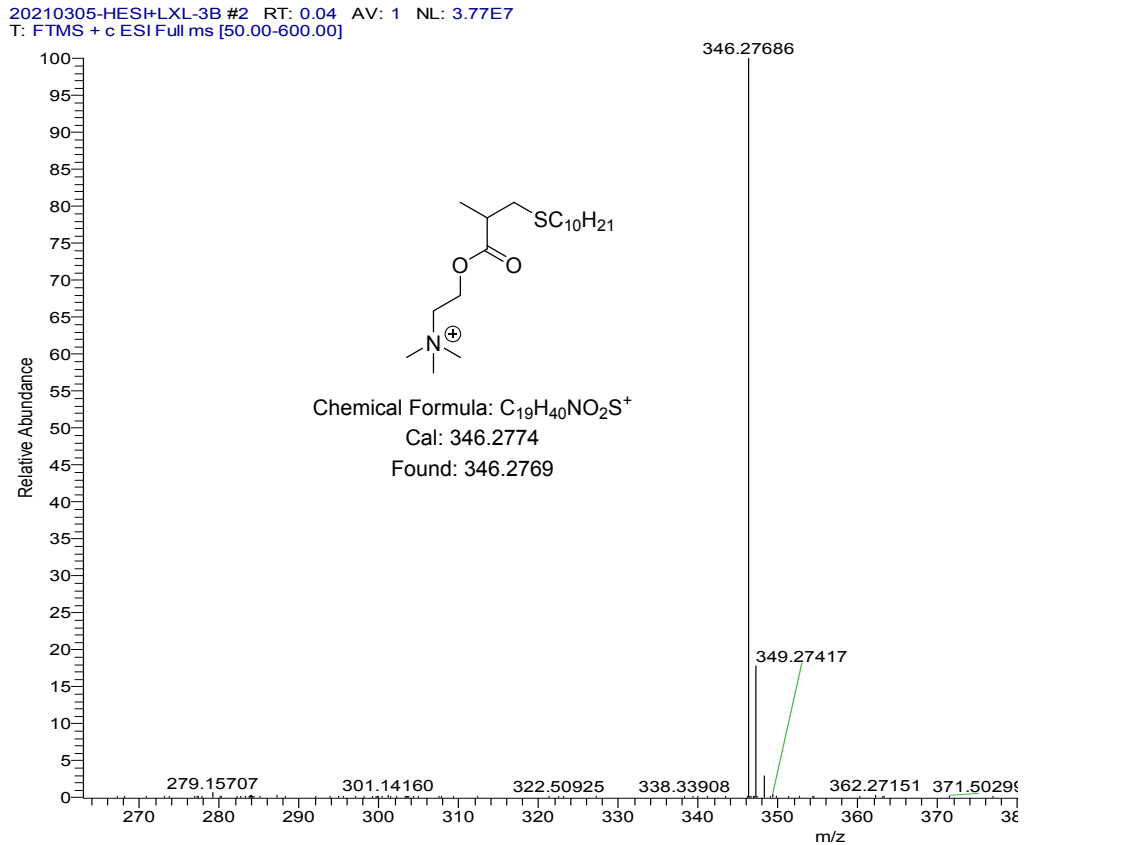


Fig S6. ESI mass spectrum of compound 3b.

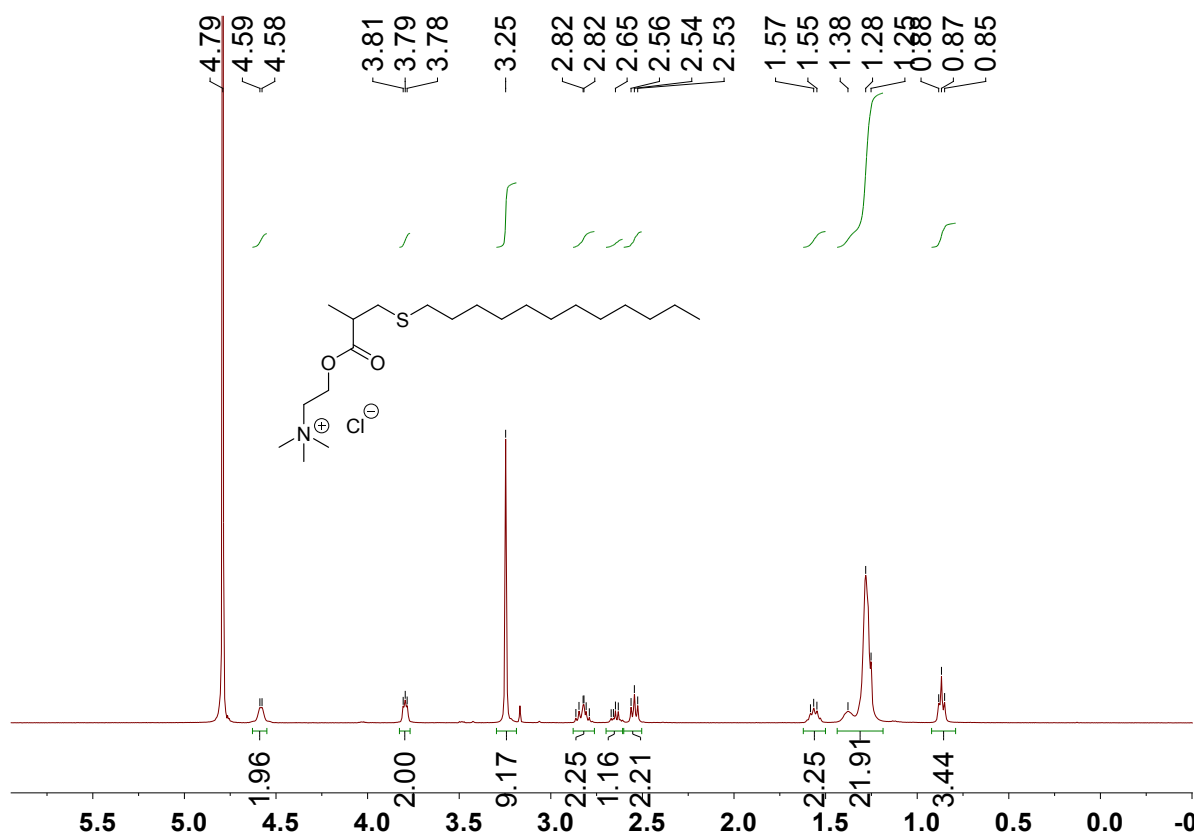


Fig S7. ¹H NMR spectrum of molecule 3c in D₂O.

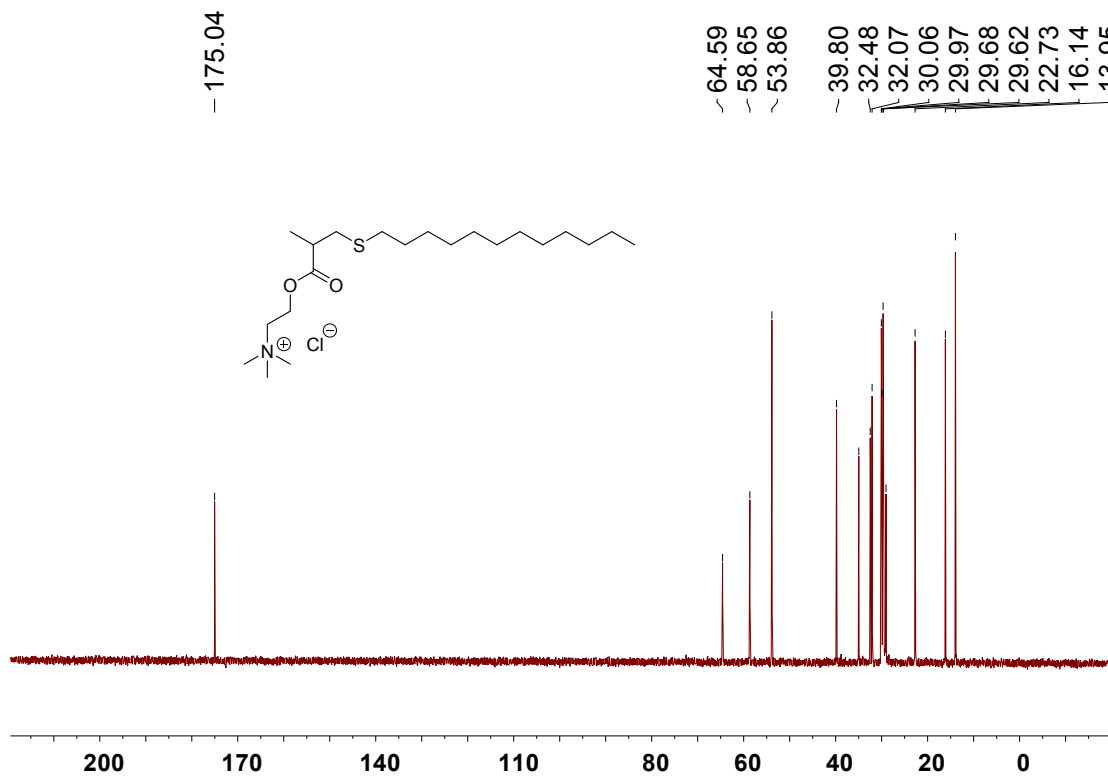


Fig S8. ^{13}C NMR spectrum of molecule **3c** in D_2O .

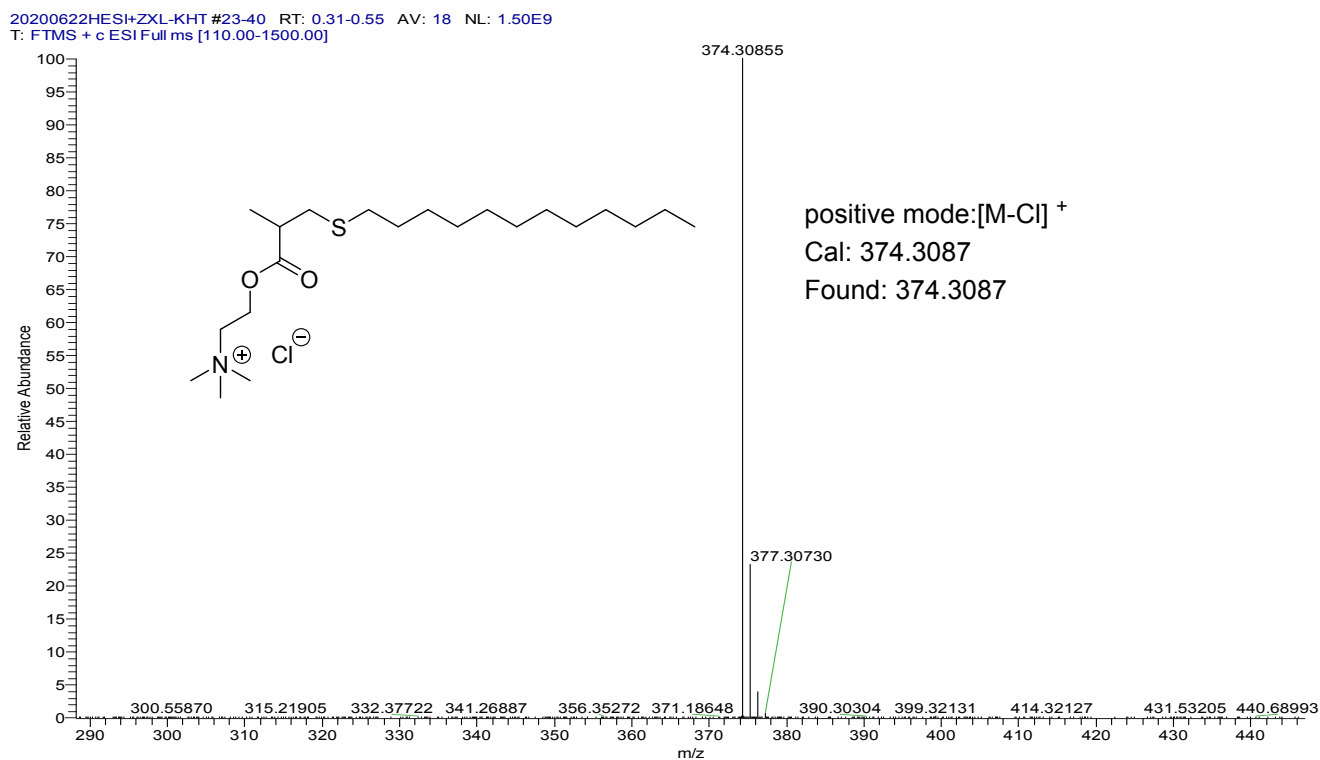


Fig S9. ESI mass spectrum of compound **3c**.

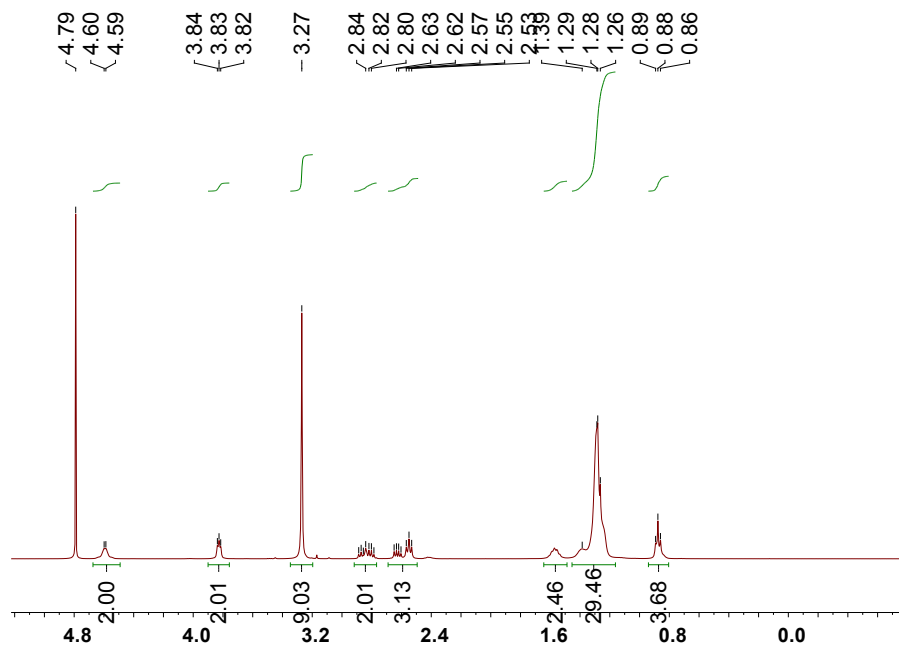


Fig S10. ^1H NMR spectrum of compound **3d** in D_2O .

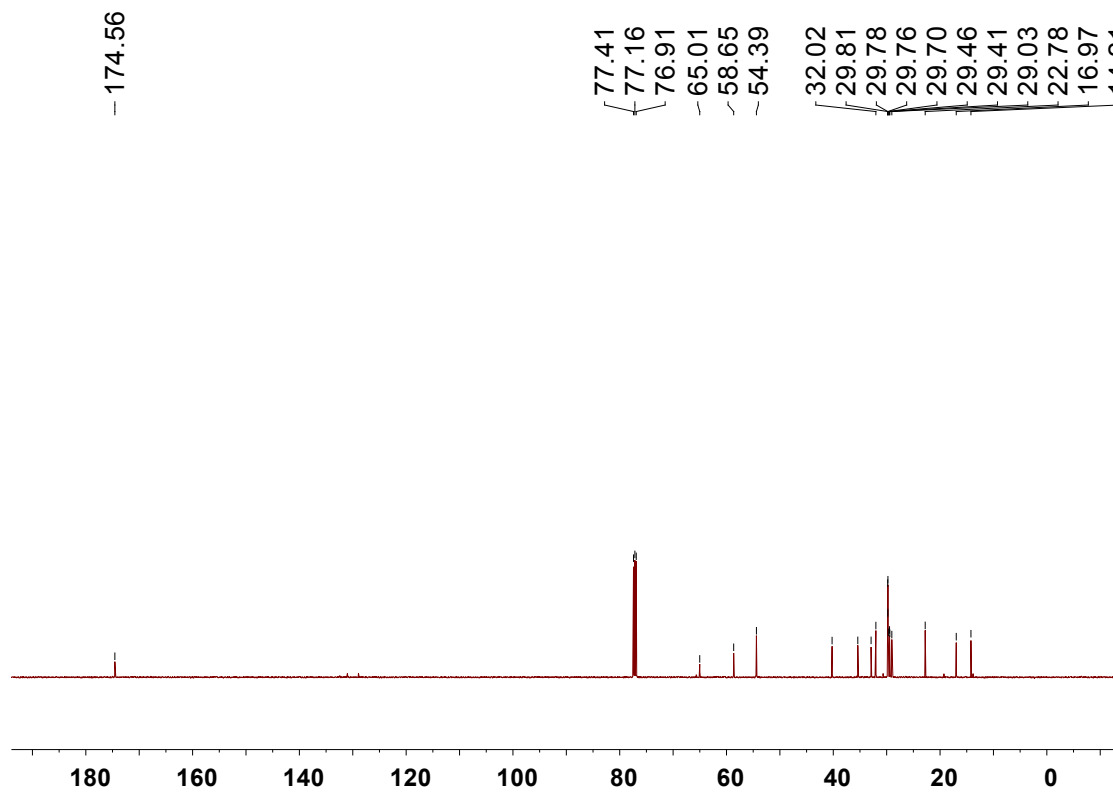


Fig S11. ^{13}C NMR spectrum of molecule **3d** in CDCl_3 .

20210305-HESI+LXL-3D #14 RT: 0.56 AV: 1 NL: 1.92E7
T: FTMS + c ESI Full ms [50.00-600.00]

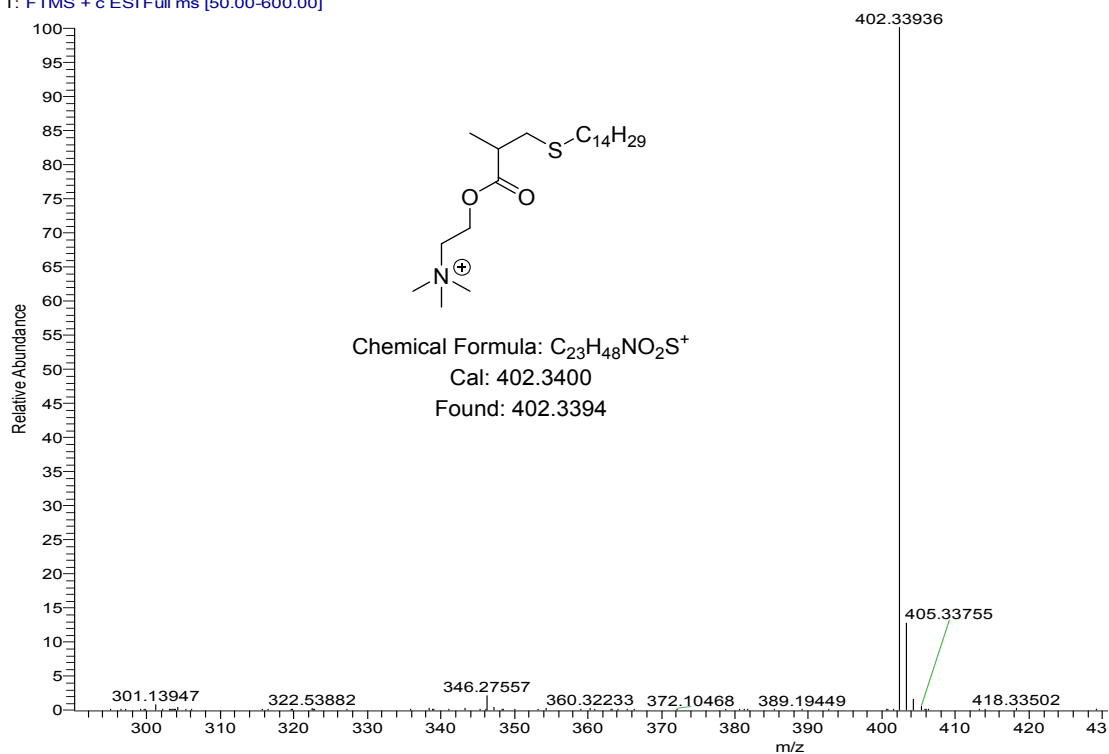


Fig S12. ESI mass spectrum of compound **3d**.

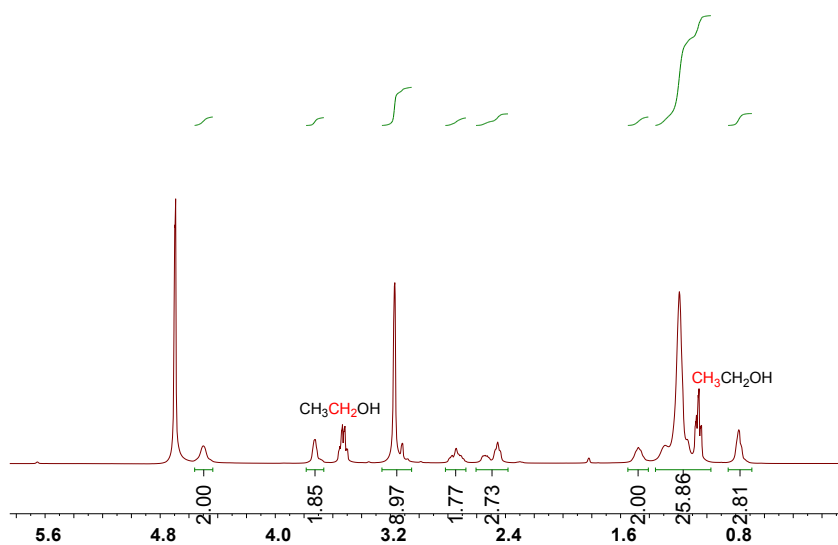


Fig S13. The product was isolated from the reaction in 50-L container and was pure by ^1H NMR spectrum in D_2O .

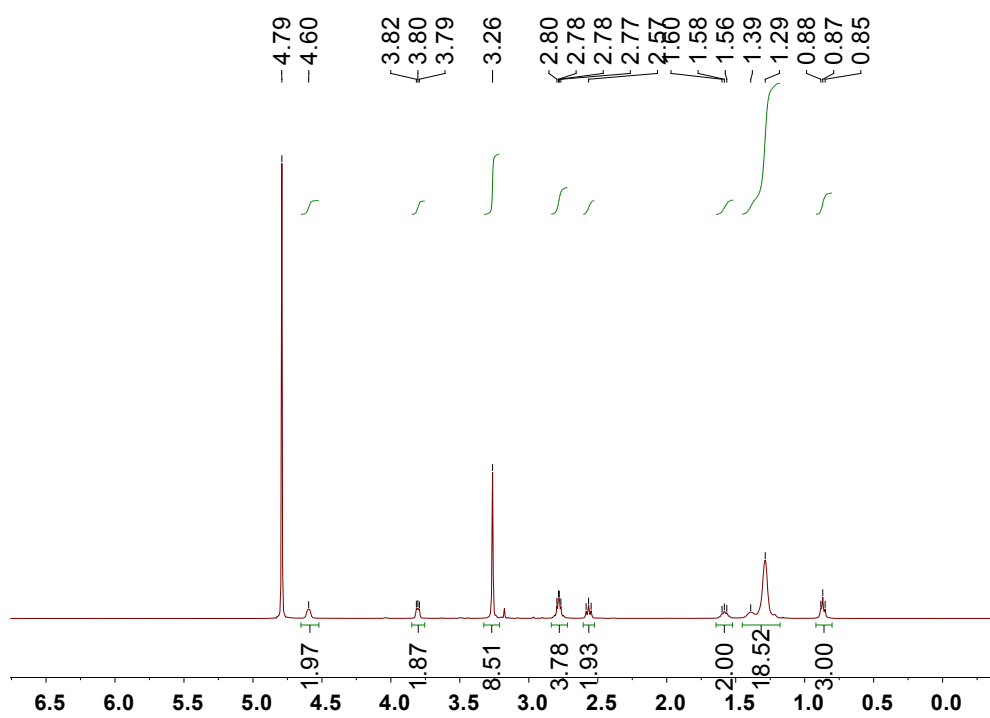


Fig S14. ^1H NMR spectrum of compound **3e** in D_2O .

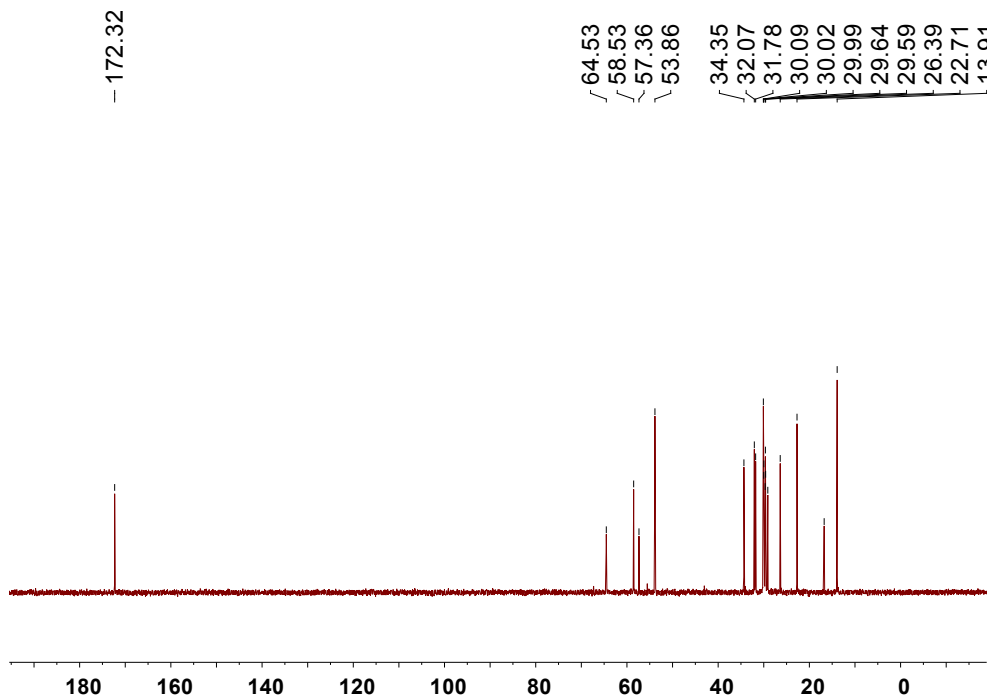


Fig S15. ^{13}C NMR spectrum of molecule **3e** in D_2O .

20210623HESI+2XL-3E #26 RT: 0.36 AV: 1 NL: 1.27E9
 T: FTMS + c ESI Full ms [50.00-800.00]

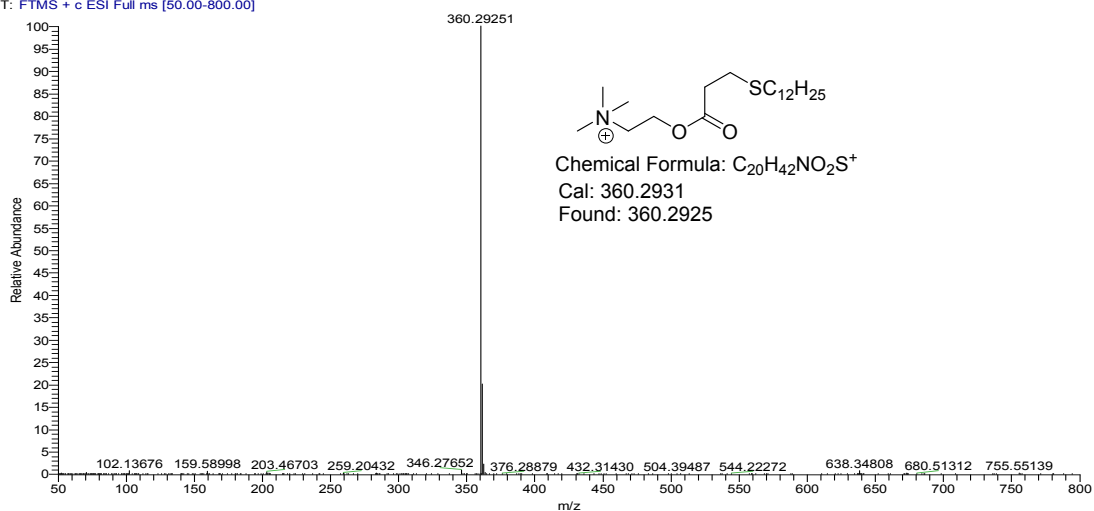


Fig S16. ESI mass spectrum of compound **3e**.

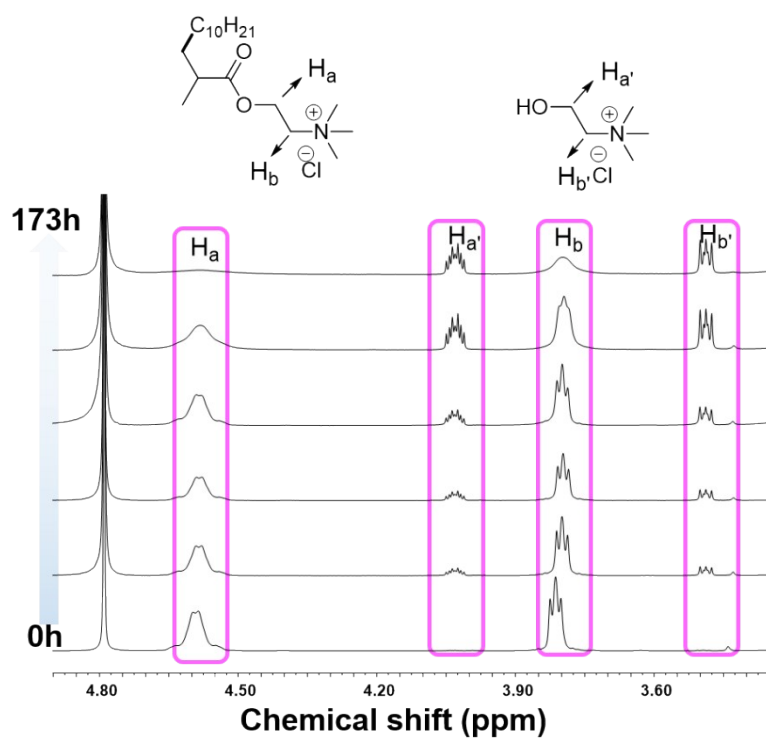


Fig S17. Partial stacked ^1H NMR spectra (400 MHz, D_2O) of compound **3b** and degradation product **4** in natural (university pond) water (1% wt, pH = 7.60, 327 K) measured at different time points.

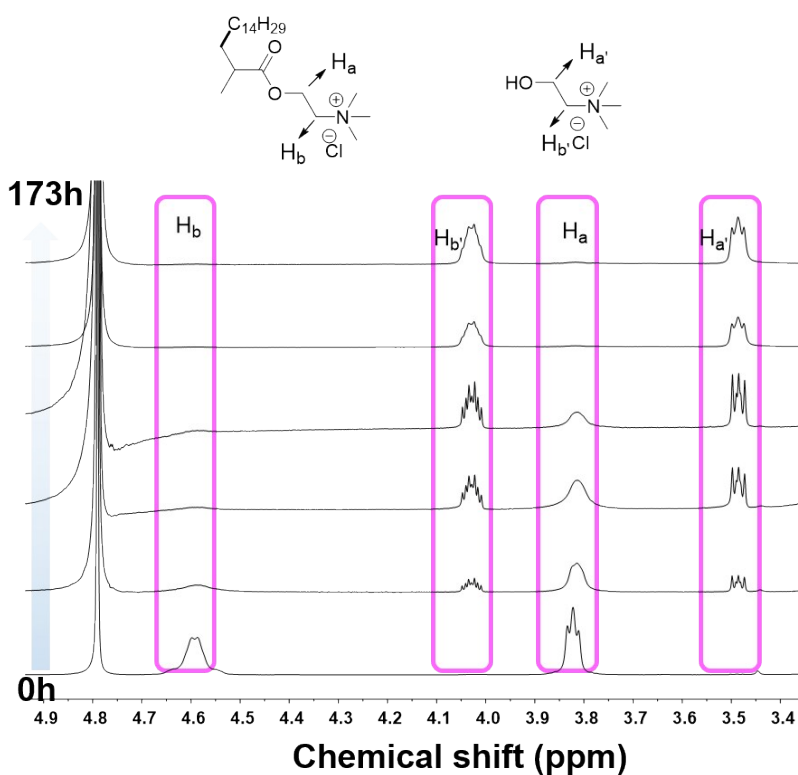


Fig S18. Partial stacked ^1H NMR spectra (400 MHz, D_2O) of compound **3d** and degradation product **4** in natural (university pond) water (1% wt, pH = 7.60, 327 K) measured at different time points.

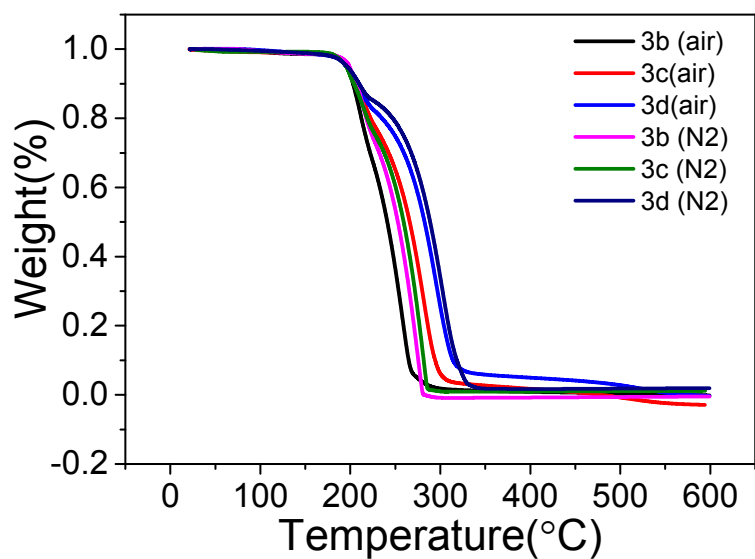


Fig S19. Thermal gravimetric analysis (TGA) graph of compound **3b**, **3c**, **3d** under N₂ or air at a temperature increase rate of 10 °C/min from 20 to 600 °C.

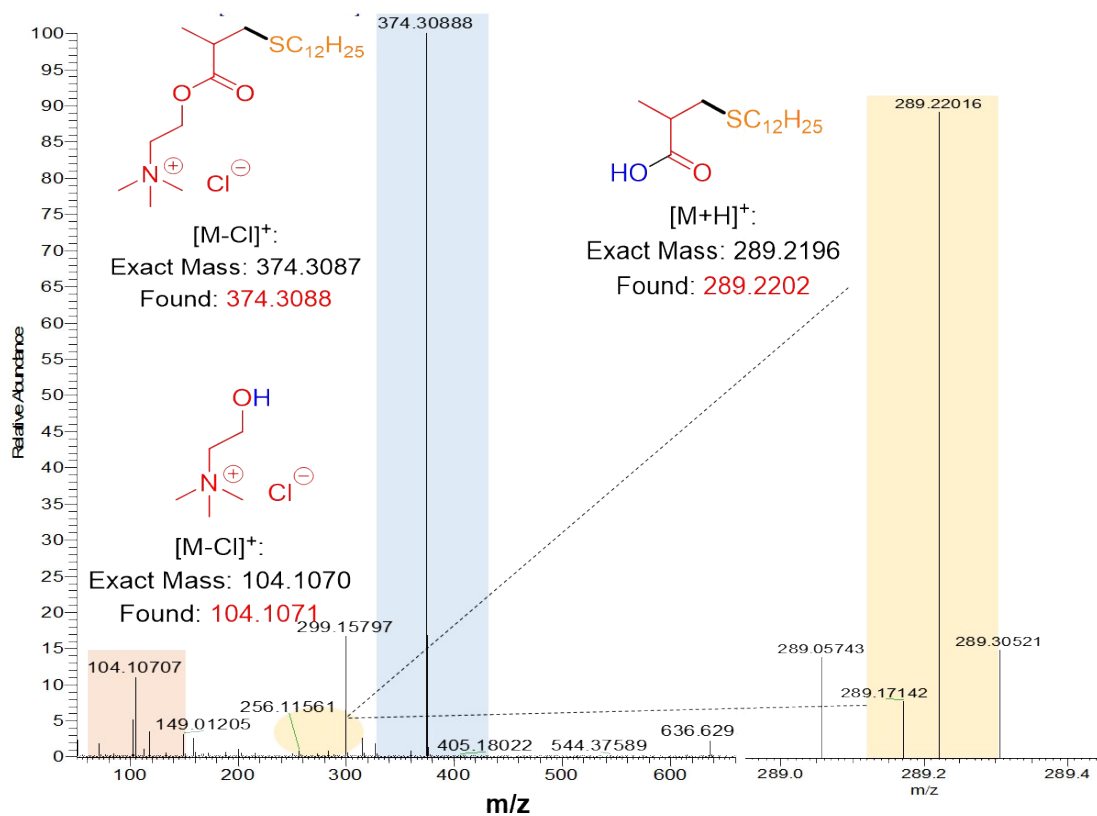


Fig S20. ESI mass spectrum of the degraded product of **3c** in natural water.

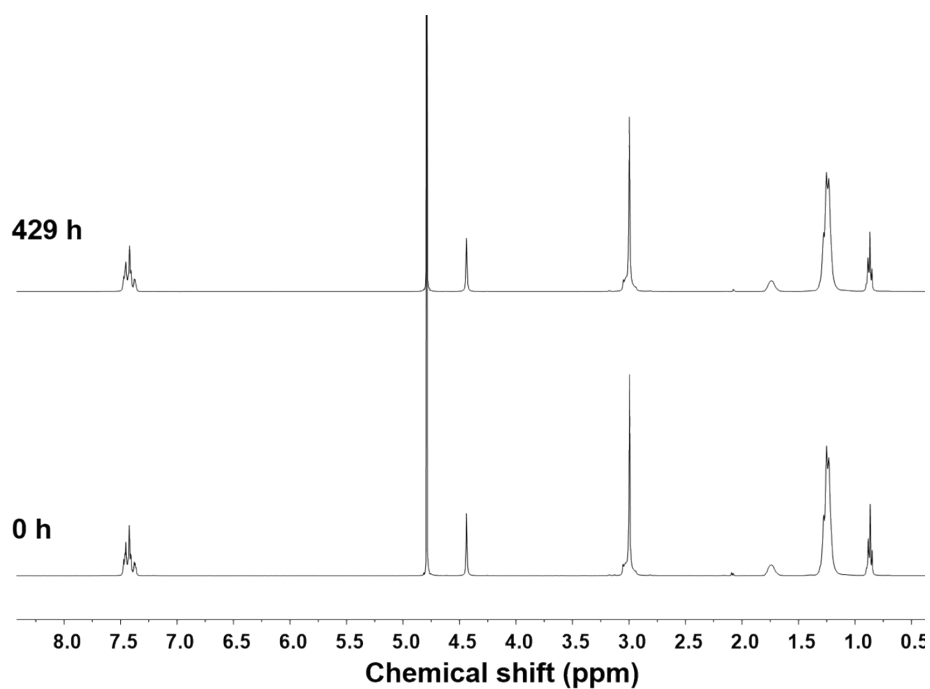


Fig S21. Partial stacked ¹H NMR spectra (400 MHz, D₂O) of benzalkonium chloride in natural (university pond) water (1% wt, pH =7.6, 327 K) measured at 0 h and 429 h. The data show that benzalkonium chloride was stable under experimental condition.

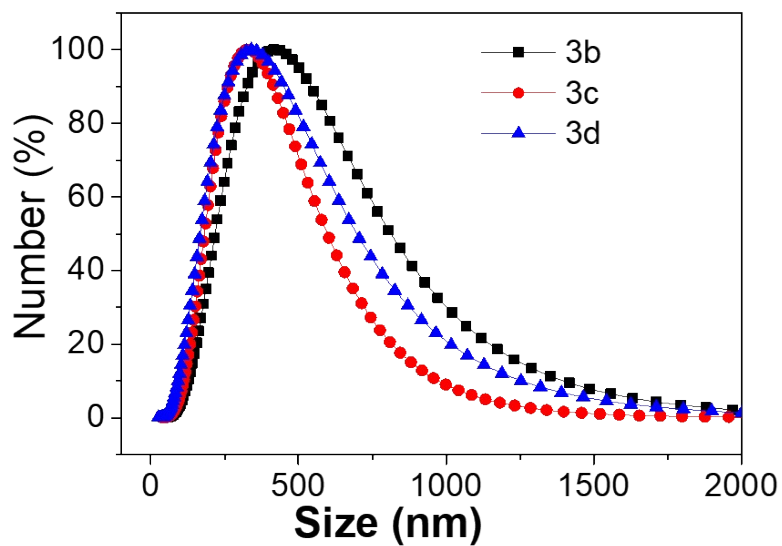


Fig S22. The DLS data of compound **3a** (1mg/mL), **3b** (1mg/mL), **3c** (1mg/mL) in natural water.

Ethanaminium,2-(3-dodecylthio-2-methyl-1-oxopropoxy)-N,N,N-trimethyl-,chloride against *Escherichia coli*

The results	Test serial number	1	2	3
Inhibitor concentration (%) and bacterial growth results	0.1	Sterile growth	Sterile growth	Sterile growth
	0.05	Sterile growth	Sterile growth	Sterile growth
	0.025	Sterile growth	Sterile growth	Sterile growth
	0.0125	Sterile growth	Sterile growth	Sterile growth
	0.00625	Sterile growth	Sterile growth	Sterile growth
	0.003125	Sterile growth	Sterile growth	Sterile growth
	0.0015625	There are bacteria growth	There are bacteria growth	There are bacteria growth
	0.00078125	There are bacteria growth	There are bacteria growth	There are bacteria growth
	0.000390625	There are bacteria growth	There are bacteria growth	There are bacteria growth
	0.0001953125	There are bacteria growth	There are bacteria growth	There are bacteria growth
0.00009765625	There are bacteria growth	There are bacteria growth	There are bacteria growth	
Average colony number of positive control group (cfu/mL)		7.55×10^5	3.60×10^6	5.95×10^5

Note: The negative control group grew aseptically.

Fig S23. Third-party report for the antimicrobial activity of **3c** (0.1% wt, 1 min) against *E. coli*.

Ethanaminium,2-(3-dodecylthio-2-methyl-1-oxopropoxy)-N,N,N-trimethyl-,chloride against *Staphylococcus aureus*

The results	Test serial number	1	2	3
Inhibitor concentration (%) and bacterial growth results	0.1	Sterile growth	Sterile growth	Sterile growth
	0.05	Sterile growth	Sterile growth	Sterile growth
	0.025	Sterile growth	Sterile growth	Sterile growth
	0.0125	Sterile growth	Sterile growth	Sterile growth
	0.00625	Sterile growth	Sterile growth	Sterile growth
	0.003125	Sterile growth	Sterile growth	Sterile growth
	0.0015625	Sterile growth	Sterile growth	Sterile growth
	0.00078125	Sterile growth	Sterile growth	Sterile growth
	0.000390625	Sterile growth	Sterile growth	Sterile growth
	0.0001953125	There are bacteria growth	There are bacteria growth	There are bacteria growth
0.00009765625	There are bacteria growth	There are bacteria growth	There are bacteria growth	
Average colony number of positive control group (cfu/mL)		4.05×10^6	6.90×10^5	8.15×10^5

Note: The negative control group grew aseptically.

Fig S24. Third-party report for antimicrobial activity of **3c** (0.1% wt, 1 min) against *S. aureus*.

Ethanaminium,2-(3-dodecylthio-2-methyl-1-oxopropoxy)-N,N,N-trimethyl-,chloride against *Candida albicans*

The results	Test serial number	1	2	3
Inhibitor concentration (%) and bacterial growth results	0.1	Sterile growth	Sterile growth	Sterile growth
	0.05	Sterile growth	Sterile growth	Sterile growth
	0.025	Sterile growth	Sterile growth	Sterile growth
	0.0125	Sterile growth	Sterile growth	Sterile growth
	0.00625	Sterile growth	Sterile growth	Sterile growth
	0.003125	Sterile growth	Sterile growth	Sterile growth
	0.0015625	Sterile growth	Sterile growth	Sterile growth
	0.00078125	There are bacteria growth	There are bacteria growth	There are bacteria growth
	0.000390625	There are bacteria growth	There are bacteria growth	There are bacteria growth
	0.0001953125	There are bacteria growth	There are bacteria growth	There are bacteria growth
0.00009765625	There are bacteria growth	There are bacteria growth	There are bacteria growth	
Average colony number of positive control group (cfu/mL)		1.15×10^6	8.70×10^5	4.80×10^6

Note: The negative control group grew aseptically.

Fig S25. Third-party report for antimicrobial activity of **3c** (0.1% wt, 1 min) against *C. albicans*.

Ethanaminium,2-(3-dodecylthio-2-methyl-1-oxopropoxy)-N,N,N-trimethyl-,chloride against *Aspergillus Niger*

The results	Test serial number	1	2	3
Inhibitor concentration (%) and bacterial growth results	0.1	Sterile growth	Sterile growth	Sterile growth
	0.05	Sterile growth	Sterile growth	Sterile growth
	0.025	Sterile growth	Sterile growth	Sterile growth
	0.0125	Sterile growth	Sterile growth	Sterile growth
	0.00625	Sterile growth	Sterile growth	Sterile growth
	0.003125	There are bacteria growth	There are bacteria growth	There are bacteria growth
	0.0015625	There are bacteria growth	There are bacteria growth	There are bacteria growth
	0.00078125	There are bacteria growth	There are bacteria growth	There are bacteria growth
	0.000390625	There are bacteria growth	There are bacteria growth	There are bacteria growth
	0.0001953125	There are bacteria growth	There are bacteria growth	There are bacteria growth
0.00009765625	There are bacteria growth	There are bacteria growth	There are bacteria growth	
Average colony number of positive control group (cfu/mL)		7.40×10^5	2.35×10^6	1.40×10^5

Note: The negative control group grew aseptically.

Fig S26. Third-party report for antimicrobial activity of **3c** (0.1% wt, 1 min) against *A. niger*.

Ethanaminium,2-(3-dodecylthio-2-methyl-1-oxopropoxy)-N,N,N-trimethyl-,chloride against *Pseudomonas aeruginosa*

The results		Test serial number	1	2	3
Inhibitor concentration (%) and bacterial growth results		0.1	Sterile growth	Sterile growth	Sterile growth
		0.05	Sterile growth	Sterile growth	Sterile growth
		0.025	Sterile growth	Sterile growth	Sterile growth
		0.0125	There are bacteria growth	There are bacteria growth	There are bacteria growth
		0.00625	There are bacteria growth	There are bacteria growth	There are bacteria growth
		0.003125	There are bacteria growth	There are bacteria growth	There are bacteria growth
		0.0015625	There are bacteria growth	There are bacteria growth	There are bacteria growth
		0.00078125	There are bacteria growth	There are bacteria growth	There are bacteria growth
		0.000390625	There are bacteria growth	There are bacteria growth	There are bacteria growth
		0.0001953125	There are bacteria growth	There are bacteria growth	There are bacteria growth
		0.00009765625	There are bacteria growth	There are bacteria growth	There are bacteria growth
Average colony number of positive control group (cfu/mL)			2.45×10^6	1.80×10^6	9.45×10^5

Note: The negative control group grew aseptically.

Fig S27. Third-party report for the antimicrobial activity of **3c** (0.1% wt, 1 min) against *P. aeruginosa*.

1. 检测项目：病毒灭活试验

1.1 检测方法：参照《消毒技术规范》2002年版

1.2 试验结果：

实验病毒及宿主	作用浓度及时间	组别	病毒滴度对数值 lgTCID ₅₀ /ml	平均病毒滴度对数值 lgTCID ₅₀ /ml	平均病毒总数 TCID ₅₀ /ml	平均灭活对数值 (KL)	病毒灭活率 %
甲型流感病毒 H1N1 宿主名称： Vero-E6 细胞	1:1 稀释 30min	对照组 1	5.57	5.52	3.31×10^5	>4.02	>99.99
		对照组 2	5.52				
		对照组 3	5.56				
		试验组 1	<1.50	<1.50	<31.6		
		试验组 2	<1.50				
		试验组 3	<1.50				

*阴性对照组细胞生长良好，试验结果符合评价规定的全部条件。

Virus/Host cell	sample	Log10 (TCID50/mL)	Mean TCID50/mL	Log10 Reduction	Reduction Rate (%)
H1N1/Vero-E6	control	1	5.57	3.31 x 10 ⁵	>4.02
		2	5.52		
		3	5.56		
	3c	1	<1.5	< 31.6	>99.99
		2	<1.5		
		3	<1.5		

Note: The cultured cells in negative control group were observed growing well.

Fig S28. The virus inactivation study of compound **3c** (0.5% wt, 15 min) against H1N1, with original report in Chinese and translated results.

1. 检测项目：病毒灭活试验

1.1 检测方法：参照《消毒技术规范》2002年版

1.2 试验结果：

实验病毒及宿主	作用浓度及时间	组别	病毒滴度对数值 lgTCID ₅₀ /ml	平均病毒滴度对数值 lgTCID ₅₀ /ml	平均病毒总数 TCID ₅₀ /ml	平均灭活对数值 (KL)	病毒灭活率 %
非洲猪瘟病毒 ASF 宿主名称： Vero-E6 细胞	1:1 稀释 30min	对照组 1	5.59	5.62	4.17×10 ⁵	>4.11	>99.99
		对照组 2	5.61				
		对照组 3	5.67				
		试验组 1	<1.50	<1.50	<31.6		
		试验组 2	<1.50				
		试验组 3	<1.50				

*阴性对照组细胞生长良好，试验结果符合评价规定的全部条件。

Virus/Host cell	sample	Log10 (TCID50/mL)	Mean TCID50/mL	Log10 Reduction	Reduction Rate (%)
ASF/Vero-E6	control	1	5.57	4.17 x 10 ⁵	>4.11
		2	5.59		
		3	5.61		
	3c	1	<1.5	< 31.6	>99.99
		2	<1.5		
		3	<1.5		

Note: The cultured cells in negative control group were observed growing well

Fig S29. The virus inactivation study of compound **3c** (0.5% wt, 30 min) against ASF, with original report in Chinese and translated results.

2. Detailed synthetic procedures for degradation products **5a**, **5b**, **5c**, and **5d** used

for antimicrobial test control group.

The obtained QACs (**3a-3d**) (25 mmol) without further purification were dissolved in water or mixture of water and ethanol in 100 mL round-bottle, then a NaOH (25 mmol, 5 mol/L in water) solution was added to the each QAC solution. The mixtures were stirred at 333 K for ca. 6 hours. Then the pH was lowered to 1-2 with a dropwise addition of HCl (12 M). The sulfide was extracted with EtOAc (30 mL×3). The organic layer was dried over anhydrous MgSO₄, filtered, and concentrated in vacuo. After evaporation, the residue was purified by chromatography on silica gel to afford the degraded product (eluent: petroleum ether/ethyl acetate : 20/1 to 5/1) .

5a, 75 %, light yellow oil, ¹H NMR (400 MHz, CHCl₃-d₁) 2.86 (dd, ²J_{H,H} = 13Hz, ³J_{H,H} = 7Hz, 1H), 2.70 (ddq, ²J_{H,H} = 13Hz, ³J_{H,H} = 7Hz, ³J_{H,H} = 7Hz, 1H), 2.59 (dd, ²J_{H,H} = 13Hz, ³J_{H,H} = 7Hz, 1H), 2.54 (t, ³J_{H,H} = 7Hz, 2H), 1.29 (d, ³J_{H,H} = 7Hz, 3H) , 1.25 (³J_{H,H} = 7Hz, 3H). ¹³CNMR (101 MHz, CHCl₃-d₁) 181.9, 40.2, 34.7, 26.5, 16.7, 14.7. HRMS (ESI+): calculated: 149.0631; found: 149.0629.

5b, 67%, white solid, ¹H NMR (400 MHz, CHCl₃-d₁) 2.85 (dd, ²J_{H,H} = 13Hz, ³J_{H,H} = 7Hz, 1H), 2.69 (ddq, ²J_{H,H} = 13Hz, ³J_{H,H} = 7Hz, ³J_{H,H} = 7Hz, 1H), 2.57 (dd, ²J_{H,H} = 13Hz, ³J_{H,H} = 7Hz, 1H), 2.51 (t, ³J_{H,H} = 7Hz, 2H), 1.56 (m, 2H), 1.37-1.25 (m, 17H) , 0.87 (³J_{H,H} = 7Hz, 3H). ¹³CNMR (101 MHz, CHCl₃-d₁) 181.9, 40.3, 35.2, 32.8, 32.0, 29.7(1), 29.6(8). 29.6(5), 29.4, 29.3, 29.0, 22.8, 16.7, 14.2. HRMS (ESI+): calculated: 261.1883; found: 261.1880.

5c, 70%, white solid, ¹H NMR (400 MHz, CHCl₃-d₁) 2.85 (dd, ²J_{H,H} = 13Hz, ³J_{H,H} = 7Hz, 1H), 2.70 (ddq, ²J_{H,H} = 13Hz, ³J_{H,H} = 7Hz, ³J_{H,H} = 7Hz, 1H), 2.58 (dd, ²J_{H,H} = 13Hz, ³J_{H,H} = 7Hz, 1H), 2.52 (t, ³J_{H,H} = 7Hz, 2H), 1.57 (m, 2H), 1.42-1.25 (m, 21H) , 0.88 (³J_{H,H} = 7Hz, 3H). ¹³CNMR (101 MHz, CHCl₃-d₁) 181.9, 40.3, 35.2, 32.9, 32.0, 29.7(9), 29.7(7), 29.7(4), 29.7(3), 29.6(6), 29.5, 29.4, 29.0, 22.8, 16.8, 14.3. HRMS (ESI+): calculated: 289.2196; found: 289.2186.

5d, 68%, white solid, ^1H NMR (400 MHz, CHCl_3-d_1) 2.86 (dd, $^2J_{\text{H,H}} = 13\text{Hz}$, $^3J_{\text{H,H}} = 7\text{Hz}$, 1H), 2.70 (ddq, $^2J_{\text{H,H}} = 13\text{Hz}$, $^3J_{\text{H,H}} = 7\text{Hz}$, $^3J_{\text{H,H}} = 7\text{Hz}$, 1H), 2.58 (dd, $^2J_{\text{H,H}} = 13\text{Hz}$, $^3J_{\text{H,H}} = 7\text{Hz}$, 1H), 2.53 (t, $^3J_{\text{H,H}} = 7\text{Hz}$, 2H), 1.57 (m, 2H), 1.42-1.25 (m, 25H), 0.88 ($^3J_{\text{H,H}} = 7\text{Hz}$, 3H). ^{13}C NMR (101 MHz, CHCl_3-d_1) 181.9, 40.3, 35.2, 32.8, 32.0, 29.8(2), 29.8(1), 29.7(8), 29.7(3), 29.7(1), 29.6(5), 29.5, 29.0, 22.8, 16.8, 14.2. HRMS (ESI+): calculated: 234.1522; found: 234.1516.

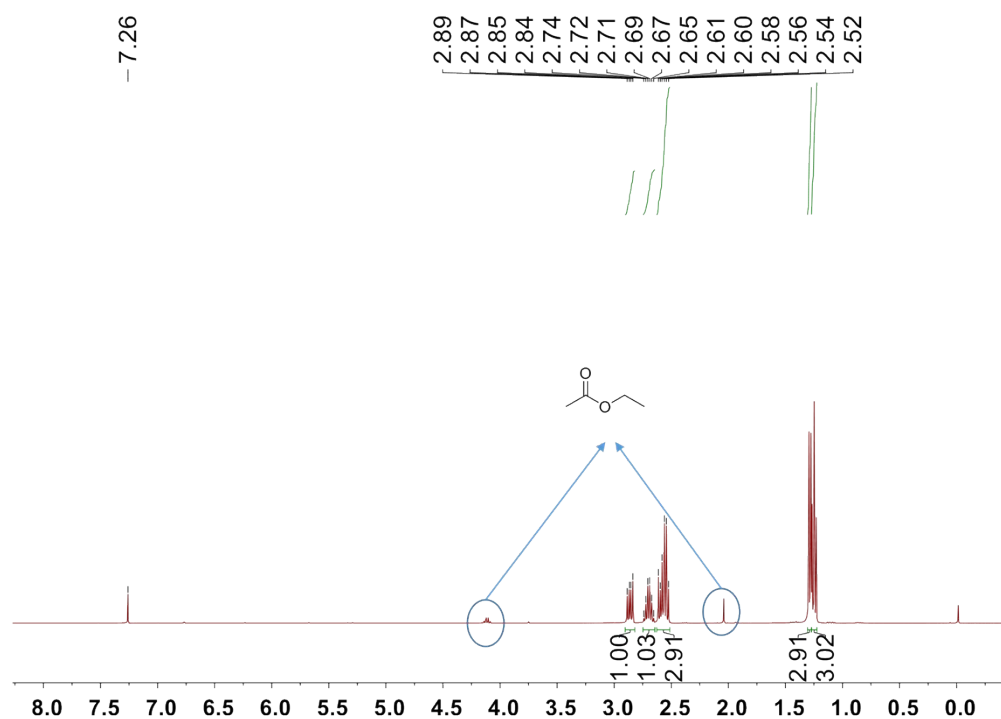


Fig S30. ^1H NMR spectrum of compound **5a** in CDCl_3 .

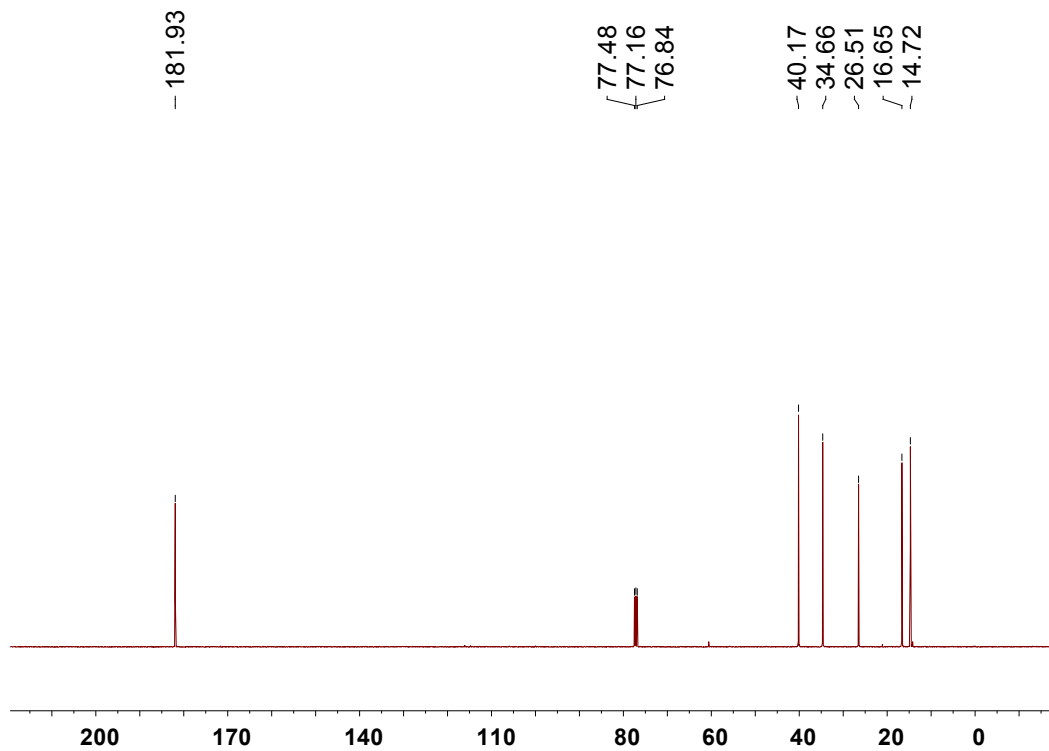


Fig S31. ^{13}C NMR spectrum of compound **5a** in CDCl_3 .

20210623HESI+2XL-5a #30 RT: 0.42 AV: 1 NL: 5.84E7
T: FTMS + c ESI Full ms [50.00-800.00]

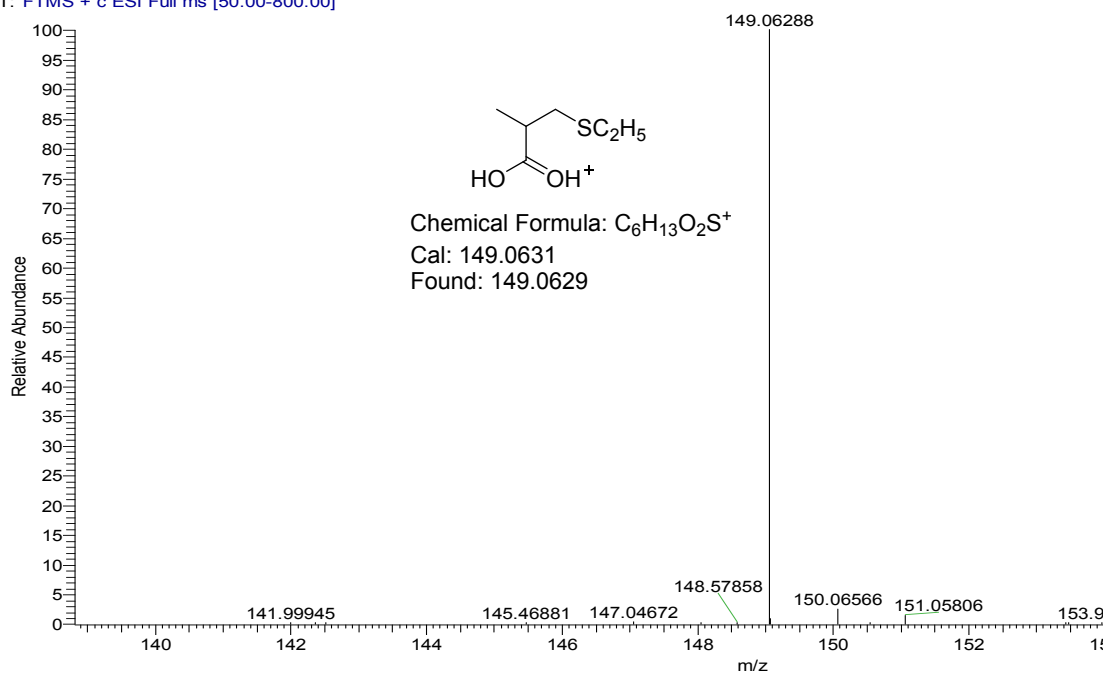


Fig S32. ESI mass spectrum of compound **5a**.

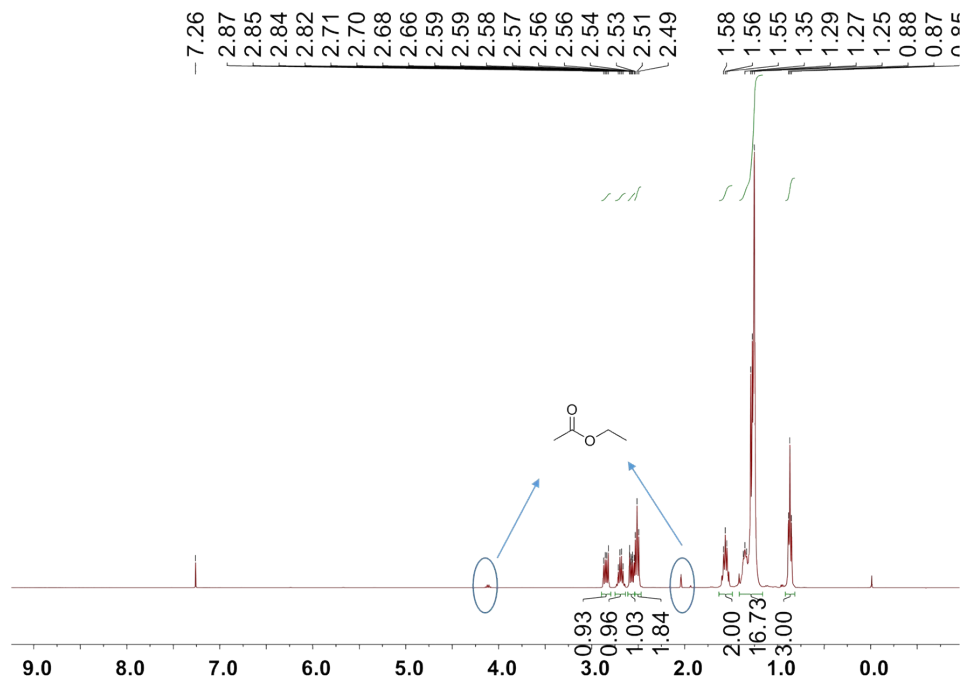


Fig S33. ^1H NMR spectrum of compound **5b** in CDCl_3 .

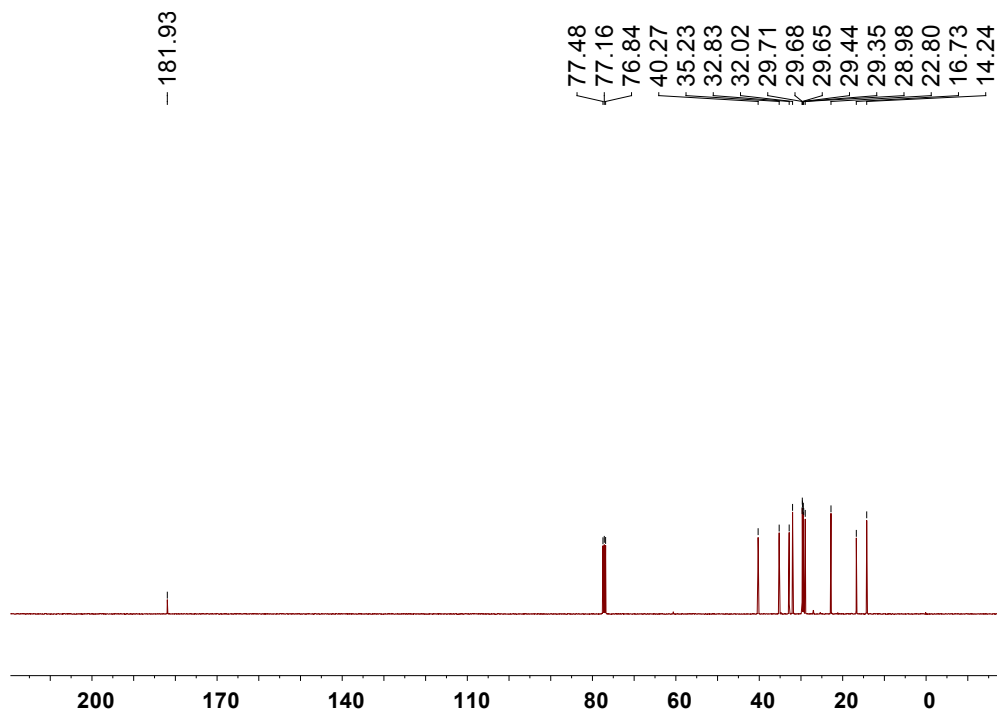


Fig S34. ^{13}C NMR spectrum of compound **5b** in CDCl_3 .

20210623HESI+2XL-5b #44 RT: 0.62 AV: 1 SB: 1 0.03 NL: 1.96E6
T: FTMS + c ESI Full ms [50.00-800.00]

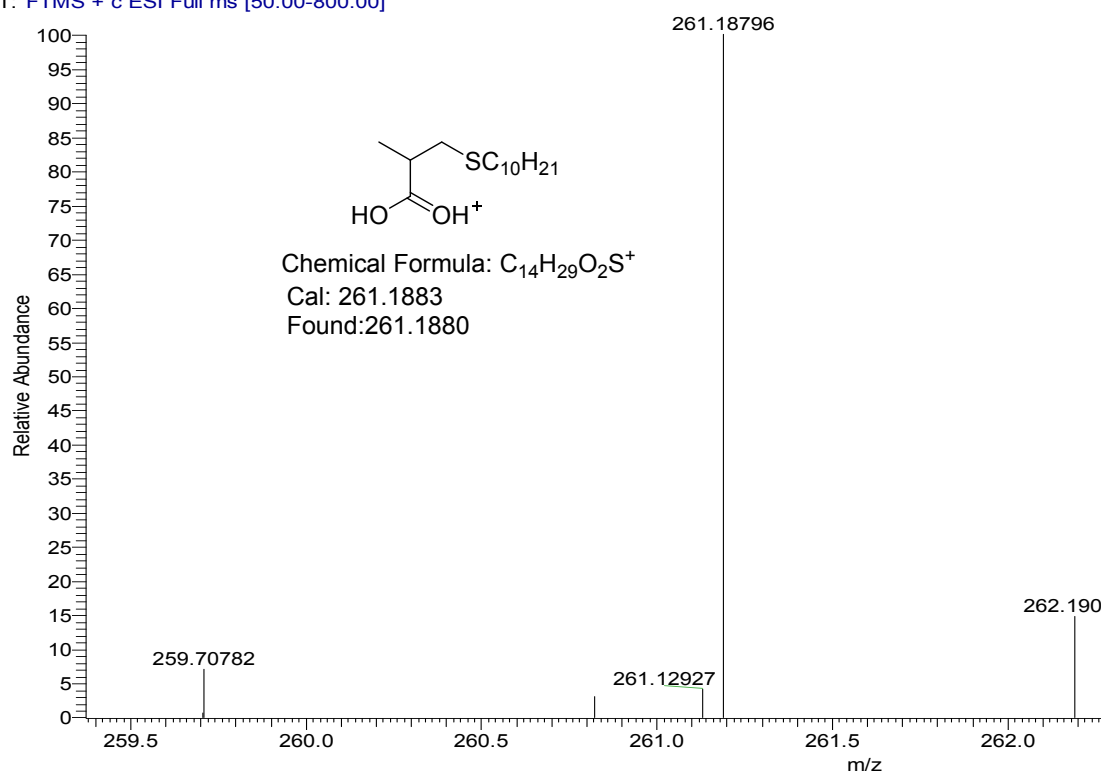


Fig S35. ESI mass spectrum of compound 5b.

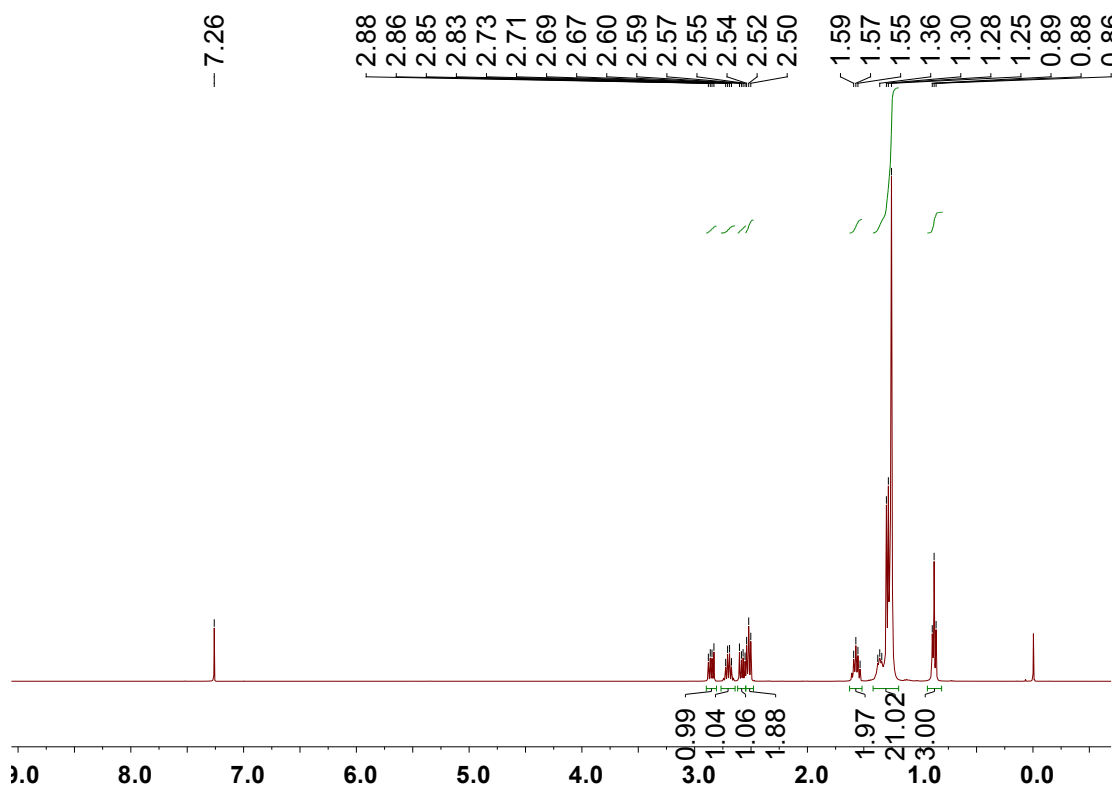


Fig S36. 1H NMR spectrum of compound 5c in $CDCl_3$.

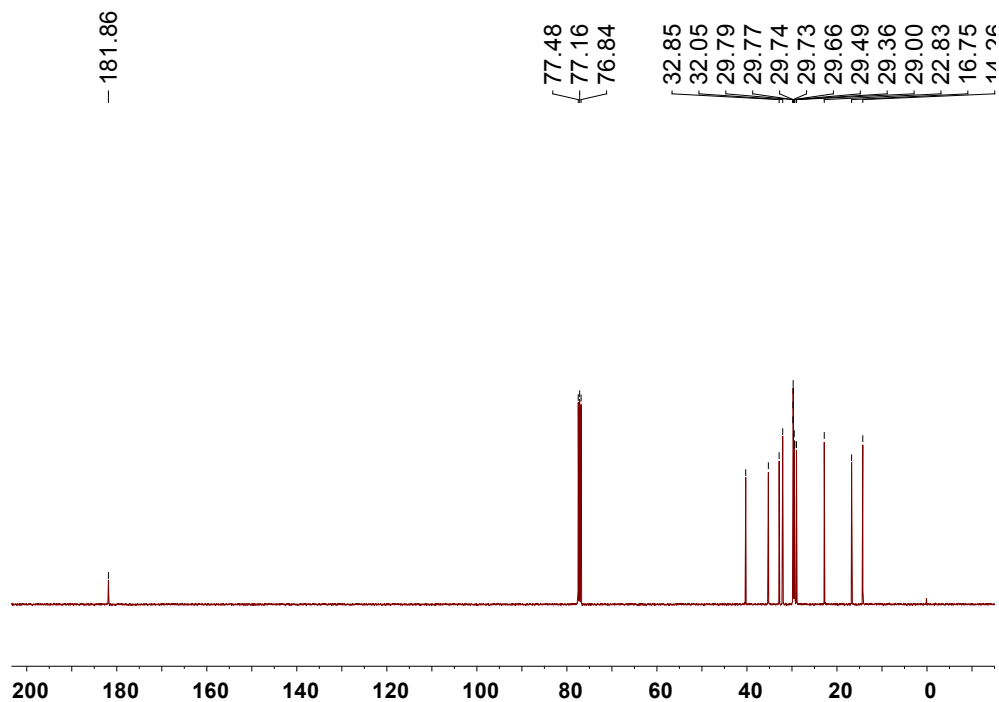


Fig S37. ^{13}C NMR spectrum of compound **5c** in CDCl_3 .

20210623HESI+2XL-5c #25-27 RT: 0.34-0.37 AV: 3 SB: 1 0.03 NL: 4.85E5
 T: FTMS + c ESI Full ms [50.00-800.00]

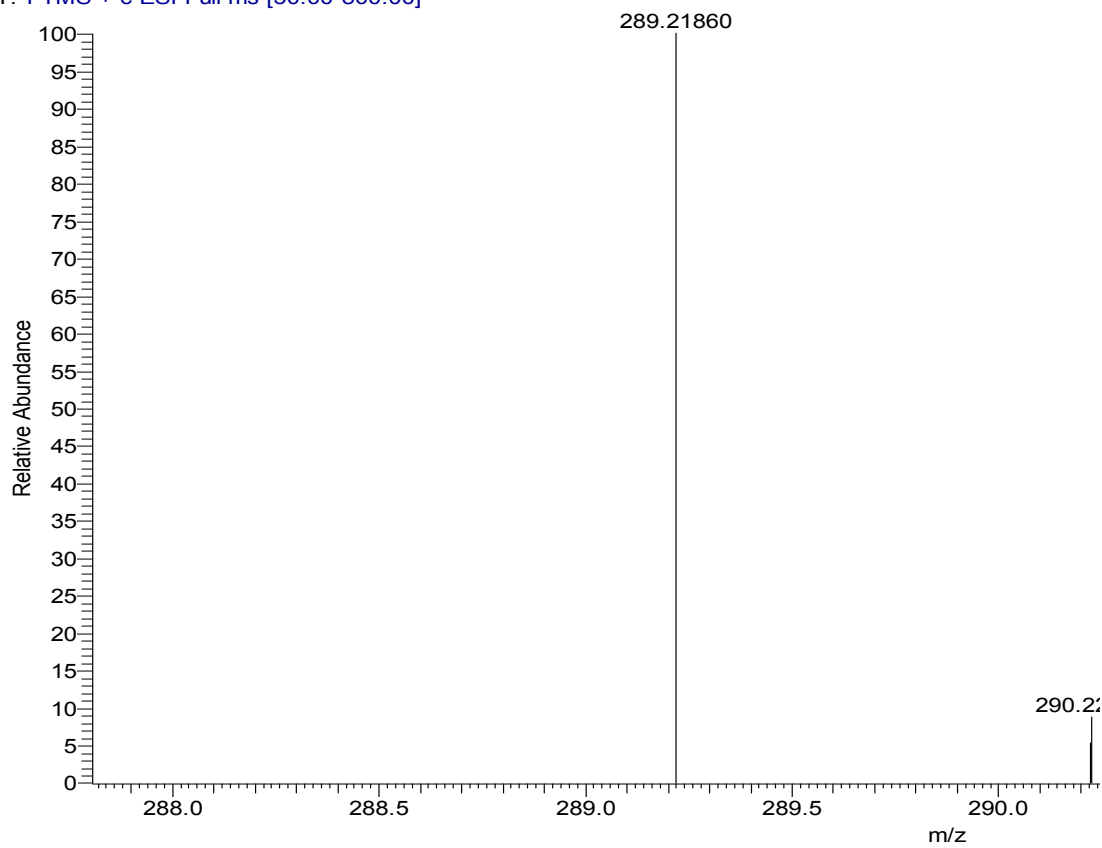


Fig S38. ESI mass spectrum of compound **5c**.

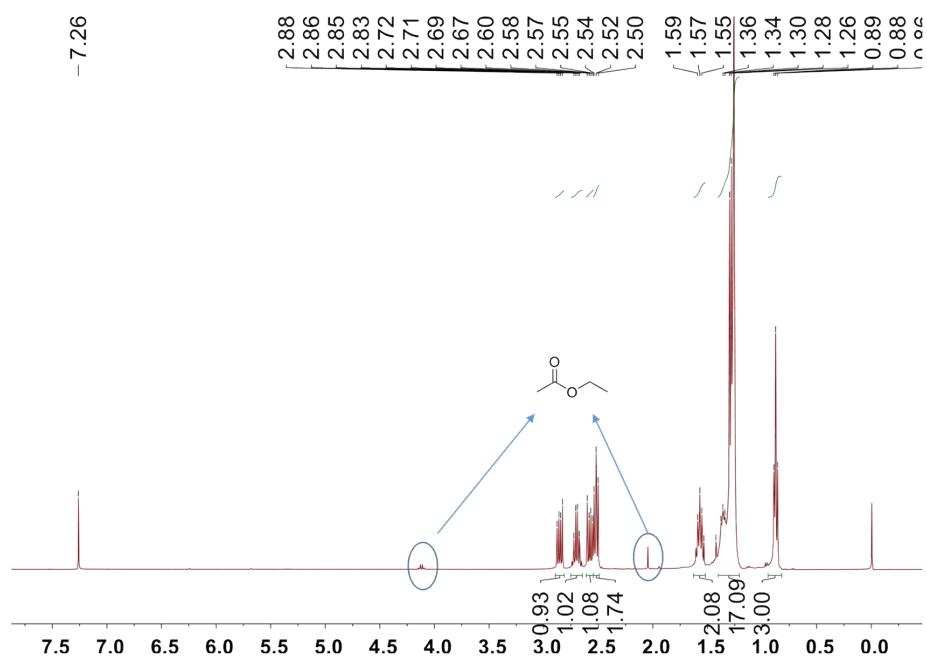


Fig S39. ^1H NMR spectrum of compound **5d** in CDCl_3 .

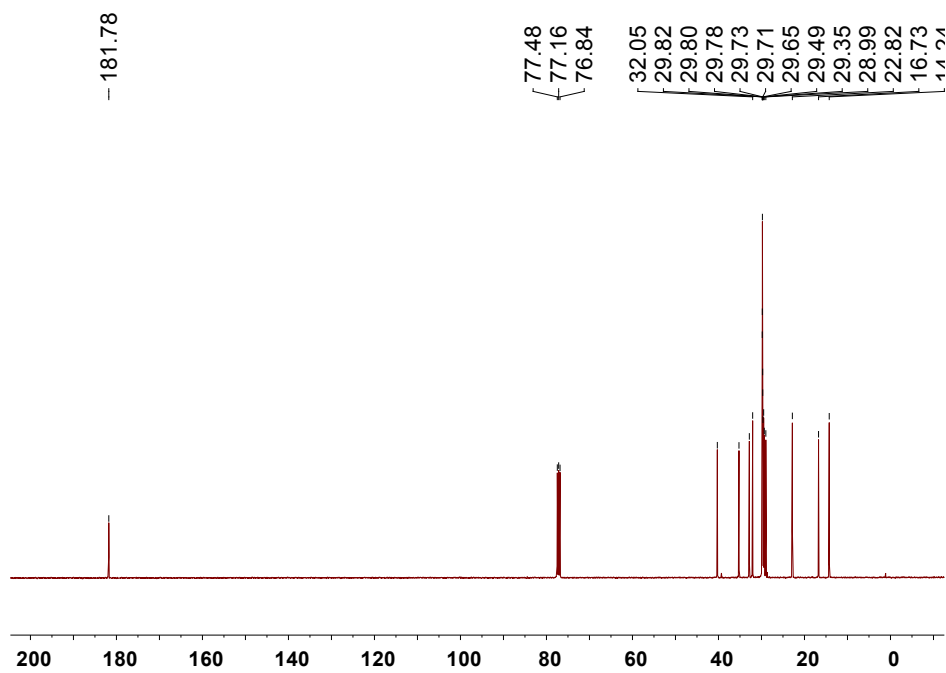


Fig S40. ^{13}C NMR spectrum of compound **5d** in CDCl_3 .

20210623HESI+2XL-5d #47 RT: 0.66 AV: 1 SB: 1 0.03 NL: 7.70E5
 F: FTMS + c ESI Full ms [50.00-800.00]

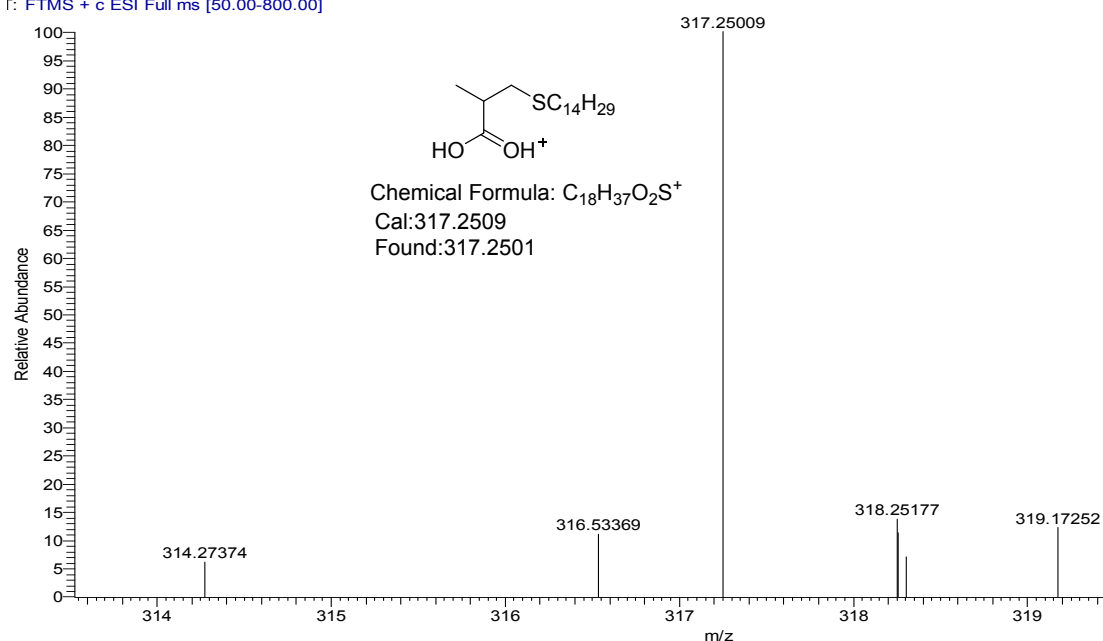


Fig S41. ESI mass spectrum of compound **5d**.

Table S1. The antimicrobial activities of degradation products **4**, **5a**, **5b**, **5c**, and **5d** against *E. coli*, and *S. aureus*.

Compound (Concentration) +Time	Bacteria	Sample	Control (CFU/mL)	Treated (CFU/mL)	Reduction Rate (%)
4 (0.1%) + 5 min	<i>E. Coli</i>	1	3.4×10^8	2.9×10^8	14.7
		2	2.5×10^8	1.1×10^8	56
	<i>S. aureus</i>	1	6.6×10^7	5.4×10^7	18.2
		2	5.7×10^7	3.2×10^7	43.9
5a (0.1%) + 5min	<i>E. Coli</i>	1	1.8×10^8	1.6×10^8	11.1
		2	3.6×10^8	3.5×10^8	2.8
	<i>S. aureus</i>	1	3.3×10^7	2.5×10^7	24.2
		2	3.6×10^7	2.1×10^7	41.7
5b(0.1%) + Dodecyl D- glucoside (0.1%) + 5 min	<i>E. Coli</i>	1	2.6×10^8	1.4×10^8	46.2
		2	2.3×10^8	1.2×10^8	47.8
	<i>S. aureus</i>	1	6.3×10^7	3.2×10^7	49.2

			2	4.2x10 ⁷	3.1x10 ⁷	26.2	
5c(0.1%) Dodecyl D- glucoside (0.1%) + 5 min	+	<i>E. Coli</i>	1	1.5x10 ⁸	1.3x10 ⁸	13.3	
			2	1.8x10 ⁸	1.6x10 ⁸	11.1	
			<i>S.aureus</i>	1	5.5x10 ⁷	2.8x10 ⁷	49.1
				2	7.2x10 ⁷	3.1x10 ⁷	56.9
5d(0.1%) Dodecyl D- glucoside (0.1%) + 5min	+	<i>E. Coli</i>	1	2.3x10 ⁸	1.2x10 ⁸	47.8	
			2	3.2x10 ⁸	3.1x10 ⁸	3.1	
			<i>S.aureus</i>	1	6.5x10 ⁷	2.9x10 ⁷	55.4
				2	6.3x10 ⁷	3.1x10 ⁷	50.8
Dodecyl D- glucoside (0.1%) + 5 min		<i>E. Coli</i>	1	1.9x10 ⁸	1.6x10 ⁸	15.8	
			2	2.1x10 ⁸	2.0x10 ⁸	4.8	
			<i>S.aureus</i>	1	5.2x10 ⁷	1.6x10 ⁷	69.2
				2	4.8x10 ⁷	3.9x10 ⁷	18.8

Table S2. The acute oral toxicity study of compound **3c** in rats.

Sex	Dose (mg/kg)	Body Weight (g)			Death
		Day 0	Day 7	Day 14	
Male (n =10)	5000	20.8 ± 1.2	20.8 ± 1.2	20.8 ± 1.2	0
Female(n =10)	5000	20.8 ± 1.2	20.8 ± 1.2	20.8 ± 1.2	0

Reference:

(1) Farley, A. J. M.; Sandford, C.; Dixon, D. J. *J. Am. Chem. Soc.*, 2015, **137**, 15992-15995.