

Fig. S1 ^1H NMR spectrum of the purified C16-4S-5OH monohydrate.

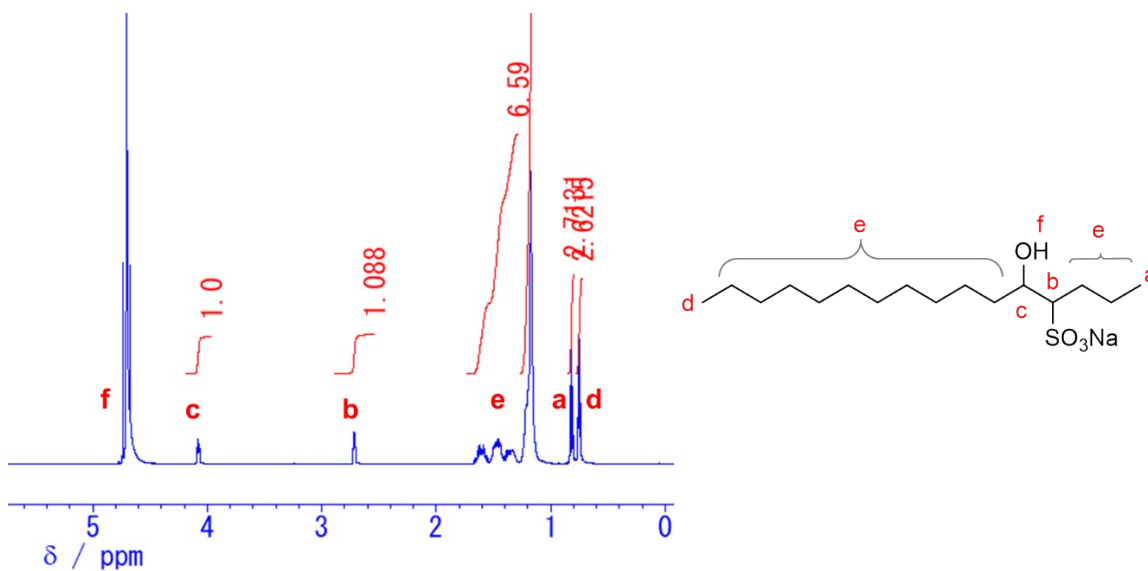


Fig. S2 LC-MS/MS Spectrum of the purified C16-4S-5OH monohydrate

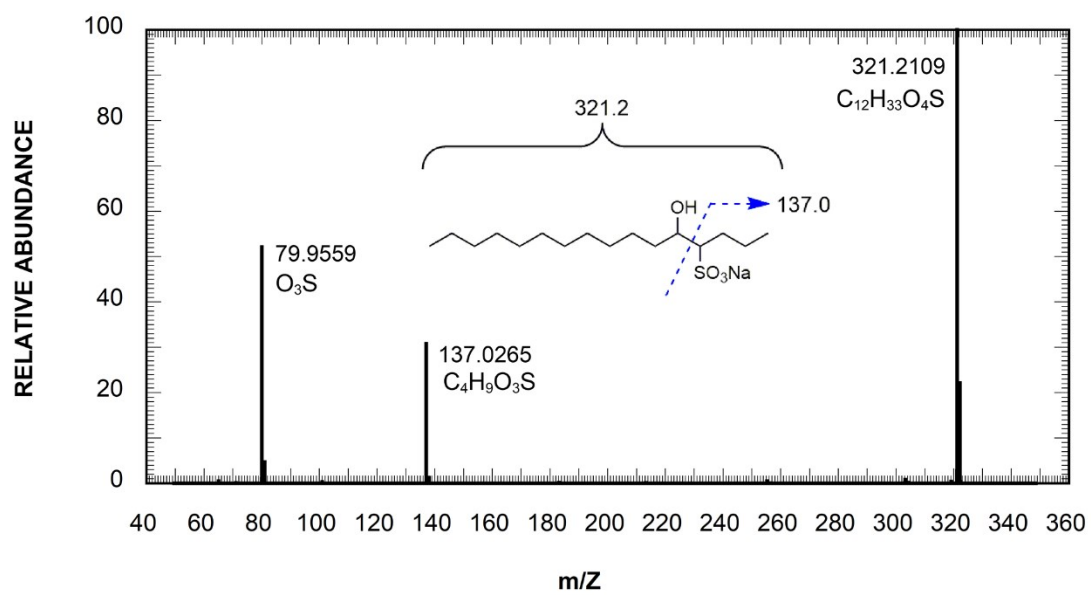


Table S1 Elemental analysis results for the purified C16-4S-5OH monohydrate

Chemical Formula: $C_{16}H_{33}O_4SNa \cdot H_2O$

Molecular Weight: 362.47

| Calculated: | C | H | N | O | S | Na |
|--------------------|------|-----|------|------|-----|-----|
| Number | 16 | 35 | 0 | 5 | 1 | 1 |
| wt% | 53.0 | 9.7 | 0.0 | 22.1 | 8.8 | 6.3 |
| Measured: | | | | | | |
| wt% | 52.4 | 9.6 | <0.3 | 22.5 | 8.8 | 6.2 |

Experimental:

C, H, N analysis. These analyses were performed using a CHN Corder MT-6 (Yanako Technical Science, Japan) with the sample, ignition and absorption zones set at 950, 850 and 500 °C, respectively.

O analysis. These analyses were performed using a varioEL III (Elementar, Germany) with the ignition zone set at 1150 °C.

S analysis. The sample was first decomposed by ignition and the gaseous products were collected in an aqueous H_2O_2 solution. After the gas volume was determined, the SO_4^{2-} concentration was measured by ion chromatography using an ICS-6000 instrument (Thermo-Fischer Scientific Inc., USA).

Na analysis. The sample was heated to ash and then dissolved in dilute HNO_3 , after which the Na concentration was determined using a 730-ES inductively coupled plasma optical emission spectroscopy apparatus (Varian Inc., USA).