

Supplementary Information

Fructose controlled ionophoric activity of a cholate-boronic acid

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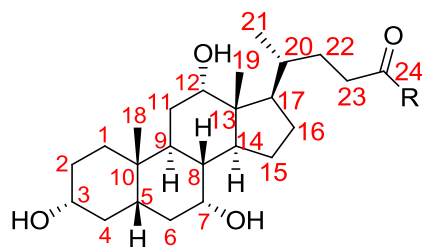
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S1: ^1H NMR and ^{13}C data for compound 3.

For the purposes of spectral assignment the steroid skeleton was assigned as follows:



The phrase ‘steroid protons’ refers to the overlapping resonances due to methylene groups at the 1, 2, 4, 6, 11, 15, 16, 22 and 23 positions and methine groups at the 5, 8, 9, 14, 17 and 20 positions.

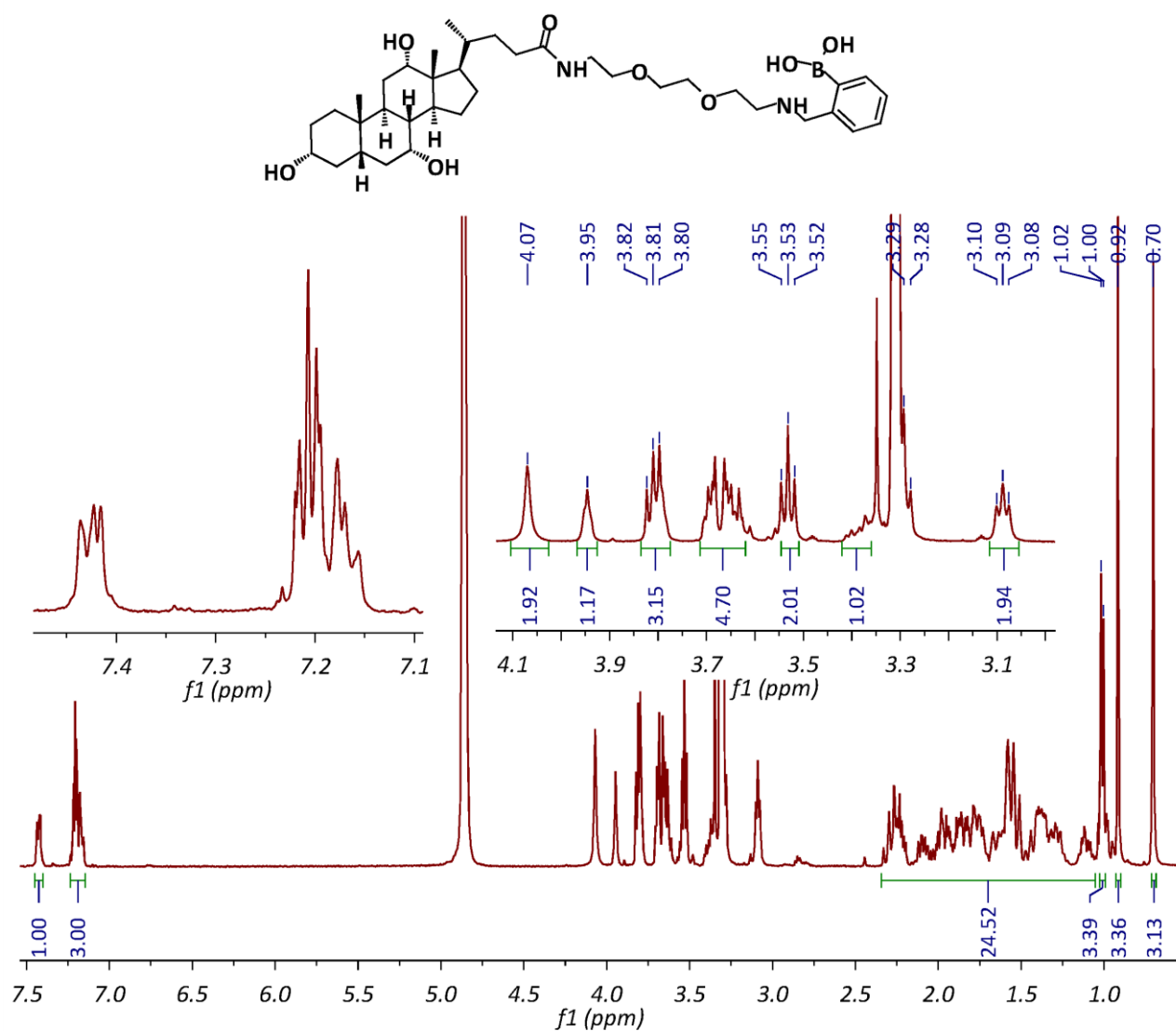
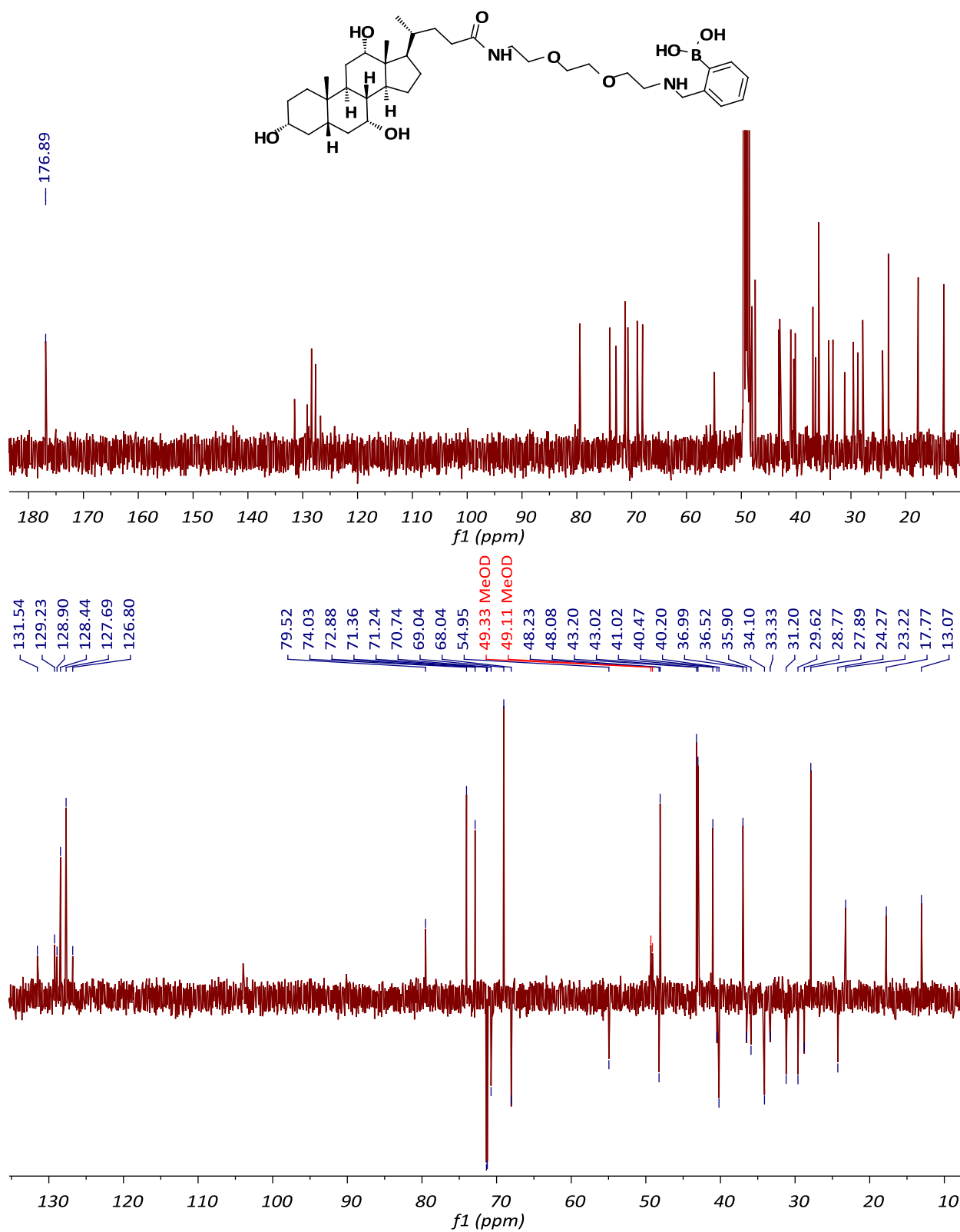


Figure S1. ^1H NMR (400 MHz) of 3 in MeOH-d_4 .

Figure S2. ^{13}C NMR (100 MHz) of 3 in MeOH-d_4

S2: Control experiment for ion transport by cholic acid **4** in the presence of 2.5 mM fructose.

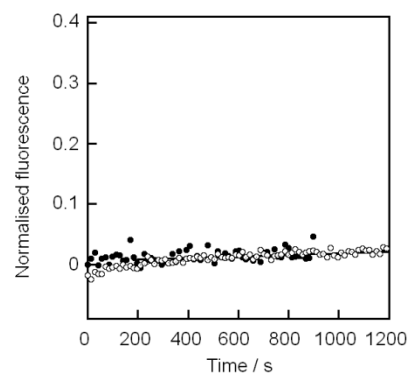


Figure S3. Transport of sodium ions across EYPC/cholesterol bilayers by cholic acid **4** ($10\ \mu\text{M}$) in the presence (empty circles) or absence (filled circles) of D-fructose (2.5 mM). Curve fits of methanol blanks have been subtracted.

S3: Ion transport by **3 in the presence of fructose.**

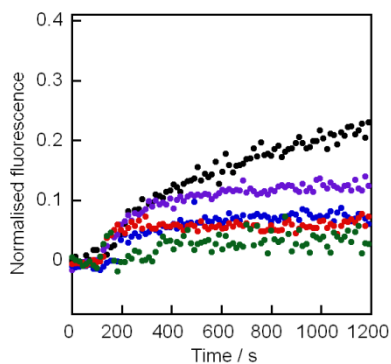


Figure S4. Transport of sodium ions across EYPC/cholesterol bilayers by cholate **3** ($10 \mu\text{M}$) in the presence of D-fructose at 0 mM (black circles), 2.5 mM (purple circles), 5 mM (blue circles), 10 mM (red circles) and 100 mM (green circles). Curve fits of methanol blanks have been subtracted.

S4: U-tube sodium picrate transport experiments.

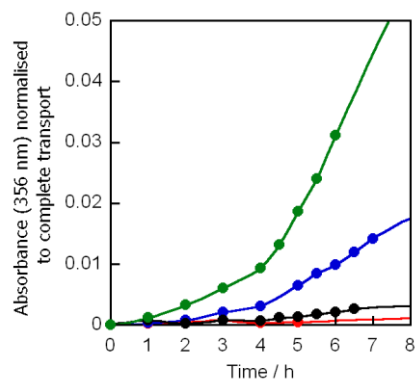


Figure S5. Time course of sodium picrate transport for 1 mM of: **2** (black, •); **3** (blue, •); cholic acid **4** (red, •); dibenzo-18-crown-6 (DB18C6 green, •).

Boronic acid **3** (1 mM) transported sodium picrate into the receiving phase at a rate comparable to DB18C6 (using $\epsilon = 15911 \text{ M}^{-1}\text{cm}^{-1}$, rates were up to $2.0 \times 10^{-10} \text{ molL}^{-1}\text{s}^{-1}$ and $6.6 \times 10^{-10} \text{ molL}^{-1}\text{s}^{-1}$ respectively). Cholate **4**, lacking the boronic acid, was unable to transport sodium through the organic phase (rates $\sim 0.1 \times 10^{-10} \text{ molL}^{-1}\text{s}^{-1}$). Boronic acid **2** was also relatively ineffective (rate up to $0.4 \times 10^{-10} \text{ molL}^{-1}\text{s}^{-1}$).

A significant lag period was observed due to slow diffusion through the chloroform phase under our experimental conditions. See A. Giannetto, S. Lanza, F. Puntoriero, M. Cordaro and S. Campagna, *Chem. Commun.*, 2013, **49**, 7611–7613. For both of the boronic acids **2** and **3**, a marked slowing of the rate of sodium picrate transport was observed at 24 h, which may be due to protodeboronation of the compounds. The maximum extent of transport after 24 hours was 3% for boronic acid-cholate conjugate **3**, 0.6% for **2**, 0.6% for cholic acid **4**, and 28% for dibenzo-18-crown-6.

S5: HPTS assays of K⁺ ion transport.

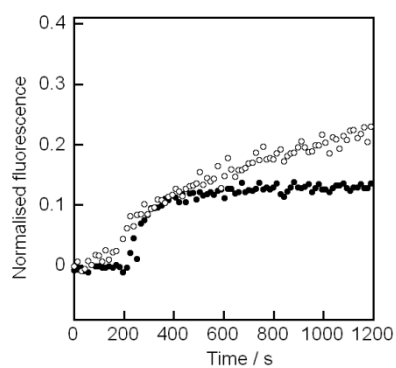


Figure S6. Transport of either potassium ions across EYPC bilayers (filled circles) or sodium ions across EYPC/cholesterol bilayers (empty circles) by cholate boronic acid **3** (10 μ M). Curve fits of methanol blanks have been subtracted.