Electronic Supplementary Information

for

A folding decalin tetra-urea for transmembrane anion transport

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1. NMR spectra of amine 8

**Figure S1.** $^1$H NMR spectrum of amine 8 in DMSO-d$_6$ (400 MHz).

**Figure S2.** $^{13}$C NMR spectrum of amine 8 in DMSO-d$_6$ (101 MHz).
Figure S3. HSQC spectrum of amine 8 in DMSO-d$_6$ (400 MHz).

Figure S4. HMBC spectrum of amine 8 in DMSO-d$_6$ (400 MHz).
Figure S5. $^{19}$F spectrum of amine 8 in DMSO-$d_6$ (377 MHz).
2. NMR spectra of decalin tetra-urea 7

**Figure S6.** $^1$H NMR spectrum of 7 in DMSO-$d_6$ (500 MHz).

**Figure S7.** $^{19}$F spectrum of 7 in DMSO-$d_6$ (377 MHz).
Figure S8. $^{13}$C NMR spectra of 7 in DMSO-$d_6$ (126 MHz).
Figure S9. HSQC spectra of 7 in DMSO-d$_6$ (500 MHz).
Figure S10. HMBC spectra of 7 in DMSO-d$_6$ (500 MHz).
Figure S11. 2D NOESY spectrum of 7 in DMSO-d$_6$ (500 MHz).

Figure S12. 2D COSY spectrum of 7 in DMSO-d$_6$ (500 MHz).
Figure S13. 2D COSY spectra of 7 in DMSO-d₆ (500 MHz).
Figure S14. $^1$H NMR spectrum of 7 in DMSO-d$_6$ (top; 600 MHz) and 1D ROESY spectrum of 7 in DMSO-d$_6$ with NH$^d$ inverted (bottom; 600 MHz).
3. Additional anion transport data and graphs

Figure S15. Comparison of the rates of anion transport by 7 with that of previously reported compounds 1a-c. All compounds were preincorporated at a transporter to lipid ratio of 1:2500 in liposomes composed of POPC and cholesterol (7:3, 0.4 mM total lipid concentration), containing lucigenin. NaNO$_3$ (225 mM) was present both inside and outside of the liposomes and the transport measurement was initiated by addition of a pulse of NaCl (25 mM).
Figure S16. Comparison of the rates of anion transport by 7 in the presence of different anions. Carrier 7 was preincorporated at a transporter to lipid ratio of 1:1000 in liposomes composed of POPC and cholesterol (7:3), containing lucigenin. Either NaNO$_3$ (225 mM), or NaHCO$_3$ (225 mM) or K$_2$SO$_4$ (225 mM) was present both inside and outside of the liposomes. The observed trends are similar as those previously found for decalin bis-ureas.$^{1,3}$

References