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Supporting Information

Structural and Functional Implications of the Interaction between Macrolide Antibiotics and Bile Acids

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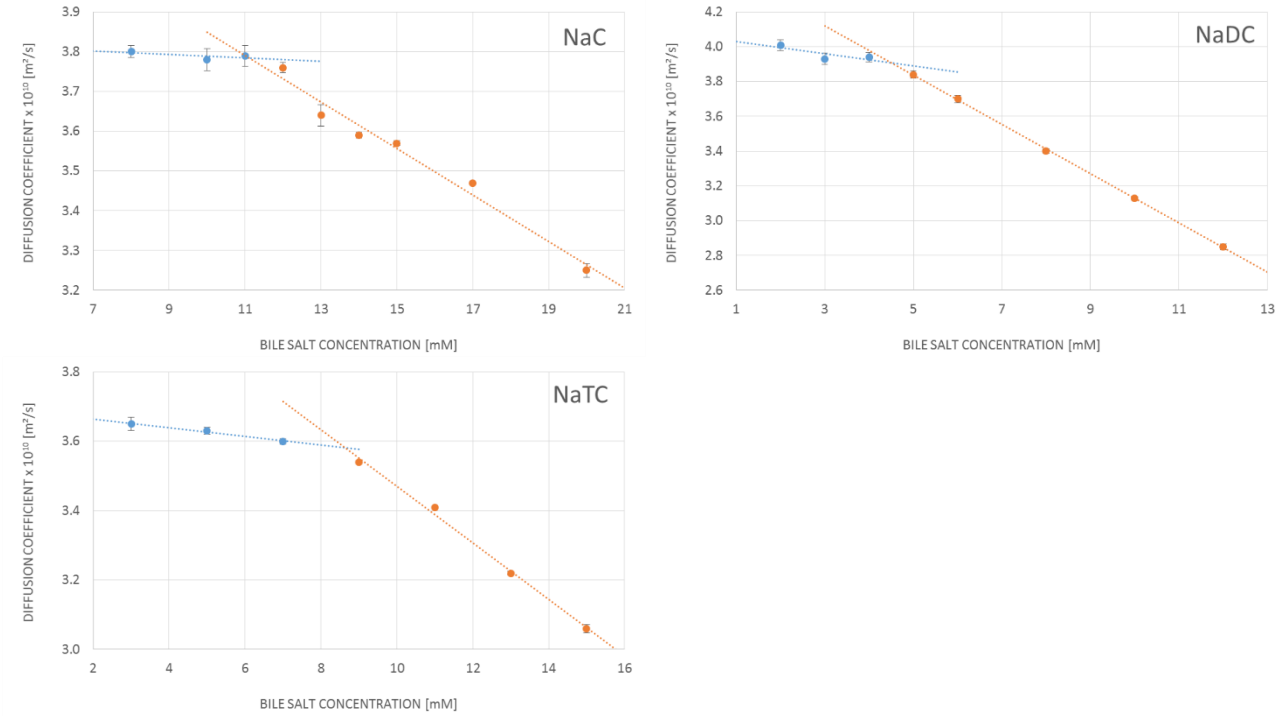
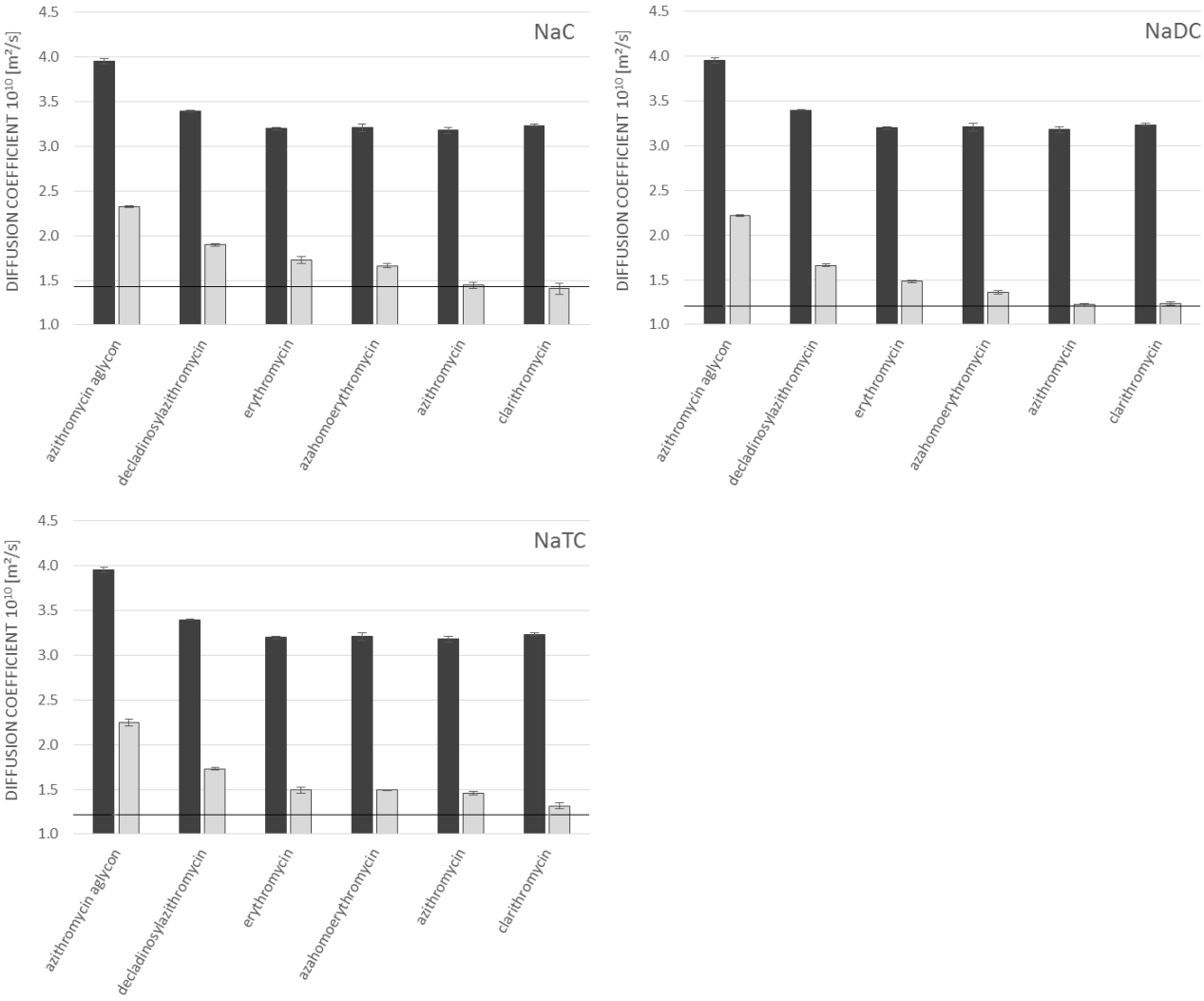
Supporting Figure 1:



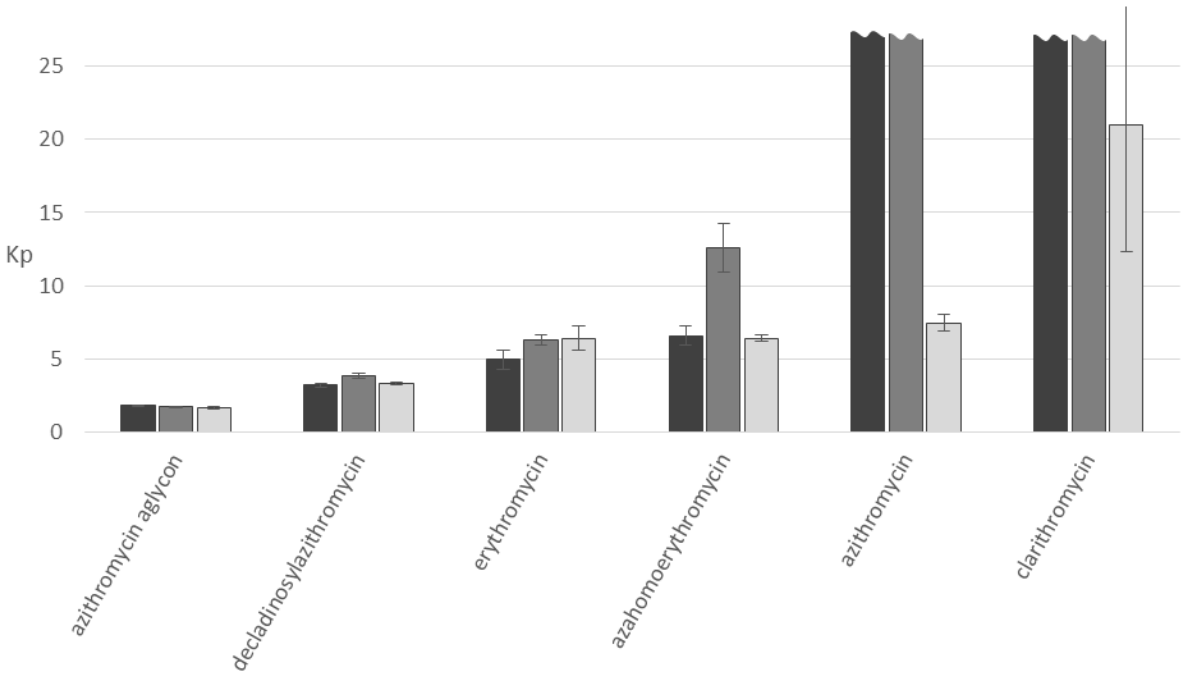
Supporting Figure 1. Diffusion values above (red) and below (blue) the cmc in pure D_2O. The point of intersection represents the cmc of NaC (~ 11 mM), NaDC (~ 4 mM) and NaTC (~ 9 mM).

Supporting Figure 2:



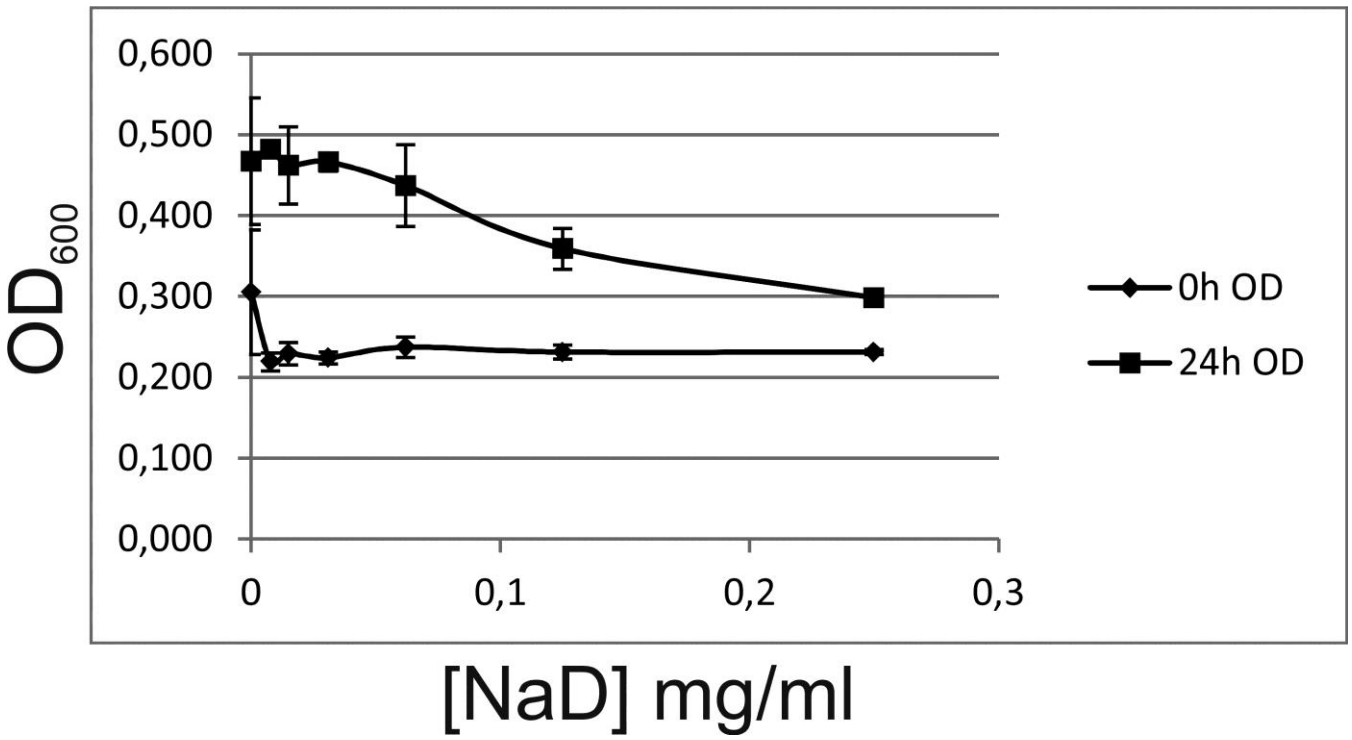
Supporting Figure 2. Diffusion coefficients of free antibiotic (black) and in bile salt (grey) in pure D_2O. The horizontal line represents the micellar diffusion D_{mic}.

Supporting Figure 3:



Supporting Figure 3. Black: NaC, dark grey: NaDC, light grey: NaTC in pure D_2O. Mole fraction partition coefficients beyond ~ 40 are ill-defined and indicated by the wave-shaped ends.

Supporting Figure 4:



Supporting Figure 4:

Optical density (at 600 nm) of ETEC (enterotoxic *E. coli*) cells right after inoculation (0h) and after 24 hours as a function of sodium cholate concentration (in mg NaD per ml).

Supporting Table 1. Mole fraction partition coefficients in NaC 100mM, NaDC 50mM and NaTC 50mM in a solvent of pure D_2O. *K_p values above ~40 are unreliable due to huge standard deviations.

	azithromycin aglycone	decladinosyl-azithromycin	erythromycin	azahomo-erythromycin	azithromycin	clarithromycin
NaC	1.82 +/- 0.04	3.22 +/- 0.12	4.94 +/- 0.64	6.60 +/- 0.63	> 42.5 *	> 60.9*
NaDC	1.71 +/- 0.03	3.83 +/- 0.16	6.29 +/- 0.38	11.6 +/- 1.66	> 68.2 *	> 41.2 *
NaTC	1.67 +/- 0.08	3.31 +/- 0.12	6.40 +/- 0.85	6.39 +/- 0.22	7.47 +/- 0.53	21.0 +/- 8.72

Experimental

NMR Spectroscopy, using pure D_2O as solvent

For the interaction studies in D_2O we used saturated solution of the macrolides. They were obtained by adding an excessive amount of the macrolide and sonicating the sample for 20-30 minutes. To get rid of the remaining solid antibiotic, the sample was centrifuged and the liquid phase was used for further experiments.