Supplemental Information

Binding Sites for Acylated Trehalose Analogs of Glycolipid Ligands on an Axtended Carbohydrate-recognition Domain of the Macrophage Receptor Mincle

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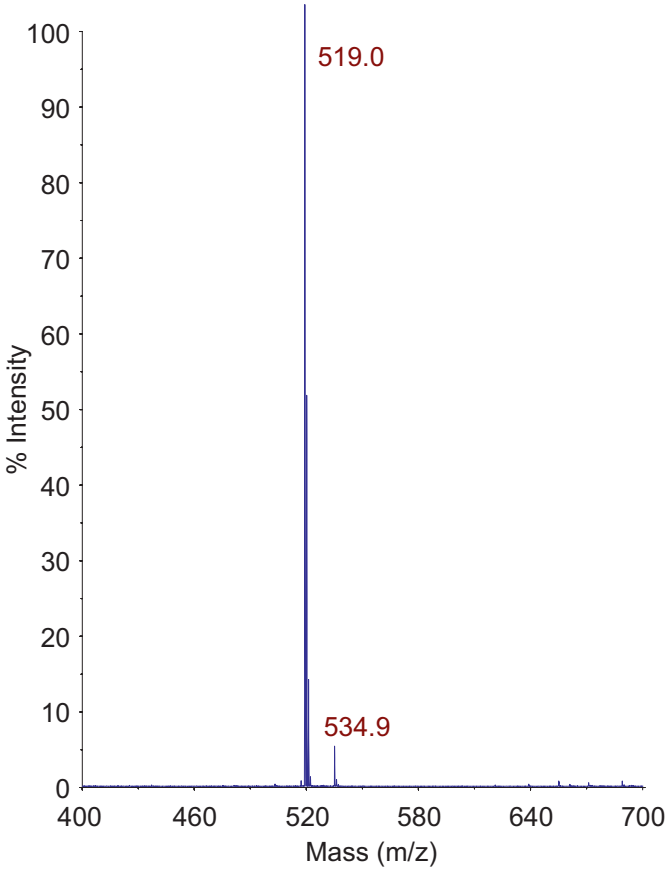
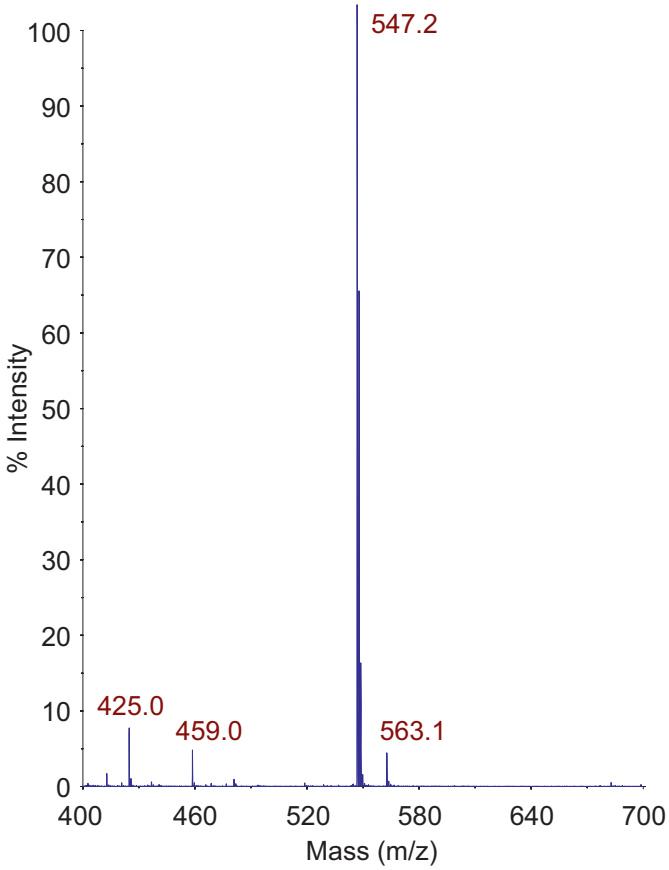
Figure S1. Mass spectrometry of acylated trehalose derivatives.

Figure S2. Proton NMR spectra of acylated trehalose derivatives.

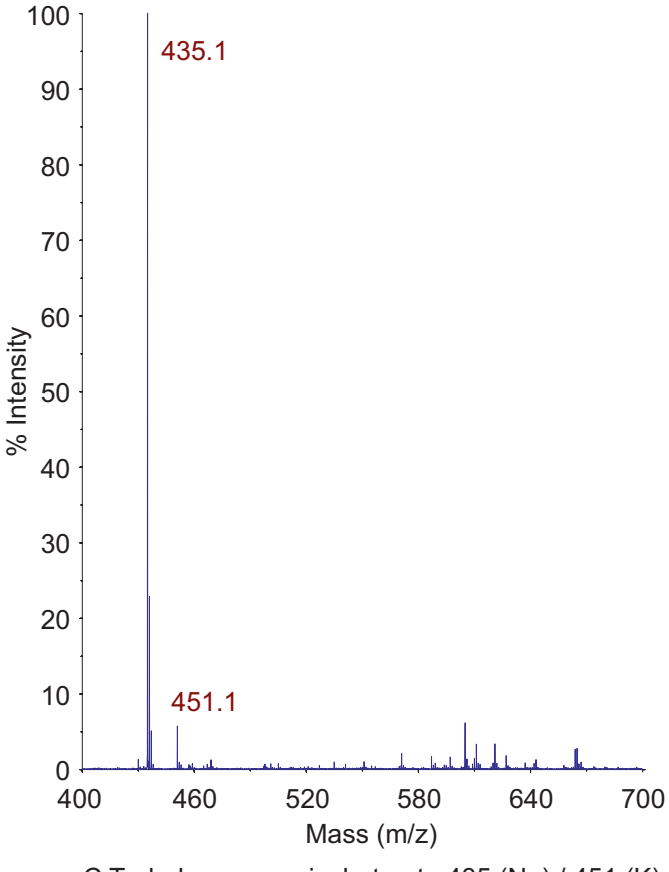
Figure S1. Mass spectrometry of di-acylated trehalose derivatives. Samples were prepared by spotting together equal volumes of matrix, 2,5-dihydroxybenzoic acid as a 10 mg/ml solution 80% methanol, and sugar derivative, dissolved at approximately 1 mg/ml in water, on a target plate. Mass spectrometry was performed on an Applied Biosystems 4800 matrix assisted-laser desorption time-of-flight mass spectrometer.



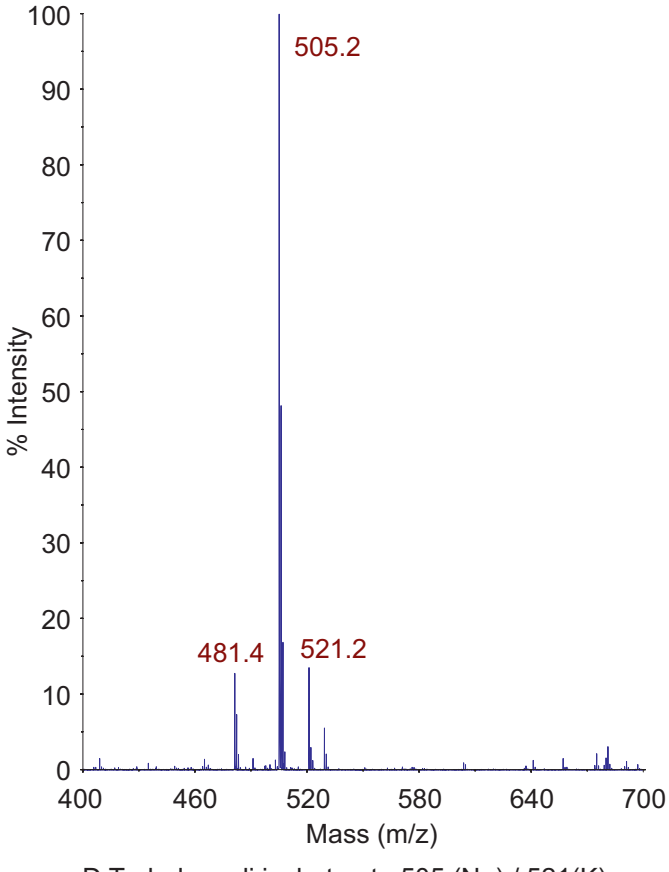
A Trehalose mono decanoate 519(Na) / 535 (K)



B Trehalose mono dodecanoate 547 (Na) / 563 (K)



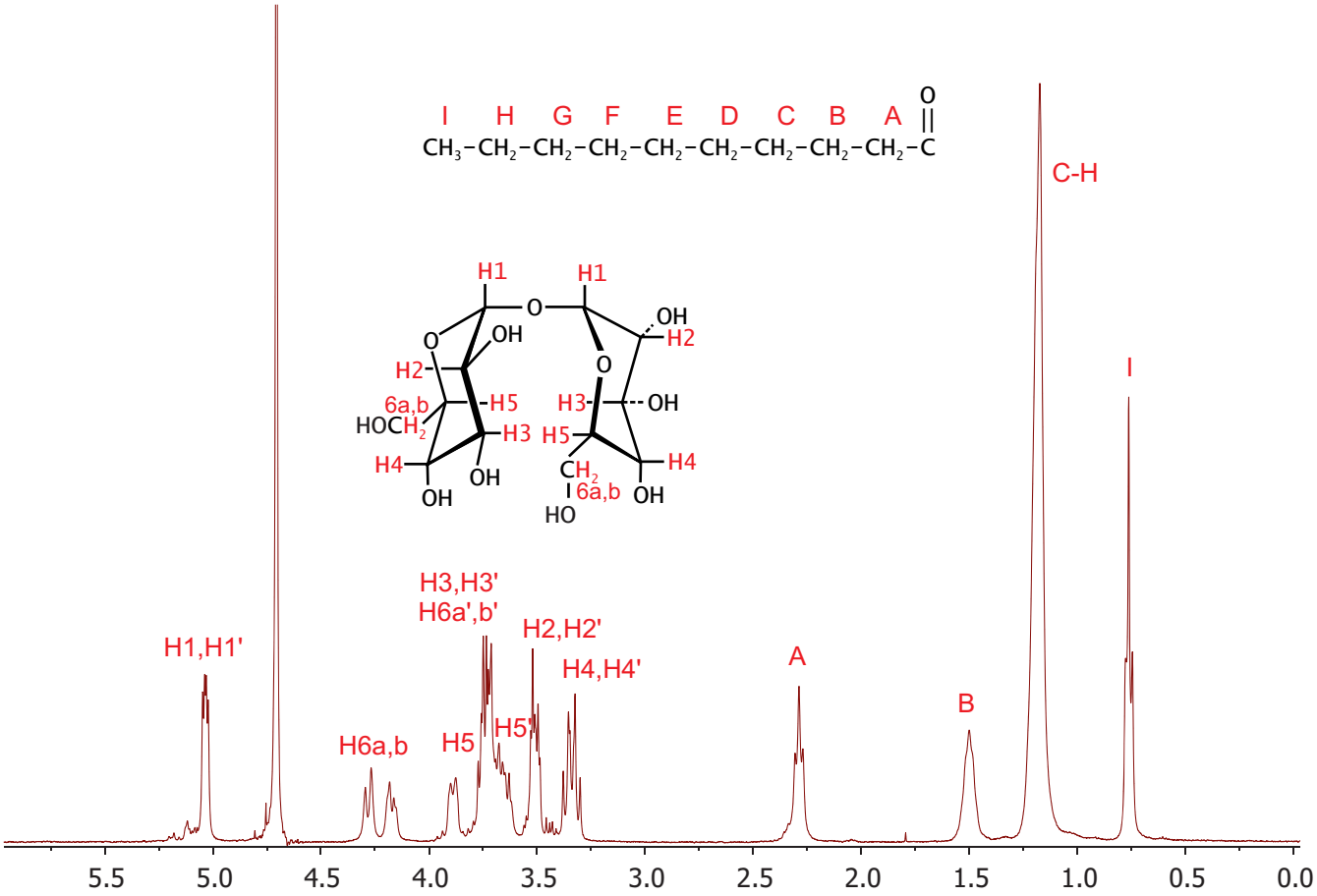
C Trehalose mono isobutyrate 435 (Na) / 451 (K)



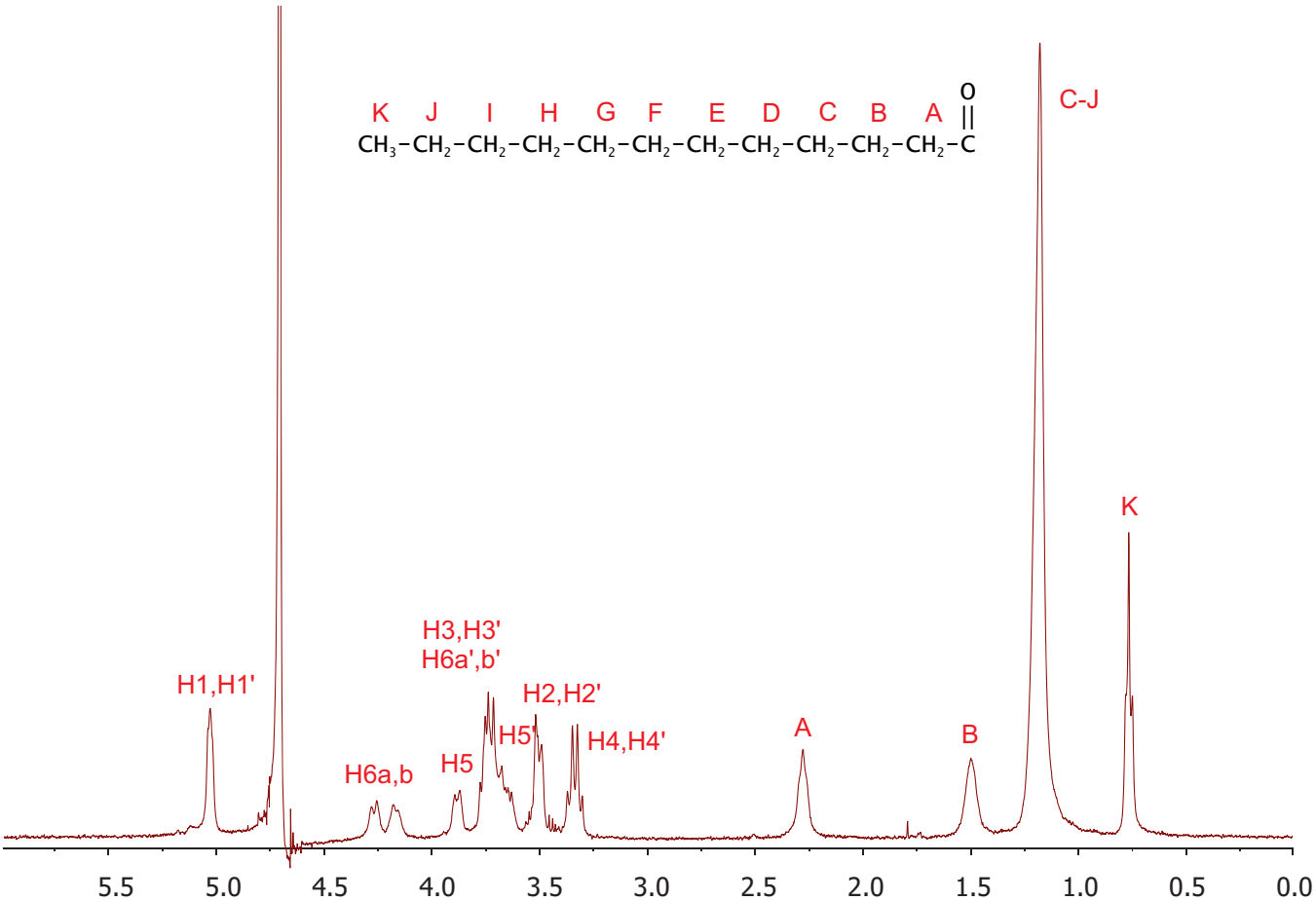
D Trehalose di isobutyrate 505 (Na) / 521(K)

Figure S2. Proton NMR spectra of acylated trehalose derivatives. Samples for NMR spectra, dissolved in D_2O at approximately 5 mg/ml, were analyzed on a Bruker 400 MHz spectrometer. Spectra are annotated to show signals from the acyl side chain (letters A-K) and key signals from trehalose. For monoacyl derivatives, signals from the non-acylated glucose residue are denoted with primes.

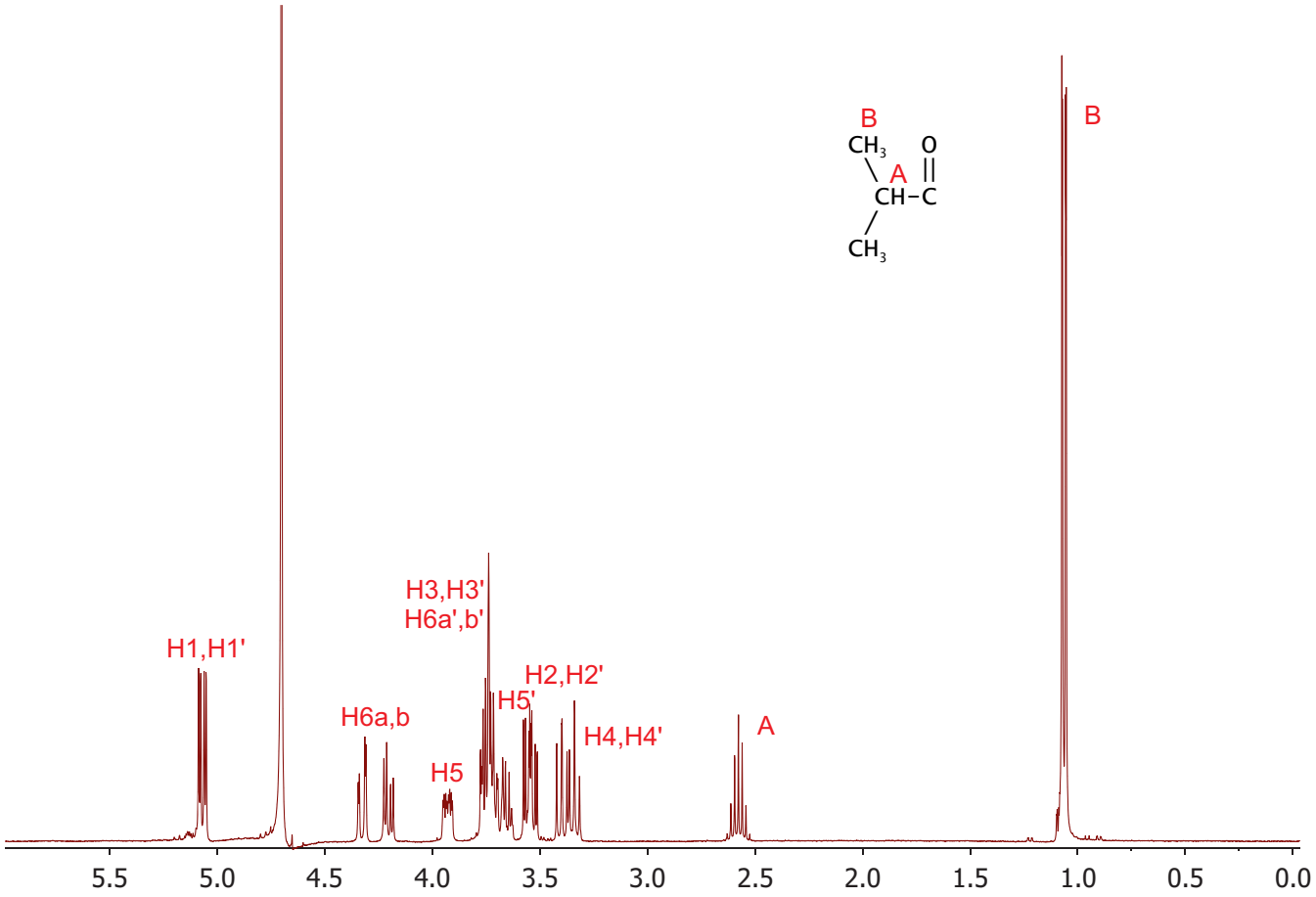
A Trehalose mono decanoate



B Trehalose mono dodecanoate



C Trehalose mono isobutyrate



D Trehalose di isobutyrate