Supplemental Information

Mechanism of interaction of human mincle with mycobacterial trehalose dimycolate probed using synthetic analogues

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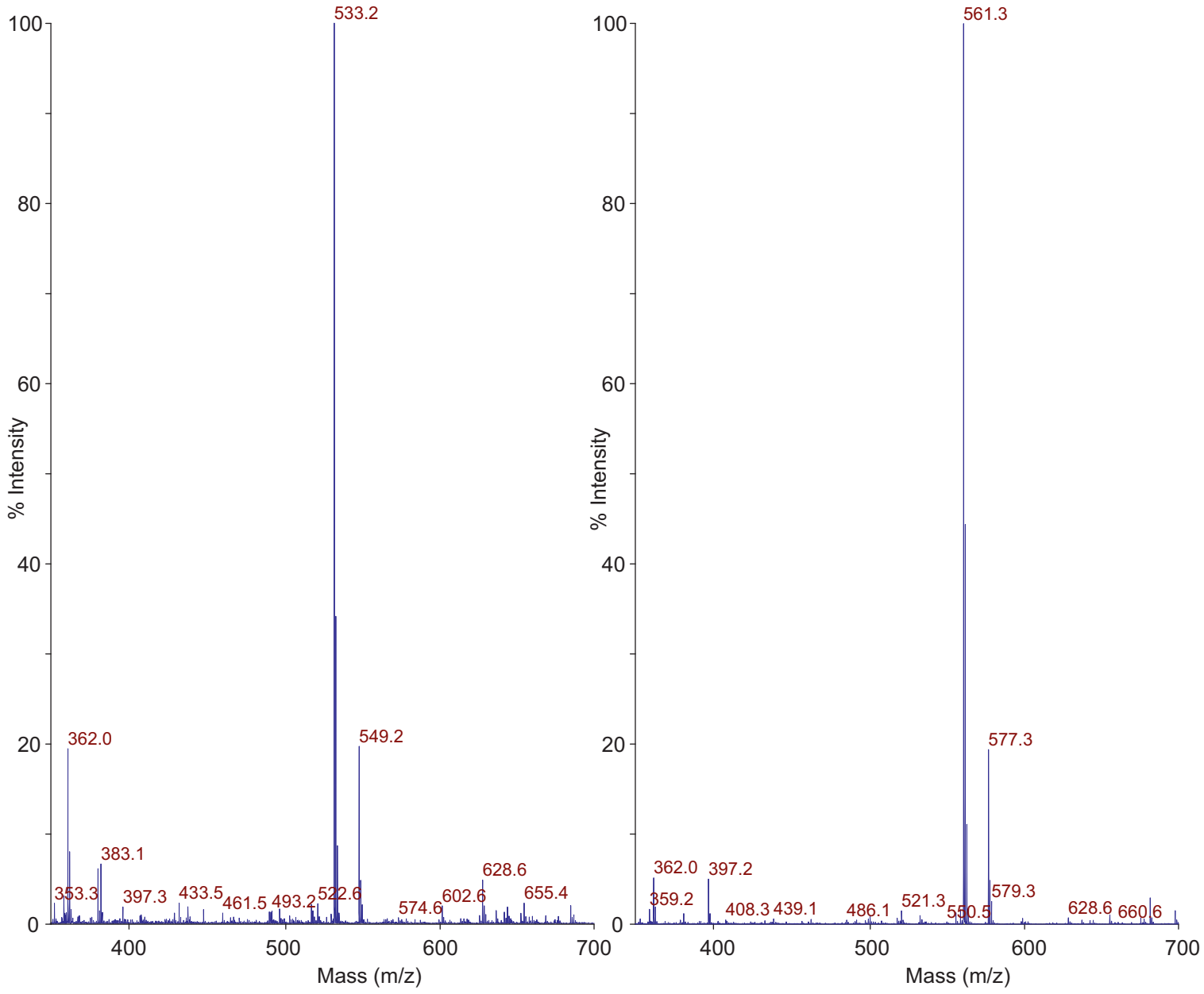
Figure S1. Mass spectrometry of novel di-acylated trehalose derivatives.

Figure S2. Proton NMR spectra of novel di-acylated trehalose derivatives.



A Trehalose divalerate 533 (Na) / 549 (K)
[Monovalerate 449 (Na)]

B Trehalose dihexanoate 561 (Na) / 577 (K)
[Monohexanoate 463 (Na)]

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.

Figure S2. Proton NMR spectra of diacylated 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-G) and key signals from trehalose.