SUPPLEMENTARY MATERIAL

Analysis of Microbial Lipids Deposited on Mars Global Simulant (MGS-1) by Geomatrix-Assisted Laser Desorption/Ionization Mass Spectrometry

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Derivatization and GC-MS analysis of lipid extract

In order to prove the presence of the free fatty acids in the lipid extract observed in the GALDI-MS spectra, analysis using gas chromatography coupled to mass spectrometry (GC-MS) were performed. Firstly, the extract was submitted to the HMDS reaction, in which the carboxylic acid groups reacted with the silylating reagent, generating trimethylsilyl esters. This procedure was required for analysing the lipid extract on the gas chromatography system available in the laboratory. The chromatogram showing the trimethylsilyl esters profile, as well as, the mass spectra and fragmentation mechanism can be seen in figure S1 and S2, respectively.

The total ion chromatogram (TIC) of the derivatized lipid extract shows a significant number of peaks. Using the NIST library, it was possible to identify the trimethylsilyl esters of all fatty acids discussed in the main manuscript.

The following trimethylsilyl esters were identified: trimethylsilyl palmitate (8.47 min), trimethylsilyl oleate (9.61 min), trimethylsilyl stearate (9.72 min) and trimethylsilyl linoleate (10.03 min). In order to corroborate with the identification using the NIST library, fragmentation mechanisms for ions of higher intensities of the presented spectra were proposed.

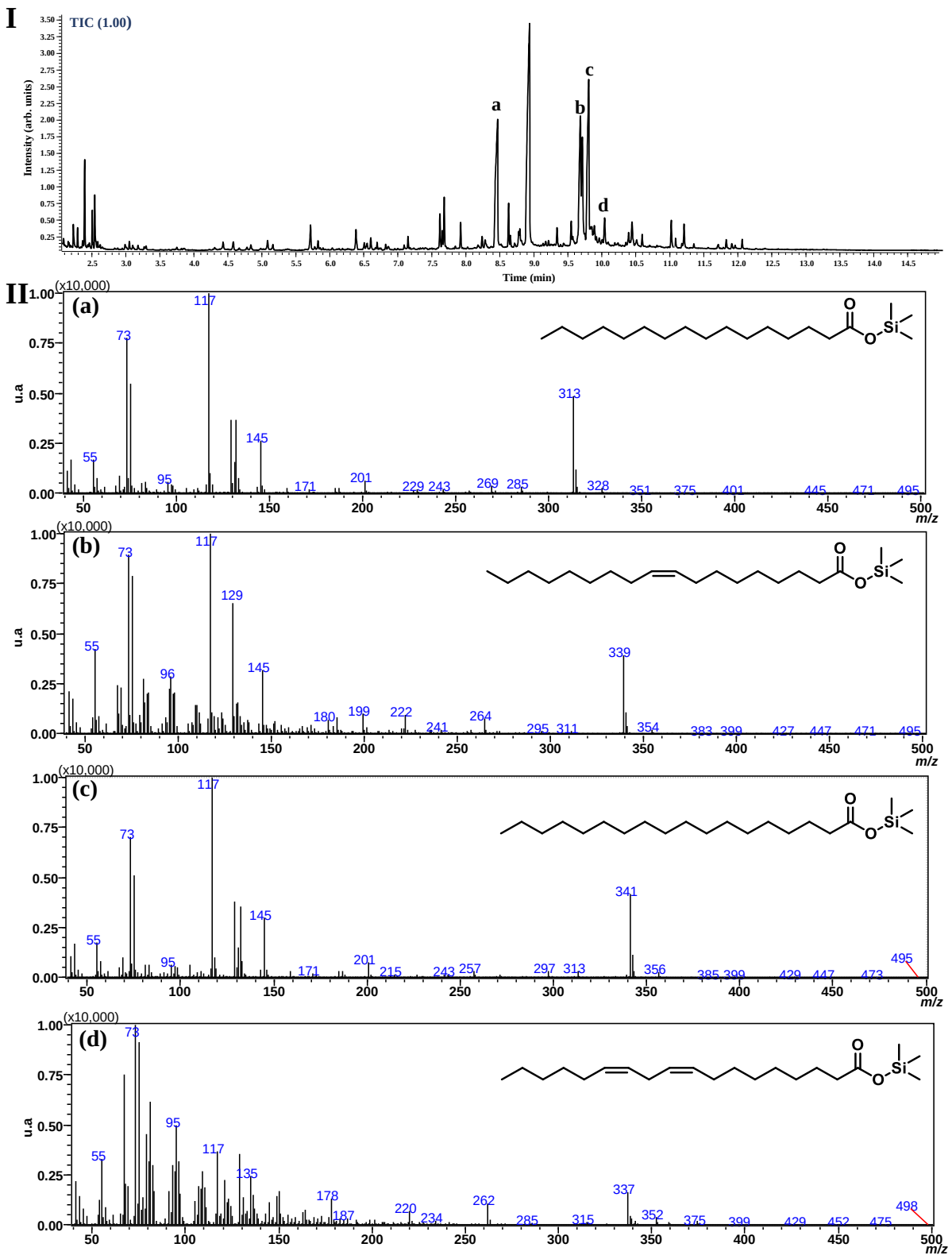

FIG. S1. (I) Total ion chromatogram of the lipid extract derivatized with HMDS. (II) Mass spectra of the peaks highlighted in the previous chromatogram.

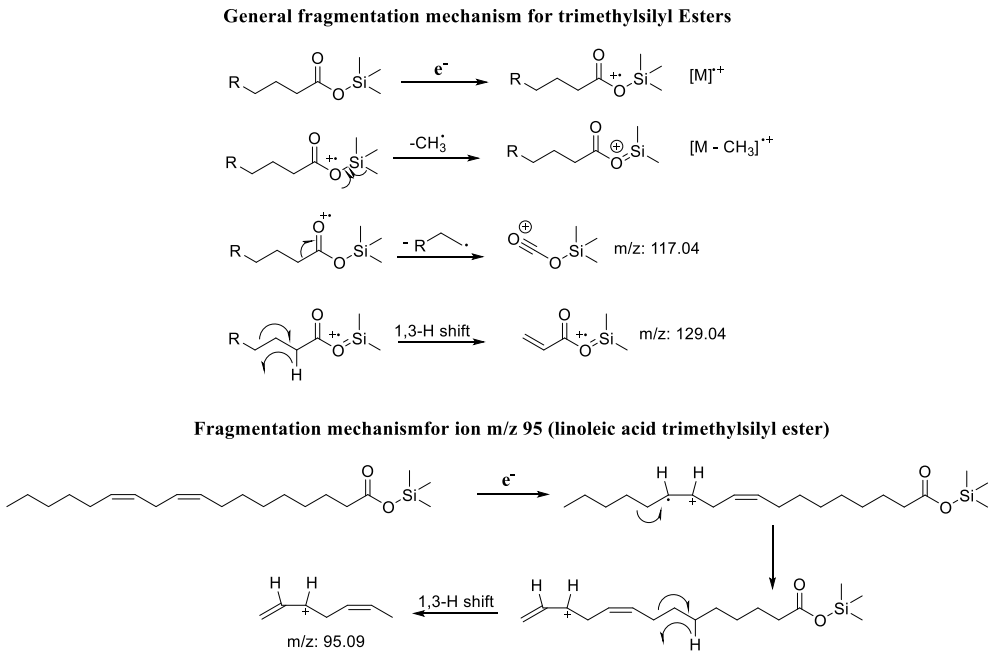

FIG. S2. Mechanistic proposal for the formation of ions of higher intensity observed in the mass spectra of trimethylsilyl esters.

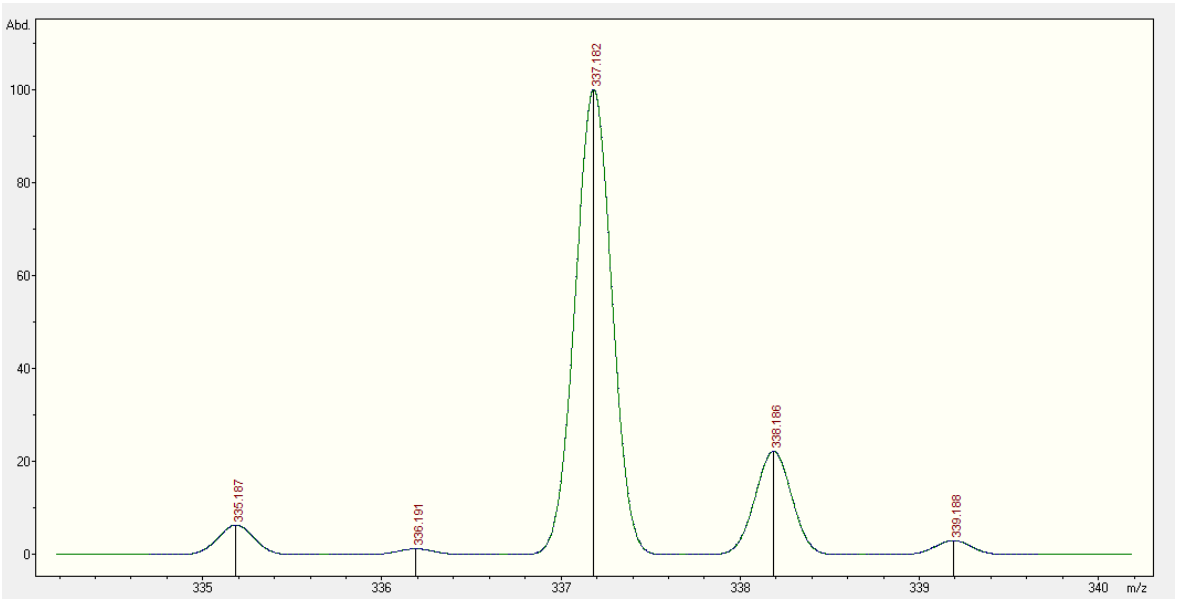

FIG. S3. Simulation of the isotopic pattern of the oleic acid iron adduct ($[C_{18}H_{34}O_2$ - H + $Fe^{2+}]^+$) by Compass IsotopePattern software.

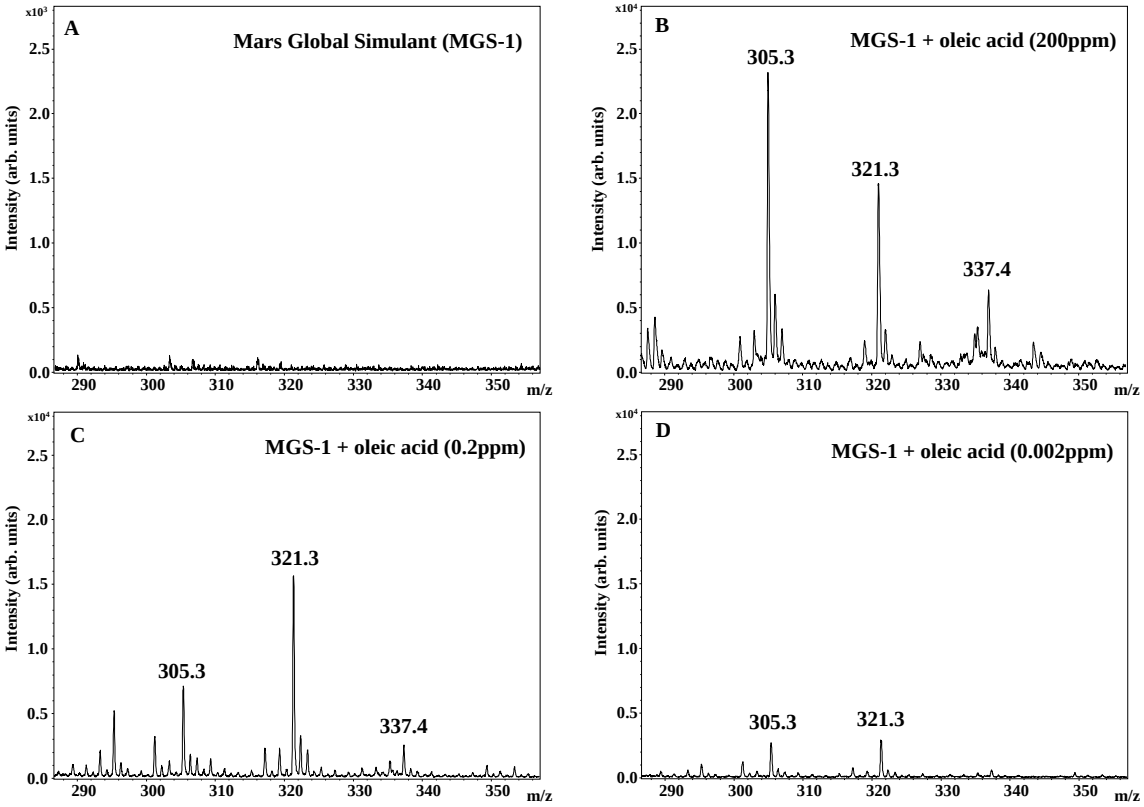

FIG. S4. GALDI-MS spectra of (A) pure MGS-1 matrix; (B), (C) and (D) Oleic acid at concentrations of 200, 0.2, and 0.002 ppm, respectively, dispersed in MGS-1 matrix.