Supplementary Material

Formation of organic acids from the gas-phase ozonolysis of terpinolene,
Yan Ma and George Marston*

Mass spectral data of the products identified from the gas-phase ozonolysis of terpinolene

The identification of the reported terpinolene ozonolysis products was made using a ThermoFinnigan gas chromatograph with mass spectrometric detection (GC-MS) in electron impact (EI, 70eV) and negative chemical ionisation (CI(–), methane) modes following derivatisation using 14% BF₃/MeOH.

Five organic acids were identified as their corresponding methyl ester derivatives, as represented by chromatographic peaks 1-5, respectively. The EI and CI(–) mass spectral data of these peaks are shown in Fig. SP1-SP5. Descriptions of the structure elucidation of these compounds are given in the main paper.

Fig. SP1 GC/EI and CI(–)-MS spectra for P1, tentatively identified as methylated terpinolic acid (a).
Fig. SP2 GC/EI and CI(–)-MS spectra for P2, tentatively identified as methylated terpinolic acid (b).

Fig. SP3 GC/EI and CI(–)-MS spectra for P3, tentatively identified as methylated terpinolalic acid (a).
Fig. SP4 GC/EI and CI(−)-MS spectra for P4, tentatively identified as methylated terpinolalic acid (b).

Fig. SP5 GC/EI and CI(−)-MS spectra for P5, tentatively identified as methylated terpinolalic acid (c).