Supplementary Material 1

Mechanisms for the formation of organic acids in the gas-phase ozonolysis of 3-carene, Yan Ma, Rachel A. Porter, David Chappell, Andrew T. Russell and George Marston*

Mass spectral data of the products identified from the gas-phase ozonolysis of 3-carene

The identification of the reported 3-carene 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% BF_3/MeOH.

Eight organic acids and two dicarbonyl compounds were identified as their corresponding methyl ester and/or acetal derivatives. These compounds were 3-caric acid, 3-caralic acid, 3-caronic acid, nor-3-caric acid, nor-3-caralic acid, nor-3-caronic acid, OH-3-caronic acid, OH-3-caralic acid, 3-caronaldehyde and nor-3-caronaldehyde; they are expected to be present in their *cis*-form due to the original *cis*-structure of 3-carene. Since no authentic standards are available, all these compounds were identified using their respective GC/EI and CI(–) mass spectral data, as shown in Fig. SP1–SP10.

For the corresponding products identified from 3-carene and α-pinene ozonolysis, the mass spectra indicate identical molecular weights and similar mass fragmentation patterns that are characteristic of the methyl ester and/or dimethoxy acetal structures. For compounds containing an acetyl group, the EI mass spectrum is also characterised by an intense peak at *m/z* 43. Thus the spectral data of 3-carene products can be interpreted in the same way as for our previously identified α-pinene ozonolysis products, described in the supplementary material for ref. 1.

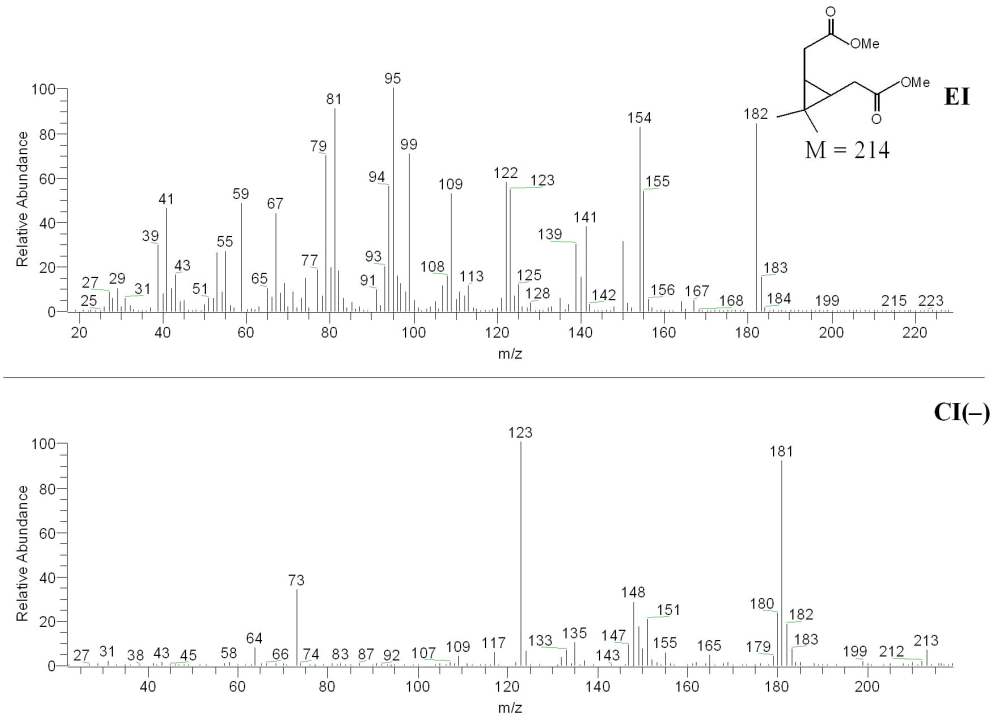

Fig. SP1: GC/EI and CI(–)-MS spectra for product peak identified as methylated *cis*-3-caric acid.

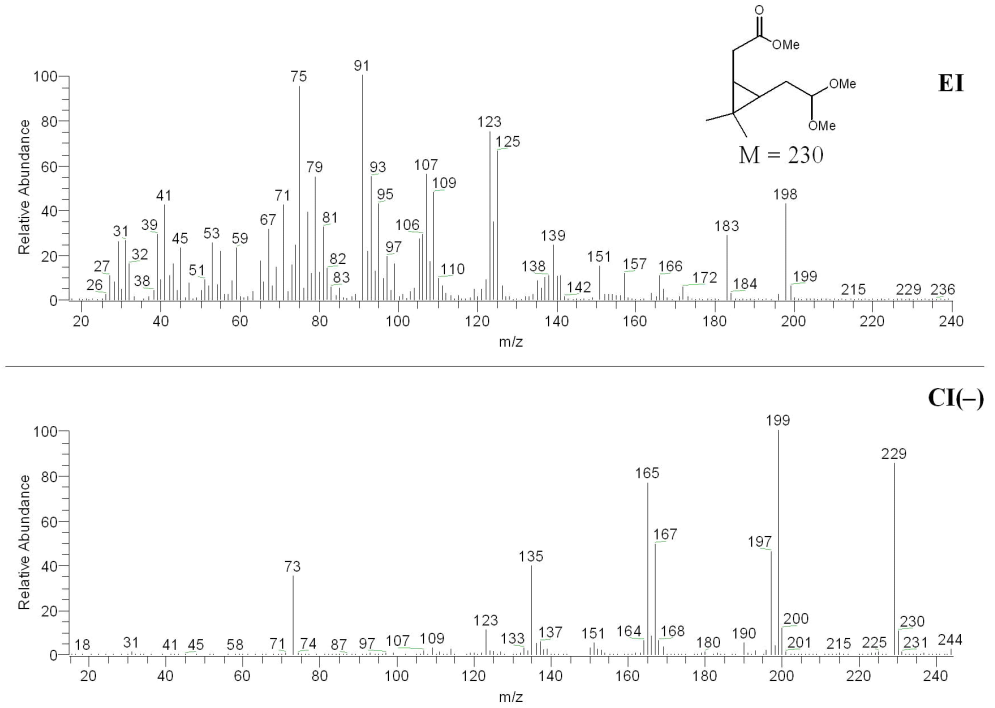

Fig. SP2: GC/EI and CI(–)-MS spectra for product peak identified as methylated *cis*-3-caralic acid.

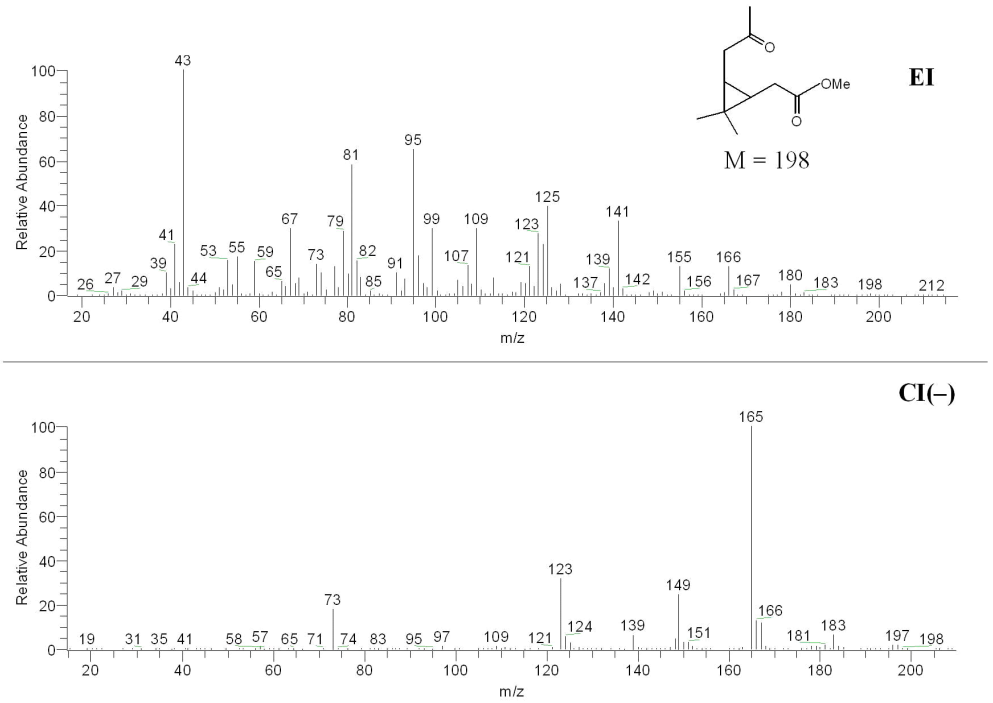

Fig. SP3: GC/EI and CI(–)-MS spectra for product peak identified as methylated *cis*-3-caronic acid.

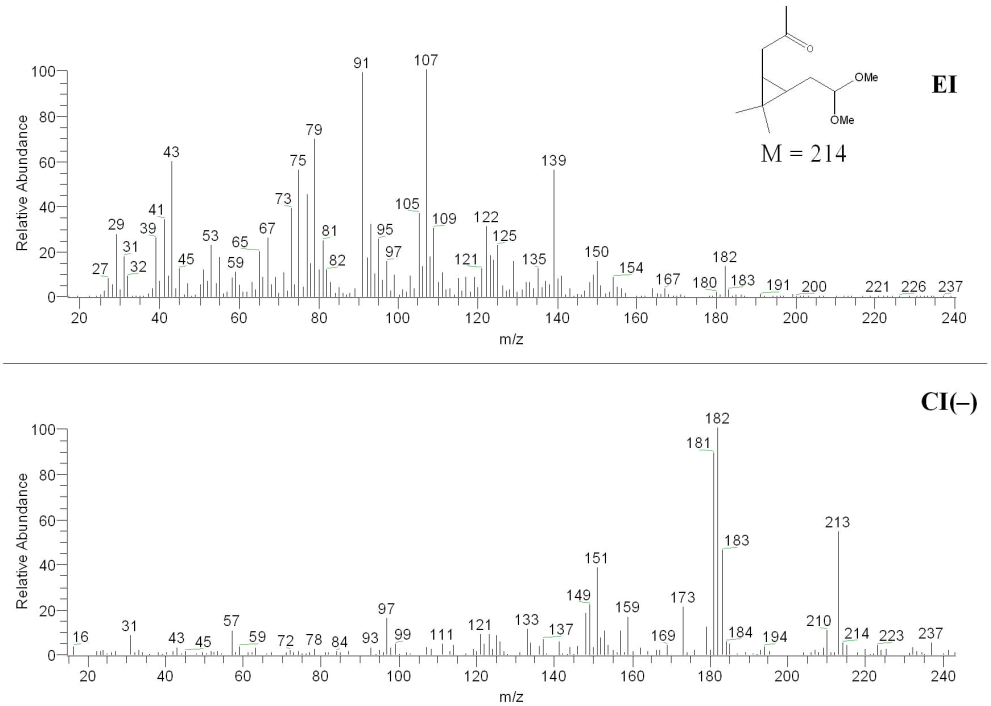

Fig. SP4: GC/EI and CI(–)-MS spectra for product peak identified as *cis*-3-caronaldehyde dimethoxy acetal.

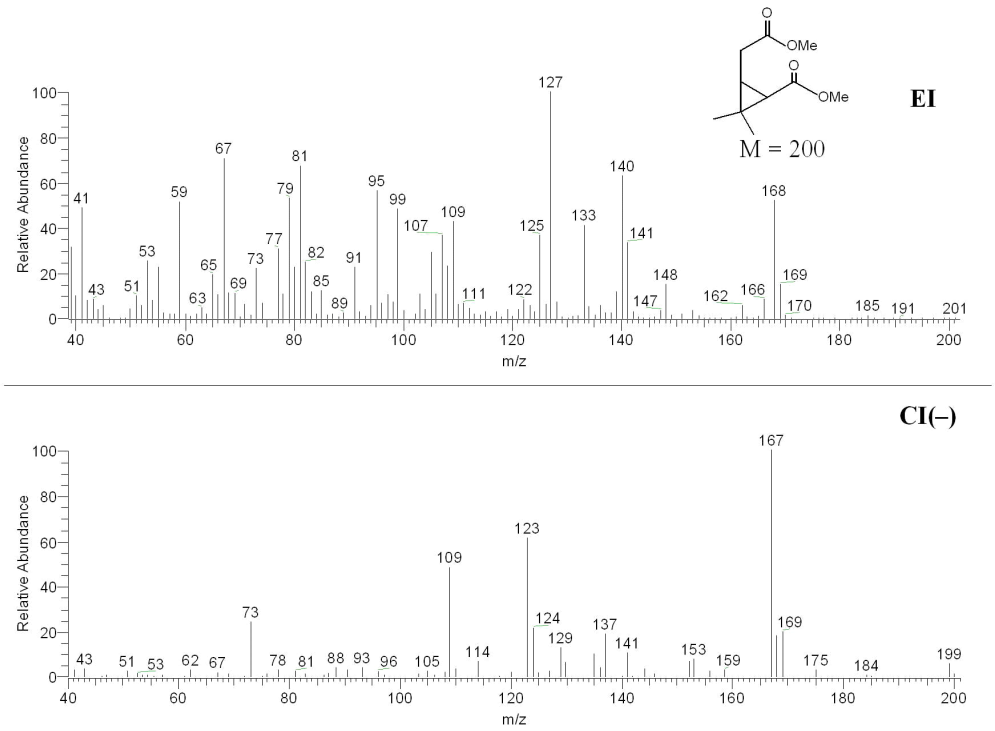

Fig. SP5: GC/EI and CI(–)-MS spectra for product peak identified as methylated *cis*-nor-3-caric acid.

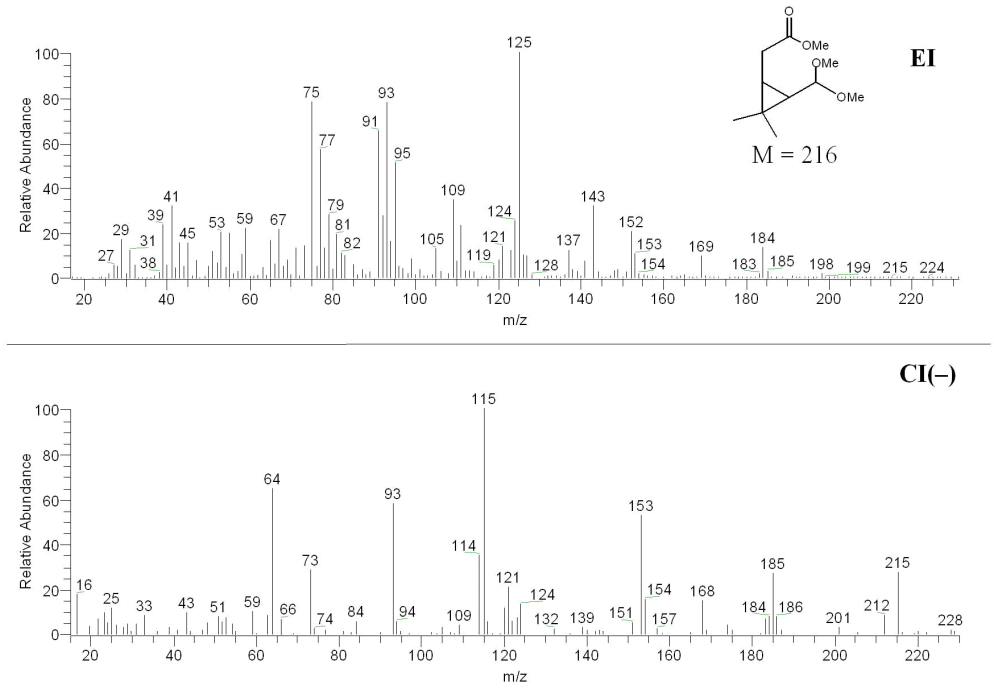

Fig. SP6: GC/EI and CI(–)-MS spectra for product peak identified as methylated *cis*-nor-3-caralic acid.

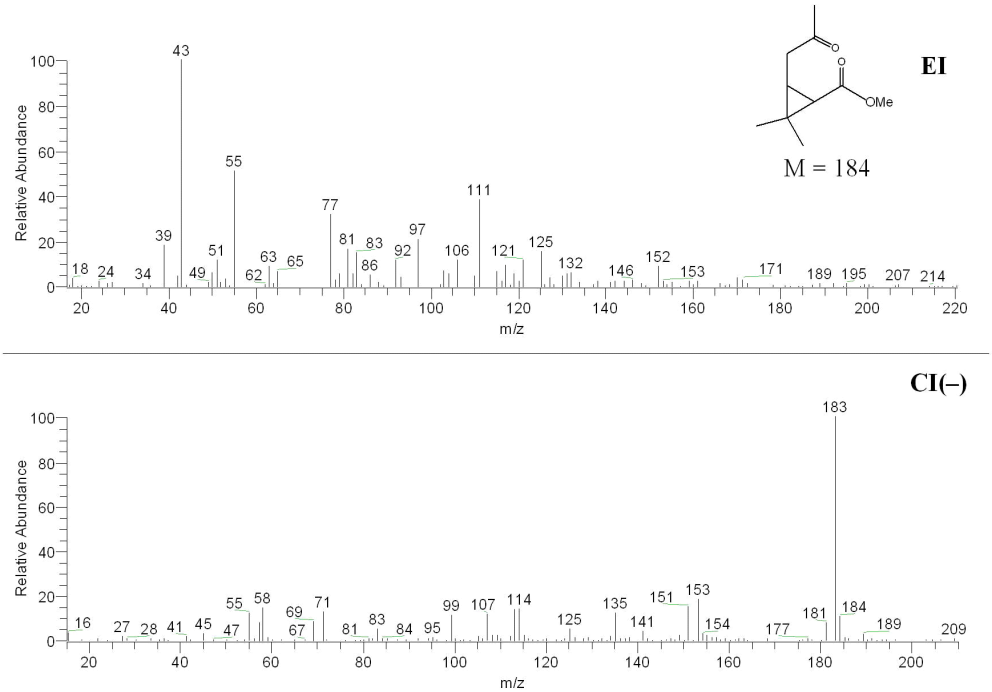

Fig. SP7: GC/EI and CI(–)-MS spectra for product peak identified as methylated *cis*-nor-3-caronic acid.

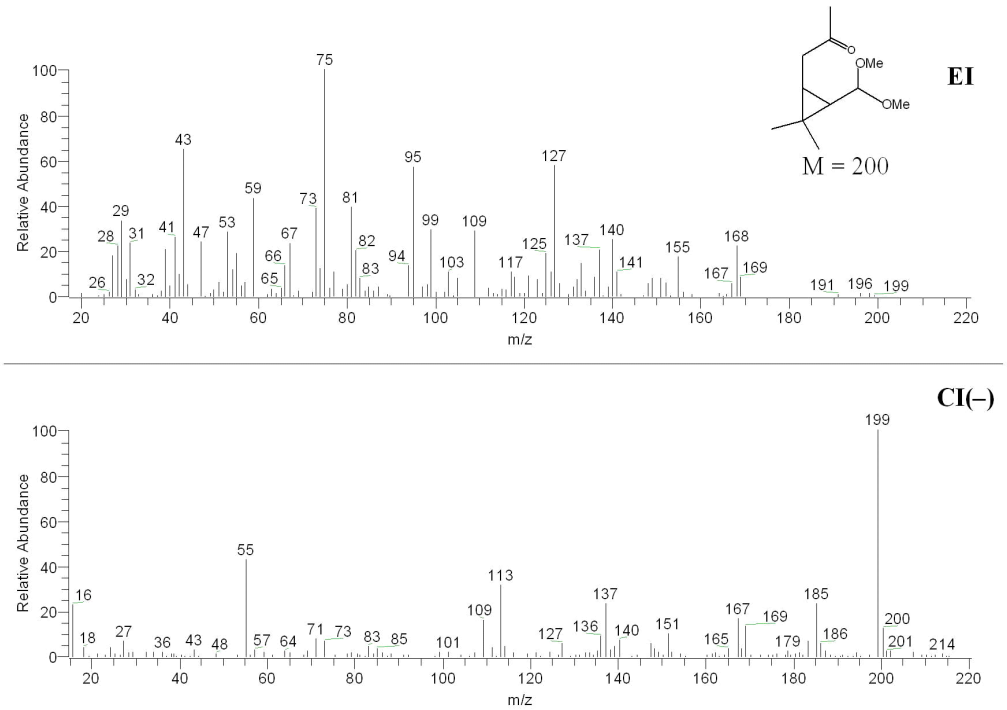

Fig. SP8: GC/EI and CI(–)-MS spectra for product peak identified as *cis*-nor-3-caronaldehyde dimethoxy acetal.

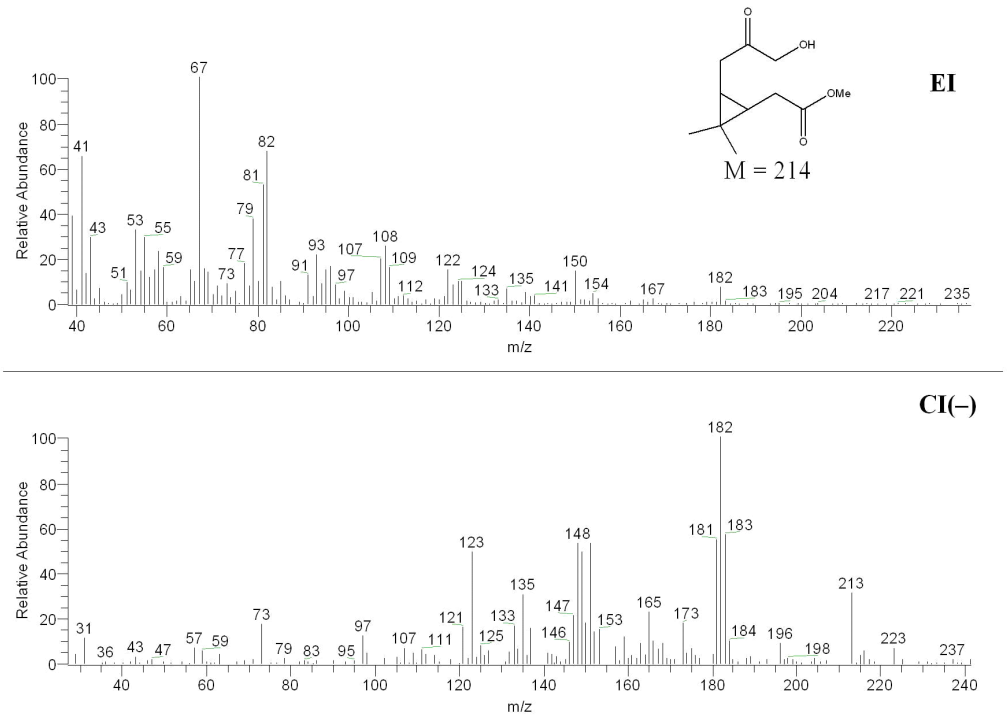

Fig. SP9: GC/EI and CI(–)-MS spectra for product peak identified as methylated *cis*-OH-3-caronic acid

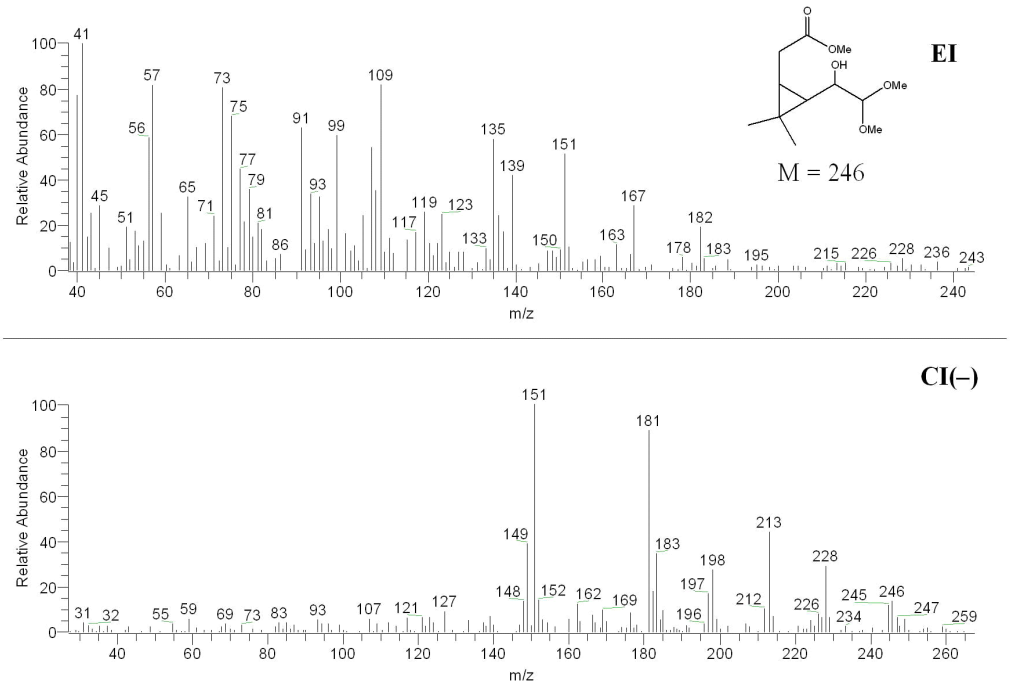

Fig. SP10: GC/EI and CI(–)-MS spectra for product peak identified as methylated *cis*-OH-3-caralic acid

1. Y. Ma, A. T. Russell and G. Marston, *Phys. Chem. Chem. Phys*., 2008, **10**, 4294.