

Electronic Supplementary Material

Real-time monitoring of exhaled volatiles using atmospheric pressure chemical
ionization on a compact mass spectrometer

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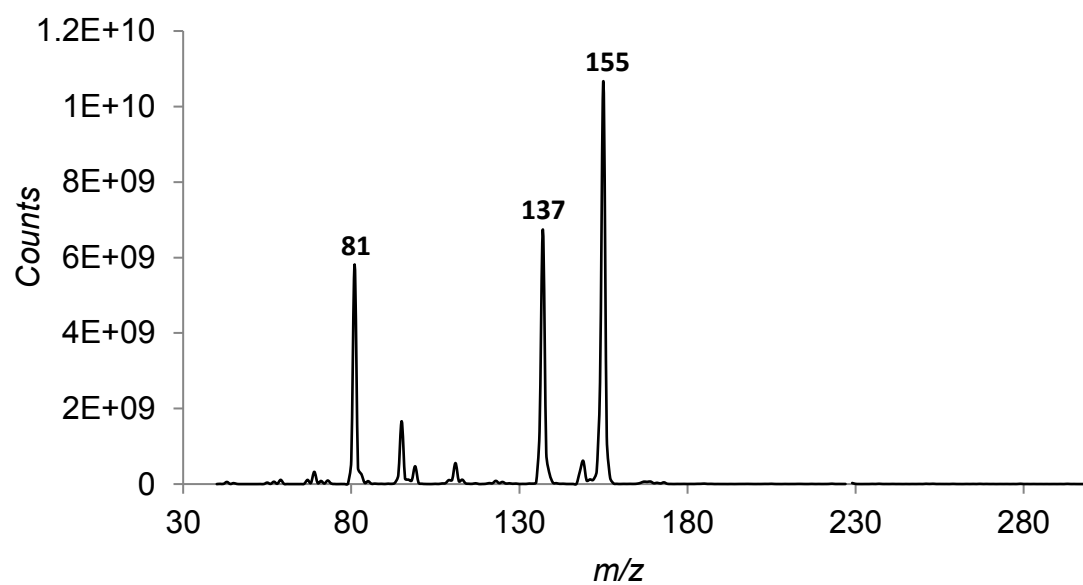


Figure S1. APCI-MS spectrum of the volatile headspace from a 1.0% menthone solution in HPLC grade water.

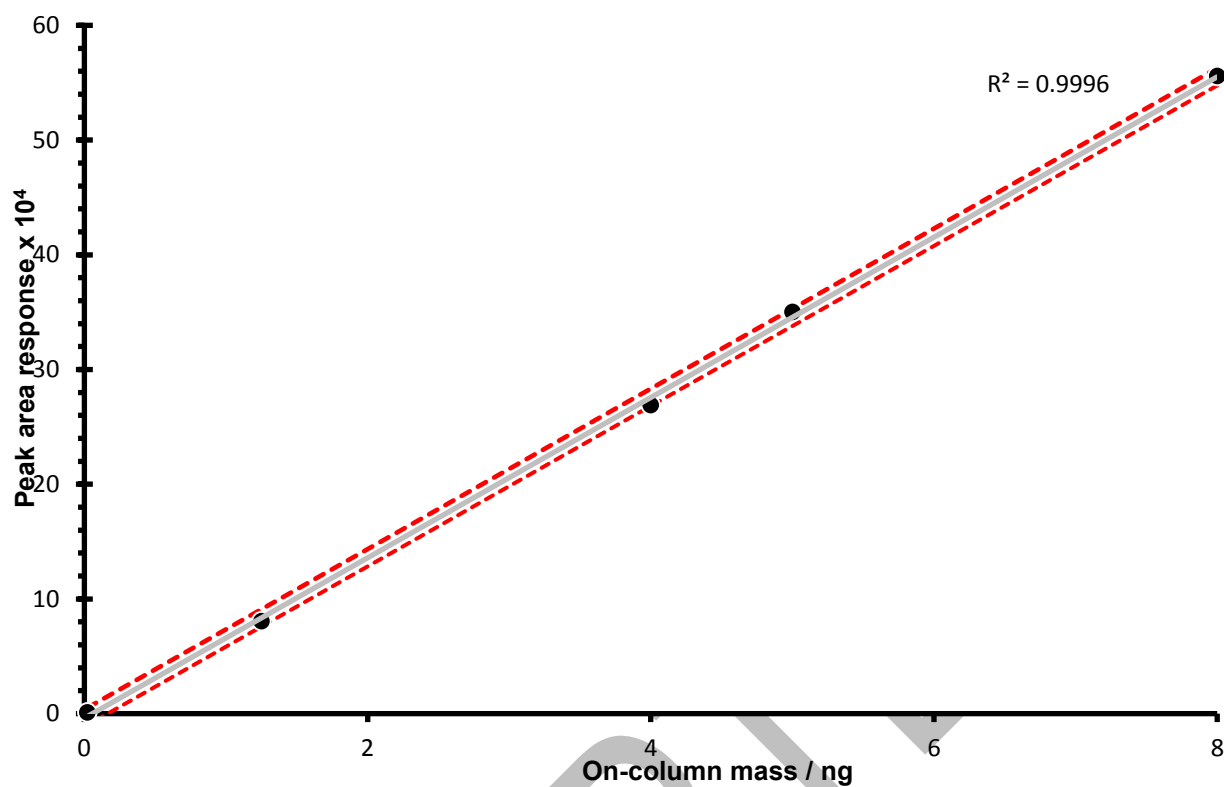


Figure S2. External calibration for the m/z 112 fragment ion of menthone from the GC-MS analysis of liquid standards spiked on Tenax/Carbograph TD tubes displaying 95% confidence limits (dotted red lines).

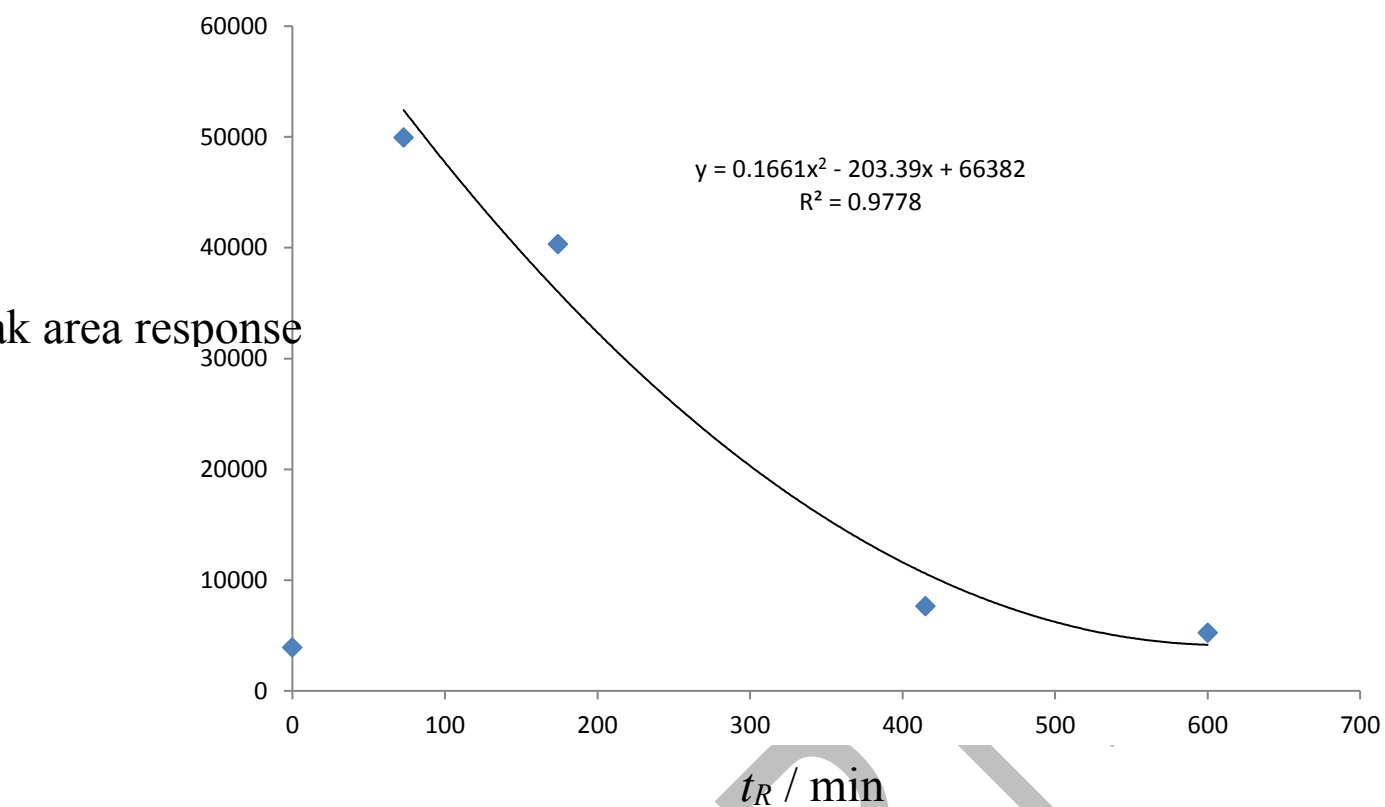


Figure S3. Graph showing the intensity of the m/z 112 ion (menthone fragment) obtained by TD-GC-MS against time over a 600 min time course post-ingestion of a peppermint oil capsule.

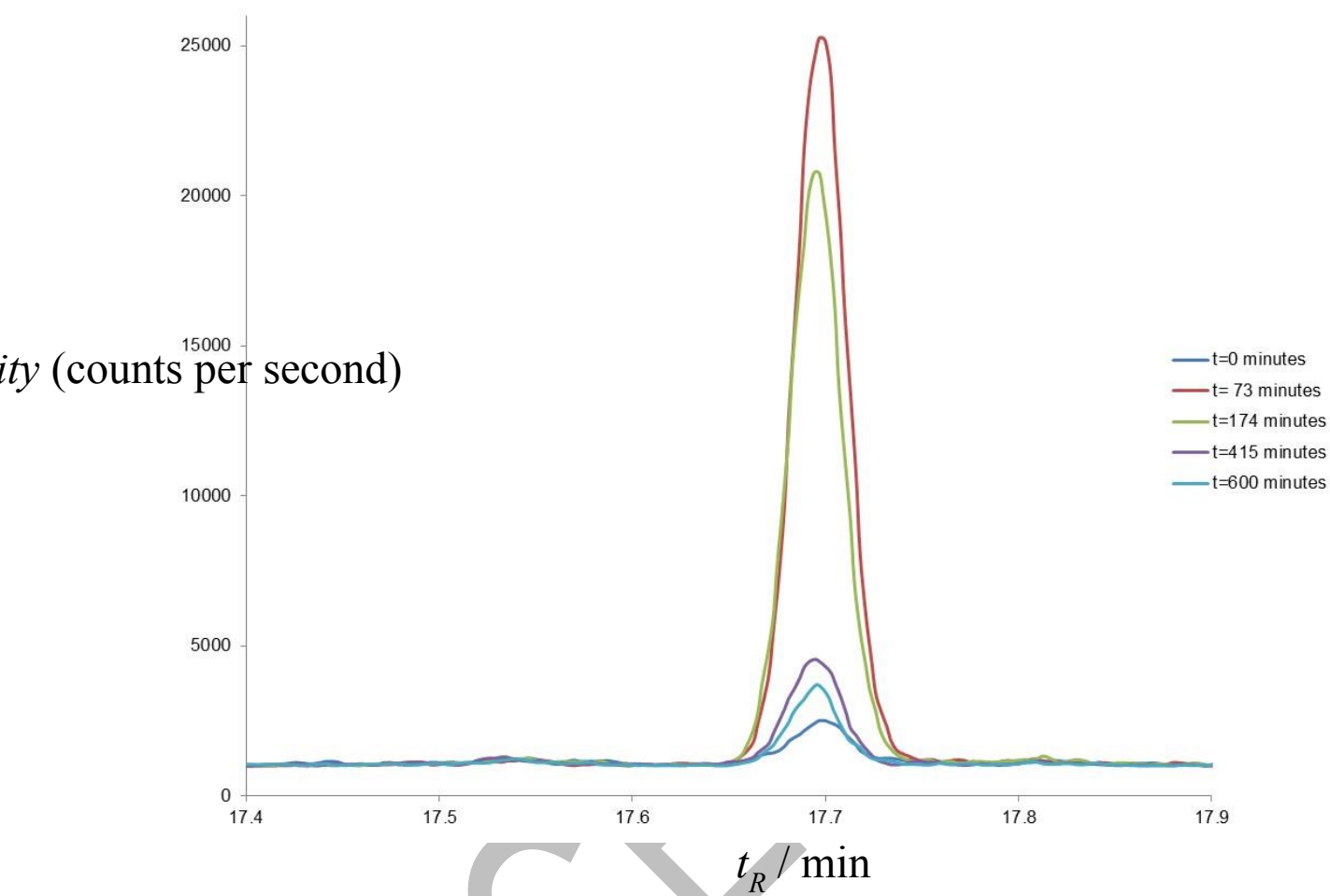


Figure S4. Overlaid TD-GC-MS extracted ion traces for the m/z 112 fragment ion of menthone from each of the 5 sampling points of the 600 min washout experiment.

Calculations

From Figure S2 at 120 minutes the peak area response for m/z 112 is calculated by:

$$y = 0.1661x^2 - 203.39x + 66382$$

$$y = (0.1661 * 120^2) - (203.30 * 120) + 66382$$

$$y = 2391.84 - 24396 + 66382$$

$$\text{Peak area response at 120 minutes} = 44378 \text{ cps}$$

On-column mass (OCM) is found by extrapolating this from the calibration graph (Figure S2) (rearranging $y = mx+c$) gives:

$$44378 + 3950.9 / 69885$$

$$\text{OCM} = 0.692 \text{ ng}$$

2 litres of breath were collected therefore the concentration of menthone per litre was 0.346 ng/L

Conversion to ppbv was accomplished using the following equation.

$$\text{Concentration in ppbv} = (\text{concentration in ng/L} \times 24.45) / \text{relative molecular mass}$$

Please note:

1 M of gas expands to fill 24.45 L at normal temperature (25 °C) and pressure (1 atm)

$$\text{RMM of menthone} = 154 \text{ amu}$$

$$\text{Concentration ppbv} = (0.346 \times 24.45) / 154$$

$$= 0.0549 \text{ ppbv} = 54.9 \text{ pptv}$$

$$\text{Menthone concentration at 120 minutes} = 54.9 \text{ pptv}$$