

## Supplement

### S1. Calculation of total uncertainties

Total uncertainties on the calibration factor values are a result from the individual uncertainties from experiments including the organic compound concentration,  $\sigma_c$ , following either Eq. (2) for Approach 1 (Heated ST) and Eq. (5) for Approach 2 (CSA), as well as the measured signals,  $\sigma_{\text{signal}}$  (one standard deviation). The various mathematical equation used for total and signal uncertainty estimation is as based on the propagation of uncertainties, as following:

$$\sigma_{C_X} = \sqrt{\sigma_c^2 + \sigma_{\text{signal}}^2}$$

$$\sigma_{\text{signal}} = \sqrt{\sigma_{\text{exp1}}^2 + \sigma_{\text{exp2}}^2 + \sigma_{\text{exp3}}^2 + \dots}$$

The equation used for quantifying the injected concentration of the organic compound from Approach 1 (heated ST) includes the gas flow rates, which were controlled by mass flow controllers (mfc, 0.6% of uncertainty) and were read using flow meters (fm, 2% of uncertainty). Uncertainties for these two latter are provided by the corresponding manufacturers. This equation also includes the vapour pressure of the organic compound, either taken from the literature with the uncertainties presented in section 3.1 for each tested compound. An exception comes for the vapour pressure experimentally found (section 2.2.2), thus including the individual uncertainty from the measuring scale (about 11% of uncertainty).

$$\sigma_c = \sqrt{\sigma_{\text{mfc}}^2 + \sigma_{\text{fm}}^2 + \sigma_{\text{Pvap}}^2}$$