

Supplementary material

Stable-isotope dilution GC-MS method for ethanol in vapour ethanol and microdialysis systems based on carbonate-catalyzed extractive pentafluorobenzoylation

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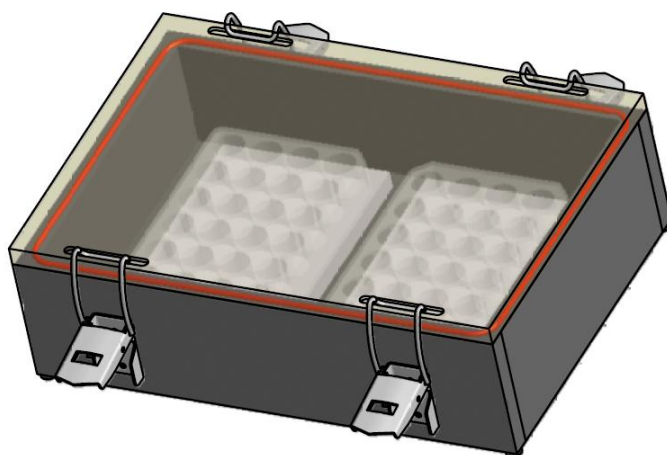
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Suppl. Figure 1

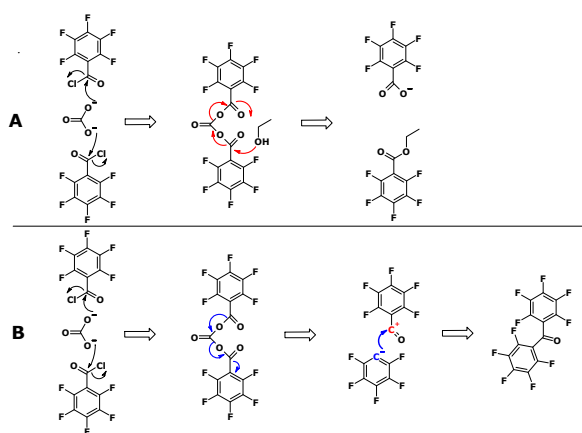
Photograph of the home-made ethanol-incubation system used in the present study. Home-made polyvinyl chloride chambers (24 cm x 16 cm x 6 cm) with tightly closable lids were used for the incubation of SH-SY5Y cells at different concentrations of ethanol and different exposure times.



Suppl. Figure 2

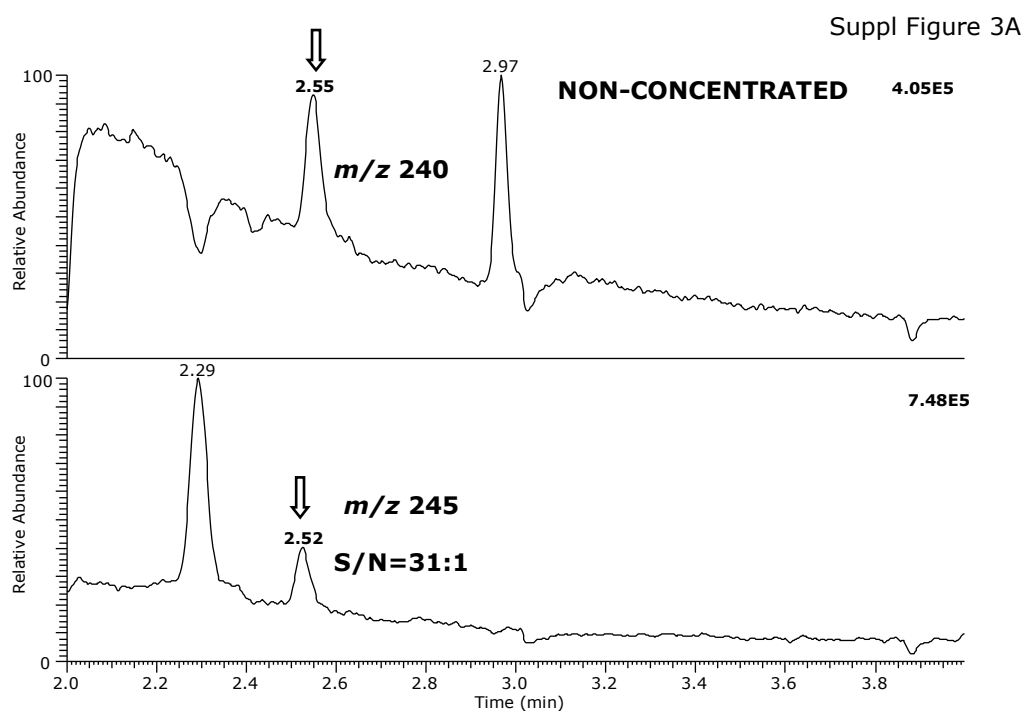
Proposal of a mechanism for the carbonate-catalyzed pentafluorobenzoylation of ethanol in the two-phase system consisting of an aqueous ethanolic phase and of a PFBz-Cl-containing toluene phase. At the aqueous/toluene boundary surface, the doubly negatively charged carbonate reacts with two PFBz-Cl molecules to form a di-pentafluorobenzoyl-carbonate which disperses in both phases. Ethanol reacts with this intermediate to form the PFBz ethanol derivative and to release carbonate.

Suppl. Figure 2

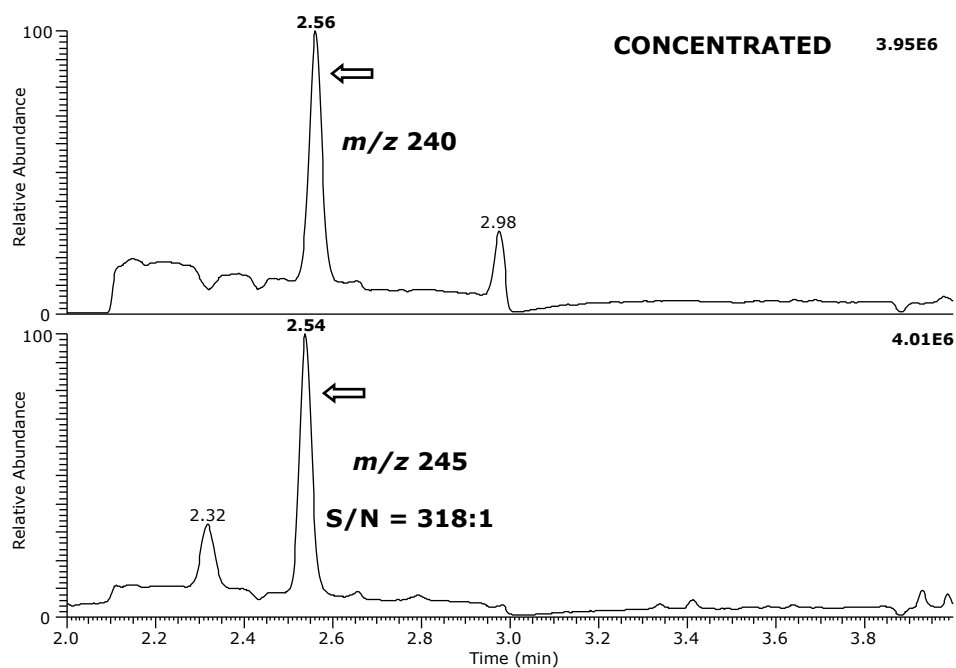


Suppl. Figure 3

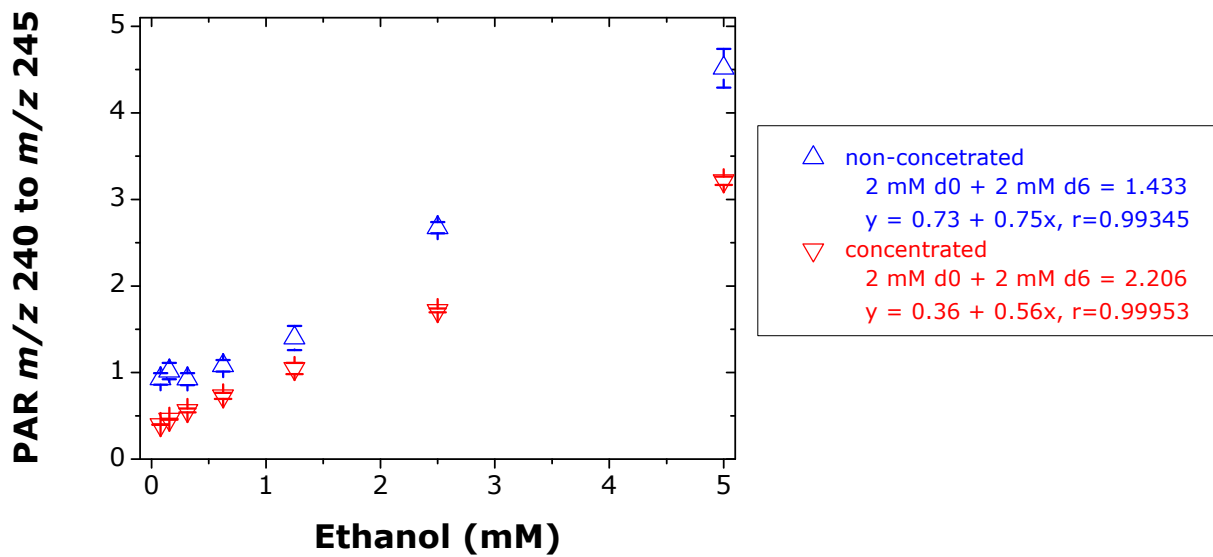
Partial GC-MS chromatograms from the quantification of ethanol in aqueous buffer before (A) and after (B) sample concentration. Numbers above the peaks indicate the retention time and number on the right of the peaks the peak area. Selected-ion monitoring of m/z 240 for unlabelled ethanol (d_0 -ethanol) and m/z 245 for the internal standard d_6 -ethanol was performed. (C) Linear regression analysis between the measured peak area ratio of m/z 240 to of m/z 245 before and after sample concentration and the ethanol concentration in the buffer subjected to derivatization. Inset shows the regression equations. The concentration of the internal standard was 2 mM in both samples.



Suppl Figure 3B

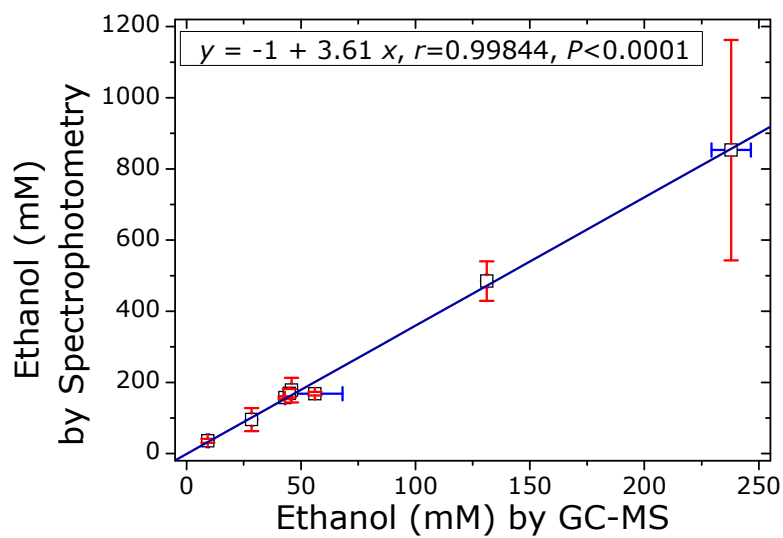


Suppl Figure 3C



Suppl. Figure 4

Correlation between ethanol concentrations measured by a commercially available spectrophotometric ethanol assay and by the GC-MS method described in this work. Data are shown as mean \pm SD from three independent experiments.



Suppl. Figure 5

Partial GC-MS chromatograms from the quantification of ethanol in the matrix fluid (A), microdialysate sample (B) and perfusion fluid (C) obtained from an in vitro microdialysis. Numbers above the solid peaks indicate the peak area. Selected-ion monitoring of m/z 240 for unlabelled ethanol (d_0 -ethanol) and m/z 245 for the internal standard d_6 -ethanol was performed after concentration of the sample by reducing the toluene volume to about 100 μ L. The concentration of the internal standard was 20 mM in all samples.

