

TECHNICAL NOTE

Concentration Estimation Equation for HAPSITE ER™

The approximate concentration of an analyte of interest that was not collected using a quantitative method can be calculated by comparing the analyte response to the HAPSITE internal standard response. Every HAPSITE ER GC/MS analysis automatically adds 0.4 mL of 5 ppm bromopentafluorobenzene (BPFB) from the internal standard canister to the collected sample.

The HAPSITE detector response to this analyte is presumed to be similar to that of BPFB. The maximum normalization number of an analyte is defined as the highest value of the most dominant mass fragment at the apex of the peak. The maximum normalization number of BPFB and the analyte are used to obtain the ratio between the two chemicals. The known quantity of BPFB and the collected sample volume are combined with this ratio to estimate the analyte concentration as shown in (1). Two examples follow.

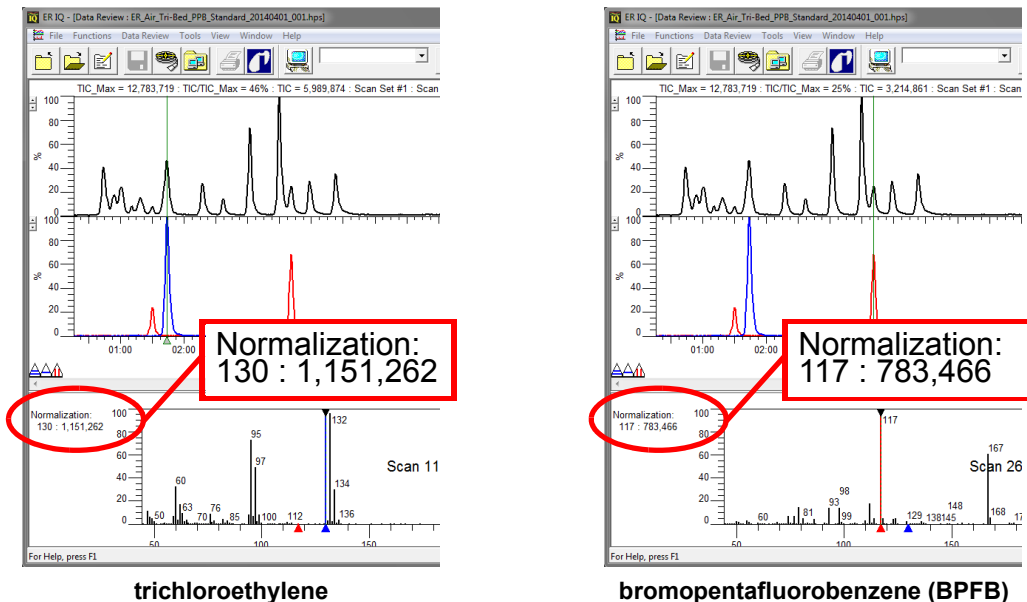
$$\frac{\text{Maximum Normalization \# of Analyte}}{\text{Maximum Normalization \# of BPFB (mass 117)}} \times \frac{(\text{Concentration of BPFB}) \times (\text{Volume BPFB})}{\text{Sample Volume}} = \text{Approximate Concentration of Analyte} \quad (1)$$

Example 1: Default method ER_Air_Tri-Bed_PPM_Standard collects a total sample volume of 5 mL. The maximum normalization number obtained for the analyte trichloroethylene is 1,151,262 for mass 130. (See Figure 1.)

The maximum normalization number for BPFB in the same analysis is 783,466 for mass 117. This information can be substituted into (1) as shown in (2). The concentration of trichloroethylene is estimated to be approximately 0.6 ppm.

$$\frac{1,151,252 \text{ (mass 130)}}{783,466 \text{ (mass 117)}} \times \frac{5 \text{ ppm} \times 0.4 \text{ mL}}{5 \text{ mL}} = 0.588 \text{ ppm} \approx 0.6 \text{ ppm} \quad (2)$$

Figure 1 Normalization Numbers

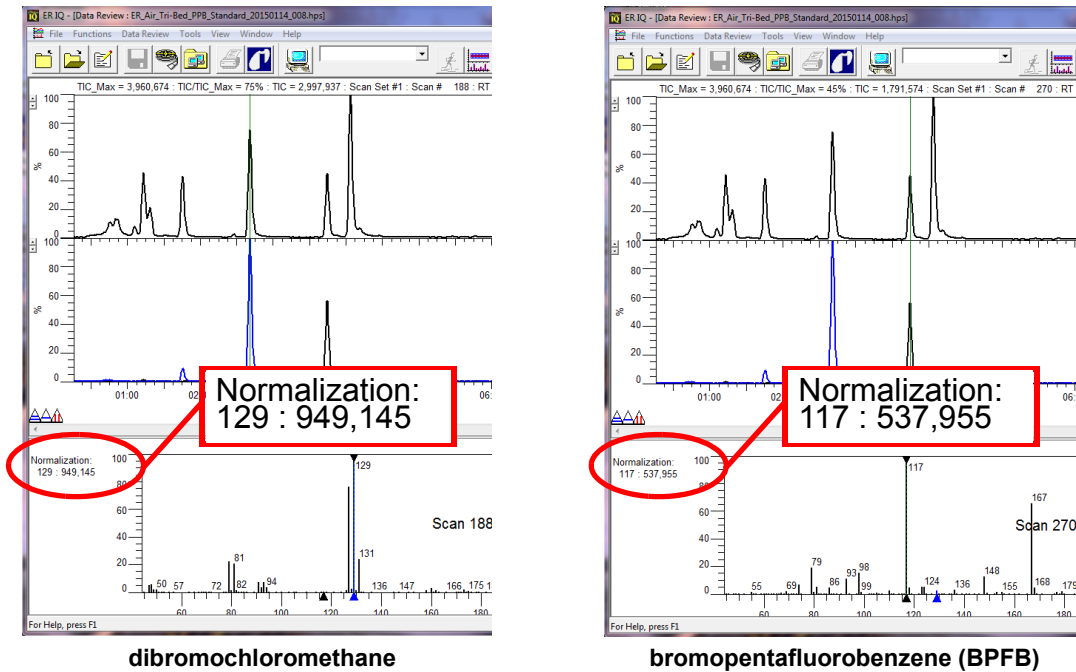


Example 2: Default method ER_Air_Tri-Bed_PPB_Standard collects a sample volume of 100 mL. The maximum normalization number for the analyte dibromochloromethane is 949,145 for mass 129. The maximum normalization number for BPFB in the same analysis is 537,955 for mass 117. (See Figure 2.)

A BPFB concentration of 5,000 ppb (5 ppm = 5,000 ppb) is used to calculate analyte concentration in ppb. Substitute the information into (1) as shown in (3). The concentration of dibromochloromethane is estimated to be approximately 35 ppb.

$$\frac{949,145 \text{ (mass 129)}}{537,955 \text{ (mass 117)}} \times \frac{5,000 \text{ ppb} \times 0.4 \text{ mL}}{100 \text{ mL}} = 35.29 \text{ ppb} \approx 35 \text{ ppb} \quad (3)$$

Figure 2 Normalization Numbers



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