

TECHNICAL NOTE

Concentration Estimation Equation for HAPSITE Smart Plus™

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 Smart Plus GC/MS analysis automatically adds 0.4 mL (0.24 second equivalent) 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 sample collection time are combined with this ratio to estimate the analyte concentration as shown in (1). Two examples follow.

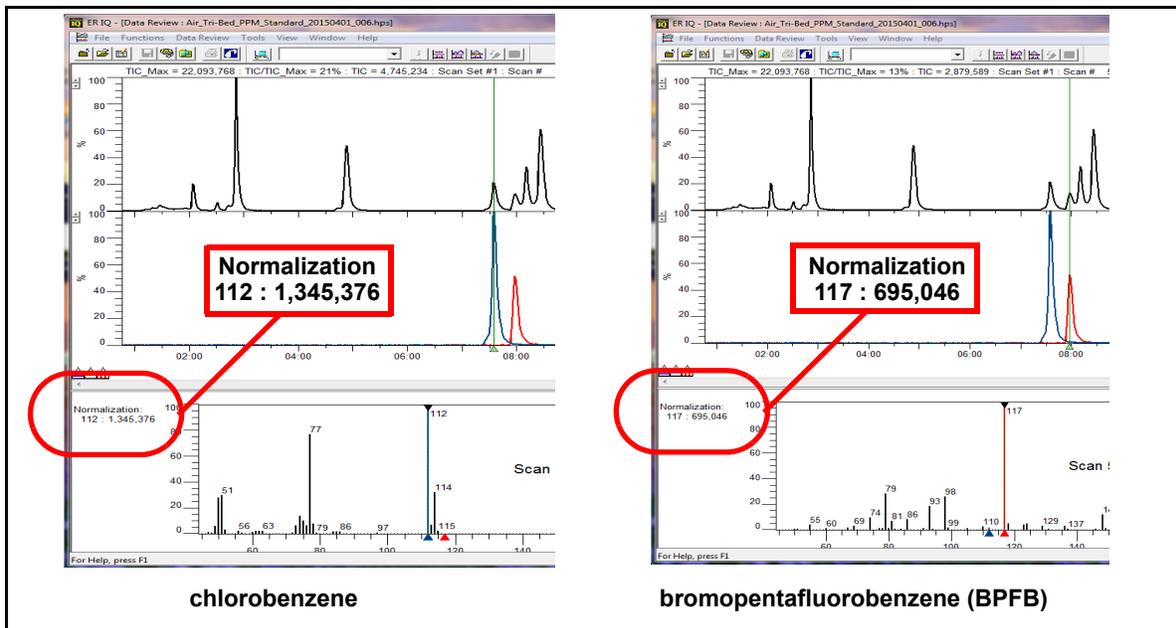
$$\frac{\text{Maximum Normalization \# of Analyte}}{\text{Maximum Normalization \# of BPFb (mass 117)}} \times \frac{(\text{Concentration of BPFb}) \times (\text{Volume BPFb})}{\text{Sample Collection Time}} = \text{Approximate Concentration of Analyte} \quad (1)$$

Example 1: Default method Air_Tri-Bed_PPM_Standard collects the sample for 3 seconds. The maximum normalization number obtained for the analyte chlorobenzene is 1,345,376 for mass 112. (See Figure 1.)

The maximum normalization number for BPFb in the same analysis is 695,046 for mass 117. This information can be substituted into (1) as shown in (2). The concentration of trichloroethylene is estimated to be approximately 0.8 ppm.

$$\frac{1,345,376 \text{ (mass 112)}}{695,046 \text{ (mass 117)}} \times \frac{5 \text{ ppm} \times 0.24 \text{ s}}{3 \text{ s}} = 0.774 \text{ ppm} \approx 0.8 \text{ ppm} \quad (2)$$

Figure 1 Normalization Numbers

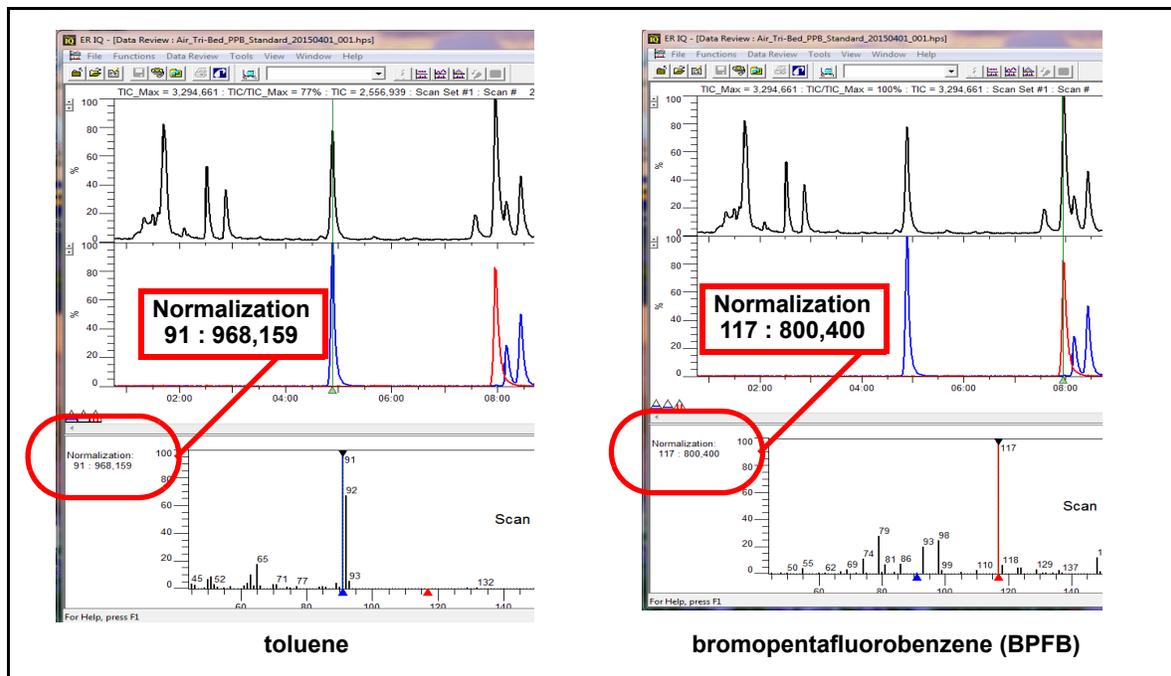


Example 2: Default method Air_Tri-Bed_PPB_Standard collects a sample for 60 seconds. The maximum normalization number for the analyte toluene is 968,159 for mass 91. The maximum normalization number for BPFB in the same analysis is 800,400 for mass 117. (See Figure 2.)

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 toluene is estimated to be approximately 24 ppb.

$$\frac{968,159 \text{ (mass 91)}}{800,400 \text{ (mass 117)}} \times \frac{5,000 \text{ ppb} \times 0.24 \text{ sec}}{60 \text{ sec}} = 24.19 \text{ ppb} \approx 24 \text{ ppb} \quad (3)$$

Figure 2 Normalization Numbers



www.inficon.com reachus@inficon.com

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