B62 Quantifying the Uncertainty of Measurement for Gas Chromatography/Mass Spectrometry (GC/MS) Acceptance Criteria

J. Tyler Davidson, MS, West Virginia University, 21 Marion Street, Apt 101, Morgantown, WV 26505; and Glen P. Jackson, PhD, West Virginia University, Dept of Forensic and Investigative Science, 208 Oglebay Hall, Morgantown, WV 26506-6121*

After attending this presentation, attendees will better understand the current acceptance criteria used for the identification of chemical substances with GC/MS. Attendees will also understand how the variability measured over more than six months in three different laboratories on five different instruments compares with recommended acceptance criteria provided by different governing bodies.

This presentation will impact the forensic science community by providing a numerical basis for the acceptance criteria generated with respect to GC/MS instrumentation. Additionally, the demonstration of a simple technique to determine the analytical uncertainty of measurement with the use of a 2 sigma (2s) criterion will assist practitioners with determining the uncertainty of measurement for their own analytical instrumentation. Finally, a demonstration of the analytical uncertainty of measurement in comparison to the published values will assist with the development of standardized language for the assessment and presentation of analytical uncertainty of measurement in court.

This research is not hypothesis driven; however, the experimental results are important and novel in the sense that the reproducibility of GC/MS results are rarely evaluated in such a detailed manner. The results provide practitioners with an appreciation for how realistic uncertainty compares with the acceptance windows recommended by different organizations.

The selectivity and confidence of compound identification by GC/MS is affected by the uncertainty in measuring the retention times and fragment ion abundances. Forensic chemists need to understand the factors that influence retention time and mass spectral measurements so that they can better present and defend the results in court.

Data analysis was conducted on GS/MS measurements collected using 13 different drug standards from three different laboratories using five different instrumental setups. An expanded uncertainty of two times the standard deviation from the mean (2σ) was used to identify the uncertainty of measurement for the retention time and relative ion abundance measurements made within these laboratories. The rationale for the use of a 2σ criterion is that this corresponds with an estimate of the 95% confidence interval, assuming normally distributed data.

Based on the numerical results, the retention time acceptance criteria currently recommended by different agencies are considerably wider than the average 2σ per week or per month determined through this study. Similarly, differences exist between recommended acceptance criteria for the uncertainty of measurement of relative ion abundances and this data set; however, when the uncertainty of measured relative ion abundances was averaged across all substances and all laboratories, the measured uncertainties agree quite well with the recommended acceptance criteria. The numerical analysis based on this data set indicates that the acceptance criteria within an instrument within a laboratory should be considerably tighter for the retention time. Also, depending on the tune frequency of the mass spectrometer, the relative ion abundance measurements should have narrower acceptance criteria than typically recommenced. The application of tighter acceptance criteria would provide more selective identification than the currently used broad-applicable recommendations.

Variability, Acceptance Criteria, GC/MS