B193 Systematic Optimization of Instrumental Conditions: Ion Mobility Spectrometry as a Model Device

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After attending this presentation, attendees will understand a method of finding optimal conditions for an ion mobility spectrometry instrument.

This presentation will impact the forensic community and/or humanity by demonstrating how to use ion mobility spectrometry as a device to detect evidence and how under optimal conditions the instrument's selectivity and sensitivity is be greatly enhanced.

This presentation presents the optimization results of an existing Solid Phase Microextraction-Ion Mobility Spectrometer (SPME-IMS) interfaced system previously developed by this group as a sampling and pre-concentration device to collect volatile drugs or explosives (or taggants) and the volatile compounds believed to be odor signatures of drugs and explosives using an IMS detector.

This group and other researchers have demonstrated that improvement in the analysis of several organic explosives and taggants is achieved by varying the drift tube temperature of the IMS instrument[1,3] by promoting adduct stability. These changes to analysis temperature lead to different product ion distributions which can be used to resolve interferences from the analytes.[2] Additionally, product ion identities can be manipulated through the addition of chemicals to produce alternative reactant ions.[2] Therefore, changes to reactant ions may also lead to different product ion distributions, and thus make these products easier to resolve in the IMS. The optimization presented varies several parameters as well as the variation of the dopant gas used for the SPME interfaced IMS instrument.

The optimization procedure developed can be used for finding the optimal operating conditions of an IMS system for any compound of interest. The search algorithm lends itself to the class of problem where the IMS instrument has a number of settings/parameters that can be varied, and therefore has a large number of possible configurations which is difficult and time consuming to evaluate exhaustively through a random search routine. The optimization procedure approach is available in a programming file and is ready to be used. Once the investigator defines a problem domain (ranges of the various operating parameters), the algorithm can be applied to optimize the detection performance of the IMS instrument for a specific compound.

This study developed a methodical and objective method of optimization to enhance selectivity and sensitivity in the IMS for a list of drugs and explosives and their volatile/semi-volatile chemical marker compounds such as DMNB, 2-E-1-hexanol, cyclohexanone, 2- nitrophenylamine, diphenylamine, methyl benzoate, piperonal, benzaldehyde, and acetic acid. Once the optimal settings of each of these compounds are found, their limits of detection were determined at their optimal settings and also presented.

References:

1 Perr J. M., Furton K.G., Almirall J.R., J. *Separation Sciences*, 2005 28(2), 177-183.

2 J.M. Perr, K.G. Furton, and J.R. Almirall, *Pro. SPIE - The Int. Soc. for Optical Engineering*, 2005, 5778, 667-672.

3 Ewing, R. G.; Atkinson, D. A.; Eiceman, G. A. *Talanta* (2001), 54(3), 515-529.

Optimization, IMS, Explosives and Narcotics

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