

Improving the Selectivity of a High Pressure Mass Spectrometer

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Mass spectrometry has been a workhorse technique for chemical analysis despite its traditional constraint to a laboratory setting. Conventional instrumentation is expensive and large, requires significant power, and must be operated by trained technicians. Recent work in this group has pushed the boundaries of portable mass spectrometry by operating at higher pressures of background gas (~1 Torr) and by using air instead of helium. These changes have greatly reduced the pumping requirements of the instrument, reducing size, weight and power (SWaP). Improvements have led to fully hand-portable devices. Portable instrumentation has provided many advantages over conventional laboratory analysis, especially in time-sensitive applications such as threat detection. Providing users with rapid information allows them to take appropriate response procedures to protect themselves from the detected threat. Many response protocols, however, require significant time and money, as well as being effective only for a given threat. Analytical selectivity is therefore an extremely important aspect of threat detection in order to eliminate false positives while maintaining low limits of detection. Mass spectrometry is inherently selective by virtue of detecting a compound's mass-to-charge ratio. This selectivity can be further improved by adding a separation and by implementing tandem mass spectrometry. Gas chromatography is appropriate for portable instruments and can achieve separations quickly. Collision induced dissociation (CID) can provide fragmentation for tandem mass spectrometry without increasing the overall footprint of the device. A gas chromatograph (GC) has been attached to the inlet of a high pressure mass spectrometer (HPMS) to demonstrate the compatibility of the techniques. Using low flow rates and fast separation times, suitable for a proposed micro-GC, many compounds, including chemical warfare agent (CWA) simulants, have been detected from complex mixtures. Tandem mass spectrometry uncovers extra chemical information about a target of interest by revealing fragmentation patterns and elucidating the chemical structure. CID has been demonstrated in microscale cylindrical ion traps ($r_0 = 170\text{-}500\ \mu\text{m}$) at pressures up to and exceeding 1 Torr of air. A wide variety of compounds have been fragmented, and studies have explored the most effective conditions for efficient fragmentation. Gas chromatography and collision-induced dissociation are shown to be effective and compatible techniques for improving the selectivity of a hand-portable device with a rapid response time.