Considerations in Nitrogen Direct Analysis in Real Time Mass Spectrometry: An Alternative to Helium

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Overview
- Helium is primarily utilized as the DART ionization gas and the current global helium shortage has increased its price and reduced its availability.
- Nitrogen is mainly used for DART in stand-by mode to improve operational cost efficiency; however, it is also a viable ionization gas.
- Nitrogen was used as the ionization gas for DART and a variety of compounds were analyzed and compared to helium.
- Results were comparable to helium with nitrogen as the ionization gas. In some instances, spectra were simpler and cleaner with nitrogen.

Introduction
- Helium has been predominantly used as the ionization gas for DART.
- Nitrogen, which can be produced by generators, is more readily available and cost-effective compared to helium. Yet nitrogen has mainly been utilized for DART in stand-by mode.
- There have been a few recent nitrogen DART studies, but at present nitrogen has not been extensively utilized or studied
- In consideration of the helium shortage, nitrogen was evaluated to determine viability as an ionization gas for DART for a variety of compounds. DART grid voltage and flow rate, as well as nitrogen purity was also examined.

Methods
- A DART-SVP ionization source was interfaced to a Waters QDa single quadrupole MS and a Thermo Q Exactive orbitrap high resolution MS.
- A PEAK Scientific NG3000A nitrogen generator was used to produce the nitrogen for DART.
- Transmission mode DART and gas temperatures of 250°C and 300°C were utilized for pesticides and drugs/explosives, respectively.
- A 2^2 full factorial design of experiment (DOE) was employed to study and identify DART parameter and nitrogen purity considerations.

Tables 1 & 2: DOE factors and their high and low levels.

<table>
<thead>
<tr>
<th>Factors</th>
<th>Level</th>
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</thead>
<tbody>
<tr>
<td>A</td>
<td>DART Grid Voltage</td>
</tr>
<tr>
<td>B Nitrogen Source</td>
<td>Cylinder</td>
</tr>
<tr>
<td>Factors</td>
<td>Level</td>
</tr>
<tr>
<td>A</td>
<td>DART Grid Voltage</td>
</tr>
<tr>
<td>B Nitrogen Flow Rate</td>
<td>2.14 l/min</td>
</tr>
</tbody>
</table>

Figure 1: PEAK Scientific NG3000A N2 generator and its specifications.

Results

Comparison between N2 Cylinder and Generator
- N2 DART spectrum of cocaine is comparable between using the generator and cylinder tank.
- Main effect plot shows higher peak area with the cylinder; however, it is not statistically significant as the effect value is within the 95% confidence level.

Effect of DART Grid Voltage and Flow Rate
- Low grid voltage increases peak area and is significant only for RDX.
- Higher flow rate increases peak area and is significant for both cocaine and RDX.

Comparison between Helium and Nitrogen
- Spectra are comparable between helium DART and nitrogen DART for all tested compounds.
- In certain instances, such as with RDX, the spectrum is simpler and cleaner with nitrogen DART.
- Replacement and oxidation occurs more frequently with nitrogen DART and is dependent on chemical structure.

Conclusions
- PEAK Scientific NG3000A is the only generator found suitable for DART and the results are comparable to those obtained using Grade 4.8-cylinder tanks.
- DART gas flow rate has a significant effect on signal response for all tested drugs whereas grid voltage has a significant effect only for explosives.
- Replacement and oxidation ion reactions occur more with nitrogen DART.

References