Application of the AMDIS Mass Spectral Deconvolution Algorithm for the GC-MS Characterization of Cigarette Smoke

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Introduction and Objective
The number of known compounds in tobacco smoke is about 4,800.
A recent study has shown that there are about 30,000 compounds in cigarette smoke samples analyzed by two-dimensional GC coupled to TOF-MS.
Chromatograms of tobacco smoke analysis suffer from severe co-elution problems.
The aim of this project is to investigate the use of a mass spectral deconvolution technique called Automatic Mass Spectral Deconvolution and Identification System (AMDIS) to unravel the spectral overlap for reliable mass spectral interpretation.

Materials and Methods
Glassware: Silanized 25 ml glass gas impinger; pore size 6-8 mm
Solvent: 20 mL Methanol
Double Take Sampler pump: 130-160 mL/min flow rate
One cigarette burns for ~ 5-7 minutes
Agilent Technologies 6890N/5973 GC-MSD

Results
GC-MS Analysis of American and Bidi Cigarette Smoke Sample

Table 1: A partial list of compounds that were exclusively identified by AMDIS with match indices greater than 80

<table>
<thead>
<tr>
<th>Name</th>
<th>R.T.</th>
<th>Total</th>
<th>Weighted Reverse</th>
</tr>
</thead>
<tbody>
<tr>
<td>1,3-Cyclopentadiene, 5,5-dimethyl-</td>
<td>3.24</td>
<td>8254</td>
<td>82</td>
</tr>
<tr>
<td>2-Propanone, 1-hydroxy-</td>
<td>3.334</td>
<td>498698</td>
<td>94</td>
</tr>
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<td>Pyrrolidine, 1-methyl-</td>
<td>3.686</td>
<td>95068</td>
<td>93</td>
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<tr>
<td>1-Hydroxy-2-butanone</td>
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Conclusion
The AMDIS program is especially effective in unraveling the spectra for the identification of ketones, aromatic amines, pyridines, alcohols, and polycyclic aromatic hydrocarbons.
About 50-300% more peaks were detected for the chromatograms of different types of cigarette smokes and 20-250% more peaks were tentatively identified with match indices better than 80 using the AMDIS software.

References

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