Identifying "Buried" Information in LC/MS Data

It is not always easy to identify minor unknown components in complex LC/MS datasets. The new DART™ ion source screened for components that were not immediately recognized in LC/MS analysis of tea samples.

LC/TOFMS datasets can contain high-resolution, exact-mass data for all ionized components of a complex mixture. Even with concurrent UV detection and chromatographic enhancement software, it is not always easy to identify all of the components that are present in the dataset. Furthermore, suppression effects may mask important information. Here, a new technique known as Direct Analysis in Real Time (DART™) was used to screen tea samples and provide elemental compositions for minor components that were "buried" in LC/MS data collected for tea analysis. DART is a powerful new ionization method that permits direct analysis of solid, liquid, or gas samples at atmospheric pressure and ground potential. DART has been applied to rapid in-situ analysis of a very wide range of materials ranging from drugs to explosives, foods, and beverages.

Experimental Conditions

Drinking-quality green tea was analyzed directly by dipping a glass rod into the liquid and placing the rod between the DART source and the mass spectrometer orifice. Analysis was complete within 30 seconds. Following the tea analysis, a piece of filter paper dipped in PEG 600 was placed in front of the DART to provide reference masses for exact mass measurements. LC/MS conditions were described in a previous application note. (http://www.lcgcmag.com/lcgc/article/articleDetail.jsp?id=87195).

Results and Conclusions

Elemental compositions for several components are given in Table 1 for several compounds identified by DART. Compositions were identified by combined exact-mass measurements and isotope pattern matching for the observed $[M+H]^+$ species. Candidate compositions were proposed by searching the mass spectral database for suitable compounds having the correct elemental composition. Following DART analysis, reconstructed ion mass chromatograms were generated from the LC/MS data for the exact mass of each component.

DART is ideal for screening because the analysis is rapid, suppression is minimal, solvent adducts are not observed, and exact mass measurements are simple and accurate. The presence of several isomers having these candidate compositions was confirmed by the RIC's. The LC/MS data shows well-separated isomers and provides quantitative information about each component.

1. $C_6H_4O_2$: Benzoquininone
2. $C_4H_4O_2$: Furanone
3. $C_5H_4O_2$: Furfural, pyranone
4. $C_6H_6O_3$: Maltol
5. $C_7H_6O_3$: Sesamol, dihydroxybenzaldehydes, salicylic acid
6. $C_{15}H_{10}O_6$: Kaempferol
7. $C_{15}H_{10}O_7$: Quercetin
8. $C_{15}H_{10}O_8$: Myricetin

Table 1. Elemental compositions and some candidate compounds identified by DART in green tea.

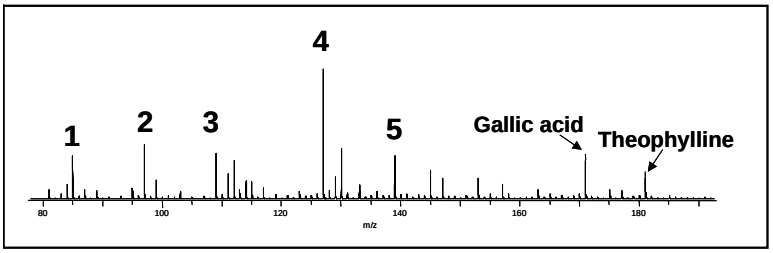

Figure 1. Portion of positive-ion DART mass spectrum for green tea sampled with a glass rod. Larger components such as #6-8, caffeine and catechin were detected but are not shown here.

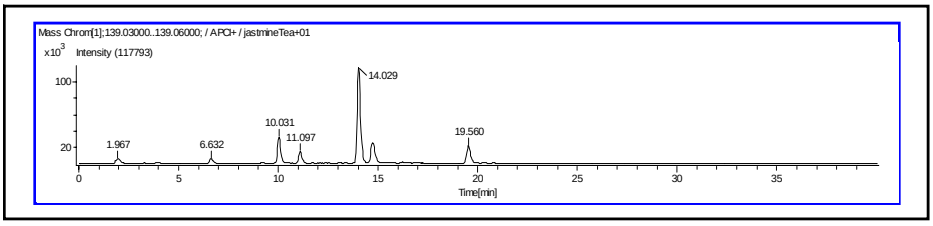

Figure 2. Reconstructed mass chromatogram for m/z 139.0395 ($C_7H_7O_3^+$).

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