

## Delta Ion Current ( $\Delta I_C$ )- A novel approach to plot total ion currents enhancing the signal from newly detected ions

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## Overview:

The novel Peak Express™ technology was evaluated and applied to natural product extracts.

Peak Express utilizes delta ion currents, a differential ion current with significantly improved signal-to-noise as well as enhanced detection ability for low abundance compounds.

## Introduction:

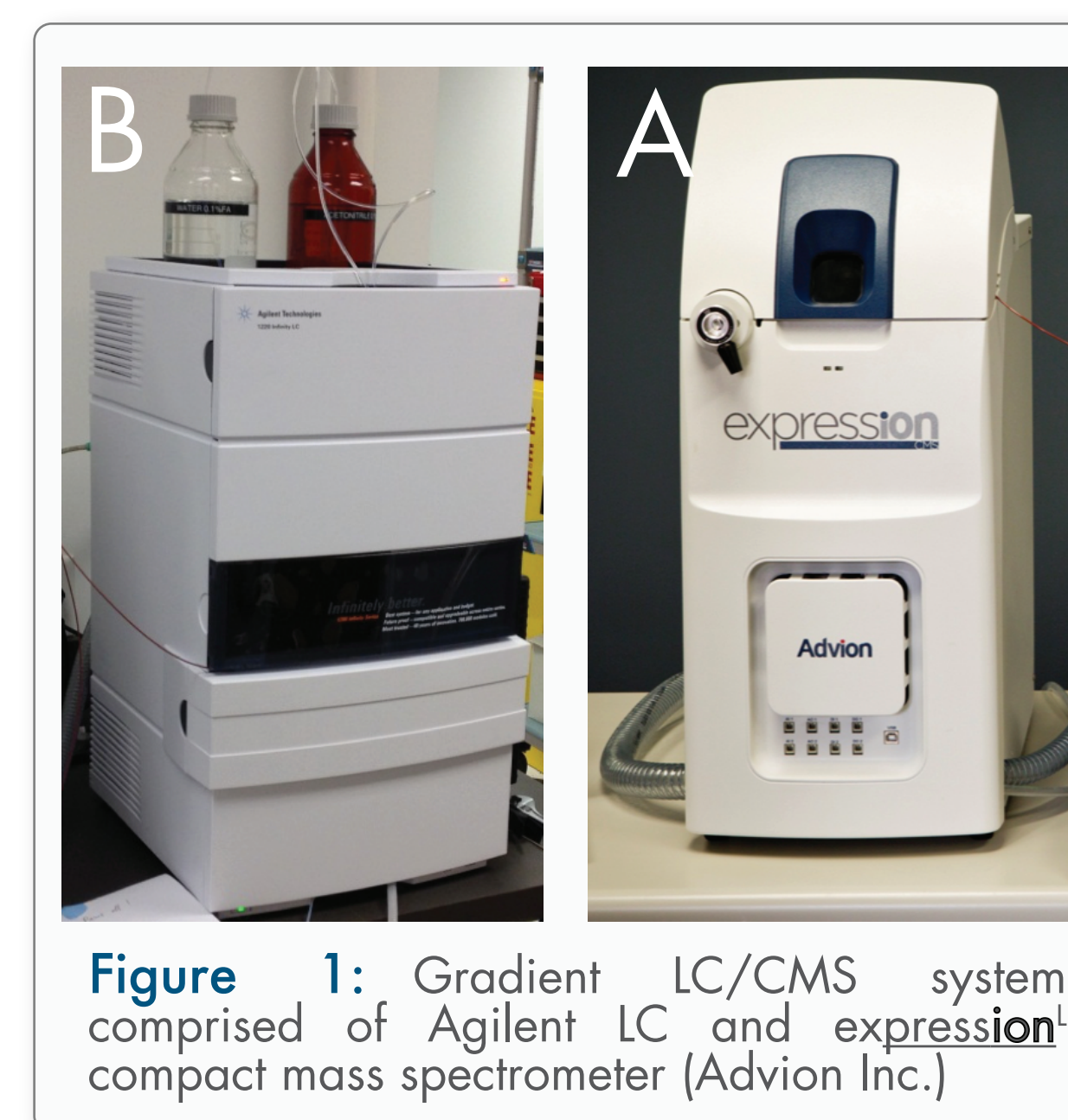
When analyzing unknown compounds on a single quadrupole mass spectrometer (MS), it is common to scan the full mass range of the mass spectrometer. Changes in Total Ion Current (TIC) or Base Peak Ion Current (BPI) are used to determine when a new compound elutes from the LC system and/or where to interrogate the data further or collect fractions for further processing.

However, even a comparatively high analyte current from a newly eluting compound may be masked in the TIC by the intensity, multitude, or random fluctuations of background ion signals. As a result, little to no discernible change in TIC might be visible (poor signal-to-noise) and the eluting compound may be missed.

Delta Ion Chromatograms ( $\Delta IC$ ) based on differential ion current plots provide new ways to enhance the signal contribution from newly detected ions while minimizing background ion signals [1]. Peak Express™ is a novel technology taking advantage of these enhancements.

## Methods and Materials:

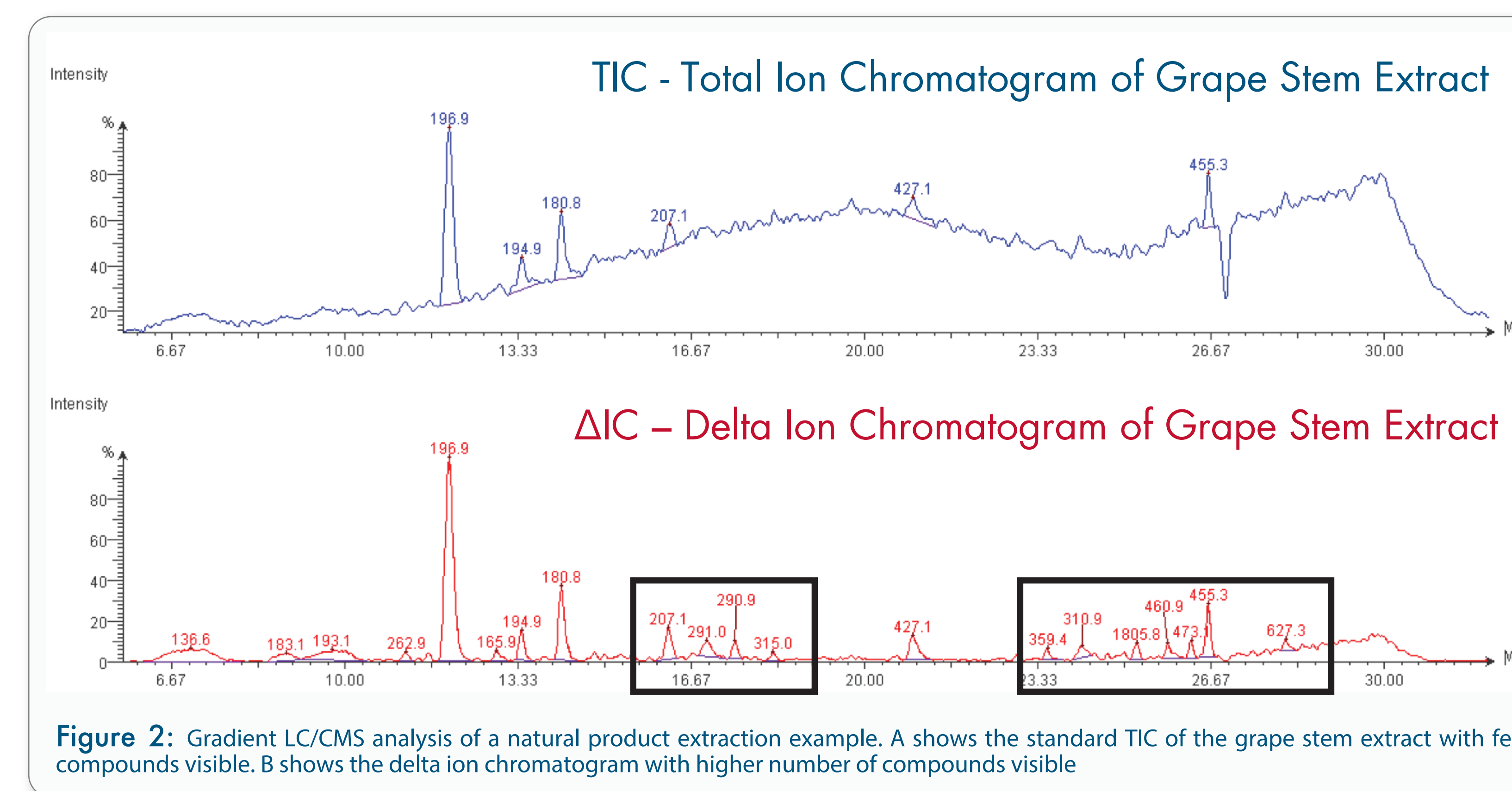
- Agilent 1220 Infinity LC System
- Flow Rate: 200  $\mu$ L/min
- Column: Supelco Titan C18 (100 X 2.1 mm, 1.9 $\mu$ m)
- Gradient using Methanol and Water with Ammonium Acetate and Acetic Acid
- Advion expression<sup>†</sup> CMS single quadrupole mass spectrometer with Peak Express™ technology using  $\Delta$ IC
- Full range scan (10-2000 m/z)
- Positive/Negative ESI



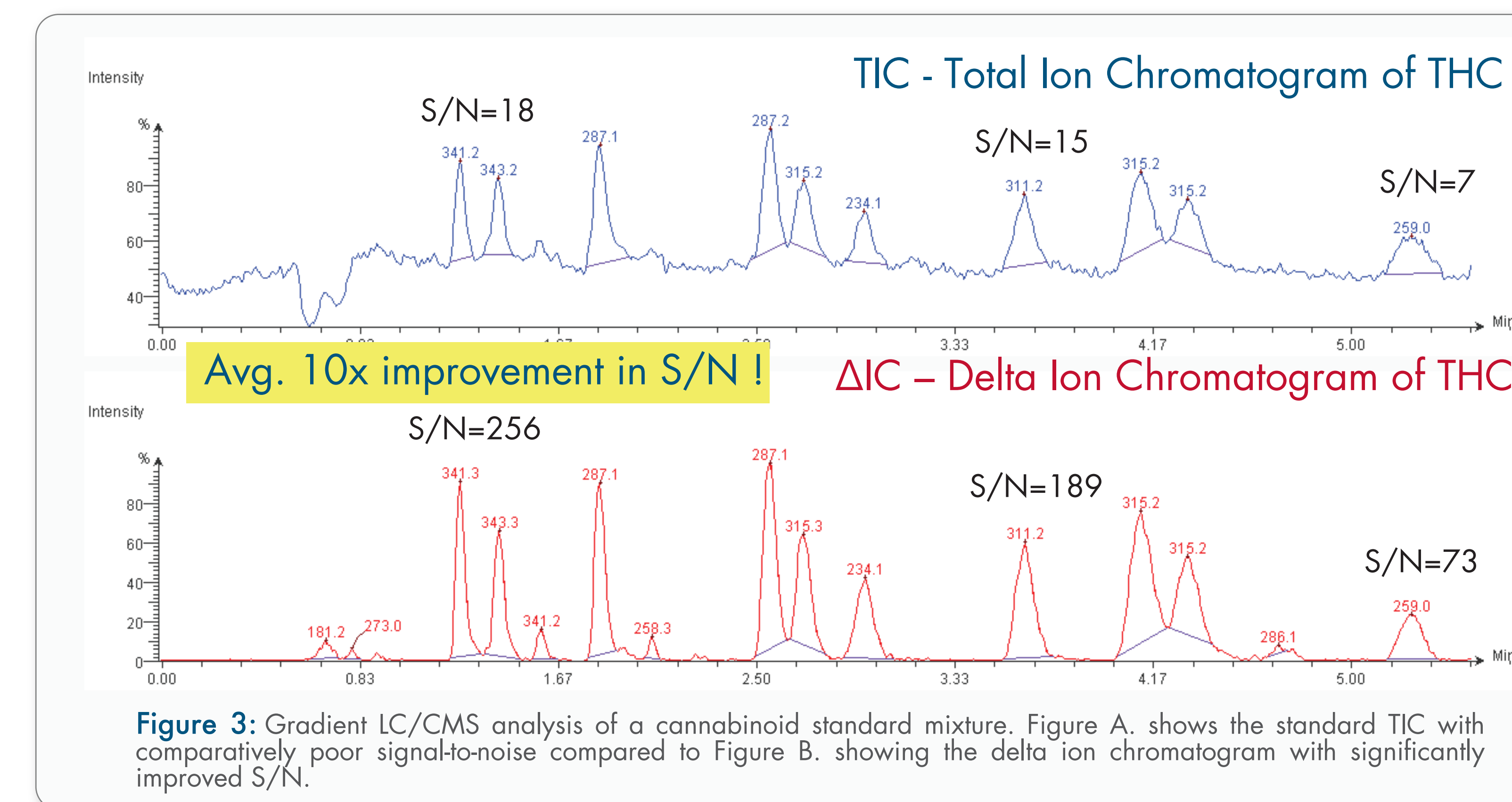
**Figure 1:** Gradient LC/CMS system comprised of Agilent LC and expression<sup>®</sup> compact mass spectrometer (Advion Inc.)

## Results:

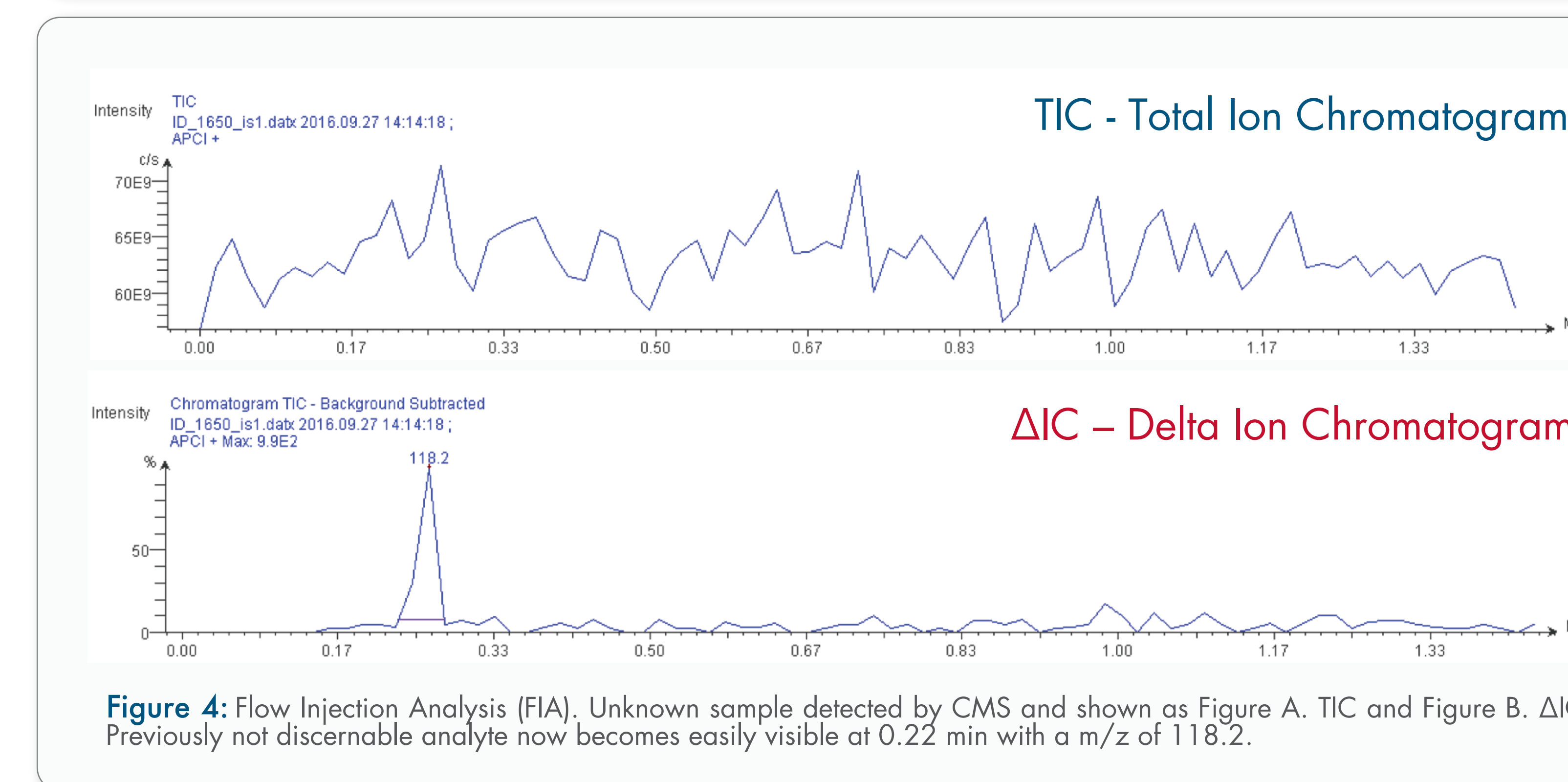
- Grape Stem Extract shows natural products in  $\Delta$ IC that are otherwise missed in TIC, these could be collected by downstream fraction collector and further investigated
- THC standard sample mix shows average 10x improvement in S/N from standard TIC to  $\Delta$ IC
- FIA analysis of an unknown compound shows sensitivity gain and simplification in the delta spectrum ( $\Delta$ S) for data analysis



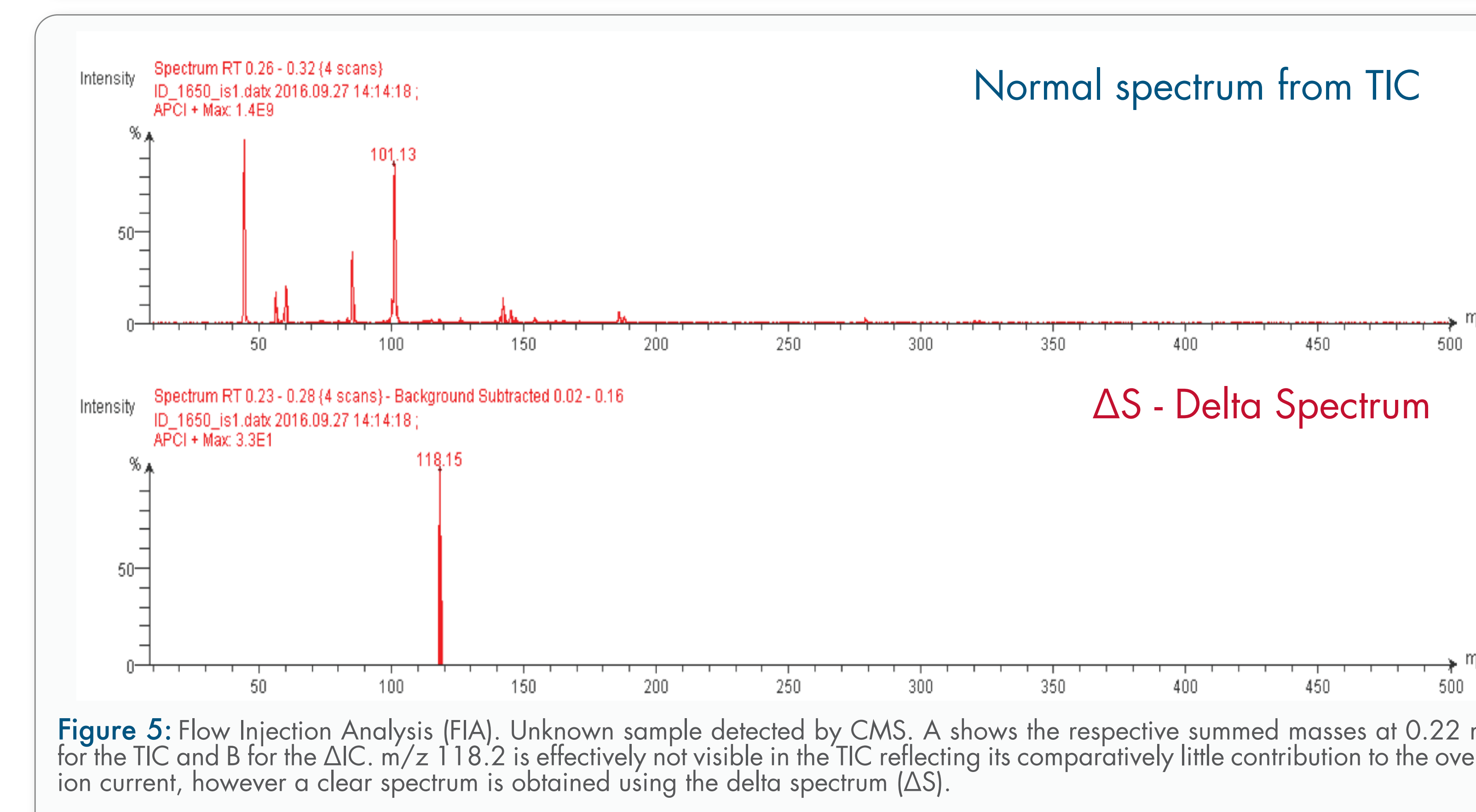
**Figure 2:** Gradient LC/CMS analysis of a natural product extraction example. A shows the standard TIC of the grape stem extract with few compounds visible. B shows the delta ion chromatogram with higher number of compounds visible



**Figure 3:** Gradient LC/CMS analysis of a cannabinoid standard mixture. Figure A. shows the standard TIC with comparatively poor signal-to-noise compared to Figure B. showing the delta ion chromatogram with significantly improved S/N.



**Figure 4:** Flow Injection Analysis (FIA). Unknown sample detected by CMS and shown as Figure A. TIC and Figure B.  $\Delta$ IC. Previously not discernable analyte now becomes easily visible at 0.22 min with a  $m/z$  of 118.2.



**Figure 5:** Flow Injection Analysis (FIA). Unknown sample detected by CMS. A shows the respective summed masses at 0.22 min for the TIC and B for the  $\Delta$ TIC.  $m/z$  118.2 is effectively not visible in the TIC reflecting its comparatively little contribution to the overall ion current, however a clear spectrum is obtained using the delta spectrum ( $\Delta$ S).

## Conclusions:

- Delta ion chromatograms ( $\Delta$ IC) based on a differential ion current greatly improve signal-to-noise compared to classical TIC plots in both LC/MS as well as FIA/MS.
- Some eluents that could not be seen in the TIC plot at all are readily discernable within the  $\Delta$ IC plot and can automatically be labelled for improved data analysis.
- Delta Spectrum ( $\Delta$ S) shows a clear and easy to interpret mass spectrum devoid of background signal
- Consequently,  $\Delta$ IC and  $\Delta$ S help to detect more analytes in complex mixtures, especially otherwise elusive low abundance compounds.
- Peak Express™ technology and its  $\Delta$ IC and  $\Delta$ S are valuable tools when working with unknown compound mixtures such as natural product extracts.

### Literature and Acknowledgements:

[1] Klecha L: GENERATION OF DISCOVERY ION CURRENTS AND MASS SPECTROMETRY AND USES THEREOF (2017). USPTO Application 15/408,146

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