

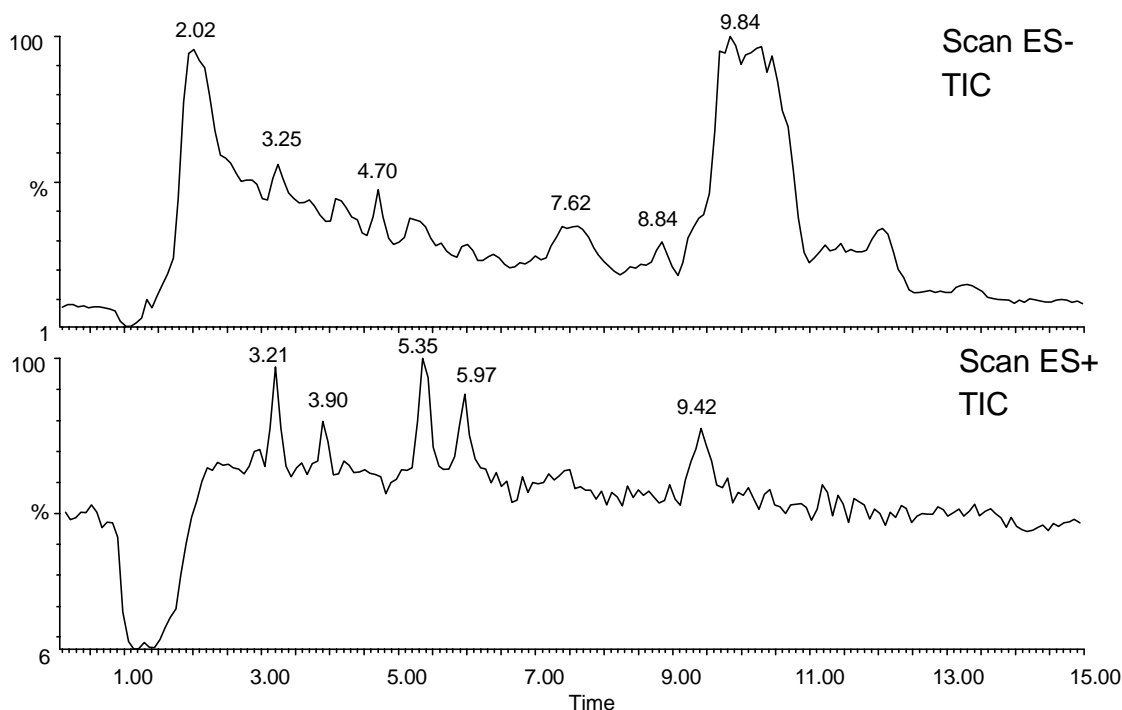
# Waters Alliance™ Systems for LC/MS ESI/APCI Applications

## LC/MS: Simultaneous Positive and Negative Ion Detection

**Highlights:** LC/MS methods development requires choosing an ionization technique and a detection mode. Both Waters Alliance™ LC/MS systems featuring either the Platform LC or Platform LCZ detector permit positive and negative ion acquisition within the same chromatographic run using either electrospray (ESI) or atmospheric pressure chemical ionization (APCI). An example of this will be illustrated using ESI for a natural product.

### Experimental

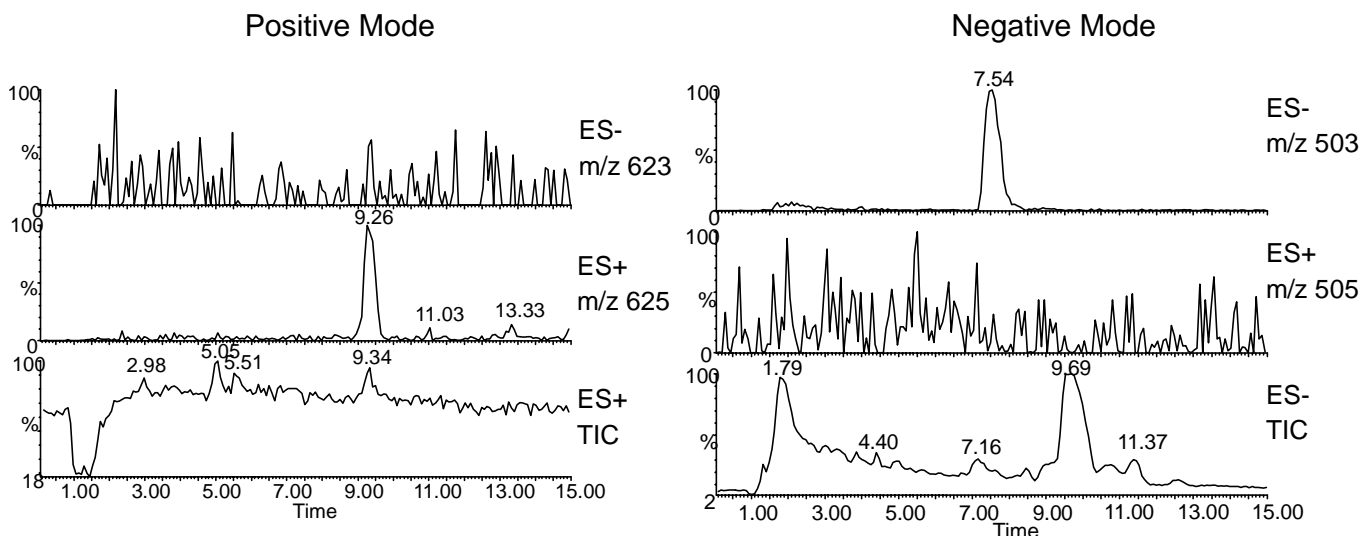
A powder from a plant was extracted in buffered methanol by sonication and filtered before injection. The sample was chromatographed on a Waters Alliance™ system with a Platform LC mass detector using a linear gradient of mobile phase containing water, acetonitrile, methanol and 1 mM triethylamine acetate, pH 7 on a Symmetry® C8 2.1x150 mm column. Ions generated by electrospray were detected by positive and negative full scans ( $m/z$  100-1000) with an interscan delay time of 0.3 seconds. Compounds with molecular weights of 504 and 624 Da were sought.



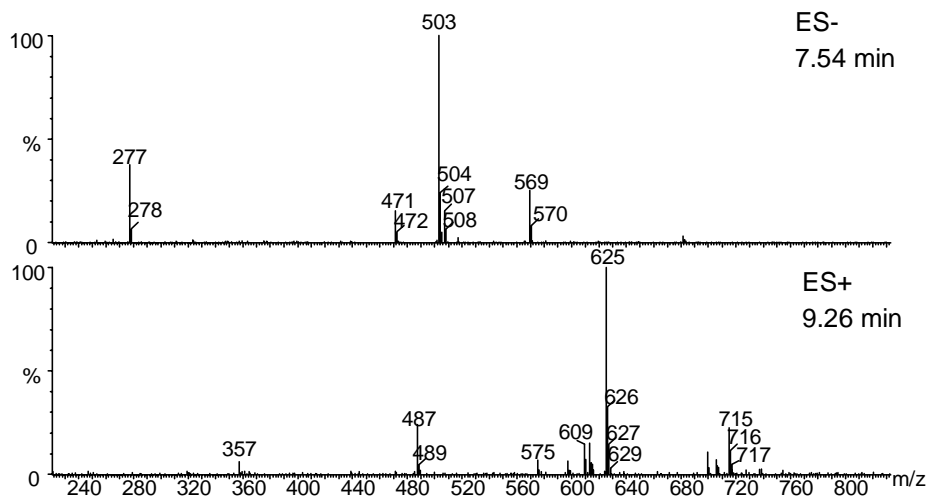
The total ion chromatograms (TIC) for scans  $m/z$  from 100 to 1000 are shown for each. Different peaks were detected by positive and negative modes.

Positive and negative ion production and sensitivity will depend on the mobile phase and the types of analytes. Ionization of acidic compounds (ESI-) will be suppressed by the addition of acid, while ionization of basic compounds (ESI+) will be suppressed by the addition of base to the mobile phase. A neutral mobile phase will be more universal.

Extracted single ion chromatograms of  $m/z$  for the two desired compounds are shown below. The compound with molecular weight 624 Da was detected by positive mode  $[M+H]^+$  625 and not detected in the negative mode  $[M-H]^-$  623. The compound with molecular weight 504 Da was detected by negative mode  $[M-H]^-$  503 and not detected in the positive mode  $[M+H]^+$  505.



### Mass Spectra of Peaks at Desired $m/z$



The mass spectra of  $m/z$  503 and  $m/z$  623 were extracted from the apexes of their respective peaks at 7.54 and 9.26 minutes.

### Summary:

The compounds in a complex sample can be separated by gradient chromatography on a Waters Alliance system with a Symmetry column. Subsequent ionization (ESI in this example) and then alternating positive and negative modes can then be performed. With a short interscan delay of 0.3 seconds, one can obtain a number of scans in each mode across each chromatographic peak. This ability to use both modes of ion polarity saves time and sample because only one injection produces data for positive and negative ions. This can speed the methods development process and shorten analysis time when both positive and negative detection modes are required for mass data.