

Waters Corporation, MS Technologies Centre, Manchester, UK

### Introduction

The Waters® LCT Premier™ Mass Spectrometer is the highest performance bench-top orthogonal acceleration time-of-flight (oa-TOF) LC/MS system available today. The innovative design and hardware enhancements to our original LCT™ Mass Spectrometer's design provide the user with the capabilities of positive/negative source ionisation capabilities on a per-injection basis, but even faster than before. With new detector and electronic components, the instrument can switch from positive to negative ion, or vice versa, in a minimum of 200 milliseconds, or 300 milliseconds for exact mass measurement.

Positive/negative ionisation switching provides the user with the capability of analyzing samples during LC/MS experiments without needing to know a compound's particular ionisation mode. This is ideal for screening applications or when multi-component mixtures are being analyzed. Even at 300 milliseconds switching time, exact mass measurements can be carried out—and all this during LC time scales.

Figure 1 shows a mass spectrum of raffinose analysed with positive/negative electrospray ionisation. With 300 milliseconds switching on the LCT Premier, the exact mass measurements are within 3 ppm. The lower spectrum shows the ES+  $[M+Na]^+$  ion of raffinose and the upper spectrum shows the ES-  $[M-H]^-$  ion. Both exact mass measurements obtained from the single LC/MS analysis are within 2 ppm of actual mass.

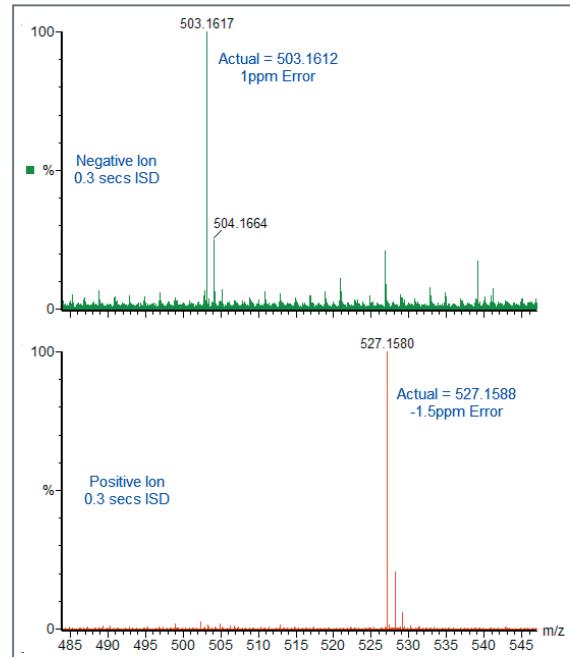


Figure 1. Positive/Negative switching analysis of Raffinose.

Figure 2 shows another example of positive/negative ionisation switching and its usefulness for complex mixture analysis. Figure 2 shows the LC/MS chromatograms for the ES+, ES- and diode array trace for a natural product extract. Figure 3a and 3b shows the simultaneous exact mass spectra obtained for both peak A (iso-orientin) and peak B (kaempferol-3-rutinoside) from the same injection. All exact mass measurements are within 2 ppm of actual providing highly specific answers.

LCT Premier: oa-TOF providing simultaneous exact mass measured positive/negative ionization.

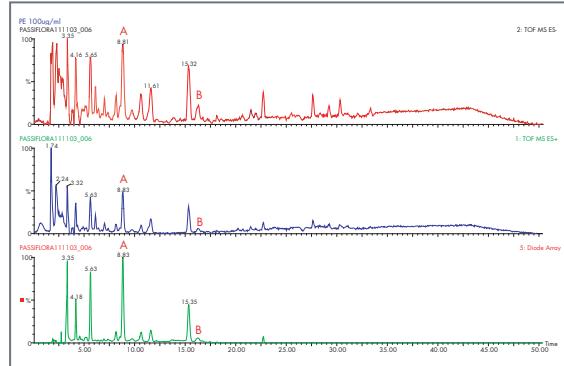


Figure 2. Positive/Negative ionisation of a Passiflora extract.

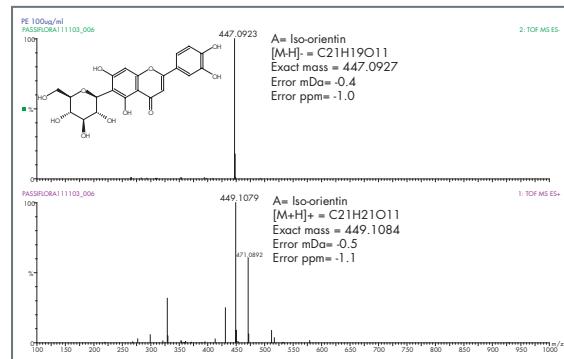


Figure 3a. Positive/Negative ionisation mass spectra of Iso-orientin (Peak A).

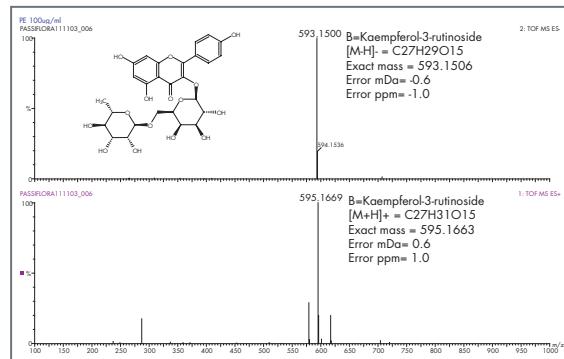


Figure 3b. Positive/Negative ionisation mass spectra of Kaempferol-3-rutinoside (Peak B).

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# Waters

WATERS CORPORATION

34 Maple St.

Milford, MA 01757 U.S.A.

T: 508 478 2000

F: 508 872 1990

[www.waters.com](http://www.waters.com)

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