

Nota applicativa

## LCT Premier: Positive/Negative Ionization Switching

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Waters Corporation

This is an Application Brief and does not contain a detailed Experimental section.

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### Abstract

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.

### Benefits

Positive/negative ionization switching provides the user with the capability of analyzing samples during LC-MS experiments without needing to know a compound's particular ionization mode

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### Introduction

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Positive/negative ionization 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.

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## Results and Discussion

Figure 1 shows a mass spectrum of raffinose analysed with positive/negative electrospray ionization. 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.

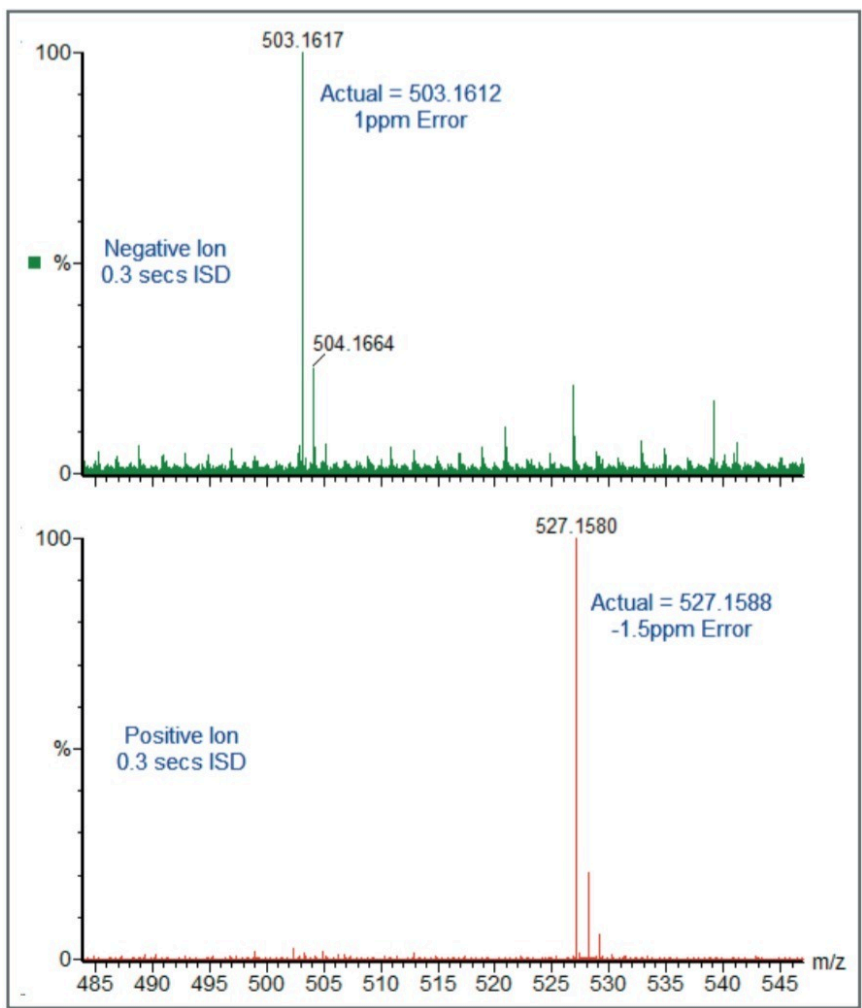


Figure 1. Positive/Negative switching analysis of raffinose.

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.

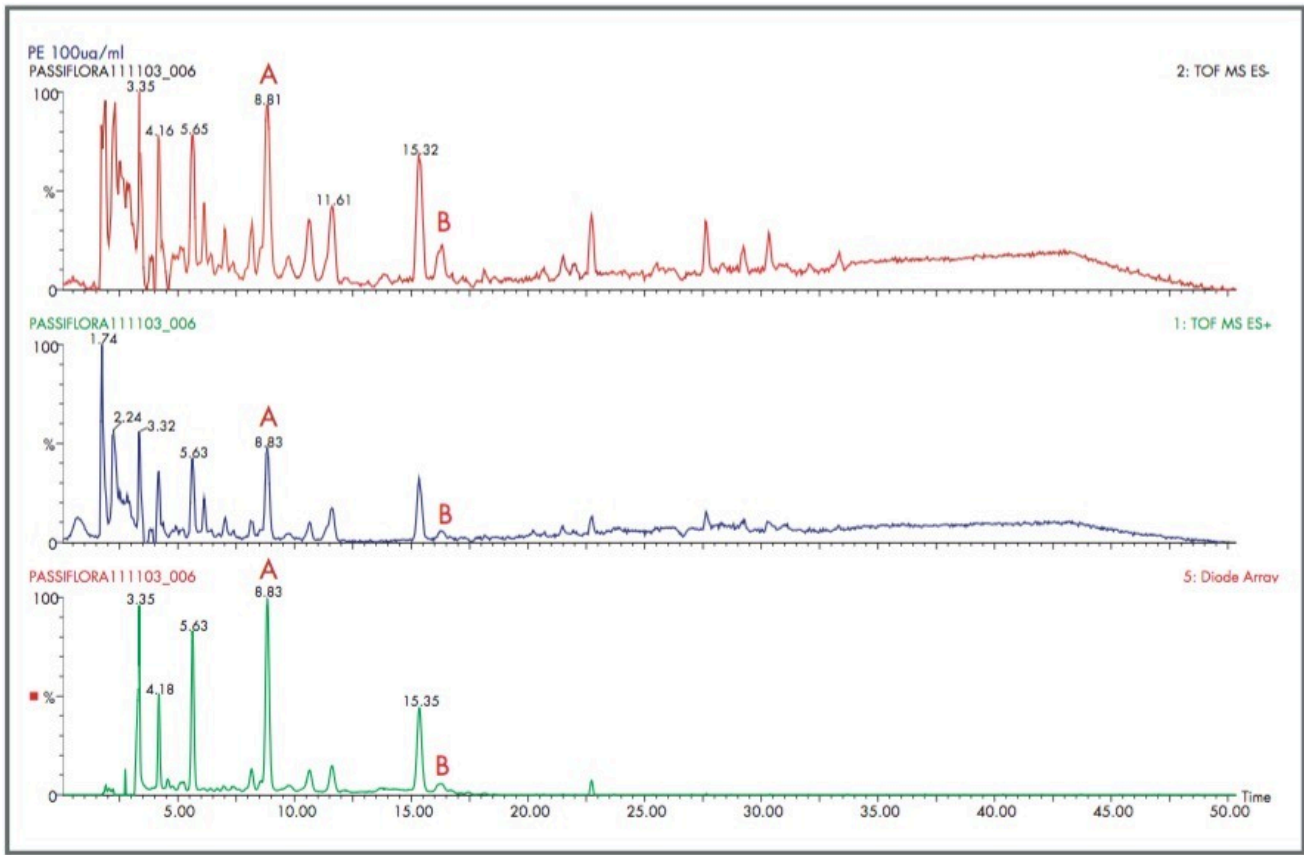


Figure 2. Positive/Negative ionization of a Passiflora extract.

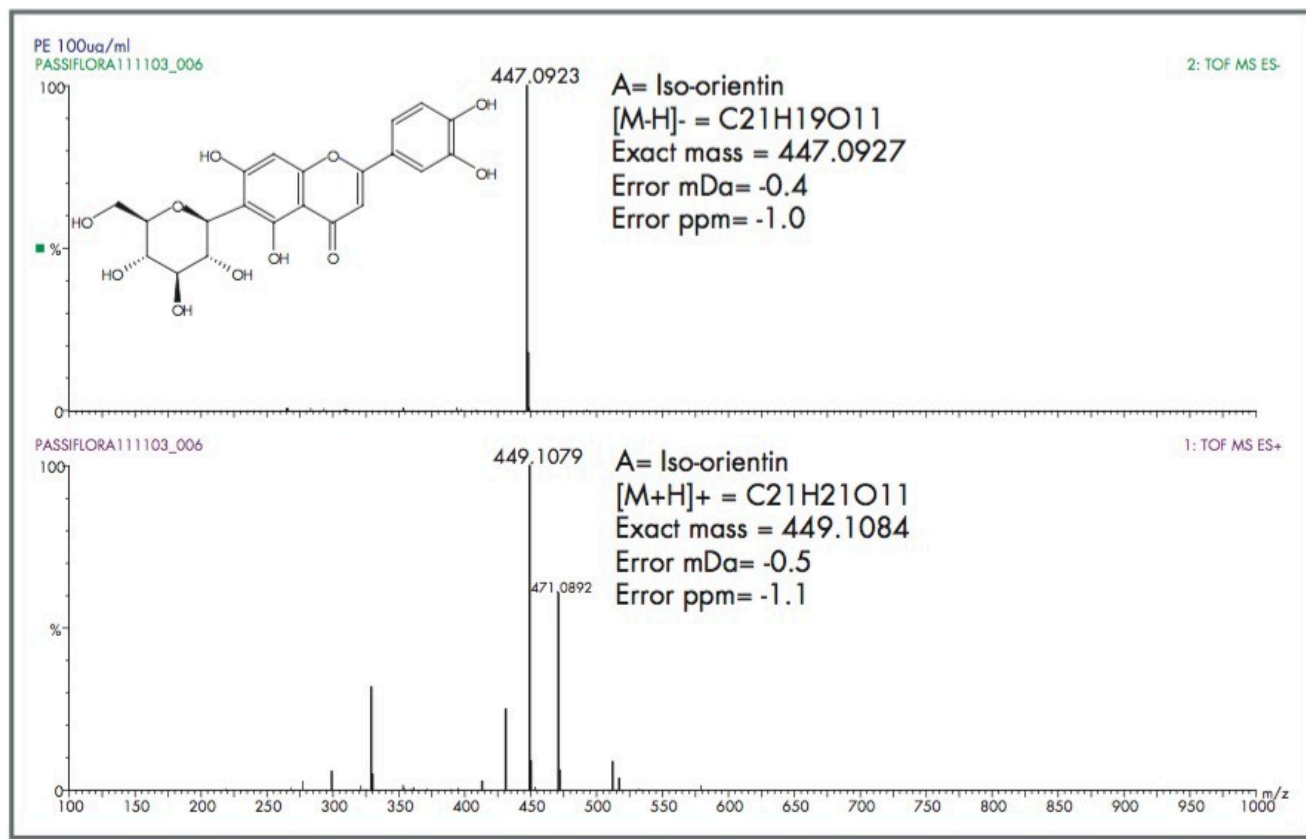


Figure 3a. Positive/Negative ionization mass spectra of Iso-orientin (Peak A).

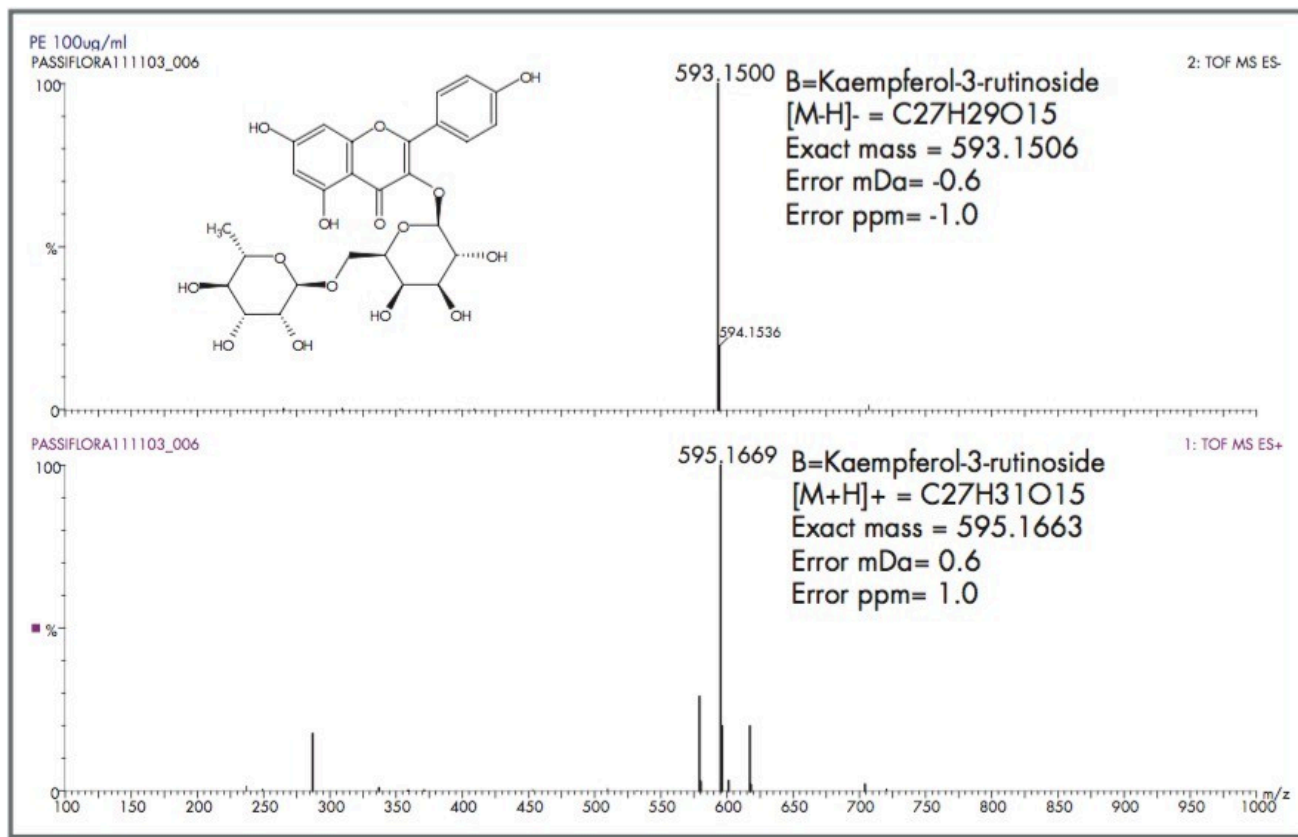


Figure 3b. Positive/Negative ionization mass spectra of Kaempferol-3-rutinoside (Peak B).

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