UltraFAIMS B1 – Suggested starting CF and DF ranges

This note outlines suggested starting values for CF ranges and DF ranges during initial method development.

CF ranges:

For DF = 0Td (no separation) – all peaks should be centred on CF=0Td. Useful CF range is probably no wider than -1 to +1 Td.

For higher DFs, peak positions depend on exact DF value an on the ion of interest. A sensible starting point for a full 2D DF sweep may be -1 to 4 Td. Once the peak positions have been observed, the range can be narrowed to allow more definition on peaks (i.e. to increase the number of MS spectra collected across the peaks in the same time interval).

If you observe peaks moving towards +4Td at intermediate DFs, and potentially being cut off or missed at the highest DFs, then increase the upper CF limit further.

If modifier gases are added to the carrier gas flow, expand initial CF range to -4 to + 4 Td, as peaks may also shift to negative CFs.

DF ranges:

Once the chip region temperature is set in the ultraFAIMS software, the instrument will calculate the maximum attainable DF. This can be observed by hovering the mouse over the "DF start" and "DF end" fields in the user interface.

Generally, little useful separation is seen at dispersion fields in the bottom half of the available range. Therefore, for an initial 2D sweep, we would suggest a range of say 0.5*max DF to max DF. For example, if maximum DF is 300Td, then a sensible initial 2D sweep might start at 150Td, end at 290Td and use CF steps of 20Td. (If good signal intensity is still seen at 290Td, you might want to then go to maximum DF of 300Td to see if separation improves further).

Timing:

Duration of sweeps is determined by the CF duration you specify. The ultraFAIMS instrument can step CF in approx 2ms and can step DF in approx 30ms. For a given CF range, the instrument will attempt to divide the range into 2000 steps to provide a smooth ramp. If the requested duration would require steps shorter than 2ms, the number of steps will be reduced (and step size increased). In general, you can assume a smooth ramp, with a sweep rate of (CF range/CF duration) Td/sec.

Note that although the ultraFAIMS instrument can sweep at this rate, your practical limit will be determined by the sampling rate of the mass spectrometer. In sweep mode, when trying to determine optimum peak positions, you ideally want to have at least 10 data points (mass spectra) sampled across a peak. As typical full width at half maximum of a peak is around 0.3Td, this would require MS samples every 0.03Td. If the MS is sampling at 1Hz, this would limit your sweep rate to 0.03Td/sec (or 100 secs for a 3Td CF window). If the MS is sampling at 5Hz, this would decrease to 20s for a 3TdCF window. (Do not use MS moving averaging in FAIMS sweep mode). Typically, FAIMS users carry out initial constant infusion experiments with analytes of interest at slow sweep rates to identify CF

and DF regions of interest. Once those are known, the sweep ranges can be narrowed and sweep duration increased, or alternatively, the static/hopping mode can be used.

In static (hop) mode, you set up a table of (CF, DF) pairs that you want to sequentially visit. For each pair, a hold time must be specified. The hold time can be from 2ms to many minutes. At each step, the instrument applies the specified CF and DF and holds them fixed for the specified hold time, effectively acting as a filter to preferentially transmit ions that are centred on the CF position for the given DF.