29<sup>th</sup> August 2014 Lauren Brown







# **NEXT** GENERATION DETECTION



• This tutorial will describe the steps required to export THE ultraFAIMS data files from Xcalibur and convert into the format required for viewing/processing data in Excel.

## **View data in Qual Browser**

• Open Qual Browser from the Xcalibur Roadmap window.



# Load RAW file in Qual Browser

- Click on the 'open data' button in the top left corner of the screen
- Select data file.



## **View data in Qual Browser**

• TIC loads in chromatogram window as standard.



## View data for ion of interest

- Ensure chromatogram window is pinned (green square indicates active window).
- Right click and select 'Ranges'.



## View data for ion of interest

- Click the box under TIC.
- Change 'Plot type' to 'Mass Range' from the drop down menu.
- Enter the m/z of the ion of interest in the 'Range(s)' box
- Press 'OK'.

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## View data for ion of interest

- Xcalibur will only allow the export of one set of data at a time.
- By default it selects the first chromatogram range.
- TIC therefore has to be de-selected to allow the ion of interest data to be exported.
- Re-load the Chromatogram Ranges window, as the previous step, and de-select the TIC.
- Hit 'OK'.

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## **Export data to Clipboard**

- Right click on the chromatogram window and click 'Export'.
- Select 'Clipboard (Chromatogram)'. This 'copies' the data and allows it to be pasted into another program.



#### Paste data into Excel

• Owlstone will provide an Excel Spreadsheet that can be used to paste the exported data into to allow data to be viewed/processed with a compensation field axis.

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## Paste data into Excel

• Right click on the 'Paste data here' cell and paste in the exported data.

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#### **Convert time axis into compensation field**

- The spreadsheet will automatically convert the time in minutes into time in seconds (column D).
- Manual input is then required to convert the time in seconds to compensation field (CF).
- This is due to the non-linear nature of ion-trap-type data acquisition.
- Automatic gain control means that the ion trap will fill for different amounts of time dependent on the number of ions present.
- However, the CF is ramped at a linear rate over a scan.
- This means the step in CF will not always be the same between different data points.
- However, CF across the compensation field scan can be back calculated using the steps in the following slides.

#### **Convert time axis into compensation field**

- First, the time taken for the total FAIMS scan must be calculated.
- In cell 'B1' change the equation to the cell where the FAIMS scan ends (in the example shown D914) minus the start of the FAIMS scan (D10 in the example shown).

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#### **Convert time axis into compensation field**

- Next, the time taken for each CF scan should be calculated.
- Divide the time taken for the FAIMS scan by the number of dispersion fields (DF) used.
  - 6 DFs were used in the example shown (cell B2).
- The number should be approximately the CF scan time inputted into the ultraFAIMS software when the data was acquired (in the example below this was 60s).

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#### **Calculate compensation field step size**

- Next, the time taken for each CF step should be calculated, based on the total time for the CF scan and the CF scan range.
- Divide the number of Td for the CF scan by the time taken to perform the CF scan, calculated in the previous step.
  - A 5 Td range (-1 Td to +4 Td) was used in the example shown (cell B4).

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# Calculate compensation field for a given time point

- A formula is inputted into cell B6 to allow the calculation of the CF at a given time point.
- This formula uses the MOD function which tells you what is the remainder after dividing one number with another.
- This allows CF to be calculated at a particular time point based on how much time has elapsed since the start of the scan.
- The CF is calculated by taking the starting CF plus the step size (in CF s<sup>-1</sup>) and multiplying it by the elapsed time.

E.g. -1+\$B\$4\*MOD(D10-\$D\$10,\$B\$2)

# Calculate compensation field for a given time point

• It is important to enter the correct starting CF and step size, as well as the correct starting time. This must be changed for each exported data file.

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• In the e.g. shown below, the CF scan starts at -1 Td, the step size is calculated in cell B4. The start time of the scan is in cell D10 and the total time taken is calculated in cell B2.

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11     0     0     0     0     0       18     5.1576     0.08596     0     0     0       19     5.55520002     0.09258667     0     0     0       20     5.9527998     0.09921333     0     0     0       21     6.305998     0.105843333     0     0     0       22     6.745998     0.11249333     0     0     0       23     7.1472     0.11912     0     0     0       24     7.5451002     0.125751667     0     0     0	17			4.35570002		0.0	72001007	0										
10     0.0057     0     0     0       19     5.55520002     0.092586667     0     0     0       20     5.95279998     0.099213333     0     0     0       21     6.3059998     0.105843333     0     0     0       22     6.7495998     0.11249333     0     0       23     7.1472     0.11912     0     0       24     7.5451002     0.125751667     0     0	18			5 1576		0.0	0.08596	0										
20     5.95279998     0.09921333     0       21     6.35059998     0.105843333     0       22     6.74559998     0.11249333     0       23     7.1472     0.11912     0       24     7.5451002     0.125751667     0	19			5 55520002		0.0	92586667	0										
21     6.35059998     0.105843333     0       22     6.74559998     0.11249333     0       23     7.1472     0.11912     0       24     7.54510002     0.125751667     0	20			5.95279998		0.0	99213333	0										
Constraint         Constra	21			6 35059998		0.1	05843333	0										
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# Convert each time point to compensation field

• The equation can be copied from cell B6 and pasted into the CF cell correlating to the start of the CF scan (E10 in this example).

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	E10	-	0	<i>f</i> <sub>x</sub> =-1+\$B\$4*M0	DD(D10-\$D\$10,\$B\$2)													×
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3						Data points: 921												
4	Step size	0.083369				Time		Intensity										
5							0.00022	4895.52										_
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14				3.56449998		0.05	9408333	0										
15				3.9621		(	0.066035	0										
16				4.35970002		0.07	2661667	0										
17				4.75999998		0.07	9333333	0										
18				5.1576			0.08596	0										
19				5.55520002		0.09	2586667	0										
20				5.95279998		0.09	9213333	0										
21				6.35059998		0.10	5843333	0										
22				6.74959998		0.11	2493333	0										
23				7.1472			0.11912	0										
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# Convert each time point to compensation field

- This can then be dragged to each subsequent cell in the example below cells D10 to D914, covering the total CF scan range.
- This then gives the data needed to be able to plot CF against intensity (Column E vs. column G).

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6	CF	-1		0.41239998		0.0	06873333	4405.703										
7				0.81130002	_	0.0	13521667	4406.505										
8				1.191	$\frown$		0.01985	4721.783										
9				1.59019998		0.0	26503333	4085.243										
10				1.97239998	-1	0.0	32873333	0										
11				2.37139998	-0.9667359	0.0	39523333	0										
12				2.76910002	-0.933580175	0.0	46151667	0										
13				3.16690002	-0.900416118	0.0	52781667	0										
14				3.56449998	-0.867268737	0.0	59408333	0										
15				3.9621	-0.834121351		0.066035	0										
16				4.35970002	-0.800973965	0.0	72661667	0										
17				4.75999998	-0.767601489	0.0	79333333	0										
18				5.1576	-0.734454103		0.08596	0										
19				5.55520002	-0.701306717	0.0	92586667	0										
20				5.95279998	-0.668159336	0.0	99213333	0										
21				6.35059998	-0.634995279	0.1	05843333	0										
22				6.74959998	-0.601731178	0.1	12493333	0										
23				7.1472	-0.568583792	1	0.11912	0										
24				7.54510002	-0.535411396	0.1	25751667	0										
25				7.94269998	0.502264015	0.1	32378333	0										
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#### Plot intensity against compensation field

• Plotting intensity against CF allows the CF scan data to be visualised.

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2	Tcf	59.97457				200614_ESI_1pMol_reserpin	e_chip(	002_180-28	80Td1+4T	d_60s_ne	DFfeede	r1_02.rav	v					
3						Data points: 921												
4	Step size	0.083369				Time	1	Intensity					3333					
5						0	.00022	4895.52			4	500						
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7				0.81130002		0.013	521667	4406.505										
8				1.191		0	.01985	4721.78			5	500						
9				1.59019998		0.026	503333	4085.243			30	000						
10				1.97239998	-1	0.032	373333	0		≥	2	500						
11				2.37139998	-0.9667359	0.0395	523333	0		isus	20	000						
12				2.76910002	-0.933580175	0.0463	151667	0		Inte	11	500						
13				3.16690002	-0.900416118	0.052	781667	0			-							
14				3.56449998	-0.867268737	0.0594	408333	0			10	000						
15				3.9621	-0.834121351	0.0	066035	0			5	500						
16				4.35970002	-0.800973965	0.072	561667	0				-0						
17				4.75999998	-0.767601489	0.0793	333333	0		-2	-1	500 <sup>(</sup>	1	2	3	4	5	
18				5.1576	-0.734454103	0	.08596	0					Compensatio	n Field (Td)				
19				5.55520002	-0.701306717	0.092	586667	0	-				9999					
20				5.95279998	-0.668159336	0.0992	213333	0										
21				6.35059998	-0.634995279	0.1058	343333	0										
22				6.74959998	-0.601731178	0.1124	493333	0										
23				7.1472	-0.568583792	0	.11912	0										
24				7.54510002	-0.535411396	0.125	751667	0										
25				7.94269998	-0.502264015	0.132	378333	0										
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# **Compare compensation field scans**

- Different CF scans can then be plotted on the same graph to allow a comparison of their CF spectra.
- E.g.

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3						Data points: 921											
4	Step size	0.083369				Time	Intensity	0.5				3333					
5						0.00022	4895.52	i r		4	500						
6	CF	-1		0.41239998		0.006873333	4405.703			4	000						
7				0.81130002		0.013521667	4406.505			-	500						
8				1.191		0.01985	4721.783			3	500						
9				1.59019998		0.026503333	4085.243			3	000						
10				1.97239998	-1	0.032873333	0		2	2	500						
11				2.37139998	-0.9667359	0.039523333	0		isu a	2	000				Analyt	e 1	
12				2.76910002	-0.933580175	0.046151667	0	101	Ĕ	1	500				-Analyt	e 2	
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14				3.56449998	-0.867268737	0.059408333	0			1			1				
15				3.9621	-0.834121351	0.066035	0				500						
16				4.35970002	-0.800973965	0.072661667	0			_	0				_		
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18				5.1576	-0.734454103	0.08596	0				0	Compensatio	n Field (Td)				
19				5.55520002	-0.701306717	0.092586667	0	2 4				0000				4:	
20				5.95279998	-0.668159336	0.099213333	0										
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23				7.1472	-0.568583792	0.11912	0										
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