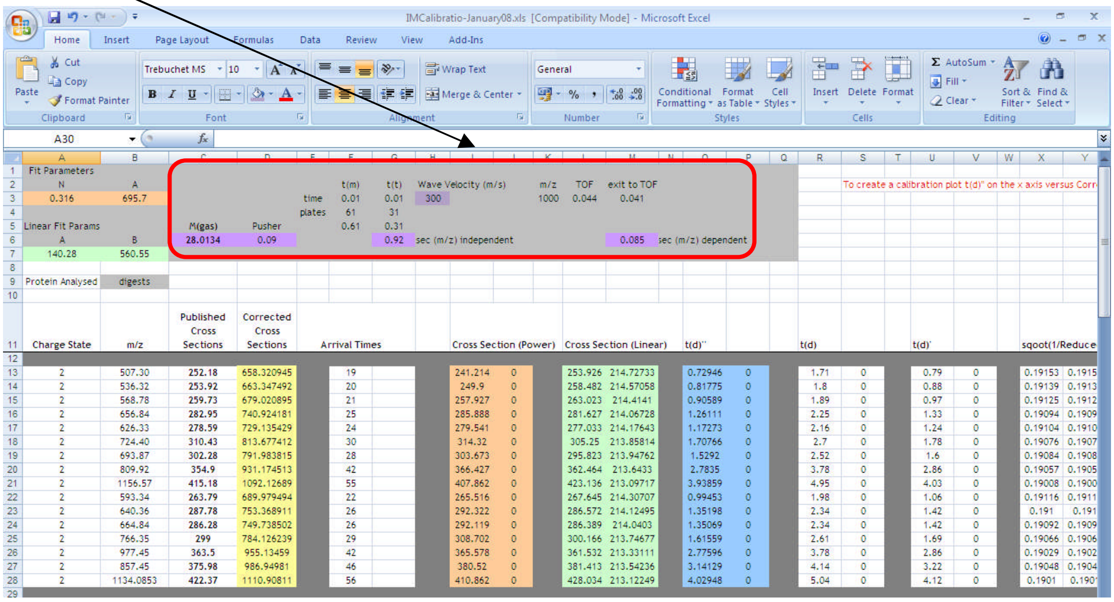
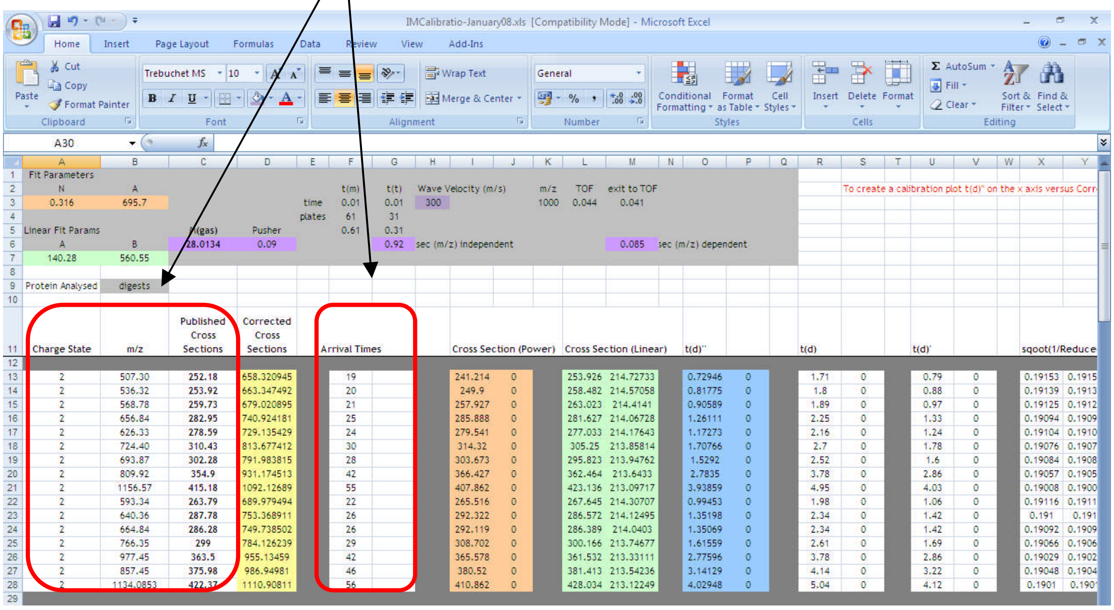
Creating a calibration

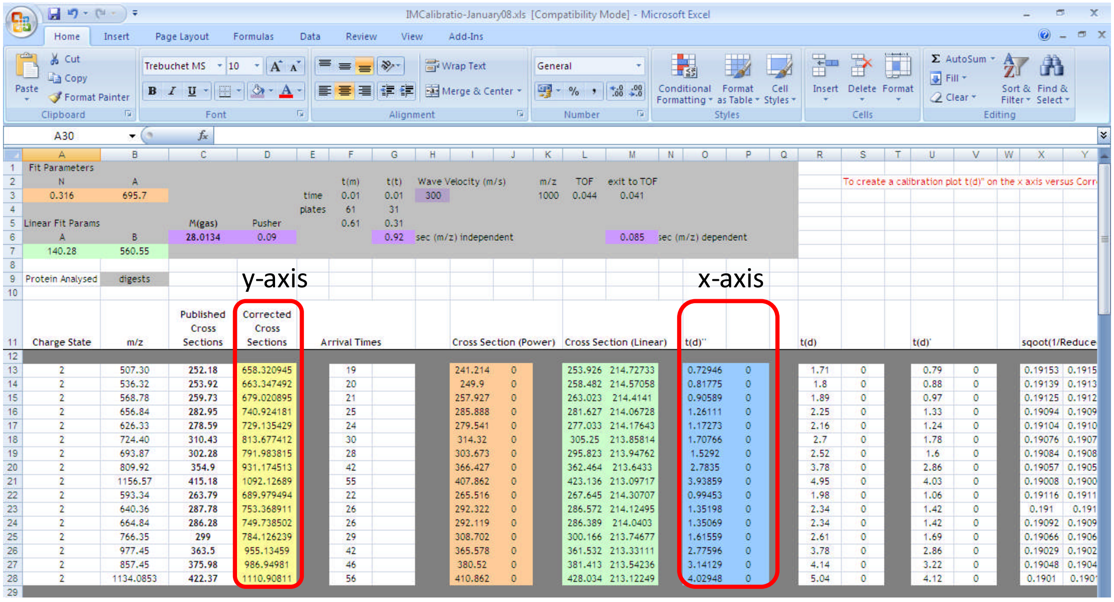
Step 1: Fill experimental parameters (purple-coloured cells)



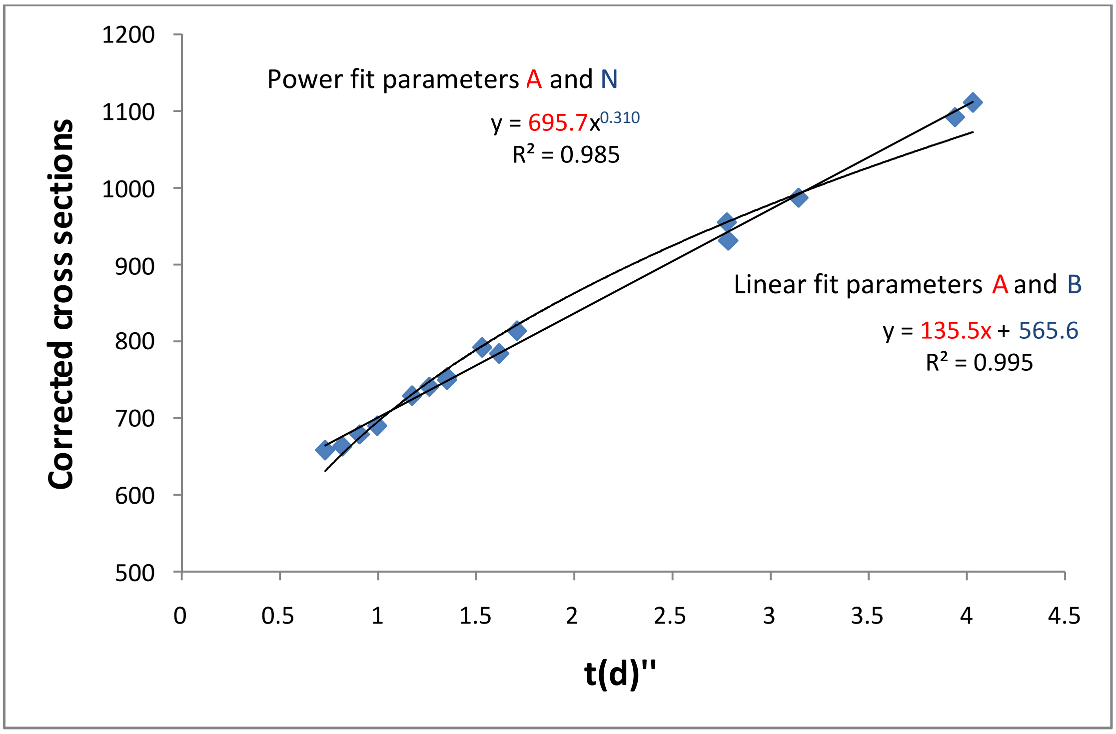
Step 2: Enter published cross section values and charge state, m/z, arrival times as measured on the Synapt



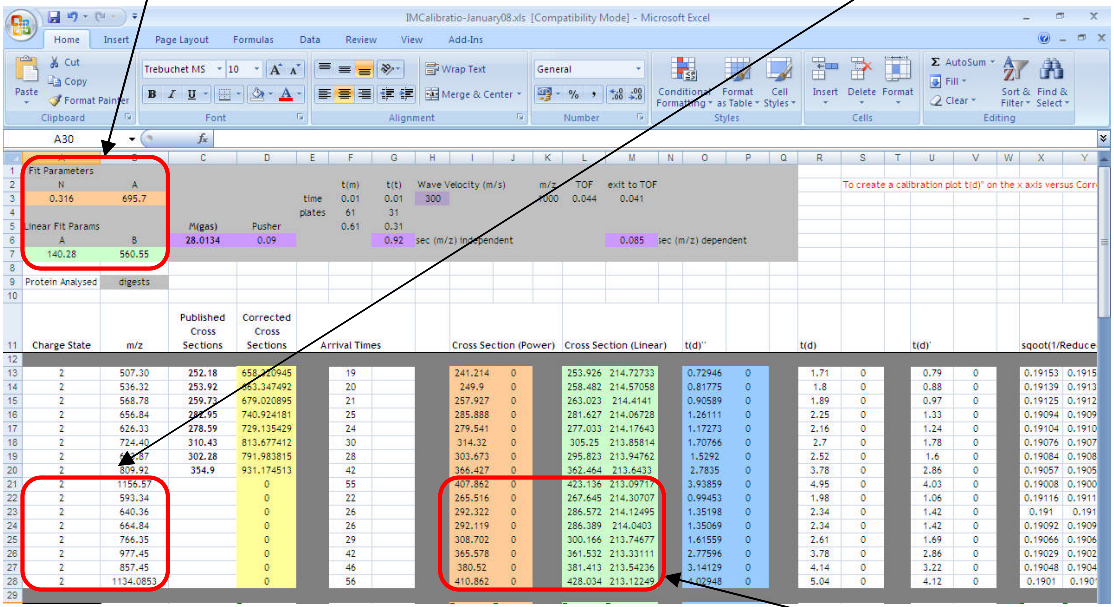
Step 3: Plot t(d)'' on the x axis versus Corrected Cross sections



Step 4: Either fit a linear or power trend. We have found that a linear trend is more suitable when analysing peptides while a power trend when analysing proteins (unpublished results). The excel sheet can handle both cases (linear calibration and results colour-coded green while power calibration and results colour -coded orange).



Step 5: Insert fit parameters and charge state, m/z, and arrival times for the ions of interest



Charge State	m/z	Published Cross Sections	Corrected Cross Sections	Arrival Times	Cross Section (Power)		Cross Section (Linear)		t(d)''		t(d)		t(d)'		sqoot(1/Reduce	
2	507.30	252.18	658.320945	19	241.214	0	253.926	214.72733	0.72946	0	1.71	0	0.79	0	0.19153	0.1915
2	536.32	253.92	663.347492	20	249.9	0	258.482	214.57058	0.81775	0	1.8	0	0.88	0	0.19139	0.1913
2	568.78	259.73	679.020895	21	257.927	0	263.023	214.4141	0.90589	0	1.89	0	0.97	0	0.19125	0.1912
2	656.84	282.95	740.924181	25	285.888	0	281.627	214.06728	1.26111	0	2.25	0	1.33	0	0.19094	0.1909
2	626.33	278.59	729.135429	24	279.541	0	277.033	214.17643	1.17273	0	2.16	0	1.24	0	0.19104	0.1910
2	724.40	310.43	813.677412	30	314.32	0	305.25	213.85814	1.70766	0	2.7	0	1.78	0	0.19076	0.1907
2	6[illegible].87	302.28	791.983815	28	303.673	0	295.823	213.94762	1.5292	0	2.52	0	1.6	0	0.19084	0.1908
2	809.92	354.9	931.174513	42	366.427	0	362.464	213.6433	2.7835	0	3.78	0	2.86	0	0.19057	0.1905
2	1156.57		0	55	407.862	0	423.136	213.09717	3.93859	0	4.95	0	4.03	0	0.19008	0.1900
2	593.34		0	22	265.516	0	267.645	214.30707	0.99453	0	1.98	0	1.06	0	0.19116	0.1911
2	640.36		0	26	292.322	0	286.572	214.12495	1.35198	0	2.34	0	1.42	0	0.191	0.191
2	664.84		0	26	292.119	0	286.389	214.0403	1.35069	0	2.34	0	1.42	0	0.19092	0.1909
2	766.35		0	29	308.702	0	300.166	213.74677	1.61559	0	2.61	0	1.69	0	0.19066	0.1906
2	977.45		0	42	365.578	0	361.532	213.33111	2.77596	0	3.78	0	2.86	0	0.19029	0.1902
2	857.45		0	46	380.52	0	381.413	213.54236	3.14129	0	4.14	0	3.22	0	0.19048	0.1904
2	1134.0853		0	56	410.862	0	428.034	213.12249	4.02948	0	5.04	0	4.12	0	0.1901	0.1901

The resulting estimated cross sections (for each type of fit) are displayed here

What calculations are performed by the spreadsheet

- Measure arrival time in scans (scan number (n))
- Convert to time (multiply by pusher time)
- t_d = n* pusher time (msecs)
- Subtract T-wave offset
- T-wave offset related to wave velocity, the time indicated on readout after wave velocity in mobility region (t_m) and transfer region (t_t) is time per pair of plates. The mobility cell has 61 pairs of plates so 61*t_m is subtracted. The transfer region has 31 pairs of plates so 31*t_t is subtracted.
- At 300 m/sec t_m and t_t are equal to 10µsec
- Subtraction would therefore be [(61*10)+(31*10)]µsec = 920µsec
- This is not *m/z* dependent!
- For these values $t_d' = t_d$ - 920µsec
- Then correct for m/z dependent time of flight.
- From Bob Bateman calculations.
- For *m/z* 1000 the TOF flight time is 44 µs and the transit time from the exit of the TriWave to the TOF is 41 µs, giving a total time of 85 µs (micro-sec) to be subtracted from the drift time. The correction time to the drift time is proportional to the square root of the m/z value.
- $td'' = td' - \sqrt{\left(\frac{m/z}{1000}\right)} \times 0.085$ msec
- This is corrected effective drift time.
- To obtain calibration coefficients use published cross section data. (Ω)
- Correct published cross sections by taking into account reduced mass and charge state.
- $\Omega' = \frac{\Omega}{e \times \left(\frac{1}{M_I} + \frac{1}{M_N}\right)^{\frac{1}{2}}}$
- e = Charge, Mi = mass of ion, MN = mass of mobility gas.
- Plot Ω' against t_d''
- Fit curve to equation type $y = Ax^N$
- Calculate A and N from fit.
- Convert experimental measurements to estimated cross sections by calculating.
- $\Omega = td''^N \times A \times e \times \left(\frac{1}{M_I} + \frac{1}{M_N}\right)^{\frac{1}{2}}$