Heterogeneity of Glycan Processing on Trimeric SARS-CoV-2 Spike Protein Revealed by Charge Detection Mass Spectrometry

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Supporting Information

CDMS Mass Resolution with 100 ms Trapping Time

In CDMS, the mass resolution has contributions from the *m/z* resolution and the charge resolution:

$$\frac{\Delta m}{m} = \sqrt{\left(\frac{\Delta[m/z]}{[m/z]}\right)^2 + \left(\frac{\Delta z}{z}\right)^2} \tag{1}$$

Where Δm, $\Delta[m/z]$, and Δz are the peak full widths at half maximum (FWHM) in the mass, *m/z*, and charge distributions. The 100 ms trapping measurements reported in the manuscript were performed on our prototype CDMS instrument.[1] On this instrument, the relative root mean square deviation (RMSD) in the *m/z* measurement, $\sigma[m/z]/[m/z]$, is around 0.0054.[2] The charge RMSD (σz) depends on both the oscillation frequency (f) and the trapping time (t_{trap}) and is given approximately by[3]

$$\sigma z = 25.58\frac{f^{-0.457}}{{t_{trap}}^{0.5}} \tag{2}$$

The oscillation frequency and m/z are related through the following equation,

$$\frac{m}{z} = \frac{C}{f^2} \tag{3}$$

where C is a constant that depends on the ion energy and trap geometry. For the spike trimer at 475 kDa in Figure 5 of the manuscript the average *m/z* is around 10,000 Da, and the average oscillation frequency is around 16,000 Hz. For a 100 ms trapping time, the charge RMSD is 0.97 e, according to Equation 2. This leads to a relative charge RMSD ($\sigma z/z$) of around 0.0205. Combining the relative RMSDs in the charge ($\sigma z/z$) and m/z ($\sigma[m/z]/[m/z]$) leads to the relative RMSD in the mass ($\sigma m/m$), which is around 0.0212. Thus, the full width at half maximum (FWHM) of the spike trimer peak at 475 kDa in Figure 5 due to instrumental resolution is $0.0212 \times 2.35 \times 475 = 23.7$ kDa, where the factor of 2.35 converts from RMSD to peak FWHM.

References

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