Metabolite Spectral Accuracy on Orbitraps

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SUPPORT INFORMATION

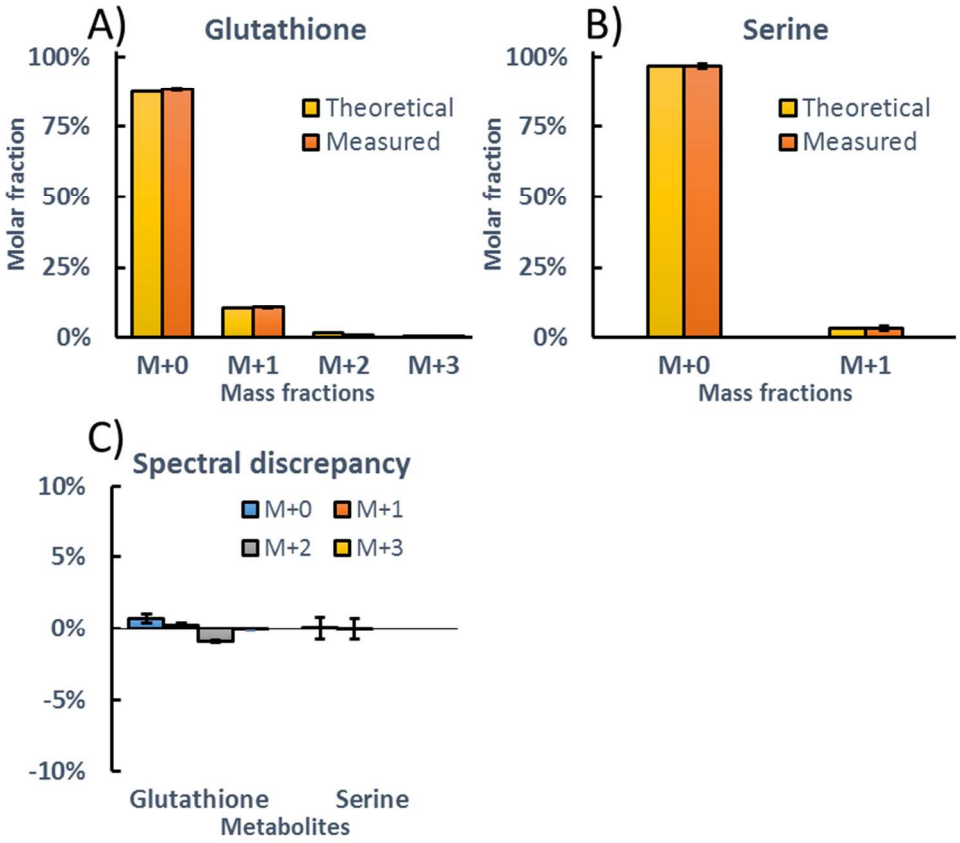

Figure S1. Spectral accuracy of glutathione (m/z 307) and serine (m/z 104). Measured and theoretical mass distribution of unlabeled A) glutathione and B) serine. C) Spectral discrepancies.

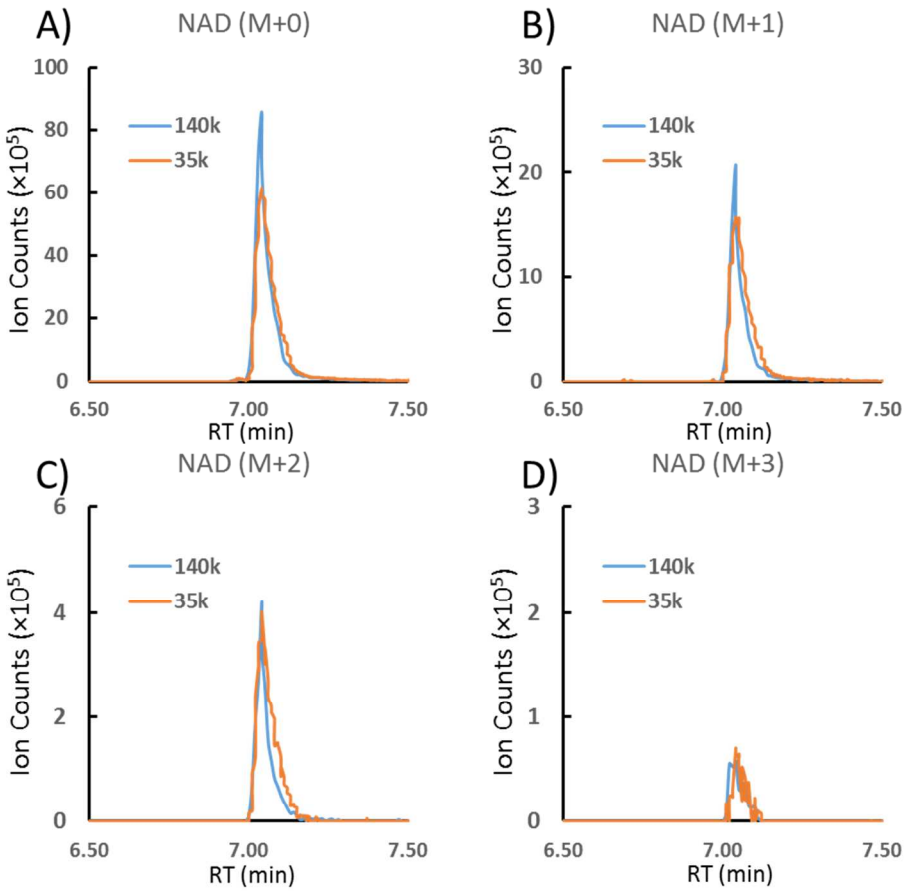

Figure S2. Extracted ion chromatograms of NAD at high and low mass resolution. A) M+0, B) M+1, C) M+2, D) M+3.

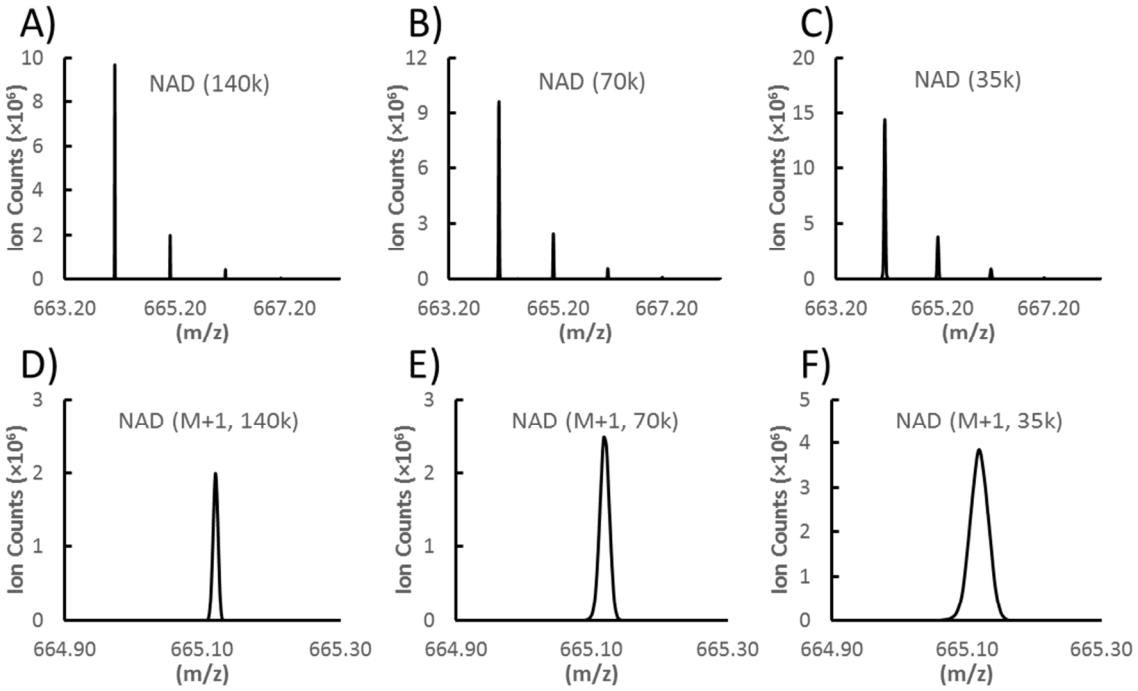

Figure S3. Mass spectra of NAD at different resolutions. A-C) Resolution 140k, 70k and 35k. D-F) Zoomed NAD M+1 peak.

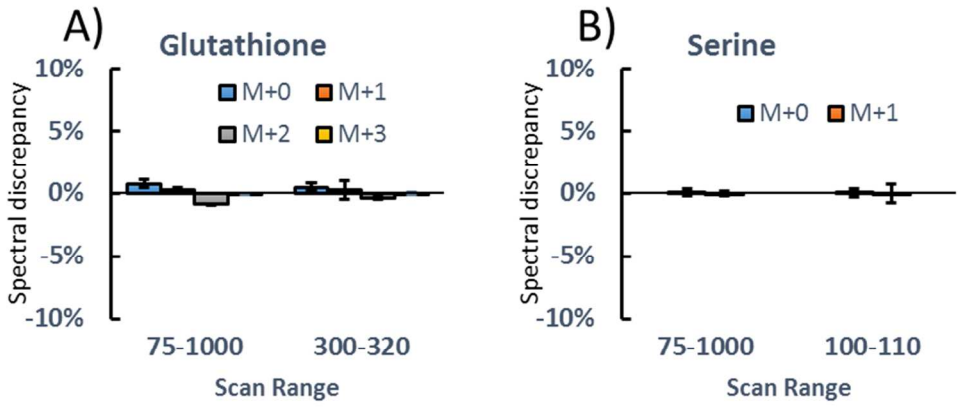

Figure S4. Spectral accuracy of A) glutathione and B) serine as a function of mass scan range.

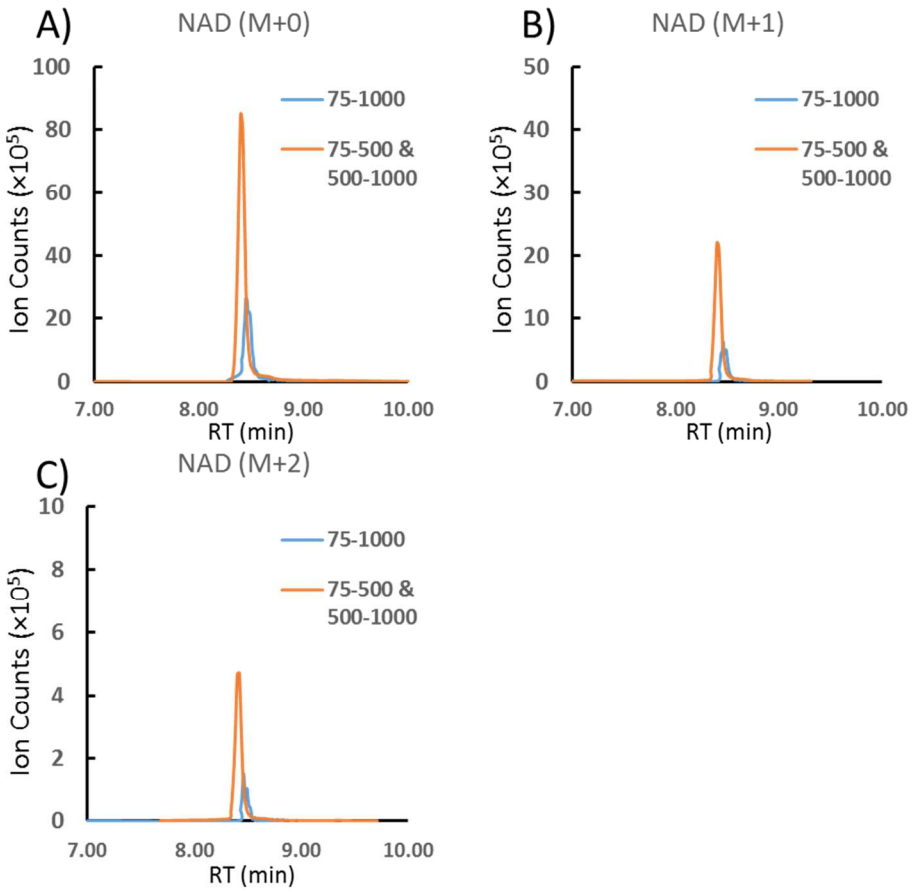

Figure S5. The extracted ion chromatogram of NAD under full scan or smaller m/z scan range (500-1000).

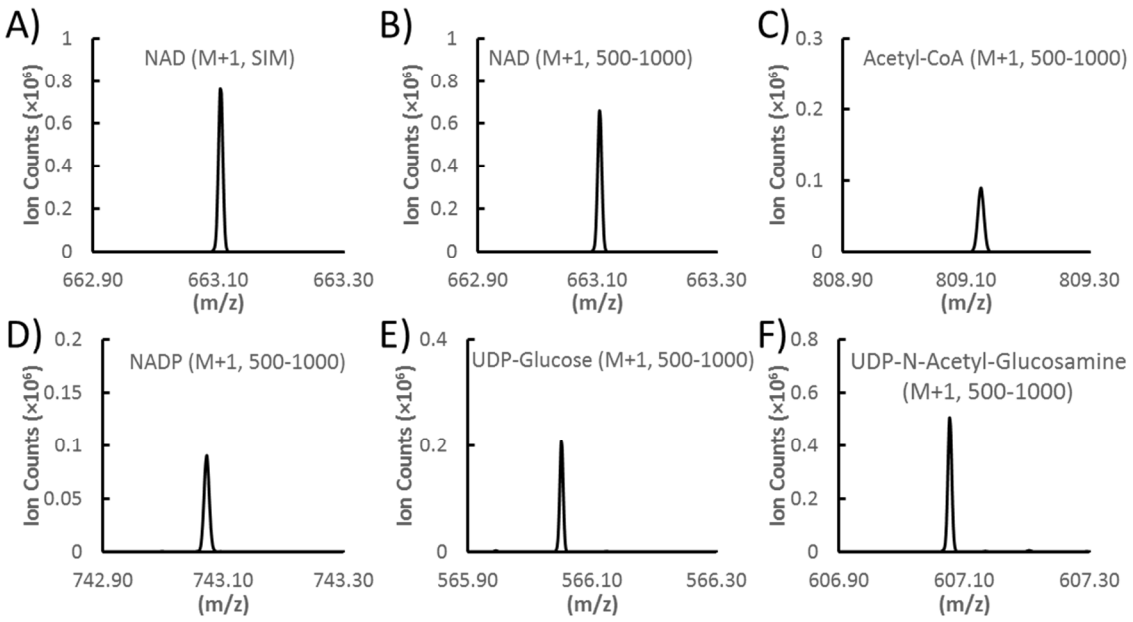

Figure S6. Zoomed mass spectra of M+1 peaks reveals no evidence of contaminating species. Values in parentheses show the scan range. A, B) NAD, C) Acetyl-CoA, D), NADP, E) UDP-glucose, F) UDP-N-acetyl-glucosamine.