Characterization of disulfide bonds by planned digestion and tandem mass spectrometry

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Supplementary Information

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Supplementary Figures

Figure S1. Annotated MS/MS spectrum of SSTSASSNYCNQMMK-CR after Asp-N/C and trypsin digestion



Figure S2. Annotated MS/MS spectrum of QHMDSSTSAASSSNYCNQMMK-CR after Asp-N/C and trypsin digestion



Figure S3. Annotated MS/MS spectrum of SSTSAASSSNYCNQMMK-CRETGSSK after Asp-N/C and trypsin digestion



Figure S4. Annotated MS/MS spectrum of QHMDSSTSAASSSNYCNQMMK-CRETGSSL after Asp-N/C and trypsin digestion



Observed=887.71(3+) MW=2660.10 basePeak (m/z=1114.8/intensity=12361) TIC=240492 peaksCount=1333

Figure S5. Annotated MS/MS spectrum of CKPVNTFVHESLA-YPNCAYK after Asp-N/C and trypsin digestion



Figure S6. Annotated MS/MS spectrum of CKPVNTFVHESLAD-YPNCAYK after Asp-N/C and trypsin digestion



Observed=1150.56(2+) MW=2299.10 basePeak (m/z=1106.4/intensity=122842) TIC=1893108 peaksCount=1431

Figure S7. Annotated MS/MS spectrum of RCKPVNTFVHESLA-YPNCAYK after Asp-N/C and trypsin digestion



Figure S8. Annotated MS/MS spectrum of CK-YPNCAYK after Asp-N/C and trypsin digestion



Observed=553.24(2+) MW=1104.47 basePeak (m/z=544.5/intensity=2231600) TIC=6322103 peaksCount=518

Figure S9. Annotated MS/MS spectrum of RCK-YPNCAYK after Asp-N/C and trypsin digestion



Figure S10. Annotated MS/MS spectrum of DRCK-YPNCAYK after Asp-N/C and trypsin digestion



Figure S11. Annotated MS/MS spectrum of CKPVNTFVHESLA-ETGSSKYPNCAYK after Asp-N/C and trypsin digestion



Figure S12. Annotated MS/MS spectrum of CK-YPNCAYKTTQANK after Asp-N/C and trypsin digestion



Observed=874.91(2+) MW=1747.80 basePeak (m/z=857.8/intensity=3354) TIC=31643 peaksCount=1033

Figure S13. Annotated MS/MS spectrum of CKPVNTFVHESLA-YPNCAYKTTQANK after Asp-N/C and trypsin digestion



Figure S14. Annotated MS/MS spectrum of NVACK-NGQTNCYQSYSTMSIT after Asp-N/C and trypsin digestion



Observed=1165.01(2+) MW=2328.00 basePeak (m/z=1105.7/intensity=37318) TIC=331067 peaksCount=1272

Figure S15. Annotated MS/MS spectrum of NVACK-NGQTNCYQSYSTMSITD after Asp-N/C and trypsin digestion



Figure S16. Annotated MS/MS spectrum of NVACKNGQTNCYQSYSTMSIT after Asp-N/C and trypsin digestion



Figure S17. Annotated MS/MS spectrum of NVACKNGQTNCYQSYSTMSITD after Asp-N/C and trypsin digestion



Figure S18. Annotated MS/MS spectrum of VQAVCSQK-HIIVACEGNPYVPVHF after Asp-N/C and trypsin digestion

VQAVCSQK HIIVACEGNPYVPVHF P*v14++ 1202.9 100 P*b12++ 1078.8 P*b15(3+) 830.8 P*b6(3+) intensity(%) P*b1 1176.9 <mark>у7</mark> 858.4 499.3 P*b11+ P*y15++ γ5 Т Y2 y5++ ¹⁷v12v9 P? 1096.8 <mark>ру2</mark> 303.3 b5 1029.1061.7 b2 ЬЗ Ъ4 v8 146.6 1259 4 813.7 598.4 1214.7 534.5 972.6 251.0275, 299.2 364.2 430.0⁴ . իստեր L ա և 1 1 دادتان m/z 300 400 500 600 700 800 900 1000 1100 1200

Observed=885.45(3+) MW=2653.34 basePeak (m/z=1202.9/intensity=150453) TIC=1772728 peaksCount=1095

Figure S19. Annotated MS/MS spectrum of VQAVCSQK-HIIVACEGNPYVPVHF after Asp-N/C and trypsin digestion



Figure S20. Annotated MS/MS spectrum of VQAVCSQK-HIIVACEGNPYVPVHFDASV after Asp-N/C and trypsin digestion



Figure S21. Annotated MS/MS spectrum of VQAVCSQK-TTQANKHIIVACEGN PYVPVHF after Asp-N/C and trypsin digestion



Figure S22. Annotated MS/MS spectrum of VQAVCSQK-TTQANKHIIVACEG NPYVPVHFD after Asp-N/C and trypsin digestion



Figure S23. Annotated MS/MS spectrum of DVQAVCSQK-HIIVACEGNPYVPVHFD after Asp-N/C and trypsin digestion



Figure S24. Annotated MS/MS spectrum of PVNTFVHESLADVQAVCSQK-HIIVACEGNPYVPVHF after Asp-N/C and trypsin digestion

Observed=1322.00(3+) MW=3962.99 basePeak (m/z=1733.9/intensity=3137) TIC=47275 peaksCount=1022



Figure S25. Annotated MS/MS spectrum of PVNTFVHESLADVQAVCSQK-HIIVACEGNPYVPVHFD after Asp-N/C and trypsin digestion



Figure S26. Annotated MS/MS spectrum of PVNTFVHESLADVQAVCSQK-HIIVACEGN PYVPVHF after Asp-N/C and trypsin digestion

