

**Figure S3.** NSI fragmentation spectra of ion  $1415^{+4}$  derived from reduced and alkylated cal12.b. Excellent coverage of the peptide is exhibited with the b and y ion series. The inset shows the  $y_6$  ion showing the bromine isotopic distribution. C = cysteine with carbamidomethyl group.  $\underline{W} = bromotryptophan$ . O = hydroxyproline.