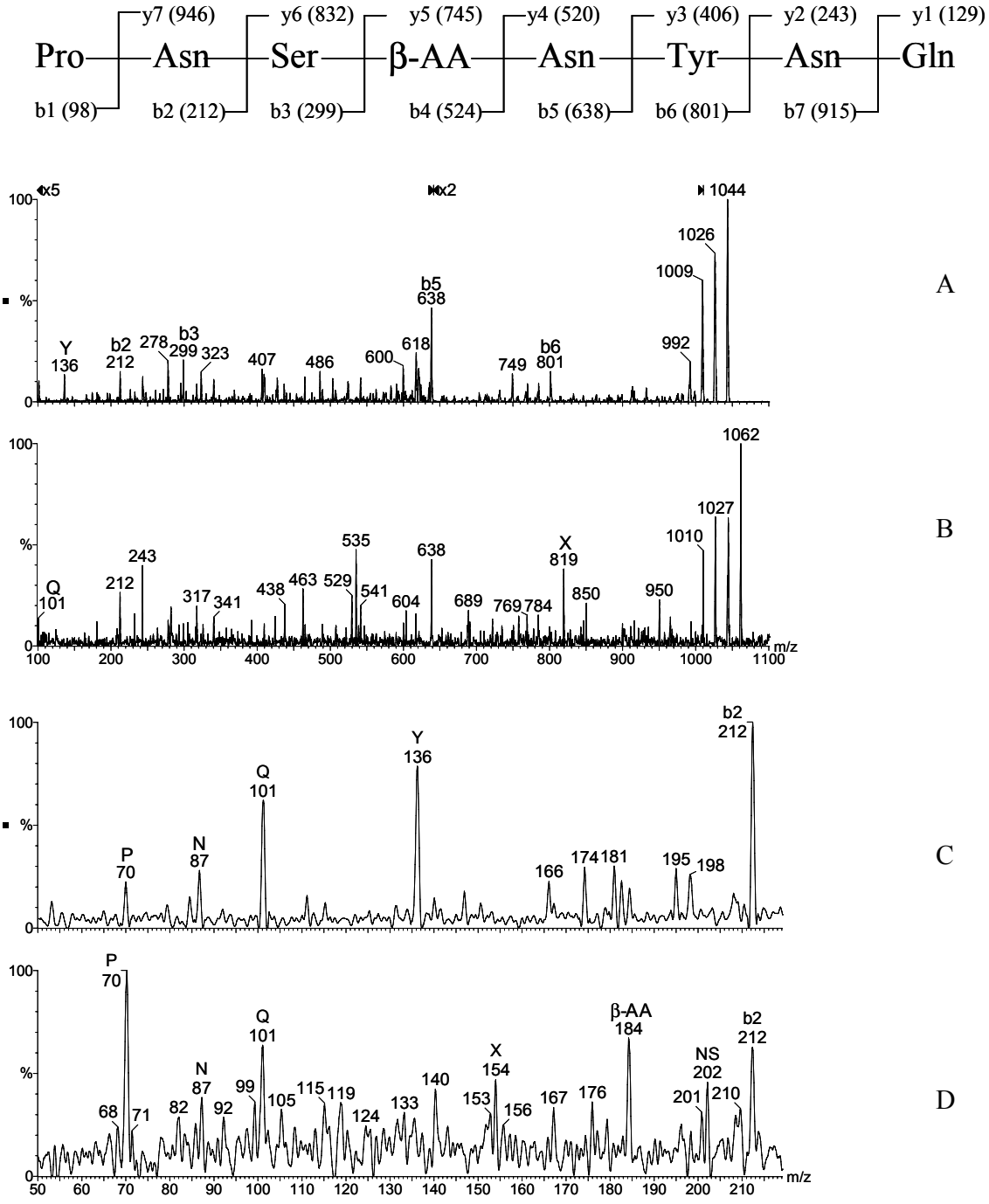
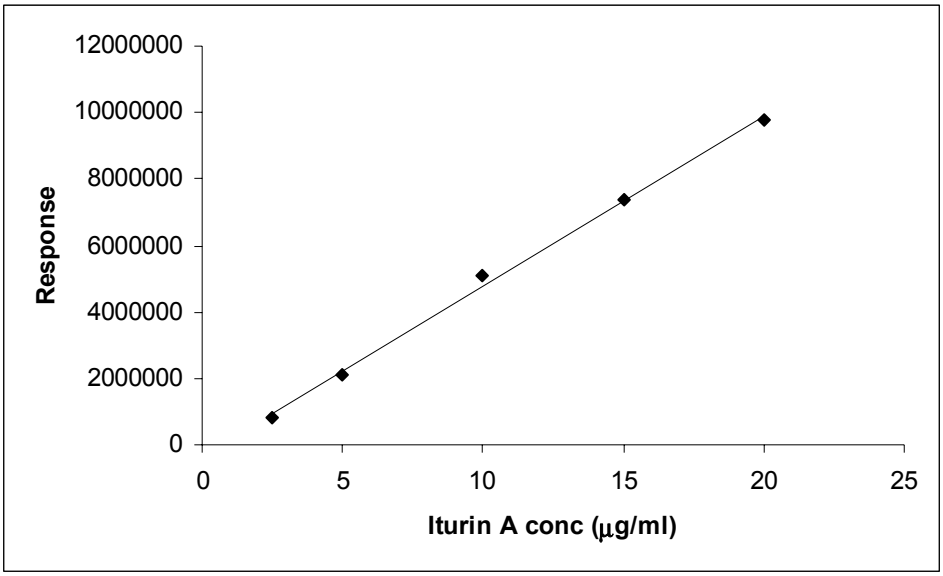


Comparison of the MS/MS spectra of protonated C-14 iturin A and C-14 fluoroiturin (A and B, respectively). The possible b- and y-fragment ions of linear iturin A are shown above the mass spectra[1]. β-AA indicates the iturinic acid. Of particular interest is the presence of the b6 ion (*m/z* 801) in spectrum A, which corresponds to the fragment containing the tyrosine residue, and its absence in spectrum B; a new ion fragment, *m/z* 819, is observed in spectrum B (indicated by x) corresponding to the fluorotyrosine-containing peptide. The lower mass regions of the MS/MS spectra for iturin and fluoroiturin are also shown (C and D, respectively). The immonium ions of the constituent amino acids are present in spectrum C: Pro (*m/z* 70), Asn (*m/z* 87), Gln (*m/z* 101), Tyr (*m/z* 136) and β-AA (*m/z* 184); in the spectrum for fluoroiturin (D), tyrosine is replaced by fluorotyrosine (*m/z* 154).



Calibration graph of authentic iturin A as determined by LC-MS; the responses of ions *m/z* 1043.5 and *m/z* 1057.5 were combined.

1. M. Gong, J-D. Wang, J. Zhang, X-F. Lu, Y. Pei and J-Q. Cheng, *Acta Biochimica et Biophysica Sinica,* 2006, **38**, 233-240.