Figure 1 – Examples of spectra predicted by the Bayesian neural network model:
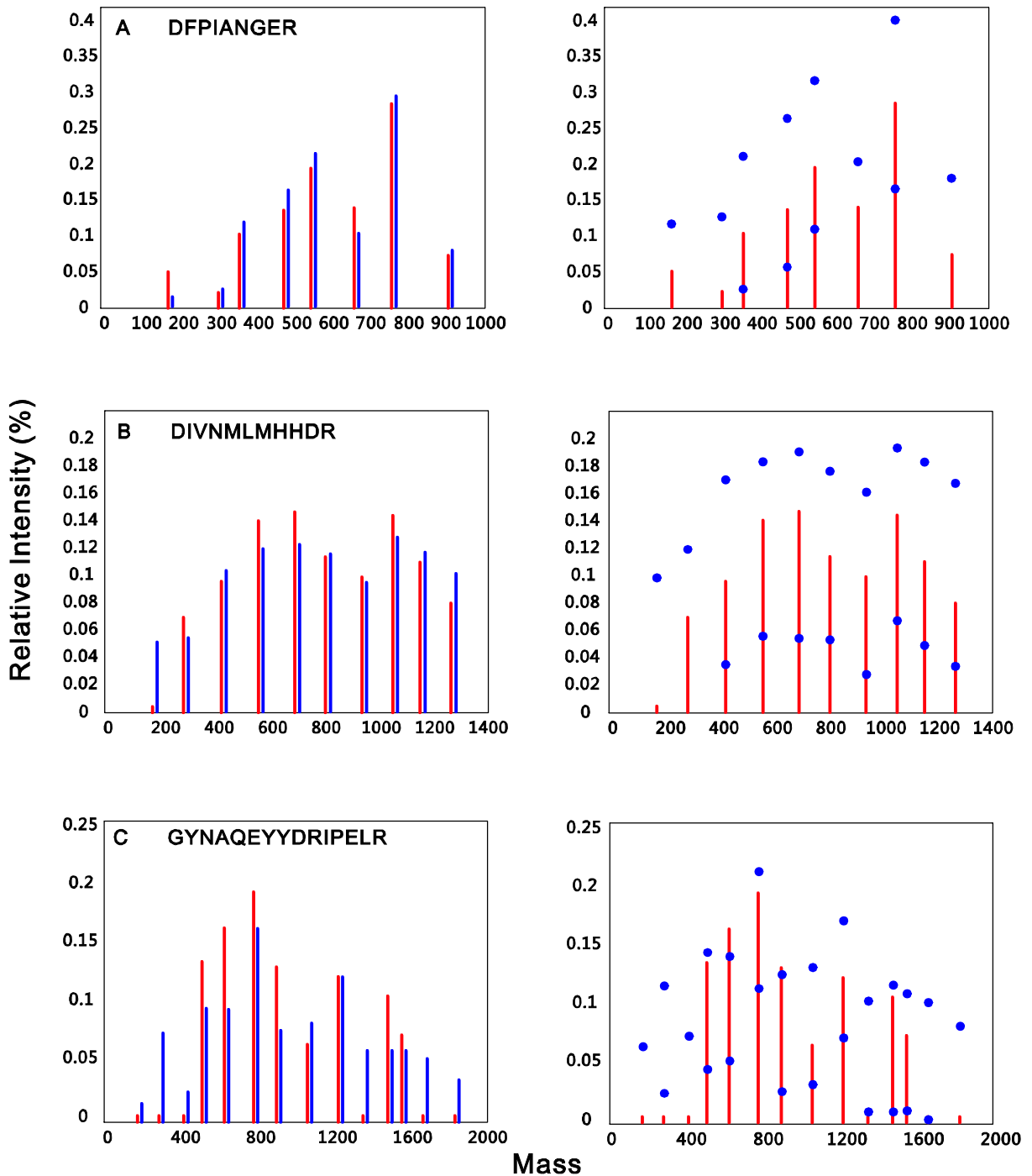

Figure 1-A: Mobile peptide with residue Asp and Pro. Similarity score: 9.32.

Figure 1-B: Partial-mobile peptide with Asp. Similarity score: 8.19.

Figure 1-C: Non-mobile peptide with Asp and Pro. Similarity score: 14.64.

Experimental spectra are log-transformed and indicated in red. Predicted spectra are indicated in blue. Both types of spectra are subject to total ion current normalization. Blue dots indicate the interval [mean intensity – SD, mean intensity + SD] within which intensities of the ions are supposed to lie.