1 Representing uncertainty in common mass-spectrometry quantities

One quantity that we frequently interested in mass-spectrometry is the sequence of a peptide. There is some uncertainty in a peptide sequence given the relevant spectra. If we quantified the probability in this sequence, we could plot the probability that one amino acid proceeds another as a heatmap, example below:

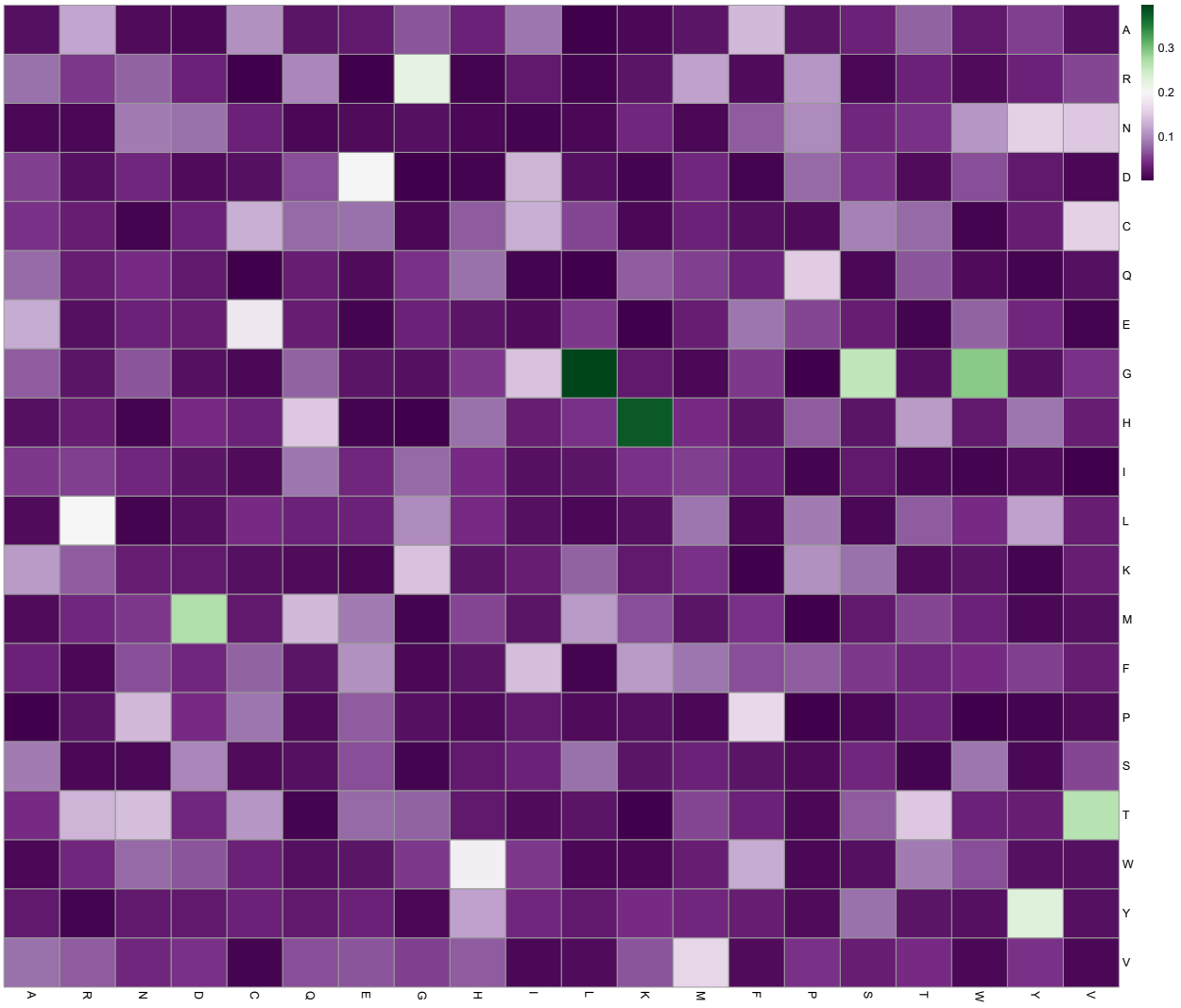

Figure 1: **Heatmap of amino-acid probabilities.** A heatmap where the the $(i, j)^{th}$ entry represents the probability that amino acid i is followed by amino acid j

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Another quantity is the uncertainty in a spectra. The following are 9 MS1 spectra which are all compatible with peptide PARRDABZJARA with total intensity 1000.

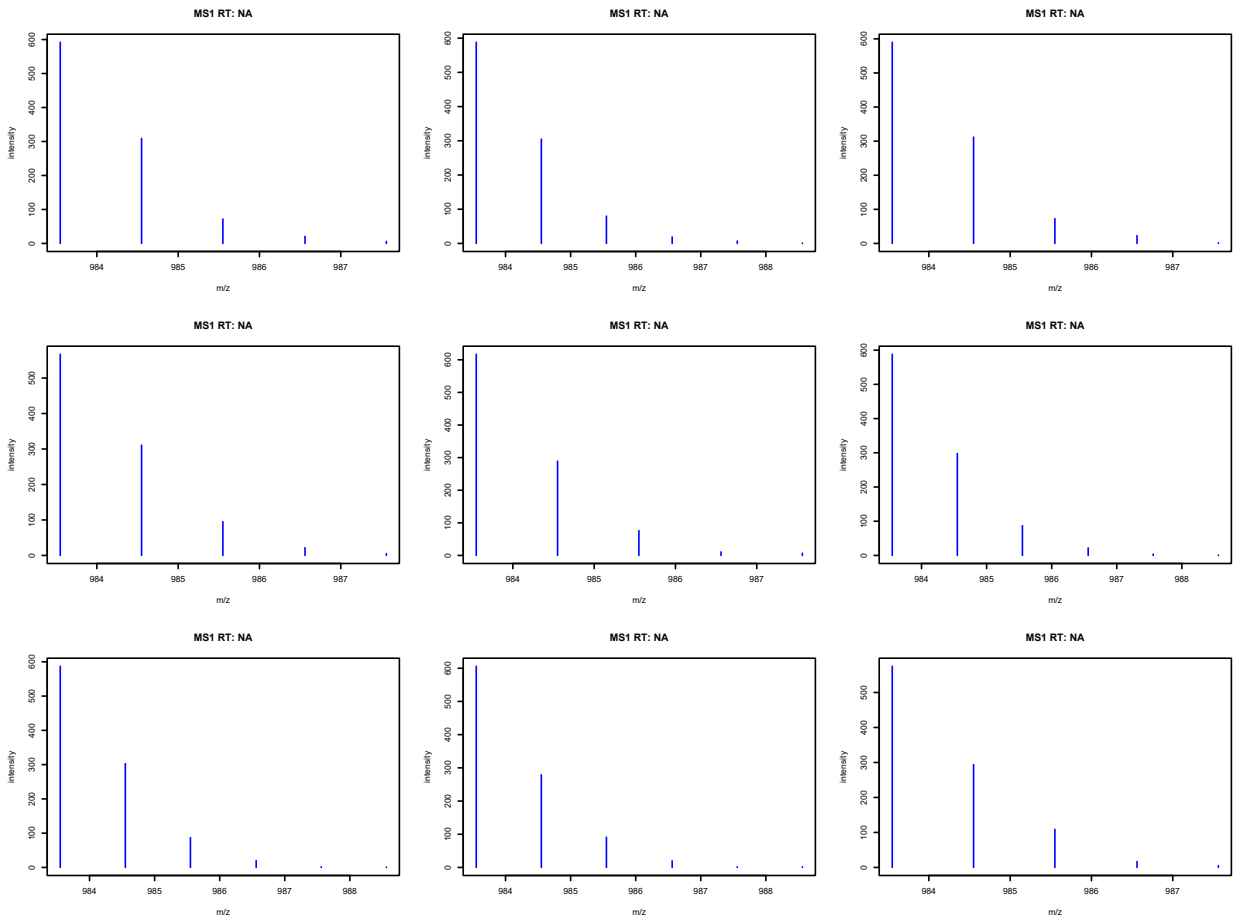

Figure 2: **Spectra of PARRDABZJARA.** Spectra diagrams showing spectra compatible with the MS1 spectra of PARRDABZJARA

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It is infeasible to plot the 1000's of spectra that are compatible with MS1 spectra of an amino-acid sequence. Hence, we can use a contour plot which capture the local density of the spectra locations and heights. A typical spectra is overlaid for reference in white.

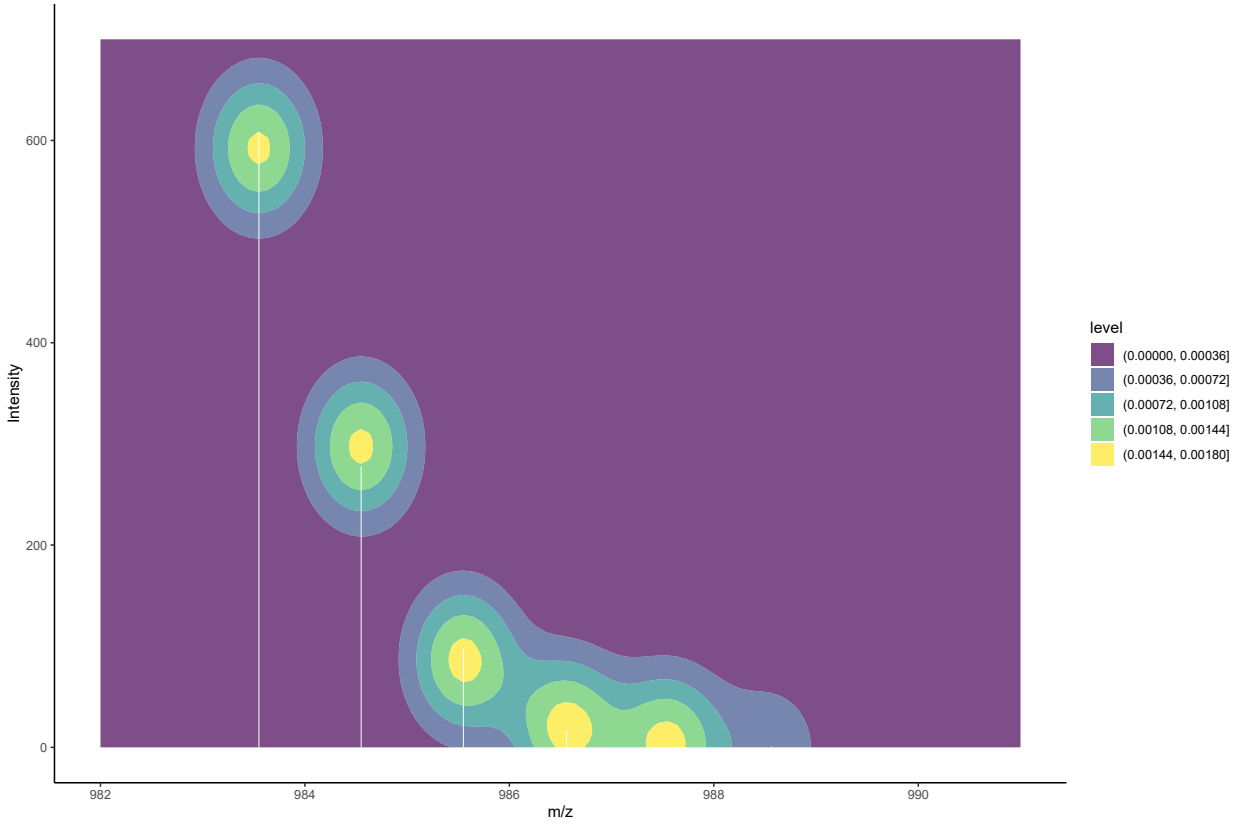

Figure 3: **Contour Spectra of PARRDABZJARA.** A contoured Spectra diagrams showing the densities compatible with the MS1 spectra of PARRDABZJARA. Colour bar indicated relative probability. Example spectra overlaid in white.