POISSON APPROXIMATION BASED MONOISOTOPIC PEAK FINDING IN MASS SPECTRA OBTAINED BY COMBINED FRACTIONAL DIAGONAL CHROMATOGRAPHY

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Breen *et al.* (2000) proposed a method for finding monoisotopic peptide peaks in mass spectra based on an approximation of the distribution of different isotopic variants of a peptide by a Poisson distribution. They developed the method using all protein sequences from SWISS-PROT database. Mass spectra obtained by a COmbined FRActional DIagonal Chromatography (COFRADIC) approach, developed by Gevaert *et al.* (2003), target a specific subset of peptides, in this case the N-termini. One can therefore ask the question whether the original results of Breen *et al.* apply to spectra generated by this particular COFRADIC method. We investigate whether the proposed approximation holds for N-termini. We also evaluate whether ignoring sulphur atoms while developing the approximation, as proposed by Breen *et al.*, does not increase the risk of missing monoisotopic peaks corresponding to sulphur-containing peptides. Finally, we check sensitivity of the quality of the approximation to optimization criteria used in the development process.