A compositional data model to predict the isotope distribution for average peptides using a compositional spline model.

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Abstract

We propose an updated approach for approximating the isotope distribution of average peptides given their monoisotopic mass. Our methodology involves in-silico cleavage of the entire UNIPROT database of Human reviewed proteins using Trypsin, generating a theoretical peptide dataset. The isotope distribution is computed using BRAIN. We apply a compositional data modelling strategy that utilizes an additive log-ratio transformation for the isotope probabilities followed by a penalized spline regression. Furthermore, due to the impact of the number of Sulphur atoms on the course of the isotope distribution, we develop separate models for peptides containing zero up to five Sulphur atoms. Additionally, we propose three methods to estimate the number of Sulphur atoms based on an observed isotope distribution. The performance of the spline models and the Sulphur prediction approaches is evaluated using a mean squared error and a modified Pearson's χ^2 goodness-of-fit measure on an experimental UPS2 data set. Our analysis reveals that the variability in spectral accuracy contributes more to the errors than the approximation of the theoretical isotope distribution by our proposed average peptide model. Moreover, we find that the accuracy of predicting the number of Sulphur atoms based on the observed isotope distribution is limited by measurement accuracy.

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