A Strategy to Automatically Infer Precursor Charge States of Electron Transfer Dissociation Tandem Mass Spectra

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Electron Transfer Dissociation (ETD) is a new method to dissociate highly charged ions in the mass spectrometer. It cleaves randomly along the polypeptide backbone and is indicated when trying to pinpoint the location of protein posttranslational modifications. Efficient analysis of ions dissociated with ETD requires accurate determination of charge states for calculation of molecular weight. We created a computational strategy to assign the charge state of ions often used for ETD to be used in large-scale proteomic experiments. The program, *Charge Prediction Machine* (CPM), uses Bayesian decision theory to account for different charge reduction processes encountered in ETD, and can also handle multiplex spectra (co-fragmentation of different ion species). CPM correctly assigned charge states to 99% of the 13,097 MS2 spectra from a combined dataset of four experiments while a competing program, Charger (ThermoFisher) only assigned 86% of the charges correctly. As far as we know, CPM is the only freely available software for academic use for this purpose.

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