mspms: a R package and graphical interface for the processing and analysis of multiplex substrate profiling by mass spectrometry for proteases (MSP-MS) data.

Abstract:

MSP-MS is a powerful method for determining the sequence specificity profile of proteases and has been used as a starting point for rational drug design. Analysis of this MS based data is a multistep process involving normalization, outlier detection, imputation, and cleavage sequence identification. This can be challenging, especially for biologists/ mass spectromitrists with limited programming experience. To overcome these issues, we provide the mspms R package alongside a companion graphic user interface to facilitate the analysis of MSP-MS data with good software practices.

Introduction:

Results:

Discussion: