Brief User Guide of the extended Ascore

(3/18/2018)

Introduction

We extended the original Ascore (http://ascore.med.harvard.edu/ascore.php) to allow for the localization of any modification mass to any type of amino acids. The extended Ascore was written in Matlab.

Parameter

There are seven parameters to be specified.

(1) Input_file: peptide identification file, see next section of "Input" for details.

(2) Output_path: the file path of Ascore results

(3) Dataset_path: The file path of data set. Now it only supports 'mgf' format.

(4) Fragment_tol: fragment ion tolerance, unit is Da

(5) Fragment_charge_mode: Available values are 1 and 2. 1 means that only one-charged theoretical fragment ions will be generated no matter what the precursor charge is, and 2 means that the maximal charge of fragment ions dependents on the precursor charge state as original Ascore version.

(6) Restrictive: Availabe values are 0 and 1. 0 means unrestrictive localization, and 1 means restrictive localization.

(7) AA: only useful when the parameter of restrictive is 1. The candidate amino acids for target modification. Available values is 20 kinds of amino aicds, case sensitivity.

Input

The extended Ascore now only supports our specific format of input file.

(1) Dataset: the data set name where the spectrum comes;

(2) Spectrum: the spectrum name, the same as the 'TITLE' in 'mgf' formatted data set;

(3) Sequence: the identified peptide sequence;

(4) Charge: the precursor charge of experimental spectrum;

(5) Other Identified modifications: identified modifications except for target modification, e.g., phosphorylation. Each of these modifications must be specified as the format: 'pos, name;', e.g., '1, Oxidation[M];' or '1, Oxidation[M]; 3, Deamidated[N];'. Note that the comma and semicolon are necessary for each modification.

(6) Mass Shift: the mass of target modification.

Output

The extended Ascore output localization results with the following properties:

(1) Ascore

(2) Site_1: the most optimal site, i.e., the localized site;

(3) Site_2: the suboptimal modification site;

(4) Site_1_N: the number of site determining ions for 'Site_1';

(5) Site_2_N: the number of site determining ions for 'Site_2';

(6) Depth: the number of peaks per 100-Da window that generates the greatest difference of 'Peptide Score' between 'Site_1' and 'Site_2'.