Phosphate Localization Score

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As published in Albuquerque et al, MCP 2008, the Phosphate Localization Score (PLS) is our way of quantifying the certainty of placement for a phosphate on the peptide sequence. Details of the algorithm are both in the paper, and in the code. This tutorial goes over how to use the script and understand the output.

- Preparing your input file
- Using Inspect's toolkit
- Understanding the output

Preparing your input file

Input and output formats are a hassle. Not just for you as a user, but for programmers everywhere. The problem is that they keep making up more of them, and changing the ones that already exist. I can't write code to parse everyone's output. So I'm going to make it as simple as possible and hope that other people follow my cue. The format that I expect here is either Inspect's native format or a super simple three column format: spectrum file, spectrum number (sometimes called scan number), peptide annotation. Put these three in a tab-delimited text file and that's it. It should look like this

May07/MM2D-02.mzXML	14063	M.ANSphosESSSSPVNEEENSQR.I
May07/MM2D-02.mzXML	15094	*.MQPTphosETSQPAPSDQGR.R
May07/MM2D-02.mzXML	15194	A.ATphosAVPESAEEGDNSGK.L
May07/MM2D-02.mzXML	16482	M.ADTphosEMQEQDVPSGTK.G
May07/MM2D-02.mzXML	17580	*.M+16DESphosGGDSGSVATPVQQR.A
May07/MM2D-02.mzXML	17758	M.SphosDGDSTTTSAMEISGDK.I

One note is that the string should not have brackets. If you are specifying a modification, please follow this format.
1. Phosphorylated residues are denoted as "Sphos" meaning the serine is phosphorylated
2. Other PTMs are denoted with their mass shifts, e.g. M+16 is oxidized methionine

Using Inspect's Toolkit

To use the PLS scoring scripts, you must properly install python and the inspect toolkit (see the Inspect tutorial). Once you've done this the script is rather easy. At the command line

>python PhosphateLocalization.py -r InputFile –w OutputFile –m SpectraDirectory

If that didn't make sense, read the Inspect tutorial and the advanced tutorial. I go over the command line and how to use it.

Understanding the output

The output of the script is very basic. It tells you for each input line (spectrum and annotation) what the PLS is, and if there was a better annotation than the one that you gave.