

SUPPLEMENTARY MATERIAL

Reviewing Spectra Using the SpectrumLook Software Package. We have written a software package called SpectrumLook that allows readers to inspect the fragmentation (MS/MS) spectra for the phosphopeptides identified in this study. Using this software, readers can visually browse the MS/MS spectra that led to the phospho-peptide identifications, including viewing annotations for the identified b and y ions, and neutral loss ions where appropriate. This software is supported by the Microsoft Windows platform. There are six files included with the SpectrumLook package that can be accessed at <http://ncrr.pnl.gov/Data>.

Note: To access the file, right click on the above link and select "Open Weblink in Browser".

1. SpectrumLook_Installer.msi - the installer. To install, double click on the file and follow the installation prompts. During installation, a shortcut to run the SpectrumLook program is placed at Start->Programs->PAST Toolkit->SpectrumLook. Alternatively, navigate to the C:\Program Files\SpectrumLook\ folder and double-click file "SpectrumLook.exe".
2. MT_Human_PP5_grouped.mzXML - the phosphopeptide spectra in mzXML format.
3. MT_Human_PP5_grouped_syn.txt - a summary of the identifications determined by SEQUEST. See the Readme.txt file for a description of the columns in this file.
4. MT_Human_PP5_grouped.ini - a parameter file that specifies the appropriate parameters for these data when browsing them with SpectrumLook.
5. Readme.txt and RevisionHistory.txt - text files that describe the SpectrumLook software.