

Continued progress reports:

Scott:

Posted mass spectrometer code to Github, repository here:

<https://github.com/sbordyak/MassSpecMCMC-matlab>

Changed the directories to make them internally consistent.

Jim will wait until it can handle the five-isotope data stream

Jim:

Been plugging away at creating more 1D arrays (vectors) in preparation for the MCMC algorithm machinery.

At the top level: the notion of mass spectrometers. Mass spectrometer interface serves as the template for inputting data/metadata specific to each.

Noah:

If W_B is the width of the ion beam at the focal plane, W_C is the width of the collector opening, and R_{eff} the effective radius of the magnet, then the width of the top of the peak W_T in units of amu for a given mass

$$W_T = \frac{(W_C - W_B) \cdot \text{mass}}{R_{\text{eff}}}$$

And the width of the entire peak W_P in units of amu is

$$W_P = \frac{(W_C + W_B) \cdot \text{mass}}{R_{\text{eff}}}$$

For instance, for commonly used values $W_B = 0.35$ mm, $W_C = 1$ mm, $R_{\text{eff}} = 540$ mm, then W_T is