Supporting Information

The alphabet projection of spectra

Patrick A. Kreitzberg,† Marshall Bern,‡ Qingbo Shu,¶ Fuquan Yang,§ and Oliver

Serang*,†

†Department of Computer Science, University of Montana, Missoula, MT, USA

‡Protein Metrics Inc., Cupertino, CA, USA

¶Biodesign Institute, Arizona State University, Tempe, AZ, USA

§Institute of Biophysics, Chinese Academy of Sciences, Beijing, China

E-mail: oliver.serang.@umontana.edu

Supporting Information Available

The following files are available free of charge.

- S-1 Zip file of source code; organized as follows:
 - /data/ directory includes both datasets used in paper.
 - /src/mcmc/ directory includes source code for the Gibbs sampler method used and a README.txt with instructions.
 - /src/annotate-spectra directory includes code for a *de novo* sequencing script
 written in Python 2.7 which was used to create figures in the paper.
 - /src/elemental-decomposition directory includes source code for an elemental decomposition script written in C++.