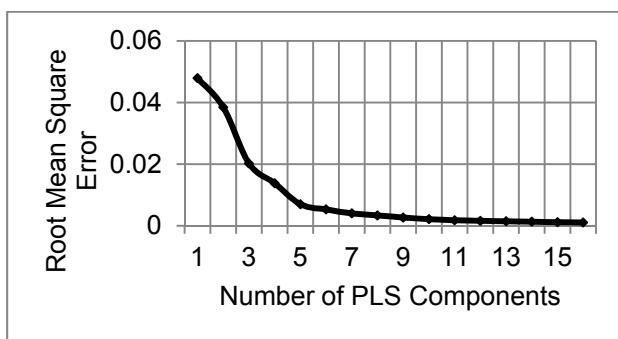
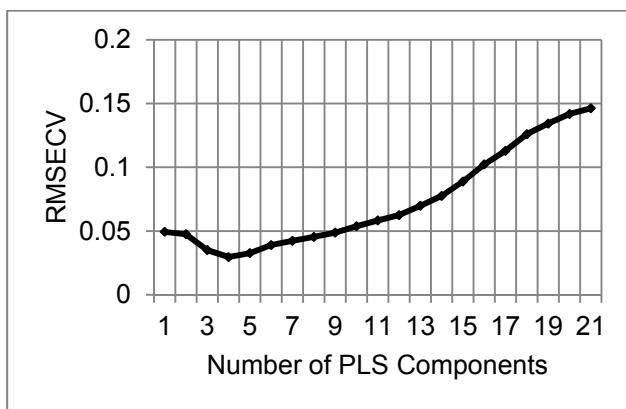


SI Figure 1. Explained y variance of α -helix content for analysis of the Amide I region as a function of number of components.



SI Figure 2. RMSEC vs. number of components for α -helix prediction from the Amide I region.



SI Figure 3. Cross-validation: 4 PLS components only are required to fit the α -helix model for proteins in H_2O using Amide I data.