

Supplementary Information

A simulation-guided fluorescence correlation spectroscopy tool to investigate the protonation dynamics of cytochrome c oxidase

A. Wolf, C. Schneider, T. Y. Kim, K. Kirchberg, P. Volz, and U. Alexiev

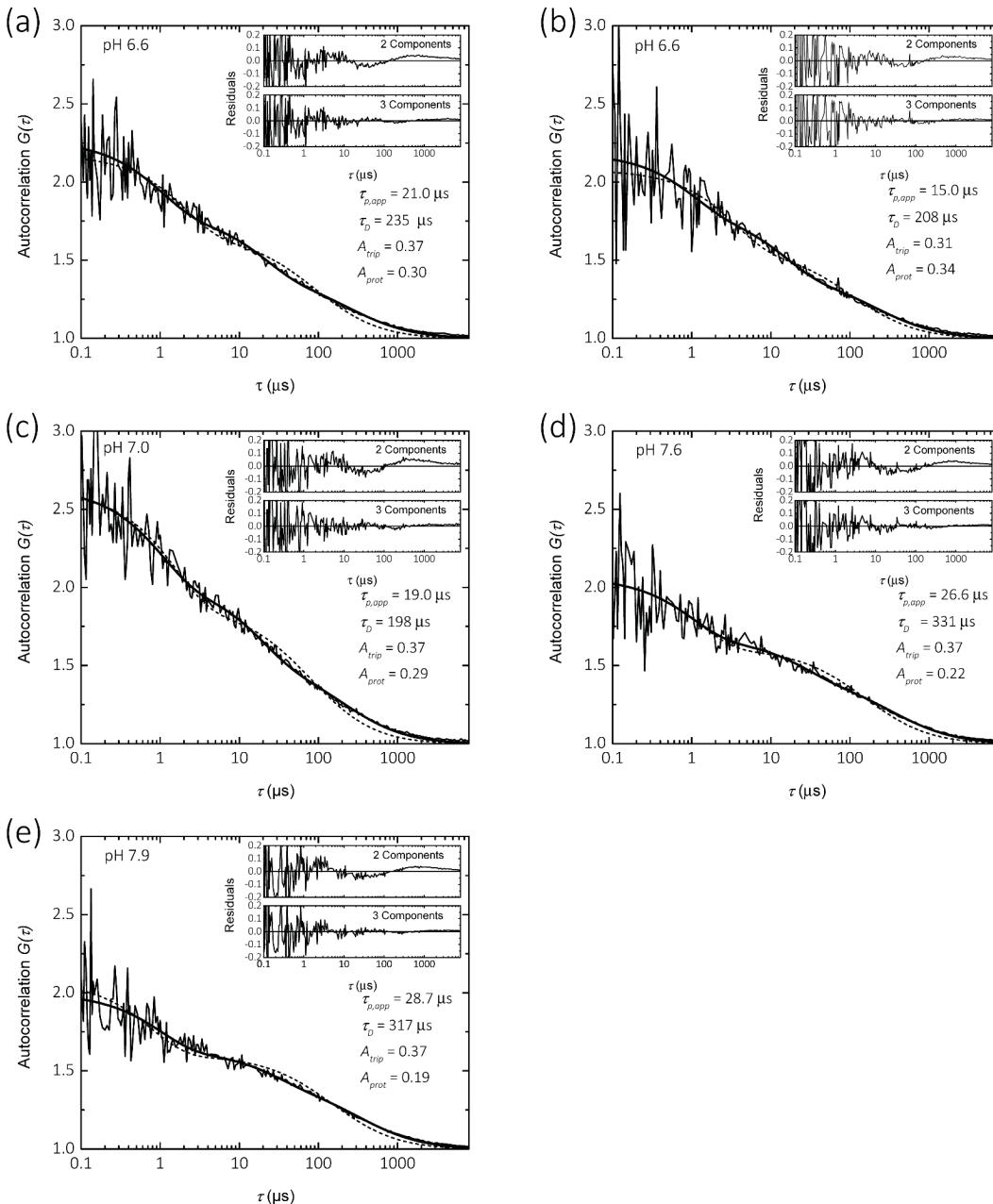


Figure S1 FCS curves of CcO CS-P301C-AF. Fits according to eq. 4 in the manuscript with two exponential components in the autocorrelation function are plotted in dashed lines and for 3 components in straight lines. The corresponding residuals are shown in the insets. Fit parameters are given in each panel; the triplet time constant was 1 μs .

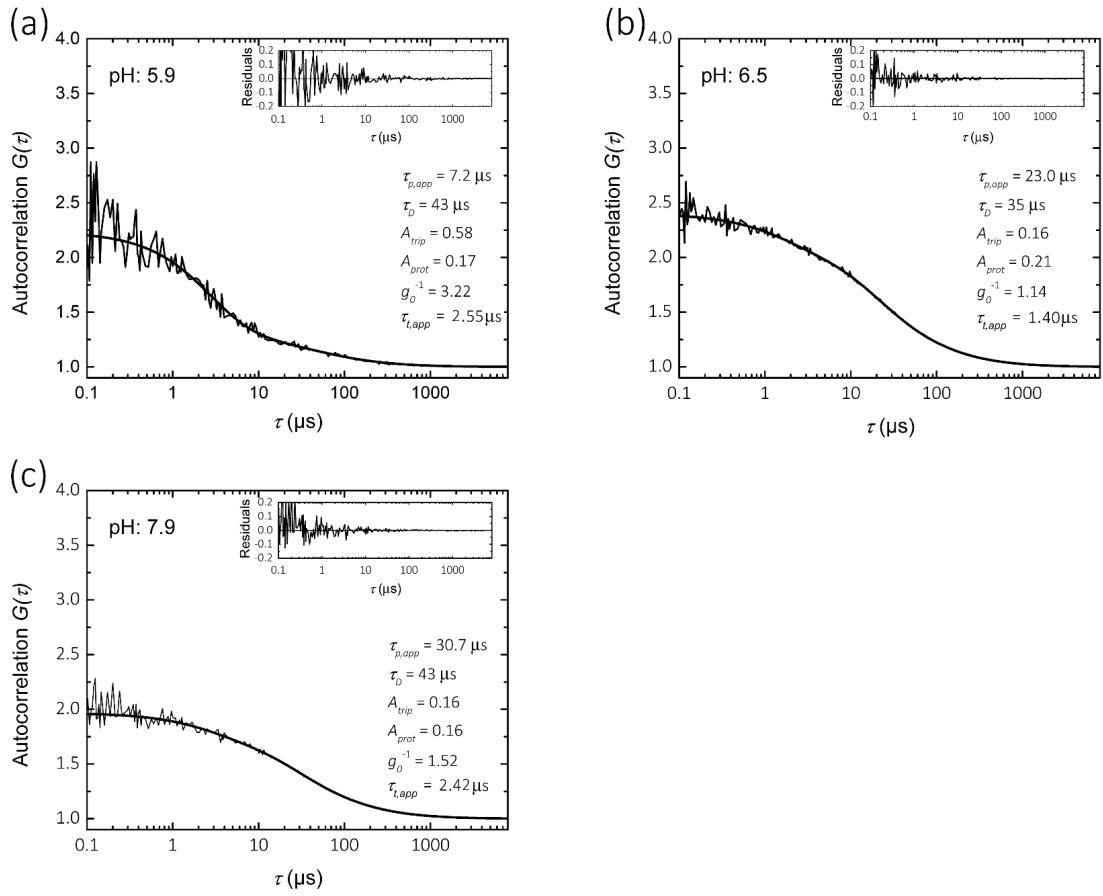


Figure S2 FCS curves for selected pH values of fluorescein sodium salt in solution for data plotted in Figure 5 of the manuscript. Fits are according to eq. 4 in the manuscript. Fit residuals are shown in the insets. Fit parameters are given in each panel.

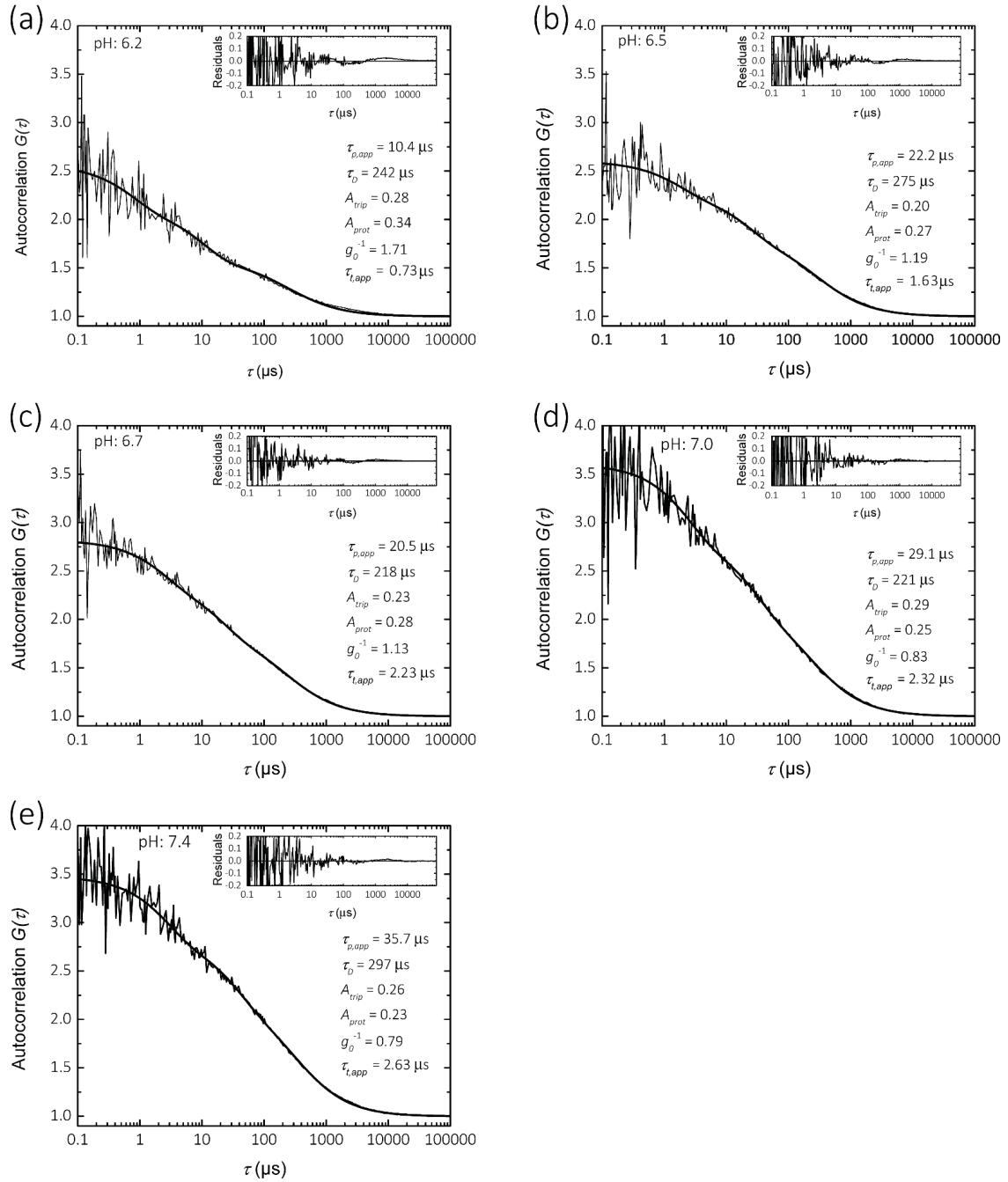


Figure S3 FCS curves for selected pH values of CcO CS-K299C-AF. Fits are according to eq. 4 in the manuscript. Fit residuals are shown in the insets. Fit parameters are given in each panel.