Quantitative, label-free and site-specific monitoring of molecular recognition: A multivariate resonance Raman approach

Stephan Niebling, Hannes Y. Kuchelmeister, Carsten Schmuck and Sebastian Schlücker

Supplementary Information

1. Experimental electronic absorption spectrum of the receptor CBS-KKF

2. Experimental UV resonance Raman binding study

3. Calculated contributions of free receptor and complex to the experimental spectrum of CBS-KKF and 1.2 eq. of the ligand AE_3.

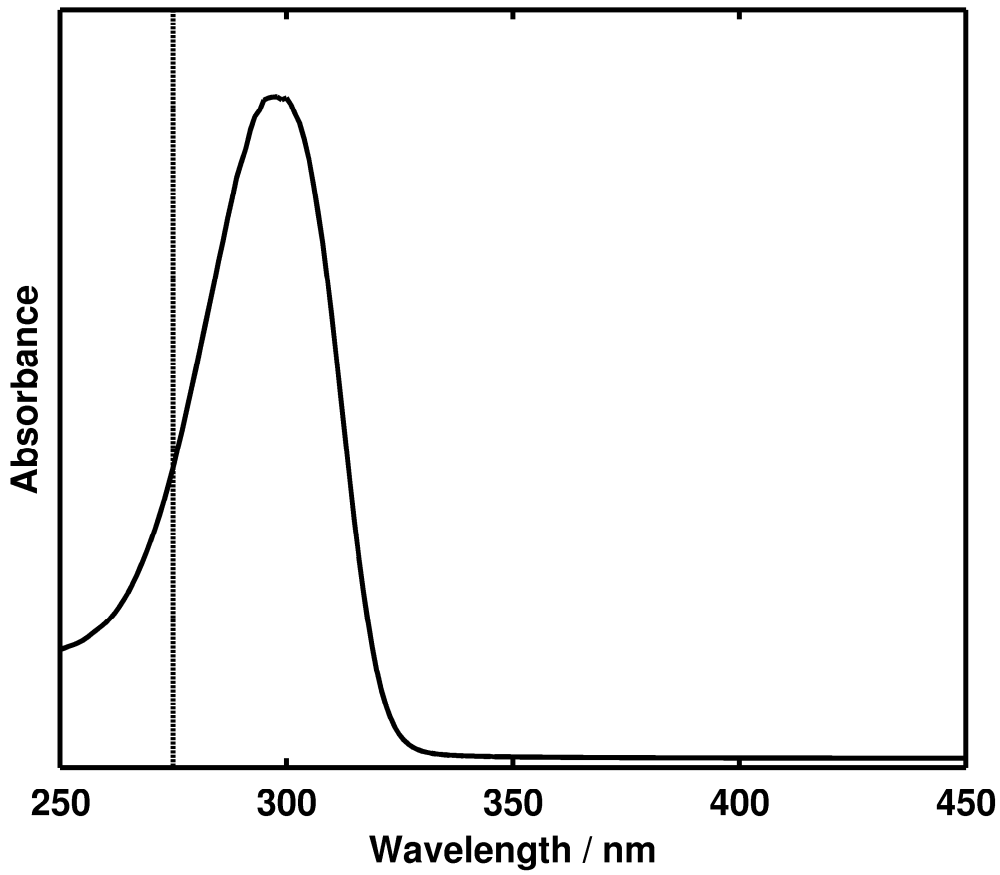

Fig. S1 Experimental electronic absorption spectrum of the receptor CBS-KKF

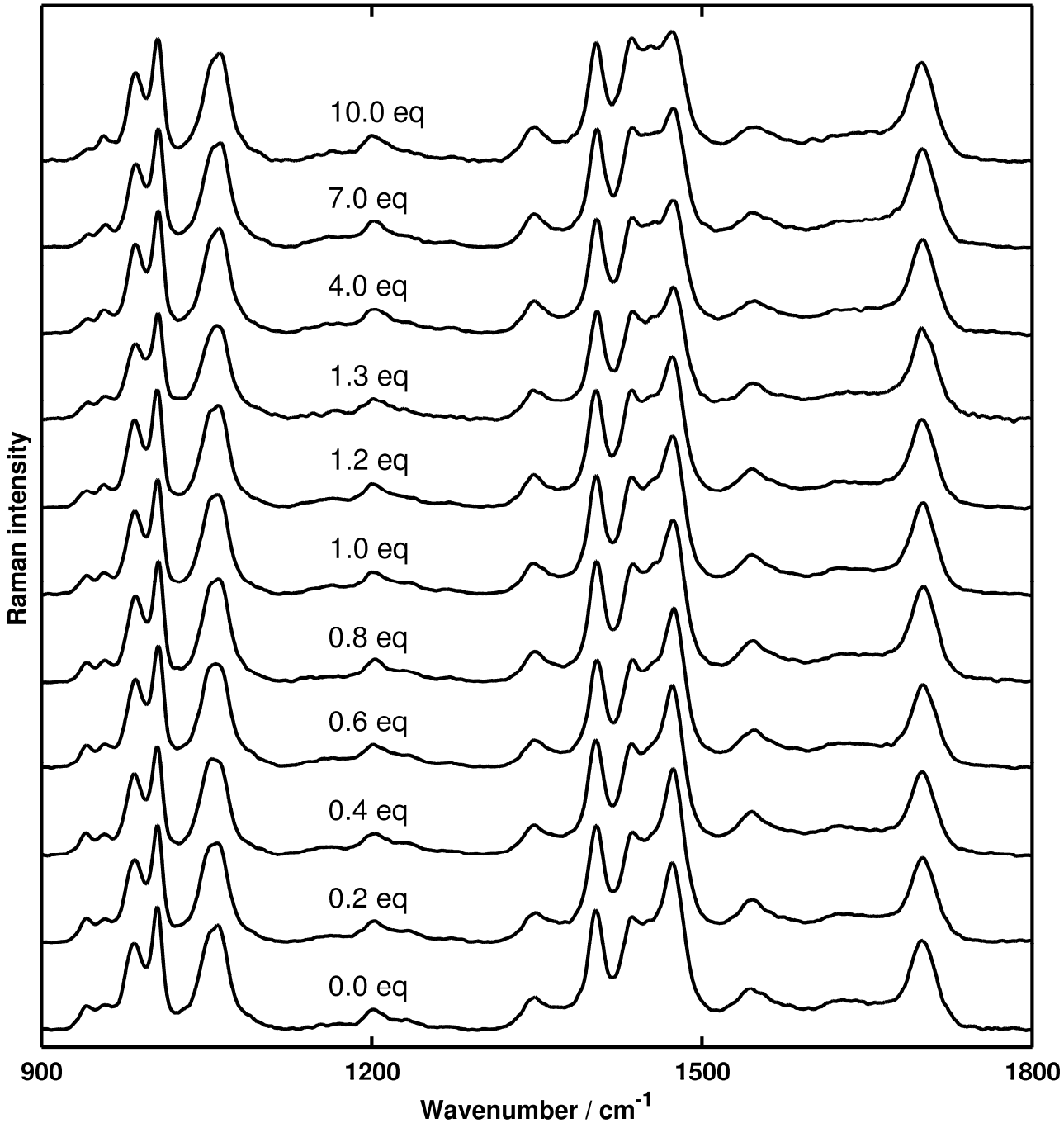

Fig. S2 Experimental UV resonance Raman spectra (λ_{exc} = 275 nm) of the peptide receptor CBS-KKF (c = 1 mM) at different ligand concentrations ranging from 0 to 10 mM.

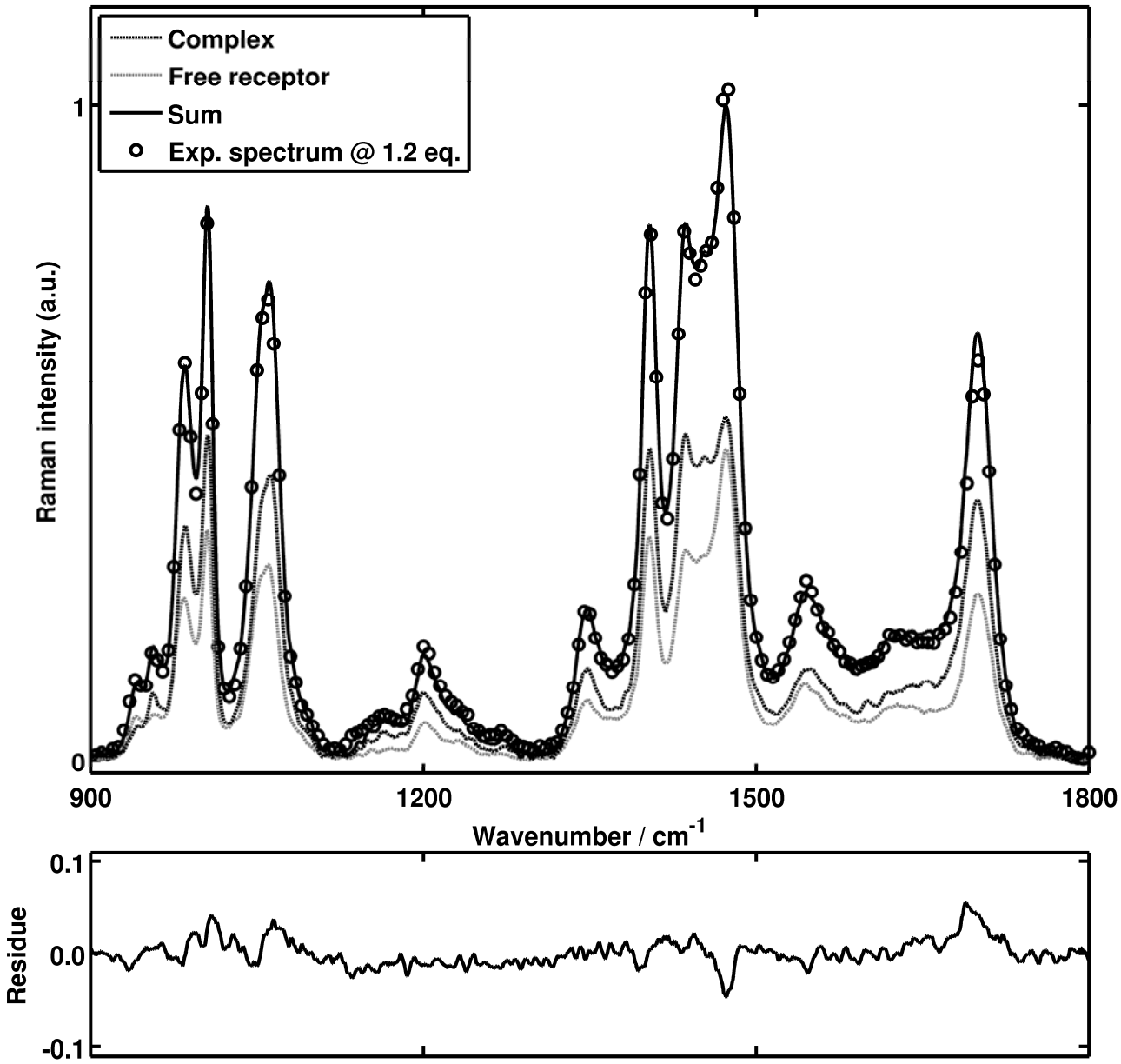

Fig. S3 Top: Experimental UV resonance Raman spectrum of CBS-KKF (c = 1 mM) in the presence of 1.2 equivalents of the ligand AE_3 (circles). The contributions of the free receptor and the complex, as determined by non-negative matrix factorization, are denoted as dashed lines, the sum of these contributions is shown as solid line. Bottom: Difference between the sum of the NMF component spectra and the experimental spectrum.