Supporting Information

Kinetic and Conformational Insights of Protein Adsorption onto Montmorillonite Revealed Using in Situ ATR-FTIR/2D-COS

Michael P. Schmidt and Carmen Enid Martínez*

Soil and Crop Sciences Section, School of Integrative Plant Science, Cornell University, Ithaca, NY 14853, United States

Corresponding author: Carmen Enid Martínez
906 Bradfield Hall
Soil and Crop Sciences Section
School of Integrative Plant Sciences, SIPS
Cornell University
Ithaca, New York 14853
Tel.: 607-255-0895
E-mail address: cem20@cornell.edu (C.E. Martínez)

Supporting Information
Contains 3 tables and 9 figures. This material is available free of charge via the Internet at http://pubs.acs.org.

Table S1 Pseudo-first order model parameters for each experimental concentration

Concentration (µM)	k_1 (min^{-1})	RMSE
1.50	0.0274	1.64×10^{-2}
3.75	0.0271	2.37×10^{-2}
7.50	0.0311	2.83×10^{-2}
15.0	0.0282	3.56×10^{-2}

Table S2 Pseudo-second order model parameters for each experimental concentration

Concentration (µM)	k_2 (min^{-1})	q_e	h (min^{-1})	RMSE
1.50	0.627	0.148	0.0137	4.38×10^{-3}
3.75	0.246	0.264	0.0171	9.34×10^{-3}
7.50	0.303	0.281	0.0239	8.99×10^{-3}
15.0	0.323	0.306	0.0302	9.64×10^{-3}

Table S3 Intraparticle diffusion model parameters for each experimental concentration

Concentration (µM)	k_d (a.u. $min^{-1/2}$)	RMSE
1.50	0.0150	1.98×10^{-2}
3.75	0.0250	2.49×10^{-2}
7.50	0.0280	3.43×10^{-2}
15.0	0.0312	4.13×10^{-2}

Figure S1. FTIR spectrum of cleaned SWy-2 bentonite used in ATR-FTIR experiments

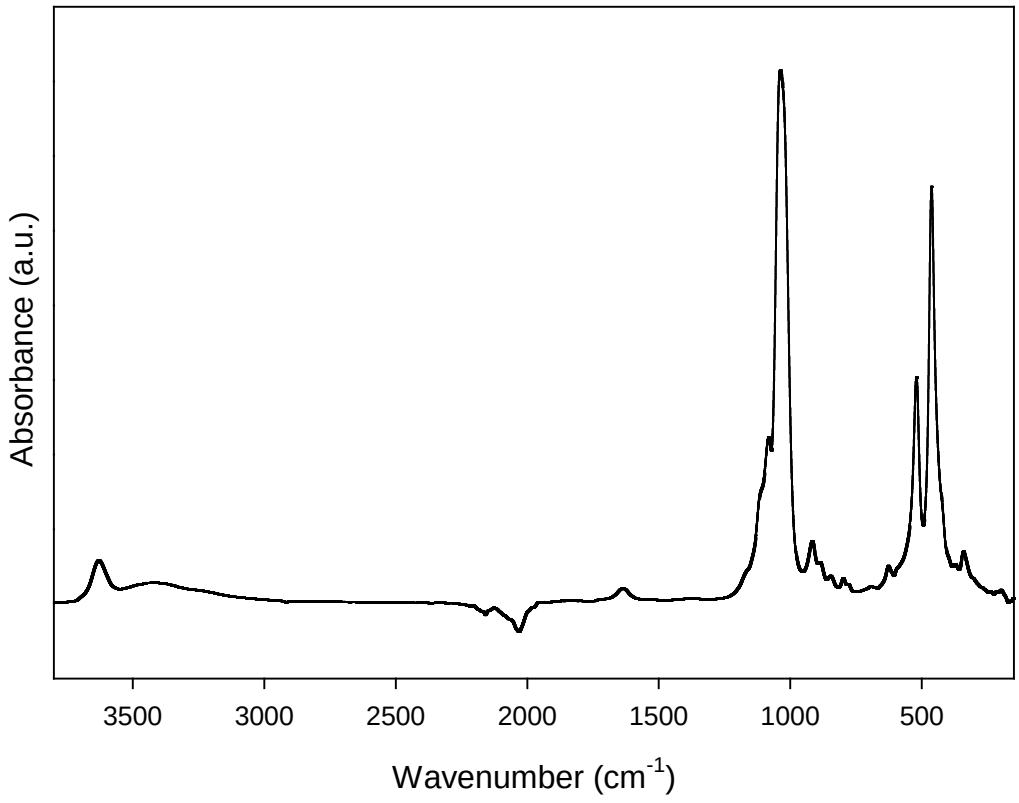

Figure S2. FTIR spectra from an adsorption experiment ([BSA] = 15.0 µM). Shown spectra were collected at ≈20 minute intervals from t = 3 minutes until t =120 minutes. The red line represents the FTIR spectrum of 15.0 µM BSA over a bare diamond IRE.

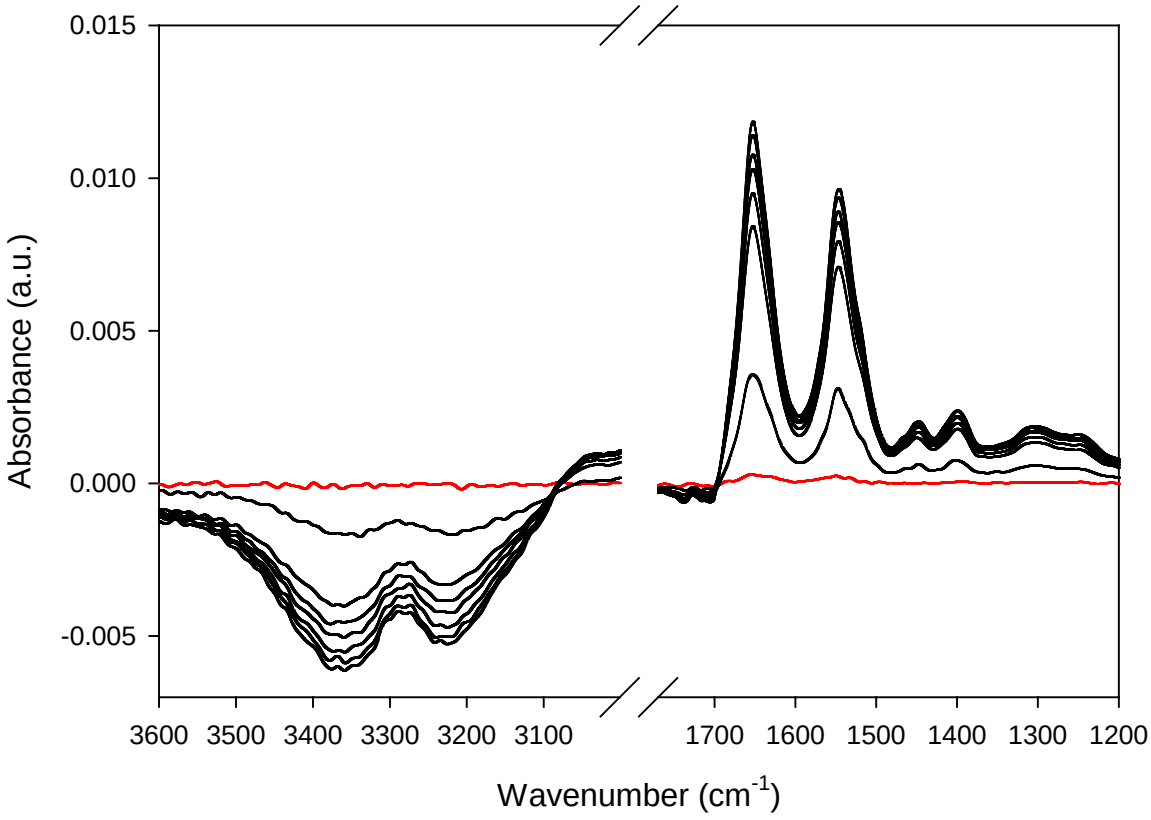

Figure S3. Elovich rate plot (q_t vs. ln(t)) for each experimental BSA concentration. [BSA] = 1.50 (yellow squares), 3.75 (red x), 7.50 (green circles) and 15.0 µM (orange triangles). Linear regression for each set is shown as solid line of corresponding color.

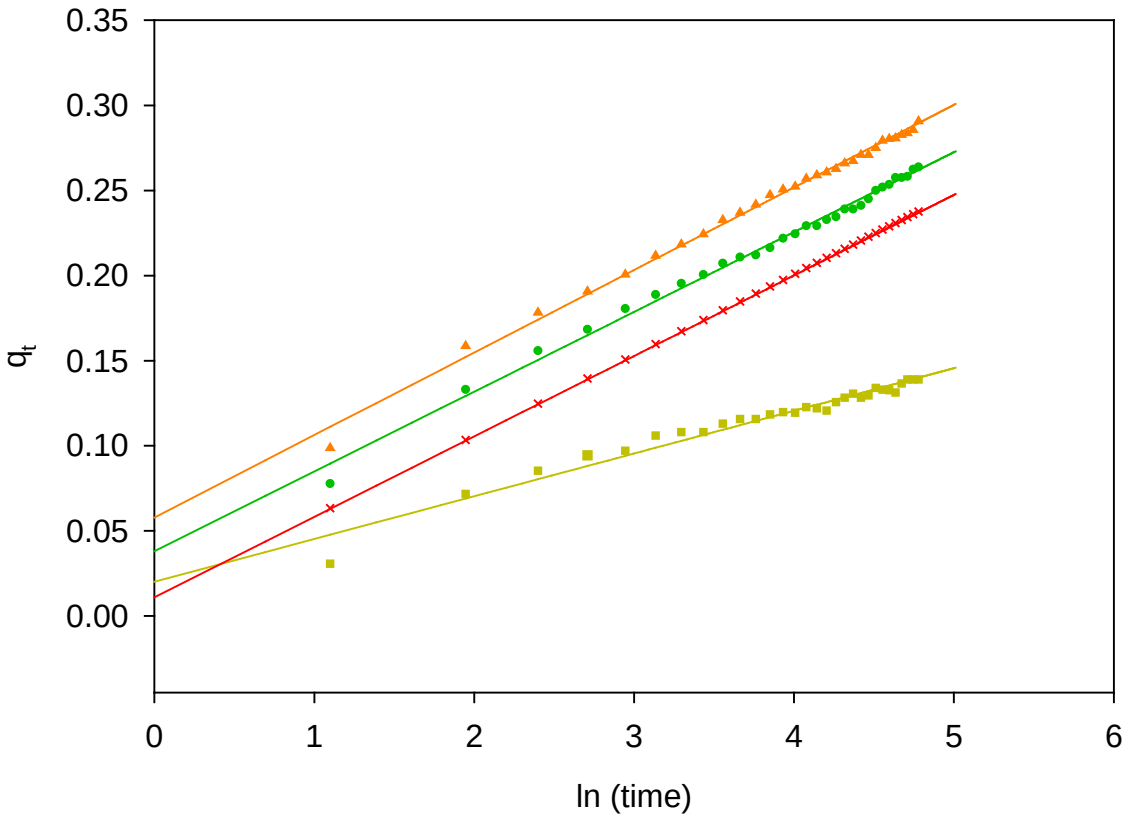

Figure S4. Pseudo-first order rate plot ($\ln(q_e-q_t)$ vs. t) for each experimental BSA concentration. [BSA] = 1.50 (yellow squares), 3.75 (red x), 7.50 (green circles) and 15.0 µM (orange triangles). Linear regression for each set is shown as solid line of corresponding color.

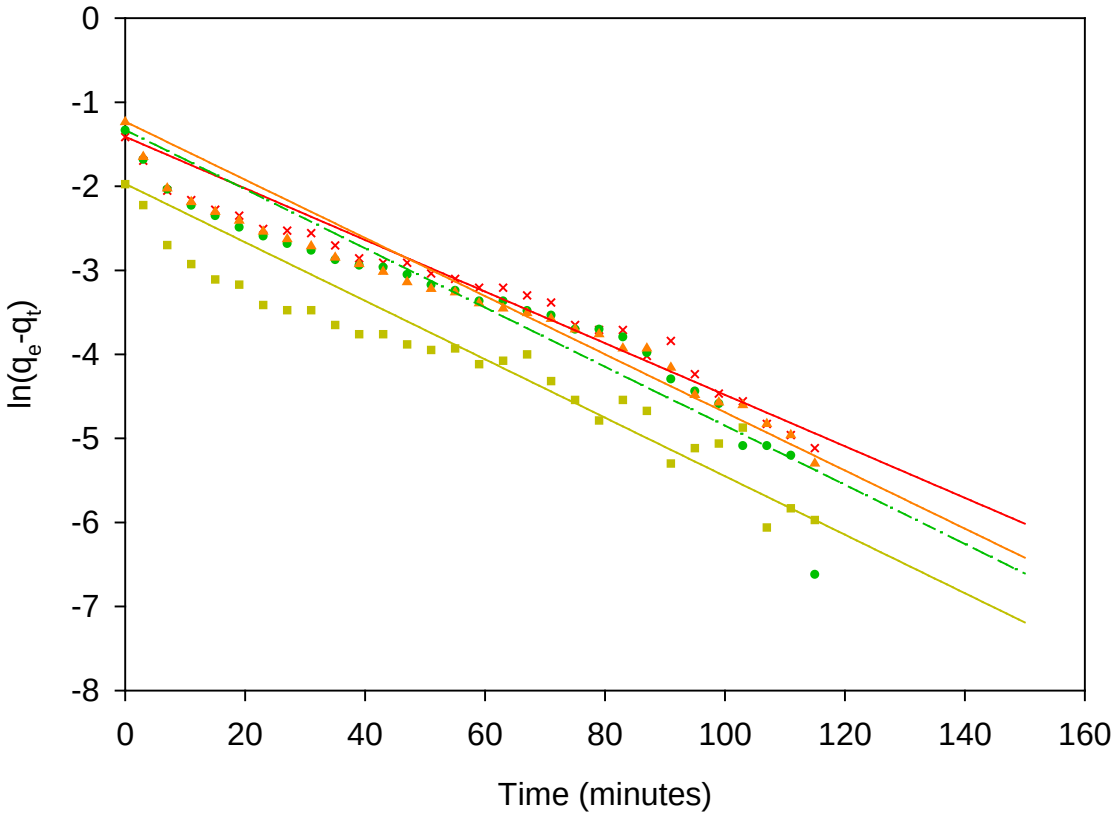

Figure S5. Pseudo-second order rate plot (t/q_t vs. t) for each experimental BSA concentration. [BSA] = 1.50 (yellow squares), 3.75 (red x), 7.50 (green circles) and 15.0 µM (orange triangles). Linear regression for each set is shown as solid line of corresponding color.

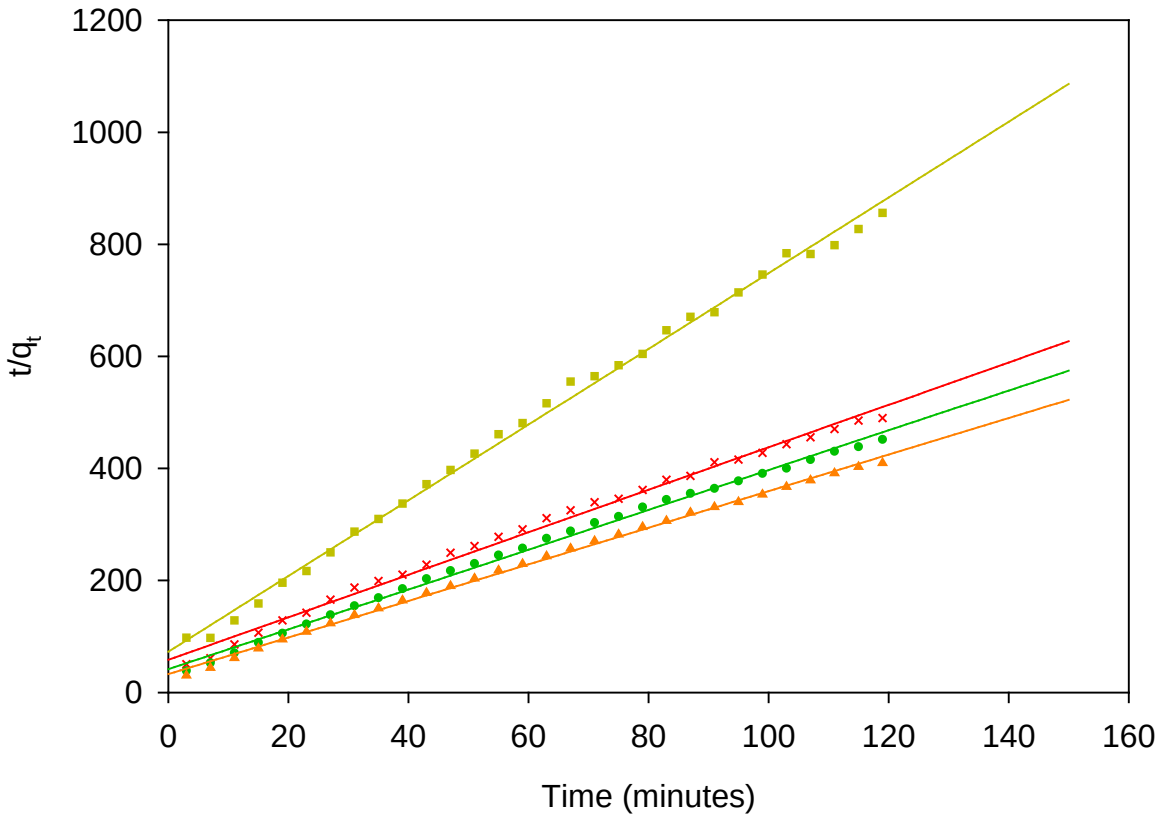

Figure S6. Intraparticle diffusion rate plot (q_t vs. $\sqrt{t}$) for each experimental BSA concentration. [BSA] = 1.50 (yellow squares), 3.75 (red x), 7.50 (green circles) and 15.0 µM (orange triangles). Linear regression for each set is shown as solid line of corresponding color.

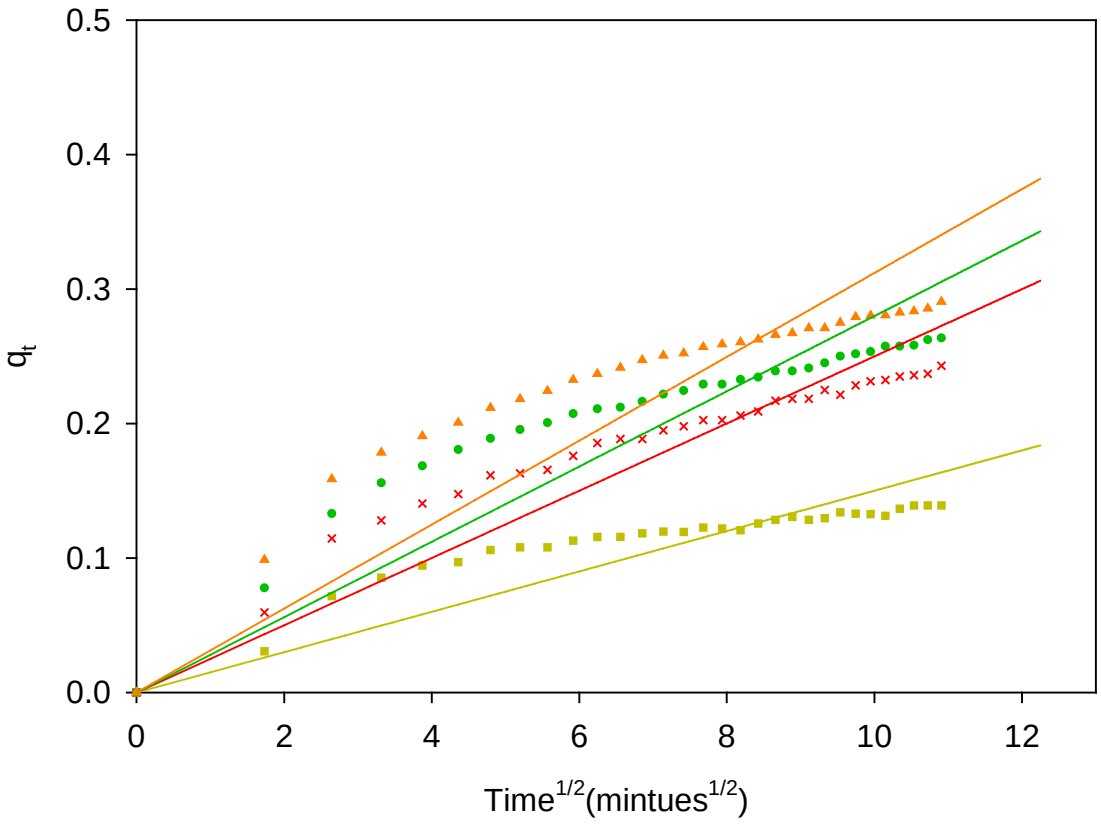

Figure S7 a) Synchronous 2D-COS plot for [BSA] = 1.50 µM with corresponding autocorrelation spectrum and labelled peaks in the amide I band. Legend presents correlation values.

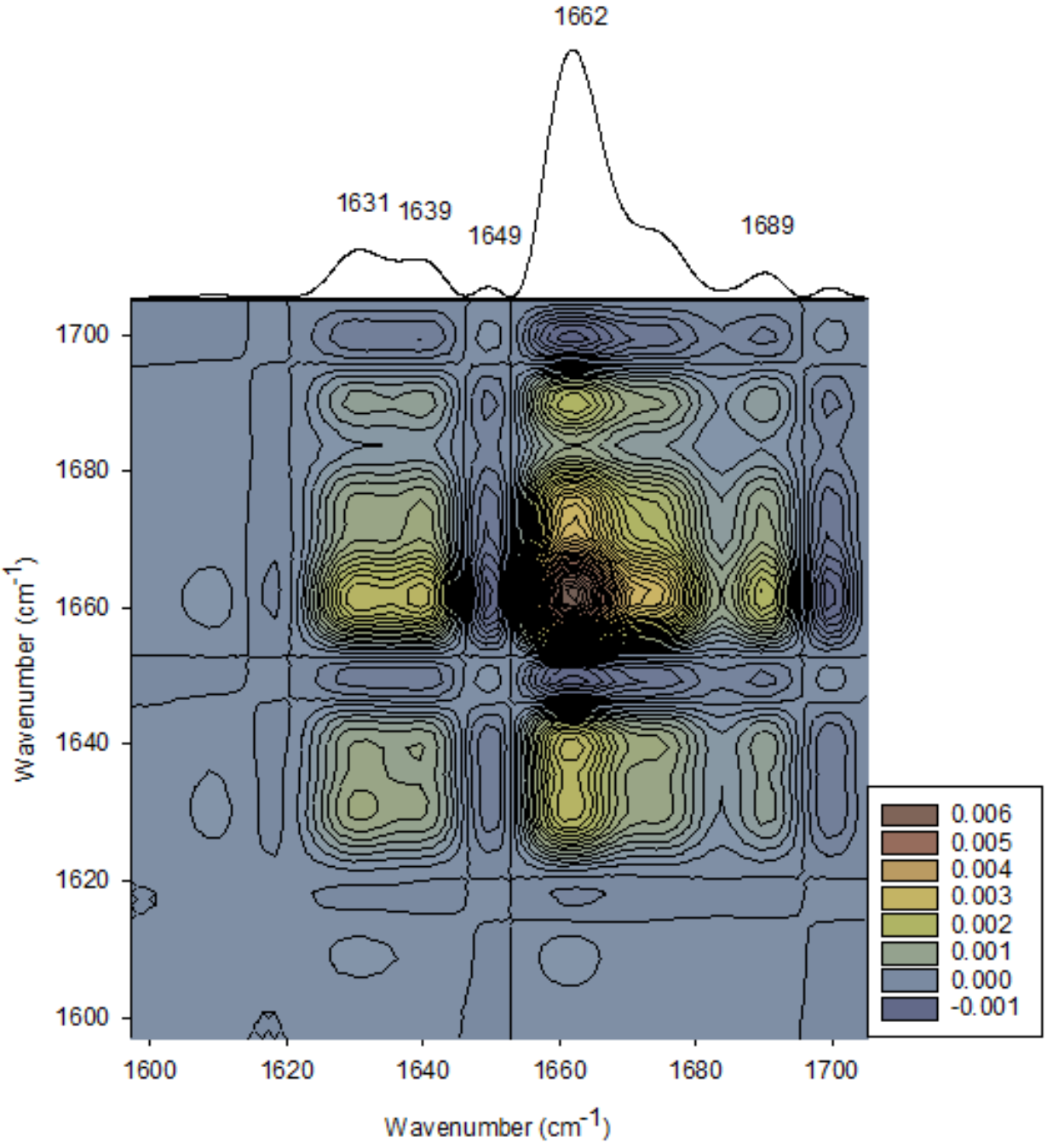

Figure S7 b) Asynchronous 2D-COS plot for [BSA] = 1.50 µM. Correlation values are shown in the legend.

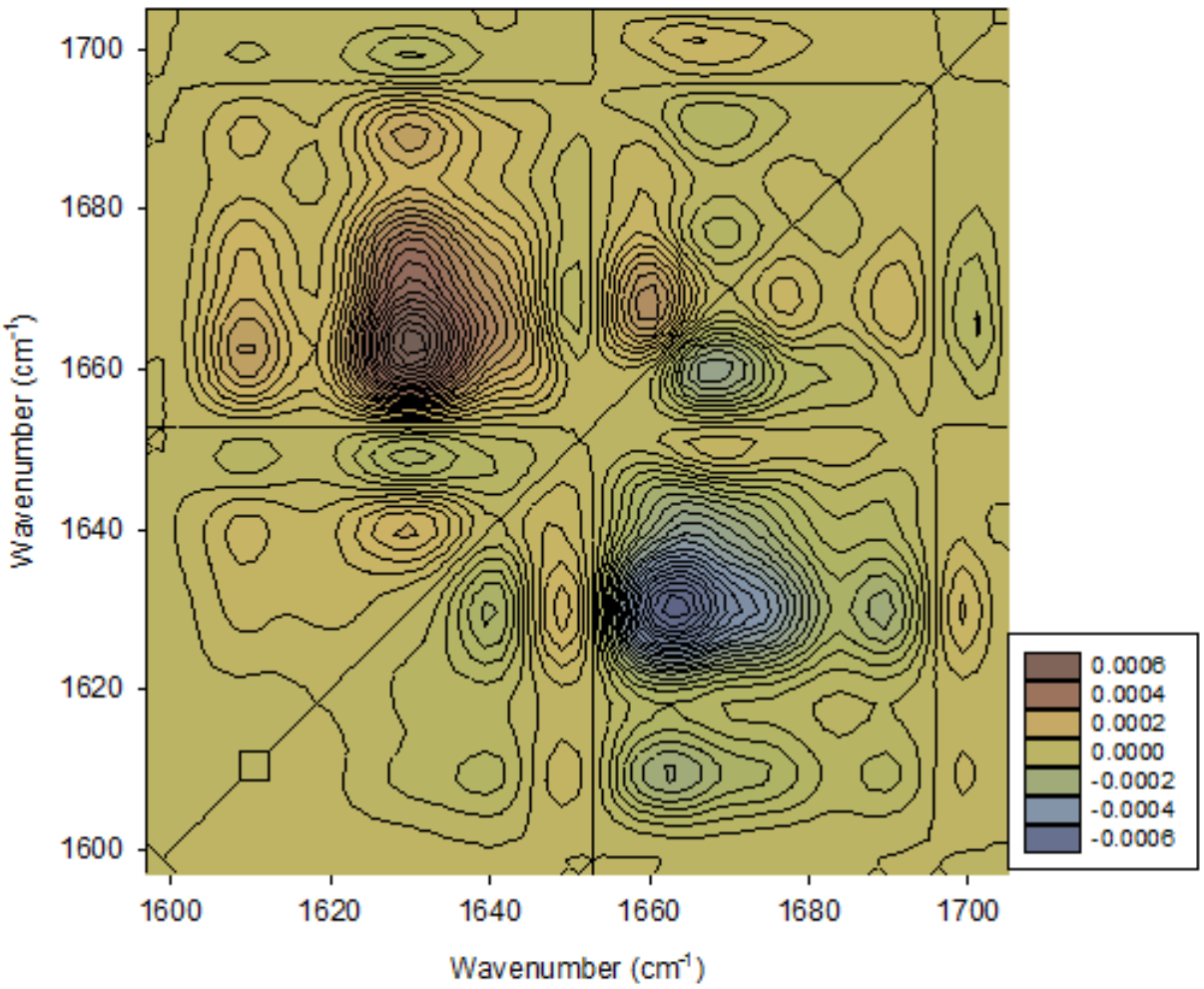

Figure S8 a) Synchronous 2D-COS plot for [BSA] = 7.50 µM with corresponding autocorrelation spectrum and labelled peaks in the amide I band. Legend presents correlation values.

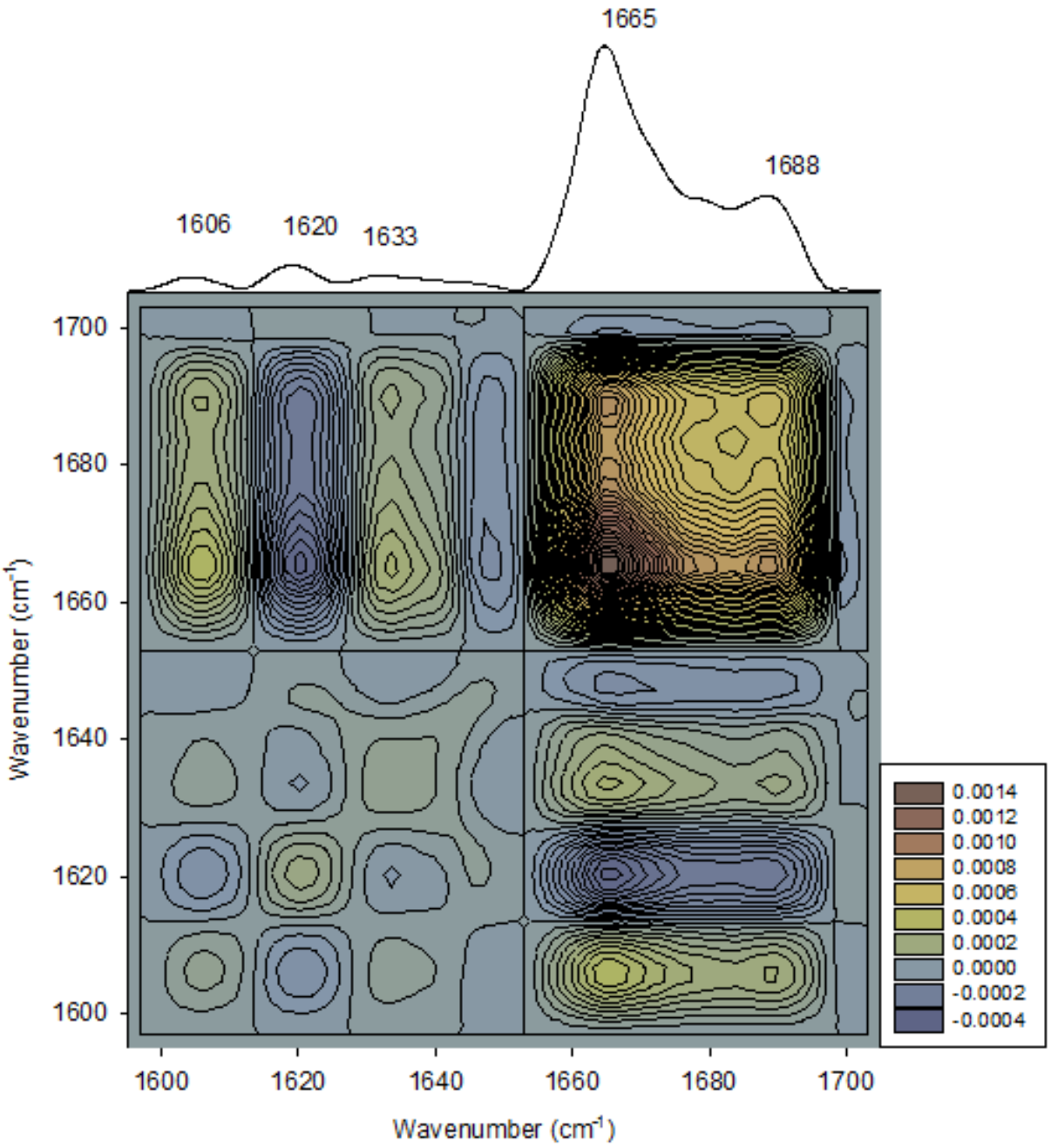

Figure S8 b) Asynchronous 2D-COS plot for [BSA] = 7.50 µM. Correlation values are shown in the legend.

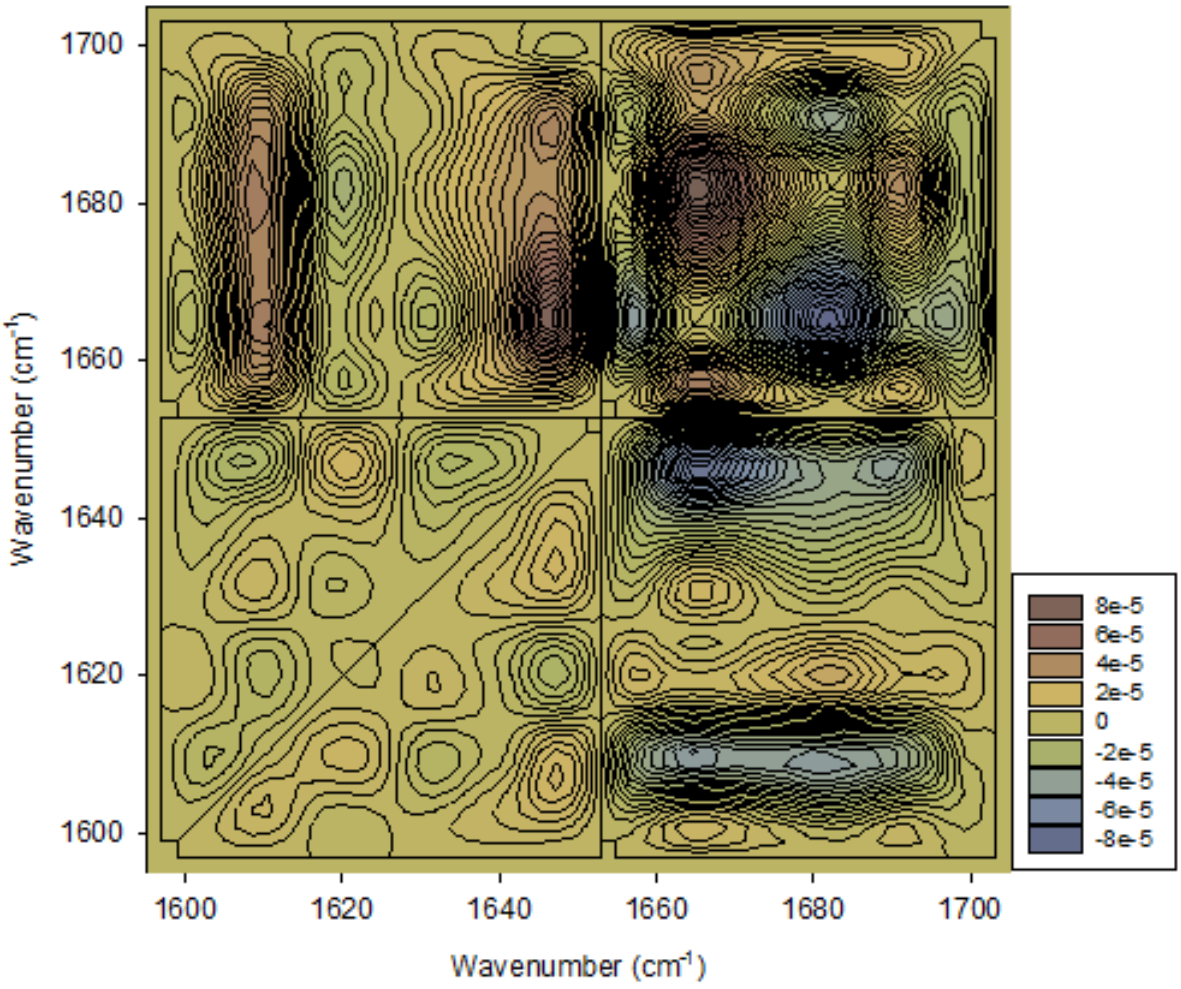

Figure S9 a) Synchronous 2D-COS plot for [BSA] = 15.0 µM with corresponding autocorrelation spectrum and labelled peaks in the amide I band. Correlation values are shown in the legend.

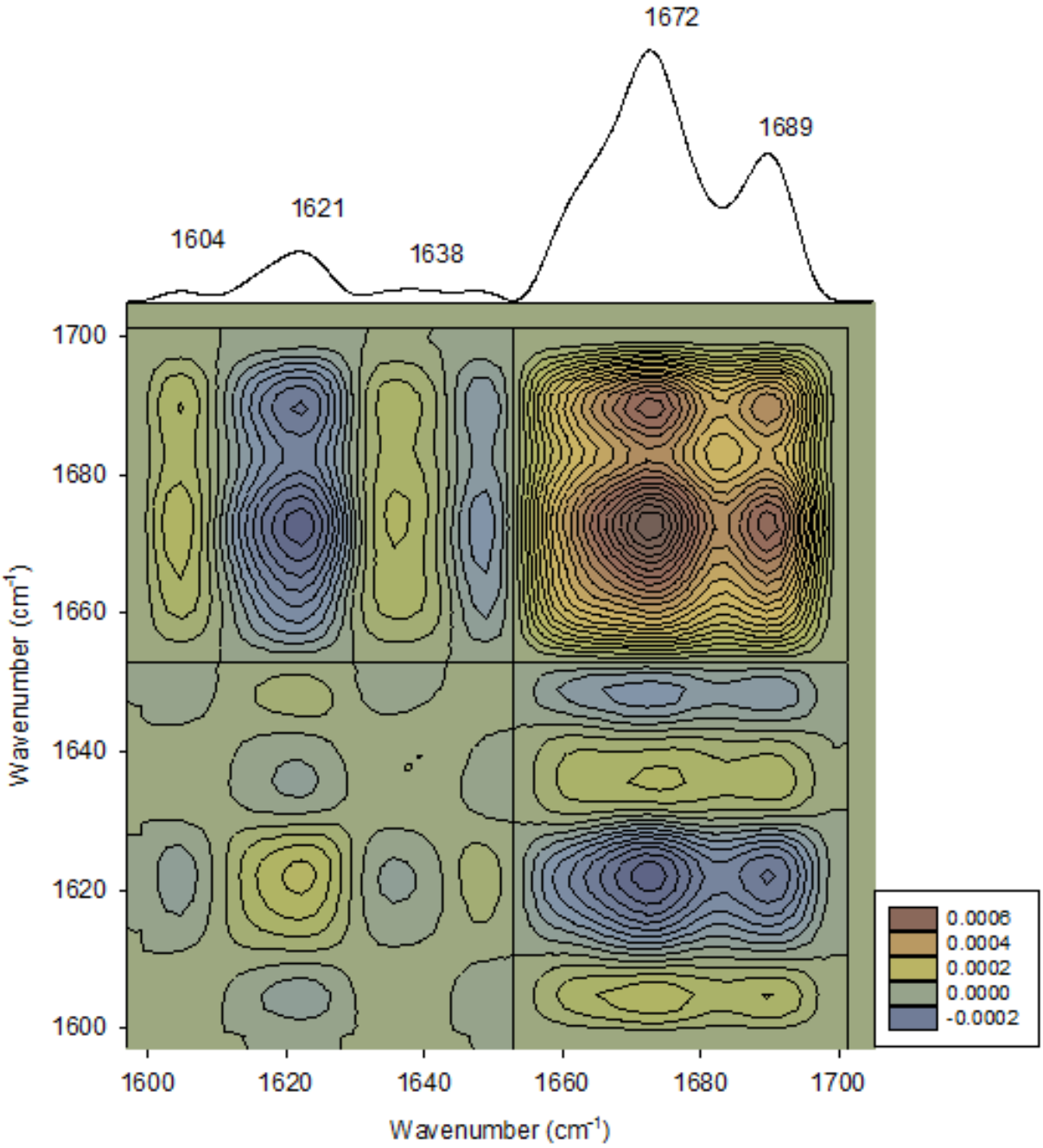

Figure S9 b) Asynchronous 2D-COS plot for [BSA] = 15.0 µM. Correlation values are shown in the legend.