Supplementary material

# Behavior of weakly adsorbing protein impurities in flow-through ion-exchange chromatography

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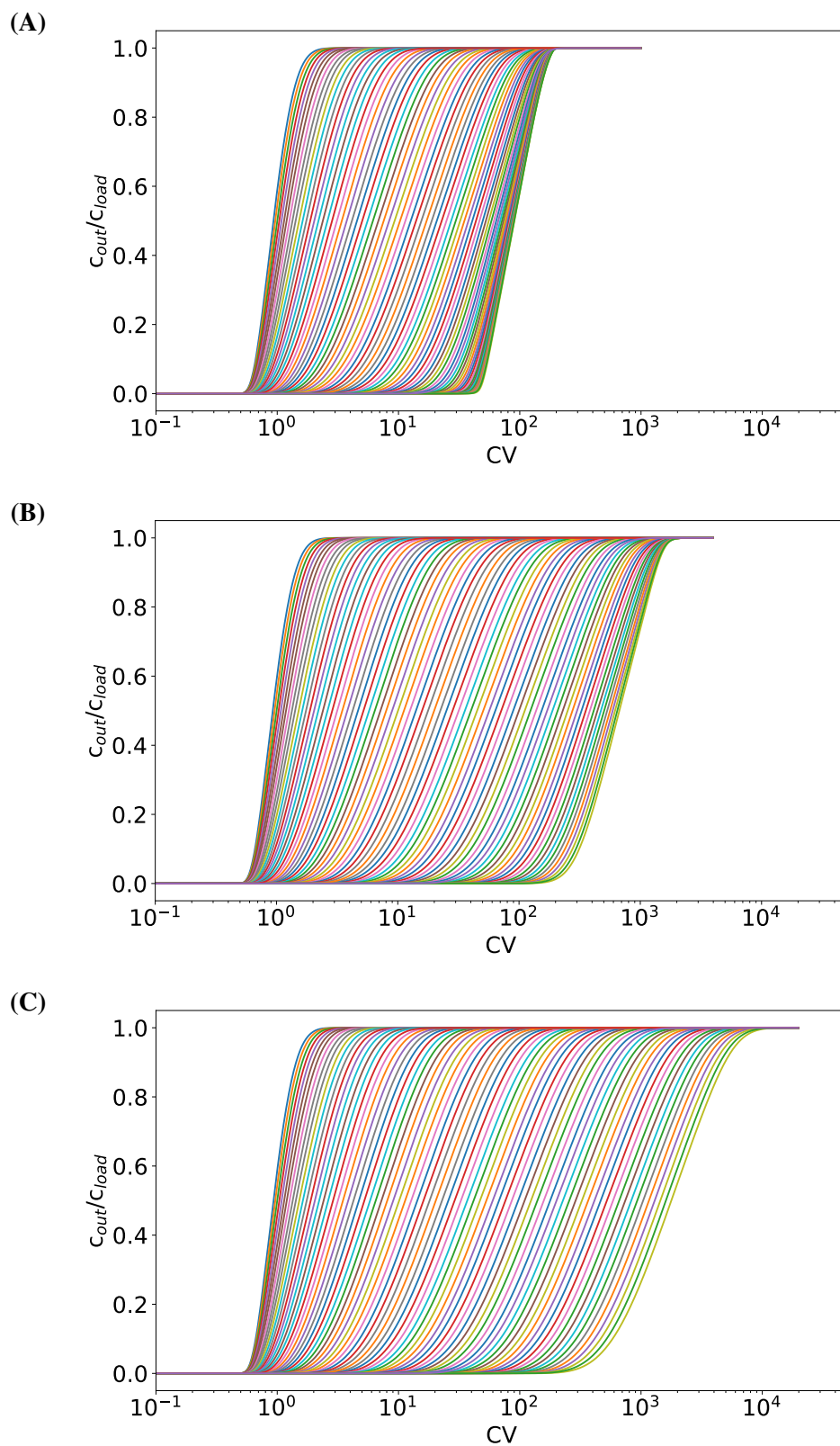Zheng Jian Li, and Abraham M. Lenhoff

**Figure S1:** Breakthrough profiles from a simulation of solute loading at (A) 1 mg/ml, (B) 100 $\mu$g/ml, and (C) 10 $\mu$g/ml. Lines correspond to simulations with different $K_{eq}$, which increases by 4 orders of magnitude from left to right. Note that $q_{max}$ was fixed at 100 mg/ml of packed column for all simulations, and the abscissa is on a logarithmic scale.
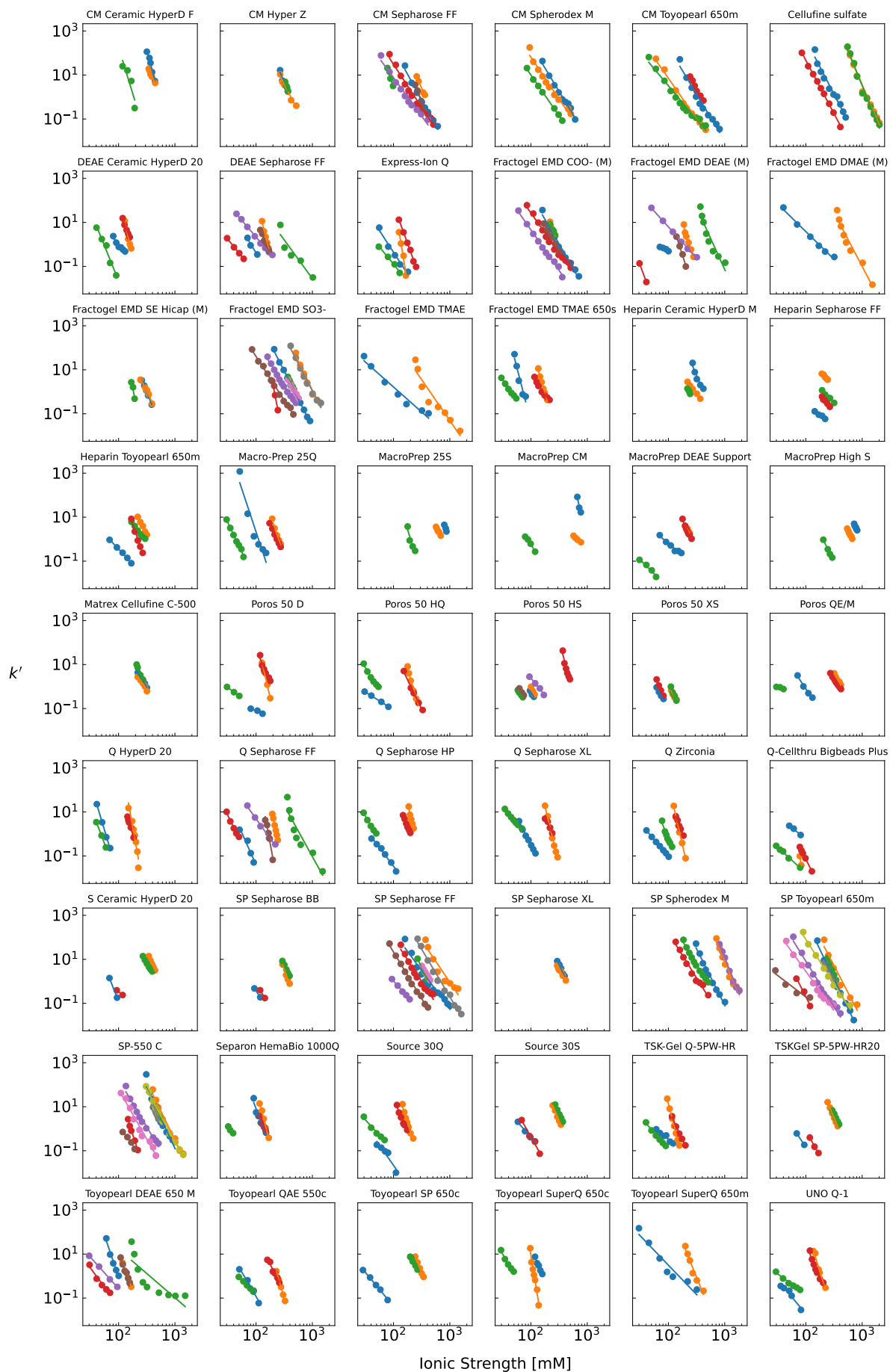
**Figure S2:** Isocratic $k'$ data that were consolidated from the literature. Each series represents a unique protein-pH-resin combination, and lines represent quasi-SDM fits to the data. These data, which are available in the `Supplementary_table_S2.xlsx` file, were acquired by digitizing plots (using the Engauge Digitizer software), which may introduce some error into the precise $k'$ values.

**Table S1:** Simulation parameters.

| Variable | Figures 1, 2, and S1 | Figure 3 |
|---|---|---|
| $L_{col}$ [cm] | 4.2 | 5.0 – 20.0 |
| $r_p$ [$\mu$m] | 25.0 | 2.5 – 100.0 |
| $\varepsilon_c$ [ - ] | 0.49 | 0.49 |
| $\varepsilon_p$ [ - ] | 0.40 | 0.40 |
| $u$, superficial velocity [cm/h] | 300 | 100 – 200 |
| $D_{ax}$ [m$^2$/s] | $1.25 \times 10^{-7}$ | Function of $u$ |
| $k_{film}$ [m/s] | $1.0 \times 10^{-3}$ | $1.0 \times 10^{-3}$ |
| $D_p$ [m$^2$/s] | $1.0 \times 10^{-11}$ | $5.0 \times 10^{-12} - 4.0 \times 10^{-11}$ |
| $a$ [m$^2$/s] (in $D_s = aK_{eq}^b$) | $7.76 \times 10^{-12}$ | $1.66 \times 10^{-12}$ |
| $b$ [ - ] (in $D_s = aK_{eq}^b$) | $-1.54$ | $-0.24$ |
| $K_{eq}$ [ - ] | $1.0 - 1.0 \times 10^4$ | $1.0 - 1.0 \times 10^4$ |
| $q_{max}$ [mg/ml column] | 100 | 100 |
| $c_{load}$ [mg/ml] | $1.0 \times 10^{-3} - 1.0 \times 10^1$ | $1.0 \times 10^{-3}$ |