Supplemental materials for:

Comparing Normalization Methods and the Impact of Noise

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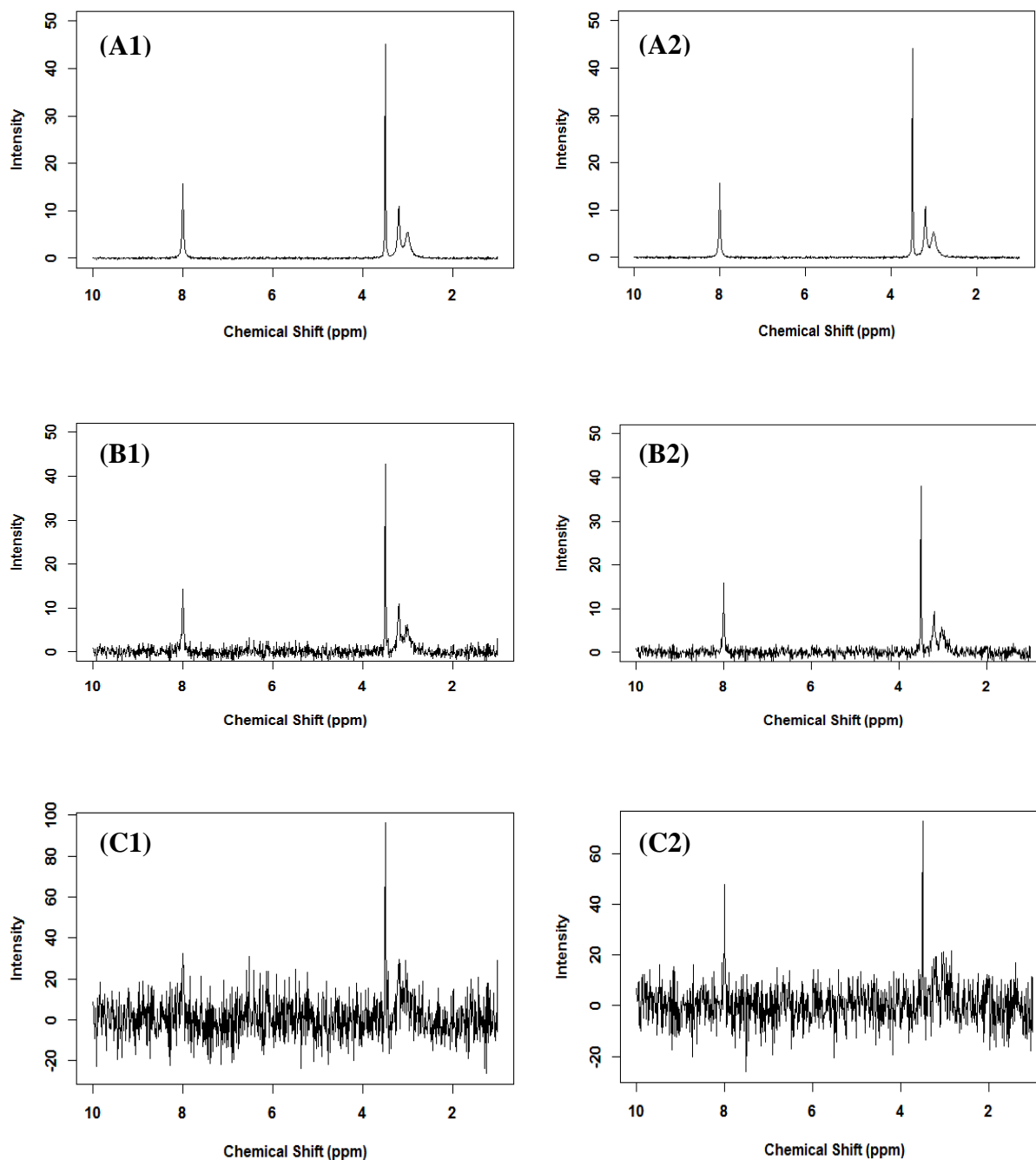
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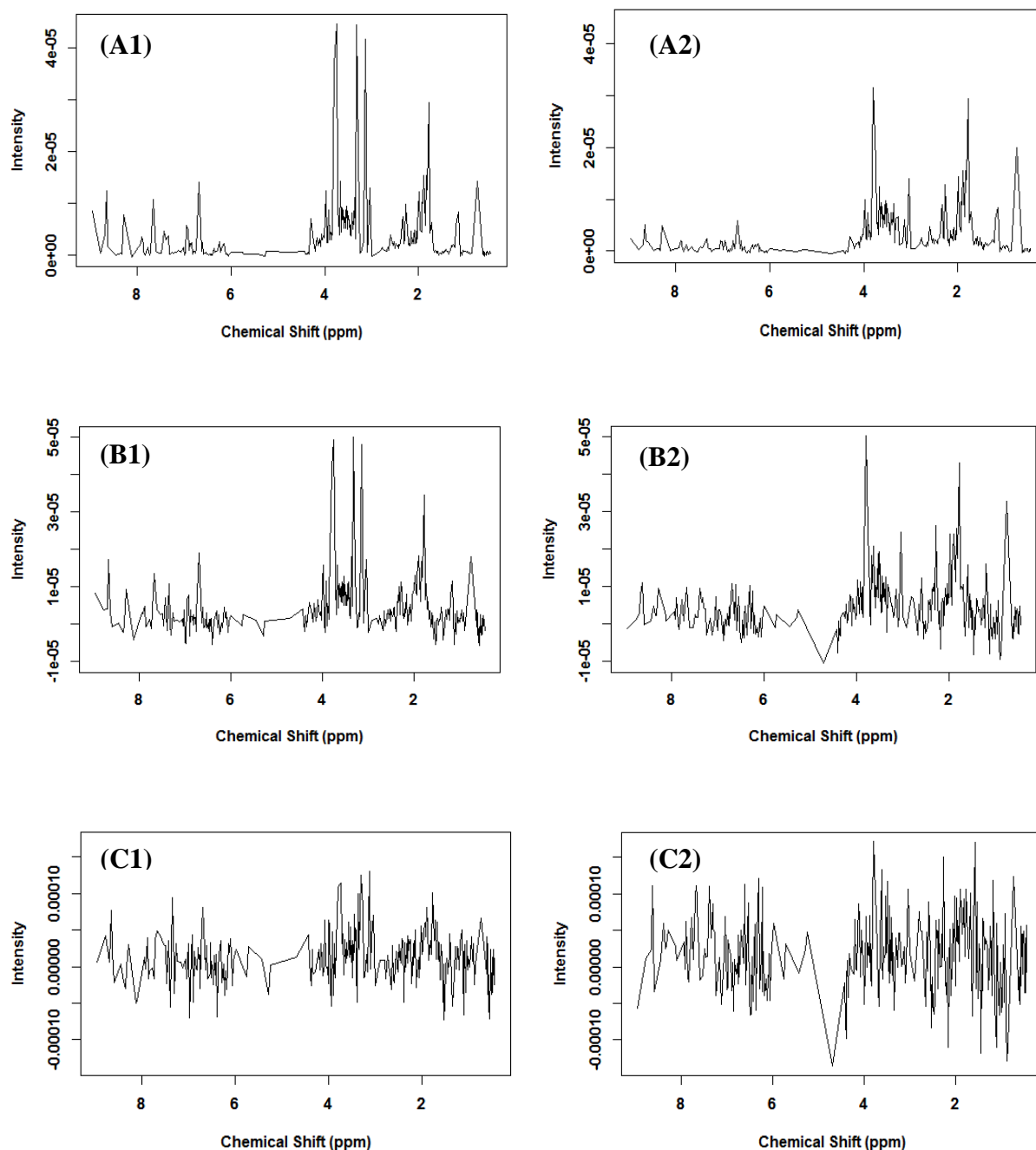
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Figure S1. Representative simulated spectra with added noise. At modest level of added Gaussian noise (5%), **(A1)** and **(A2)** correspond to noisy spectra at the lower end and upper end of the dilution factor range (0.9, 1.1), respectively. At a medium level of added Gaussian noise (50%), **(B1)** and **(B2)** correspond to noisy spectra at the lower end and upper end of the dilution factor range (0.5, 1.5), respectively. At the highest level of added Gaussian noise (200%), **(C1)** and **(C2)** correspond to noisy spectra at the lower end and upper end of the dilution factor range (0.001, 5) respectively.

Figure S2. Representative coffee spectra with added noise. At modest level of added Gaussian noise (5%), **(A1)** and **(A2)** correspond to noisy spectra at the lower end and upper end of the dilution factor range (0.9, 1.1), respectively. At a medium level of added Gaussian noise (50%), **(B1)** and **(B2)** correspond to noisy spectra at the lower end and upper end of the dilution factor range (0.3, 1.7), respectively. At the highest level of added Gaussian noise (200%), **(C1)** and **(C2)** correspond to noisy spectra at the lower end and upper end of the dilution factor range (0.001, 5) respectively.
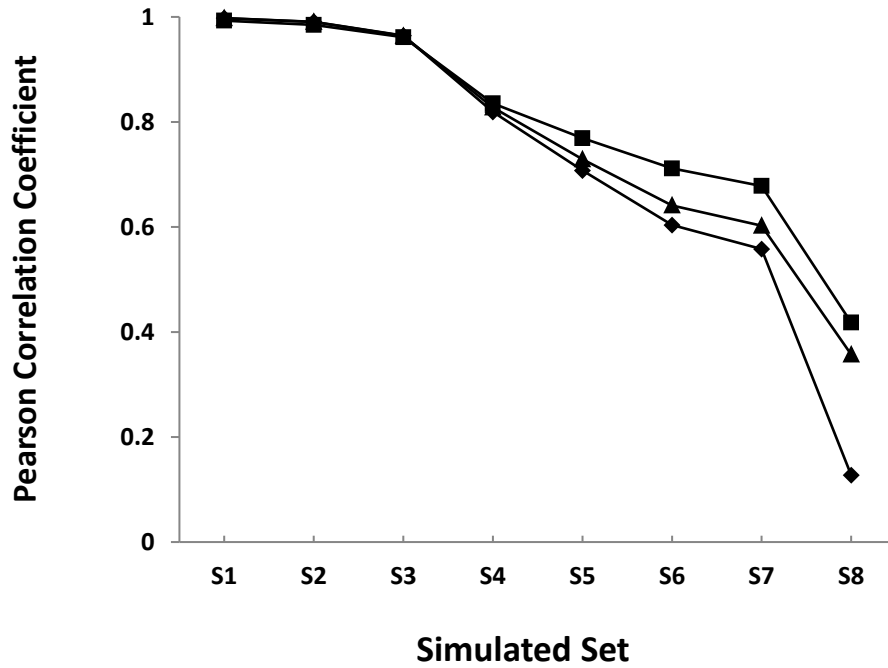
Figure S3. Pearson correlation coefficients between estimated first loadings and true first loadings of 8 simulated sets after being normalized with CS (♦), PQ (■), and ROI (▲) respectively. The amount of signal variance introduced into the coffees dataset is described in **Table 1**.