

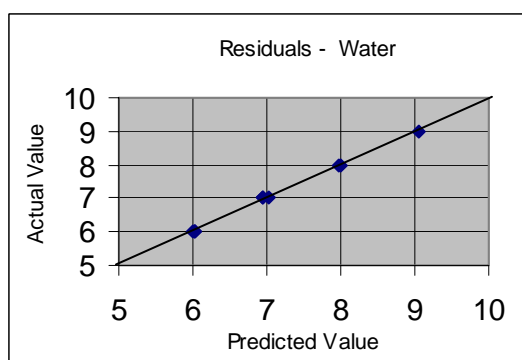
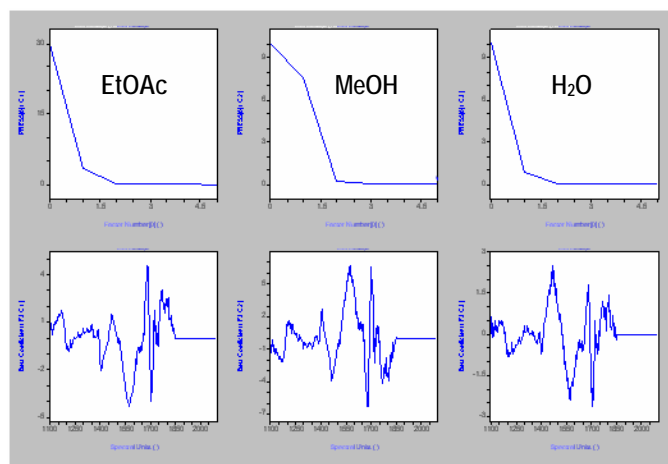
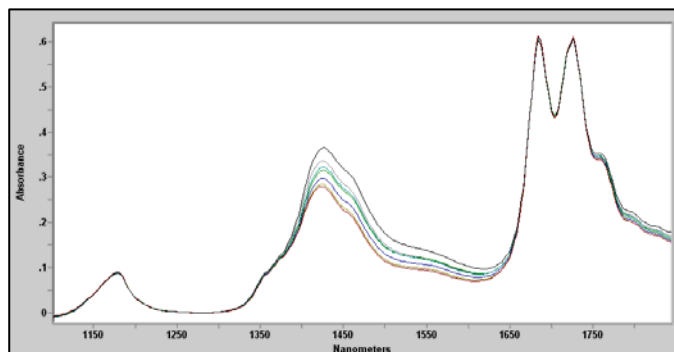
Application Note — Solvent Recovery Using a Near-Infrared ChemView® Photometer

Purpose: To measure the concentrations of ethyl acetate (EtOAc - 80-90%), methanol (MeOH - <10%) and water (<10%) for continuous control of a solvent recovery process to reduce distillation time and processing costs.

Approach: Use our PS-2E diode array spectro-photometer to collect the NIR spectra at 30 °C in a 2 mm cuvette in our Heater-Cell accessory. Perform a partial least-squares (PLS) analysis. Use the number of PLS Factors and the Beta Coefficients to determine the number and locations of the wavelengths to use in an MLR model. Extract the absorbance data at those wavelengths and import them into Microsoft® Excel®. Use our OutlierDetect™ Excel® add-in to determine the MLR coefficients and perform the outlier analysis.

Results: The NIR spectra are shown above right. The PLS results are shown at right. The PRESS plots (upper row) indicate that 3 factors are generally required for all three species, and the Beta Coefficients (bottom row) show strong contributions at 1460, 1580 and 1680 nm. The MLR observed vs. predicted plot for water is shown below and the MLR results for all coefficients are also presented.

Our OutlierDetect™ program indicated that no calibration sample was an outlier, each having M (Mahalanobis Distance) and Q (Sum of Squares Error) well below their 95% confidence limits. With 1 mAU photometric drift, ChemView® should be stable to <0.05% change per month.



	EtOAc	MeOH	H ₂ O
R ²	0.9993	0.9973	0.9990
Std. Error of Calibration	0.06	0.07	0.04
Number of Samples	10	10	10
Std. Error of Prediction	0.10	0.07	0.05
Number of Samples	7	7	7

Conclusions: These results indicate that a ChemView® photometer and fiber optic probe can be used to monitor solvent recovery operations. ChemView® can continuously calculate, output and alarm based upon M and Q outlier values, as measures of the confidence of the predicted concentrations. Full System Life Cycle documentation and IQ/OQ are available. A multiplexed version of the ChemView®, the ChemViewMx™, can analyze up to 8 fiber optic probes.