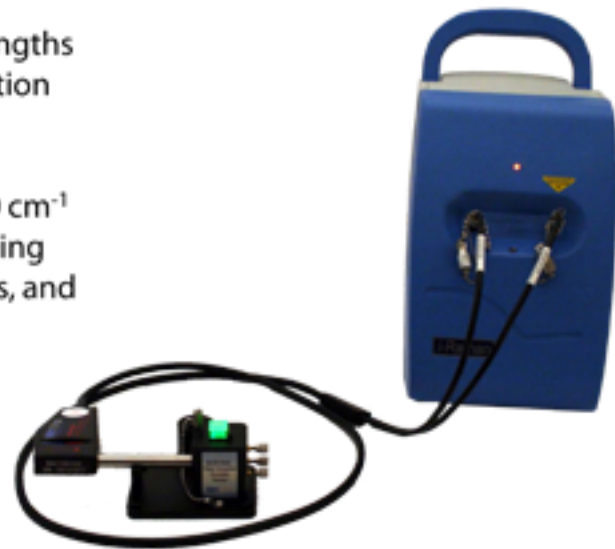


Chemometric Modeling to Determine Concentrations of Methanol in Tertiary Mixtures Using a High Resolution Portable Raman Spectrometer

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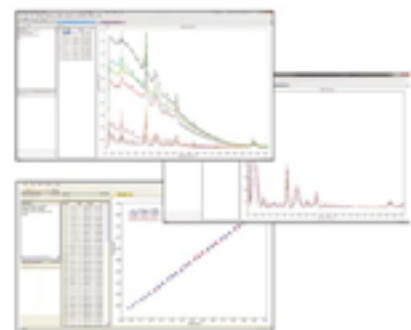
i-Raman® High Resolution Raman Spectrometer

- 785nm or 532nm Excitation Wavelengths
- Patented CleanLaze® Laser Stabilization
- High Throughput F/2 Spectrograph
- Spectral Resolution as Fine as 3cm⁻¹
- Spectral Range from 65cm⁻¹ to 4000 cm⁻¹
- Fiber Optic Probe for Flexible Sampling
- Sampling Stages, Video Microscopes, and Cuvette Holders Available
- 830 nm Excitation Now Available
- Deeper TE Cooling Now Allows for Integration Time Up to 4 minutes for Demanding Samples



Instrumentation

BWQ™ Chemometrics Software Package



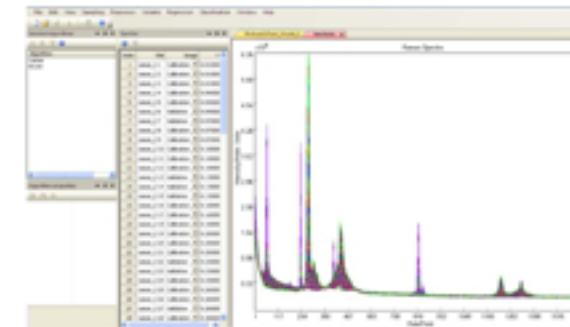
- Provides Powerful Techniques for Classification and Regression.
- Range of Methods and New Computational Algorithms that provide High Accuracy, High Speed and Less Memory Usage
- State-of-the-art Pretreatment Methods for Spectral Smoothing and Baseline Correction
- Enhanced Multivariable Methods
- Vector Processing for Non-linear Datasets
- Chemometric Modeling Markup Language (CMML) for Model Storage and Sharing.

1. Experimental Setup and Data Collection

The i-Raman® and BWQ™ were used to determine unknown methanol concentrations in a tertiary mixture of methanol, acetonitrile, and water. Known methanol, acetonitrile, and water standards were prepared for development of a calibration curve.

Acquisition parameters :

- 532nm Excitation Wavelength
- Laser Power – 30 mW
- Integration Time – 7.5 seconds
- Averaging – 1, Single Acquisition



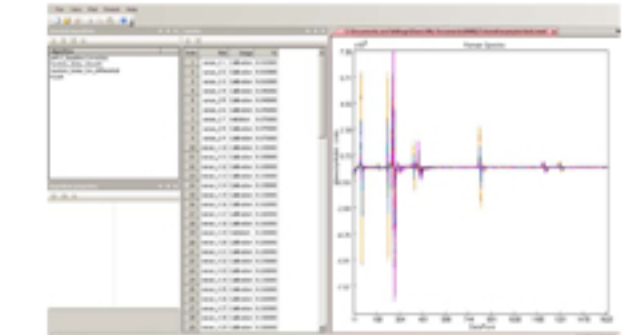
94 Overlaid Raman Spectra

Experiment & Conclusion

2. Preprocessing and Regression

A total of 94 spectra were collected with varying concentrations of the three components. Of those, 70 were randomly chosen for use in creating the calibration curve and the remaining 24 were used for validation.

- The following preprocessing functions were used:
 - airPLS Baseline Correction
 - Sovitzky-Golay Smooth
 - Sovitzky-Golay 1st Differential
- PLS1 regression was used to model this three component system

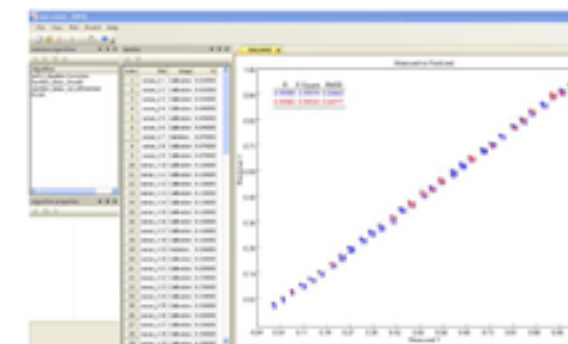


Preprocessed Raman Spectra

3. Calibration Curve Creation and Validation

After applying preprocessing and regression to the data, the measured vs. predicted concentrations were plotted to determine the accuracy of the model.

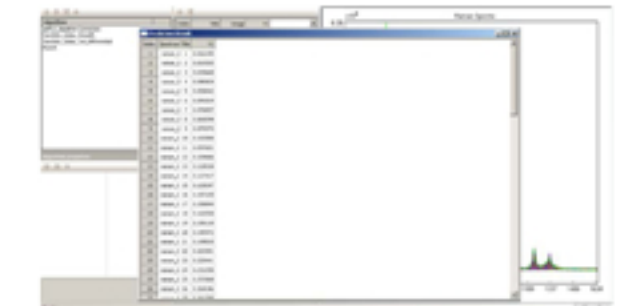
The R² value was calculated to be greater than 0.999 for both the measured and predicted concentrations. Similarly, the RMSE was calculated to be less than 0.008 for both.



Calibration Curve With Validation Data

4. Prediction and Conclusion

Lastly, samples were prepared with unknown methanol concentrations in a tertiary mixture of methanol, acetonitrile, and water. These samples were then measured by the i-Raman® and fed into BWQ™ which determined the concentration using the previously developed model.



Prediction of Unknown Concentrations

In conclusion, we have shown that the i-Raman® high resolution portable Raman spectrometer can be used with BWQ™ to successfully develop a model to determine the concentration of methanol in tertiary mixtures of methanol, acetonitrile, and water.