# ChemWiz® Analyzer Development Kit

Full spectrum **chemometric analysis** for multiple components can now be performed using the ChemWiz® Analyzer Development Kit (ADK). This software toolkit, when combined with StellarNet spectrometer instrumentation and SpectraWiz operating software, enables rapid development of complex analyzers needed to provide custom measurement solutions for many applications.

Real-time spectral data is used as input to measure concentrations of up to 6 components such as moisture, fat, protein, alcohols, acids, or chemicals such as pesticides. Alternatively, the ChemWiz® ADK can be used to identify samples, such as the types of plastic.

The toolkit includes a model builder which is used to process spectra from a set of known component concentrations. Here the spectral preprocessing techniques are selected such as multivariate scatter correction (MSC), smoothing, derivatives, and mean centering. The multivariate analysis type is then selected such as partial least squares (PLS). Finally a cross validation technique is chosen and used to improve the reported statistics indicating accuracy and *fitness* of the calibration model created.

The ADK includes a runtime engine that performs the analysis in real-time with little to no sample preparation. The measurement results are displayed on the SpectraWiz Application panel for "Chemometric Predictor" which is also provided in our LabVIEW software program for OEM developers.

Each Analyzer system would need to be configured with appropriate sampling accessories and references, for measuring liquids or solids or powders. Solid reflectance works well using the RED-Wave NIR spectrometer (see the DWARF-Star model, cooled InGaAs diode array). For liquid analyzers, sample absorbance is measured in flow cells or dip probes via UV-VIS BLACK-Comet or BLUE-Wave UV spectrometers. Now there's no need to hire a spectral "Chemistry Wizard", just use ours!
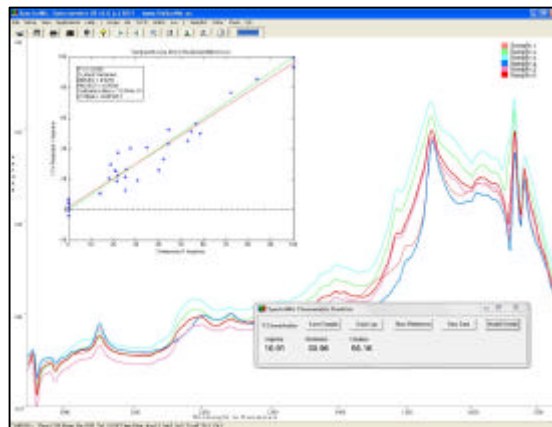
Real-time spectral display of sample measurements include concentration values of multiple components.

➢ **Multivariate algorithms for Quantitative analysis**
   Partial Least Squares PLS, Principle Component Regression PCR

➢ **Discriminant methods for Qualitative analysis**
   Principle Component Analysis PCA, and MDR

➢ **Preprocessing options to stablize data**
   Sample averaging, Spectral smoothing, First or second derivative with gap select, Multiplicative scatter correction, Mean centering, and lots more preprocessing options.

➢ **Visual graphs and Model cross validation**

➢ **Applications** include:
   Food Safety
   Packaging / Process
   Beverage QC
   Agriculture Feed
   Pharmaceutical
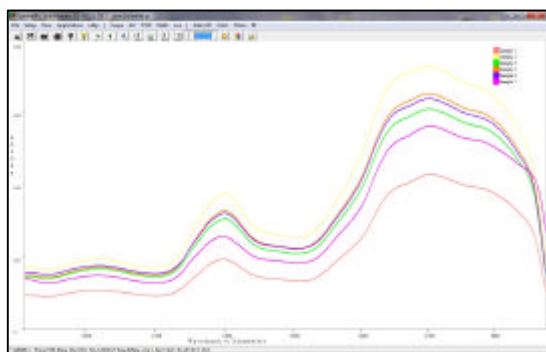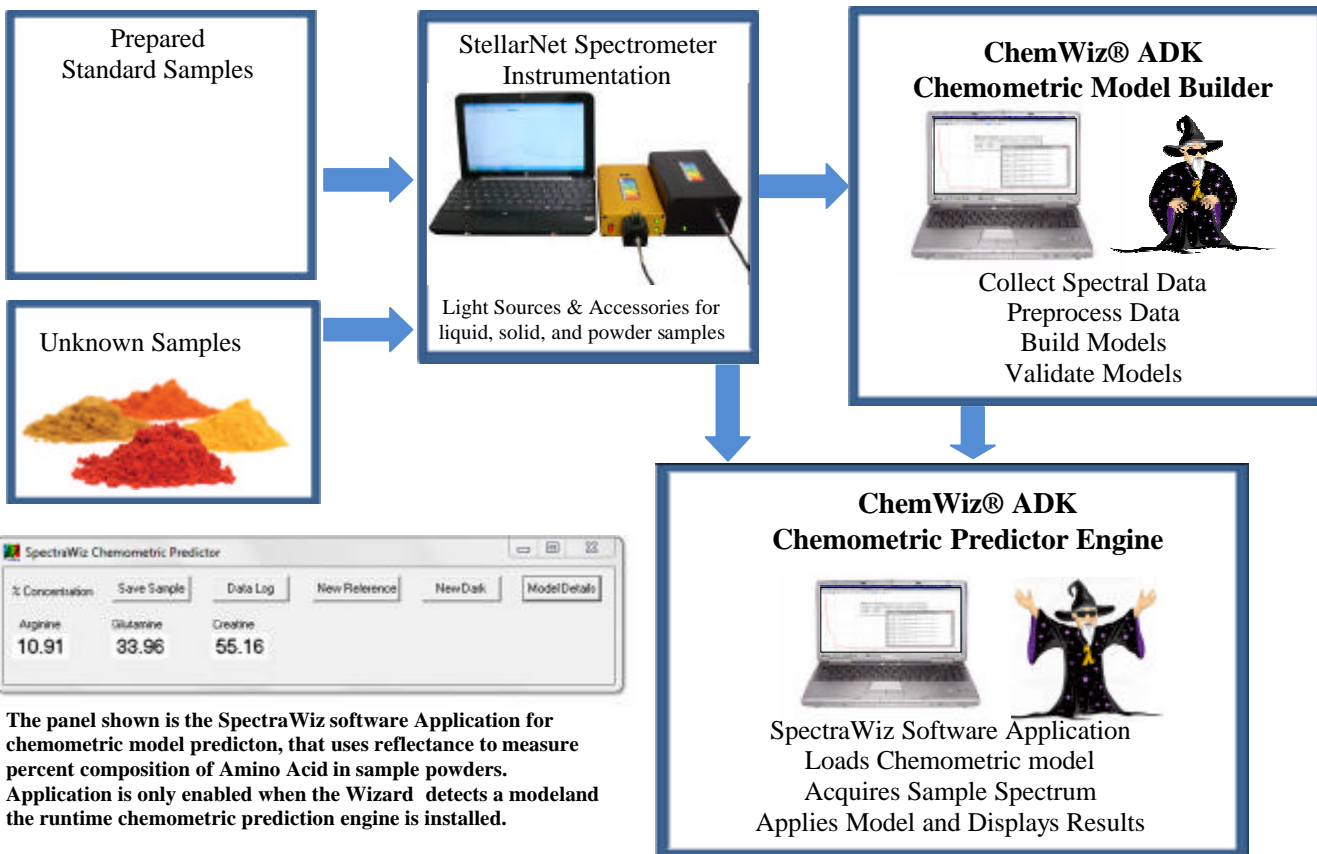   Oil & Chemical
   Plastics

ChemWiz® Analyzer Development Kit

Item	Description	Price
ChemWiz-ADK	Chemometric model builder plus Wizard runtime predictor engine	$3500 *
Wizard-runtime	Predictor engine for chemometric models – one license only	$1500 *

* Contact StellarNet application scientist as price will vary with choice of 3rd party vendor for model and predictor engine

Specifications

Operating System	WinXP, Vista, Win 7	Runtime speed	3Hz max
Runtime	SpectraWiz v5.0 or higher	**Full Spectrum Measures**	Concentrations or Classification
Spectral range	190 – 2500nm	**Analysis (typical)**	PLS or PCA/MDR

ChemWiz® Analyzer Development Kit

Prepared Standard Samples	StellarNet Spectrometer Instrumentation	ChemWiz® ADK Chemometric Model Builder
		Collect Spectral Data
		Preprocess Data
Unknown Samples	Light Sources & Accessories for liquid, solid, and powder samples	**Build Models**
		Validate Models

ChemWiz® ADK
Chemometric Predictor Engine

SpectraWiz Software Application
Loads Chemometric model
Acquires Sample Spectrum
Applies Model and Displays Results

SpectraWiz Chemometric Predictor

% Concentration	Save Sample	Data Log	New Reference	New Dark	Model Details

Arginine	Glutamine	Creatine
10.91	33.96	55.16

The panel shown is the SpectraWiz software Application for chemometric model predicton, that uses reflectance to measure percent composition of Amino Acid in sample powders. Application is only enabled when the Wizard detects a modeland the runtime chemometric prediction engine is installed.
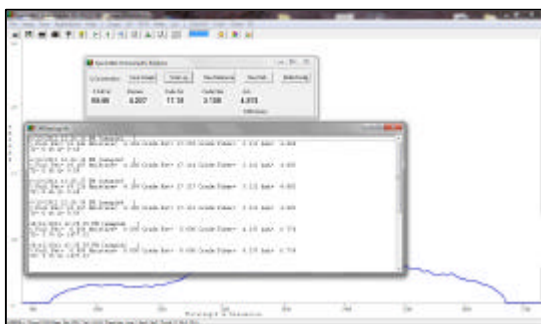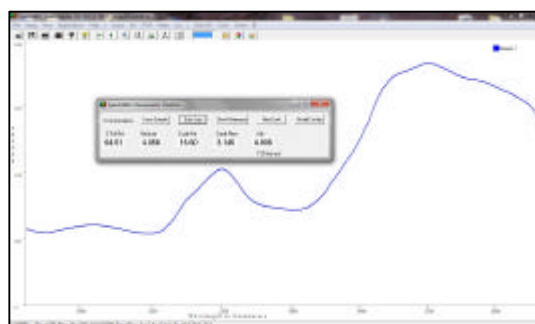
Step 1 - import spectra dataset taken from calibrated samples and select usable wavelength range
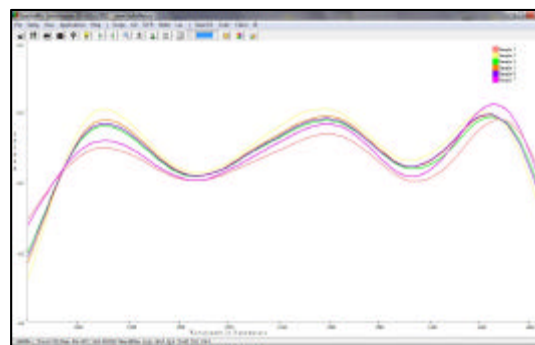
Step 2 – Select reprocessing needed for sample type such as scatter correction, smoothing, 2nd derivative

Step 3 - build model and perform cross validation until statistics indicate excellent prediction performance

Step 4 – install model on real-time system with prediction engine and StellarNet spectrometer used to collect data