



# **P/ACE™ MDQ**

# **Basic Training Workbook**

**32 Karat™ 8.0**

A33116AB  
November 2009

Beckman Coulter, Inc.  
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## Foreword

### Welcome

Welcome to the Basic level of the Beckman Coulter training program for P/ACE™ MDQ with 32 Karat™ Software. During this training, our engineer will guide you through the basic operation of the system, review safety and maintenance guidelines, and review optional accessories that provide optimum performance for your system.

The purpose of basic training is to introduce you to the system and ensure that you are able to perform basic functions. However, the training is not intended to include creating custom applications. For advanced training options, please contact your sales office.

The following prerequisites have been defined to ensure a successful basic training:

1. The operator must be available without interruption for the entire training session.
2. No more than two operators will be trained as part of the installation.

The system operation requires a basic knowledge of Windows XP. The operator must be familiar with the following terms and skills:

- Creating, opening, saving, editing, moving, and copying files

## **Training Overview**

The training is organized in thirteen sections. Your instructor will guide you through each section. At the end of most sections, a skill check is provided to help you evaluate your progress.

### **System Overview**

- Overview
- Hardware Terminology
- Software Terminology

### **Safety**

- Safety Features
- Safety Notices
- Chemical and Biological Safety
- Electrical Safety
- Electrostatic Discharge

### **Software Setup and Initialization**

- Accessing 32 Karat Software
- Configuring 32 Karat Software
- Starting the Instrument
- Skill Check

### **Reviewing Detectors**

- UV Detectors
- PDA Detectors
- LIF Detectors

### **Using Direct Control**

- Accessing Direct Control
- Using Direct Control Screens
- Skill Check

### **Working with Methods**

- Using the Method Wizard
- Creating a Method
- Saving a Method
- Editing a Method
- Printing a Method
- Other Method Functions
- Skill Check



## Running a Sample

- Running a Single Sample
- Stopping or Aborting a Method
- Displaying Data
- Skill Check

## Analyzing and Integrating Data

- Opening Data Files
- Optimizing Integration
- Defining and Naming Peaks
- Identifying Peaks Based on Migration Time
- Identifying Peaks Based on Mobility
- Skill Check

## Using Sequence Tables

- Using the Sequence Wizard
- Viewing a Sequence
- Editing a Sequence
- Saving a Sequence
- Running a Sequence
- Skill Check

## Creating Calibrations

- Editing the Peak ID table
- Creating a Calibration Sequence with the Sequence Wizard
- Running a Calibration Sequence
- Reviewing Calibration Curves
- Final Skill Check

## Preparing Custom Reports

- Accessing and Editing a Custom Method Report
- Creating a Custom Method Report
- Skill Check

## Summary

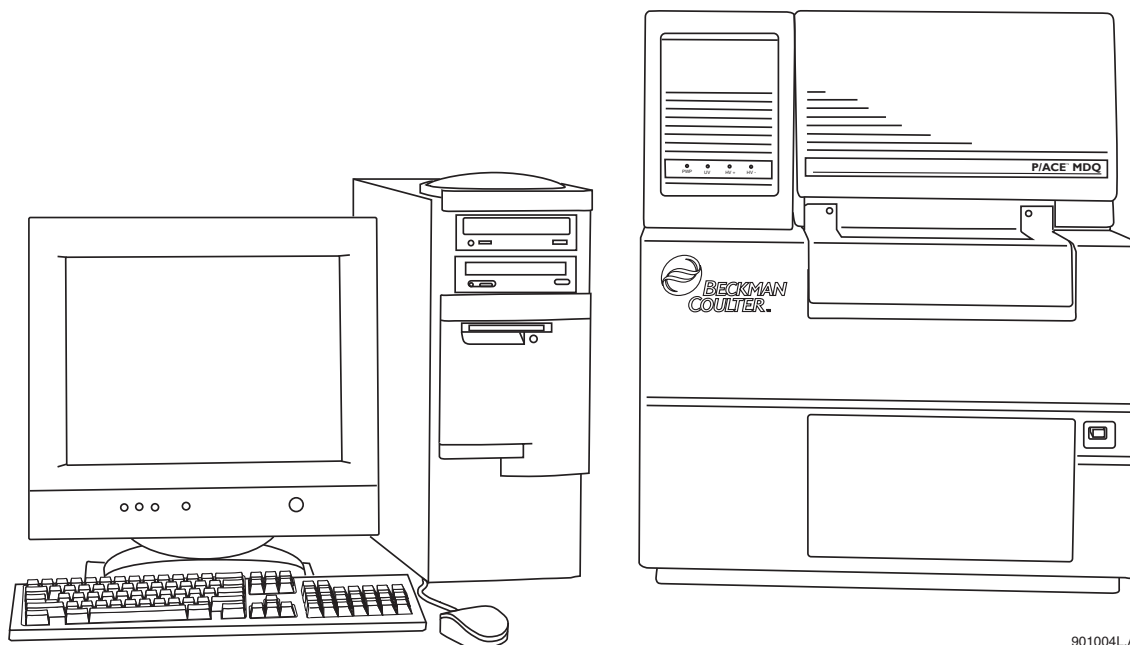
- Advancing your skill
- Record of Operator Training



## System Overview

### 1.1 Overview

This section describes the hardware components of P/ACE MDQ system. You will learn the operation considerations for each module and terms commonly used for the software and hardware.



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Figure 1.1 P/ACE MDQ System

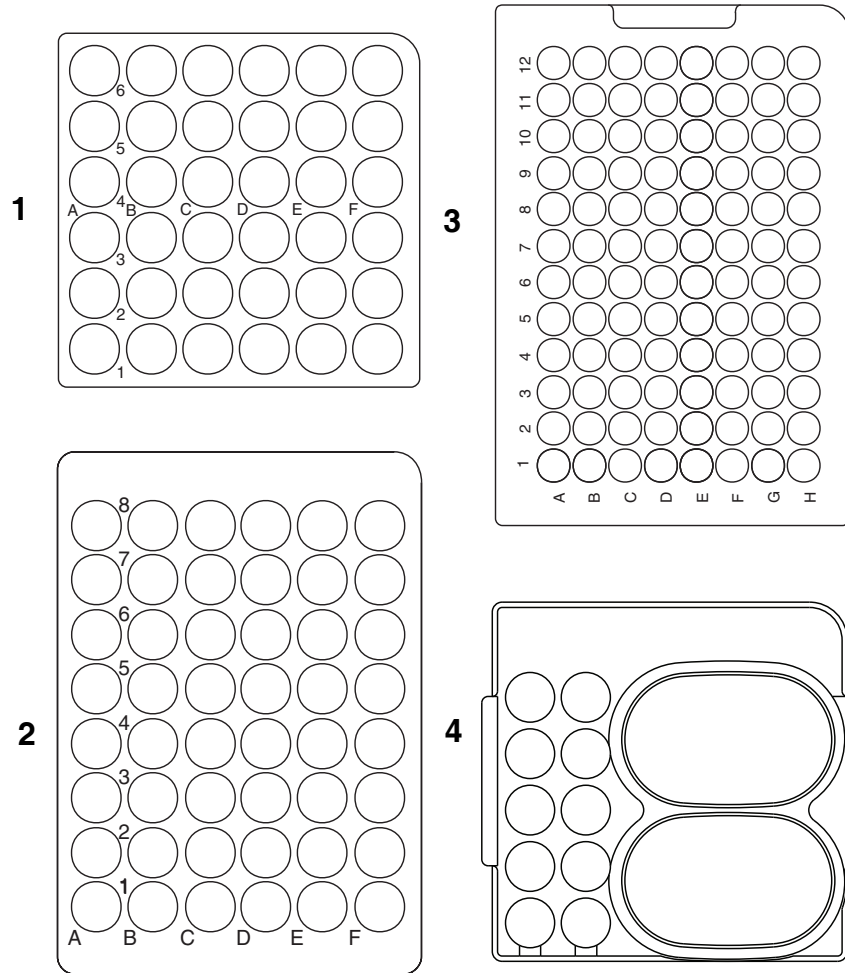
## Hardware Terminology

### System

- Power Switch
  
- Front Panel LEDs and Indicator lights
  
- Communications cables
  
- Remote hook-ups
  
- Other detectors
  
- Spare parts and consumables list

## Trays

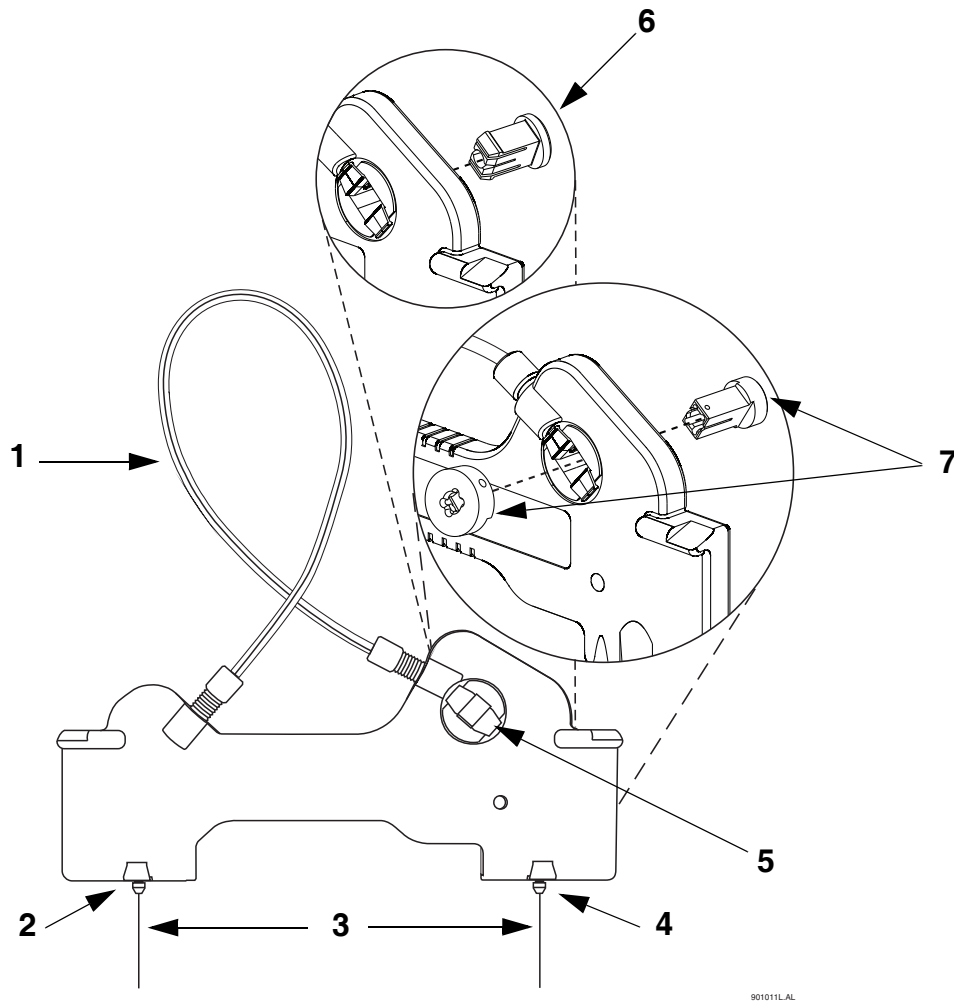
- Tray Cover and Capillary Cartridge Cover
- Tray Racks
- Sample Tray and Sample Cooling
- Tray Name and Format



901018L.A1

1. Buffer Tray	2. 48 Vial Sample Tray
3. 96 Position Sample Tray	4. Large Volume Buffer Reservoir

## Capillary Cartridge



1. Coolant tubing with capillary inside	2. Inlet Side
3. Capillary	4. Outlet Side
5. Detector Window and Aperture	6. Aperture for UV and PDA cartridge
7. Aperture and Stabilizer Plug for LIF cartridge	

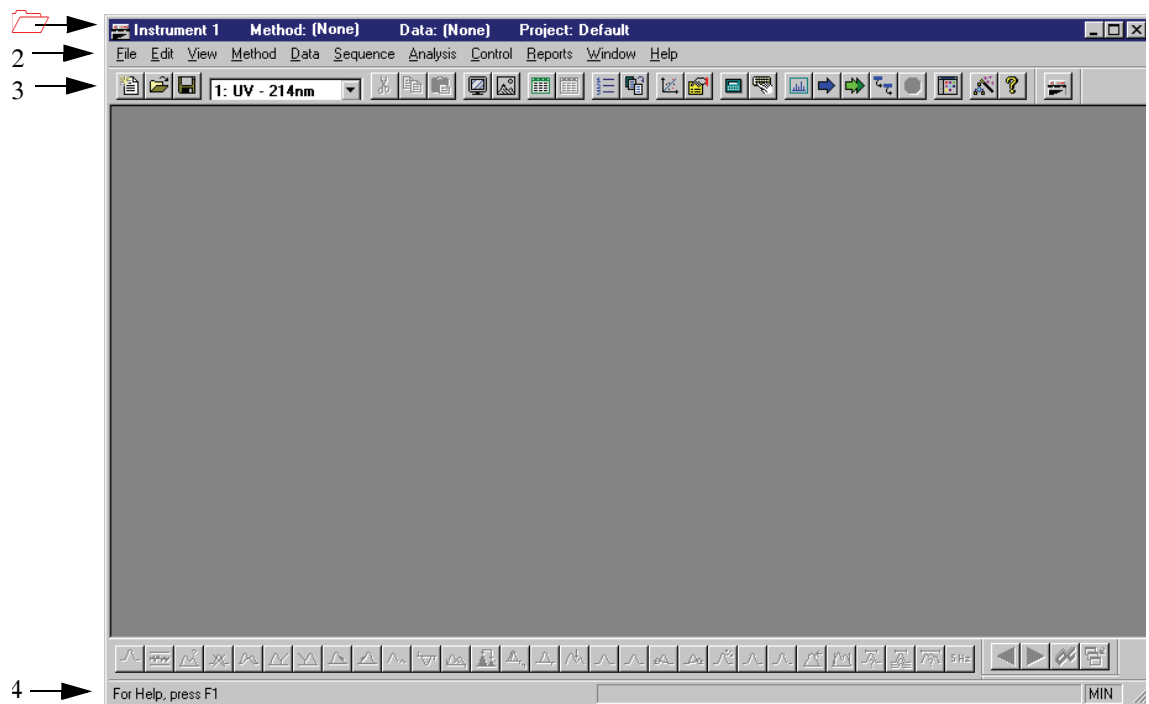
## Detectors (UV, PDA or LIF)

### Lamp

- Hours
- Change procedure
- Diagnostics

## Software Terminology

### Window



- Title Bar
- Menu Bar
- Toolbar
- Status Line

### **Main Menu**

- New Instrument
  
- System Configuration
  
- Interface Configuration
  
- Online/Offline System Administration

### **Summary**

This section introduced you to an overview of P/ACE MDQ system. Now you are ready to learn the details required for successful operation. Refer to "[Safety](#)" on [page 2-7](#) before proceeding.



## Safety

### 2.1 Overview

This section provides safety instructions for P/ACE MDQ hardware and accessories. You will review:

- Safety Feature
- Safety Notices
- Chemical and biological safety
- Electrical safety
- Moving parts
- Instrument safety features
- Release Notes

### 2.2 Safety Information for P/ACE MDQ and 32 Karat Software

All safety instructions should be read and understood before installation, operation, maintenance or repairs are attempted.

See the MDQ User's Guide for Safety Information regarding this system.

#### Safety Features

Review the location and action of the following safety features:

- ON/OFF switch
- Fuse replacement and voltage selection

#### Safety Notices

Review meaning and placement:

- International safety symbols
- High voltage symbol

## Chemical and Biological Safety

Normal operation of the system involves the use of many solvents and reagents, which may be toxic, flammable or biologically harmful.

- Observe all cautionary information printed on the original solution containers prior to use.
- Operate the system in an appropriate enclosure and take all necessary precautions when using pathologic, toxic, or radioactive materials to prevent the generation of aerosols.
- Observe the appropriate cautionary procedures as defined by your safety officer when using flammable solvents in or near the powered-up instrument.
- Wear appropriate lab attire (safety glasses, gloves, lab coat, and breathing apparatus) when working with hazardous materials.
- Remember that solvents may be flowing under high pressure.

## Electrical Safety

- Always disconnect power to the system before performing maintenance operations.
- Refer servicing that requires removal of covers to qualified personnel.

## Electrostatic Discharge

- Ground yourself before working with system.
- Carpeting in a building can influence static charge. Use caution when working in this environment.
  - Contact Beckman Coulter Field Service if you have questions.

## Release Notes

The Release Notes contain important information that became available after the 32 Karat Software manuals were printed:

- Read and review the information contained in this file
- Print the file and place in binder, if necessary

## Summary

This completes the safety portion of the basic training. For more detailed information regarding safety, refer to the P/ACE MDQ Installation and Maintenance Guide.

**WARNING** Do not use the product in any manner other than specified. The safety and performance of the equipment will be impaired.

## Software Setup and Initialization

### 3.1 Overview

This section considers the start-up process for the 32 Karat Software. We will discuss:

- Accessing 32 Karat Software
- The Enterprise Screen (Main Menu)
- Configuring 32 Karat Software
- Screen Layout
- Skill Check

### 3.2 Accessing 32 Karat Software

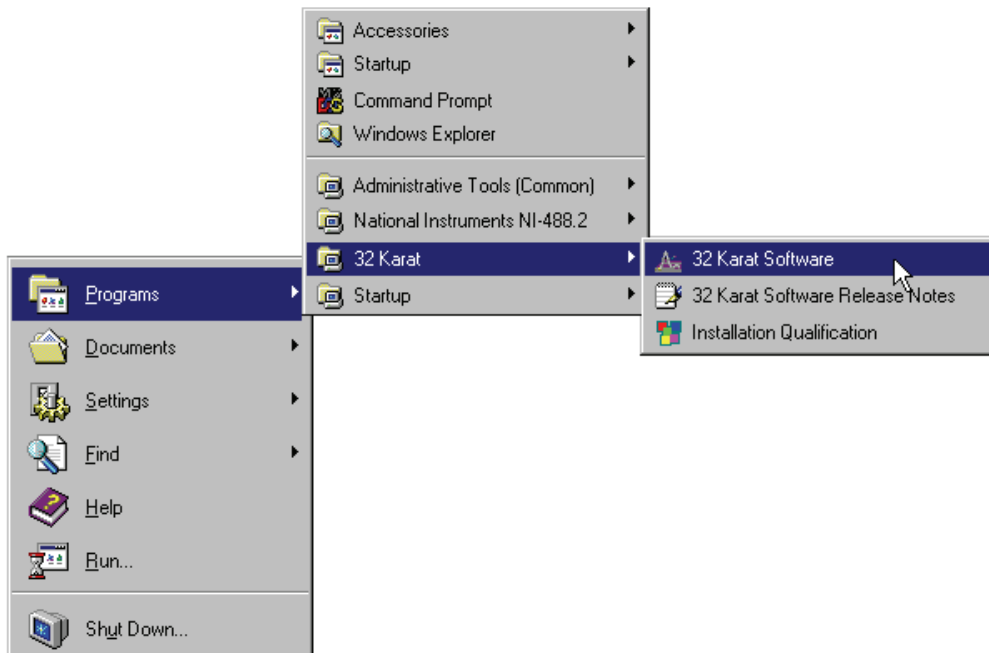


Figure 3.1 Accessing 32 Karat Software through Startup Menu

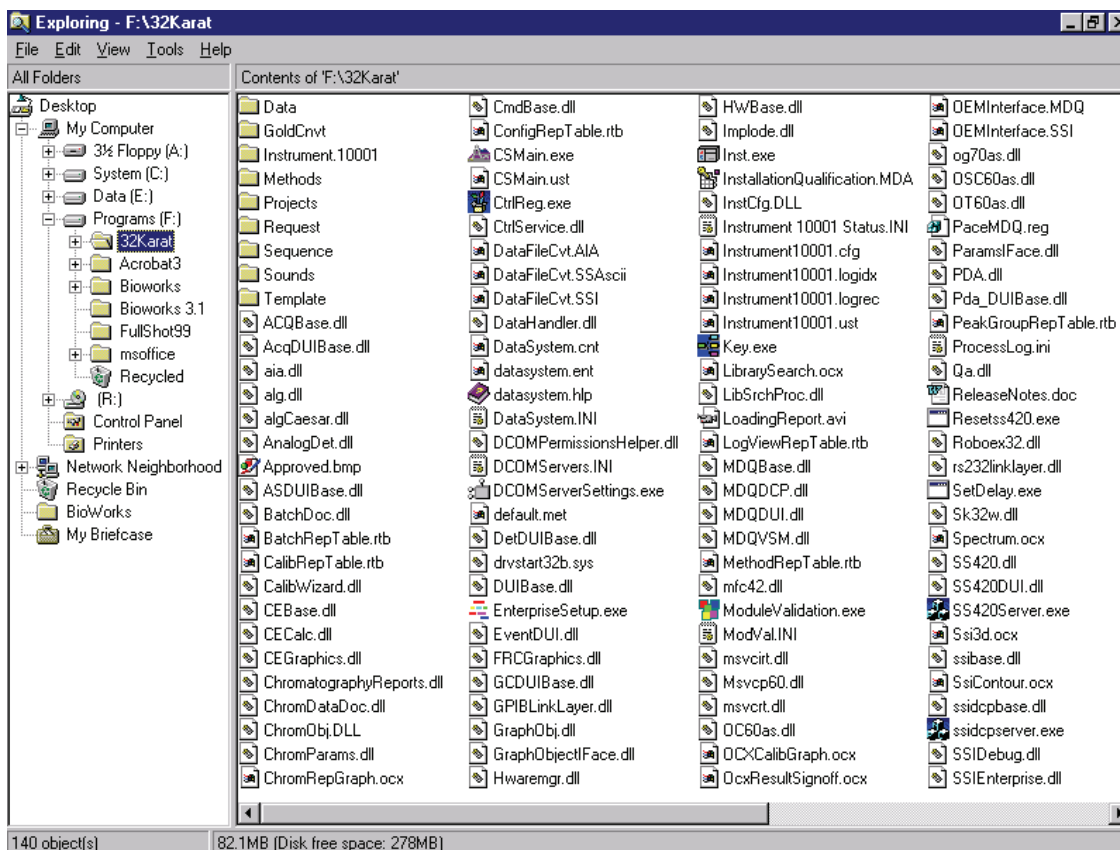
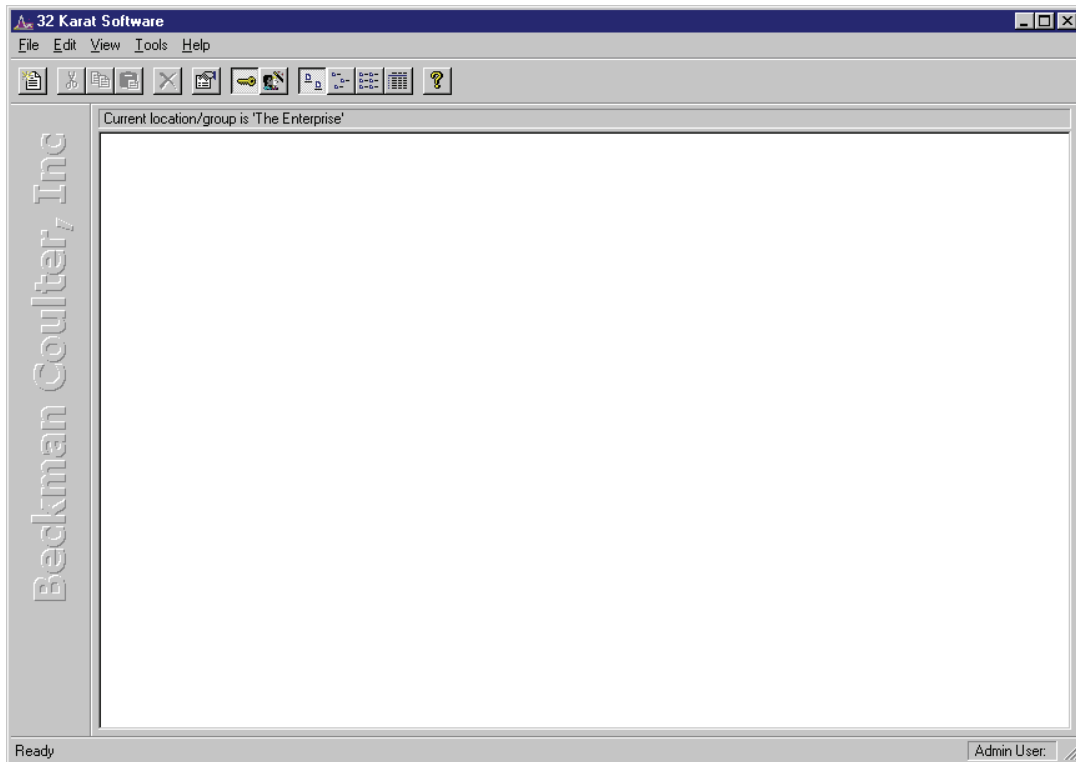


Figure 3.2 Accessing 32 Karat Software through Windows



**Figure 3.3 32 Karat Software Enterprise Screen (Main Menu)**

- Creating an Instrument
- Online Instruments (for control of system)
- Offline Instruments (for multitasking)
- System Administration
- System Administration Wizard
- Users

### **3.3 Instrument Configuration**

- Naming the Instrument
- When and how to auto-configure
- Selecting system options
- SS420A/D Board or SS420x A/D Device

### 3.4 Module Configuration: Selecting Options

- ❑ Naming the Detectors

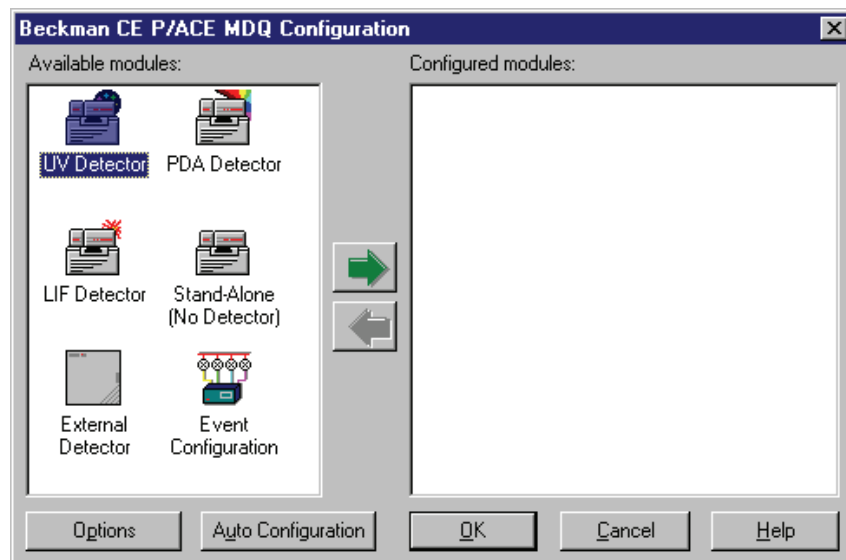


Figure 3.4 P/ACE MDQ System Configuration dialog

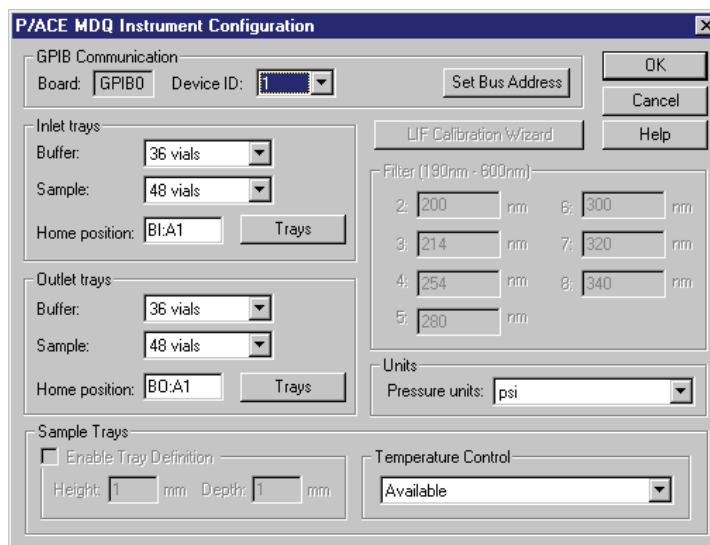
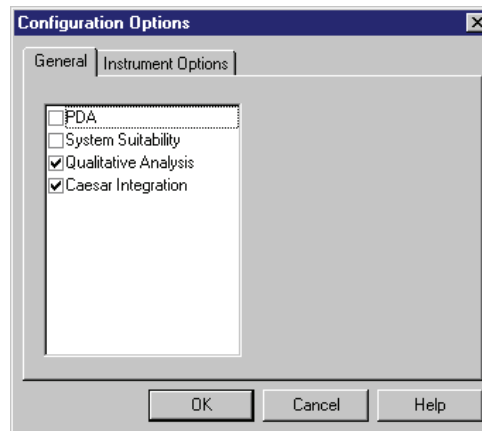


Figure 3.5 Instrument Configuration dialog

- ❑ GPIB Communication
- ❑ Inlet/Outlet Trays
- ❑ Sample Trays

- LIF Calibration Wizard
- Filters
- Units
- Temperature Control



**Figure 3.6 Configuration Options dialog**

- PDA
- System Suitability
- Qualitative Analysis
- Caesar Integration

### 3.5 Starting the Newly Configured Instrument

#### Instrument Wizard

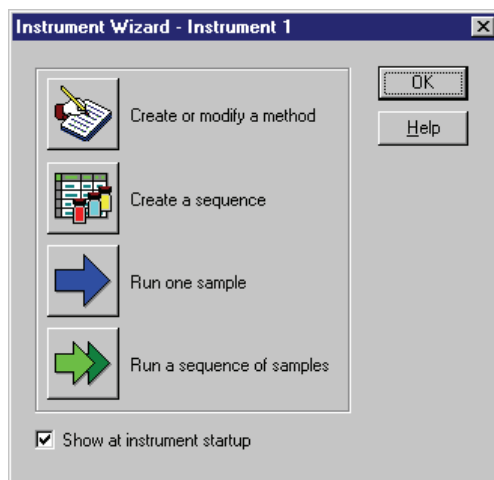


Figure 3.7 Instrument Wizard dialog

#### Instrument Window Screen Layout

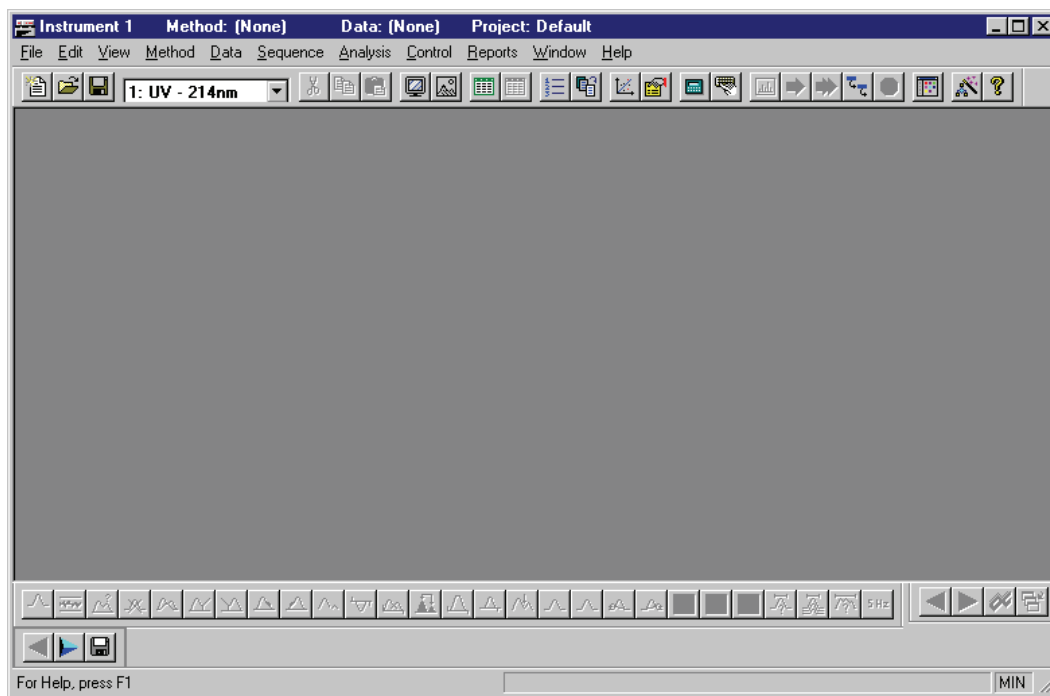


Figure 3.8 Instrument Window

 Instrument Window



- Title Bar
- Menu Bar
- Tool Bar
- Status Line

### 3.6 Skill Check

Upon completion of this section, you should be able to do the following:

1. Start the computer.
2. Log on to the Windows operating system.
3. Start 32 Karat Software.
4. Create an Instrument.
5. Auto Configure the instrument.
6. Open the Instrument Window.

### 3.7 Summary

This completes the software setup portion of the training. The software should now be started and configured.

The next section covers the various types of detectors. You will review the information that pertains to the configuration of your instrument. Only one detector type will be covered.



## Reviewing Detectors

### 4.1 Overview

Depending on the configuration of your system, the function of the detector(s) varies. This section focuses on the important setup and functions of each detector. Some of these relate to report options you will learn in Section 12. In this section we will discuss:

- UV Initial Conditions Tab
- UV Data Display
- PDA Initial Conditions Tab
- The PDA Setup Window
- PDA Data Display
- LIF Initial Conditions Tab
- LIF Data Display
- LIF Calibration Wizard

### 4.2 UV Detector

#### UV Initial Conditions

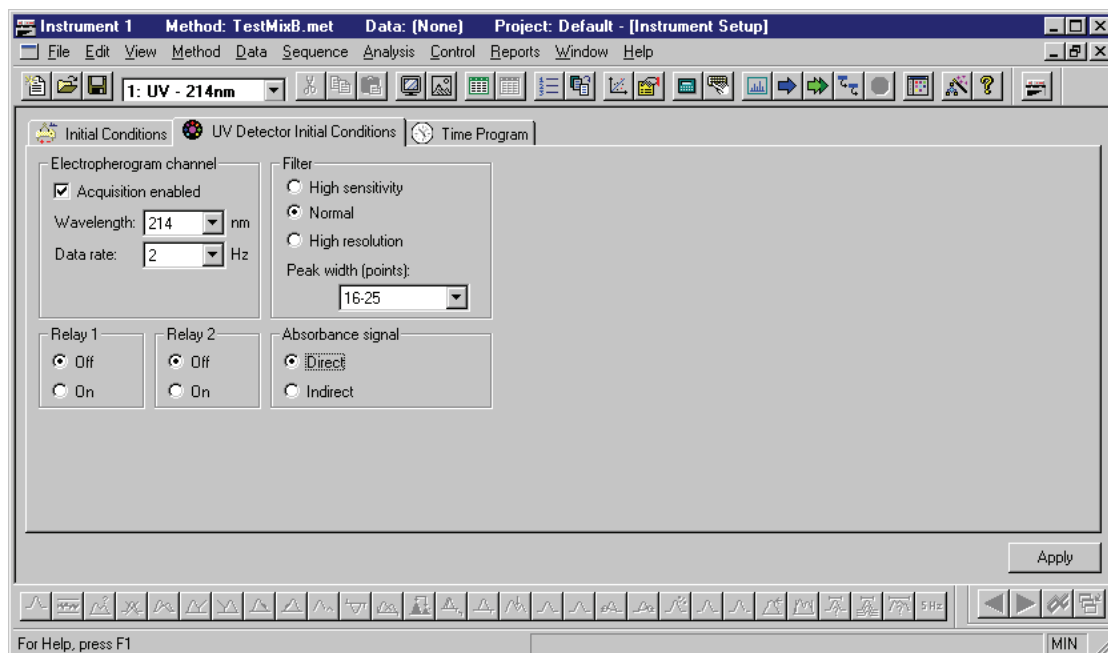


Figure 4.1 UV Initial Conditions tab

### Electropherogram Channel

- Wavelength
- Data Rate

### Filter Settings

- Peak width

### Relays

- On/Off

### Absorbance signal

- Direct
- Indirect

### UV Data Display

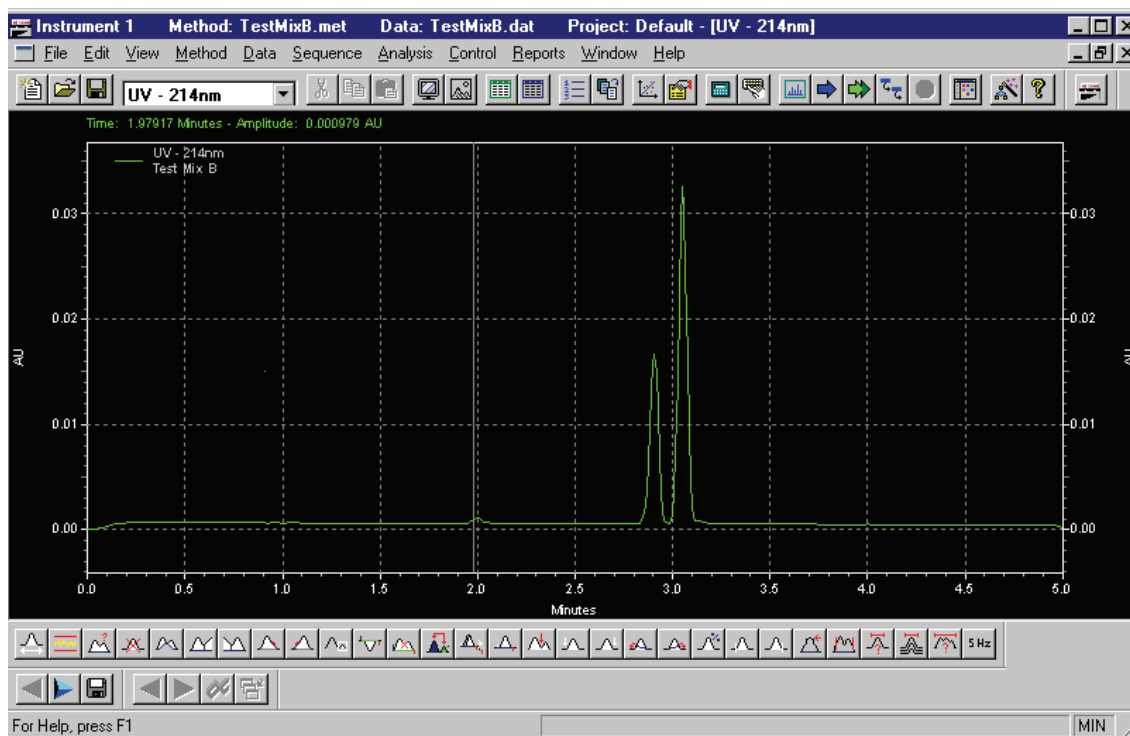


Figure 4.2 Instrument Window with UV data displayed

## 4.3 PDA Detector

### PDA Initial Conditions

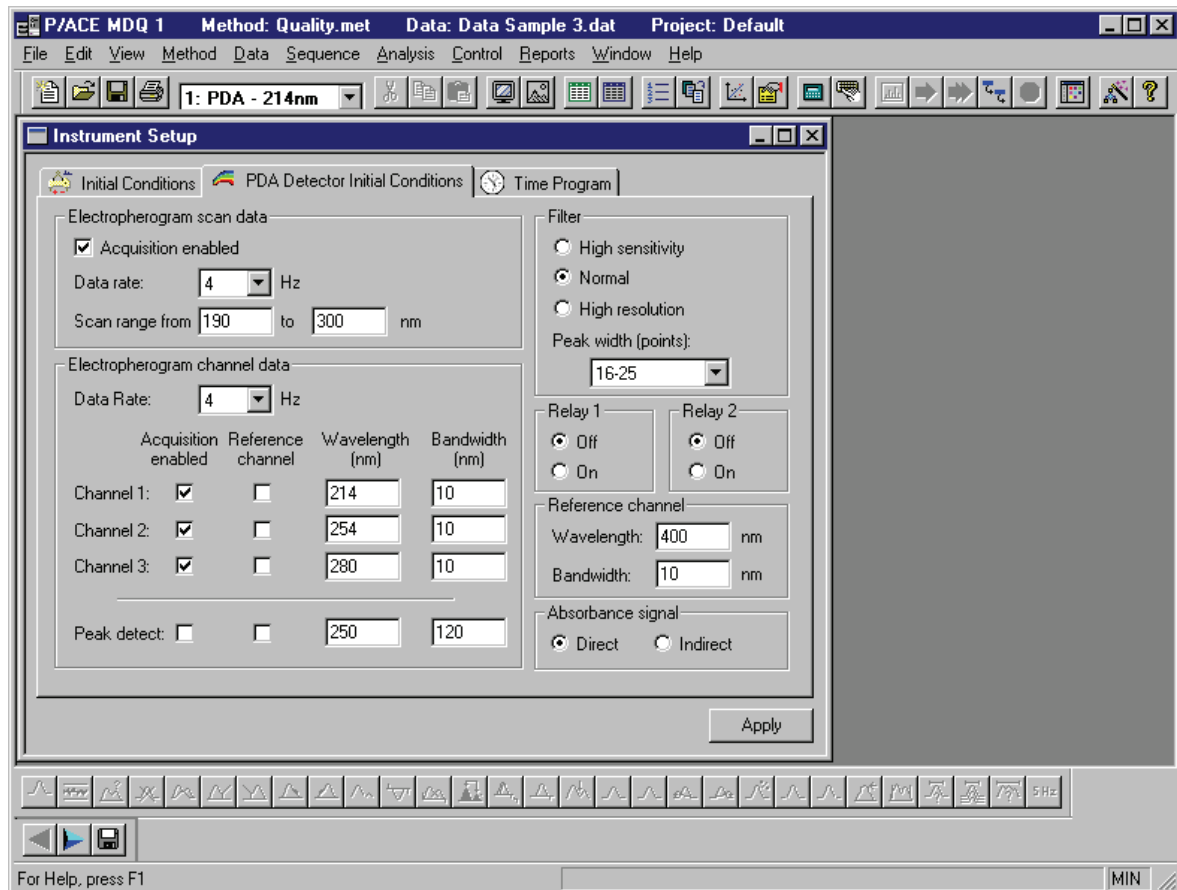


Figure 4.3 PDA Initial Conditions tab

#### Electropherogram scan data

- Data rate
- Scan range

#### Electropherogram channel data

- Data rate
- Channel Definition
- Peak detect

#### Filter Settings

- Peak width

### Fraction Collector /Relays

- On
- Off

### Reference Channel

- Wavelength
- Bandwidth

### Absorbance signal

- Direct
- Indirect

## 4.4 PDA Setup

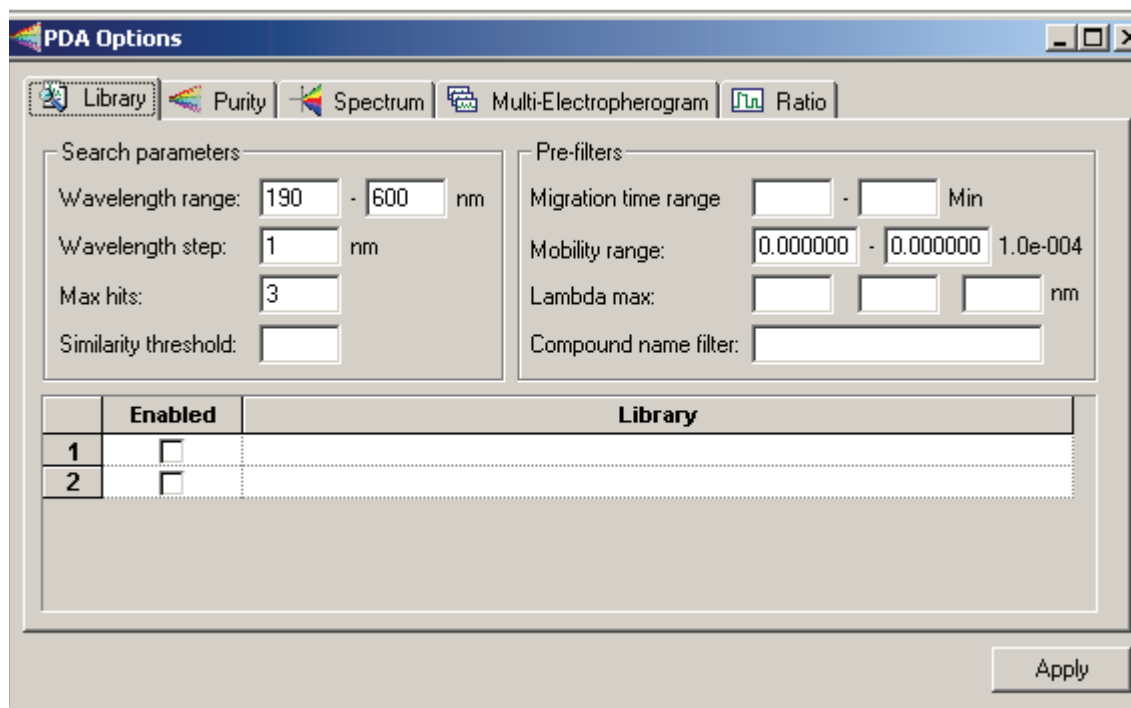


Figure 4.4 PDA Options with Library tab selected

- Library Search Parameters

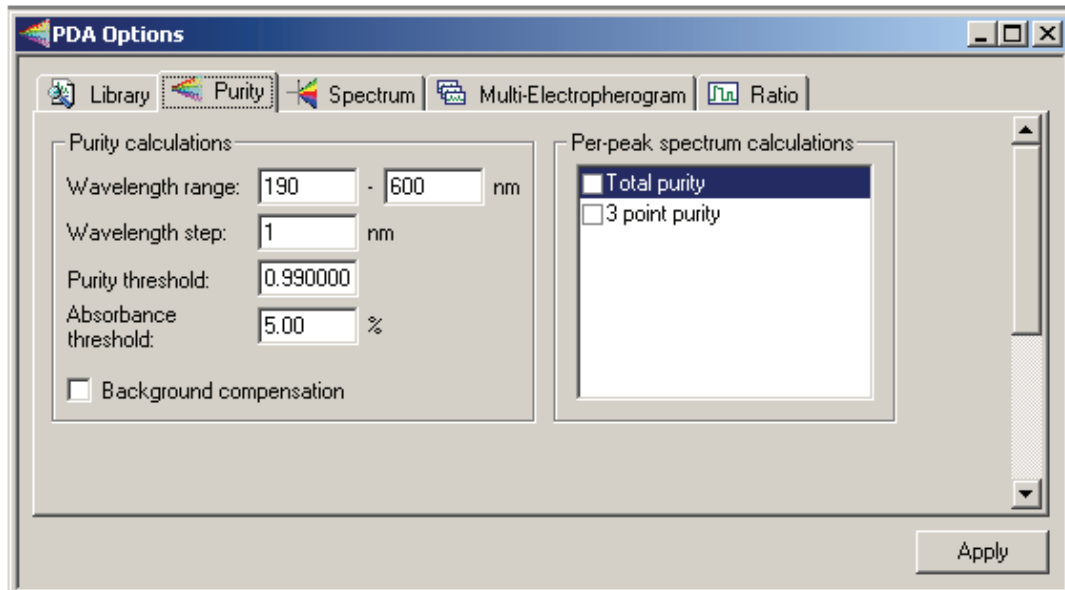


Figure 4.5 PDA Options with Purity tab selected

- Purity Calculations

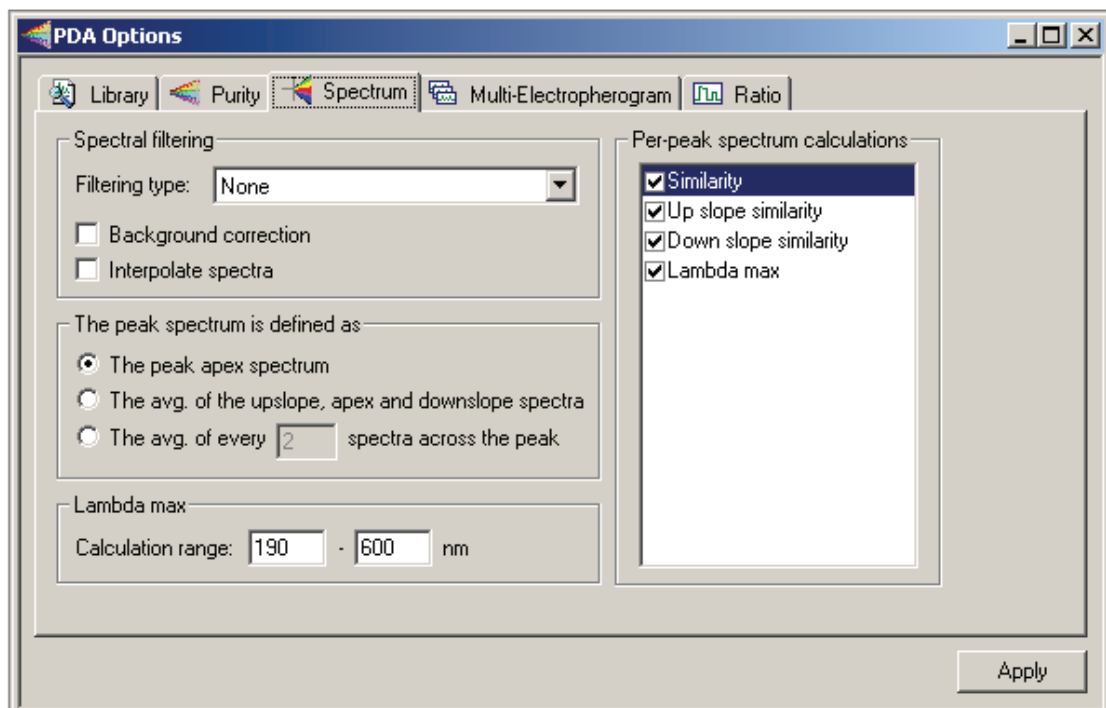


Figure 4.6 PDA Options with Spectrum tab selected

- Spectral Filtering

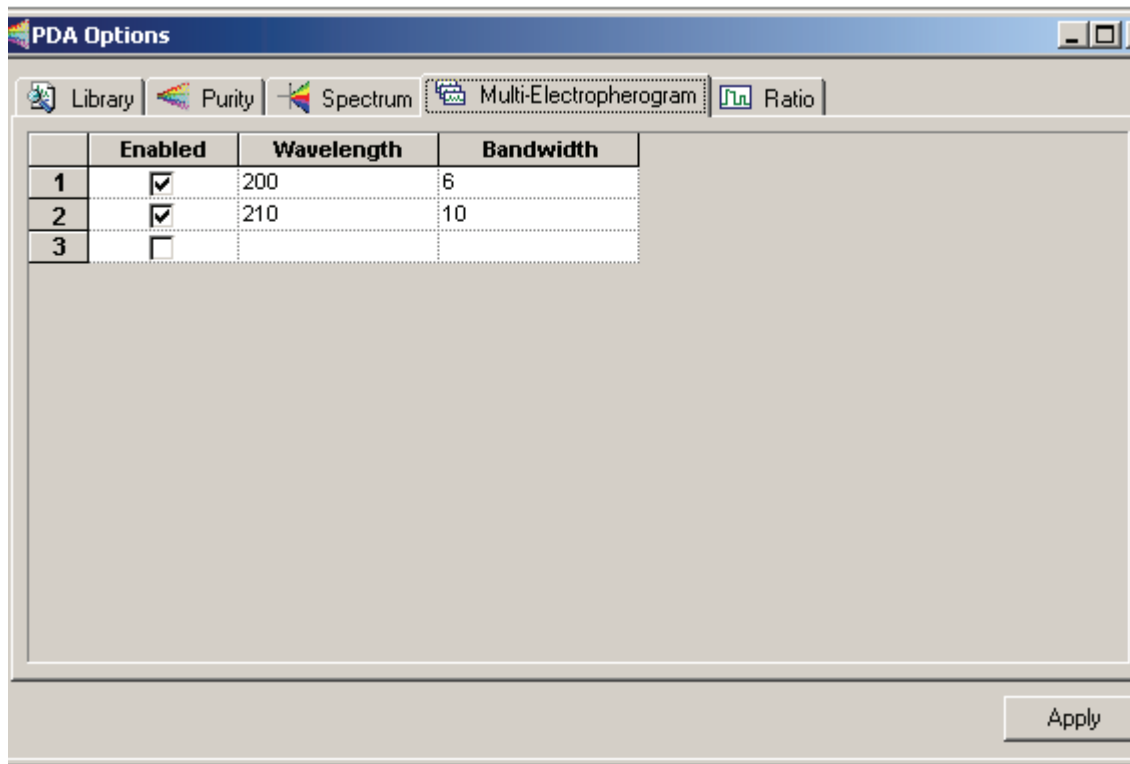


Figure 4.7 PDA Options with Multi-Electropherogram tab selected

- Enabled
- Wavelength
- Bandwidth



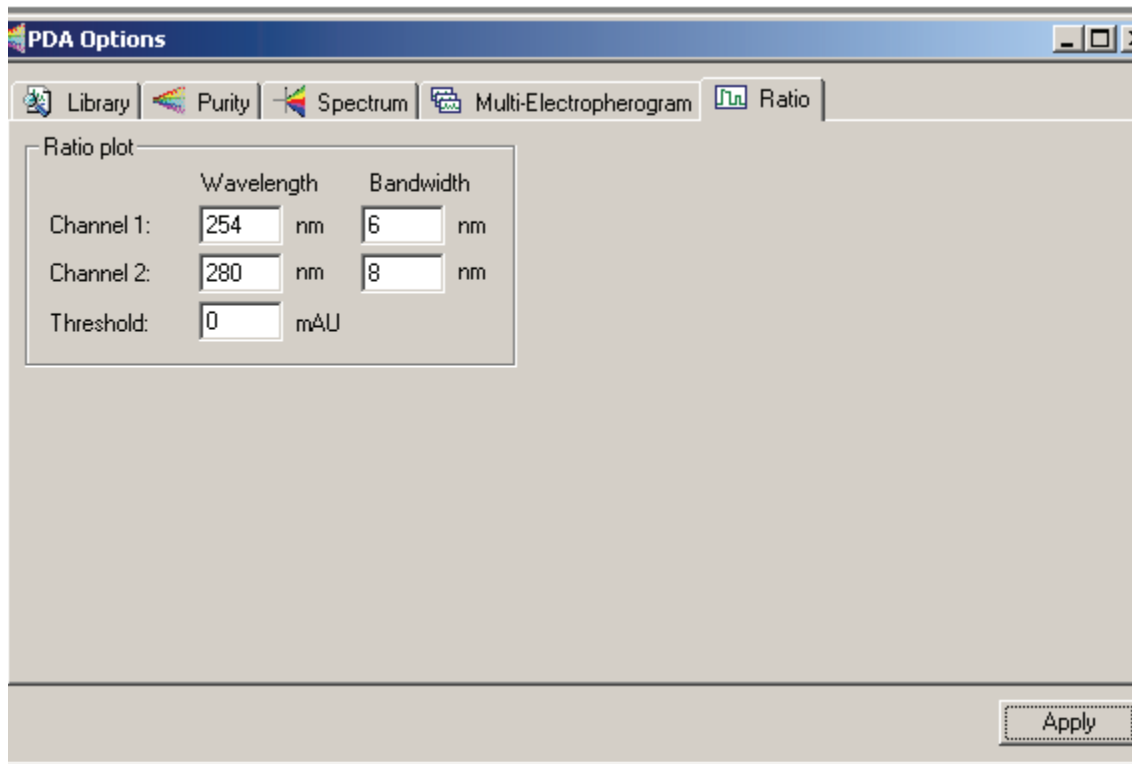


Figure 4.8 PDA Options with Ratio tab selected

- Wavelength
- Bandwidth

## 4.5 PDA Data Display

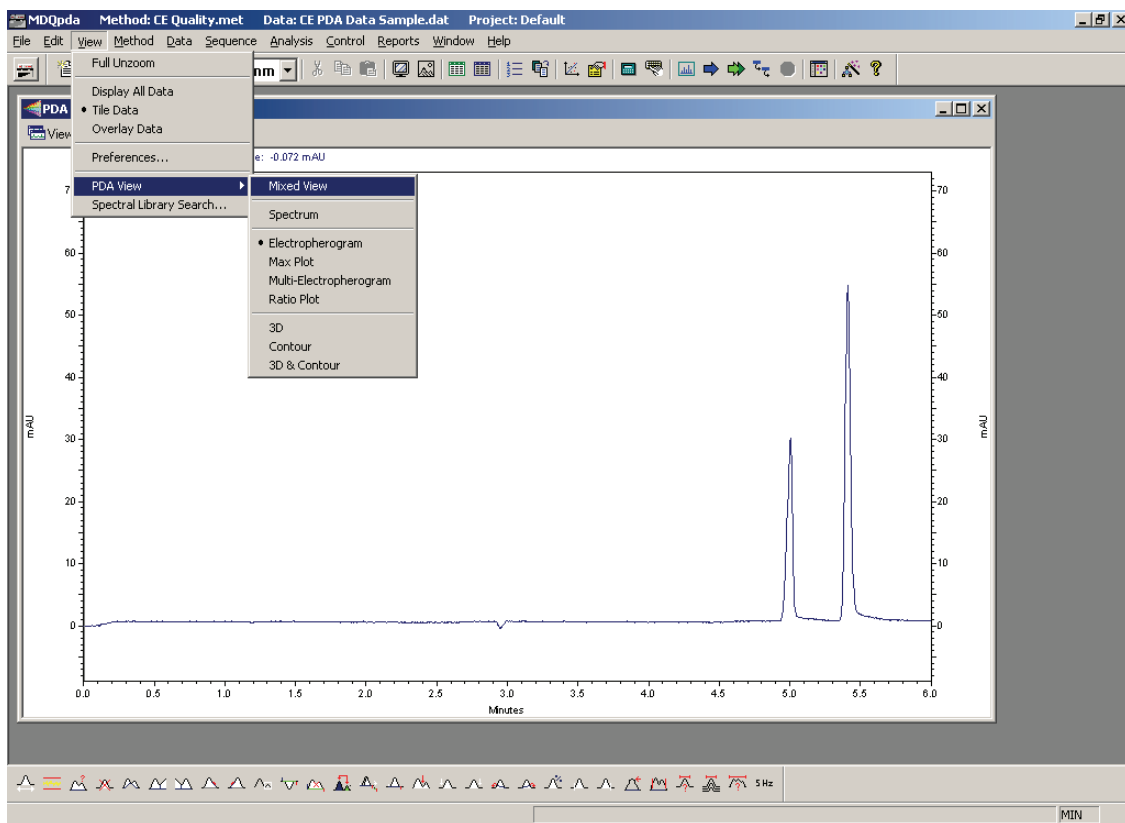


Figure 4.9 Instrument Window with PDA data file open; View menu open and PDA View selected

- Photo Diode Array data features
- PDA View

## View Options

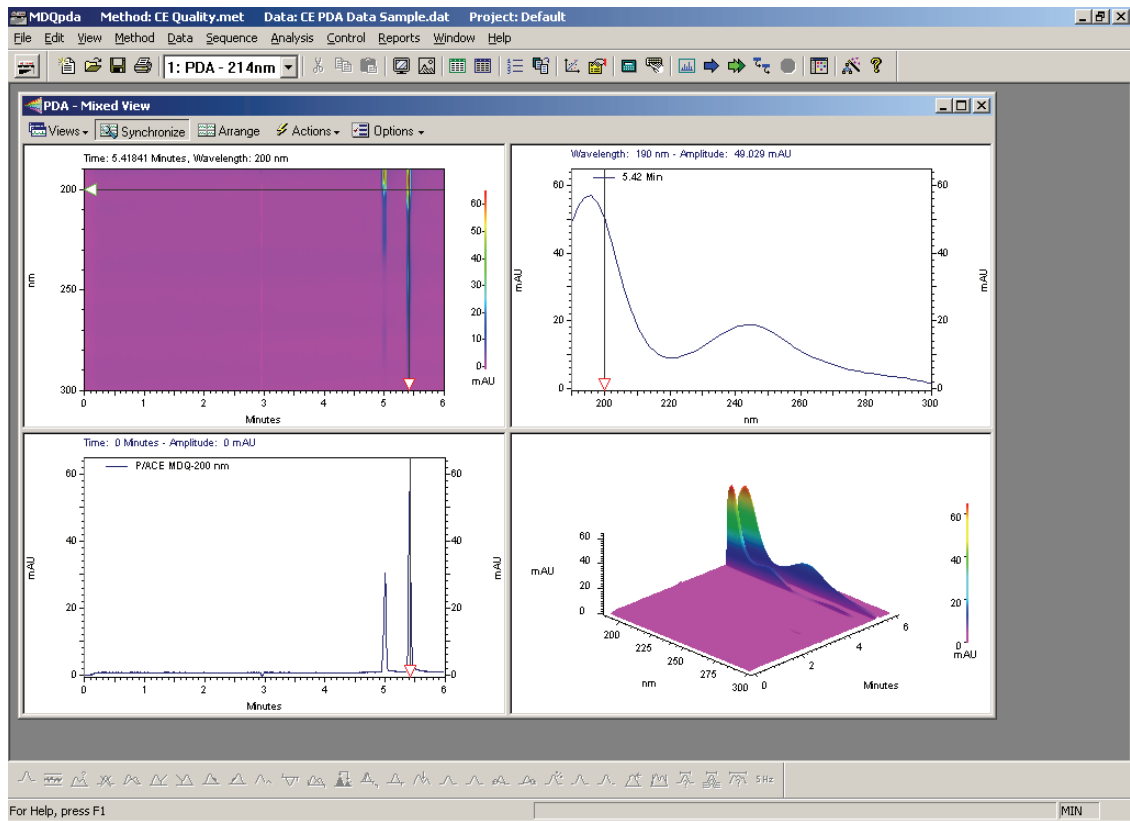


Figure 4.10 Photo Diode Array data

## 4.6 LIF Detector

### LIF Initial Conditions

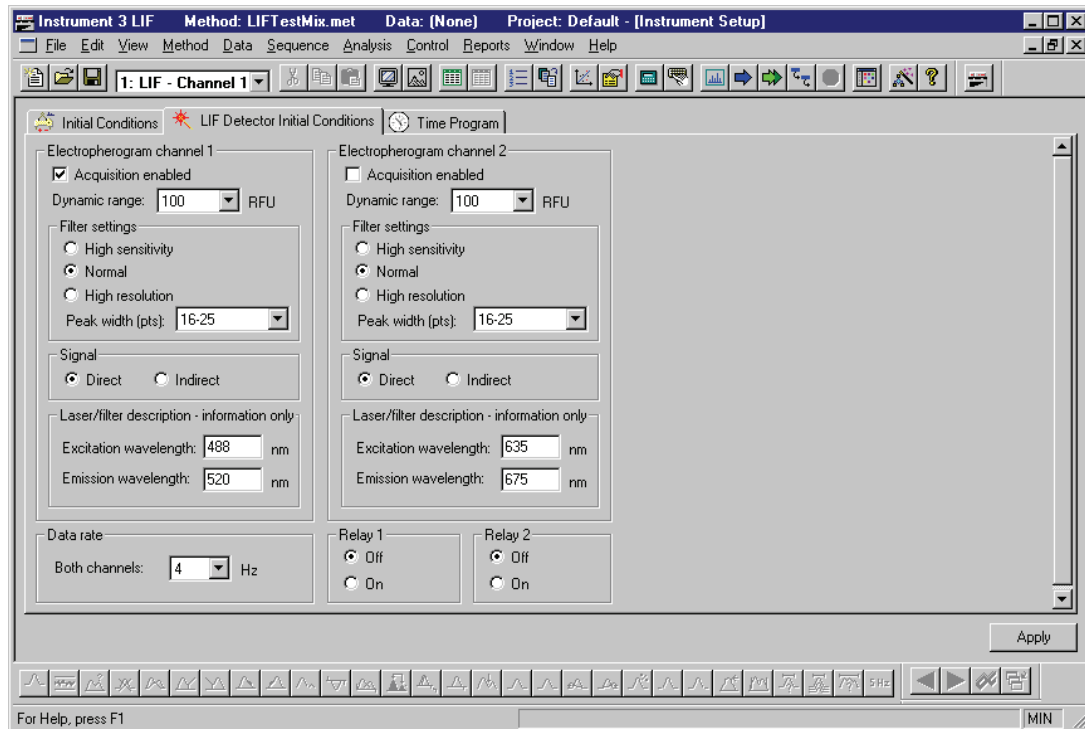


Figure 4.11 LIF Initial Conditions tab

#### Electropherogram Channels

- Dynamic range
- Filter Settings
- Peak width
- Signal

#### Laser/Filter Descriptions

- Excitation wavelength
- Emission wavelength

## 4.7 Data Rate

### Relays

On/Off

### LIF Data Display

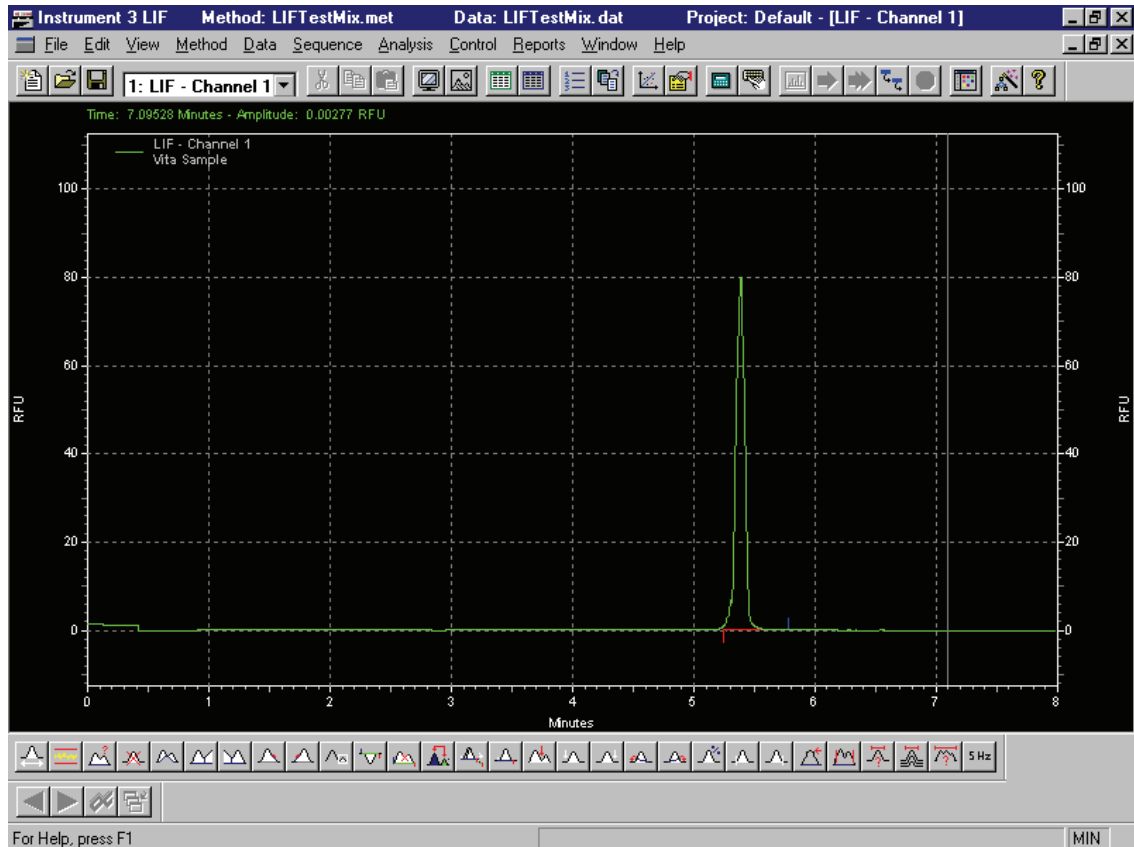


Figure 4.12 Instrument Window with LIF data file open; right mouse click menu open

## LIF Calibration Wizard

- Accessing LIF Calibration Wizard

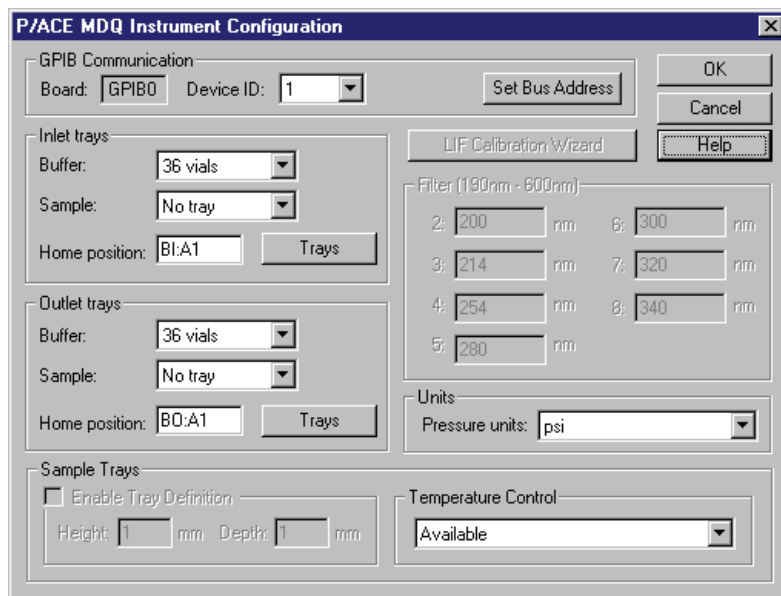


Figure 4.13 Instrument Configuration dialog

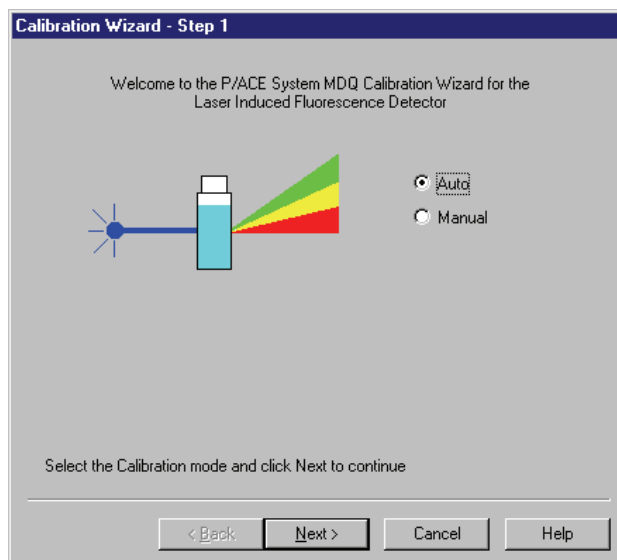


Figure 4.14 LIF Detector Calibration Wizard - Step 1

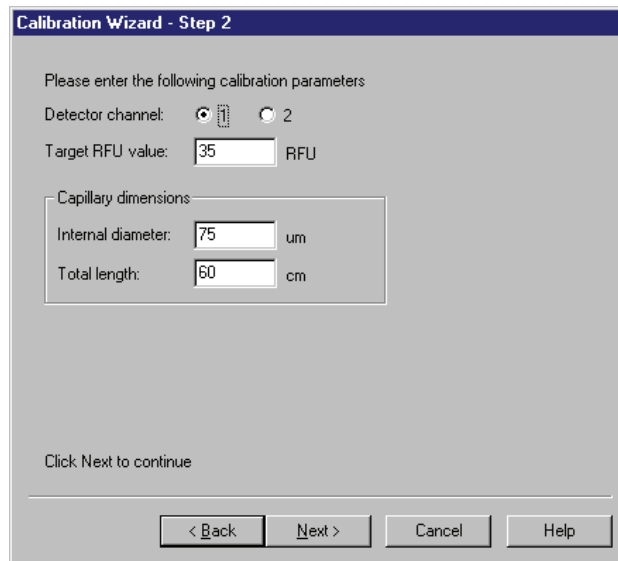


Figure 4.15 LIF Detector Calibration Wizard - Step 2

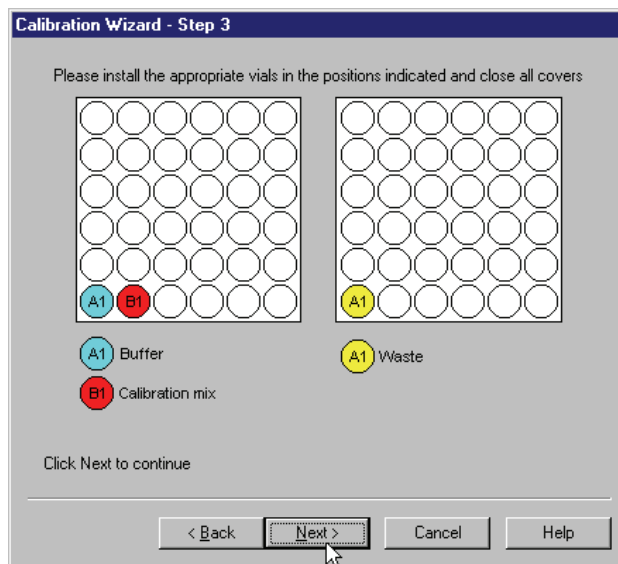


Figure 4.16 LIF Detector Calibration Wizard - Step 3

## 4.8 Summary

This completes the detector portion of the 32 Karat Software Basic Instrument Training. You are ready to use the Direct Control feature.





## Using Direct Control

### 5.1 Overview

This section covers the start up process and parameter control for P/ACE MDQ system. You will establish initial running conditions for each component.

We will discuss:

- Accessing Direct Control
- Direct Control screens
- Controlling module parameters
- Skill Check

### Accessing Direct Control

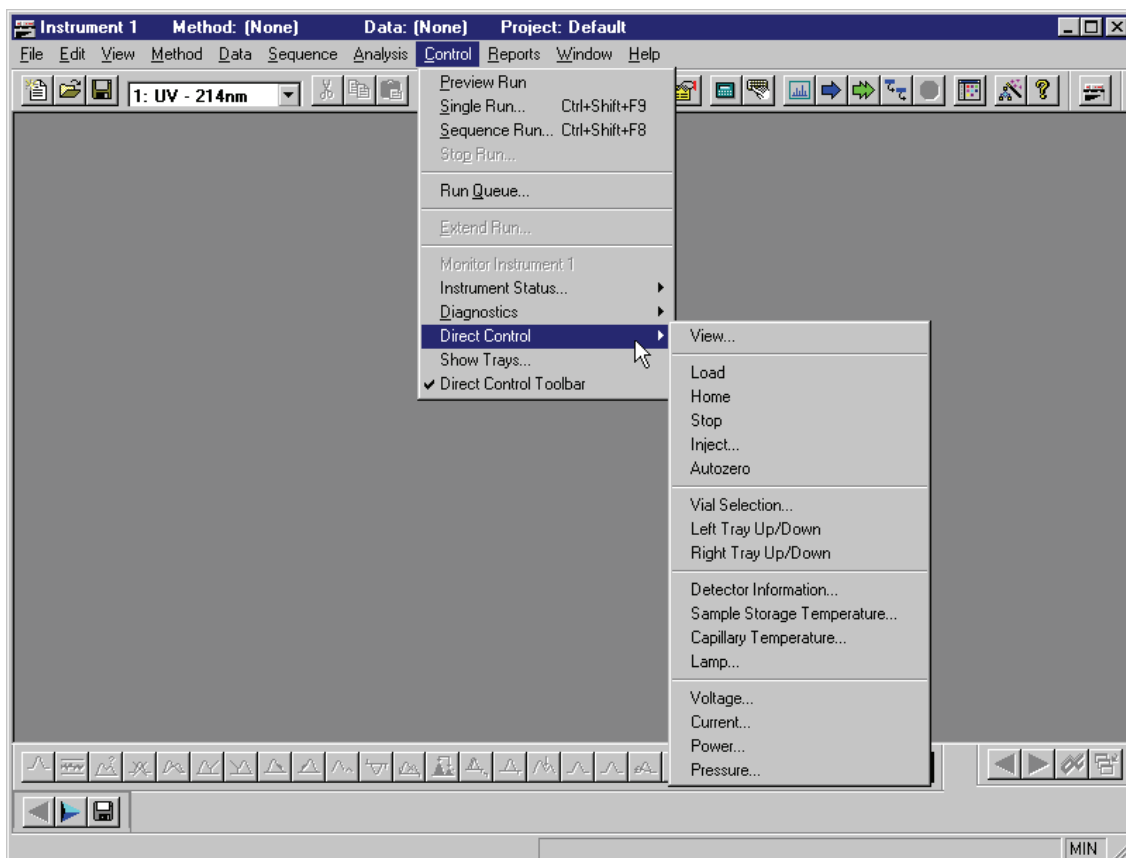


Figure 5.1 Instrument Window with Control | Direct Control selected

## 5.2 Using Direct Control

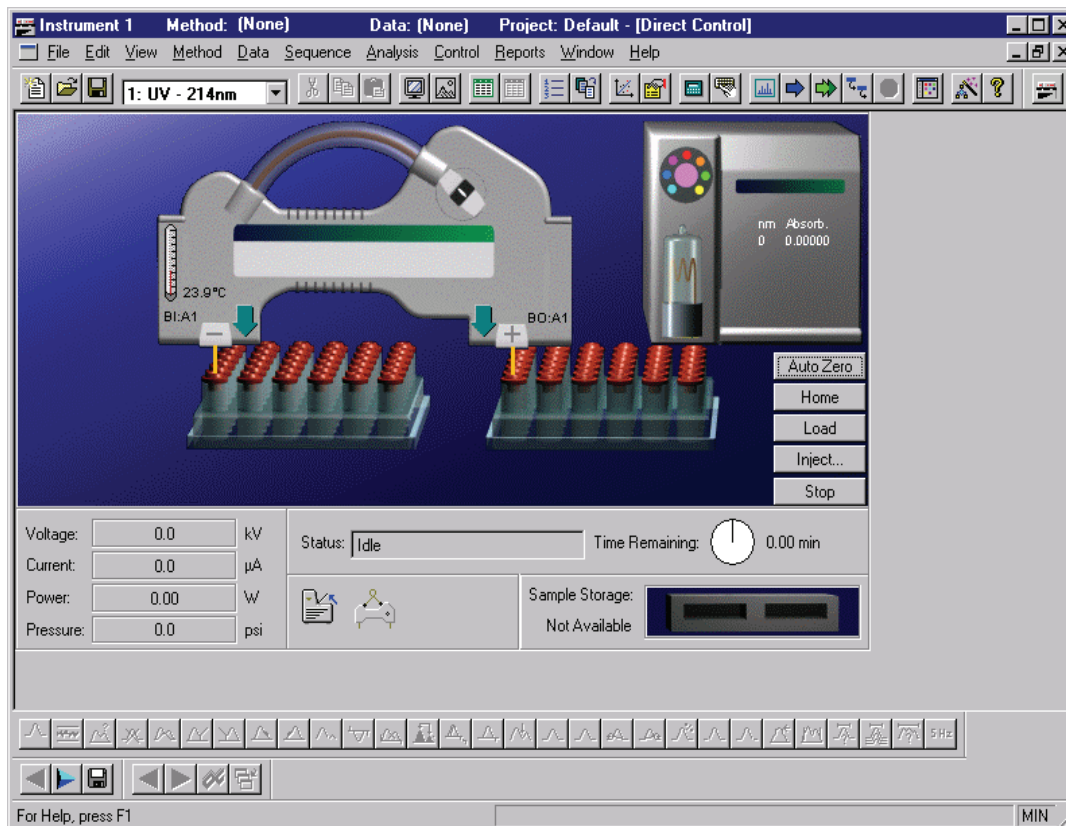


Figure 5.2 Direct Control Screen

### Cartridge Coolant Temperature

- Set Temperature

### Sample Storage Temperature

- Set Temperature

### Capillary Information

- Capillary Description
- Capillary Lot Number

## Rinse

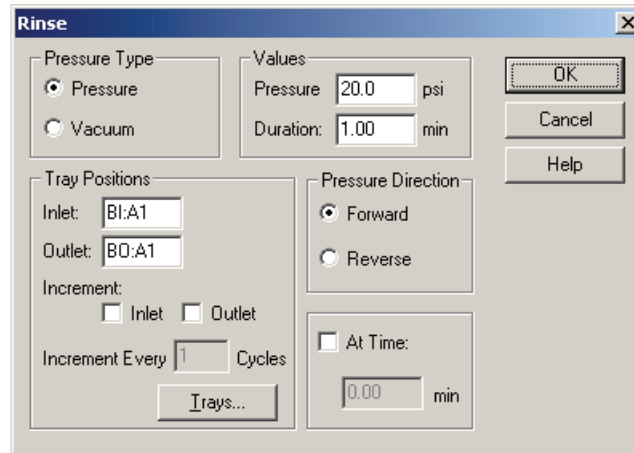


Figure 5.3 Rinse dialog

## Inject

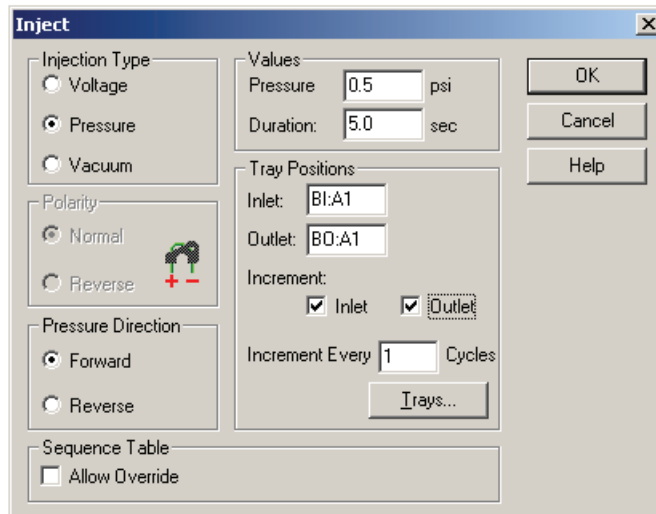


Figure 5.4 Inject dialog

## Separate

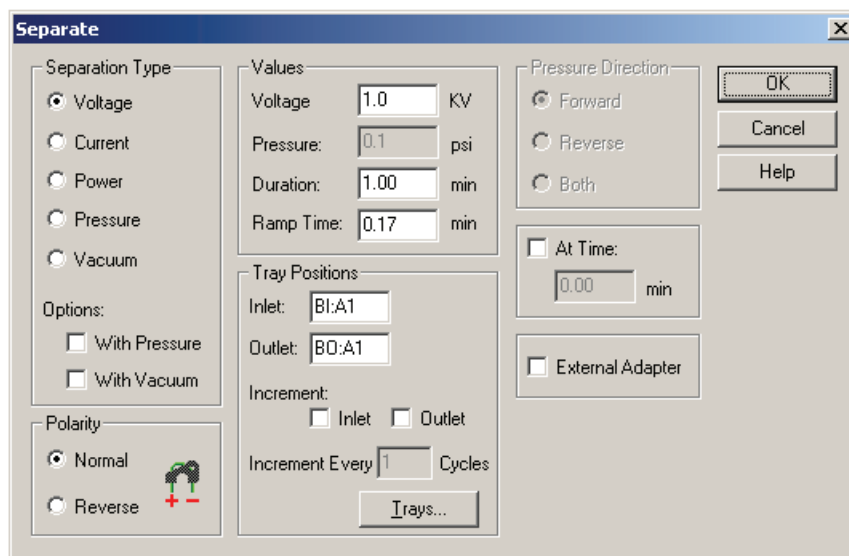


Figure 5.5 Separate dialog

## Detector Settings

### Common Parameters

- Data Filters
- Peak Width
- Relays
- Detection Signal
- Data Acquisition

### UV Detector Parameters

- Wavelength selection
- Data Rate
- Filter Positions

### PDA Detector Parameters

- Channel data
- Scan Data

- Reference Channel
- Shutter

### **LIF Detector Parameters**

- Electropherogram Channels 1 and 2
- Dynamic Range
- Data Rate
- Laser / Filter Description

### **Lamp Status**

- On/Off

### **Laser Status**

- On/Off

### **Tray Position**

- Graphical display

### **Voltage Settings**

- Voltage
- Duration
- Ramp Time
- Voltage Max
- Current Max
- Tray Positions
- External Adapter
- Polarity
- Pressure

### **Current Settings**

- Current
- Duration

- Ramp Time
- Voltage Max
- Current Max
- Tray Positions
- External Adapter
- Polarity
- Pressure

### **Power Settings**

- Power
- Duration
- Ramp Time
- Voltage Max
- Current Max
- Tray Positions
- External Adapter
- Polarity
- Pressure

### **Pressure**

- Pressure / Vacuum
- Duration
- Tray Positions
- Direction
- Pressure Type

### **Time Remaining**

- Graphical display

## Status

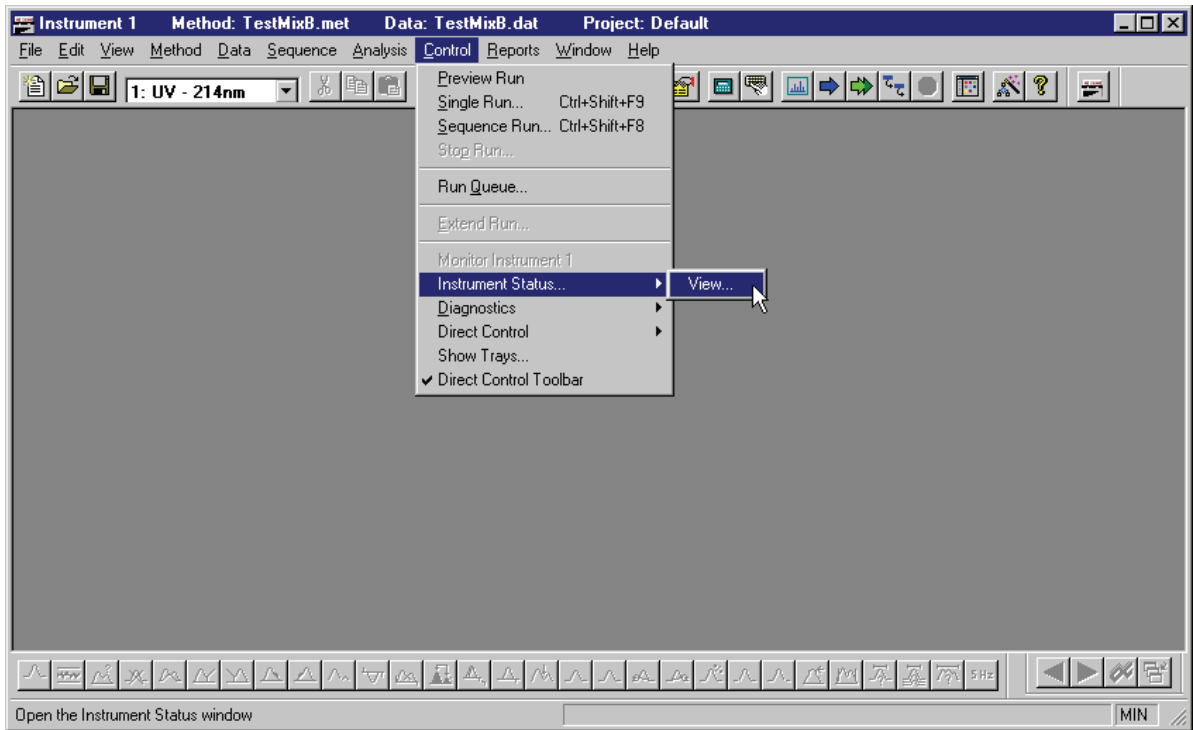


Figure 5.6 Instrument Window with Control | Instrument Status | View selected

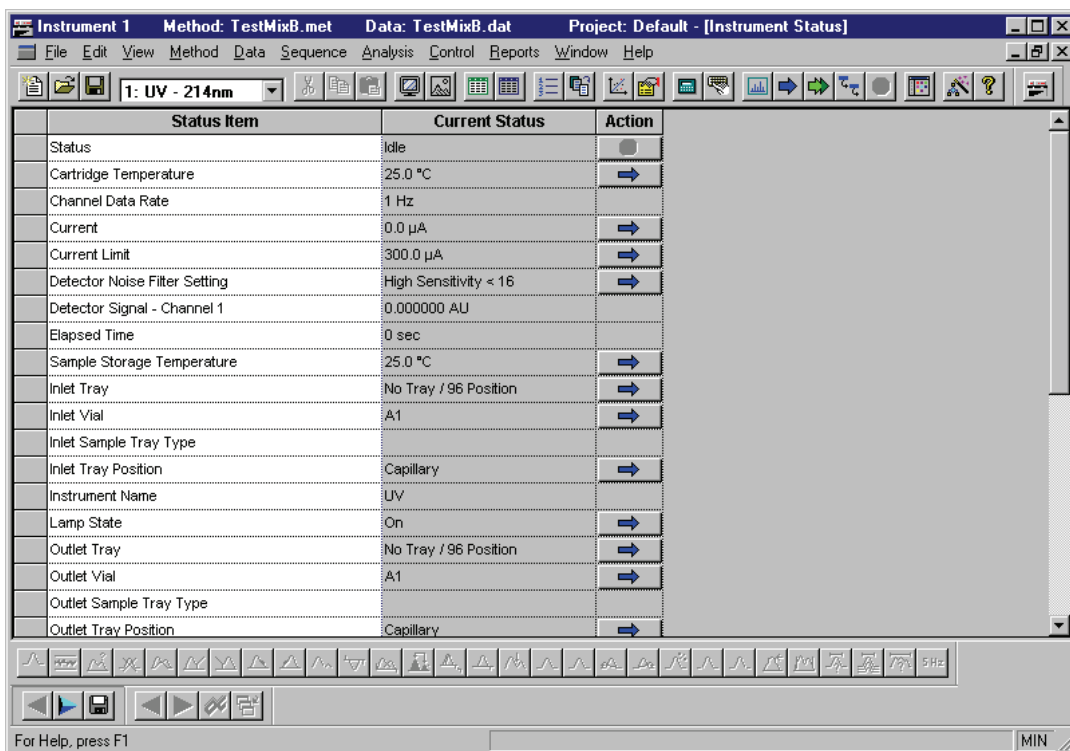


Figure 5.7 Status Window

- Status Item
- Current Status
- Action

### 5.3 Skill Check

Upon completion of this section, you should be able to do the following:

- Access Direct Control.
- Program and run a rinse.
- Program and run an injection.
- Program and run a separation.

### Summary

This completes the Direct Control portion of 32 Karat Software Basic Instrument Training. When the system finishes equilibrating, you will prepare a method to run.



## Working with Methods

### 6.1 Overview

In this section we will explain procedures for building and editing a method. A method automates all of the hardware functions as well as data collection.

Later we will talk about editing, analysis parameters, and report generation). In this section, we will discuss:

- Method Wizard
- Creating a Method
- Saving a Method
- Editing a Method
- Printing a Method
- Other Method Properties
- Skill Check

### Using the Method Wizard



**Figure 6.1** Method Window dialog

- Creating a new method
- Modifying the current method
- Modifying a method on disk

## Creating a Method

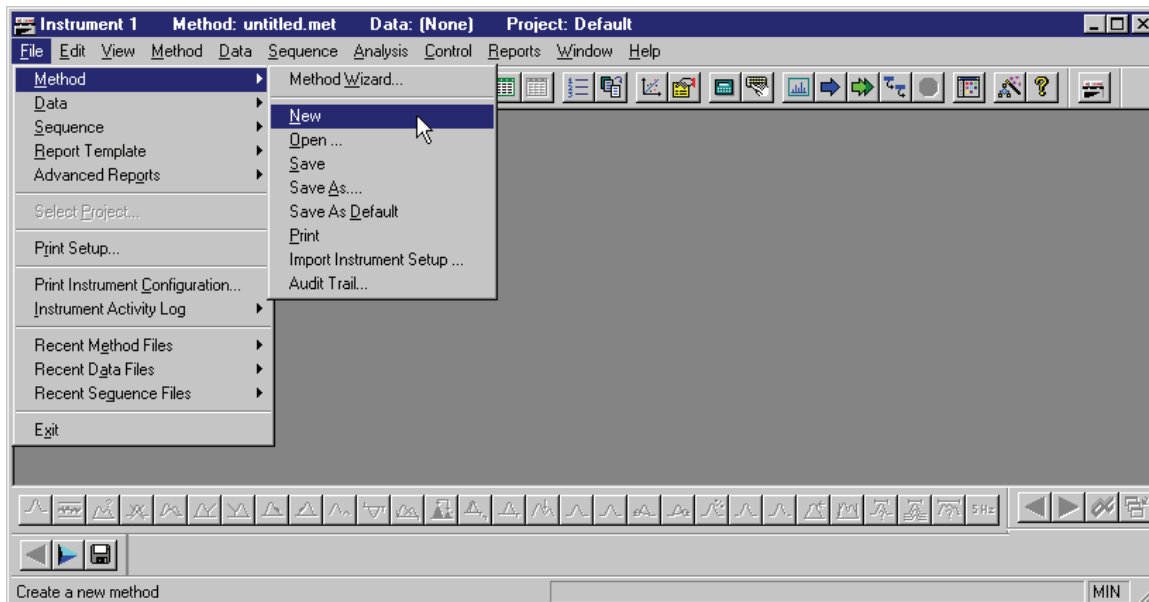


Figure 6.2 Instrument Window with File | Method | New selected

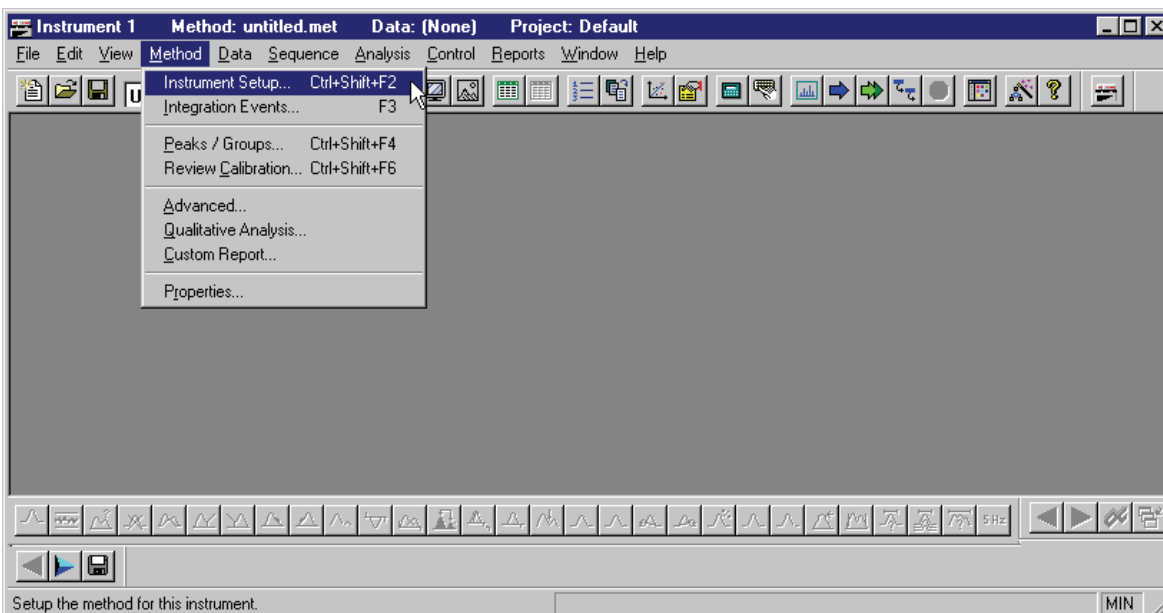


Figure 6.3 Instrument Window with Method | Instrument Setup selected

## Instrument Setup

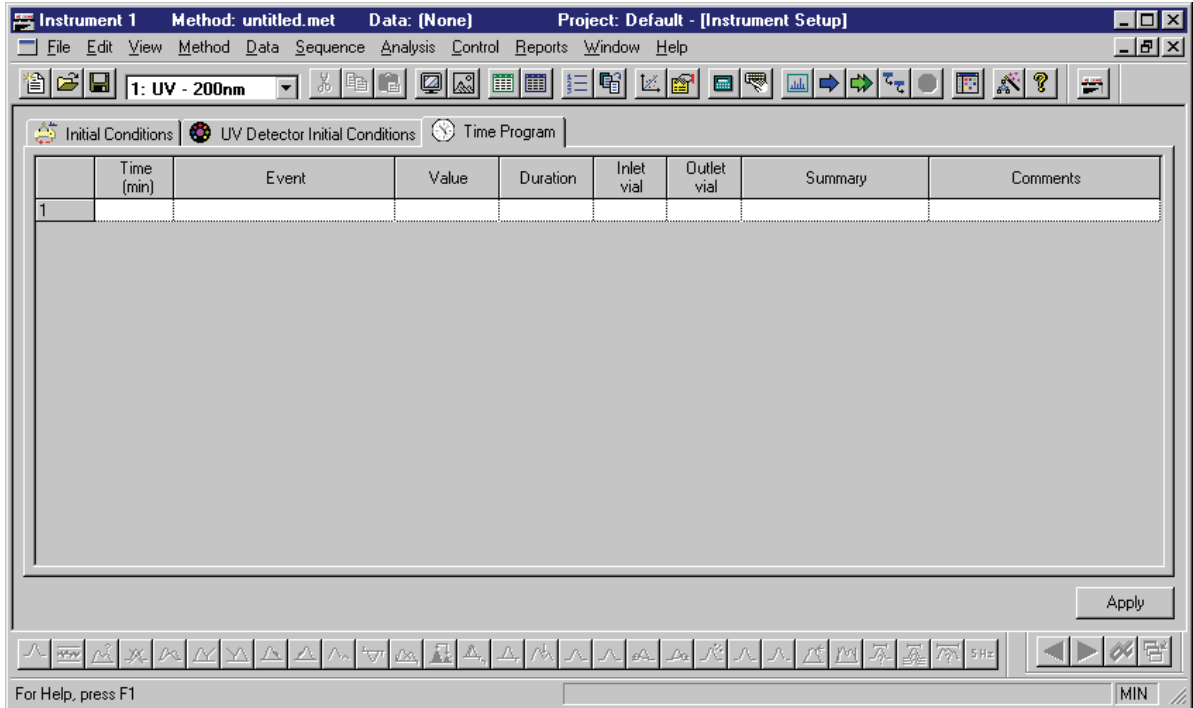


Figure 6.4 Instrument Setup Window with Time Program tab

## Initial Conditions Tabs

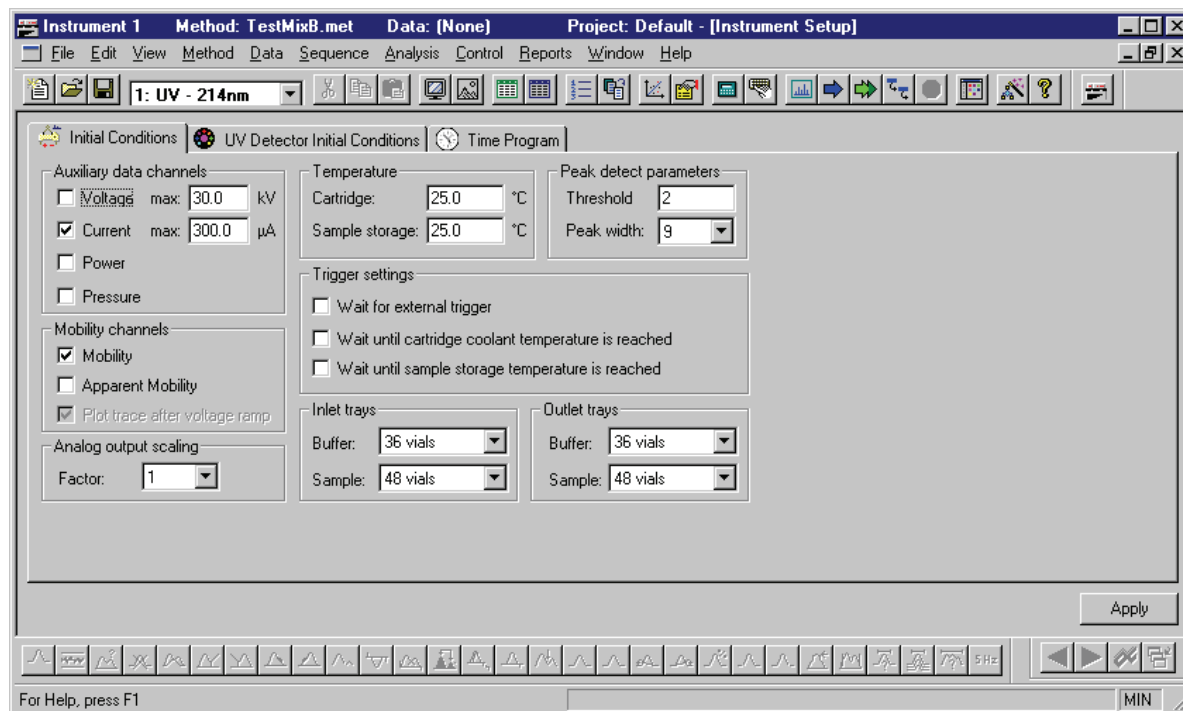
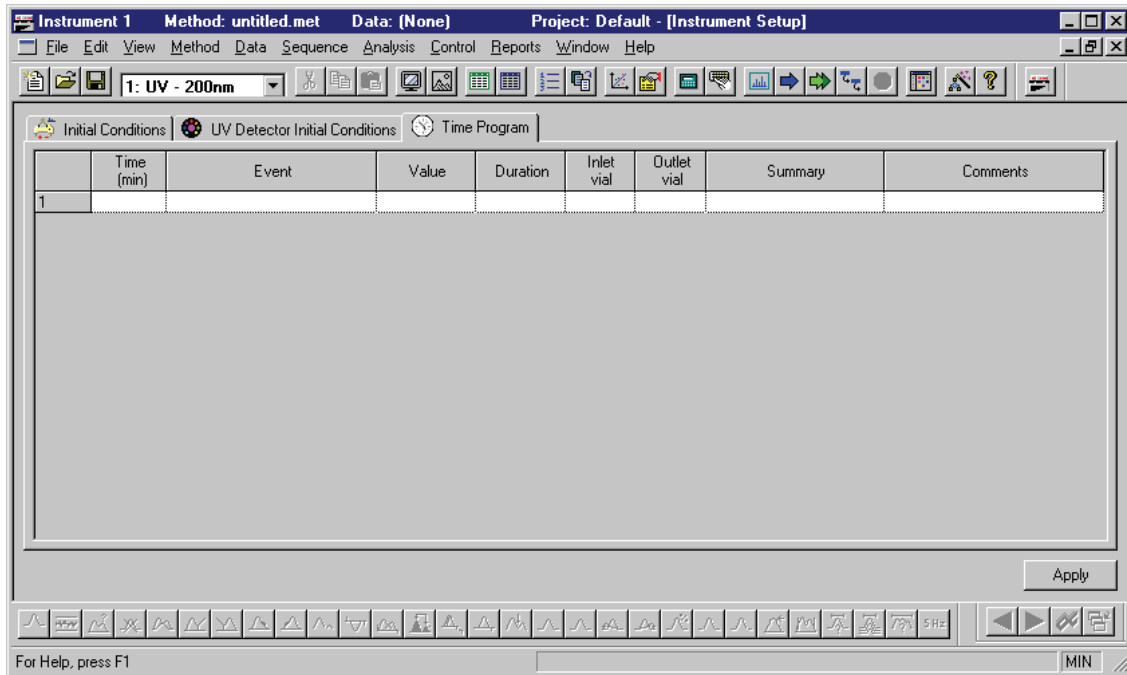


Figure 6.5 Initial Conditions tab

- Auxiliary data channels
- Mobility Channels
- Temperature
- Peak detect parameters
- Trigger settings
- Tray type selection
- Analog output scaling

## Time Programming



### Time Programming tab

- Time
- Event
- Value
- Duration
- Inlet Vial/Outlet Vial
- Summary
- Comments

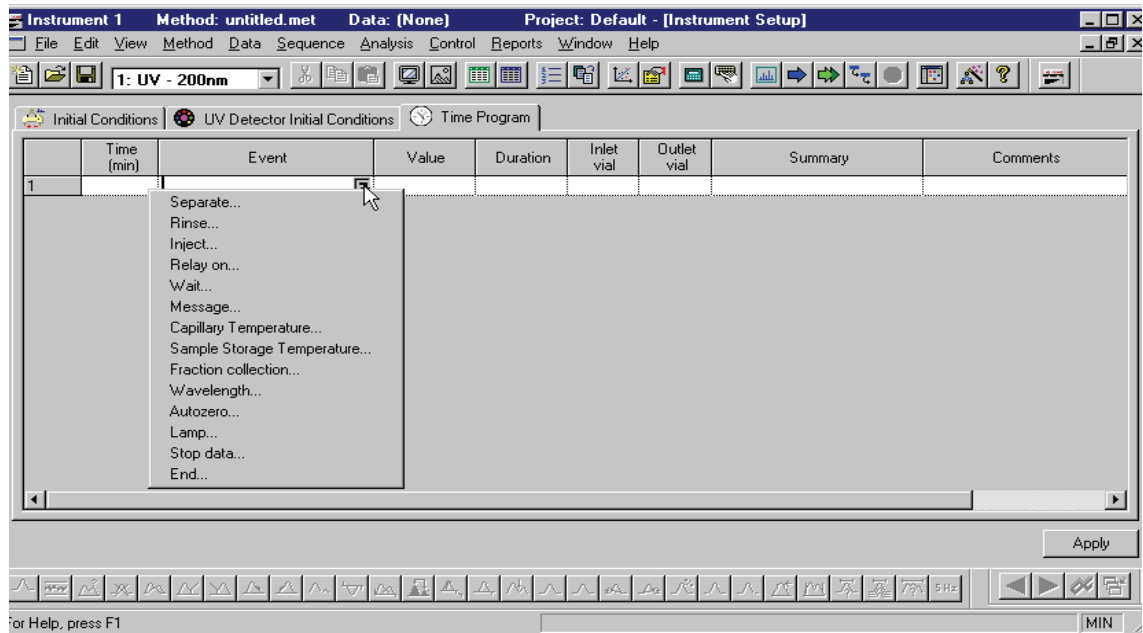


Figure 6.6 Time Program tab with available Event list displayed

### Events

- Rinse
- Inject
- Separate

### UV Detector

- Associated Event dialog boxes

### PDA Detector

- Associated Event dialog boxes

### LIF Detector

- Associated Event dialog boxes

### External Detector

- Selecting an External Detector Adapter

## Saving a Method

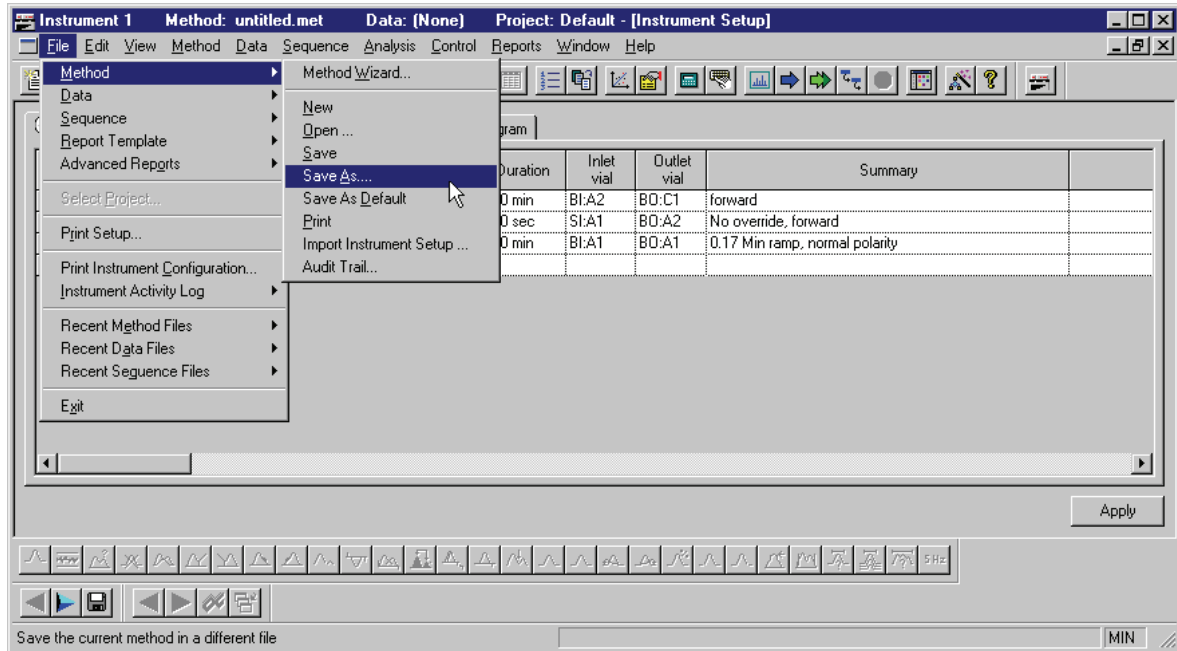


Figure 6.7 Instrument Window with File | Method | Save selected

- Save Method As
- Save As Default

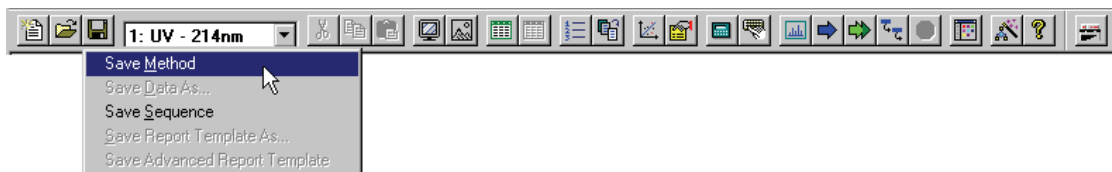


Figure 6.8 Save icon with Method selected

- Naming and saving a new method
- Saving an existing method

## Editing a Method

- Method Wizard
- Open method



Figure 6.9 Open Method File dialog

- Make changes
- Save Method or Save Method As



## Printing a Method

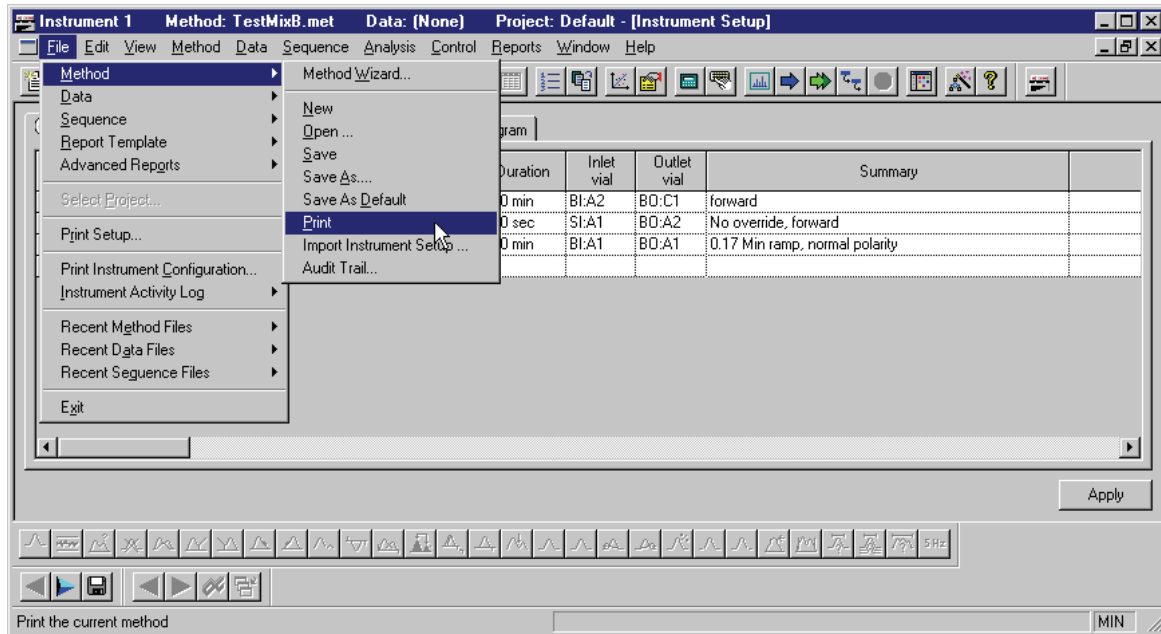


Figure 6.10 Instrument Window with File | Method | Print selected

## Other Method Functions Properties

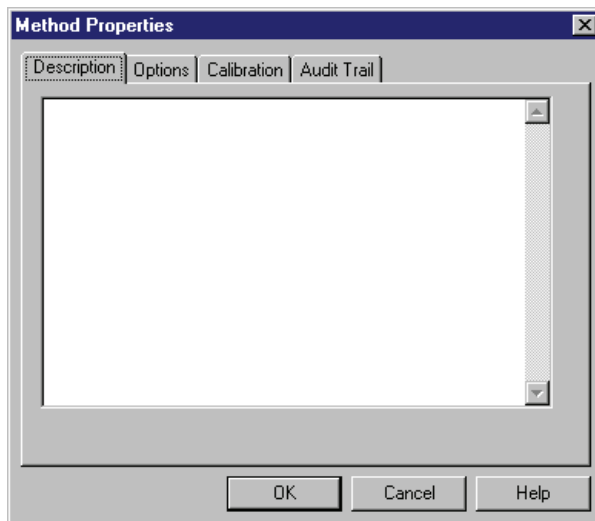


Figure 6.11 Description tab

- Method Description

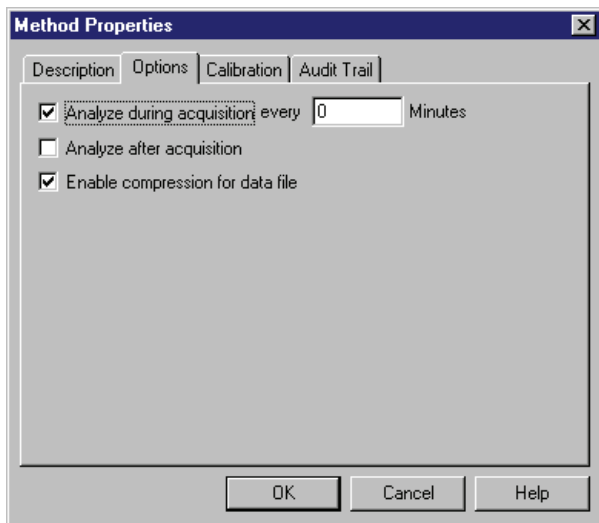


Figure 6.12 Options tab

- Analysis
- Data Compression

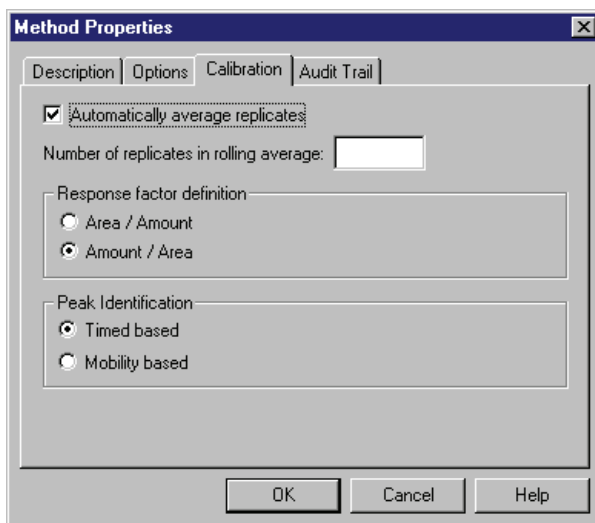


Figure 6.13 Calibration tab

- Automatically Average Replicates
- Response Factor Definition
- Peak Identification Options

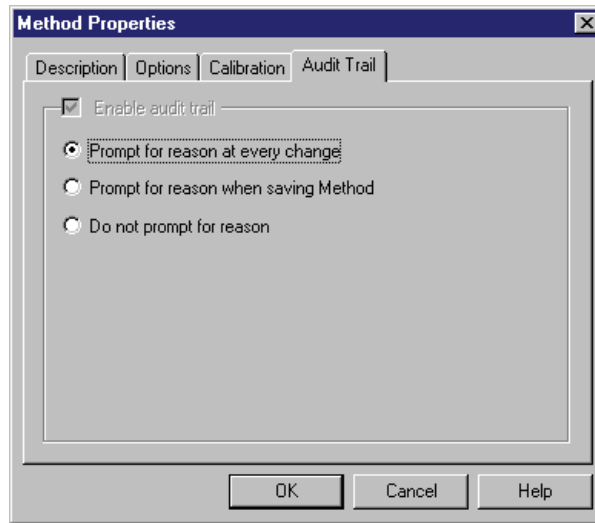


Figure 6.14 Audit Trail tab

Audit Trail

## 6.2 Skill Check

Upon completion of this section, you should be able to do the following:

1. Create a new method for a constant voltage separation in a 60 cm, 75  $\mu\text{m}$  I.D. capillary.
2. Prepare the following 2 mL vials for inlet and outlet vial positions and for rinses:

Vial	Contents	Volume	Position
Rinse	Run Buffer A	2 mL	BI:B1
Injection	Run Buffer A	1 mL	BO:B1
Separation	Run Buffer A	2 mL	BI:A1
Separation	Run Buffer A	2 mL	BO:A1
Waste	N/A	0	BO:A3

S = Sample; B = Buffer

I = Inlet; O = Outlet

A1 through F6 indicate Vial Positions

3. For UV and PDA detectors, fill one 2 mL vial with Beckman Coulter Test Mix B and place in the SI:A1 position. If you are using an LIF detector, fill the 2 mL vial with Beckman Coulter LIF Detector Test Mix. (Prepare LIF Detector Test Mix according to the Test Mix directions.)
4. Set the initial temperature to 23°C.
5. Program an un-timed pre-rinse (with a duration of at least two minutes at 20-30 psi) of Run Buffer A (BI:B1) to the waste vial (BO:A3).
6. Program a 10 second forward pressure injection of Beckman Coulter Test Mix (SI:A1) at 0.5 psi to the injection buffer vial (BO:B1).
7. Program a 30.0 kV constant voltage separation using a 0.17 minute ramp time and a duration of 6.0 minutes. Select the At Time check box and enter 0.00 minutes.
8. If you are using a UV detector, set the wavelength to 214 nm. If you are using a PDA, set the wavelength to 214 nm with a 10 nm bandwidth. If you are using an LIF detector make sure that the appropriate filters are in place.
9. Save the method you have created as `TestMixB.met`.

### Summary

This completes the methods development portion of the 32 Karat Software Basic Instrument Training. We are ready to run an actual separation.

## Running A Sample

### 7.1 Overview

We will now use the method you prepared in the previous lesson to generate an electropherogram of Beckman Coulter Test Mix. We will discuss:

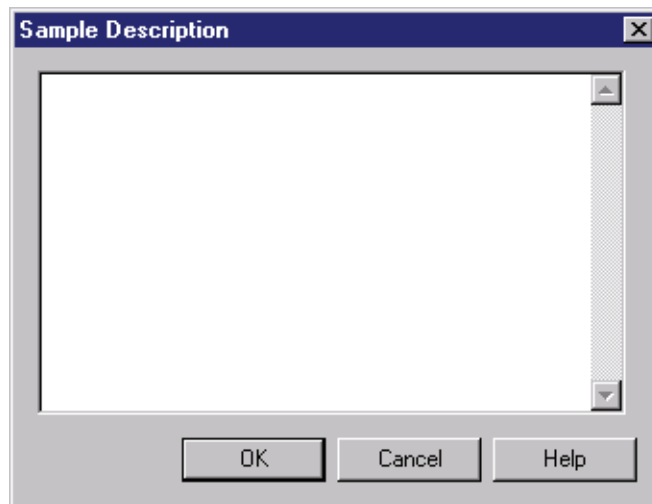
- Running a Single Sample
- Stopping / Aborting Method
- Data Display
- Skill Check

### 7.2 Running a Single Sample

Figure 7.1 Single Run Acquisition dialog

- Sample ID
- Method
- Data path
- Data file

- Description



**Figure 7.2 Sample Description dialog**

- Start

### **7.3 Stopping / Aborting Method**

- Stop Run
- Abort Run

## 7.4 Displaying Data

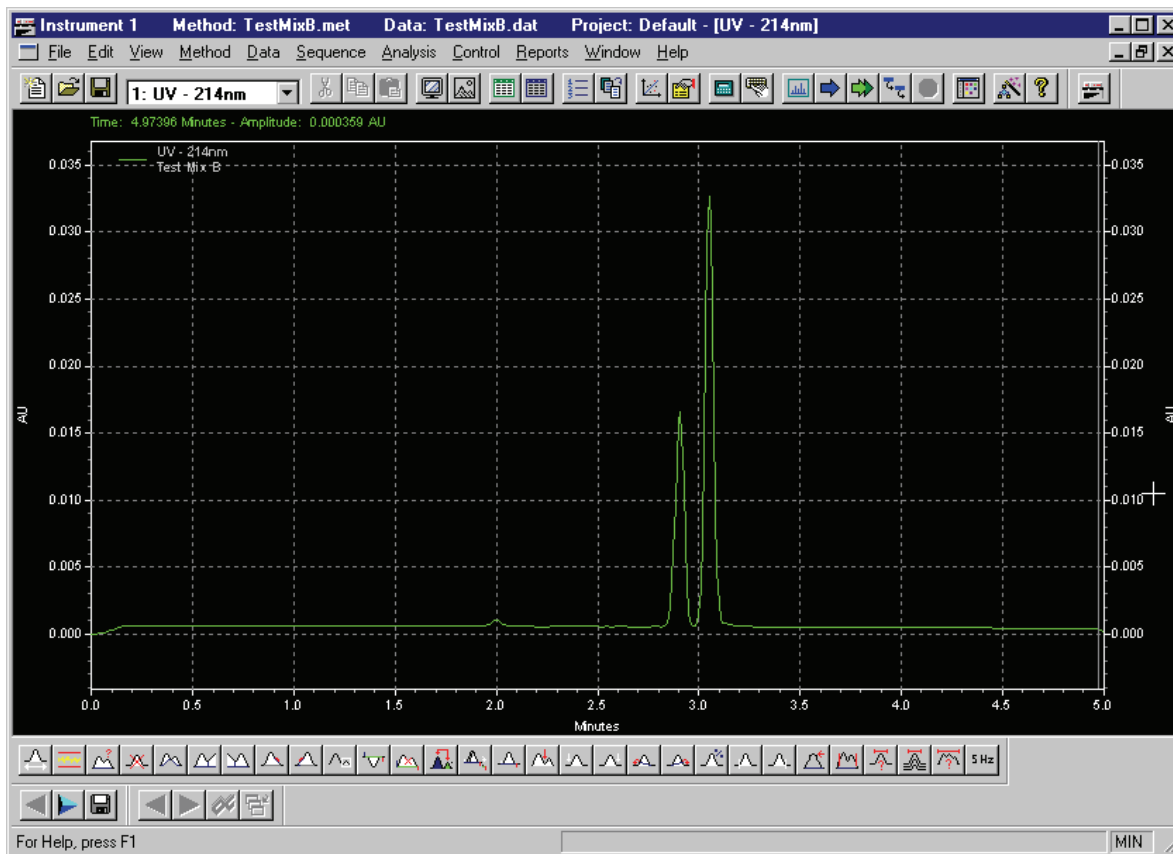


Figure 7.3 Instrument Window with *TestMixB.dat* open

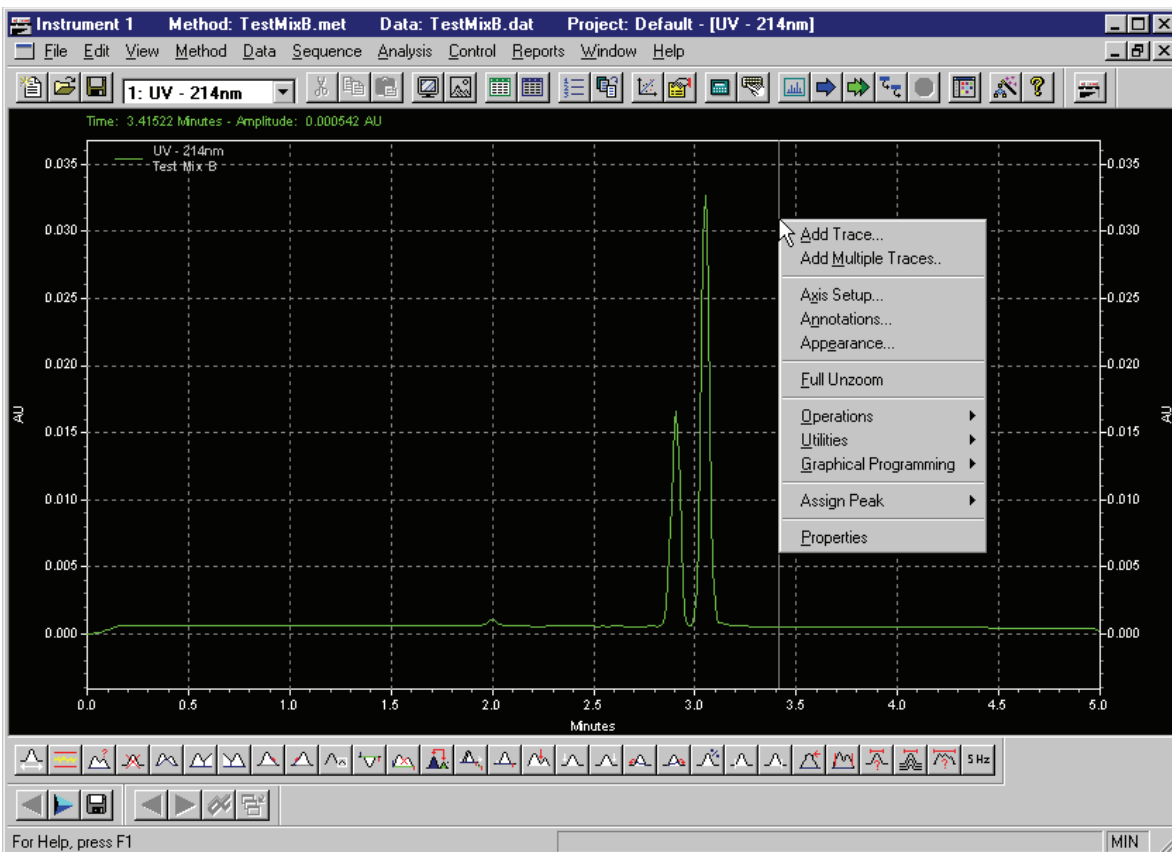


Figure 7.4 Instrument Window with data file open and right mouse click menu open

## Add Trace

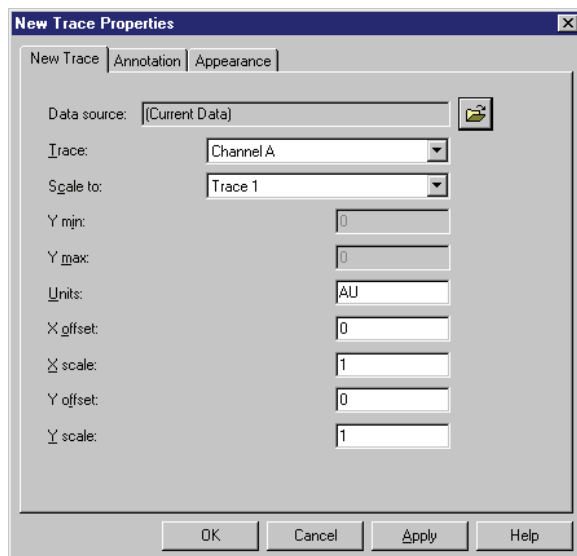


Figure 7.5 New Trace Properties dialog



- New Trace
- Annotation
- Appearance

### Add Multiple Traces

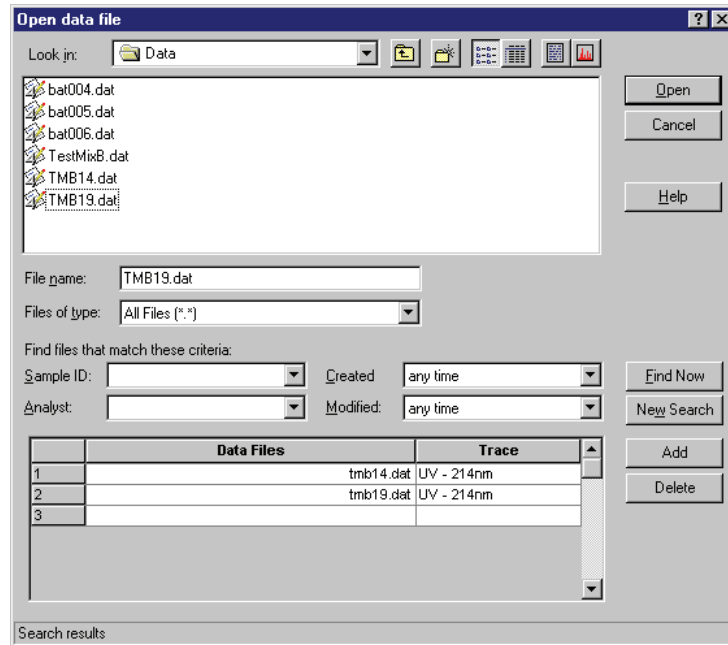


Figure 7.6 Open Data File dialog

## Axis Setup

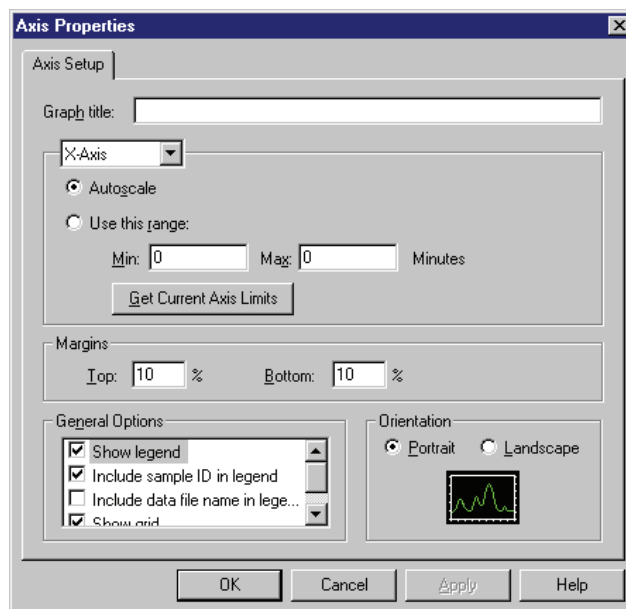


Figure 7.7 Axis Properties Setup dialog

- Axis Setup
- Graph Title
- Autoscale
- Range
- Margins
- General Options
- Orientation

## Annotations

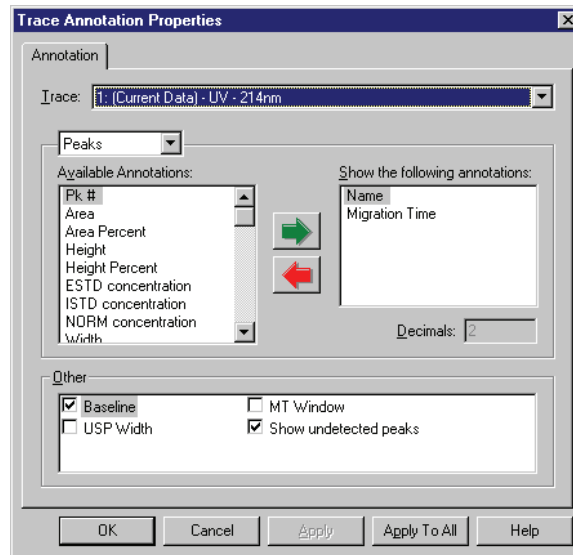


Figure 7.8 Trace Annotation Properties dialog

- Traces
- Available Annotations list box
- Other options

## Appearance

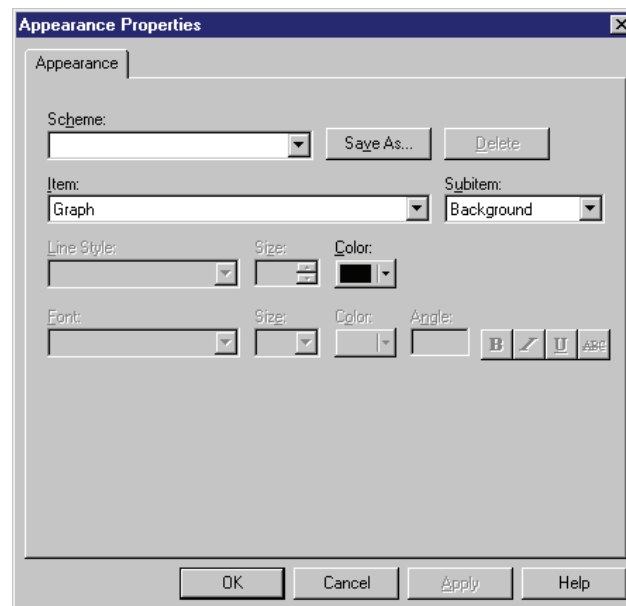


Figure 7.9 Appearance Properties dialog

- Scheme
- Line Style
- Item
- Font

## Full Unzoom

### Operations

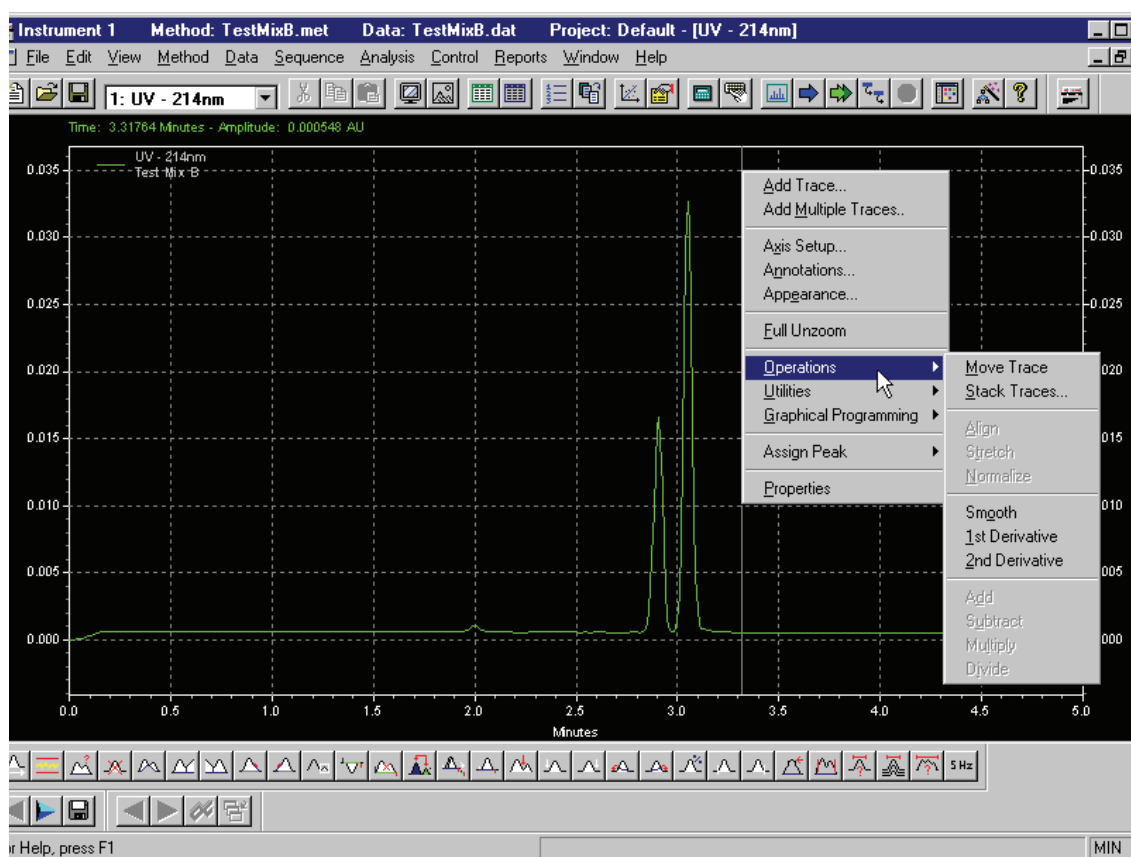


Figure 7.10 Operations Sub-menu

## Utilities

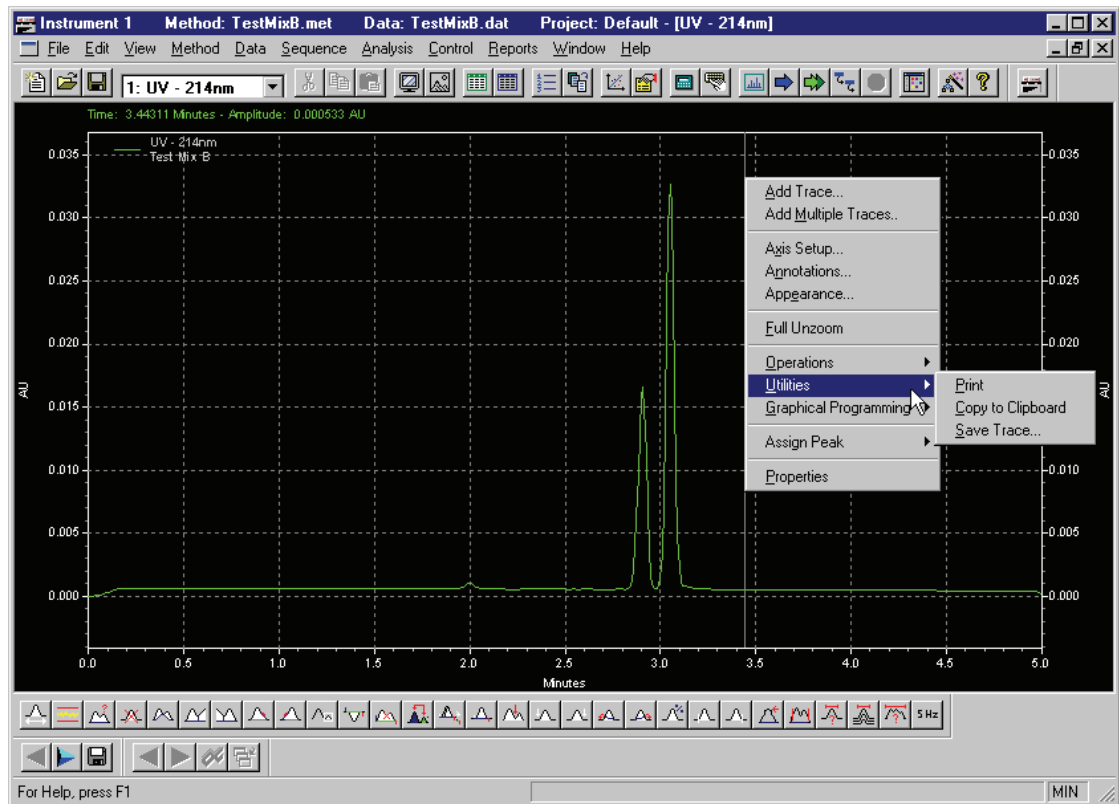


Figure 7.11 Utilities Sub-menu

## Properties

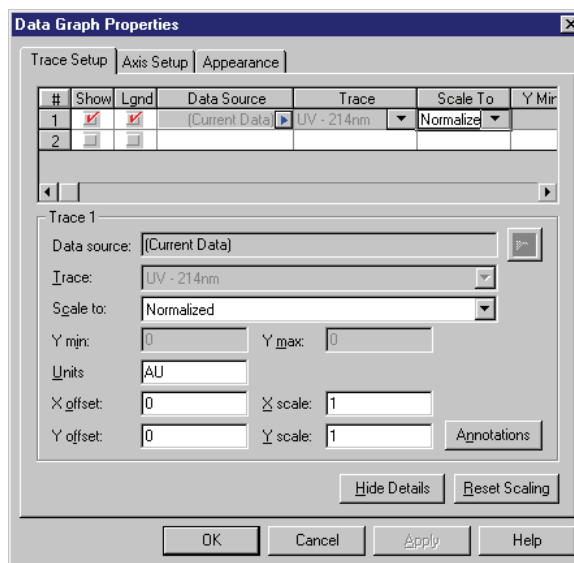


Figure 7.12 Data Graph Properties dialog

## 7.5 Skill Check

Upon completion of this section, you should be able to do the following:

1. Run the method `TestMixB.met`.
2. Zoom the display scale.
3. Auto zero from the status window.
4. Change the selections in the status window.
5. Save the data as `TestMixB.dat`.

### Summary

Congratulations! You have just generated your first electropherogram with your new P/ACE MDQ system. Next we will learn how to analyze the data.

## Analyzing and Integrating Data

### 8.1 Overview

Now that we have collected some actual run data, we will use the integration features of 32 Karat Software to begin analysis of the sample.

We will discuss:

- Opening data files
- Graphical integration events programming
- Defining and Naming Peaks
- Identifying Peaks based on Migration Time
- Identifying Peaks based on Mobility
- Annotation of the on-screen Display
- Skill Check

### 8.2 Opening Data Files

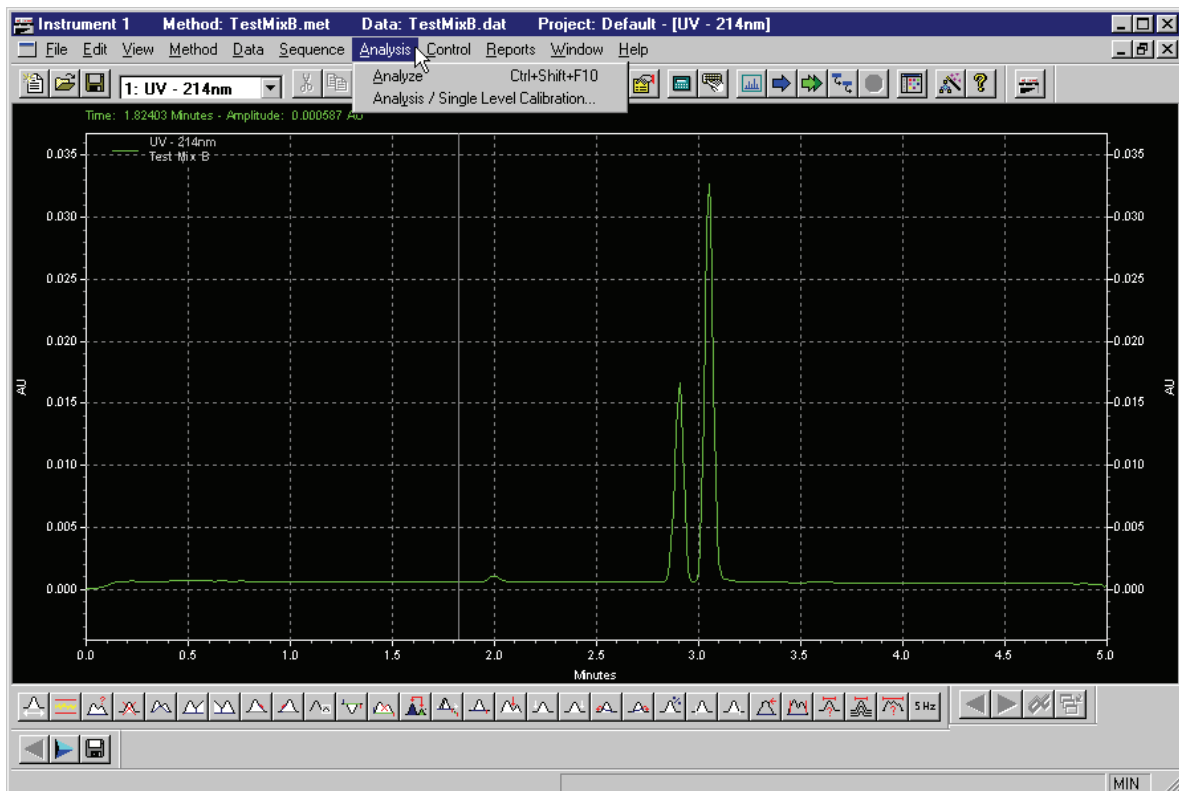


Figure 8.1 Instrument Window with data file open and Analysis menu selected



Figure 8.2 Analyze icon

## Graphical Programming

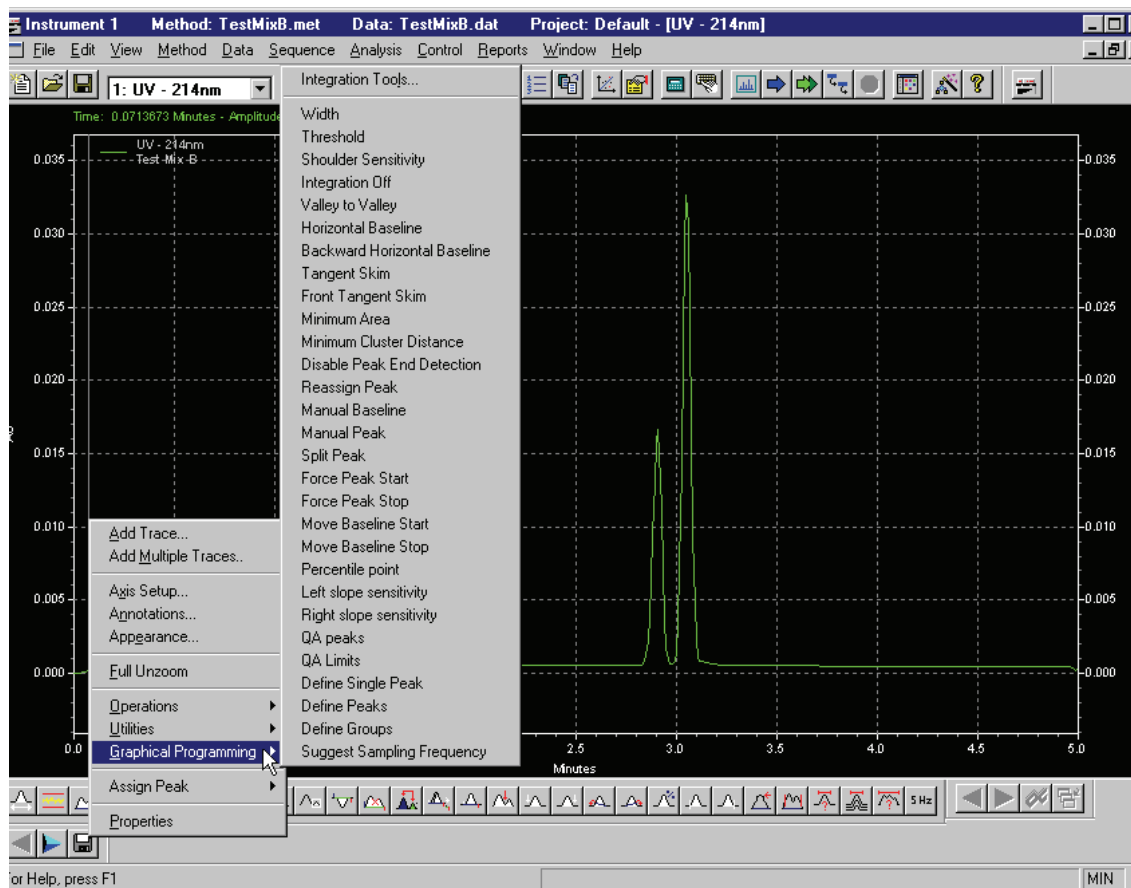


Figure 8.3 Graphical Programming Sub-menu

- Define Peaks



### Analyzed electropherogram

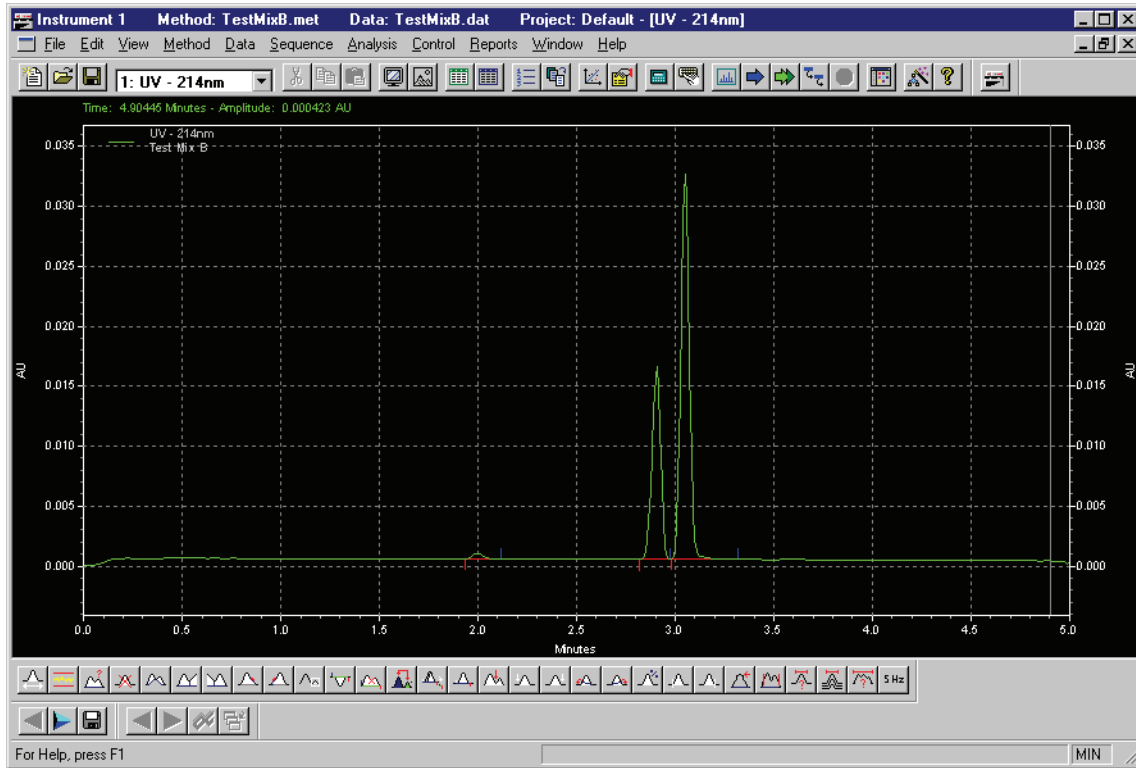


Figure 8.4 Instrument Window with an analyzed data file open

### 8.3 Optimizing Integration

The Integration Tool bar is located at the bottom of the Instrument window or, from the right mouse button-click menu and select Graphical Programming.



Figure 8.5 Integration Events Toolbar

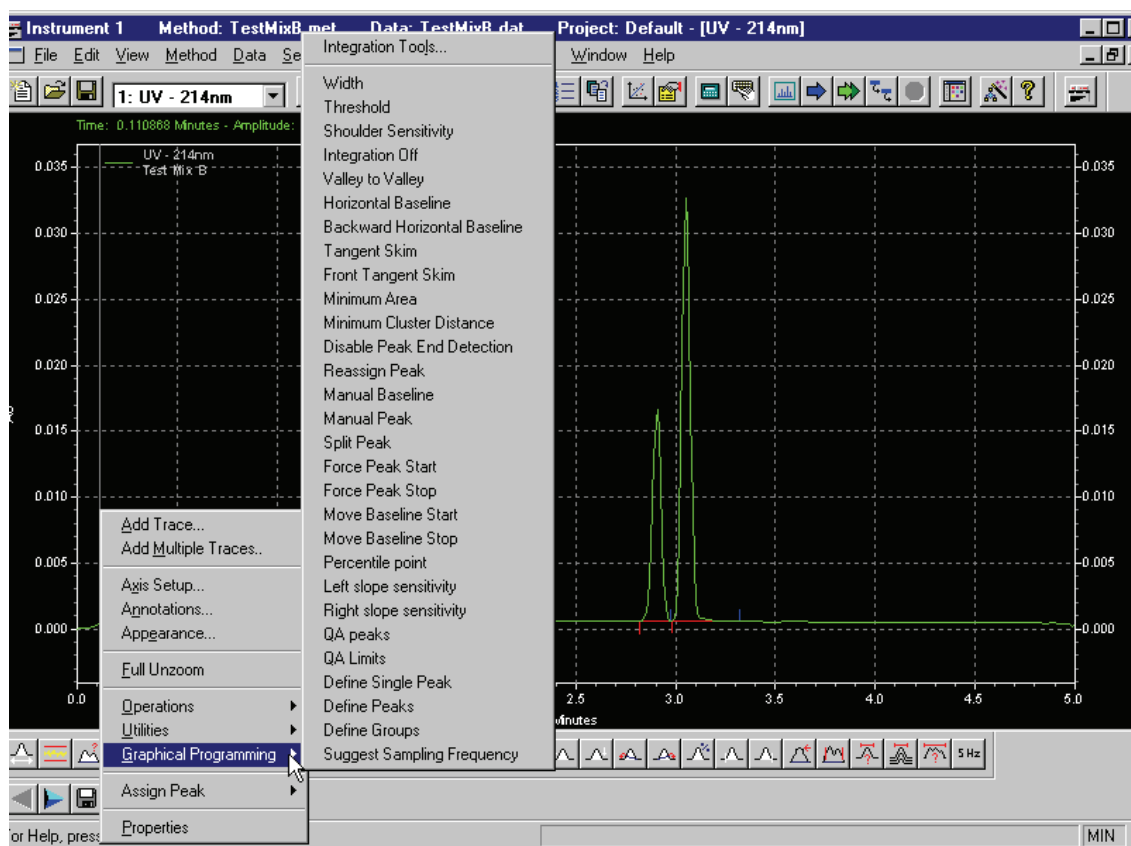


Figure 8.6 Instrument Window with right mouse click menu open and Graphical Programming selected

- Set Width
- Set Threshold
- Integration Off

- Manual Integration Fixes vs. Integration Events Table
- Valley to Valley
- Horizontal Baseline
- Backward Horizontal Baseline
- Tangent Skim
- Front Tangent Skim
- Minimum Area
- Negative Peak
- Disable Peak End Detection
- Reassign Peak
- Manual Baseline
- Manual Peak
- Split Peak
- Force Peak Start
- Force Peak Stop
- Move Baseline Start
- Move Baseline Stop
- Percentile Point
- Left Slope Sensitivity
- Right Slope Sensitivity
- Define Single Peak
- Define Peaks
- Define Groups

- ❑ Suggest Sampling Frequency

## 8.4 Defining and Naming Peaks

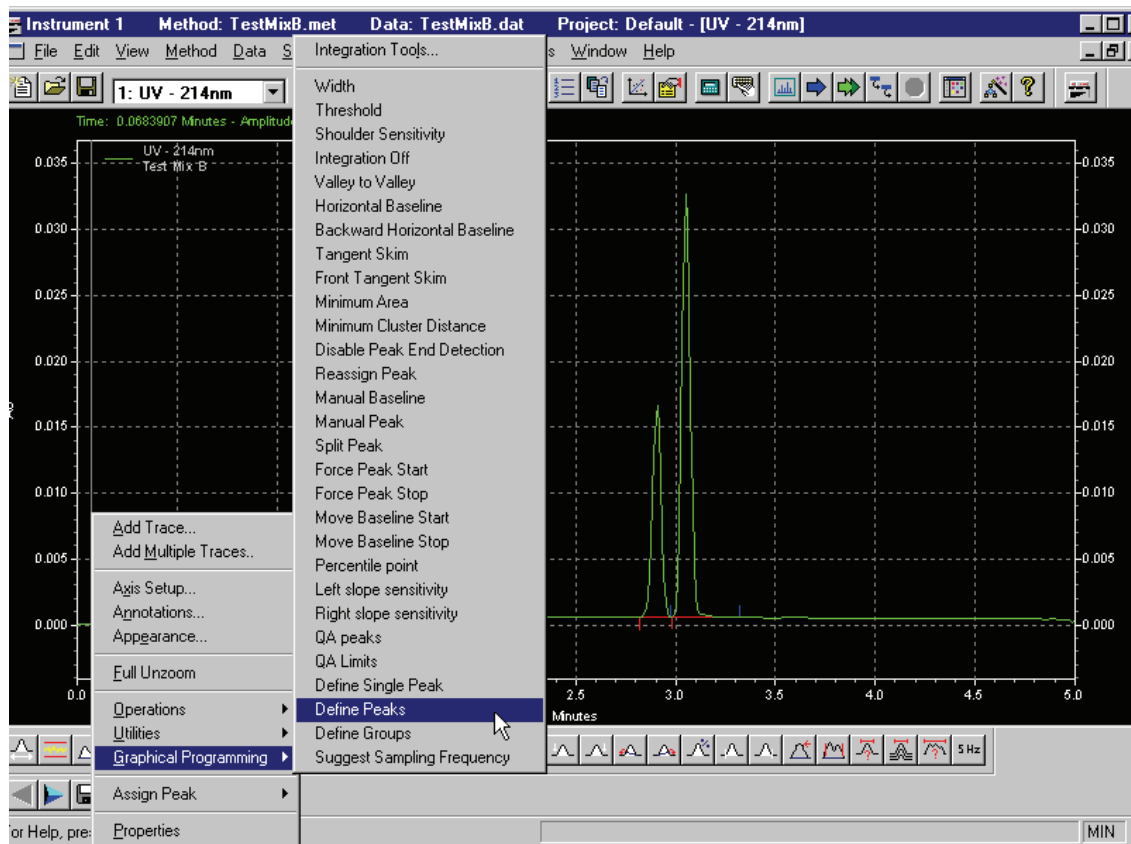


Figure 8.7 Instrument Window with Define Peaks selected

- ❑ Define Peaks



Figure 8.8 Define Peaks icon

- ❑ Select Start of Named Peak Range
- ❑ Select End of Named Peak Range

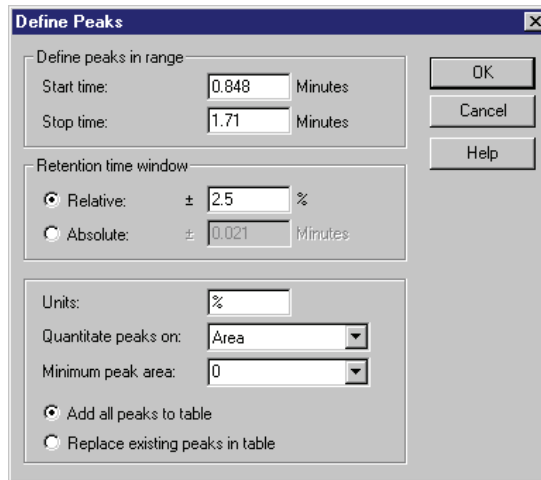


Figure 8.9 Define Peaks dialog

- Define peaks in range
- Retention time window
- Units
- Quantitate on Area or Height

### Identifying Peaks based on Migration Time

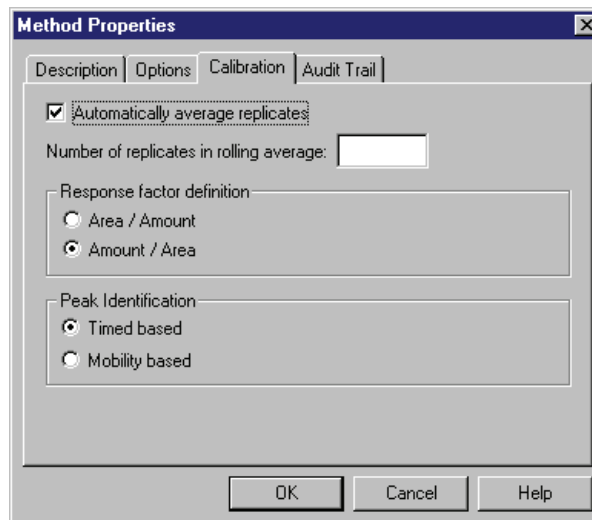


Figure 8.10 Method Properties dialog

- Defining Peaks
- Viewing Peak ID Table

The screenshot shows a software window titled "Instrument 1" with a menu bar (File, Edit, View, Method, Data, Sequence, Analysis, Control, Reports, Window, Help) and a toolbar. Below the toolbar is a "Named Peaks" tab with a "Groups" sub-tab. The main area contains a table with the following data:

#	Name	ID	Mig. Time	MT Window	Ref. ID #	ISTD. ID #	Units	Mobility Marker	N
1	OH Benzoate	1	2.90833	0.145417	2	0	ug/ml		
2	OH Phenylacetic Acid	2	3.05		4	2	0 ug/ml		
3									

Below the table is a large empty area and a toolbar with various icons. At the bottom, there is a status bar with the text "For Help, press F1" and a "MIN" button.

Figure 8.11 Peak ID Table

- Enter peak names in Peak ID Table

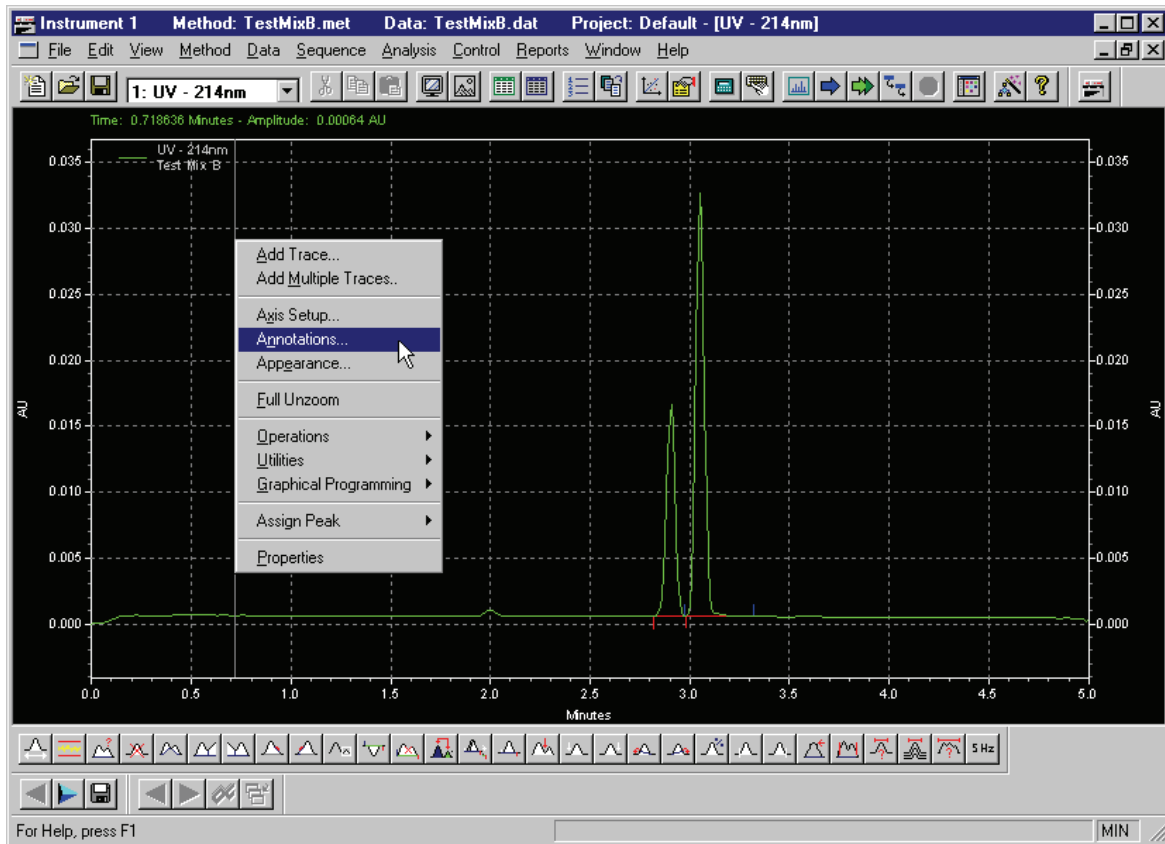


Figure 8.12 Instrument Window with the right mouse click menu and Annotations highlighted

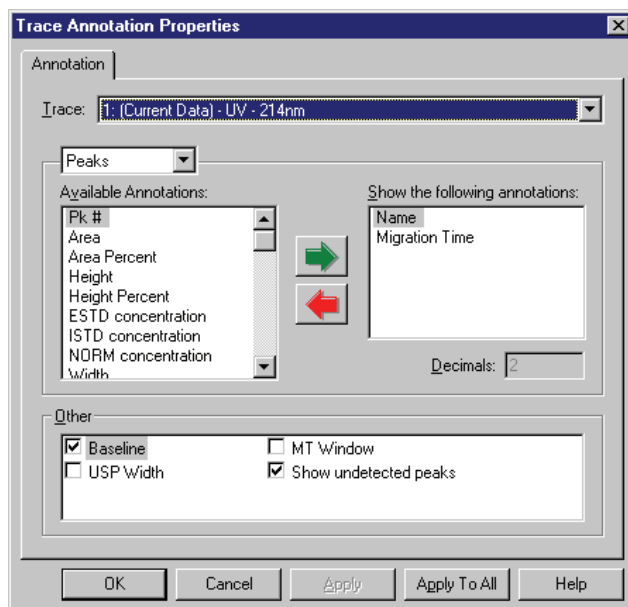


Figure 8.13 Trace Annotation Properties dialog

- Annotation of on-screen display

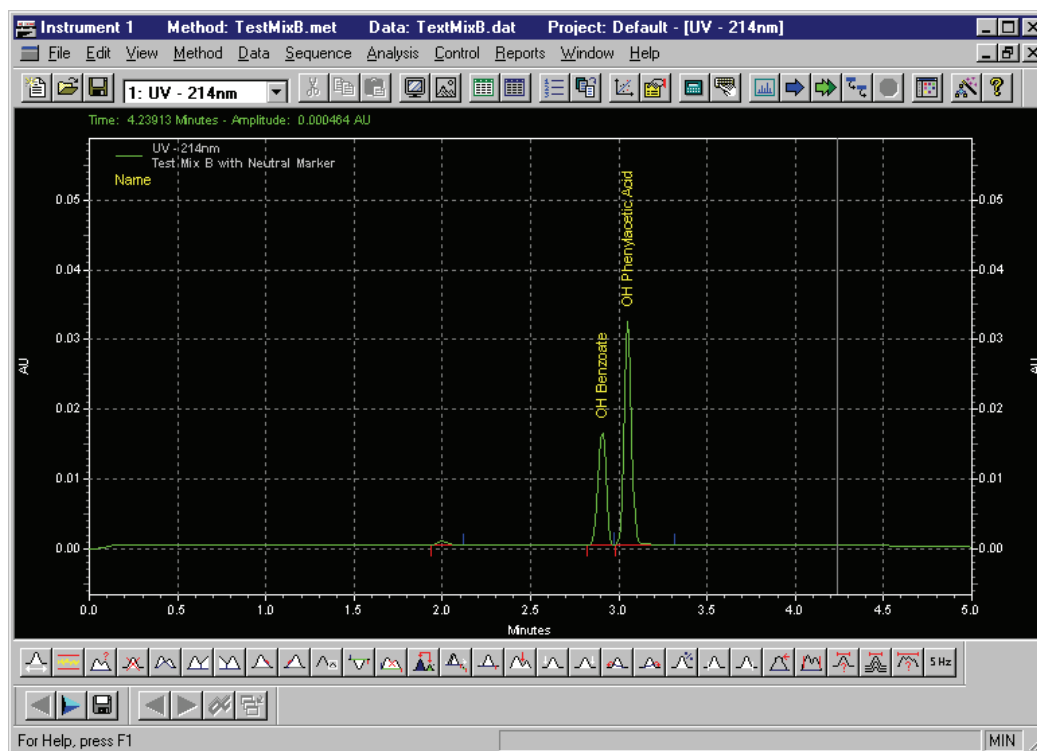


Figure 8.14 Data Display with Annotations for Time-Based Peak Identification



### Identifying Peaks based on Mobility

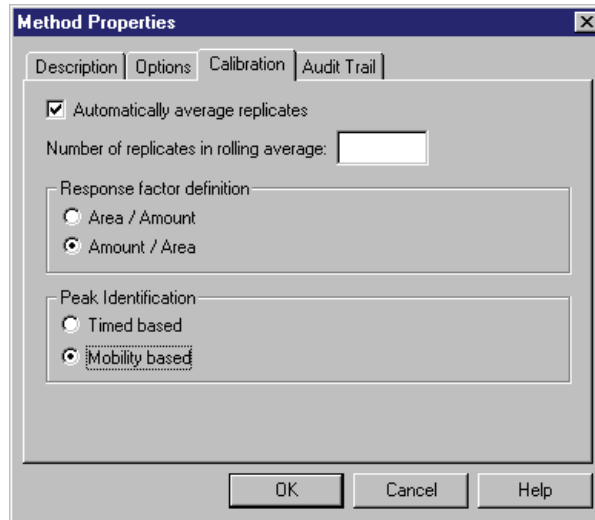


Figure 8.15 Method Properties dialog

### Defining Peaks

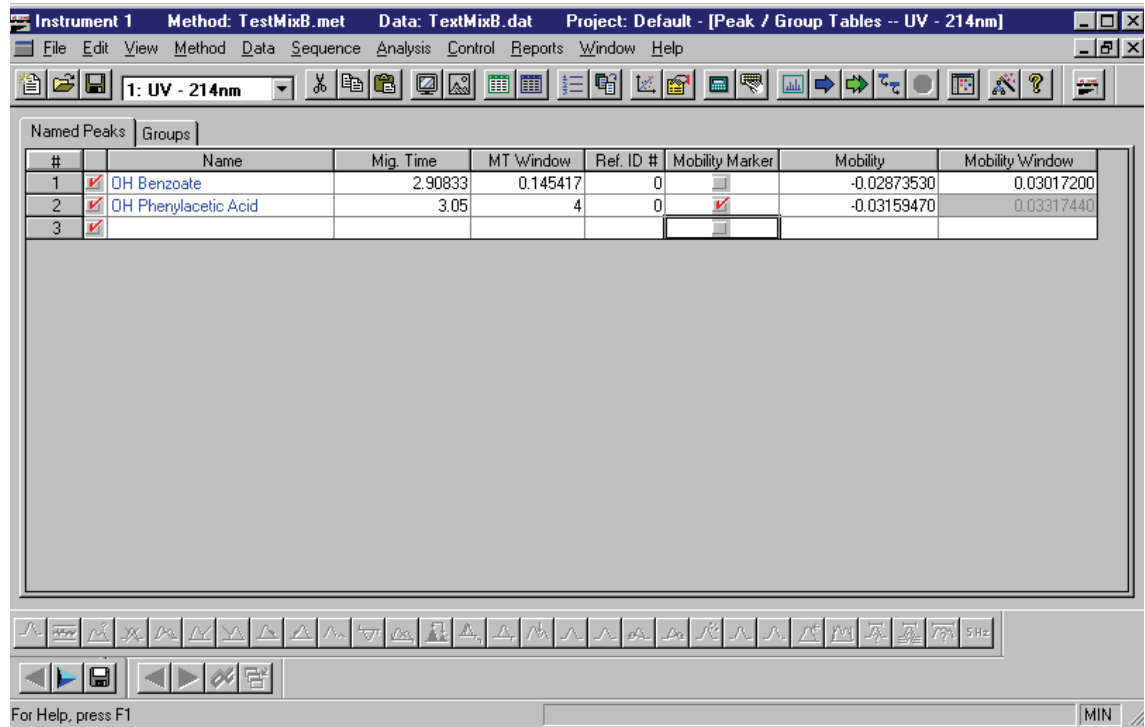


Figure 8.16 Peak ID Table with Mobility Marker selected

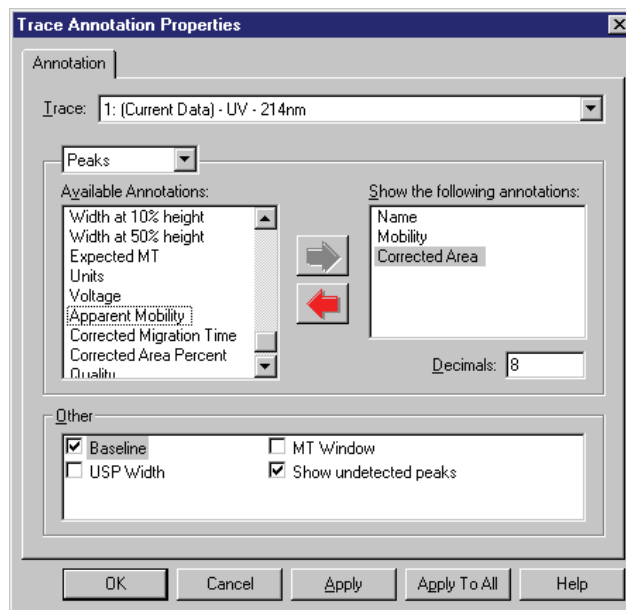


Figure 8.17 Trace Annotations Properties dialog

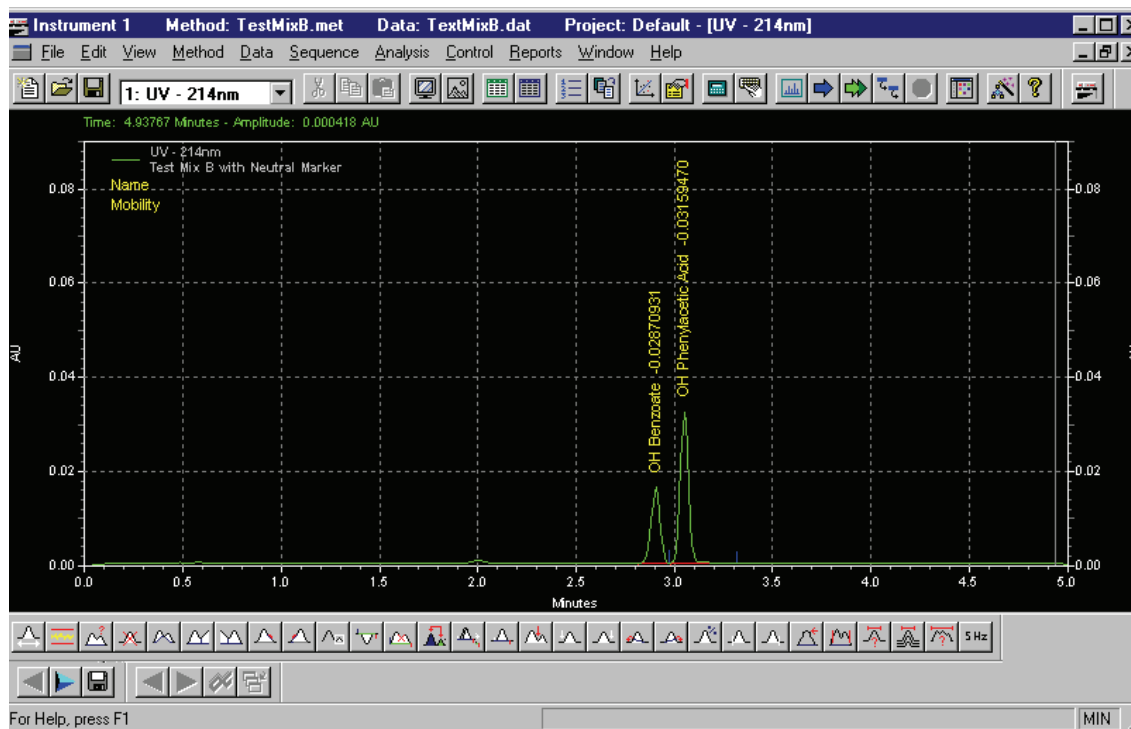


Figure 8.18 Data Display with Annotations for Mobility - Based Peak identification

## 8.5 Skill Check

Upon completion of this section, you should be able to do the following:

1. Open the `Test Mix B.dat` data file.
2. After data collection, add a **Peak ID Table** to identify the two peaks.
3. Analyze the data.
4. Set the peak width and threshold to obtain acceptable integration of both peaks.
5. Build a table to name the peaks. (The elution order is Benzoic acid and then Phenyl acetic acid.)
6. Make sure **Time based** is selected in the **Options** tab of the Method Properties dialog.
7. Set the parameters in the **Peak ID** table to identify peaks based on migration time.
8. Analyze the data and apply annotations to show names, migration times and corrected areas on the on-screen electropherogram display.
9. Change the selection in the **Options** tab to **Mobility based**.
10. Change the parameters in the **Peak ID** table to identify peaks based on mobility.
11. Reanalyze the data.
12. Apply the appropriate annotations to the data display.

### Summary

This completes the Analysis and Integration portion of the Basic Instrument Training. Be sure to come back and explore all the various integration and peak identification options to find the ones that best suit your own work.

Next we will automate groups of consecutive runs using Sequence Tables.



## Using Sequence Tables

### 9.1 Overview

In this section we will further automate the system by defining a sequence of methods and samples to run unattended. This is accomplished using a Sequence Table. We will discuss:

- Sequence Wizard
- Editing Sequence Tables
- Saving Sequence Tables
- Running Sequence Tables

### 9.2 Using the Sequence Wizard

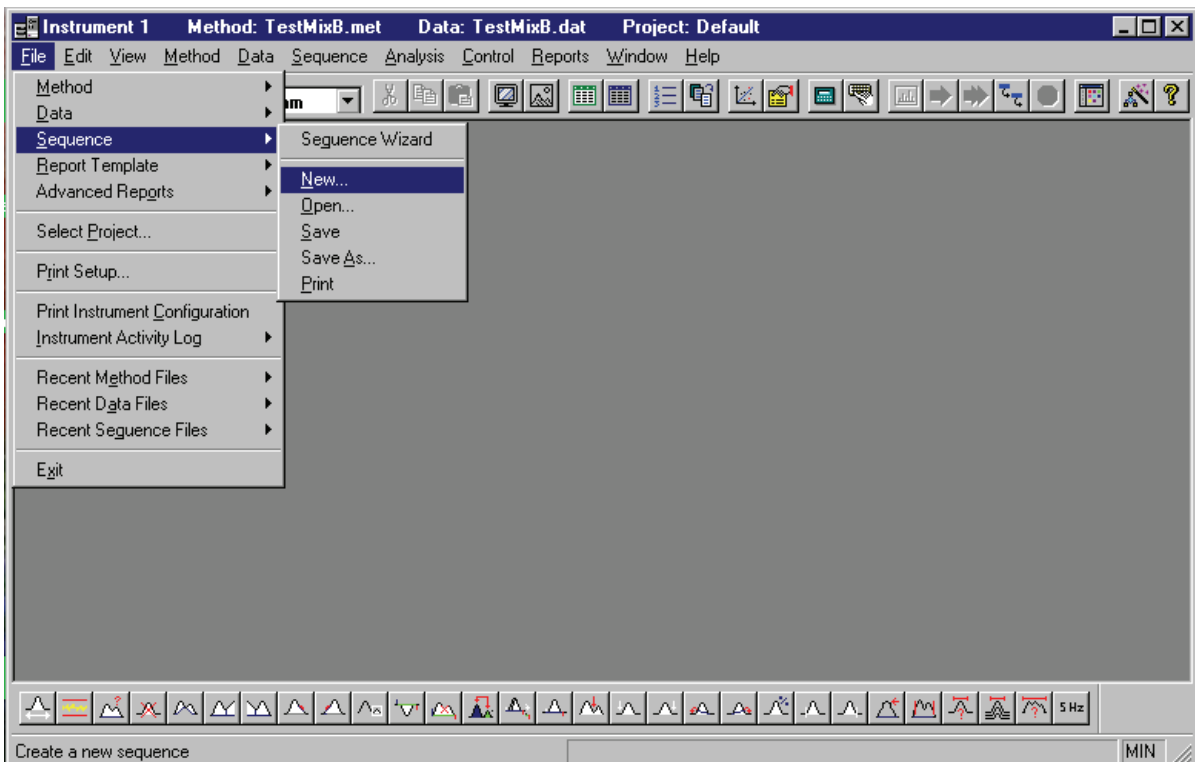


Figure 9.1 Instrument Window with File | Sequence | New selected

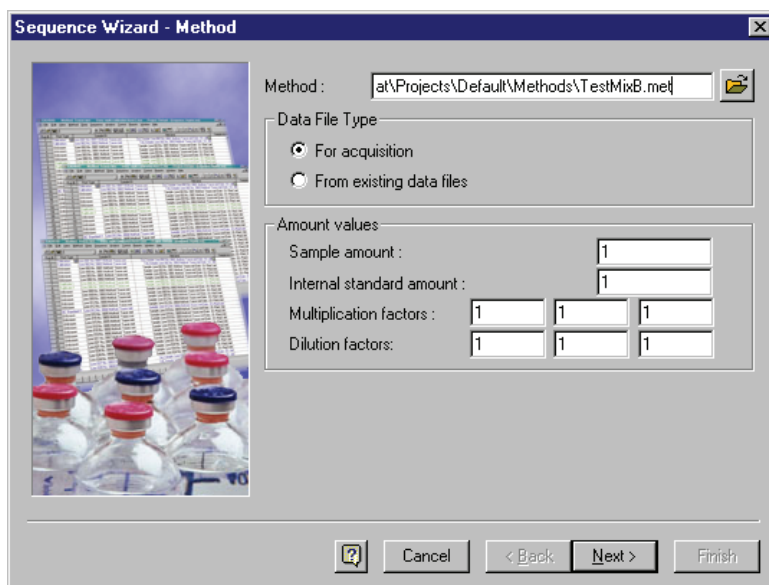


Figure 9.2 Sequence Wizard - Methods dialog

- Method Information
- Data File Type
- Amount values

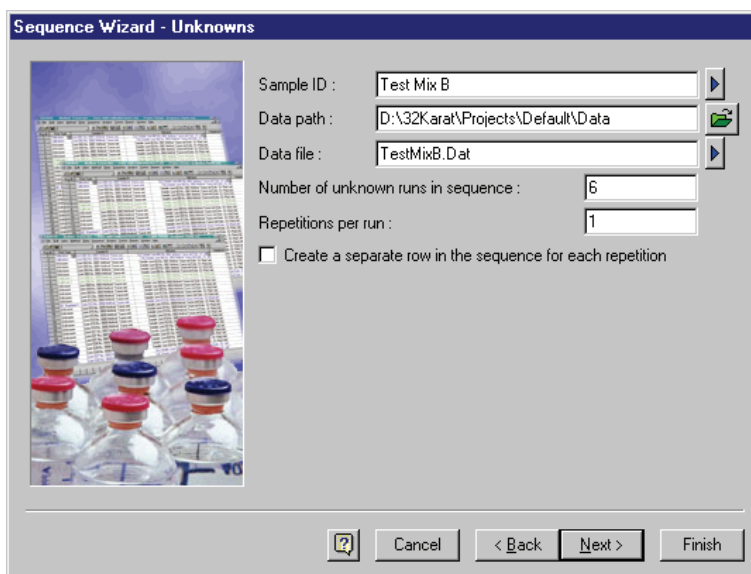


Figure 9.3 Sequence Wizard - Unknowns dialog

- Information about unknown and data file

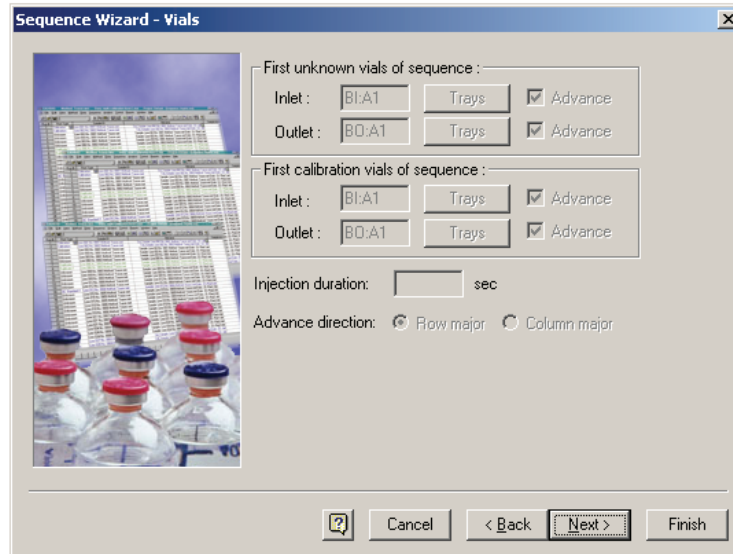


Figure 9.4 Sequence Wizard - Vials dialog

- Information about vials

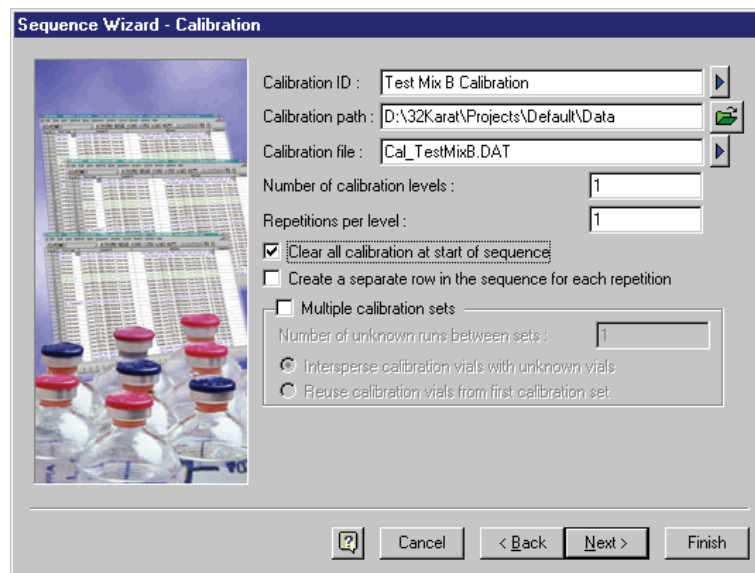
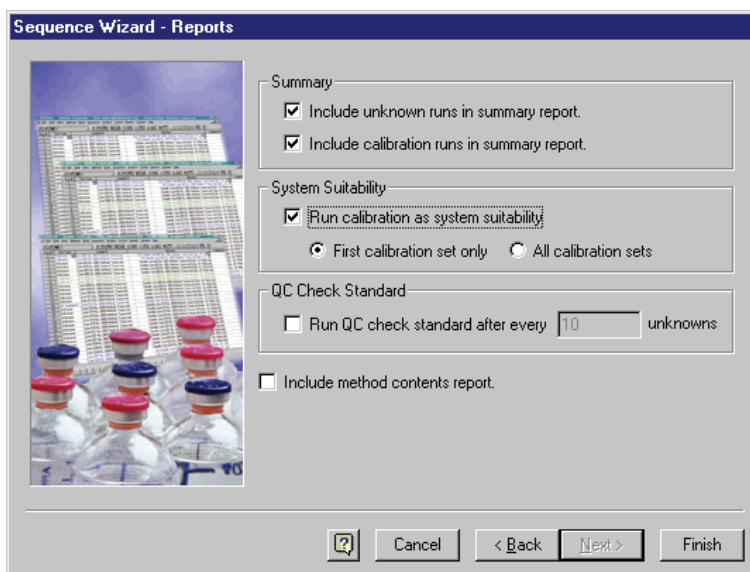


Figure 9.5 Sequence Wizard - Calibration dialog

- Calibration Information



**Figure 9.6 Sequence Wizard - Reports dialog**

- Reports Information
- Summary
- System Suitability
- QC Check Standard



### 9.3 Viewing a Sequence

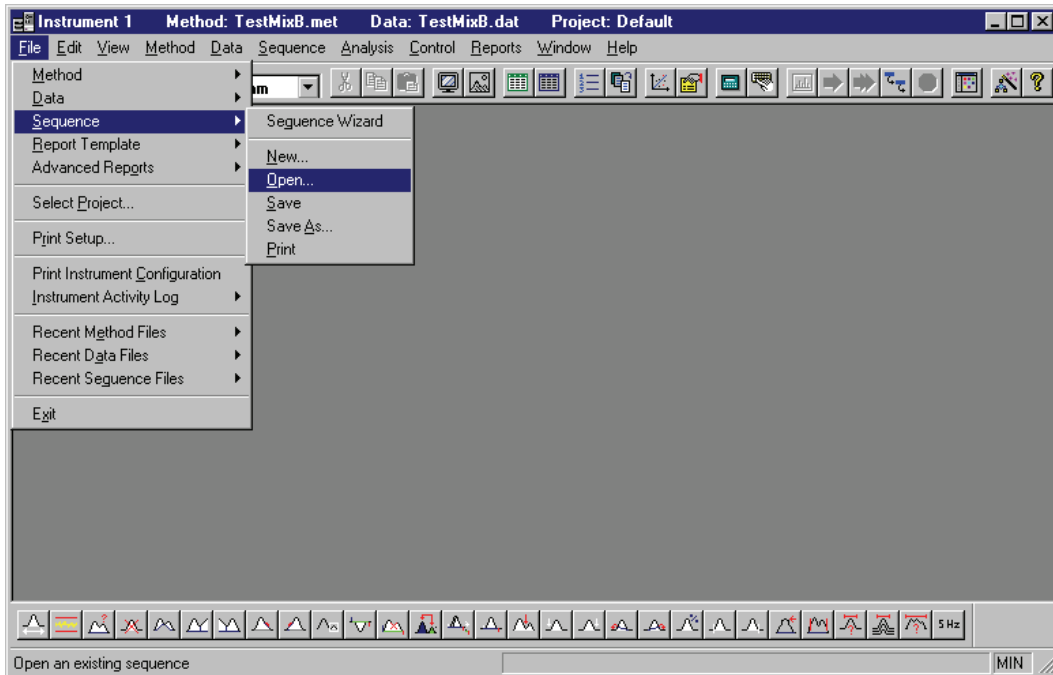


Figure 9.7 Instrument Window with File | Sequence | Open selected

The screenshot shows the Instrument software interface with a sequence table displayed. The title bar indicates 'Instrument 1', 'Method: TestMixB.met', 'Data: TestMixB.dat', and 'Project: Default - [Sequence: Tbatch.seq]'. The 'Sequence' menu is open, and '1: UV - 214nm' is selected. The table below shows the sequence details.

Run #	Status	Run Type	Level	Conc Override	Reps	Sample Inject Inlet	Sample Inject Outlet	Sample Inject Duration	Other Inject
1		Summary Begin		0 n/a	1	SI:A1	BO:A2	10	
2		Summary Run		0 n/a	1	SI:A1	BO:A2	10	
3		Summary Run		0 n/a	1	SI:A1	BO:A2	10	
4		Summary Run		0 n/a	1	SI:A1	BO:A2	10	
5		Summary Run		0 n/a	1	SI:A1	BO:A2	10	
6		Summary End		0 n/a	1	SI:A1	BO:A2	10	
7									

Figure 9.8 Sequence Table

- Status
- Run Type

## Using Sequence Tables

### *Viewing a Sequence*

Clear All Calibration	Begin Summary
Clear Calibration at Level	Summary Run
Print Calibration Report	End Summary
Average Replicates	Vial Summary
Clear Replicates	QC Check Standard
Begin Loop	Unspiked
End Loop	Spiked
Shutdown	Spike 1 of 2
Print Additional Reports	Spike 2 of 2
Begin System Suitability	Duplicate
System Suitability Standard	Begin Calibration
End System Suitability	End Calibration

- Level
- Concentration Override
- Repetitions
- Sample ID
- Method
- Filename
- Sample Amount
- ISTD Amount
- Multiplier
- Action
- Description

## 9.4 Editing a Sequence

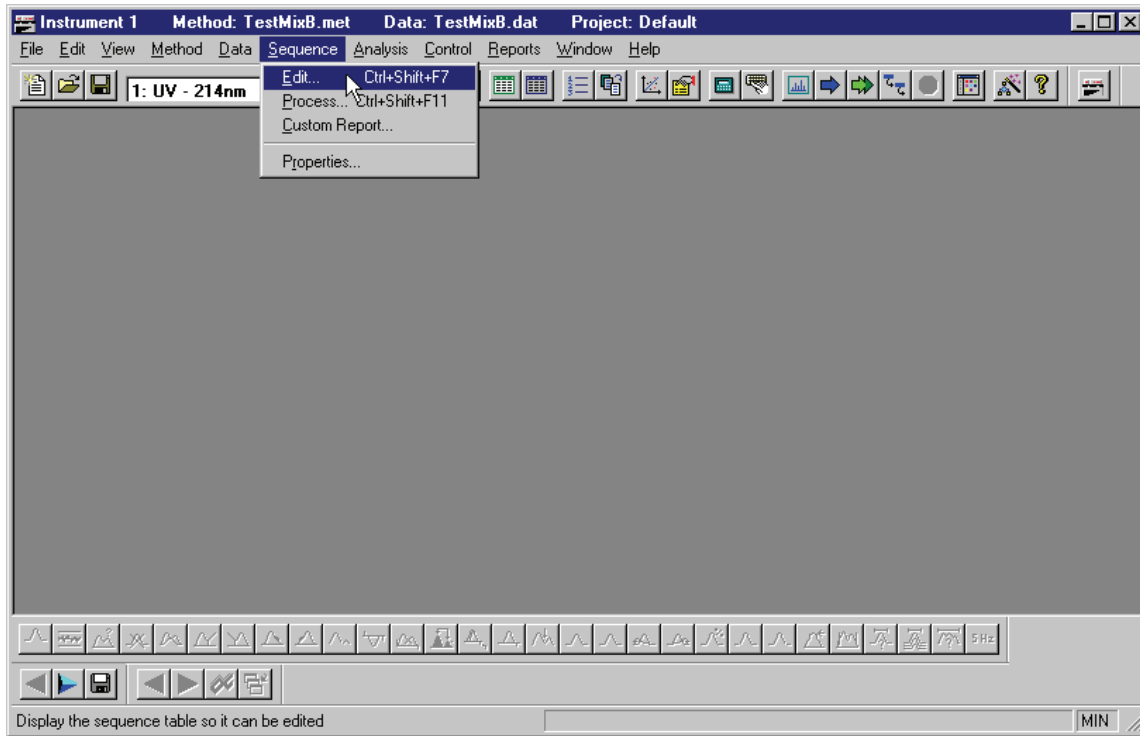


Figure 9.9 Instrument Window with Sequence | Edit selected



Figure 9.10 Edit Sequence icon

## 9.5 Saving a Sequence

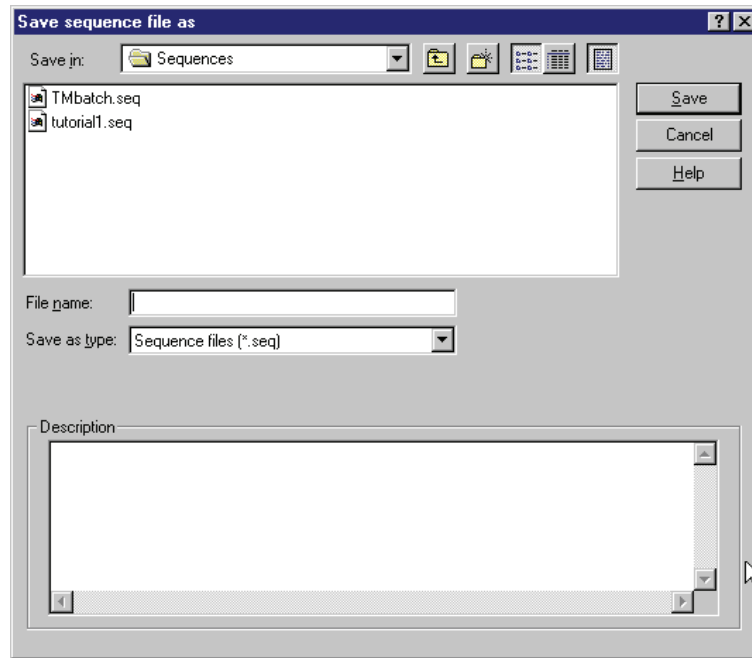


Figure 9.11 Saving Sequence dialog

- Save Sequence
- Save Sequence As

## 9.6 Running a Sequence

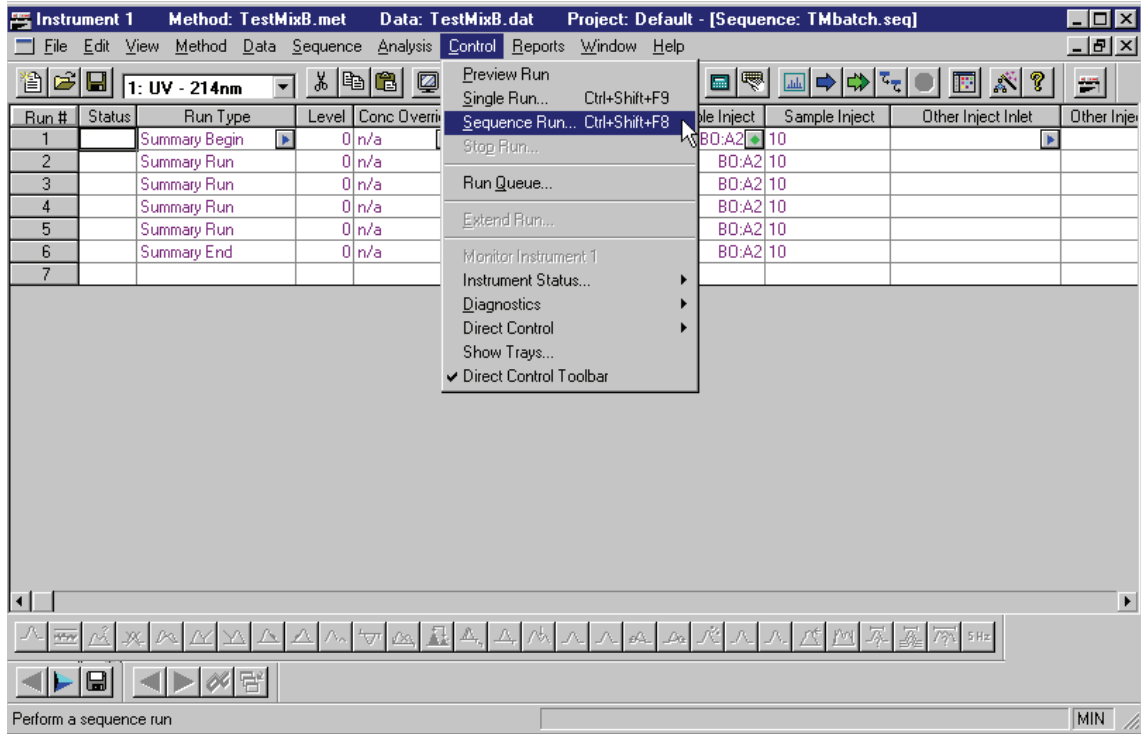


Figure 9.12 Instrument Window with Control | Sequence Run selected



Figure 9.13 Sequence Run icon

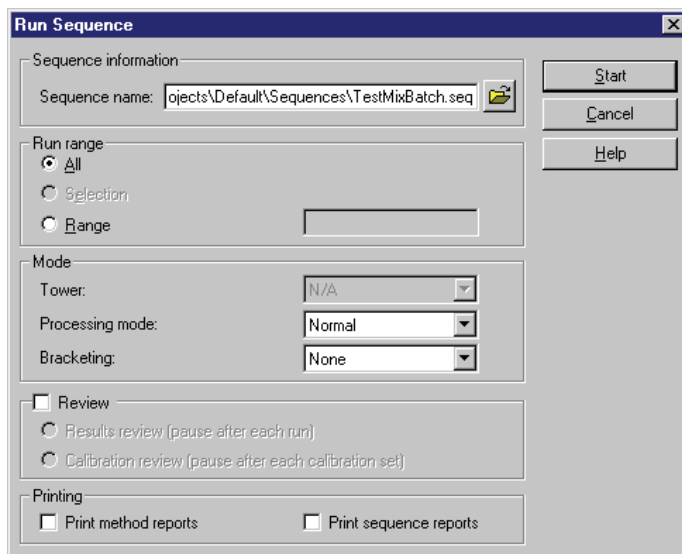


Figure 9.14 Run Sequence dialog

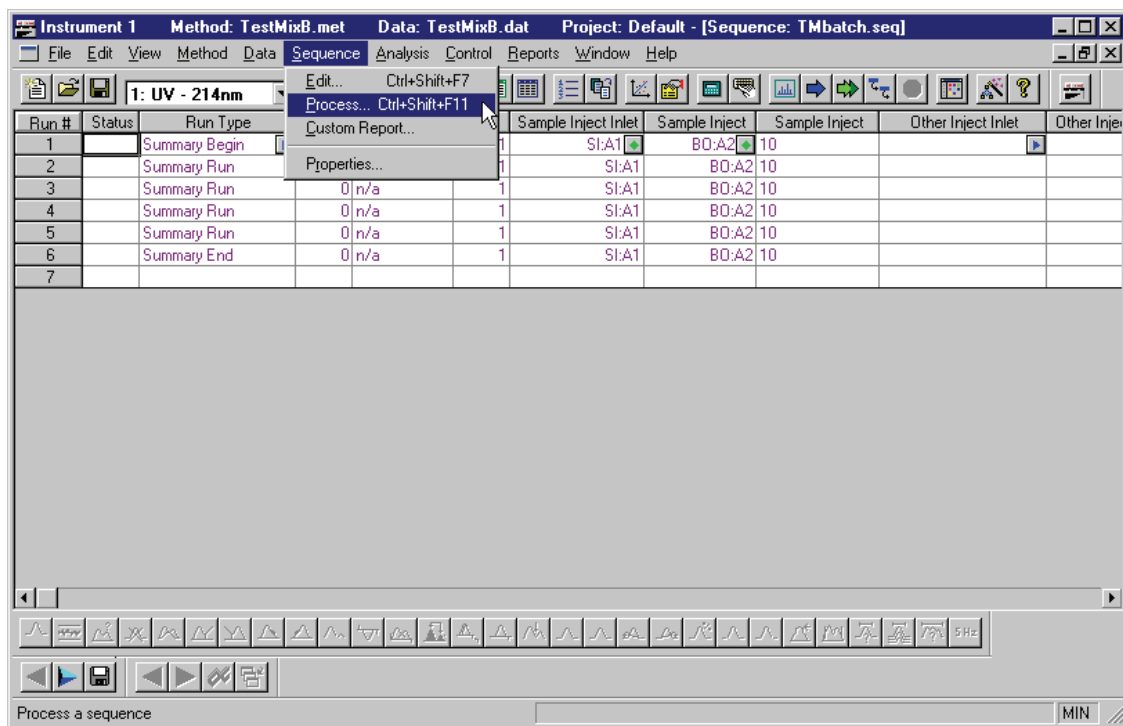


Figure 9.15 Instrument Window with Sequence | Process selected

Process

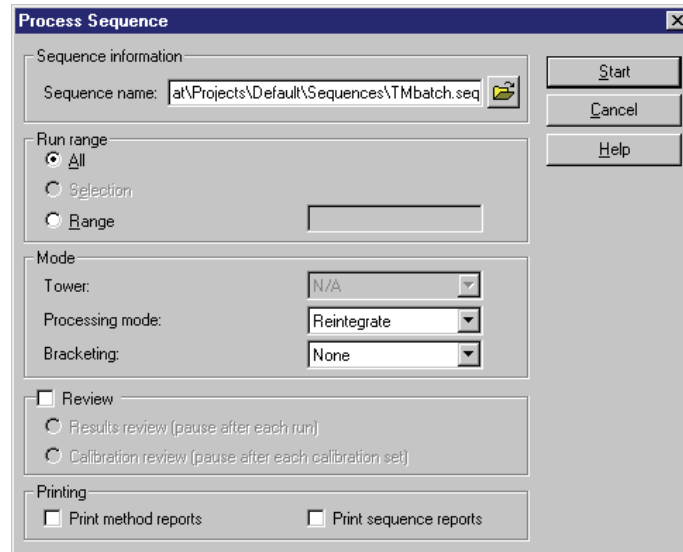


Figure 9.16 Process Sequence dialog

- Sequence Information
- Run Range
- Mode
- Review
- Printing

## 9.7 Skill Check

Upon completion of this section, you should be able to do the following:

1. Run the same method (TestMixB.met) three times.
2. Specify sample vial SI:A1 as the sample for line 1, vial SI:F10 as the sample for line 2 and vial SI:C8 as the sample for line 3.
3. Specify sequential file names for the data.
4. Do NOT run the sequence table at this time.

### Summary

This completes the Sequence portion of the 32 Karat Software Basic Instrument Training. We can now automate running and processing the data of multiple samples.

In the next section we will take a look at the steps necessary to automatically generate and apply calibration data.



## Creating Calibrations

### 10.1 Overview

The Peak ID and Sequence Tables have entry columns that we have not yet discussed. These parameters are used for generating and updating the calibration data for a given method. To generate a calibration curve we will:

- Edit a Peak ID Table for calibration
- Create a Calibration Sequence Table
- Run a Single Level Calibration Sequence
- Review Calibration Curves
- Final Skill Check

### 10.2 Editing the Peak ID Table

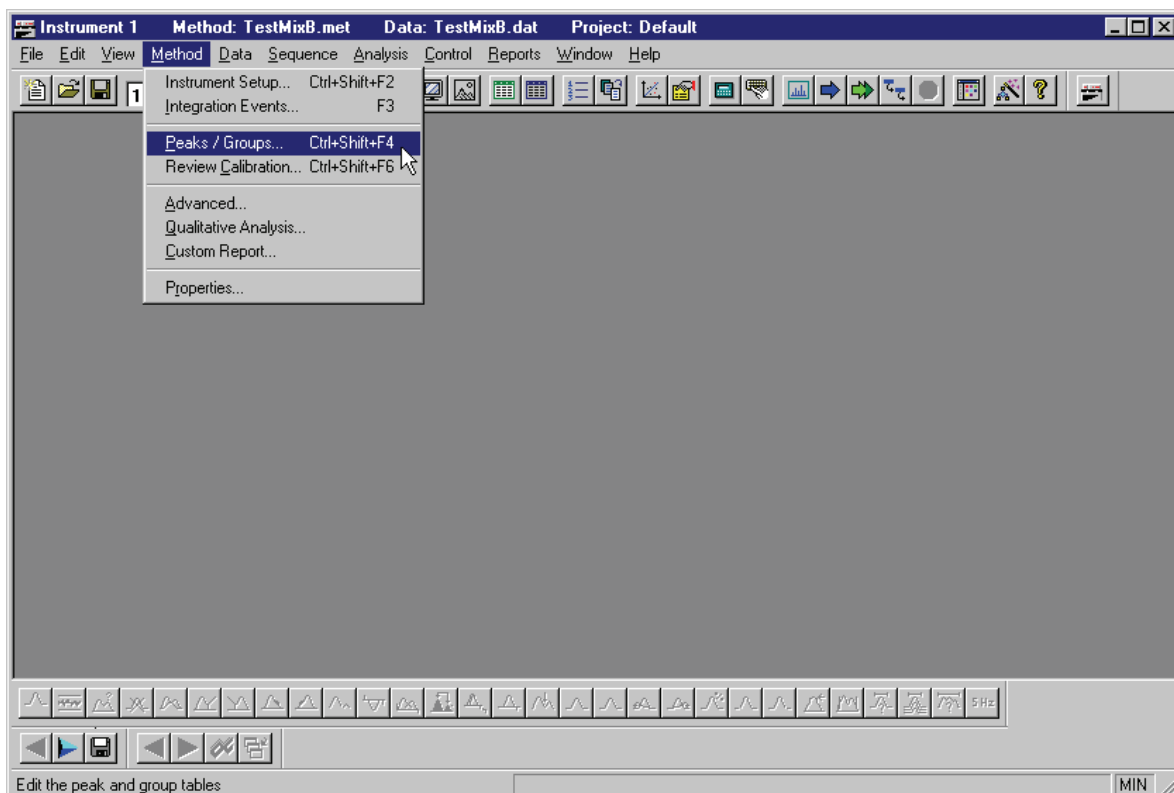
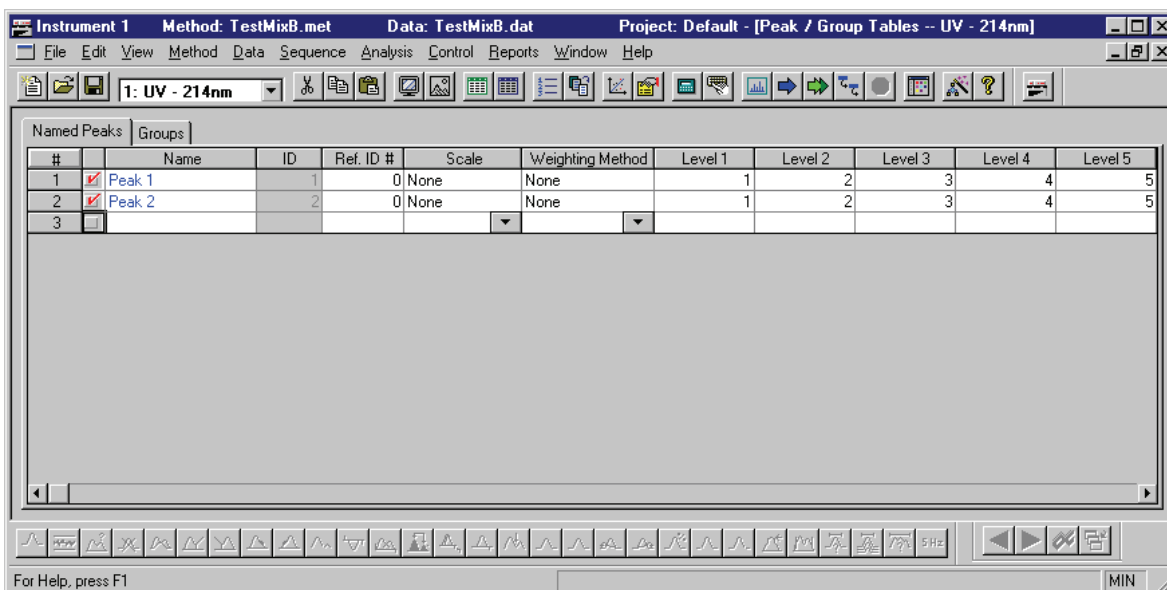


Figure 10.1 Instrument Window with Method | Peaks | Groups selected



**Figure 10.2 Peak ID Table set for Calibration**

- Properties - Select parameters

**Parameter Options**

Name	Weighting Method
ID	10 Levels
Ref ID #	STD ID #
ISTD ID #	STD Mult.
Units	Low Conc
Analysis Channel	High Conc
Quantitate	Check Std 1 Conc
Fit Type	Check Std 1%RD
Zero	Spike 1 Amount
Calib Flag	Spike 2 Amount
Calib Weight	Dup %RD Limit
% Calib Margin	RF %RSD Limit
Scale	

### 10.3 Creating a Calibration Sequence with the Sequence Wizard

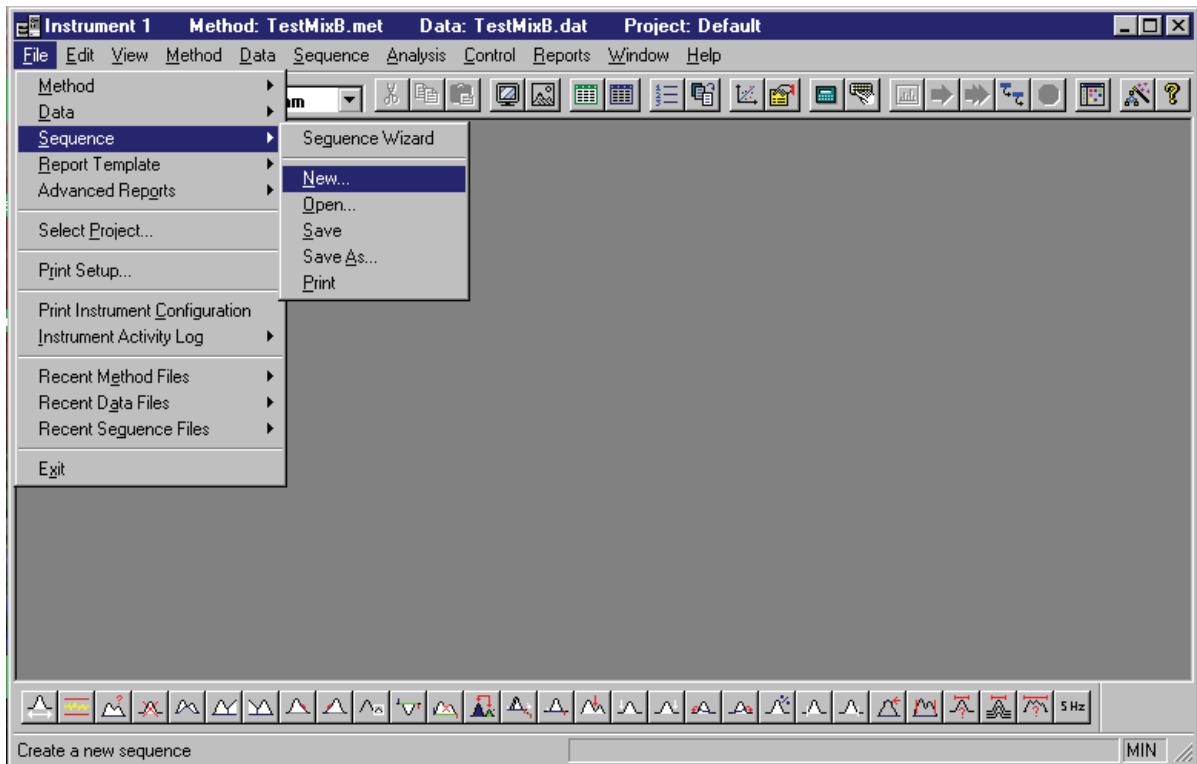


Figure 10.3 Instrument Window with File | Sequence | New selected

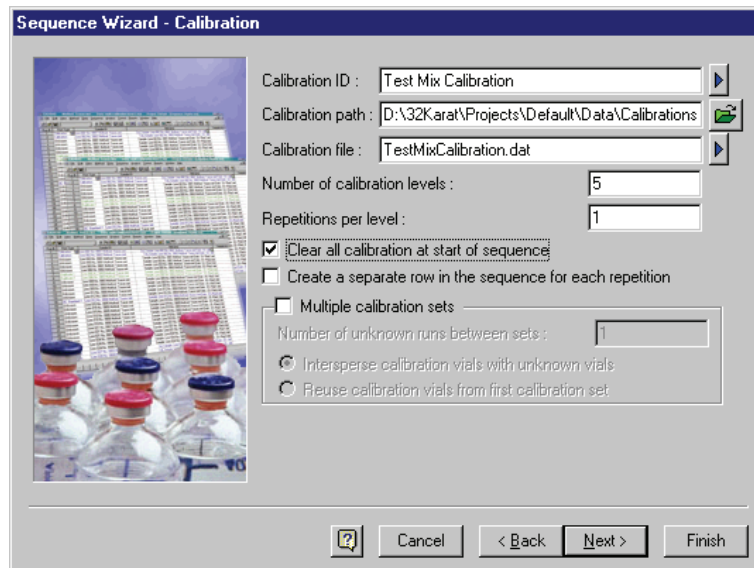


Figure 10.4 Sequence Wizard - Calibration dialog

- Calibration ID
- Calibration Path

## Creating Calibrations

### Creating a Calibration Sequence with the Sequence Wizard

- Calibration file
- Number of levels
- Number of Repetitions per level

Run #	Status	Run Type	Level	Reps	Sample ID	Method	Filename
1	Completed	CAL CCA	1	1	Test Mix Calibration	TestMixB.met	TestMixCalibration1.dat
2	Completed	Calibration	2	1	Test Mix Calibration	TestMixB.met	TestMixCalibration2.dat
3	Completed	Calibration	3	1	Test Mix Calibration	TestMixB.met	TestMixCalibration3.dat
4	Completed	Calibration	4	1	Test Mix Calibration	TestMixB.met	TestMixCalibration4.dat
5	Completed	Calibration	5	1	Test Mix Calibration	TestMixB.met	TestMixCalibration5.dat
6							

Figure 10.5 Completed Sequence

## 10.4 Running a Calibration Sequence

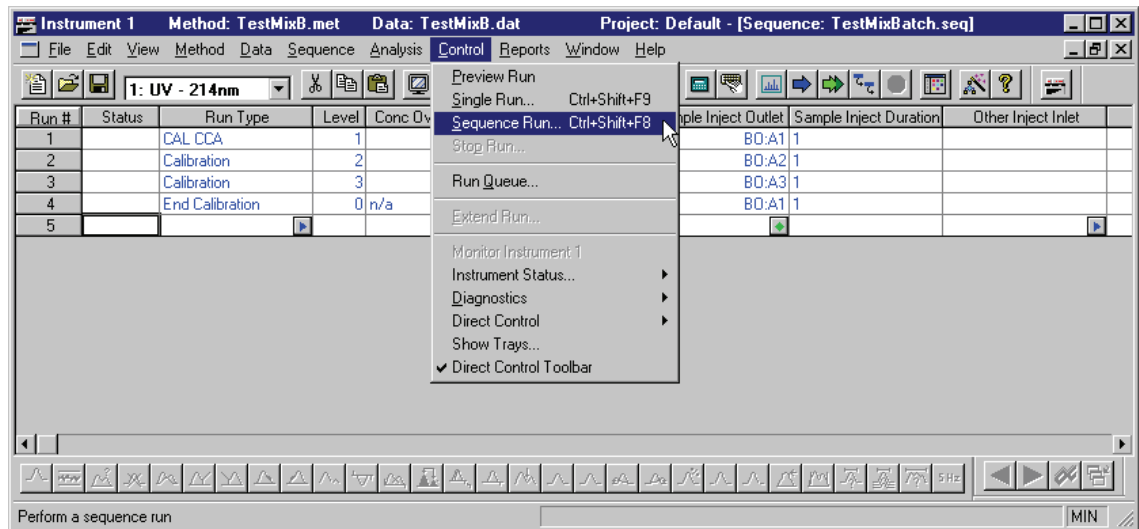


Figure 10.6 Instrument Window with Control | Sequence Run selected



Figure 10.7 Run Sequence icon

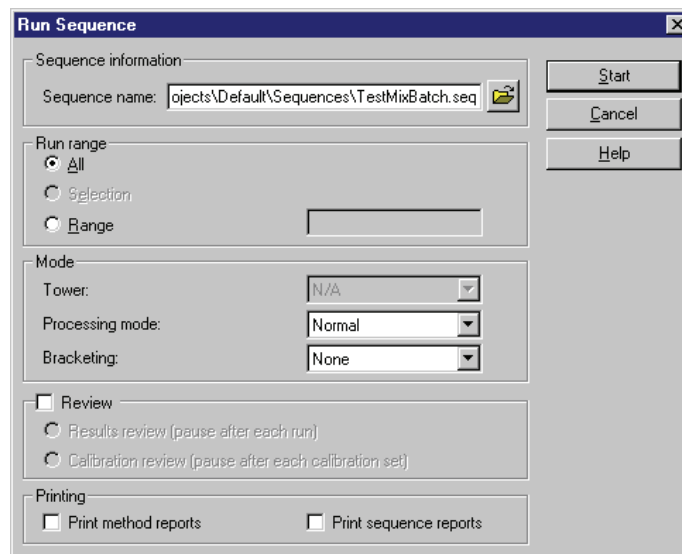


Figure 10.8 Run Sequence dialog

## 10.5 Reviewing Calibration Curves

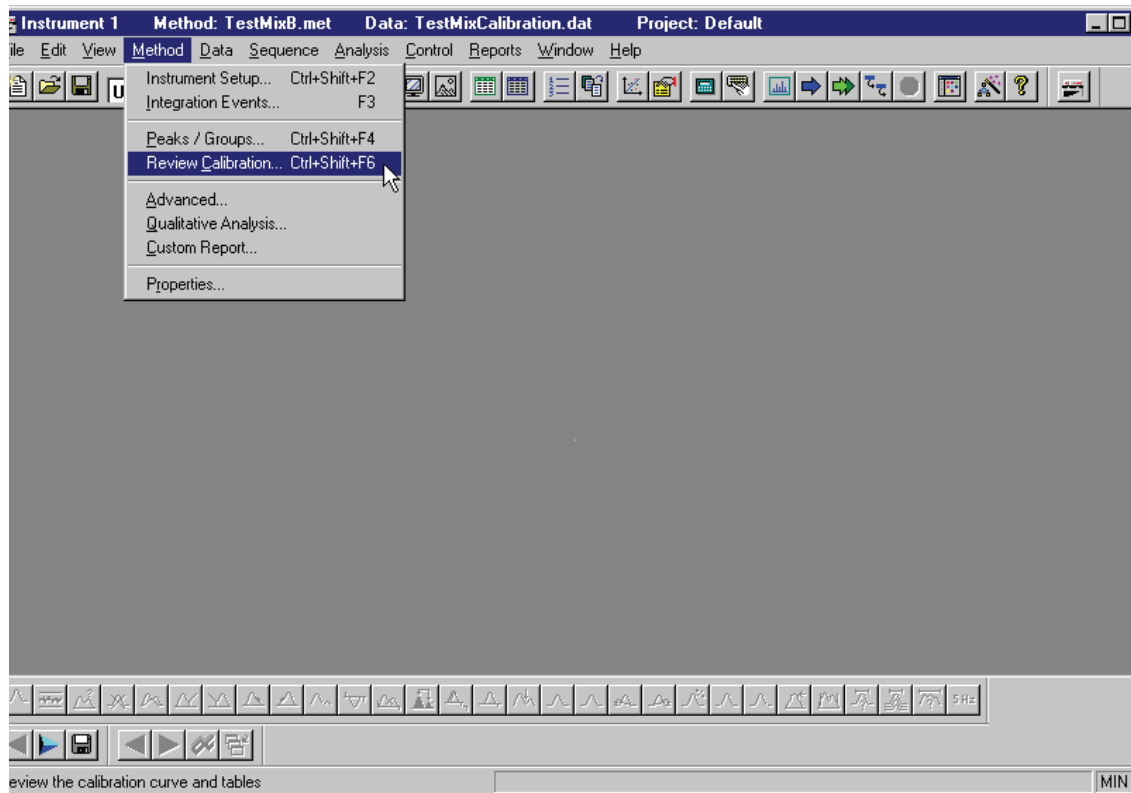


Figure 10.9 Instrument Window with Method | Review Calibration selected



Figure 10.10 Review Peak Calibration icon

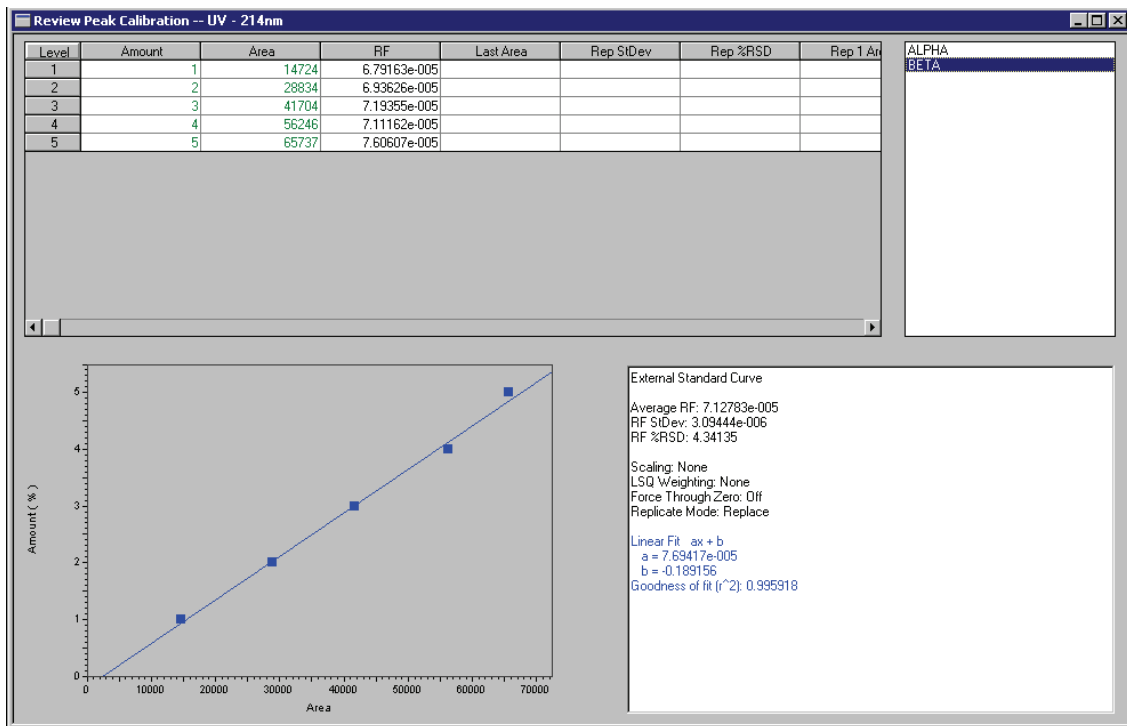


Figure 10.11 Review Peak Calibration Window

- Selecting a curve to review
- Deleting data points
- Equation and goodness of fit

## 10.6 Final Skill Check

Upon completion of this section, you should be able to do the following:

1. Edit the peak ID table in your method to specify three calibration levels. (Five level calibration is shown in this section.)
2. Modify the sequence table you created in the previous section to specify the run types as calibration (enter the level number in the Level column to change run type from Unknown to Calibration).
3. Dilute the test mix to create three levels of concentrations for calibration.
4. Specify sequential file names for the calibration standards.
5. Use **Direct Control** to bring the trays to the load position. Verify that the Test Mix vials are in the appropriate positions.
6. Run the **Sequence table**.
7. When the run is complete, review your calibration data.

### Summary

You now know the basics of generating, analyzing and reporting electrophoretic data. Next we will set up customized reports and sequence reports.



## Preparing Custom Reports

### 11.1 Overview

This section considers the creation of custom reports. We will discuss:

- Accessing a Custom Report
- Editing a Custom Report
- Creating a Report
- Skill Check

### 11.2 Accessing and Editing a Custom Method Report

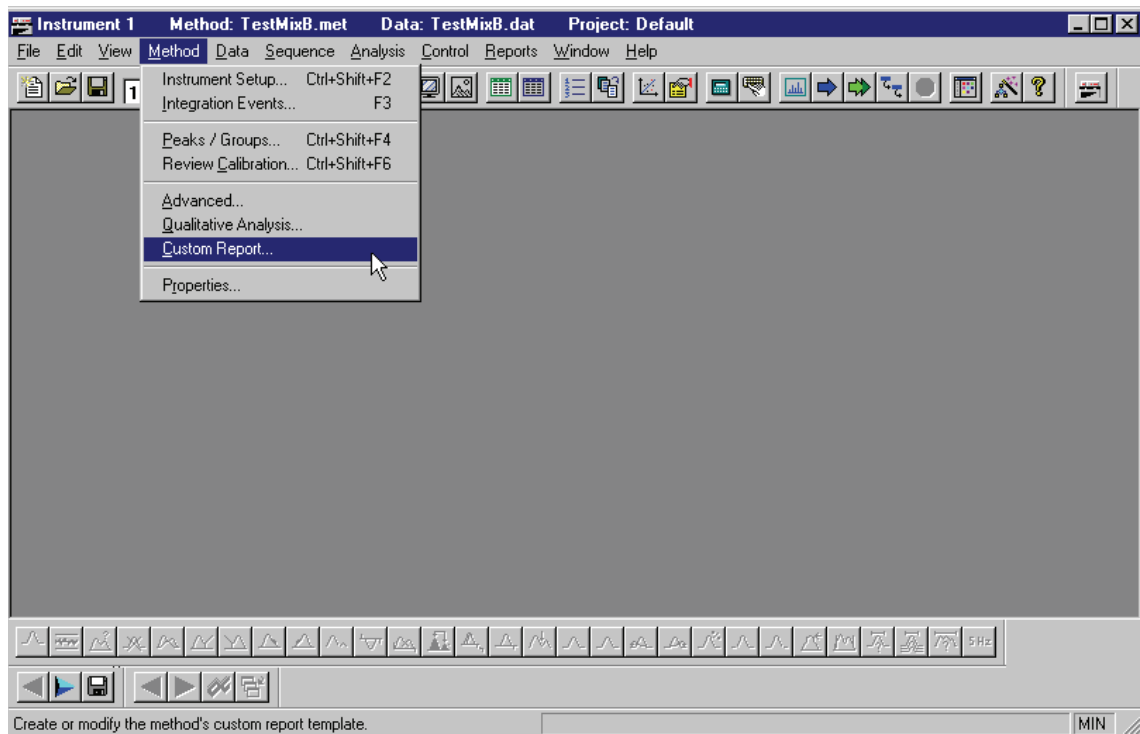


Figure 11.1 Instrument Window with Method | Custom Report selected

## Preparing Custom Reports

### Accessing and Editing a Custom Method Report

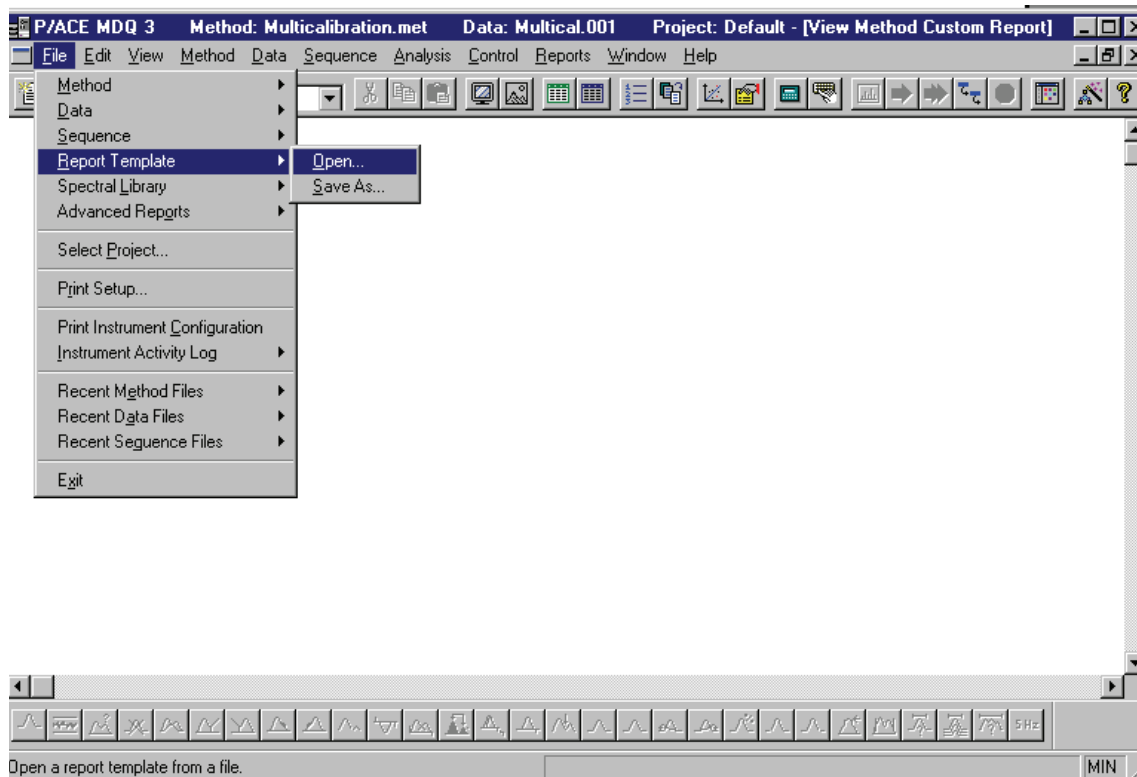


Figure 11.2 Instrument Window with File | Report Template selected

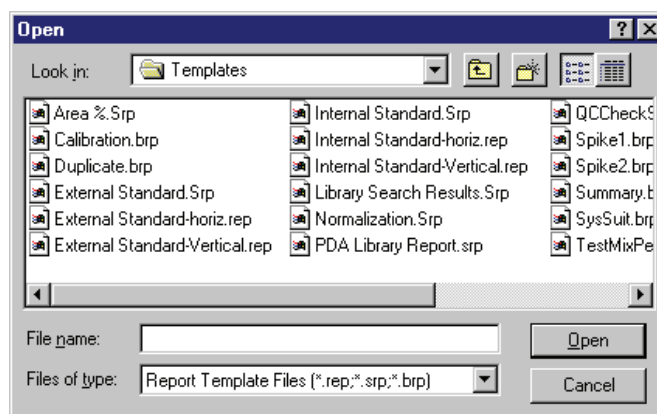


Figure 11.3 Report Template Open dialog

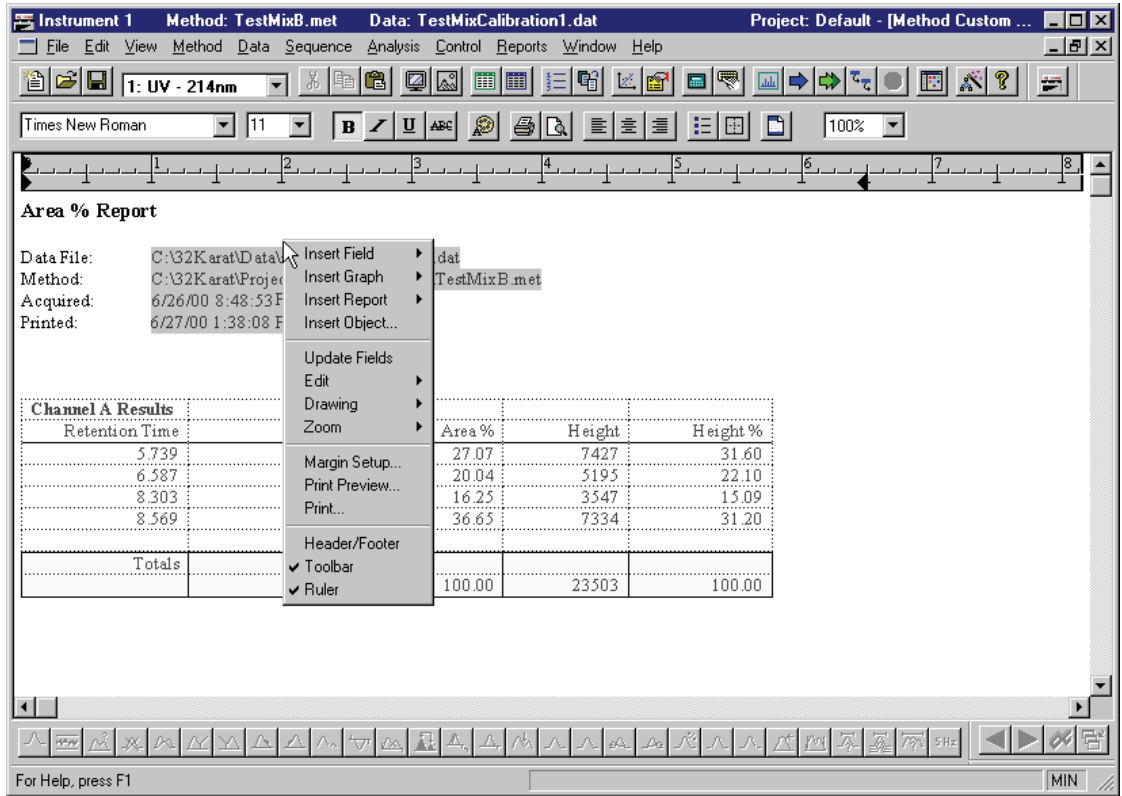


Figure 11.4 Method Report Template with right-click menu displayed

### 11.3 Creating a Custom Method Report

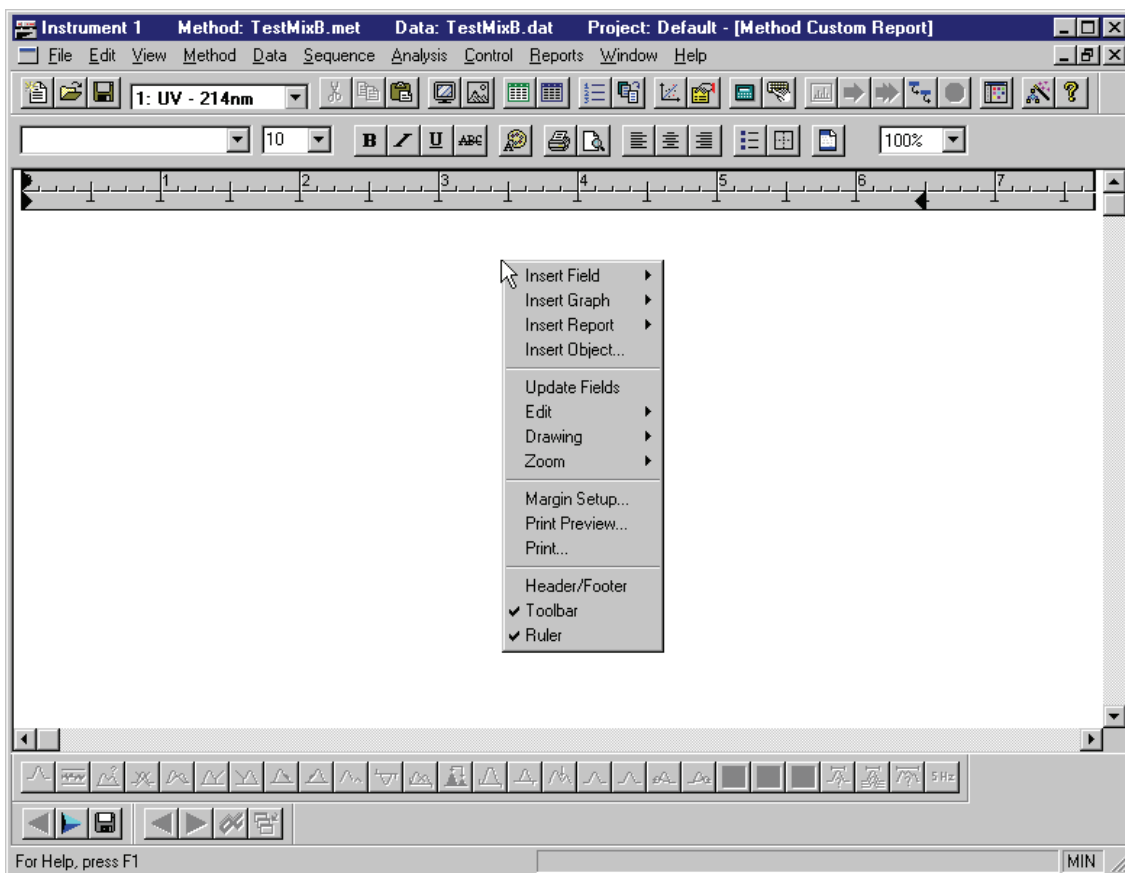
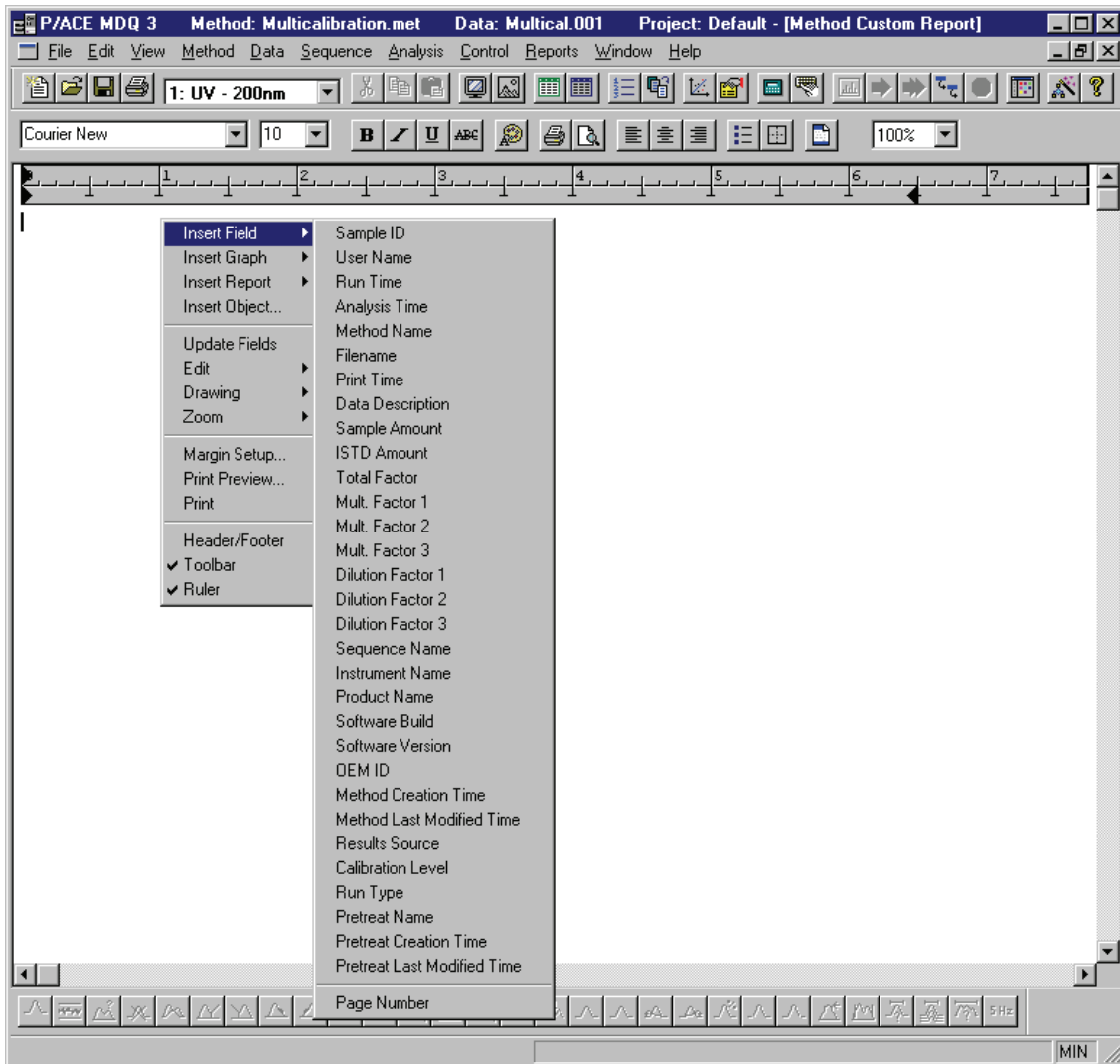


Figure 11.5 Instrument Window - Custom Report, right-click menu displayed



Instrument Window - Custom Report, right-click menu, Insert Field selected

❑ Inserting a Field

## Preparing Custom Reports

### Creating a Custom Method Report

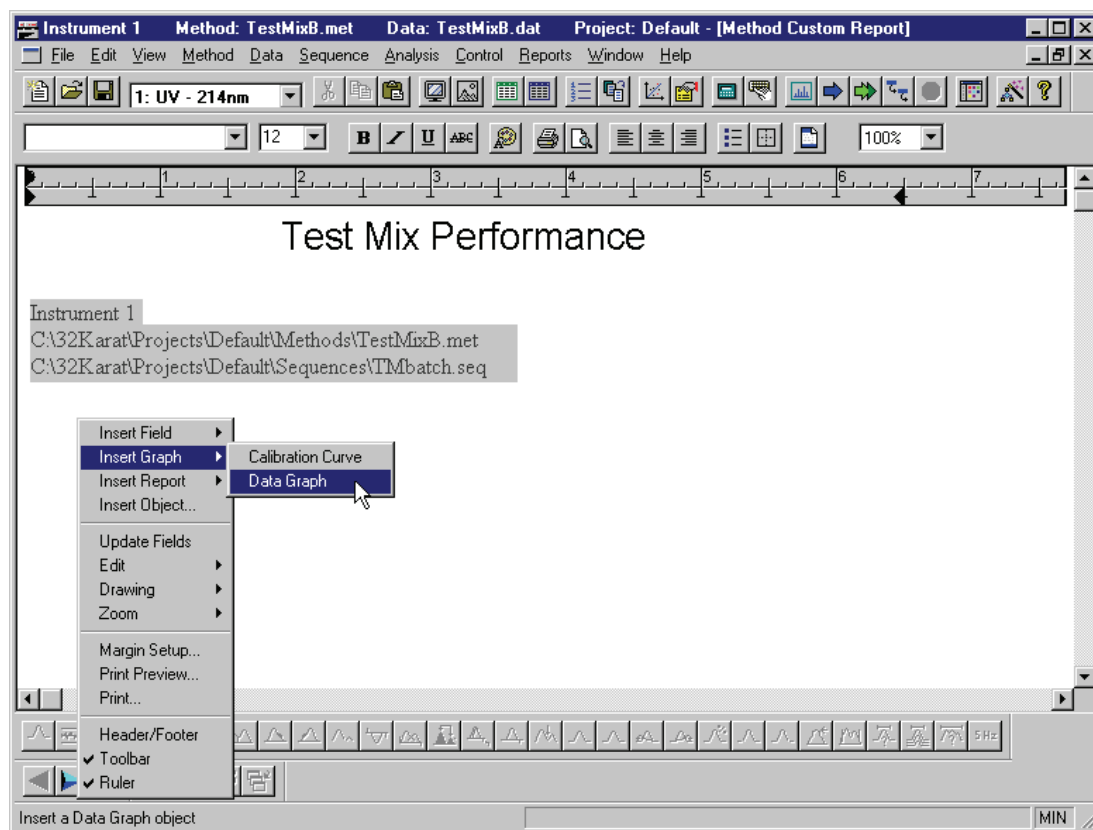


Figure 11.6 Instrument Window - Custom Report; right-click menu, Insert Graph selected

❑ Inserting a Graph

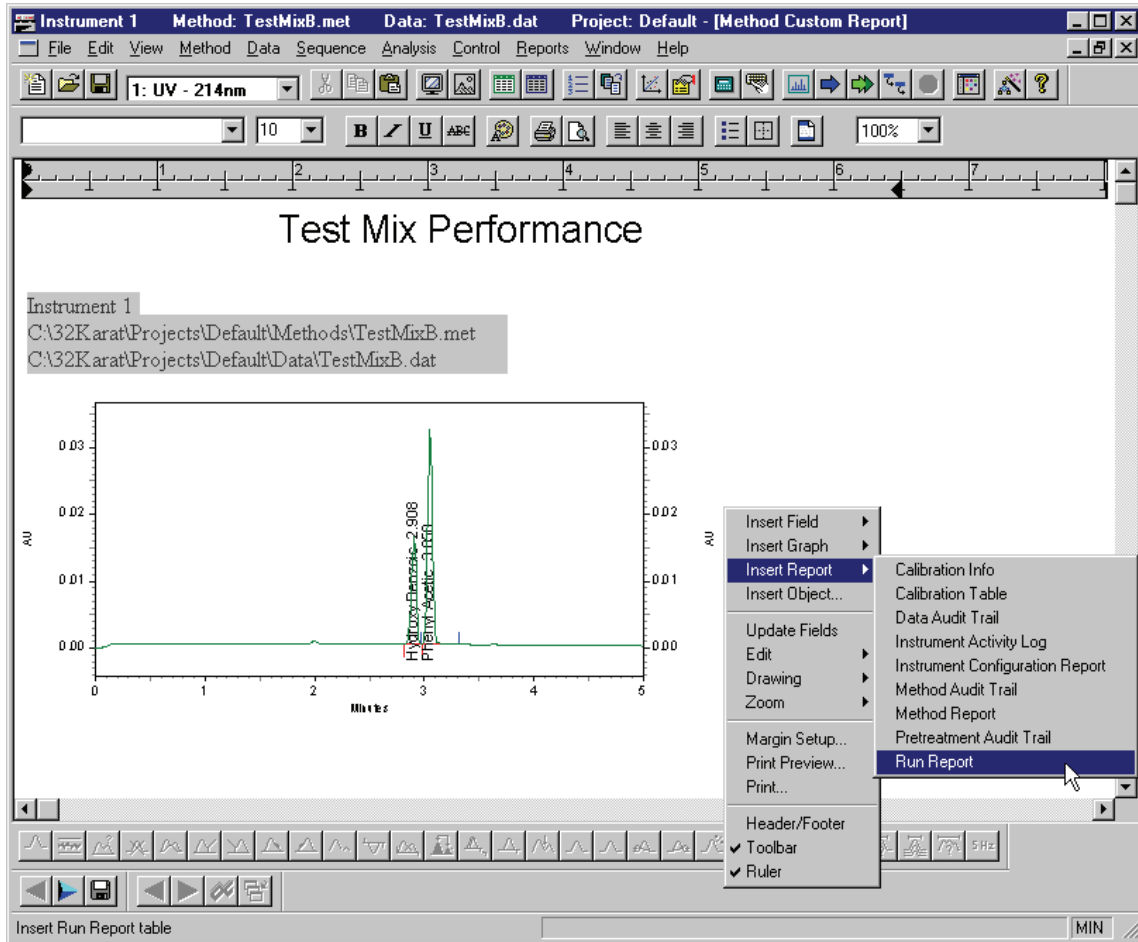
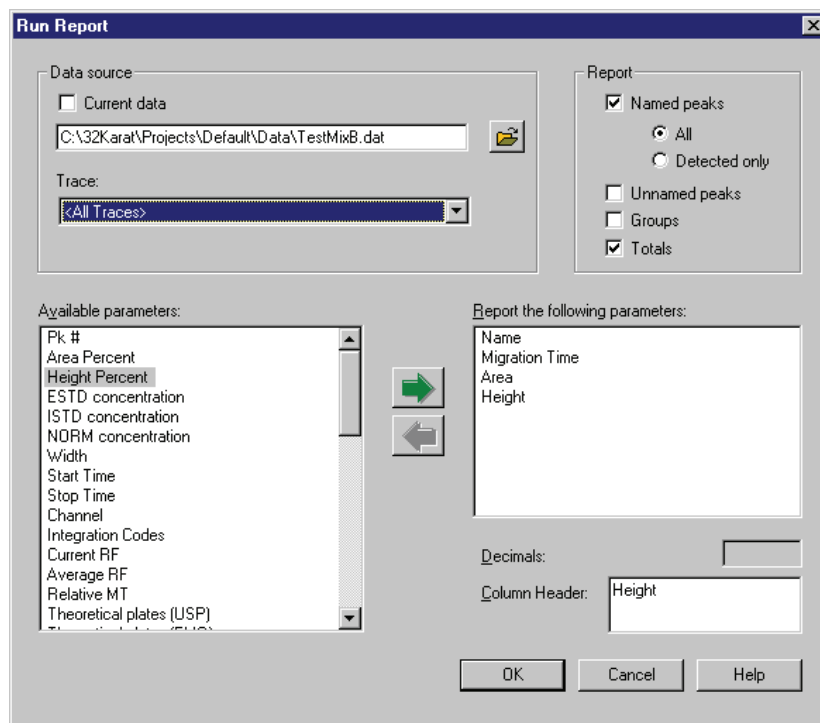


Figure 11.7 Instrument Window - Custom Report; right-click menu, Insert Report Selected

- Inserting a report
- Format columns

## Preparing Custom Reports

### Creating a Custom Method Report



Run Report dialog

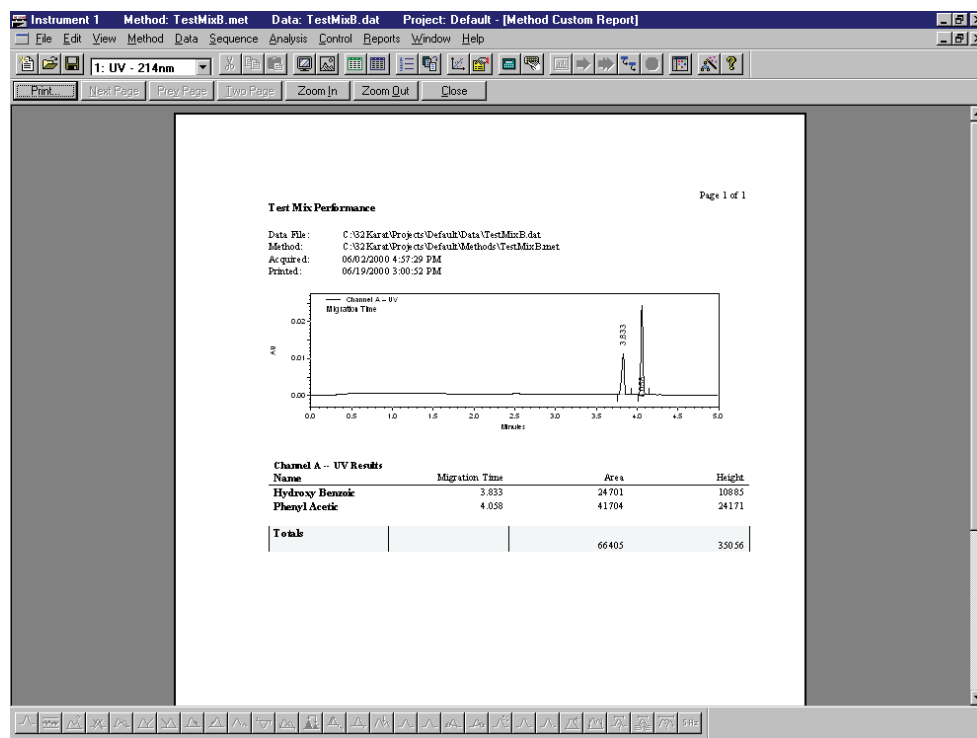


Figure 11.8 Formatted Custom Report



## 11.4 Skill Check

Upon completion of this section, you should be able to do the following:

1. Start and configure 32 Karat Software.
2. Establish initial conditions to run the method used to generate your first electropherogram.
3. Run a sample of test mix.
4. Analyze the data and generate a custom report that includes:
  - A header and footer
  - Information fields
  - An electropherogram with identified peaks (data graph)
  - A run report
5. Save the report as a template and print the final report.

### Summary

Congratulations! You have successfully completed 32 Karat Software Basic Instrument Training. We suggest that you repeat these exercises on your own before beginning work with your own methods and samples.



## Summary

### 12.1 Advancing Your Skill

We sincerely hope that you are pleased with your new P/ACE MDQ system.

32 Karat Software has many additional features and functions that are beyond the scope of this introduction. These include:

- System Administration
- System Suitability
- Data Export
- User-defined data manipulation

To help you benefit from these advanced features, we have provided you with Online Help. This Help is also available as an on-line manual which can be found on the 32 Karat Software Manual CD-Rom.

Please take some time to familiarize yourself with these references. If you would like to enroll in one of our advanced seminars or purchase additional in-lab training, please contact your local service representative.

## **12.2 Record of Operator Training**

### **Training Summary**

The following pages list the contents of 32 Karat Software Basic Training Workbook. Items initialed by the instructor are relevant to the system trained and were covered. Items marked with an “x” are not relevant to the system trained and were not covered.

Instructor Name \_\_\_\_\_

Operator Name \_\_\_\_\_

Operator Name \_\_\_\_\_

**Checklist:**

- |   |  |
|---|--|
| <input type="checkbox"/> System Overview                      | <input type="checkbox"/> Optimizing Integration                              |
| <input type="checkbox"/> Hardware Terminology                 | <input type="checkbox"/> Defining and Naming Peaks                           |
| <input type="checkbox"/> Safety Features                      | <input type="checkbox"/> Identifying Peaks using Migration                   |
| <input type="checkbox"/> Safety Notices                       | <input type="checkbox"/> Identifying Peaks using Mobility                    |
| <input type="checkbox"/> Chemical/Biological Safety           | <input type="checkbox"/> UV, PDA or LIF Initial Conditions                   |
| <input type="checkbox"/> Electrical Safety                    | <input type="checkbox"/> PDA Setup   |
| <input type="checkbox"/> Electrostatic Discharge              | <input type="checkbox"/> UV, PDA or LIF Data Display                         |
| <input type="checkbox"/> Windows Explorer                     | <input type="checkbox"/> LIF Calibration Wizard                              |
| <input type="checkbox"/> Accessing 32 Karat Software          | <input type="checkbox"/> Using the Sequence Wizard                           |
| <input type="checkbox"/> Configuring 32 Karat Software        | <input type="checkbox"/> Viewing a Sequence                                  |
| <input type="checkbox"/> Starting Newly Configured Instrument | <input type="checkbox"/> Editing Sequences                                   |
| <input type="checkbox"/> Accessing Direct Control             | <input type="checkbox"/> Saving Sequences                                    |
| <input type="checkbox"/> Using Direct Control                 | <input type="checkbox"/> Running Sequences                                   |
| <input type="checkbox"/> Using the Method Wizard              | <input type="checkbox"/> Accessing Custom Reports                            |
| <input type="checkbox"/> Creating a Method                    | <input type="checkbox"/> Creating Custom Reports                             |
| <input type="checkbox"/> Saving a Method                      | <input type="checkbox"/> Editing Peak ID Table for Calibration               |
| <input type="checkbox"/> Editing a Method                     | <input type="checkbox"/> Creating Calibration Sequences with Sequence Wizard |
| <input type="checkbox"/> Printing a Method                    | <input type="checkbox"/> Running Calibration Sequences                       |
| <input type="checkbox"/> Other Method Functions               | <input type="checkbox"/> Reviewing Calibration Curves                        |
| <input type="checkbox"/> Running a Single Sample              | <input type="checkbox"/>   |
| <input type="checkbox"/> Stopping / Aborting Methods          | <input type="checkbox"/>   |
| <input type="checkbox"/> Displaying Data                      | <input type="checkbox"/>   |
| <input type="checkbox"/> Opening Data Files                   | <input type="checkbox"/>   |

**Signatures:**

Operator \_\_\_\_\_ Date \_\_\_\_\_

Operator \_\_\_\_\_ Date \_\_\_\_\_

The person(s) listed above have received basic instruction from the representative signed below.

Instructor \_\_\_\_\_ Date \_\_\_\_\_