
**Compound Independent Calibration Enhancements for the
GC-AED**

CICQuant

Version 1.0

By Diablo Analytical, Inc.

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Getting Started

System Requirements

CICQuant requires an installed and operational GC-AED ChemStation with version A.01.02 or greater AED software.

Technical Support

Technical support is available directly from Diablo Analytical using one of the following modes of communications:

Phone

Call **(925) 609-1150** to speak directly with technical support.

Fax

Fax a description of your problem to **(925) 609-9360**.

E-mail

Send an e-mail to **support@diab.com** with a description of your problem.

Mail

You can send your technical support questions via mail to the following address:

Diablo Analytical, Inc.
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1110 Burnett Avenue, Ste C
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Introduction

What is CICQuant

CICQuant is an enhancement to the Compound Independent Calibration functionality that is built into Hewlett-Packard's GC-AED ChemStation.

Summary of Features

- Allows Compound-Independent Calibration calculations and reports to be generated automatically during a sequence or from data analysis.
- Helps reduce the need for manual data analysis and Excel Spreadsheet calculations for analyses using Compound-Independent Calibration.
- Can be configured to generate peak area, weight, and/or element ratio results tables automatically. Results can be sent to either a screen viewer, or the printer.

About Diablo Analytical, Inc.

*Mt. Diablo is a well-known
San Francisco Bay Area
Mountain*

CICQuant was written by Diablo Analytical, Inc. Diablo Analytical is an analytical application development company located in Concord, CA. We specialize in the development of custom analytical solutions for a broad range of industries.



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Hewlett-Packard Channel Partner

Diablo Analytical is a Hewlett-Packard Channel Partner for analytical application development and system integration.



Using CICQuant

Loading the CICQuant Macro

In order to configure and use CICQuant you will need to load the CICQuant ChemStation macro each time you restart the ChemStation.

1. Start the AED ChemStation and switch to the Data Analysis view by selecting "Data Analysis" from the ChemStation "View" menu.
2. Execute the command, **Macro "cicquant.mac"**, from the command line at the bottom of the ChemStation window. If the command line is not visible, select "Command Line" from the ChemStation "View" menu.
3. After the macro has loaded, you should find two new menu options added to the bottom of the "AED_CIC" ChemStation menu: "Display CICQuant Setup...", and "Start Auto CICQuant".

Configuring CICQuant

To configure CICQuant, select "Display CICQuant Setup..." from the AED_CIC menu. The following dialog box is displayed.

The screenshot shows the "Diablo Analytical CICQuant" dialog box. It has a title bar with a close button. The main area contains several sections: "Result File Name (default is CIC_RPT1.TXT in the Data Directory)" with a "File Name:" text box; "CIC Quant File Name (default is DEF_CAL.CIC in the Method Directory)" with "File Name:" and "Directory:" text boxes; "Save and Print Results:" with three checked checkboxes for "Area", "Weight", and "Ratio", and a "Browse CIC Quant File" button; "Text Results:" with radio buttons for "Printer" (selected) and "Screen"; "Print Chromatogram:" with radio buttons for "yes" (selected) and "no"; "Ref. Element:" with a dropdown menu showing "C"; and "Wt. Units (7 max):" with a text box showing "ng". At the bottom are "OK" and "Cancel" buttons, and a copyright notice: "(c) Copyright 1997-98, Diablo Analytical, Inc."

CICQuant Configuration Dialog Box

Result File Name

By default, CICQuant saves the CIC Results tables to the file "CIC_RPT1.TXT" that is located in the individual data file's data directory. If you would like to use a different file name, it may be specified in this text box. Leave the text box blank if you want to use the default result file name.

CIC Quant File Name

By default, CICQuant uses a CIC Calibration file with a name of "DEF_CAL.CIC" that is located in the current method directory. This allows different methods in a sequence to use a different calibration table. If you would like all methods to use the same calibration table, use the "Browse CIC Quant File" button to select the calibration table. The directory path and file name will be placed in the respective text boxes automatically. Leave both text boxes blank to use the default calibration table.

Save and Print Results

These check boxes allow the user to select which CIC results will be calculated, saved and printed.

Text Results

Use these radio buttons to select whether the CIC results will be sent to the printer or to an on-screen text file viewer.

Print Chromatograms

If you would like to have each of the element chromatograms printed along with your CIC results, click the "Yes" option. CICQuant will automatically scale the chromatograms, and print them.

Ref Element

A reference element is needed for the Element Ratio result table. All other elements will be ratioed to the reference element. A new reference element can be selected from the drop down list box. The Default is C for Carbon as the reference element.

Wt. Units

The Units that you want displayed in the Weight result table can be entered here. The Default if this text field is blank is ng.

OK

Pressing the OK button will cause the current CICQuant configuration to be saved.

Cancel

Pressing the Cancel Button will close the CICQuant Configuration dialog box without saving any of the changes that were made.

Running CICQuant from Data Analysis

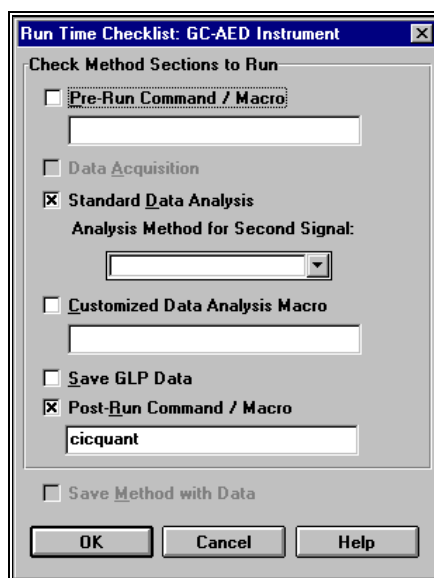
You can generate a CICQuant report directly from data analysis by using the following procedure.

1. Configure CICQuant with the desired options.
2. Make sure that you have either specified a valid CIC calibration file in the CICQuant configuration, or have a valid calibration file with the name "DEF_CAL.CIC" saved in the current method directory.
3. Load the desired signal.
4. Integrate all desired signals.
5. Evaluate suppression and the integration results, and make corrections if necessary.
6. Select "Start Auto CICQuant" from the ChemStation "AED_CIC" menu.

CICQuant will automatically apply the specified CIC calibration to each of the loaded signals, and print the specified CIC result tables to either the screen, or the printer.

Running CICQuant from a Method or Sequence

In order to have the CICQuant reports generated automatically after each run in a sequence, the CICQuant macro must be loaded, and the command "cicquant" needs to be specified as the "Post-Run Command / Macro" for each method in the sequence.



Procedure

1. Make sure that the CICQuant macro has been loaded.

2. Switch to the "Method and Run Control" View of the ChemStation by selecting "Method and Run Control" from the ChemStation "View" menu.
3. Load the method to which you want to add CICQuant reporting
4. Display the "Run-Time Checklist" dialog box by selecting "Run-Time Checklist" from the ChemStation "Method" Menu.
5. Click the "Post-Run Command / Macro" check box, and add the command "cicquant" to the text box as shown above.
6. Click the "OK" button
7. **Important:** Save the method before starting the sequence to ensure that your changes take effect.
8. Make sure that there is a CIC Calibration file named "DEF_CAL.CIC" located in the method directory, or, you have specified an alternate CIC Calibration table in the CICQuant Setup dialog box.

Appendix

Creating a CIC Calibration Table

The following steps describe how to create a CIC Calibration Table using the AED_CIC menu options that are part of the GC-AED ChemStation. For additional information on using the AED_CIC menu options, see the on-line help that can be accessed by selecting "AED_CIC Help" from the ChemStation "AED_CIC" menu.

1. Run a calibration standard that contains analytes with the element(s) of interest. For each of the analytes you will need to know the Molecular Formula, and the weight of analyte injected in ng.
2. Integrate the calibrant peaks in each of the elemental chromatograms. Make sure to evaluate suppression and integration quality, and correct any problems before proceeding
3. If you are creating a new calibration table, select "Create New Table" from the AED_CIC "Calibration Table" menu option. If you want to add to a calibration table that you have already saved to disk, select "Load Table" instead.
4. For each calibrant peak in your standard chromatogram select "Calibrate Peak" - "Select Peak" from the AED_CIC menu. Click on

the peak that you want to calibrate. You will be presented with a dialog box to confirm that you have selected the correct peak.

5. Enter the molecular formula and the amount of calibrant injected in the subsequent dialog box. Make sure that you enter the *entire* molecular formula, not just the elements you will calibrate.
6. In the next dialog box, select the elements that you want to calibrate, as well as the calibration mode (new, replace, average, normalize).
7. Finally, after you have calibrated all the peaks of interest in your standard, save the CIC Calibration Table to disk using the "Save Table" option of the CIC Cal table menu option. By default, CICQuant uses a CIC Calibration Table named "DEF_CAL.CIC" located in the current method directory.