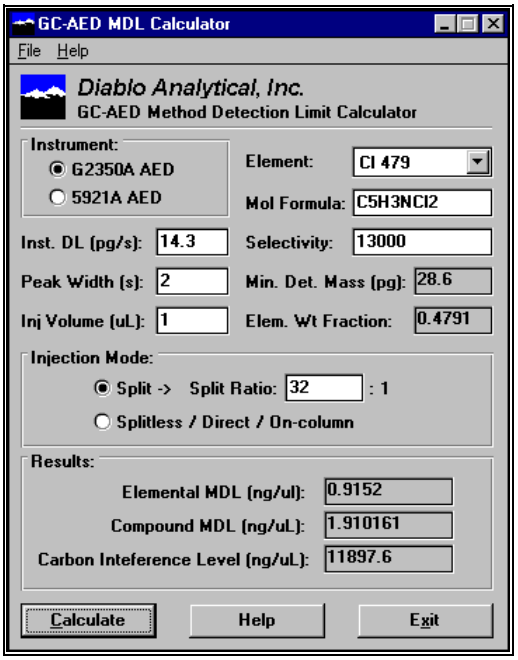
A Diablo Analytical Custom Software Application

AED MDL Calculator

By Diablo Analytical, Inc.



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Introduction

About the AED Method Detection Limit Calculator

This program was written by Diablo Analytical, Inc. to help GC-AED users with method development and in evaluating new applications for the AED. We are distributing the application as unsupported "Freeware". You are free to distribute the unaltered setup file or diskette to anyone who might find it useful.

About Diablo Analytical, Inc.

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Diablo Analytical, Inc. is an analytical application development company located in Concord, CA. We specialize in application development and training for Agilent Technologies Atomic Emission Detector for Gas Chromatography (GC-AED). We provide the following AED-related services as an Agilent Technologies Channel Partner:

GC-AED Application Development

Diablo Analytical has a complete G2350A GC-AED system in our development laboratory for use in method and application development projects.

Custom Software for the GC-AED

We are experienced in developing custom software programs for analytical applications.

- Custom macros for data acquisition and data analysis for both the DOS and Pascal ChemStations
- Simplified user interfaces for the DOS ChemStation
- Pascal - to -DOS ChemStation transition assistance

GC-AED Training

Diablo Analytical is the authorized provider of GC-AED technical training in North America. We provide both regularly scheduled GC-AED training courses across the country, as well as customized on-site training courses at customer's facilities. Our training courses apply to both the 5921A GC-AED as well as the G2350A GC-AED.

Analytical Application Development

In addition to our services for the GC-AED, we also provide analytical application development services and custom software applications for technologies such as gas and liquid chromatography and mass spectrometry. Additional information on our capabilities and services can be found on our web page at http://www.diabloanalytical.com.

The AED MDL Calculator

Getting Started

Installing the Application

The AED MDL Calculator is distributed both electronically and CD-ROM.

CD-ROM

If you received the AED MDL application from Diablo Analytical on a CD-ROM, insert the CD into your diskette drive and run the program "SETUP.EXE". The installation program will prompt you for any information it needs to install the application files correctly.

Electronic Distribution

If you received the AED MDL application from Diablo Analytical electronically via e-mail, or by downloading from our web page, simply run the "MDLSETUP.EXE" program. The installation program will prompt you for any information it needs to install the application files correctly.

Starting the Application

By default, an icon is created in the "Diablo AED MDL Calculator" program group. Double click on this icon to start the AED MDL Calculator. If you can't find the icon, you can run the application MDLCALC.EXE from the directory into which you installed the application files.

Calculating a Method Detection Limit

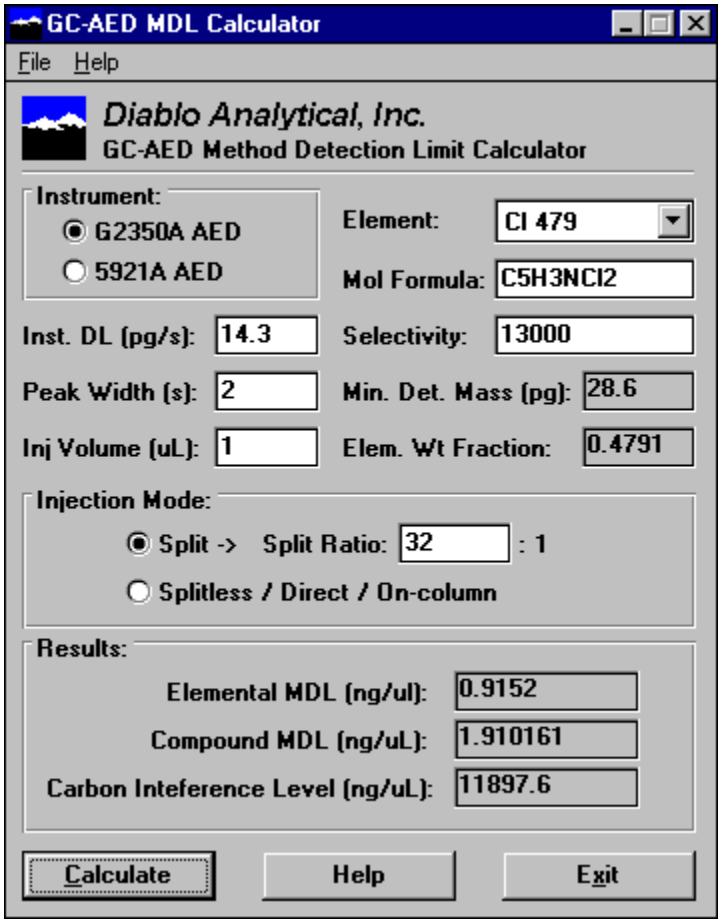
Follow these steps to calculate an MDL for a GC-AED Application

1. Select the type of AED Instrument (G2350A or 5921A) for which you are calculating the MDL.
2. Use the *Element* list box to select the element and wavelength combination for which you would like to calculate an MDL.

3. If you know the molecular formula of the compound containing the element, enter it in the *Mol. Formula* text box. Please note that the molecular formula entry is case sensitive. This means you must use the proper combination of upper and lower case letters for the elements (e.g CH3Br).
4. Enter the expected width (in seconds) of the chromatographic peak for the compound of interest into the *Peak Width* text box.
5. Enter the volume (in uL) of sample you will be injecting into the gas chromatograph into the *Inj Volume* text box.
6. Select the injection mode that you will be using. If the injection mode is "Split", make sure to enter your split ratio.
7. Press the *Calculate* button to calculate and display the MDL results. The following values are calculated:

   Elemental MDL
   Compound MDL
   Carbon Interference Level

Overview of the Main Screen Functions



Screen Shot of the GC-AED MDL Calculator

Instrument

There are two kinds of GC-AED instruments: The current HP/Agilent G2350A model and the older HP 5921A model. The instrumental detection limits vary between these two instruments. Select the instrument for which you will be calculating the MDL.

Element

Use this list box to select the element and wavelength for which you want to calculate an MDL. Each combination of element and wavelength (known as a recipe) will have a different instrumental detection limit and selectivity. When you make a selection using this list box, the default values for instrumental detection limit and selectivity are copied into their respective text boxes. The default values for both the G2350A and 5921A AEDs are taken from the Hewlett-Packard Application Note 228-363, "A Comparison of the HP G2350A AED vs. HP 5921A AED for Average Values of MDL and Selectivity for Selected Elements".

Mol Formula

Enter the molecular formula of a compound containing the selected element if you want to have a compound MDL calculated.

Important: The molecular formula is case-sensitive. This means that formulas must be entered using the proper combination of upper/lower case characters for the elements: Br *not* BR for Bromine (e.g. C6H2Br2Cl2).

Inst D.L. (pg/s)

This is the instrumental detection limit in pg/s for this element and wavelength combination (recipe) taken from Hewlett Packard Application Note 228-363. You may enter your own value in the text box.

Selectivity

This is the selectivity of this element and wavelength recipe with respect to carbon interference taken from Hewlett Packard Application Note 228-363. Selectivity values are only available for non-carbon and non-hydrogen elements. You may enter your own value in the text box.

Peak Width

Enter the width, in seconds, of the chromatography peaks for which you are calculating the MDL.

Min. Det. Mass (pg)

The calculated instrumental minimum detectable mass in pg. Calculated by multiplying the instrumental detection limit by the chromatographic peak width.

Inj. Volume

Enter the volume of sample injected into the gas chromatograph in μL.

Elem. Wt. Fraction

This is the weight fraction of the selected element in a compound having the molecular formula you entered into the Mol Formula text box: (g of element in

compound / molecular weight of compound). This value is multiplied by the Elemental MDL to calculate the Compound MDL.

Injection Mode

Select the mode of chromatographic injection. If using split injection, enter the split ratio.

Elemental MDL

This is the calculated method detection limit for the selected element in ng/uL (ppm) of sample injected into the gas chromatograph.

Compound MDL

This is the calculated method detection limit in ng/uL (ppm) of sample injected for the compound for which you have entered a molecular formula. The compound MDL assumes you are using the selected element and wavelength recipe for quantitation.

Carbon Interference Level

This is the concentration of carbon in ng/uL above which a detectable peak on the selected element's signal chromatogram will be observed.

Calculate

Press this button to calculate the MDL(s) using the current parameters.

Help

Press this button to activate this help file. Alternatively, press the "F1" key.

Exit

Press this button to exit the GC-AED MDL Calculator. The current values for Instrument, Peak Width, Injection Mode, Split Ratio, and Injection volume will automatically be saved as the defaults for the next time you use the MDL Calculator.