

ClearView™ Quick Start Guide

For more detailed installation instructions and information on parameter settings, please refer to "Getting started with ClearView™" (below)

1. Open the installation folder and run the setup.exe file. Follow the on-screen prompts to install ClearView.
2. **Note:** If installing to update an existing version:
 - a. Save a copy of the ClearView .ini file.
 - b. *Uninstall* existing software.
 - c. Following installation, ClearView .ini file should be placed in ClearView directory
3. Once installed, run the software. It will prompt you to enter some user-related details. A **.bin** file is then created that must be e-mailed to clearview@markes.com. This file is located in the following directory: **../Program Files/ALMSCO/Clearview**
4. On receipt, the ClearView team will reply directly with the unlock code. *Entering this code will register the software for the installation PC.*
5. Launch ClearView *via* shortcut or start menu.
6. Set '**Noise Counts**' and '**Window Width [s]**' parameter settings (Default settings work well for most standard capillary GC/MS data).
7. Click on '**File**' to open dropdown menu. This enables selection of the chromatogram format for processing.
8. Select chromatograms by clicking on the list (selections will become highlighted), then click on '**Select**'.
9. Chromatogram will automatically appear in the display window. The buttons displayed beneath the chromatogram, at the end of the process, will prompt the user to '**Select New Files**', '**Reprocess selected files**' or '**Exit**'.

Getting started with ClearView™

1. Introduction

Chromatograms produced by conventional GC/MS systems are often affected by background contamination and/or baseline anomalies. The most common sources of background ions and baseline disturbances are capillary column bleed, contaminated carrier gas, air/water background and valve switching.

Background ions interfere with mass ion fragmentation patterns of chromatographic peaks. This leads to poor match quality factors for target compounds, and/or incorrect matches with library spectra, especially for trace compounds. Baseline disturbances make it difficult to reproducibly identify peak starts and peak ends, thus affecting integration and quantitation.

Standard approaches (*with limitations*) for addressing these problems are:

- Scanning from 45 amu upwards to remove any contribution from air/water. *This can remove key ions and make positive identification of light compounds troublesome.*
- Performing spectral subtractions on the apex of a peak compared to the peak start to remove background. *This is difficult to automate.*
- Selecting an area of particularly high background and performing a global background subtraction over the whole chromatogram. *This can remove signal of interest in areas of low background.*

ClearView™ software uses sophisticated proprietary dynamic background compensation (DBC) algorithm to rapidly identify and minimise these varying background ion contributions throughout the total ion or extracted ion chromatogram. Single or multiple data files can be selected within ClearView for batch processing. The original data files remain unaltered and separate ClearView reprocessed GC/MS data files are produced for comparison and analysis.

ClearView™ software supports ChemStation (HP/Agilent), Thermo .raw and ANDI (.cdf) GC/MS data file formats. It also supports SIM/scan data. ClearView will also work with these file formats for LC/MS data files.

Registered users will have access to additional file formats free of charge, as and when they become available.

2. Software Installation

Software is delivered as a web download or CD.

There are two versions of ClearView™ – this 30-day free trial version and the full version.

Both versions require electronic registration and can be opened after the unique workstation serial number, subsequently provided by Markes International, has been entered. Full software functionality is then available.

Note: If installing to update an existing version of ClearView, users should first save a copy of the ClearView .ini file. *Uninstall* existing software. Following installation, ClearView .ini file should be placed in the ClearView directory (please contact clearview@markes.com to resolve any issues).

Open the installation folder and run the setup.exe file. Follow the on-screen prompts to install ClearView.

Default parameters will install the program to the following directory: **../Program Files/ALMSCO/Clearview**, and place shortcuts on your desktop and start menu.

Once installed, it will prompt you to enter some user-related details. A **.bin** file is then created that must be e-mailed to clearview@markes.com (Figure 2.1).

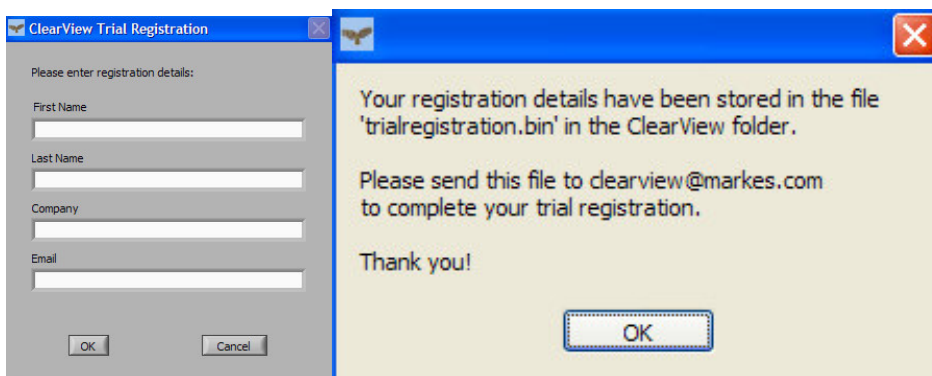


Figure 2.1: ClearView registration process

On receipt of this file, the ClearView team will reply directly with the unlock code. *On entering this code the software will then be registered for the PC it is installed on.*

3.1 Getting started with ClearView

Launch ClearView *via* the desktop shortcut, or from the start-menu.

Set 'Noise Counts' and 'Window Width [s]' parameter settings. Default settings for noise counts (100) and window width (40) work well for most standard capillary GC/MS data (Figure 3.1.1). Use the dropdown file menu to select the chromatogram format for processing as shown in figure 3.1.2. See 3.2 for more information on parameter settings.

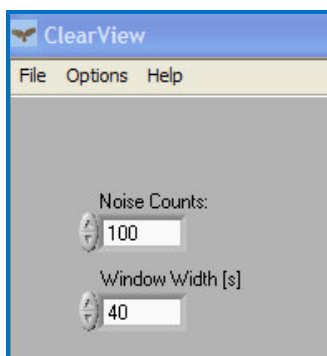


Figure 3.1.1: Default settings for most standard capillary GC/MS data analyses

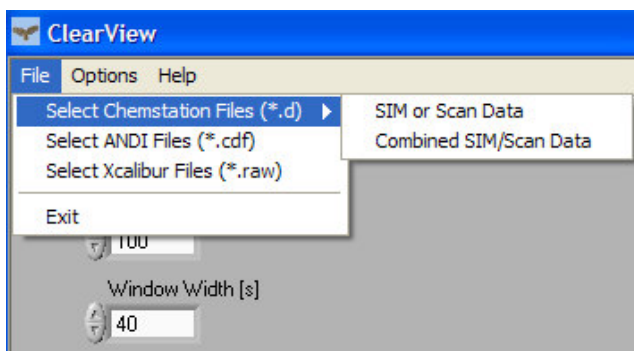


Figure 3.1.2: ClearView user interface showing chromatogram file formats

Select chromatograms by clicking on those listed (they will become highlighted), then click 'Select' (figure 3.1.3).

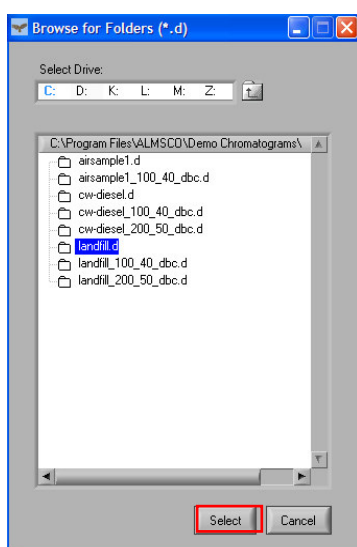
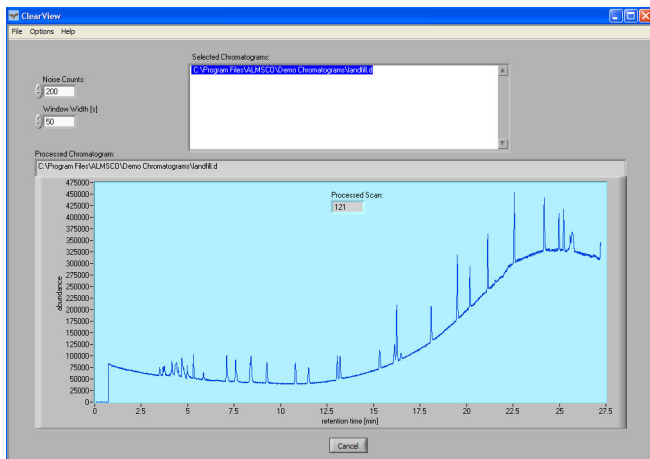


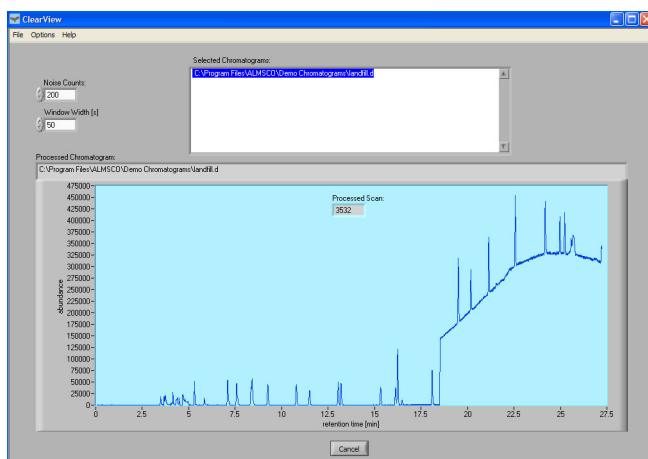
Figure 3.1.3: Selection of chromatograms for ClearView processing

Selected chromatogram will automatically appear in the display window. The buttons displayed beneath the chromatogram, at the end of the process, will prompt the user to 'Select New Files', 'Reprocess selected files' or 'Exit'. Figure 3.1.4 shows snapshots of a landfill chromatogram being processed.

(1)



(2)



(3)

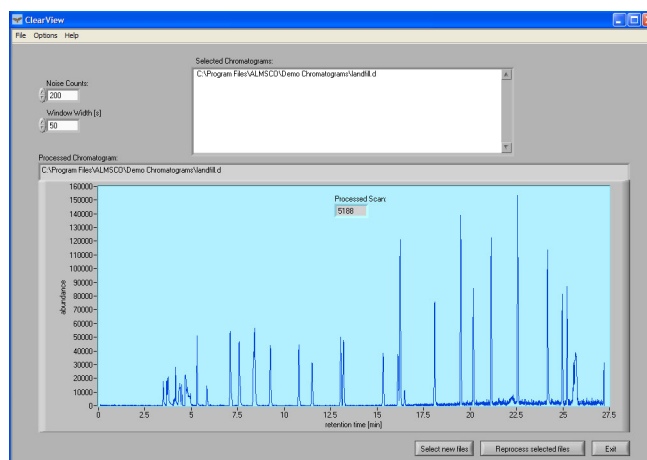


Figure 3.1.4: Progress (1-3) of ClearView analysis on a landfill .d chromatogram

After ClearView processing, data files created have their parameter values (noise counts and window width) assigned, followed by **_dbc** in their filenames. In the example the original file is called **landfill.d**. Browsing to this location will now show a new file called **landfill_100_40_dbc.d**. Critically, the original file is unaltered.

Both files may now be reprocessed in any compatible GC/MS data processing software (e.g. Chemstation). Figure 3.1.5 shows a comparison of dbc and non-dbc data. The mass ion fragmentation patterns for the small thiophene peak at 16.483 minutes are highlighted.

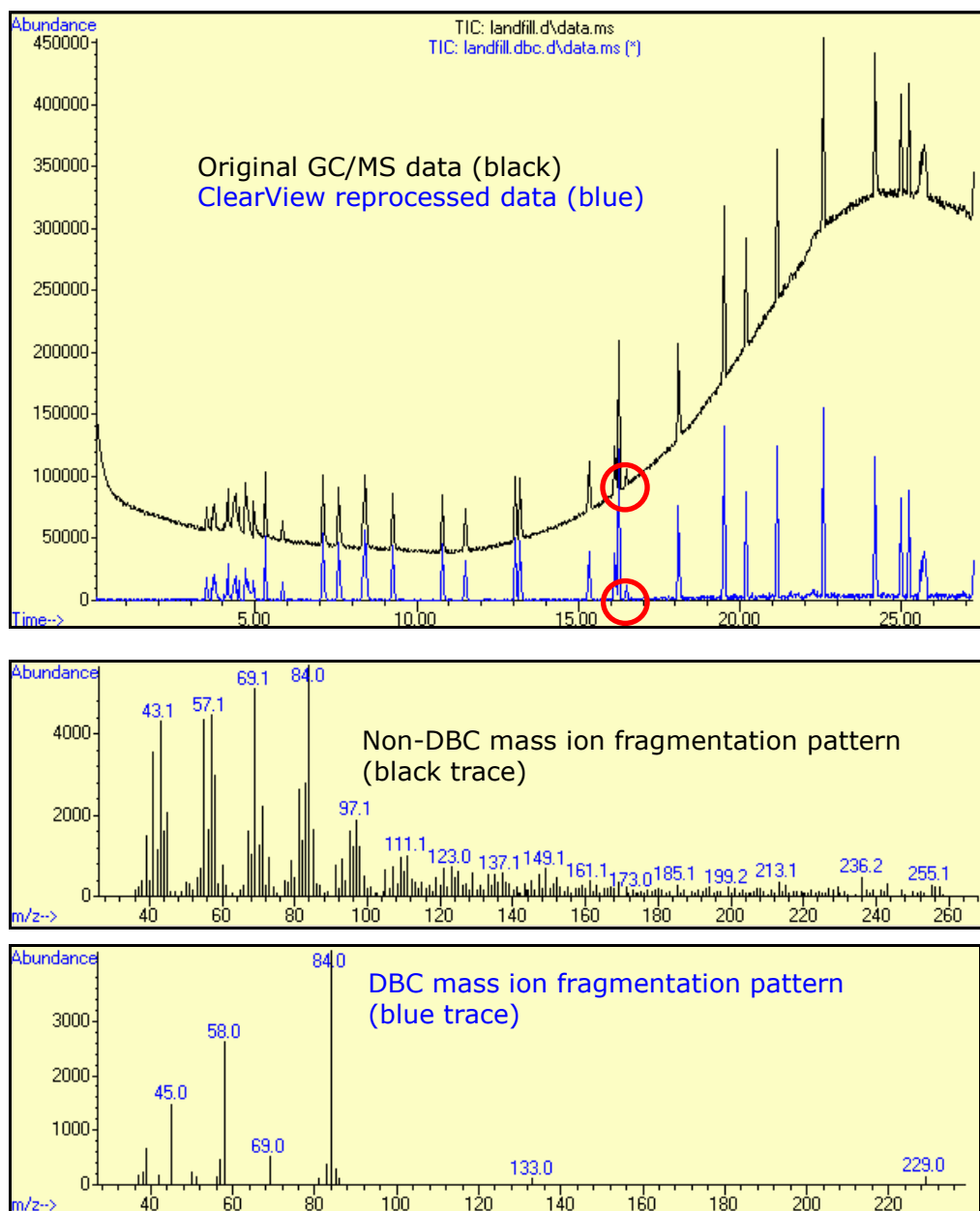


Figure 3.1.5: Comparing files in GC/MS data processing software

To process another GC/MS data file, select it, click 'Display Selected Chromatogram' button and click 'Process'.

Changing the 'Noise Counts' and Window Width' settings must be done *prior* to selecting and displaying the next chromatogram.

3.2 Parameter settings

'Noise Counts' sets a threshold. Setting it too low will lead to a higher number of low abundance ions in your mass ion fragmentation patterns. Setting it too high will begin to remove lower intensity ions of interest and make compound identification less selective.

'Window Width [s]' refers to the "time slice" of a chromatogram that ClearView considers when separating signal from background. A good starting point is ten times the average peak width at base. Decreasing the value will gradually truncate peaks, with the effect becoming very noticeable as the window width approaches that of the peak width at base.

4. Purchasing a full copy of ClearView

We hope that you have been impressed with the ClearView software capabilities.

If you think that the spectral purity, integration and automation enhancements offered by ClearView would be useful in your laboratory, purchasing a full copy could not be easier.

The full package can be obtained on CD or via electronic delivery (see contact details below). On installation it will prompt you to enter some user-related details. It will then create a **.bin** file that you e-mail to clearview@markes.com. The ClearView team will then contact you within one working day to confirm price and payment terms, and then send you (by return e-mail) the unlock code **unique to the PC** on which ClearView has been installed.

Contact information is as follows:

- UK Tel: +44 (0) 1443 233920 (ALMSCO International)
 +44 (0) 1443 230935 (Markes International Ltd)
- US Tel: 1-866-483-5684
- E-mail: clearview@markes.com

We accept payment by Visa or MasterCard. Alternatively, if you have an account with us, ClearView can be added and payment processed in the normal way.

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- iii. the results that may be obtained from the use of the software will be effective, accurate or reliable
- iv. the quality of the software will meet your expectations
- v. any errors in the software will be corrected

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