

A Web-Based Search Engine for Chromatography Applications

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INTRODUCTION

Chromatography applications are run daily in laboratories worldwide and many of these applications can be reused by other laboratories working in the same area. Method developers like to share their results to accelerate development and to ensure that their work is not duplicated; analysts also require a quick way to find chromatography methods for the compounds they are analyzing.

To effectively compare and evaluate applications, the following data must be stored and also be easily accessible:

- Results such as peak name and peak resolution
- Information about the instrument used, such as detector and pump type
- Column details, such as manufacturer, length, internal diameter, packing material, and particle size
- Method details, such as flow rate, gradient table, injection volume, column temperature, and detector wavelength
- Raw data to allow visualization of the chromatogram

Dionex offers a new web service for a quick and easy search/view of chromatography applications using a web browser.

The new service will allow the user to browse applications and download all relevant information directly into the Chromeleon® Chromatography Data System (CDS).

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A CHROMATOGRAPHY APPLICATION

A chromatography application is the analysis and determination of certain properties of a sample, such as the amount of a compound of interest. The process consists of the following details:

- Instrument used for analysis
- Instrument settings including flow, injection volume, and detector wavelength
- Raw data including chromatograms, UV spectra
- Calculated peak results including retention times, area, and plates

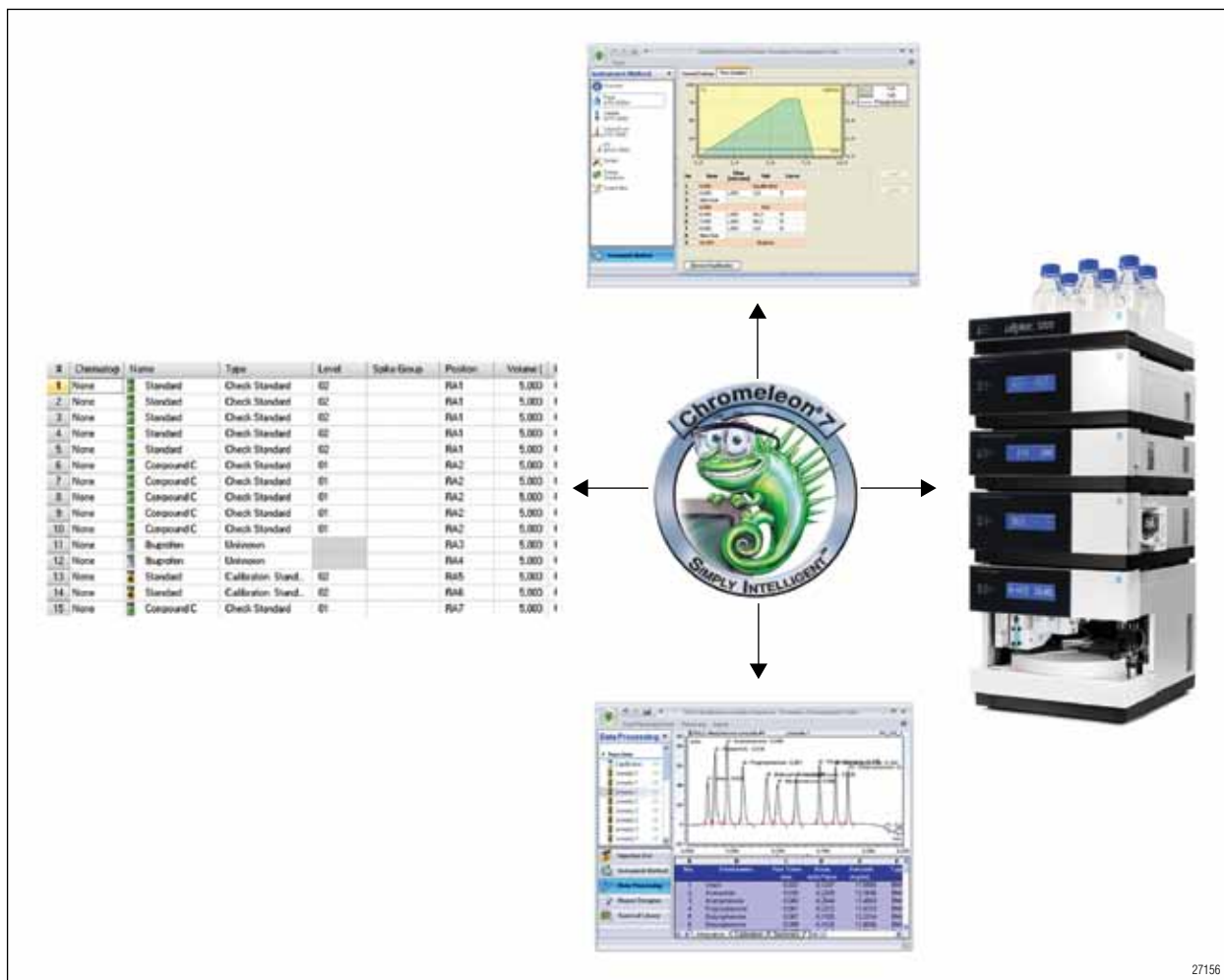
All details are stored in the chromatography data system. However, the information is distributed in several places:

- Raw data file
- Instrument settings in the configuration file or audit trail
- Sample information in the database
- Result information in the database or file

To describe a chromatography application consistently, all the information needs to be collected and synthesized in a format that is easily accessible to the analyst.

THE CHROMELEON CDS CONTAINS ALL RELEVANT INFORMATION

All the information describing an application is available in the Chromeleon software. The software's reporting capabilities are used to create an XML file with all the data required to describe the application (Figure 1). The resulting XML file is then uploaded into the application search database.



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Figure 1. Application details available in the Chromeleon CDS.

THE SEARCH VIEW

In the normal search view, customers can enter text to search. Figure 2 shows the resulting display of a simple search for the word *analysis*. The result list shows a chromatogram thumbnail, title and description, instrument type, market, matrix, and run time for each application found.

When results are displayed, keyword hits in the result list are highlighted. The highlighting is also maintained when viewing an application from the result list.

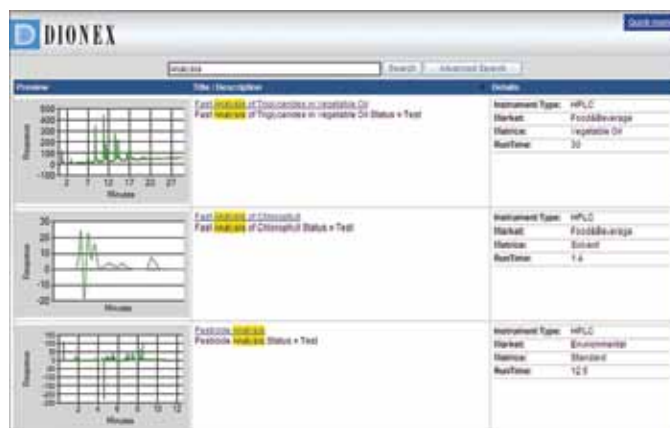


Figure 2. Search view.

ADVANCED SEARCH

A more detailed search is available when opening the *Advanced Search* feature (Figure 3). This includes:

- Full text search in title and description
- Market and matrix
- Method run time
- Instrument type, such as HPLC, IC, etc.
- Column manufacturer, model, length, internal diameter, packing material, and particle size
- Compound name and class



Figure 3. Advanced search.

By default, all conditions must be met when entering multiple conditions. If required, the logical condition can be changed to *OR*. It is possible to enter a range for numeric parameters, such as the application run time or the particle size. When only a minimum value is given, values larger than this are considered; when the maximum is set, only smaller values are considered.

Where applicable, available choices are shown in a list box (Figure 4). This list narrows as more words are typed.

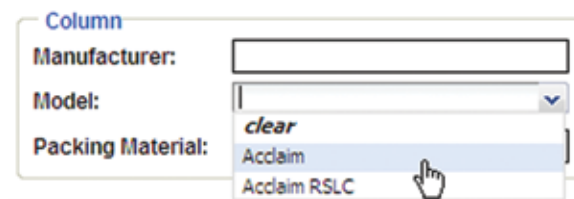


Figure 4. List of available choices.

VIEWING AN APPLICATION

An application can be viewed in detail by a click on the title or the chromatogram thumbnail (Figure 5).

The application view (seen in Figure 5) shows a chromatogram and the result table for each channel of interest on the left side. The chromatogram plot allows zooming, and the peak name and results for that peak are highlighted when hovering over the index mark of a peak.

On the right side of the application view, the description and the most important instrument parameters, such as wavelength and oven temperature, are also shown.

The gradient table, column details, and instrument model numbers are available through separate tabs (Figures 6–8).

On the lower right side, web links with related information and downloadable files, such as a template sequence or an eWorkflow (patent pending), can be provided (Figure 9).

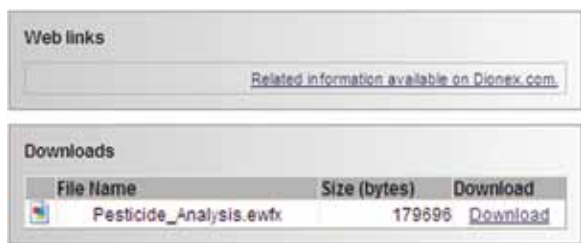


Figure 9. Links and downloads.

CONCLUSION

Here, a new, fast, and simple application service to browse through applications offered by Dionex is presented. Applications can be searched by name, description, instrument type and model, matrix, market, compound, and column details. All details of an application can be viewed online in a web browser. This includes details about the HPLC system, the column, gradient, and other instrument parameters. The web interface lists the integration results and a chromatogram view for each channel. This allows zooming into the chromatogram and investigating the data. Once a suitable application is found, a ready-to-run sequence template including report, instrument, and processing methods can be downloaded into the Chromeleon Chromatography Data System. This new application service provides the fastest way to find an application and start work in a few easy steps.

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