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Université Libre de Bruxelles Selects Agilent ELN to Manage Research Data

- January 2010

The Institute for Medical Immunology (IMI), a research institute of the Faculty of Medicine of the Université Libre de Bruxelles (ULB) has chosen Agilent Electronic Notebook (ELN) as the solution to manage their research data.

IMI users found Agilent ELN simple, powerful and intuitive to use. They were convinced from the start by both the architecture of the product and the support by the Agilent ELN team.

"The Agilent ELN is the perfect set of tools for organizing the large amounts of data generated by our scientists," said Dominique Demonté, deputy

director of the IMI. "It will also be helpful regarding the application of our internal intellectual property policy. We based our decision largely on the Agilent system's ease-of-use, architecture, and also on the level of support provided by the Agilent team."

Agilent ELN enables labs to share information and results digitally, helping them to become more connected, streamlined and productive. ELN makes it easy for managing scientific data and is flexible for capturing a variety of experiments. ELN's web based architecture was a key factor in ULB's decision to choose Agilent.



The IMI has been created with the support of the Walloon Region and GSK Biologicals to build a knowledge platform dedicated to medical immunology. This platform aims at delivering new concepts of immunointervention for human diseases by integrating basic and clinical research.

Announcements

New Releases - Now Available!

- Agilent ELN v4.0 SP2
- Wiley Registry 9th Edition with NIST09
- OpenLAB ICM v3.3.2 SP3

Upcoming Releases

- Lab Advisor B.01.03 SP2 - Early 2010

Upcoming Events

- PITTCON 2010 - Orlando, Florida
March 1-4, 2010
- IQPC Events
 - Smart Lab Exchange - Brussels, Belgium
March 17-18, 2010
 - Lab Informatics Forum - Boston
March 29-31, 2010



Announcing OpenLAB Empower 2 Interface Support for Empower 2 Feature Release 5 (FR5)

- Brad Snyder, OpenLAB ECM Product Manager

After working closely with the Waters Empower development team and completing a full customer validation testing cycle, Agilent is announcing the availability of the OpenLAB ECM Empower 2 Interface with support for the Waters Empower 2 Feature Release 5 (FR5).

What's New:

• FR5 Support:

- Agilent has tested the compatibility for customers that want to use the interface with the Empower FR5 release

• Removal of Empower 2 Toolkit Dependency:

- Toolkit is no longer required

• FULL compatibility with legacy (Empower 1) Data:

- Handles SampleSet and ResultSet retrieval situations where there are sample sets with no injections associated

- Fixed the situation where project uploads from the Empower 2 Workstation generated an incorrect project integrity error

• Minor updates to the documentation including:

- Updated Release Notes
- Updated IQ/OQ

For more information

To download the OpenLAB ECM Empower 2 Data Interface data sheet, visit the website at:

http://www.chem.agilent.com/en-US/Search/Library/_layouts/Agilent/PublicationSummary.aspx?whid=57318&iid=397

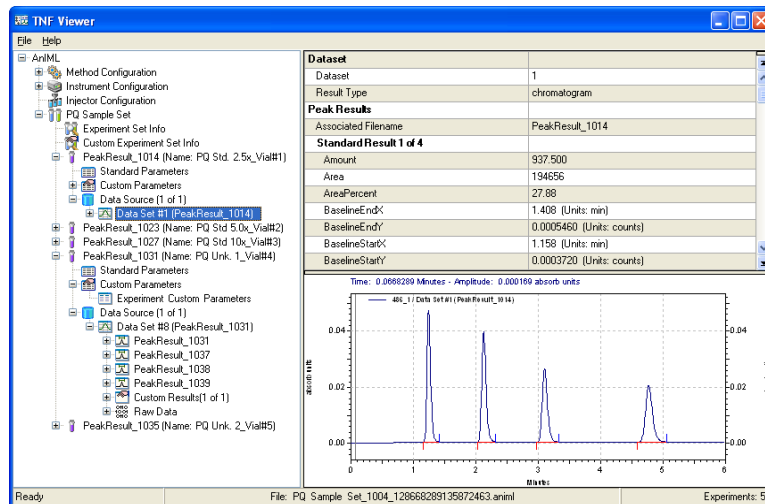


Figure 1: Empower data viewed from OpenLAB ECM

New Version of the Wiley/NIST Mass Spectral Library Now Released

- Anthony Gray, GC/MS Software Product Manager

Wiley-Blackwell and Agilent are pleased to announce the release of the Wiley Registry®, 9th Edition/NIST 2008 Mass Spectral Library (Wiley 9th/NIST08). The combined Wiley 9th/NIST08 library

contains compounds covering a wide range of applications – including pathology, food safety, food quality, environmental science, and general chemical analysis.

The release of the 9th edition celebrates the 40th anniversary of Wiley publishing the Wiley Registry® with Dr. Fred McLafferty.

The new library has a significant increase in the number of compounds, the number of spectra, and number of structures from the previous version of the Wiley/NIST combination library. The combined library contains (approximately):

- 796,000 spectra,
- 667,000 compounds,
- 746,000 spectra with chemical structures, and
- 2.9 million names

The combined Wiley 9th/NIST08 library is the largest mass spectral library ever commercially available. As seen in

Figure 1, the combined library contains more than three times the number of spectra in the NIST 2008 library.

The Wiley 9th/NIST08 was released January, 2010.

System requirements: Windows XP SP3, Windows VISTA SP2, Windows 7, DVD drive, 2GB free disk space. The Wiley Library is compatible with both MSD ChemStation (G1701EA & G1710EA) and MassHunter Workstation.

For more information

For more information please contact your local Agilent representative.

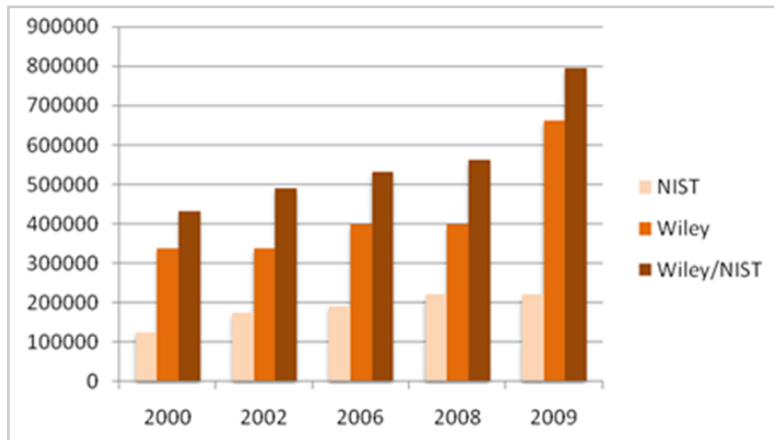


Figure 1: Library Spectral Content - 2000 to 2009



Post-Run Adjustment for Retention Time Variability

- Brian Rohrback / Infometrix, Inc.
- Jon Welsh, EZChrom C/S Product Manager
- Chet Sharrar, GC Software Product Manager
- Ute Bober, ChemStation Product Manager

All forms of chromatography are subject to column and sampling variability. In many applications, this fluctuation forces the operator to review and occasionally intervene to insure precise, reproducible peak identification and quantitation. As a result, eliminating retention time variability has been an oft-stated goal where accurate identification is required for improved data analysis.

It is possible to use a software mechanism for correcting shifts in retention time resulting from normal operation of a GC or HPLC. The LineUp™ version 3.0 software is available from Infometrix, Inc. and can be integrated into both Agilent chromatography systems: EZChrom Elite and ChemStation. LineUp uses a form of the external standard approach, where a reference chromatogram is used as a target and adjustments are made to the current chromatogram to match the target as closely as possible. The original data file is retained and a companion, aligned chromatogram is created, adding to the EZChrom .DAT file or the ChemStation .D directory.

Because this approach requires no intervention by the operator, it can be run as part of an unattended chromatographic sequence. Interestingly, the proper handling of retention time shifts appears to minimize the need to recalibrate for most applications. Expected retention windows for integration can be tightened as there is less chromatographic drift to account for run-to-run. For instance, a quality control run on fuel-grade kerosene is compared to the product standard within EZChrom, shown in figure 1.

Additionally, in figure 1, the QC sample is shown in blue with the target

reference in red. LineUp adjusts the retention axis to match the “gold standard” for this analysis by creating a companion chromatogram in the EZChrom binary file; this aligned profile is shown in green. The software can do this alignment process for up to two independent columns, as shown above. It is useful to note that the alignment does not depend on a constant shift, shift in a single direction, nor the presence of marker peaks within the chromatogram. Peak populations must be similar, but not all peaks need to be present and the peaks do not have to display consistent relative concentrations. Variance in solvent mixing (HPLC) or temperature programming (GC) can cause peaks to shift in different directions within the same chromatogram, but this is also accounted for by the algorithm.

With alignment in place, it is practical to compare chromatograms from multiple instruments as long as they are running substantially the same method and use similar columns and conditions. Even data from the historical record can be retrieved and brought into alignment with a more modern gold standard. This allows a company to create a consistent world-wide database, completely eliminating variability caused by instrument-to-instrument and time-to-time differences. You can mine a multi-year chromatographic data set for associated trends and groupings much more easily. This also means that standards run on one instrument can be shared *as data files* with any other instrument, thus minimizing calibration requirements.

To demonstrate, a set of three different chromatographs with nominally identical methods and configuration were given the same sample to

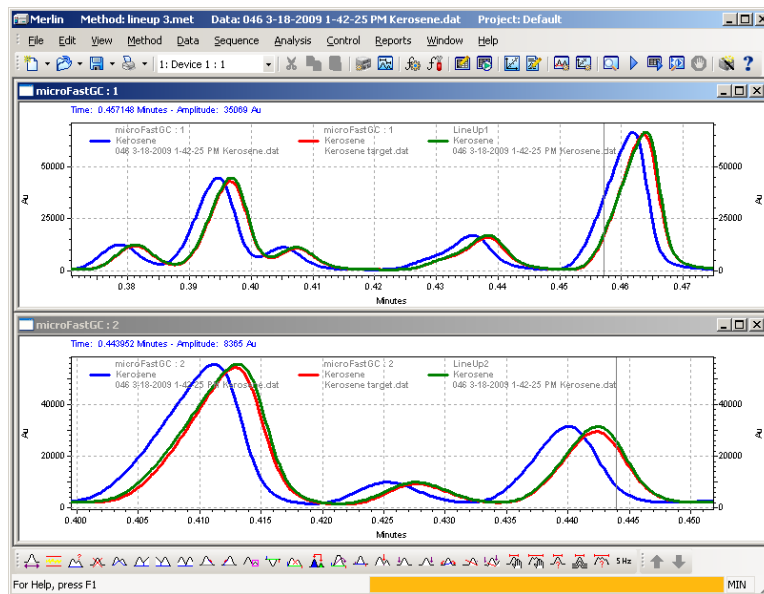


Figure 1: Quality control run on fuel-grade kerosene is compared to the product standard within EZChrom.

process. Applying the alignment algorithm, the differences in retention time are insignificant, allowing direct comparison of the chromatographic traces. In this case, the retention time shift is between one and two peak widths. Experience has shown that variations up to six peak widths can be handled by LineUp without creating a delay in the data processing (see figure 2 below).

For the latest releases of EZChrom Elite (version 3.3.1 or later), the LineUp parameters can be set inside the Elite Instrument Setup to completely integrate alignment into the method. ChemStation integration requires System Version A.06 or later and can handle 5890s, 6850s, 6890s and 7890s.

For more information

For information on EZChrom Elite C/S, please contact Jon Welsh at: jon_welsh@agilent.com

For information on GC Software, please contact Chet Sharrar at: chet_sharrar@agilent.com

For information on ChemStation, please contact Ute Bober at: ute_bober@agilent.com

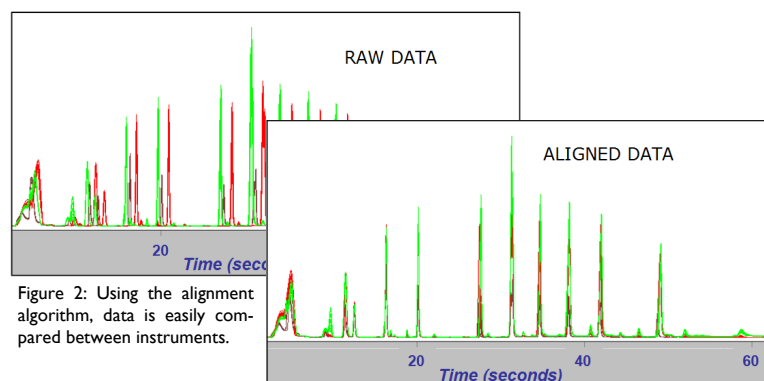


Figure 2: Using the alignment algorithm, data is easily compared between instruments.

