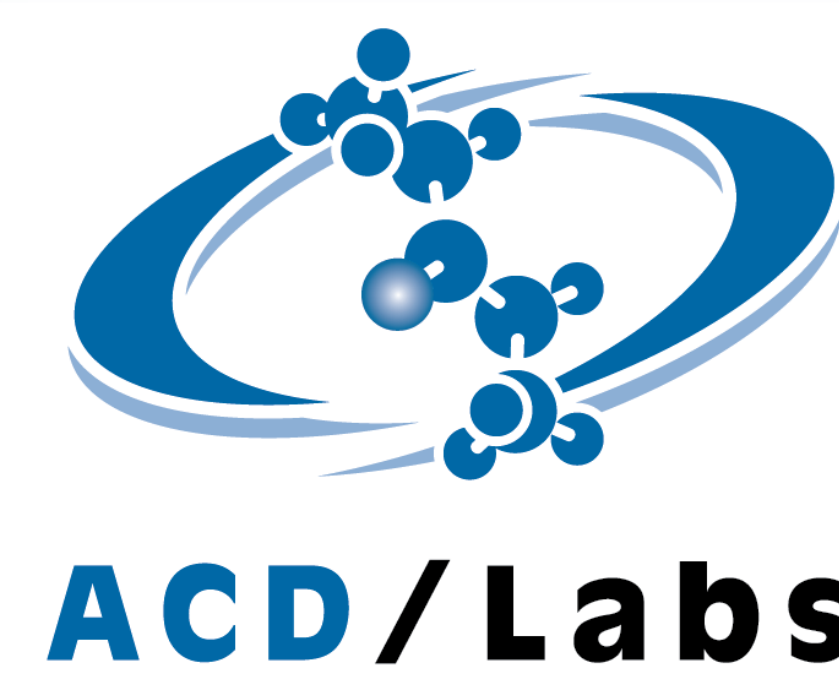


Can a Unified Laboratory Intelligence Approach be Applied to E&L Studies?



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INTRODUCTION

Controlled extraction studies aim to obtain extensive analytical data for drug containers and medical devices, and therefore recognize compounds and materials that may generate safety and performance concerns. It is, however, a challenge to sift and interpret data to find extractable signals from different instruments, especially when using a variety of hyphenated chromatography–mass spectrometry analyses. Therefore informatics technologies and software automation of workflows are becoming key strategic considerations for identification, elucidation, and characterization of extractables and leachables (E&L).

This work describes how an informatics platform embodying unified laboratory intelligence (ULI) can be applied to managing, analyzing, and interpreting GC, LC, and other analytical data; then using it to create and search a knowledgebase of identified compounds. Data processing workflows can be automated, and such a knowledgebase allows for simplified review of results and creation of summary reports and data packages.

THE UNIFIED LABORATORY INTELLIGENCE (ULI) PLATFORM

Scientific insights stem from analysis of new and existing data, so the variety of analytical instruments and informatics systems poses a real challenge for many organizations to manage data into a digital, standardized, accessible, and easily reusable format. Automated conversion into a standardized, normalized, structured format in a homogeneous environment is one foundational aspect of unified laboratory intelligence. When unified chemical, structural, and analytical information is stored this way it provides chemical content (what) with context (why), which reduces information related costs, inconveniences, or risks, and offers a platform for more agile decision making. Figure 1 indicates how ACD/Spectrus provides a software platform on which raw and processed data from different instruments within and across laboratories can be collected and converted to homogeneous structured data with metadata, automatically.

DISCUSSION

The vendor instruments used to collect data for extractables studies are typically GC with FID and MS detectors to enable semi-quantitation and compound identification by spectral matching. LC with UV and MS is used to find polar and GC labile compounds. Data may thus be in a variety of different file formats, which ACD/Labs specializes in handling as shown in Figure 1. Algorithms like ACD/Labs IntelliXtract and IntelliTarget can be used manually or with automation to automate LC non-targeted and targeted screening compounds, while ACD/IXCR can help with GC/MS, with an output exported to a database shown in Figure 2.

In addition to advanced tools for characterization and identification of compounds using LC/UV/MS and GC/MS data, ACD/MS Workbook Suite also facilitates knowledge-sharing through the creation of libraries of structures, spectra, and chromatograms, and customized reporting capabilities. An example of LC/UV/MS data handling in the processing interface is indicated for a plastic bottle extract shown in Figure 3. Key data can be extracted to the knowledgebase as shown for GC in Figure 2. Other types of data can be included, as indicated in Figure 4, which shows a set of polymer UV spectra including some spectral assignments. Client views are configurable.

FIGURE 2. GC Data (Grob Mixture) Processed and Results in Knowledgebase Client Interface

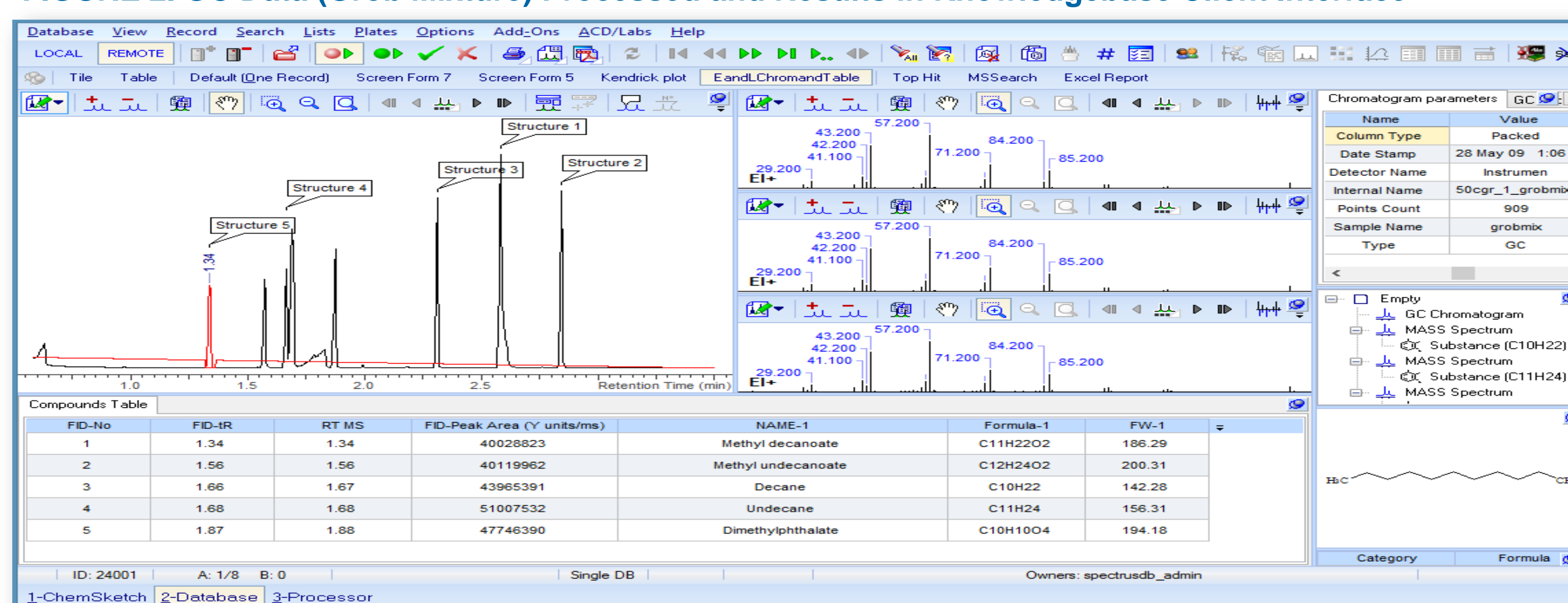


FIGURE 3. LC Data (Bottle Extract) in Client Interface

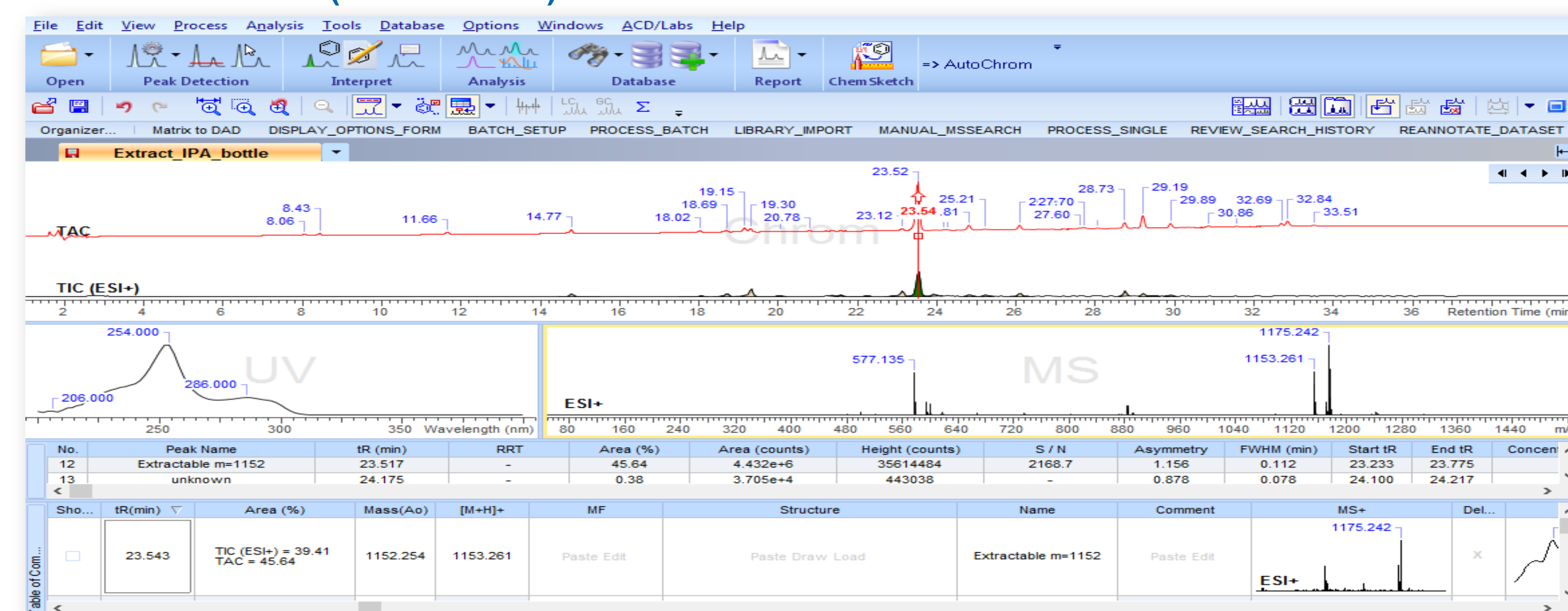


FIGURE 4. UV Data (Polymer) in Knowledgebase Client Interface

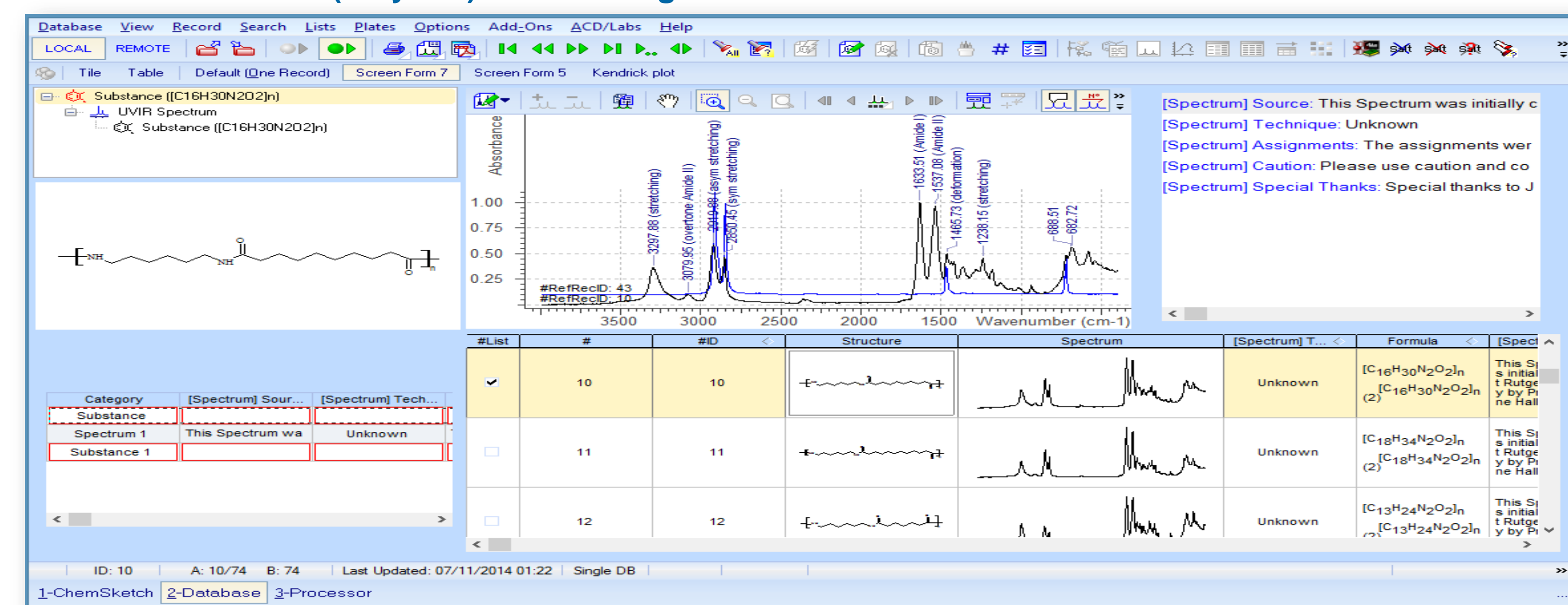
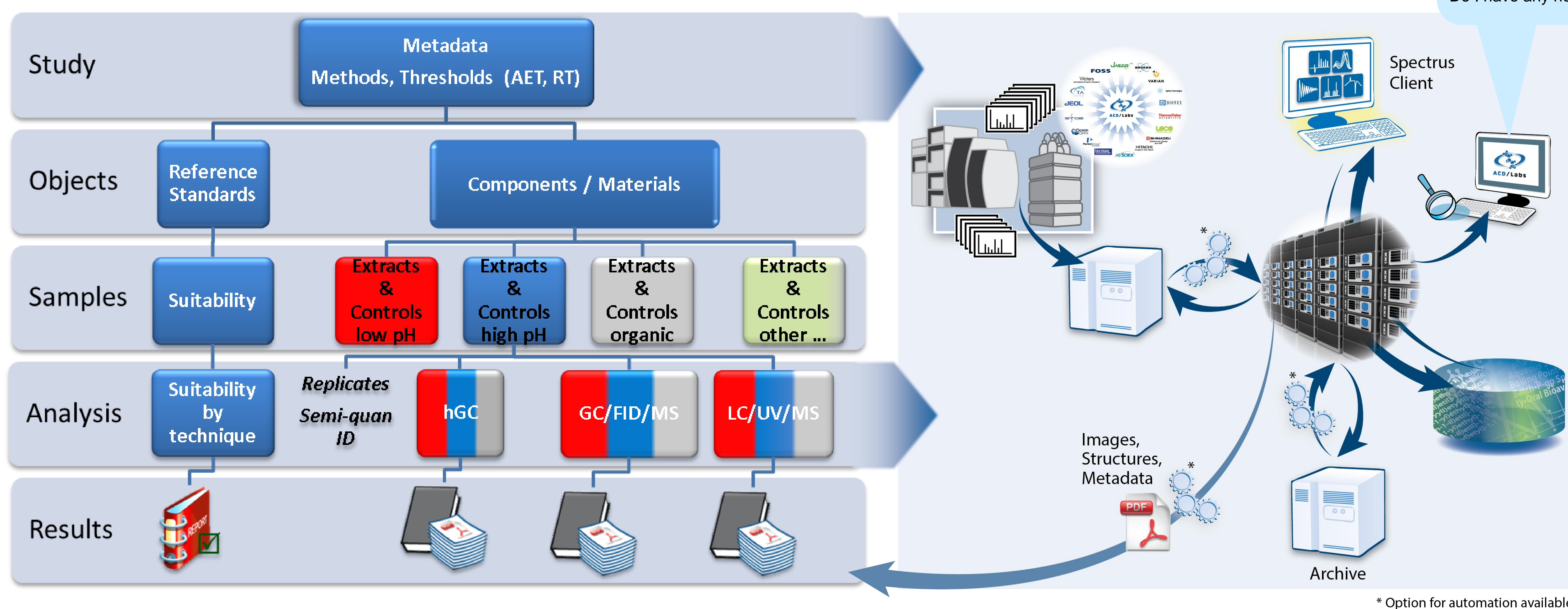


FIGURE 1. ULI Enables Data Generation Workflows to Provide Knowledge Management with Access to Live Data and Information

The platform enables data processing, manual to automated, with scripting configuration to handle aspects of comparisons, semi-quantitation, collation of data, and results. Identification steps are aided by powerful algorithms for extracting features and conducting searches against databased information, whether spectra from commercial libraries or self-built ones. Data, structures, and results are stored in the knowledgebase and can be queried to find or recognize already known information. Reports can be generated and also stored in the knowledgebase.

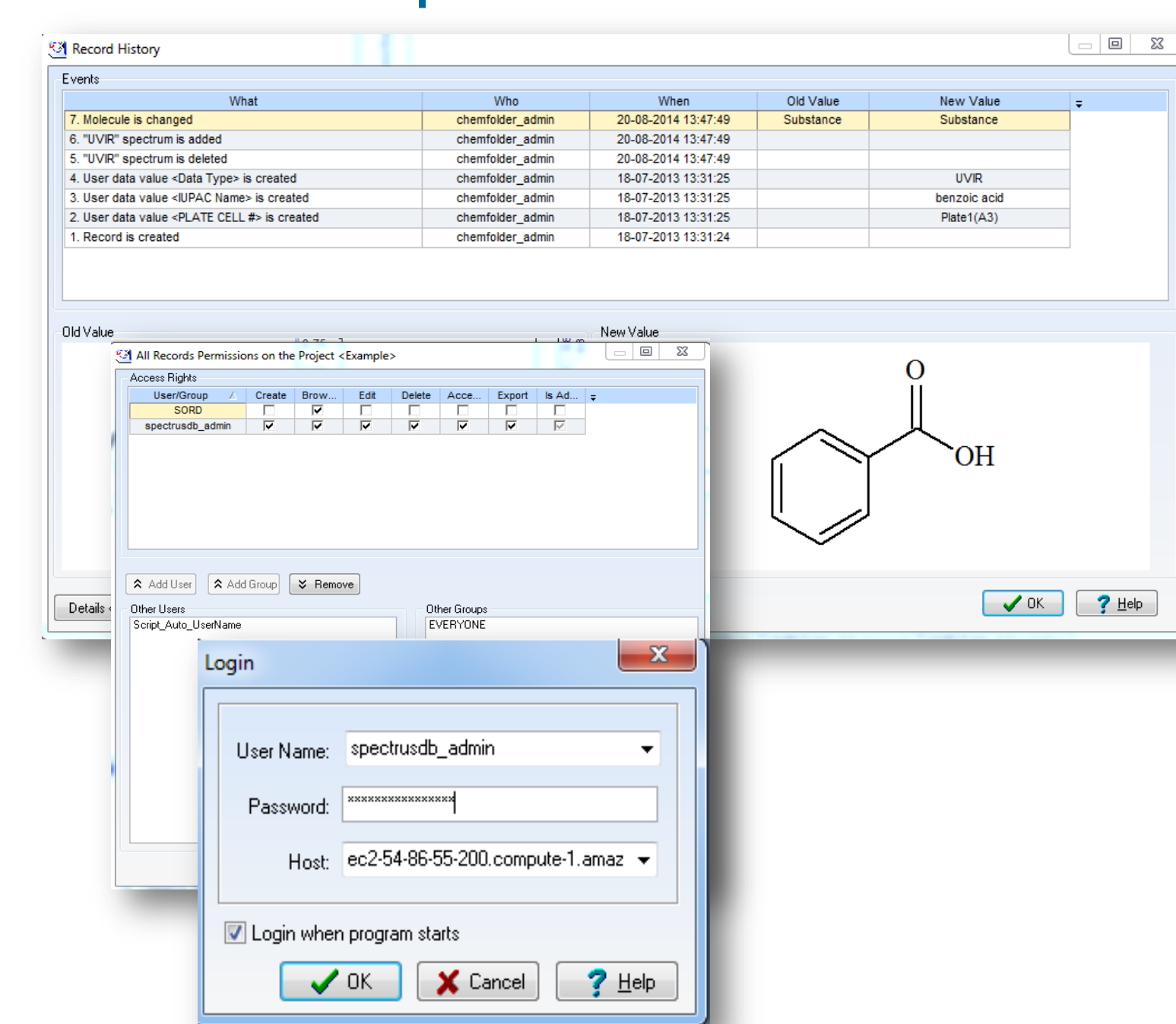


Where have I seen this extractable before?
Have I seen this peak or spectrum before?
Do I have any new concerns?

SUMMARY

- The platform allows manual and automated data handling
- A variety of types and formats of data can be handled
- Workflows can be configured
- Summaries and reports can be generated using templates and through automation
- Features of the ACD/Spectrus Platform provide user access control, permissions controls, audit trail via record histories, and electronic signature capabilities (see Figure 5)

FIGURE 5. Compliance Related Features



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