Allotrope Connect Virtual Workshop
MassSpec ADF: a full data “round-trip” - From raw data conversion from Sciex Analyst to reopen ADF
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Data-centric System Architecture

Escape interfacing gridlock in – Unlock Data from Apps

Status quo (examples)

// bilateral interfaces
// Raw data is locked in source systems
// changes costly and difficult

Target state

// separation of apps & data
// standardizing data access
// streamlined interfacing
// interlink data assets
SCIEX ADF Viewer

• Stand-alone application
• Creates ADF files from SCIEX Analyst® mass spectrometry data
  – Includes:
    • Raw spectra
    • Method information
    • Quantitated data
    • Audit trails
    • Native files
• Uses SCIEX Analyst®-specific model
SCIEX ADF Viewer

- Reads (SCIEX) ADF files
- Displays data in tabular and hierarchical format
- Displays Total Ion Chromatograms, Extracted Ion Chromatograms
- Exports data description to Turtle (ttl) and XML format
SCIEX ADF Viewer

• Uses SCIEX-specific vocabulary
• Vocabulary is customizable
  – Allows administrative user to customize URIs
    • Vocabulary URIs
    • Unit URIs
SCIEX ADF Viewer

• Demo
Work planned or in-process

- Integration with ADF Explorer
- Harmonization with MS Data Shape
- Documentation
- GLP Support (e.g., software validation)
- Support for SCIEX Multiquant, SCIEX OS software
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