Creating ADF output from Chromeleon

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What is Chromeleon CDS?

Chromeleon Chromatography Data System

- Industry-leading multi-vendor instrument control
- Robust enterprise deployment
- Simple workflows with one-click sequence creation
- Admin-controls ensure data integrity and enable GxP compliance
- Full integration with SampleManager LIMS
## High-level Use Cases

<table>
<thead>
<tr>
<th>Injection</th>
<th>Sequence</th>
<th>Experiment</th>
<th>Project</th>
</tr>
</thead>
</table>
| • ADF created as soon as injection has acquired  
  • Automatic generation at end of injection  
  • Raw data only  
  • Minimal processing | • ADF created after all samples in sequence have acquired  
  • Automatic generation at end of sequence  
  • Raw data, processed results | • ADF created after one or multiple Sequence(s) have been acquired and analysed  
  • Manual export action  
  • Raw data, processed results, reports | • ADF created after completion of all analyses in a project  
  • Manual / batch export action  
  • Raw data, processed results, cross-sequence reports, etc |
• The Console shows all sequences available for export
An “Export” option is available from the context menu.
Data Export

- “Allotrope data file format (*.adf)” option available from the Export dialog

- The output file name can be configured according to a defined formula

* This slide contains forward-looking statements based on current expectations and assumptions which involve risks and uncertainties that could cause actual results to vary materially from those stated or implied.
• Dialogs appear to inform the user of progress

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• ADF created for each Sequence selected
• Data Description for each injection includes: name, type, method names, vial position, injection volume, status and time

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Viewing the ADF file – Data Cubes

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Viewing the ADF file – Data Package

- Basic information is written to the Data Package

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Automated ADF creation

- For routine output in ADF, select “Export report” option in Sequence Properties
- Choose “After whole sequence” or “After each injection”
- Select ADF as output file type in Report Template
- Enforce auto-export option in Instrument Properties

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Next steps

• Plan to increase content of ADF output:
  • Full Sequence data
  • Processing methods
  • Full Processing results
  • Instrument methods
  • Mass Spec data and results
  • Report contents

• Incorporate feedback from today and from yesterday’s poster and group sessions

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These use-cases are all prototyped in Chromeleon – need to increase the ADF content - release timeframe is currently in planning

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QUESTIONS?