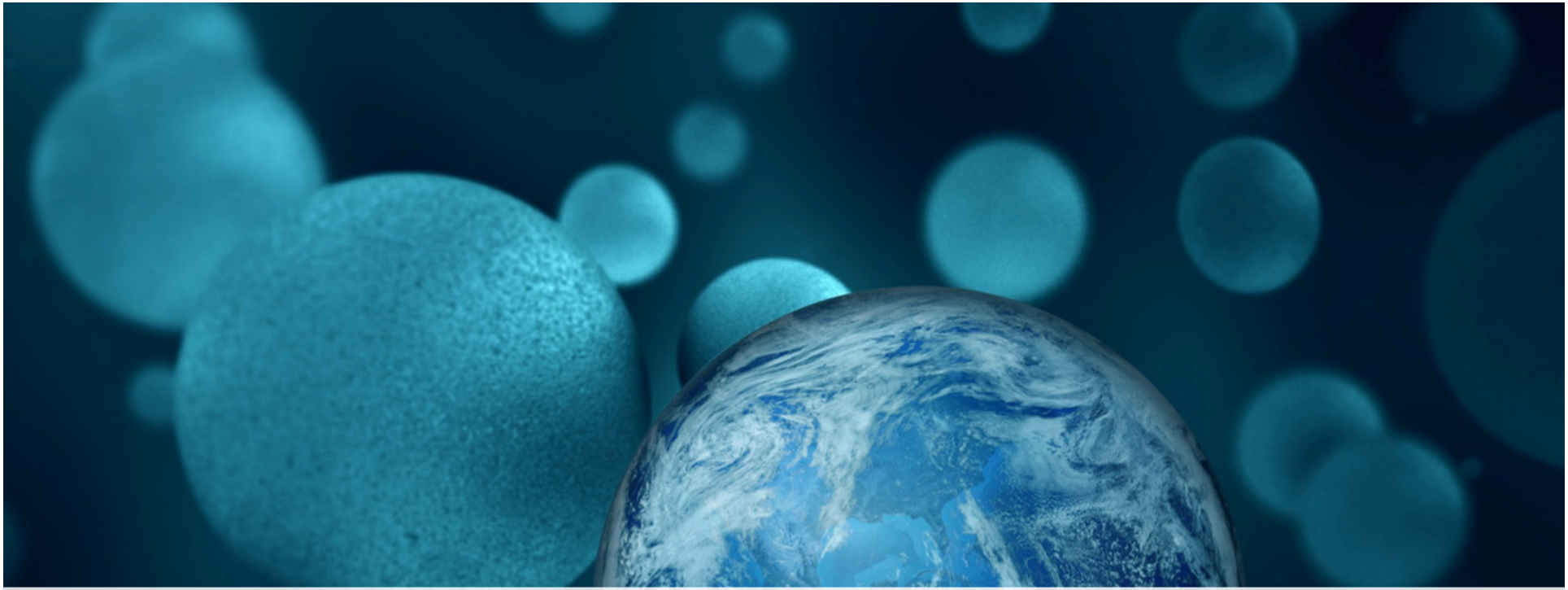

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Creating ADF output from Chromeleon

Greg Whitaker
Chromatography Software Product Manager
25-April-2018

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

Injection

- ADF created as soon as injection has acquired
- Automatic generation at end of injection
- Raw data only
- Minimal processing

Sequence

- ADF created after all samples in sequence have acquired
- Automatic generation at end of sequence
- Raw data, processed results

Experiment

- ADF created after one or multiple Sequence(s) have been acquired and analysed
- Manual export action
- Raw data, processed results, reports

Project

- ADF created after completion of all analyses in a project
- Manual / batch export action
- Raw data, processed results, cross-sequence reports, etc

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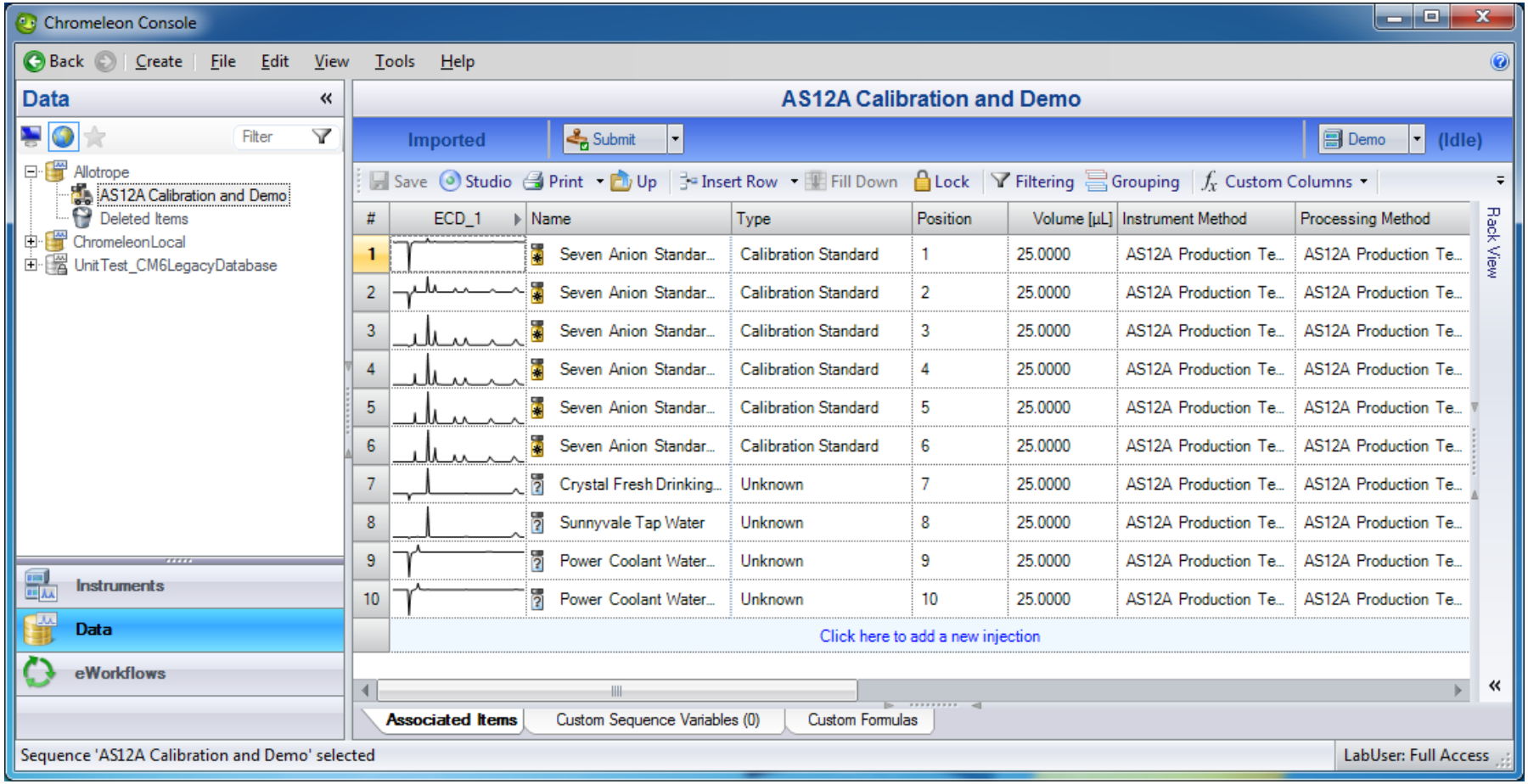
Chromeleon Console

- The Console shows all sequences available for export



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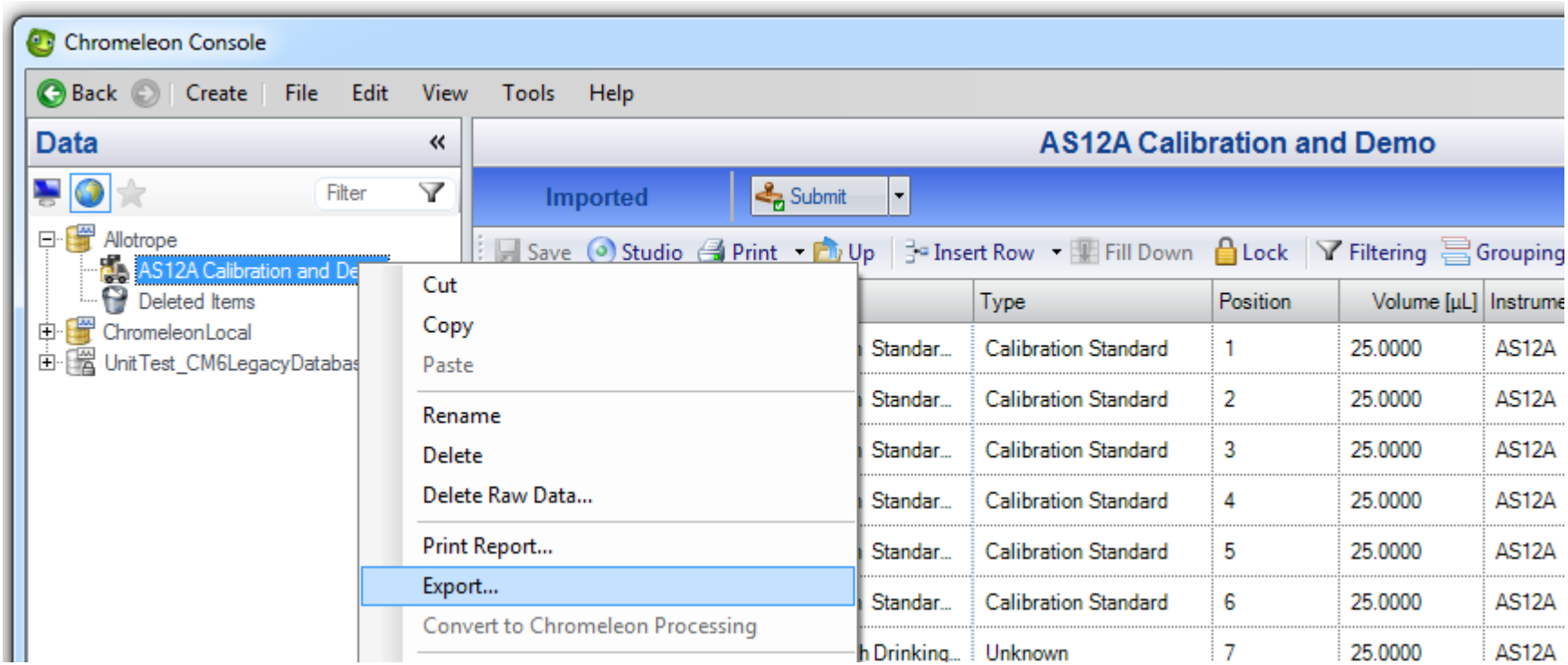
Chromeleon Console

- An “Export” option is available from the context menu



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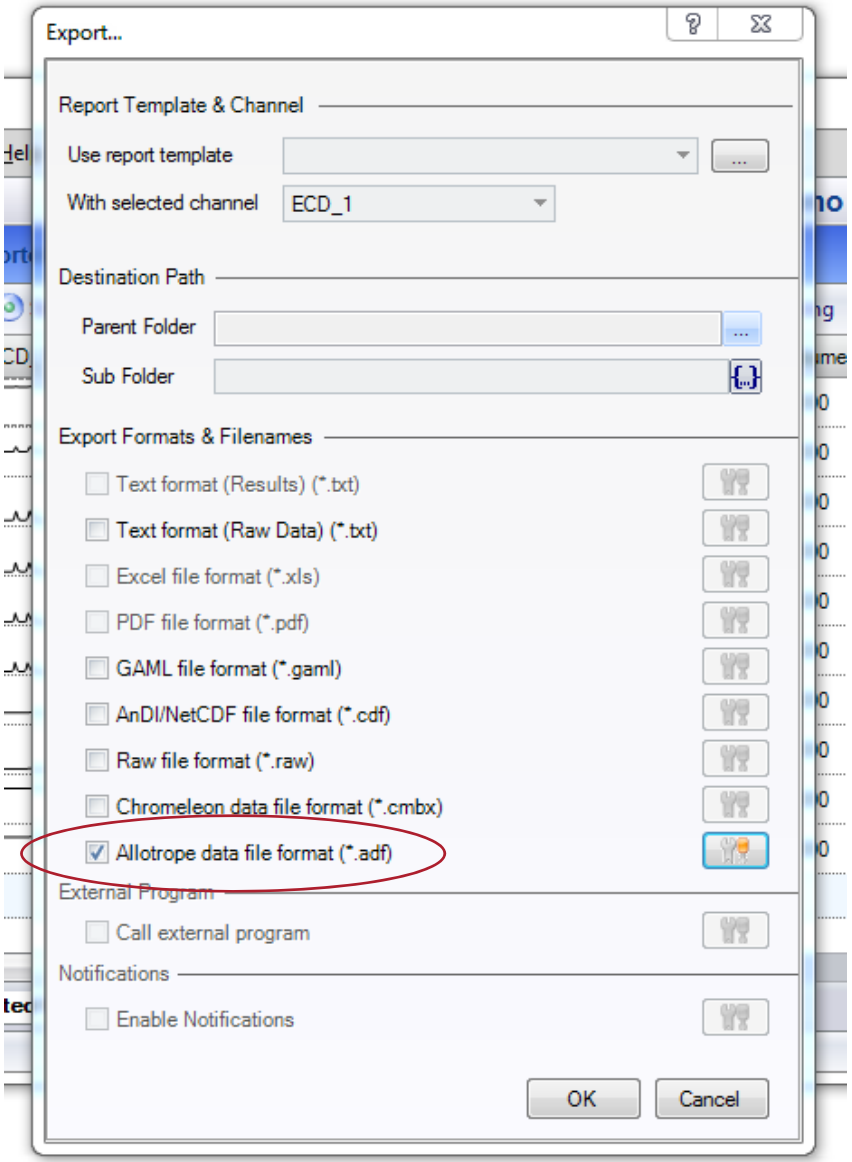
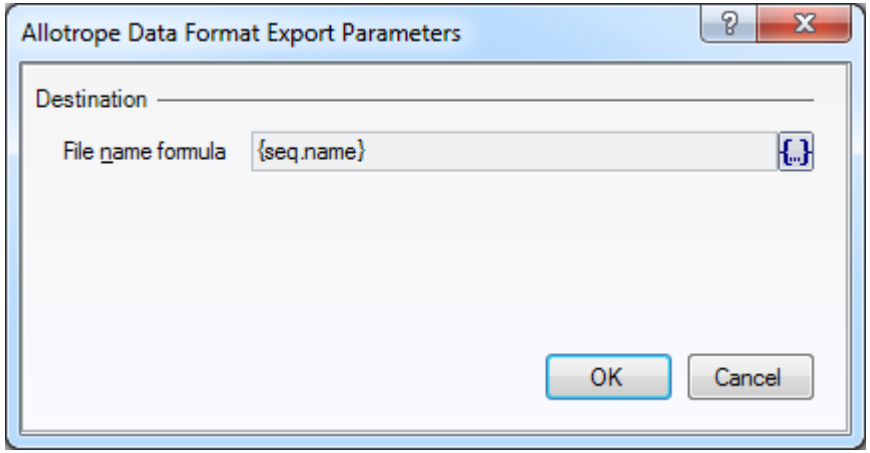
Data Export



- "Allotrope data file format (*.adf)" option available from the Export dialog
- The output file name can be configured according to a defined formula



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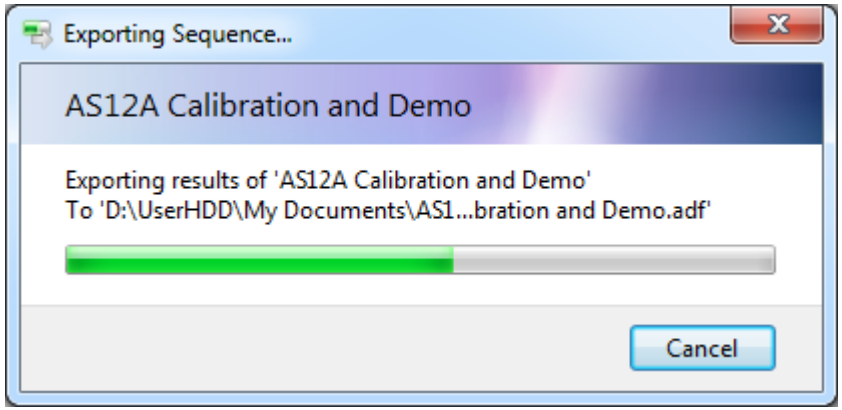
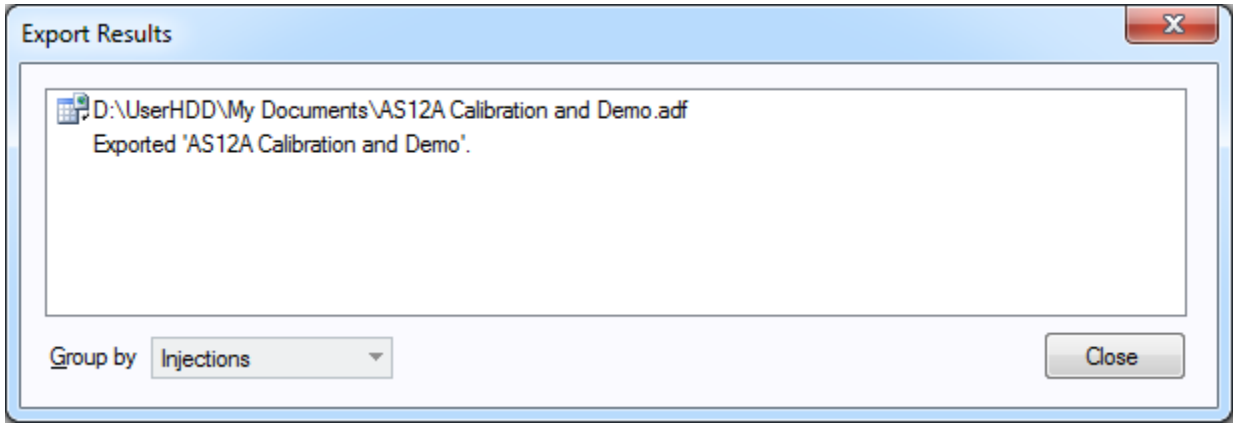
Data Export

- Dialogs appear to inform the user of progress





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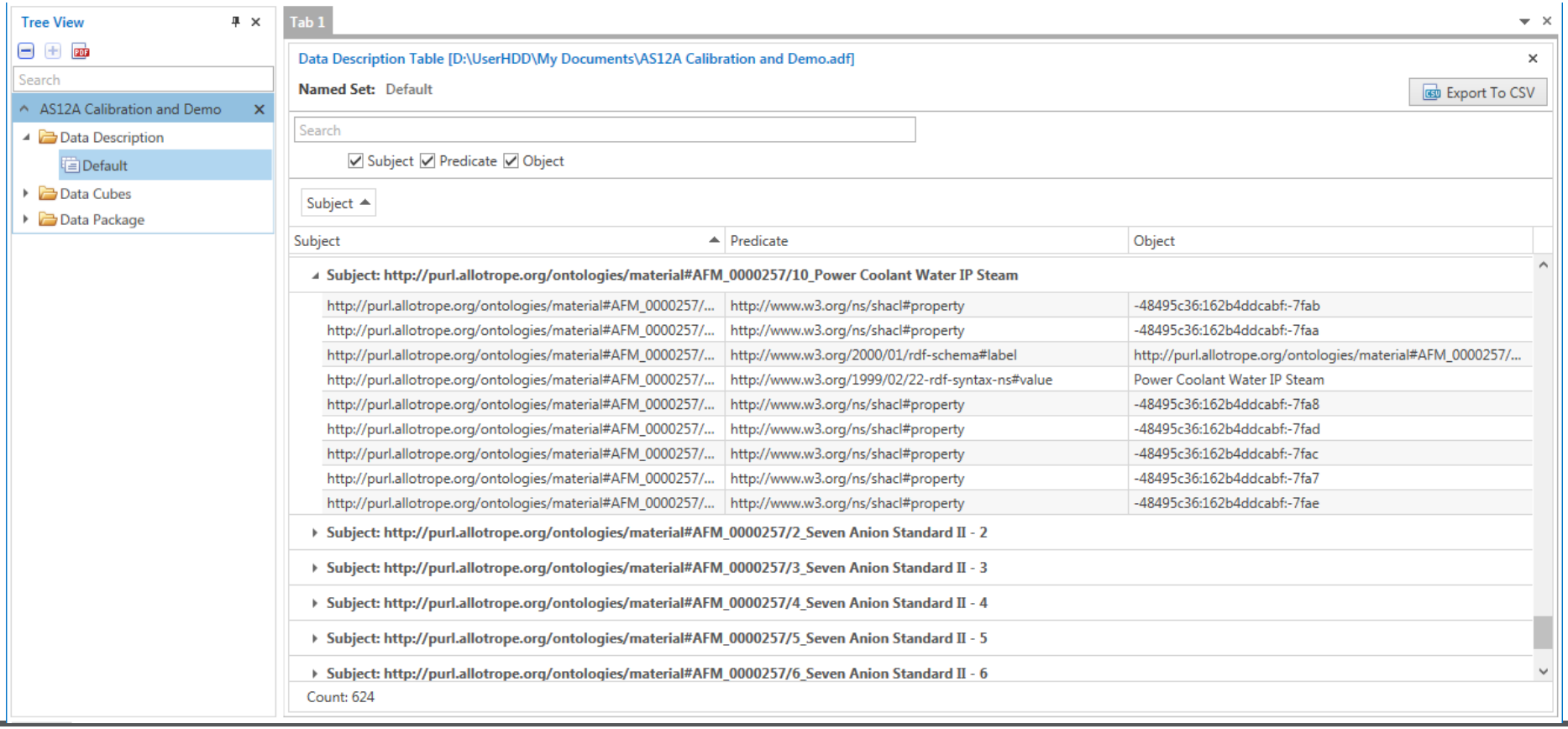
Viewing the ADF file – Data Description

- 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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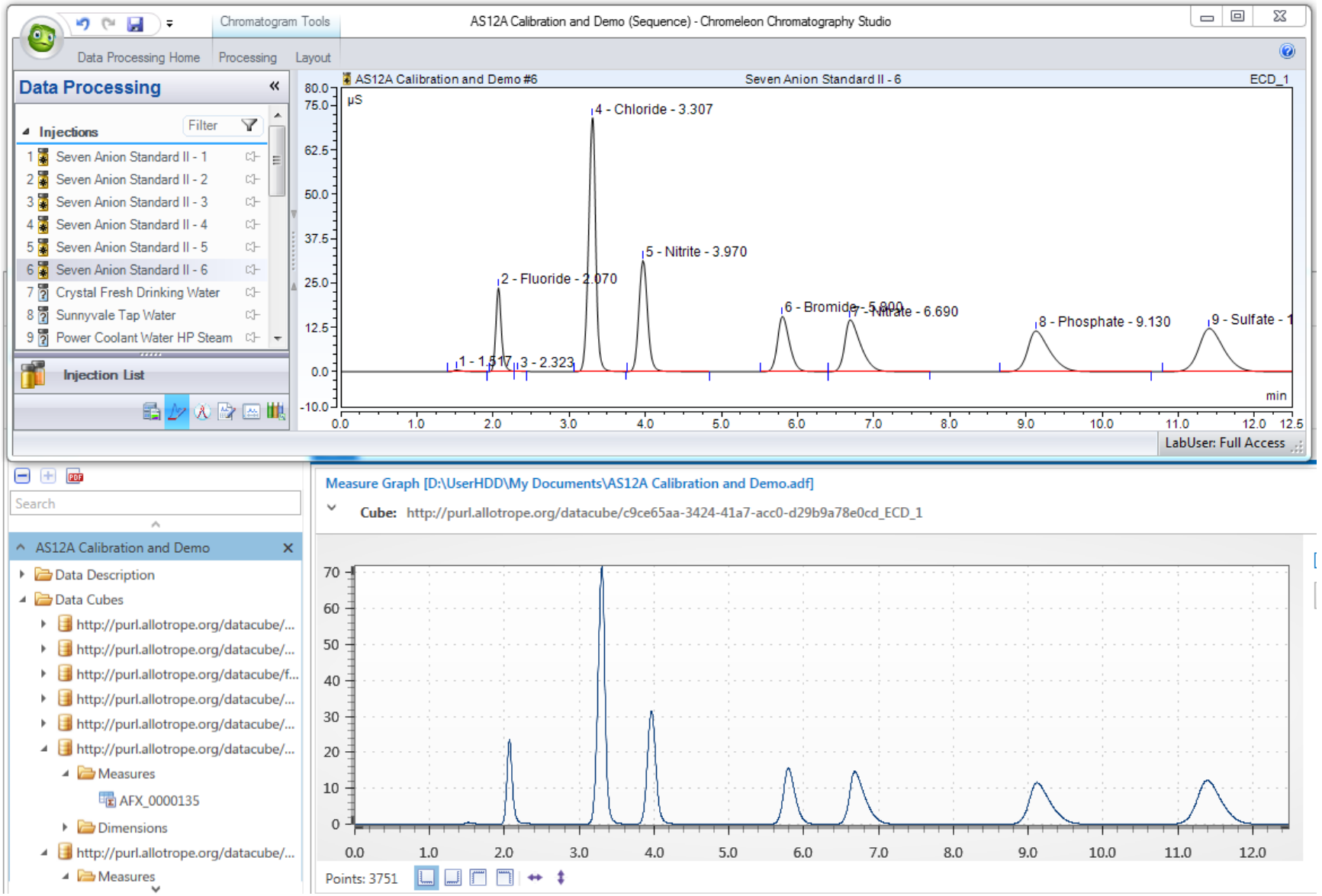
Viewing the ADF file – Data Cubes



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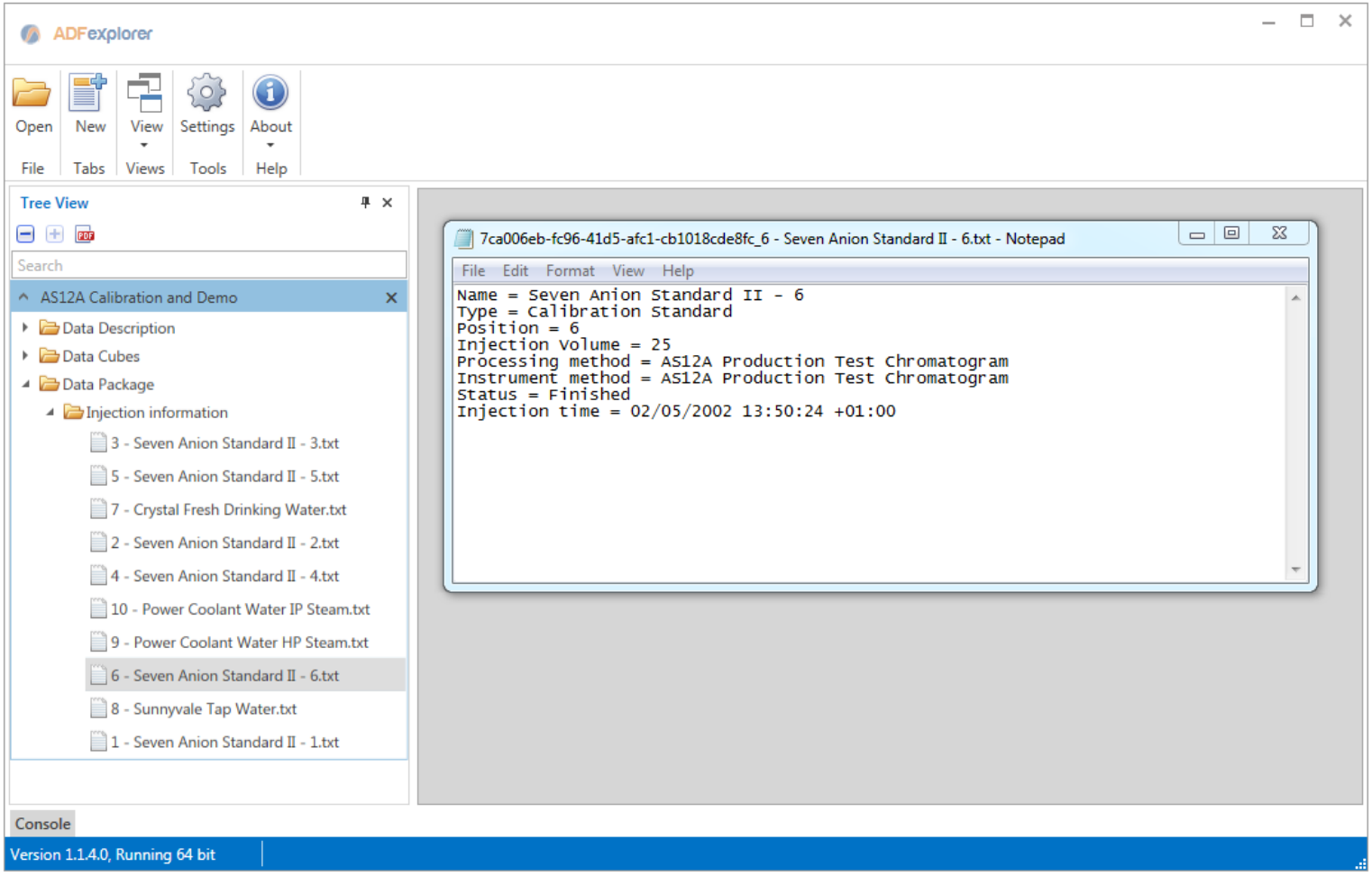
Viewing the ADF file – Data Package

- Basic information is written to the Data Package



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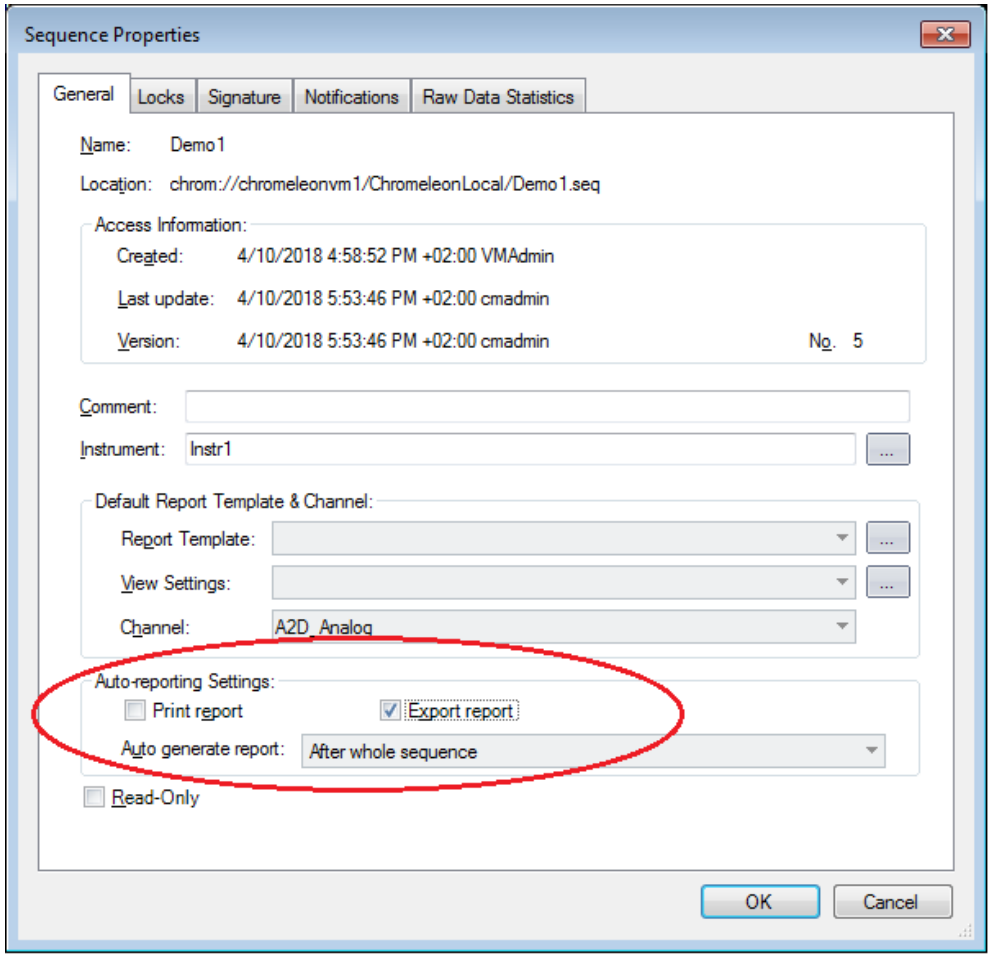
Automated ADF creation

- 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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