

ThermoFisher
S C I E N T I F I C

Creating ADF output from Chromeleon

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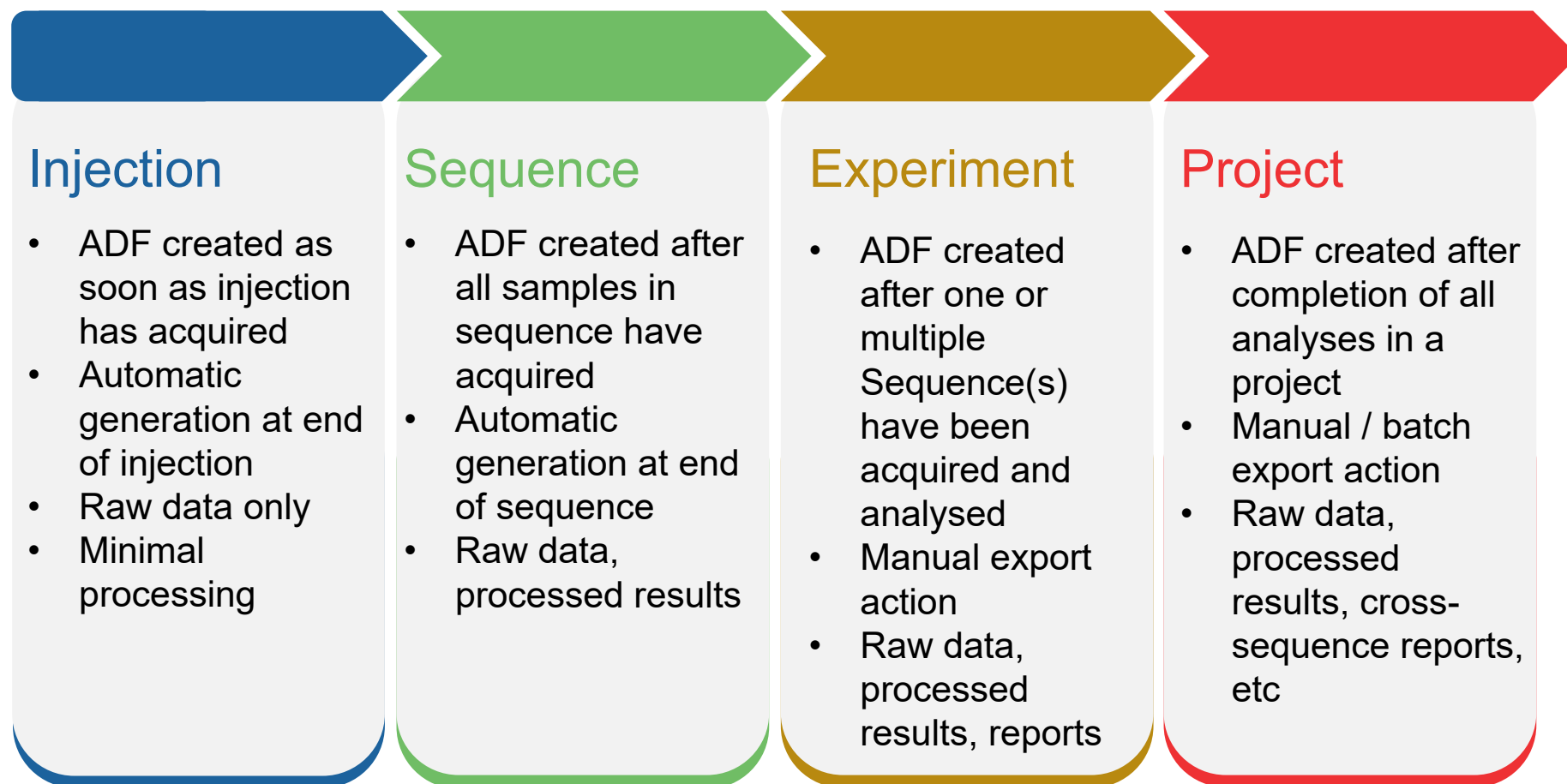
What is Chromeleon CDS?



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



Chromeleon Console

- The Console shows all sequences available for export

The screenshot displays the Chromeleon Console software interface. The main window is titled 'AS12A Calibration and Demo'. On the left, a 'Data' sidebar shows a tree view with folders like 'Allotrope', 'AS12A Calibration and Demo', 'Deleted Items', 'ChromeleonLocal', and 'UnitTest_CM6LegacyDatabase'. The main area features a table of sequences with columns: #, ECD_1, Name, Type, Position, Volume [μL], Instrument Method, and Processing Method. The table lists 10 sequences, including 'Seven Anion Standar...' (Calibration Standard) and 'Crystal Fresh Drinking...' (Unknown). A 'Rack View' sidebar is on the right. At the bottom, a status bar shows 'Sequence 'AS12A Calibration and Demo' selected' and 'LabUser: Full Access'.

#	ECD_1	Name	Type	Position	Volume [μL]	Instrument Method	Processing Method
1		Seven Anion Standar...	Calibration Standard	1	25.0000	AS12A Production Te...	AS12A Production Te...
2		Seven Anion Standar...	Calibration Standard	2	25.0000	AS12A Production Te...	AS12A Production Te...
3		Seven Anion Standar...	Calibration Standard	3	25.0000	AS12A Production Te...	AS12A Production Te...
4		Seven Anion Standar...	Calibration Standard	4	25.0000	AS12A Production Te...	AS12A Production Te...
5		Seven Anion Standar...	Calibration Standard	5	25.0000	AS12A Production Te...	AS12A Production Te...
6		Seven Anion Standar...	Calibration Standard	6	25.0000	AS12A Production Te...	AS12A Production Te...
7		Crystal Fresh Drinking...	Unknown	7	25.0000	AS12A Production Te...	AS12A Production Te...
8		Sunnyvale Tap Water	Unknown	8	25.0000	AS12A Production Te...	AS12A Production Te...
9		Power Coolant Water...	Unknown	9	25.0000	AS12A Production Te...	AS12A Production Te...
10		Power Coolant Water...	Unknown	10	25.0000	AS12A Production Te...	AS12A Production Te...

Click here to add a new injection

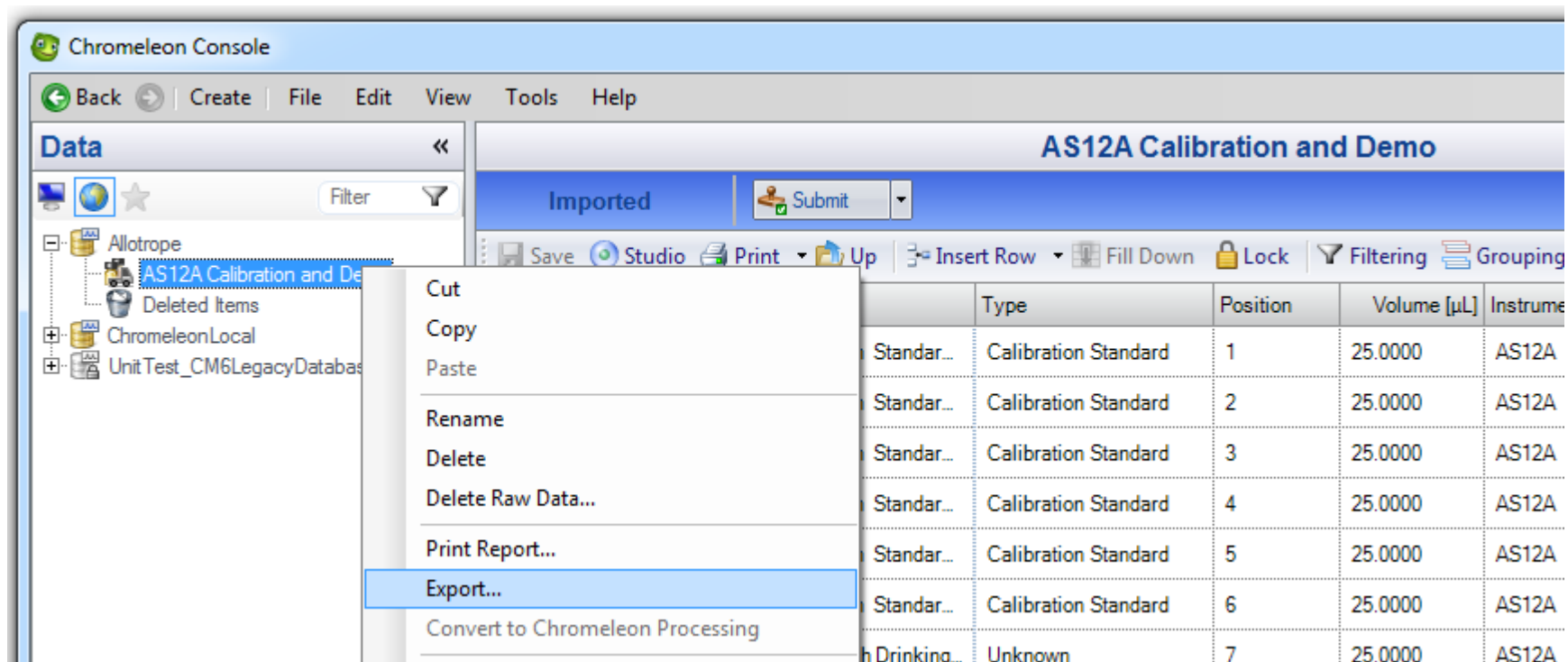
Associated Items: Custom Sequence Variables (0) Custom Formulas

Sequence 'AS12A Calibration and Demo' selected

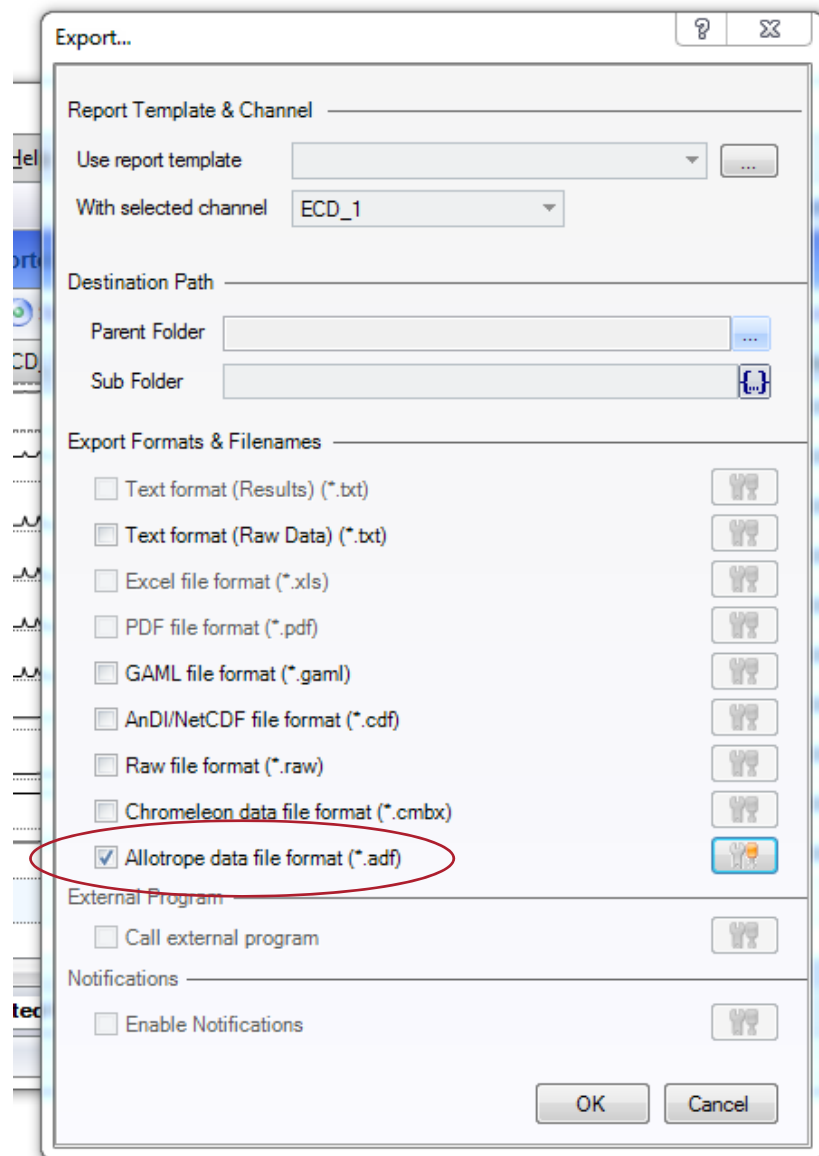
LabUser: Full Access

Chromeleon Console

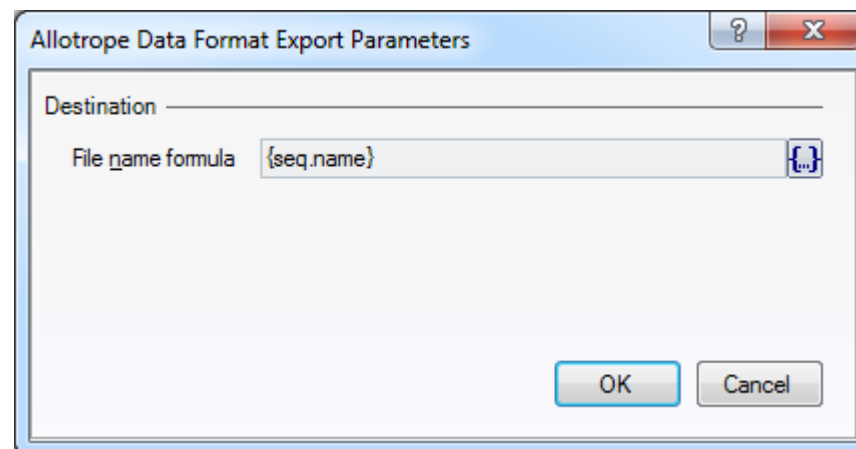
- An “Export” option is available from the context menu



Data Export

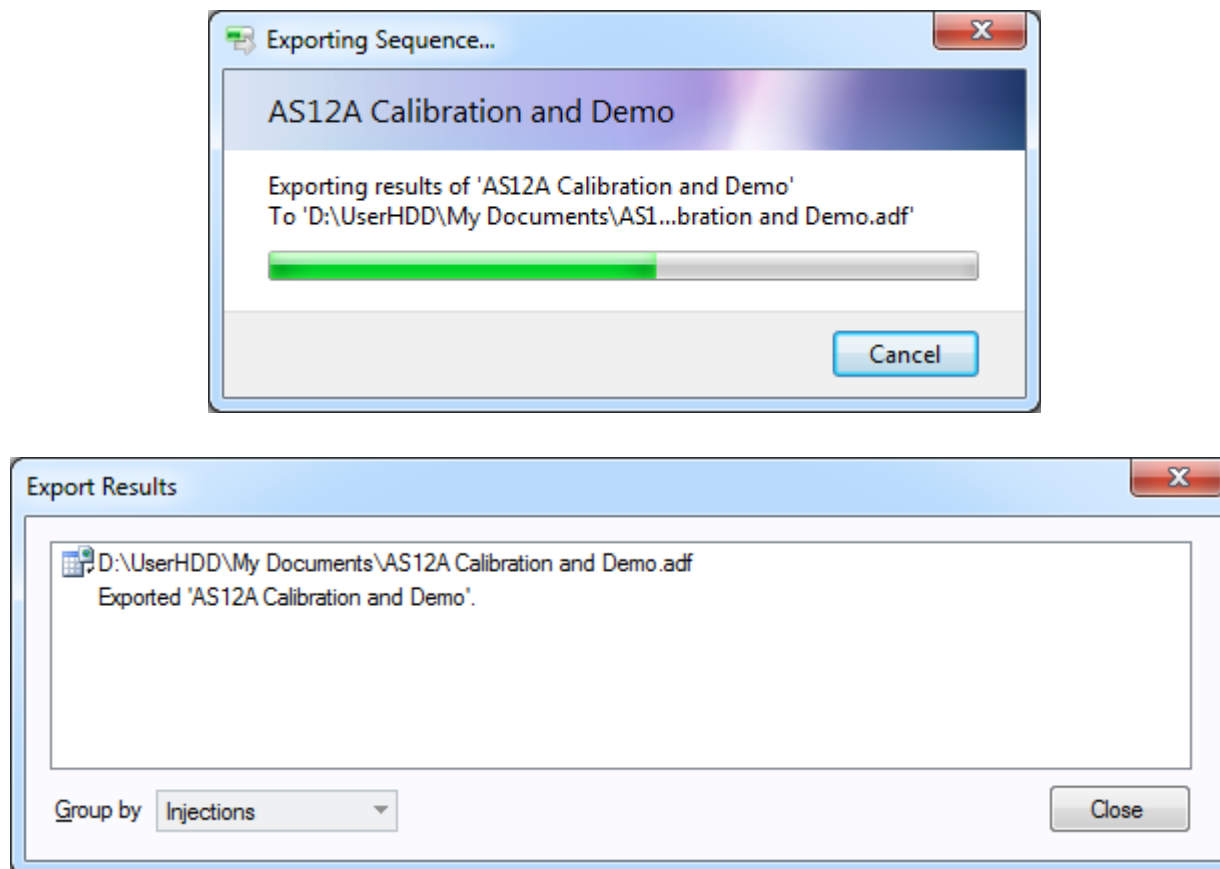


- “Allotrope data file format (*.adf)” option available from the Export dialog
- The output file name can be configured according to a defined formula



Data Export

- Dialogs appear to inform the user of progress



Viewing the ADF file – Data Description

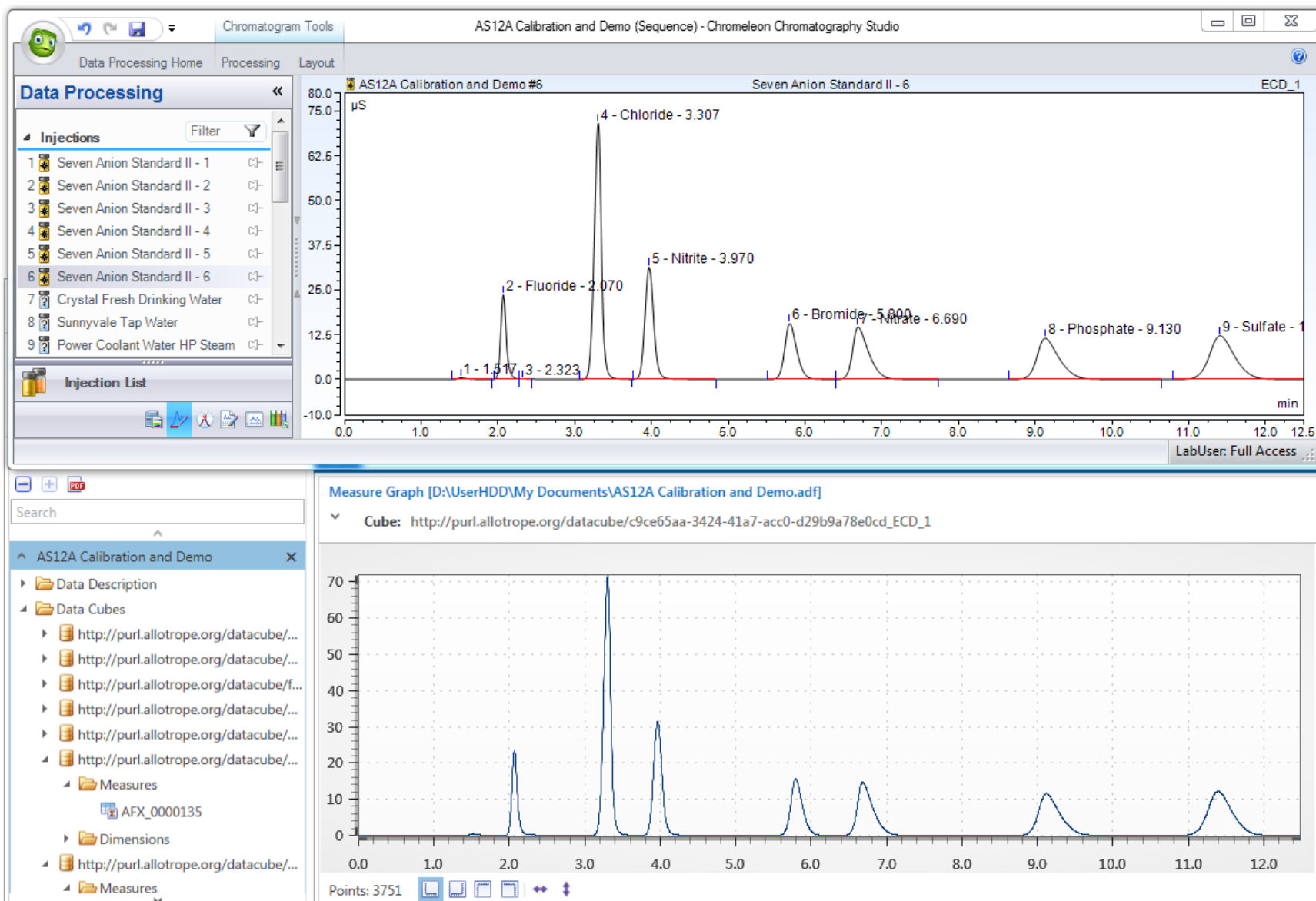
- ADF created for each Sequence selected
- Data Description for each injection includes: name, type, method names, vial position, injection volume, status and time

The screenshot displays the 'Data Description Table' window in the software. On the left, a 'Tree View' pane shows the file structure: 'AS12A Calibration and Demo' (selected), 'Data Description' (expanded), 'Default' (selected), 'Data Cubes', and 'Data Package'. The main window, titled 'Tab 1', shows the 'Data Description Table [D:\UserHDD\My Documents\AS12A Calibration and Demo.adf]'. It includes a 'Named Set: Default' dropdown, a search bar, and checkboxes for 'Subject', 'Predicate', and 'Object'. Below these, a table lists data entries. The first entry is expanded, showing a list of rows with columns for Subject, Predicate, and Object. The 'Subject' column contains URIs for various materials, the 'Predicate' column contains URIs for properties, and the 'Object' column contains specific values. The table ends with a 'Count: 624' label.

Subject	Predicate	Object
Subject: http://purl.allotrope.org/ontologies/material#AFM_0000257/10_Power Coolant Water IP Steam		
http://purl.allotrope.org/ontologies/material#AFM_0000257/...	http://www.w3.org/ns/shacl#property	-48495c36:162b4ddcabf:-7fab
http://purl.allotrope.org/ontologies/material#AFM_0000257/...	http://www.w3.org/ns/shacl#property	-48495c36:162b4ddcabf:-7faa
http://purl.allotrope.org/ontologies/material#AFM_0000257/...	http://www.w3.org/2000/01/rdf-syntax#label	http://purl.allotrope.org/ontologies/material#AFM_0000257/...
http://purl.allotrope.org/ontologies/material#AFM_0000257/...	http://www.w3.org/1999/02/22-rdf-syntax#value	Power Coolant Water IP Steam
http://purl.allotrope.org/ontologies/material#AFM_0000257/...	http://www.w3.org/ns/shacl#property	-48495c36:162b4ddcabf:-7fa8
http://purl.allotrope.org/ontologies/material#AFM_0000257/...	http://www.w3.org/ns/shacl#property	-48495c36:162b4ddcabf:-7fad
http://purl.allotrope.org/ontologies/material#AFM_0000257/...	http://www.w3.org/ns/shacl#property	-48495c36:162b4ddcabf:-7fac
http://purl.allotrope.org/ontologies/material#AFM_0000257/...	http://www.w3.org/ns/shacl#property	-48495c36:162b4ddcabf:-7fa7
http://purl.allotrope.org/ontologies/material#AFM_0000257/...	http://www.w3.org/ns/shacl#property	-48495c36:162b4ddcabf:-7fae
Subject: http://purl.allotrope.org/ontologies/material#AFM_0000257/2_Seven Anion Standard II - 2		
Subject: http://purl.allotrope.org/ontologies/material#AFM_0000257/3_Seven Anion Standard II - 3		
Subject: http://purl.allotrope.org/ontologies/material#AFM_0000257/4_Seven Anion Standard II - 4		
Subject: http://purl.allotrope.org/ontologies/material#AFM_0000257/5_Seven Anion Standard II - 5		
Subject: http://purl.allotrope.org/ontologies/material#AFM_0000257/6_Seven Anion Standard II - 6		

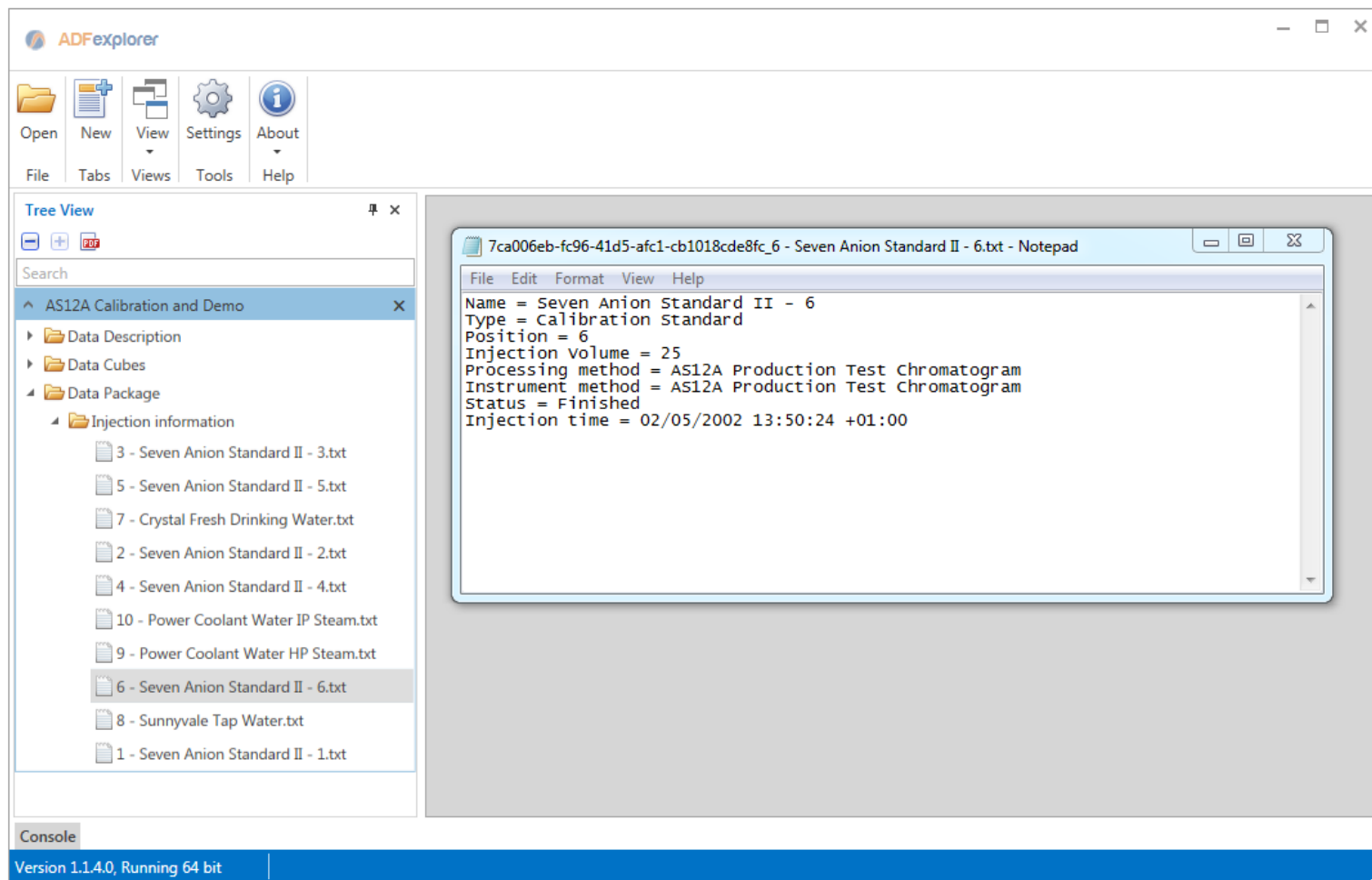
Count: 624

Viewing the ADF file – Data Cubes



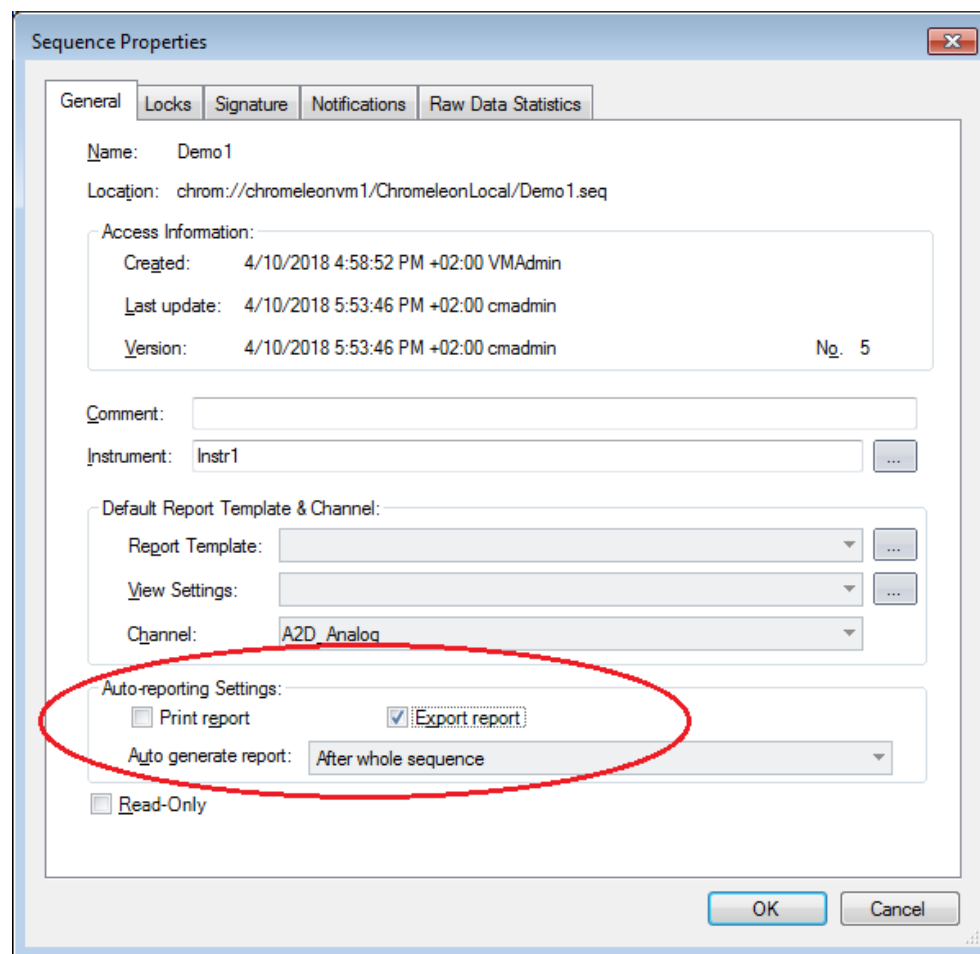
Viewing the ADF file – Data Package

- Basic information is written to the Data Package



Automated ADF creation

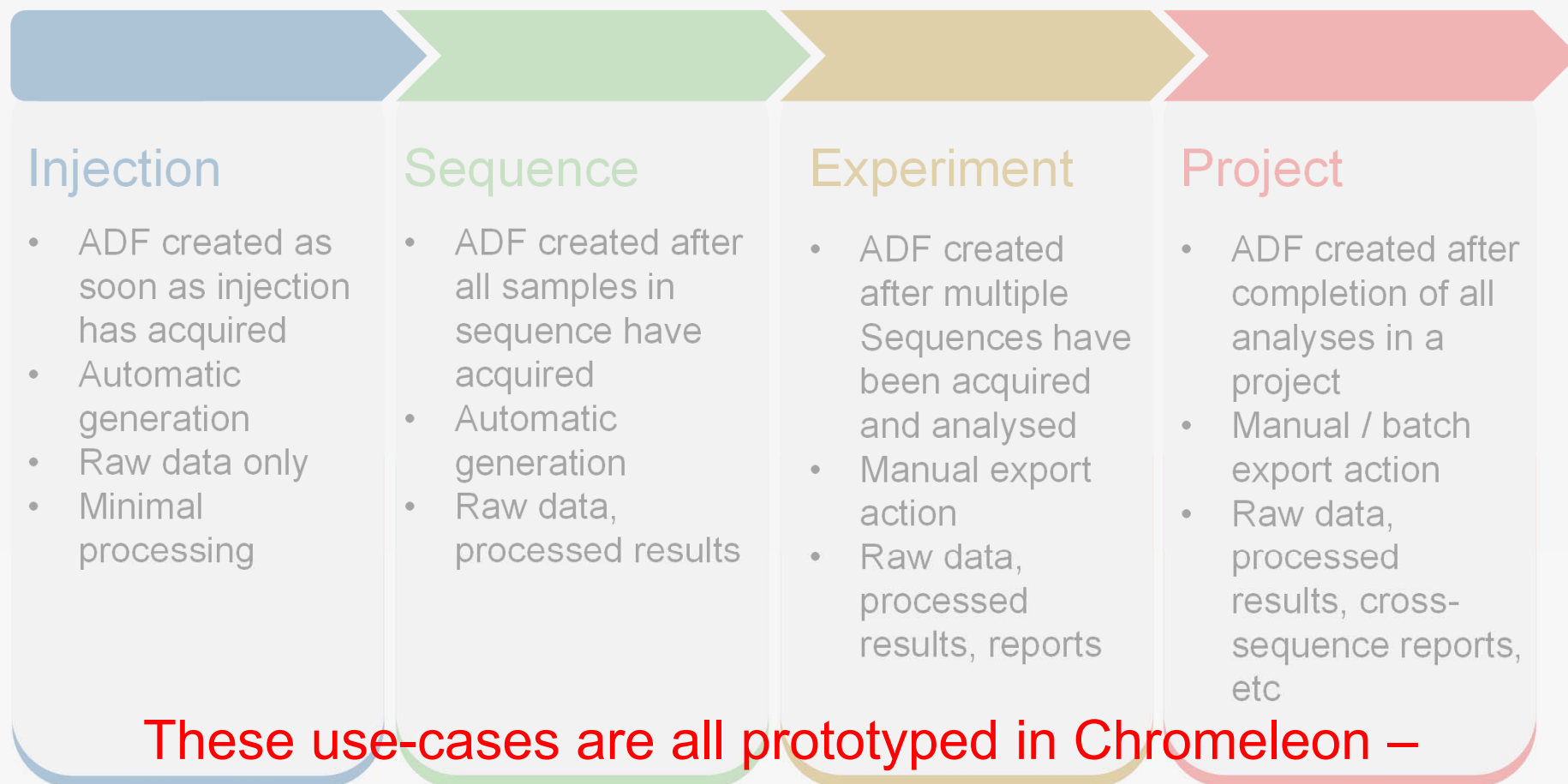
- For routine output in ADF, select “Export report” option in Sequence Properties
- Choose “After whole sequence” or “After each injection”
- Select ADF as output file type in Report Template
- Enforce auto-export option in Instrument Properties



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

High-level Use Cases



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

Q₁₀ U₁ E₁ S₁ T₁ I₁ O₁ N₁ S₁ ?₁