

	Standard Operating Procedure HPLC Data Handling and Naming Conventions using Chromeleon Series 7.X Software		SOP Number D-813	Revision 5
			Effective Date 01/27/23	Page Page 1 of 5
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1.0 Purpose

The purpose of this procedure is to provide guidelines for storing and managing Chromeleon Series 7.X software electronic files.

2.0 Scope

This procedure applies to data files created, stored and altered on lab computer(s) dedicated to the Dionex HPLC system(s). This procedure applies specifically to the Chromeleon Series 7.X software. This procedure describes the naming conventions for each of the critical file types used by the U3000 HPLC.

3.0 Responsibility

- 3.1 It is the responsibility of QC and Analytical Chemists to follow this procedure.
- 3.2 It is the responsibility of QC Laboratory Management to implement this procedure and to ensure that the procedure is being followed.
- 3.3 It is the responsibility of QC Laboratory Management and/or Analytical Development to keep this procedure current with the latest Ion Labs practices.

4.0 Definitions

- 4.1 QC – Quality Control

5.0 References

- 5.1 Chromeleon Series 7.X User's Guide

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6.0 General Guidelines

6.1 The five created and/or modified file types used by the Chromeleon Series 7.X software are:

6.1.1 Instrument Method files

6.1.2 Processing Method files

6.1.3 Sequence files

6.1.4 Report Template files

6.1.5 Spectral Library files

6.2 The basic unit of data in Chromeleon is a Sequence. The Sequence contains all the data and meta-data that are necessary to recreate the results. The official record of a chromatographic test is the Sequence. Finished Sequences are Submitted and Reviewed / Approved in the Chromeleon software. Submitted Sequences cannot be changed.. Electronic and hardcopies of all generated data are saved for a period of five years.

6.3 File Types

6.3.1 Instrument Method Files

6.3.1.1 Include the operating parameters of the HPLC components.

6.3.1.2 Instrument Method files are to be named with the following structure:
“D-XXX, analyte(s)”

Example: D-710.0 Dextromethorphan HBr

6.3.1.3 For sub programs related to a specific SOP or Method Validation, the following nomenclature is added: “D-XXX, analyte(s), (a,b,c or distinguishing feature-Isocratic, gradient, pH, etc.)

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Example: D-728 Folic acid gradient

6.3.1.4 Instrument Method files will be stored in instrument specific **Instrument Methods** file folders.

6.3.2 Processing Method Files

6.3.2.1 Processing Method files include, for example, integration parameters for quantification of peaks and system suitability requirements, single and multi-level standard concentrations and associated spectral libraries.

6.3.2.2 Processing Method files are to be named with the same nomenclature as described in 6.3.1.2 to 6.3.1.3 and the files will be differentiated by file type icon.

Example: D-710.0 Dextromethorphan HBr

6.3.2.3 Processing Method files will be stored in instrument specific **Processing Methods** file folders.

6.4.1 Sequence Files

6.4.1.1 Sequence files contain the sequential list of individual chromatographic tests. The tests themselves are contained within the sequence file. Sequence Files also / can also contain Instrument Methods, Processing Methods, Report Templates, Spectral Libraries, etc. as Associated Items.

6.4.1.2 Subfolders in instrument specific **Sequences** file folders will be made each month and named by Numerical designator for month, month and year.

Example: 01 January 2015, 02 February 2015, etc

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6.4.1.3 Individual sequences will be named with the following nomenclature:

- Date in format: Year_Month_Day
- To distinguish multiple runs in a single day add: seq(1,2,3,etc)
- Add: Analyte(s)
- Add: Batch# or R#(s)

Example of complete name: 2017_04_13 seq1 niacin 420503_R7628

6.5.1 Report Template Files

6.5.1.1 Report Template files are spreadsheet-like files that define how data are printed or exported. When the template is applied on a sequence (to view, print or export the results) the output is referred to as the report.

6.5.1.2 Report Template files are to be named with the following nomenclature:

- The SOP or Method Validation number.
- The analyte(s).

Example of complete name: D-727 Raspberry Ketone

6.6.1 Spectral Library Files

6.6.1.1 Spectral Library files are collections of spectra used for peak identification and matching.. These files may be created using the linearity injections performed during method validation, or they may be extracted from appropriate standard injections in a given sequence.

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6.6.1.2 The UV Spectral Library view of the Chromatography Studio provides tools for managing and comparing spectra extracted from 3D field data. Spectral Library files are saved as Associated Items in Submitted Sequences.

6.6.1.3 Spectral Library files are to be named with the following structure: “D-XXX, analyte(s).”

- The Spectral Library file will include the chromatographic conditions under which the spectra were generated.
- The Spectral Library will link the injections to the actual sequence in which they were generated.
- The Spectral Library will include the actual concentrations of the standards that were injected to generate the file.

Example of complete name: D-710.0 Dextromethorphan HBr

6.7.1 Printed Data

6.7.1.1 Data displayed as Interactive Results, Chromatograms, Peak Properties, UV-Vis Spectra, etc. will be printed and pasted into the Laboratory Notebook.

7.0 Revision History

Revision	Date	Description of Changes	CCR #	By
0	05/06/10	New	-	-
1	01/24/12	Updated SOP	-	-
2	03/07/13	Updated SOP format, defined new naming guidelines, expanded file types to address.	13-0 129	B. Johns
3	02/19/15	Scheduled review: updated SOP format. Increased Clarity.	15-0175	B. Johns
4	01/02/19	Scheduled review: updated SOP to Chromeleon 7 software.	19-0015	J. Maignan
5	01/16/23	Scheduled review: updated responsibilities. Changed logo. Updated document format.	CC-23-0026	K. Burris