

ACCQPrep™ Sample Queue List Programmer's Reference Guide



Chromatography Technical Note
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Summary

This document describes the file format used to import a list of samples into the sample queue on ACCQPrep systems with AutoSamplers. This list is created by any software that generates text files. The ability to generate sample lists outside of the ACCQPrep allows improved automation between analytical HPLC systems, electronic notebooks, and laboratory information management systems. The files can be generated using JAVA, C, C++, Python, Visual Basic, or Visual Basic for Applications.

Note that a Microsoft Excel file containing Visual Basic for Applications code is available from the Teledyne ISCO web site. Although this file is intended for use by non-programmers, it is a useful programming example.

The data files can be loaded into the ACCQPrep using a USB drive or uploaded via the instrument web interface.

Creating a sample list to upload into an ACCQPrep requires two steps:

1. Download the list of installed columns and methods
2. Uploading the list of samples, including the column and method to be used for each run

Columns, methods, and instrument identification download from ACCQPrep

First, retrieve a list of columns and their associated methods from the ACCQPrep to avoid errors when the columns and methods sent back to a system don't match the internal data. The file from the ACCQPrep also contains the instrument name and a MAC (media access control) address unique to each ACCQPrep. This MAC address is needed for the ACCQPrep to accept a list as this verifies the data is intended for a particular system. This data is accessed via the EXPORT COLUMN/METHOD LIST button on the queue screen which prompts for a file path. Data is stored on a USB drive from the ACCQPrep, or into a computer drive from a web browser. The data is stored as an ASCII text file.

The data has the following format (note that the quotation marks are present in the file):

A header with the fields:

"Instrument_Name", "MAC_Address", "Extra_Field"

After the header, there will be a line for each column, containing the column name and methods stored with that column:

"Column_Name", "Method_1", "Method_2", "Method_3", ...

Only the columns that can be run will be listed in the file, there can be up to 4 columns if the optional column

switcher is installed. Each field is in double quotes, separated by a comma.

FIELD NAME	COMMENTS
Instrument_Name	This may be exported as an empty string. It is a user-friendly identification of the instrument. It is set up in the Instrument Configuration tab of the configuration screen.
MAC_Address	This is unique to the instrument, and serves to identify the instrument that exported the list of columns and methods. Letters in the MAC address should be entered in upper case. It is listed when a user selects "Help", followed by "About PeakTrak" from the instrument.
Extra_Field	This field is enabled in the Instrument Configuration tab of the configuration window under Queue Screen Custom Parameters. The values from the ACCQPrep are: "null" meaning this field is not configured "UVThreshold" indicates that a threshold needs to be set for each sample to trigger peak detection "DetectionIons" indicates a sample may provide mass spectrometer detection ion information
Column_Name	This is the name of the column as entered into PeakTrak.
Method	This is a method associated with a column; there may be several methods for each column. There will be at least one method associated with each column.

Sample list file upload

The sample list sent to the ACCQPrep is an ASCII text file with the following order and format:

A header with the following information:

"Instrument_Name", "MAC_Address", "Extra_Field"

Lines of text with the data listed below:

"Sample_Name", "Column_Name", "Method", "Extra_Field_Value", "Total_Sample_Volume", "Number_Of_Injections", "Sample_Position", "Next_Rack_Or_Tube", "Bracketed_Sample_Injection", "Post_Separation_Pause"

The data to the ACCQPrep is an ASCII file, the data is in quotes and comma delimited. Each line is terminated with a carriage return. The quotation marks shown above are expected to surround the data in the generated file.

The various field names are like those in the ACCQPrep sample queue screen and have the same limitations.

The fields contain the following information:

FIELD NAME	COMMENTS
Instrument_Name	Optional. This may be an empty string. It is a user-friendly identification of the instrument. It is set up in the Instrument Configuration tab of the configuration screen. This data came from the ACCQPrep download
MAC_Address	Required. This is unique to the instrument, and serves to identify the instrument that exported the list of columns and methods. Letters in the MAC address should be entered in upper case. It is listed when a user selects "Help", followed by "About PeakTrak" from the instrument. It is also part of the download file, and should be sent back in the same format
Extra_Field	Required. This field must match the configuration in the instrument and is sent by the instrument with the columns and methods in the download file. The values from the ACCQPrep are: "None" meaning this field is not configured "UVThreshold" indicates that a threshold needs to be set for each sample to trigger peak detection "DetectionIons" indicates a sample may provide mass spectrometer detection ion information
Sample_Name	This is a unique name for the sample. If a sample with the same name exists on the ACCQPrep, the list will be rejected by the system. If an empty string is submitted, a name will be assigned by the ACCQPrep.
Column_Name	Required. One of the columns exported from the instrument as part of the download file.
Method	Required. One of the methods associated with the column above, and was exported as part of the download file.
Extra_Field_Value	The value in this field depends on the Extra_Field setting: If "None", the value is ignored If "UVThreshold", then a value greater than 0 should be sent. If there is no value, a threshold of 0 will be used. If "DetectionIons": This may be blank (no mass spectrometer detection), or a numeric value within the range of the mass spectrometer. Multiple masses (up to 6) may be defined, each mass is separated by a space. A range may be defined, with the ends of the range separated by a colon ":" symbol. Use a dash "-" to indicate negative masses. For negative ranges put the dash only before the first mass in the range. All masses must be the same polarity.
Total_Sample_Volume	Required. This is the total volume of sample in ml for all injections.
Number_Of_Injections	Required, a whole number must be greater or equal to 1. It is the number of injections from the sample.
Sample_Position	Required. It is the position in the sample rack on the AutoSampler. Values may range from 1 to 28. If a half-rack is used, the number is preceded by "G:" for the front rack, or "H:" for the rear rack. If no letter is provided, the front rack is assumed.
Next_Rack_Or_Tube	Required. Send "Next Tube" if the next tube is to be used following the last sample, or "Next Rack" if this sample will be run on its own fraction rack.
Bracketed_Sample_Injection	Required. Values are "Yes" or "No"
Post_Separation_Pause	Required, values are "Yes" or "No"

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