

Result File Rules

August 12, 2020

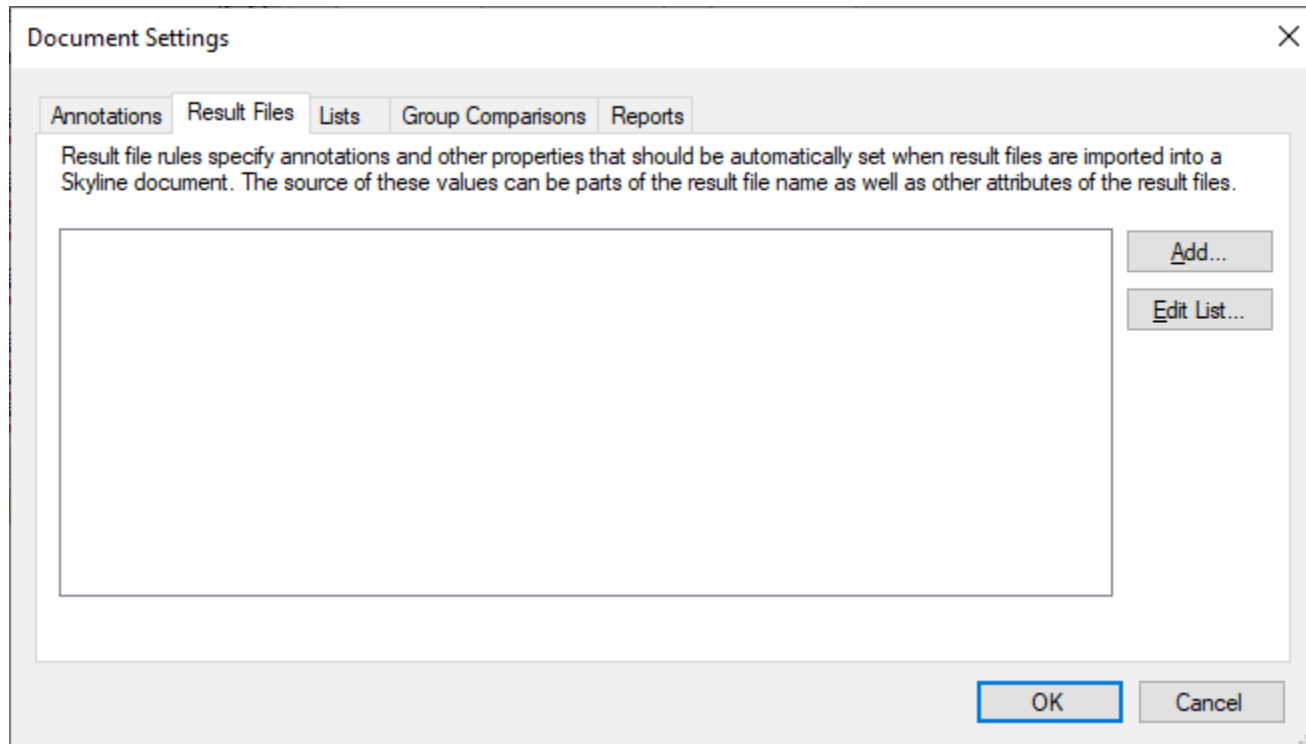
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New feature: Result File Rules

- Skyline version 20.2 will have a new feature which allows you to automatically set annotations and other properties based on parts of the result file names and other features of the result files.

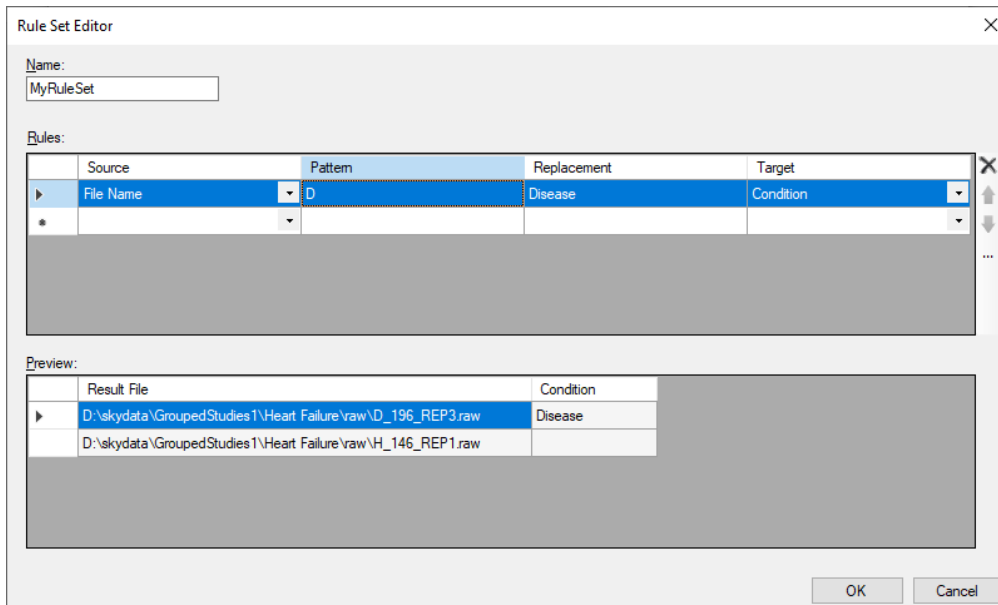
Defining a Result File Rule Set

- Result file rule sets are listed on the “Result Files” tab of the Document Settings dialog



Defining Rule Sets

- Rule Sets have a list of rules which set Result File and Replicate properties from parts of the result file name and other attributes of the Result File

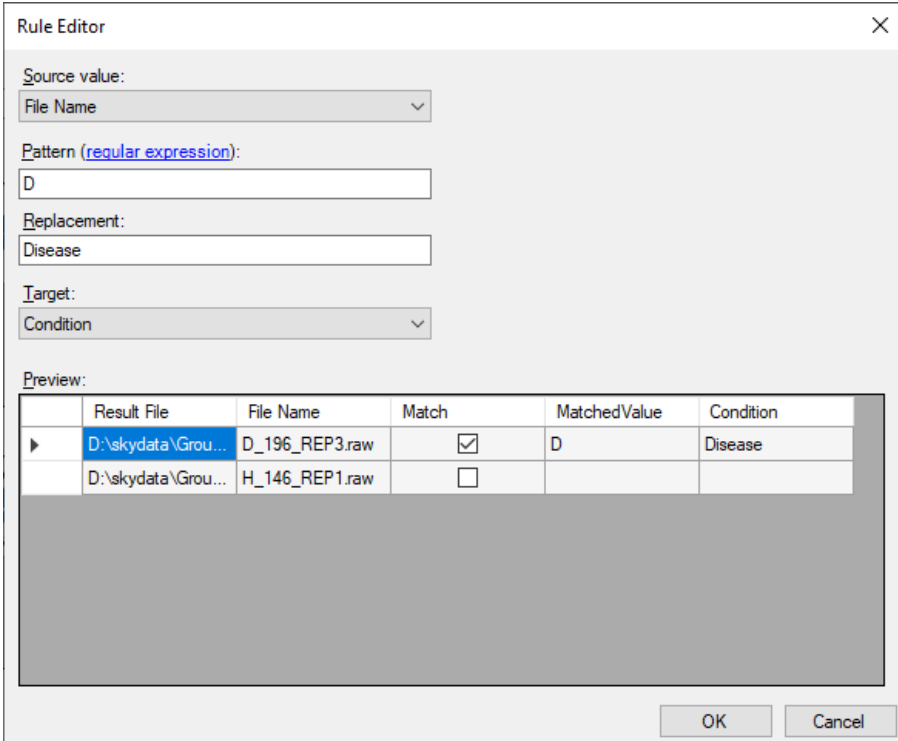


- You can either add or modify rules by changing the values in the Rules grid, or you can press the “...” button to bring up the more detailed Rule Editor

Detailed Rule Editor

- The Rule Editor shows you the intermediate values from matching a regular expression and performing a replacement

The rule shown here says that any file name which contains the letter “D” should result in the “Condition” annotation being set to “Disease”



The screenshot shows the 'Rule Editor' dialog box with the following configuration:

- Source value: File Name
- Pattern (regular expression): D
- Replacement: Disease
- Target: Condition

The Preview table shows the following data:

	Result File	File Name	Match	MatchedValue	Condition
▶	D:\skydata\Grou...	D_196_REP3.raw	<input checked="" type="checkbox"/>	D	Disease
	D:\skydata\Grou...	H_146_REP1.raw	<input type="checkbox"/>		

Buttons: OK, Cancel

Regular Expressions

- The “Pattern” in a rule is a regular expression which can be used to match parts of the source value.
- In this documentation, the following regular expressions are used:
 - [DH]: matches either the letter “D” or “H”
 - [0-9]+: matches one or more numerical digits in a row
 - Parentheses: putting parentheses around something in the regular expression makes it into a “group” which can be referenced in the Replacement Text using “\$” followed by a number

Replacement text

- The replacement text specifies what value to use when the regular expression has matched part of the source value.
- If the replacement text is blank, then the replacement value is the entire value matched by the regular expression
- The replacement text can refer to groups in parentheses using “\$” followed by the number of the group.
- “\$0” refers to the entire part matched by the regular expression
- “\$1” refers to the text matched by the first group in the regular expression

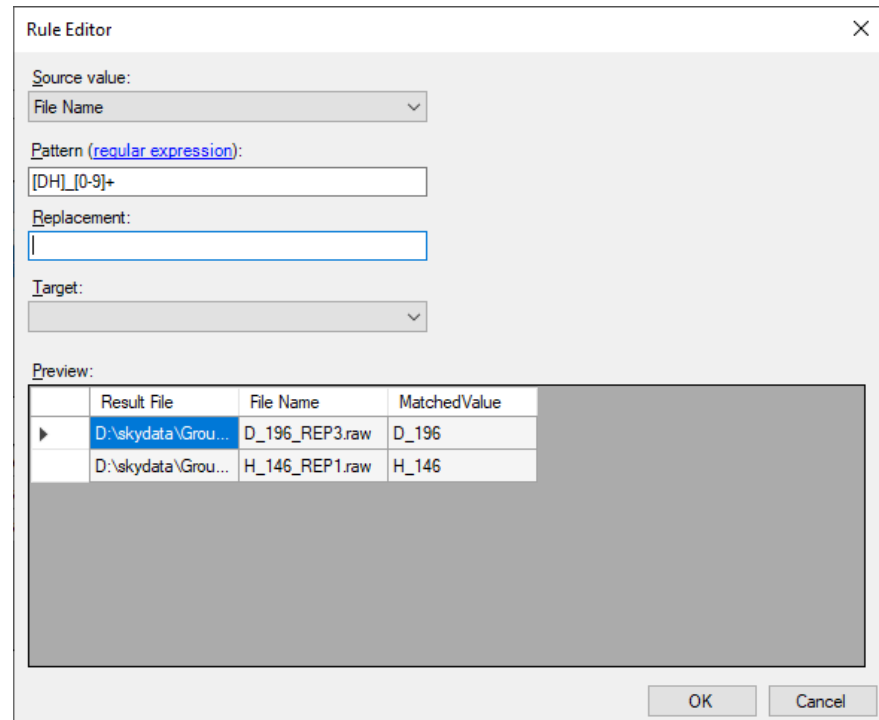
Regular expression example: Removing the underscore in the middle of a value

- In this example, we have files named
“D_196_REP3.raw” and “H_146_REP1.raw”

The regular expression:

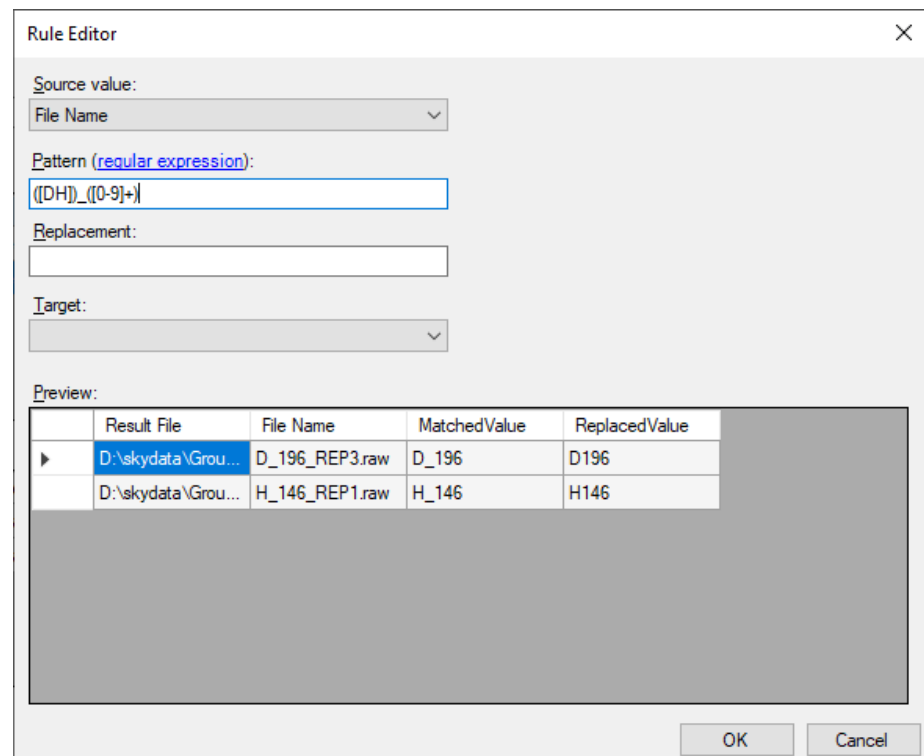
`[DH]_[0-9]+`

will match the letter “D” or “H”,
followed by an underscore,
followed by 1 or more digits



Adding parentheses to define groups in the regular expression

- We can add parentheses to the regular expression in order to define groups which can be referred to in the replacement text. The parentheses in the regular expression do not typically affect what text gets matched by the regular expression



The screenshot shows a 'Rule Editor' dialog box with the following fields:

- Source value:** File Name
- Pattern (regular expression):** `((DH))_([0-9]+)`
- Replacement:** (empty)
- Target:** (empty)

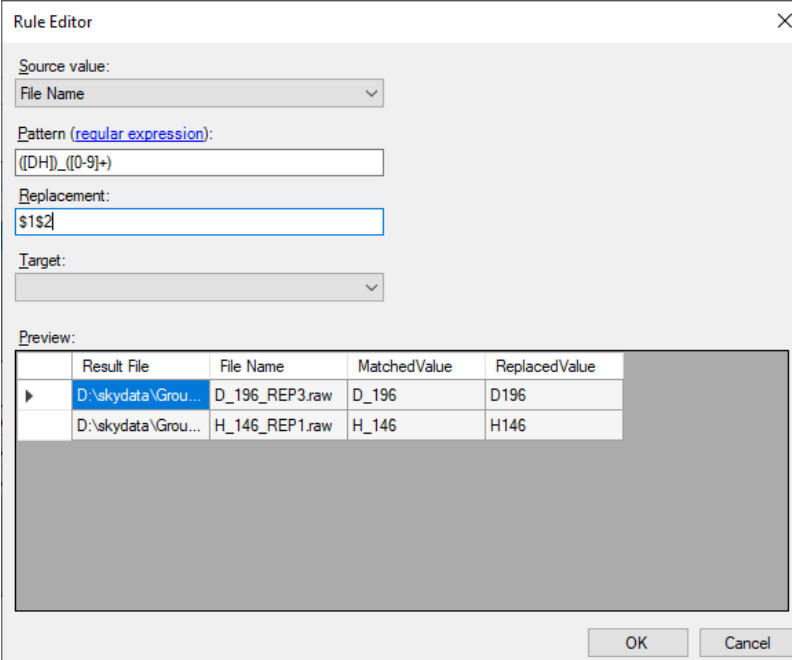
The **Preview:** section contains a table with the following data:

	Result File	File Name	MatchedValue	ReplacedValue
▶	D:\skydata\Grou...	D_196_REP3.raw	D_196	D196
	D:\skydata\Grou...	H_146_REP1.raw	H_146	H146

Buttons: OK, Cancel

Using dollar signs to refer to groups in the regular expression

- If we set the replacement text to “\$1\$2”, then the replaced value will become the concatenation of the two matched groups



The screenshot shows a 'Rule Editor' dialog box with the following fields and values:

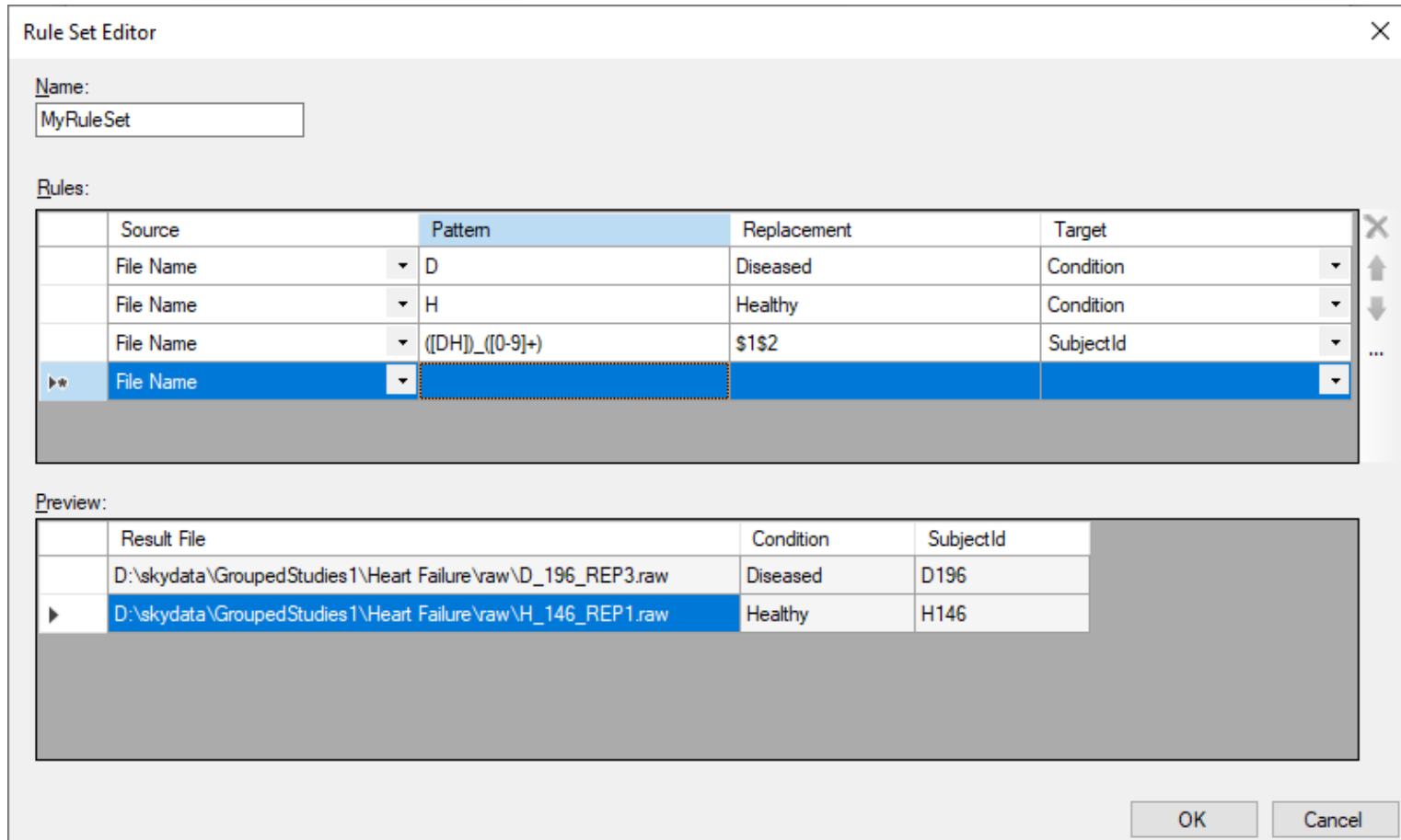
- Source value: File Name
- Pattern (regular expression): `((DH))_([0-9]+)`
- Replacement: `$1$2`
- Target: (empty)

The Preview section contains a table with the following data:

	Result File	File Name	MatchedValue	ReplacedValue
▶	D:\skydata\Grou...	D_196_REP3.raw	D_196	D196
	D:\skydata\Grou...	H_146_REP1.raw	H_146	H146

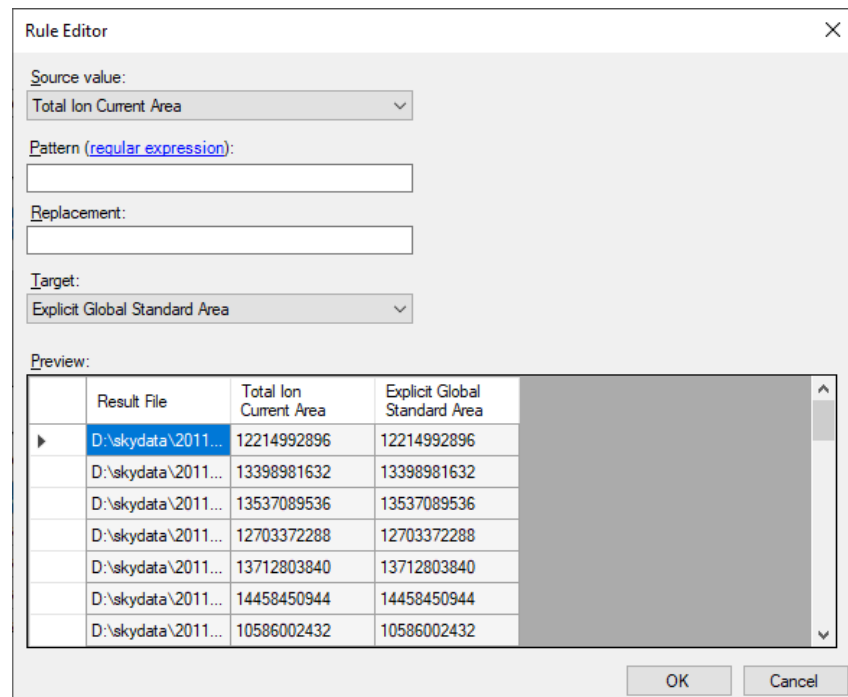
Buttons: OK, Cancel

Rule Sets contain multiple rules



Setting Explicit Global Standard Area from the Total Ion Current Area

- Result file rules can also be used to automatically set the Explicit Global Standard Area from the Total Ion Current Area that Skyline calculates when extracting chromatograms



Rule Editor

Source value:
Total Ion Current Area

Pattern (regular expression):

Replacement:

Target:
Explicit Global Standard Area

Preview:

	Result File	Total Ion Current Area	Explicit Global Standard Area
▶	D:\skydata\2011...	12214992896	12214992896
	D:\skydata\2011...	13398981632	13398981632
	D:\skydata\2011...	13537089536	13537089536
	D:\skydata\2011...	12703372288	12703372288
	D:\skydata\2011...	13712803840	13712803840
	D:\skydata\2011...	14458450944	14458450944
	D:\skydata\2011...	10586002432	10586002432

OK Cancel