

 Empower™ing you | **ACHIEVE MORE**  
*by* **DOING LESS**

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APAC Informatics Marketing

24 September 2020

## House Rules



- If you have any questions during the webinar, please feel free to post them in the Q&A Feature.
  - We will address these questions at the end of the webinar
- Post-webinar, we will send these to your registered email:
  - PDF slides of the presentation
  - PDF summary of the presentation
  - Q&A summary
- I would be happy to have further discussions via email at:  
[haining\\_pee@waters.com](mailto:haining_pee@waters.com)

ACHIEVE  
MORE



*by* **DOING LESS**



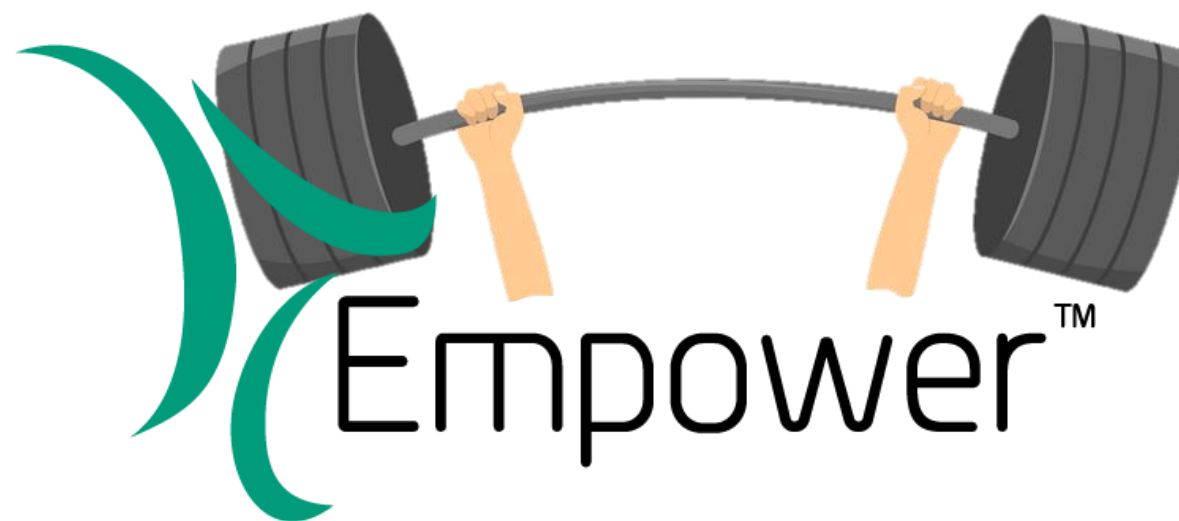
## INTERACTIVE SYSTEM SUITABILITY

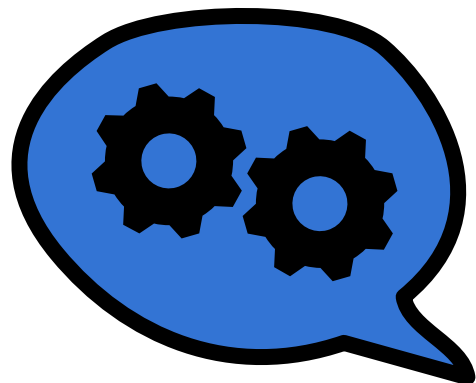
automated processing of system suitability criteria



## CUSTOM FIELDS

make multiple tailored calculations & quick decisions





# Interactive System Suitability



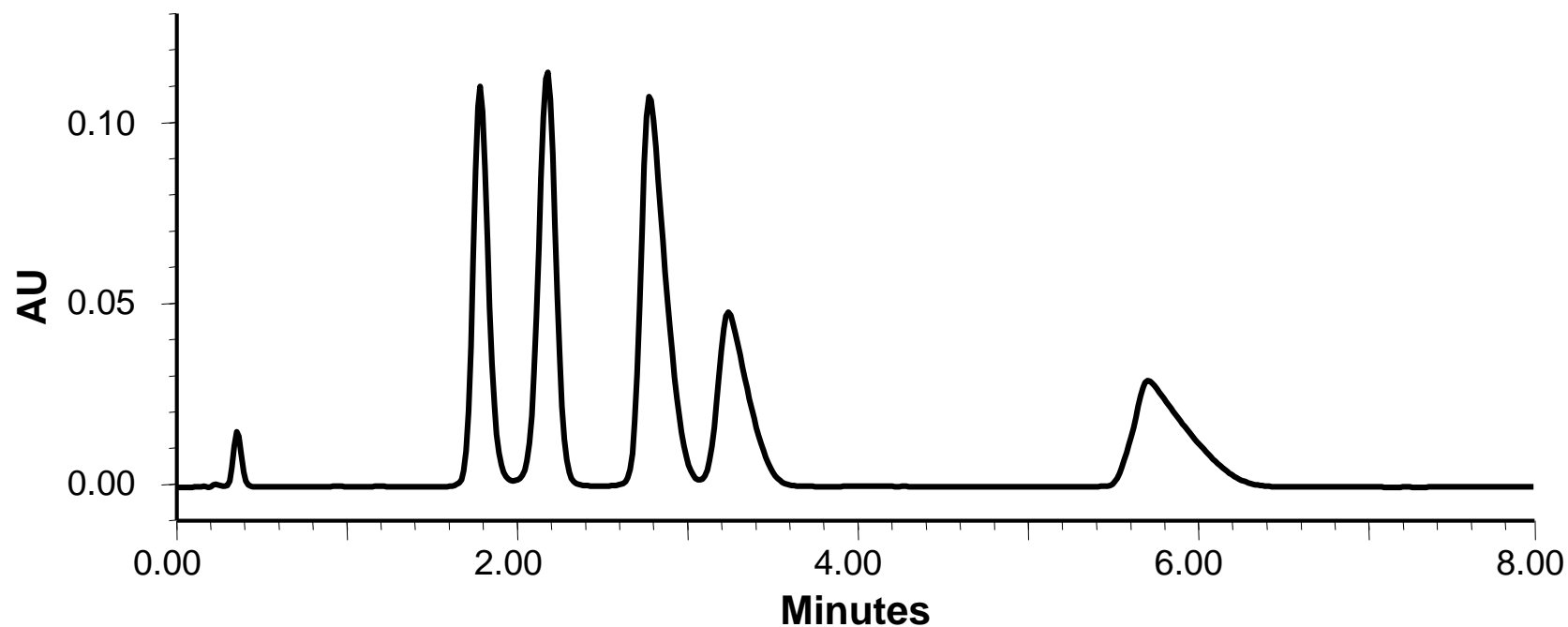


# INTERACTIVE SYSTEM SUITABILITY

What is Suitability?



**System Suitability (SysSuit)** is a series of injections to determine the suitability and effectiveness of chromatographic system before use

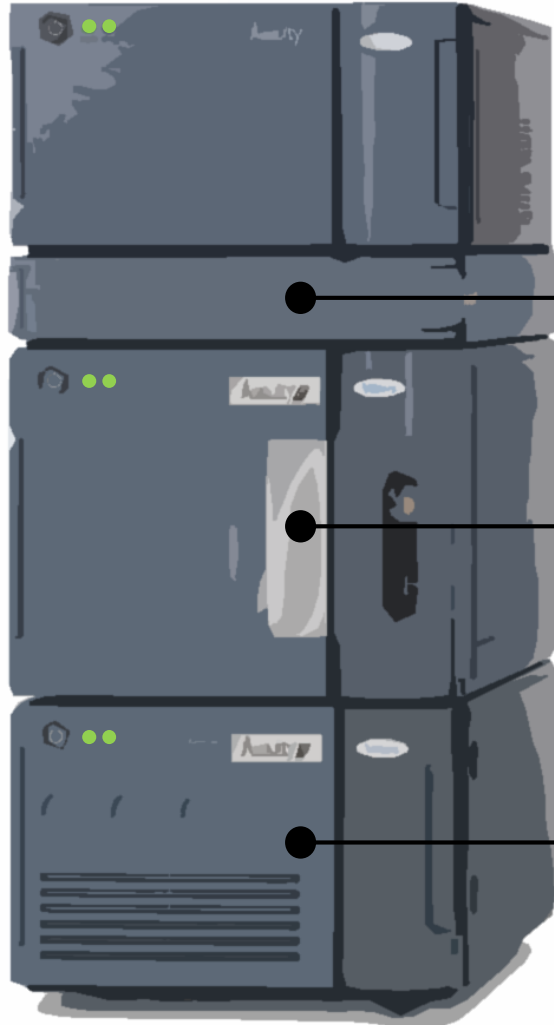




# INTERACTIVE SYSTEM SUITABILITY

What is Suitability?

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| A **system suitability** testing mixture can be injected to test:

**Column Performance:**

Plate count, S/N ratio,  
Resolution, etc.

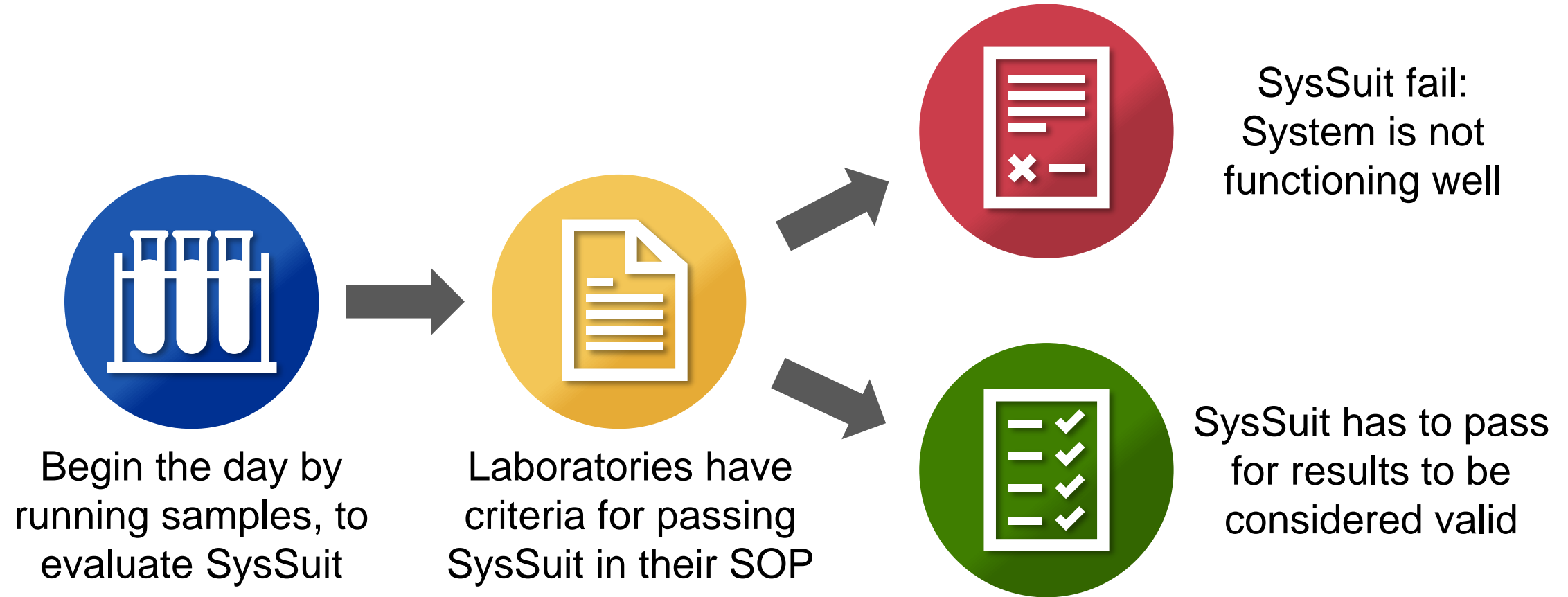
**Injector Performance:**

Injection Repeatability, etc.

**Mobile Phase Preparation:**

Resolution, USP Tailing, etc.

This is the typical analytical laboratory workflow:

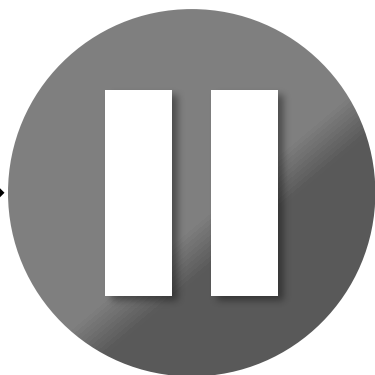
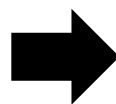




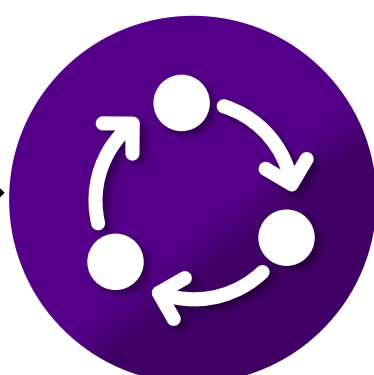
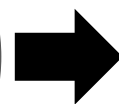
However, to evaluate these System Suitability Criteria, the Analyst has to:



Run samples to  
evaluate SysSuit



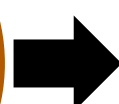
Pause  
Sample Run



Process  
samples to  
determine RT



Manually enter  
RT of 6 inj to  
check for %RSD

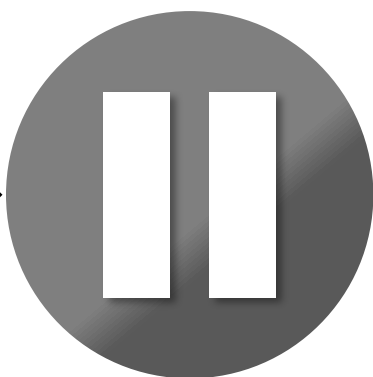
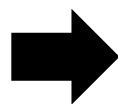


Restart Sample  
Run if SysSuit  
passes

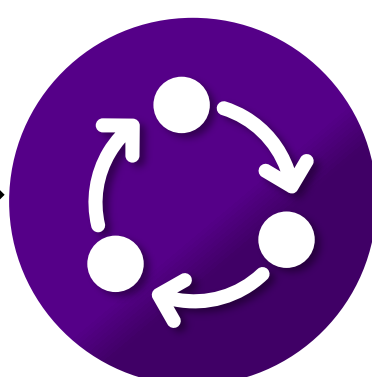
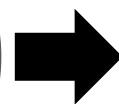
With **Interactive System Suitability**, to evaluate these SysSuit Criteria:



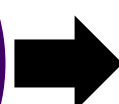
Run samples to  
evaluate SysSuit



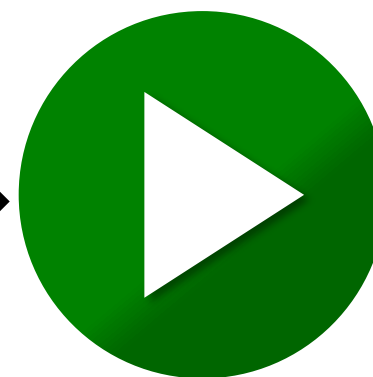
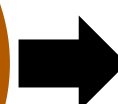
Pause  
Sample Run



Process  
samples to  
determine RT

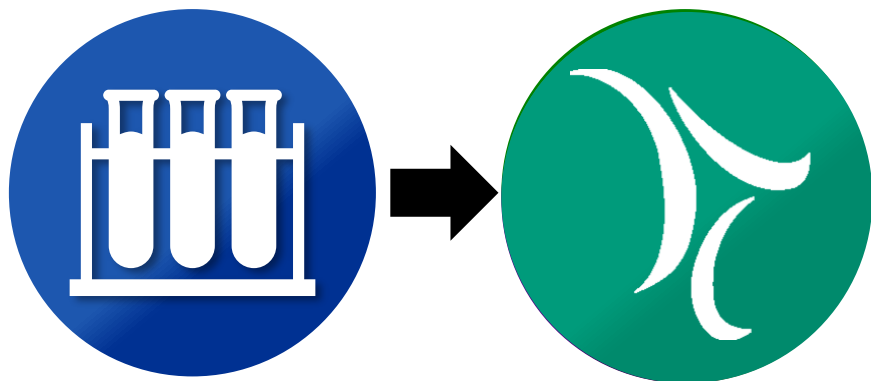


Manually enter  
RT of 6 inj to  
check for %RSD



Restart Sample  
Run if SysSuit  
passes

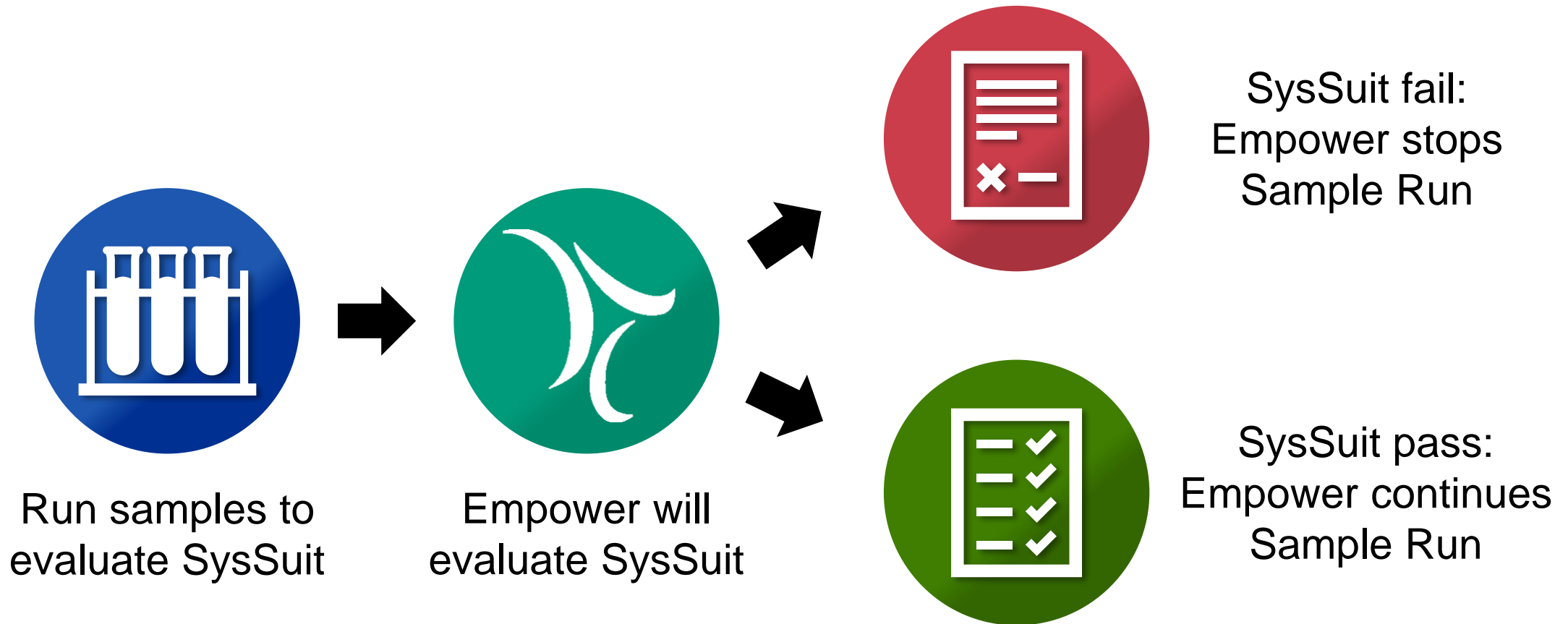
With **Interactive System Suitability**, to evaluate these SysSuit Criteria:



Run samples to  
evaluate SysSuit

Empower will  
evaluate SysSuit

With **Interactive System Suitability**, to evaluate these SysSuit Criteria:

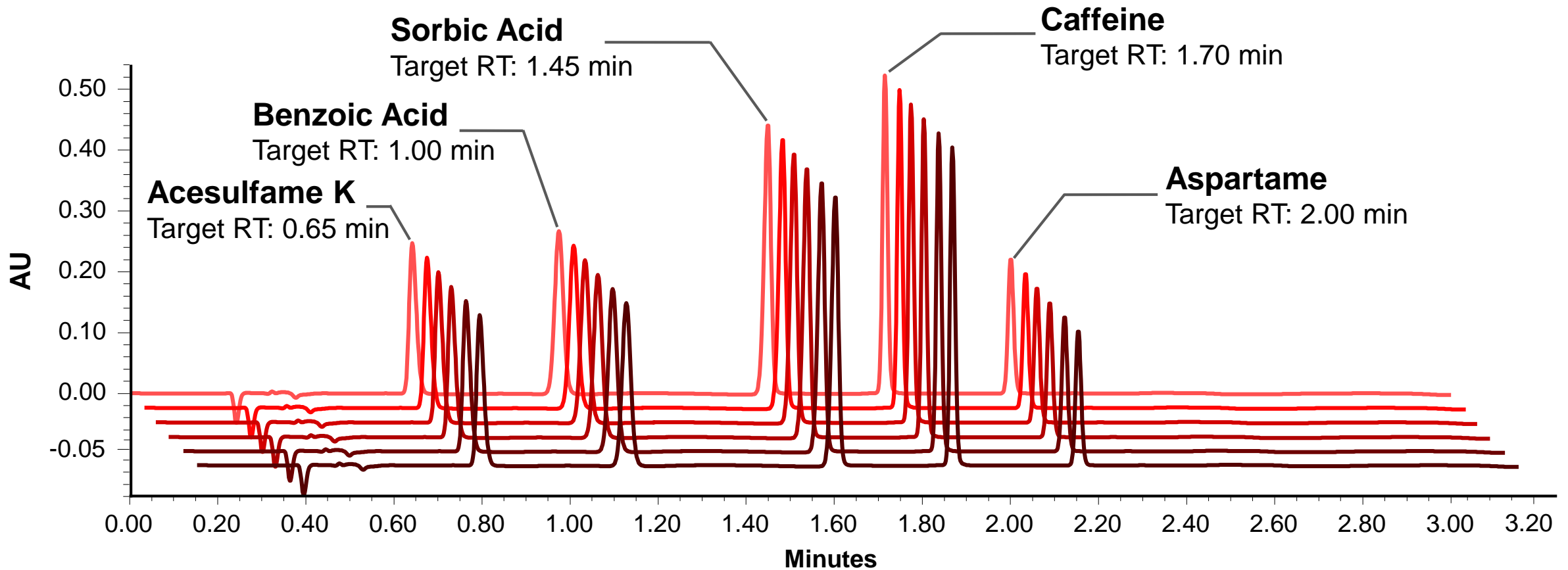




# INTERACTIVE SYSTEM SUITABILITY

## Setting up Interactive System Suitability

In this example, 6 SysSuit samples will be analyzed

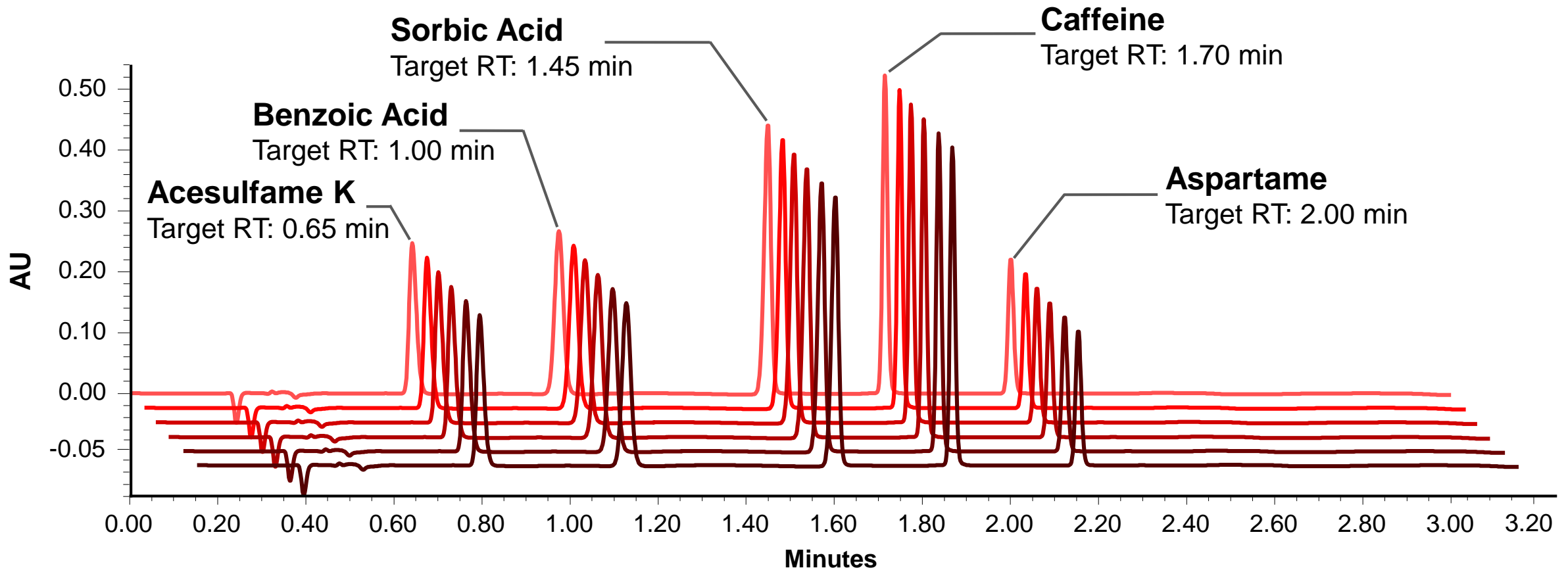




# INTERACTIVE SYSTEM SUITABILITY

## Setting up Interactive System Suitability

Analyte retention time must fall  $\pm 3\%$  of Target RT





# INTERACTIVE SYSTEM SUITABILITY

## Setting up Interactive System Suitability – Processing

System Suitability Criteria is set up in the Processing Method

Named Groups | Timed Groups | **Suitability** | Limits | Noise and Drift

Calculate Suitability Results

Calculate Suitability Results for Unknown Peaks

System and Separation Efficiency

Void Volume Time (min)

US Pharmacopoeia       European Pharmacopoeia

Japanese Pharmacopoeia       All

Tangent Percent for USP Resolution

Tangent Percent for USP Plate Count

Calculate USP, EP, and JP s/n

Use noise centered on peak region in blank injection

Half Height Multiplier for USP s/n Noise Region

Half Height Multiplier for EP s/n Noise Region

Half Height Multiplier for JP s/n Noise Region

Noise Value for s/n

- For System Suitability: Processing Method > Suitability Tab
- Examples of Sys Suit calculations:
  - USP Plate Count
  - USP Noise
  - USP Resolution



# INTERACTIVE SYSTEM SUITABILITY

Setting up Interactive System Suitability – Processing

◀ ▶

Named Groups | Timed Groups | **Suitability** | Limits | Noise and Drift

Calculate Suitability Results

Check *Calculate Suitability Results* <sup>§</sup>

System and Separation Efficiency

Void Volume Time (min)

US Pharmacopoeia       European Pharmacopoeia  
 Japanese Pharmacopoeia       All

Tangent Percent for USP Resolution

Tangent Percent for USP Plate Count





# INTERACTIVE SYSTEM SUITABILITY

## Setting up Interactive System Suitability – Processing

Integration | Smoothing/Offset | Components | Impurity | Peak Ratios (MS Ion Ratios) | Default Amounts/Purity | Named Groups | Timed Groups | Suitability | **Limits** | Noise and Drift

Flag Values Outside Limits

Suitability Components

	Name	Calculate Suit Results	Flag Outside Limits
1	Acesulfame K	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
	Benzoic Acid	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
3	Sorbic Acid	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
4	Caffeine	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
5	Aspartam	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>

Click on your target *Component*

Suitability Limits

Field Name	Target	Error %	Lower Error Limit (LCL)	Upper Error Limit (UCL)	Warning %	Lower Warning Limit	Upper Warning Limit	Ignore Blank Values	Check Limits

Select the parameter(s) you wish to monitor and assign limit(s) to that parameter(s)



# INTERACTIVE SYSTEM SUITABILITY

## Setting up Interactive System Suitability – Processing

Flag Values Outside Limits

Suitability Components		
Name	Calculate Suit Results	Flag Outside Limits
1 Acesulfame K	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
2 Benzoic Acid	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
3 Sorbic Acid	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
4 Caffeine	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
5 Aspartame	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>

Repeat for the rest of the *Components*

Suitability Limits									
Field Name	Target	Error %	Lower Error Limit (LCL)	Upper Error Limit (UCL)	Warning %	Lower Warning Limit	Upper Warning Limit	Ignore Blank Values	Check Limits



# INTERACTIVE SYSTEM SUITABILITY

## Setting up Interactive System Suitability – Processing

Integration   Smoothing/Offset   Components   Impurity   Peak Ratios (MS Ion Ratios)   Default Amounts/Purity   Named Groups   Timed Groups   Suitability   <b>Limits</b>   Noise and Drift										
<input checked="" type="checkbox"/> Flag Values Outside Limits										
Suitability Components										
E	Name	Calculate Suit Results					Flag Outside Limits			
1	Acesulfame K	<input checked="" type="checkbox"/>					<input checked="" type="checkbox"/>			
2	Benzoic Acid	<input checked="" type="checkbox"/>					<input checked="" type="checkbox"/>			
3	Sorbic Acid	<input checked="" type="checkbox"/>					<input checked="" type="checkbox"/>			
4	Caffeine	<input checked="" type="checkbox"/>					<input checked="" type="checkbox"/>			
5	Aspartame	<input checked="" type="checkbox"/>					<input checked="" type="checkbox"/>			
Suitability Limits										
E	Field Name	Target	Error %	Lower Error Limit (LCL)	Upper Error Limit (UCL)	Warning %	Lower Warning Limit	Upper Warning Limit	Ignore Blank Values	Check Limits



# INTERACTIVE SYSTEM SUITABILITY

## Setting up Interactive System Suitability – Processing

Integration   Smoothing/Offset   Components   Impurity   Peak Ratios (MS Ion Ratios)   Default Amounts/Purity   Named Groups   Timed Groups   Suitability   <b>Limits</b>   Noise and Drift										
<input checked="" type="checkbox"/> Flag Values Outside Limits										
Suitability Components										
E	Name	Calculate Suit Results					Flag Outside Limits			
1	Acesulfame K	<input checked="" type="checkbox"/>					<input checked="" type="checkbox"/>			
2	Benzoic Acid	<input checked="" type="checkbox"/>					<input checked="" type="checkbox"/>			
3	Sorbic Acid	<input checked="" type="checkbox"/>					<input checked="" type="checkbox"/>			
4	Caffeine	<input checked="" type="checkbox"/>					<input checked="" type="checkbox"/>			
5	Aspartame	<input checked="" type="checkbox"/>					<input checked="" type="checkbox"/>			
Suitability Limits										
E	Field Name	Target	Error %	Lower Error Limit (LCL)	Upper Error Limit (UCL)	Warning %	Lower Warning Limit	Upper Warning Limit	Ignore Blank Values	Check Limits



# INTERACTIVE SYSTEM SUITABILITY

## Setting up Interactive System Suitability – Processing

<input checked="" type="checkbox"/> Flag Values Outside Limits										
Suitability Components										
	Name	Calculate Suit Results					Flag Outside Limits			
1	Acesulfame K	<input checked="" type="checkbox"/>					<input checked="" type="checkbox"/>			
2	Benzoic Acid	<input checked="" type="checkbox"/>					<input checked="" type="checkbox"/>			
3	Sorbic Acid	<input checked="" type="checkbox"/>					<input checked="" type="checkbox"/>			
4	Caffeine	<input checked="" type="checkbox"/>					<input checked="" type="checkbox"/>			
5	Aspartame	<input checked="" type="checkbox"/>					<input checked="" type="checkbox"/>			
Suitability Limits										
	Field Name	Target	Error %	Lower Error Limit (LCL)	Upper Error Limit (UCL)	Warning %	Lower Warning Limit	Upper Warning Limit	Ignore Blank Values	Check Limits

After the System Suitability limits are set, run the System Suitability Samples





# INTERACTIVE SYSTEM SUITABILITY

## Setting up Interactive System Suitability – Run Samples

Run Only
Continue on Fault

Sample Set Method: Soft Drink Analysis

	Vial	Inj Vol (uL)	# of Injs	Label	SampleName	Function	Method Set / Report or Export Method	Label Reference	Processing	Run Time (Minutes)
1	1	5.0	1		Blank	Inject Samples	Soft Drink Analysis ACQ		Ignore Faults	3.00
2	2	5.0	6	SST	System Suitability Standard	Inject Samples	Soft Drink Analysis ACQ		Normal	3.00
3						Summarize Custom Fields			Normal	
4	3	5.0	1		Standard 1	Inject Sta			Normal	3.00
5	4	5.0	1		Standard 2	Inject Sta			Normal	3.00
6	5	5.0	1		Standard 3	Inject Sta			Normal	3.00
7	6	5.0	1		Standard 4	Inject Standards	Soft Drink Analysis ACQ		Normal	3.00
8	7	5.0	1		Standard 5	Inject Standards	Soft Drink Analysis ACQ		Normal	3.00
9	8	5.0	1		Sample A	Inject Samples	Soft Drink Analysis ACQ		Ignore Faults	3.00
10	9	5.0	1		Sample B	Inject Samples	Soft Drink Analysis ACQ		Ignore Faults	3.00
11	10	5.0	1		Sample C	Inject Samples	Soft Drink Analysis ACQ		Ignore Faults	3.00

Sys Suit will only be evaluated for System Suitability Standard



# INTERACTIVE SYSTEM SUITABILITY

## Setting up Interactive System Suitability – Run Samples

Run Only    Continue on Fault

Run Only  
Run and Process  
Run and Report

Sample Set Method: So

Vial	Inj Vol (uL)	# of Injs	Label	SampleName	Function	Method	Label	Processing	Run Time (Minutes)
1	1	5.0	1	Blank					3.00
2	2	5.0	6	SST	System Suitability Standard	Inject Samples	Soft Drink Analysis ACQ	Normal	3.00
3					Summarize Custom Fields			Normal	
4	3	5.0	1	Standard 1	Inject Standards	Soft Drink Analysis ACQ		Normal	3.00
5	4	5.0	1	Standard 2	Inject Standards	Soft Drink Analysis ACQ		Normal	3.00
6	5	5.0	1	Standard 3	Inject Standards	Soft Drink Analysis ACQ		Normal	3.00
7	6	5.0	1	Standard 4	Inject Standards	Soft Drink Analysis ACQ		Normal	3.00
8	7	5.0	1	Standard 5	Inject Standards	Soft Drink Analysis ACQ		Normal	3.00
9	8	5.0	1	Sample A	Inject Samples	Soft Drink Analysis ACQ		Ignore Faults	3.00
10	9	5.0	1	Sample B	Inject Samples	Soft Drink Analysis ACQ		Ignore Faults	3.00
11	10	5.0	1	Sample C	Inject Samples	Soft Drink Analysis ACQ		Ignore Faults	3.00

Choose Run and Process or Run and Report for online data processing



# INTERACTIVE SYSTEM SUITABILITY

## Setting up Interactive System Suitability – Run Samples

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Choose *Interactive System Suitability* Settings

Run and Process

Continue on Fault

- Continue on Fault
- Stop on Fault
- Reinject on Fault
- Next Sample on Fault
- Next Sample Set on Fault

What's a Fault?  
This is a *System Suitability Fail*

Vial	Inj Vol (uL)	# of Injs	Label	SampleName	Function	Method Set / Report or Export Method	Re			
1	1	5.0	1		Blank	Inject Samples	Soft Drink Analysis ACQ		Ignore Faults	3.00
2	2	5.0	6	SST	System Suitability Standard	Inject Samples	Soft D			
3					Summarize Custom Fields					
4	3	5.0	1		Standard 1	Inject Standards	Soft Drink Analysis ACQ		Normal	3.00
5	4	5.0	1		Standard 2	Inject Standards	Soft Drink Analysis ACQ		Normal	3.00
6	5	5.0	1		Standard 3	Inject Standards	Soft Drink Analysis ACQ		Normal	3.00
7	6	5.0	1		Standard 4	Inject Standards	Soft Drink Analysis ACQ		Normal	3.00
8	7	5.0	1		Standard 5	Inject Standards	Soft Drink Analysis ACQ		Normal	3.00
9	8	5.0	1		Sample A	Inject Samples	Soft Drink Analysis ACQ		Ignore Faults	3.00
10	9	5.0	1		Sample B	Inject Samples	Soft Drink Analysis ACQ		Ignore Faults	3.00
11	10	5.0	1		Sample C	Inject Samples	Soft Drink Analysis ACQ		Ignore Faults	3.00





# INTERACTIVE SYSTEM SUITABILITY

## Setting up Interactive System Suitability – Run Samples

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Sample Set Method: Soft Drink Ana

	Vial	Inj Vol (uL)	# of Injs	Label	SampleName	Function	Report or Export Method	Label Reference	Processing	Time (Minutes)
1	1	5.0	1		Blank	Inject Samples	Soft Drink Analysis ACQ		Ignore Faults	3.00
2	2	5.0	6	SST	System Suitability Standard	Inject Samples	Soft Drink Analysis ACQ		Normal	3.00
3						Summarize Custom Fields			Normal	
4	3	5.0								3.00
5	4	5.0								3.00
6	5	5.0	1		Standard 3	Inject Standards	Soft Drink Analysis ACQ		Normal	3.00
7	6	5.0	1		Standard 4	Inject Standards	Soft Drink Analysis ACQ		Normal	3.00
8	7	5.0	1		Standard 5	Inject Standards	Soft Drink Analysis ACQ		Normal	3.00
9	8	5.0	1		Sample A	Inject Samples	Soft Drink Analysis ACQ		Ignore Faults	3.00
10	9	5.0	1		Sample B	Inject Samples	Soft Drink Analysis ACQ		Ignore Faults	3.00

Press to Start Run



# INTERACTIVE SYSTEM SUITABILITY

## Stops Run Automatically Upon Suitability Failure

# Waters

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The screenshot displays the Waters software interface during a sample run. The main window title is "Alliance in Empower Marketing Demos\Empower for Food\_Custom Fields as System/Administrator - QuickStart - [Run Samples]". The menu bar includes File, Edit, View, Inject, Actions, Tools, Customize, Diagnostics, Manage, and Help. The toolbar shows various icons for file operations and system control, with "Run and Process" and "Stop on Fault" dropdown menus. The active sample set is "Soft Drink Analysis".

Vial	Inj Vol (uL)	# of Injs	Label	SampleName	Function	Method Set / Report or Export Method	Label Reference	Processing	Run Time (Minutes)
1	5.0	1		Blank	Inject Samples	Soft Drink Analysis ACQ		Ignore Faults	3.00
2	5.0	6	SST	System Suitability Standard	Inject Samples	Soft Drink Analysis ACQ		Normal	3.00
3					Summarize Custom Fields			Normal	
4	5.0	1		Standard 1	Inject Standards	Soft Drink Analysis ACQ		Normal	3.00
5	5.0	1		Standard 2	Inject Standards	Soft Drink Analysis ACQ		Normal	3.00
6	5.0	1		Standard 3	Inject Standards	Soft Drink Analysis ACQ		Normal	3.00
7	5.0	1		Standard 4	Inject Standards	Soft Drink Analysis ACQ		Normal	3.00
8	5.0	1		Standard 5	Inject Standards	Soft Drink Analysis ACQ		Normal	3.00
9	5.0	1		Sample A	Inject Samples	Soft Drink Analysis ACQ		Ignore Faults	3.00
10	5.0	1		Sample B	Inject Samples	Soft Drink Analysis ACQ		Ignore Faults	3.00

The bottom right of the interface shows a chromatogram plot with the y-axis labeled "AU" (Absorbance Units) ranging from 0.00 to 1.00 and the x-axis labeled "Minutes" ranging from -1.00 to 0.00. The plot area is currently empty. The status bar at the bottom left indicates "For Help, press F1".



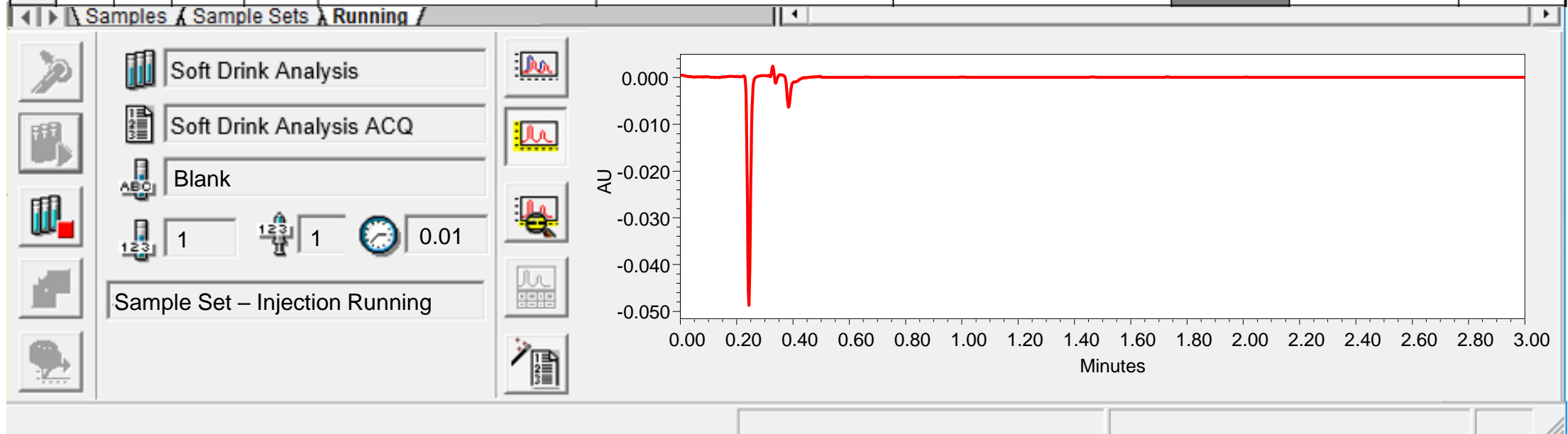
# INTERACTIVE SYSTEM SUITABILITY

## Stops Run Automatically Upon Suitability Failure

# Waters

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	Vial	Inj Vol (uL)	# of Injs	Label	SampleName	Function	Method Set / Report or Export Method	Label Reference	Processing	Run Time (Minutes)
1	1	5.0	1		Blank	Inject Samples	Soft Drink Analysis ACQ		Ignore Faults	3.00
2	2	5.0	6	SST	System Suitability Standard	Inject Samples	Soft Drink Analysis ACQ		Normal	3.00
3						Summarize Custom Fields			Normal	
4	3	5.0	1		Standard 1	Inject Standards	Soft Drink Analysis ACQ		Normal	3.00
5	4	5.0	1		Standard 2	Inject Standards	Soft Drink Analysis ACQ		Normal	3.00





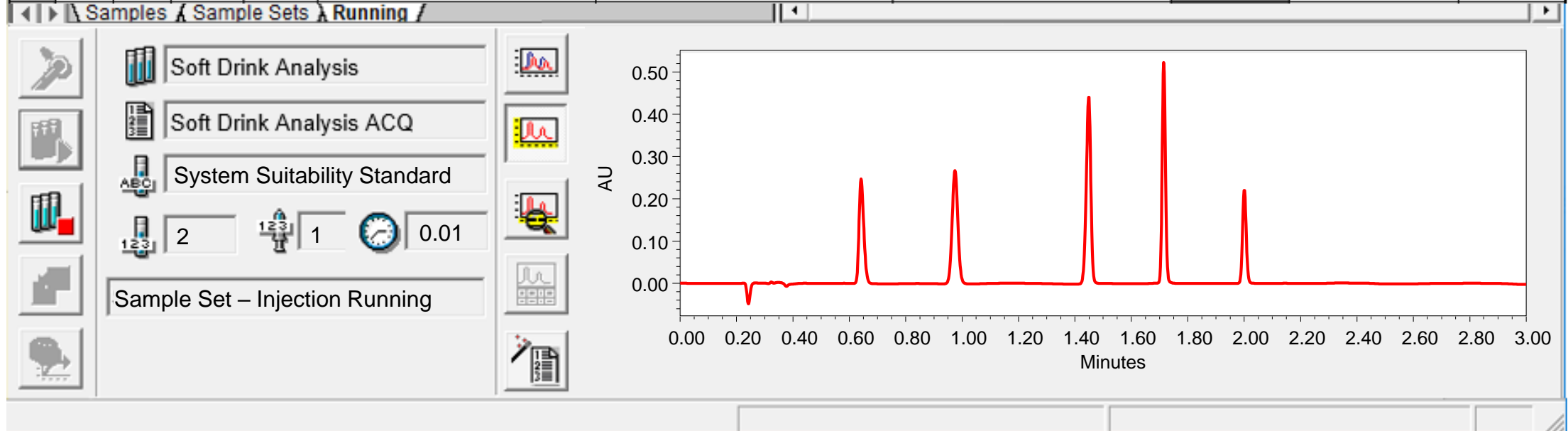
# INTERACTIVE SYSTEM SUITABILITY

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	Vial	Inj Vol (uL)	# of Injs	Label	SampleName	Function	Method Set / Report or Export Method	Label Reference	Processing	Run Time (Minutes)
1	1	5.0	1		Blank	Inject Samples	Soft Drink Analysis ACQ		Ignore Faults	3.00
2	2	5.0	6	SST	System Suitability Standard	Inject Samples	Soft Drink Analysis ACQ		Normal	3.00
3						Summarize Custom Fields			Normal	
4	3	5.0	1		Standard 1	Inject Standards	Soft Drink Analysis ACQ		Normal	3.00
5	4	5.0	1		Standard 2	Inject Standards	Soft Drink Analysis ACQ		Normal	3.00





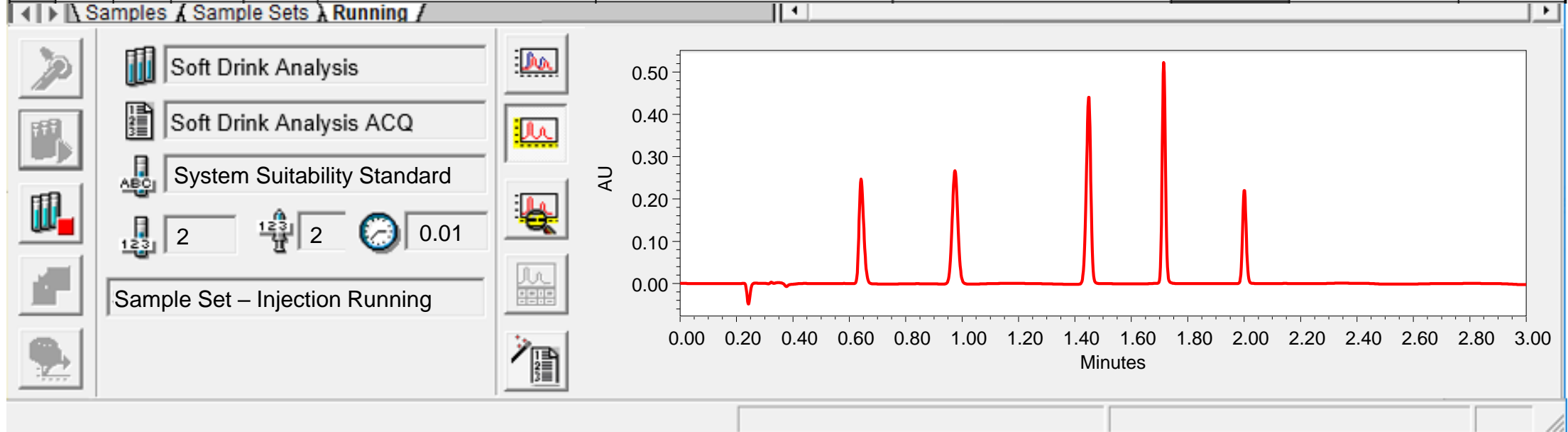
# INTERACTIVE SYSTEM SUITABILITY

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	Vial	Inj Vol (uL)	# of Injs	Label	SampleName	Function	Method Set / Report or Export Method	Label Reference	Processing	Run Time (Minutes)
1	1	5.0	1		Blank	Inject Samples	Soft Drink Analysis ACQ		Ignore Faults	3.00
2	2	5.0	6	SST	System Suitability Standard	Inject Samples	Soft Drink Analysis ACQ		Normal	3.00
3						Summarize Custom Fields			Normal	
4	3	5.0	1		Standard 1	Inject Standards	Soft Drink Analysis ACQ		Normal	3.00
5	4	5.0	1		Standard 2	Inject Standards	Soft Drink Analysis ACQ		Normal	3.00





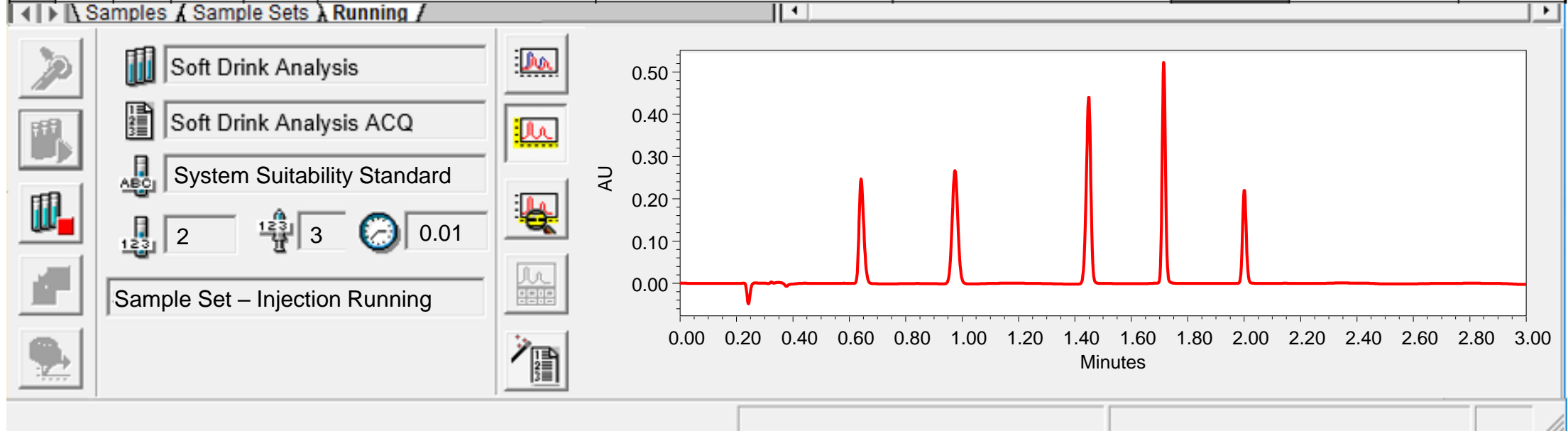
# INTERACTIVE SYSTEM SUITABILITY

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	Vial	Inj Vol (uL)	# of Injs	Label	SampleName	Function	Method Set / Report or Export Method	Label Reference	Processing	Run Time (Minutes)
1	1	5.0	1		Blank	Inject Samples	Soft Drink Analysis ACQ		Ignore Faults	3.00
2	2	5.0	6	SST	System Suitability Standard	Inject Samples	Soft Drink Analysis ACQ		Normal	3.00
3						Summarize Custom Fields			Normal	
4	3	5.0	1		Standard 1	Inject Standards	Soft Drink Analysis ACQ		Normal	3.00
5	4	5.0	1		Standard 2	Inject Standards	Soft Drink Analysis ACQ		Normal	3.00





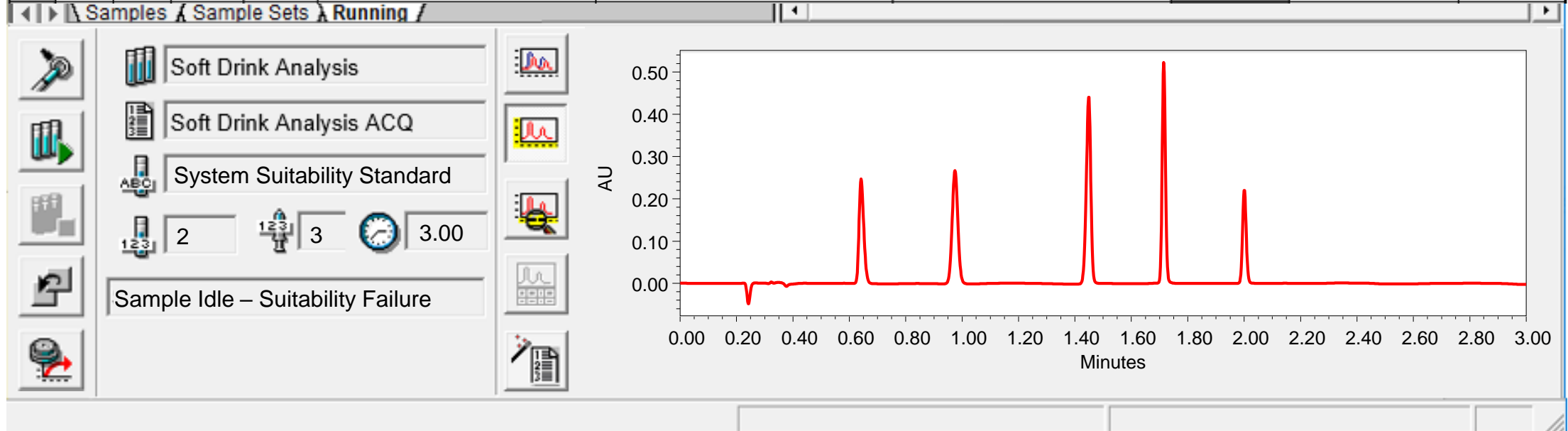
# INTERACTIVE SYSTEM SUITABILITY

## Stops Run Automatically Upon Suitability Failure

# Waters

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	Vial	Inj Vol (uL)	# of Injs	Label	SampleName	Function	Method Set / Report or Export Method	Label Reference	Processing	Run Time (Minutes)
1	1	5.0	1		Blank	Inject Samples	Soft Drink Analysis ACQ		Ignore Faults	3.00
2	2	5.0	6	SST	System Suitability Standard	Inject Samples	Soft Drink Analysis ACQ		Normal	3.00
3						Summarize Custom Fields			Normal	
4	3	5.0	1		Standard 1	Inject Standards	Soft Drink Analysis ACQ		Normal	3.00
5	4	5.0	1		Standard 2	Inject Standards	Soft Drink Analysis ACQ		Normal	3.00





# INTERACTIVE SYSTEM SUITABILITY

## Stops Run Automatically Upon Suitability Failure

# Waters

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	Vial	Inj Vol (uL)	# of Injs	Label	SampleName	Function	Method Set / Report or Export Method	Label Reference
	1	5.0	1		Blank	Inject Samples	Soft Drink Analysis ACQ	
	2	5.0	6	SST	System Suitability Standard	Inject Samples	Soft Drink Analysis ACQ	
	3					Summarize Custom Fields		
	4	5.0	1		Standard 1	Inject Standards	Soft Drink Analysis ACQ	
	5	5.0	1		Standard 2	Inject Standards	Soft Drink Analysis ACQ	

← Samples / Sample Sets / Running /

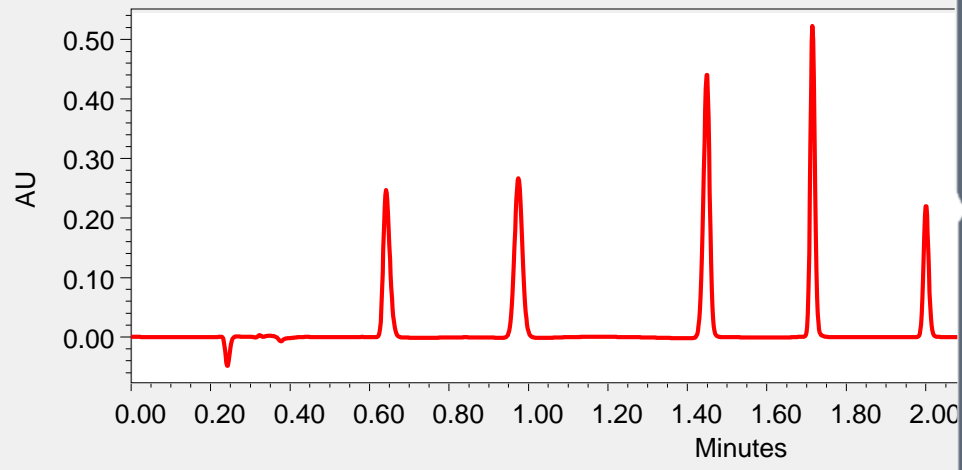
Soft Drink Analysis

Soft Drink Analysis ACQ

System Suitability Standard

2 3 3.00

**Sample Idle – Suitability Failure**





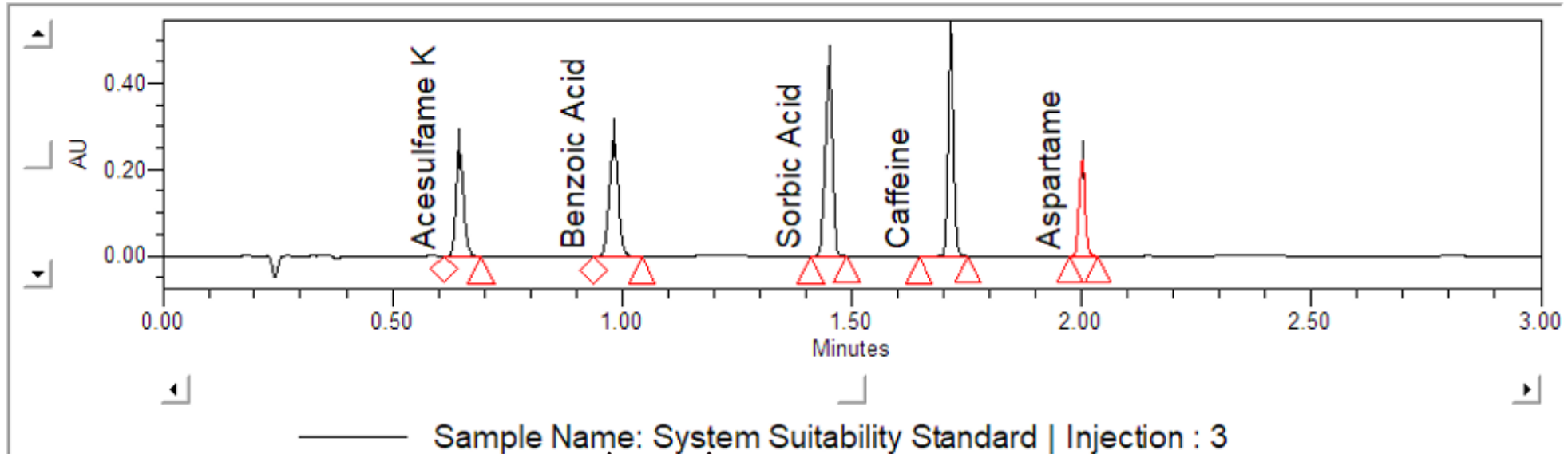


# INTERACTIVE SYSTEM SUITABILITY

## Stops Run Automatically Upon Suitability Failure

# Waters

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Name	Retention Time (min)	Area	Height (μV)	Int Type	Amount	Units	Peak Type
1 Acesulfame K	0.645	294068	248749	VB	50.000	mg/L	Found
2 <b>Benzoic Acid</b>	<b>0.968</b>	384068	272845	VB	50.000	mg/L	Found
3 Sorbic Acid	1.451	497416	497416	VB	75.000	mg/L	Found
4 Caffeine	1.716	428613	428613	VB	75.000	mg/L	Found
5 Aspartame	2.001	201227	221723	BB	75.000	mg/L	Found



In the Results Review Window, Empower flags **SysSuit failures**.



# INTERACTIVE SYSTEM SUITABILITY

## Conclusion

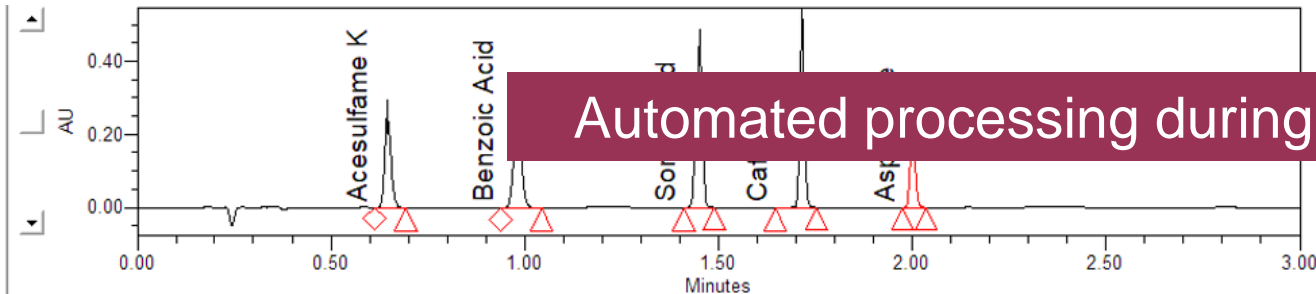
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System Suitability parameters are set up in the processing method

Suitability Components									
Name	Calculate Suit Results					Flag Outside Limits			
1 Acesulfame K	<input checked="" type="checkbox"/>					<input checked="" type="checkbox"/>			

Suitability Limits									
Field Name	Target	Error %	Lower Error Limit (LCL)	Upper Error Limit (UCL)	Warning %	Lower Warning Limit	Upper Warning Limit	Ignore Blank Values	Check Limits
1 Retention Time	0.650	3.00	0.631	0.670				<input type="checkbox"/>	During Quantitation



Name	Retention Time (min)	Area (μV*sec)	% Area	Height (μV)	Int Type	Amount	Units	Peak Type
2 <b>Benzoic Acid</b>	<b>0.968</b>	384068	21.32	272845	VB	50.000	mg/L	Found

Automatically stops a run when System Suitability parameters fail





# INTERACTIVE SYSTEM SUITABILITY

We're Empowered! Can Empower Do More?

**Interactive System Suitability** can also be set up for:

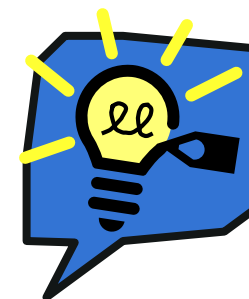
- **Calibration Standards**

- Calibration Curve Linearity ( $R^2$ )
- Percent Difference between calibration standards
- % Deviation

- **Repeat injections of System Suitability Standards**

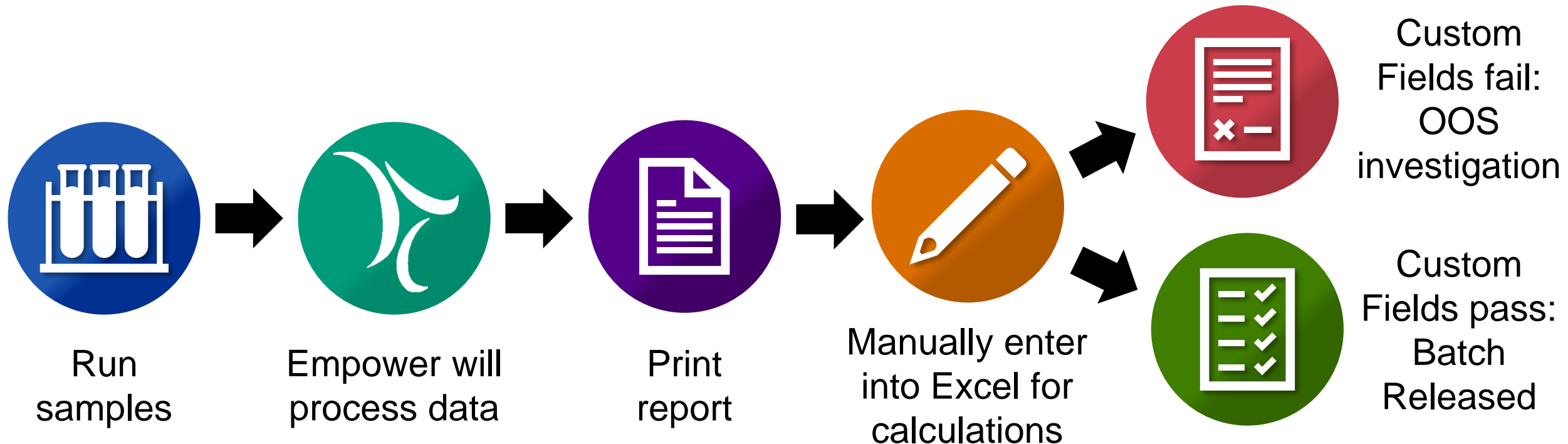
- Average / %RSD of peak area, retention time
  - Can be done with intersample summary custom fields



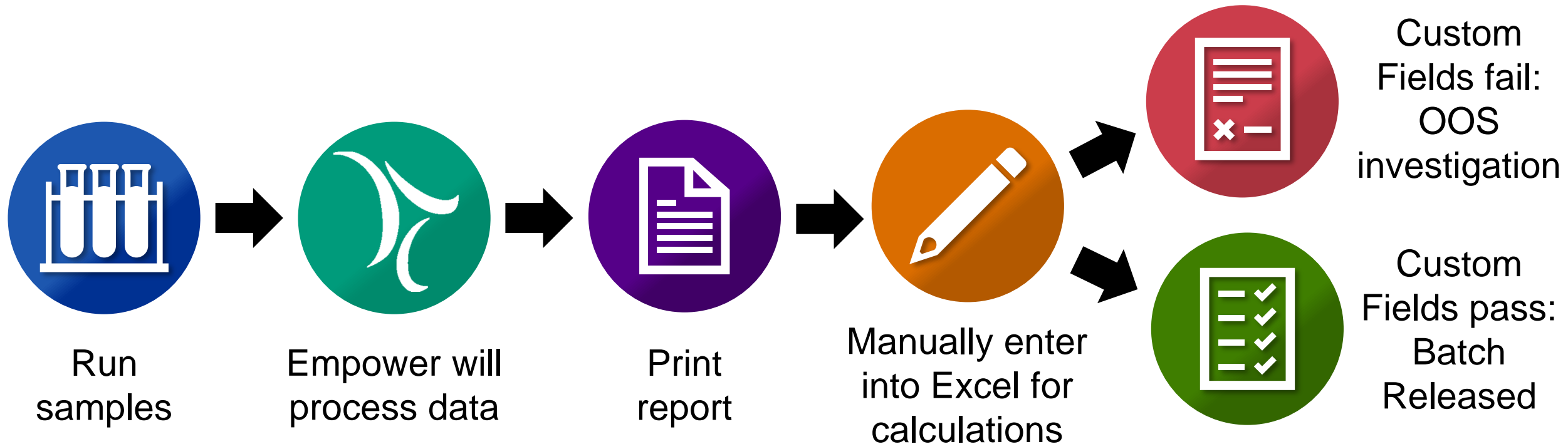


## Custom Fields

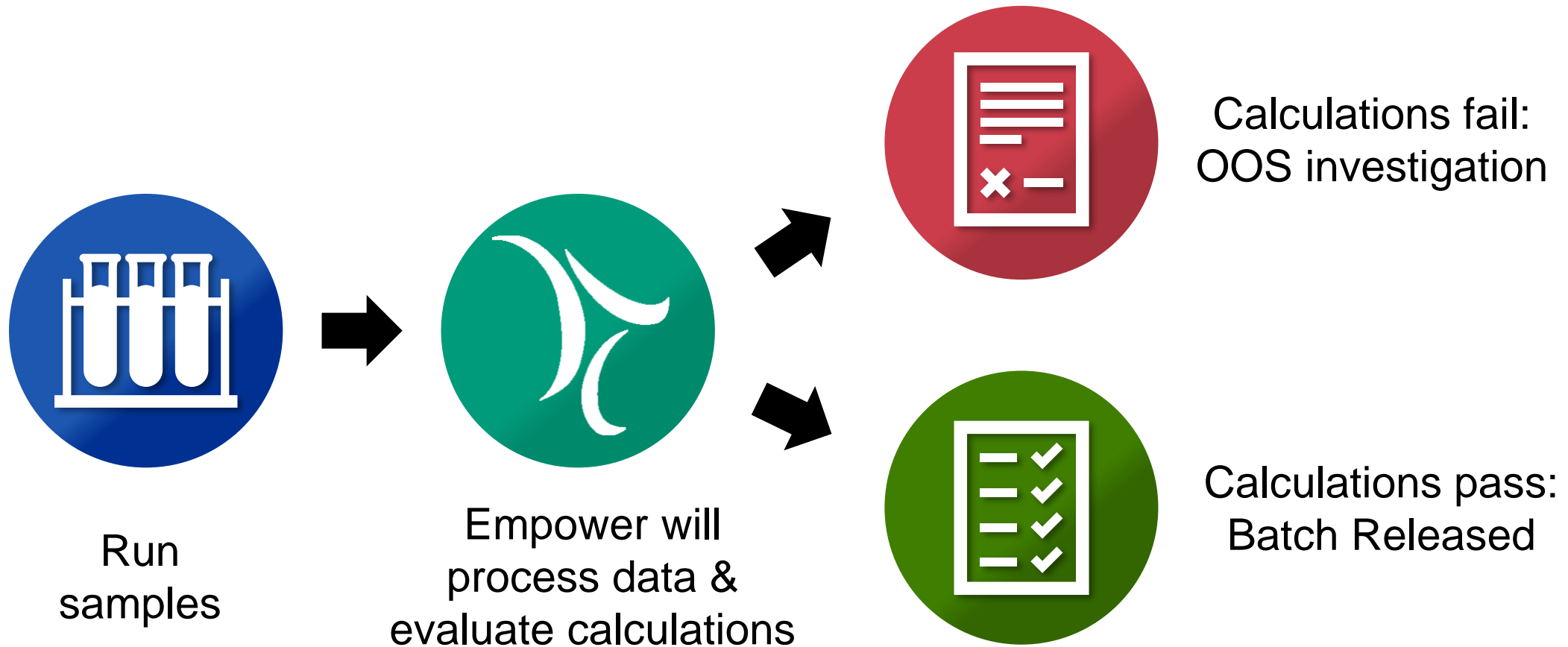
This is the typical analytical laboratory workflow for assay calculations:



With **Custom Fields**, the Analyst can streamline their workflow to:



With **Custom Fields**, the Analyst can streamline their workflow to:





# TAILORED CALCULATIONS

## What are Custom Fields?

Custom Fields are user-defined fields.

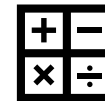
### DESCRIPTORS



*Fields that store data*

- Retrieve and sort data
- Track data entry
- Report data

### CALCULATIONS



*Fields that perform calculations*

- Minimize manual transcription and perform automated calculations
- Track calculations
- Lock calculation formulae
- Report calculated custom fields





# TAILORED CALCULATIONS

Setting up Custom Fields



How much Aspartame is in the drink?

What is the deviation?

Is deviation within target specs?



# TAILORED CALCULATIONS

Setting up Custom Fields



## CUSTOM FIELD 1: TARGET AMOUNT

*Input* Target Amount of Asp expected



How much Aspartame is in the drink?

What is the deviation?

Is deviation within target specs?



# TAILORED CALCULATIONS

Setting up Custom Fields



## CUSTOM FIELD 1: TARGET AMOUNT

Input Target Amount of Asp expected

How much Aspartame is in the drink?



## CUSTOM FIELD 2: PERCENT DIFFERENCE

Calculate Percent Difference based on the measured and Target Amount

What is the deviation?

Is deviation within target specs?





# TAILORED CALCULATIONS

## Setting up Custom Fields



### CUSTOM FIELD 1: TARGET AMOUNT

Input Target Amount of Asp expected

How much Aspartame is in the drink?



### CUSTOM FIELD 2: PERCENT DIFFERENCE

Calculate Percent Difference based on the measured and Target Amount

What is the deviation?



### CUSTOM FIELD 3: ASP PERCENT DIFFERENCE

Compare Percent Difference against the max acceptable specs to give pass/fail outcome

Is deviation within target specs?



# TAILORED CALCULATIONS

## Setting up Custom Fields

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**CREATING CUSTOM FIELDS IN EMPOWER**

Configuration Manager > Right Click on Project > Project Properties > Custom Fields Tab > New

No.	Field Name	Purpose of Field	Input / Output	Field Type	Data Type	Formula
1	Target Amount		Input <input type="checkbox"/> Calculated <input type="checkbox"/>	Sample <input type="checkbox"/> Result <input type="checkbox"/> Peak <input type="checkbox"/> Sample Set <input type="checkbox"/> Component <input type="checkbox"/> Distribution <input type="checkbox"/>	Integer <input type="checkbox"/> Text <input type="checkbox"/> Boolean <input type="checkbox"/> Real <input type="checkbox"/> Date <input type="checkbox"/> Enumerated <input type="checkbox"/>	
2	Percent Difference		Input <input type="checkbox"/> Calculated <input type="checkbox"/>	Sample <input type="checkbox"/> Result <input type="checkbox"/> Peak <input type="checkbox"/> Sample Set <input type="checkbox"/> Component <input type="checkbox"/> Distribution <input type="checkbox"/>	Integer <input type="checkbox"/> Text <input type="checkbox"/> Boolean <input type="checkbox"/> Real <input type="checkbox"/> Date <input type="checkbox"/> Enumerated <input type="checkbox"/>	
3	Asp Percent Difference		Input <input type="checkbox"/> Calculated <input type="checkbox"/>	Sample <input type="checkbox"/> Result <input type="checkbox"/> Peak <input type="checkbox"/> Sample Set <input type="checkbox"/> Component <input type="checkbox"/> Distribution <input type="checkbox"/>	Integer <input type="checkbox"/> Text <input type="checkbox"/> Boolean <input type="checkbox"/> Real <input type="checkbox"/> Date <input type="checkbox"/> Enumerated <input type="checkbox"/>	
4	Percent Difference Crit		Input <input type="checkbox"/> Calculated <input type="checkbox"/>	Sample <input type="checkbox"/> Result <input type="checkbox"/> Peak <input type="checkbox"/> Sample Set <input type="checkbox"/> Component <input type="checkbox"/> Distribution <input type="checkbox"/>	Integer <input type="checkbox"/> Text <input type="checkbox"/> Boolean <input type="checkbox"/> Real <input type="checkbox"/> Date <input type="checkbox"/> Enumerated <input type="checkbox"/>	
5	Batch Release Decision		Input <input type="checkbox"/> Calculated <input type="checkbox"/>	Sample <input type="checkbox"/> Result <input type="checkbox"/> Peak <input type="checkbox"/> Sample Set <input type="checkbox"/> Component <input type="checkbox"/> Distribution <input type="checkbox"/>	Integer <input type="checkbox"/> Text <input type="checkbox"/> Boolean <input type="checkbox"/> Real <input type="checkbox"/> Date <input type="checkbox"/> Enumerated <input type="checkbox"/>	
6			Input <input type="checkbox"/> Calculated <input type="checkbox"/>	Sample <input type="checkbox"/> Result <input type="checkbox"/> Peak <input type="checkbox"/> Sample Set <input type="checkbox"/> Component <input type="checkbox"/> Distribution <input type="checkbox"/>	Integer <input type="checkbox"/> Text <input type="checkbox"/> Boolean <input type="checkbox"/> Real <input type="checkbox"/> Date <input type="checkbox"/> Enumerated <input type="checkbox"/>	
7			Input <input type="checkbox"/> Calculated <input type="checkbox"/>	Sample <input type="checkbox"/> Result <input type="checkbox"/> Peak <input type="checkbox"/> Sample Set <input type="checkbox"/> Component <input type="checkbox"/> Distribution <input type="checkbox"/>	Integer <input type="checkbox"/> Text <input type="checkbox"/> Boolean <input type="checkbox"/> Real <input type="checkbox"/> Date <input type="checkbox"/> Enumerated <input type="checkbox"/>	

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Follow along with the  
**Webinar #3 Worksheet!**



# TAILORED CALCULATIONS

Setting up Custom Fields



## CUSTOM FIELD 1: TARGET AMOUNT

*Input* Target Amount of Asp expected

- Input: Keyboard
- Field Type: Component
- Data Type: Real





# TAILORED CALCULATIONS

Setting up Custom Fields



## CUSTOM FIELD 2: PERCENT DIFFERENCE

Calculate Percent Difference based on the measured and Target Amount

- Output: Calculated
- Field Type: Peak
- Data Type: Real

- Formula: 
$$\frac{|Target\ Amount - Amount|}{Amount} * 100$$





# TAILORED CALCULATIONS

Setting up Custom Fields



## CUSTOM FIELD 3: ASP PERCENT DIFFERENCE

Compare Percent Difference against the max acceptable specs to give pass/fail outcome

- Output: Calculated
- Field Type: Peak
- Data Type: Boolean
- Formula:  $LT(\text{Percent Difference}, 15)$ 
  - Formula Output: If Percent Difference  $< 15$ , Pass.  
If Percent Difference  $\geq 15$ , Fail.







# TAILORED CALCULATIONS

Automatically Calculates Custom Fields Upon Processing

- Upon processing, all custom calculations are automatically processed.

	Sample Name	Inj	Peak Name	RT	Amount	Units
1	Soft Drink Sample A	1	Aspartame	1.999	53.018	mg/L
2	Soft Drink Sample A	2	Aspartame	1.997	53.430	mg/L
3	Soft Drink Sample B	1	Aspartame	1.995	90.106	mg/L
4	Soft Drink Sample B	2	Aspartame	1.990	90.382	mg/L
5	Soft Drink Sample C	1	Aspartame	1.994	90.566	mg/L
6	Soft Drink Sample C	2	Aspartame	1.991	91.348	mg/L
7	Soft Drink Sample D	1	Aspartame	1.992	78.614	mg/L
8	Soft Drink Sample D	2	Aspartame	1.992	78.009	mg/L

*Amount* is automatically calculated by Empower



# TAILORED CALCULATIONS

Automatically Calculates Custom Fields Upon Processing

- Upon processing, all custom calculations are automatically processed.

	Sample Name	Inj	Peak Name	RT	Amount	Units	Target Amount
1	Soft Drink Sample A	1	Aspartame	1.999	53.018	mg/L	85.000
2	Soft Drink Sample A	2	Aspartame	1.997	53.430	mg/L	85.000
3	Soft Drink Sample B	1	Aspartame	1.995	90.106	mg/L	85.000
4	Soft Drink Sample B	2	Aspartame	1.990	90.382	mg/L	85.000
5	Soft Drink Sample C	1	Aspartame	1.994	90.566	mg/L	85.000
6	Soft Drink Sample C	2	Aspartame	1.991	91.348	mg/L	85.000
7	Soft Drink Sample D	1	Aspartame	1.992	78.614	mg/L	85.000
8	Soft Drink Sample D	2	Aspartame	1.992	78.009	mg/L	85.000

*Target Amount* was entered into Empower



# TAILORED CALCULATIONS

Automatically Calculates Custom Fields Upon Processing

- Upon processing, all custom calculations are automatically processed.

	Sample Name	Inj	Peak Name	RT	Amount	Units	Target Amount	Calculated Percent Difference (%)	Aspartame Percent Difference (Range: 0 - 15%)
1	Soft Drink Sample A	1	Aspartame	1.999	53.018	mg/L	85.000	37.625	Fail
2	Soft Drink Sample A	2	Aspartame	1.997	53.430	mg/L	85.000	37.142	Fail
3	Soft Drink Sample B	1	Aspartame	1.995	90.106	mg/L	85.000	6.008	Pass
4	Soft Drink Sample B	2	Aspartame	1.990	90.382	mg/L	85.000	6.331	Pass
5	Soft Drink Sample C	1	Aspartame	1.994	90.566	mg/L	85.000	6.549	Pass
6	Soft Drink Sample C	2	Aspartame	1.991	91.348	mg/L	85.000	7.469	Pass
7	Soft Drink Sample D	1	Aspartame	1.992	78.614	mg/L	85.000	7.513	Pass
8	Soft Drink Sample D	2	Aspartame	1.992	78.009	mg/L	85.000	8.224	Pass

*Percent Difference* is automatically calculated, with a decision automatically generated



# TAILORED CALCULATIONS

Setting up Custom Fields



## CUSTOM FIELD 1: TARGET AMOUNT

Input Target Amount of Asp expected

How much Aspartame is in the drink?



## CUSTOM FIELD 2: PERCENT DIFFERENCE

Calculate Percent Difference based on the measured and Target Amount

What is the deviation?



## CUSTOM FIELD 3: ASP PERCENT DIFFERENCE

Compare Percent Difference against the max acceptable specs to give pass/fail outcome

Is deviation within target specs?



# TAILORED CALCULATIONS

Setting up Custom Fields – Extended



## CUSTOM FIELD 1: TARGET AMOUNT

Input Target Amount of Asp & Ace K

How much Asp & Ace K is in the drink?



## CUSTOM FIELD 2: PERCENT DIFFERENCE

Calculate Percent Difference based on the measured and Target Amount

What is the deviation?



## CUSTOM FIELD 3: ASP PERCENT DIFFERENCE

Compare Percent Difference against the max acceptable specs to give pass/fail outcome

Is deviation within target specs?



# TAILORED CALCULATIONS

Setting up Custom Fields – Extended



## CUSTOM FIELD 1: TARGET AMOUNT

Input Target Amount of Asp & Ace K

How much Asp & Ace K is in the drink?



## CUSTOM FIELD 2: PERCENT DIFFERENCE

Calculate Percent Difference based on the measured and Target Amount

What is the deviation?



## CUSTOM FIELD 3: PERCENT DIFFERENCE CRIT

Compare Percent Difference against the max acceptable specs to give pass/fail outcome

Is deviation within target specs?



# TAILORED CALCULATIONS

Setting up Custom Fields – Extended



## CUSTOM FIELD 1: TARGET AMOUNT

Input Target Amount of Asp & Ace K

How much Asp & Ace K is in the drink?



## CUSTOM FIELD 4: BATCH RELEASE DECISION

Output Batch Release Decision based on Asp & Ace K Percent Difference Crit outcomes



## CUSTOM FIELD 2: PERCENT DIFFERENCE

Calculate Percent Difference based on the measured and Target Amount

What is the deviation?



## CUSTOM FIELD 3: PERCENT DIFFERENCE CRIT

Compare Percent Difference against the max acceptable specs to give pass/fail outcome

Is deviation within target specs?



# TAILORED CALCULATIONS

Setting up Custom Fields – Extended



## CUSTOM FIELD 1: TARGET AMOUNT

*Input Target Amount of Asp & Ace K*

- Input: Keyboard
- Field Type: Component
  - Since Target Amount is a Component field, a different value can be entered for each Component
- Data Type: Real







# TAILORED CALCULATIONS

Setting up Custom Fields – Extended



## CUSTOM FIELD 2: PERCENT DIFFERENCE

Calculate Percent Difference based on the measured and Target Amount

- Output: Calculated
- Field Type: Peak
- Data Type: Real

- Formula: 
$$\frac{|Target\ Amount - Amount|}{Amount} * 100$$





# TAILORED CALCULATIONS

Setting up Custom Fields – Extended



## CUSTOM FIELD 3: PERCENT DIFFERENCE CRIT

Compare Percent Difference against the max acceptable specs to give pass/fail outcome

- Output: Calculated
- Field Type: Peak
- Data Type: Boolean
- For **ASP PERCENT DIFFERENCE**

Formula:  $LT(\text{Percent Difference}, 15)$

– Formula Output: If Percent Difference  $< 15$ , Pass.

If Percent Difference  $\geq 15$ , Fail.

– However, this is a fixed Percent Difference threshold





# TAILORED CALCULATIONS

Setting up Custom Fields – Extended



## CUSTOM FIELD 3: PERCENT DIFFERENCE CRIT

Compare Percent Difference against the max acceptable specs to give pass/fail outcome

- Output: Calculated
- Field Type: Peak
- Data Type: Boolean
- Formula:  $LT(\text{Percent Difference}, CConst1)$ 
  - Set different threshold for different components
  - CConst is entered in the Processing Method
  - E.g. For Aspartame,  $CConst1 = 15$   
For Acesulfame K,  $CConst1 = 10$
  - Formula Output: If  $\text{Percent Difference} < CConst$ , Pass.  
If  $\text{Percent Difference} \geq CConst$ , Fail.





# TAILORED CALCULATIONS

Setting up Custom Fields – Extended



## CUSTOM FIELD 4: BATCH RELEASE DECISION

Output Batch Release Decision based on Asp & Ace K Percent Difference Crit outcomes

- Output: Calculated
- Field Type: Peak
  - Data Type: Boolean
- Formula:  $LT(CCompRef1[Percent\ Difference], CConst1) \& LT(CCompRef2[Percent\ Difference], CConst2)$ 
  - CCompRef & CConst are entered in the Processing Method
  - E.g. CCompRef1 = Aspartame, CConst1 = 15  
CCompRef2 = Acesulfame K, CConst2 = 10
  - Formula Output: If both Asp and Ace K pass, Batch Release.

If either/both Asp/Ace K fail, Out of Specifications



# TAILORED CALCULATIONS

Automatically Calculates Custom Fields Upon Processing

- Different specifications for different analytes can be performed easily

Sample Name: Soft Drink Sample A

	Sample Name	Inj	Name	RT	Amount	Units	Target Amount	Calculated Percent Difference (%)	Acesulfame K Percent Difference (Range: 0-10%) Aspartame Percent Difference (Range: 0 - 15%)	Batch Release Decision
1	Soft Drink Sample A	1	Acesulfame K	0.645	62.236	mg/L	48.000	29.657	Fail	Out of Specifications
2	Soft Drink Sample A	1	Aspartame	1.999	53.018	mg/L	85.000	37.625	Fail	
3	Soft Drink Sample A	2	Acesulfame K	0.643	63.042	mg/L	48.000	31.337	Fail	Out of Specifications
4	Soft Drink Sample A	2	Aspartame	1.997	53.430	mg/L	85.000	37.142	Fail	

1 Field for *Percent Difference* calculates for both Acesulfame K and Aspartame



# TAILORED CALCULATIONS

Automatically Calculates Custom Fields Upon Processing

- With the use of generic peak names & constants, custom fields can become highly flexible

Sample Name: Soft Drink Sample B

	Sample Name	Inj	Name	RT	Amount	Units	Target Amount	Calculated Percent Difference (%)	Acesulfame K Percent Difference (Range: 0-10%) Aspartame Percent Difference (Range: 0 - 15%)	Batch Release Decision
1	Soft Drink Sample B	1	Acesulfame K	0.647	20.357	mg/L	48.000	57.589	Fail	Out of Specifications
2	Soft Drink Sample B	1	Aspartame	1.995	90.106	mg/L	85.000	6.008	Pass	
3	Soft Drink Sample B	2	Acesulfame K	0.646	20.016	mg/L	48.000	58.301	Fail	Out of Specifications
4	Soft Drink Sample B	2	Aspartame	1.990	90.382	mg/L	85.000	6.331	Pass	

1 Field to make a *Decision* for both Acesulfame K and Aspartame



# TAILORED CALCULATIONS

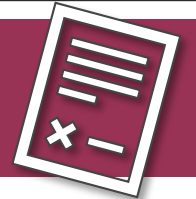
Automatically Calculates Custom Fields Upon Processing

- Boolean calculations enable Empower to generate a batch release decision based on multiple outcomes

Sample Name: Soft Drink Sample B

	Sample Name	Inj	Name	RT	Amount	Units	Target Amount	Calculated Percent Difference (%)	Acesulfame K Percent Difference (Range: 0-10%) Aspartame Percent Difference (Range: 0 - 15%)	Batch Release Decision
1	Soft Drink Sample B	1	Acesulfame K	0.647	20.357	mg/L	48.000	57.589	Fail	Out of Specifications
2	Soft Drink Sample B	1	Aspartame	1.995	90.106	mg/L	85.000	6.008	Pass	
3	Soft Drink Sample B	2	Acesulfame K	0.646	20.016	mg/L	48.000	58.301	Fail	Out of Specifications
4	Soft Drink Sample B	2	Aspartame	1.990	90.382	mg/L	85.000	6.331	Pass	

1 Field to consolidate Batch Release decisions based on the outcome of both Acesulfame K and Aspartame





# TAILORED CALCULATIONS

Automatically Calculates Custom Fields Upon Processing

- Boolean calculations enable Empower to generate a batch release decision based on multiple outcomes

Sample Name: Soft Drink Sample C

	Sample Name	Inj	Name	RT	Amount	Units	Target Amount	Calculated Percent Difference (%)	Acesulfame K Percent Difference (Range: 0-10%) Aspartame Percent Difference (Range: 0 - 15%)	Batch Release Decision
1	Soft Drink Sample C	1	Acesulfame K	0.646	50.358	mg/L	48.000	4.914	Pass	Batch Release
2	Soft Drink Sample C	1	Aspartame	1.994	90.566	mg/L	85.000	6.549	Pass	
3	Soft Drink Sample C	2	Acesulfame K	0.643	50.106	mg/L	48.000	4.388	Pass	Batch Release
4	Soft Drink Sample C	2	Aspartame	1.991	91.348	mg/L	85.000	7.469	Pass	

**1** Field to consolidate Batch Release decisions based on the outcome of both Acesulfame K and Aspartame

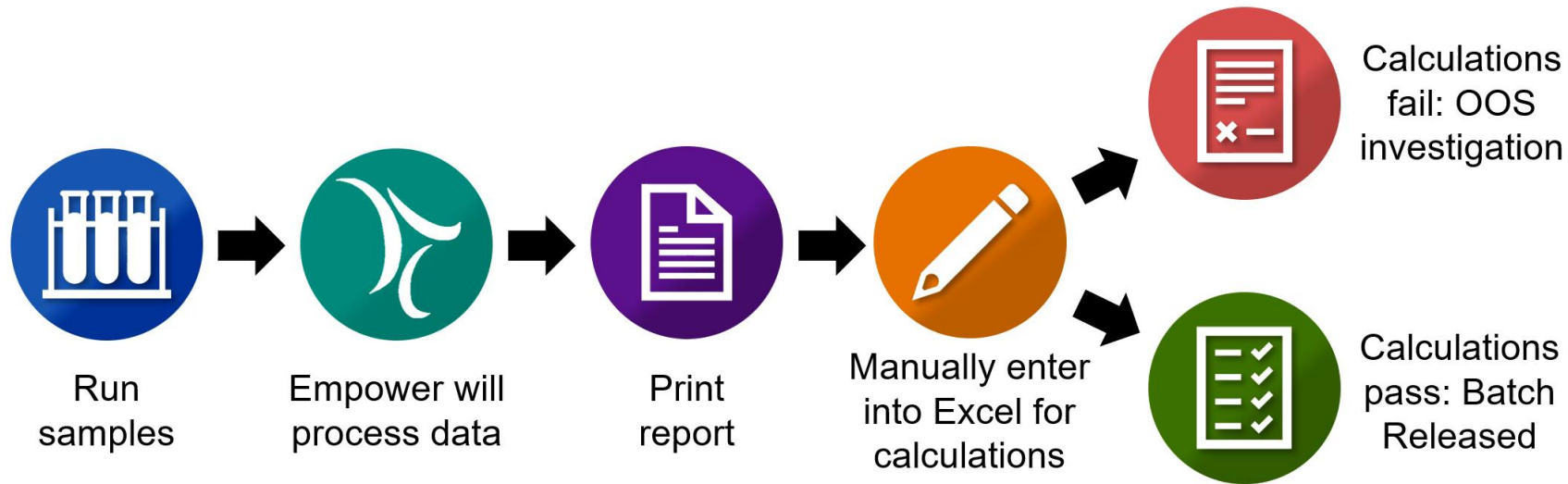






# TAILORED CALCULATIONS

## Conclusion



- Custom Fields allow for automated calculations
  - Eliminates transcription errors, increases laboratory efficiency
  - Quick decisions based on multiple outcomes
- Custom Fields can also be used for data recording
- Ensure traceability of results: Each generated calculation is recorded



# TAILORED CALCULATIONS

We're Empowered! Can Empower Do More?

Tailored calculations can also be set up to obtain:

## ■ User-defined conclusions

- Pass/Fail, Yes/No, etc
- Display actual value
  - E.g. If  $s/n$  is  $< 10$ , formula output: Below LOQ
  - If  $s/n$  is  $\geq 10$ , formula output: Actual  $s/n$  value

## ■ Generate 3 or more conclusions

- E.g. OOS (Low), Batch Release, OOS (High)

## ■ OR Boolean

- E.g. If either/both Asp and Ace K pass, Batch Release



# ACHIEVE MORE



- Interactive System Suitability
  - Automated online processing of system suitability criteria
  - Automatically stops/reinjects upon system suitability failure
- Custom Fields
  - Evaluate multiple components with 1 formula
  - Automated calculations
  - Quick decision making

One-time set up for an immediate,  
long term boost in productivity

*by* **DOING LESS**

## Conclusion

- For more information:
  - Interactive System Suitability (Tip #14): <https://tinyurl.com/interactive-sys-suit>
  - Custom Fields (Tip #82–90, 92, 99): <https://blog.waters.com/get-empowered-review-window-and-the-processing-method-tip-82-custom-fields>
  - Empower 3 Software Automated Tailored Calculations (720000576EN)
  - Empower Custom Fields for Assay Calculations in Food (720006974EN)
  
- Empower for Food Project on Waters Marketplace (Project with Notes):  
<https://marketplace.waters.com/apps/309174/empower-food-project#!overview>

## Learnt Something New Today? Please Help Us!

- Please help us create content that is more relevant for you by filling in the post-webinar survey on this webinar page
- If you like to learn more Empower tips, please visit: <https://waters.com/empowertips>



Survey

\*1. The webinar met my expectation  
Select a Choice

\*2. The subject matter was presented effectively  
Select a Choice

\*3. The duration of the webinar was sufficient for the material covered  
Select a Choice

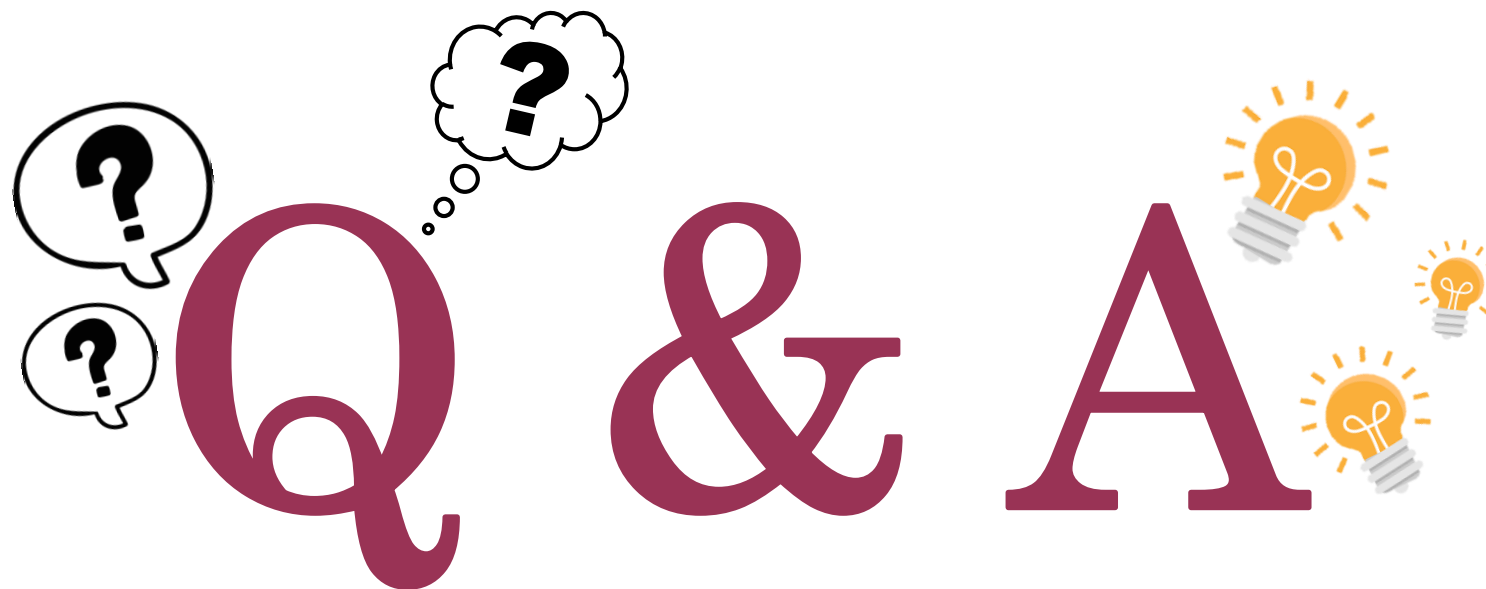
4. Are the Empower tips presented valuable to your laboratory operation?

5. What other Empower topics would you like to learn more about in the future?



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Let us know your questions and concerns!