



S88 IN THE LAB NOT JUST FOR BATCH PROCESSING

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3DEXPERIENCE®



WHAT AND WHY S88?

- ▶ S88, shorthand for ANSI/ISA88, is a standard addressing batch process control. It began as part of the ISA's standardization activity started in 1988.
- ▶ Design philosophy for describing equipment, and procedures (Recipes & Methods)
- ▶ Provides a comprehensive and modular methodology for designing, implementing, and managing batch processes.
- ▶ Defines what the main building blocks of a recipe (procedure, unit procedure, operation, and phase) look like and how they interact
- ▶ Streamlines process authoring and standardize structured data capture

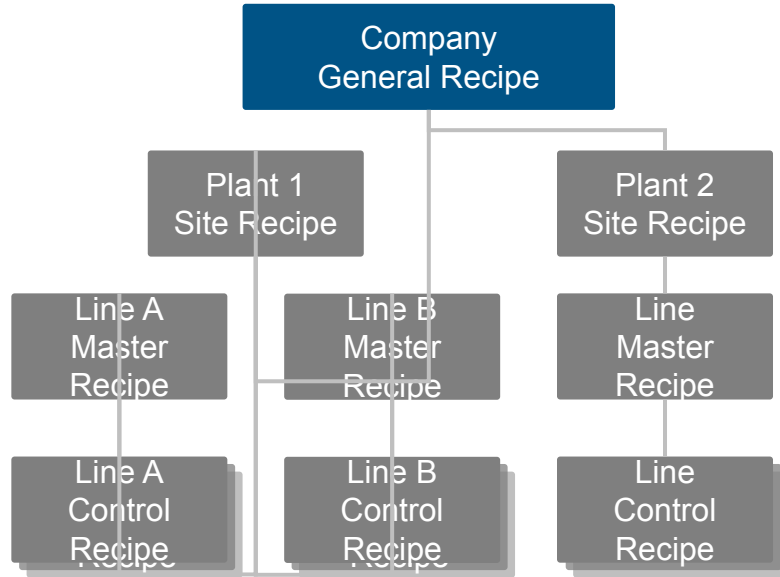
<https://en.wikipedia.org/wiki/ISA-88>



Meaning of Angel Number 88

Angel number 88 is a sign of great success, abundance, and prosperity. When this number keeps appearing in your life, it indicates that exciting and positive changes are on the horizon. Your guardian angels or spirit guides are trying to prepare you for the wonderful opportunities that lie ahead.

S88 CONCEPTS FOR RECIPE AUTHORIZING

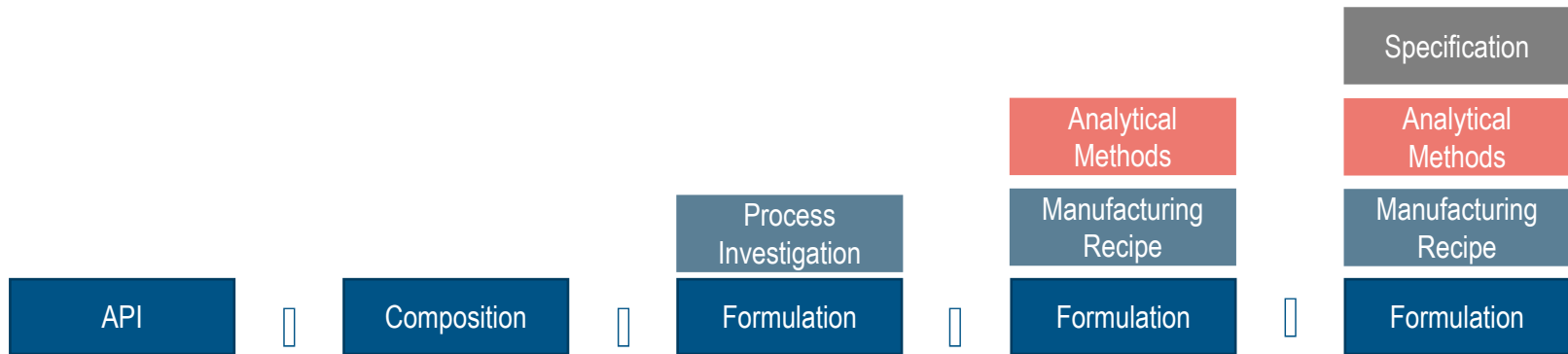


- ▶ Enterprise / Site / Master / Control levels for proper harmonization.
- ▶ Process / Stage / Operation / Action building blocks for proper parametrization.
- ▶ Enables Tech Transfer from Development to Manufacturing.

DIGITAL PRODUCT DEVELOPMENT □ DIGITAL TECH TRANSFER

Development

Manufacturing



CERTIFICATE OF ANALYSIS

Product: My Product	Specification: 31004	Lot: 31004
Regulatory Reference: 123456789	Manufacturer: ABCDEF	Control: GHIJKL
Material: 123456789	Amount: 1000 g	Equipment: MNO PQR
Material: 987654321	Amount: 2.1 g	Equipment: STU VWX
Material: 456789012	Amount: 1880 g	Equipment: YZ A B C D E F G H I J K L M N O P Q R S T U V W X Y Z

Experiment

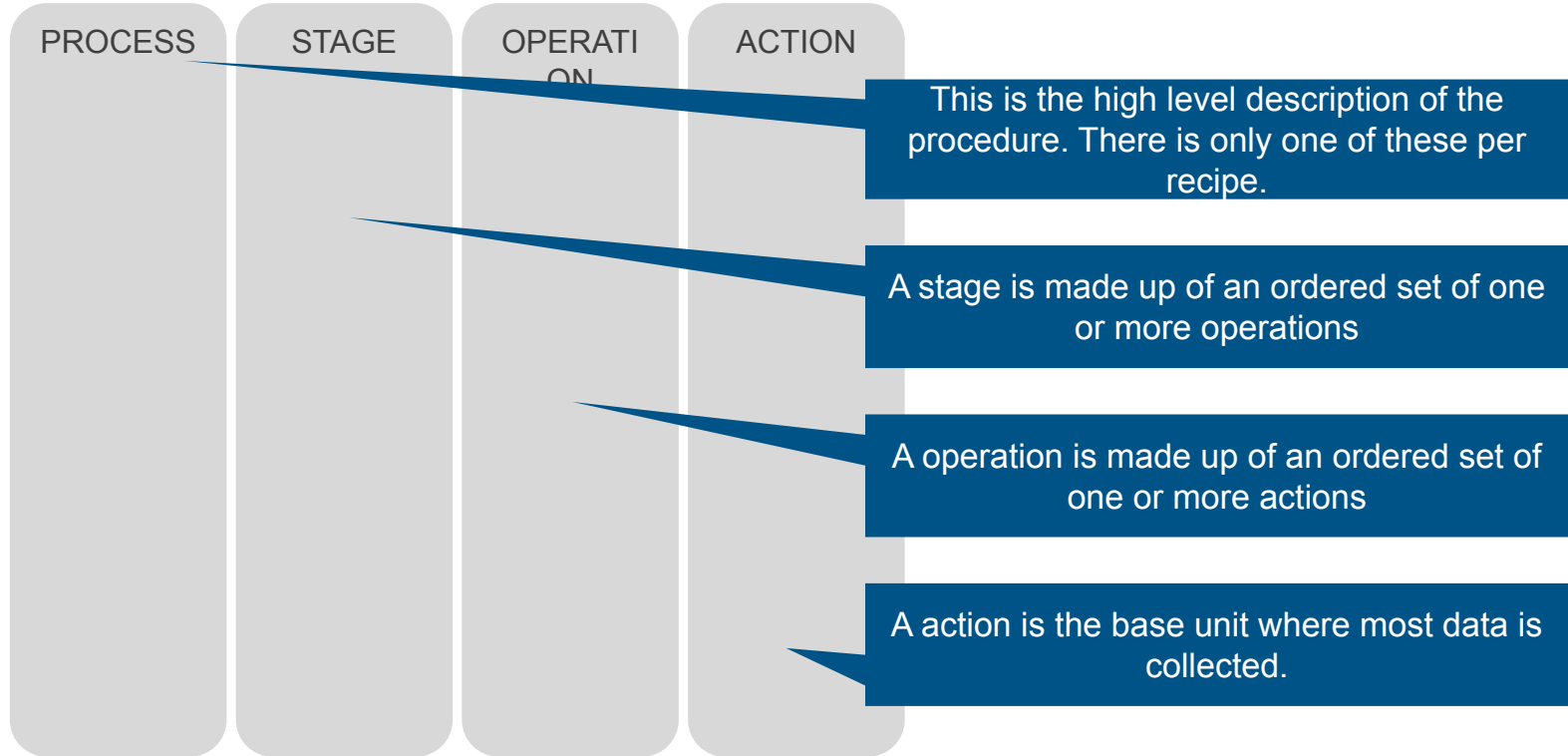
Process



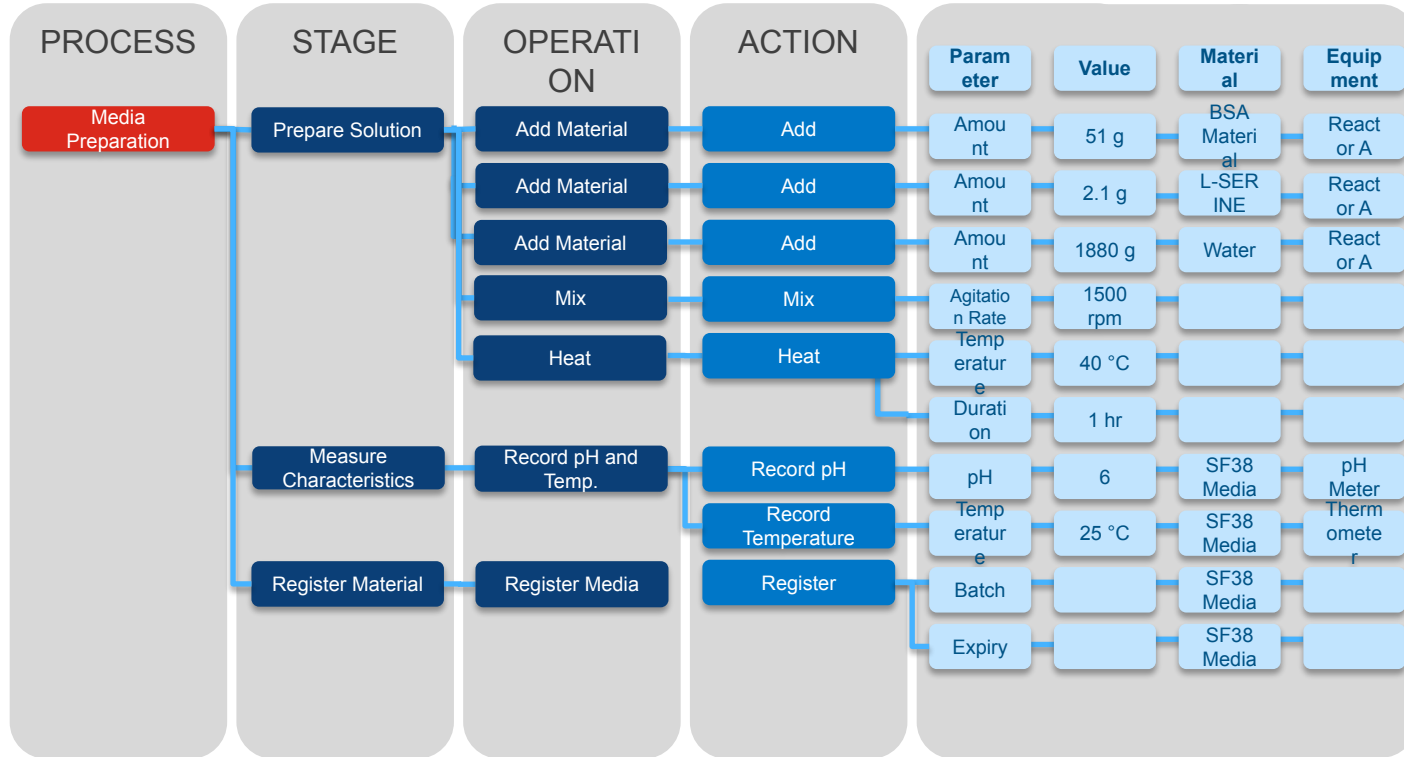
Ontology



S88 CONCEPTS FOR PROCESS AUTHORIZING



S88 CONCEPTS FOR PROCESS AUTHORING



ONTOLOGIES FOR LIFE SCIENCE

Upstream Thinking

Unmet Medical Need

Biological Target
Drug landscape
Therapeutic Indication

Population

Cohort
Subject
Characteristics

Living System

Biological Entity
Biological Function
Organism
Organ
Tissue
Cell
System
Influence

Company / Organization

Business Interaction
Pipeline
Drug Portfolio
Location

Research & Development

Material Substance

Cell Line
Nucleic Acid
Protein
Sequence
Conjugate
Small molecule
Structure

Materials

Material
Composition
Characteristics
Supplier
Package
Lot
Container
Chain of Custody

Resources

Equipment
Measurement
People
Skills
Capacity
Schedule

Experiments

Study
Experiment
Plan
Expectations
Parameters
Result
Analysis
Outcome

Process

Process
Stage
Operation
Action
Method
Formulation
Recipe
Ingredient
Reaction
Reaction Scheme
Process Transfer Doc

Clinical Trials

Clinical Site
Patient
Prescriber
Trial Protocol
Trial Master File

Regulatory

IND Authorization
Common Technical Document (CTD)

Product

Part
Assembly
Label
Artwork
Packaging

Specification

QTPP

Manufacturing

Plant

Manufacturing Site
Production line
Production unit
Equipment

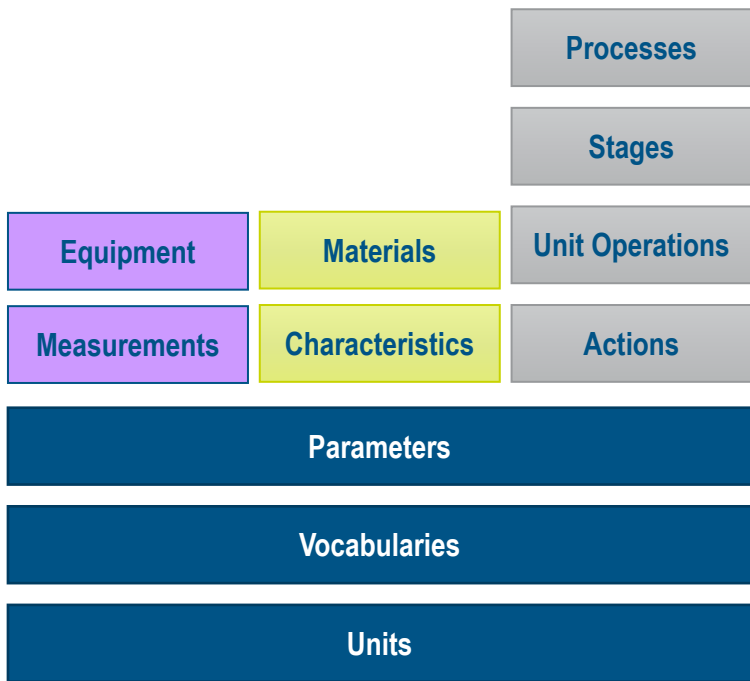
Quality/change control

Incident
Deviation
CAPA

Pharmaceutical Product

Active Pharmaceutical Ingredient (API)
Administration Route
Administrable Dose Form
Mode of Action
Batch Record

REFERENCE DATA



BIOVIA

Admin and Settings

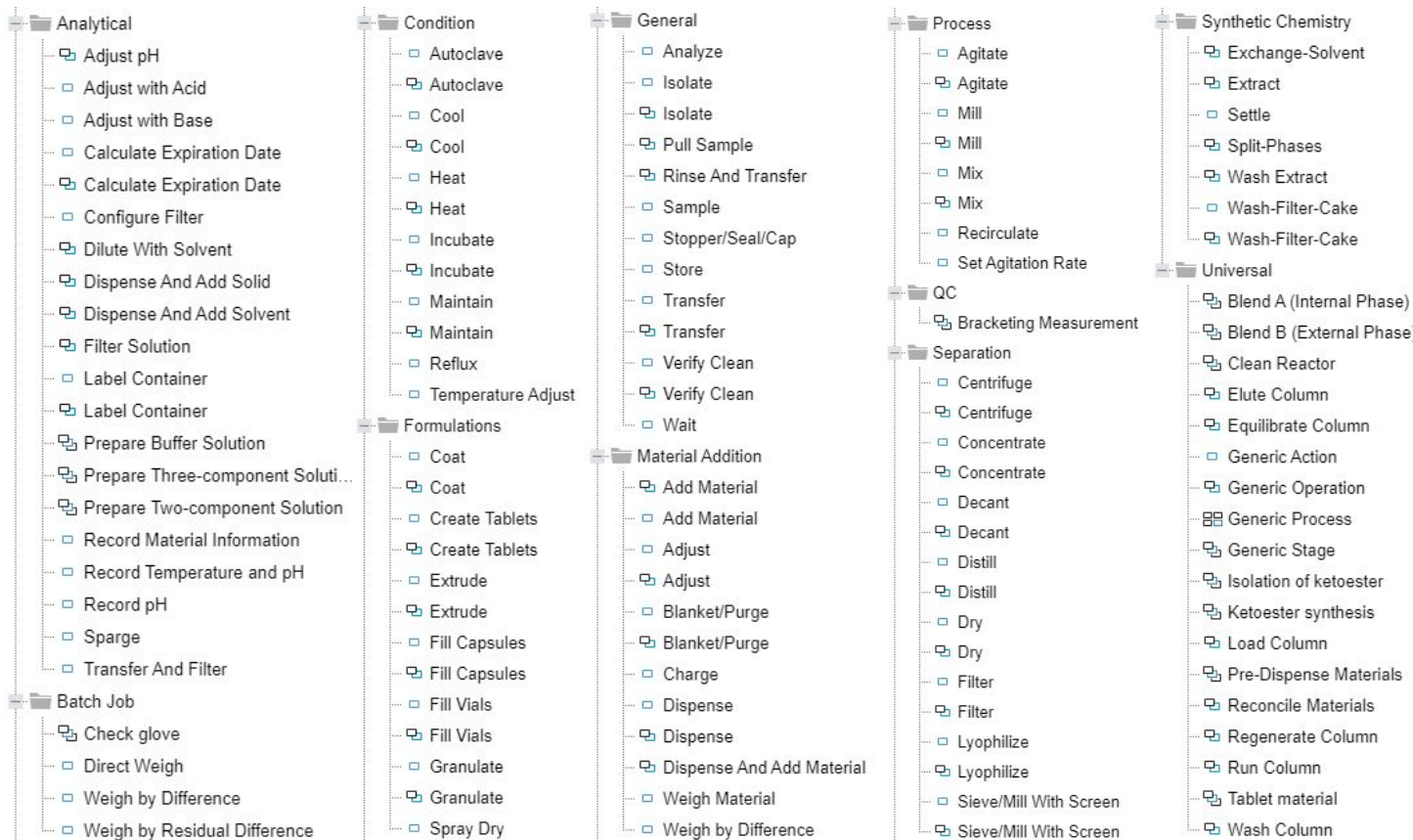
- Security Events
- Trusted Certificates
- Users
- Resources**
- Activity Plans
- Data Packets
- Equipment
- Locations
- Organizations
- Parameter Templates
- Projects
- Sequence Templates
- Unit Types
- Vocabularies

Equipment measurements & parsing

Process parameters

Units and Vocabularies

STANDARD UNIT OPERATIONS



RECIPE AND METHOD MANAGEMENT

Create and store recipes and methods with standardized libraries of operations

- S88/S95 standard design for procedure authoring
- Harmonization of recipes and methods:
- Process elements library managed by super-users (master data)
- Generic method capabilities to optimize procedure management
- Enabling deployment scalability

The screenshot displays the BIOVIA Compose software interface. The top navigation bar includes 'Production | Default (Author) | SOULES Margaux' and 'Karl Fischer (v.1.1, updated 31-Mar-2021 19:36)'. The main interface is divided into several panels:

- Toolbox:** A hierarchical tree view of process elements under 'Process Library', including categories like Analytical, Batch Job, Condition, Formulations, General, Material Addition, Process, QC, Separation, and Synthetic Chemistry.
- Process Tree:** A table listing process steps with columns for '#', 'Name', and 'Pr...'. The steps include: 1. Water Content by KF, 2. Record Test Date & Verify SOP, 3. Record Titrant, 3.1. Prepare Samples, 3.2. Add Sample and Dilute, 4. Vortex, 4.1. Analyze, 4.1.1. Inject Samples, 4.2. Weigh and Inject Sample (highlighted), 4.2. Import KF Results, and 4.2.1. KF Result.
- Weigh and Inject Sample:** A detailed view of the selected step, showing parameters for 'Tare Wt', 'Residual Wt', and 'Net Wt'. Each parameter has a 'Value' field, a unit dropdown (e.g., 'mg'), a 'Display Method' dropdown (e.g., 'SigFigs'), a 'Rounding Rule' dropdown (e.g., 'Half-Up (USF)'), and a '# figs' dropdown (e.g., '5').

THE MAIN CHALLENGE IMPLEMENTING A LAB EXECUTION SYSTEM (LES)

Digitizing the processes to run electronically in the solution



#	Name	Predecessor	Add	Remove	Copy
1	Prepare growth medium		<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
2	Check Cells		<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
3	Prepare cell suspension		<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
3.1	Use aseptic technique for all steps		<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
3.2	Plate cells		<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
3.3	Warm culture medium		<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
3.4	Pour off media		<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
3.5	Replace cells		<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
3.6	Scope cells		<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
3.7	Mix		<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
4	Calculate Cell Density		<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
5	Plate cells		<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>

THE MAIN CHALLENGE IMPLEMENTING AN LES

Simplified HPLC method as an example

HPLC Method

Abstra

ct
Materia

ls
Reagen

ts

Buffer – R1 +R1

Diluent A – R1

Eluent A – R1 +

Eluent B– R3 +

R4

Std Washes – R5 +

prep
R6

Std1 – diluent + std

Refstd – diluent +

refstd

Sample

prep

Sample Weight 1 – diluent +
sample

Sample Weight 2 - diluent +
sample

Conditio

ns

Wavelength

Injection

Time

Result

ts

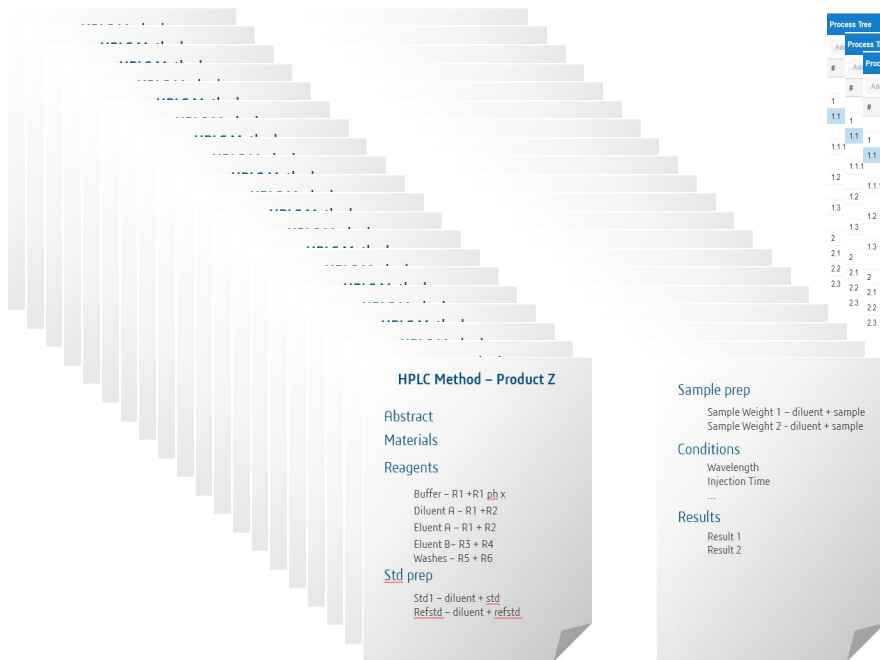
Result

1

Result

2

CREATE AN ELECTRONIC VERSION



The screenshot displays a complex software interface for method development. On the left, a 'Process Tree' shows a hierarchical structure of steps, with each step having an 'Input Parameter Details' window. The tree includes steps like 'Start Parallel', 'End Parallel', 'Solution Preparation', 'Read RI Barc.', and 'Transfer 01'. The right side of the interface shows a detailed view of a specific step, 'Input Parameter Details', with tabs for 'Details', 'Parameters', 'Samples', 'Materials', 'Equipment', 'Process', 'Forecast', and 'Instr.'. The 'Parameters' tab is active, showing a list of parameters such as 'pH Limit', 'Verify Method Id', and 'Range Monitor', each with a 'Role' column (e.g., 'Input', 'Output', 'Control'). A 'Version' table is also visible, showing a list of versions for the method.

100's of
methods

EACH METHOD NEEDS TO BE QUALIFIED FOR USE

HPLC Method – Product A

Process Tree

Abstract

Material

Reagen

Bu

Dil

Elu

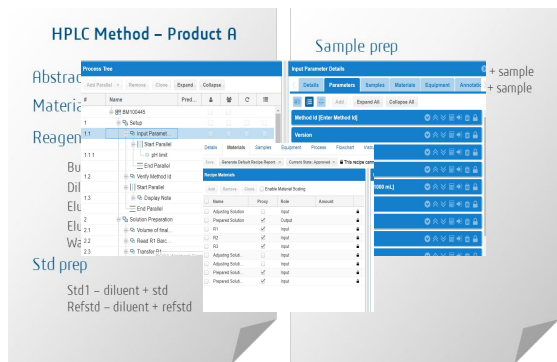
Wa

Std prep

Std1 – diluent + std
Refstd – diluent + refstd

Sample prep

+ sample
+ sample



HPLC Method – Product B

Process Tree

Abstract

Material

Reagen

Bu

Dil

Elu

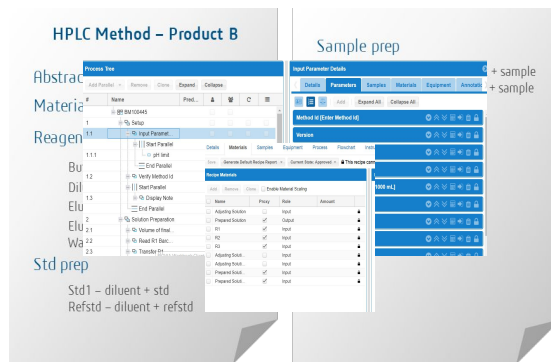
Wa

Std prep

Std1 – diluent + std
Refstd – diluent + refstd

Sample prep

+ sample
+ sample



HPLC Method – Product C

Process Tree

Abstract

Material

Reagen

Bu

Dil

Elu

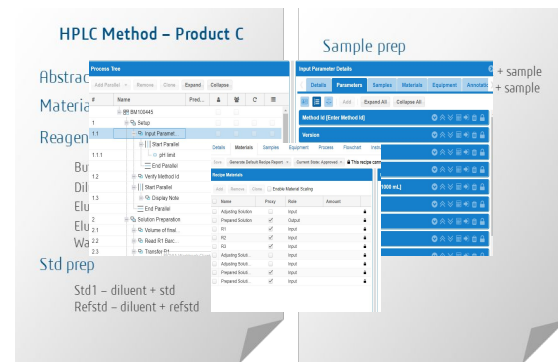
Wa

Std prep

Std1 – diluent + std
Refstd – diluent + refstd

Sample prep

+ sample
+ sample



Qualify each
method

Repeat for all the different processes that are executed for
each product

LET US LOOK AT THE SIMPLIFIED HPLC AGAIN

Simplified HPLC method as an example

HPLC Method

Abstra

ct
Materia

ls
Reagen

ts

Buffer – R1 +R1

Diluent A – R1

Eluent A – R1 +

Eluent B– R3 +

R4

Std Washes – R5 +

prep
R6

Std1 – diluent + std

Refstd – diluent +

refstd

Sample

prep

Sample Weight 1 – diluent +
sample

Sample Weight 2 - diluent +
sample

Conditio

ns

Wavelength

Injection

Time

Result

ts

Result

1

Result

2

BREAK UP THE METHOD

HPLC Method

Abstract
Materials
Reagents

2 component operation

Buffer – R1 +R1
Diluent A – R1
Eluent A – R1 +
Eluent B – R3 +
R4

Standards

HPLC Std operation

Std1 – diluent + std
Refstd – diluent +
refstd

HPLC Sample operation

Sample
preps

Sample Weight 1 – diluent +
sample

Sample Weight 2 - diluent +
sample

Conditions

Wavelength
Injection
Time

Results

Result
1
Result
2

GENERIC TEMPLATE CONCEPT

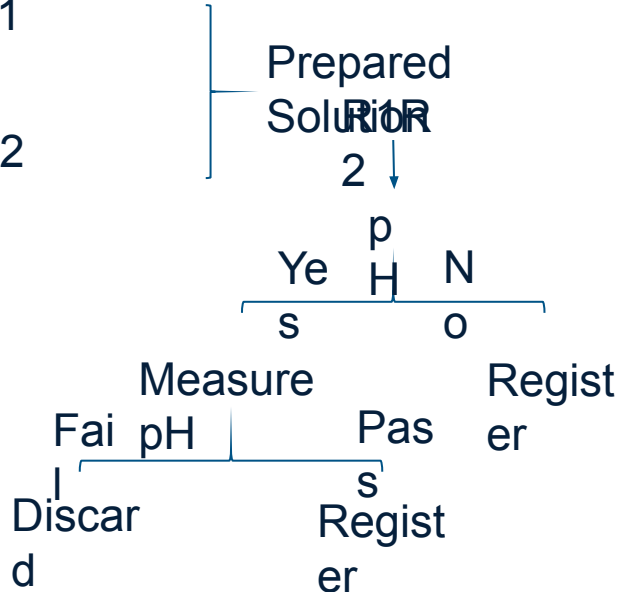
• Solution Preparation

Workflow

W

Reagent 1
(liquid) +

Reagent 2
(liquid)



Input

Parameters

- The Name of the Reagents/Materials
- How much you are making
- The volume to add (the scaling factor)
- The units
- The format
- Does it need a pH?
- Yes
- ...

DIGITAL TRANSFORMATION FROM DEVELOPMENT TO MANUFACTURING

