

Recipe driven, data visualization from lab to commercial

Presented by **Barry Higgins** and **Koen Paeshuyse**



Agenda

- Introduction
- Goal and Challenges
- S88 recipe strategy
- Recipe integration into systems
- OSIsoft PI AF/EF setup
- Data visualization
- Conclusions

Introduction



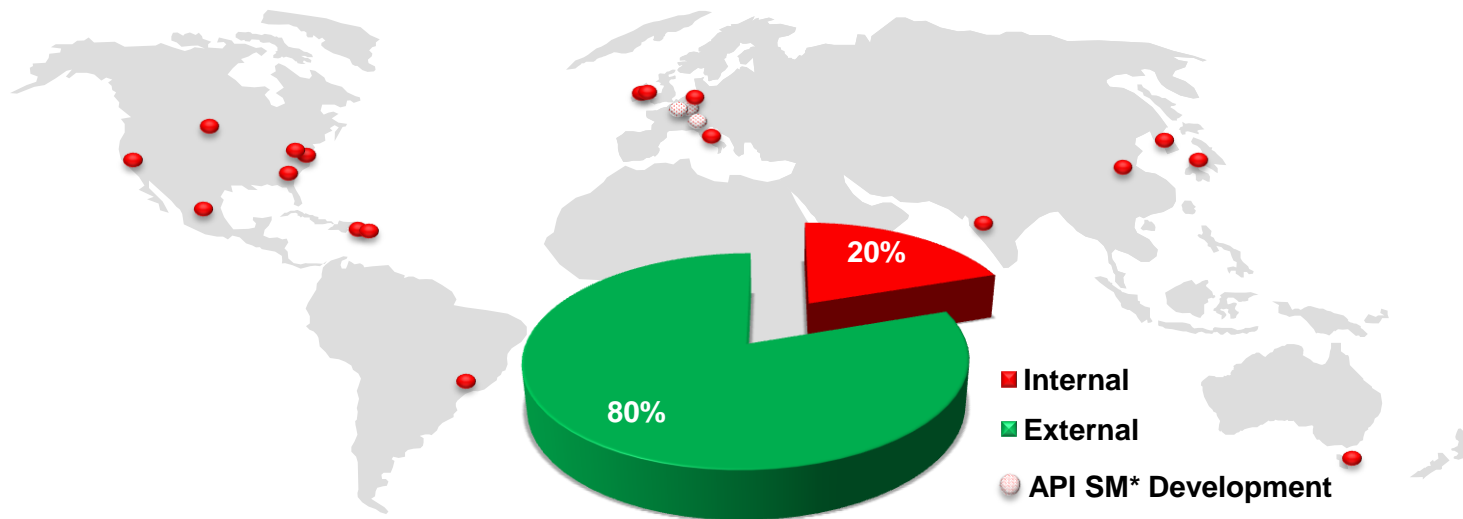
Cardiovascular
& Metabolism

Immunology

Infectious
Diseases &
Vaccines

Neuroscience

Oncology



■ Internal

■ External

● API SM* Development

* API: Active Pharmaceutical Ingredient
SM: Small Molecules

Goal and Challenges

Building a Knowledge Based Organization

Common Recipe Approach
Ensures that we all “speak the same language” promoting consistency



Common Data Warehouse
Enables leveraging of information across systems to help drive data driven decisions



API



DPD



AD



Electronic
Lab Notebook



Data
Infrastructure



Data
Visualization

S88 – What is it?

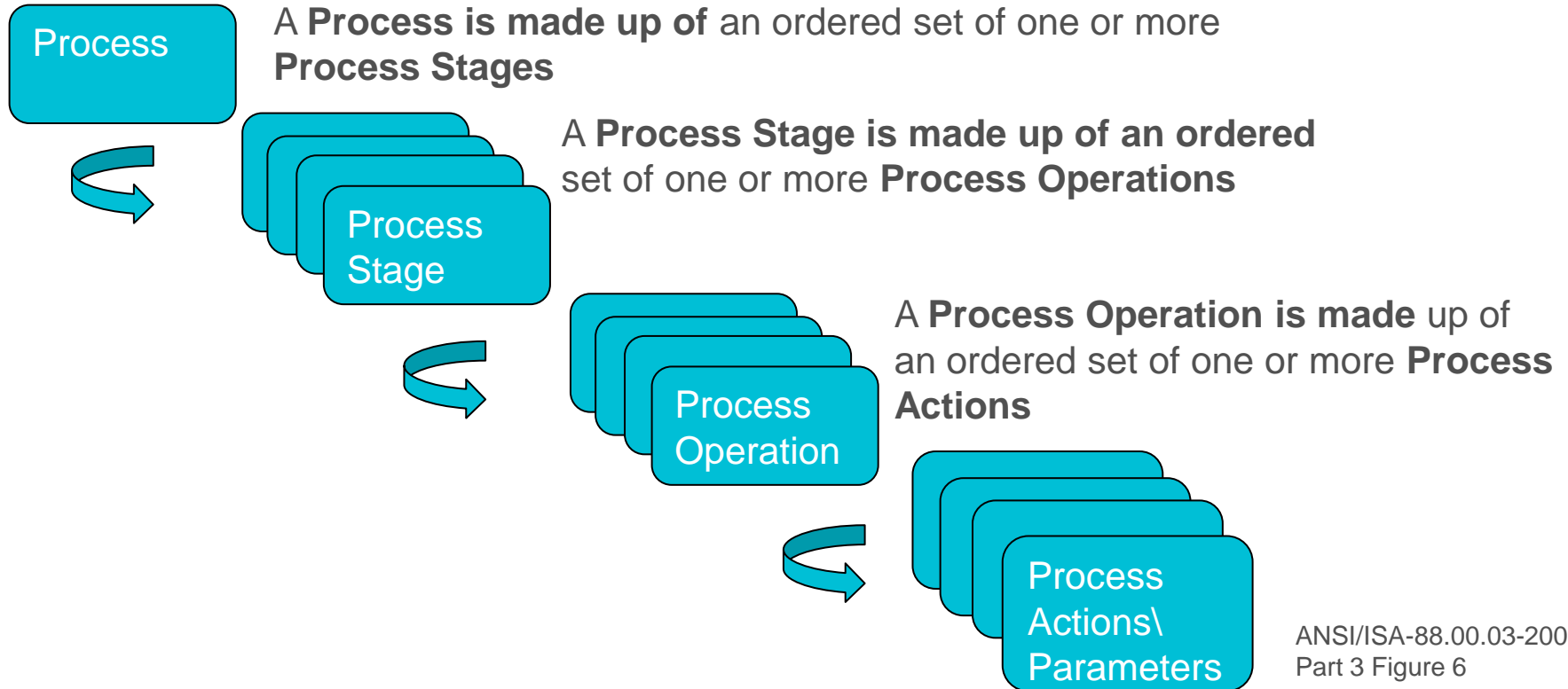
Short for ANSI/ISA-88

- ANSI is American National Standards Institute
- ISA is Instrumentation, Systems, and Automation Society

An industry standard addressing batch process control

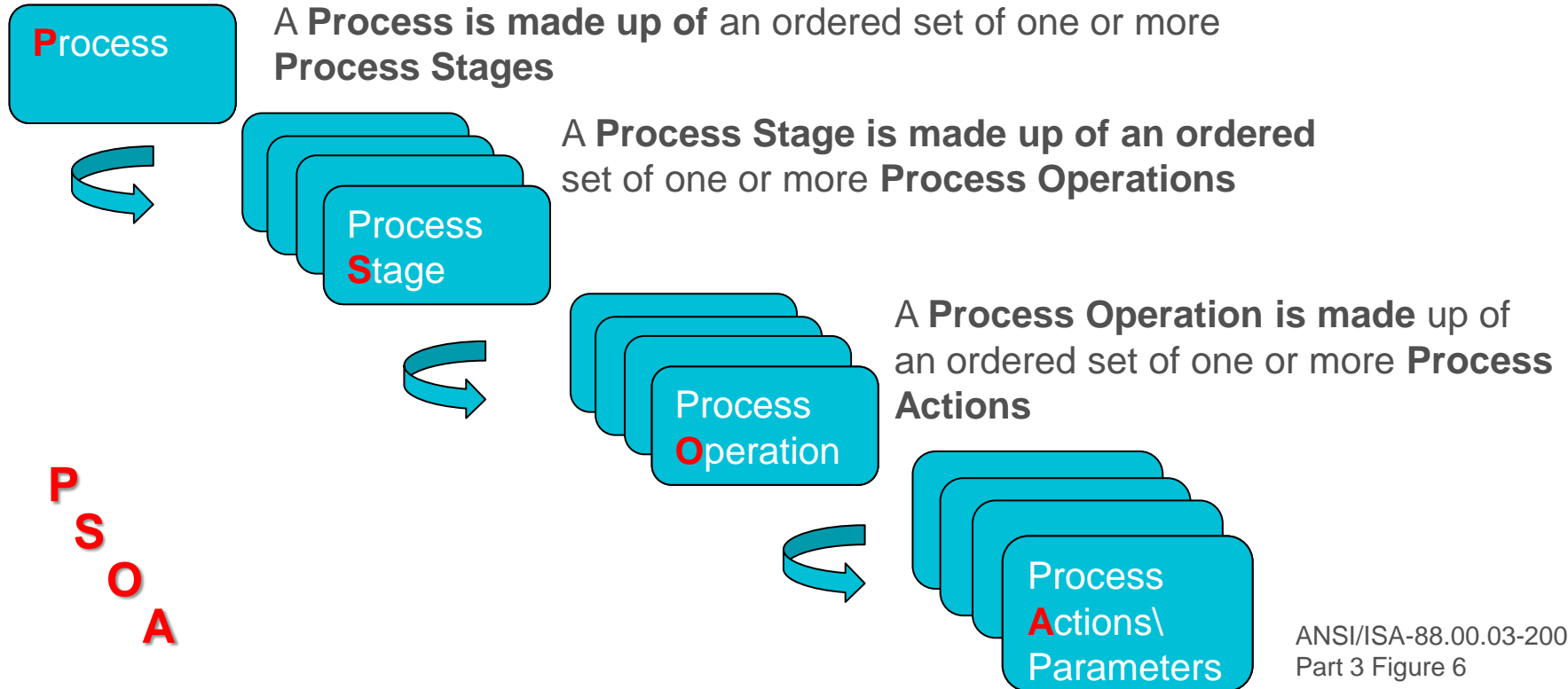
S88 provides a consistent set of standards and terminology for batch control

S88 – Process Model



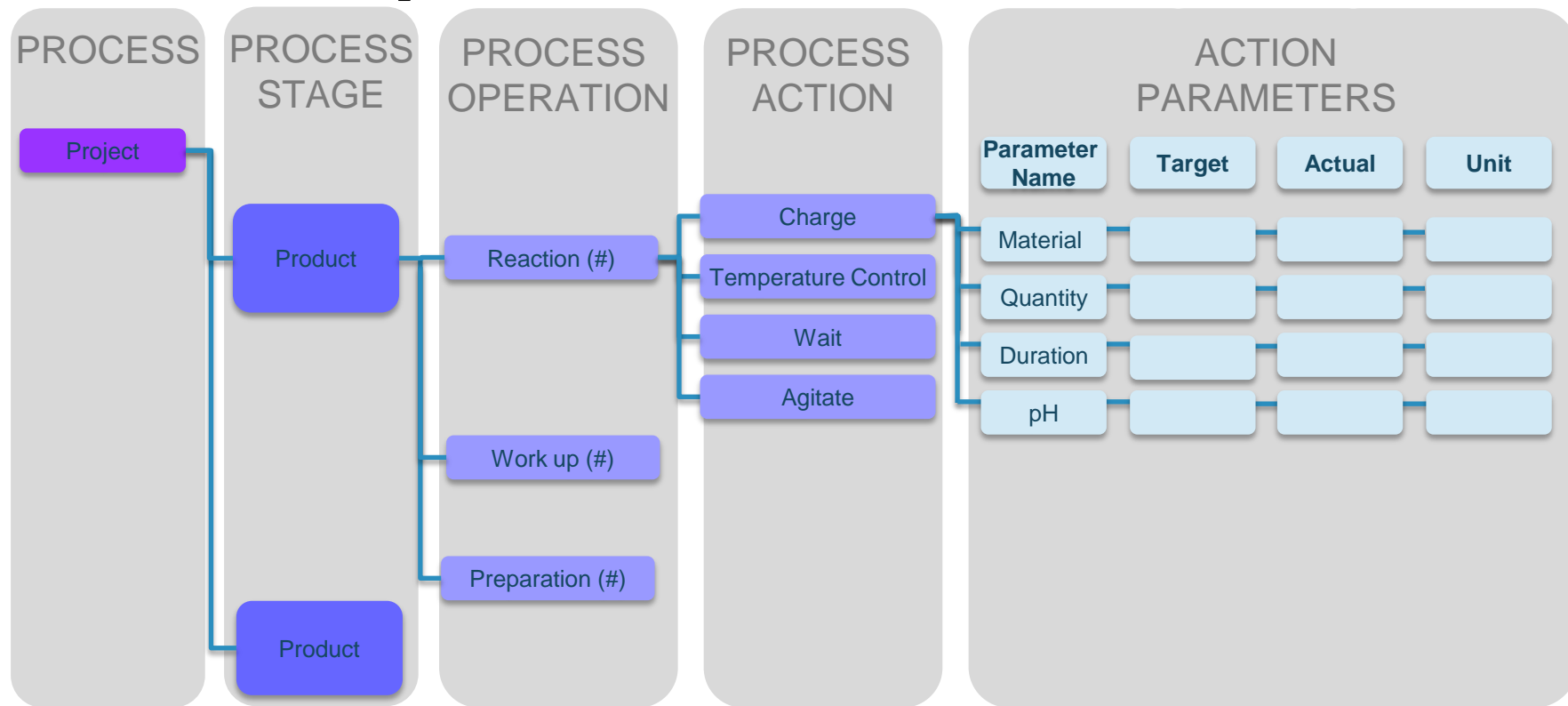
ANSI/ISA-88.00.03-2003
Part 3 Figure 6

S88 – Process Model



ANSI/ISA-88.00.03-2003
Part 3 Figure 6

S88 recipe model for API SM Dev



S88 recipe model for API SM Dev

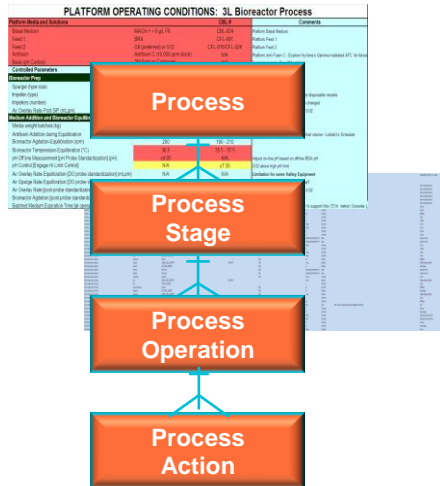


S88 Recipe KM* Strategy

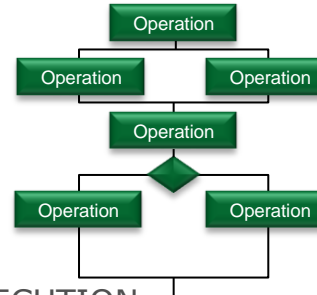
Regulatory Filing = General Recipe

CONTENT

Critical Parameters and Steps
Structured in S88 Format



Site Executable Recipe



EXECUTION

Data generated in S88 Format
Contains additional site details



VISUALIZATION
Critical Parameters and Steps
Context rich data

* KM: Knowledge Management

Dataflow in the Process Chemistry lab

OFFICE

Initiates ELN experiment in Symyx Notebook



Scientist



Chemistry Table

Experiment	Reaction	Time	Yield	Purity	Notes
1	Reaction 1	10 min	95%	98%	Good
2	Reaction 2	15 min	90%	95%	Good
3	Reaction 3	20 min	85%	92%	Good

S88 Executed Recipe

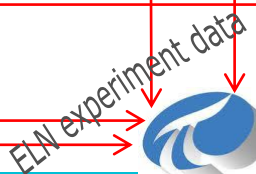
Based on Approved Operations and Actions

Analytical results

LC
KF
NMR



View/Reprocess on Client
Automatic update on server

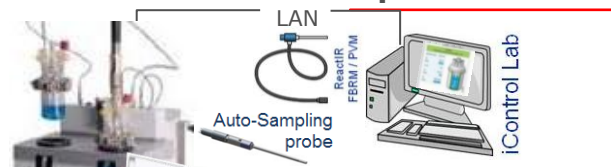


IDM

OSIsoft®

LAB

Execute experiment



Start experiment on
Automate Lab Reactor

Samples during experiment
incorporated in same ELN
experiment

Experiment done

SERVER

iC Data Center by Mettler

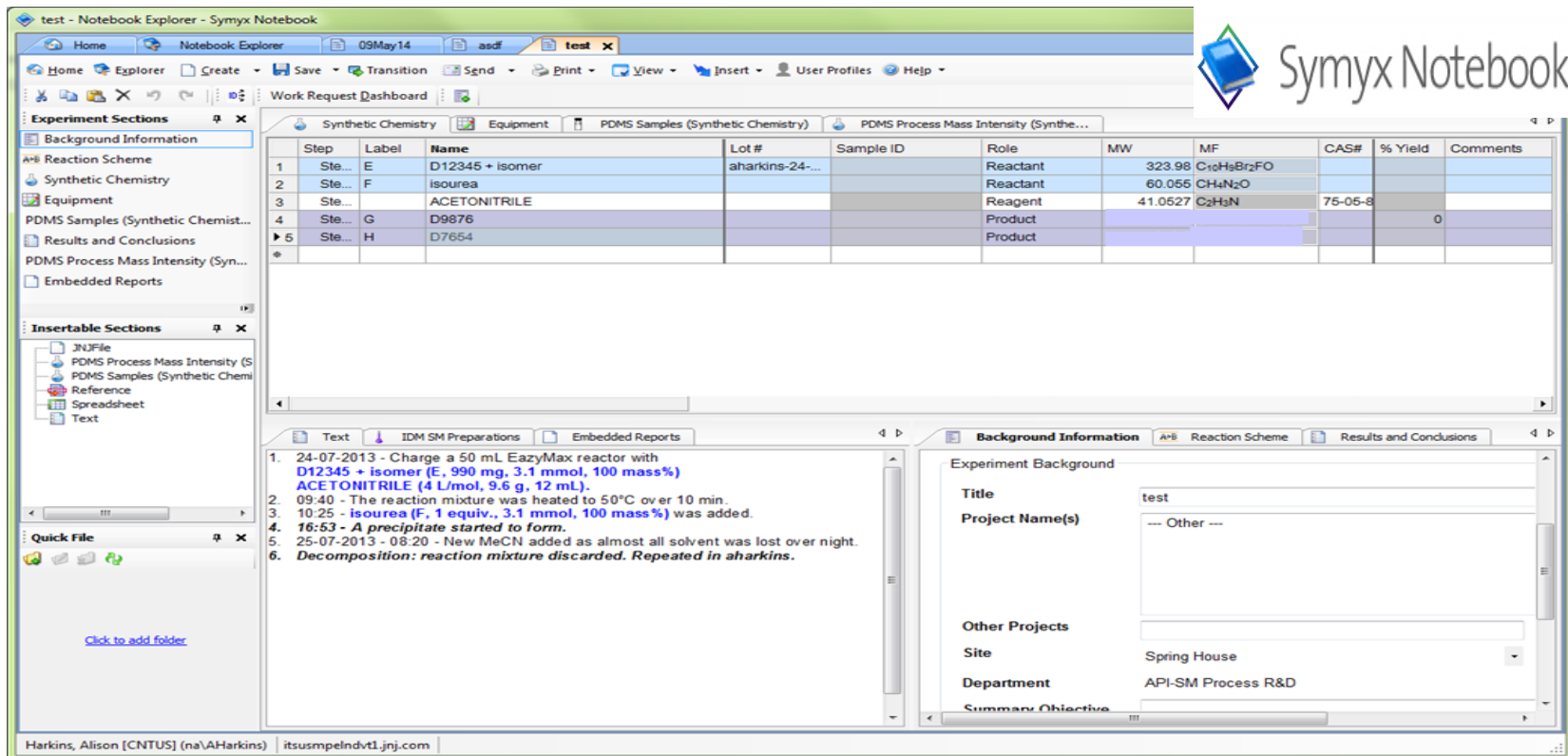
Output files



csv file contains ALR recipe
and data (to be XML format)

ALR and PAT data

S88 integration in ELN



test - Notebook Explorer - Symyx Notebook

Home Notebook Explorer 09May14 asdf test x

Home Explorer Create Save Transition Send Print View Insert User Profiles Help

Work Request Dashboard

Experiment Sections

- Background Information
- Reaction Scheme
- Synthetic Chemistry
- Equipment
- PDMS Samples (Synthetic Chemist...)
- Results and Conclusions
- PDMS Process Mass Intensity (Syn...)
- Embedded Reports

Insertable Sections

- JNFile
- PDMS Process Mass Intensity (S
- PDMS Samples (Synthetic Chemi
- Reference
- Spreadsheet
- Text

Quick File

Click to add folder

Step	Label	Name	Lot #	Sample ID	Role	MW	MF	CAS#	% Yield	Comments
1	Ste...	E	D12345 + isomer	aharkins-24-...	Reactant	323.98	C ₁₀ H ₉ Br ₂ FO			
2	Ste...	F	isourea		Reactant	60.055	CH ₄ N ₂ O			
3	Ste...		ACETONITRILE		Reagent	41.0527	C ₂ H ₃ N	75-05-8		
4	Ste...	G	D9876		Product				0	
5	Ste...	H	D7654		Product					

1. 24-07-2013 - Charge a 50 mL EazyMax reactor with D12345 + isomer (E, 990 mg, 3.1 mmol, 100 mass%) ACETONITRILE (4 L/mol, 9.6 g, 12 mL).

2. 09-40 - The reaction mixture was heated to 50°C over 10 min.

3. 10-25 - isourea (F, 1 equiv., 3.1 mmol, 100 mass%) was added.

4. 16:53 - A precipitate started to form.

5. 25-07-2013 - 08:20 - New MeCN added as almost all solvent was lost over night.

6. Decomposition: reaction mixture discarded. Repeated in aharkins.

Background Information

Experiment Background

Title test

Project Name(s) --- Other ---

Other Projects

Site Spring House

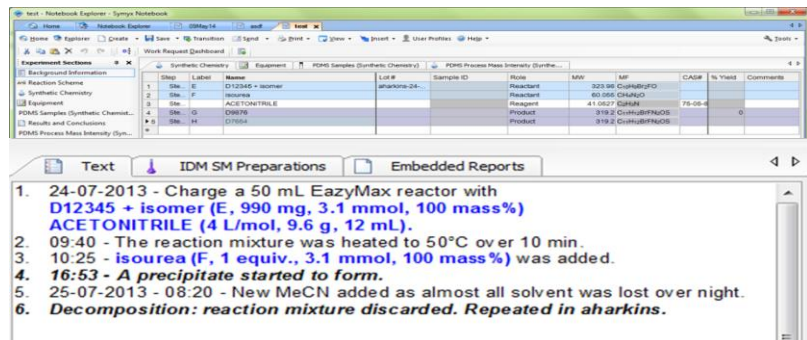
Department API-SM Process R&D

Summary Objective

Harkins, Alison [CNTUS] (na\AHarkins) itsusmpelndvt1.jnj.com

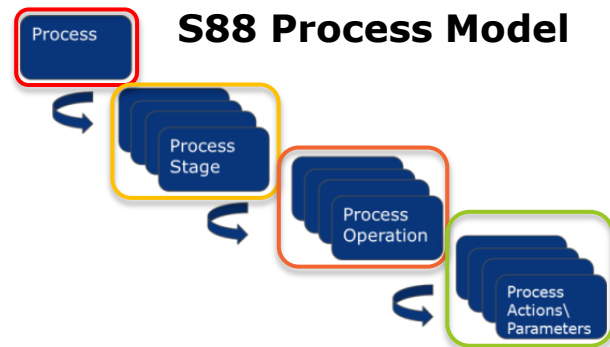


S88 integration in ELN



Text

- 24-07-2013 - Charge a 50 mL EazyMax reactor with D12345 + isomer (E, 990 mg, 3.1 mmol, 100 mass%) ACETONITRILE (4 L/mol, 9.6 g, 12 mL).
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- 25-07-2013 - 08:20 - New MeCN added as almost all solvent was lost over night.
- Decomposition: reaction mixture discarded. Repeated in aharkins.



Text

IDM SM Preparations

Embedded Reports

Process	Lot #	Batch Id	Expiry Date
RED-3 Cathepsin Time 9400115.9001	Recipe 1		

Components	Note	Stage	Operation	Action	Parameter	Setpoint	Unit	Material	Instruction
D20417, D20492		Reaction			COMMENTS				
D20417, D20492		Reaction	Charge:1		MATERIAL			THIOUREA	Charge of THIOUREA (1 equiv., 0.23 g,)
D20417, D20492		Reaction	Charge:1		ELN QUANTITY				
D20417, D20492		Reaction	Charge:2		MATERIAL			D20623 + isomer	Charge of D20623 + isomer (990 mg, 0.99 g,)
D20417, D20492		Reaction	Charge:2		ELN QUANTITY				
D20417, D20492		Reaction	Temperature Adjust		CONTROL TYPE	Delta T			Temperature Adjust with Delta T to 100 °C at Delta T 10 °C
D20417, D20492		Reaction	Temperature Adjust		CURVE FACTOR				
D20417, D20492		Reaction	Temperature Adjust		TEMPERATURE DELTA	10	°C		
D20417, D20492		Reaction	Temperature Adjust		END TEMPERATURE	100	°C		
D20417, D20492		Reaction	Temperature Adjust		RAMP TIME		min		
D20417, D20492		Reaction	Agitate		SPEED	30	rpm		Agitate for 100 min at 30 rpm
D20417, D20492		Reaction	Agitate		ELAPSED TIME	100	min		

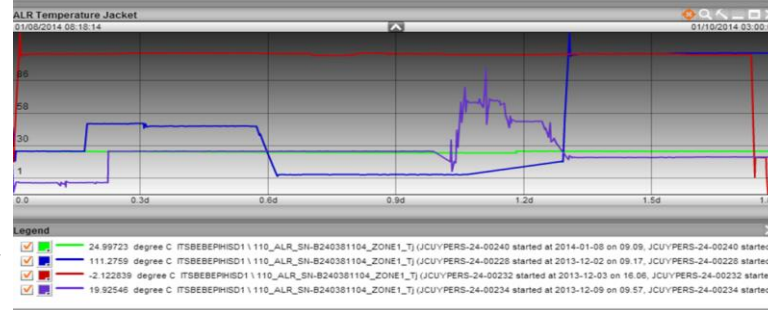
unstructured

structured

Text		IDM SM Preparations	Embedded Reports				
Process		Lot #	Batch Id	Expiry Date			
1 - RED-3 Cathepsin Time 9400115.9001		Recipe 1					
Components		Note					
Stage	Operation	Action	Parameter	Setpoint	Unit	Material	Instruction
D20417, D20492	Reaction		COMMENTS				
D20417, D20492	Reaction	Charge.1	MATERIAL			THIOUREA	Charge of THIOUREA (1 equiv., 0.23 g.)
D20417, D20492	Reaction	Charge.1	ELN QUANTITY				
D20417, D20492	Reaction	Charge.2	MATERIAL			D20623 + isomer	Charge of D20623 + isomer (990 mg, 0.99 g.)
D20417, D20492	Reaction	Charge.2	ELN QUANTITY				
D20417, D20492	Reaction	Temperature Adjust	CONTROL TYPE	Delta T			Temperature Adjust with Delta
D20417, D20492	Reaction	Temperature Adjust	CURVE FACTOR				
D20417, D20492	Reaction	Temperature Adjust	TEMPERATURE DELTA	10	°C		
D20417, D20492	Reaction	Temperature Adjust	END TEMPERATURE	100	°C		
D20417, D20492	Reaction	Temperature Adjust	RAMP TIME		min		
D20417, D20492	Reaction	Agitate	SPEED	30	rpm		Agitate for 100 min at 30 rpm
D20417, D20492	Reaction	Agitate	ELAPSED TIME	100	min		

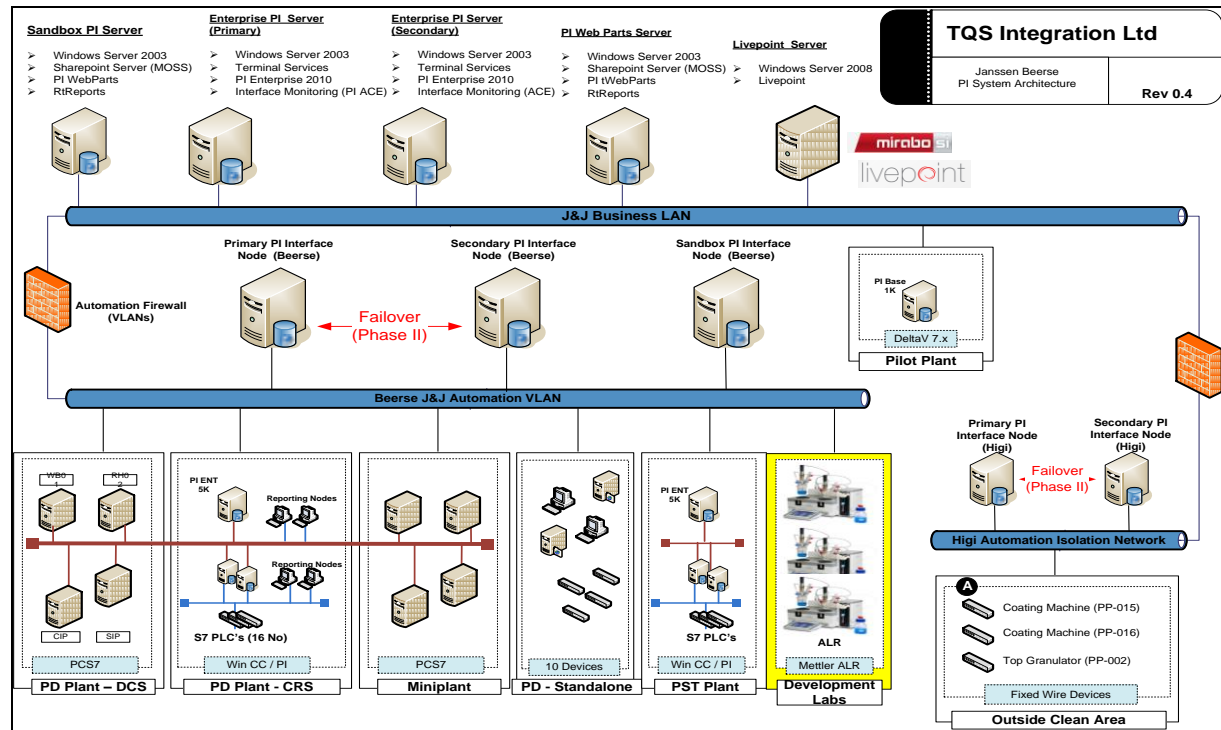


A diagram showing a power supply unit (PSU) connected to a probe. A black cable runs from the PSU to the probe. A large orange arrow points from the PSU towards the right, indicating the direction of power flow or the path of the signal.

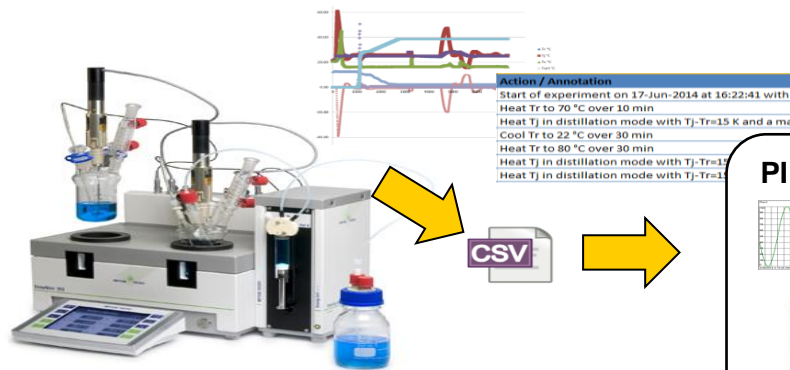


OSIsoft PI System Architecture

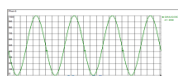
- Existing infrastructure utilized.
- Development and Production environments.
- 74 Automated Lab Reactors (ALRs) across 20 of labs.



PI Event Frames Addition

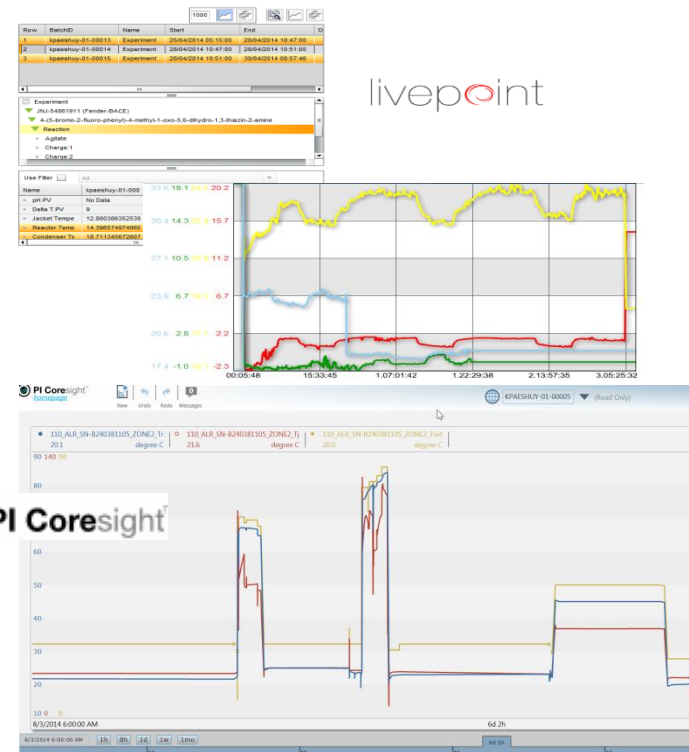


PI Interfaces



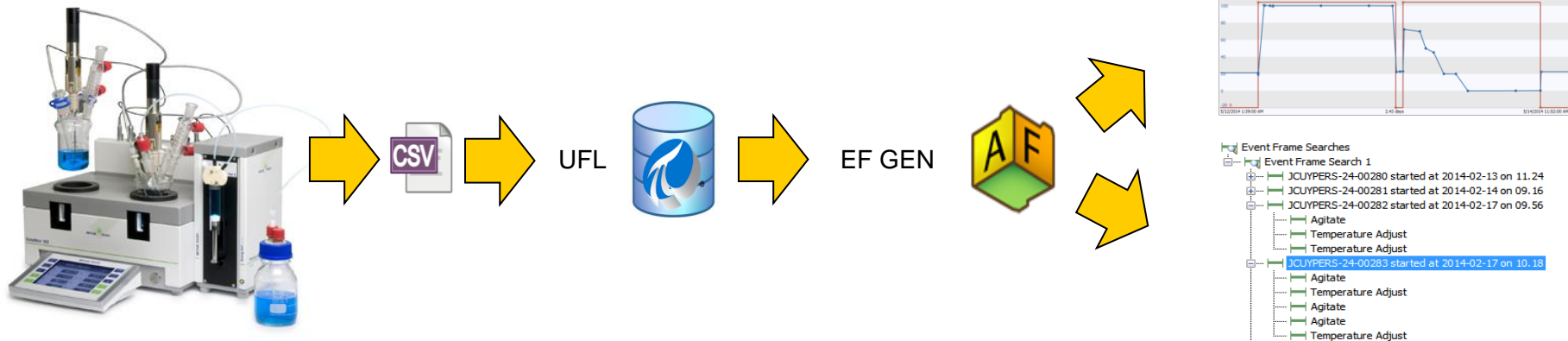
CHARGE TEMP ADJUST

Text		IDM SM Preparations	Embedded Reports					
Process		Lot #	Batch Id		Expiry Date			
RED-3 Cathexis Time 9400115.9001		Recipe 1						
Components Note								
Stage		Operation	Action	Parameter	Setpoint	Unit	Material	Instruction
D20417, D20482		Reaction	Charge:1	COMMENTS			THIOUREA	Charge of THIOUREA (1 equiv., 0.23 g.)
D20417, D20482		Reaction	Charge:1	ELN QUANTITY				
D20417, D20482		Reaction	Charge:2	MATERIAL			D20623 + isomer	Charge of D20623 + isomer (990 mg, 0.99 g.)
D20417, D20482		Reaction	Charge:2	ELN QUANTITY				
D20417, D20482		Reaction	Temperature Adjust	CONTROL TYPE	Delta T			Temperature Adjust with Delta T to 100 °C at Delta T 10 °C
D20417, D20482		Reaction	Temperature Adjust	CURVE FACTOR				
D20417, D20482		Reaction	Temperature Adjust	TEMPERATURE DELTA	10	°C		
D20417, D20482		Reaction	Temperature Adjust	END TEMPERATURE	100	°C		
D20417, D20482		Reaction	Temperature Adjust	RAMP TIME		min		
D20417, D20482		Reaction	Agitate	SPEED	30	rpm		Agitate for 100 min at 30 rpm
D20417, D20482		Reaction	Agitate	ELAPSED TIME	100	min		



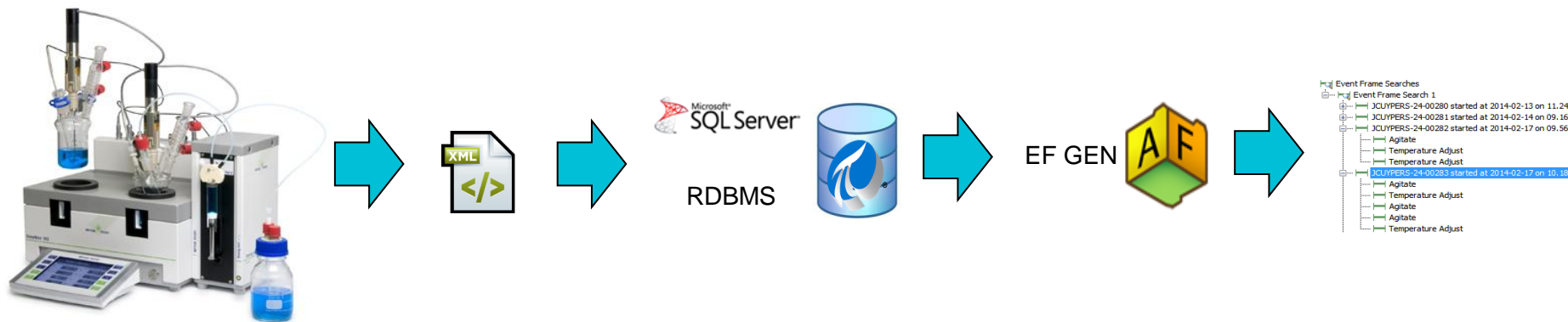
PI Event Frames 1 – ALR Data

- CSV generated from ALR, containing both continuous and event data.
- PI UFL Interface developed to write data to tags.
- PI System configured to generate PI Event Frames



PI Event Frames 2 – ELN Data

- XML output from ELN exported every night.
- Stored Procedures run via PI RDBMS.

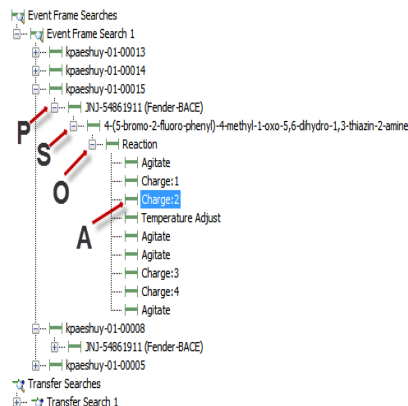


PI Event Frames 3 – ELN and ALR Data

- **Challenge** – ELN and ALR data are **not** time linked.
- **Goal** – Create a single event frame that contains and combines the ELN and ALR actions and all its data for analysis

PI Event Frames 3 – Bringing it all together

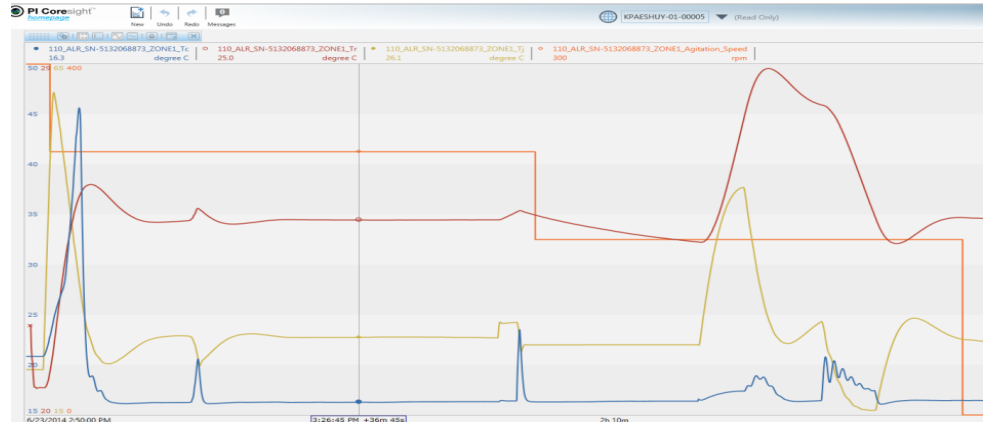
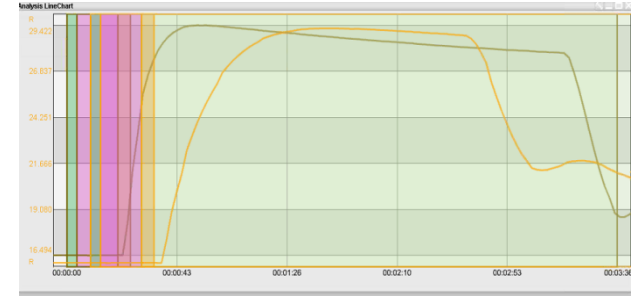
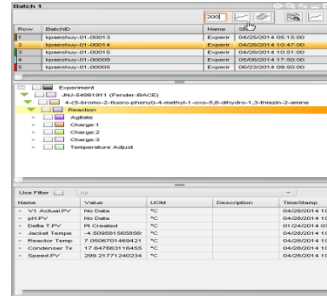
- Data and action timestamps.
- ELN Timestamps adjusted.
- Stored procedure call writes to PI System.
- Entire experiment is captured in one event.



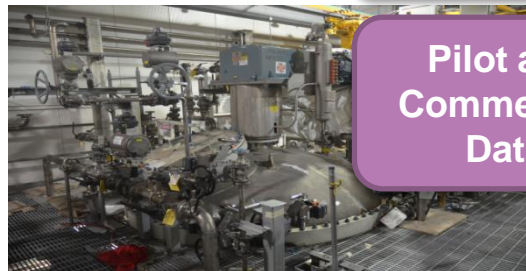
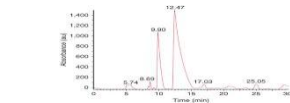
General Child Event Frames Referenced Elements Attributes		
Filter		
Name	Value	
Category: <None>		
Condenser Temperature.PV	17.3575534820557 °C	
Delta T.PV	9 °C	
EQUIPMENT	ISN-8240381104_Zone2	
Jacket Temperature.PV	17.6289119720459 °C	
MATERIAL.CAS#		
MATERIAL.LOT	9720	ELN Data
MATERIAL.MF	C18 H16 Br F N2 O S	ELN Data
MATERIAL.MW	407.3	ELN Data
MATERIAL.PLAN AMOUNT	0	
MATERIAL.PLAN AMOUNT UNIT	0	
MATERIAL.PV AMOUNT	0	
MATERIAL.PV AMOUNT UNIT	0	
MATERIAL.ROLE	Reactant	
MATERIAL.SAMPLE ID	11	
pH.PV	8.17	ALR Data
QUANTITY.PV	17	
QUANTITY.SP	18	ALR Data
Reactor Temperature.PV	18.1716957092285 °C	ALR Data
Speed.PV	11.7340278625488 °C	

Visualizing the data

- Ability to view, analyze and share experiment data away from the lab.
- Web based tools preferred.
- PI Coresight live point.



PI System lab data integration overview future



PAT

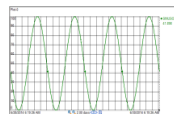
iControl,
touch panel

ELN

Analytical
Data

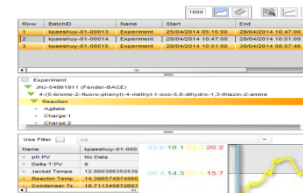
Pilot and
Commercial
Data

PI Interfaces

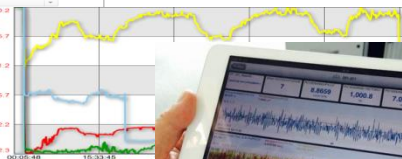


CHARGE

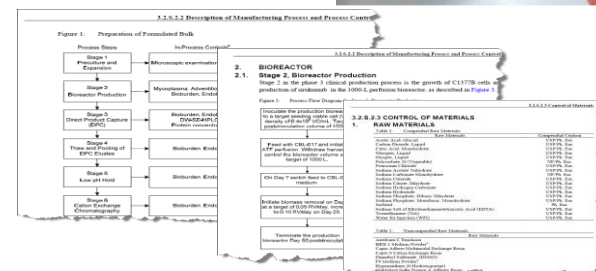
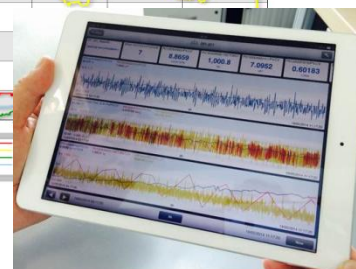
TEMP
ADJUST



livepoint

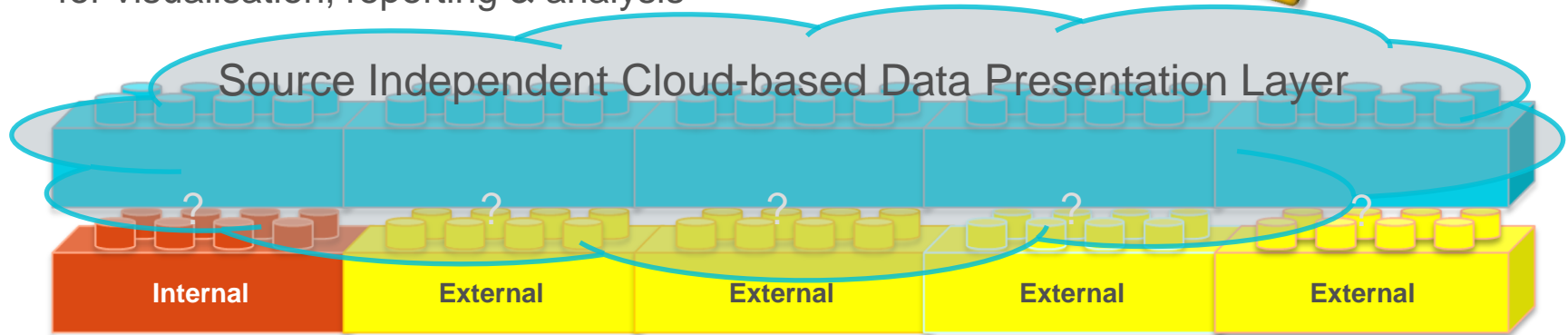
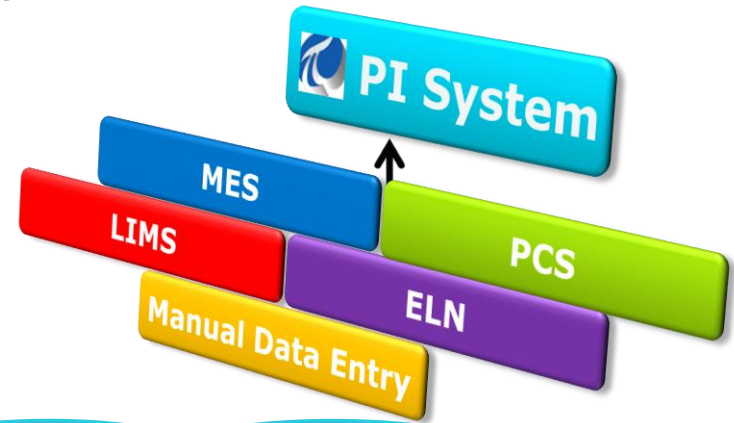


PI Coresight



Value of the OSIsoft PI System: Future

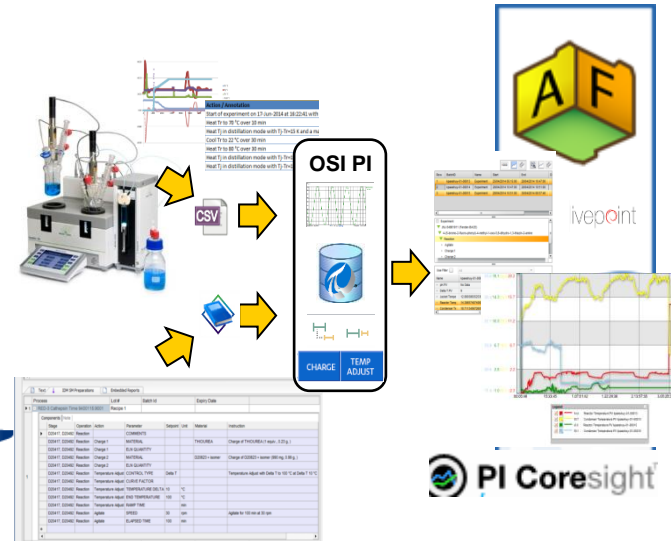
- Very disparate systems landscape – now including MES, ELN, Manual Data Entry...
- Ability to share contextualized process data with external partners is critical.
- Require capability to capture and aggregate data for visualisation, reporting & analysis



Recipe driven, data visualization from lab to commercial

- Enabling scientists to generate and capture consistent process data in a standard recipe context to generate information and knowledge from experiments.
- Enabling efficient transfer from the lab through our pilot plants, commercial operations and ultimately to our patients, capturing and building knowledge throughout.

Janssen
PHARMACEUTICAL COMPANIES
OF *Johnson & Johnson*



Business Challenge

- Streamline and implement the S88 recipe strategy in the different variety on lab systems we have in place
- Combining the data from multiple data sources

Solution

- OSIsoft PI System as our global Data Infrastructure is the key enabler towards this recipe concept.
- PI Asset Framework and PI Event Frames components to bring the data together

Results and Benefits

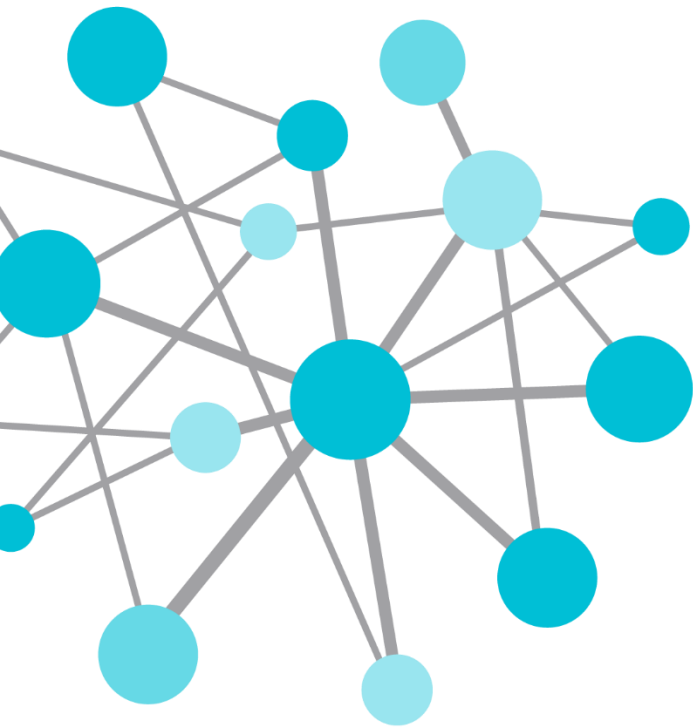
- Visualizing the data outside of the lab.
- By applying the S88 structure, lab to commercial comparisons are possible

Acknowledgments

Ryan Bass, Nick Dani, Adam Fermier, Alison Harkins, Jim Kenyon, Mike McGorry, Luc Moens, Terry Murphy, Chris Nichols, Gaby Wevers
...and many others

Thanks

- Barry Higgins – bhiggin2@its.jnj.com
- Koen Paeshuyse – kpaeshuy@its.jnj.com
- Janssen PDMS

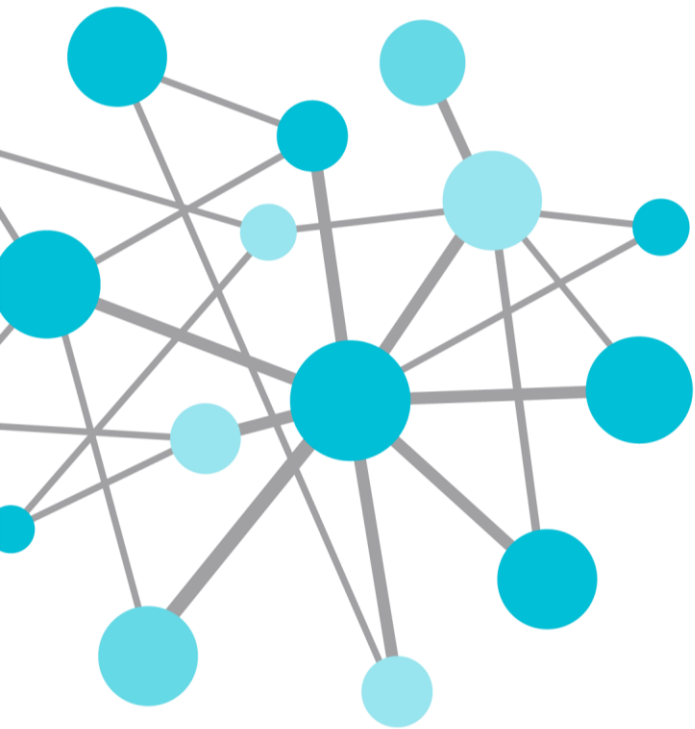


Questions

Please wait for
the **microphone**
before asking
your questions



State your
**name &
company**



THANK
YOU

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