Seamless Integration of OpenLab CDS with ZONTAL Space – Implementing the Pistoia Method Model

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Target Definition for Methods Database

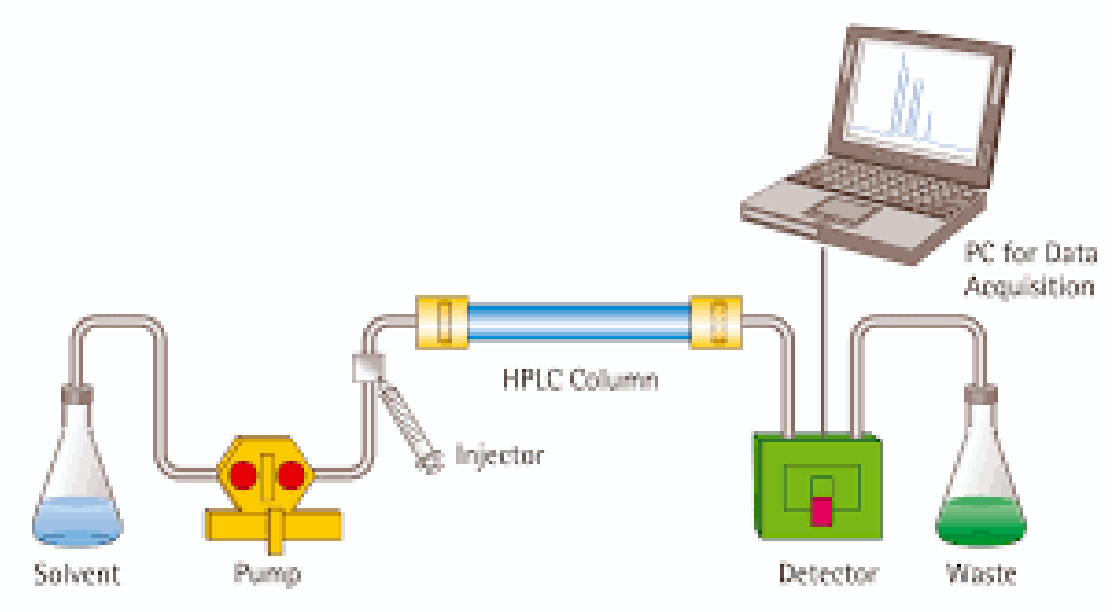
METHODS DATABASE
PISTOIA ALLIANCE & ALLOTROPE FOUNDATION

The transformation of paper-based method descriptions into digital instruction sets for different analytical methods and instrument types, including a common digital format and an ontology for analytical chemistry methods:

Return on Investment

- Reproducibility of methods is expected to be significantly improved while time and resources to re-establish a method in a different lab will be drastically reduced.
- From a cyber security perspective, a centralized storage location will create a much more resilient environment.

Common Parameters for HPLC



Pump:

Flow rate
Solvent lines
Pressure limits
Solvent % at time

Sampler:
Cooler Temp
Injection volume
Offset
Draw speed
Needle wash
Seal wash

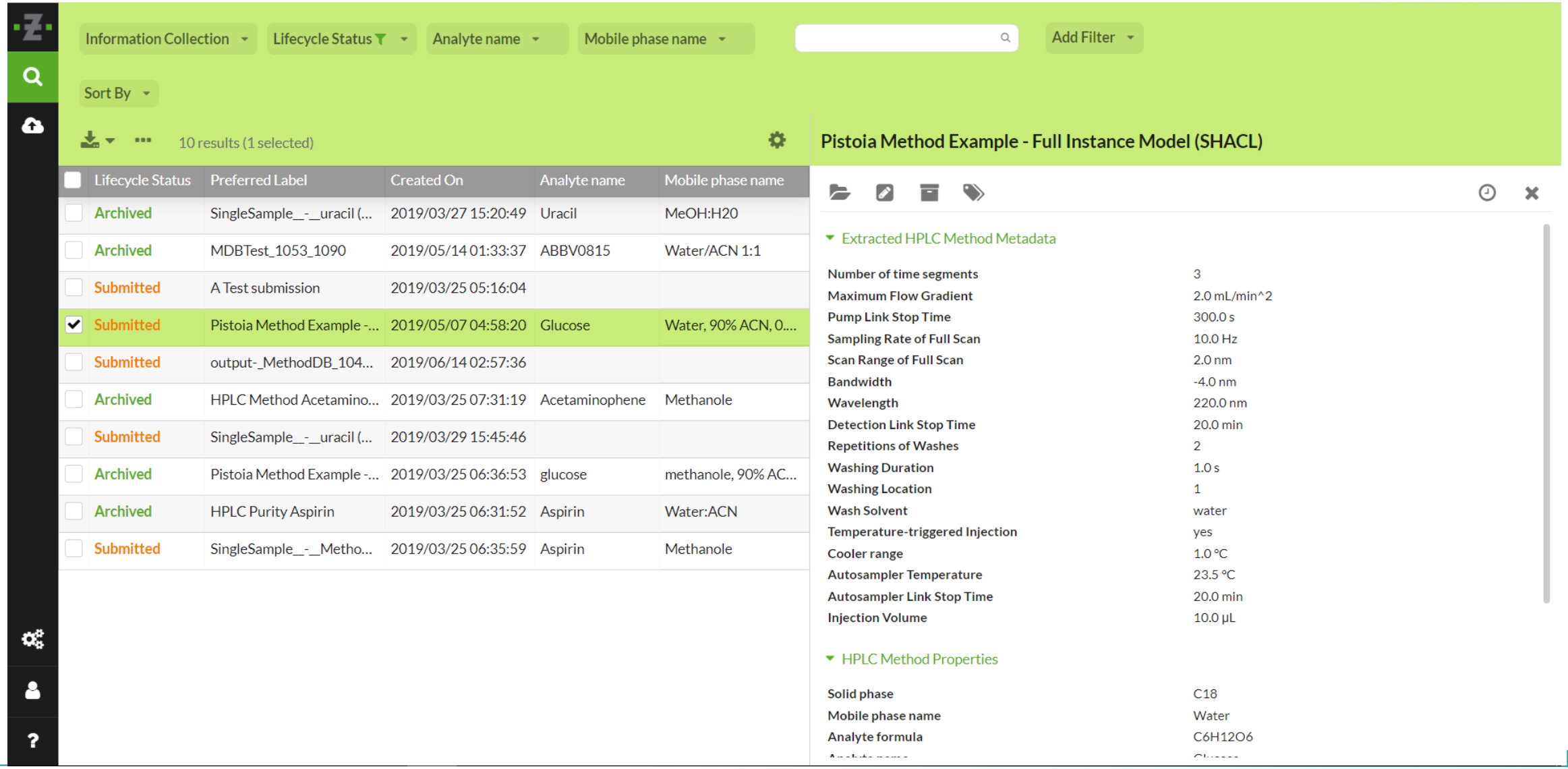
Column Compartment:

Temperature control
Valve position
Valve position at time

DAD:
Full scan option
Range
Full scan (step)
Select Channels (wavelength)
Select channels (bandwidth)
Peak width (sampling rate)
Analog output attenuation

Methods Database PoC 2019

METHODS DATABASE
PISTOIA ALLIANCE & ALLOTROPE FOUNDATION



Human Readable Method Report

METHODS DATABASE
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Pistoia Method Report

A. Solutions

The volume of these solutions may be scaled up or down as appropriate for testing.

1. Phosphoric Acid 85 wt% in water
2. Diluent A (Acetonitrile:Water - 80:20 v/v)
3. Diluent B (Acetonitrile:Water - 30:70 v/v)
4. Mobile Phase A: Pipet 2.0 mL of phosphoric acid and 2.0 mL of 5000 ppm sodium sulfite solution into a suitable container containing 2 L of water.
5. Mobile Phase B (Acetonitrile)

B. Chromatographic Conditions

Column: Octadecyl silane bonded to porous silica (USP column type L1) or equivalent, 150 x 4.6 mm, 3-5 µm particle size or equivalent

Column Temperature: 20 °C

Flow Rate: 1.5 mL/minute

Detection: UV absorbance at 220 nm

Injection volume: 10.0 µL

Run Time: 25min data acquisition + 5min re-equilibration

Time (min)	%A	%B
0	90	10
2	80	20
20	40	60
25	10	90
25.1	90	10
30	90	10

H. Instrument Method

1. Autosampler method

Injection volume: 10.0 µL

Autosampler link stop time: 20.0 min

Number of washes before injection: 2

Prewash duration: 1.0 s

Prewash vial position: 1

Prewash solvent: water

Number of washes after injection: 2

Postwash duration: 1.0 s

Postwash vial position: 1

Postwash solvent: water

Autosampler temperature: 23.5 degC

Injection trigger: true

Injection trigger temperature minimum: 23.0 degC

Injection trigger temperature maximum: 25.0 degC

Injection trigger temperature tolerance minimum: -1.0 degC

Injection trigger temperature tolerance maximum: 1.0 degC

2. DAD method

DAD link stop time: 20.0 min

Fullscan sampling rate: 10.0 Hz

Fullscan range minimum: 280.0 nm

Fullscan range maximum: 700.0 nm

Fullscan range step: 2.0 nm

Channels

channel	setting	value	unit
1	wavelength	220.0	nm
1	bandwidth	-4 to 4	nm
2	wavelength	440.0	nm
2	bandwidth	-4 to 4	nm

3. Pump method

Pump link stop time: 20.0 min

Maximum flow gradient: 2.0 mL/min^2

Solvent name: 90% ACN, 0.01%TFA

Gradient start: 300.0 s

Solvent lines

index	time	unit	A	unit	B	unit	flow	unit	pressure	unit
1	0.0	s	100.0	%	0.0	%	1.0	mL/min	2.0	bar
2	300.0	s	50.0	%	50.0	%	1.0	mL/min	2.0	bar
3	600.0	s	0.0	%	100.0	%	1.0	mL/min	2.0	bar

Methods on Demand, Pistoia Alliance

Business Challenge

- Method descriptions are still mainly text-based documents
- Reproducibility of methods limited by interpretation of free text
- Descriptions use different terminology and levels of detail
- Version control often difficult because of number of copies

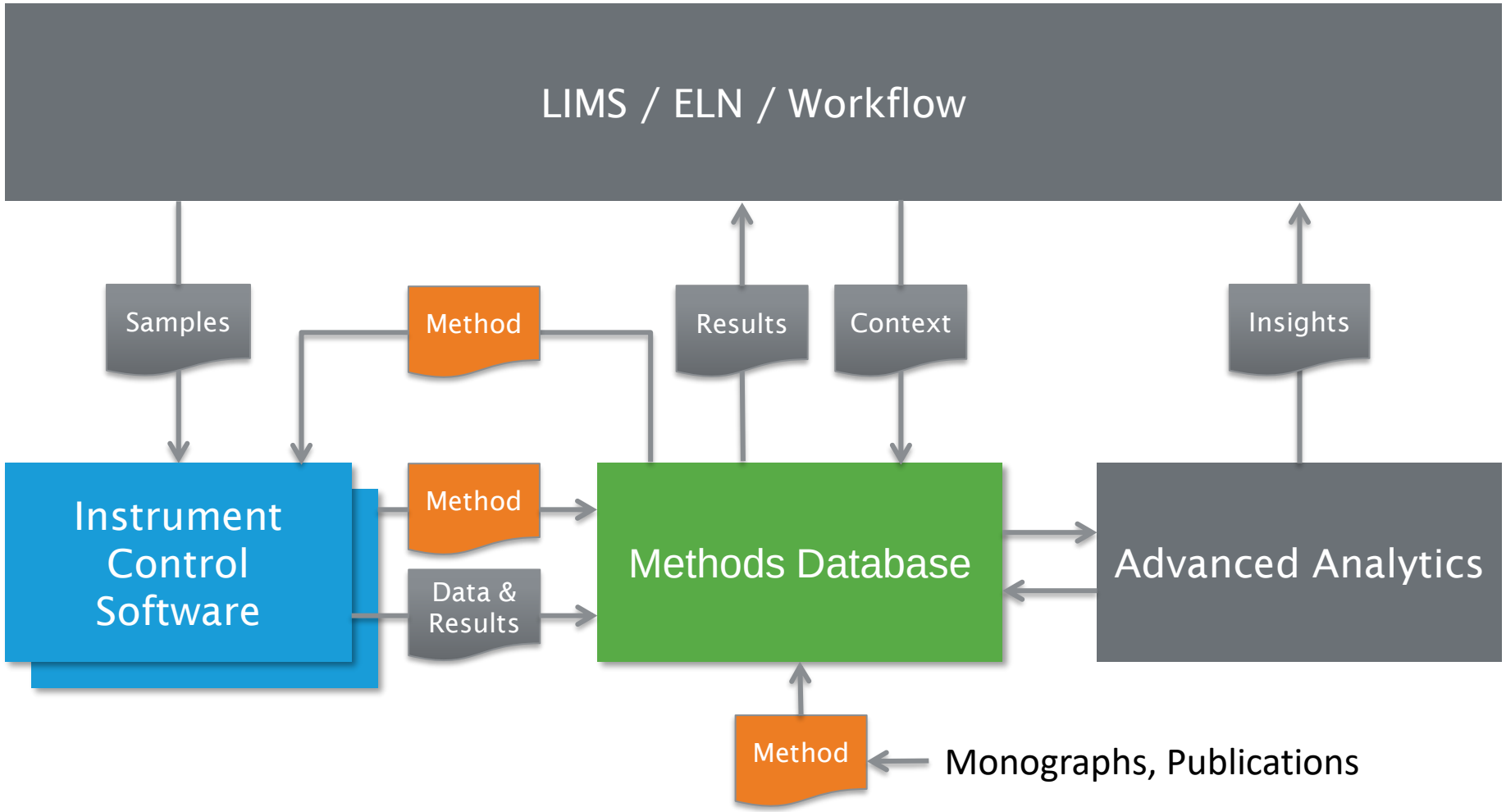
Objectives

- Parse methods from public and private monographs and academic publications (Natural Language Processing, NLP)
- Extension of method model from instrument method to complete analytical method

Contributors

- Pharma Member Companies, USP (US Pharmacopeia), BP (British Pharmacopeia), CAS, a division of the American Chemical Society (MethodsNow), Elsevier, Pistoia, Allotrope, OSTHUS

Methods Database Context



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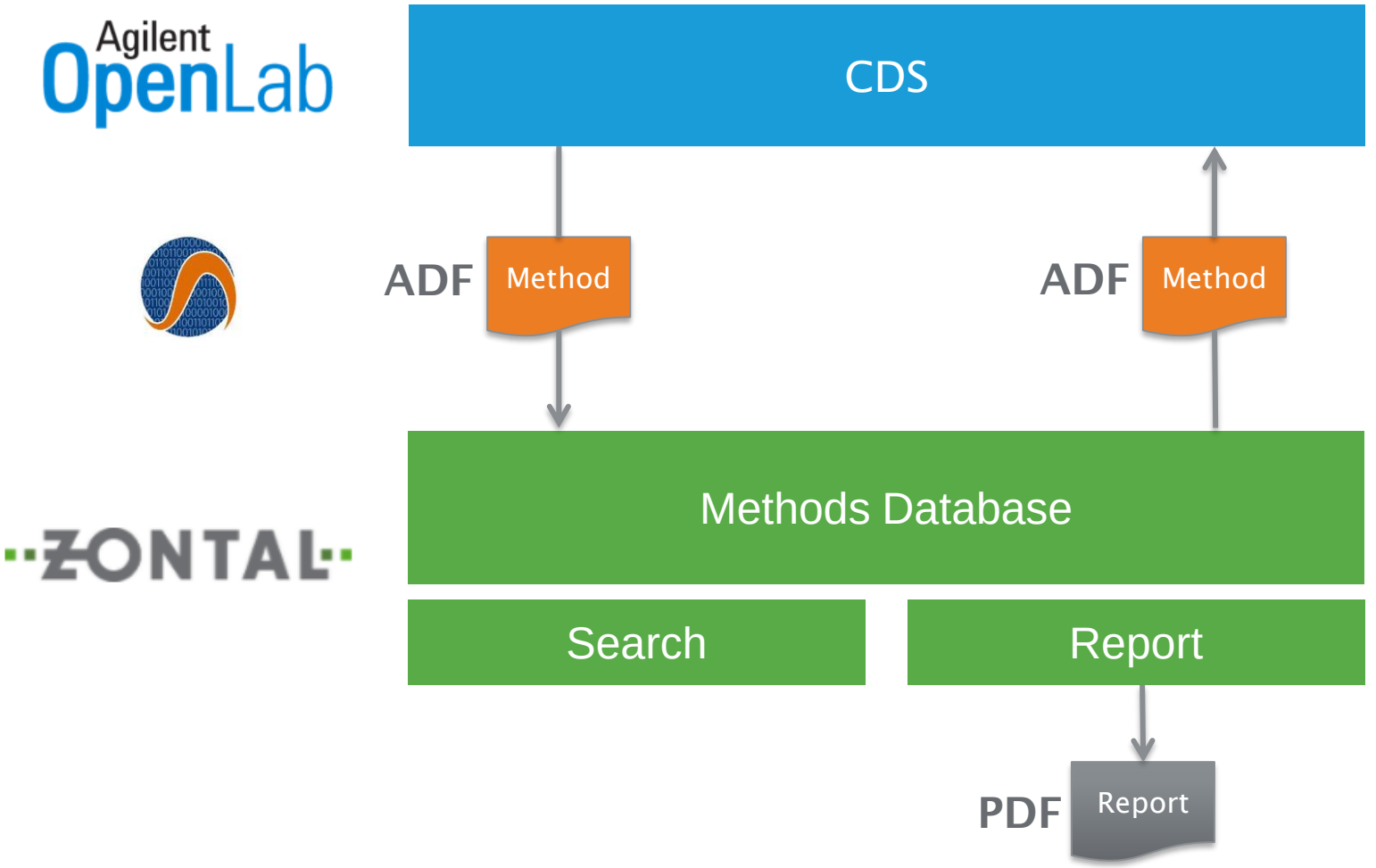
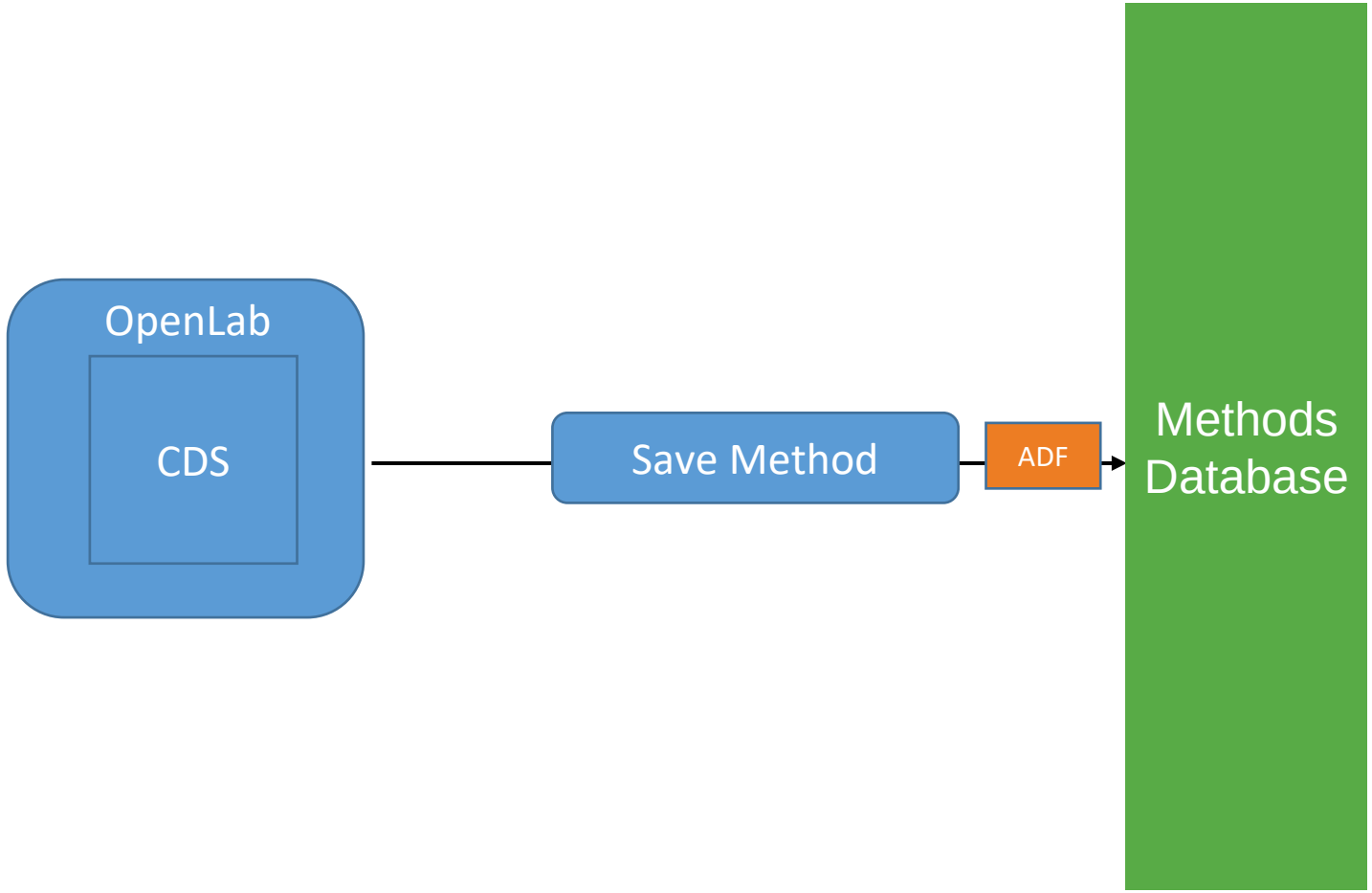
Solution Architecture



Demo Workflow 1

Saving a Method into the Methods Database



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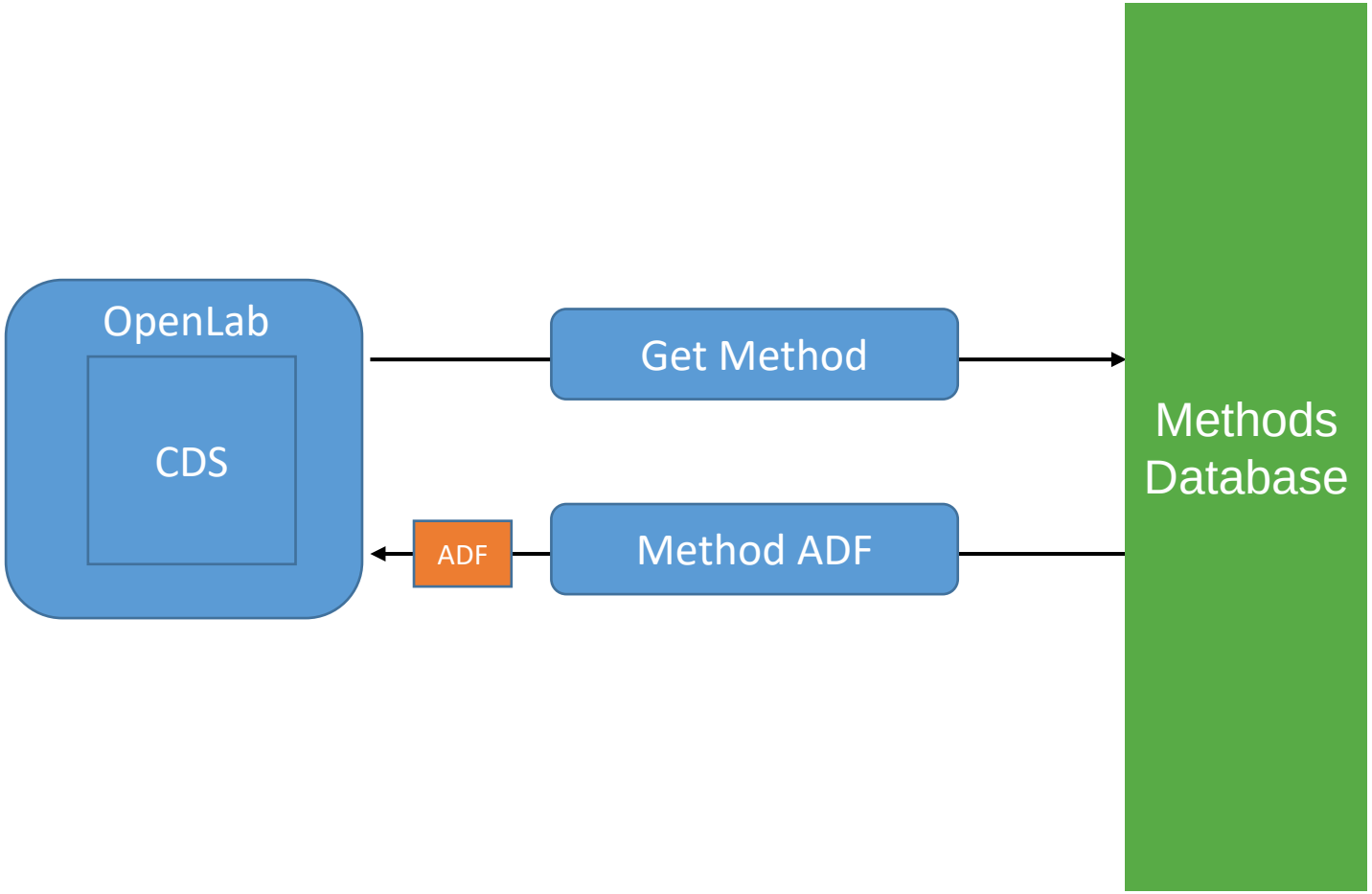
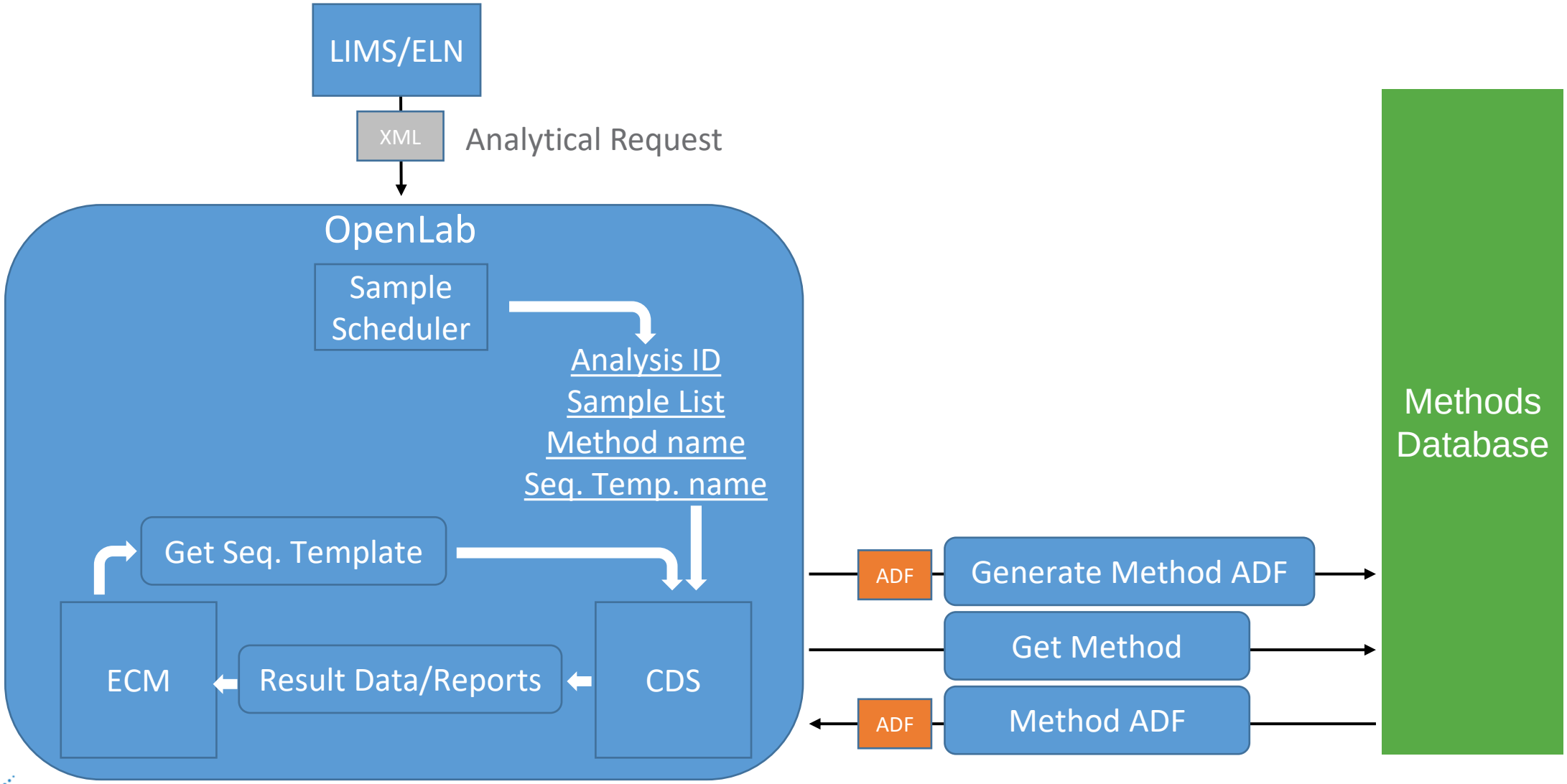
Demo Workflow 2

Retrieving a Method from the Methods Database

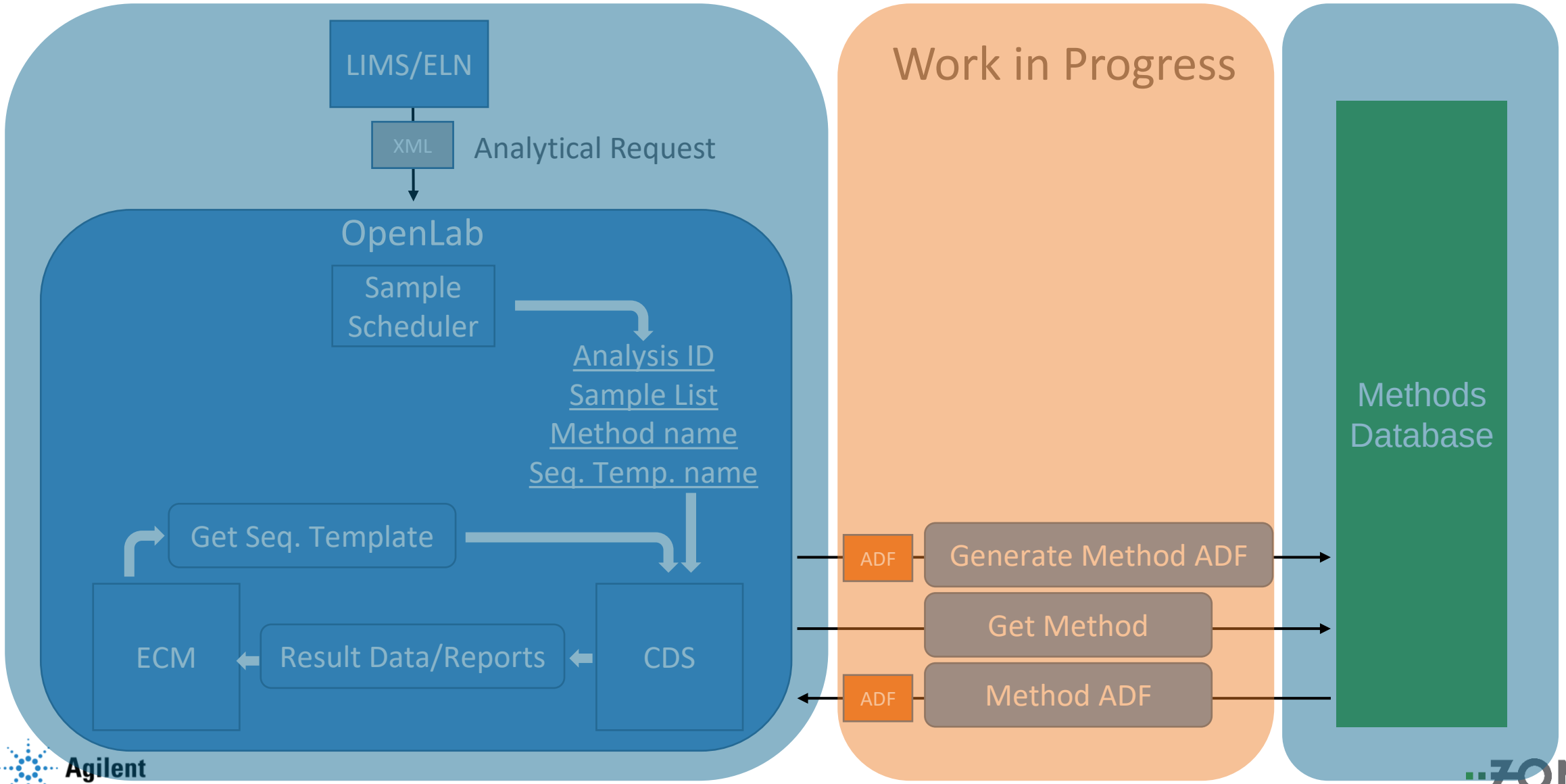


DEMO

Outlook: Completing the QA/QC Routine Lab Workflow



Commercialized today : QA/QC Routine Lab Workflow



Q&A