Emerald Cloud Lab

Elevating Science with Cloud Laboratories

Louis Sintasath, MSc, MBA
Senior Director, Business Development

Jake Hostetler
Account Manager – West Coast

What is a Cloud Lab?

A physical laboratory which scientists can access remotely via software over the internet which provides the same level of control as a scientist would have in a traditional lab environment

Emerald Cloud Lab

1. Remote, On-demand Experimentation

A Cloud Lab must allow customers to remotely conduct experiments on-demand, 24/7/365 via a computer interface without ever requiring the customer to physically visit the lab or communicate additional instructions outside of the computer interface.

2. On Demand Control of Every Experiment

A Cloud Lab must allow customers to fully specify any and all aspects of experiments conducted remotely, providing the same flexibility they would have standing in front of the instrument itself, without any lead time or the involvement of software or automation engineers to reconfigure programs or hardware.

3. Comprehensive Instrumentation

A Cloud Lab must provide customers on-demand access to instrumentation covering the full scope of laboratory work they will be performing, obviating the need to perform any of your daily lab work outside of the cloud laboratory.

4. Comprehensive Sample Preparation

A Cloud Lab must allow customers to perform all aspects of sample preparation, storage, and handling remotely. At a minimum, sample preparation capabilities must include liquid handling ranging from microliter to liter scale, solid handling from grams to kilograms, interoperability with any container form factor, indefinite sample storage in typical storage conditions, and operations in specific environments such as biosafety cabinets, fume hoods and glove boxes.

5. One Software Interface for the Entire Lab

A Cloud Lab interface must allow customers to script experiments (including connecting multiple experiments) as well as process, analyze, visualize and interpret all of the data generated by the interface without requiring third party software or involvement of software or automation engineers to reconfigure software or hardware.

McKinsey & Company

March 8, 2023 Article

Share Print Download Save

Laboratory technology has been a steady runner in the world of pharmaceuticals, rather than a racing star—until now. A series of innovations points toward exponential gains in R&D productivity.

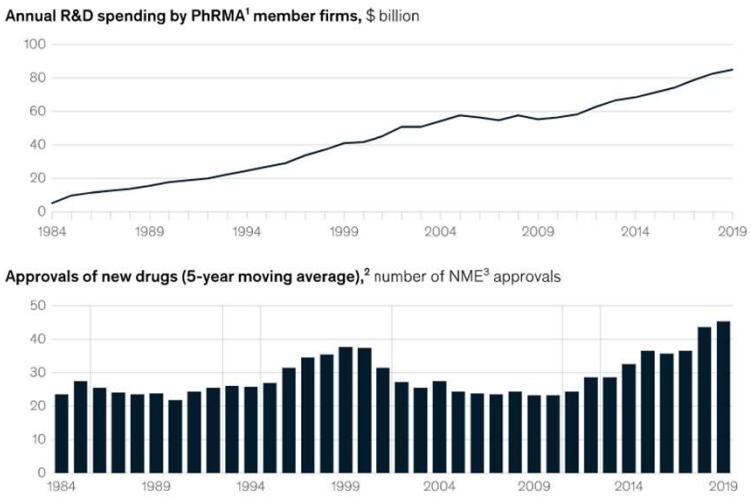
McKinsey & Company – Listen to the article: From bench to bedside: Transforming R&D labs through automation SOUNDCLOUD

McKinsey & Company

March 8, 2023 Article

Exhibit 1

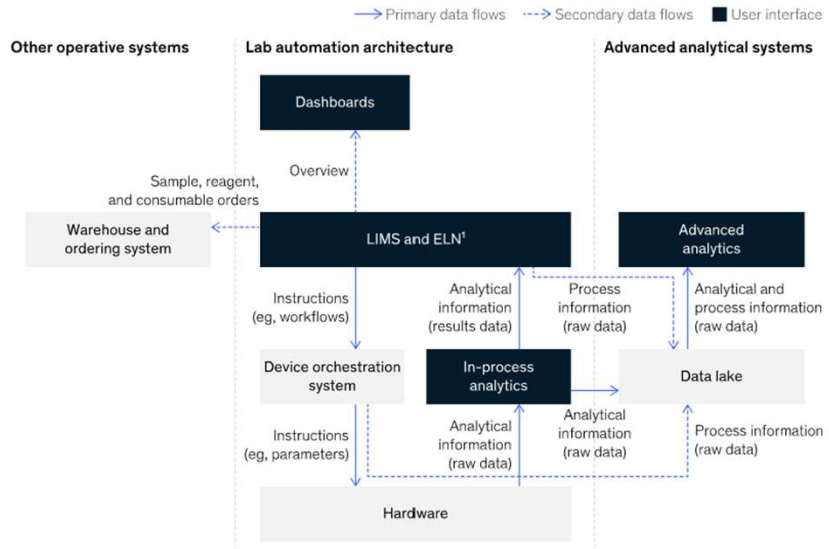
US R&D spending more than doubled from 2001 to 2019, but the number of newly developed drugs has increased only marginally.



[1]Pharmaceutical Research and Manufacturers of America.
[2]A 5-year moving average replaces the value for each year in an annual data series with an average over 5 consecutive years. (Here the arithmetic mean of each annual value and the preceding 4 is used.) A moving average is smoother than the underlying data series and is useful for reducing year-to-year changes unrelated to overall trends in the data.
[3]New molecular entity.

Exhibit 2

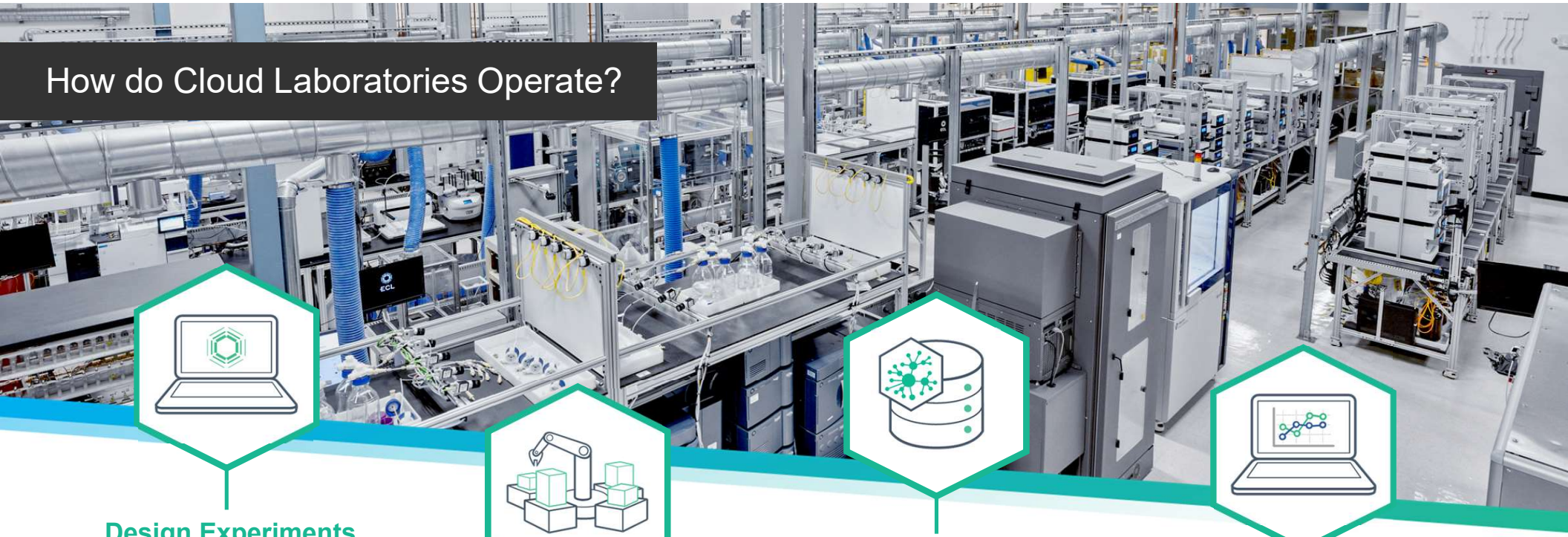
Software capabilities can be integrated into a holistic lab software architecture.



[1]Laboratory information management systems and electronic lab notebooks.
Source: McKinsey analysis

McKinsey & Company

How do Cloud Laboratories Operate?



Design Experiments

Ship (or drop off) samples and design your experiments in software using the Command Center application. All activities in the lab can be orchestrated by a series of commands.

Run Experiments

The shared cloud lab facility remotely executes your experiment commands in parallel, to your exact specifications, in a 24/7 environment (without you ever needing to set foot in it)

Organize and Connect Data

Both primary and ancillary data is automatically organized into a searchable scientific graph database with fixed ontologies for every type of data generated

Explore, Analyze, & Share

Command Center includes an extensive suite of tools for data analysis and visualization as well as tools for sharing notebooks and database access to experimental programs with other users

Automating the Lab of the Future

Classifying levels of automation in the lab and providing examples of the capabilities they enable

Comprehensive Data Capture Enables Automation

Proceduralization and capture of all steps performed in the laboratory directly drive degree to which a lab can be automated

Closed-loop Experimentation

Creating a full-featured cloud lab enables real closed-loop experimentation that can be driven autonomously

Level 0: Manual Unit Operations

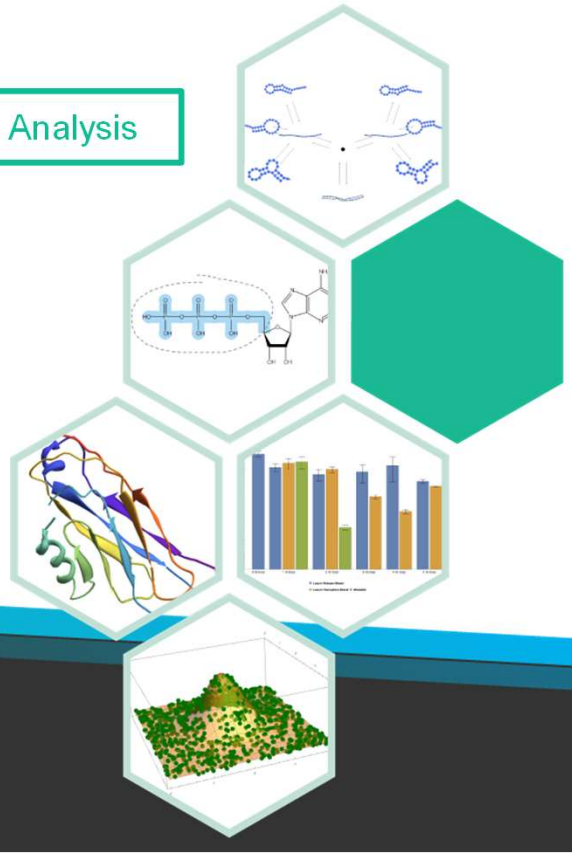
Manual Sample Handling / Prep

Level 1: Automated Unit Operations

Automated Sample Handling / Prep

Instrument

Data Analysis



Emerald Cloud Lab

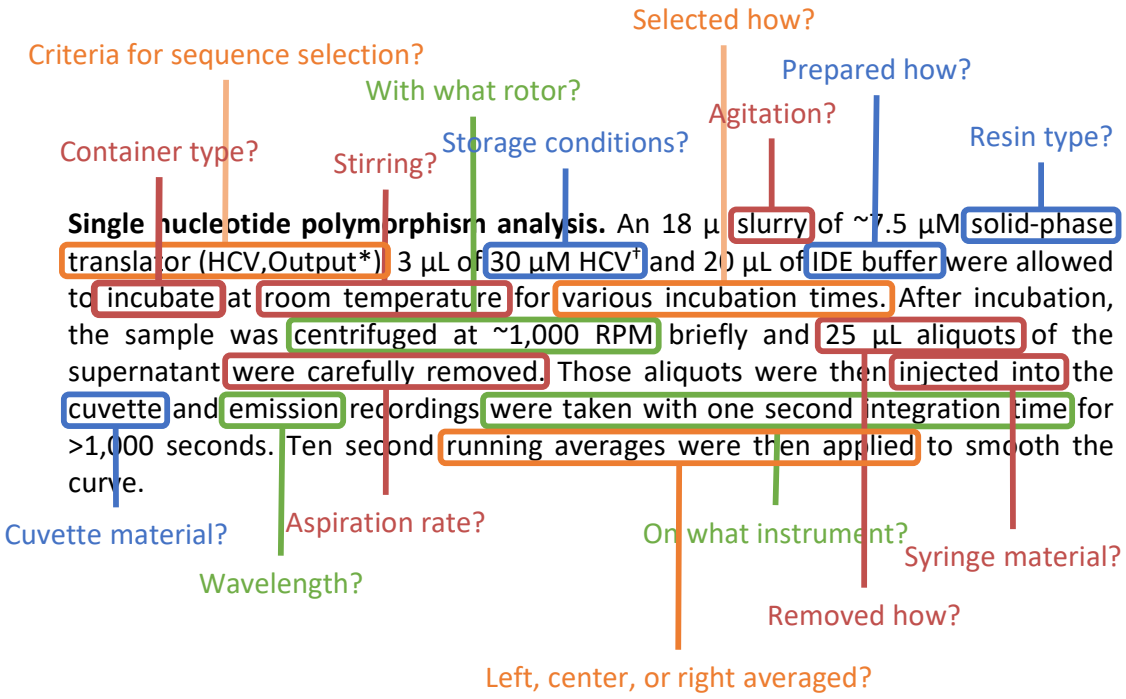
Manual Sample Handling / Prep

Level 2: Semi-automated Experiment

Automated Sample Handling / Prep — Instrument — Data Analysis

Reproducibility

Codifying experiments provides push-button reproducibility of any experiments run on the ECL



ECL Codifies Experiments

```
ExperimentFluorescenceKinetics[
  "Reaction Mixture",
  PreparatoryUnitOperations->{
    Transfer[
      Source->Model[Sample,StockSolution,"IDE Buffer"],
      Destination-> Model[Container,"2mL Tube"],
      Amount->20 Microliter,
      Label->"Reaction Mixture"
    ],

    Transfer[
      Source->Model[Sample,"7.5uM HCV Translator"],
      Destination->"Reaction Mixture",
      Amount->18 Microliter,
      AspirationMixVolume->10 Microliter,
      NumberOfAspirationMixes->10,
      AspirationMixRate-> 100 Microliter/Second
    ],

    Transfer[
      Source->Model[Sample,"30uM HCV RNA"],
      Destination->"Reaction Mixture",
      Amount-> 3 Microliter
    ],

    Incubate[
      Sample->"Reaction Mixture",
      Time->5 Minute,
      Temperature->Ambient,
      MixType->Pipette,
      NumberOfMixes->10,
      MixVolume->30 Microliter,
      MixRate-> 100 Microliter/Second
    ],

    Centrifuge[
      Sample->"Reaction Mixture",
      Intensity->800G,
      Rotor->Model[CentrifugeRotor,"20R FA361.5"],
      Time->10 Second
    ]
  },

  AliquotVolume->25 Microliter,
  AliquotContainer->Model[Container,Cuvette,"2mL UV
  Quartz"],
  AssayVolume->2 Milliliter,
  ExcitationWavelength->355 Nanometer,
  EmissionWavelength->420 Nanometer,
  ReadTime->1 Second,
  RunTime->1000 Second
]
```

Emerald Cloud Lab

J. Am. Chem. Soc. 131, 9368 (2009)

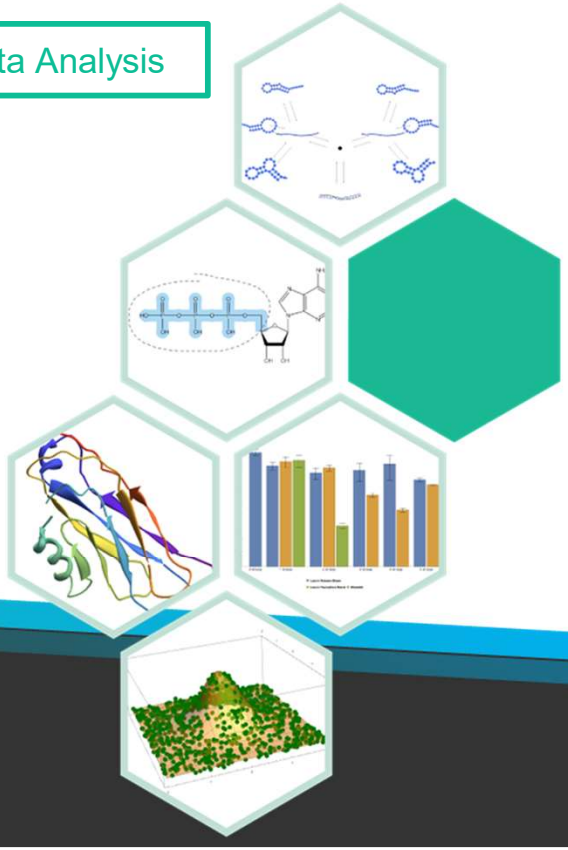
Level 3: Automated Experiment

Manual Sample Handling / Prep

Automated Sample Handling / Prep

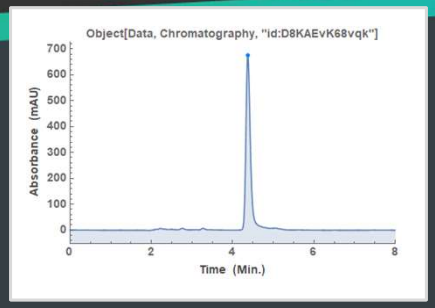
Instrument

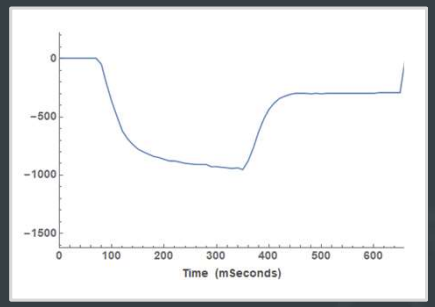
Data Analysis

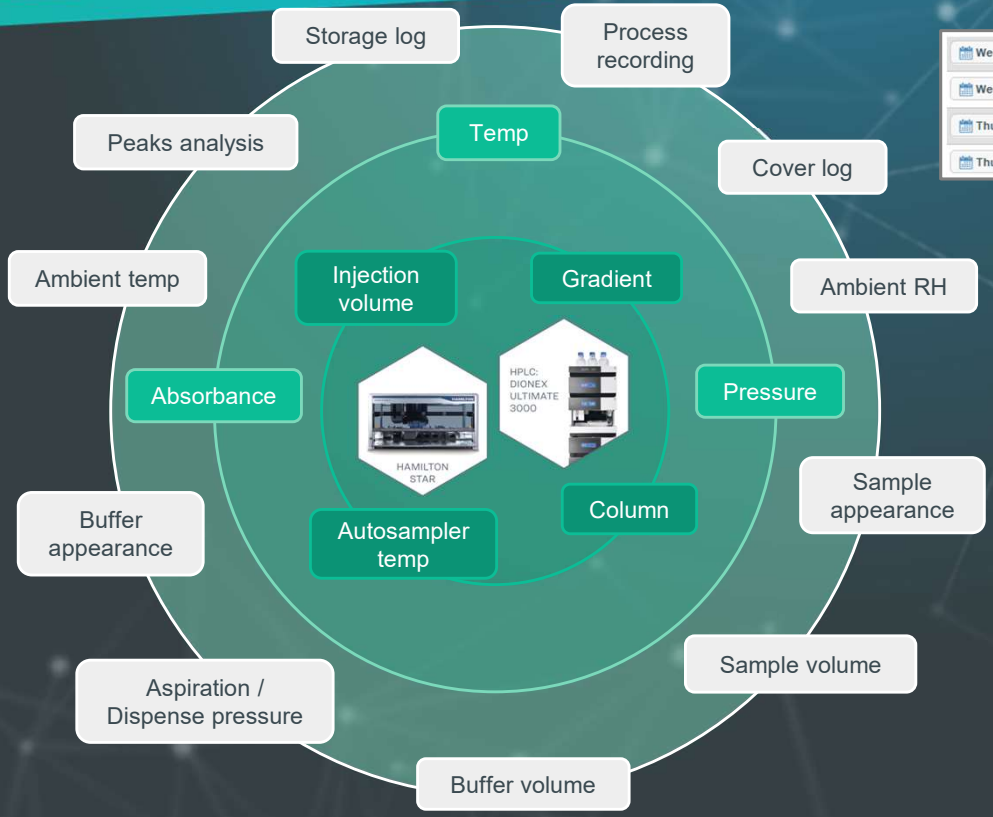


Primary data are the tip of the iceberg

Complete capture of experimental parameters, primary data, analysis, and metadata







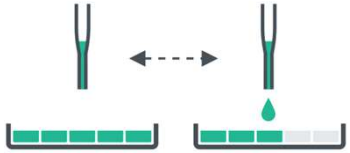
Wed 7 Sep 2022 15:20:40 GMT−4.	Out	Null	Null
Wed 7 Sep 2022 15:20:40 GMT−4.	In	Object[Container, Vessel, id:n0k9mGkY8Y8k]	A1
Thu 22 Sep 2022 06:54:04 GMT−4.	Out	Object[Container, Vessel, id:n0k9mGkY8Y8k]	A1
Thu 22 Sep 2022 06:54:04 GMT−4.	In	Object[Container, Vessel, id:O81aEB1Pdmqp]	A1

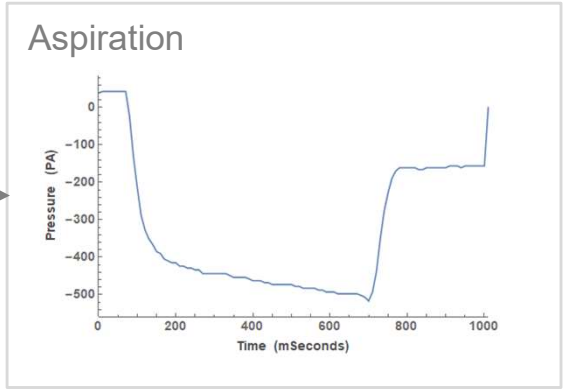
Emerald Cloud Lab

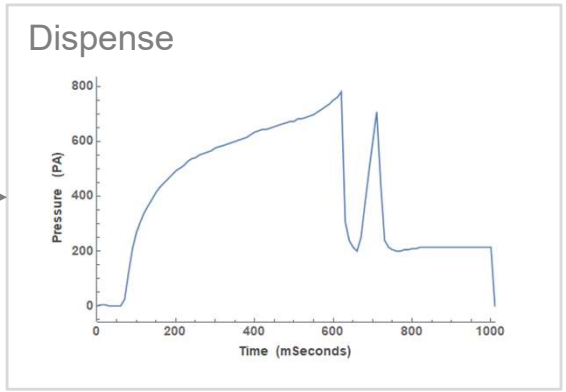
Automating metadata analysis

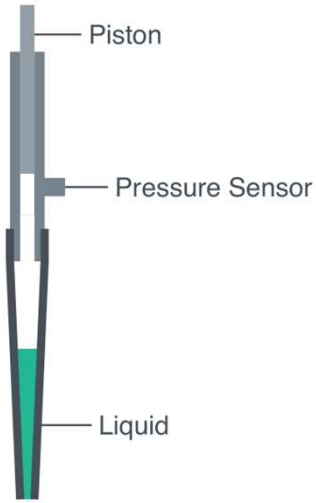
ML-driven scoring of pipetting success by aspiration/dispense pressure

Automated Sample Handling / Prep





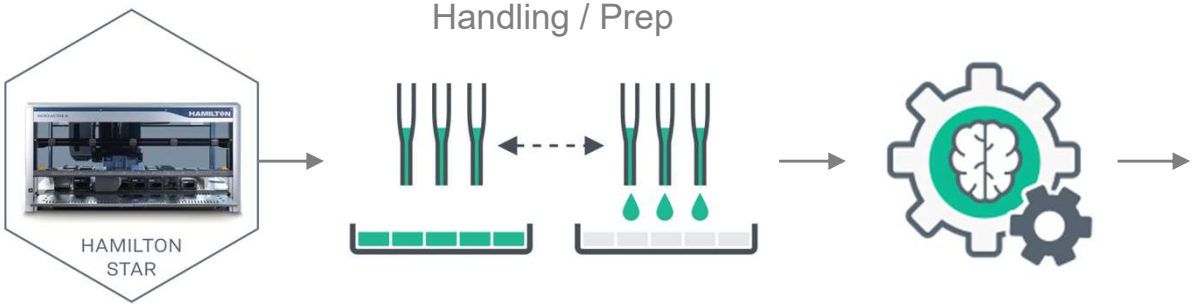


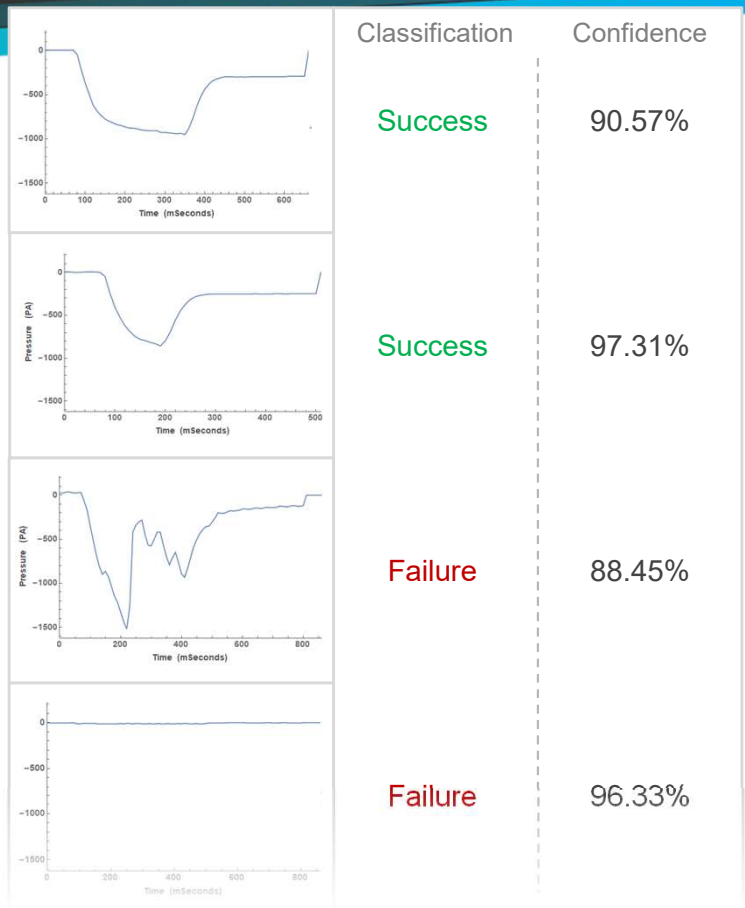


Emerald Cloud Lab

Automating metadata analysis

ML-driven scoring of pipetting success by aspiration/dispense pressure

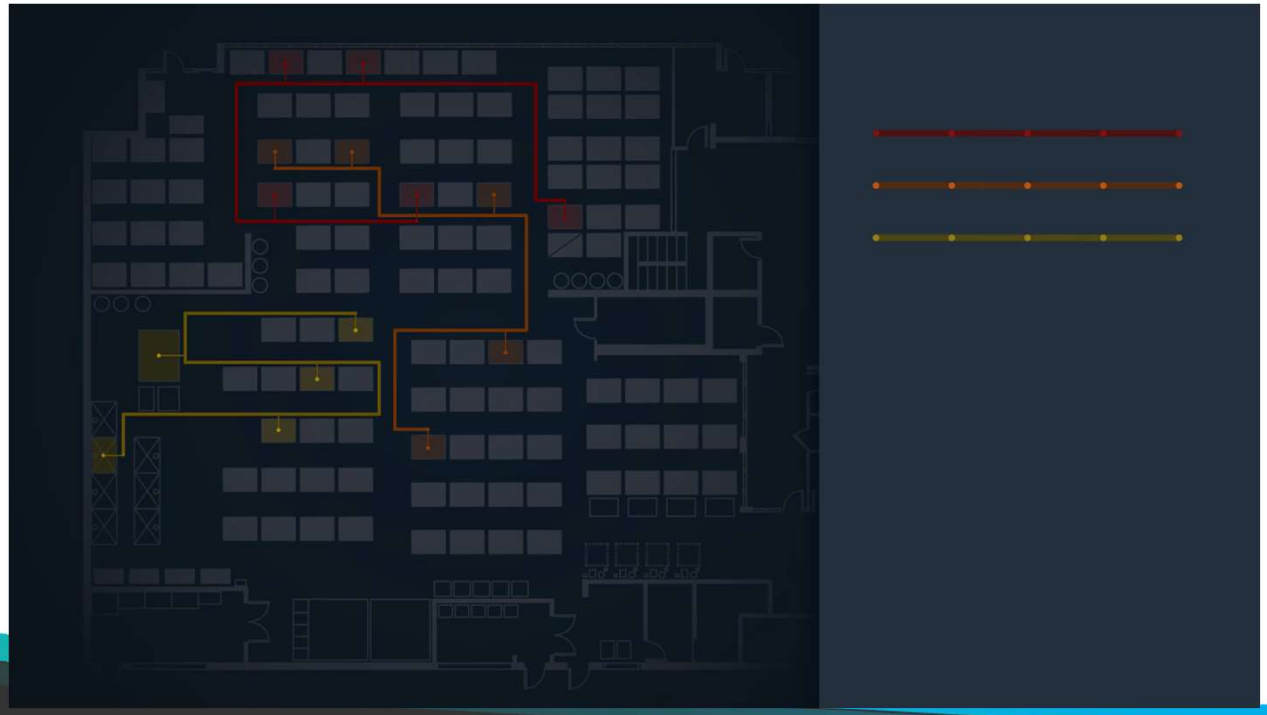




Emerald Cloud Lab

Level 4: Full Lab Automation

- Cloud lab enabled
  - Unified software application allows users to design experiments, run them, automate the analysis
  - Scripts can be written to run an experiment, process the data and, using logic statements, select the next run's conditions and queue the experiment
  - Universal data format required by a cloud lab drives interoperability between disparate experiments



Example: # Stability study

Scientists can quickly transfer new methods to the ECL and combine any number of individual experiments using scripts. This allows for complete, multi-armed, multi-timepoint stability studies, with automated analysis of analytical data, and custom reporting to be controlled from a few blocks of code.

Manage and queue your entire stability protocol from a single script

Samples are stored, pulled and analyzed automatically in the ECL

Automated data analysis and fully customizable reporting to close out your study quickly

Preparation and Storage

Intake of materials

Ship materials to ECL

```
sampleShipment = ShipToECL[
 {Model[Sample, "Stability Formulation 1"]},
 {"Stability formulation 1 tube"},
 ContainerModel → Model[Container, Vessel, "50mL Tube"],
 Volume → 20 Milliliter
 ]
```

Generate aliquots (one per time point per condition)

Retrieve and name shipped samples

```
shippedSamples = sampleShipment[SamplesOut]
UploadName[shippedSamples, {"Stability Formulation 1 Sample 1"}]
```

Aliquot each received sample

Make 12 aliquots, one for each stability condition (3) and time point (4) combination:

```
aliquotProtocol = ExperimentAliquot[
 Repeat[Object[Sample, "Stability Formulation 1-1"], 12],
 Amount → 1 Milliliter
 ]
aliquotedSamples = aliquotProtocol[SamplesOut];
```

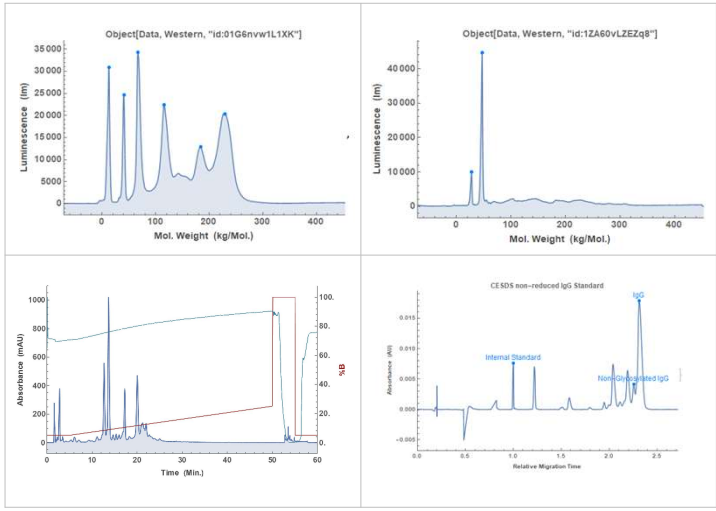
Store aliquots in each of the conditions

```
aliquots4C = aliquotedSamples[[1 ;; 4]];
aliquots25C = aliquotedSamples[[5 ;; 8]];
aliquots37C = aliquotedSamples[[9 ;; 12]];

StoreSamples[
 Join[
  aliquots4C,
  aliquots25C,
  aliquots37C
  ],
 Join[
  Repeat[Model[StorageCondition, "Stability Chamber 4C"], 4],
  Repeat[Model[StorageCondition, "Stability Chamber 25C"], 4],
  Repeat[Model[StorageCondition, "Stability Chamber 37C"], 4]
  ]
 ]
```

Set up sampling time points

1. Ship to ECL
2. Liquid Handler
3. Environmental Chambers
4. Analytical Package



Emerald Cloud Lab

Level 5: Closed loop experimentation

- Building on a fully automated lab, the integration of AI/ML tools will allow scientists to close the loop on experimentation
- Allows scientists to focus on the direction of their research instead of the minutae
- Scientists define optimization objectives, direction, constraints
- AI/ML tools to manage the details – determining the series of experiments, automating data analysis, identifying outliers or abberant data, leveraging historical data, updating models as data is generated

- Example
  - Target to maximize peak separation on an HPLC
  - Variables – gradient concentration, column temperature, column type
  - Directly integrate machine learning models to explore the parameter space to help make better decisions on what to run next
  - Data is added to the model as experiments are run which can minimize the number of experiments needed to meet an objective

Unique Features of ECL

- Every piece of data is captured, organized in ECL Constellation, and associated with relevant experiments
- Scientists are assisted to fully define their method or protocol up front in ECL Command Center, and the system ensures the instruction set is not ambiguous
- Experiments can be scripted together
- Command Center is a complete programming language built on Mathematica, so logic can be inserted in-line with scripted experiments


FACILITY TOUR

Louis Sintasath
Senior Director, Business Development
Louis.Sintasath@emeraldcloudlab.com
858-344-8398
https://www.linkedin.com/in/louissintasath/

Emerald Cloud Lab