Dotmatics
Virscidian

Allotrope Simplified Model Automatic Creation

We’re all about…

Drug discovery software from synthesis to registration & HTS

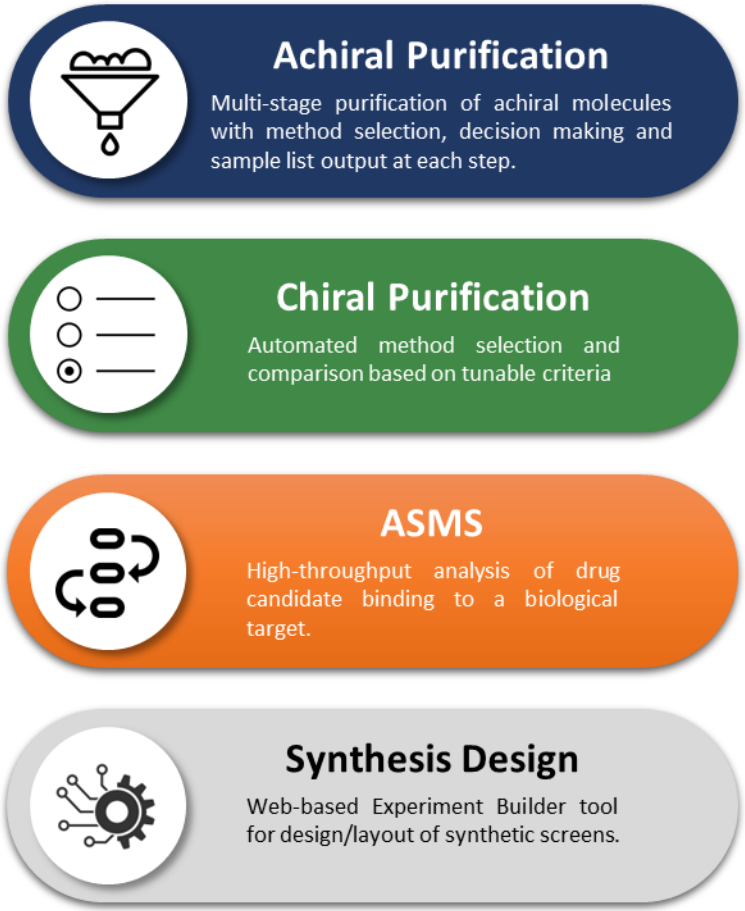
Automating workflows

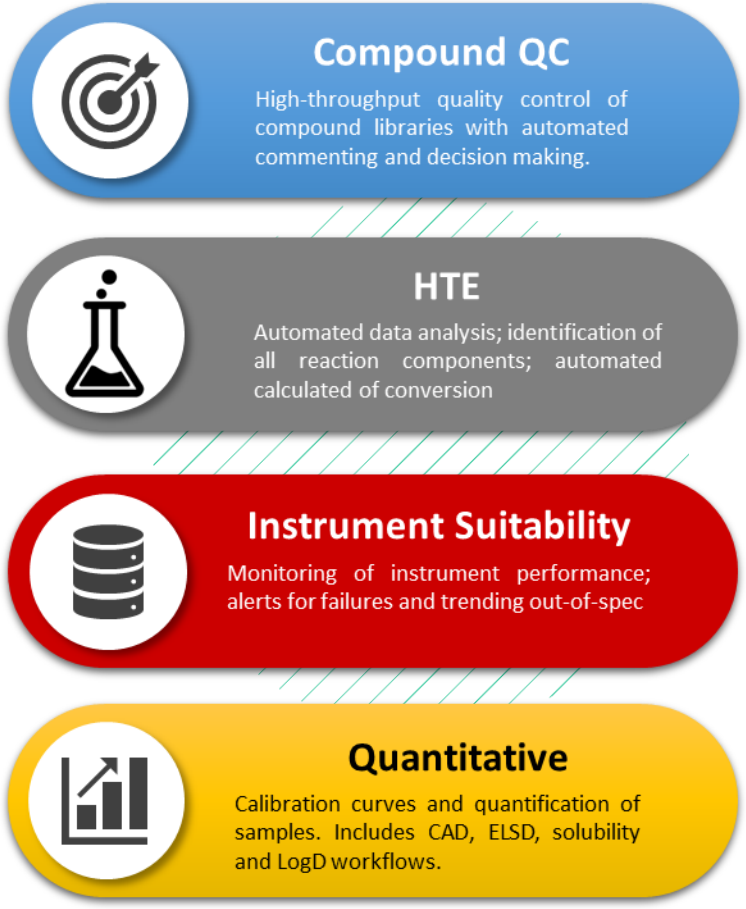
Desktop and enterprise level products for any sample throughput

Best-in-class LC-MS data processing

Virscidian
=
Virtual (Vir)
Scientific (sci)
Decisions (dian)

Many drug discovery workflows...





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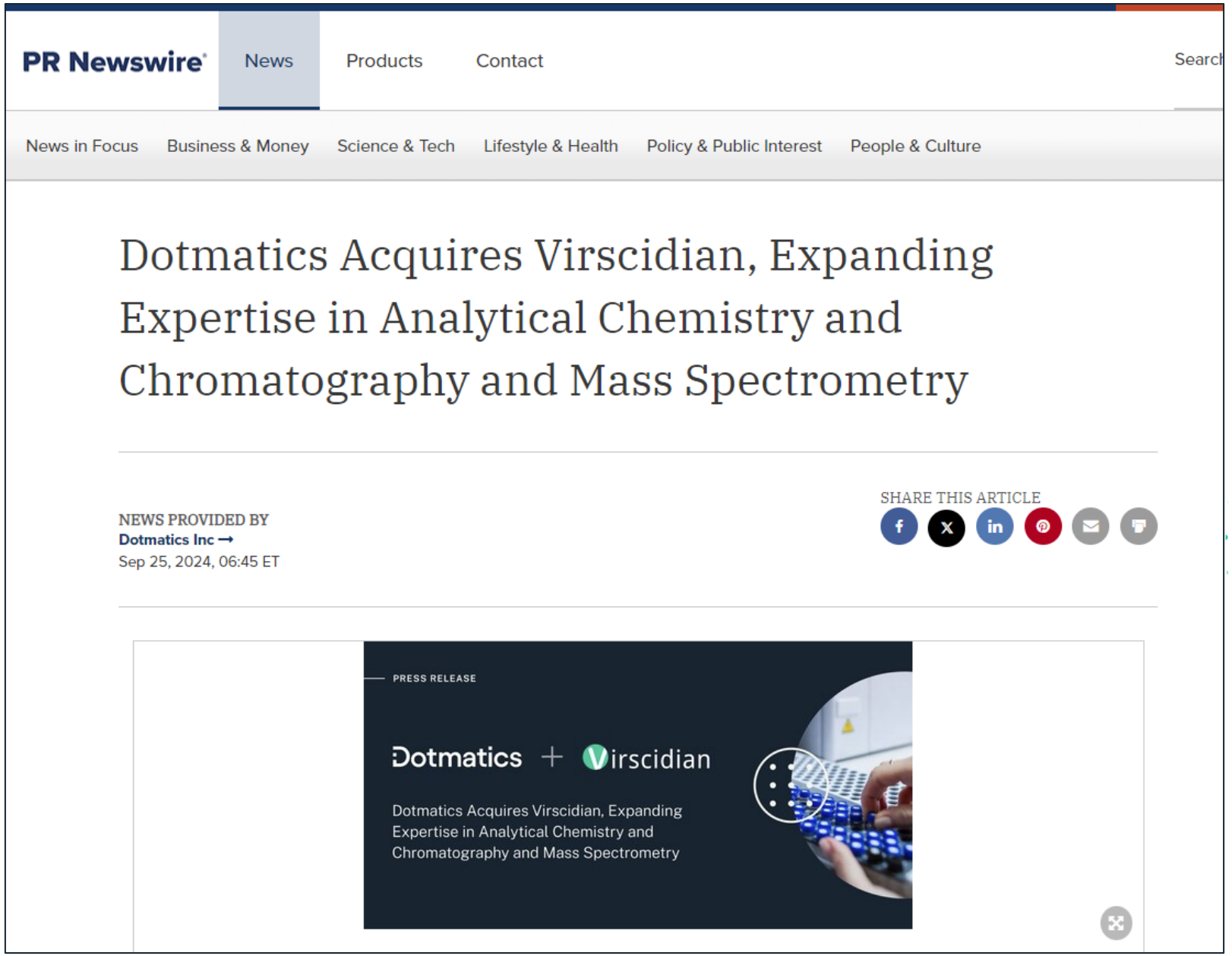
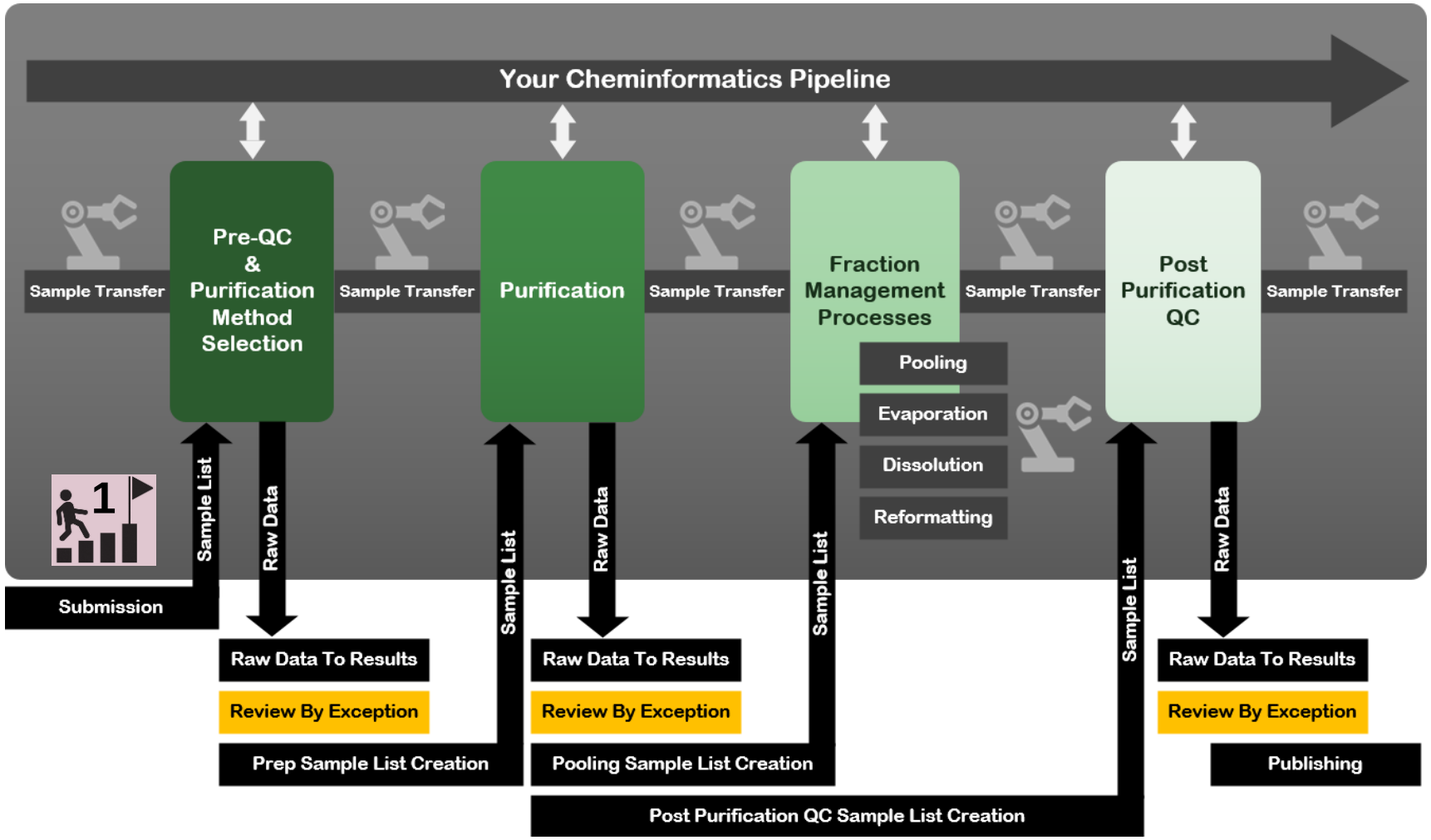


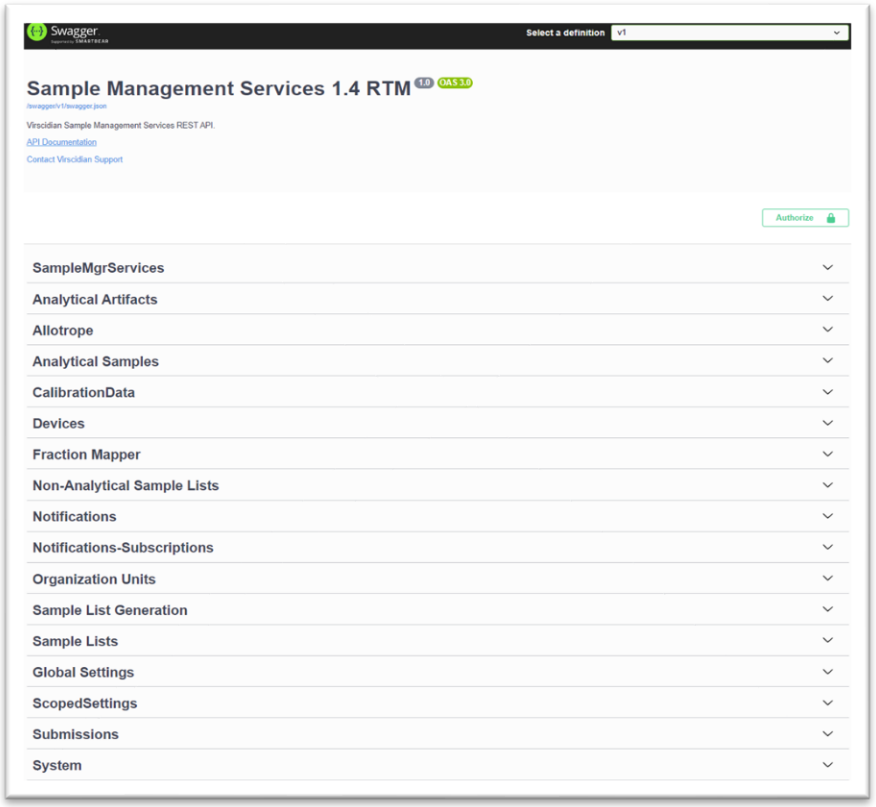
https://www.prnewswire.com/news-releases/dotmatics-acquires-virscidian-expanding-expertise-in-analytical-chemistry-and-chromatography-and-mass-spectrometry-302257760.html

Where are the short-term challenges to solve?

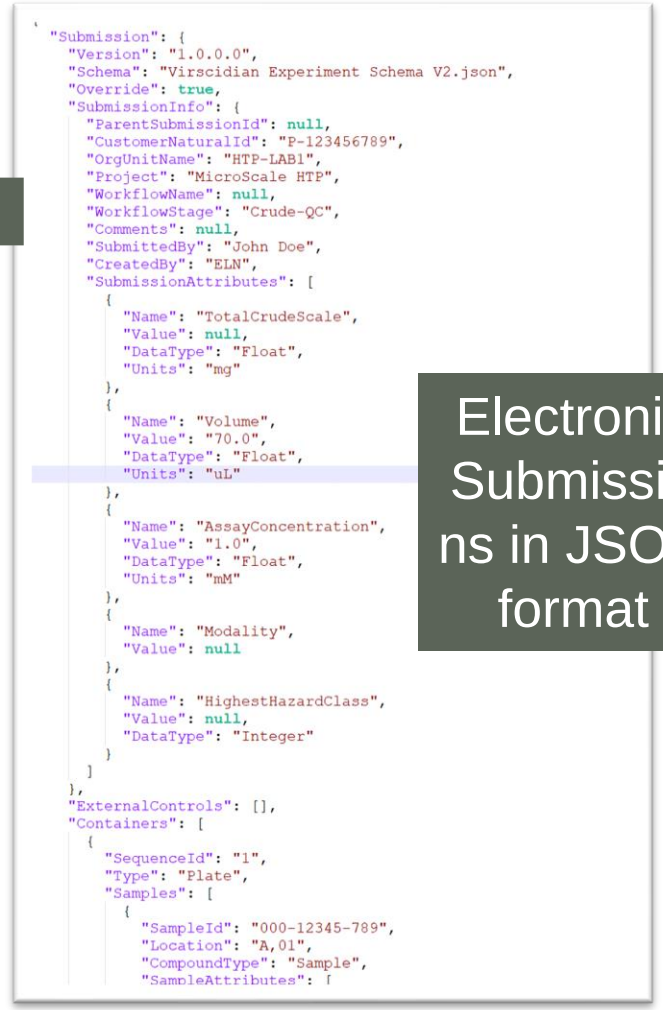


How to get the right metadata, in the right place, at the right time?

Electronic Submissions – Sample Management APIs



New API Integration



Electronic Submissions in JSON format

Third party - On demand sample list generation

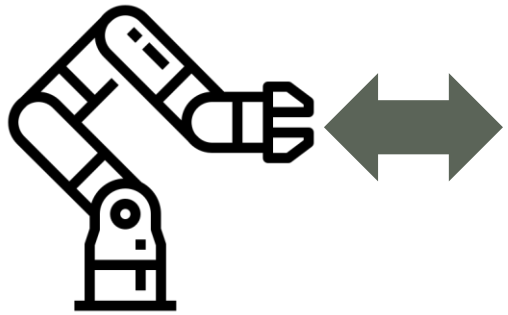
How to put the configuration of what goes into a sample list in the hands of the scientists AND continue to optimize complex automated robotics workflows without software redevelopment?

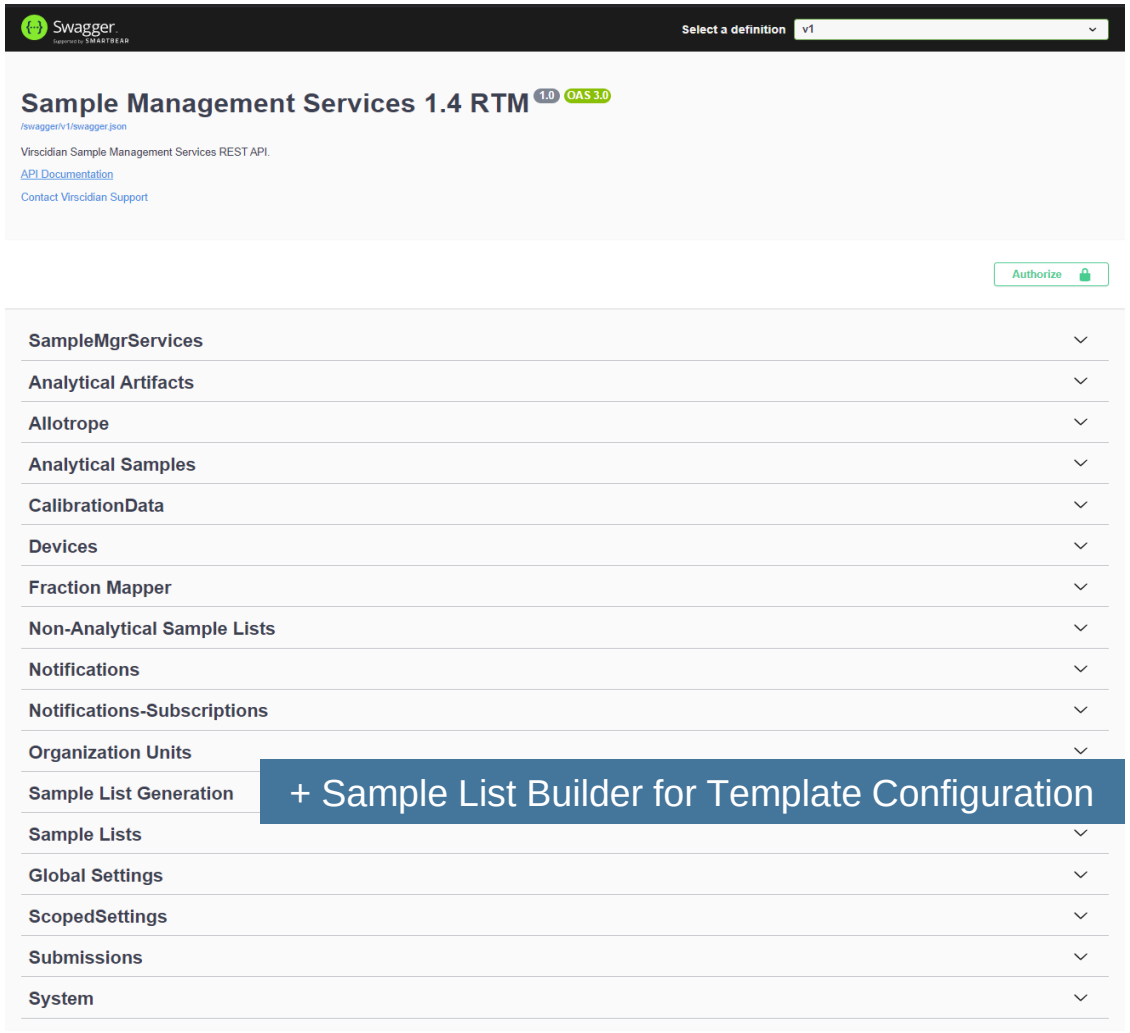
Biosero GBG™

- Multiple projects delivered / In progress

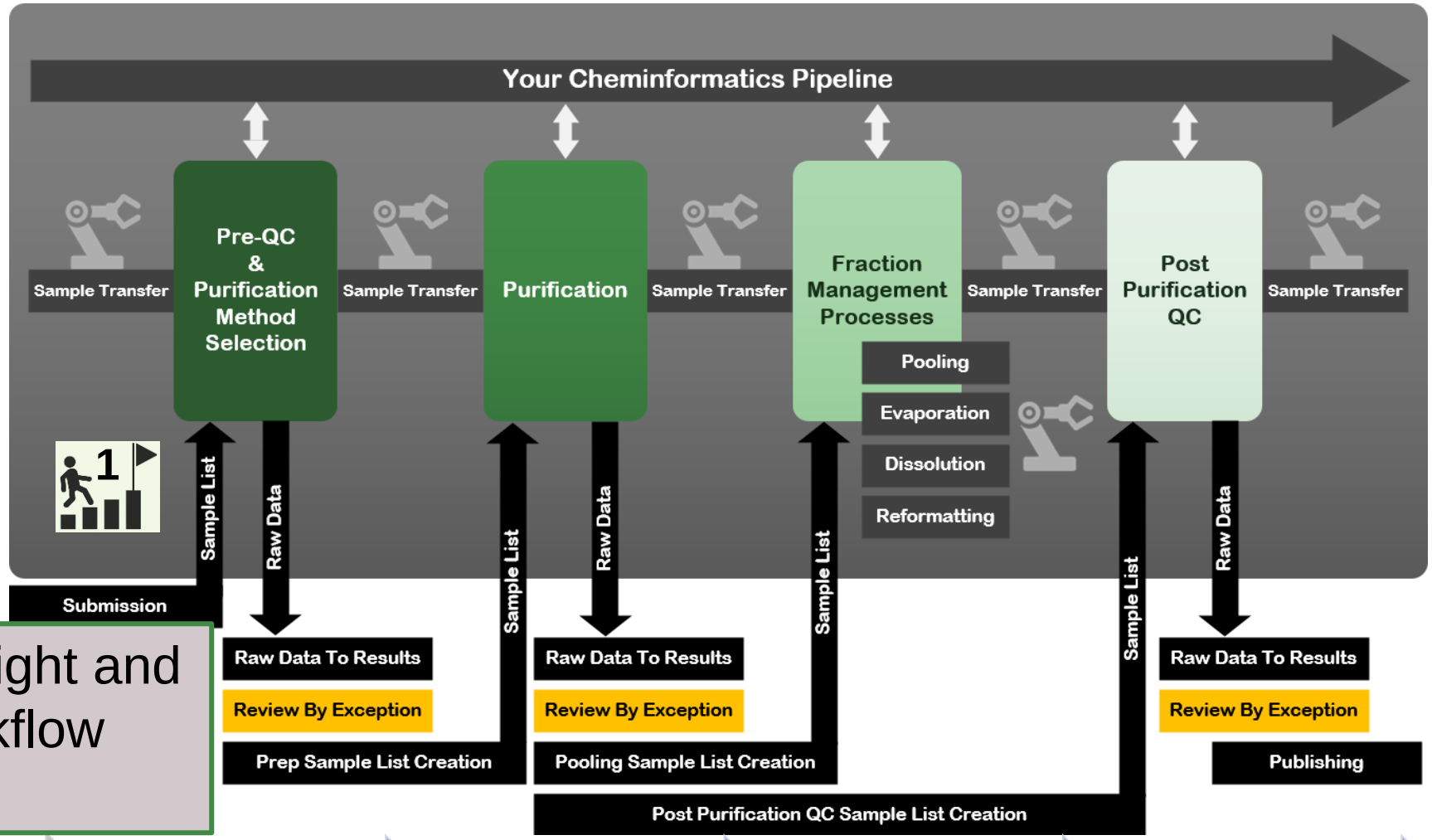
HighRes BioSolutions™

- Multiple projects in progress

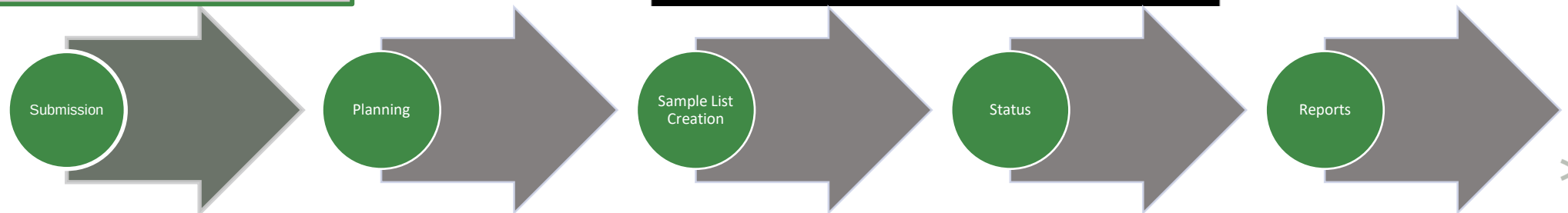




Where are the short-term challenges to solve?



Lack of oversight and stepwise workflow execution



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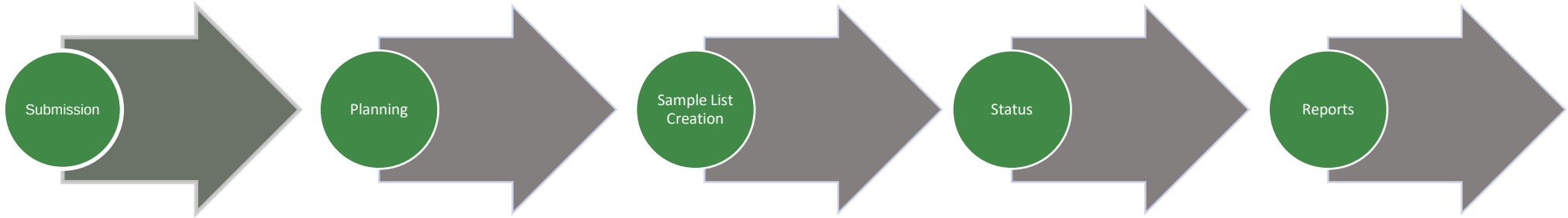


Analytical Studio - Sample List

Planning
Submissions Dashboard

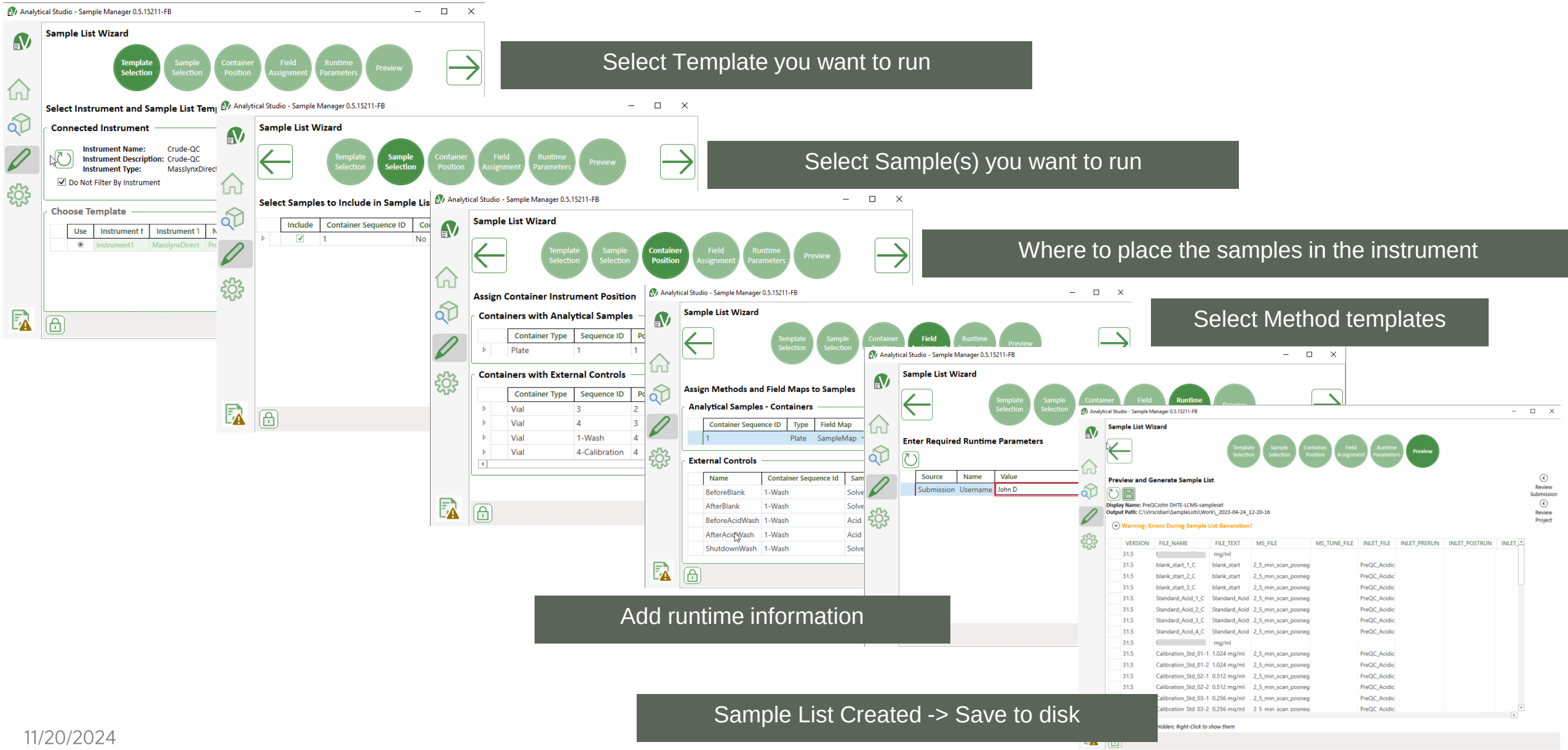
Reporting
Lineage

Execution
Create Sample List Wizard

Execution
Sample List Dashboard

Execution
Submission Information

Sample List Creation Wizard - Execution



Active Status Information – Informing Project Teams

Oversight Execution Reporting

Submissions View

Submission Browser

Submissions Dashboard

Submission ID	Parent Submission ID	Submission State	Priorit
1	0	Completed	
2	1	Completed	
3	2	Completed	
4	0	Acquisition Pending	
5	0	Completed	
6	5	Completed	
7	6	Completed	
8	0	Acquisition Pending	

Submission Dashboard - Status

Sample List - Status

Sample Lists View

Sample List Browser

Sample Lists Dashboard

group by area Drag a field here to group by that field

Submission ID	Sample List State	Sample List ID	Sample Completed Count	Samples Processed	Customer Natural Id	Samples Not Processed
1	Acquired	1	25 / 25			
2	Acquired	2	25 / 25			
3	Acquired	3	21 / 21			
4	Unknown	4	0 / 25			
5	Acquired	5	25 / 25			
6	Acquired	6	27 / 27			
7	Acquired	7	23 / 23			
4	Pending Acquisition	8	0 / 25			

Sample- Status

Samples Submission Artifacts

Submission Id	Sample List Id	Analytical Sample Id	Express Sample Id	Workflow Stage	Sample Id	State
5	5	97	339	PreQC		Processed
5	5	98	337	PreQC		Processed
5	5	99	334	PreQC		Processed
5	5	100	335	PreQC		Processed
5	5	101	341	PreQC		Processed
5	5	102	340	PreQC		Processed
5	5	103	338	PreQC		Processed
5	5	104	336	PreQC		Processed
5	5	105	343	PreQC		Processed
5	5	106	348	PreQC		Processed
5	5	107	347	PreQC		Processed
5	5	108	342	PreQC		Processed
5	5	109	344	PreQC		Processed
5	5	110	346	PreQC		Processed
5	5	111	349	PreQC		Processed

Status – Accessible via the API

Closing the Loop – Aggregated Report Via API→ ELN

Reporting

Crude Screening Results

Prep Fraction Results

Fraction QC &/OR FinalQC Results

Version 1.0

- Sample Results
- Chromatographic Peak Results
- Chromatogram Images
- Expressions
- Fractions

Version xx

- ++ Spectrum Results
- ++ Spectrum Images
- ++ Graphed Results
- ++ Graphed Images

Notifications

Supported Topics

- Submission Created
- Artifact Uploaded
- Artifacts Uploaded (Filter available)
- Batch Task Completed

Output/Subscribers

- Publish-Subscriber Pattern
- Client
- Email
- File Drop

The Problem...

How do we produce standardized output that can be taken by a consumer, from various instruments in an automated fashion?

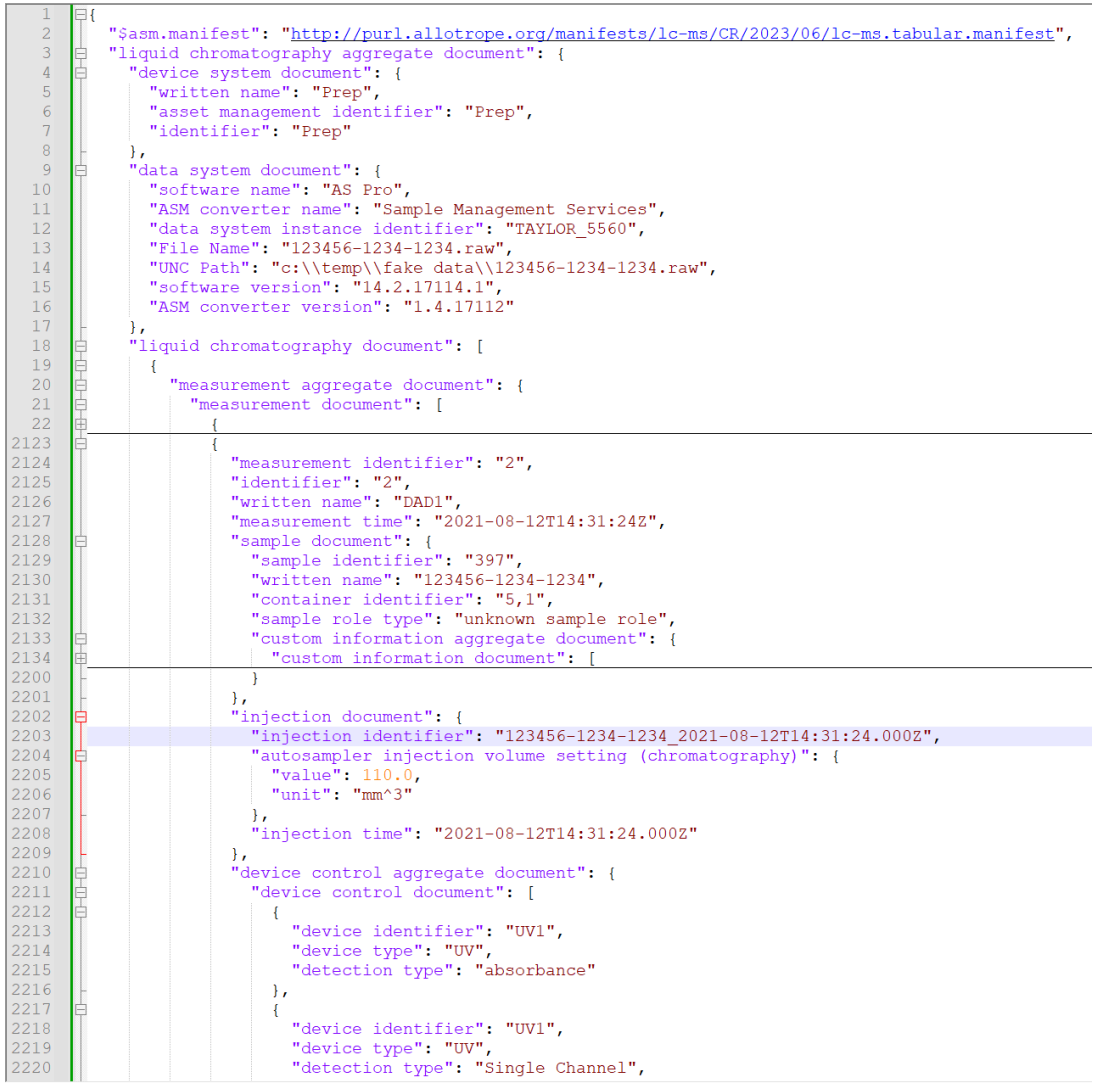
“The Allotrope Simple Model (ASM) is a JavaScript Object Notation (JSON)-based standard for the structure of instrument data. Through its use of JSON, the de facto standard by which computers on the internet share data, the data in an ASM is designed to be easy to read, write, and transmit by any modern software system. “ - https://www.allotrope.org/asm

The Solution…

Through our software suite we can take raw data from an instrument to produce analytical results and through SMS can transform it into the ASM which is then output to a subscriber to be consumed…

1. Working with the allotrope guidelines and the allotrope members we created the data model internally that is version controlled.
2. We needed to match our analytical results within the standardized definitions of the ASM.
3. Then we created a mechanism that allows users to define the settings needed to output the ASM JSON.
4. Through our suite of software once the raw data is captured, we create results and publish them through SMS which can produce the ASM automatically as a notification for use by consumers.

Information Rich Generic Output– Allotrope ASM JSON




```
{
  "$asm.manifest": "http://purl.allotrope.org/manifests/lc-ms/CR/2023/06/lc-ms.tabular.manifest",
  "liquid chromatography aggregate document": {
    "device system document": {
      "written name": "Prep",
      "asset management identifier": "Prep",
      "identifier": "Prep"
    },
    "data system document": {
      "software name": "AS Pro",
      "ASM converter name": "Sample Management Services",
      "data system instance identifier": "TAYLOR_5560",
      "File Name": "123456-1234-1234.raw",
      "UNC Path": "c:\\temp\\fake data\\123456-1234-1234.raw",
      "software version": "14.2.17114.1",
      "ASM converter version": "1.4.17112"
    },
    "liquid chromatography document": [
      {
        "measurement aggregate document": {
          "measurement document": [
            {
            {
              "measurement identifier": "2",
              "identifier": "2",
              "written name": "DAD1",
              "measurement time": "2021-08-12T14:31:24Z",
              "sample document": {
                "sample identifier": "397",
                "written name": "123456-1234-1234",
                "container identifier": "5,1",
                "sample role type": "unknown sample role",
                "custom information aggregate document": {
                  "custom information document": [
                }
              },
              "injection document": {
                "injection identifier": "123456-1234-1234_2021-08-12T14:31:24.000Z",
                "autosampler injection volume setting (chromatography)": {
                  "value": 110.0,
                  "unit": "mm^3"
                },
                "injection time": "2021-08-12T14:31:24.000Z"
              },
              "device control aggregate document": {
                "device control document": [
                  {
                    "device identifier": "UV1",
                    "device type": "UV",
                    "detection type": "absorbance"
                  },
                  {
                    "device identifier": "UV1",
                    "device type": "UV",
                    "detection type": "Single Channel",
```


Allotrope JSON output

- Backwards compatibility generic format

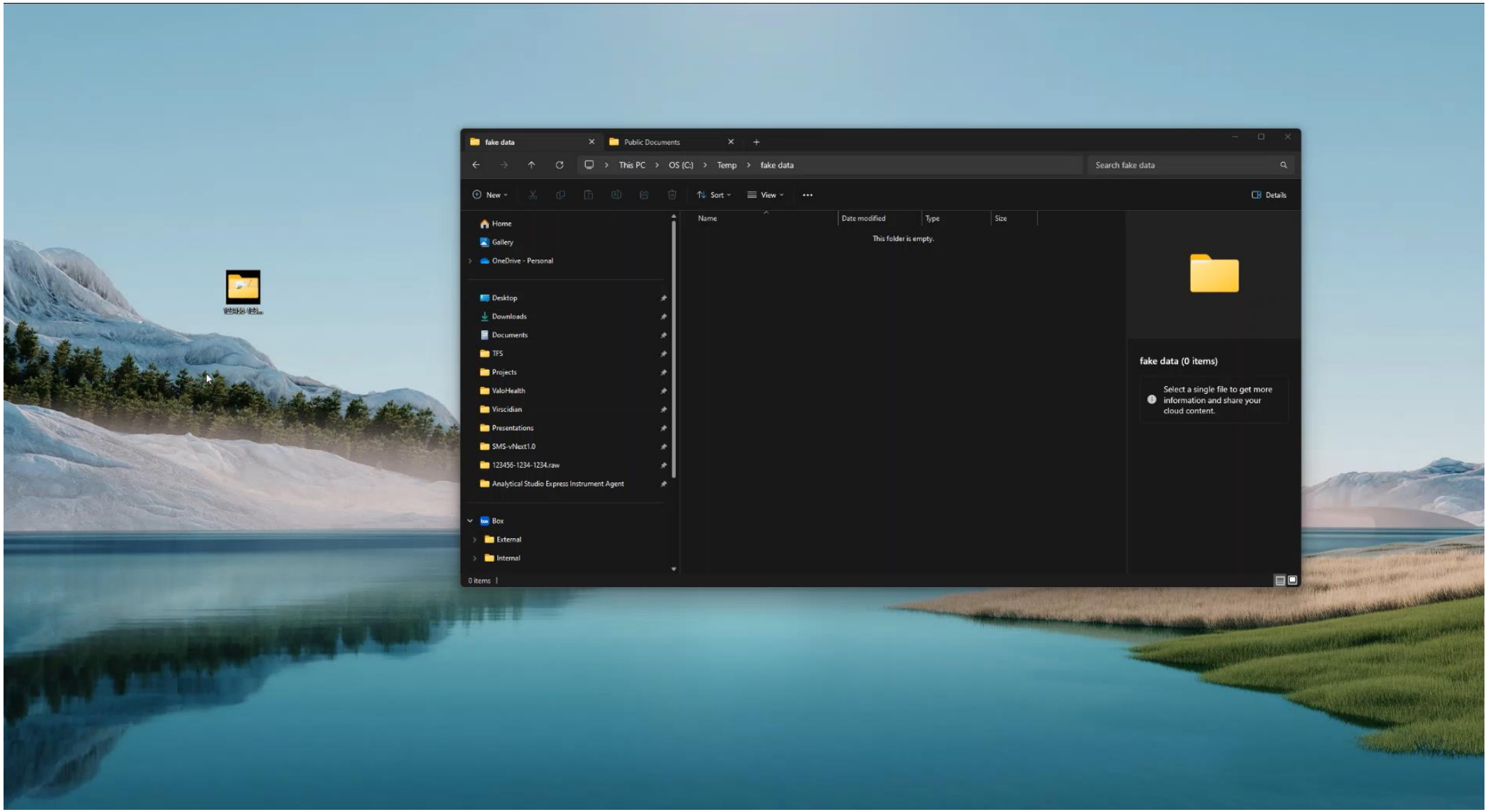
Rich extensible metadata

- Sample metadata
- Result metadata
- Processing metadata
- Substance metadata
- Expressions metadata
- Chromatogram x,y values
- Spectrum x,y values

To be added

- Fraction/dissolution/Replating results metadata
- Focused Gradient Metadata

Demo



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Challenges

1. Modeling and producing a valid ASM based on updating schemas.
2. Matching definitions to Allotrope. Raw data from instrument > Processing > ASM output.

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Thank you!

Get in touch:

Info@virscidian.com
Virscidian.com