



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...




Achiral Purification
Multi-stage purification of achiral molecules with method selection, decision making and sample list output at each step.




Chiral Purification
Automated method selection and comparison based on tunable criteria




ASMS
High-throughput analysis of drug candidate binding to a biological target.



Synthesis Design
Web-based Experiment Builder tool for design/layout of synthetic screens.




Compound QC
High-throughput quality control of compound libraries with automated commenting and decision making.



HTE
Automated data analysis; identification of all reaction components; automated calculated of conversion



Instrument Suitability
Monitoring of instrument performance; alerts for failures and trending out-of-spec

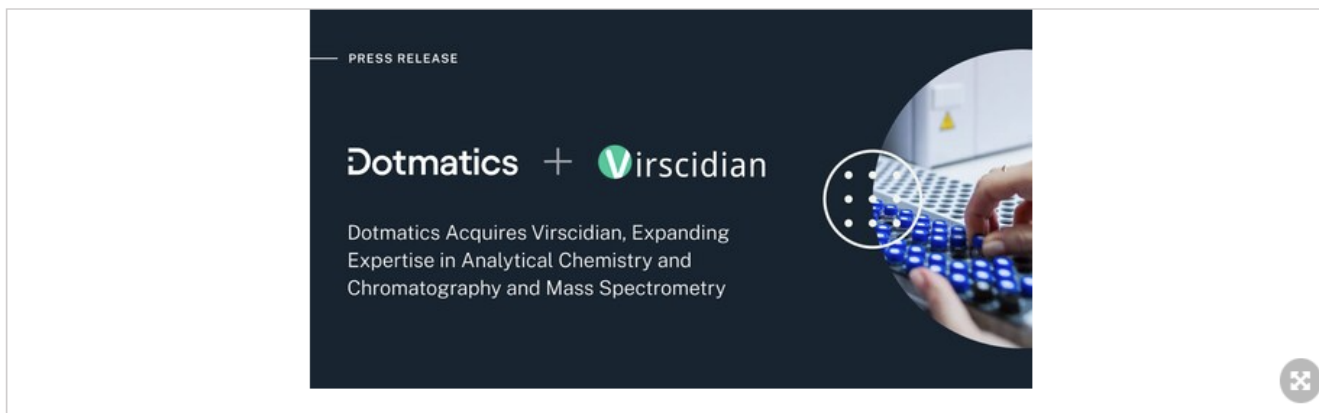


Quantitative
Calibration curves and quantification of samples. Includes CAD, ELSD, solubility and LogD workflows.

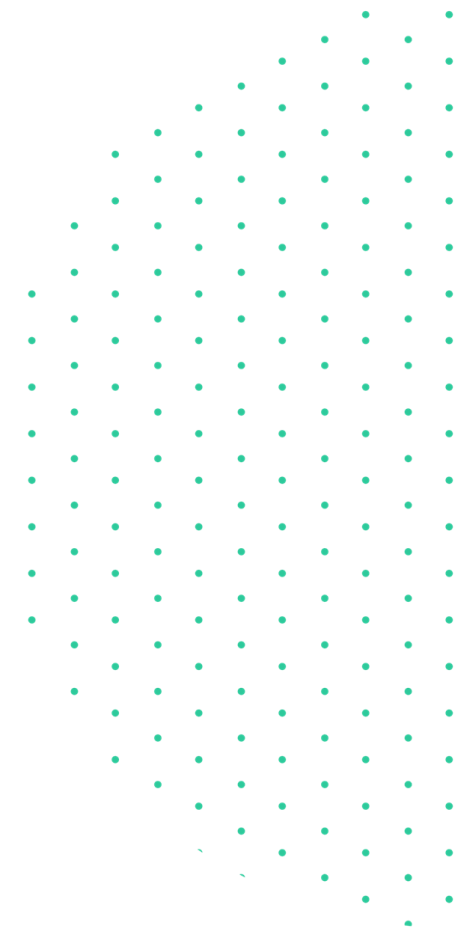
Dotmatics Acquires Virscidian, Expanding Expertise in Analytical Chemistry and Chromatography and Mass Spectrometry

NEWS PROVIDED BY
Dotmatics Inc →
Sep 25, 2024, 06:45 ET

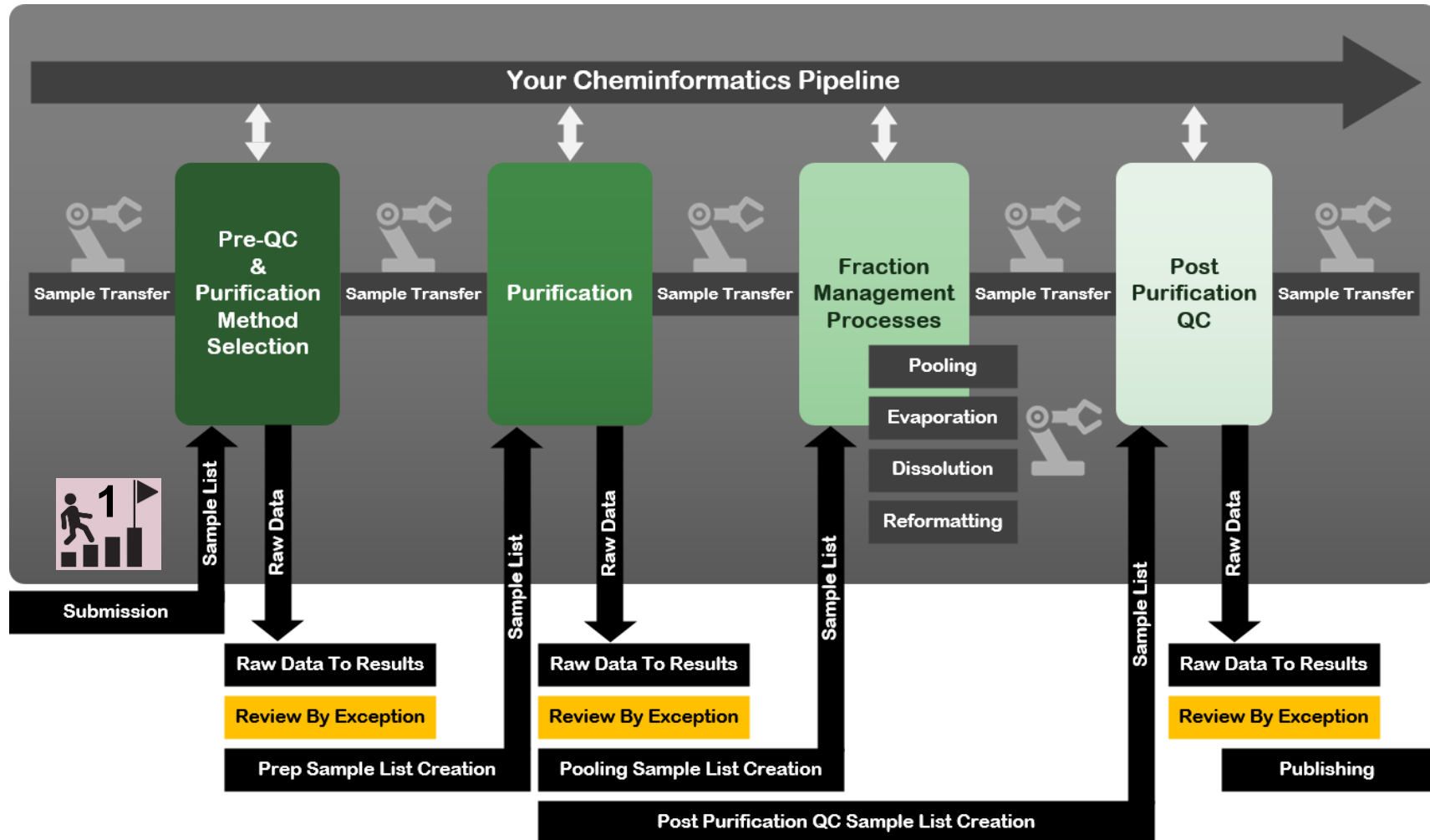
SHARE THIS ARTICLE



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

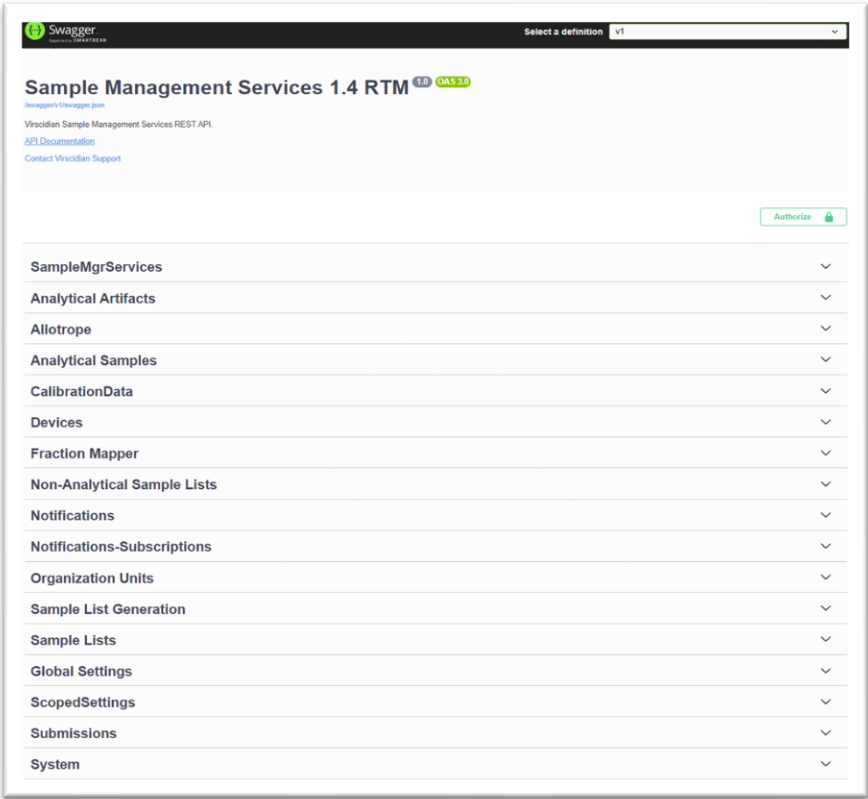


Where are the short-term challenges to solve?



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

Electronic Submissions – Sample Management APIs



New API Integration



```
"Submission": {
  "Version": "1.0.0.0",
  "Schema": "Virscidian Experiment Schema V2.json",
  "Override": true,
  "SubmissionInfo": {
    "ParentSubmissionId": null,
    "CustomerNaturalId": "P-123456789",
    "OrgUnitName": "HTP-LAB1",
    "Project": "MicroScale HTP",
    "WorkflowName": null,
    "WorkflowStage": "Crude-QC",
    "Comments": null,
    "SubmittedBy": "John Doe",
    "CreatedBy": "ELN",
    "SubmissionAttributes": [
      {
        "Name": "TotalCrudeScale",
        "Value": null,
        "DataType": "Float",
        "Units": "mg"
      },
      {
        "Name": "Volume",
        "Value": "70.0",
        "DataType": "Float",
        "Units": "uL"
      },
      {
        "Name": "AssayConcentration",
        "Value": "1.0",
        "DataType": "Float",
        "Units": "mM"
      },
      {
        "Name": "Modality",
        "Value": null
      },
      {
        "Name": "HighestHazardClass",
        "Value": null,
        "DataType": "Integer"
      }
    ]
  },
  "ExternalControls": [],
  "Containers": [
    {
      "SequenceId": "1",
      "Type": "Plate",
      "Samples": [
        {
          "SampleId": "000-12345-789",
          "Location": "A_01",
          "CompoundType": "Sample",
          "SampleAttributes": {
```

Electronic Submissions in JSON format

Third party - On demand sample list generation

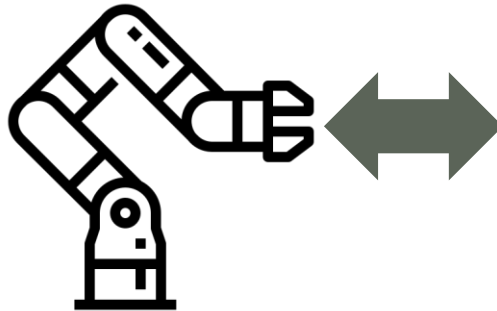
How to put the configuration of what goes into a sample list in the hands of the scientists AND continue to optimize complex automated robotics workflows without software redevelopment?

Biosero GBG™

- Multiple projects delivered / In progress

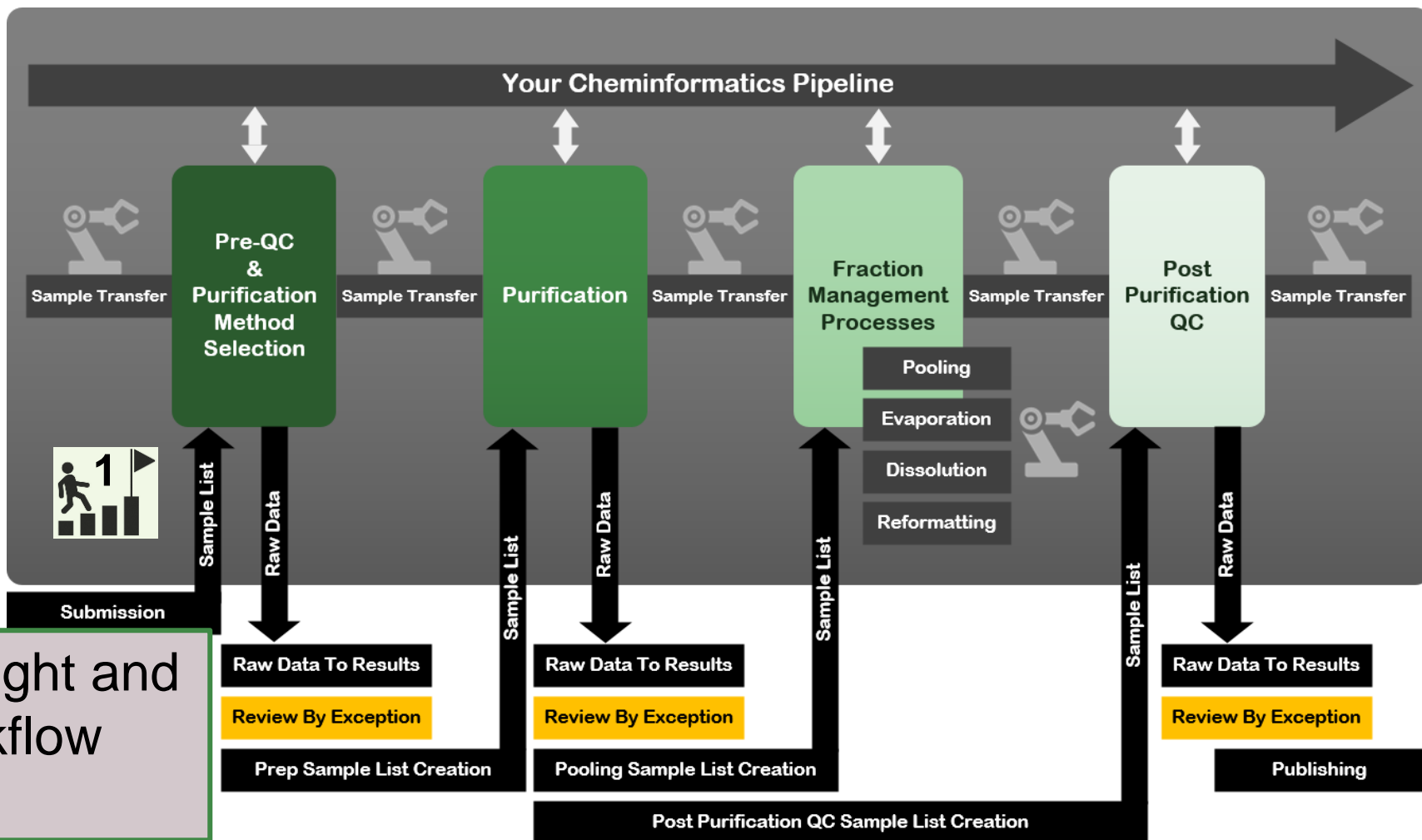
HighRes BioSolutions™

- Multiple projects in progress

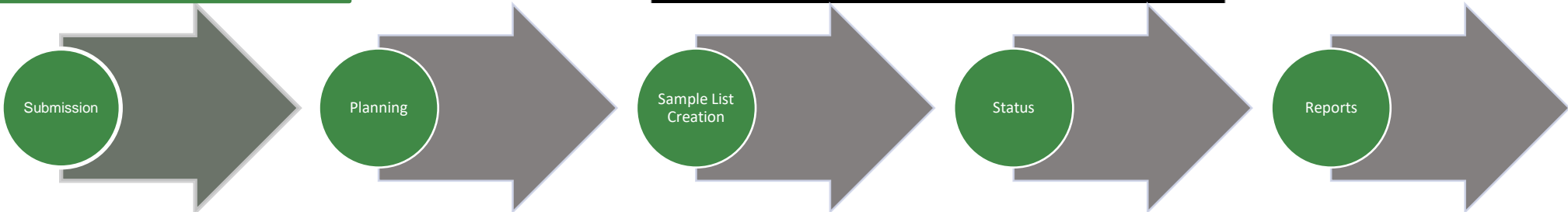


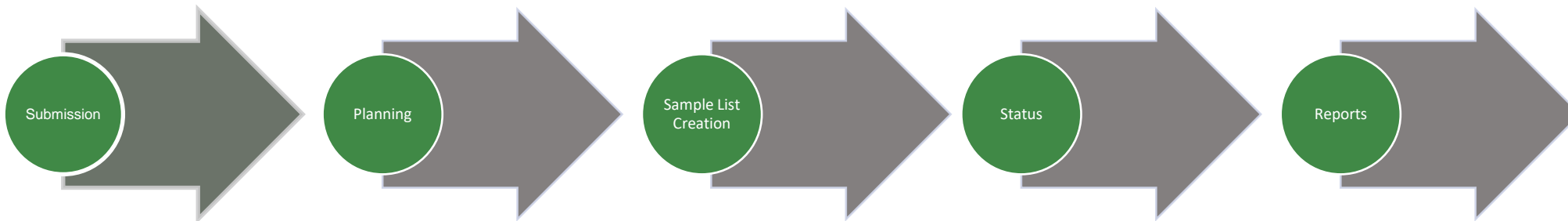
A screenshot of the Swagger API documentation interface. At the top, it says "Swagger" and "Select a definition v1". The main title is "Sample Management Services 1.4 RTM" with a "1.0 OAS 3.0" badge. Below the title, there are links for "API Documentation" and "Contact Virscidian Support". An "Authorize" button is visible on the right. A list of API endpoints is shown on the left, including "SampleMgrServices", "Analytical Artifacts", "Allotrope", "Analytical Samples", "CalibrationData", "Devices", "Fraction Mapper", "Non-Analytical Sample Lists", "Notifications", "Notifications-Subscriptions", "Organization Units", "Sample List Generation", "Sample Lists", "Global Settings", "ScopedSettings", "Submissions", and "System". A blue callout box highlights the "Sample List Generation" endpoint with the text "+ Sample List Builder for Template Configuration".

Where are the short-term challenges to solve?



Lack of oversight and stepwise workflow execution





Analytical Studio - Sample List

Planning

Submissions Dashboard

Submission ID	Parent Submission ID	Submission State	Priority	Project	Workflow Name	Workflow Stage Alias	Needed By	Submitted By	Created By	Last Updated By	Created Time
1		0 Completed		0 Project-Test	Normal Scale	CrudeQC		Mark B	Dotmatics	Composite Workflow	3/23/2023 1:47
2		1 Completed		0 Project-Test	Normal Scale	Prep		Mark B	Virscidian	Composite Workflow	3/23/2023 1:48
3		2 Completed		0 Project-Test	Normal Scale	FinalQC		Mark B	Virscidian	Composite Workflow	3/23/2023 1:49
4		0 Acquisition Pending		0 Project-Test	Normal Scale	CrudeQC		Mark B	Dotmatics	MARK-DESKTOP	3/27/2023 5:14
5		0 Completed		0 Project-Test	Normal Scale	CrudeQC		Mark B	Dotmatics	Composite Workflow	3/27/2023 5:25
6		5 Completed		0 Project-Test	Normal Scale	Prep		Mark B	Virscidian	Composite Workflow	3/27/2023 5:26
7		6 Completed		0 Project-Test	Normal Scale	FinalQC		Mark B	Virscidian	Composite Workflow	3/27/2023 5:27
8		0 Acquisition Pending		0	Solubility	Other		testadmin	Dotmatics	MARK-DESKTOP	4/5/2023 8:38

Reporting

Lineage

Execution

Create Sample List Wizard

Instrument Vendor	Instrument Name	Created Time	Last Updated Time	Sample List ID	File Name	Display Name	Sample Completed Count	Samples Processed	Samples Not Processed	Artifacts Count	Customer Natural Id	Project	Created By	Last Update
MasslynxDirect		3/23/2023 1:49 PM	4/1/2023 10:29 AM	3				0	0	0		MARK-DESKTOP	EPA.MARK-DES	

Execution

Sample List Dashboard

Submission ID	State	Sample List ID	Completed Count	Samples Processed	Customer Natural Id	Not Processed	Created Time
1	Acquired		1 25 / 25	25			0 3/23/2023 1:47 PM
2	Acquired		2 25 / 25	25			0 3/23/2023 1:48 PM
3	Acquired		3 21 / 21	21			0 3/23/2023 1:49 PM
4	Unknown		4 0 / 25	0		25	3/27/2023 5:15 PM
5	Acquired		5 25 / 25	25			0 3/27/2023 5:26 PM
6	Acquired		6 27 / 27	27			0 3/27/2023 5:27 PM
7	Acquired		7 23 / 23	23			0 3/27/2023 5:27 PM
4	Pending Acquisition		8 0 / 25	0		25	4/3/2023 6:31 PM

Execution

Submission Information

Property	Value
Created By	Dotmatics
Created Time	3/27/2023 5:25:45 PM
Customer Natural Id	Library 5-1
Last Updated By	Composite Workflow
Last Updated Time	3/29/2023 11:53:12 AM
Needed By	
Parent Submission Id	0
Priority	0
Project	Project-Test
State	Completed
State Raw	Completed
Submission Id	5
Submitted By	Mark B
Workflow Name	Normal Scale
Workflow Stage	PreQC
Workflow Stage Alias	CrudeQC

Sample List Creation Wizard - Execution

Sample List Wizard

Template Selection | Sample Selection | Container Position | Field Assignment | Runtime Parameters | Preview

Select Instrument and Sample List Template

Connected Instrument
Instrument Name: Crude-QC
Instrument Description: Crude-QC
Instrument Type: MasslynxDirect
 Do Not Filter By Instrument

Choose Template

Use	Instrument 1	Instrument 2
<input checked="" type="radio"/>	Instrument1	MasslynxDirect

Sample List Wizard

Template Selection | Sample Selection | Container Position | Field Assignment | Runtime Parameters | Preview

Select Samples to Include in Sample List

Include	Container Sequence ID	Container
<input checked="" type="checkbox"/>	1	No

Sample List Wizard

Template Selection | Sample Selection | Container Position | Field Assignment | Runtime Parameters | Preview

Assign Container Instrument Position

Containers with Analytical Samples

Container Type	Sequence ID	Position
Plate	1	1

Containers with External Controls

Container Type	Sequence ID	Position
Vial	3	2
Vial	4	3
Vial	1-Wash	4
Vial	4-Calibration	4

Sample List Wizard

Template Selection | Sample Selection | Container Position | Field Assignment | Runtime Parameters | Preview

Assign Methods and Field Maps to Samples

Analytical Samples - Containers

Container Sequence ID	Type	Field Map
1	Plate	SampleMap

External Controls

Name	Container Sequence ID	Sample
BeforeBlank	1-Wash	Solve
AfterBlank	1-Wash	Solve
BeforeAcidWash	1-Wash	Acid
AfterAcidWash	1-Wash	Acid
ShutdownWash	1-Wash	Solve

Sample List Wizard

Template Selection | Sample Selection | Container Position | Field Assignment | Runtime Parameters | Preview

Enter Required Runtime Parameters

Source	Name	Value
Submission	Username	John D

Sample List Wizard

Template Selection | Sample Selection | Container Position | Field Assignment | Runtime Parameters | Preview

Preview and Generate Sample List

Display Name: PreQCJohn D\TE-LCMS-sampleset
Output Path: C:\msc\clan\SampleLists\Work\2023-04-24_12-20-16

Warning: Errors During Sample List Generation!

VERSION	FILE_NAME	FILE_TEXT	MS_FILE	MS_TUNE_FILE	INLET_FILE	INLET_PRERUN	INLET_POSTRUN	INLET
31.5		mg/ml						
31.5	blank_start_1_C	blank_start	2_5_min_scan_posneg		PreQC_Acidic			
31.5	blank_start_2_C	blank_start	2_5_min_scan_posneg		PreQC_Acidic			
31.5	blank_start_3_C	blank_start	2_5_min_scan_posneg		PreQC_Acidic			
31.5	Standard_Acid_1_C	Standard_Acid	2_5_min_scan_posneg		PreQC_Acidic			
31.5	Standard_Acid_2_C	Standard_Acid	2_5_min_scan_posneg		PreQC_Acidic			
31.5	Standard_Acid_3_C	Standard_Acid	2_5_min_scan_posneg		PreQC_Acidic			
31.5	Standard_Acid_4_C	Standard_Acid	2_5_min_scan_posneg		PreQC_Acidic			
31.5		mg/ml						
31.5	Calibration_Std_01-1	1.024 mg/ml	2_5_min_scan_posneg		PreQC_Acidic			
31.5	Calibration_Std_01-2	1.024 mg/ml	2_5_min_scan_posneg		PreQC_Acidic			
31.5	Calibration_Std_02-1	0.512 mg/ml	2_5_min_scan_posneg		PreQC_Acidic			
31.5	Calibration_Std_02-2	0.512 mg/ml	2_5_min_scan_posneg		PreQC_Acidic			
31.5	Calibration_Std_03-1	0.256 mg/ml	2_5_min_scan_posneg		PreQC_Acidic			
31.5	Calibration_Std_03-2	0.256 mg/ml	2_5_min_scan_posneg		PreQC_Acidic			

Hidden: Right-Click to show them

Active Status Information – Informing Project Teams

Oversight
Execution
Reporting

Sample List - Status

Sample- Status


Submission Dashboard - Status

Status – Accessible
via the API

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	

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			

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

Closing the Loop – Aggregated Report Via API → ELN

```
1 {
2   "AggregatedResults": {
3     {
4       "SampleId": "XXXXXXXXXX",
5       "WorkflowStages": [
6         {
7           "Name": "PreQC",
8           "Alias": null,
9           "SampleResults": [
10            {
11              "Artifacts": {
12                "SampleMetadata": {
13                  "Expression": {
14                    "Gradient": {
15                      "Fraction": {
16                        "Chromatogram": {
17                          "Substance": {
18                            "WorkflowStage": "PreQC",
19                            "SubmissionId": 4,
20                            "SampleId": "XXXXXXXXXX",
21                            "AnalyticalSampleId": 813,
22                            "CreatedTime": "2023-04-21T12:43:15.13"
23                          }
24                        }
25                      }
26                    }
27                  }
28                }
29              },
30              "WorkflowStage": "PreQC",
31              "SubmissionId": 4,
32              "SampleId": "XXXXXXXXXX",
33              "AnalyticalSampleId": 813,
34              "CreatedTime": "2023-04-21T12:43:15.13"
35            }
36          ],
37          "Name": "Prep",
38          "Alias": null,
39          "SampleResults": [
40            {
41              "Artifacts": {
42                "SampleMetadata": {
43                  "Expression": {
44                    "Gradient": {
45                      "Fraction": {
46                        "Chromatogram": {
47                          "Substance": {
48                            "WorkflowStage": "Prep",
49                            "SubmissionId": 5,
50                            "SampleId": "XXXXXXXXXX",
51                            "AnalyticalSampleId": 874,
52                            "ParentAnalyticalSampleId": 813,
53                            "CreatedTime": "2023-04-21T12:41:43.637"
54                          }
55                        }
56                      }
57                    }
58                  }
59                }
60              },
61              "WorkflowStage": "Prep",
62              "SubmissionId": 5,
63              "SampleId": "XXXXXXXXXX",
64              "AnalyticalSampleId": 874,
65              "ParentAnalyticalSampleId": 813,
66              "CreatedTime": "2023-04-21T12:41:43.637"
67            }
68          ],
69          "Name": "FractionQC",
70          "Alias": null,
71          "SampleResults": [
72            {
73              "WorkflowStage": "FractionQC",
74              "SubmissionId": 7,
75              "SampleId": "XXXXXXXXXX-02",
76              "AnalyticalSampleId": 904,
77              "ParentAnalyticalSampleId": 874
78            },
79            {
80              "WorkflowStage": "FractionQC",
81              "SubmissionId": 7,
82              "SampleId": "XXXXXXXXXX-03",
83              "AnalyticalSampleId": 905,
84              "ParentAnalyticalSampleId": 874
85            }
86          ]
87        }
88      ]
89    }
90  ]
91 }
92 }
```

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

```
1  {}
2  "Sasm.manifest": "http://purl.allotrope.org/manifests/lc-ms/CR/2023/06/lc-ms.tabular.manifest",
3  "liquid chromatography aggregate document": {
4    "device system document": {
5      "written name": "Prep",
6      "asset management identifier": "Prep",
7      "identifier": "Prep"
8    },
9    "data system document": {
10     "software name": "AS Pro",
11     "ASM converter name": "Sample Management Services",
12     "data system instance identifier": "TAYLOR_5560",
13     "File Name": "123456-1234-1234.raw",
14     "UNC Path": "c:\\temp\\fake data\\123456-1234-1234.raw",
15     "software version": "14.2.17114.1",
16     "ASM converter version": "1.4.17112"
17   },
18   "liquid chromatography document": [
19     {
20       "measurement aggregate document": {
21         "measurement document": [
22           {
2123          "measurement identifier": "2",
2124          "identifier": "2",
2125          "written name": "DAD1",
2126          "measurement time": "2021-08-12T14:31:24Z",
2127          "sample document": {
2128            "sample identifier": "397",
2129            "written name": "123456-1234-1234",
2130            "container identifier": "5,1",
2131            "sample role type": "unknown sample role",
2132            "custom information aggregate document": {
2133              "custom information document": [
2134                {
2200                }
2201              ]
2202            },
2203            "injection document": {
2204              "injection identifier": "123456-1234-1234_2021-08-12T14:31:24.000Z",
2205              "autosampler injection volume setting (chromatography)": {
2206                "value": 110.0,
2207                "unit": "mm^3"
2208              },
2209              "injection time": "2021-08-12T14:31:24.000Z"
2210            },
2211            "device control aggregate document": {
2212              "device control document": [
2213                {
2214                  "device identifier": "UV1",
2215                  "device type": "UV",
2216                  "detection type": "absorbance"
2217                },
2218                {
2219                  "device identifier": "UV1",
2220                  "device type": "UV",
2221                  "detection type": "Single Channel",
```

Allotrope JSON output

- Backwards compatibility generic format

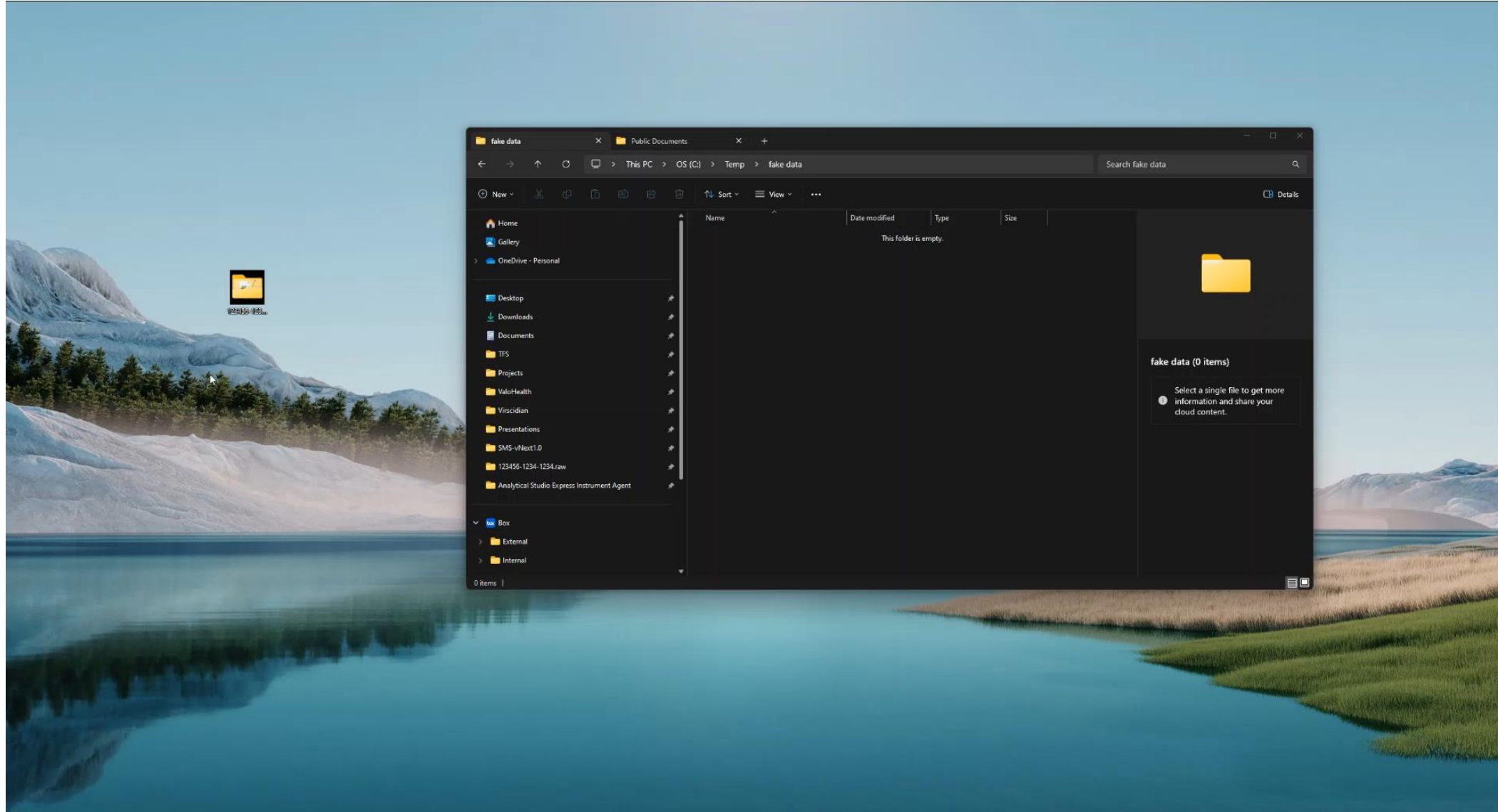
Rich extensible metadata

- 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



Challenges

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



Dotmatics

Virscidian

Thank you!

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