



Allotrope[®] Technology Implementation Update

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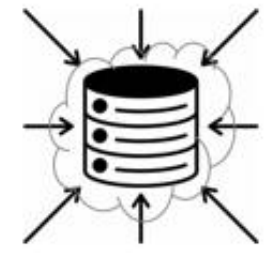
Instrument Data (Re)use Problem Statement

Experiment & measurement data are heterogeneous and not well connected

- Creates tremendous friction executing E2E workflows (capture to consumption)
- Limits (re)use of data, which limit value created from key asset
- Heterogeneity leads to friction, which slows science



Reusable capabilities to be addressed in various E2E workflows



Data Movement and Storage
Instrument to Cloud



Data Standardization
Consistent representation

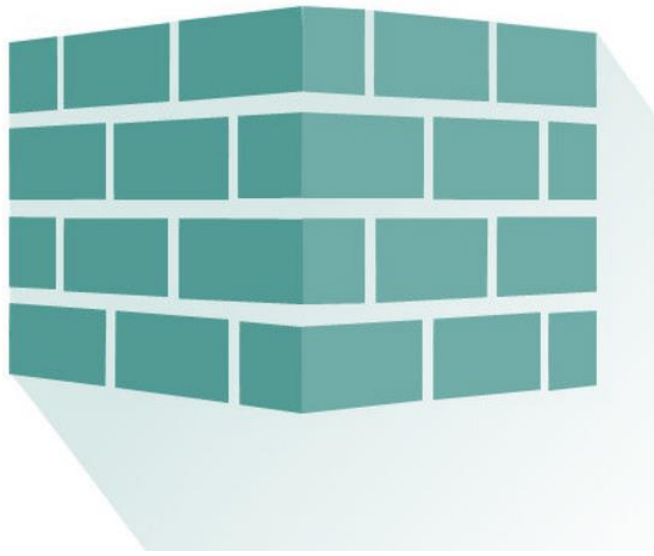


Data Consumption
Simpler to use

Instrument Data Standardization via ASM is viewed as a foundational capability required to achieve many digital goals

Provide frictionless flow of data from instruments to insights through modern foundational data platforms and provide a great user experience

Instrument data capture



High quality, accessible data

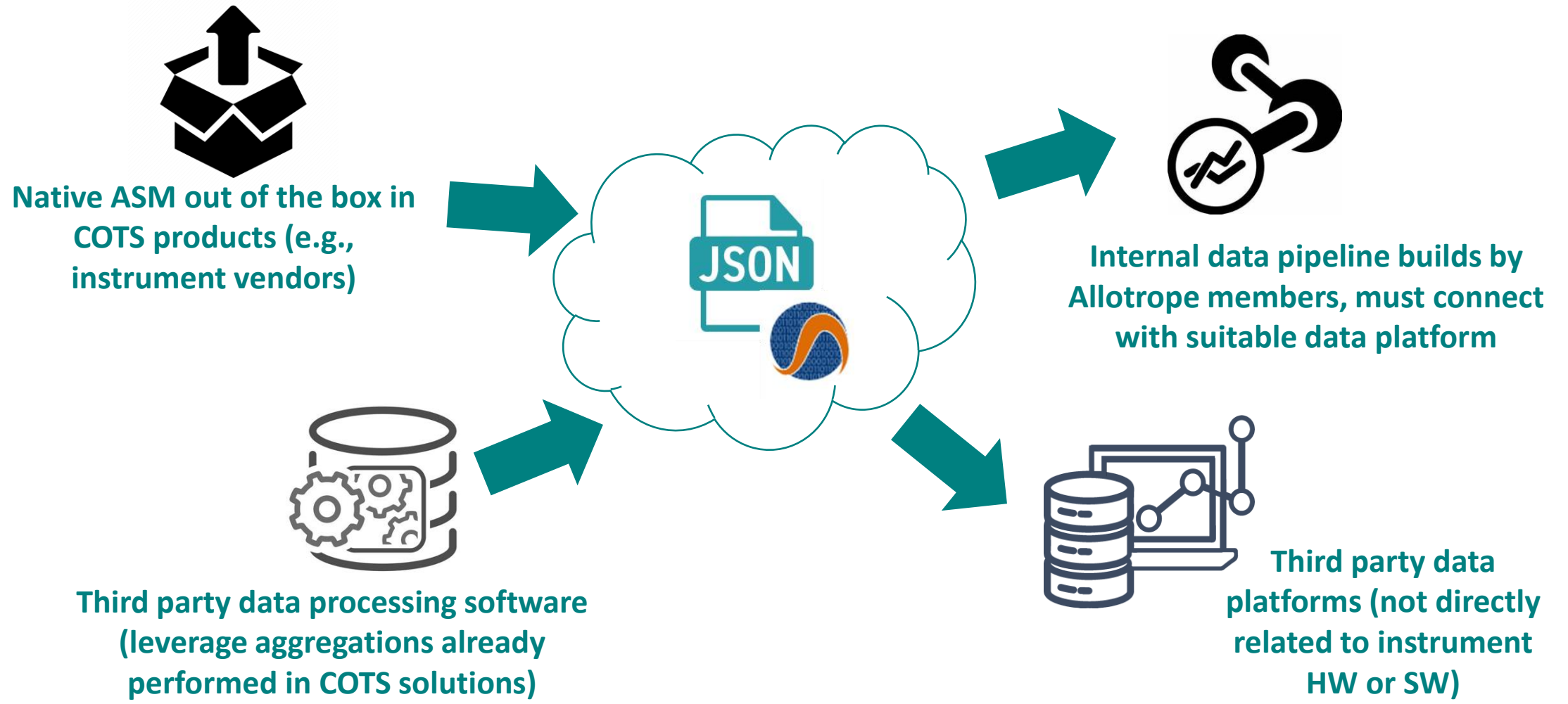


Highly reusable data



ASM = Allotrope® Simple Model

Landscape is evolving with multiple paths to ASM production



Extract, Transform, Move, Store, & Analyze

Evolution of needs during the Allotrope[®] journey

Multiple Personas



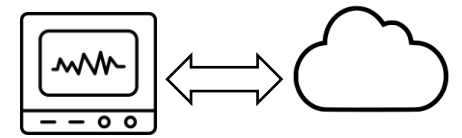
- **Laboratory Personnel:** Data producers and first line data consumers
- Need simple and on demand tools that are ready to use



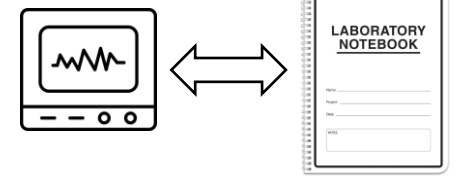
Data Scientists:

- Data consumers doing modeling and workflow development
- Need easy and rapid access to cloud data endpoints

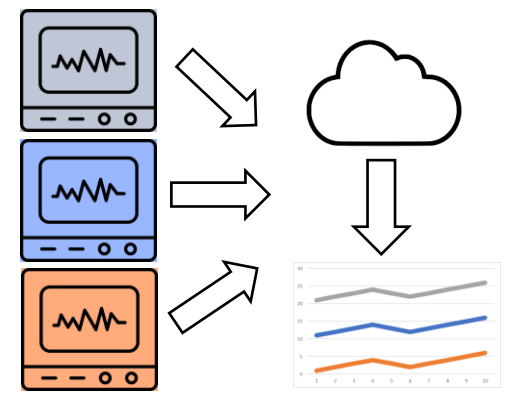
Use Cases



On demand search with consistent controlled terms



Automated and efficient data sharing across key IT systems in a value stream



Simplified visualization, analysis, and data dashboarding within and across data sources

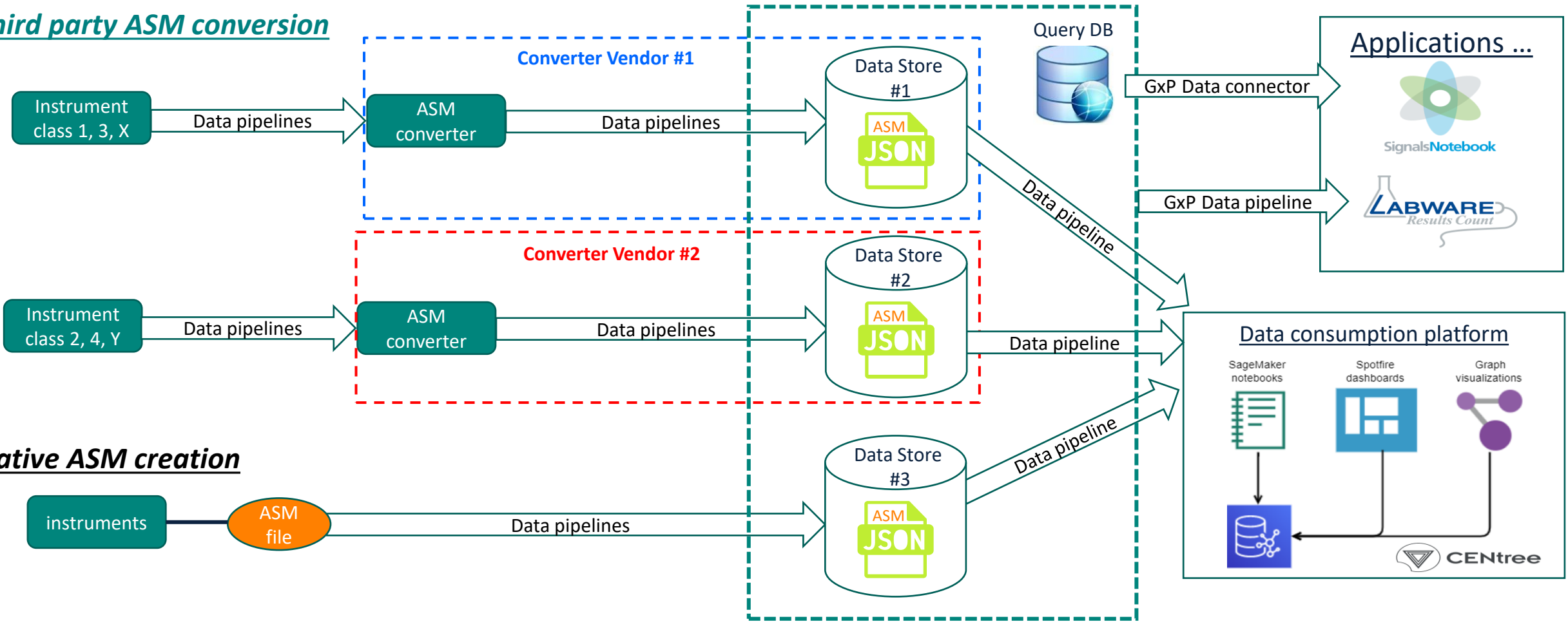
High Level Architecture Overview

Data Sources

Data Stores / Data Products

Sharing & Analytics

Third party ASM conversion



Note: Ability for a converter to be able to ingest native ASM files and/or of a data store platform to export files can reduce total # of data stores.

MSD accomplishments to date with ASM – May 2024

Infrastructure



*Expected to
be in place
by the end
of 2024*

ASM Conversion Pipelines

- Chromatography
 - Empower (implemented), AKTA = Unicorn (implemented), Chemstation (developed, implement by mid 2024), Chromeleon (developed)
- Plate readers
 - Envision (developed)
- Evaluating additional ASM conversion tools / platforms

Native ASM Output

- Virscidian (implemented for Agilent ChemStation, MassLynx, MassHunter)
- Mestranova (in-progress for Bruker, target end Q2 2024)
- Mettler Toledo (in discovery)

ASM Data Store (independent of data conversion tools)

- PoC in progress; solution to be implemented ~Q3 2024

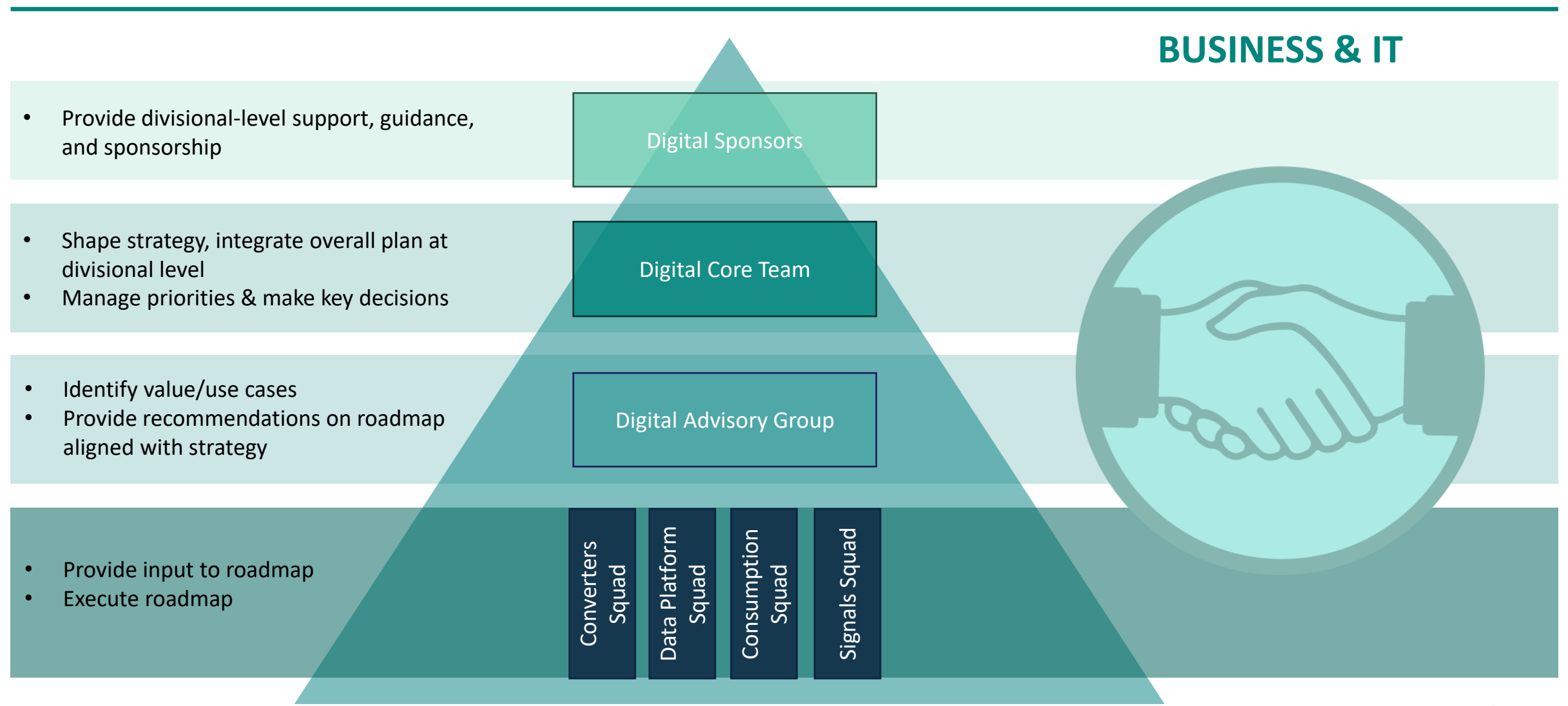
ASM Integration Capabilities

- PoC Integration of Signals to Empower with in house tool; in production in mid 2024

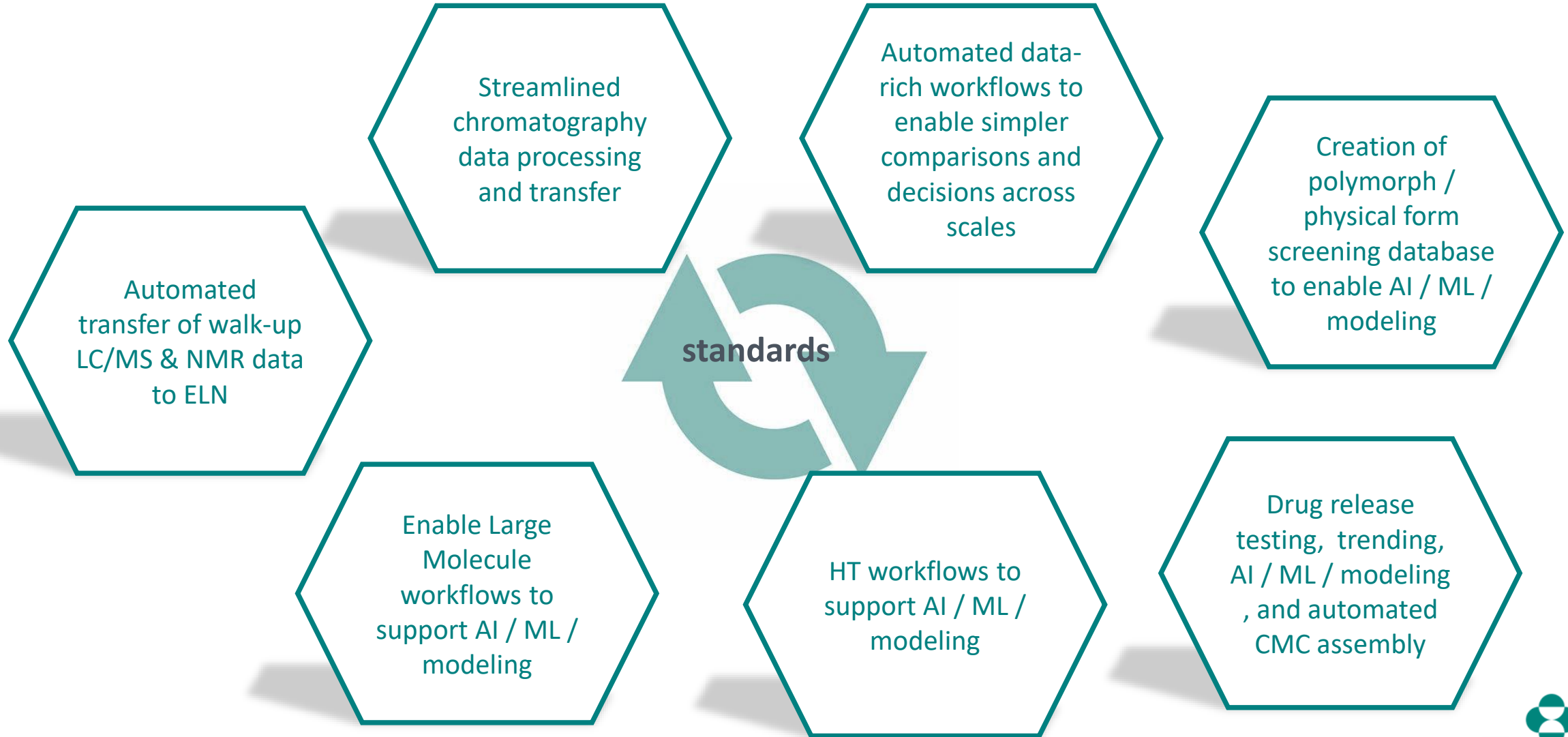
ASM Consumption Capabilities

- PoC AWS Neptune knowledge graph (implement in production in mid 2024)
- Spotfire visualization PoC for chromatography ASMs (implement in production in mid 2024)
- Data scientist AWS toolkit demonstrated (Jupyter NB interface, SPARQL queries, etc.)

Instrument data standardization (ASM) governance has now been established



Target Use Cases for ASM Enablement – The Road Ahead



Instrument classes in ASM required for these use cases

Instrument Classes (# vendors targeted in parentheses)	
Plate Readers & UV (7)	DSC (2)
Cell Counting (6)	TGA (2)
Filtration (4)	Particle Size Distribution (3)
Automated Reactors (3)	Scintillation Counters (1)
qPCR (2)	Surface Area Analysis (1)
Electrophoresis (4)	Spectroscopy (TBD)
Refractometer / Multi-Angle Light Scattering –MALS (1)	Titration (3)
XRPD (2)	

