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# The Empower CDS Allotrope Community Project

Community Presentation

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Justin VanDuine  
Vincent Chan

Principal Scientist  
Product Manager

[justin.vanduline@pfizer.com](mailto:justin.vanduline@pfizer.com)  
[vchan@tetrascience.com](mailto:vchan@tetrascience.com)



# Background



# Empower Community Project



- Since the beginning of Allotrope...
  - Top Priority: Chromatography Data...
- Empower Working Group
  - Formed in July 2016
  - Released RFP Q4 2017
  - What's a Community Project?
  - APN Selection / Interview / Paperwork
  - Funding: Initially 4 Companies... then 5... **6**... ← Tipping point funding/resources
- Today – 7 AF Member companies + TetraScience!



# Potential Use Cases Beyond Today...

- Why do we want a CDS ADF?
  - Downstream analytics/integration: Spotfire, ACD, etc...
  - Long-term archiving: No software/version dependences
  - CDS mix match... Empower to Chromeleon to Empower...
  - Method development: Use/reuse the data from 100+ runs
- Many things we haven't even imagined yet will be possible once we are able to access data freely
- Out of scope of this project



# Business Case for a Chromatography ADF

- Use case brainstorming at an Allotrope F2F
- As a scientist I need to be able to...
  - Identify user entered input parameters
  - Identify how the experiment was set up
  - Identify system captured metadata
  - Identify parameters (system and user entered)
  - Provide results
  - Identify what system parameters were used to run instrument



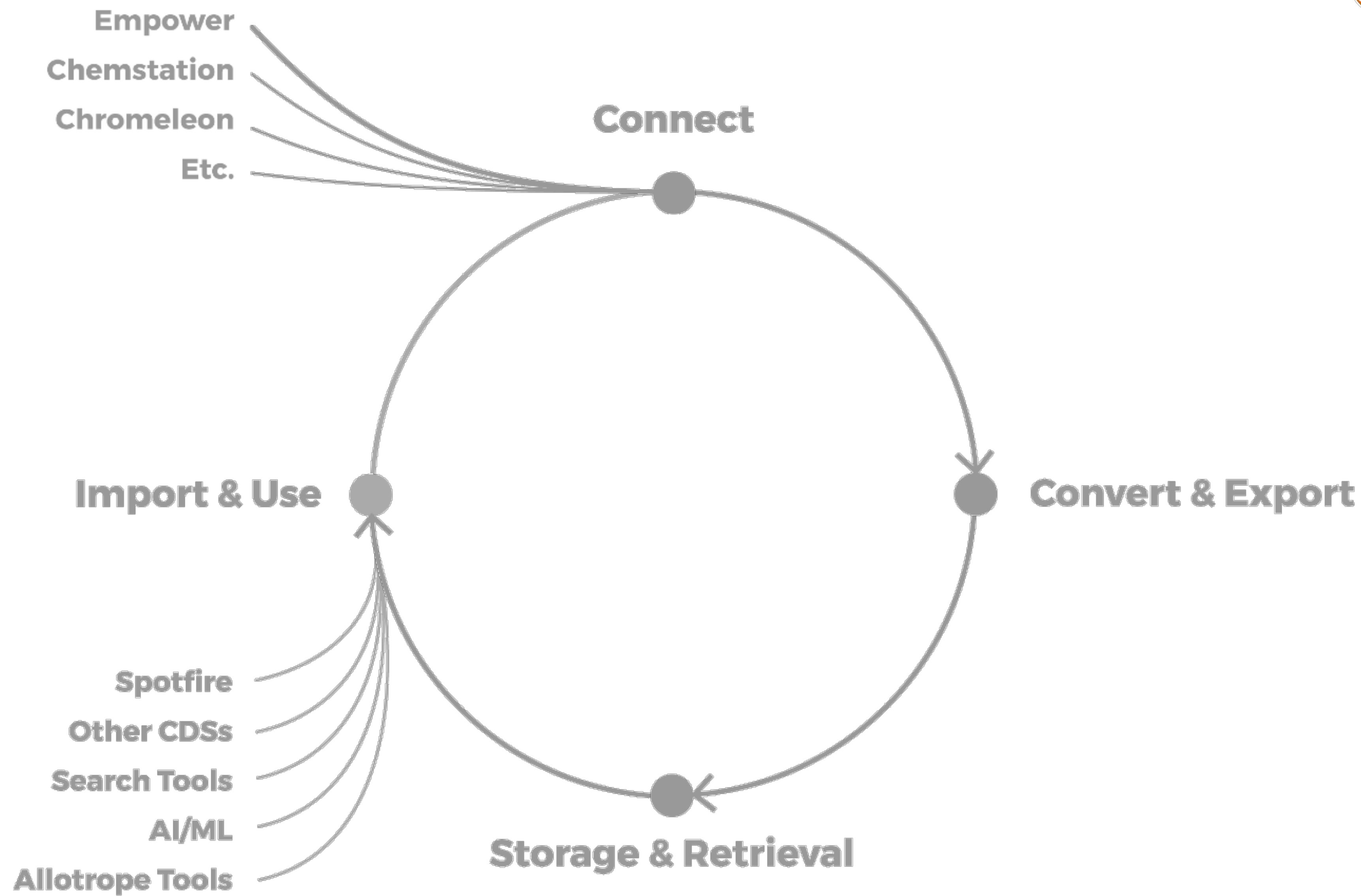
# Use Cases from 50K Feet

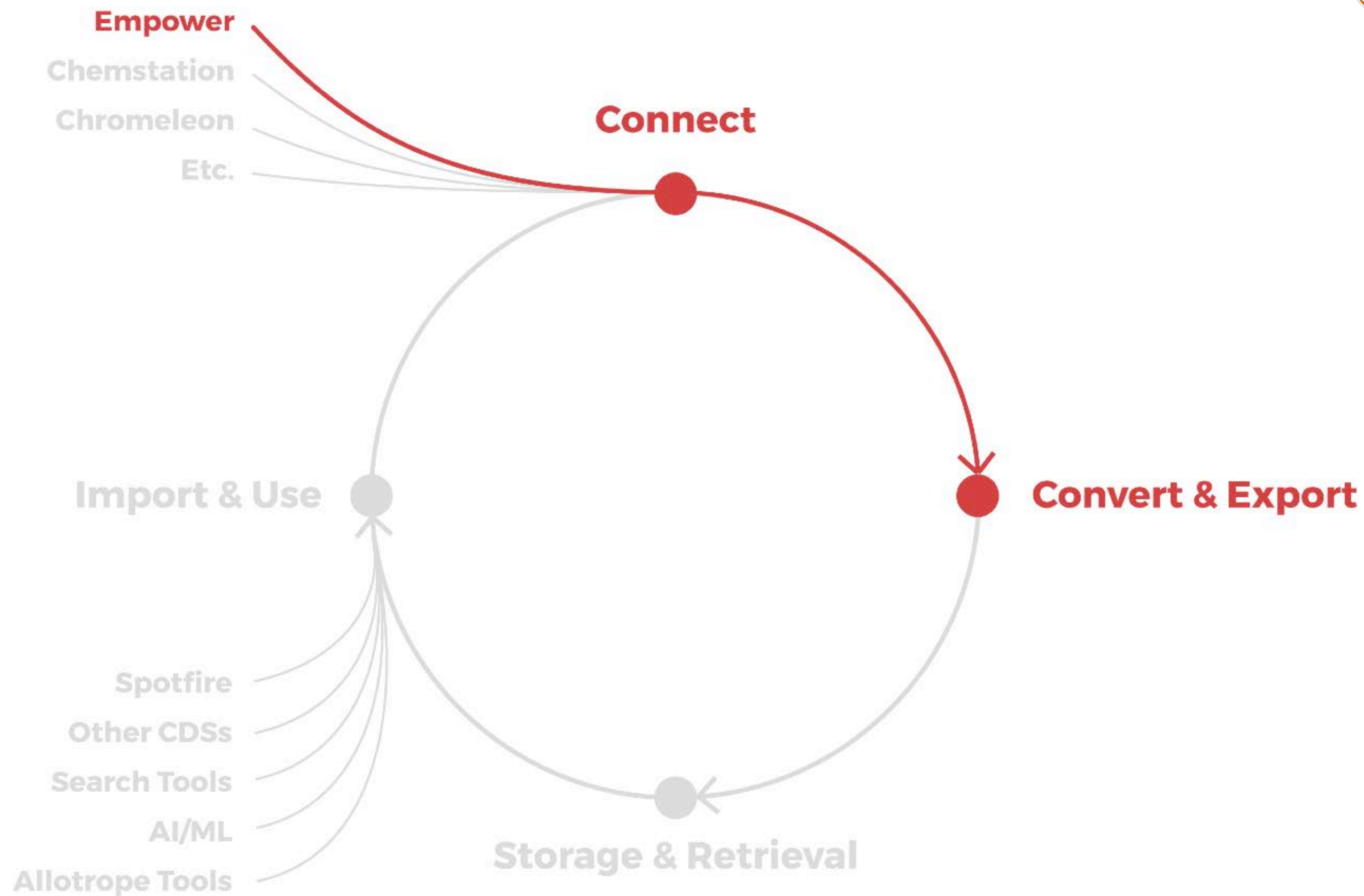
- **2 Broad Categories:** Routine Activities / Long Term Archive
  - Routine: Use cases from previous slide... the details
    - Business as usual how do I make my data available for further downstream activities
    - Support regulatory filing - Today
  - Archive:
    - Automation of legacy data conversion
    - Support regulatory filing – Tomorrow, emerging markets

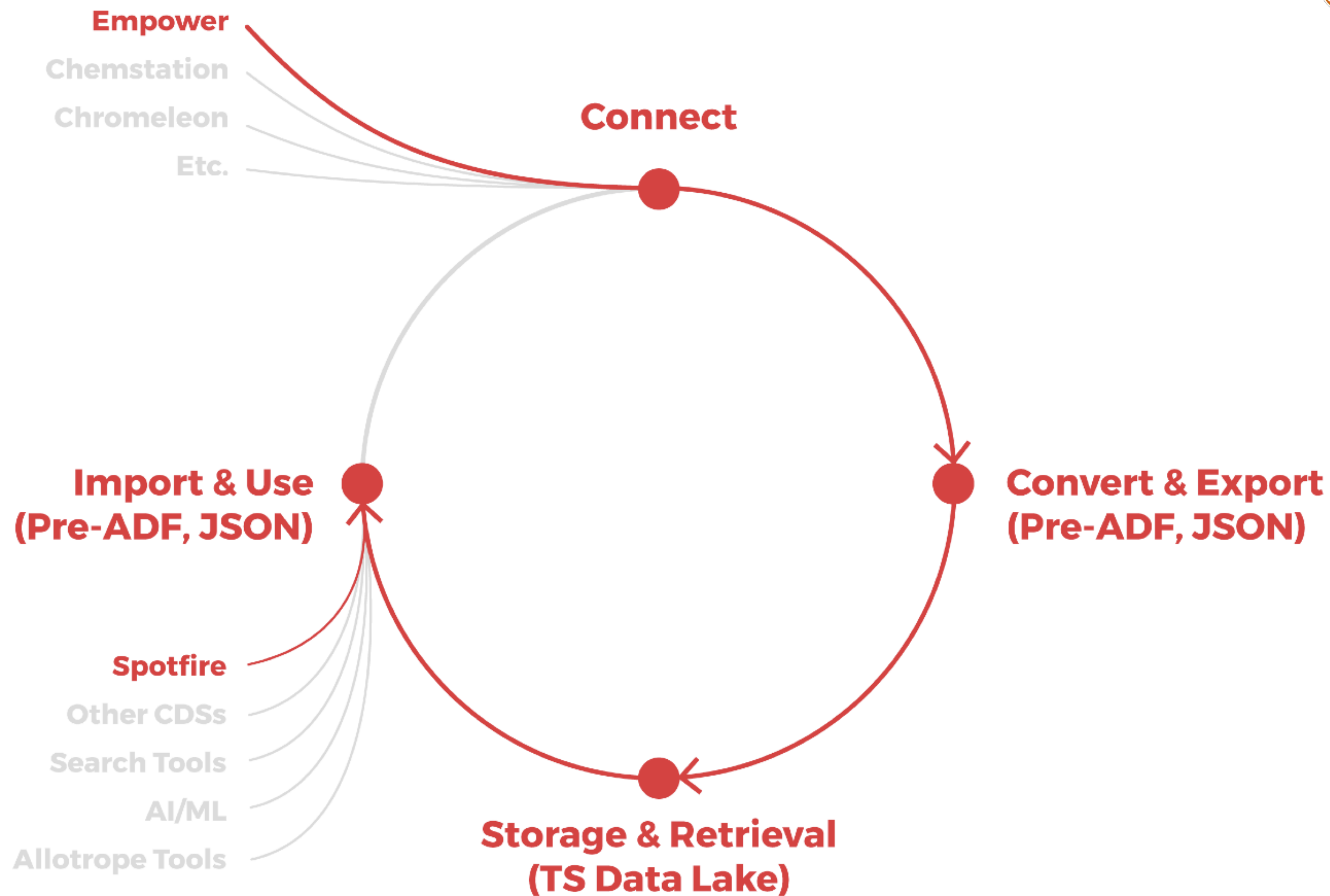


# **TetraScience**

## **The ADF Lifecycle for CDS's**





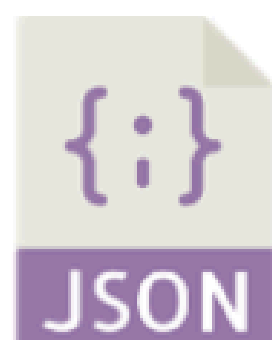
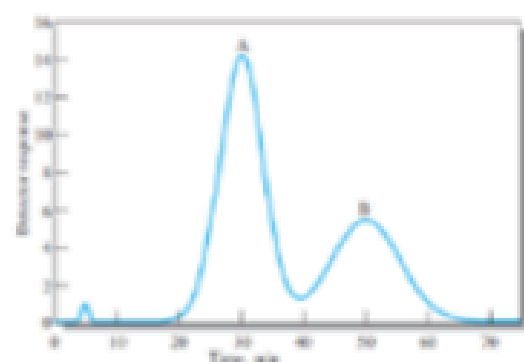




# The Pre-ADF

## PRE-ADF FILE

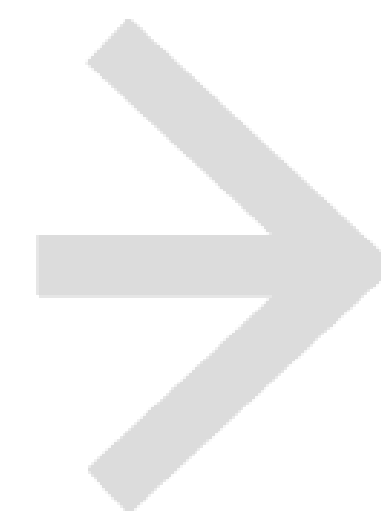
Modeled via  
JSON in the  
data package



**Data  
Description**

**Data Cube**

**Data Package**

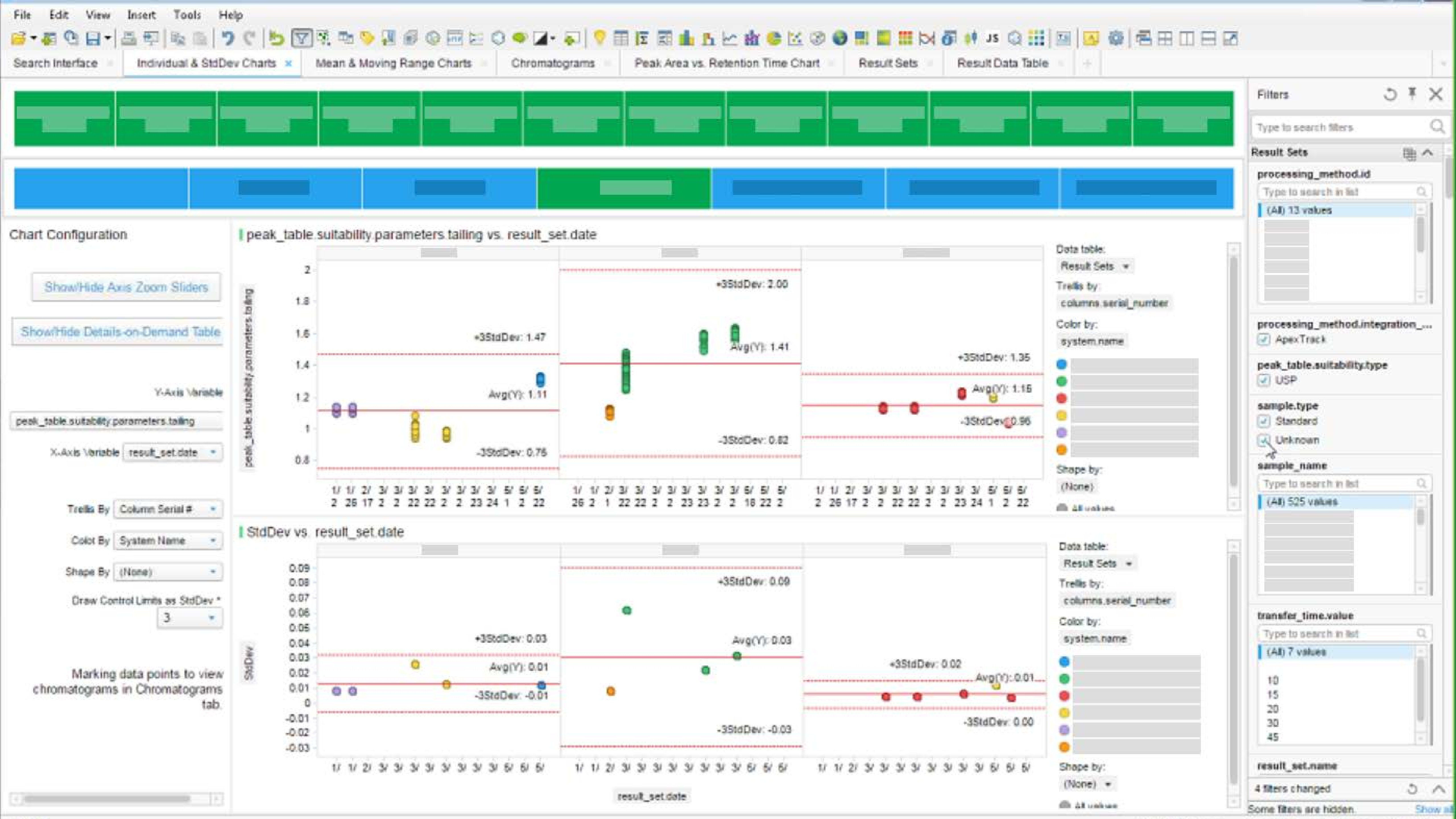


## ADF FILE

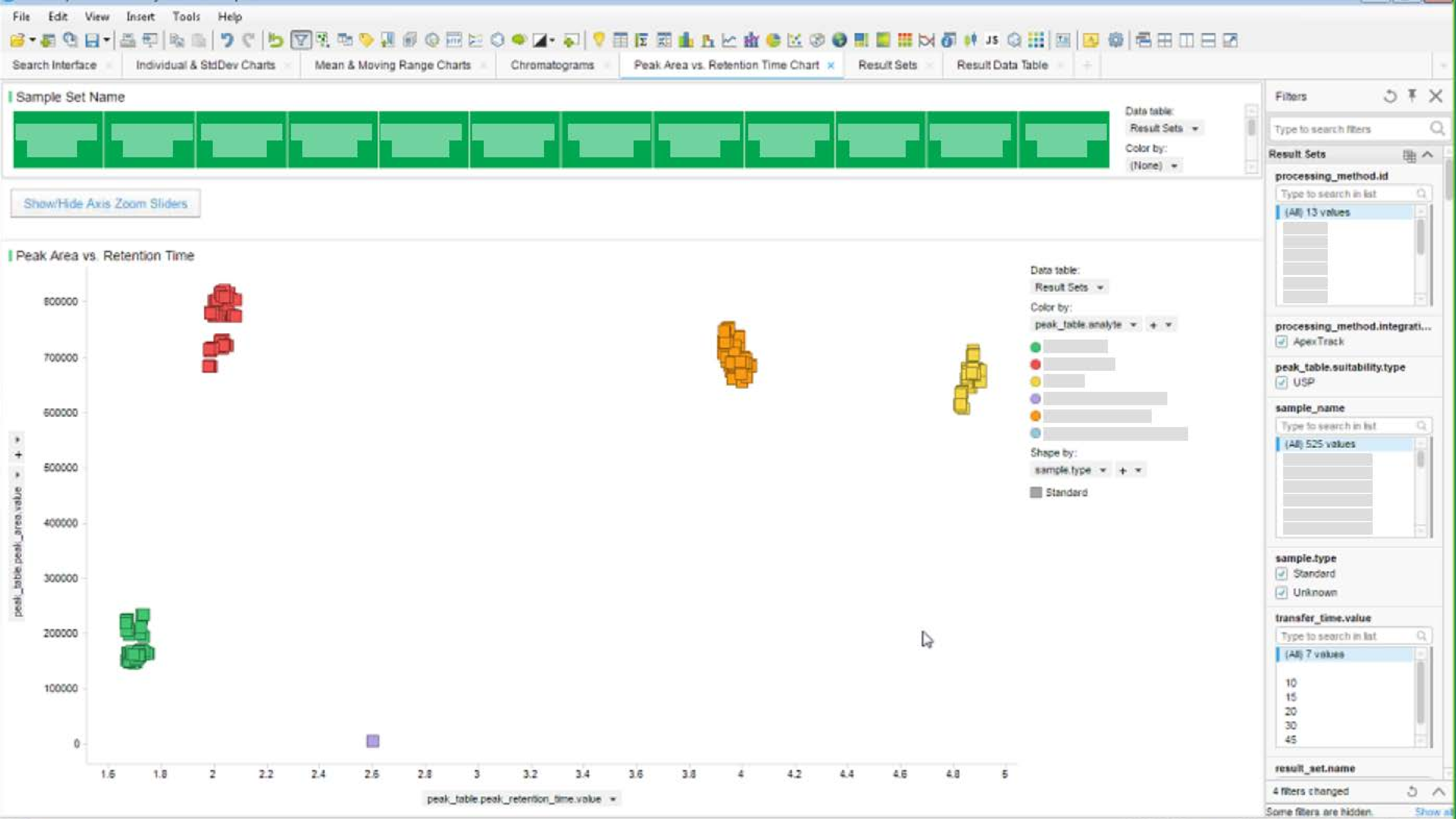
**Data  
Description**

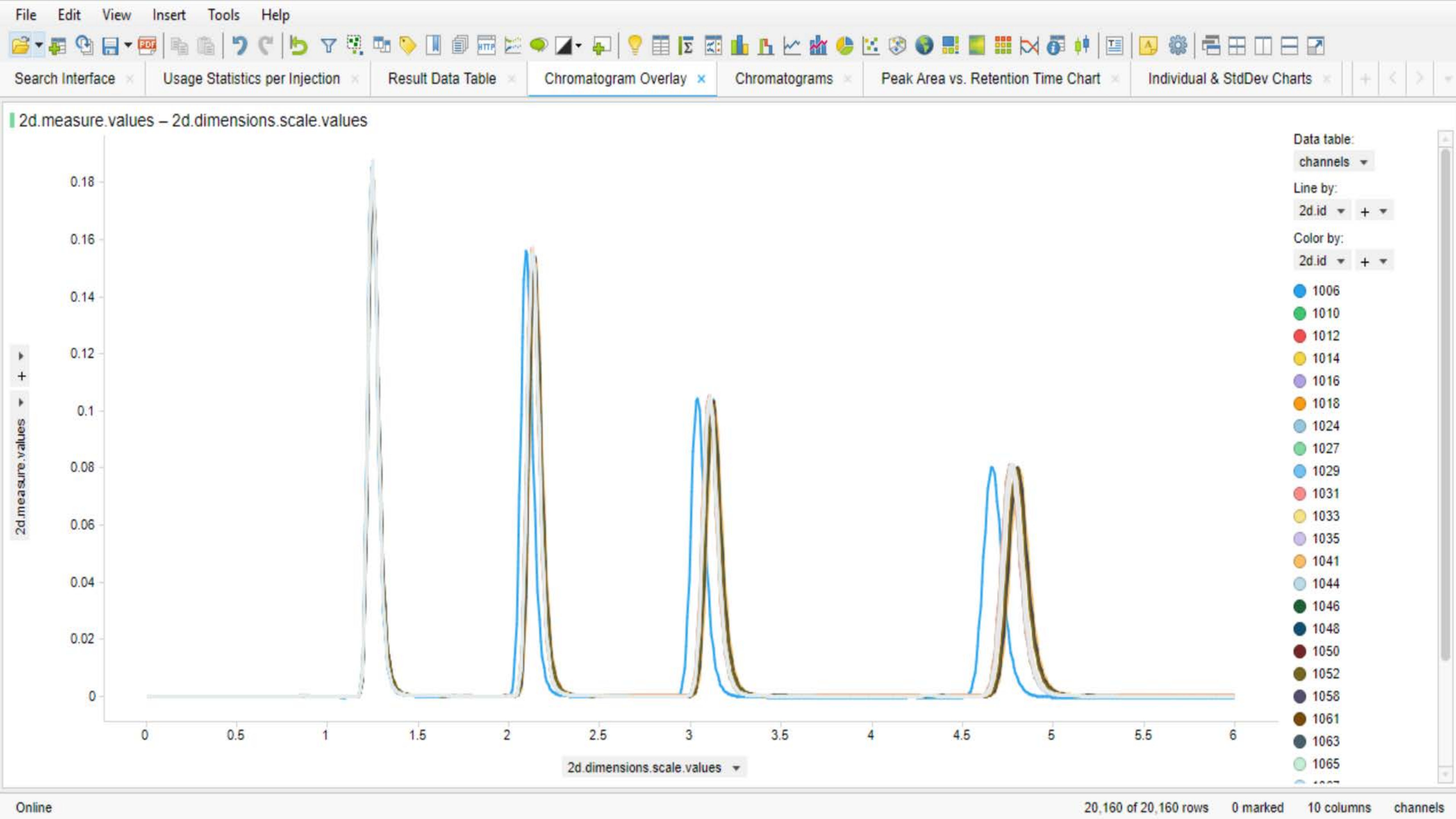
**Data Cube**

**Data Package**











## **Special Thanks to the Merck Team for making this happen**

Michael Fernando (IT Team Lead)

Chintan Patel (Lab SME)

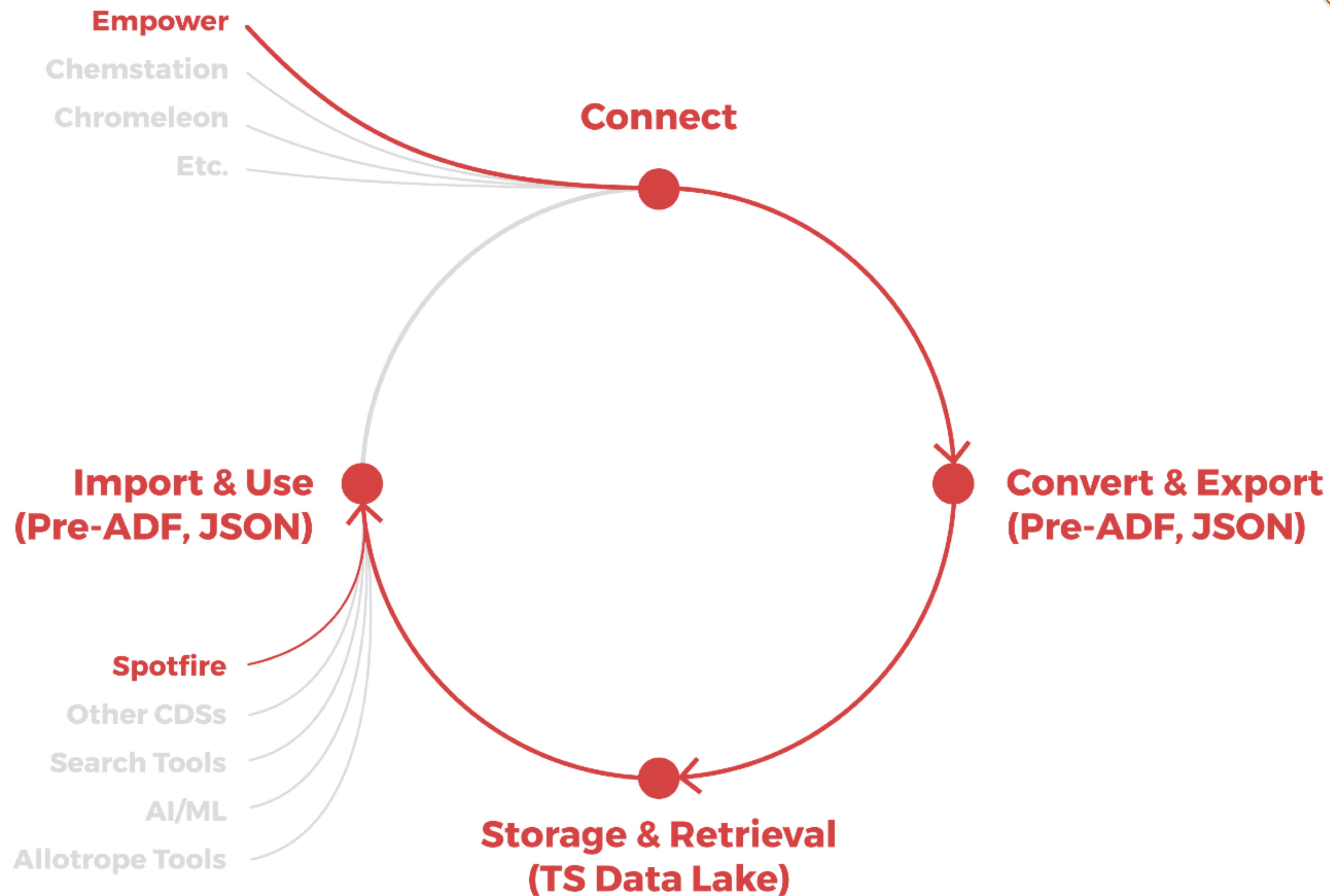
Antonio Oliveira (Lab SME)

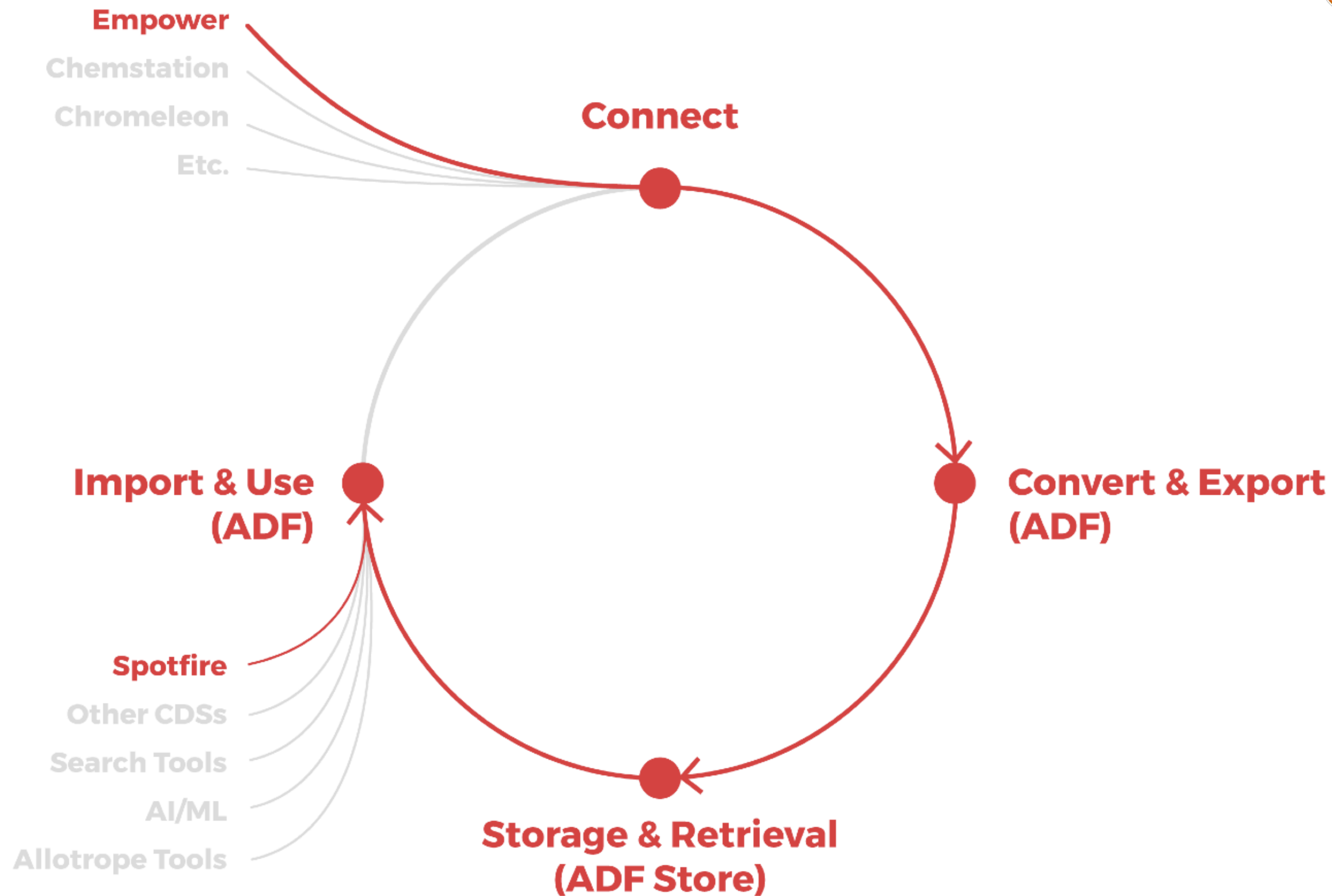
Dong Min Shen (Spotfire lead)

Zdenek Hribal (Empower team)

Michael McClellan (Empower team)

Jeff Feist (Cloud computing)

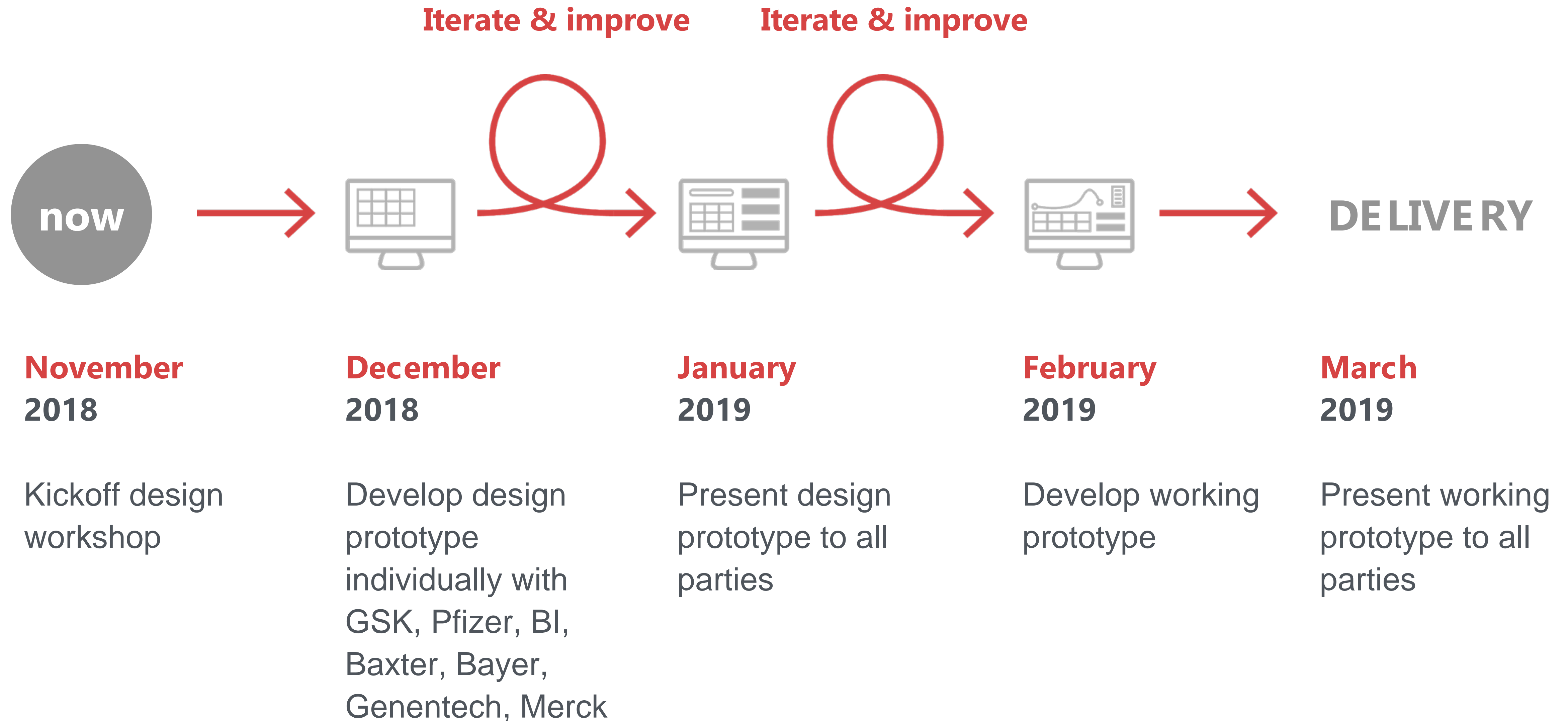






# Project Plan (Design Process)

# Empower/ADF Converter App Design Process





# Thank You/Questions?



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