



# Automated Workflow for Building a Compound Structure Database Using ACD/Spectrus Platform

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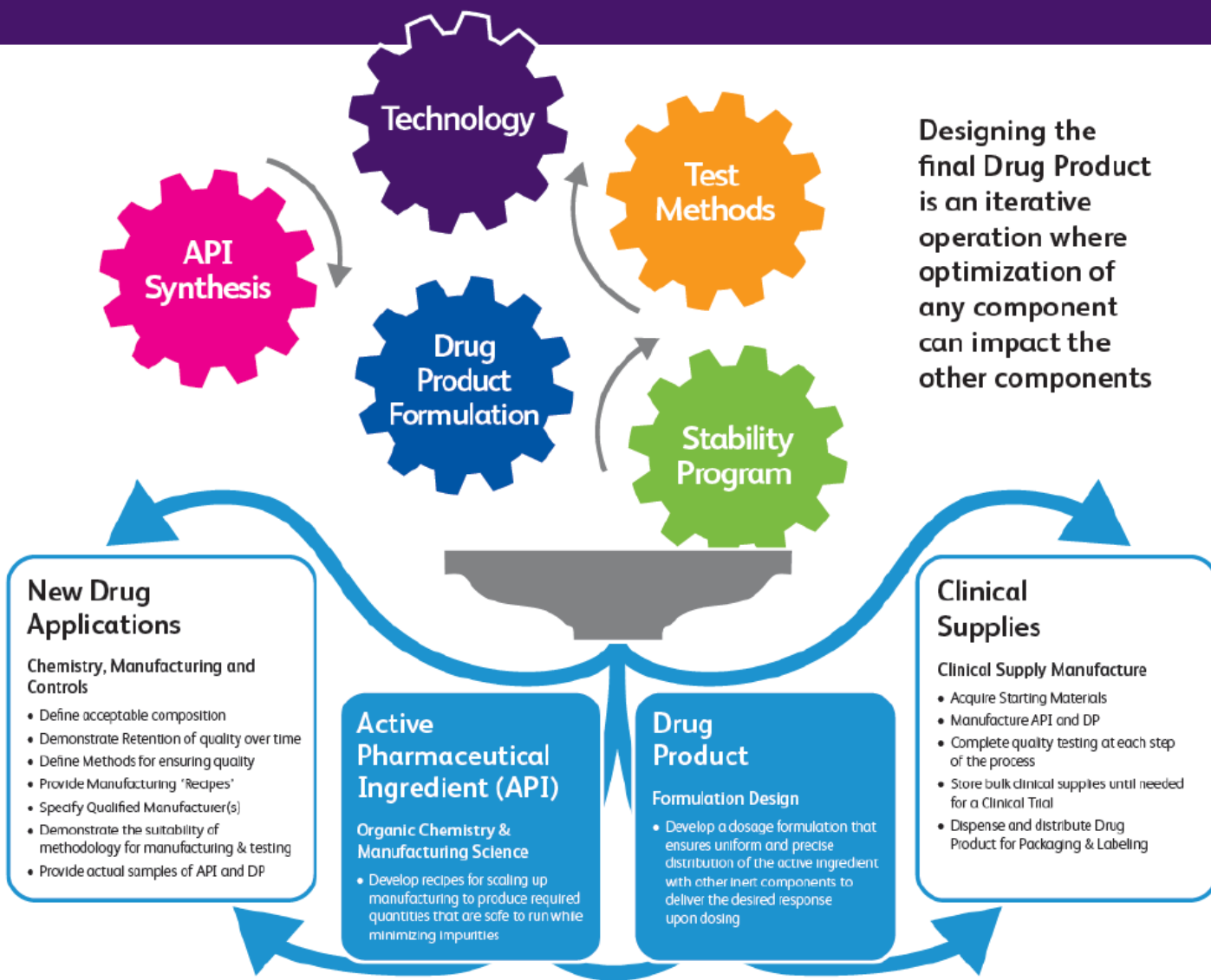
Pfizer Groton-Structure Elucidation Group

Mass Spectrometry Specialist

# PHARMSCI SMALL MOLECULE

Leader in the design, development and clinical manufacture of innovative medicines

Ensuring robustness and repeatability throughout the development process to deliver new medicines to patients across the globe



## Process, Product & Analytical Development

Processes are designed, developed and constantly tweaked to yield a safe, reproducible, cost effect path to a stable, manufacturable Drug Product Formulation with optimal bioperformance. Developing technologies are utilized in all aspects of the development process, while scientific knowledge in these areas is utilized to aid in the selection of the final drug molecule.

## Manufacturing

Requires identification and sourcing of Raw Materials, execution of multiple organic synthesis and formulation steps and in-process analysis to ensure the manufacture is proceeding as expected.

## Analytical Test Methods

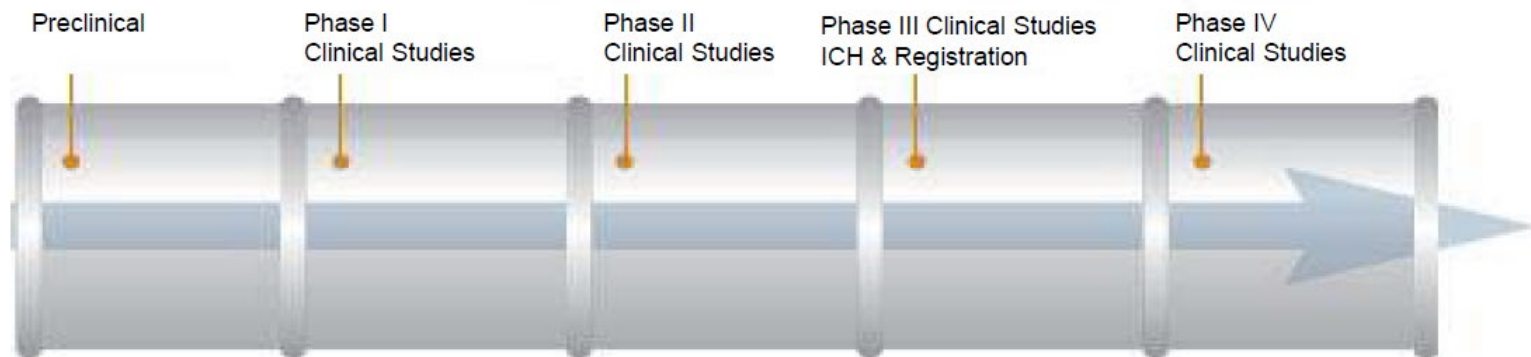
Developed to match each step of the manufacturing process, testing is utilized to confirm quality of a drug and its precursors. Approximately 70 tests are completed for each Drug Product lot released.

## Stability Program


Allows for identification of degradation products and the pathways that create them for both API and Drug Product. Also yields information regarding the usable lifespan of a manufactured dose.

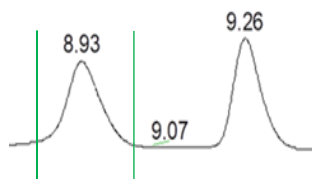
# Analytical Research and Development (ARD)

- Development of analytical methods
- Characterization of structures
- Specifications and control strategies to enable API & drug product development
- Clinical supply release testing, and shelf-life assignment
- Support for all phases of development

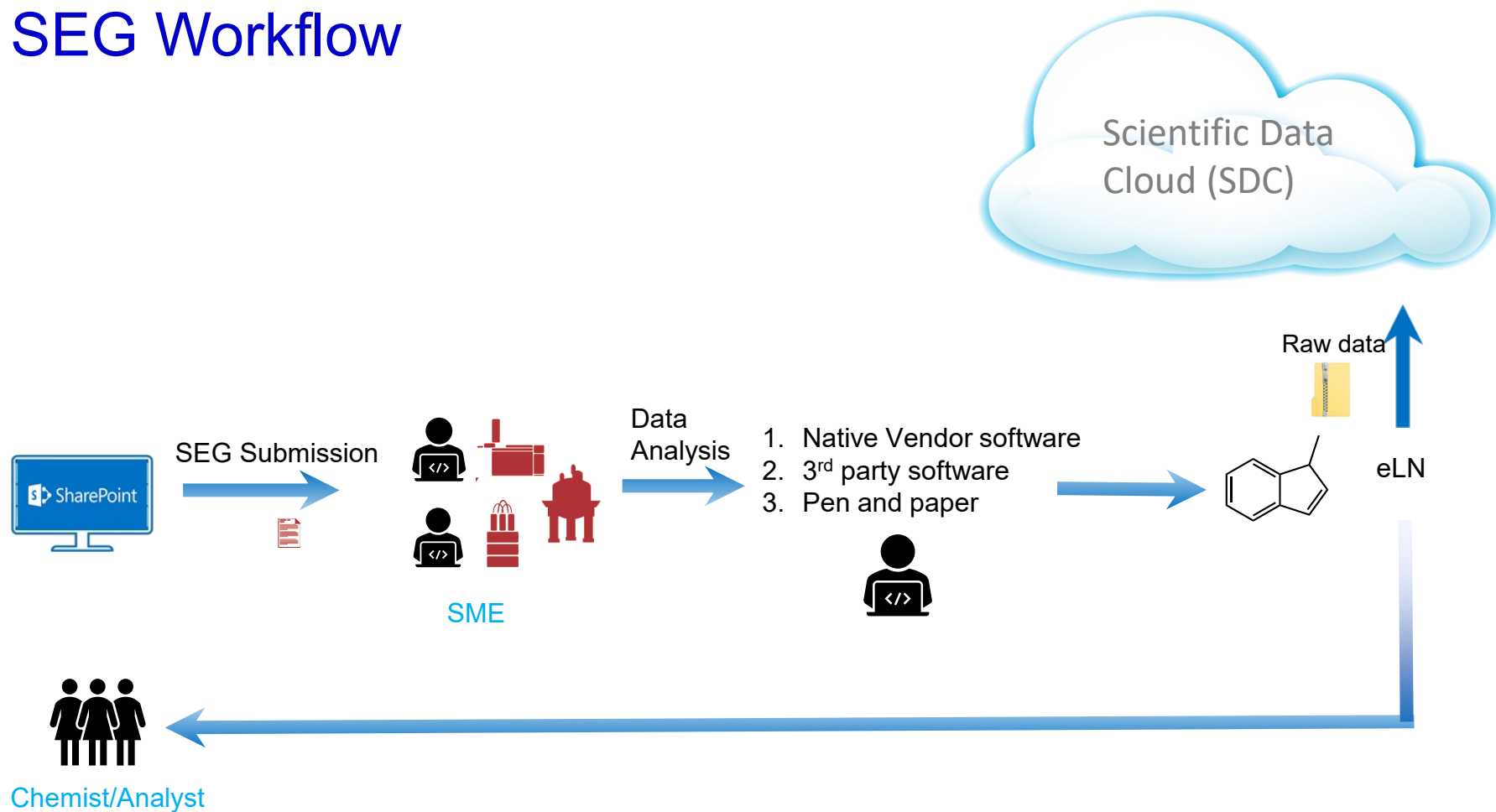


# Pfizer Structure Elucidation Group (SEG)

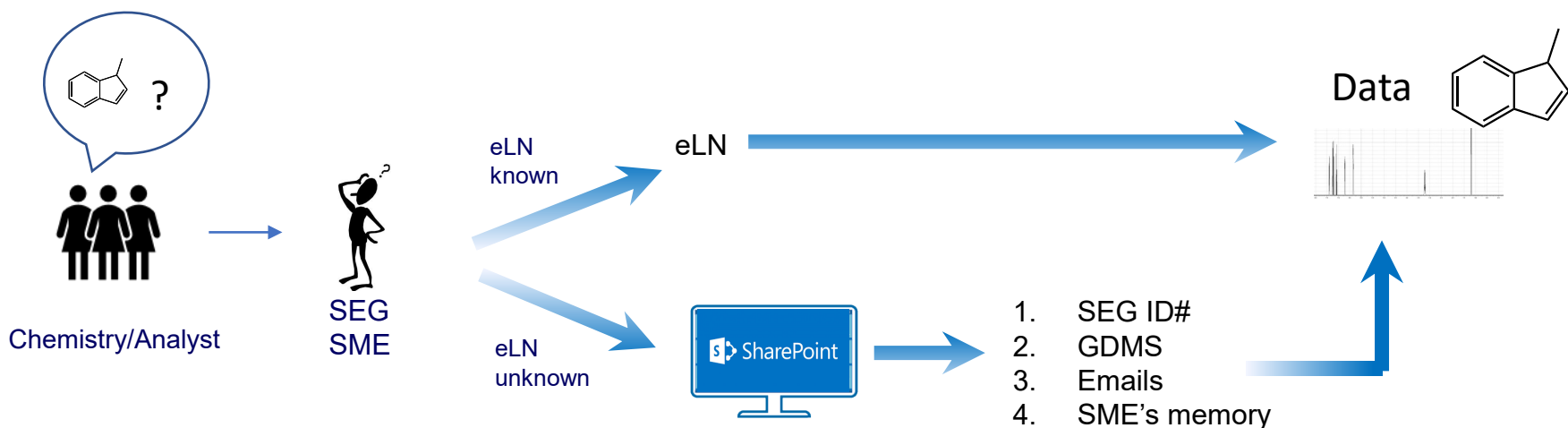
- Global partners in small molecule Structure characterization
- Active pharmaceutical ingredients (APIs), synthetic intermediates, byproducts, process related impurities and degradants.
- Support through discovery, development, late stage, and manufacturing
- Two sites, Groton US and Sandwich UK 
- Purification, MS, NMR, enabling technologies
- >600 structure elucidation requests per year



# SEG Workflow

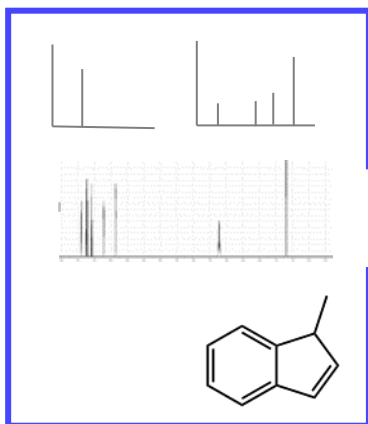


# Challenges



- Limited data searchability
- Inefficient process to respond to queries, and data investigations
- Duplication of structure elucidation efforts
- Limited data sharing between sites
- Multiple data formats

# Solution: Structure Database

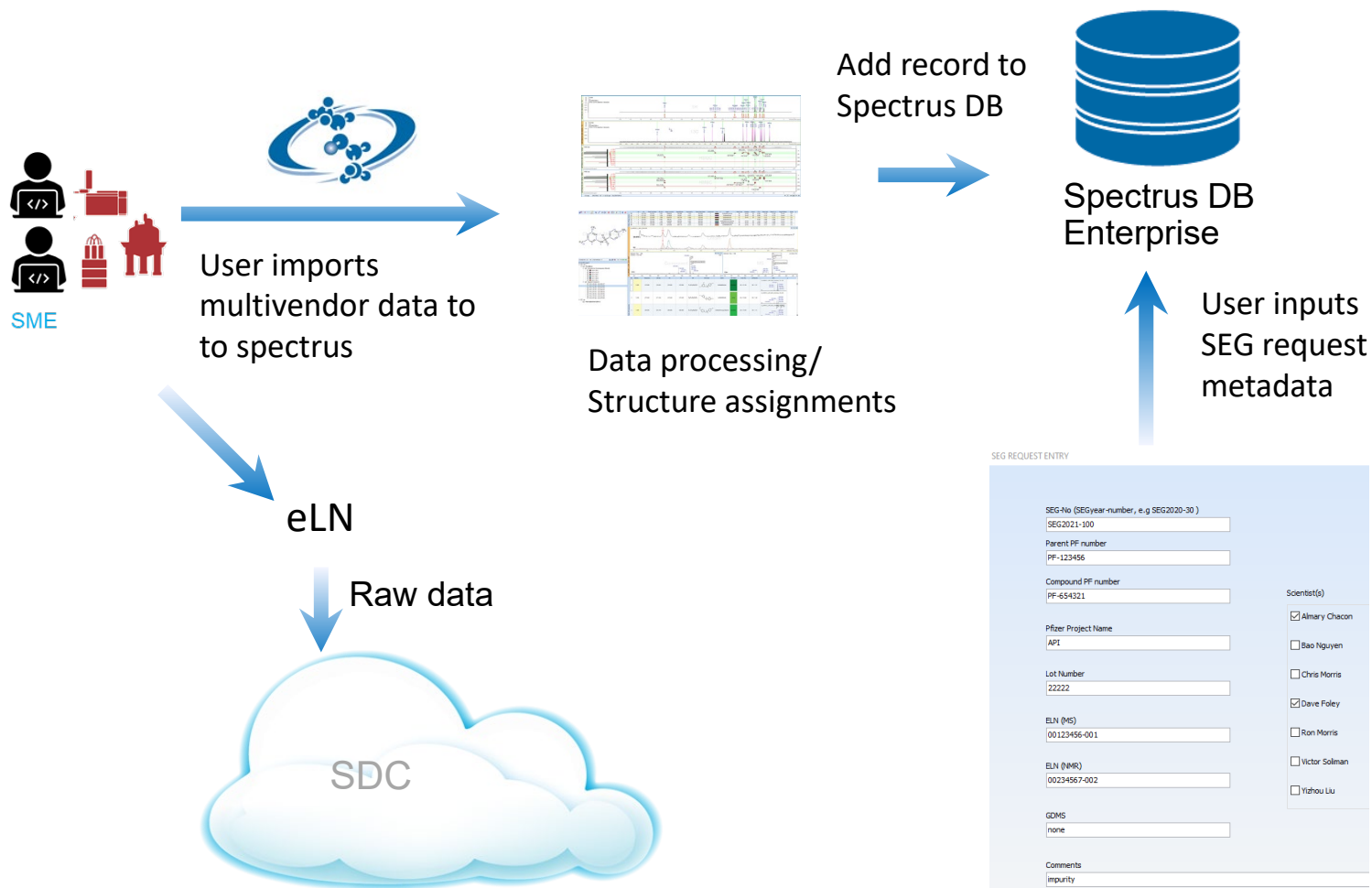


SEG ACD Spectrus DB

- Search by structure, PF-# and any other meta data
- Search by spectra
- Access to other site's data
- Analyst/chemist access to data



# ACD Spectrus DB workflow



SEG REQUEST ENTRY

SEG-No (SEGyear-number, e.g SEG2020-30 )	<input type="text" value="SEG2021-100"/>
Parent PF number	<input type="text" value="PF-123456"/>
Compound PF number	<input type="text" value="PF-654321"/>
Pfizer Project Name	<input type="text" value="API"/>
Lot Number	<input type="text" value="2222"/>
ELN (MS)	<input type="text" value="00123456-001"/>
ELN (NMR)	<input type="text" value="00234567-002"/>
GDMS	<input type="text" value="none"/>
Comments	<input type="text" value="impurity"/>

Scientist(s)

- ☒ Almary Chacon
- ☐ Bao Nguyen
- ☐ Chris Morris
- ☒ Dave Foley
- ☐ Ron Morris
- ☐ Victor Solomon
- ☐ Yihou Liu





# Implementation

- Slow process
  - Users must perform several extra steps to add data to DB
- Up to user how much metadata is captured in records
  - Inconsistencies across record set leads to impaired searching
- Still one DB per site
  - Different workflows
  - Different metadata captured

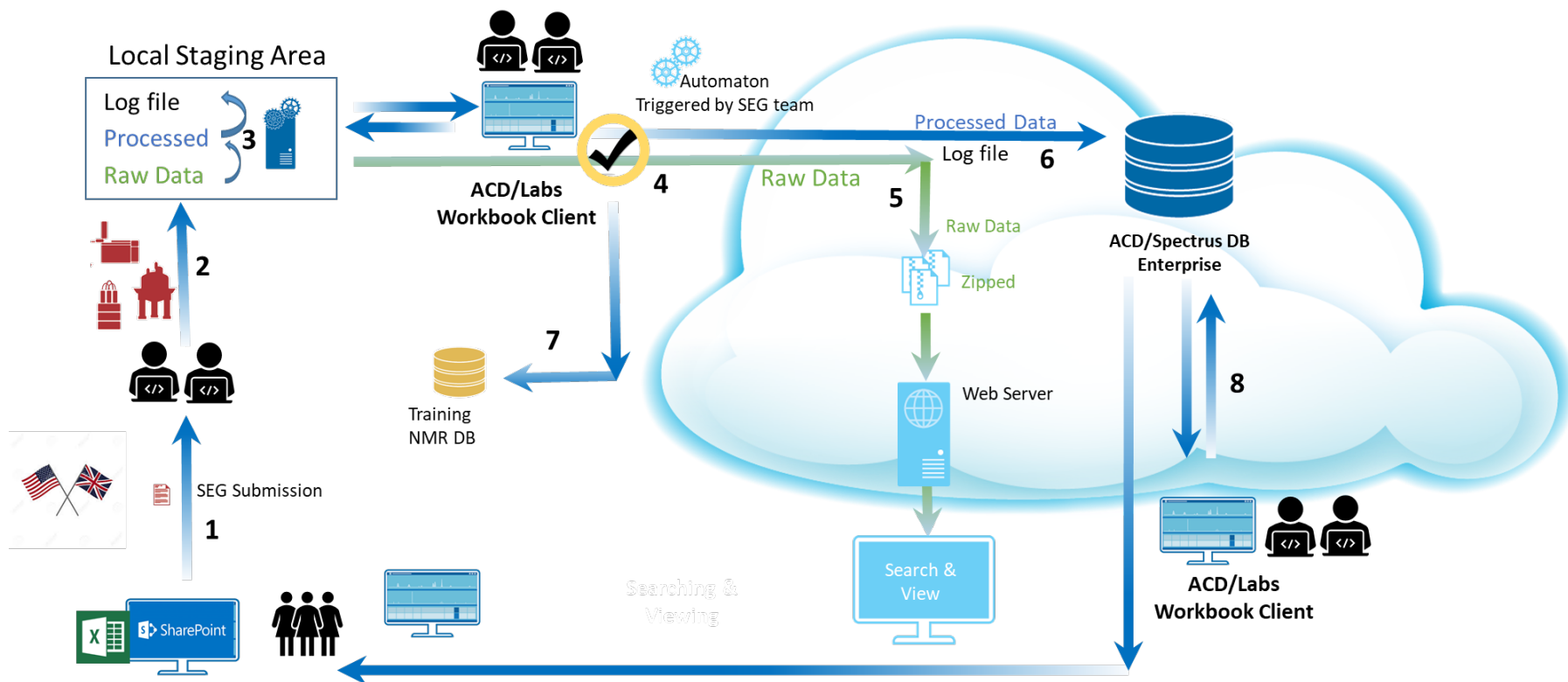
Need for automation



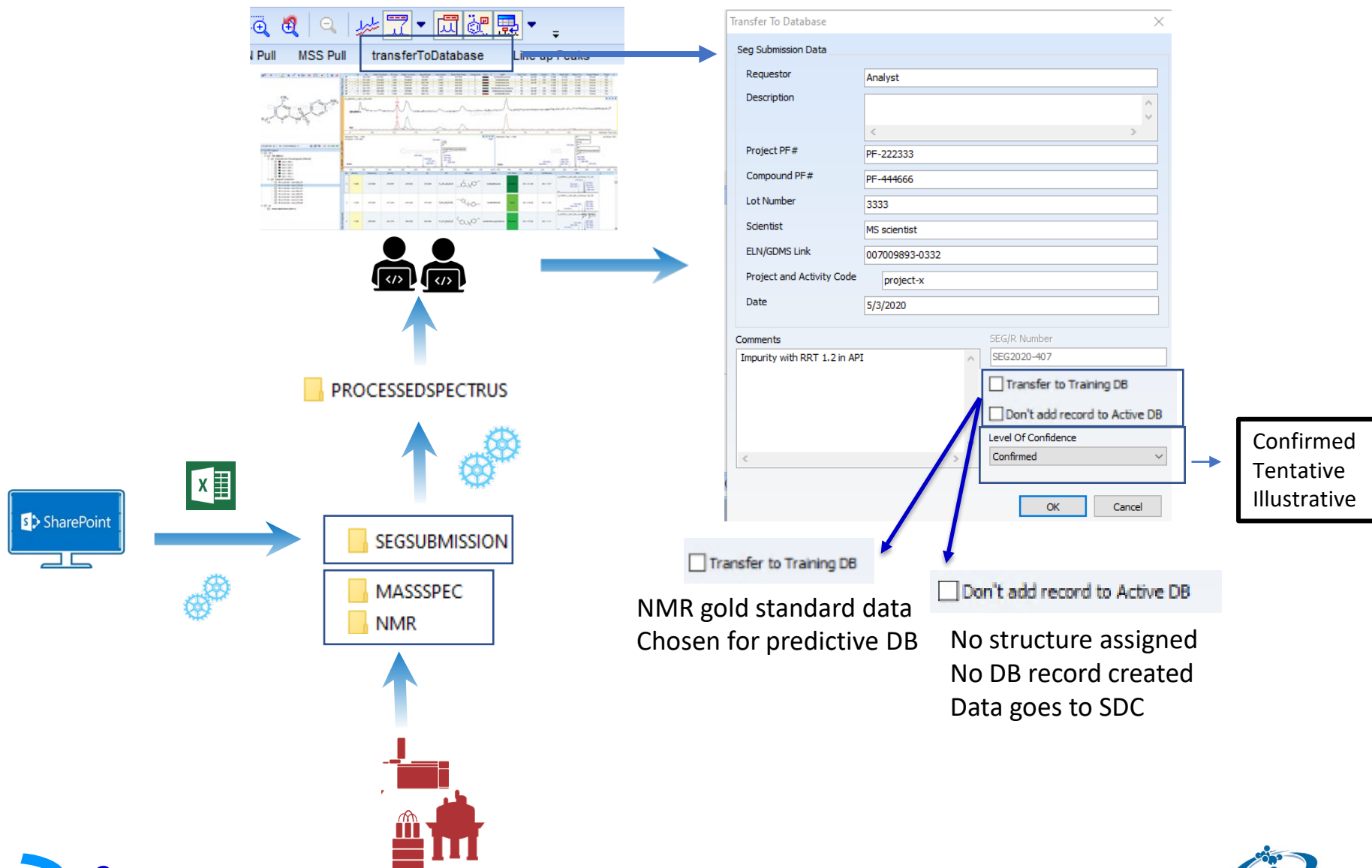
## Goals for Automation

- Harmonization of SEG workflows (Global SEG DB)
- Sample submission metadata automatically captured
- Raw data automatically converted to spectrus files for data processing
- Results uploaded to global DB via push of a button
- MS, NMR data, and sample submission metadata married into one record for each structure
- Raw data, full spectrus files, and processed spectrus files automatically transferred to SDC
- Selected gold standard NMR data added to an NMR prediction training DB
- Access to spectrus data in SDC via web viewer.

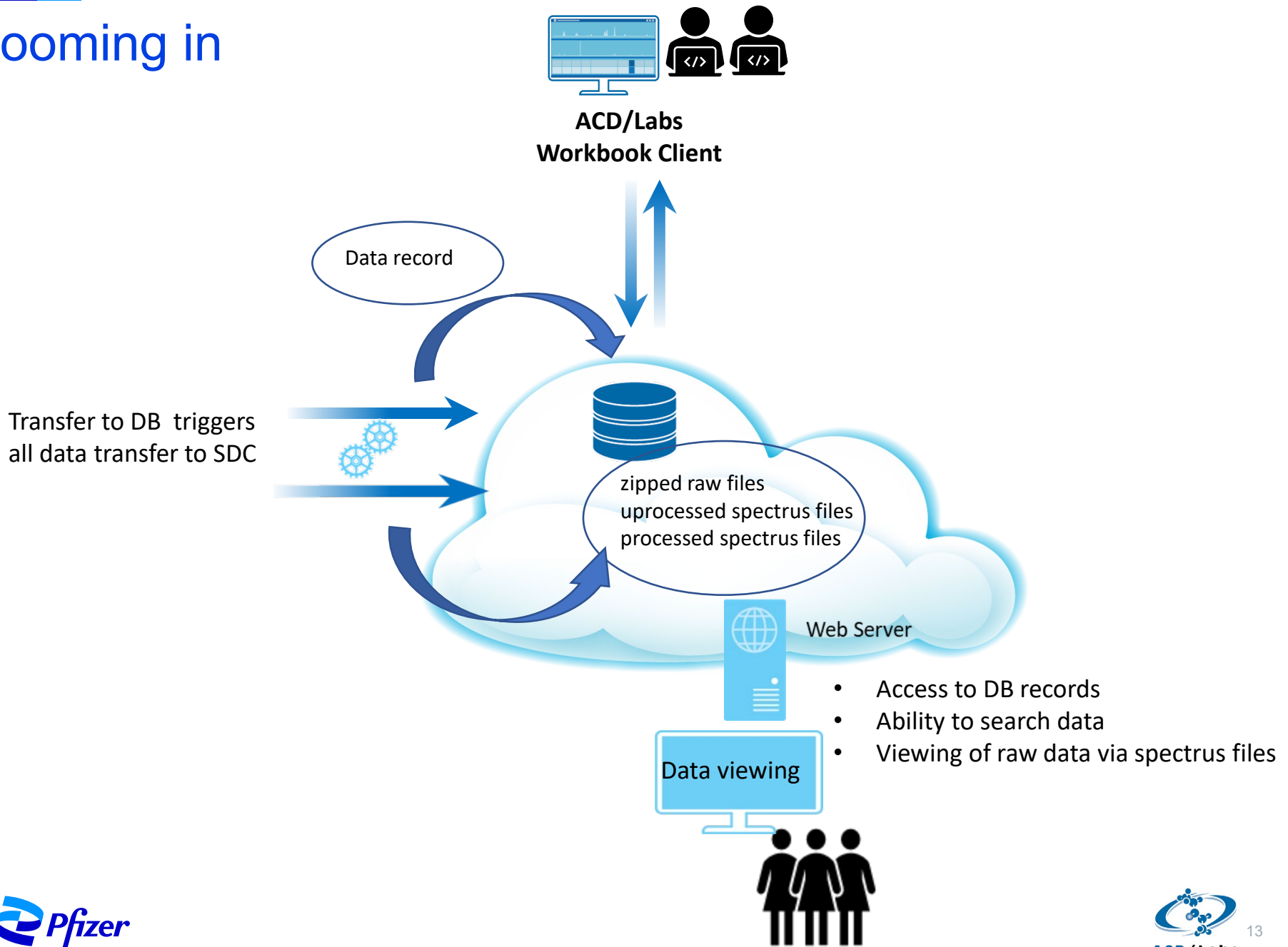
# Automated Workflow Overview



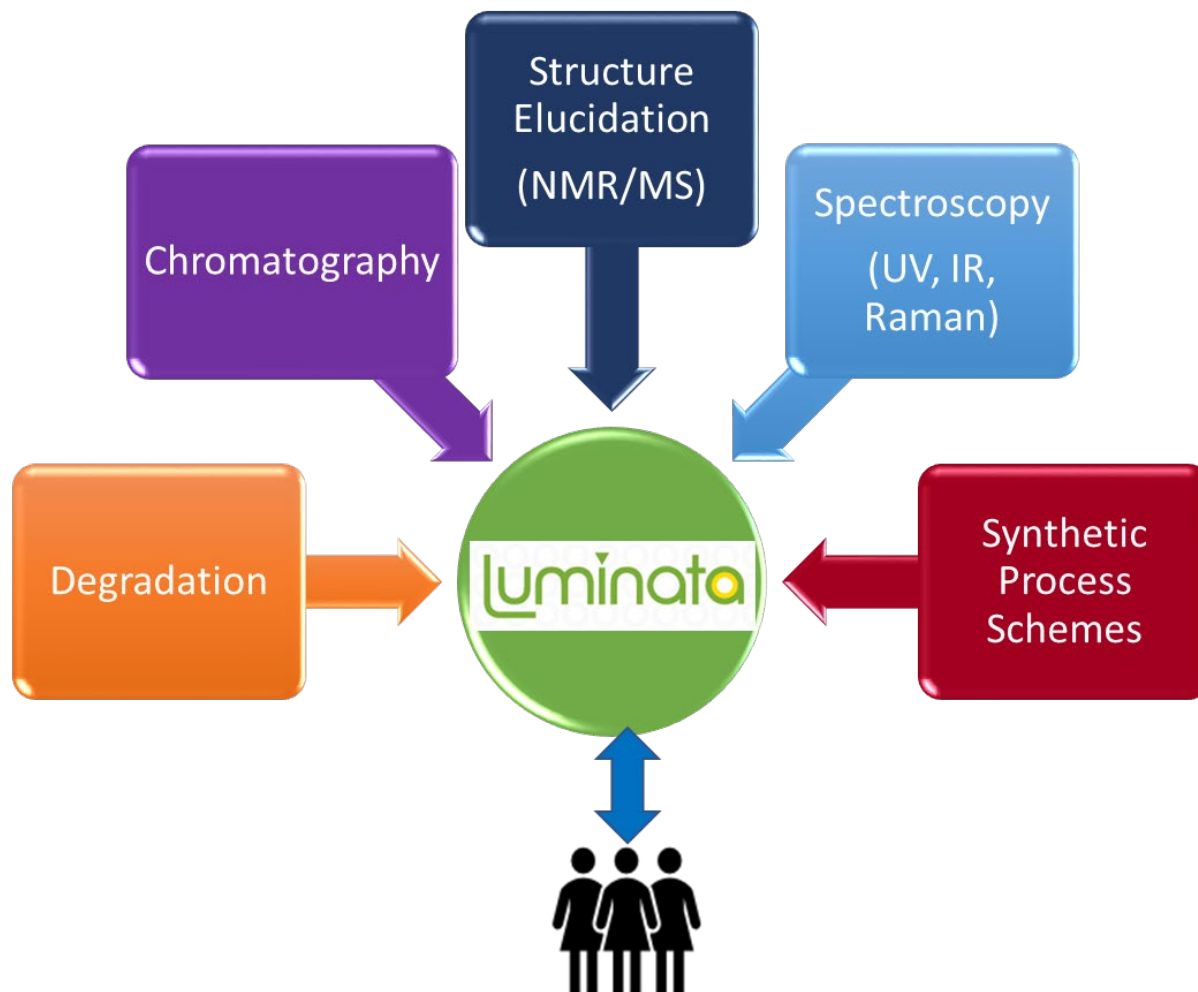
# Zooming in



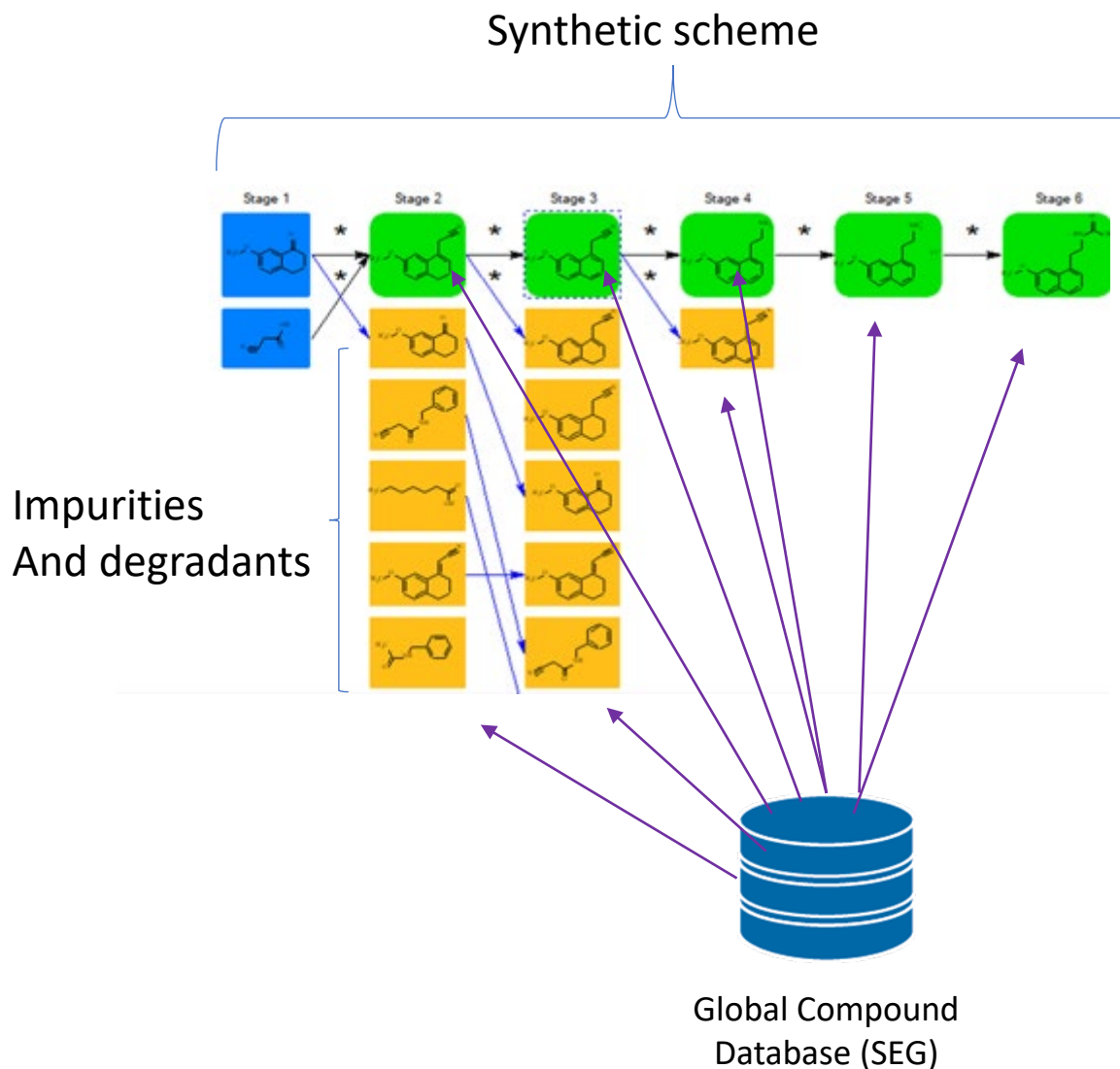
# Zooming in



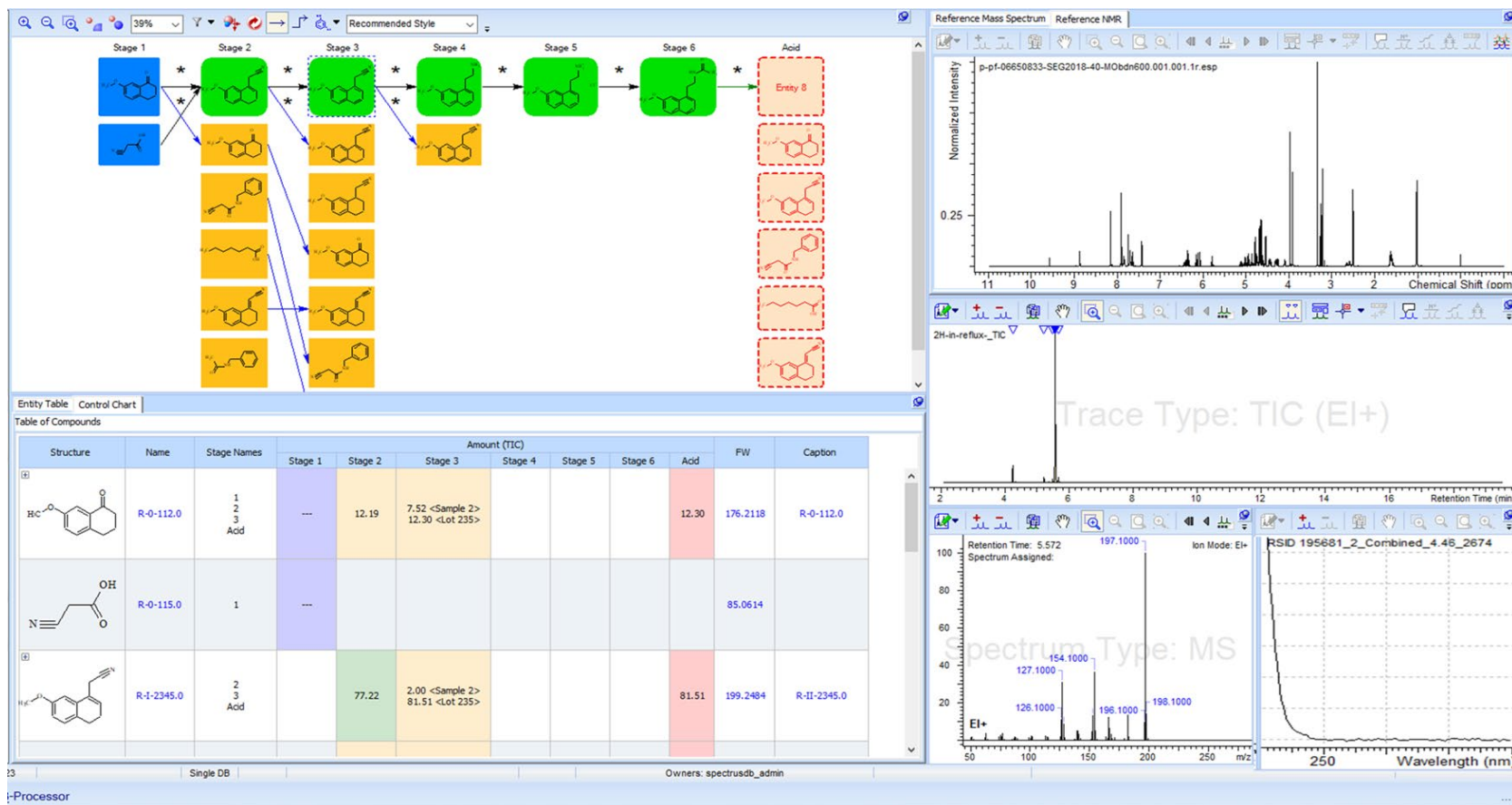
# Looking Forward



# Global SEG DB Integrated with all Project data

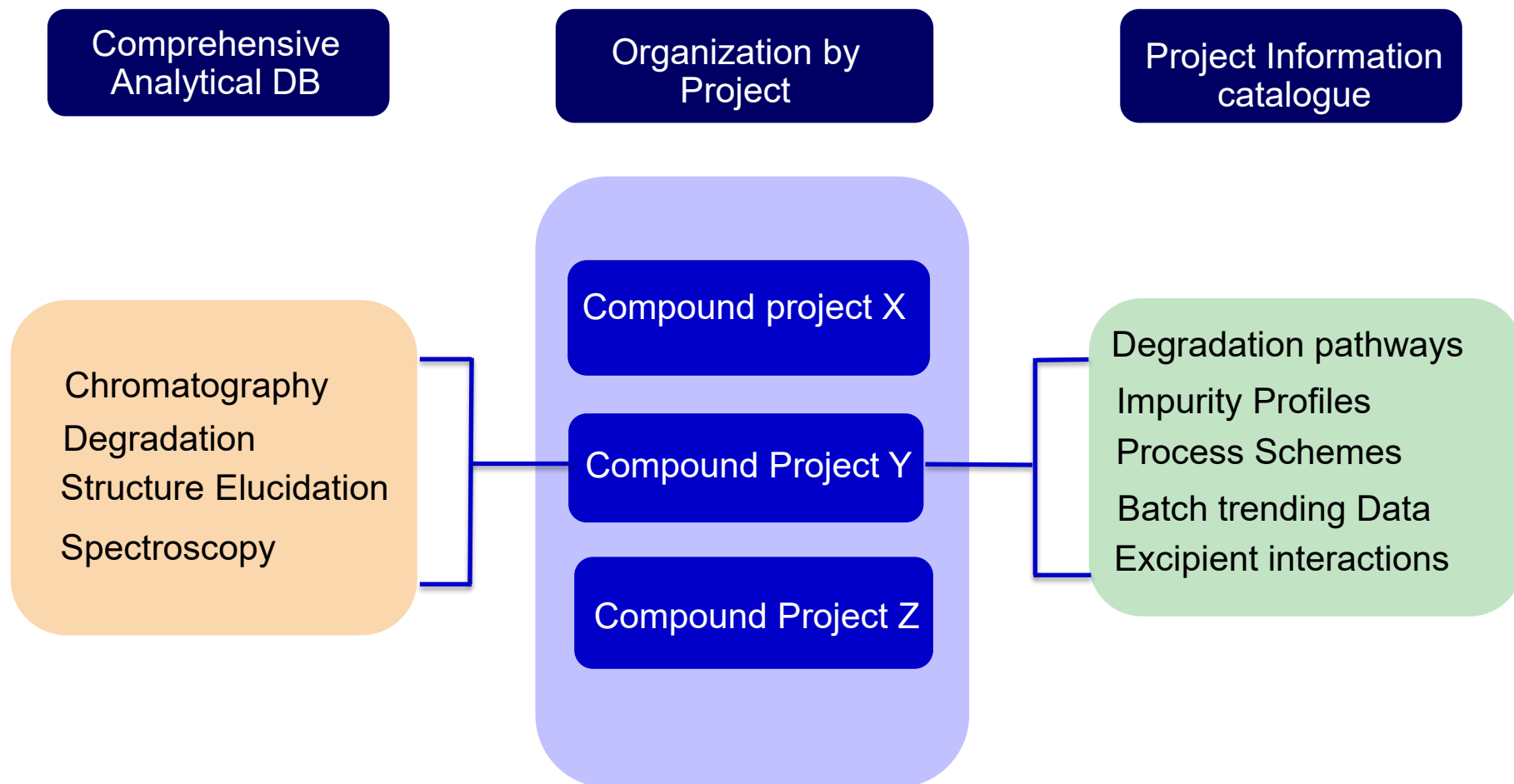


# Luminata





# Information Library



# Acknowledgements

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## Pfizer SEG

- David Foley
- Ruth Boetzel
- Drew Gibson
- Rajesh Mishra

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## Pfizer Digital

- Rajesh Mishra
- Bo Du
- Kingsley Sumner
- John Henrikson
- Pennie Fox

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## ACD Team

- Karim Kassam
- Ashley Di Fruscia
- Hans De Bie
- Terry Chu
- Linda Bean