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Project team data visualization and decision support solutions: core requirements and must-have features

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Project Team Data Visualization and Decision Support Solutions

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Core requirements and must-have features

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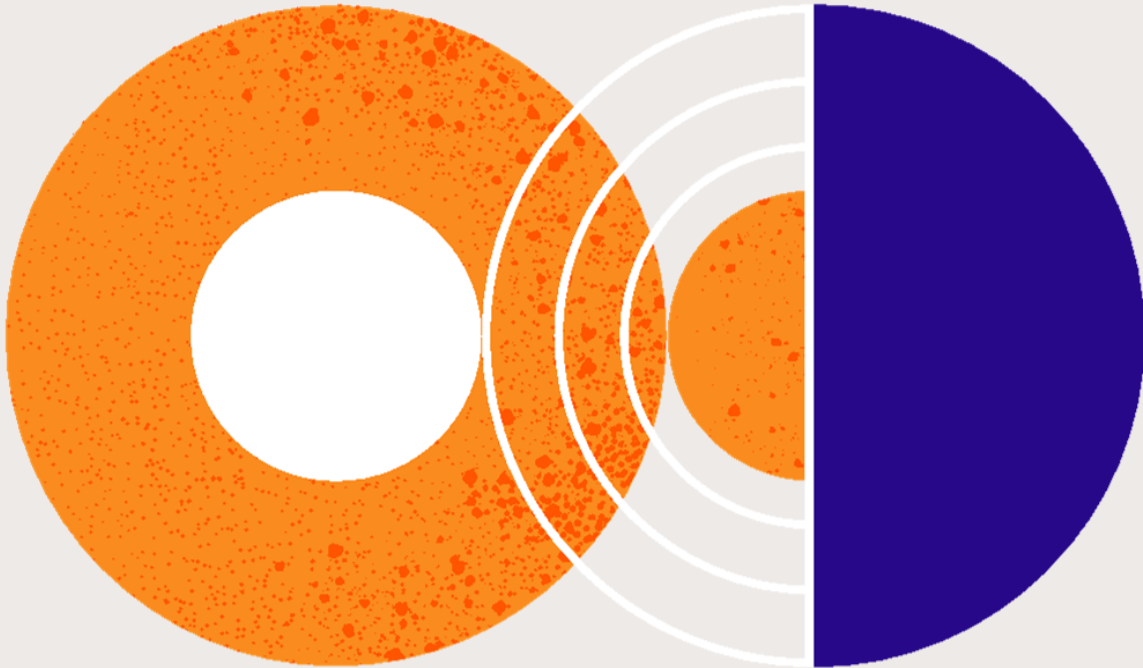

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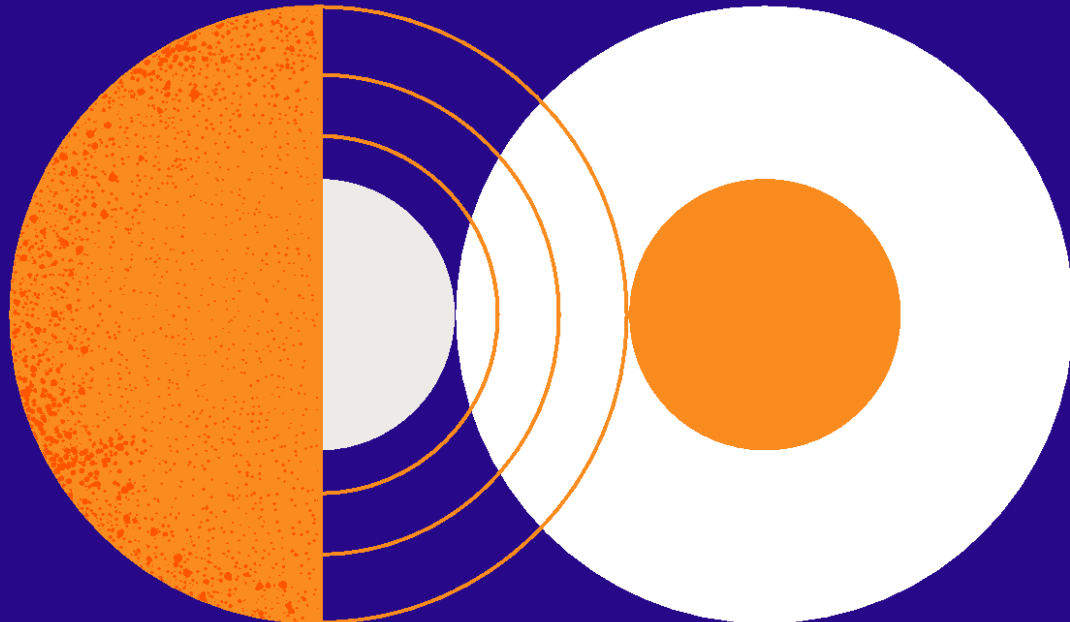
Organizing Requirements



Science to Inform Decisions

All the effort and expense of research is only useful when it generates data that drives good decisions

Project Teams Members are Specialists

- Each discipline, like Medicinal Chemistry, Assay Biology, and Pharmacology, requires specialist analysis tools
- Project teams and members also need specialized project-analysis tools
- Each team member will need both discipline-specific tools and project team tools

Project Team Roles and Goals

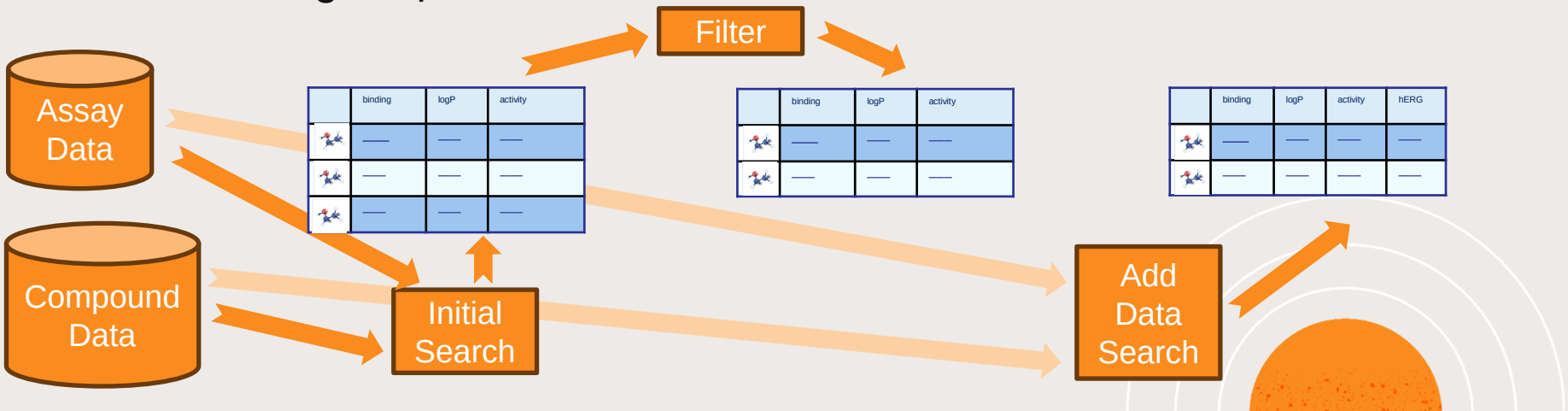
Small molecule drug discovery examples

- **Project leader goals**
  - Track program execution
  - Prioritize compounds to synthesize and test
  - Determine if compounds meet requirements to clear a project gate
- **Project team member**
  - Select the best datasets for making project decisions
  - Reach a shared understanding of current project information
  - Understand which aspects of a compound's performance as a drug must be improved to meet project goals
  - Collaboratively recommend compound synthesis and assay priorities
- **Medicinal chemist goals**
  - Understand how compound structure impacts all aspects of its performance as a drug
  - Understand if specific batches of the same parent structure behave differently
  - Propose new compounds that improve specific qualities or overall performance
- **Pharmacologist goals**
  - Understand how compound structure affects pharmacology
  - Understand if specific salt forms of the same parent structure behave differently
  - Verify data are properly curated and presented to the project team with sufficient context to correctly interpret it
- **Computational chemist goals…**

Each goal may require specialized software tools and data drill-down

Search vs Filter

- **Initial search requirements are not the same as filtering**
  - But they often overlap – e.g. search by substructure then filter by substructure
- Commonly missed requirement: Filter by assay condition for late-stage experiments



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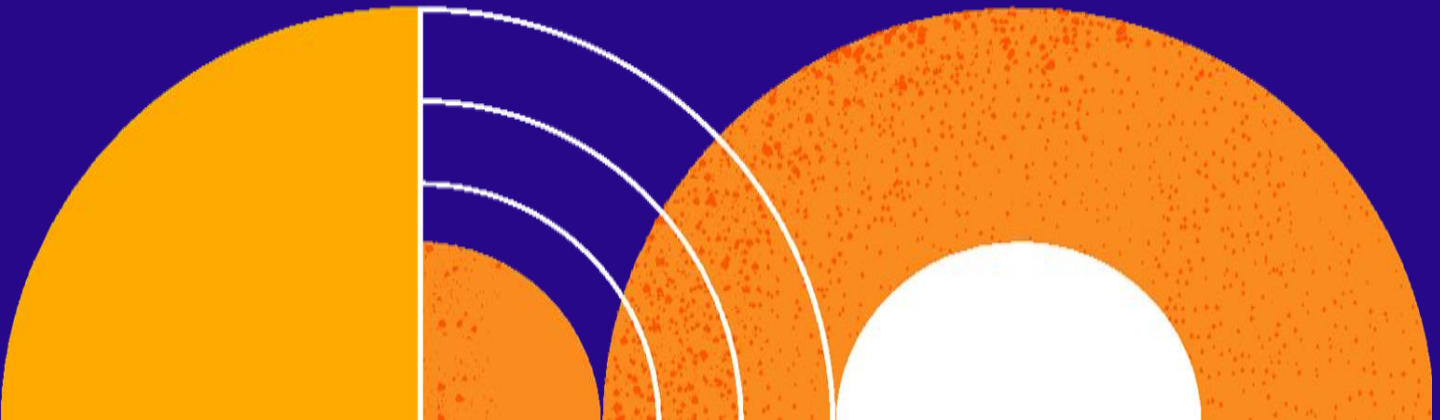
Derived Requirements

Commonly missed requirements



Row Aggregation

“Average” results for the “same” assay and compound

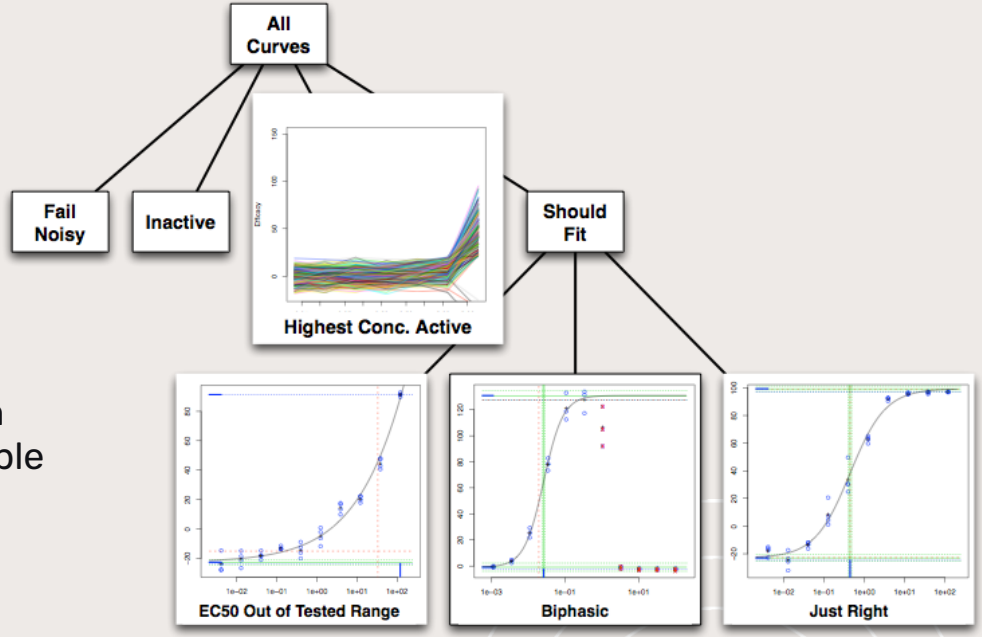
- Same “Compound” depends on the purpose
  - Same structure averaged for multiple lots is common, but sometimes you care about lot variability
  - Common aggregations use-cases
    - By lot
    - By parent
    - By salt
  - Less common use cases
    - By formulation
    - By assay condition
- “Averaging” must be mathematically correct for each endpoint type
  - Different data types require different operations, log avg, avg, etc.
  - Only average comparable* assays

*This topic could be a whole presentation

Dose-Response Curves

In early research, clean sigmoids are the exception

- Many of these curve categories fit results require ‘<‘ or ‘>’ in the EC50
  - The tools must sort numerically with operators
- Plots must be rendered for scientific interpretation
- Aggregated rows require overlaid curves
- Curves must be rendered in 30-40ms each to have good scrolling performance of a table with a few thousand rows of data and 3-4 curve data columns
  - Because of overlays, not all curves can be pre-rendered or cached



Assay and Endpoint Aliasing

Consensus is not always possible

Problems

- Assay names vary by CRO, lab, and scientist
- The same assay may be a primary-screen for one project but a counter-screen for another
- Endpoint names may not be standardized
- There is always project history and team needs evolve
- Some team members want the assay type in the name, while others need assay conditions

Solutions

- Allow assay name aliases
  - The name shown in report is not the same as assay name in the database
  - Ideally, alias by project
- Same for endpoint names
- Configurable assay trees
  - Ideally multiple user-selectable trees
    - by condition or by assay type

Collaborative Requirements

- Access controls
  - By project, by lot, & by assay
- Shared project team reports
  - Repositories of institutional knowledge
    - e.g. Just because data has the project target, does not mean the project team currently uses it for decision making
  - Evolve as the program progresses
    - e.g. Initially solubility is not important, but it will become important
  - Templates
    - Read, edit, clone

Team A Visible

	Lot Project	logP	Target A Activity	Target B Activity
	A	—	—	—
	A	—	—	—
	All	—	—	—
	B	—	—	—
	B	—	—	—

Team B Visible

	Lot Project	logP	Target A Activity	Target B Activity
	A	—	—	—
	A	—	—	—
	All	—	—	—
	B	—	—	—
	B	—	—	—

“And you may ask yourself, well, how did I get here?”*

Understanding the context of past decisions

- How do we learn from prior projects?
- What if we could restore our collaborative decision space to the exact state as when we discontinued a structure series, or approved a candidate?
  - The same sorting, filtering, analysis tools, but on historic data

*From “Once in a Lifetime” by Talking Heads and Brian Eno

Summary

Intelligence Amplification

- Our job as informatics providers is to deliver tools that
  - Stuff as much information as possible into project team member's big, wet, neural nets
  - Reduce distracting or confusing information
  - Eliminate mental gymnastics to remember caveats and context
  - Support a project from inception to clinic
  - **Help project teams make excellent decisions and brilliant leaps of inductive logic**

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Thank you

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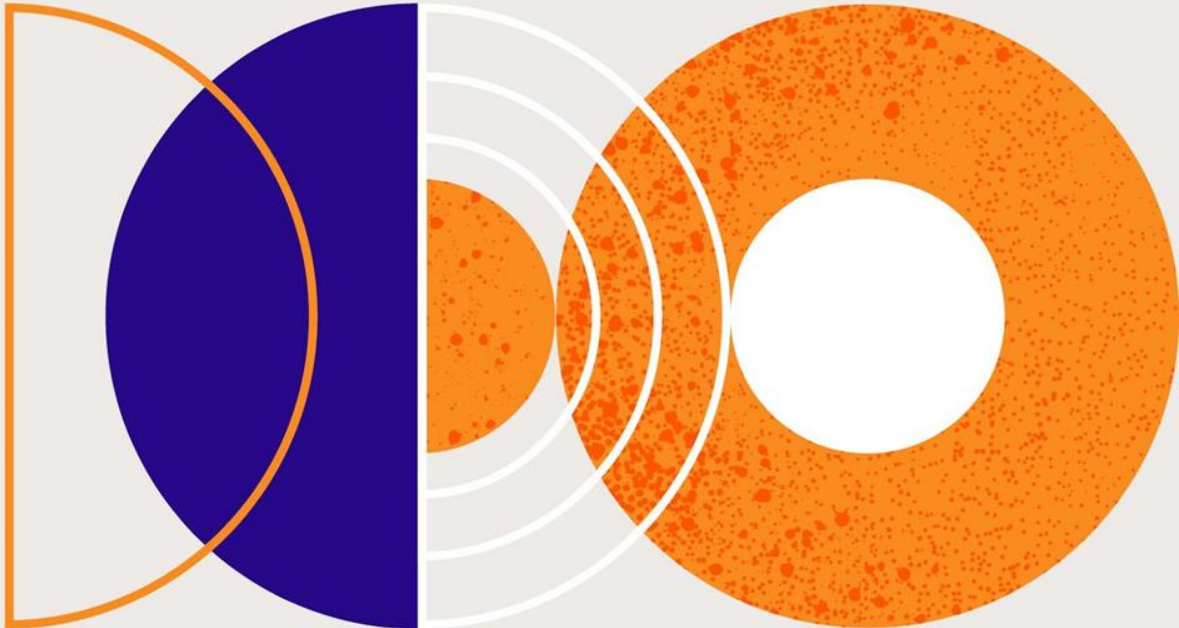
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