

Population Pharmacokinetics with Pipeline Pilot

1. Overview of Pipeline Pilot
2. Application Examples

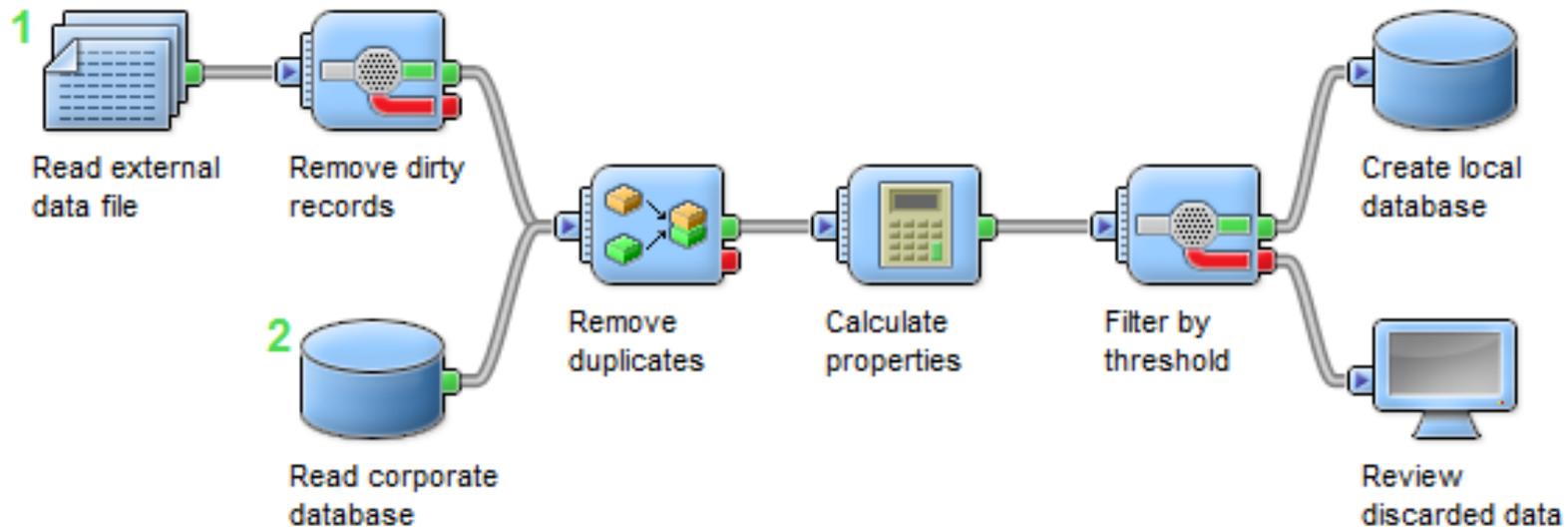


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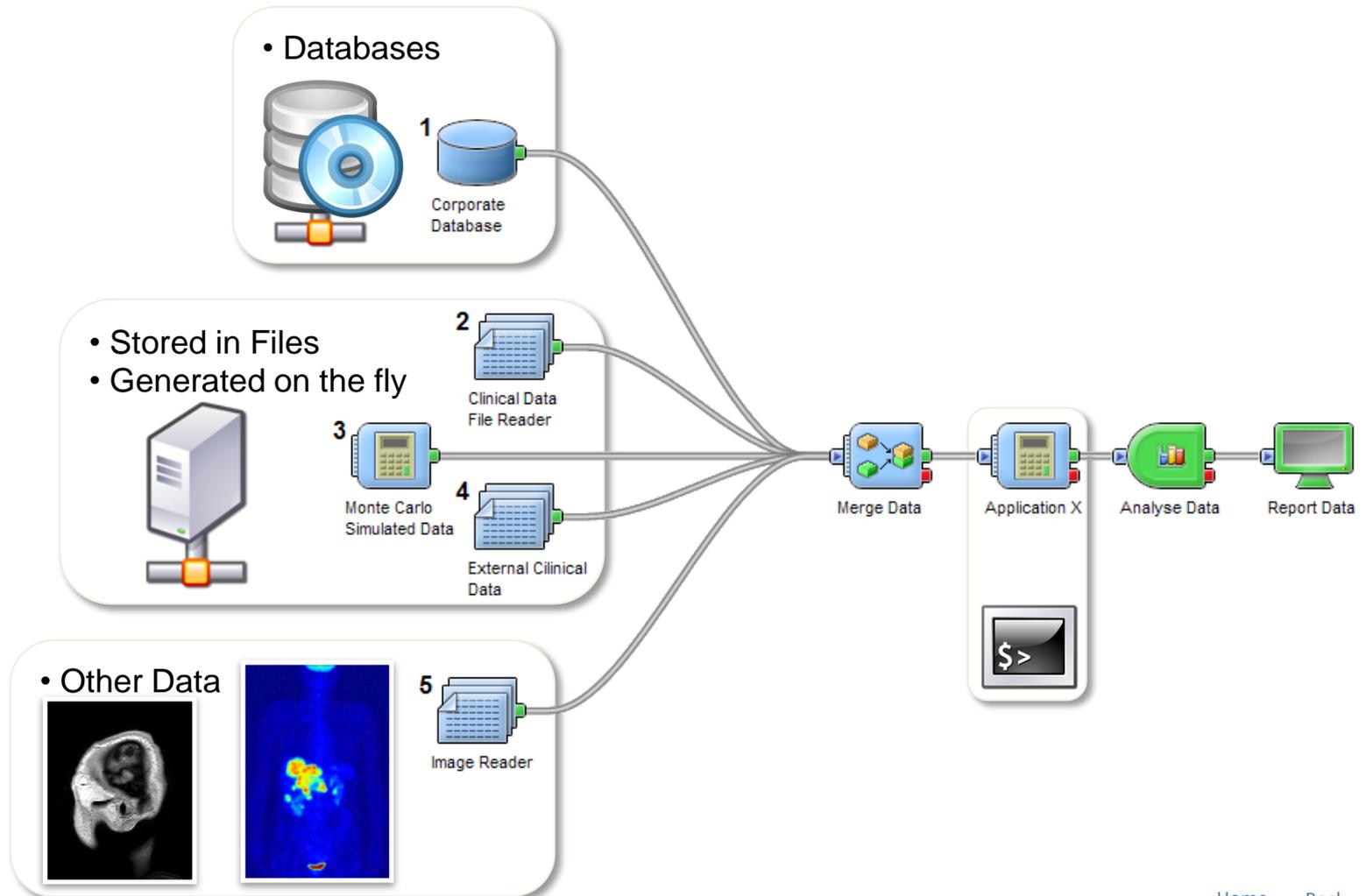
1. Overview of Pipeline Pilot
2. Application Examples



- A powerful new paradigm for data processing
- Pipelines guide the flow of data through a network of modular computational components



- Access disparate research data locked in silos



- Access disparate research data locked in silos
- Automate the scientific analysis

Command Line

ORACLE (CDISC)

SAS

R

MATLAB

Perl

Java

Python

VBScript

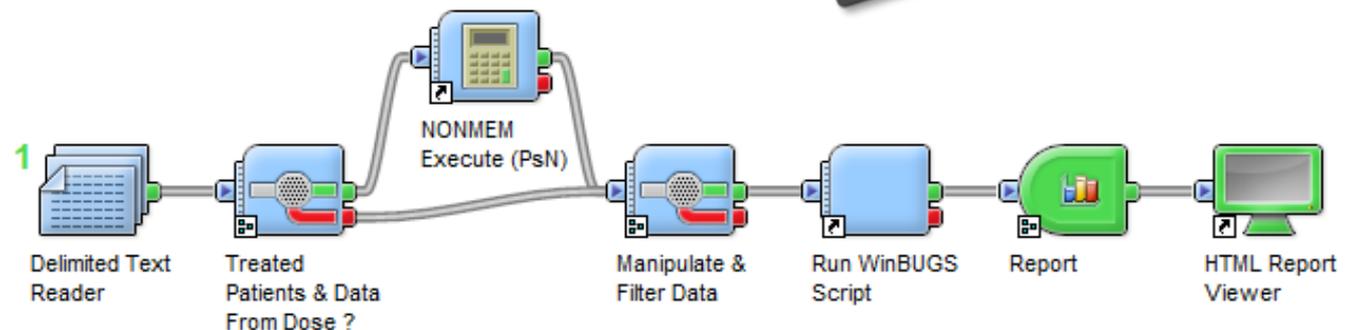
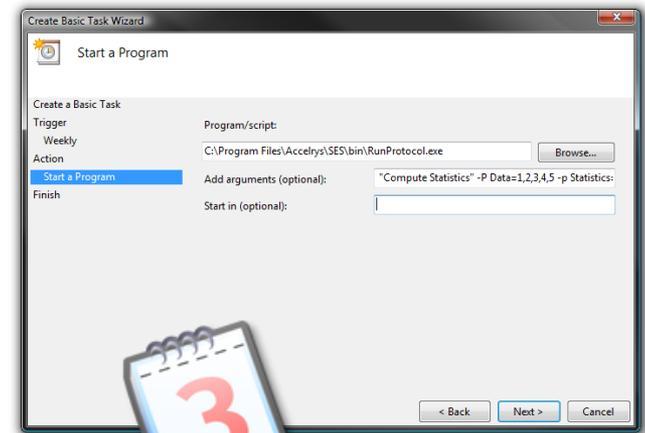
NONMEM (PsN, Xpose)

WinBUGS

Monolix

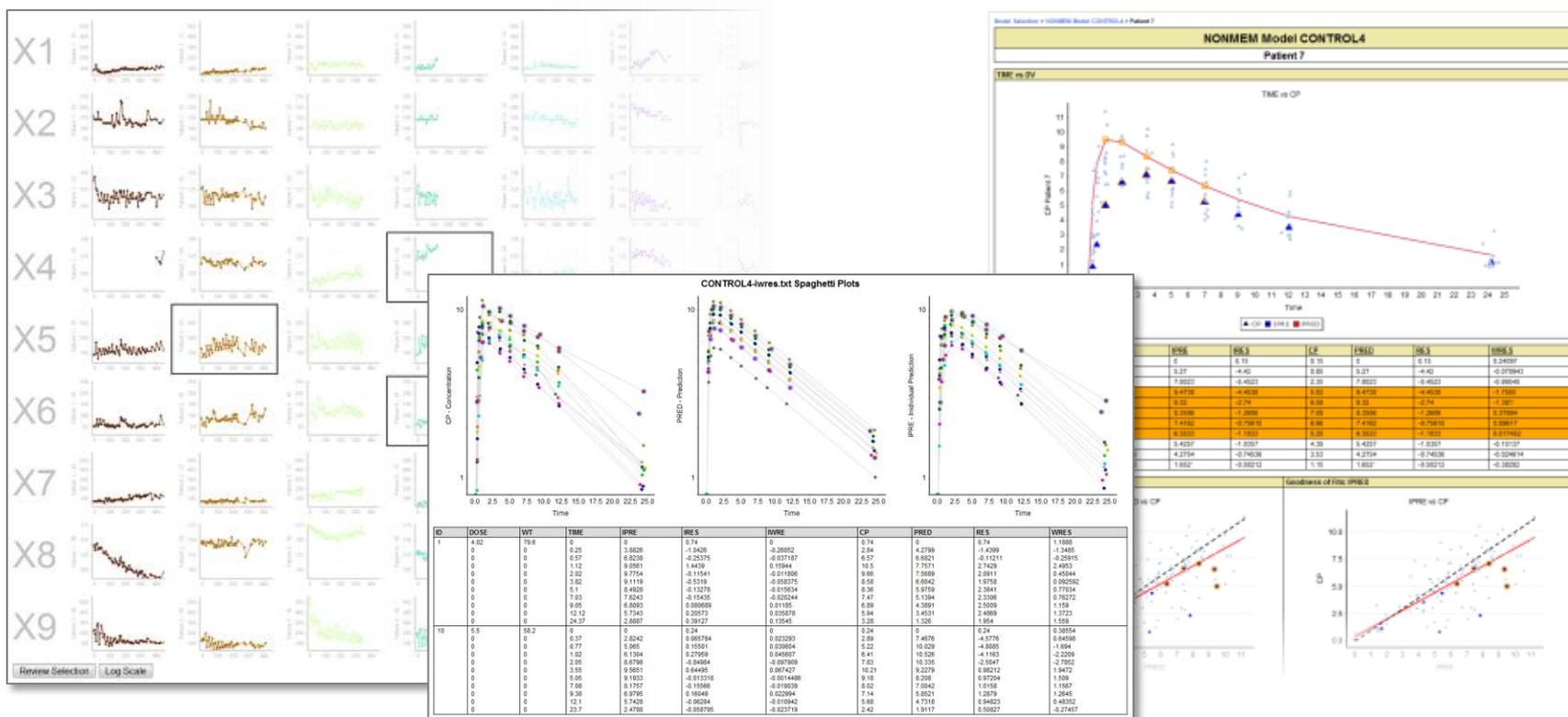
WinNonlin, Phoenix

Simcyp



With Pipeline Pilot

- Access disparate research data locked in silos
- Automate the scientific analysis
- Explore, visualize and report research results



Merge Data

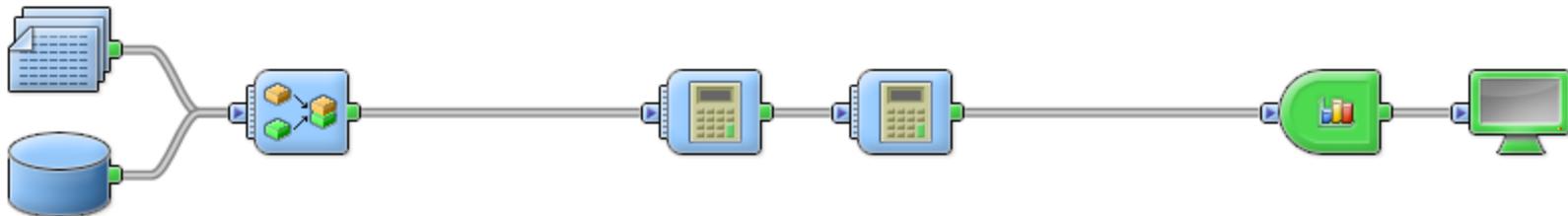
- Extract knowledge
- Fewer errors

Automate Applications

- Extract knowledge
- Fewer errors
- Save time
- Focus on Science

Report & Deploy

- Extract knowledge
- Fewer errors
- Save time
- Focus on Science
- Educate decisions
- Collaborate



Materials M&S



[Materials](#)

[Polymer Properties \(Synthia\)](#)

Life Science M&S



[Catalyst \(Pharmacophore\)](#)

[CHARMm \(Simulations\)](#)

Chemistry



[Chemistry](#)

[ADMET](#)

[Cheminformatics](#)

Biology



[Sequence Analysis](#)

[Gene Expression](#)

[Mass Spectrometry for Proteomics](#)

[Next Generation Sequencing](#)

Laboratory



[Plate Data Analytics](#)

[Analytical Instrumentation](#)

Imaging



[Imaging](#)

[Advanced Imaging](#)

Analysis & Statistics



[Modeling](#)

[Advanced Modeling](#)

[R-Statistics](#)

Document Search & Analysis



[Text Analytics](#)

[Chemical Text Mining](#)

Database & Application Integration



[Integration](#)

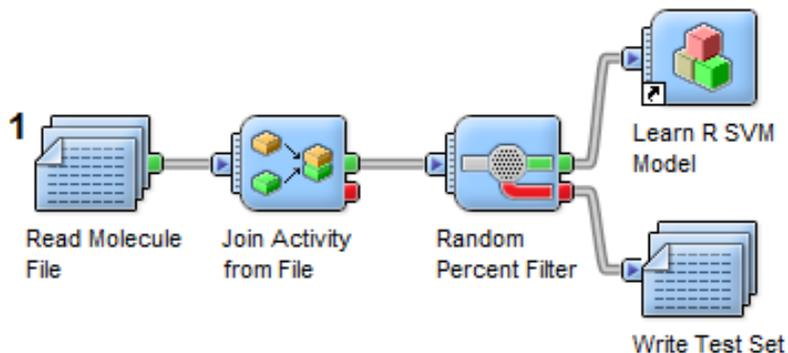
Reporting & Visualization



[Reporting](#)



(non R experts)
Scientists use R tools
without scripting

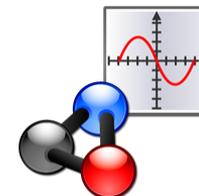


R experts customise R
script within Pipeline
Pilot

```
Script  
1 boxplot ($ (Y) ~ $ (Category),  
2   data = AllData,  
3   col = "$ (Box Color) ",  
4   main = "$ (Chart Options Title)" )
```

OK
Cancel
Apply
Help

Synergies between statistically-aware R & scientifically-aware Pipeline Pilot

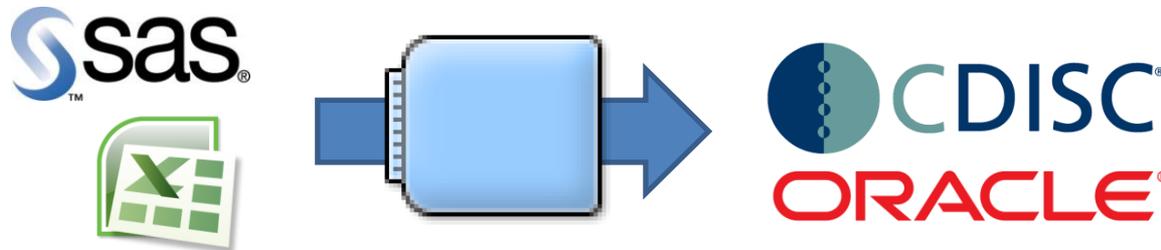


Population Pharmacokinetics with Pipeline Pilot

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- Acadia ClinPK internal PP development
- Transform and migrate human clinical trial data
 - From multiple locations, including SAS transport files and Excel spreadsheets
 - Into a consolidated CDISC* compliant Oracle database
 - Cross-study querying and reporting

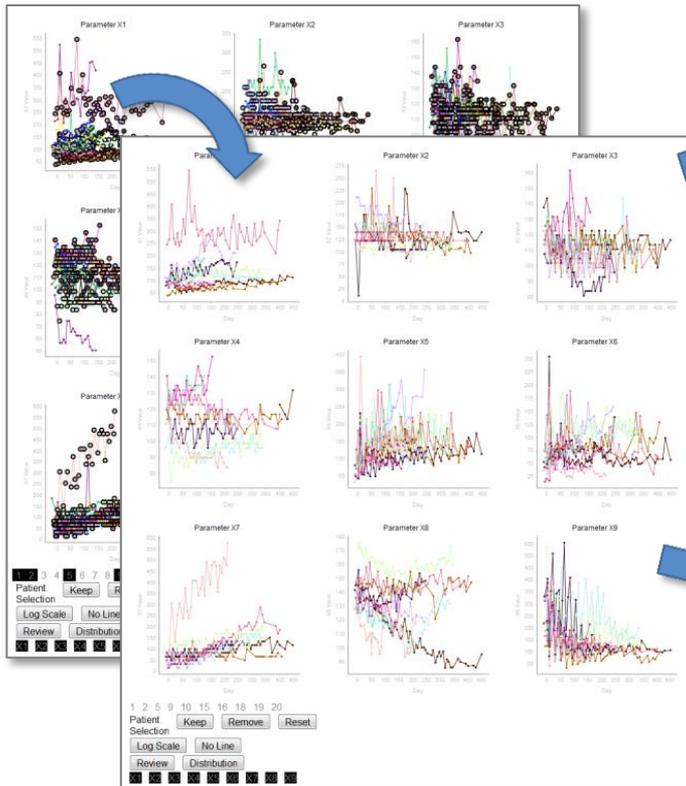


* CDISC = Clinical Data Interchange Standards Consortium

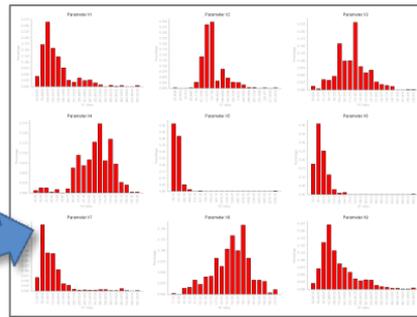
Use case 2 - Data Exploration

1. Data Overview

- Keep/Remove Patients
- Linear/Log Scale



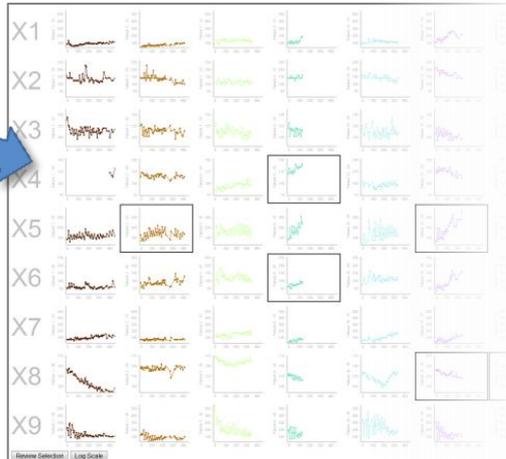
2. Data Distribution



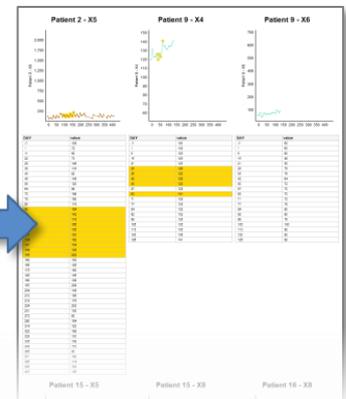
- Remove/keep outliers
- Select parameters
- Linear and log scales
- Show/hide lines

3. Patient vs Parameter

- Select to review in detail
- Linear/Log Scale



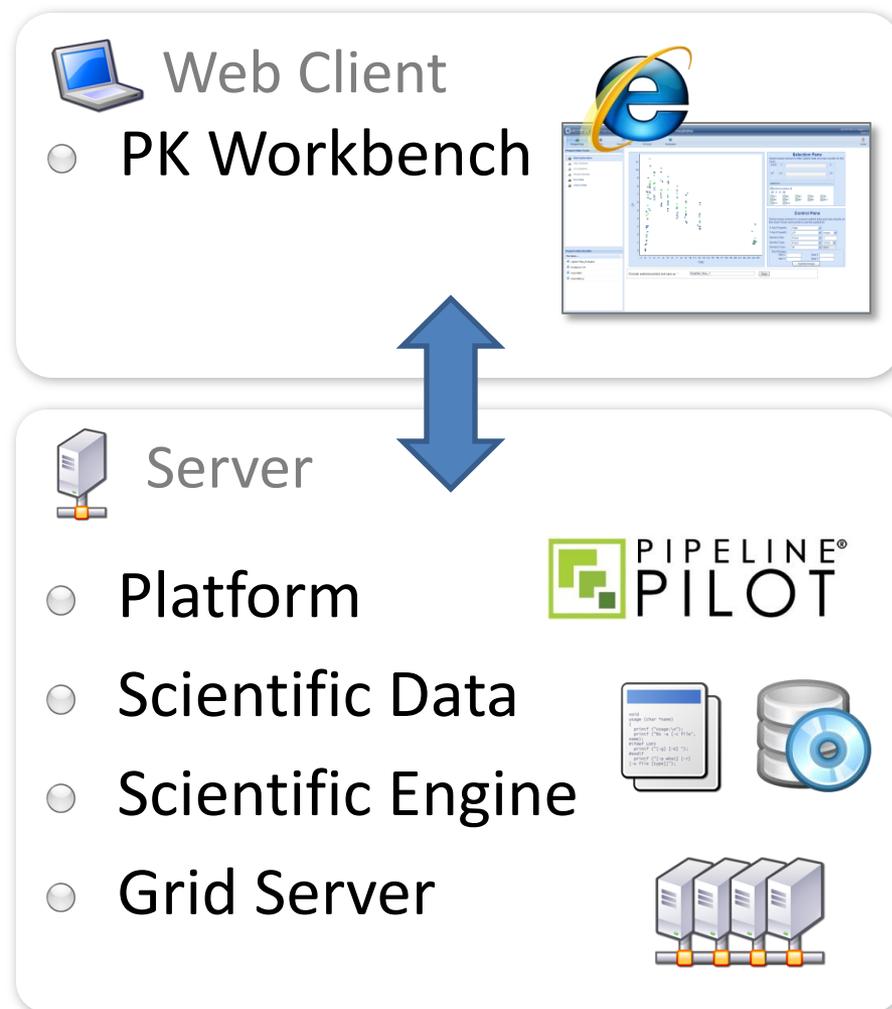
4. Data Details



Use Case 4 – Pharmacokinetics Workbench

- Web environment for modeling & simulation
- Create, share, run and compare models & scripts
- Track, log and replay!

- Enables capture and sharing of **best practice**
- Ensures **repeatability** by recording workflows
- Enables automation of workflow leading to **time saving**



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 - Extract knowledge
 - Fewer errors
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 - Save time
 - Focus on Science
- Explore, visualize and report research results
 - Educate decisions
 - Collaborate

Questions & Comments

Accelrys Web Site

 www.accelrys.com

Accelrys Community Forum

 www.accelrys.org

Accelrys Advantage

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