
Application of SIMDAT technologies in Pharma R&D

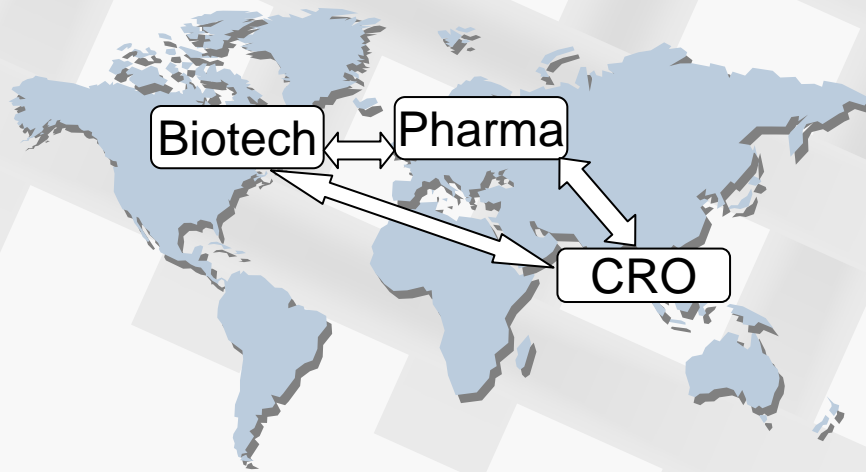
Moustafa Ghanem
Director of Research, InforSense Ltd

SIMDAT Pharma WP Partners

- Application partners
 - GSK
 - Galapagos (Inpharmatica)
 - EMBL Heidelberg
 - ULB
- Technology partners
 - IIT Innovation, University of Southampton
 - University of Karlsruhe
 - InforSense Ltd.
 - NEC Research Europe

Towards supporting key trends business trends in Pharma R&D

- **Virtualisation**
 - Strategy to tap into external knowledge and expertise through a network of external alliances sharing the risk, reward and control
- **Globalisation**
 - Strategy to be able to create organisational alliances with the wealth of knowledge development in the global market.



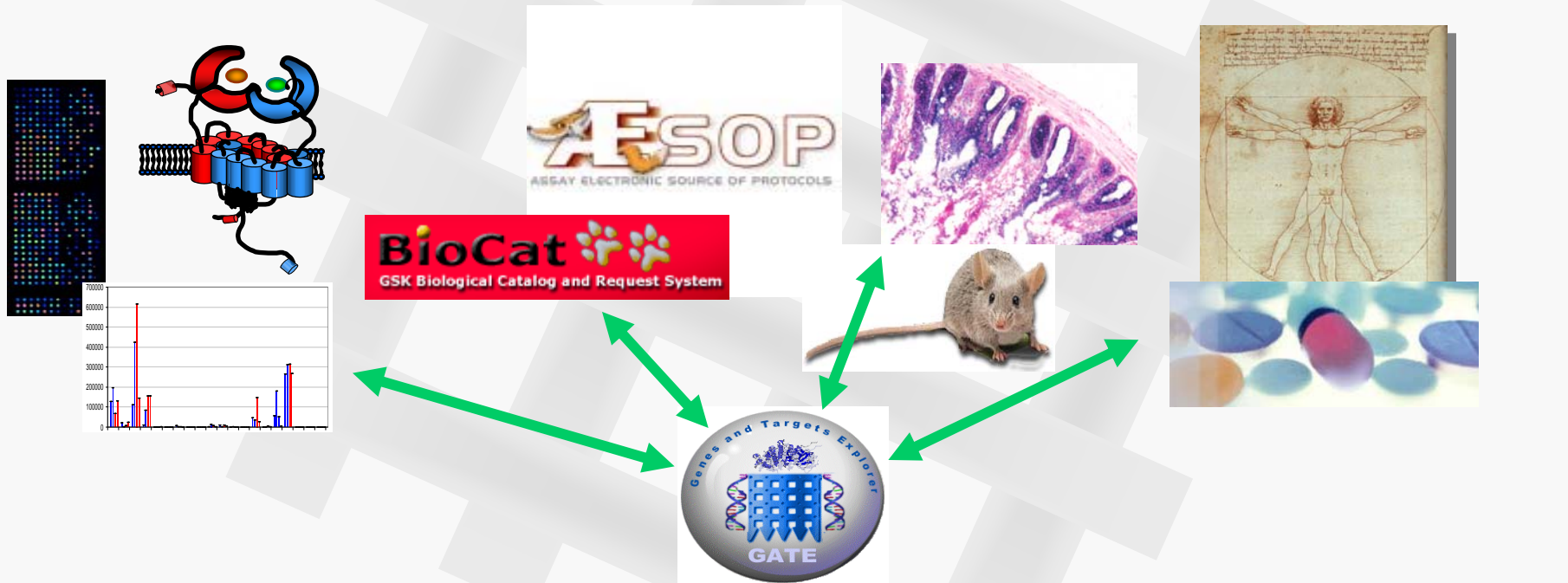
Pharma R&D: an informatics perspective

TARGETS

SCREENS

CANDIDATES

DRUGS

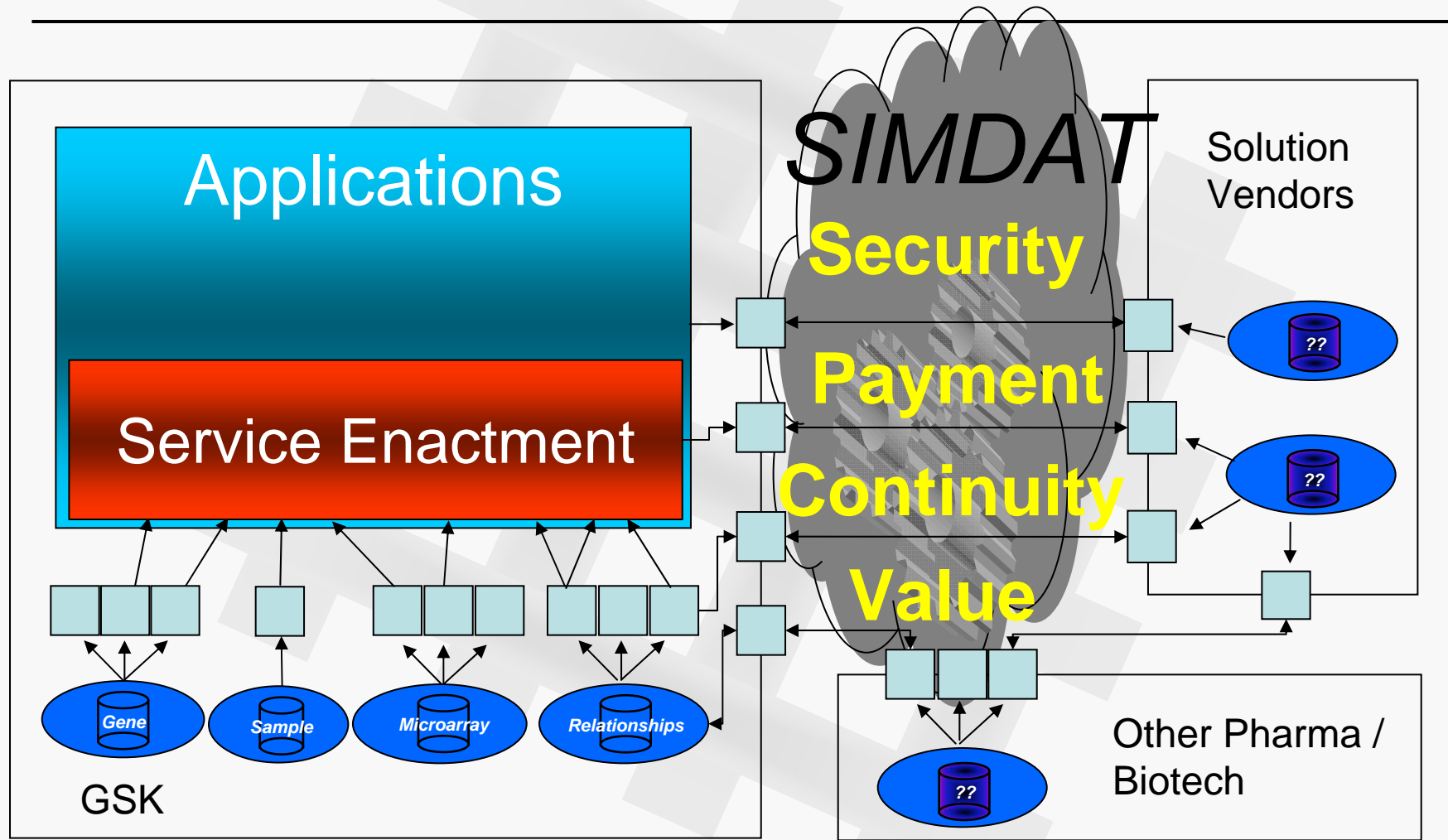


But all these tools are typically built and integrated only within the Organisation

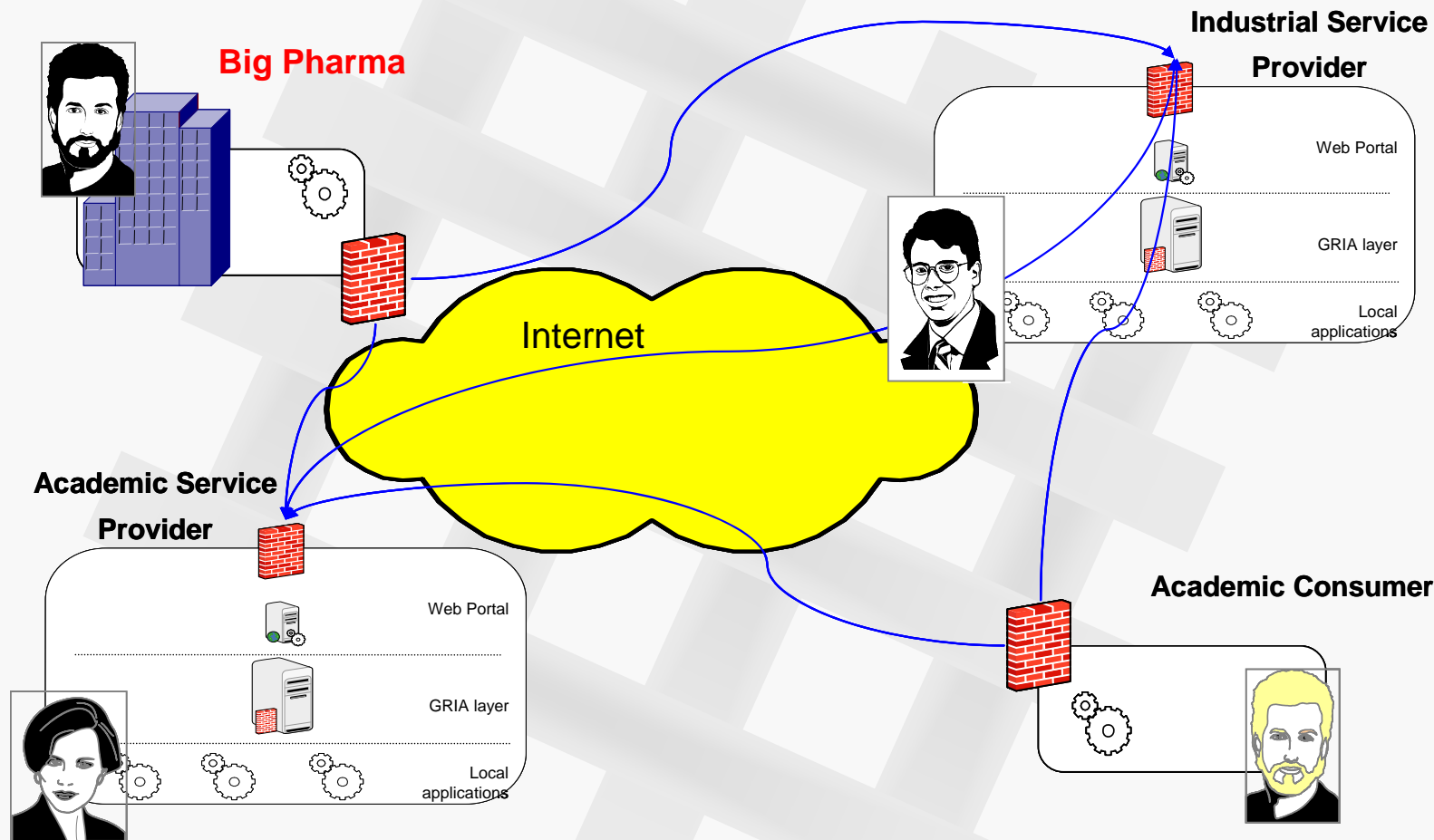
The informatics challenge

- Business trend is away from the “fortress” towards an “ecosystem”
- IT environments are not currently designed for this
- Significant overhead required to integrate this new approach into R&D processes
- Most IT solutions are “bolted on” to current infrastructure
- **SIMDAT technologies can now be used as a means to augment this Evolution**

The SIMDAT SOA Approach



SIMDAT: Business to Academic Prototype



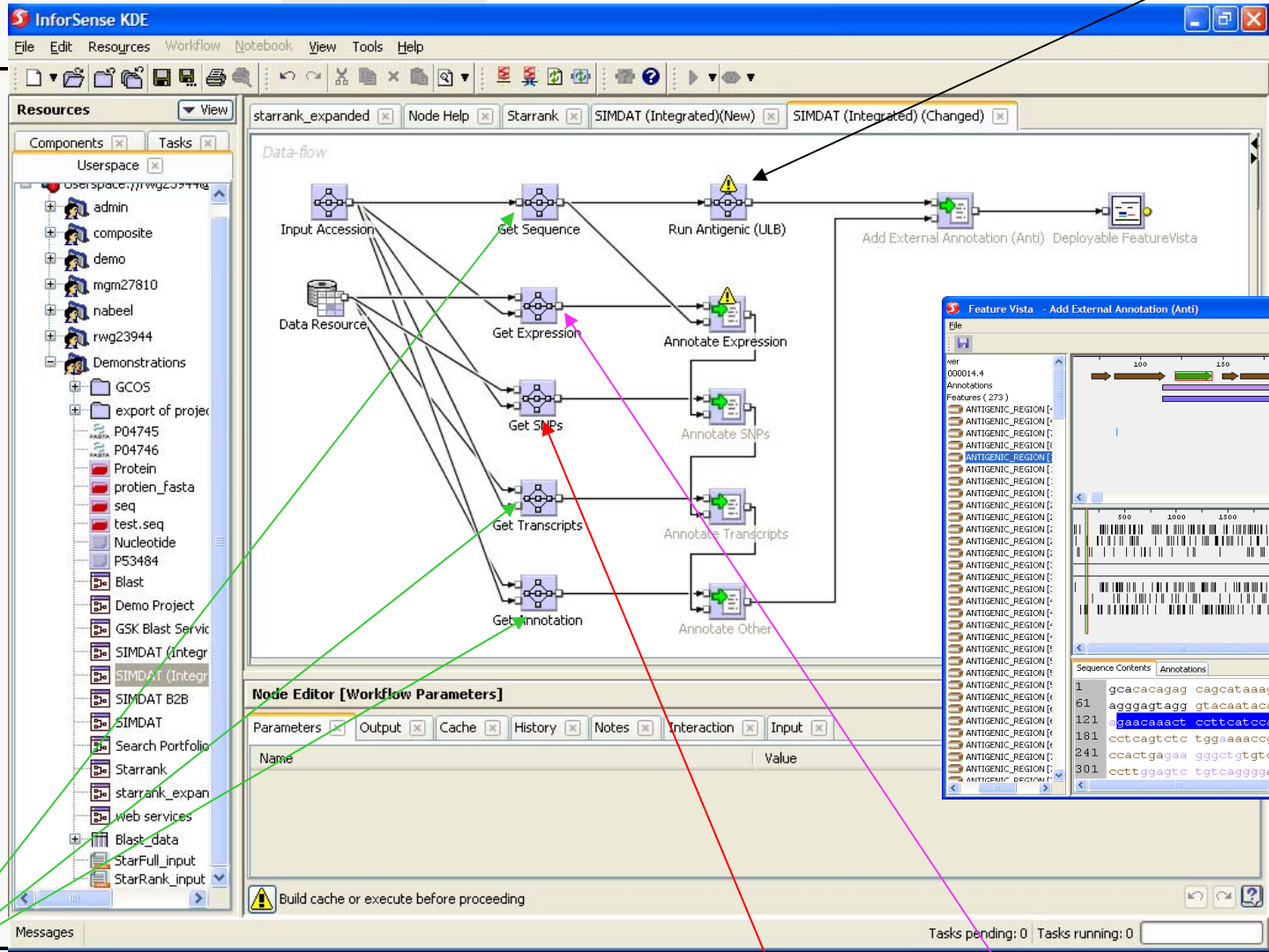
SIMDAT provides Pharma R&D with

- Framework for Service Consumption
 - Specialised Software Granularity
 - Data and Algorithm Services
 - Accounting and Consumption Model
 - Open Service Market
 - Service Orchestration
- Relationship Management
 - Good Fit with current partnering models
 - Focused Licensing
 - Zero Setup (reduce IT overheads in partnerships)
 - Negotiated Catalogue

The SIMDAT Prototype: Master Sequence Analysis Pipeline

- Prototype Virtualised Workflow
- Sequence analysis using both internal and external analysis tools
 - University of Brussels (ULB)
 - Sequence analysis tools
 - Galapagos (Inpharmatica)
 - Druggability portal

ULB (Resource Services)



GSK STV
(Gene Service)

GSK RTP
(Polymorphism Service)

GSK UM
(Expression Service)

Demonstration

Full demo webcast available on

<http://www.inforsense.com/company/webcasts>

Demonstration

SIMDAT: The GSK Experiences

- Initially a novelty – Now highly relevant
- Strong partnership with technology experts
 - Workflow
 - Service Orchestration
 - Security
- Ability to build “fit for purpose” demonstrators
- Applications immediately available within the organisation

Conclusions

- SIMDAT supports the move towards Virtualisation
 - Novel Tools & Contacts
 - Demonstrators of the service based approach
- Security requirements adequately addressed
- Grid Technologies lower the barrier of building a business relationship
- Access to new markets
- Faster deployment of analysis tools
- Development of new business Models

Acknowledgements

- Rob Gill – GSK
- John Armstrong - GSK
- Bart Ailey – formally GSK

- Nabeel Assam – InforSense

- David Gee – Galapagos (Inpharmatica)

- Richard Kamuzinzi - ULB

- Falk Zimmermann - NEC

- Mike Boniface et al – IT Innovation

Backup Slides

InforSense KDE

File Edit Resources Workflow Notebook View Tools Help

Resources View

Userspace x
Tasks x
Components x

- Import-Export
- Preprocess
- Normalization
- Statistics
- Association
- Classification
- Clustering
- Multivariate
- FeatureAnaly
- Assess
- BioSense
- Visualization
- TextSense
- Oracle
- SparseVector
- Utilities
- Deployment
- WebServices
- Reporting
- Scripting
- ControlFlow
- XML
- Gria

SIMDAT (Integrated) (Changed) x NetworksWareHouse x NetworksWareHouse_Table x SIMDAT (B2B) x

Data-flow

Actions View

Select Action...

Description...

Parameters

Execute

Node Editor [Add Annotation or Feature] Annotate Other View

Parameters x Output x Cache x History x Notes x Interaction x Input x

Name	Value
Type	feature
Sequence ID	TRANSCRIPT ACC
Feature Type	FEATURE TYPE

Locked. Maybe because a visualizer is open or a task is running.

Messages Add External Annotation (Anti) of SIMDAT (Integrated) (08:17:54.458 24/01/08) Failed Tasks pending: 0 Tasks running: 0

InforSense KDE

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SIMDAT (Integrated) (Changed) NetworksWareHouse NetworksWareHouse_Table SIMDAT (B2B) Group Node: Run Antigenic (ULB) (Changed)

Data-flow

```

    graph LR
      Input[abc def  
Input Text  
[Cached]] --> G1((G))
      G1 --> G2((G))
      G2 --> G3((G))
      G3 --> Read[Read File]
      Read --> Import[Import Text to Table (2)]
      Import --> Derive[Derive (3) (2) (3)]
      G3 --> G2
  
```

Sequence Collection to Text [Cached] Export Text to Server File [Cached] 888UploadDataStager [Cached] 888Execute Job [Cached] 888DownloadDataStager

Read File Import Text to Table (2) Derive (3) (2) (3)

Actions View

Select Action...

Description...

Parameters

Execute

Node Editor [Workflow Parameters] View

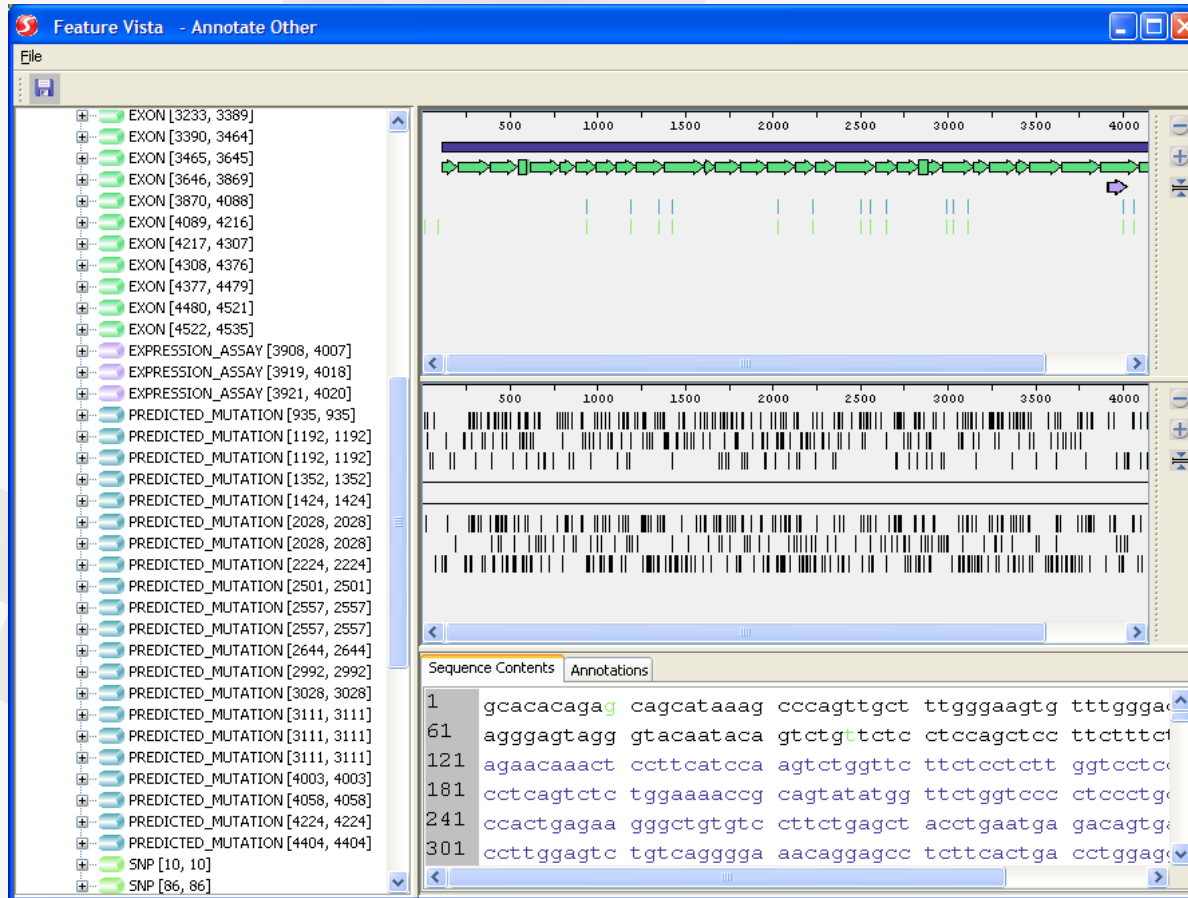
Parameters Output Cache History Notes Interaction Input

Name	Value

Build cache or execute before proceeding

Messages Add External Annotation (Anti) of SIMDAT (Integrated) (08:17:54.458 24/01/08) Failed Tasks pending: 0 Tasks running: 0





Resources

View

Components Tasks

Userspace

- mgn27810
- nabeel
- rwg23944
- Demonstrations
- GCOS
- export of project start
- P04745
- P04746

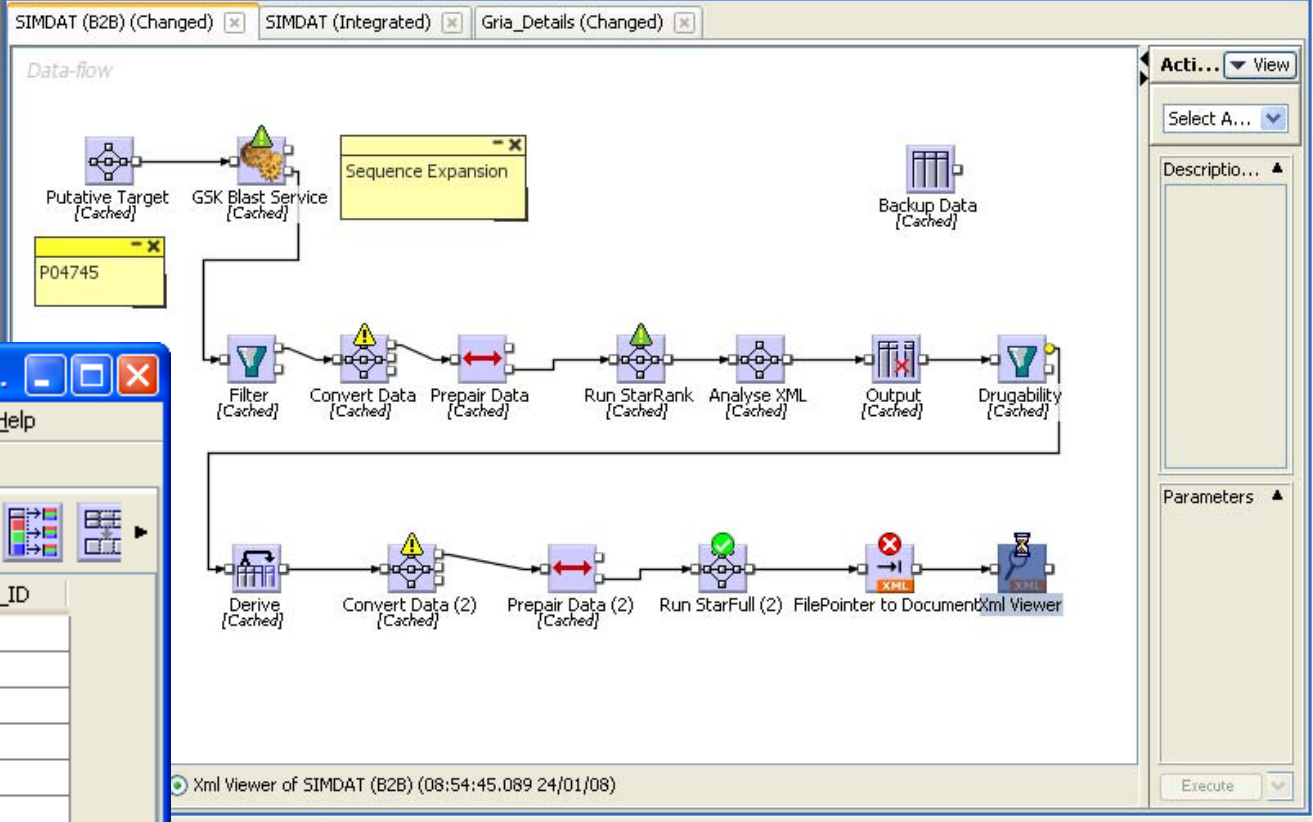


Table Editor - launched fr...

Graph DataSet Selection Tools Help

Table Editor Statistics Summary

Item	Rank	Taxon_ID
P04745	1	9606
P19961	1	9606
P04746	101	9606
P00690	1	9606
P00687	1	9606
P00688	1	9606
P00689	1	9606
P83053	1	9606

Displaying 8/8 rows (24 cells)

Undo Cancel Commit

Viewer] Xml Viewer

View

Output Cache History Notes Interaction Input

Failed

Tasks pending: 0 Tasks running: 0