

Extensible Informatics

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Limitations of Current Products

- Narrowly Scoped
 - Registration
 - HTS
 - In-vivo
- Insufficiently flexible
 - Difficult to incorporate
 - New science
 - New processes
 - Processes change to fit product
 - Product does not change to fit process
 - Aka “shoehorning”
- Do not address operational needs

• Drug Discovery: A Multi-Faceted Domain •

- Assay Complexity and Organization Is Extremely Varied
 - HTS:
 - Small number of technologies/SOP's
 - Simple system
 - Many compounds
 - Cell Based
 - Varied procedures
 - Few compounds
 - Multiple "targets"
 - In Vivo
 - Complex system
 - Multiple formulations
 - Varied readouts
- Salient Features Change as the Compound Nears The Clinic
 - Structure/salt-Form
 - Formulation
- Relevant science changes over time
 - New assays/measurement
 - New paradigms e.g. pathway based analysis

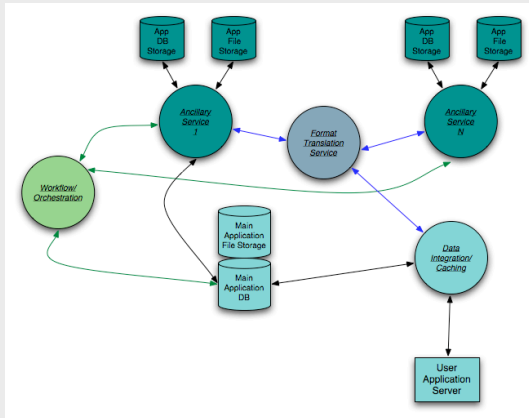
Desired Characteristics

- Flexible
 - Extensible core entities
 - Support multiple, overlapping hierarchies
 - Ability to adapt to changing scientific needs
 - Play well with others
 - Will not be the only application
 - May not even be the core application
- Integrateable Architecture, Integrated Operation
 - Security
 - Event queues
 - Workflow
 - Rules engines
 - Clear transaction model
- Integrateable Data
 - Unique, stable identifiers
 - Support cross system identifier synonyms
 - E.g., x in system A == y in system B

Principles

- Convention over configuration
- Modular, extensible, even at the DB level
 - Core entity tables, with (almost) no foreign keys
 - No forced hierarchy/relationship
 - Hierarchy handled by join tables
- Operational debugging/diagnostics
 - Logging of time for execution
 - Operation performed
 - Tunable log level
 - Time line analysis
 - Early warning systems
- Monitoring and management via web interface
 - Quickly reflect changes in code tables etc..

Operation



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