The fastest, most productive way for life sciences research groups to find the optimal lead.
To make critical decisions, users need to
- Overview
- Query
- Drill down

To make critical decisions, users need
- Domain specific tools
- Task Specific tools

Data is located everywhere within and outside the enterprise. Users need access to
- Any data source
- From any where
- without any programming.
Premium eAnalytic Application for Lead Discovery

Helps researchers decide “What do we test next?”

...make next?

What’s the next best step?

What data do I have?

What do others know?

Compound profiling, Structure browsing
Data mining

Decision

ISIS
Oracle
IDdb3
Spotfire role-configured e-Analytic application

Featuring a web-enabled collection of
- High impact analytics for compound profiling
- Information interaction services

And
- Spotfire’s dynamic user experience
Spotfire DecisionSite

Information interaction services
Role-based services

Patented visualization engine and interactive displays

Query Devices
1 Item Slider
2 Range Slider
3 Radio Buttons
4 Full text search
5 Check Boxes

Details-on-Demand Window

Legend

Visualization Window(s)
**High impact analytics for compound profiling**

- Structure search proprietary, commercial and web sources
- Compound profiling and structure data mining
  - Cross assay analysis
  - Structure-based analysis
  - List management
  - Data reduction methods
    - Cluster analysis
- Analyze the results of Rgroup decomposition
- High quality SAR reports
High impact analytics for compound profiling

Which compounds have profiles similar to this lead?

Which compounds in the corporate library contain this substructure?

What is the optimal incubation time for this new assay?

How do the hits in these assays compare structurally?

Do similar compounds show up in MDDR or CMC?
Information interaction services

- Retrieve information from multiple critical sources
  - Oracle
  - ISIS

- Merge new information into your data set
  - New columns
  - From local files or database

- Access Web sources, such as IDdb3
Which compounds tested in this assay have this substructure?

Show me all the hits in this assay

Are the hits structurally similar?

Show me the results for these plates

Show me last night’s results
Now let’s take a closer look...
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Query structure data

- ISIS formatted databases
  - ISIS/Base
    - Project DBs
  - ISIS/Host
    - Corporate DB
    - Inventory
    - Commercial
      - E.g. MDDR, CMC, ACD, …

- Search types
  - SSS, SIM, ID
- Portfolios become central
  - Store ISIS results
  - Store ABase results
- List management
  - Boolean operations
  - Familiar drag/drop operations
  - Persistence
- Easily view the structure for any stored compound or list
High Quality SAR Reports

- Organize and report results
  - Sortable
  - Printable

- Select columns
  - Choose columns from DecisionSite
  - Choose fields from ISIS

- Support for 3rd party chemically aware spreadsheet
  - ISIS for Microsoft Excel

SAR reports in Excel
Vector drawings provide clarity
Analytical methods: Cluster analysis

- Hierarchical clustering
- Data
  - Column data
  - ISIS structure keys
- Bi-directional clustering
- Auto-creation of information rich views
  - Heatmaps
  - Parallel coordinate charts
  - Trellis plots
- Auto creation of new query devices

- Methods
  - Complete and single linkage
  - Wards method
  - Weighted and unweighted average methods
- Distance metrics
  - Correlation (signed and unsigned), Cosine, Euclidean, CityBlock, Tanimoto
- Normalization
  - Z-score
  - STD
  - Simple scaling
  - No normalization
- Formats
  - Tall/skinny
  - Short/wide
Current Drugs IDdb3 patent and literature info

Find information on related projects and compounds

• Search IDdb3
  • Drug name or synonym
  • Supports IDdb3 structure search

• Retrieve
  • Drug reports
    • Patent references
    • Synthesis
    • SAR
    • Pharmacology
    • Metabolism
    • Toxicity
    • Clinical reports
    • Bioactivity listings
  • Patent reports

Find information on related projects and compounds
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Information Interaction Service

- Allows end users to ask and save complex database queries with no knowledge of SQL
  - Static
  - Parametrized queries
  - Sequential queries
  - Source transparency
- Information Library preconfigured for ActivityBase
  - Sequential queries
- Define Information Library targeted to custom databases
Query biology data

• An example:

**ActivityBase schema**

- Select
  - Study
  - Protocol
  - Run

- Filter options
  - Completion Date
  - Plate ID
  - Compound ID
  - Value range

- Data formats
  - Pivot function
- Access to any information sources
  - Cut & Paste, Text files, Excel files, Access databases, ODBC database access, OLEDB database access, Oracle/Sybase/SQL Server,
- Integrated data conditioning
- Role based information access
- Programming Interface
- Web based administration tool for designing and maintaining the Information Interaction Model
- Map of databases
- Element workbench
- Map of Information Interaction Model

Source databases
Tables and Columns
Element definition instructions
Information Interaction Model

Workbench UI for each interaction element
Reporting information

- Word
- Web
- PowerPoint
Configured to suit your best practices

- **API**
  - New methods
  - New data sources
  - New best practices

- **Extensible**
  - Added by Spotfire Professional Services
  - Added by your own developers
• **Spotfire role-configured e-Analytic application**

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  - Information interaction services

  And
  - Spotfire’s dynamic user experience
Spotfire’s Newest View Types help you make sense of the results of your data

- Heatmaps
- Parallel coordinate plots
- Trellis plots
Data-driven visualizations

Profile compounds across experiments

Automatically generated visualizations based on user-specified data format and selected analysis options

Assess relationships among variables as well as among compounds
● **Spotfire role-configured e-Analytic application**

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DecisionSite for Lead Discovery benefits

- Simplified access to critical primary and secondary data
- High impact analytics for compound profiling
- List management including list logic
- Ability to communicate results via SAR reports, Web reports, dynamic presentations, Word and Powerpoint export
- Analytical power of Spotfire visual discovery
DecisionSite for Lead Discovery benefits

- Most useable and flexible end-user analytic environment in Life Sciences

- Programming-free database queries and data integration

- Open, flexible, and configurable for rapid integration with other environments

- Only Web-delivered analysis environment updated quarterly

- Only “New Leads Discovery” solution with support for microarray analysis, and clinical trial analysis
Role-based services across discovery

- **Genomics**
  - Expression analysis

- **Lead Discovery**
  - SAR

- **Chemogenomics**
  - SER
    - Structure Expression Relationships
    - Toxicity Profiling
    - Differential expression in response to exogenous compounds

- **Clinical studies**
  - Trial data analysis
Spotfire® DecisionSite for Lead Discovery™.