From Custom R&D Web Implementations to Fully Operational E-commerce Sites: Technology and Examples

Sheila Ash, Judith Bandy
Agenda

From Custom R&D Web Implementations to Fully Operational E-commerce Sites: Technology and Examples

• Needs for e-R&D and e-commerce
• Pharmacopeia e-Solutions
• Variety of Examples
According to a study of large and medium-sized U.S. corporations by GartnerGroup, the average cost of a commerce-enabled Web site is US $1 million, with 79 percent of the costs going toward labor.

Today's question:
According to the study, what is the average amount of time it takes to build an e-commerce Web site from start to finish?

Related Web site:
http://www.gartnergroup.com

©1999 Rick Broadhead/XPLANE Corp. Distributed by United Feature Syndicate, Inc. 10/25a

graphics by xplane.com
What is the Need?
e-commerce

- Business to Business e-Commerce to Reach $8.5tn in 2005 - Gartner
- Sigma-Aldrich Internet Website
  - Today accepts orders of $2.5m/month = 5% sales
  - Expects to handle 50% sales through site by end 2003
e-R&D

“"If the industry is to exploit the real power of e-R&D, it must invest in innovative new technologies, build networked organizations and harness its knowledge capital.”"

- Pharma 2005. Silicon Rally: The Race to e-R&D - PriceWaterhouseCoopers
- E-R&D: computerisation of the R&D process
Issues Facing...

Chemistry Vendors

• You need to provide customers with easy access to chemical data
• Your company’s needs are unique - you require cost-effective custom applications
• You need fast, cost-effective deployment and easy learning for customers
Issues Facing...

Discovery Operations

• Your scientists and managers need easy access to chemical and biological data in Oracle
• Your company’s needs are unique - you require cost-effective custom applications
• You need fast, cost-effective deployment and easy learning for users
What is the Solution?
Enterprise Solutions based on RS³ Discovery

• ORACLE Database Server
• Chemistry and Biology Search Engine
• High Performance, Open, Scalable Architecture
• Enterprise-wide Information Management Solutions

RS³ Powered Solutions

RS³ Discovery Server

ORACLE 8

Synopsys, Oxford Molecular, MSI. Subsidiaries of Pharmacopeia, Inc.
RS³ Intranet Application Builder

• Add-on module for RS³ Discovery / HTS
  – Enables you to build and deploy chemically-aware browser-based applications
  – Enables you to easily create your own intranet applications that meet your exact needs

Solutions
RS³ IAB Applications

Technology
Web Server
RS³ Discovery Server
ORACLE 8
RS³ IAB

• You need:
  – A web server
  – Some knowledge of HTML and Oracle
  – Some programming ability / enthusiasm
  – User-machines with Web Browsers (PC or Mac)
RS3 IAB

• Create HTML pages with any HTML editor
• Appearance, layout, style etc exactly as you want them
• Page content is dynamic - write HTML pages & insert tags where data is required
• Java Server Pages (JSP) tag library provided
RS³ IAB - JSP Tag Library

• Java Server Pages (JSP) tag library manages:
  – Oracle & RS³ connections, the chemical database functions
  – Execution of SQL statements & stored procedures
  – Access & display of chemical structures
  – Transfer of data between pages
  – Simple programmatic constructs like loops and decisions

...<tr>
  <td style="border-bottom:solid 2px; border-right: hidden">STRUCTURE: </td>
  <td style="border-bottom:solid 2px">
    <oxmol:DisplayMol id="compDisp" structure="<%=compstructure%>" width="200" height="150" allowEdit="false"/>
  </td>
</tr>…
Key Concepts

• A Java Server Page is a HTML page + JSP file extension
  – Java can be embedded. Server-side HTML tags can be embedded.
  – Is compiled by JSP Servlet Engine into a Java Servlet.

• A Java Servlet is a Server-side Java program.
  – Only one instance of a Servlet resides in memory.
  – A call is made to a servlet for each HTTP request.
  – A Servlet is multi-threaded.

• A Servlet Engine
  – A Java program that manages multiple Servlets.
  – Acts as an intermediary between a Servlet and the Web Server
A traditional Intranet

HTTP request (URL) sent to web server

Web server locates page from URL

HTML Pages

Page posted to the browser
JSP Operation

HTTP request (URL) sent to web server

Web Server delegates request to JSP engine

Servlets

Servlet negotiates with database

Corporate Oracle Database

HTML Page + Java Code Compiled into a Servlet

Web Server

Servlets

HTML sent on to the browser

HTML passed on to the web server
RS³ IAB: Advantages of JSP

• You develop HTML pages
• You concentrate on presentation not content generation
• Pages are auto-compiled into Servlets for efficiency
• Can mix’n’match with other tag libraries and Servlets
• It is an industry standard
RS³ IAB: benefits

• Quick and easy to build your own, custom cheminformatics applications
  – Precisely fit your needs
  – Easy to change
  – Excellent for creating task specific applications
  – Cheap to deploy
  – Integrate with other resources on the company Intranet
Intra/Internet Applications
Chemistry & Biology Workflow

HTS
Secondary
*In vivo*

- Assay Plate/Matrix Setup
- Data Capture
- Calculation
- Data Reduction
- Validation
- Robotics
- Plate Formatting
- Curve Fitting
- Data Analysis and Posting
- lead Compound Drug Candidate

- Batch Tracking
- Compound Management
- Analysis

- Natural Products
- Single Synthesis
- Generic Structures Polymers
- CombiChem Synthesis
- Registration
- Compound Catalogs
- Formulations
- 3rd party Collaboration

- Assay Protocols
- Database Setup

- Natural Products
- Lead Compound Drug Candidate
Where Our Applications Fit

- CombiChem
  - Single Synthesis
  - Generic Structures
  - Polymers
  - Natural Products

- Sigma-Aldrich
  - Formulations
  - 3rd party Collaboration

- Specs

- Ferring
  - Assay Protocols
  - Assay Plate/Matrix Setup

- Rs3 Inventory
  - Database Setup
  - Robotics

- Screening
  - Data Capture
  - Calculation
  - Data Reduction
  - Validation

- HTS Secondary
  - In vivo

- Analysis
  - Compound Selection
  - Data Analysis and Posting

- Lead Compound Drug Candidate
Exploiting RS$^3$ Discovery Architecture
Sigma-Aldrich

Synopsys, Oxford Molecular, MSI. Subsidiaries of Pharmacoepia, Inc.
Chemistry/Substance: pyridine

Registration Date: 2000-02-28T12:13:00

Show Audit  Show Properties  Show Security
Combichem

Synopsys, Oxford Molecular, MSI. Subsidiaries of Pharmacopeia, Inc.
Inventory
From this page you can retrieve information about plates stored in our central RS³/FLIMS database.

Get information about a plate:

Please choose the plate ID using the "Scientist" and "Notebook Reference" buttons, select the plate wells you want to retrieve information about, then press the "Retrieve Plate" button.
Screening

Send Request To:

Items Required: List2 - Project002

Format of Samples: 96 Well Plate (IC50)

Required For: IC50

Required By Date: Priority (5 working days)

Send Order To: Default user name

Change lists: 

View Orders: 

Oxford Molecular
Solutions for Discovery Research

Synopsys, Oxford Molecular, MSI. Subsidiaries of Pharmacopeia, Inc.
SpecsNet

Synopsys, Oxford Molecular, MSI. Subsidiaries of Pharmacopeia, Inc.
<table>
<thead>
<tr>
<th>Structure</th>
<th>Compound ID</th>
<th>Availability</th>
<th>Amount</th>
<th>Price</th>
<th>In Basket</th>
<th>Add</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image1" alt="Structure" /></td>
<td>AA 516259012161</td>
<td>1180 mg</td>
<td>100 mg</td>
<td>USD 118.00</td>
<td>100 mg</td>
<td><img src="image2" alt="Add" /></td>
</tr>
</tbody>
</table>

**Molecular Weight:** 224.28

**LogP:** 1.19

<table>
<thead>
<tr>
<th>Structure</th>
<th>Compound ID</th>
<th>Availability</th>
<th>Amount</th>
<th>Price</th>
<th>In Basket</th>
<th>Add</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image3" alt="Structure" /></td>
<td>AA 516259012168</td>
<td>1232 mg</td>
<td>100 mg</td>
<td>USD 116.00</td>
<td>100 mg</td>
<td><img src="image4" alt="Add" /></td>
</tr>
</tbody>
</table>

**Molecular Weight:** 155.19

**LogP:** 0.97

<table>
<thead>
<tr>
<th>Structure</th>
<th>Compound ID</th>
<th>Availability</th>
<th>Amount</th>
<th>Price</th>
<th>In Basket</th>
<th>Add</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image5" alt="Structure" /></td>
<td>AR 35238316170</td>
<td>244 mg</td>
<td>0 mg</td>
<td>USD 6.00</td>
<td>0 mg</td>
<td><img src="image6" alt="Add" /></td>
</tr>
</tbody>
</table>

**Molecular Weight:** 268.34

**LogP:** 2.54

<table>
<thead>
<tr>
<th>Structure</th>
<th>Compound ID</th>
<th>Availability</th>
<th>Amount</th>
<th>Price</th>
<th>In Basket</th>
<th>Add</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image7" alt="Structure" /></td>
<td>AC 3075909764</td>
<td>347 mg</td>
<td>100 mg</td>
<td>USD 116.00</td>
<td>100 mg</td>
<td><img src="image8" alt="Add" /></td>
</tr>
</tbody>
</table>

**Molecular Weight:** 293.94

**LogP:** 3.64

<table>
<thead>
<tr>
<th>Structure</th>
<th>Compound ID</th>
<th>Availability</th>
<th>Amount</th>
<th>Price</th>
<th>In Basket</th>
<th>Add</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image9" alt="Structure" /></td>
<td>AC 9075909492</td>
<td>265 mg</td>
<td>0 mg</td>
<td>USD 6.00</td>
<td>0 mg</td>
<td><img src="image10" alt="Add" /></td>
</tr>
</tbody>
</table>

**Molecular Weight:** 244.63

**LogP:** 2.35

<table>
<thead>
<tr>
<th>Structure</th>
<th>Compound ID</th>
<th>Availability</th>
<th>Amount</th>
<th>Price</th>
<th>In Basket</th>
<th>Add</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image11" alt="Structure" /></td>
<td>AC 9075909632</td>
<td>15 mg</td>
<td>0 mg</td>
<td>USD 6.00</td>
<td>0 mg</td>
<td><img src="image12" alt="Add" /></td>
</tr>
</tbody>
</table>

**Molecular Weight:** 210.19

**LogP:** 1.81
Summary

• Complements existing tools and applications
  – Easy to build simple interfaces for specific tasks

• Puts you in control
  – Create your own company-specific tools, change them as often as you need

• Make data available where it is needed
  – Build your own “cheminformatics data portal”

• Cost-effective
  – Development is fast
  – Easy to deploy to every desktop
  – Short learning curve for users
According to a study of 350 sites by GartnerGroup, the average site is US $1 million, with 79 percent of the costs going toward labor. According to a study of large and medium-sized U.S. corporations by GartnerGroup, the average cost of an e-commerce-enabled Web site is US $5.4 million, with 79 percent of the costs going toward labor.

Today's question:
According to the study, what is the average amount of time it takes to build an e-commerce Web site from start to finish?

Answer: 5 months
Advantages of RS³ powered Intranet and Internet Applications

• Fast and Easy to Develop
  – simple applications take a few hours

• Fast and Easy to Deploy
  – no need to modify user’s desktop

• Browser-based Applications are Easy to Learn
  – data made accessible

• Applications Meet Organisation's Requirements
  – no shrink-wrapped constraints
sash@oxmol.co.uk
jbandy@oxmol.co.uk
mherron@oxmol.com

Pharmacopeia Cheminformatics
sash@oxmol.co.uk
jbandy@oxmol.co.uk
mherron@oxmol.com

Pharmacopeia’s Software Division