Riding the Mobile Wave

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It'll simplify a lot of tasks you never had to do before.
Presentation Agenda

• Background

• Mobile-to-cloud Infrastructure

• App examples w/demos

• Lessons learned
Apple's iPad Sales Blow Past Projections

San Jose Business Journal  March 14, 2011

Apple sold 14.8M iPads in 2010

During the release of the iPad 2 in March 2011, Steve Jobs said that just under 15 million iPads had been sold in the device’s first nine months on the market — more than all other tablet PCs combined.

Apple iPad Sales Projected to Hit 28 Million in 2011

http://tech.fortune.cnn.com/2010/10/05/how-many-ipads-has-apple-really-sold/
Mobile-Cloud Infrastructure

- Internet Connection (Wi-Fi or 3G)

- **Database/WebServer** (e.g. kinasedata.com: GoDaddy/HostGator)
  - Apache + php
  - mysql

- **StructureSearch/Application Server** *(Amazon Cloud-LAMP)*
  - Apache + php, EC2 instances
  - mysql, RDS instances
  - ChemAxon JChem + JChemWebServices (includes tomcat/axis2, etc.)
  - Chemene JSDraw (javascript)/ MMDS (objective-C library)

- RICE.....
In January 2008, Amazon announced that the Amazon Web Services consume more bandwidth than its entire global network of Amazon.com retail sites.

Source: http://aws.typepad.com/aws/2008/05/lots-of-bits.html
Nov 1, 2010: Amazon announced AWS Free Usage Tier

New AWS customers will be able to run a free Amazon EC2 Micro Instance for a year, while also leveraging 5 GB of Amazon S3 storage, and free tiers of Amazon Elastic Block Store, Amazon Elastic Load Balancer, and AWS data transfer.
Cloud Computing - In Practice

### Amazon EC2 Console Dashboard

#### Getting Started

To start using Amazon EC2 you will want to launch a virtual server, known as an Amazon EC2 instance.

- **Launch Instance**

**Note:** Your instances will launch in the US East (Virginia) region.

#### Service Health

<table>
<thead>
<tr>
<th>Current Status</th>
<th>Details</th>
</tr>
</thead>
<tbody>
<tr>
<td>Amazon EC2 (US East - N. Virginia)</td>
<td>Service is operating normally</td>
</tr>
</tbody>
</table>

- **View complete service health details**

### My Resources

You are using the following Amazon EC2 resources in the US East (Virginia) region:

- 1 Running Instance
- 1 Elastic IP
- 1 EBS Volume
- 4 EBS Snapshots
- 2 Key Pairs
- 2 Security Groups
- 0 Load Balancers

### Related Links

- Documentation
- All EC2 Resources
- Forums
- Feedback
- Report an Issue

### My Instances

- **EC2 Instance:** i-294bf742

**Description**

Graphs are for 1 instance that has monitoring enabled. Times are displayed in UTC.

**Time Range:** 0 last hour

- **Avg CPU Utilization (Percent)**
- **Avg Disk Reads (Bytes)**
- **Avg Disk Writes (Bytes)**
- **Max Network In (Bytes)**
- **Max Network Out (Bytes)
Eidogen-Sertanty’s iPhone and iPad Apps

* Reaction101 and Yield101 - built collaboratively with Molecular Materials Informatics, Inc.*
Welcome back to iKinase!

With iKinase update 5 and having registered, you have access to over 500K datapoints! Max: 8.92

Be sure to check out the new MobileReagents integration. Simply touch-hold briefly on a structure to see the MobileReagents menu item. If you don’t have MobileReagents on your device, you can download it for free in the App store.

PKC [Cell-Based Assay]...
Cytotoxicity Activity (HeLa S3 Cells) cytotoxicity 0.004 nM (pval: 11.388)

SLK
Inhibition of SLK Kinase Activity
Kd 0.00002 uM (pval: 10.699)
iKinase iPhone Demo
iKinasePro (iOS4 and iPad) - 3/10 (v1) ... 6/11 (v5.51)
iKinasePro (iOS4 + iPad) Demos

http://www.youtube.com/watch?v=p_wyys4Tkxk
Accessing TIP content through iProtein

Through iProtein, the TIP database can be surveyed by Sequence, Structure/Model, Site, head-nodes (i.e., protein family), and by bound ligand structure searches. Simply click on any image in the main page to initiate a search. Future versions of iProtein may enable more complex searching – e.g., protein structure search, site-search, etc. So stay tuned....

Structure/Model Searches (cont)

Click on the arrow (when present) to see more data. You can click the arrow (“>”) to see more detail. If there is a bound ligand, you can initiate ligand-based searches.
iProtein iPad Demo
Mobile Reagents (iOS4) - 10/5/10 (v1) ... 6/1/11 (v5.51)
Addition of alcohols to alkynes
Addition of hydrogen cyanide to alcohol oxidation with Corey rea...
Yield101 (iOS4) 4/11 (v1) ... 6/11 (v1.02)

**Reactants**
- Molecular Formula: C₆H₈O₃
- Molecular Weight: 158.121 g/mol
- Equivalents: 1
- Mass: 10 g
- Volume: 6.93001 mL (calculated)
- Moles: 0.072004 mol (calculated)
- Density: 1.443 g/mL

(Primary Reactant)

**Products**
- Molecular Formula: C₆H₈O₃
- Molecular Weight: 158.121 g/mol
- Equivalents: 1
- Mass: 11.5 g
- Moles: 0.0638331 mol (calculated)
- Yield: 86.1667 % (calculated)

\[
PMI = \frac{\text{(Mass of raw materials input)}}{\text{(Mass of desired output)}}
\]

Eidogen-Sertanty’s iPhone and iPad Apps

- iKinase
- iKinasePro
- Mobile Reagents
- iProtein
- Reaction101
- Yield101

*Reaction101 and Yield101 - built collaboratively with Molecular Materials Informatics, Inc.*
Lessons Learned...

• Devices are worldwide and pervasive
  ➡ Millions of people surf the app store!!!

• Development environment is very good
  ➡ Large activation energy to start, Apple’s CDAs can be a hindrance (contrasted with LAMP)

• Don’t expect large app revenues
  ➡ People prefer free apps (in app purchase woes)

• Apps can be phenomenal marketing vehicles
  ➡ People come to you

• Patience is important…
  ➡ It is tough to keep up with Apple innovation speed
Enter Drawing for an iPhone or iPad App

Send an e-mail to:

To: mobileapps@eidogen-sertanty.com
Subj: ACS Denver {iPod or iPhone or iPad}

10 of each will be given away
Acknowledgements

- Dr. Rajan Sharma and Prof. Stephan Schurer

- Dr. Maurizio Bronzetti

- Dr. Alex Clark
  - MMDSLib:

- Dr. Tony Yuan
  - Chemene:
About Eidogen-Sertanty, Inc.

- **Knowledge-Driven Solutions Provider**
  - Sertanty established in 2003, acquired Libraria assets
  - Sertanty acquired Eidogen/Bionomix in 2005 → Eidogen-Sertanty
  - $20M invested: Libraria ($6M), Eidogen/Bionomix ($12M), Sertanty/ES ($2M)
  - 15 distributed FTE’s (5 US and 10 India)
  - Worldwide (bio)pharmaceutical customer base
  - Cash-positive since 2006

- **Databases & Software – Annual Subscriptions**
  - *TIP*™ - Protein Structural Informatics Platform
  - *KKB*™ - Kinase SAR and Chemistry Knowledgebase
  - *CHIP*™ - Chemical Intelligence Platform

- **DirectDesign™ Fee-For-Service**
  - In Silico Target Screening (“Target Fishing” and Repurposing)
  - Target and compound prioritization services
  - Fast Follower Design: Novel, Patentable Leads
## Introduction – PMI by industry

<table>
<thead>
<tr>
<th>Industry</th>
<th>Typical PMI</th>
<th>Annual Production tonnage</th>
</tr>
</thead>
<tbody>
<tr>
<td>Oil refining</td>
<td>~1.1</td>
<td>$10^6 - 10^8$</td>
</tr>
<tr>
<td>Bulk chemicals</td>
<td>&lt;2 to 6</td>
<td>$10^4 - 10^6$</td>
</tr>
<tr>
<td>Fine chemicals</td>
<td>6 to &gt;50</td>
<td>$10^2 - 10^4$</td>
</tr>
<tr>
<td>Pharma</td>
<td>26 to &gt;100</td>
<td>$10 - 10^3$</td>
</tr>
</tbody>
</table>

**Pharma: Rapid product launches (unmet medical needs, patent life)**

*Constrains development time for process optimization*