Building a business with and without scientific computing: The five W's and one H

(why, when, who, what, where and how)

Steven Muskal, Ph.D
Chief Executive Officer
Eidogen-Sertanty, Inc

Chemical Information for Small Businesses & Startups
Dr. Steven Muskal
25 years (bio)pharmaceutical industry

- ’84–’88 - Engineering Chemistry/Computer Science (Colorado School of Mines)
- ’88–’91 - Ph.D. Biophysical Chemistry (UC Berkeley)
- ’91–’95 Molecular Design Ltd. (MDL) (Project manager, BizDev)
- ’95–’00 Affymax-Glaxo (Unit Director - lead optimization (ADME), and research computing)
- ’00–present Eidogen-Sertanty (CEO)
Learning from Hobbies

(Communicate, Collaborate and Digging-out of Failure)
Baba Shiv: Failure is the Mother of Innovation

Startups may embrace the “fail-fast” mantra, but many leaders are risk-adverse.

March 2, 2016 | by Eilene Zimmerman
1) Why: business with(out) scientific computing

Dr. Alejandro Zaffaroni (1923-2014)

ALZA, DNAX, Affymax/Affymetrix, Symyx, Maxygen, Alexza, etc.
2) When (can you afford it?)

**Startup Financing Cycle**

- **Valley of Death**
- **Seed Capital**
- **Break even**
- **Early Stage**
- **1st**
- **2nd**
- **3rd**
- **Mezzanine**
- **Later Stage**
- **VCs, Acquisitions/Mergers & Strategic Alliances**
- **IPO**
- **Secondary Offerings**
- **Public Market**
3) Who: Your Network

414,000,000+
REGISTERED MEMBERS
Drug Industry Layoffs: 300,000 in the last decade!

<table>
<thead>
<tr>
<th>Year</th>
<th>Number of jobs cut</th>
</tr>
</thead>
<tbody>
<tr>
<td>2000</td>
<td>2,453</td>
</tr>
<tr>
<td>2001</td>
<td>4,736</td>
</tr>
<tr>
<td>2002</td>
<td>11,488</td>
</tr>
<tr>
<td>2003</td>
<td>28,519</td>
</tr>
<tr>
<td>2004</td>
<td>15,640</td>
</tr>
<tr>
<td>2005</td>
<td>26,300</td>
</tr>
<tr>
<td>2006</td>
<td>15,638</td>
</tr>
<tr>
<td>2007</td>
<td>31,732</td>
</tr>
<tr>
<td>2008</td>
<td>43,014</td>
</tr>
<tr>
<td>2009</td>
<td>61,109</td>
</tr>
<tr>
<td>2010</td>
<td>53,636</td>
</tr>
<tr>
<td>2011 (First three months)</td>
<td>3,385</td>
</tr>
<tr>
<td><strong>TOTAL</strong></td>
<td><strong>297,650</strong></td>
</tr>
</tbody>
</table>

Source: Challenger, Gray & Christmas, Inc. ©
3) Who (cont.): The World...

The Earth-sized talent pool for enterprise

Fingertip access to designers, developers, writers, translators, customer support pros, lead gen specialists, and more.

Forbes (5May 2015): Elance-oDesk Becomes 'Upwork' In Push To Build $10B In Freelancer Revenues
4) **What:** Access, Buy...then Build

Software and resources for computational medicinal chemistry

Liao C, Sitzmann M, Pugliese A, Nicklaus MC.

Annotating and mining the ligand-target chemogenomics knowledge space

Ansgar Schuffenhauer and Edgar Jacoby

5) Where: The cloud...

The Power of the Cloud
The Cloud: Amazon AWS

AWS Usage Growth

Today: AWS bandwidth usage 30% greater than Amazon.com global websites

2007: AWS bandwidth usage surpassed Amazon.com global websites
The Cloud: Amazon S3 (Amazon Simple Storage Service)

The Cloud Scales: Amazon S3 Growth

Peak Requests:
650,000+
per second

Total Number of Objects Stored in Amazon S3
<table>
<thead>
<tr>
<th>Service</th>
<th>Feature Description</th>
<th>AWS Free Tier Details</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Amazon EC2</strong></td>
<td>Resizable compute capacity in the Cloud.</td>
<td>750 hours per month of Linux, RHEL, or SLES t2.micro instance usage</td>
</tr>
<tr>
<td></td>
<td></td>
<td>750 hours per month of Windows t2.micro instance usage</td>
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<tr>
<td></td>
<td></td>
<td>For example, run 1 instance x 1 month or 2 instances x half a month</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Expires 12 months after sign-up.</td>
</tr>
<tr>
<td><strong>Amazon S3</strong></td>
<td>Highly scalable, reliable, and low-latency data storage infrastructure.</td>
<td>5 GB of Standard Storage</td>
</tr>
<tr>
<td></td>
<td></td>
<td>20,000 Get Requests</td>
</tr>
<tr>
<td></td>
<td></td>
<td>2,000 Put Requests</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Expires 12 months after sign-up.</td>
</tr>
<tr>
<td><strong>Amazon DynamoDB</strong></td>
<td>Fast and flexible NoSQL database with seamless scalability.</td>
<td>25 GB of Storage</td>
</tr>
<tr>
<td></td>
<td></td>
<td>25 Units of Write Capacity</td>
</tr>
<tr>
<td></td>
<td></td>
<td>25 Units of Read Capacity</td>
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<tr>
<td></td>
<td></td>
<td>Enough to handle up to 200M requests per month. Does not expire at the end of your 12 month AWS Free Tier term.</td>
</tr>
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</table>
Amazon: Cloud Simplification

EC2

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

- 5 Running Instances
- 12 Volumes
- 5 Key Pairs
- 1 Placement Group
- 5 Elastic IPs
- 12 Snapshots
- 0 Load Balancers
- 5 Security Groups

Create Instance
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 (N. Virginia) region.

Service Health

Service Status:
- US East (N. Virginia):
  - This service is operating normally

Availability Zone Status:
- us-east-1a:
  - Availability zone is operating normally
- us-east-1b:
  - Availability zone is operating normally
- us-east-1c:
  - Availability zone is operating normally
- us-east-1d:
  - Availability zone is operating normally
- us-east-1e:
  - Availability zone is operating normally

RDS

Resources
You are using the following Amazon RDS resources in the US East (N. Virginia) region:

- DB Instances (4)
- DB Snapshots (41)
- DB Parameter Groups (4)
- DB Security Groups (1)

- Reserved DB Purchases (5)
- Recent Events (10)
- Supported Platforms: EC2, VPC

Create Instance

Amazon Relational Database Service (RDS) makes it easy to set up, operate, and scale a relational database in the cloud. You can click the button below to launch a Database (DB) Instance in minutes with automated backups, turnkey Multi-AZ replication and free monitoring metrics. Amazon RDS gives you access to a familiar MySQL, Oracle, or SQL Server database to facilitate compatibility with existing code, applications, and tools.

Launch a DB Instance

Note: Your DB Instances will launch in the US East (N. Virginia) region.

Service Health

Current Status
- Amazon Relational Database Service (N. Virginia)
  - Service is operating normally

View complete service health details
How: Engage an Individual

Recent example:

° Past colleague contacted me (i.e. stay connected!)

° Company has a lead, need backup(s) (i.e. business critical)

° Target(s) and structure(s) known, some SAR but binding site(s) unknown (i.e. Science needed)

° Want to identify potential binding sites and enable chemical idea generation (i.e. Technology integration needed)

° Small budget, need workflow tool (i.e. public domain tools, delivered in cloud)
e.g. HotSpot Identification

AutoDock Vina Multiple Docking (http://vina.scripps.edu/download.html)

Multivariate Analysis with |STAT Statistical Data Analysis (http://oldwww.acm.org/perlman/stat/)

PyMOL (https://sourceforge.net/projects/pymol/files/pymol/1.8/)
e.g. Workflow WebApp

*MarvinJS, dropzoneJS, etc.*
Lovastatin lactone may improve constipation in Irritable Bowel Syndrome (IBS) by inhibiting enzymes in the archaeal methanogenesis pathway

Muskal S, *† Sliman J, † Kokai-Kun J, † Pimentel M ‡, Wacher V, † Gottlieb K. †

† Eidogen-Sertanty, 3460 Marron Road Suite 103-475, Oceanside, CA 92056
‡ Synthetic Biologics, 9605 Medical Center Dr. Suite 270, Rockville, MD 20850
§ Cedars-Sinai Medical Center, 8730 Alden Drive, Room E-220, Los Angeles, CA, 90048

Service engagements can leverage a wide spectrum of tools
Summary

- Why: Fail into success
- When: When you can afford it
- Who: Leverage your network
- What: Many available tools
- Where: The cloud
- How: Your project/workflow...
One More Thing...
SERIAL ENTREPRENEURS
HOW TO PURSUE MULTIPLE OPPORTUNITIES
by Anna Vital

Do most entrepreneurs

TRY MANY IDEAS? OR GO FOR ONE BIG IDEA?

Let's look at world's top entrepreneurs...
...the self-made billionaires

Of the world's 1,426 billionaires in 2013, 960 are self-made

830 made money from multiple businesses
130 made money from one business

Some are particularly notable for starting multiple businesses.

HOW DID THEY DO IT?

Richard Branson
Mark Cuban
Sheldon Adelson
Eric Lefkovsky
Elon Musk

http://fundersandfounders.com/
We Know Protein!

12 years World-wide advances
### Outsourcing Trends

#### Pharma R&D outsourcing

<table>
<thead>
<tr>
<th>Extent of Outsourcing</th>
<th>Activities Outsourced</th>
<th>Operating Model</th>
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<tbody>
<tr>
<td></td>
<td>Competitive Intelligence</td>
<td>Captive + Outsourcesd</td>
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<tr>
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<td>Only Captive</td>
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<tr>
<td></td>
<td>Discovery chemistry</td>
<td>Captive + Outsourced</td>
</tr>
<tr>
<td></td>
<td>Preclinical</td>
<td>Captive + Outsourced</td>
</tr>
<tr>
<td></td>
<td>Material Preparation</td>
<td>Captive</td>
</tr>
<tr>
<td></td>
<td>Analytics</td>
<td>Outsourced</td>
</tr>
</tbody>
</table>

**Activities Outsourced**
- **Competitive Intelligence**
  - Pipeline analysis
  - Clinical trial mapping
- **Functional Genomics**
  - Specialized chemistry
  - Bioinformatics support
- **Discovery chemistry**
  - Lead verification
  - Lead optimization
  - Chemical synthesis
  - Hit/lead optimization
- **Preclinical**
  - Bioanalytics
  - Pharmacokinetics
  - Toxicology studies
- **Clinical Trials**
  - Programming/scheduling
  - Data management
  - Site management
  - Clinical statistics
- **Material Preparation**
  - Dossier production
  - CD production
- **Analytics**
  - Commercial analytics
  - Sales force analytics
  - Brand modeling and forecasting

**Operating Model**
- Captive + Outsourced
- Only Captive
- Captive + Outsourced
- Captive + Outsourced
- Captive
- Outsourced

**Regulation**
- Most outsourced
- Least outsourced

Source: KPMG  Outsourcing in the pharmaceutical industry: 2011 and beyond