

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

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 Eidoagen-Sertanty (CEO)



Learning from Hobbies

(Communicate, Collaborate and Digging-out of Failure)

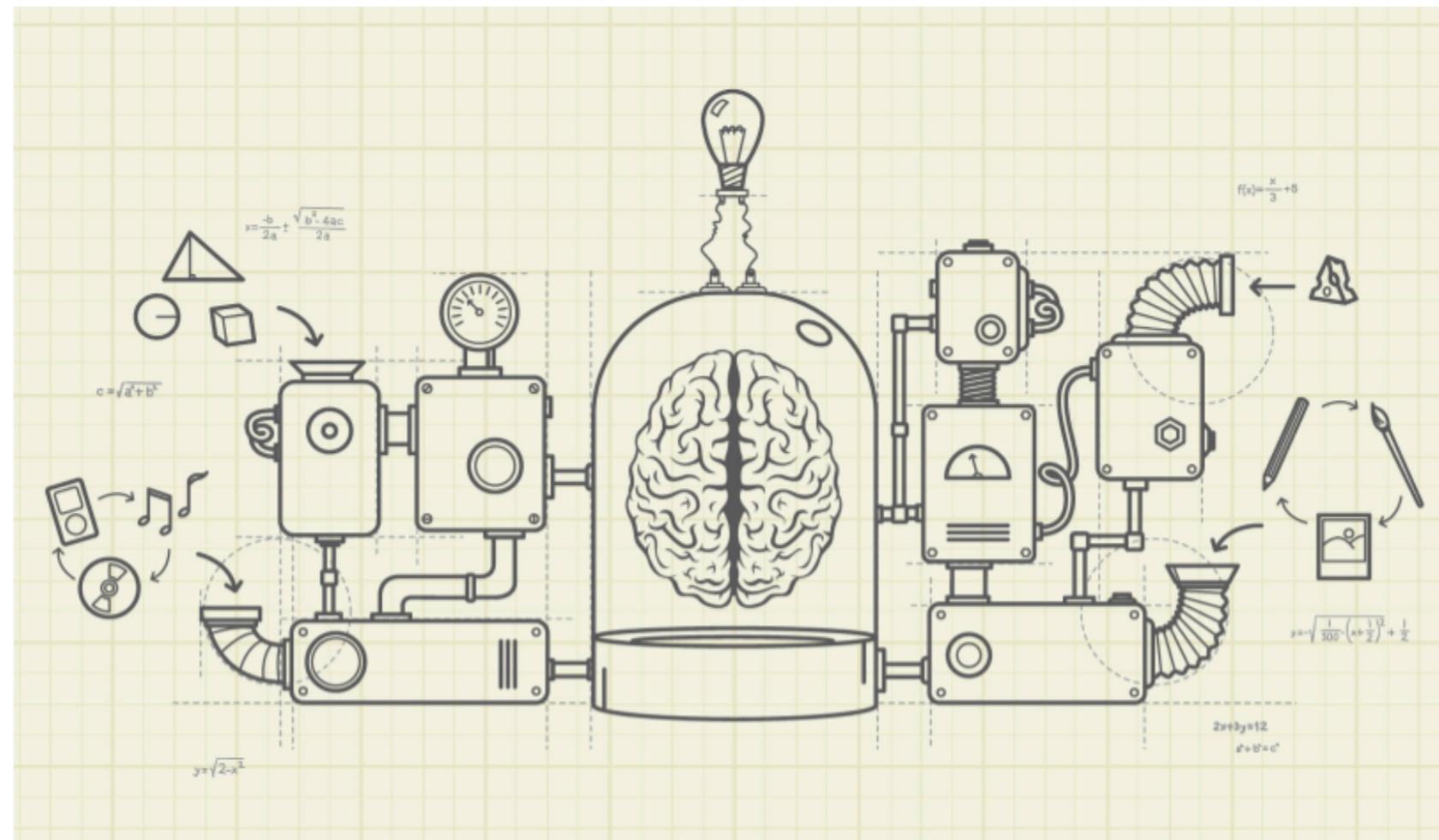


Entrepreneurship, Management

Baba Shiv: Failure is the Mother of Innovation

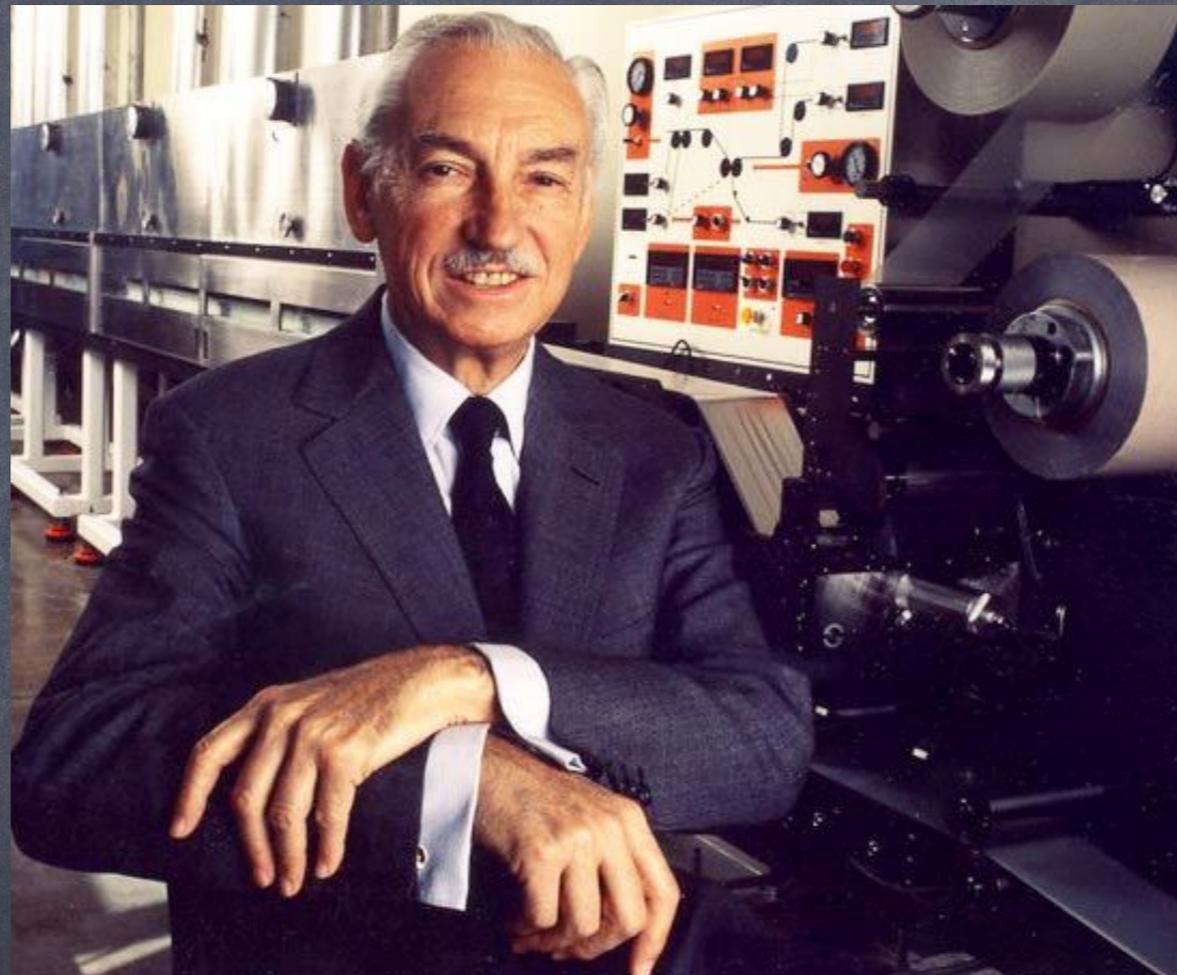
Startups may embrace the “fail-fast” mantra, but many leaders are risk-adverse.

March 2, 2016 | by Eilene Zimmerman



Innovation requires plenty of trial and error. | iStock/mustafahacalaki

1) Why: business with(out) scientific computing



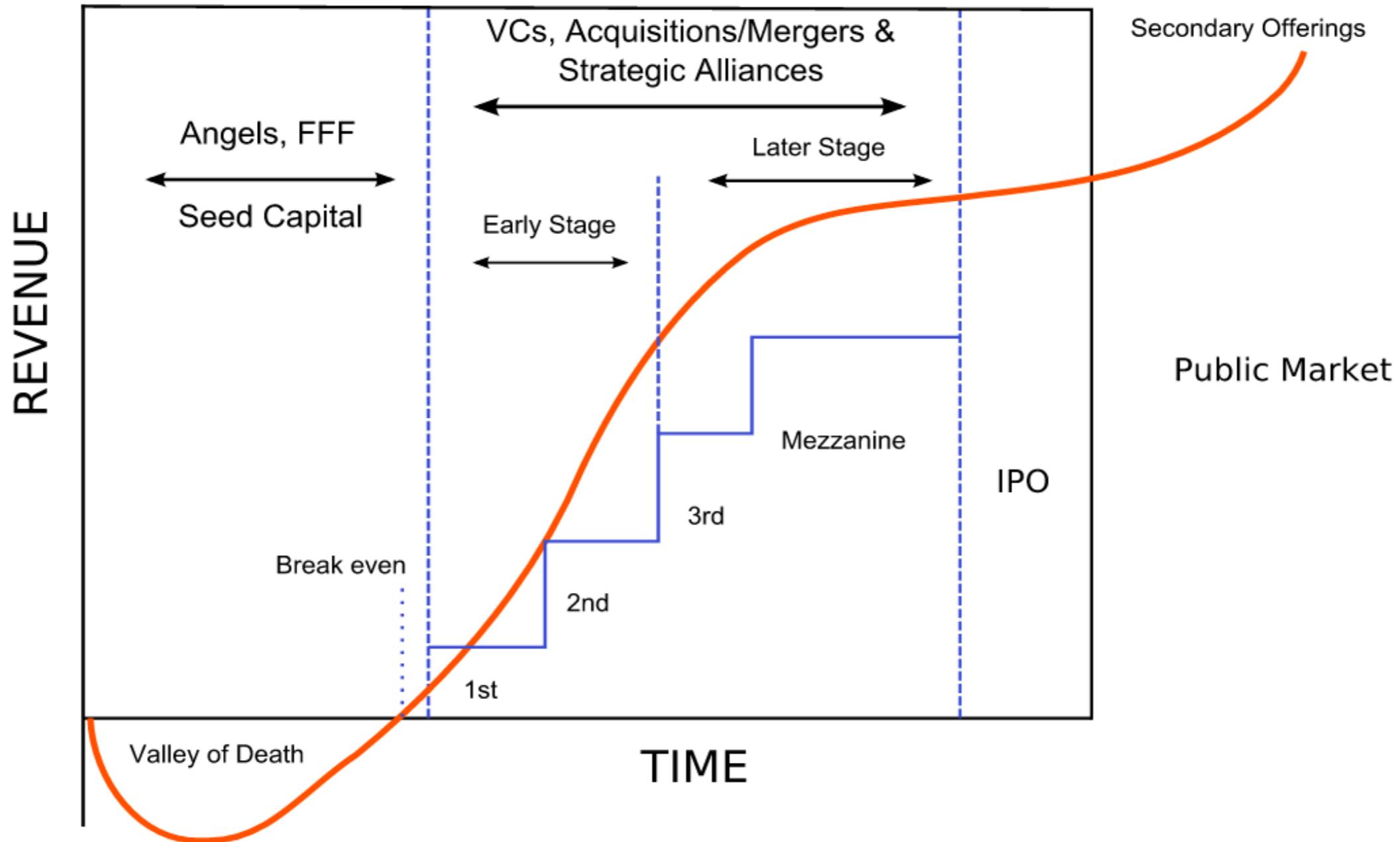
Dr. Alejandro Zaffaroni (1923-2014)

ALZA, DNAX, Affymax/Affymetrix, Symyx, Maxygen, Alexza, etc.



2) When (can you afford it?)

Startup Financing Cycle

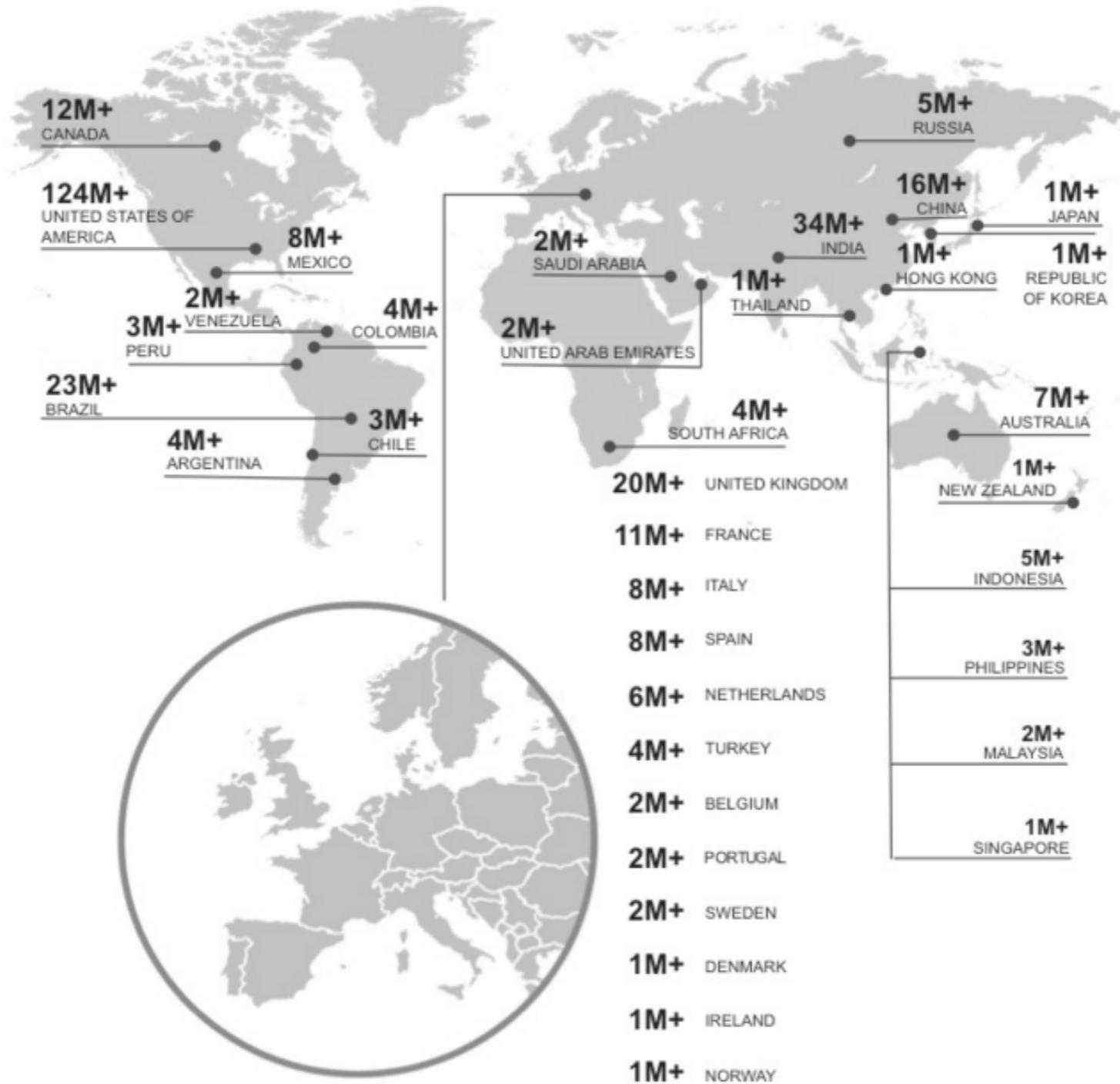


3) Who: Your Network

LinkedIn



414,000,000+
REGISTERED MEMBERS



Drug Industry Layoffs: 300,000 in the last decade!

A Decade In Drug Industry Layoffs	
Year	Number of jobs cut
2000	2,453
2001	4,736
2002	11,488
2003	28,519
2004	15,640
2005	26,300
2006	15,638
2007	31,732
2008	43,014
2009	61,109
2010	53,636
2011 (First three months)	3,385
TOTAL	297,650

Source: Challenger, Gray & Christmas, Inc. ©

3) Who (cont.): The World...

Upwork enterprise™

OVERVIEW

PRODUCT

SERVICES

BENEFITS

PRICING

RESOURCES

Get in Touch

Become a Freelancer

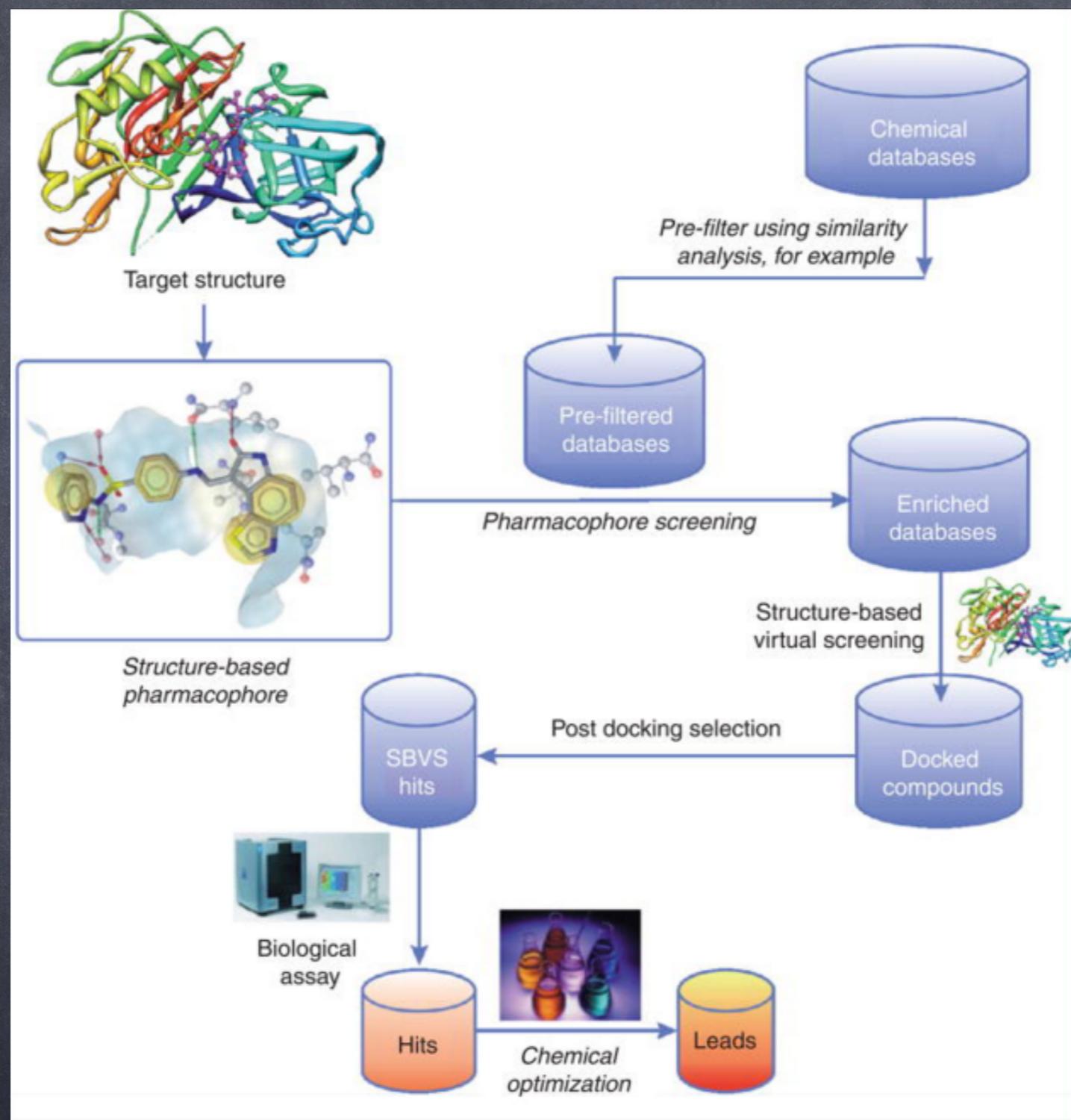
The **Earth-sized** talent pool for enterprise

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



Forbes (5 May 2015): Elance-oDesk Becomes 'Upwork' In Push To Build \$10B In Freelancer Revenues

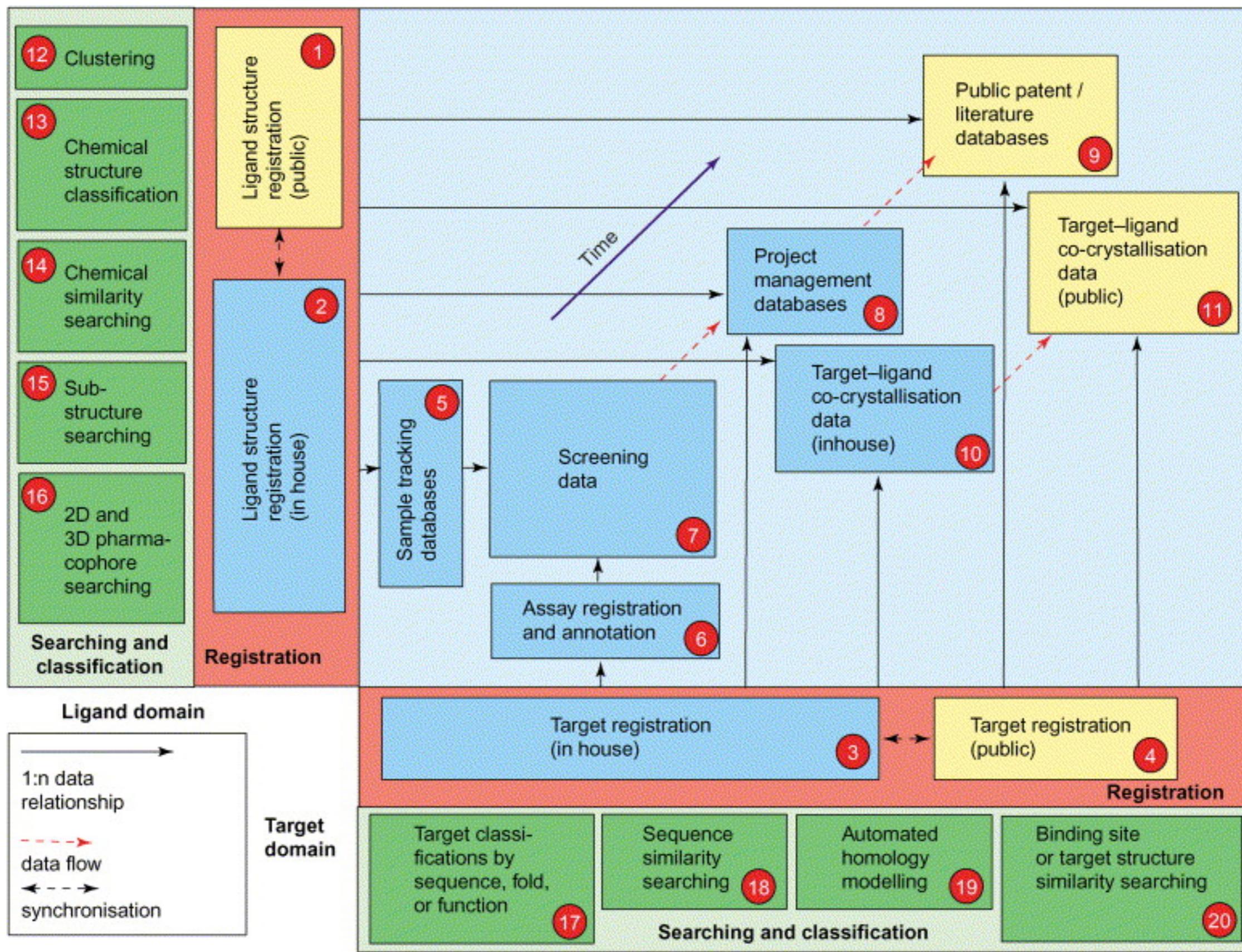
4) What: Access, Buy...then Build



Software and resources for computational medicinal chemistry

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

Future Med Chem. 2011 Jun;3(8):1057-85



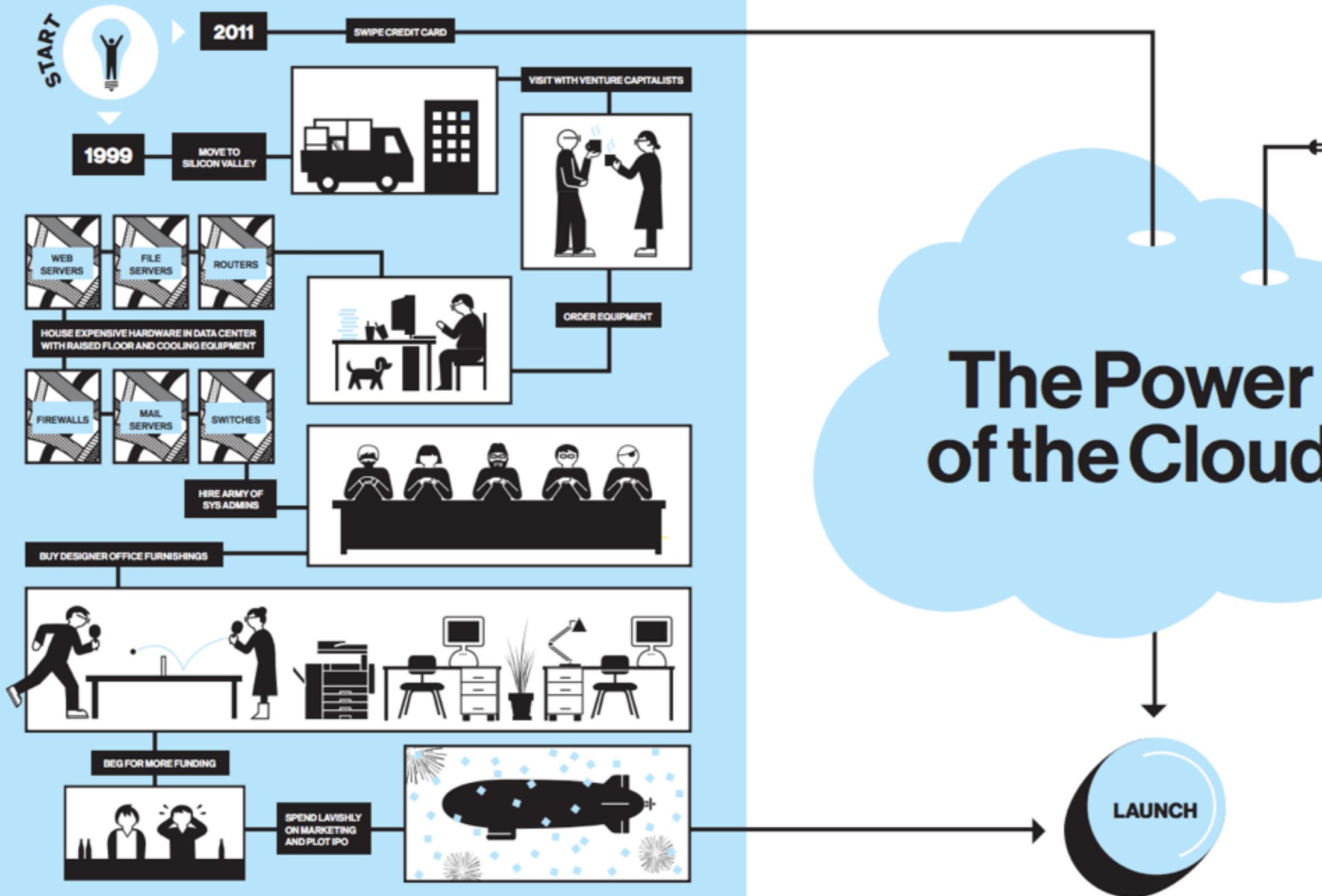
Annotating and mining the ligand-target chemogenomics knowledge space

Ansgar Schuffenhauer and Edgar Jacoby

Drug Discovery Today: BIOSILICO Volume 2, Issue 5, September 2004, Pages 190-200

5) Where: The cloud...

**Bloomberg
Businessweek**



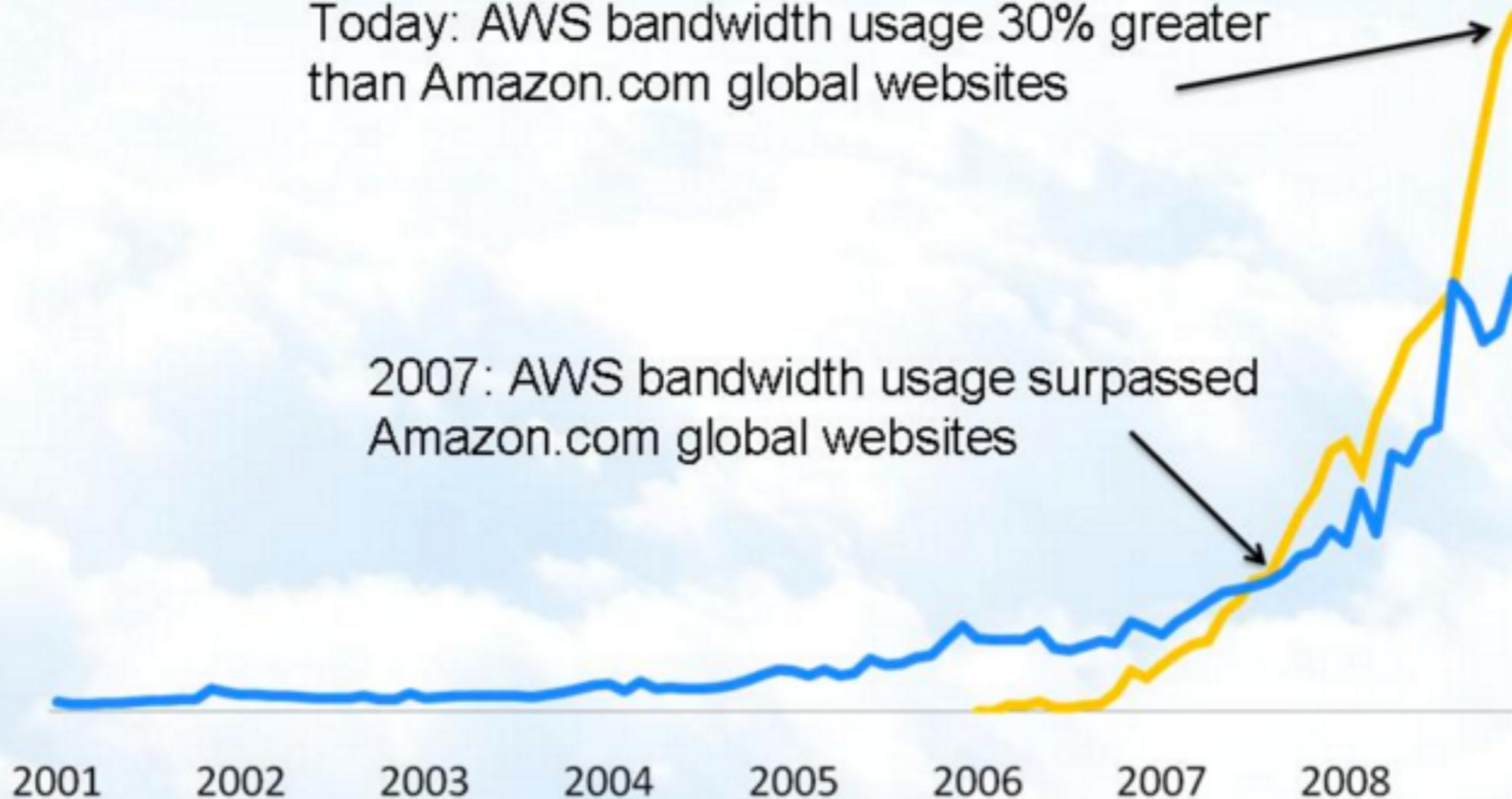
The Cloud: Amazon AWS

(Amazon Web Services)

AWS Usage Growth

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

2007: AWS bandwidth usage surpassed Amazon.com global websites

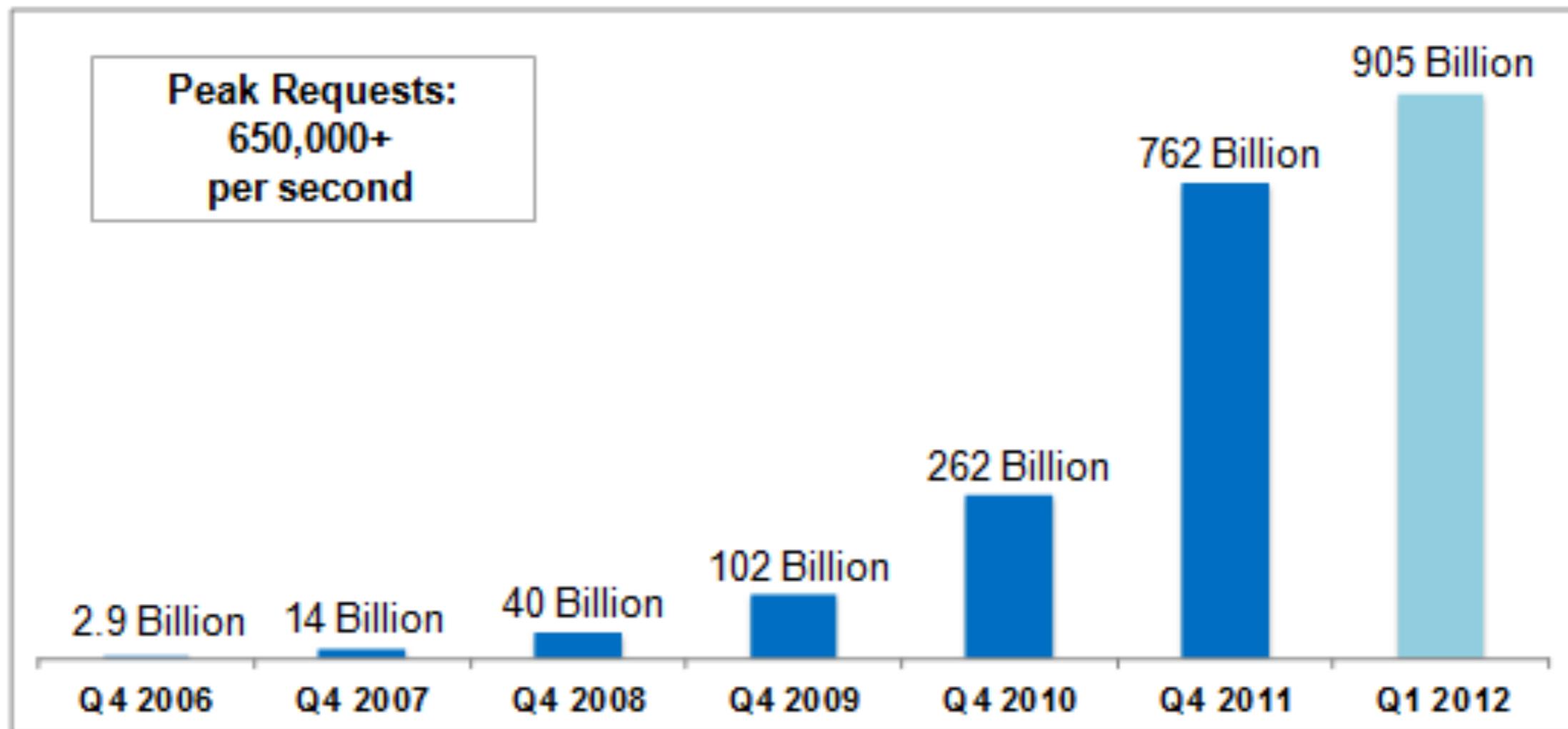


Bandwidth Usage: — AWS — Amazon.com



The Cloud: Amazon S3 (Amazon Simple Storage Service)

The Cloud Scales: Amazon S3 Growth



Total Number of Objects Stored in Amazon S3

Amazon AWS Free Tier



Amazon EC2

Resizable compute capacity in the Cloud.

[Learn More »](#)

750 hours per month of Linux, RHEL, or SLES t2.micro instance usage

750 hours per month of Windows t2.micro instance usage

For example, run 1 instance x 1 month or 2 instances x half a month

Expires 12 months after sign-up.



Amazon S3

Highly scalable, reliable, and low-latency data storage infrastructure.

[Learn More »](#)

5 GB of Standard Storage

20,000 Get Requests

2,000 Put Requests

Expires 12 months after sign-up.



Amazon DynamoDB

Fast and flexible NoSQL database with seamless scalability.

[Learn More »](#)

25 GB of Storage

25 Units of Write Capacity

25 Units of Read Capacity

Enough to handle up to 200M requests per month.

Does not expire at the end of your 12 month AWS Free Tier term.

Amazon Web Services

Compute

-  **EC2**
Virtual Servers in the Cloud
-  **EC2 Container Service**
Run and Manage Docker Containers
-  **Elastic Beanstalk**
Run and Manage Web Apps
-  **Lambda**
Run Code in Response to Events

Storage & Content Delivery

-  **S3**
Scalable Storage in the Cloud
-  **CloudFront**
Global Content Delivery Network
-  **Elastic File System** PREVIEW
Fully Managed File System for EC2
-  **Glacier**
Archive Storage in the Cloud
-  **Import/Export Snowball**
Large Scale Data Transport
-  **Storage Gateway**
Hybrid Storage Integration

Database

-  **RDS**
Managed Relational Database Service
-  **DynamoDB**
Managed NoSQL Database
-  **ElastiCache**
In-Memory Cache
-  **Redshift**
Fast, Simple, Cost-Effective Data Warehousing
-  **DMS** PREVIEW
Managed Database Migration Service

Networking

-  **VPC**
Isolated Cloud Resources
-  **Direct Connect**
Dedicated Network Connection to AWS
-  **Route 53**
Scalable DNS and Domain Name Registration

Developer Tools

-  **CodeCommit**
Store Code in Private Git Repositories
-  **CodeDeploy**
Automate Code Deployments
-  **CodePipeline**
Release Software using Continuous Delivery

Management Tools

-  **CloudWatch**
Monitor Resources and Applications
-  **CloudFormation**
Create and Manage Resources with Templates
-  **CloudTrail**
Track User Activity and API Usage
-  **Config**
Track Resource Inventory and Changes
-  **OpsWorks**
Automate Operations with Chef
-  **Service Catalog**
Create and Use Standardized Products
-  **Trusted Advisor**
Optimize Performance and Security

Security & Identity

-  **Identity & Access Management**
Manage User Access and Encryption Keys
-  **Directory Service**
Host and Manage Active Directory
-  **Inspector** PREVIEW
Analyze Application Security
-  **WAF**
Filter Malicious Web Traffic
-  **Certificate Manager**
Provision, Manage, and Deploy SSL/TLS Certificates

Analytics

-  **EMR**
Managed Hadoop Framework
-  **Data Pipeline**
Orchestration for Data-Driven Workflows
-  **Elasticsearch Service**
Run and Scale Elasticsearch Clusters
-  **Kinesis**
Work with Real-Time Streaming Data
-  **Machine Learning**
Build Smart Applications Quickly and Easily

Internet of Things

-  **AWS IoT**
Connect Devices to the Cloud

Game Development

-  **GameLift**
Deploy and Scale Session-based Multiplayer Games

Mobile Services

-  **Mobile Hub**
Build, Test, and Monitor Mobile Apps
-  **Cognito**
User Identity and App Data Synchronization
-  **Device Farm**
Test Android, FireOS, and iOS Apps on Real Devices in the Cloud
-  **Mobile Analytics**
Collect, View and Export App Analytics
-  **SNS**
Push Notification Service

Application Services

-  **API Gateway**
Build, Deploy and Manage APIs
-  **AppStream**
Low Latency Application Streaming
-  **CloudSearch**
Managed Search Service
-  **Elastic Transcoder**
Easy-to-Use Scalable Media Transcoding
-  **SES**
Email Sending and Receiving Service
-  **SQS**
Message Queue Service
-  **SWF**
Workflow Service for Coordinating Application Components

Enterprise Applications

-  **WorkSpaces**
Desktops in the Cloud
-  **WorkDocs**
Secure Enterprise Storage and Sharing Service
-  **WorkMail**
Secure Email and Calendaring Service

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

[Service Health Dashboard](#)

Scheduled Events

US East (N. Virginia):
No events

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 (9)
- Recent Events (10)
- Supported Platforms EC2,VPC
- Default Network none

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	Details
Amazon Relational Database Service (N. Virginia)	Service is operating normally
View complete service health details	

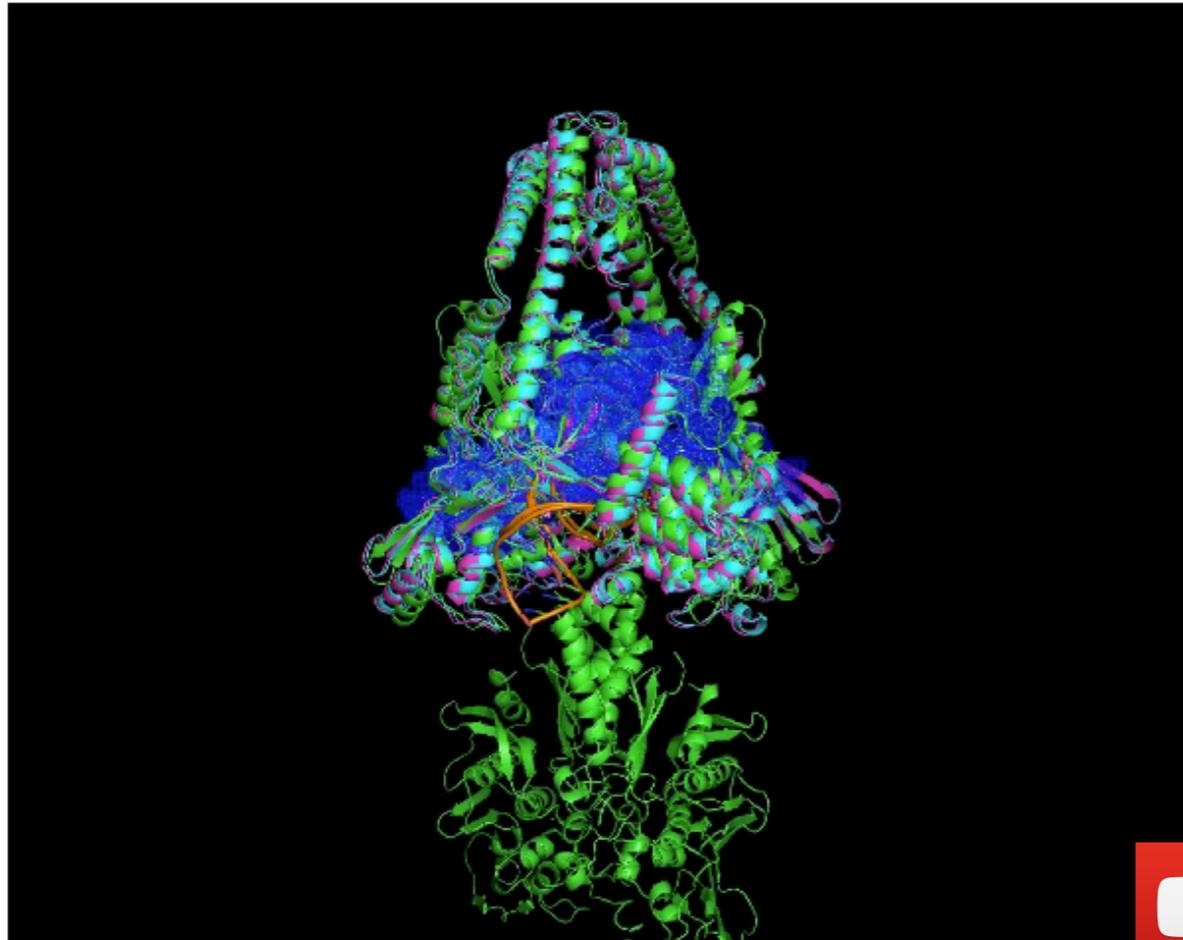
How: Engage an Individual

Recent example:

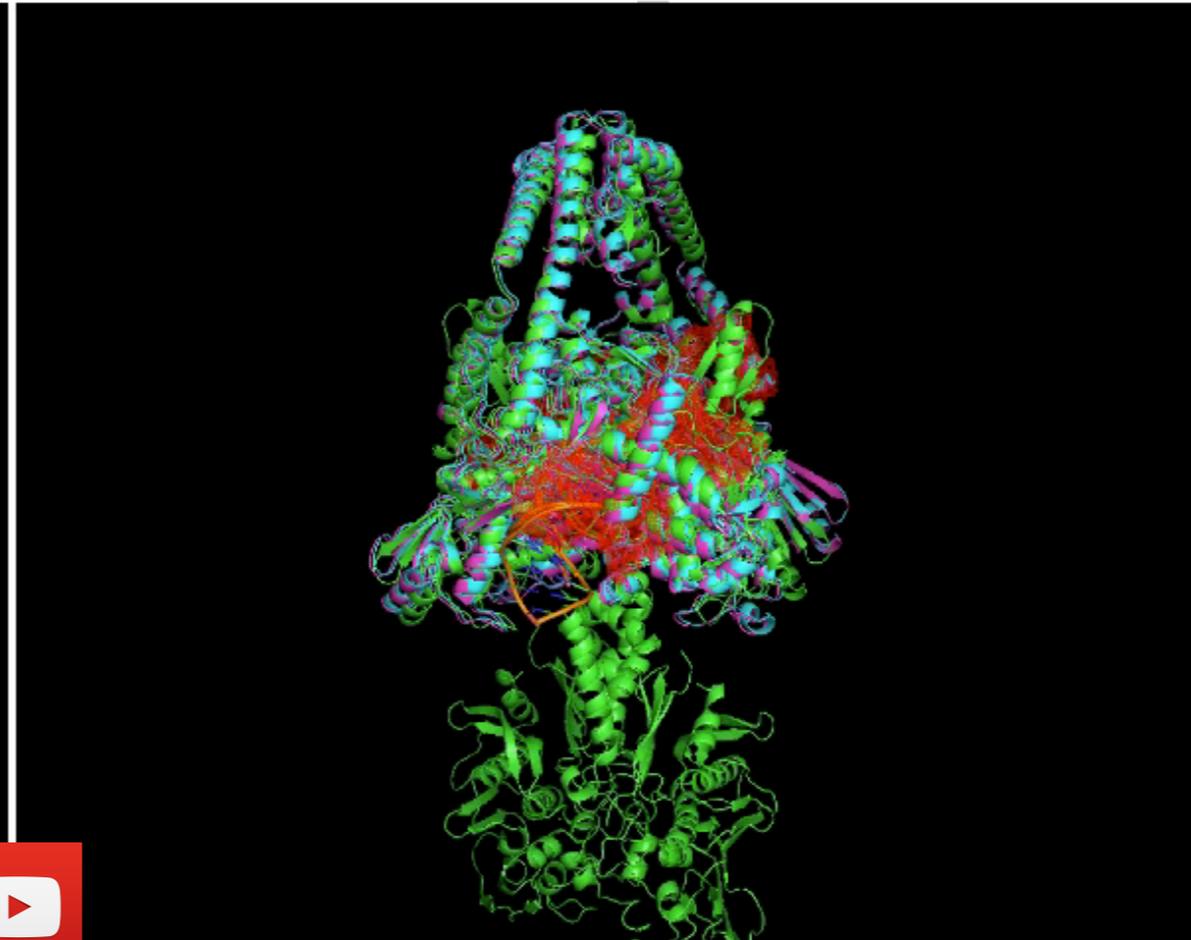
- Past colleague contacted me (i.e. stay connected!)
- Company has a lead, need backup(s) (i.e. business critical)
- Target(s) and structure(s) known, some SAR but binding site(s) unknown (i.e. Science needed)
- Want to identify potential binding sites and enable chemical idea generation (i.e. Technology integration needed)
- Small budget, need workflow tool (i.e. public domain tools, delivered in cloud)

e.g. HotSpot Identification

Top 10 Predicting α hotspots



Top 10 Predicting β hotspots



HotSpots

HotSpot	$Q\alpha$	$Q\beta$
hs-88	0.86	0.64
hs-83	0.83	0.36
hs-27	0.83	-0.06
hs-140	0.81	0.49
hs-76	0.80	0.56
hs-144	0.80	0.31
hs-22	0.80	0.84
hs-70	0.80	0.75
hs-138	0.80	0.21
hs-79	0.79	0.70
-	-	-
hs-22	0.80	0.84
hs-33	0.77	0.78
hs-70	0.80	0.75
hs-112	0.52	0.73
hs-79	0.80	0.70
hs-63	0.71	0.69
hs-7	0.64	0.69
hs-23	0.65	0.67
hs-88	0.86	0.64
hs-1	0.54	0.64



- AutoDock Vina Multiple Docking (<http://vina.scripps.edu/download.html>)
- Multivariate Analysis with ISTAT Statistical Data Analysis (<http://oldwww.acm.org/perlman/stat/>)
- PyMOL (<https://sourceforge.net/projects/pymol/files/pymol/1.8/>)

e.g. Workflow WebApp

Reference pages:
[Top-hotspots](#)

Result Files:

AND/OR, drop molfile(s) into the below box

Drop files here to upload

Project

Select one or more hotspot(s)

09Mar2016

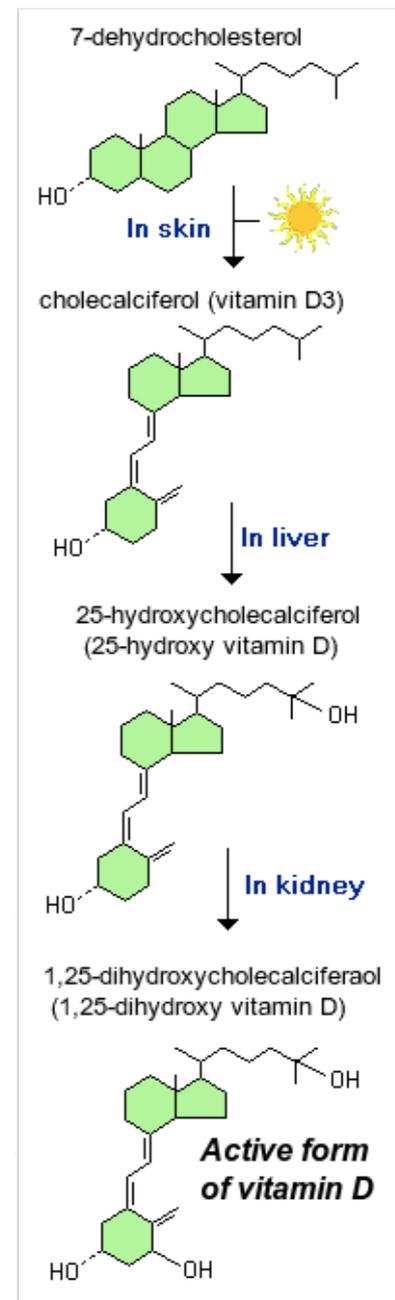
hs-88
hs-22

Alpha

Beta

Process

Purge



*MarvinJS, dropzoneJS, etc.



How: Engage a s/w Company

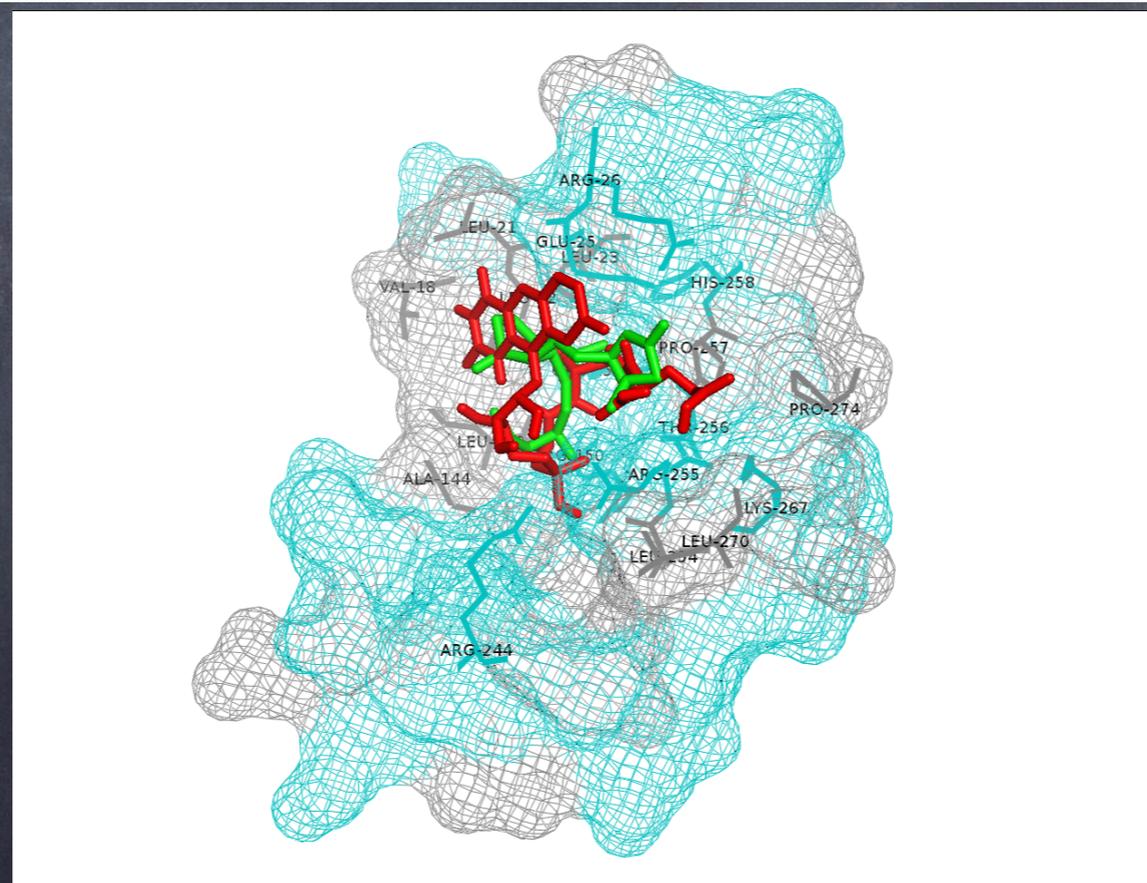
Lovastatin lactone may improve constipation in Irritable Bowel Syndrome (IBS) by inhibiting enzymes in the archaeal methanogenesis pathway

Muskal S, *† Sliman J, ‡ Kokai-Kun J, ‡ Pimentel M §, Wachter 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

Building a business with and without scientific computing

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



Some are particularly notable for starting multiple businesses.

HOW DID THEY DO IT?



Richard Branson



Mark Cuban



Sheldon Adelson



Eric Lefkovsky



Elon Musk

We Know Protein!



12 years World-wide advances



Outsourcing Trends

Pharma R&D outsourcing

