

# Standing on the Shoulders of Giants:

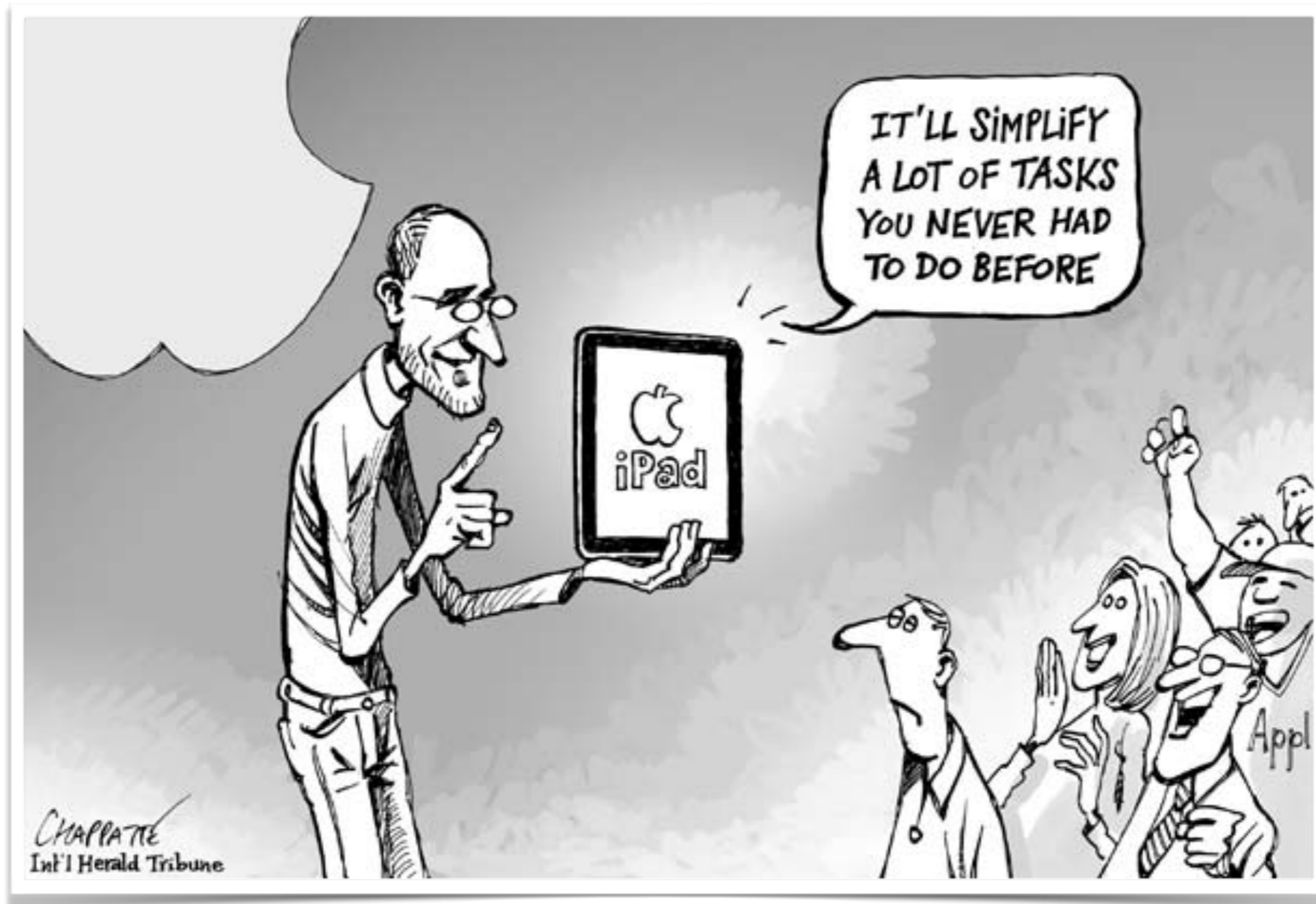
New strategies to involve more of the world with data mining and intelligence extraction.

**Dr. Steven Muskal**

Chief Executive Officer

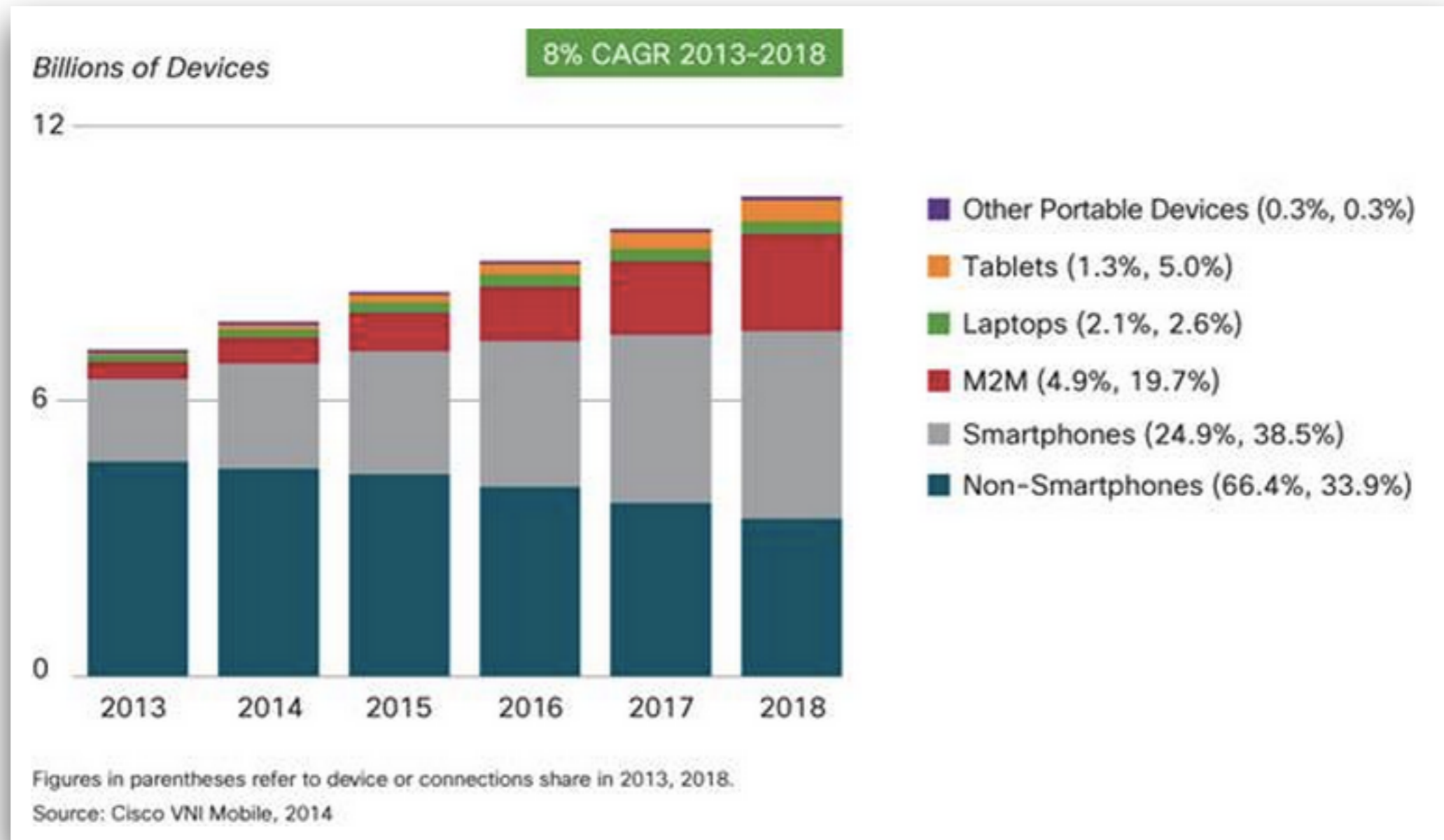
Eidogen-Sertanty, Inc

[smuskal@eidogen-sertanty.com](mailto:smuskal@eidogen-sertanty.com)



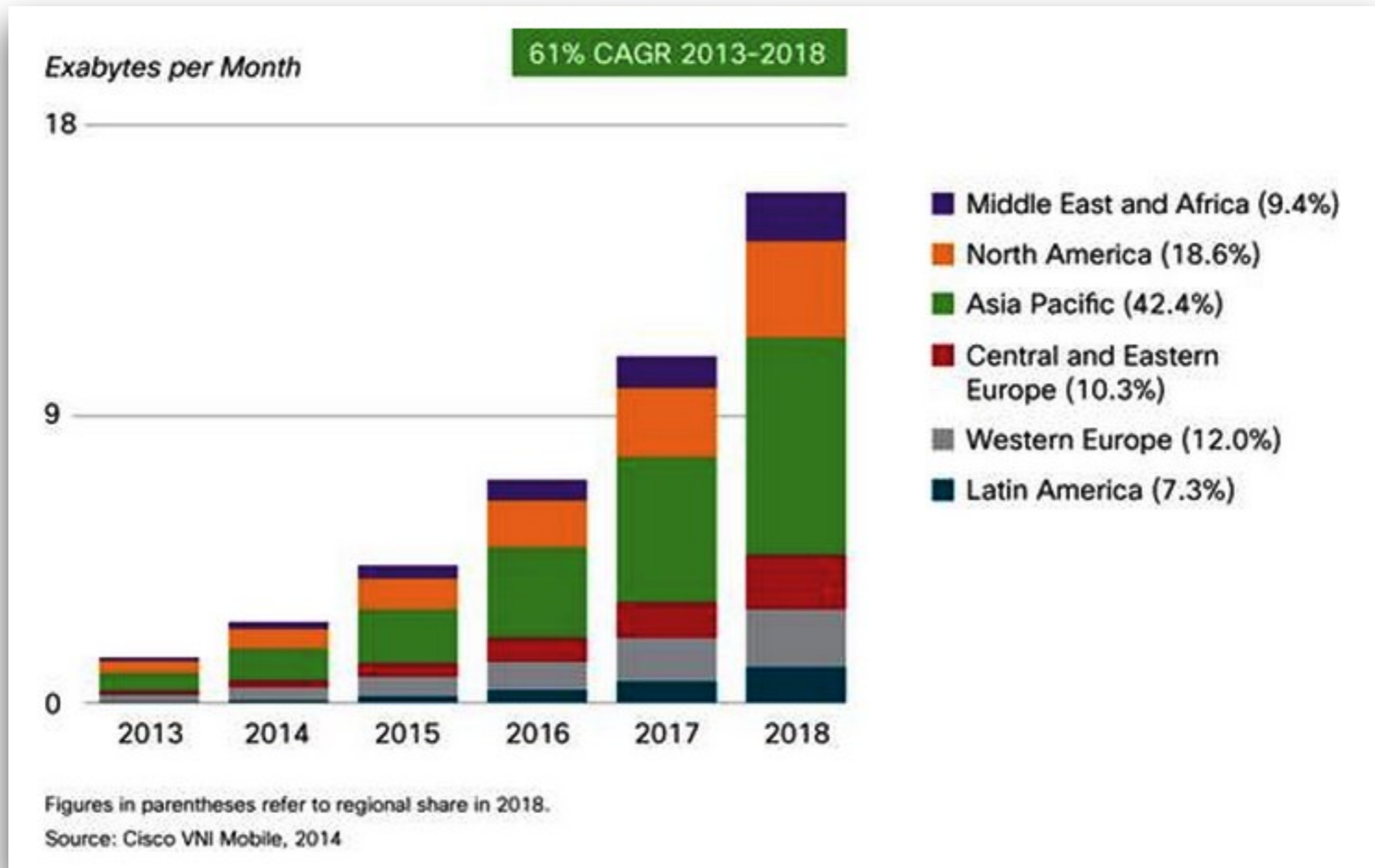
\* Apple's iPad was first released in April 2010.

# 70% of World's Population Uses Mobile Devices

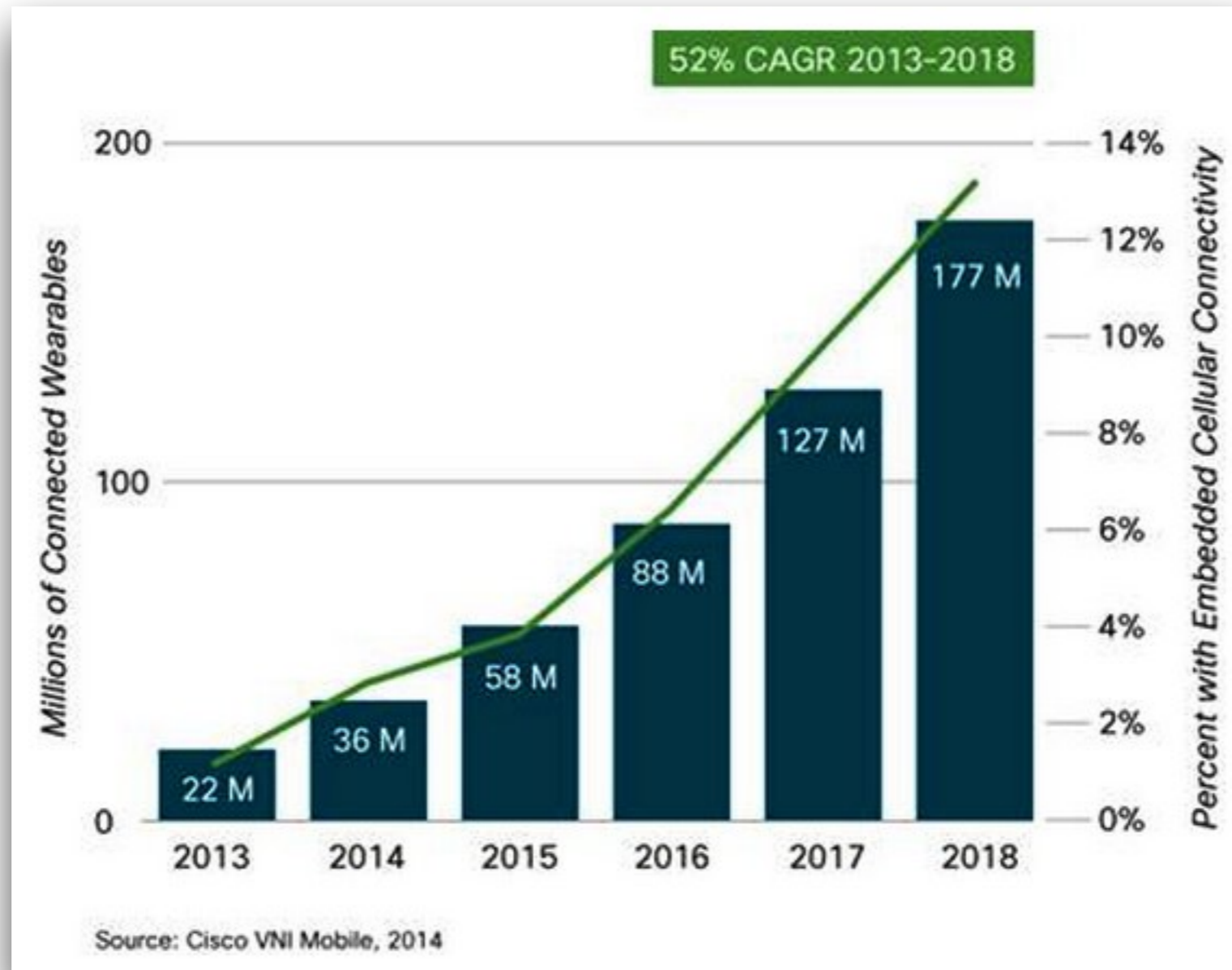


**Over half a billion mobile devices and connections were added in 2013**

# Growing World Demand for Connectivity

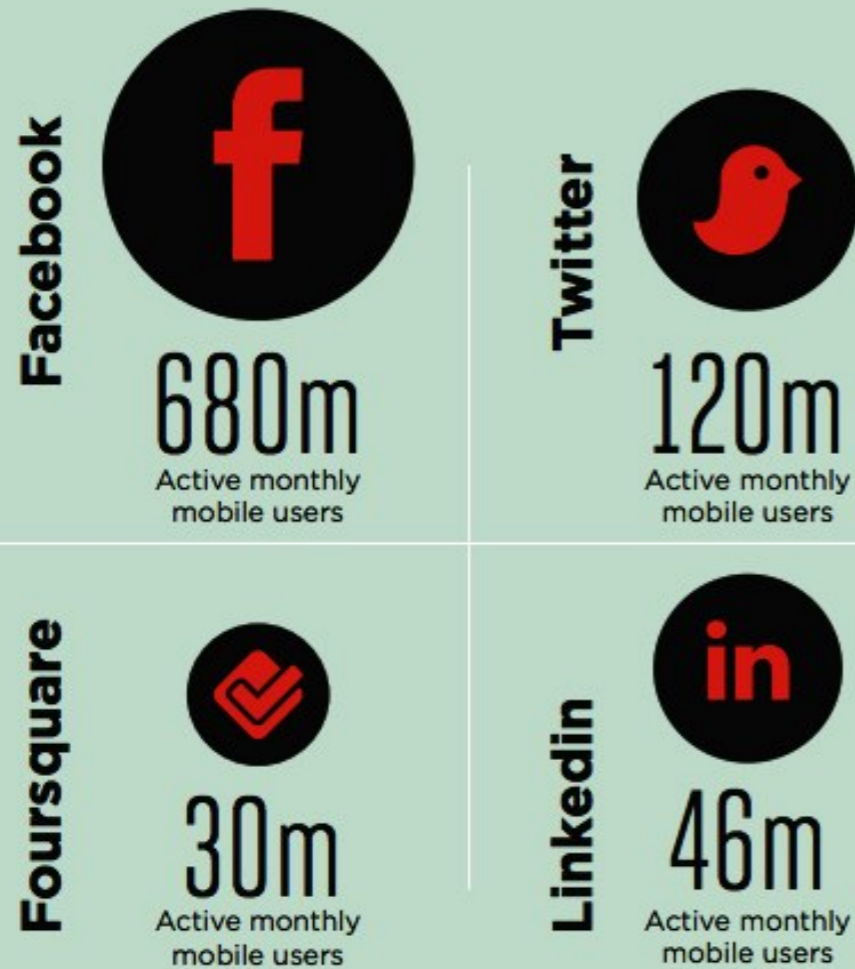


# Spoiler Alert: Wearables



# Mobile Social Networking

## Explosion of Mobile Data Services and Social Media



The advent of the smartphone, combined with the widespread deployment of mobile broadband networks, has led to an explosion of mobile data services

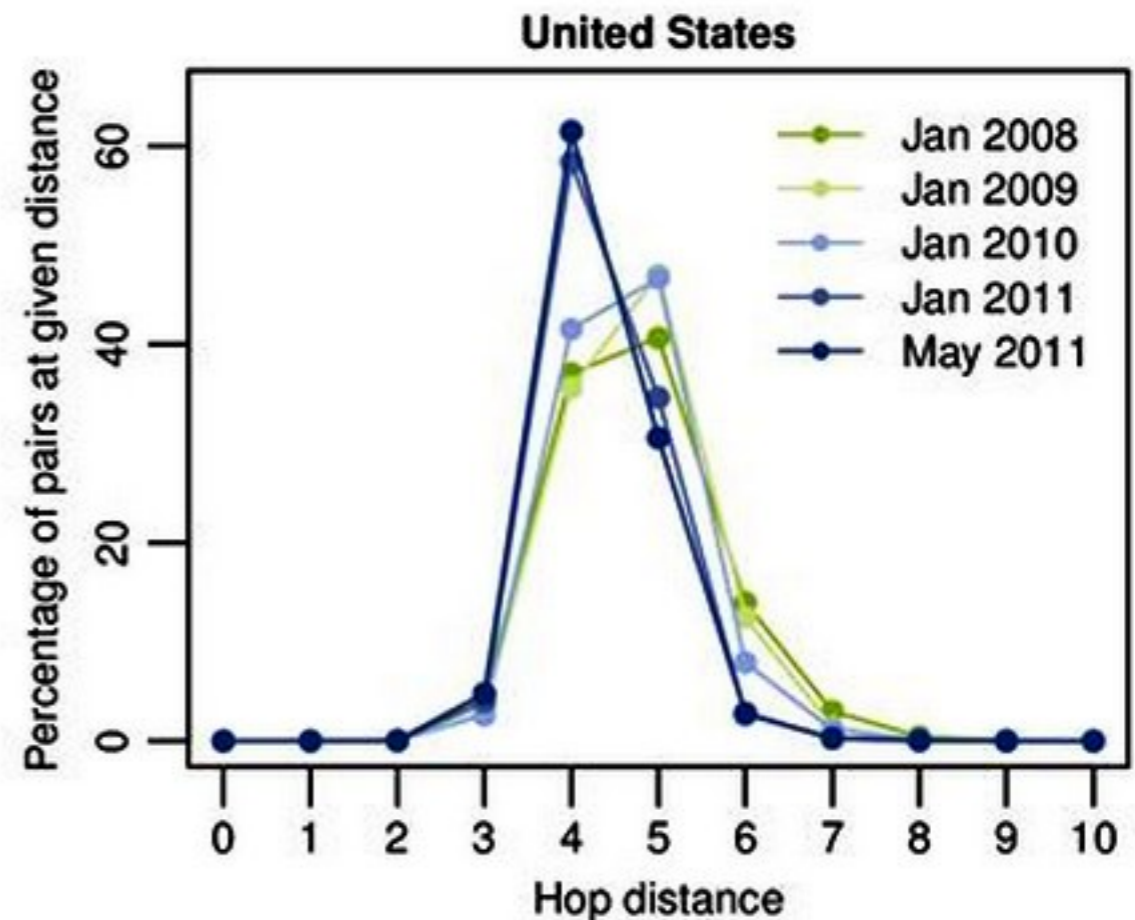
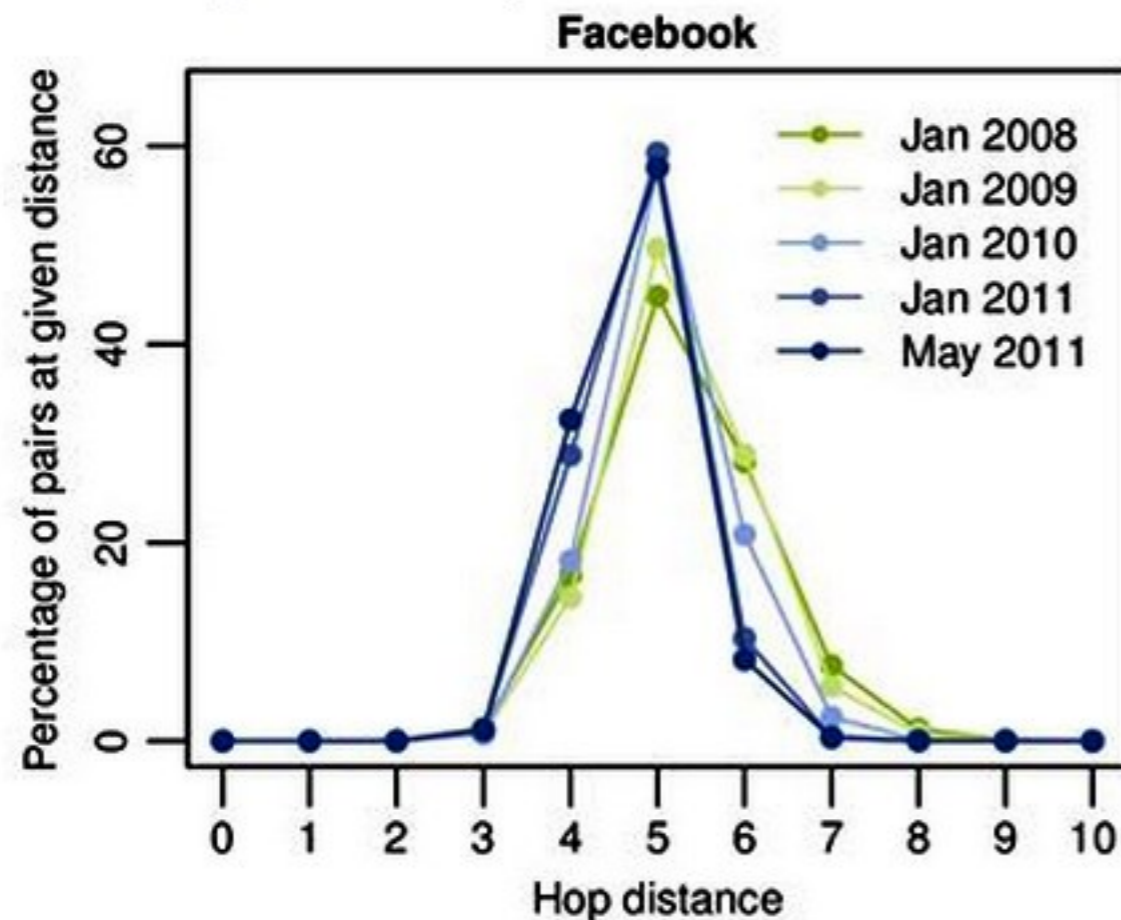


SOURCE: A.T. KEARNEY, CISCO 2013 MOBILE VNI STUDY, GSMA INTELLIGENCE

\* March 2014: Facebook reported 1 Billion Active Mobile Users

# Less Than Four Degrees of Separation

## Four degrees of separation.

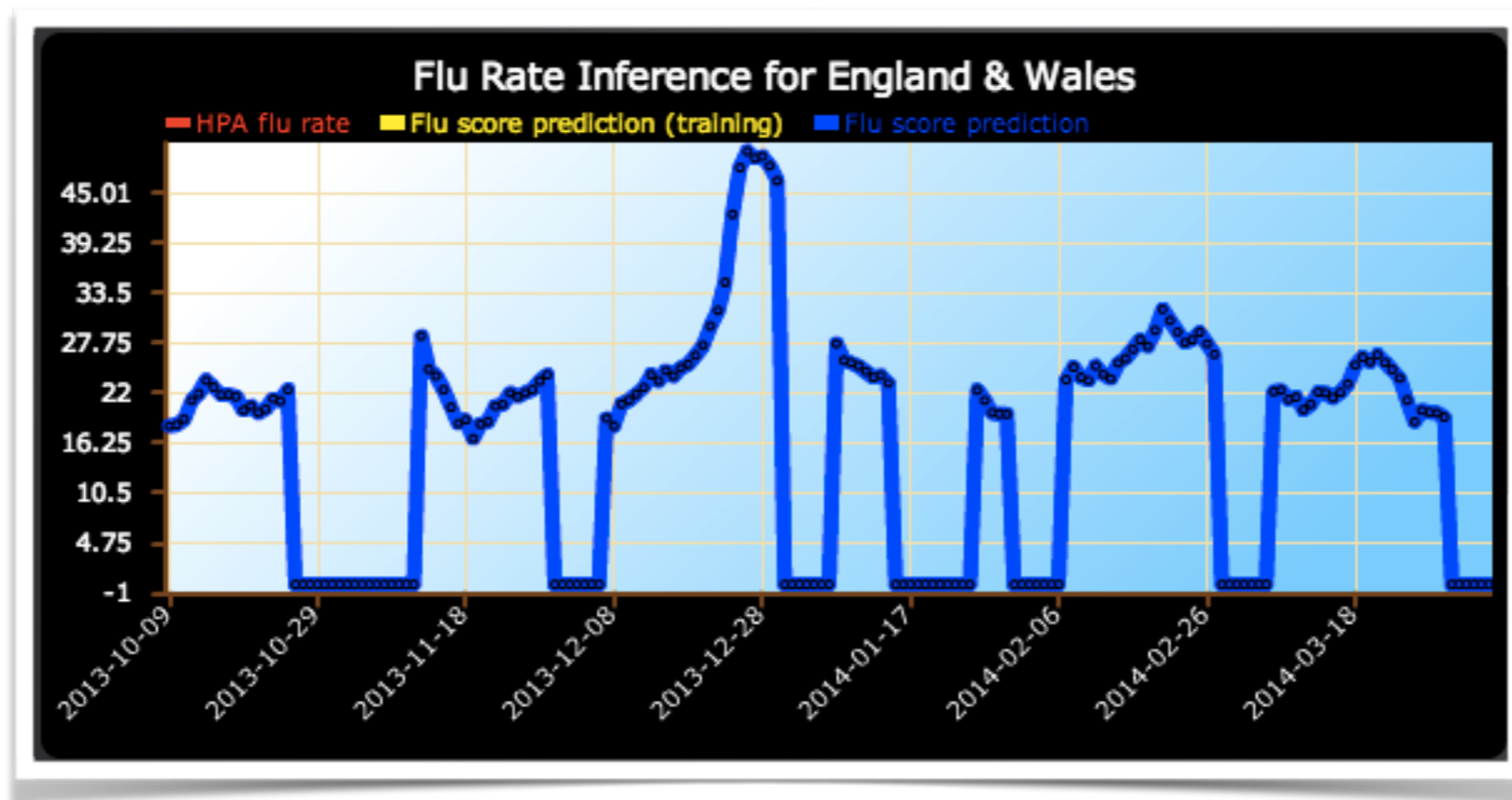


## Anatomy of Facebook

By Lars Backstrom on Monday, November 21, 2011 at 5:04pm

# Tracking Epidemics and Other Public Health Issues

## Flu Detector - Tracking Epidemics on Twitter



Machine Learning and Knowledge Discovery in Databases Lecture Notes in Computer Science Volume 6323, 2010, pp 599-602 Lampos, V. and Cristianini, N.

Tweet: “**Poor little crumb’s got fever and red spots. I feel so sorry.**”

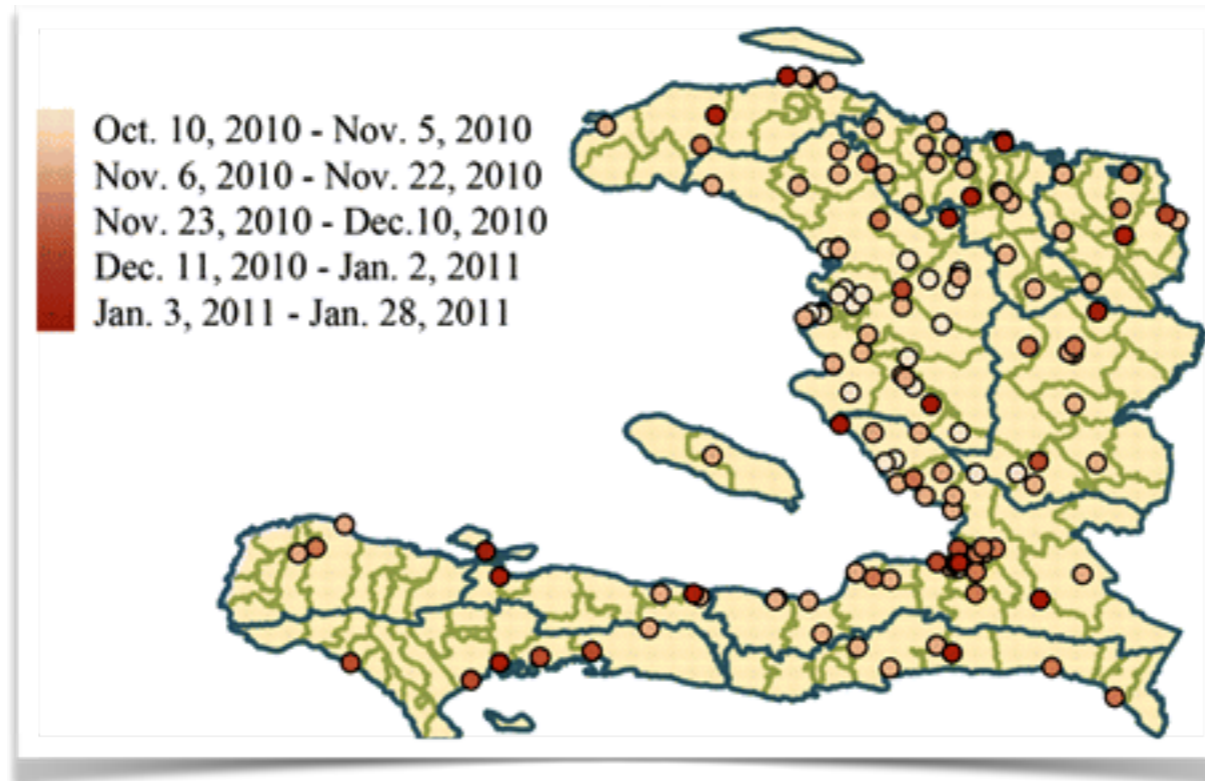
Tweet: “**Coughed the whole night. I got it bad. Flu.**”

**> 95% correlation with Health Protection Agency Data**



# Tracking Epidemics and Other Public Health Issues

## Social and News Media Enable Estimation of Epidemiological Patterns Early in the 2010 Haitian Cholera Outbreak



**HealthMap alerts for the first one hundred days of the Haiti cholera outbreak.**

- Cholera-related HealthMap news media reports, Twitter postings, and government cholera cases reported strongly correlated with official case data.
- Data from Informal sources were available up to **2 weeks earlier!**

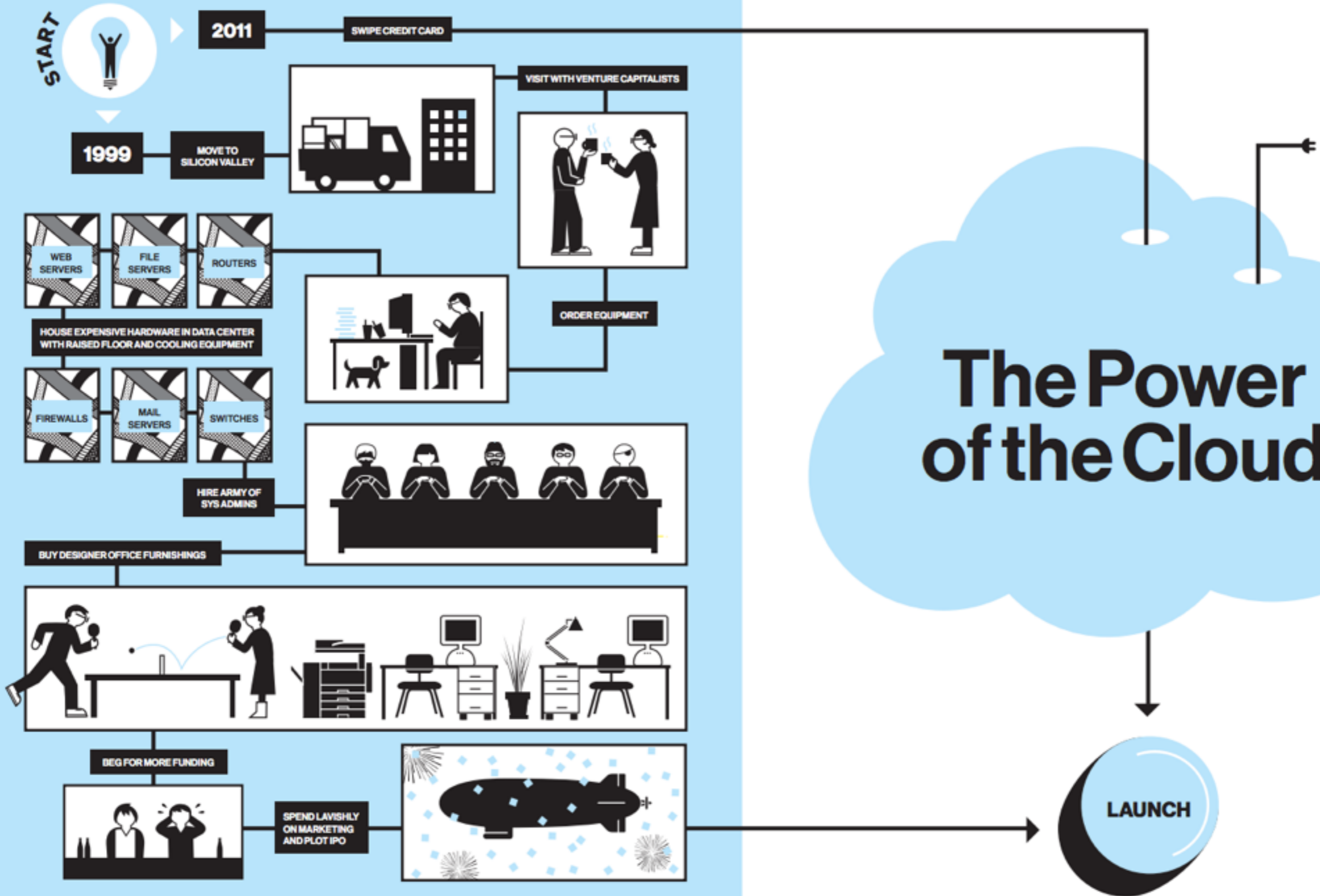
# Cloud Computing - A Revolution...

Nov 12, 2006



# Quick Poll

- How Many of You Leverage “the Cloud?”
- Gmail Users?
- Dropbox?
- Use an iPhone or iPad?



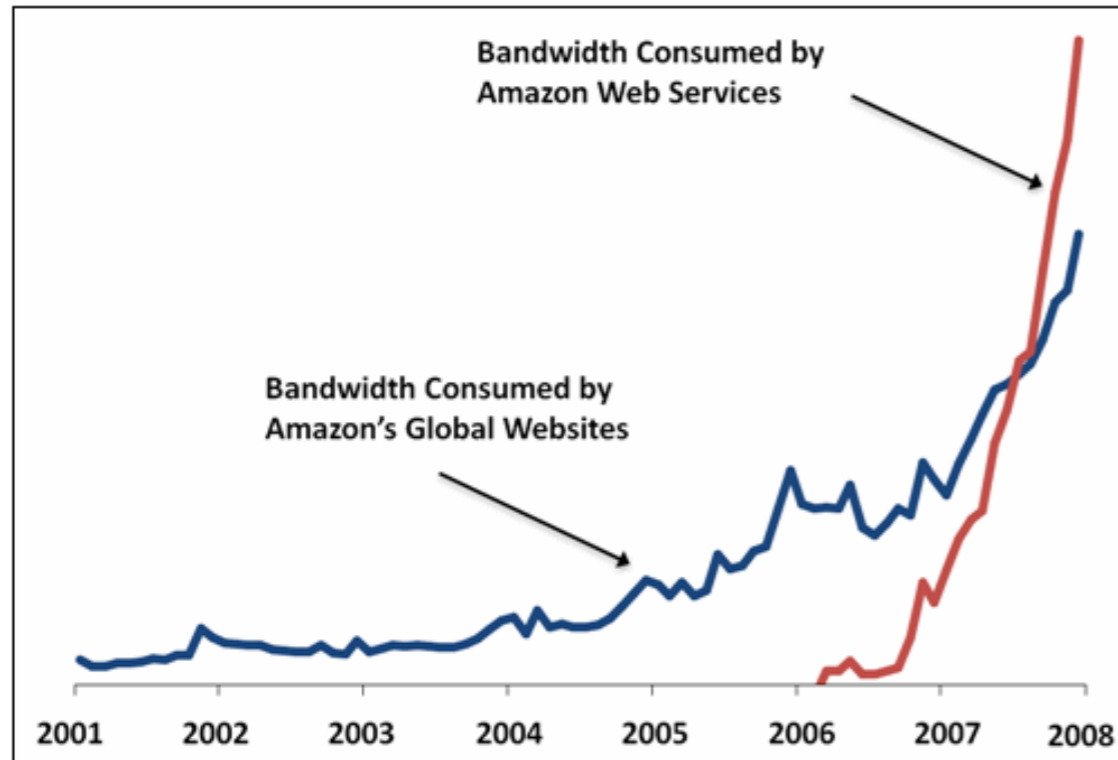
# Eidogen Cloud Migration

- 2003-2005: 3 different server rooms: 120+ servers
- 2005-2010: 1 colocation center: 5 caged racks
- 2010-2012: 1 colocation center: 3 racks + EC2/RDS cloud instances (mobile apps and migration)
- 2012-2013: EC2/RDS cloud instances (primary) + 2 legacy racks (“fallback”)



# The Cloud: Amazon AWS Growth

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



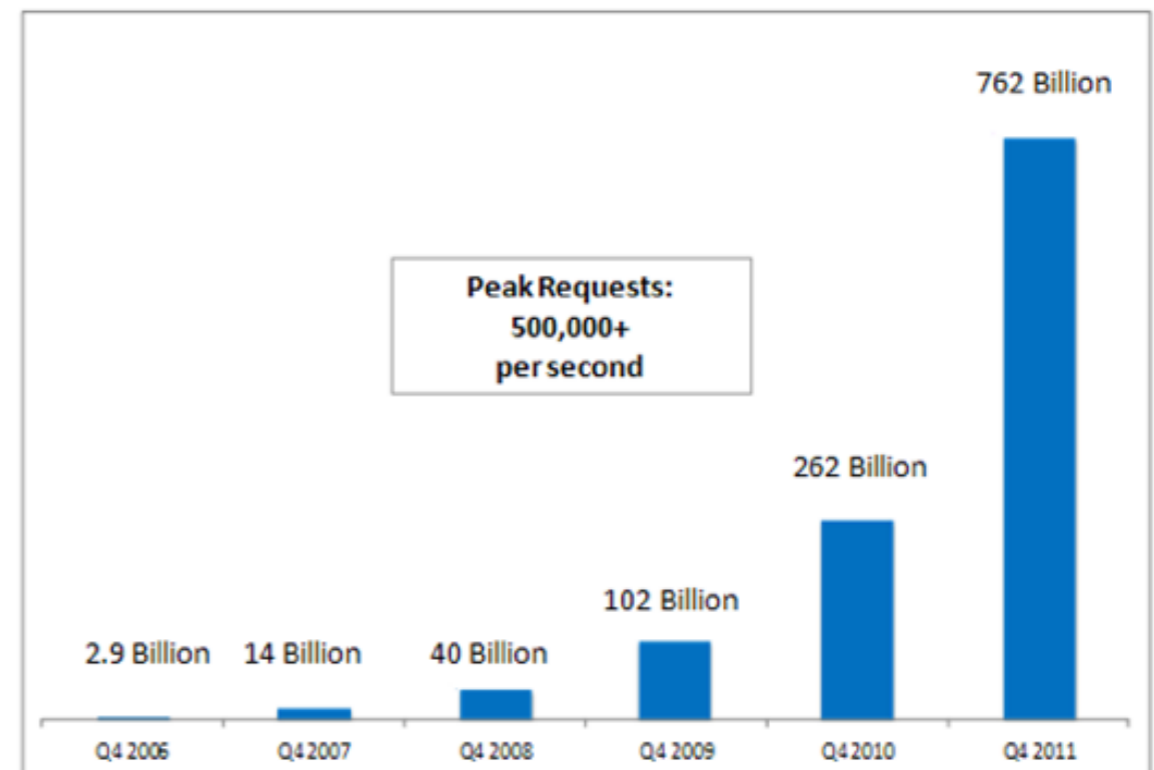
<http://aws.typepad.com/aws/2008/05/lots-of-bits.html>

AWS Free Usage Tier now includes Amazon MS-Windows Server EC2 instances

February 23, 2012

Amazon S3 grew 192% year-over-year

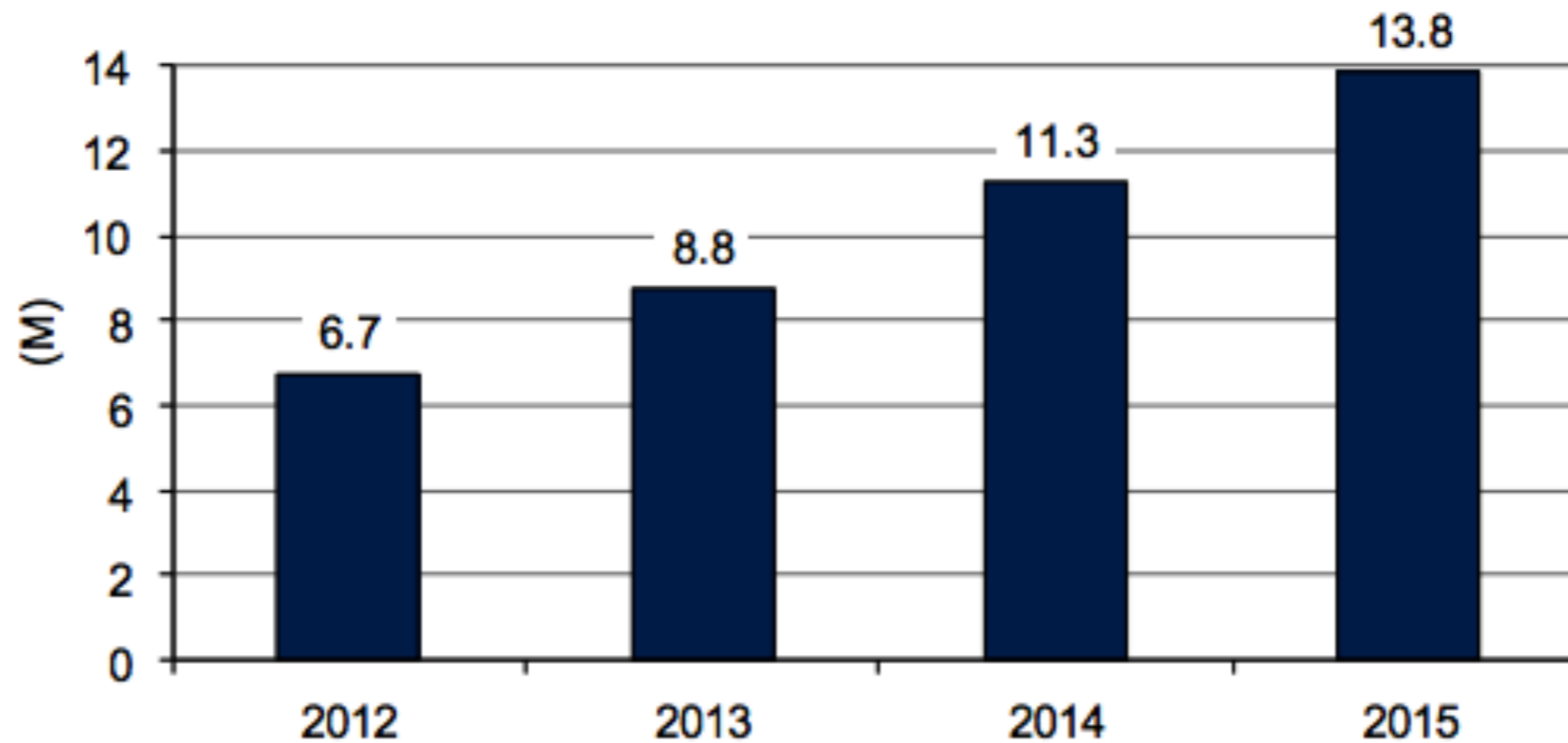
Total Number of Objects Stored in Amazon S3



<http://venturebeat.com/2012/01/31/amazon-aws-s3-growth-cloud/>

# Jobs Generated by Cloud Computing

Cloud Computing Impact on Jobs: Total Cumulative Jobs Generated by Cloud Computing Worldwide at Year-End, 2012–2015



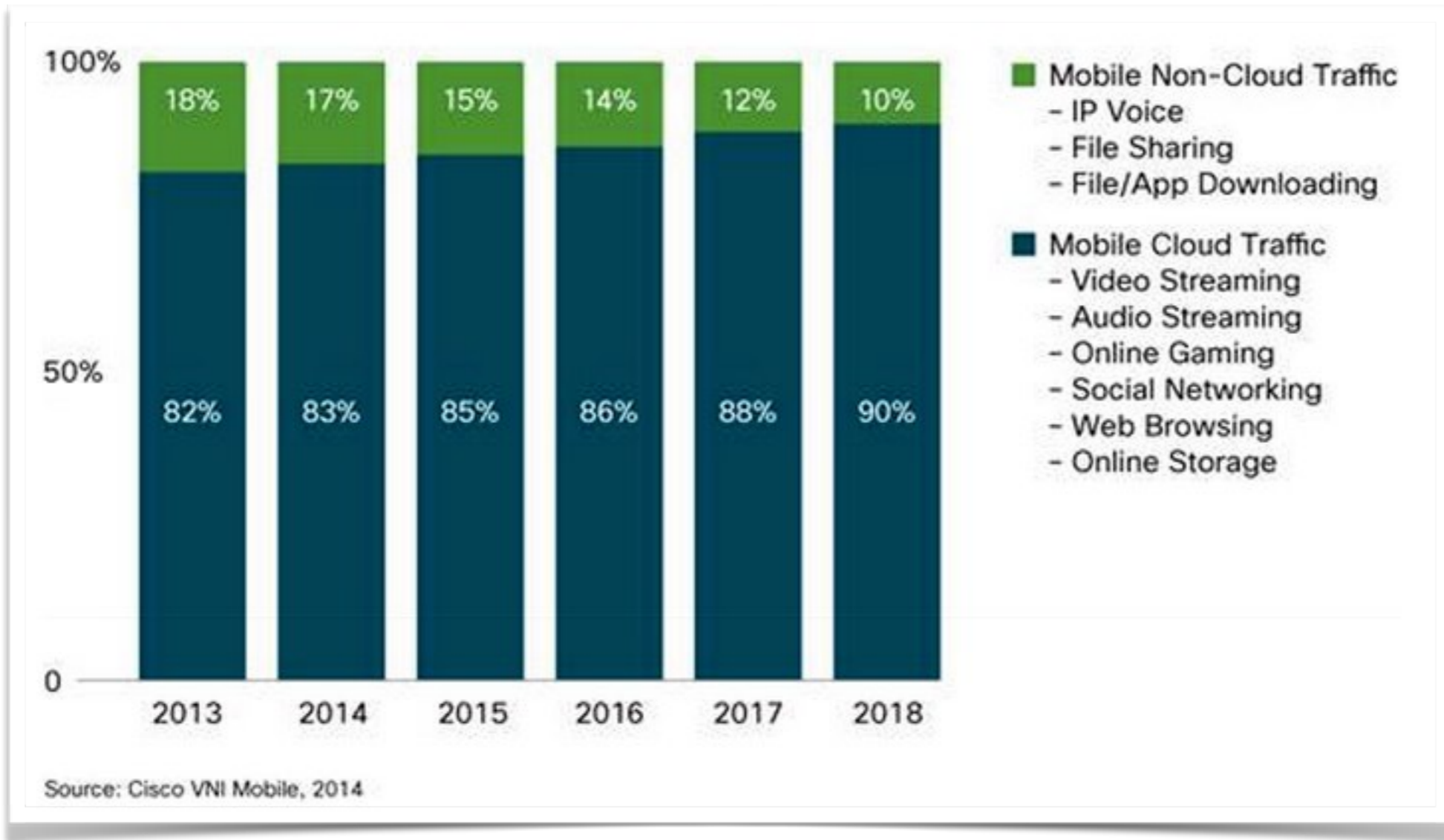
Source: IDC, 2012

**U.S. number of unemployed persons (10.5 million) - i.e. unemployment rate (6.7 percent)**

April 4, 2014: <http://www.bls.gov/news.release/empsit.nr0.htm>

# Mobile and Cloud

## Cloud Applications Will Account for 90 Percent of Mobile Data Traffic by 2018





# Many Apps, Huge Download Numbers

- Total Apps Approved for iTunes App Store: 1,542,115
- Total Active Apps (currently available for download): **1,157,279**
- Total Inactive Apps (no longer available for download): 384,836
- Number of Active Publishers in the iTunes App Store: **300,572**

March 31, 2014: <http://148apps.biz/app-store-metrics>

**> 100 Billion Downloads!**

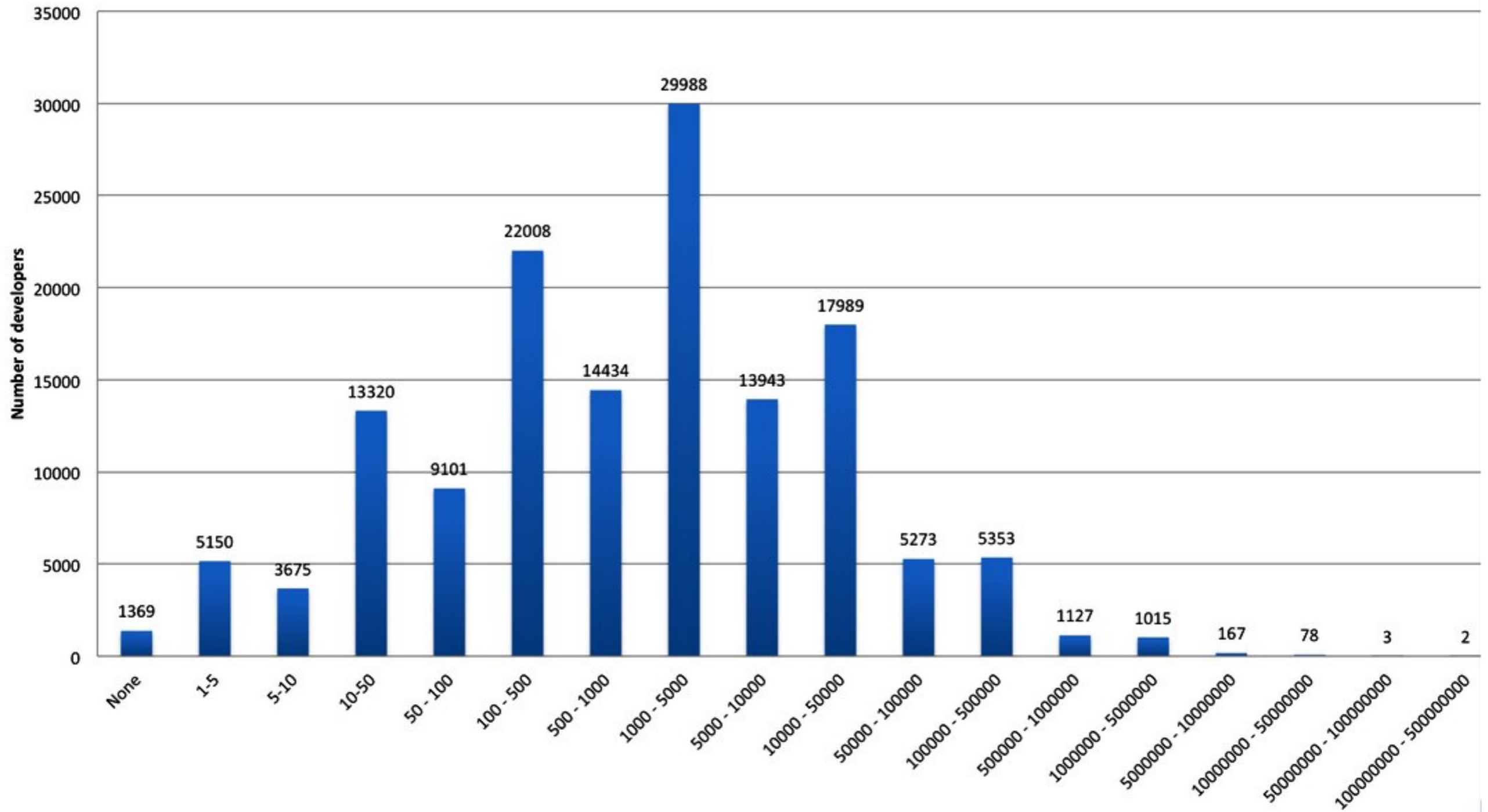
## Mobile App Store Downloads, Worldwide, 2010-2016 (Millions of Downloads)

	<b>2012</b>	<b>2013</b>	<b>2014</b>	<b>2015</b>	<b>2016</b>	<b>2017</b>
Free Downloads	57,331	92,876	127,704	167,054	211,313	253,914
Paid-for Downloads	6,654	9,186	11,105	12,574	13,488	14,778
<b>Total Downloads</b>	<b>63,985</b>	<b>102,062</b>	<b>138,809</b>	<b>179,628</b>	<b>224,801</b>	<b>268,692</b>
<i>Free Downloads %</i>	89.6	91.0	92.0	93.0	94.0	94.5

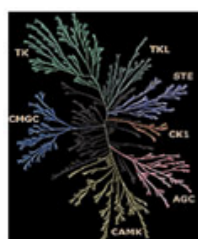
Source: Gartner (September 2013)

# However, Market Awareness Is Challenging...

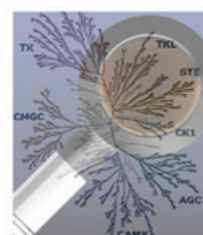
Android Developers vs. Installs



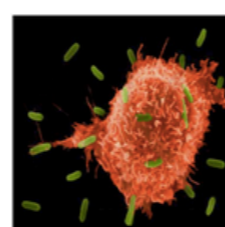
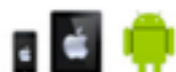
# Eidogen's Apps: More than 50K Downloads



**iKinase**



**iKinasePro**



**iOncology**



**iProtein**



**Mobile Reagents**



In partnership with Intel



**Reaction101**



**Yield101**



**SPRESImobile**



**ScienceCloud Tasks**



In partnership with Molecular Materials Informatics,

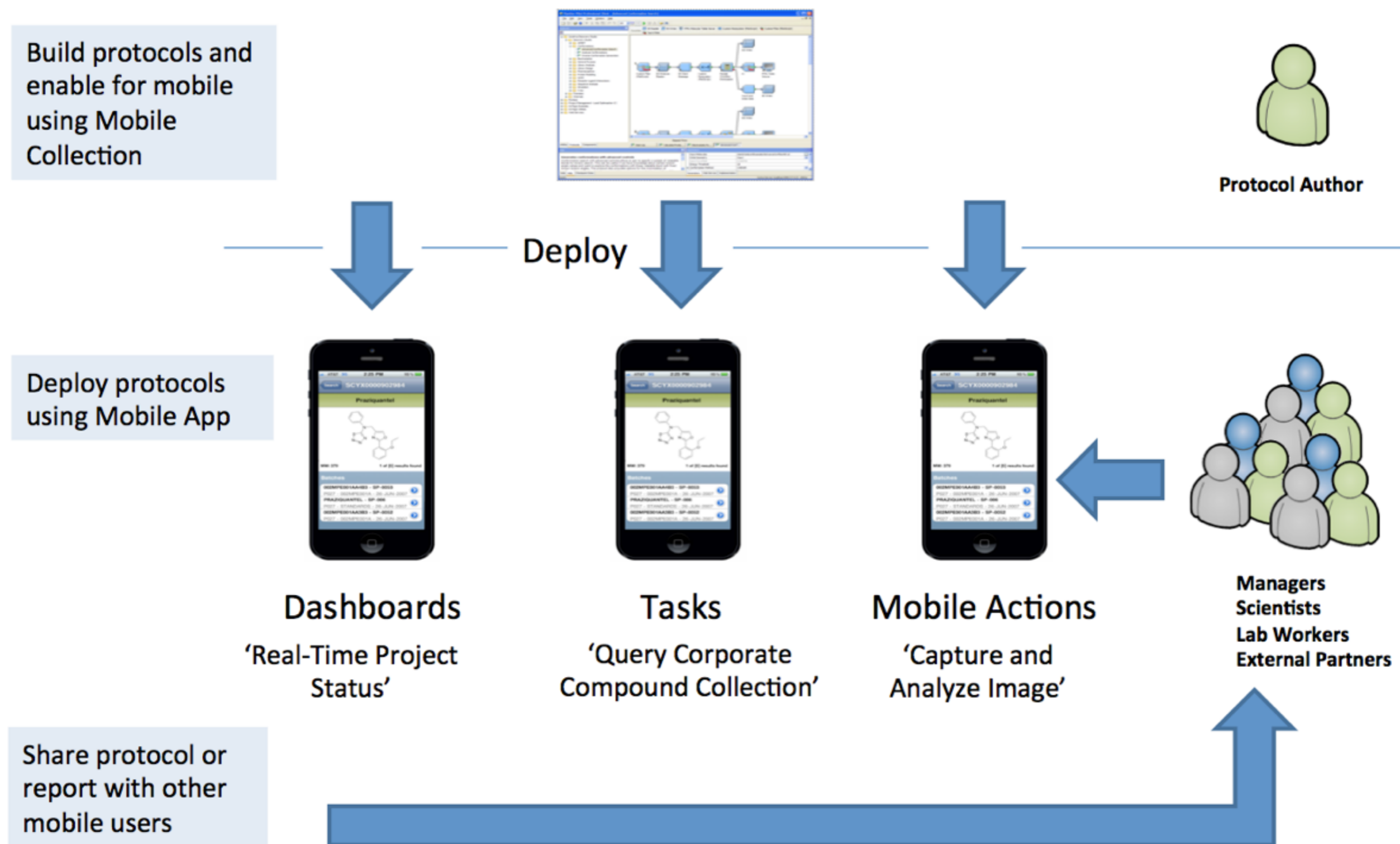
with InfoChem

In partnership with Accelrys

# Science-Cloud Tasks (Eidogen/Accelrys)

- What is it?
  - ▶ An iOS application for iPod/iPhone/iPad (Android planned)
  - ▶ A new Pipeline Pilot component collection
- What does it do?
  - ▶ Allow any Pipeline Pilot PDF and HTML report to be easily deployed to mobile devices
  - ▶ Allow authoring of new Pipeline Pilot protocols to deploy dashboards and mobile-centered tasks and actions on mobile devices
- Free App from Apple AppStore (search 'Accelrys')

# New Mobile Possibilities...



## ScienceCloud Tasks / Mobile Collection

# Pipeline Pilot Protocols are Easily 'Mobilized'

The screenshot displays the Pipeline Pilot Professional Client interface. On the left, a 'Components' tree lists various mobile input and output components. The main workspace shows a 'Protocols' tree with a selected protocol 'Where On Earth Am I'. A workflow diagram in the center shows a sequence of three components: 'Location Input (Mobile)', 'Geo Chart (Mobile)', and 'HTML Output (Mobile)'. A yellow callout box explains the process: 'We read a location from the user, then load it into a GeoChart. Simple!'. At the bottom, a 'Jobs' table lists several protocols, with 'Where On Earth Am I' highlighted as 'Not Started'. A 'Parameters' panel on the right shows 'Location' parameters: 'Latitude' and 'Longitude'.

**Components**

- Mobile
  - Inputs
    - Audio Input (Mobile)
    - Barcode Input (Mobile)
    - Camera Input (Mobile)
    - Location Input (Mobile)
    - Molecule Input (Mobile)
  - Outputs
    - Audio Output (Mobile)
    - Text to Audio Output (Mobile)
  - Reporting
    - Charts
    - Text
    - HTML Output (Mobile)
  - Utilities
    - Prototypes
      - Barcodes
      - Filters
      - Location
      - Multistep Tasks
      - Reporting
- ScienceCloud
  - Utilities
- Web Applications
  - Accelrys
  - Dependent List Boxes\_TM mod

**Protocols**

- Examples
- Mobile
  - Admin
  - Demo
    - Audio and Video
    - Chemistry
    - Fun
      - Analyzing Beers with Different Chart Types
      - City Temperature Gauges
      - Find Best Beers for your Buck
      - GeoChart Side-by-Side with Photo
      - Lookup Barcode Info
      - Manipulate My Picture Many Ways
      - Table with Inline Molecules
      - Where On Earth Am I
    - Location and Maps
    - Search
    - Developer
    - Prototypes
    - Test
  - Mobile Demo
  - Mobile Protocols
  - Mobile Services
  - Mobile Services-tests
  - Portlets
  - Stylesheets

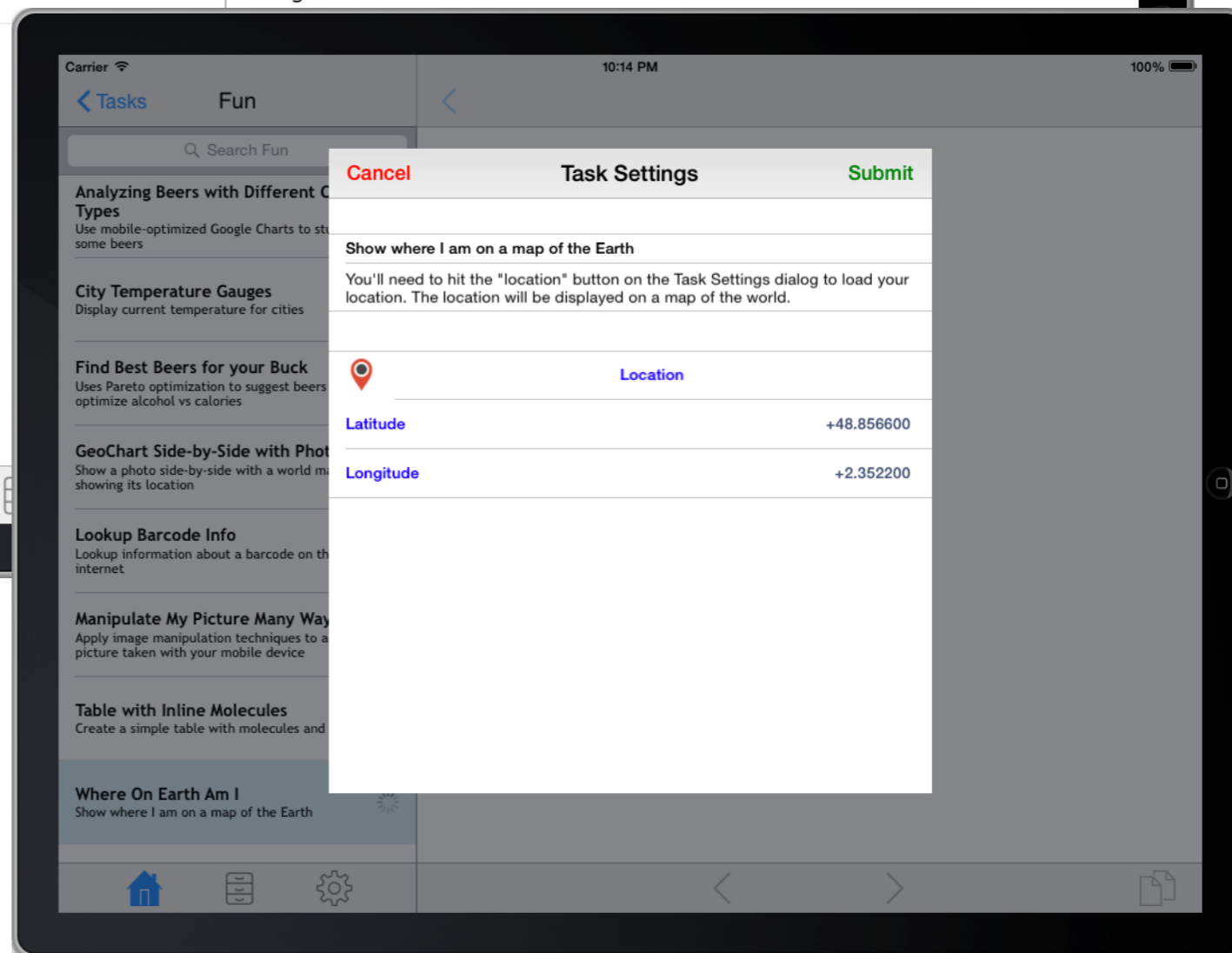
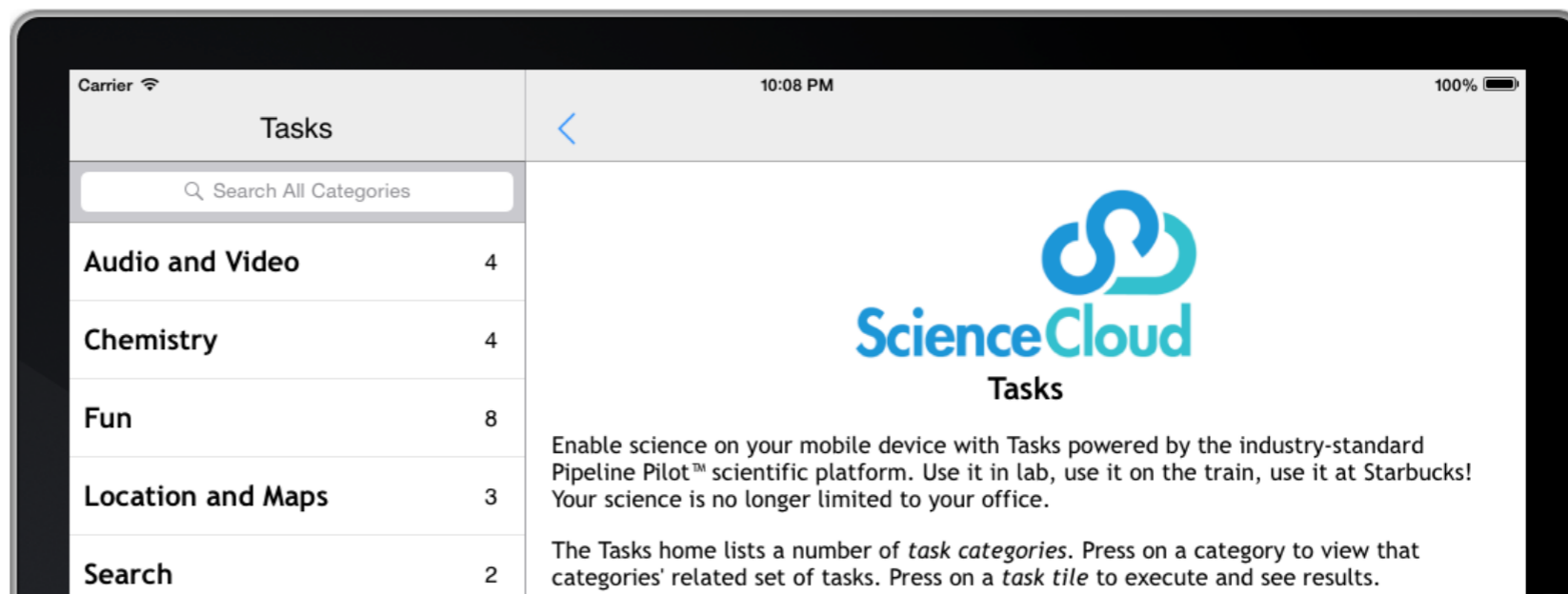
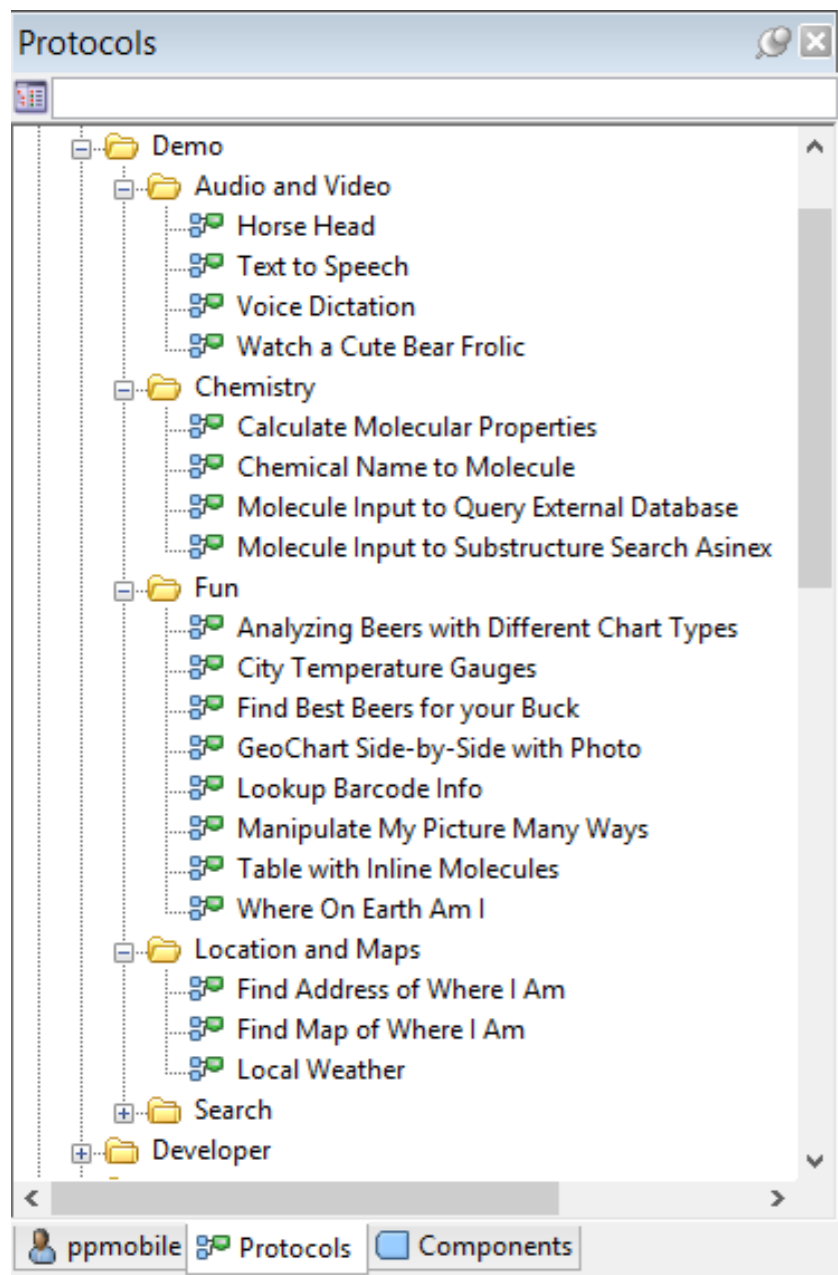
**Jobs**

Protocol Name	Status	Start Date
Horse Head	Finished	Tue Feb 18 17:21...
Manipulate My Picture Many Ways	Finished	Thu Mar 13 05:2...
New Protocol1	Finished	Thu Mar 06 07:2...
Where On Earth Am I	Not Started	

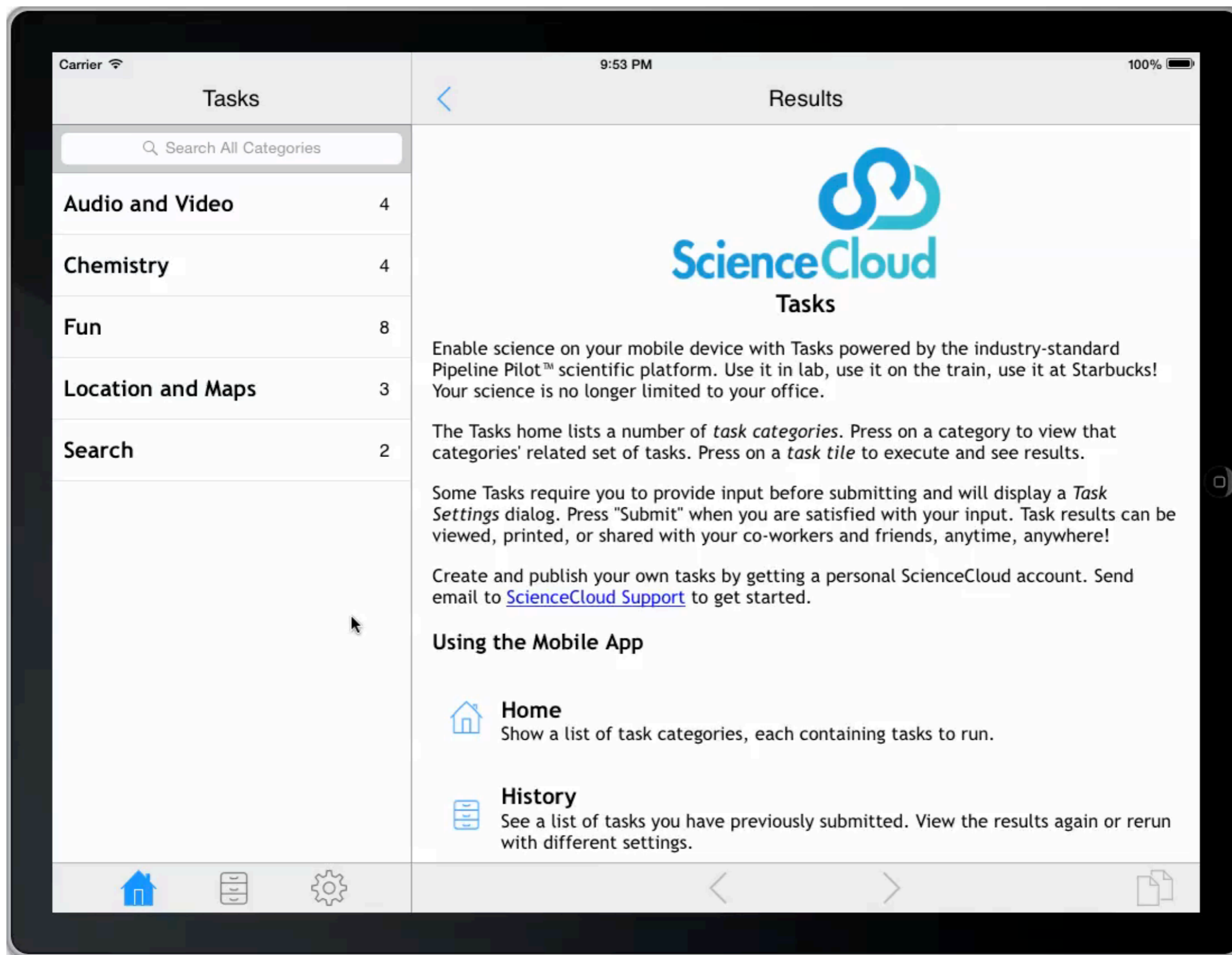
**Parameters**

- Location
  - Latitude
  - Longitude

# Protocol Folders Appear in the Tasks App

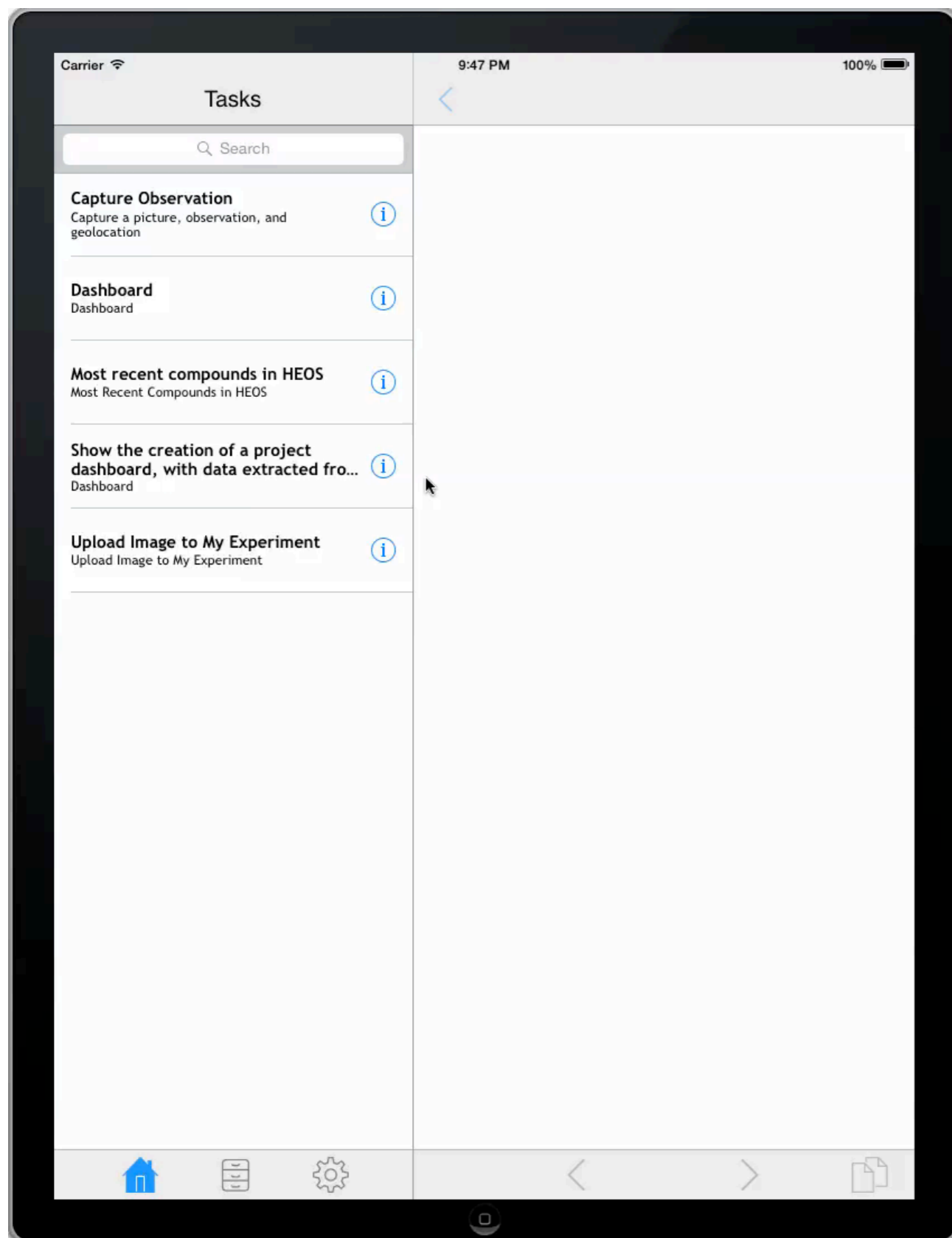


# Location Demo



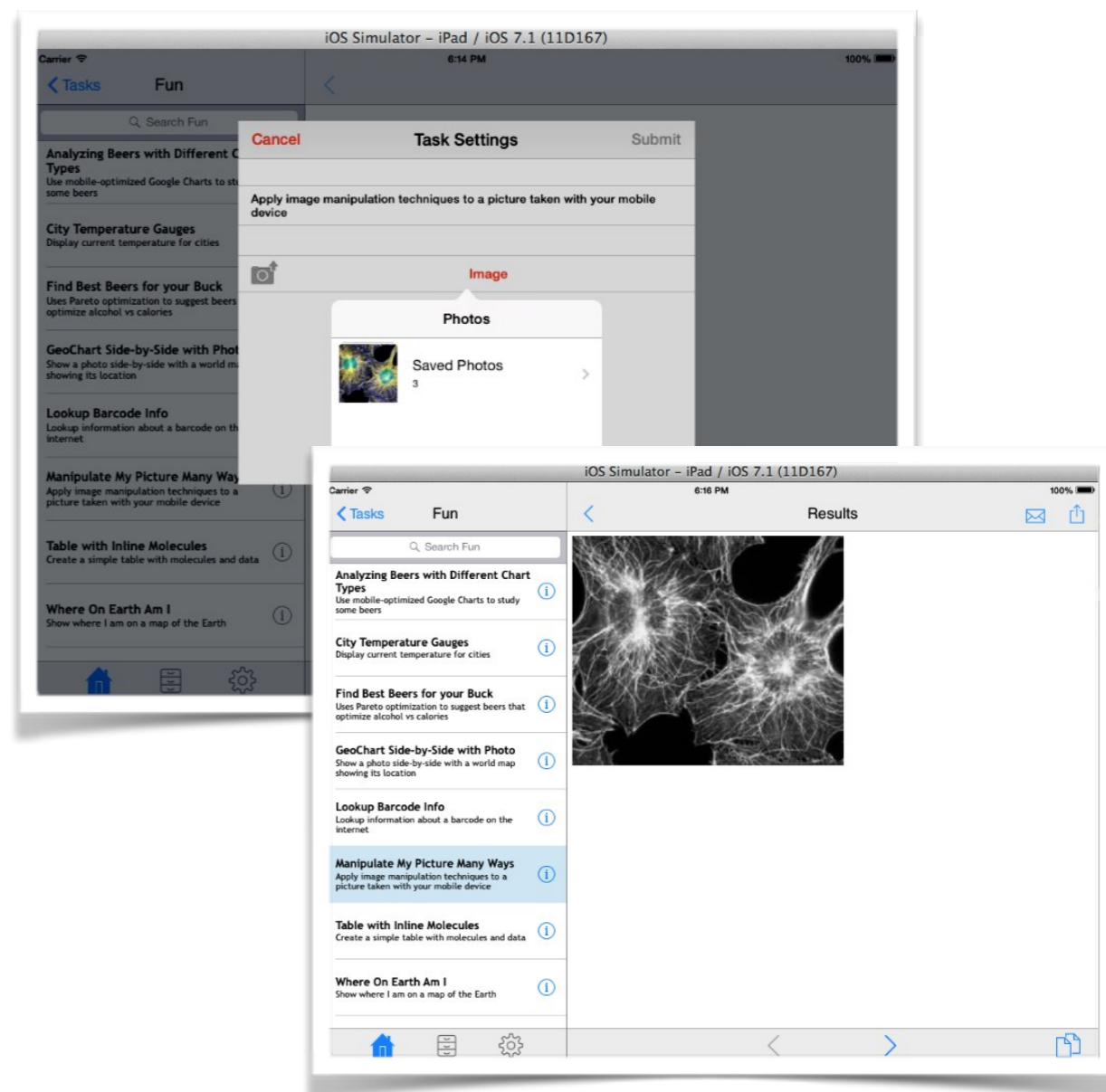


# Observation Capture (Demo)



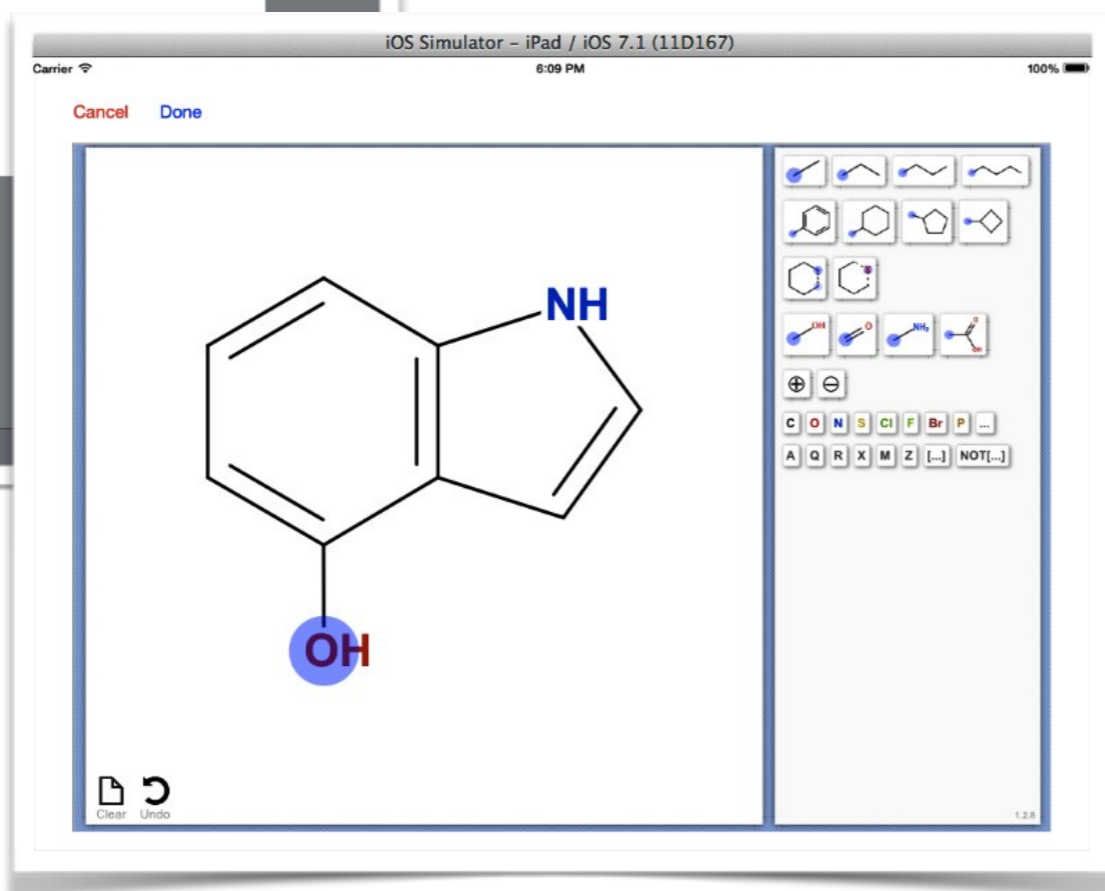
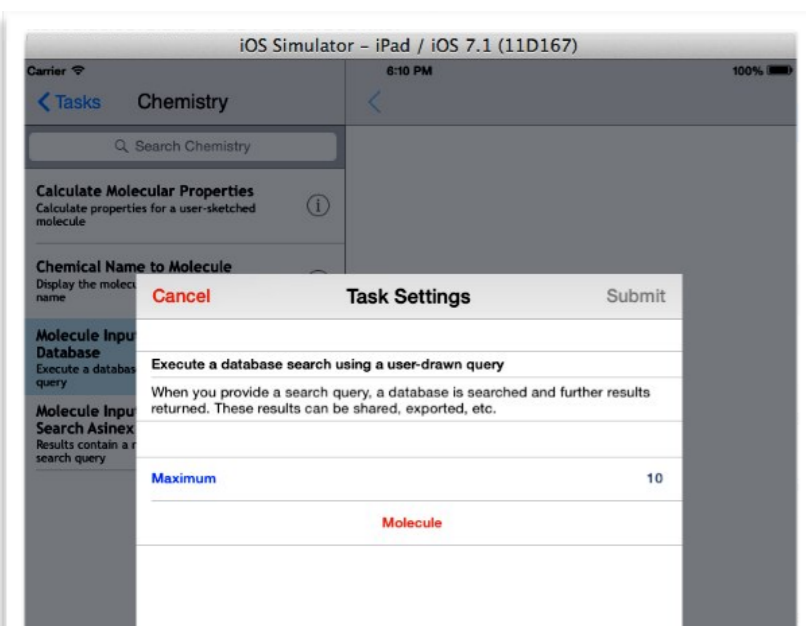
## Leverage Mobile Device Capabilities

- Camera, Audio, GPS, etc.

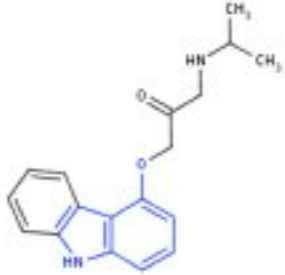


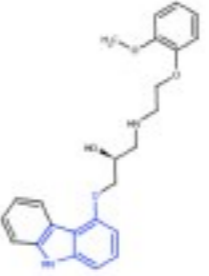


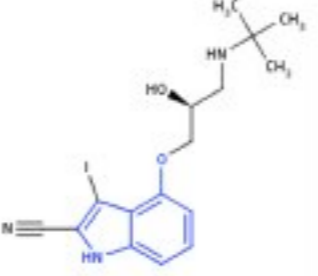
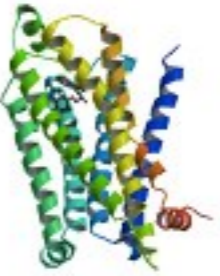
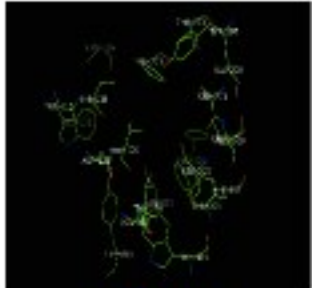


# Embed and Deploy

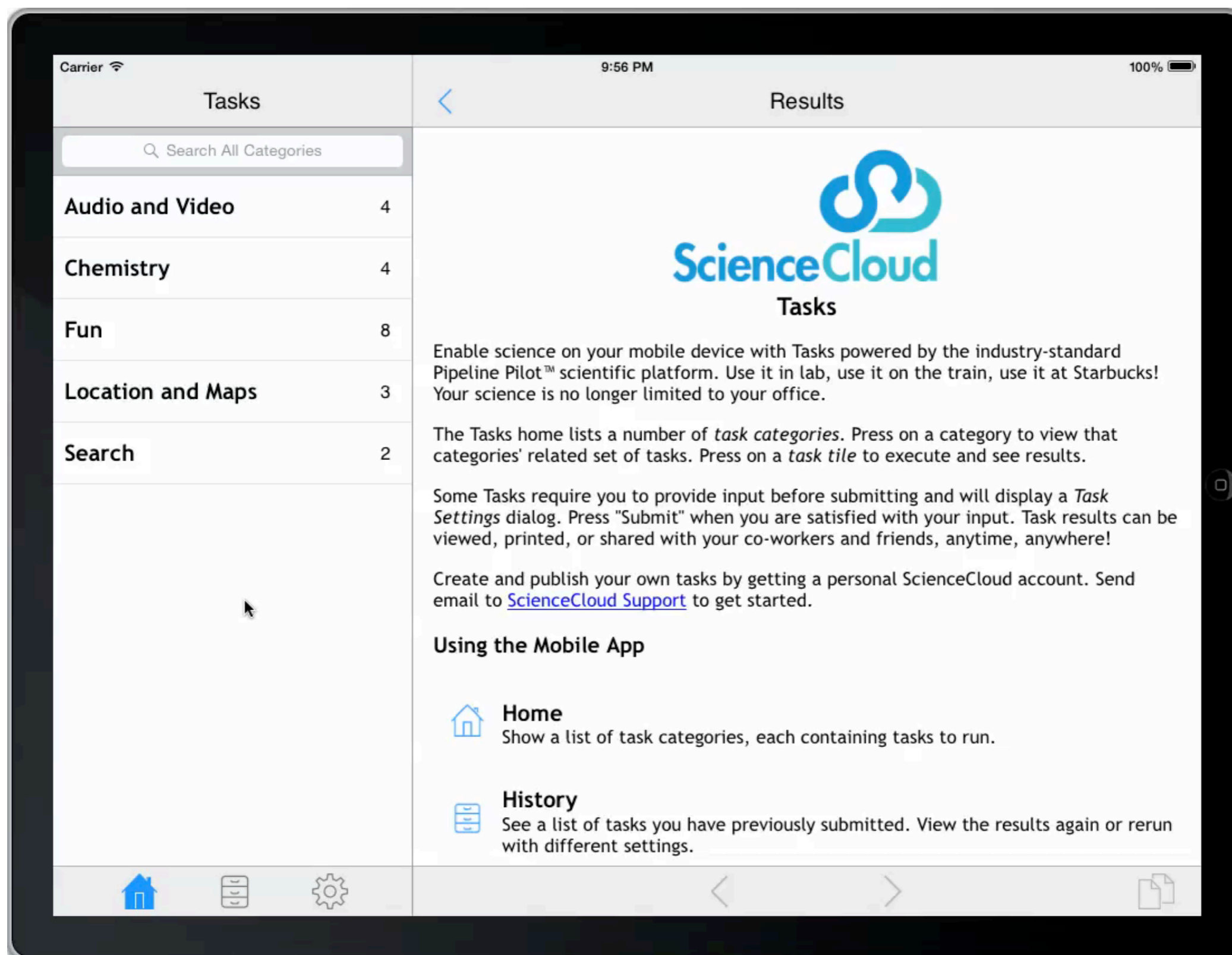
Embed full applications within Pipeline Pilot protocols and deploy to mobile users



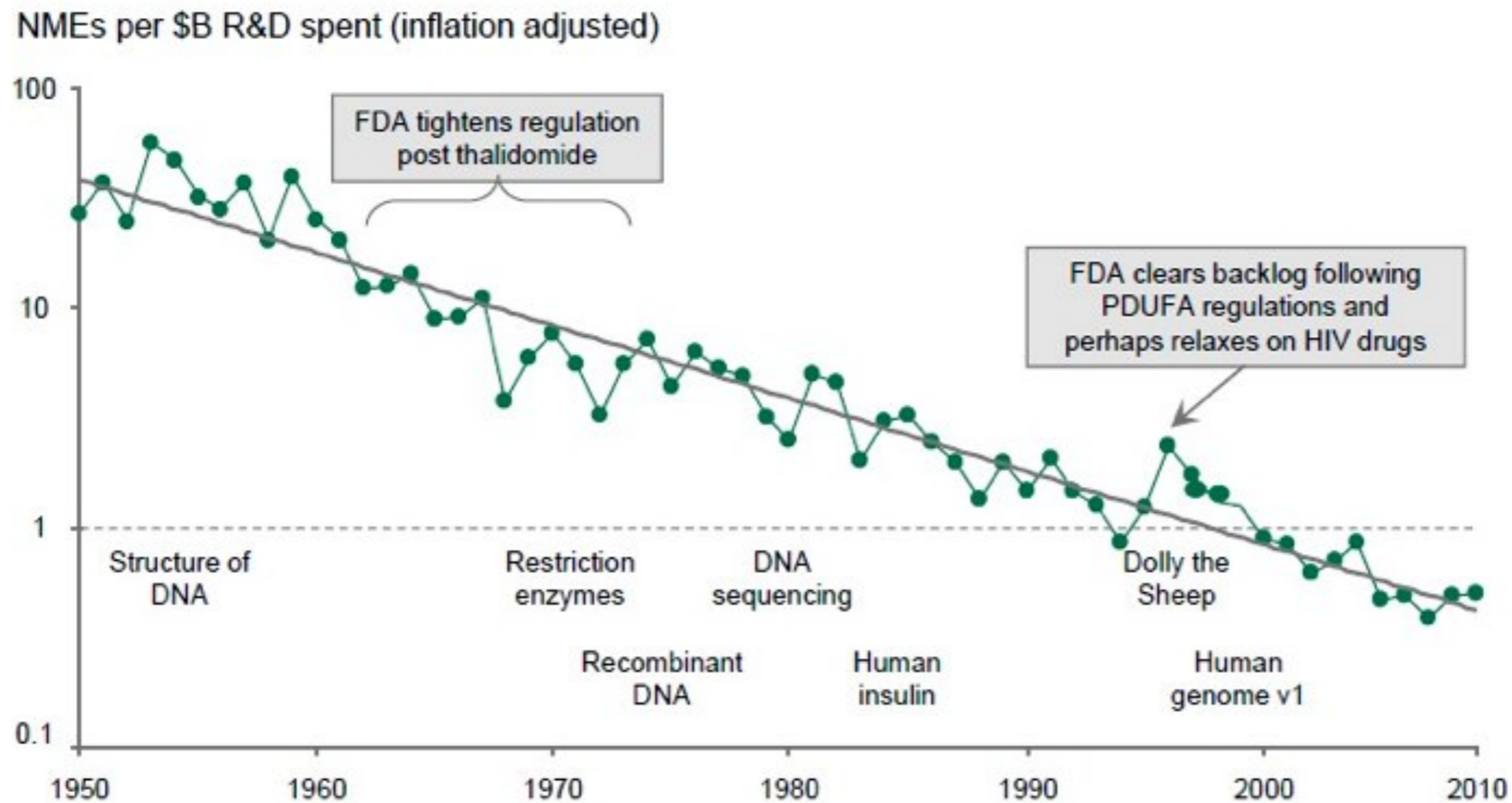
This screenshot shows the 'Results' screen of the chemistry application. It displays a table with three columns: 'Ligand Hit', 'PDB', and 'Site'. The table contains three rows of data, each showing a chemical structure, a PDB ID, and a binding site ID.

Ligand Hit	PDB	Site
 CAU	 <a href="#">2rhl</a>	 <a href="#">1276810</a>
 CVD	 <a href="#">4amj</a>	 <a href="#">2004620</a>
 I32	 <a href="#">2ycz</a>	 <a href="#">1857801</a>

# Ligand Co-Complex Search (Demo)



# R&D Productivity Has Been On The Decline



Note: R&D costs are estimated from PhRMA annual survey 2009; NMEs are the total number of small molecule and biologic approvals by the FDA

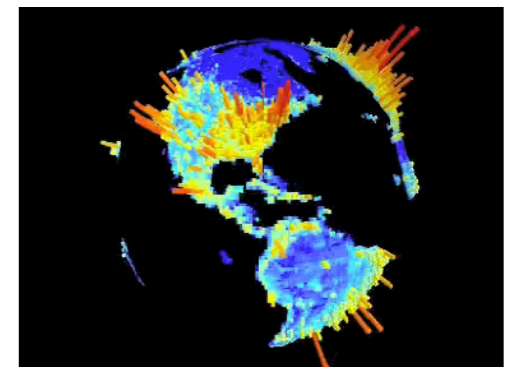
Source: Bernstein Research "The Long View - R&D Productivity" (September 30, 2010)

Life sciences R&D: Changing the innovation equation in India

THE BOSTON CONSULTING GROUP

**7 Billion** people depend on fewer than **500,000** people to discover and develop new medicines.

**Let's find a way to shift the numbers...**



# Summary

- Billions of people routinely use and connect with mobile devices.
- Massive worldwide connectivity is unprecedented.
- Well deployed social media frameworks are in-place and easy to access.
  - e.g. Facebook, Twitter, and their APIs.
- Science apps have been largely insular, vertical, and point solutions. We need to recruit more of the world!
- Cloud-based pipelining-tools, social media frameworks, and mobile devices together open many new possibilities.

# Acknowledgements

- **Accelrys**

- Matt Hahn
- Dave Rogers
- Jung Ku
- Mike Peeler
- Ton van Daelen

- Maurizio Bronzetti
- Stephan Schurer
- Alex Clark





# 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*<sup>TM</sup> - Protein Structural Informatics Platform
- *KKB*<sup>TM</sup> - Kinase SAR and Chemistry Knowledgebase
- *CHIP*<sup>TM</sup> - Chemical Intelligence Platform

## • DirectDesign<sup>TM</sup> Fee-For-Service

- In Silico Target Screening (“Target Fishing” and Repurposing)
- Target and compound prioritization services
- Fast Follower Design: Novel, Patentable Leads