

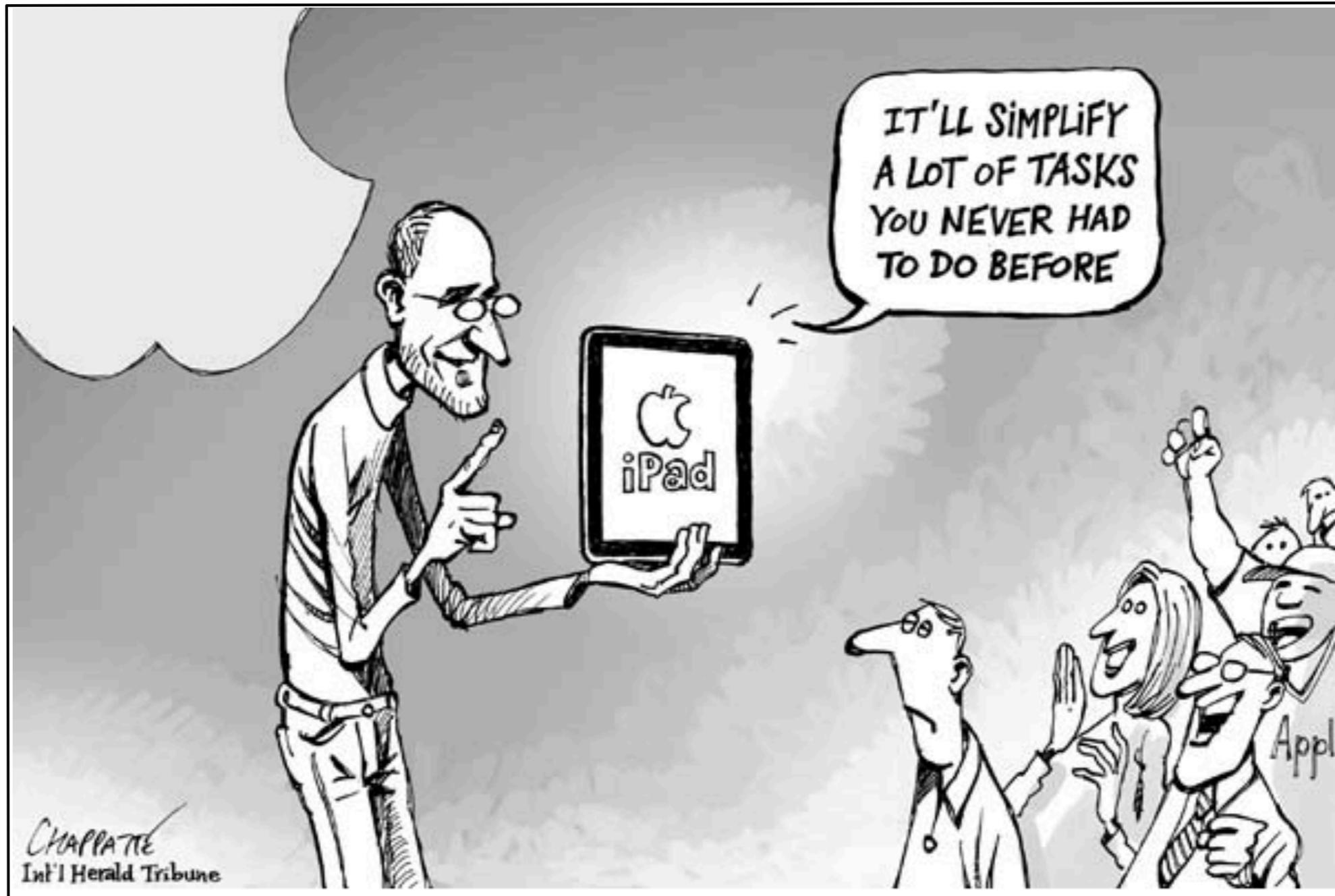
# Riding the Mobile Wave

Dr. Steven Muskal

Chief Executive Officer

Eidogen-Sertanty, Inc

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



IT'LL SIMPLIFY  
A LOT OF TASKS  
YOU NEVER HAD  
TO DO BEFORE

CHAPPATE  
Int'l Herald Tribune

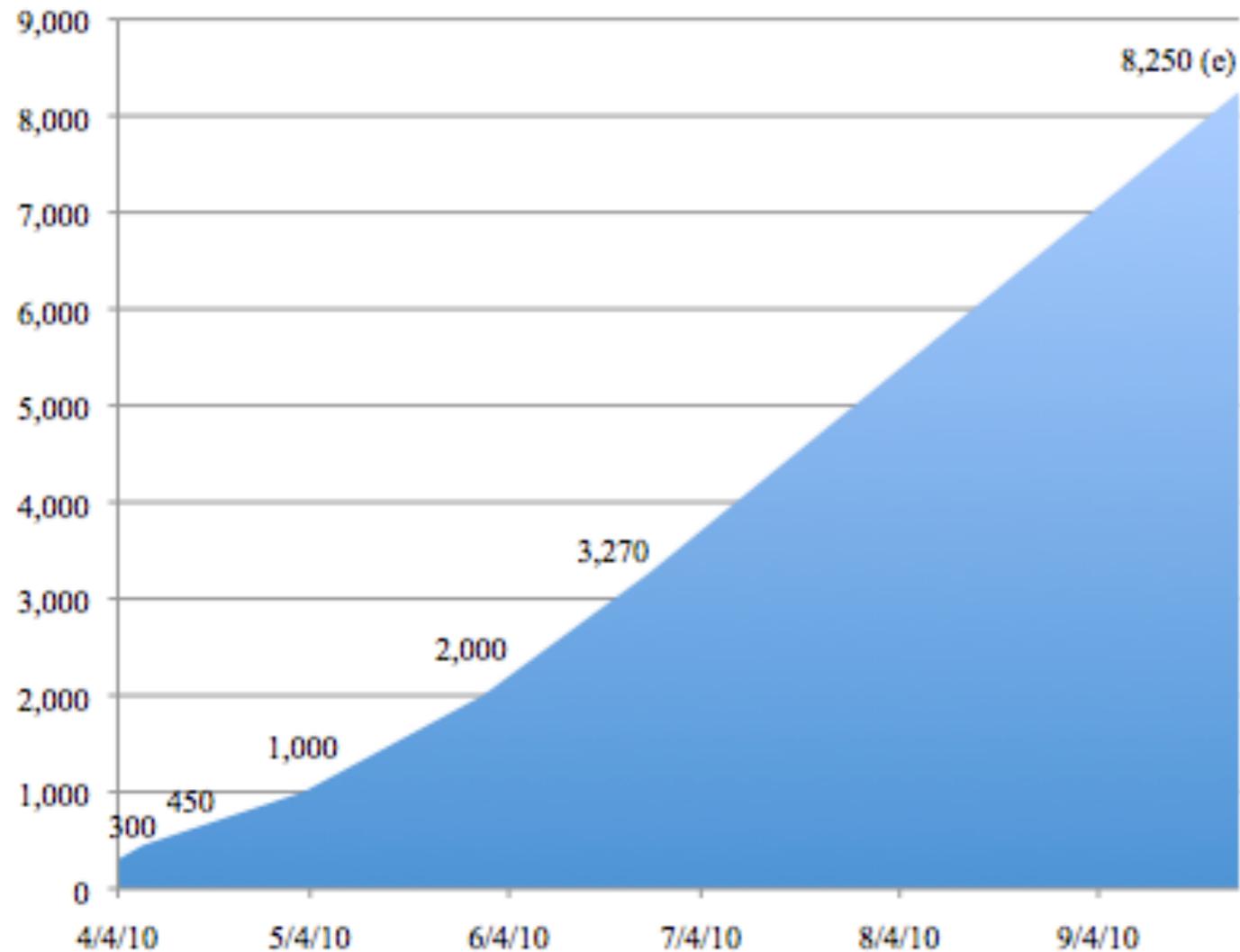
# Presentation Agenda

- 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

## iPad Sales Trajectory (000)



Sources: Company reports and the consensus estimate for Q4

**FORTUNE**

## 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

 **DailyFinance**  
An AOL Money & Finance Site

Posted 10:00 AM 09/09/10  
<http://srph.it/ak77OA>

<http://tech.fortune.cnn.com/2010/10/05/how-many-ipads-has-apple-really-sold/>

<http://www.publishersweekly.com/pw/by-topic/industry-news/financial-reporting/article/44882-ipad-total-nears-7-5-million.html>

<http://www.dailyfinance.com/story/company-news/apple-ipad-sales-projected-to-hit-28-million-in-2011/19626822/>

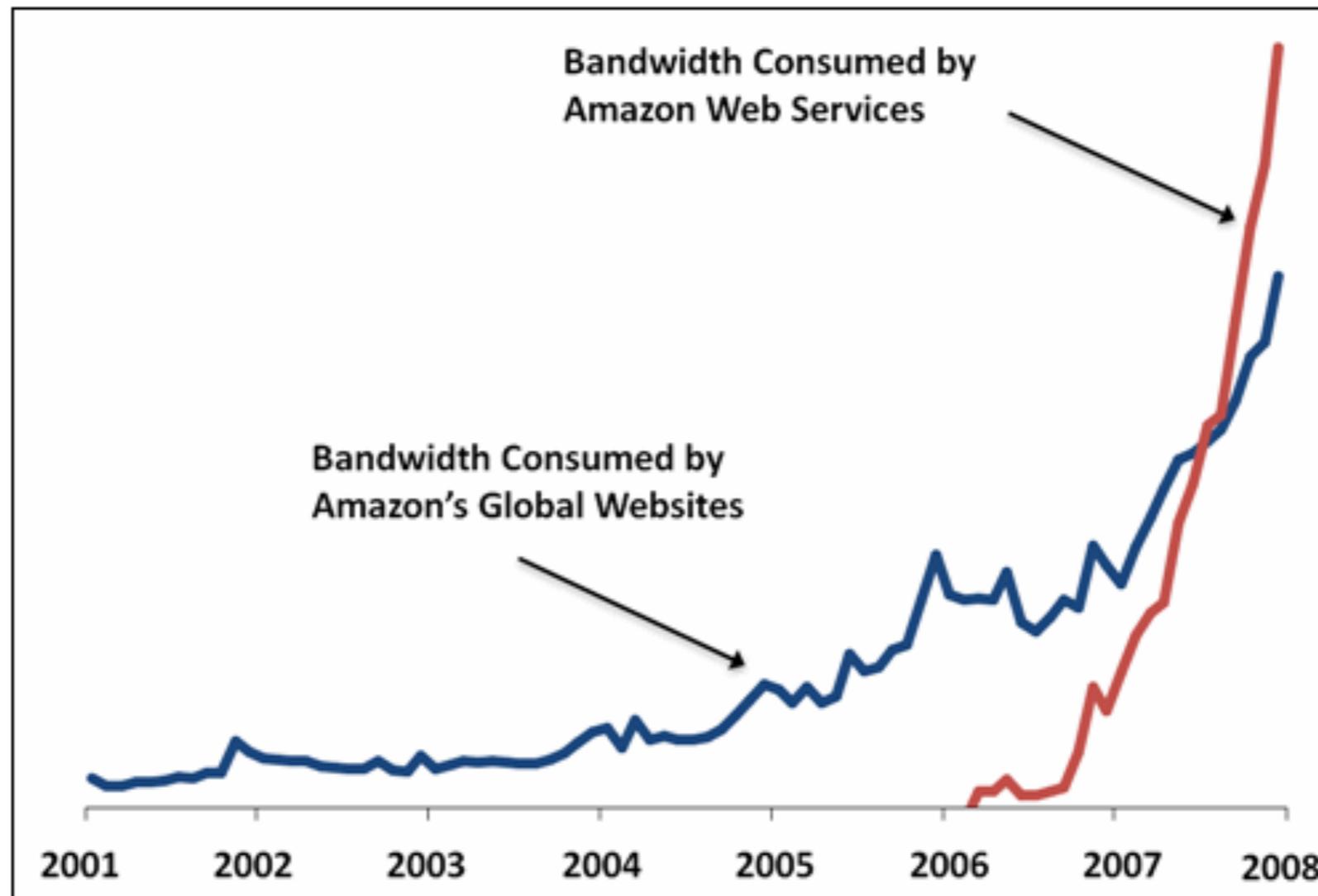
# Mobile-Cloud Infrastructure

- 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.....

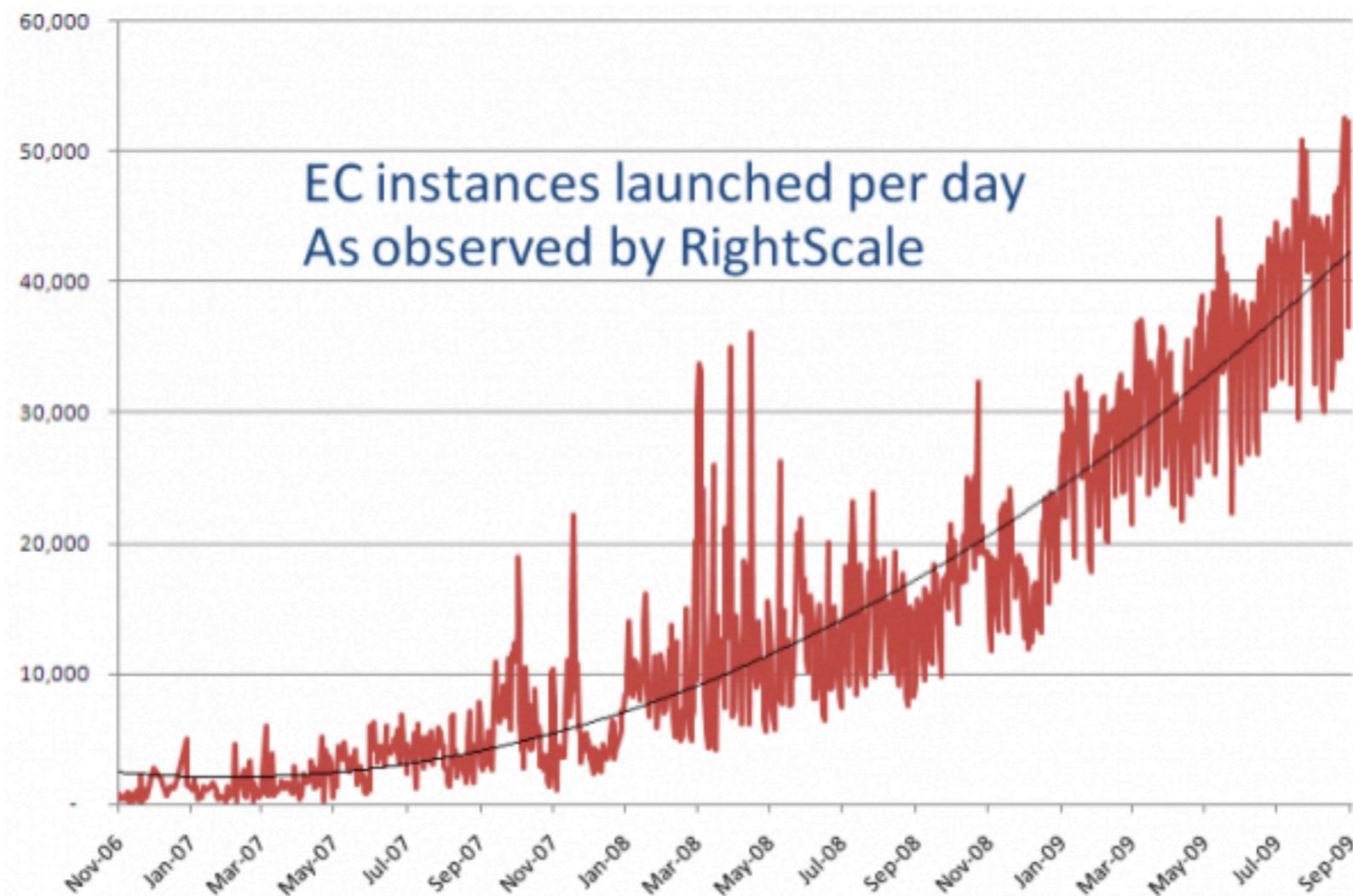


# Amazon AWS Growth

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



# Amazon AWS Growth (cont.)



Source: <http://blog.rightscale.com/2009/10/05/amazon-usage-estimates/>

## 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
Amazon Elastic MapReduce
Amazon CloudFront

**Navigation**

Region: US East

- > EC2 Dashboard
- INSTANCES
  - > Instances
  - > Spot Requests
- IMAGES
  - > AMIs
  - > Bundle Tasks
- ELASTIC BLOCK STORE
  - > Volumes
  - > Snapshots
- NETWORKING & SECURITY
  - > Elastic IPs
  - > Security Groups
  - > Key Pairs
  - > Load Balancers

## 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**

Current Status	Details
<span style="color: green;">✔</span> Amazon EC2 (US East - N. Virginia)	Service is operating normally <a href="#">View complete service health details</a>

**My Resources**

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

- 1 Running Instance1 Elastic IP
- 1 EBS Volume4 EBS Snapshots
- 2 Key Pairs2 Security Groups
- 0 Load Balancers

**Related Links**

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

---

**Navigation**

Region: US East

- > EC2 Dashboard
- INSTANCES
  - > Instances
  - > Spot Requests
- IMAGES
  - > AMIs
  - > Bundle Tasks
- ELASTIC BLOCK STORE
  - > Volumes
  - > Snapshots
- NETWORKING & SECURITY
  - > Elastic IPs
  - > Security Groups
  - > Key Pairs
  - > Load Balancers

## My Instances

[Launch Instance](#)
Instance Actions
Reserved Instances

[Show/Hide](#)
[Refresh](#)
[Help](#)

Viewing: All Instances All Instance Types

Instance	AMI ID	Root Device Type	Type	Status	Lifecycle	Public DNS	Security Groups	Key Pair Name	More	
<input checked="" type="checkbox"/>	i-294bf742	ami-2cb05345	instance-store	m1.small	● running	normal	ec2-184-73-205-197.compute-1.amazonaws.com	defaultLAMP	kinasdata	<a href="#">More</a>

**1 EC2 Instance selected**

**EC2 Instance: i-294bf742**

Time Range: Last Hour [Refresh](#)

**Avg CPU Utilization (Percent)**

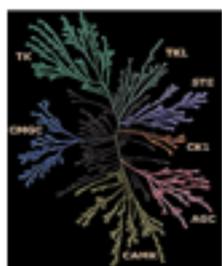
**Avg Disk Reads (Bytes)**

**Avg Disk Writes (Bytes)**

**Max Network In (Bytes)**

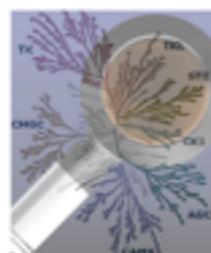
**Max Network Out (Bytes)**

# Eidogen-Sertanty's iPhone and iPad Apps



iKinase  
Eidogen-Sertanty

iKinase

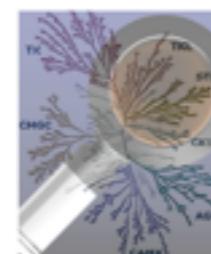


iKinasePro  
Eidogen-Sertanty

iKinasePro



Mobile Reagents



iKinasePro  
Eidogen-Sertanty

iKinasePro



iProtein



Mobile Reagents



Reaction101



Yield101



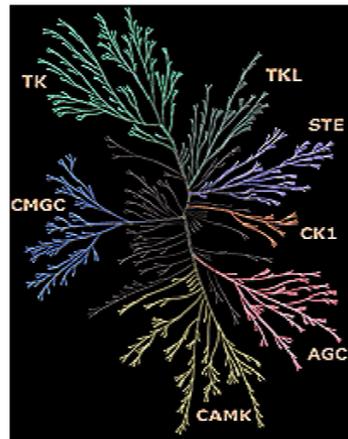
Reaction101



Yield101

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

# iKinase - 12/31/09 (v1) ... 5/5/11 (v5.1)



iKinase

Eidogen Sert@nty

Carrier 8:57 PM

KKBQ410 Tell a Friend

**Welcome back to iKinase!**

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

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.

OK

ABL DPs: 562 AVG: 5.37 STD: 1.41 Min: 2.06 Max: 9.60

ABL1 DPs: 2450 AVG: 6.51 STD: 1.14 Min: 2.82 Max: 10.52

ABL2 DPs: 57 AVG: 6.14 STD: 1.29 Min: 5.00 Max: 9.77

ACK1 DPs: 343 AVG: 5.51 STD: 1.37 Min: 4.52 Max: 8.00

ACVR1 DPs: 38 AVG: 5.27 STD: 0.53 Min: 5.00 Max: 7.13

ACVR1B DPs: 37 AVG: 5.22 STD: 0.53 Min: 5.00 Max: 7.07

ACVR2A DPs: 37 AVG: 5.08 STD: 0.30 Min: 5.00 Max: 6.68

ACVR2B DPs: 38 AVG: 5.20 STD: 0.57 Min: 5.00 Max: 9.00

Carrier 11:01 AM

KKB2010 Register

A 1.13 Min: 5.00 Max: 8.92

ABL DPs: 562 AVG: 5.37 STD: 1.41 Min: 2.06 Max: 9.60

ABL1 DPs: 2450 AVG: 6.51 STD: 1.14 Min: 2.82 Max: 10.52

ABL2 DPs: 57 AVG: 6.14 STD: 1.29 Min: 5.00 Max: 9.77

ACK1 DPs: 343 AVG: 5.51 STD: 1.37 Min: 4.52 Max: 8.00

ACVR1 DPs: 38 AVG: 5.27 STD: 0.53 Min: 5.00 Max: 7.13

ACVR1B DPs: 37 AVG: 5.22 STD: 0.53 Min: 5.00 Max: 7.07

ACVR2A DPs: 37 AVG: 5.08 STD: 0.30 Min: 5.00 Max: 6.68

ACVR2B DPs: 38 AVG: 5.20 STD: 0.57 Min: 5.00 Max: 9.00

Carrier 8:35 PM

MobileReagents Available! Register

Target EGFR

Type Enzyme Assay

Measure IC50 = 6 pM (pval: 11.222)

Carrier 8:58 PM

KKBQ410 KKBid: 66 Email SAR

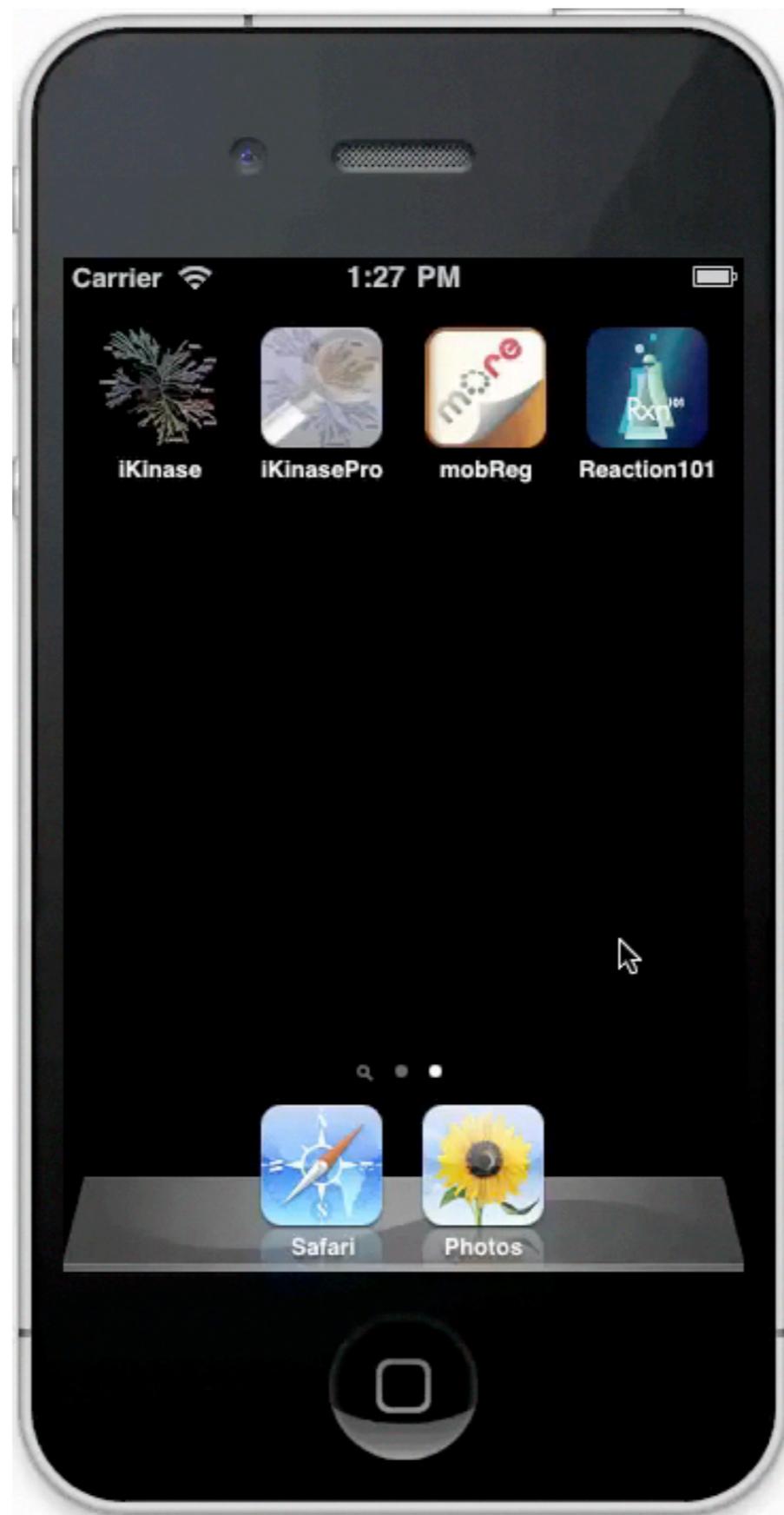
KKBid: 66

Total DataPoints: 1371

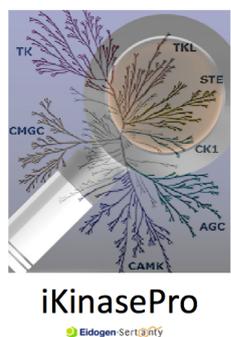
**PKC [Cell-Based Assay]...**  
Cytotoxicity Activity (HeLa S3 Cells)  
cytotoxicity 0.004 nM (pval: 11.398)

**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)



Carrier 11:34 AM

Kinase Targets Register

Search

Welcome back to iKinasePro!  
New to iKinasePro update 4:  
- iOS4.2 Multi-tasking!  
- Printing support  
- Register to gain access to over 35K additional datapoints for free!

OK

AAK1 DP: 45 AVG: 5.76 STD: 1.41 Min: 2.06 Max: 9.60  
ABL DP: 2450 AVG: 6.51 STD: 1.14 Min: 2.82 Max: 10.52  
ABL1 DP: 1.14 Min: 2.82 Max: 10.52  
ABL2 DP: 1.29 Min: 5.00 Max: 9.77  
ACVR1 DP: 38 AVG: 5.27 STD: 0.53 Min: 5.00 Max: 7.13

Rings Structure Search

Carrier 12:25 PM

Q PIK Cancel

Results

PIK3  
PIK3C2A  
PIK3C2B  
PIK3C2G  
PIK3C3

Q W E R T Y U I O P  
A S D F G H J K L  
Z X C V B N M

.?123 space Search

Carrier 12:26 PM

gleevec

Keyword(s)  
KKBid#  
Cancel

Q W E R T Y U I O P  
A S D F G H J K L  
Z X C V B N M

123 space return

Carrier 12:33 PM

Kinase... KKBid: gleevec... About Us

Target BCR/ABL  
Type Animal Model  
Measure response = 60 % (pval: )

SSSearch  
SimSearch  
SuperSimSearch  
Cancel

Carrier 11:42 AM

KKBid... KKBid: 1015... Email Alert

Edit SAR SSS Sim Super

Total DataPoints: 224

**BCR/ABL [Enzyme Assa...**  
BCR-ABL Inhibition (Substrate Phosphorylation)  
IC50 25 nM (pval: 7.602)

**PDGFRB [Cell-Based As...**  
Antiproliferation of Ba/F3.Tel-PDGFRB Cells  
IC50 0.027 uM (pval: 7.569)

Carrier 12:30 PM

KKBid: gleevec

Draw a structure and tap the button to issue a SSSearch

H  
C  
N  
O  
S  
P  
F  
Cl  
Br  
...

Carrier 12:32 PM

KKBid: gleevec

Draw Again

Example structure(s) containing selected/drawn substructure... [19 of 19]

Carrier 12:32 PM

KKBid: gleevec

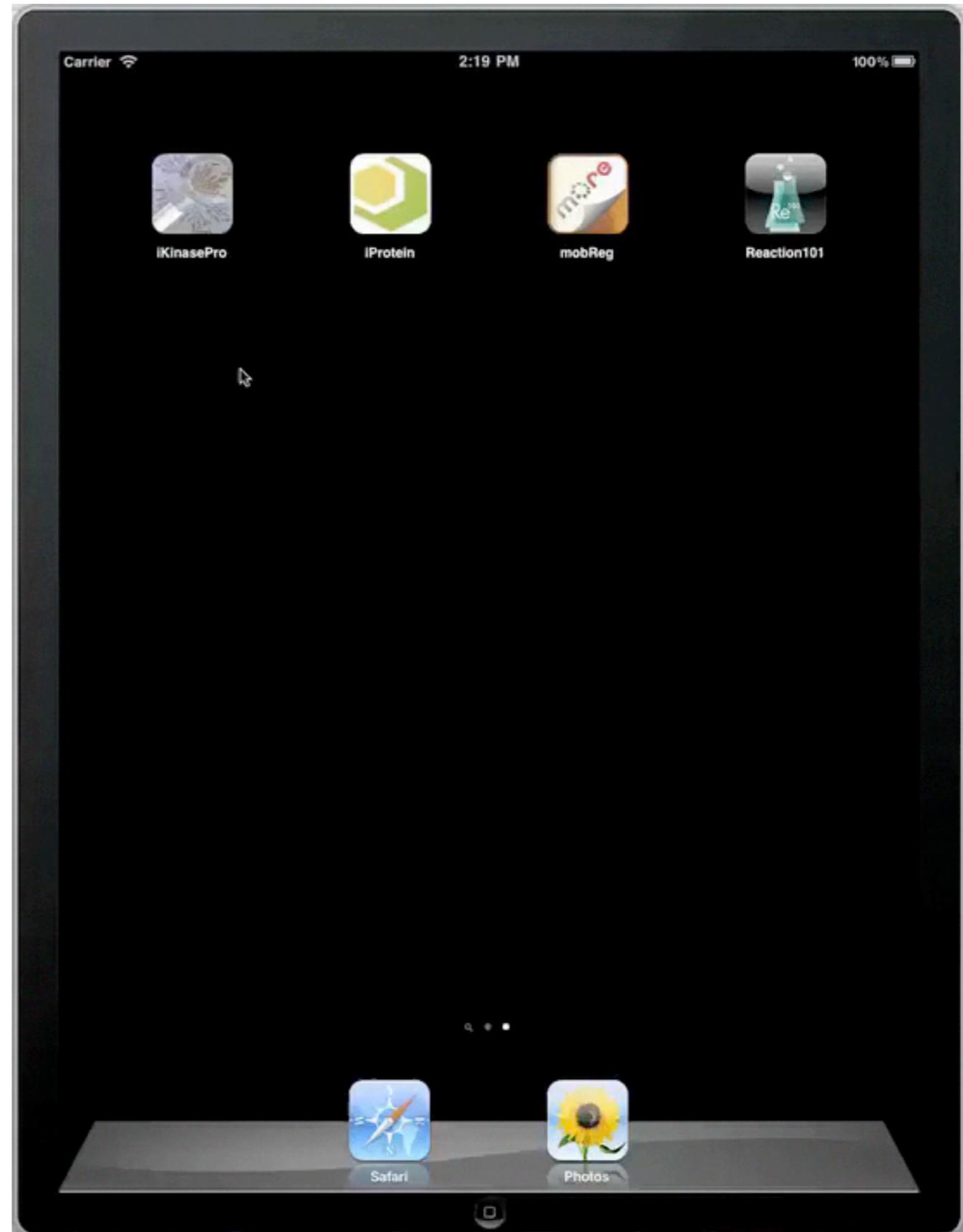
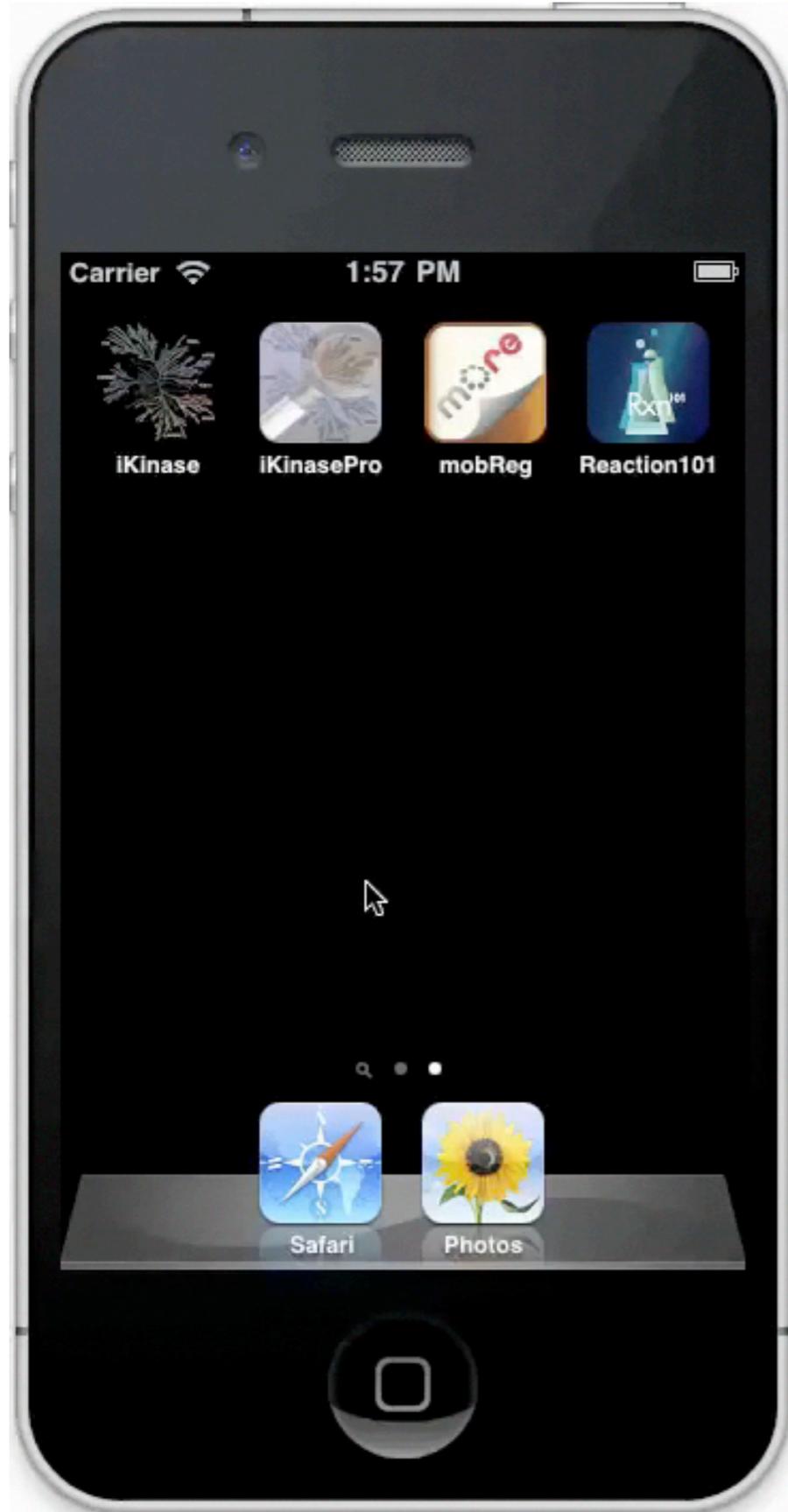
Back to Structure Grid Custom Structure Search Register for e-mail Alert

KKBid: 4194144

Target	Type	Name	Measure	Value
AURKA	Enzyme Assay	AURKA Kinase Inhibition Assay	Ki	< 0.1 uM (pval: 7.000)
GSK3B	Enzyme Assay	GSK3B Kinase Inhibition Assay	Ki	< 0.1 uM (pval: 7.000)
SRC	Enzyme Assay	SRC Kinase Inhibition Assay	Ki	Between 0.1 and 1 uM

Data extracted from the Eidogen-Sertanty Kinase Knowledgebase (KKB) as of Wed Aug 4 12:32:41 MST 2010

# iKinasePro (iOS4 + iPad) Demos

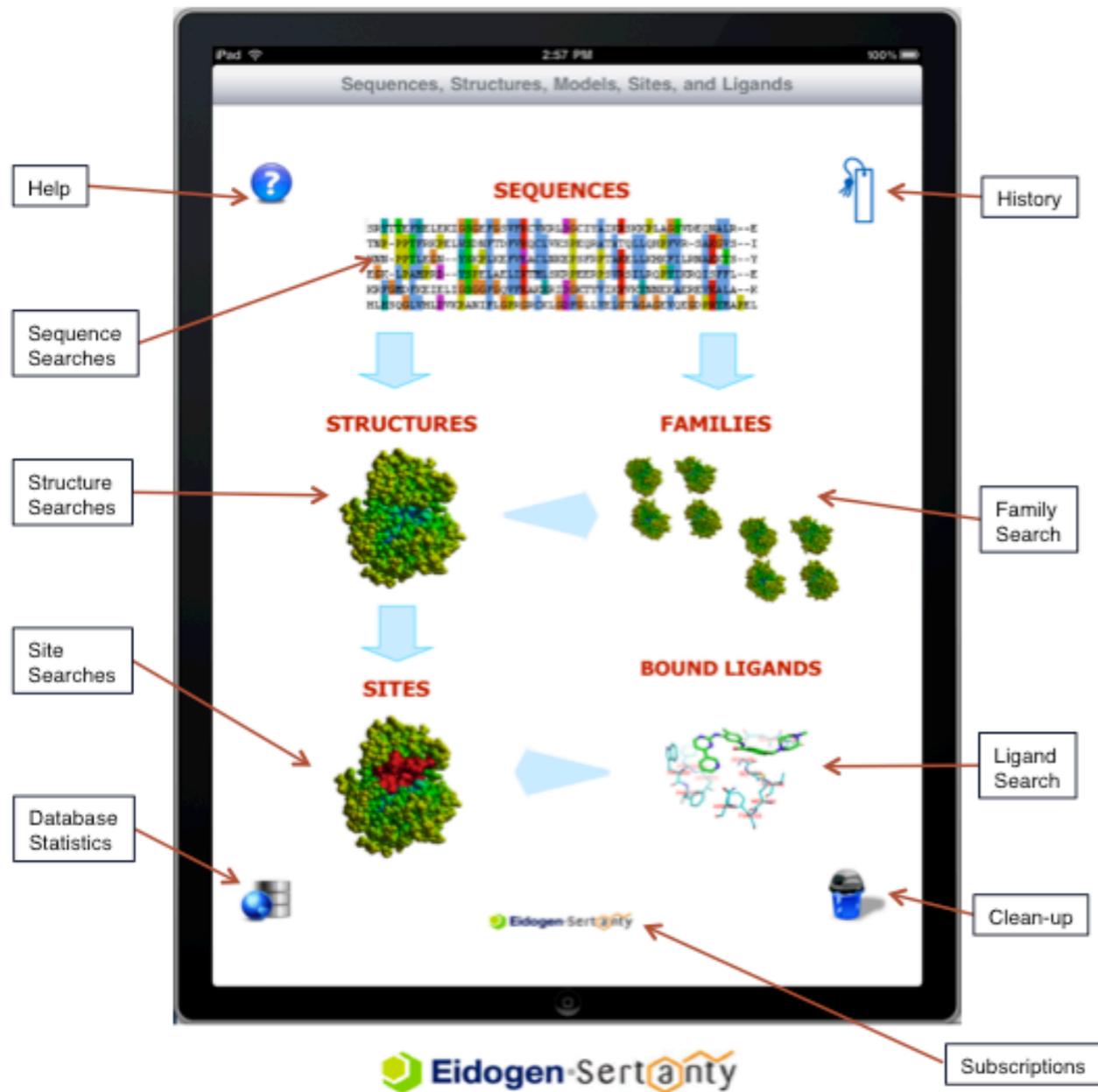


# iProtein - 8/10 (v1) ... 5/11 (v4)



## 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....

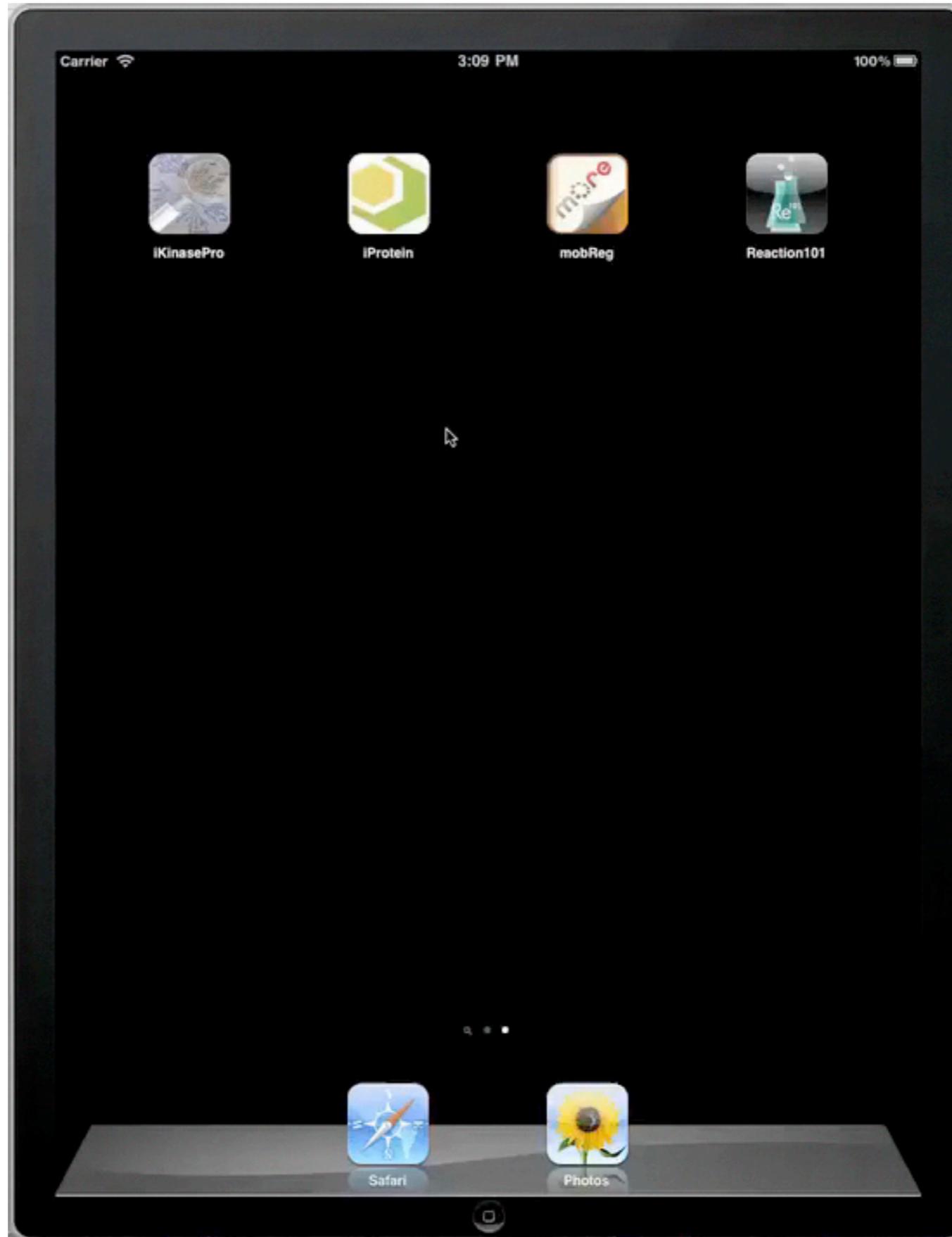


## Structure/Model Searches (cont)

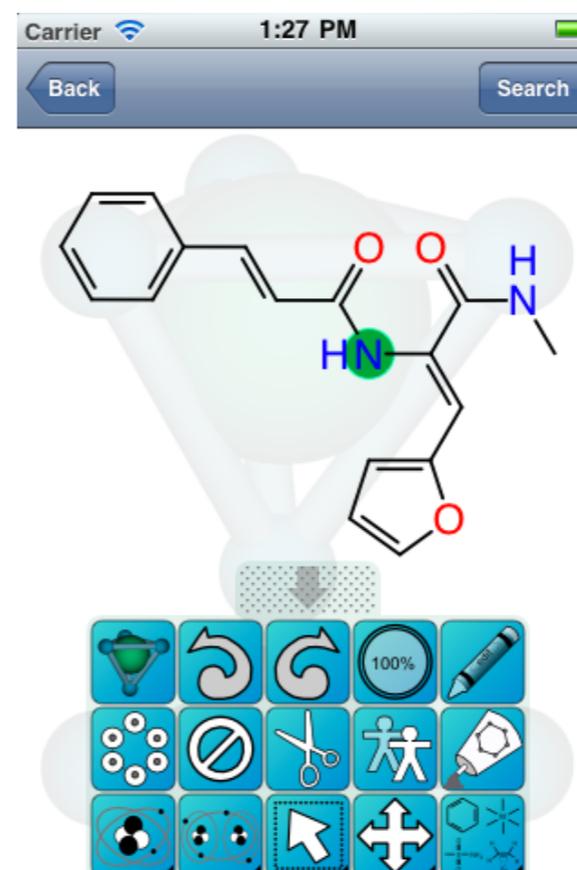
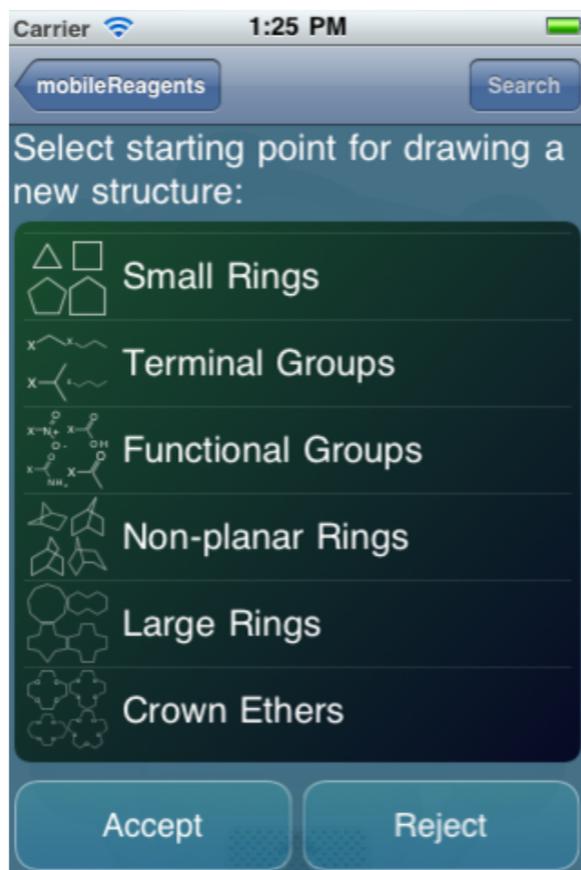
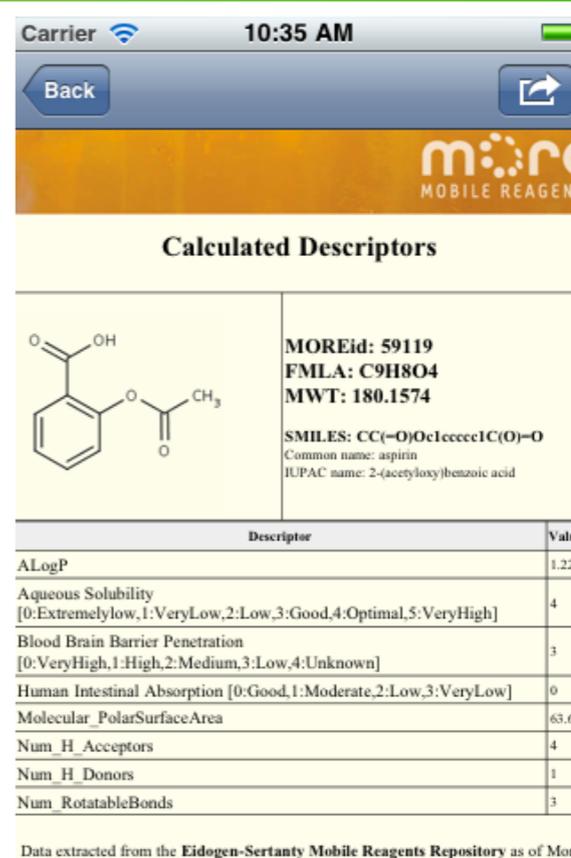
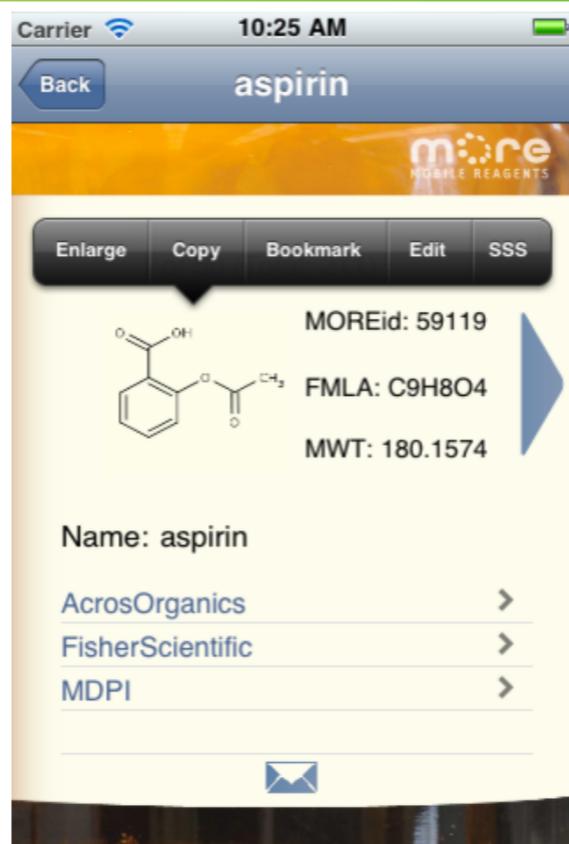
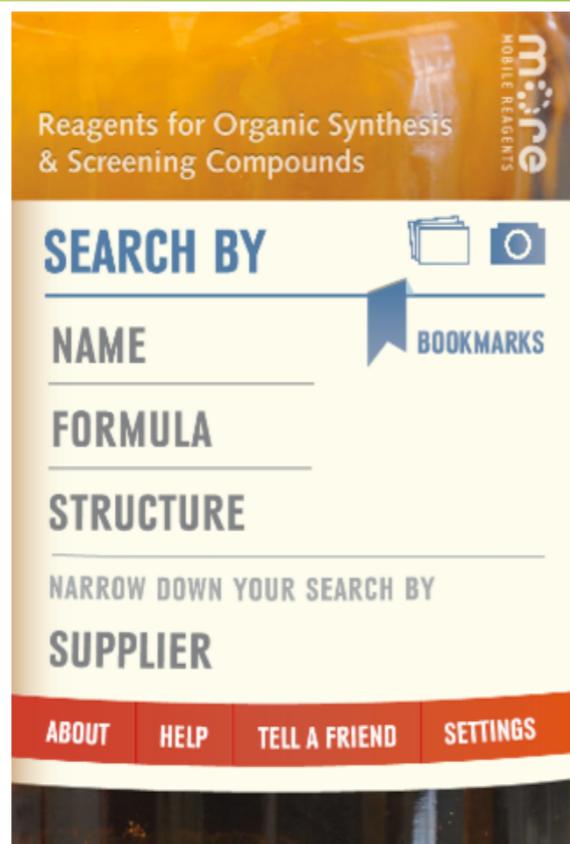
Click on the arrow (when present) to see more data. You can click the arrow (">") to see more detail. If there is a bound ligand, you can initiate ligand-based searches.



# iProtein iPad Demo



# Mobile Reagents (iOS4) - 10/5/10 (v1) ... 6/1/11 (v5.51)



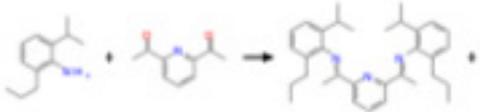
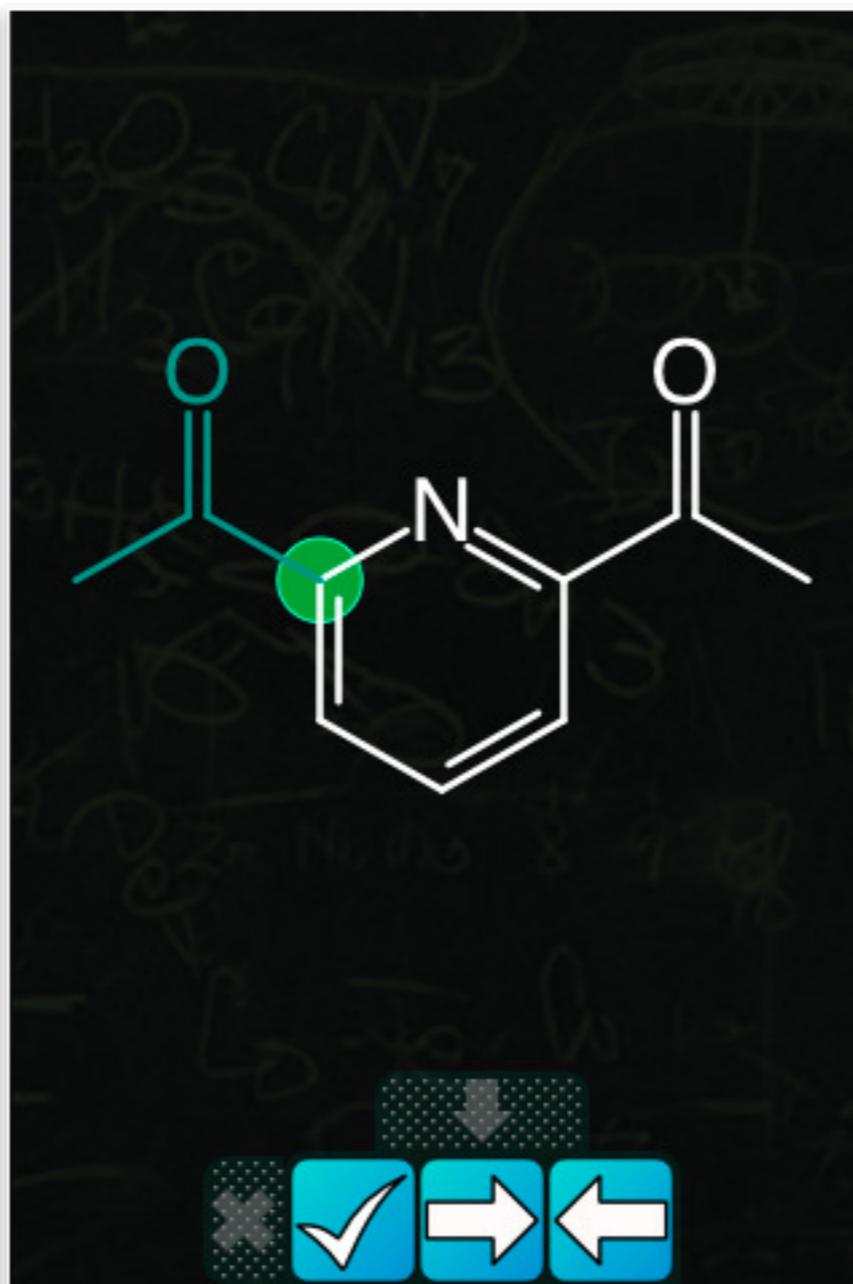
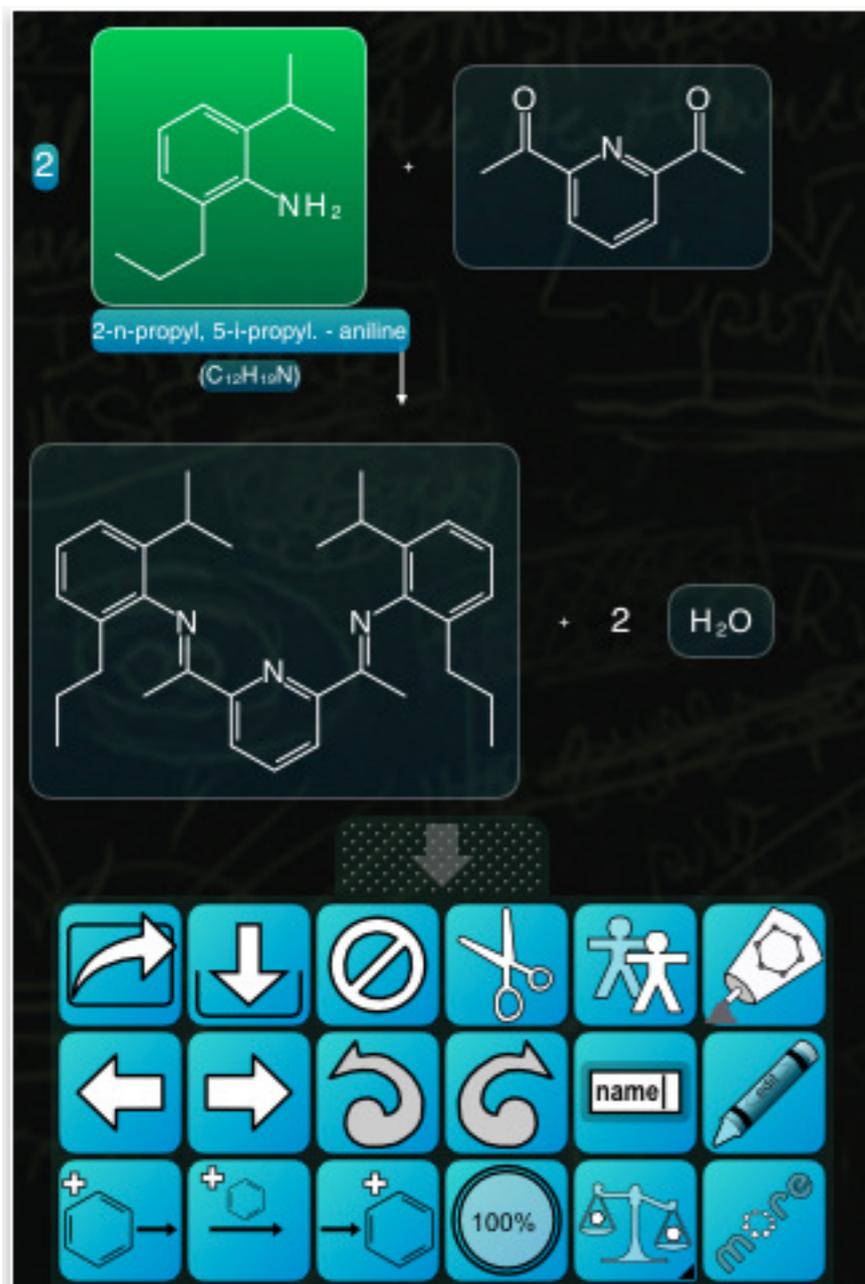
# Mobile Reagents iPhone Demo



# Reaction101 (iOS4) - 2/11 (v1) ... 3/11 (v1.01)



Reaction101



Schiff base...

Addition of alcohols to alkynes >

Addition of hydrogen cyanide to... >

alcohol oxidation with Corey rea... >

Br → Li Alkyl Lithium form...

Cl → Li Alkyl Lithium...

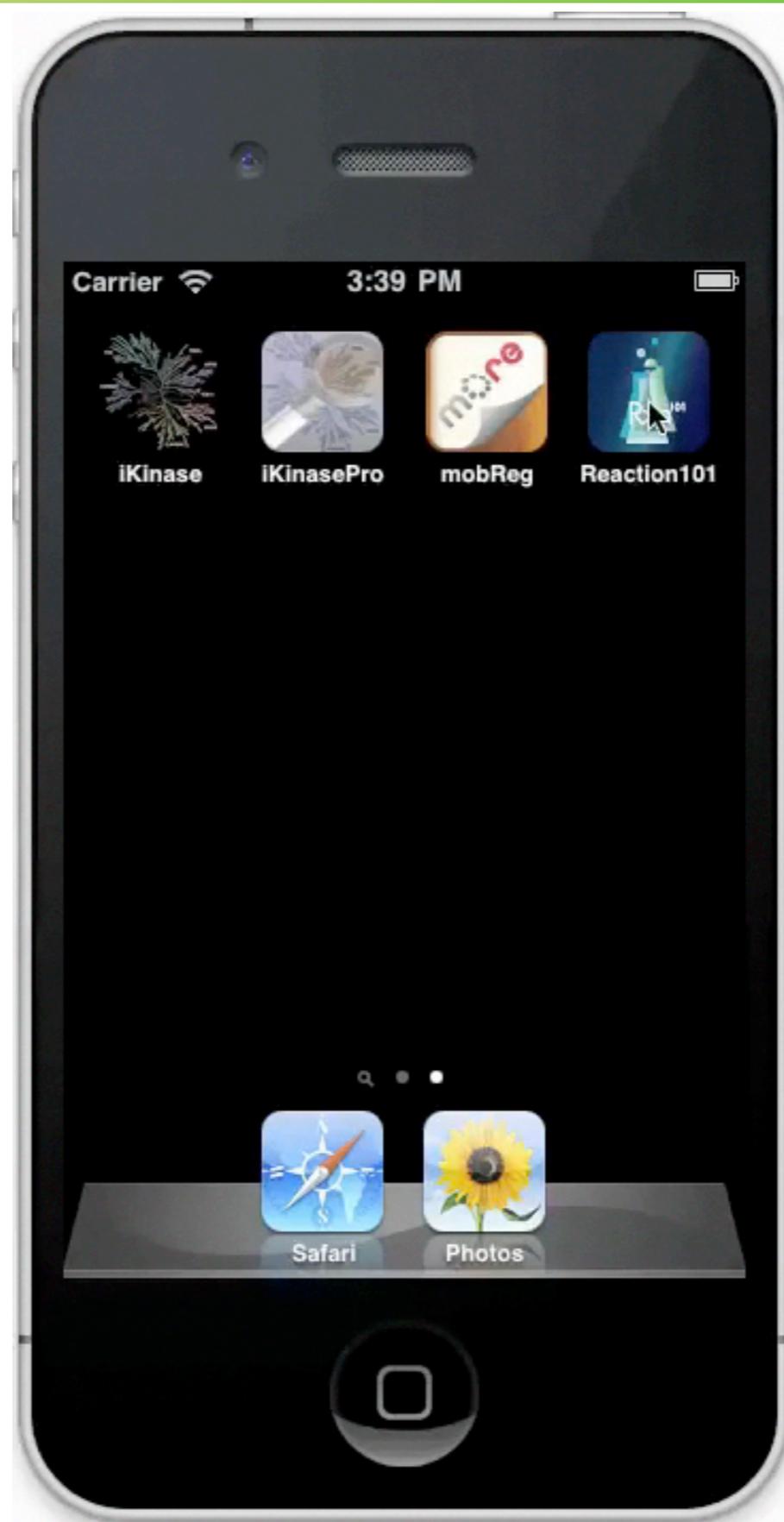
Cl → Li Alkyl Lithium forma...

Br → Li Alkyl Lithium formation...

Alkyl Lithi...

Cancel Select

# RXN101 iPhone Demo



# Yield101 (iOS4) 4/11 (v1) ... 6/11 (v1.02)



82.14 g/mol + 144.13 g/mol → 226.27 g/mol

Equiv: 1    Mass: 100 g    Volume:    Moles: 1.21738 mol    Density:    Conc:    Primary: \*

Equiv: 1    Mass: 175.455 g    Volume:    Moles: 1.21738 mol    Density:    Conc:    Primary:    Yield: 95 %

Equiv: 1    Mass: 261.683 g    Volume:    Moles: 1.15651 mol    Density:    Conc:    Yield: 95 %

Process Mass Intensity: 275.455 g / 261.683 g = 1.053

Reactants

	Molecular Formula: C <sub>7</sub> H <sub>6</sub> O <sub>3</sub>
	Molecular Weight: 138.121 g/mol
	Equivalents: 1
	Mass: 10 g
	Volume: 6.93001 mL (calculated)
	Moles: 0.0724004 mol (calculated)
	Density: 1.443 g/mL
	(Primary Reactant)

	Molecular Formula: C <sub>4</sub> H <sub>6</sub> O <sub>3</sub>
	Molecular Weight: 102.089 g/mol
	Equivalents: 1
	Mass: 7.39126 g (calculated)
	Moles: 0.0724004 mol (calculated)

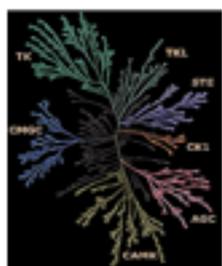
Products

	Molecular Formula: C <sub>9</sub> H <sub>8</sub> O <sub>4</sub>
	Molecular Weight: 180.157 g/mol
	Equivalents: 1
	Mass: 11.5 g
	Moles: 0.0638331 mol (calculated)
	Yield: 88.1667 % (calculated)

**PMI = Process Mass Intensity**

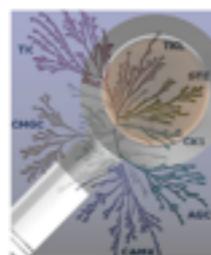
**=  $\frac{\text{Mass of raw materials input}}{\text{Mass of desired output}}$**

# Eidogen-Sertanty's iPhone and iPad Apps



iKinase  
Eidogen-Sertanty

iKinase

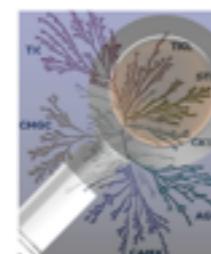


iKinasePro  
Eidogen-Sertanty

iKinasePro



Mobile Reagents



iKinasePro  
Eidogen-Sertanty

iKinasePro



iProtein



Mobile Reagents



Reaction101



Yield101



Reaction101



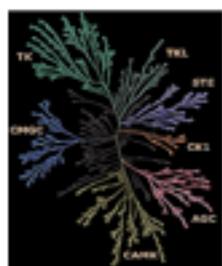
Yield101

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

# Lessons Learned...

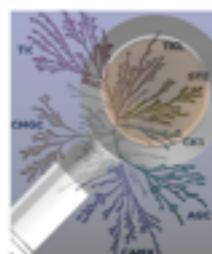
- Devices are worldwide and pervasive
  - ➔ Millions of people surf the app store!!!
- Development environment is very good
  - ➔ Large activation energy to start, Apple's CDAs can be a hindrance (contrasted with LAMP)
- Don't expect large app revenues
  - ➔ People prefer free apps (in app purchase woes)
- 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



iKinase

iKinase



iKinasePro

iKinasePro



Reaction101



Yield101

Send an e-mail to:

To: **mobileapps@eidogen-sertanty.com**

Subj: **ACS Denver {iPod or iPhone or iPad}**

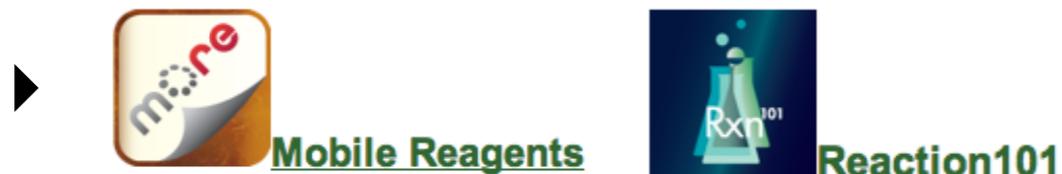
10 of each will be given away

# Acknowledgements

- Dr. Rajan Sharma and Prof. Stephan Schurer



- Dr. Maurizio Bronzetti



- Dr. Alex Clark

- ▶ MMDSLlib:



- 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*<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



# Introduction – PMI by industry

Industry	Typical PMI	Annual Production tonnage
Oil refining	~1.1	$10^6 - 10^8$
Bulk chemicals	<2 to 6	$10^4 - 10^6$
Fine chemicals	6 to >50	$10^2 - 10^4$
Pharma	26 to >100	$10 - 10^3$

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

***Constrains development time for process optimization***

References: R.A Sheldon, *Chem. Ind.*, 1997, 12-15. R.K. Henderson, J. Kindervater, J.B. Manley, "Lessons learned through measuring green chemistry performance", accessed 27-May-2009 via the ACS GCI Pharmaceutical Roundtable site.