Expanding the Reach of ChemInformatics through Mobile Computing

Dr. Steven Muskal

Chief Executive Officer

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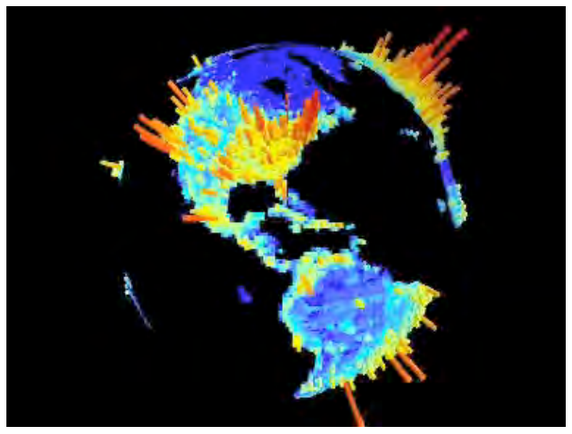
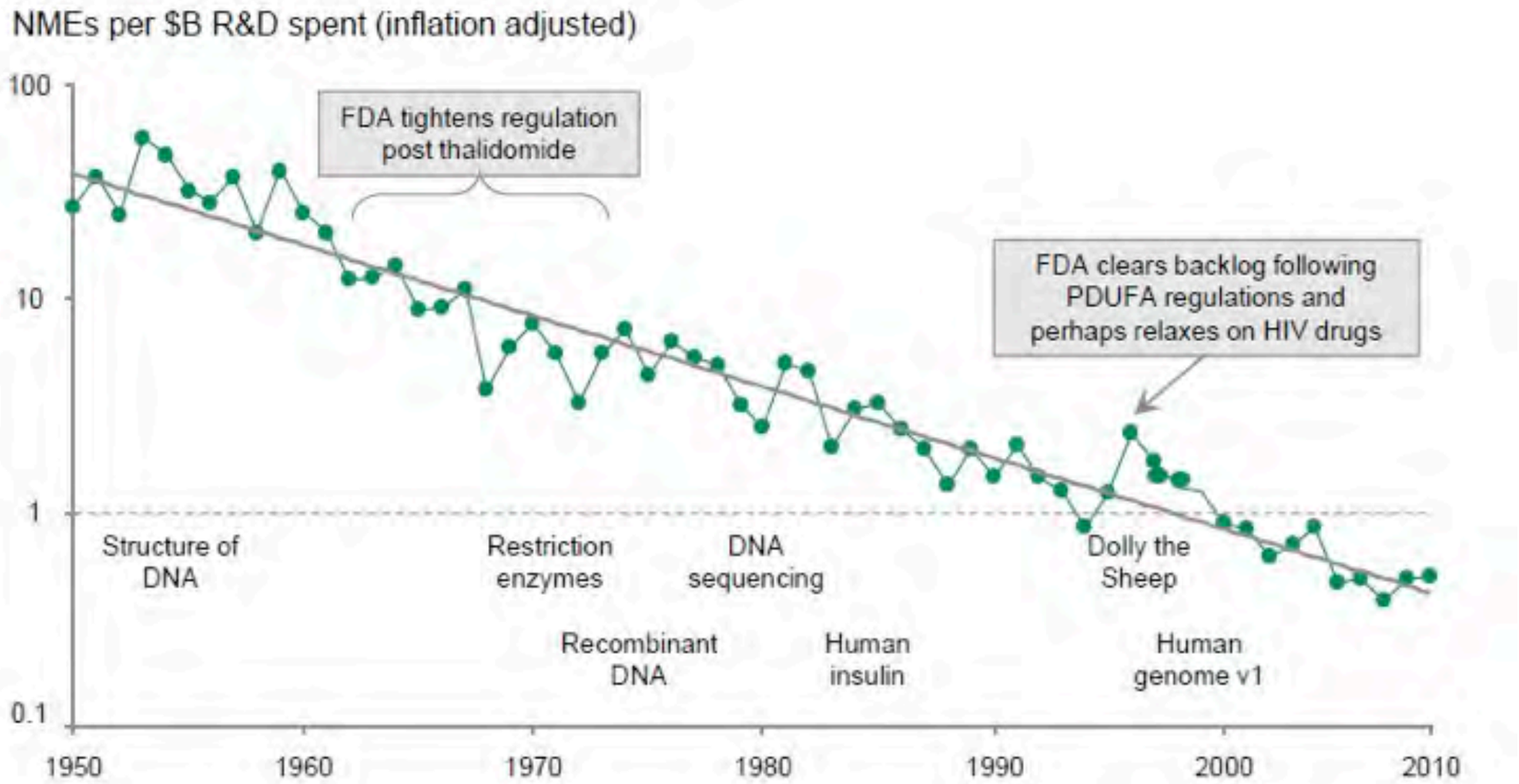
7 Billion people depend on fewer than **500,000** people to discover and develop new medicines…



World Population Density
The G-Econ project gecon.yale.edu/

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)

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

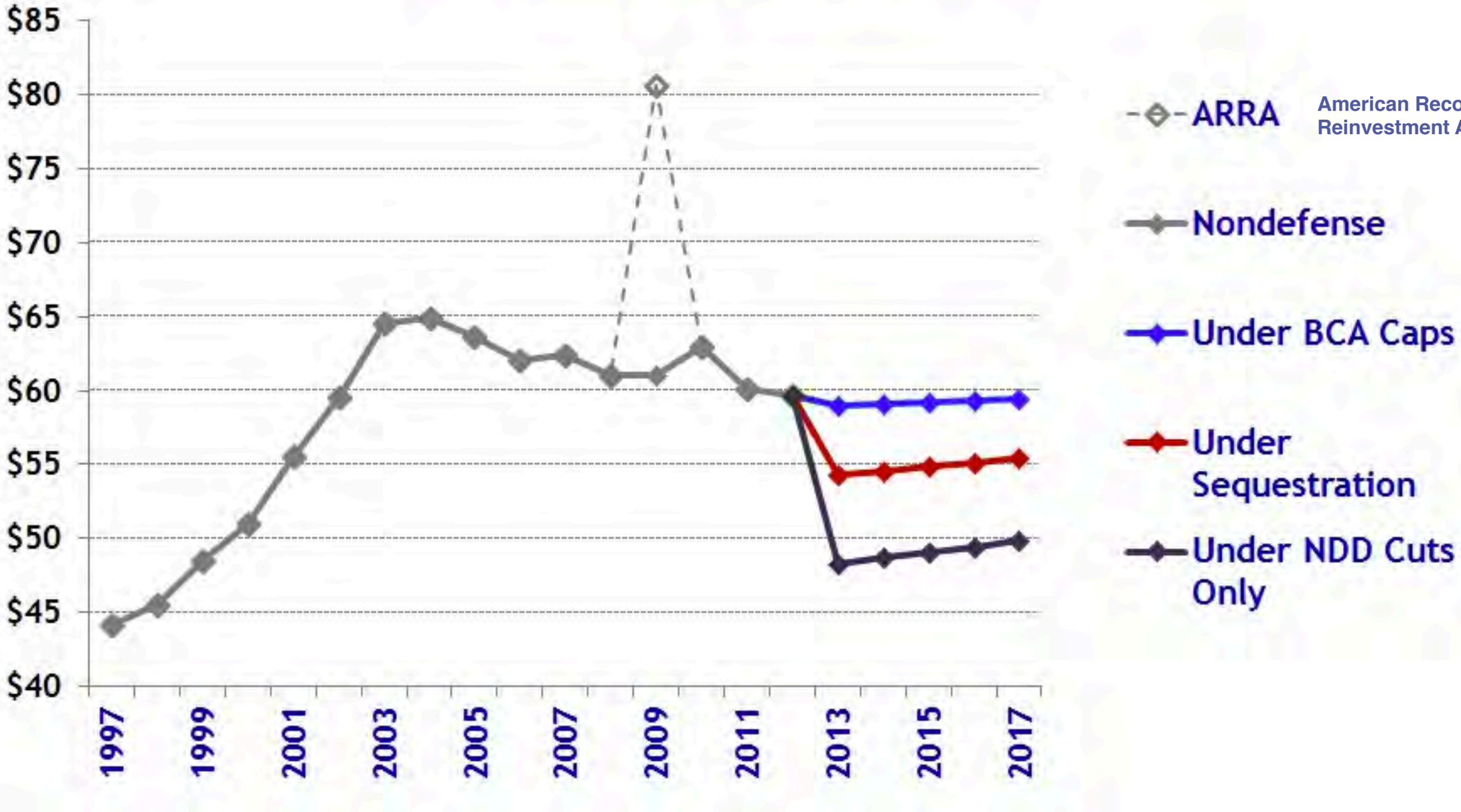
A Decade In Drug Industry Layoffs

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. ©

Federal Nondefense R&D Under BCA Caps With and Without Sequestration

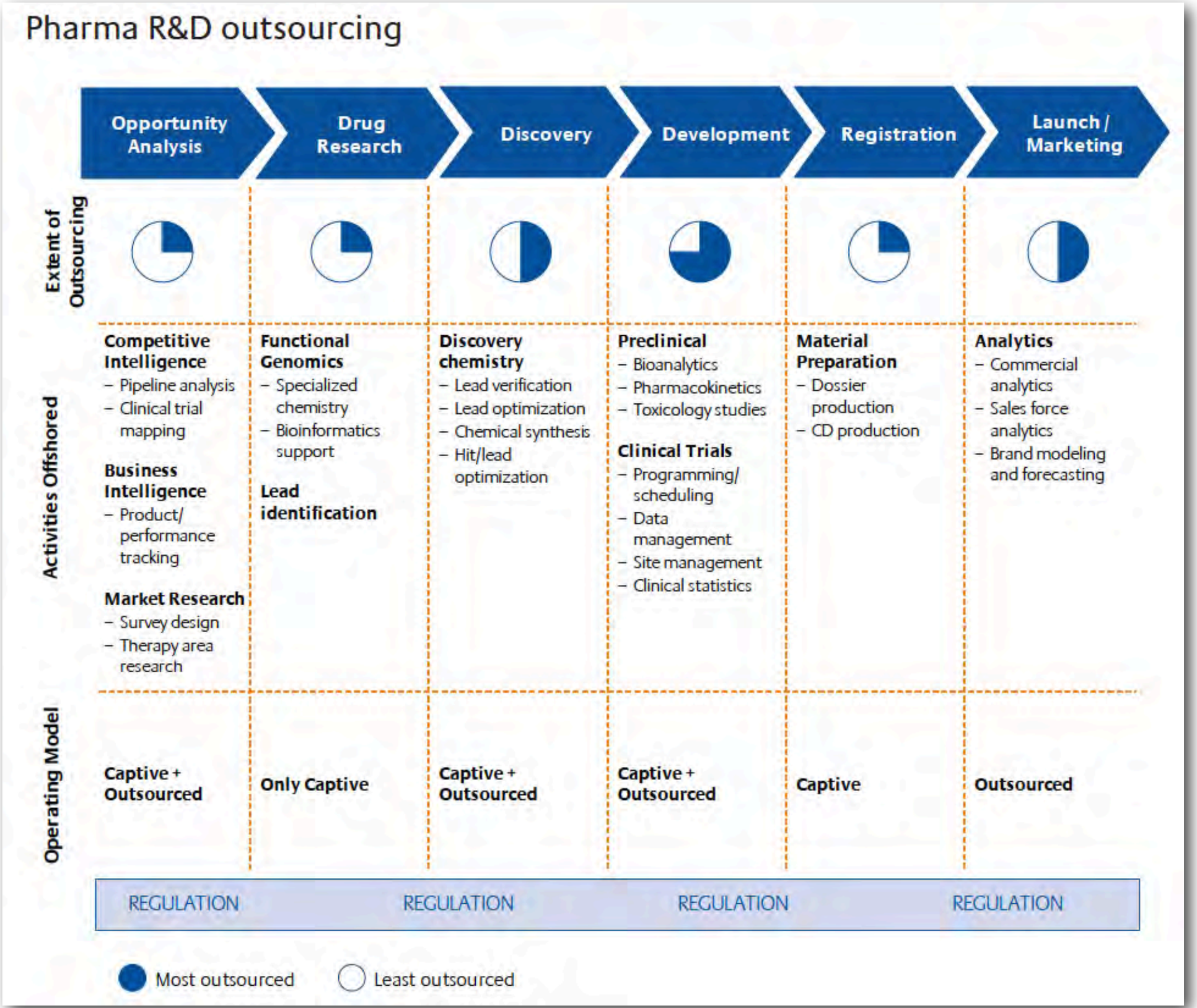
in billions of constant FY 2012 dollars



Source: Based on AAAS estimates of R&D funding and the FY 2013 budget, and CBO analyses of the Budget Control Act. http://www.aaas.org/spp/rd/fy2013/SeqBrief.pdf

Outsourcing Trends

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



Bloomberg Businessweek

START

2011 — SWIPE CREDIT CARD

1999 — MOVE TO SILICON VALLEY

VISIT WITH VENTURE CAPITALISTS

ORDER EQUIPMENT

WEB SERVERS | FILE SERVERS | ROUTERS

HOUSE EXPENSIVE HARDWARE IN DATA CENTER WITH RAISED FLOOR AND COOLING EQUIPMENT

FIREWALLS | MAIL SERVERS | SWITCHES

HIRE ARMY OF SYS ADMINS

BUY DESIGNER OFFICE FURNISHINGS

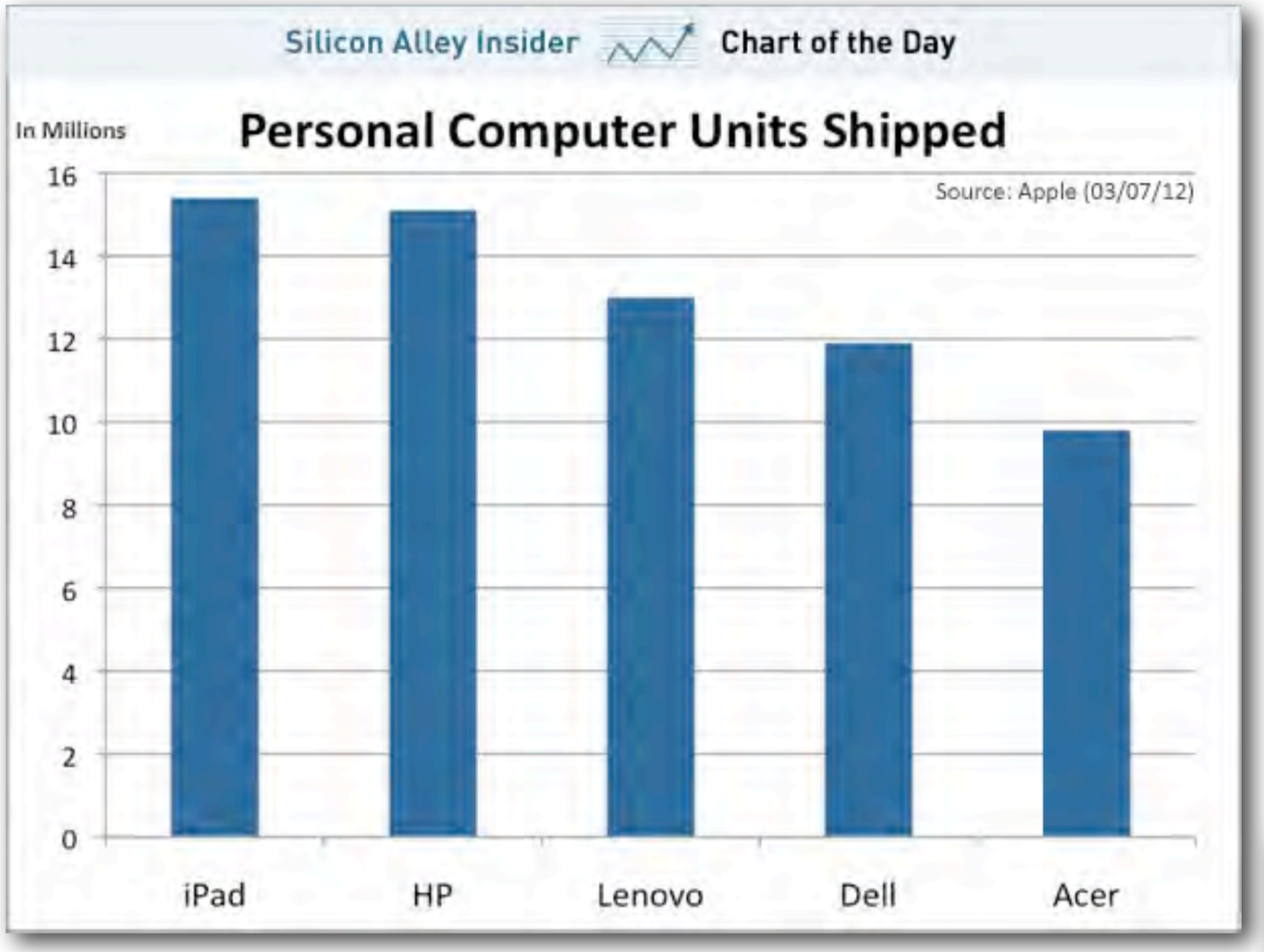
BEG FOR MORE FUNDING

SPEND LAVISHLY ON MARKETING AND PLOT IPO

The Power of the Cloud

LAUNCH

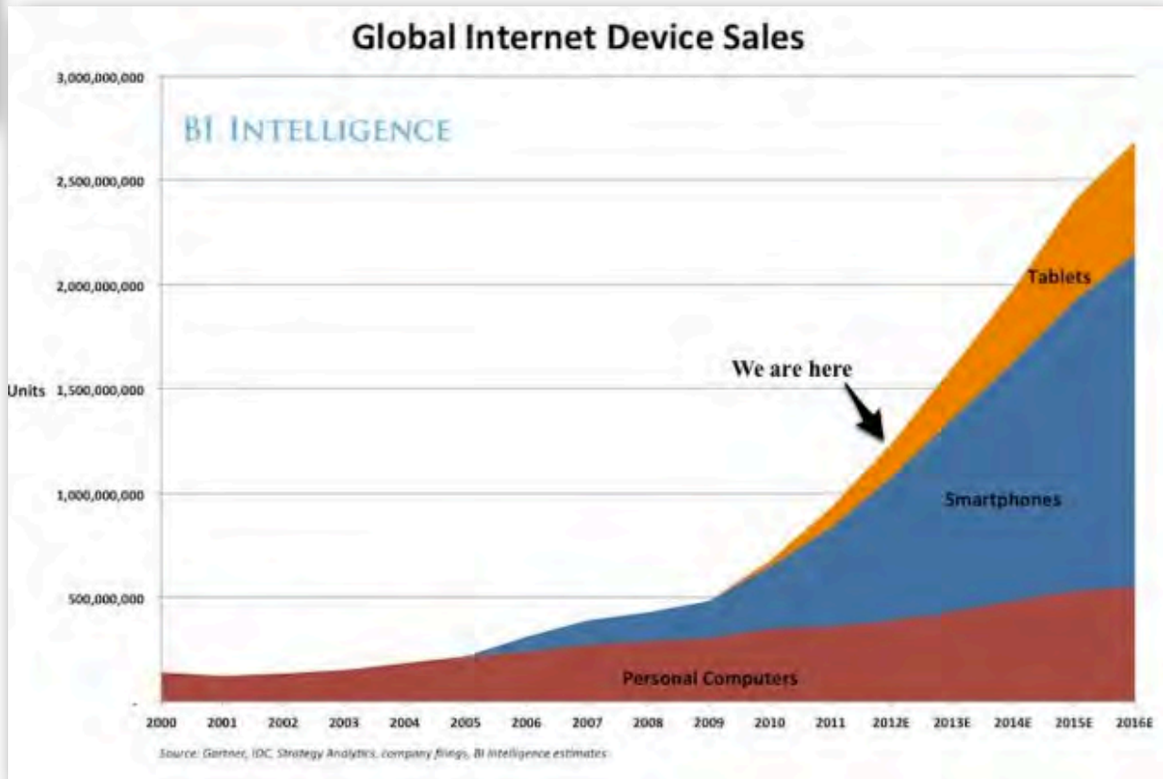
The Post-PC Revolution Is Here...



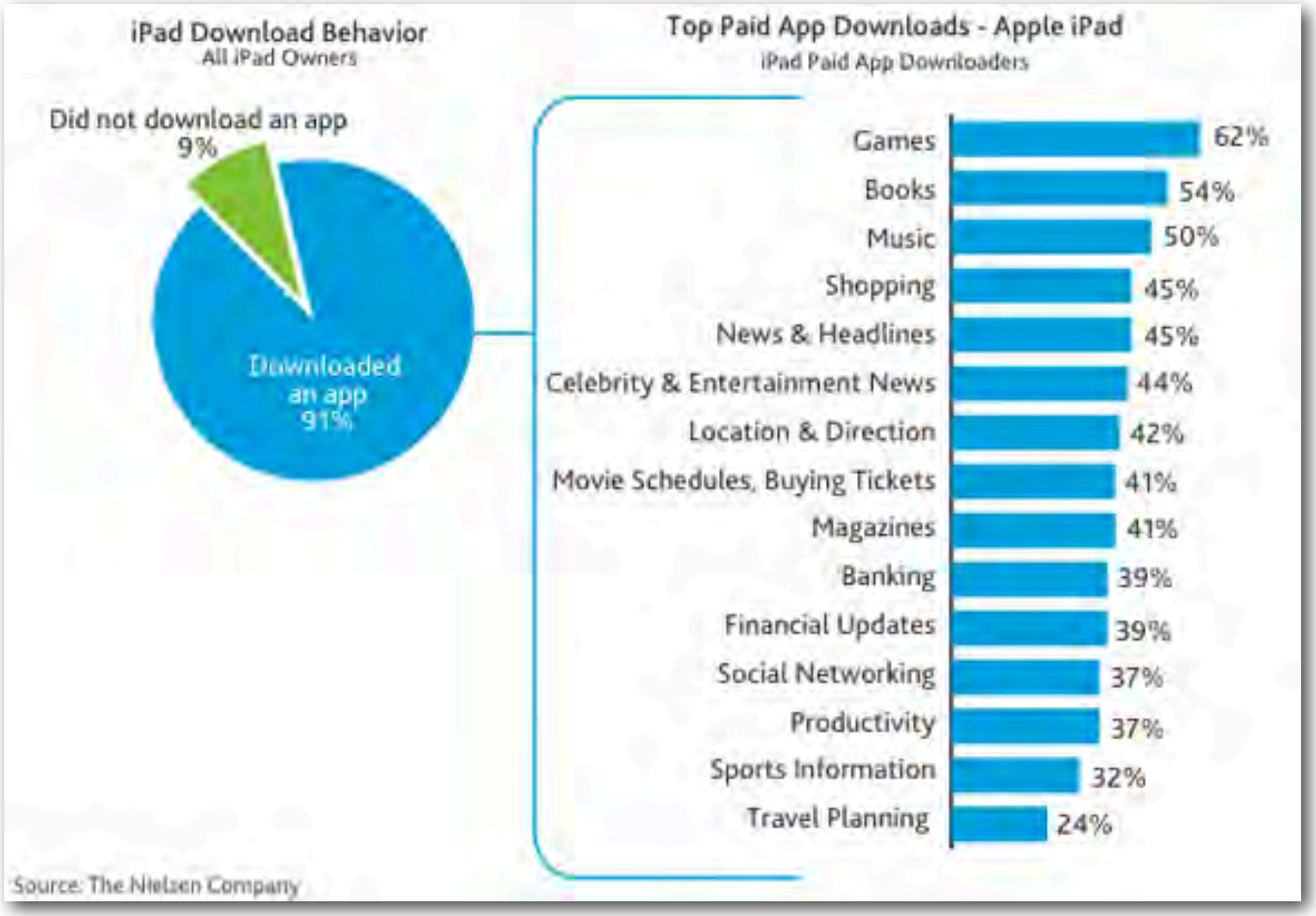
Apple Sold More iPads In Q411 Than Any Single Manufacturer Sold PC Devices

"Tablet Sales Will Blow Past PC Sales To Nearly 500 Million Units A Year By 2015"

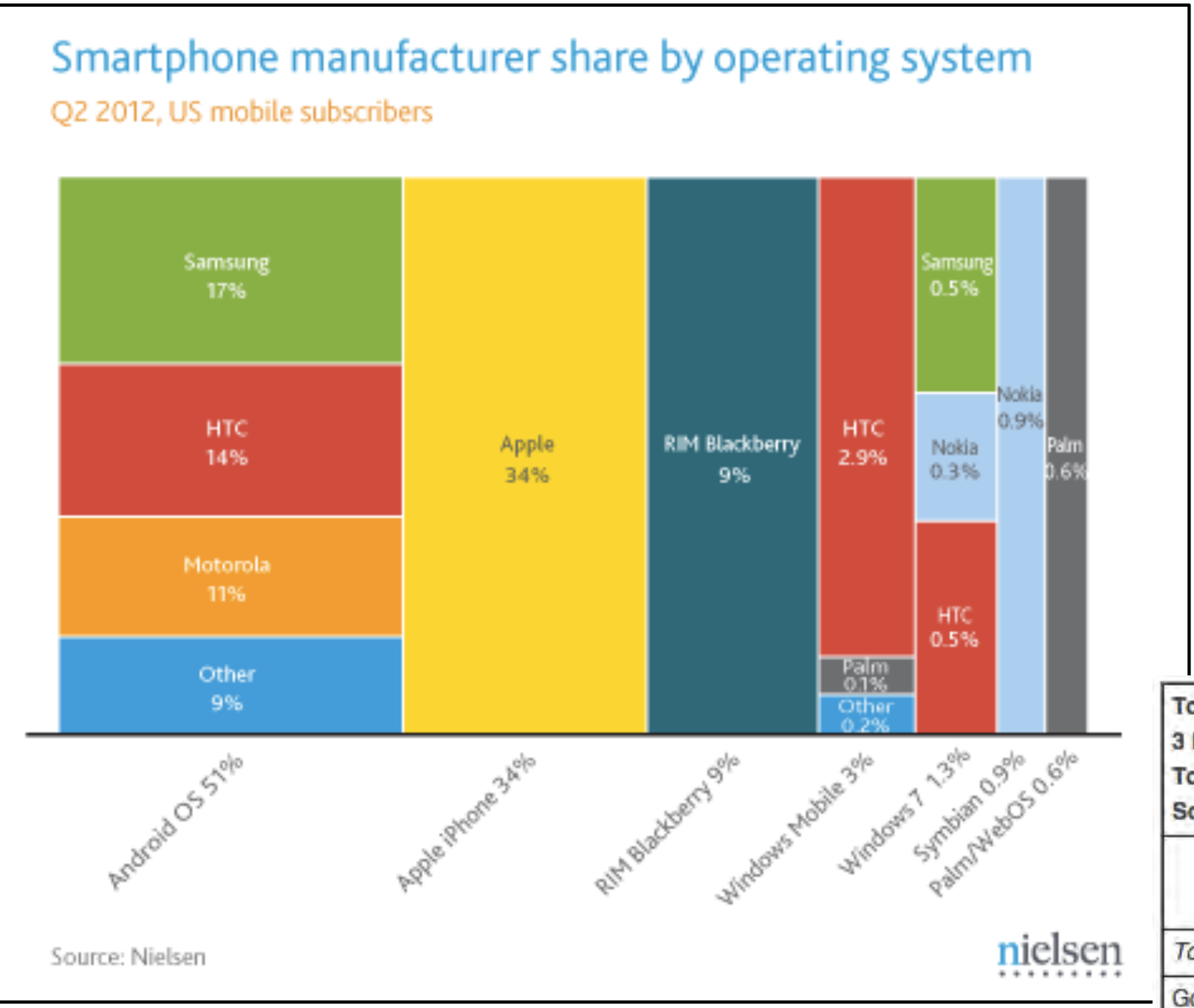
http://articles.businessinsider.com/2012-02-14/tech/31057828_1_tablet-sales-post-pc-era-lower-prices



Almost All Tablet Owners Download Apps



Top Smartphone Platforms



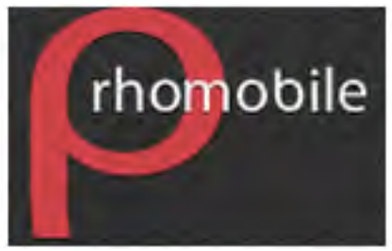
Top Smartphone Platforms
3 Month Avg. Ending Feb. 2013 vs. 3 Month Avg. Ending Nov. 2012
Total U.S. Smartphone Subscribers Age 13+
Source: comScore MobiLens

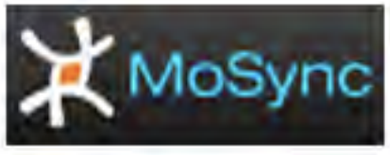
	Share (%) of Smartphone Subscribers		
	Nov-12	**Feb-13**	**Point Change**
Total Smartphone Subscribers	*100.0%*	*100.0%*	*N/A*
Google	53.7%	51.7%	-2.0
Apple	35.0%	38.9%	3.9
BlackBerry	7.3%	5.4%	-1.9
Microsoft	3.0%	3.2%	0.2
Symbian	0.5%	0.5%	0.0

http://www.zdnet.com/apple-first-samsung-second-in-u-s-smartphone-market-7000010940/

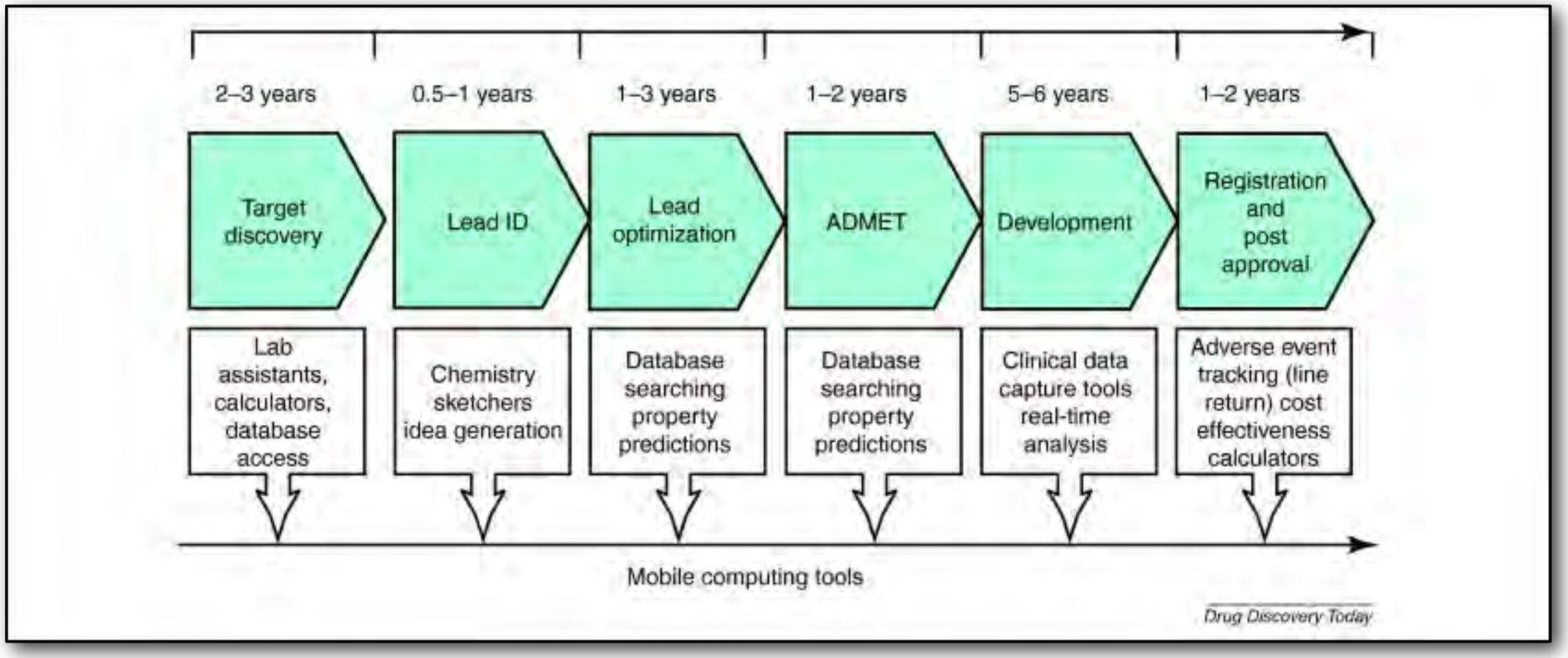
http://www.comscore.com/Insights/Press_Releases/2013/4/comScore_Reports_February_2013_U.S._Smartphone_Subscriber_Market_Share

Many Cross Platform Development “Choices”





Mobile Computing Opportunities in “Our Space”



Mobile apps for chemistry in the world of drug discovery: Volume 16, Issues 21–22, November 2011, Pages 928–939

Mobile-Cloud Infrastructure

- Int(er/ra)net Connection (Wi-Fi or 3/4G)
- Database/WebServer (e.g. GoDaddy/HostGator)
  - Apache + php
  - mysql

- Application Server (Amazon and/or BT Cloud-LAMP)
  - Apache + php, EC2 instances
  - mysql, RDS instances
  - ChemAxon JChem + JChemWebServices
  - InfoChem SPRESI Web Services
  - Accelrys Pipeline Pilot
  - JSDraw (javascript)

amazon web services

BT

Eidogen's iOS, Android, and Win8* apps

iProtein

iKinase

iKinasePro

iOncology

Mobile Reagents

*

Reaction101

Yield101

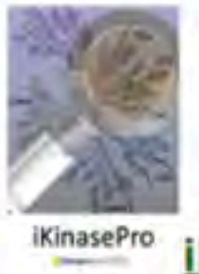
SPRESImobile

** In partnership with Intel*

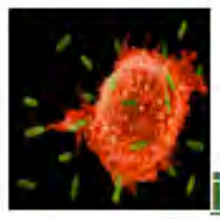
Note: Reaction101,Yield101, and SPRESImobile - built collaboratively with Molecular Materials Informatics, Inc.

MobileApps: Worldwide Access

iKinase



iKinasePro



iOncology

iProtein

Mobile Reagents

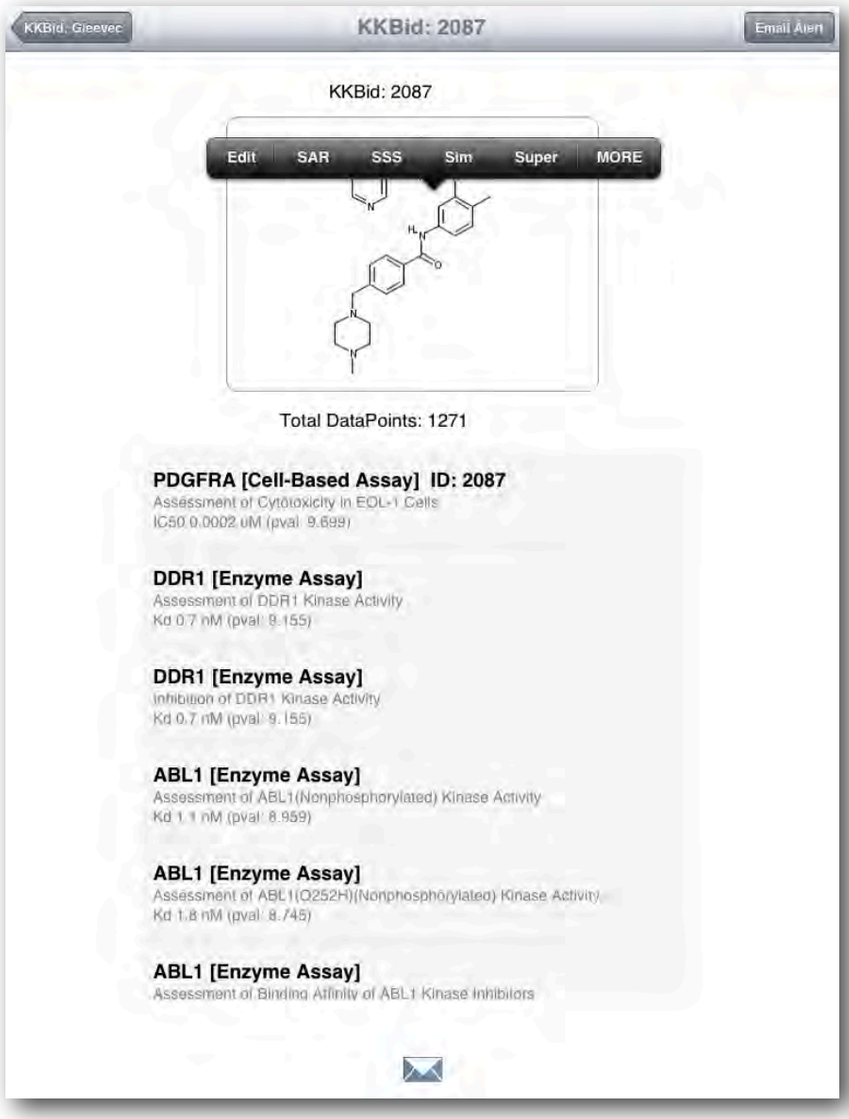
Reaction101

Yield101

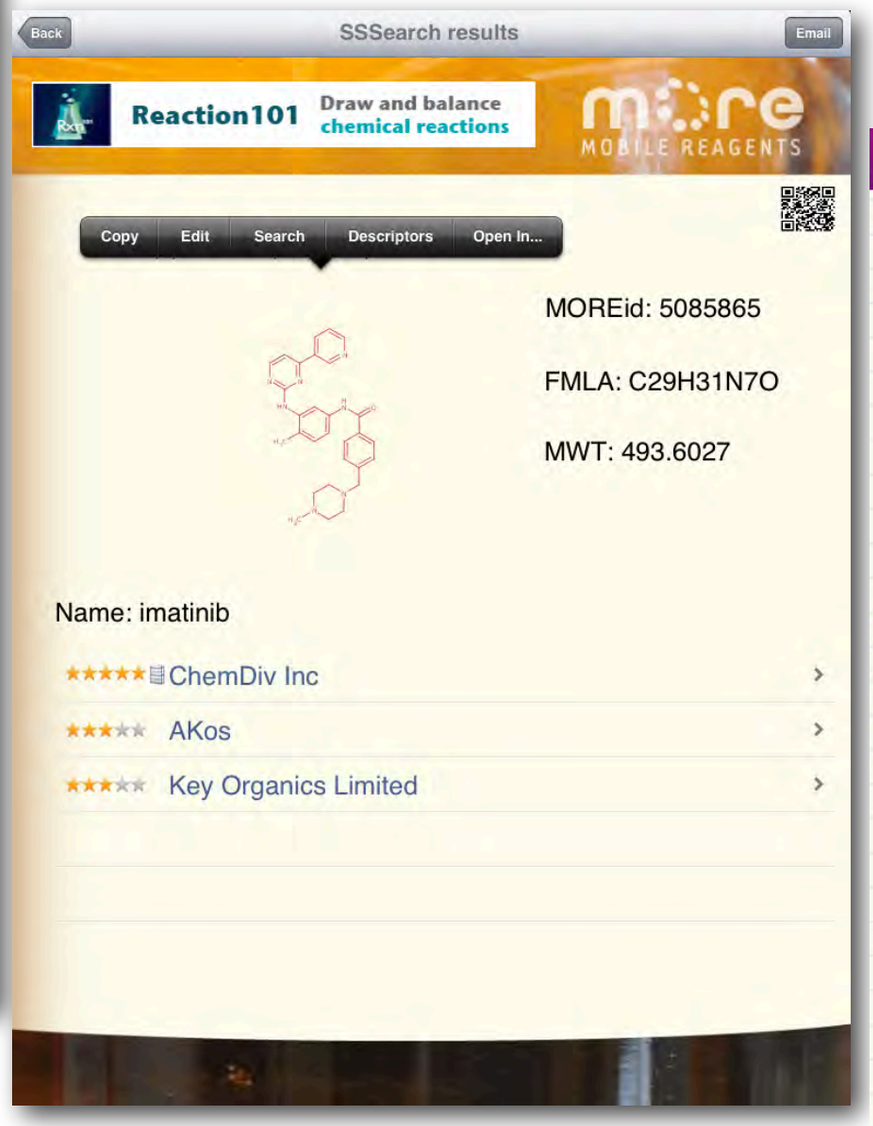
SPRESImobile

~ 30,000 People Use Eidogen Mobile Apps

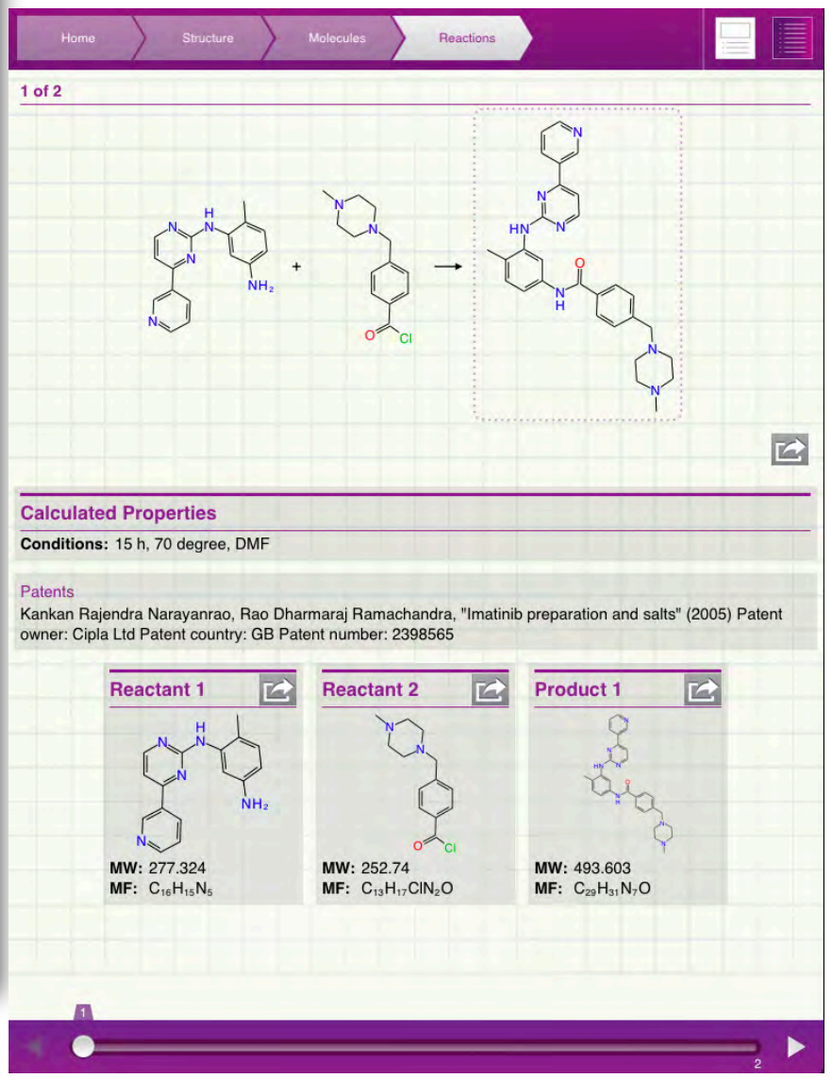
MobileApps Support Real Scientific Workflows



Bioactivity searching (e.g. kinase SAR)

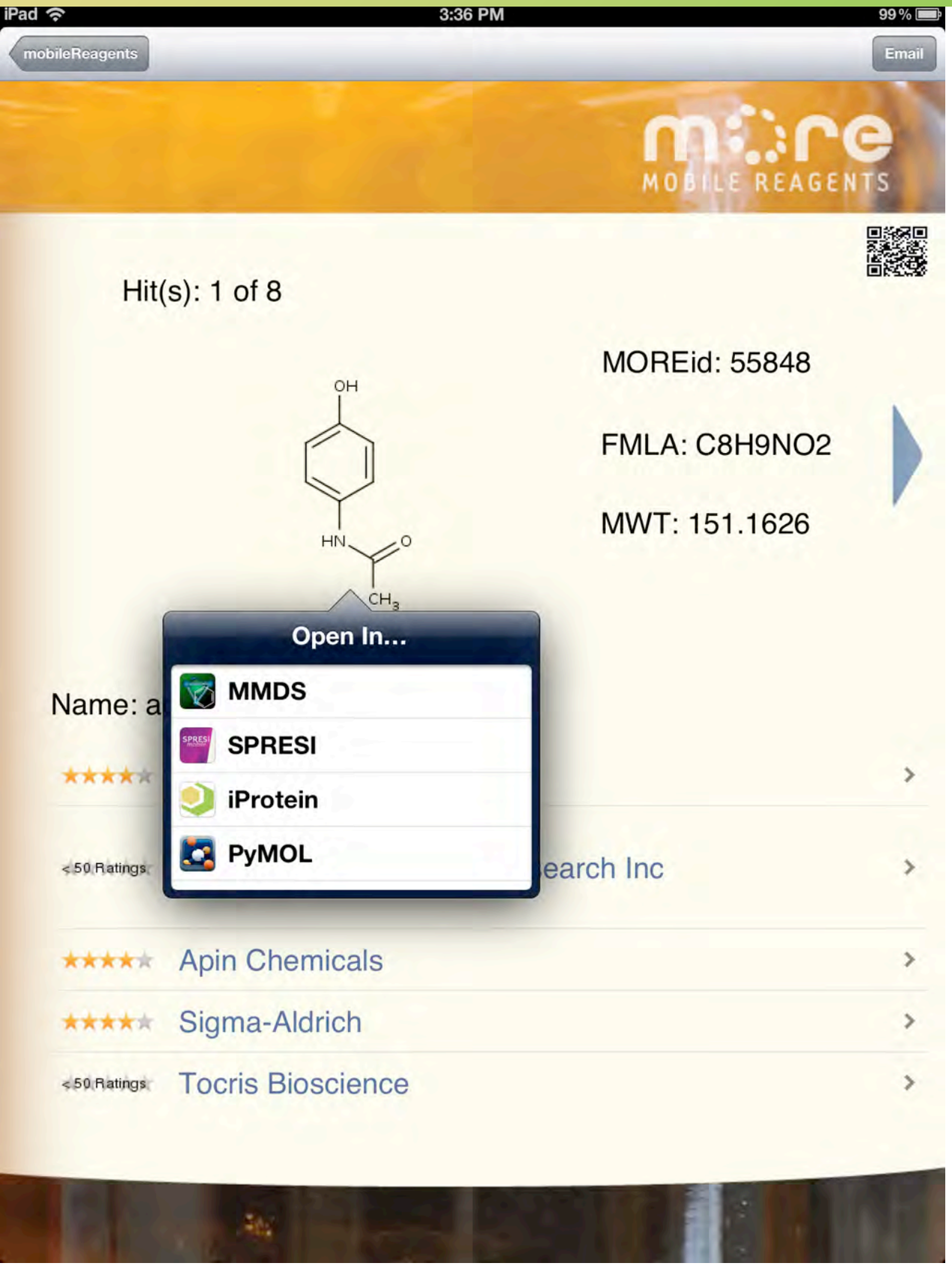


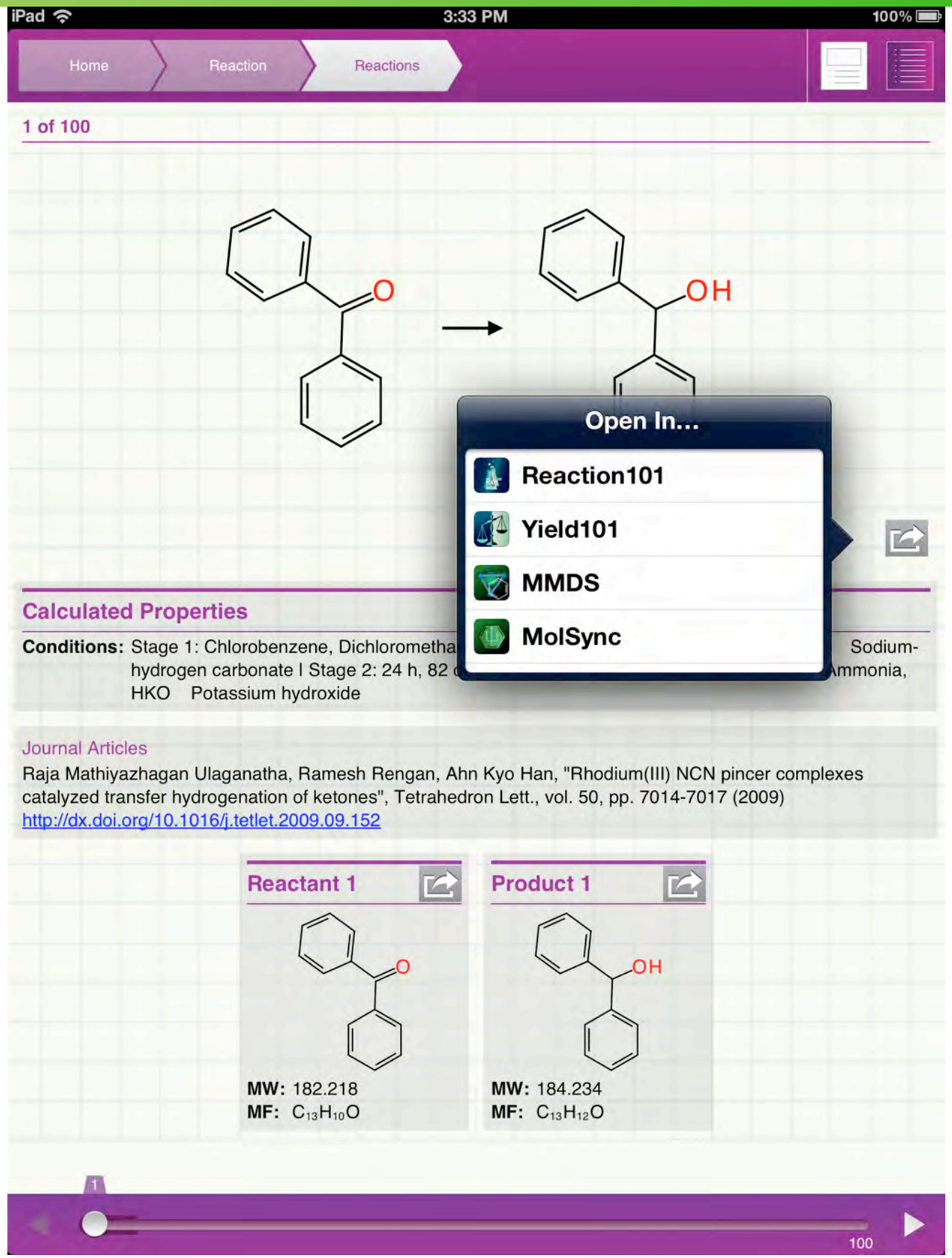
Commercial availability



Synthesis planning

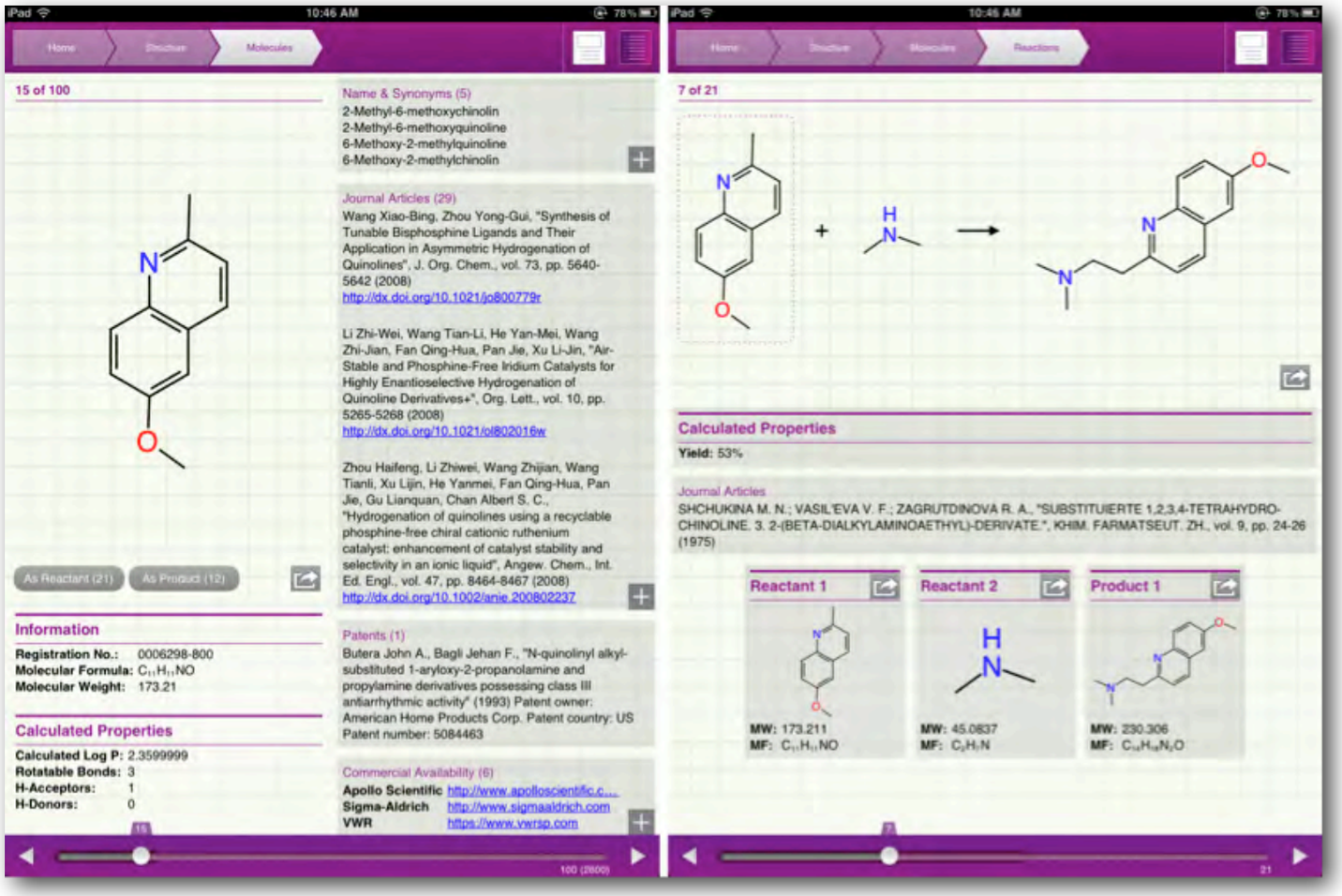
Examples of Mobile IAC (InterApplicationCommunication)

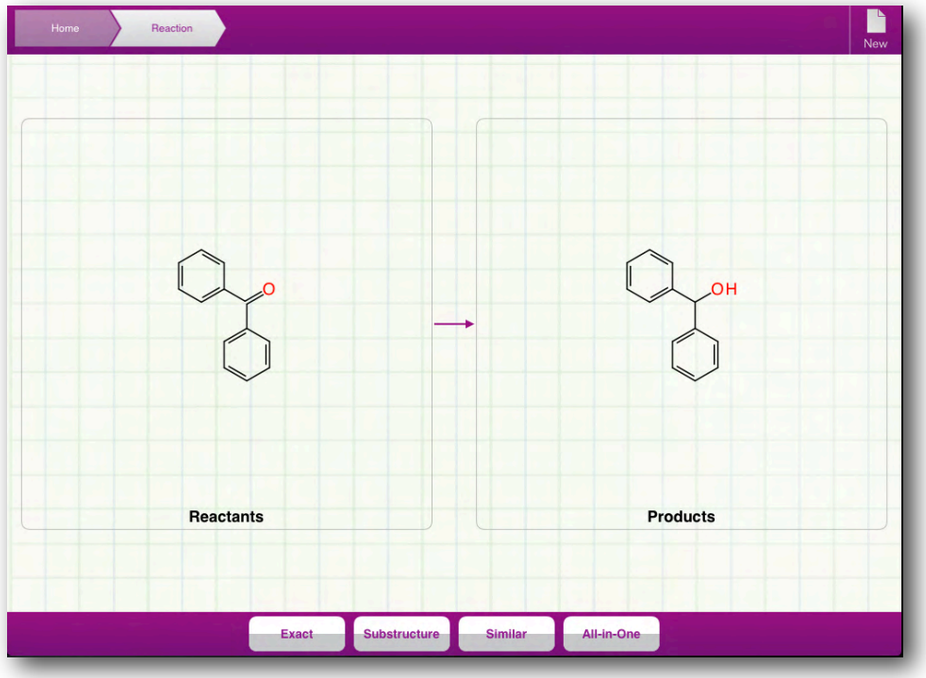


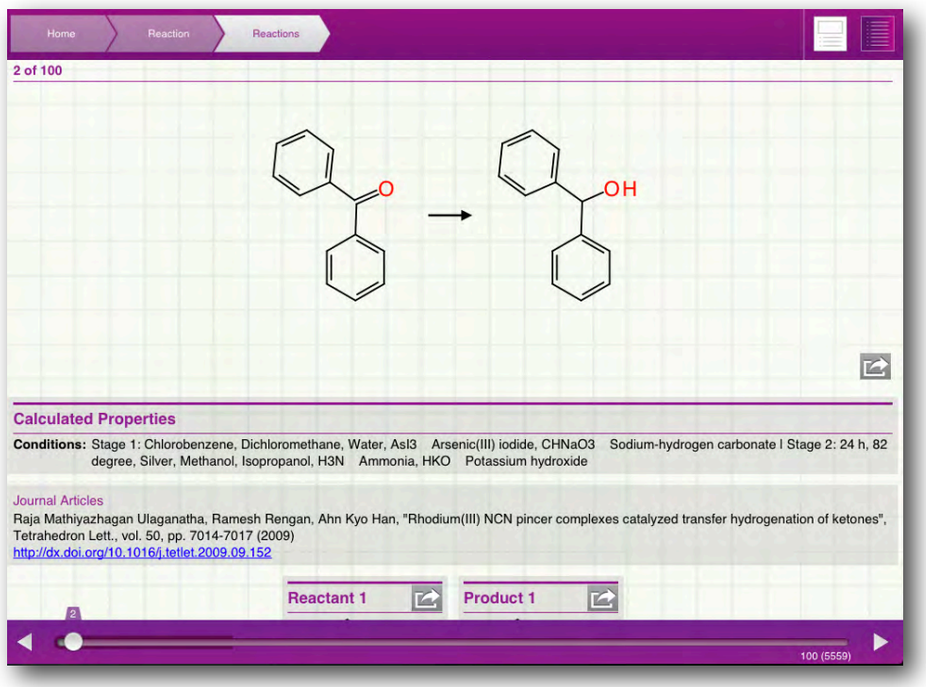


SPRESImobile - Update: Reaction Searching

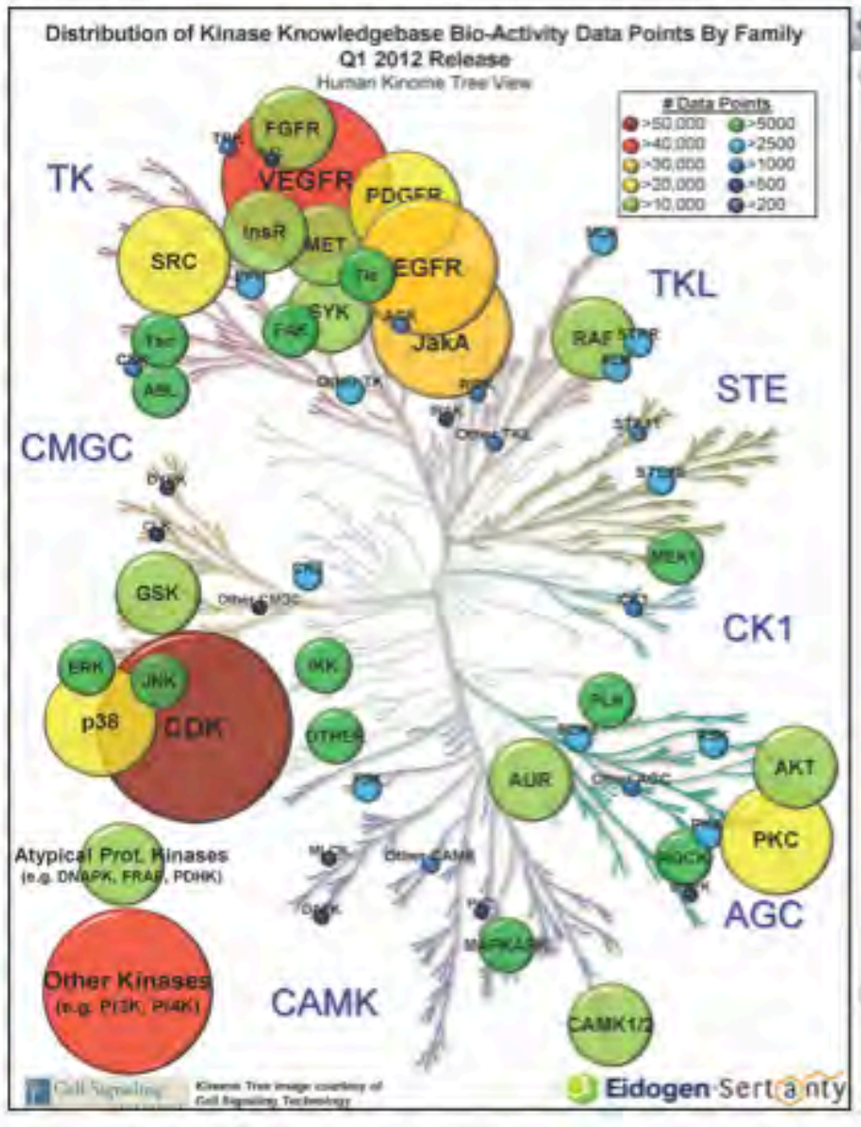
SPRESImobile: 410,000 Chemical Reactions Freely Available

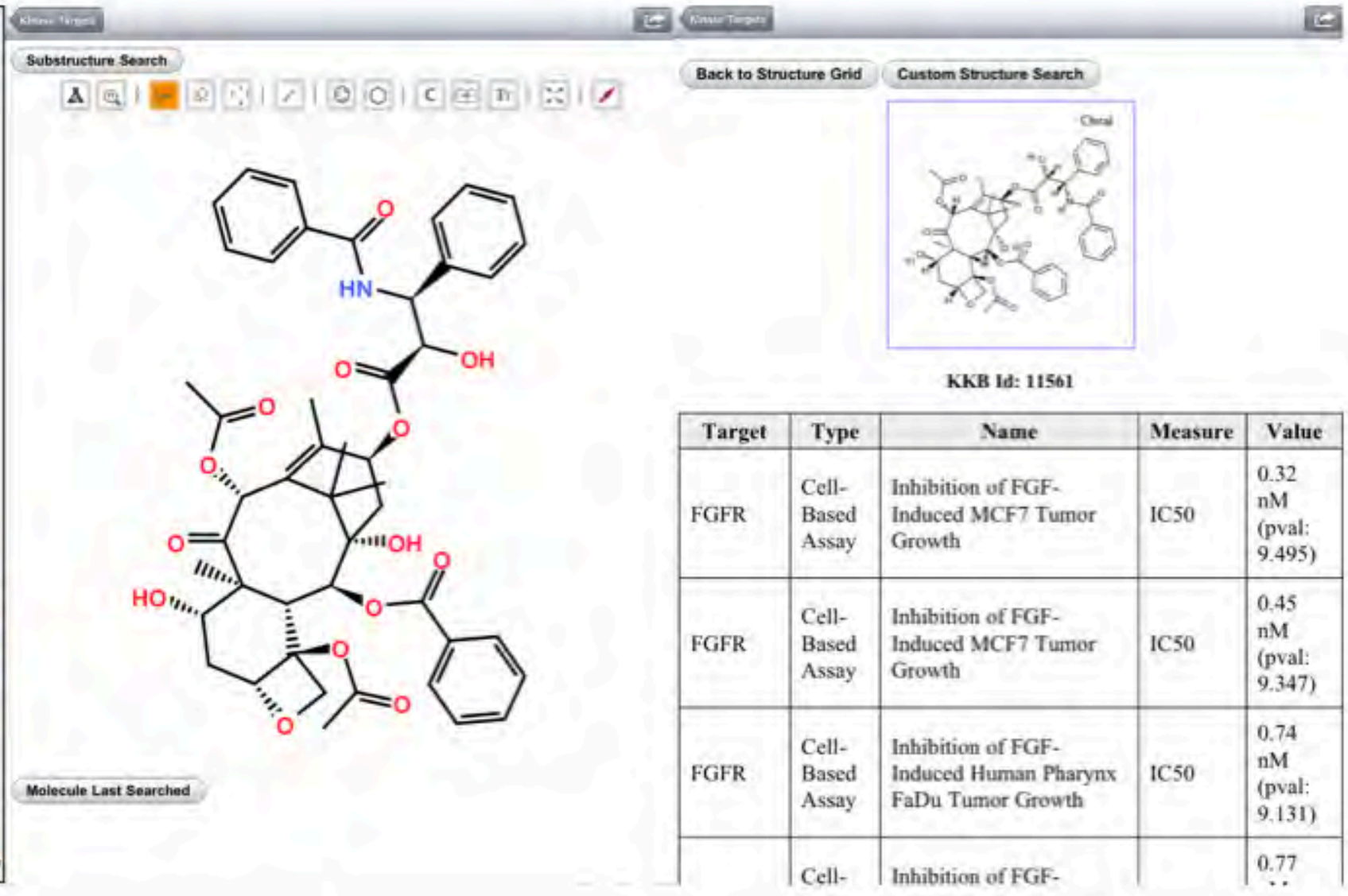






iKinasePro: Update: Android Version



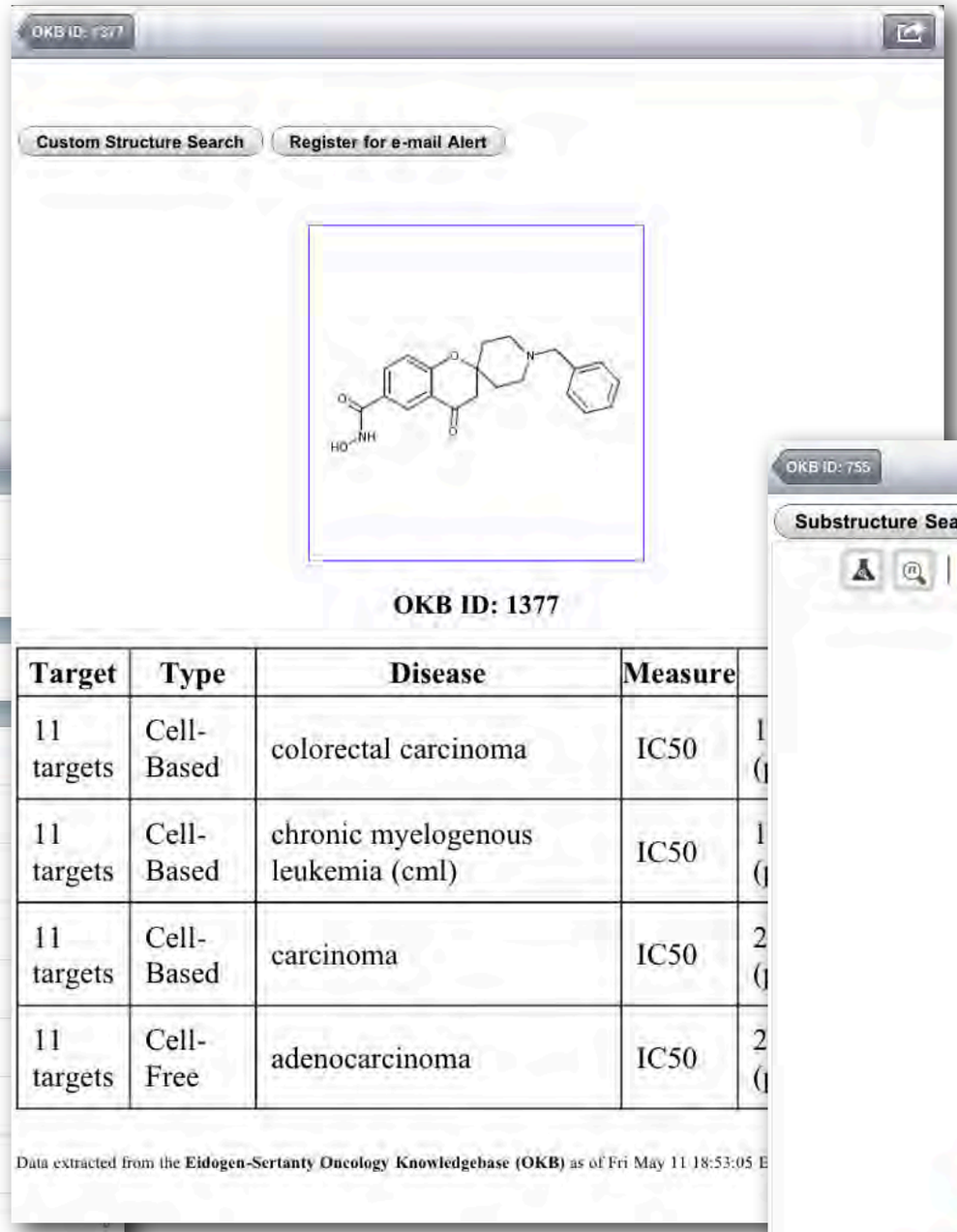


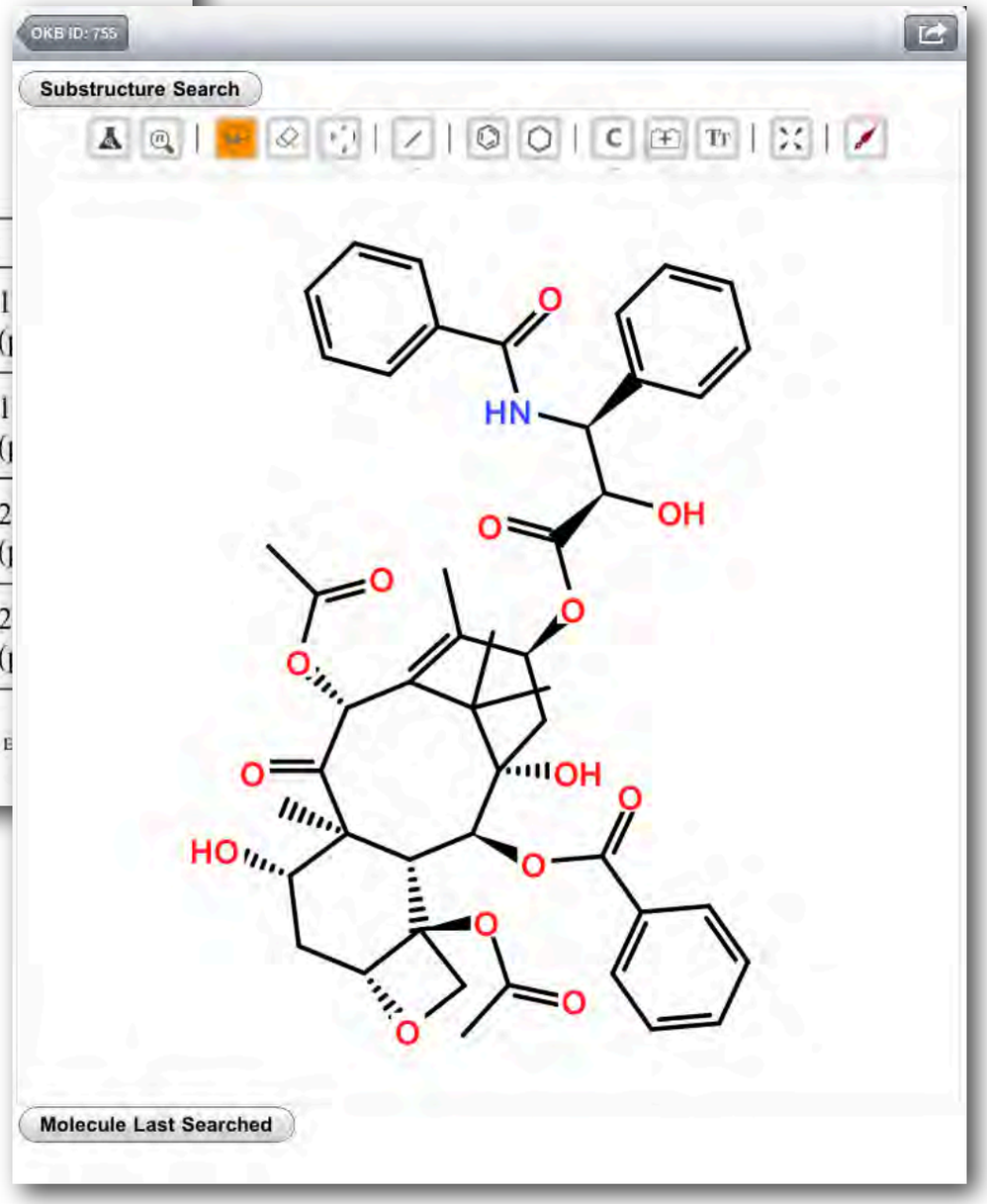
KKB Id: 11561

Target	Type	Name	Measure	Value
FGFR	Cell-Based Assay	Inhibition of FGF-Induced MCF7 Tumor Growth	IC50	0.32 nM (pval: 9.495)
FGFR	Cell-Based Assay	Inhibition of FGF-Induced MCF7 Tumor Growth	IC50	0.45 nM (pval: 9.347)
FGFR	Cell-Based Assay	Inhibition of FGF-Induced Human Pharynx FaDu Tumor Growth	IC50	0.74 nM (pval: 9.131)
	Cell-	Inhibition of FGF-		0.77

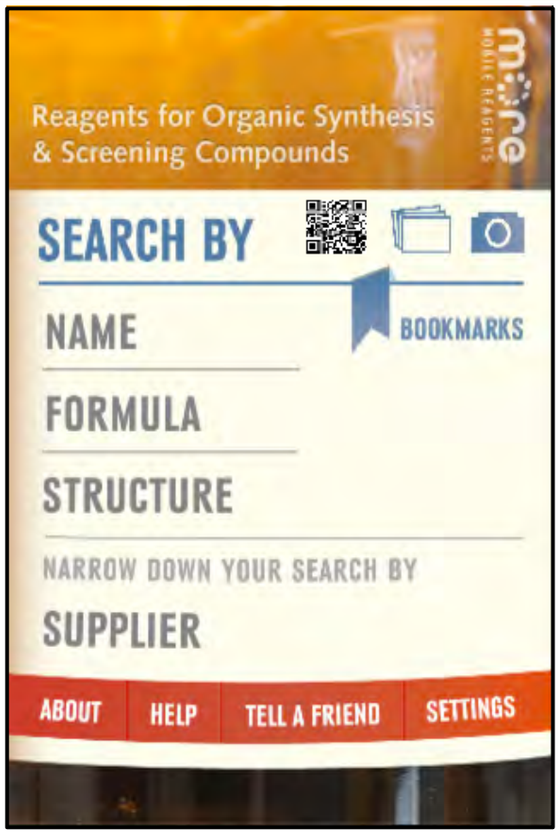
iOncology: Update: Android Version

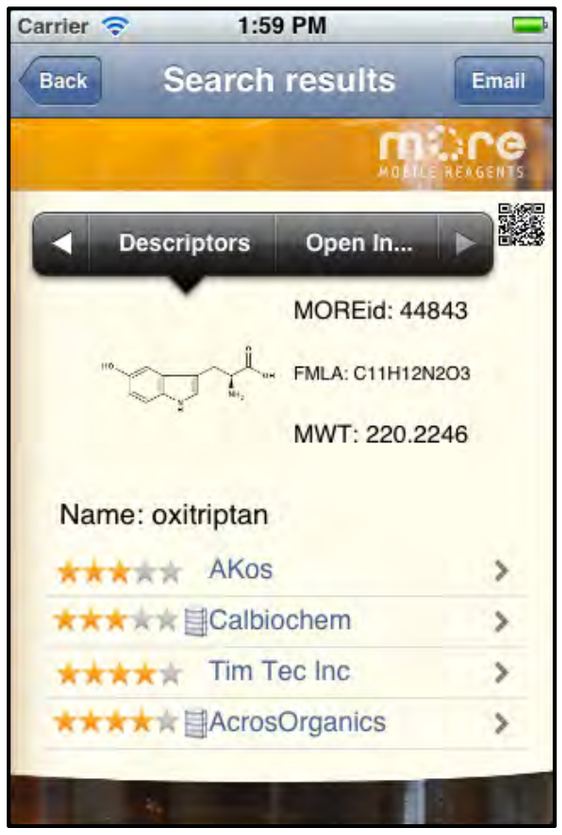
iOncology

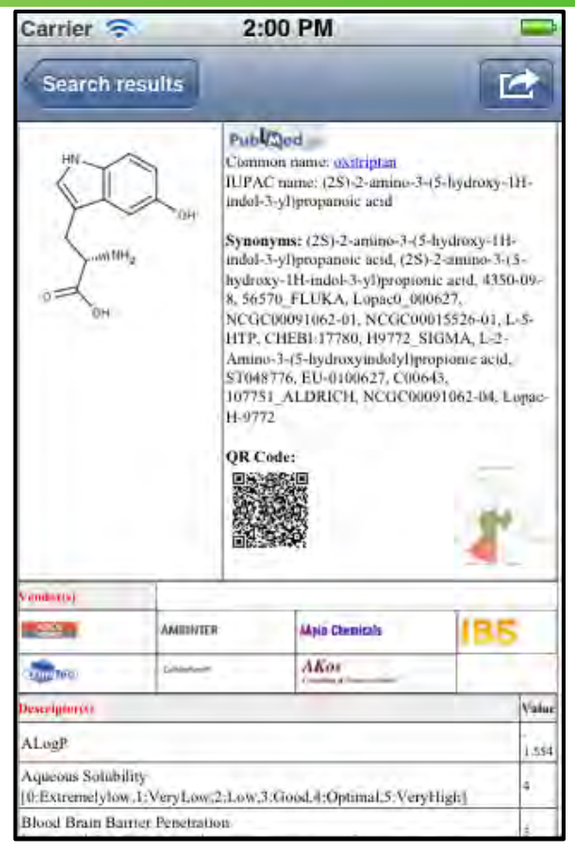


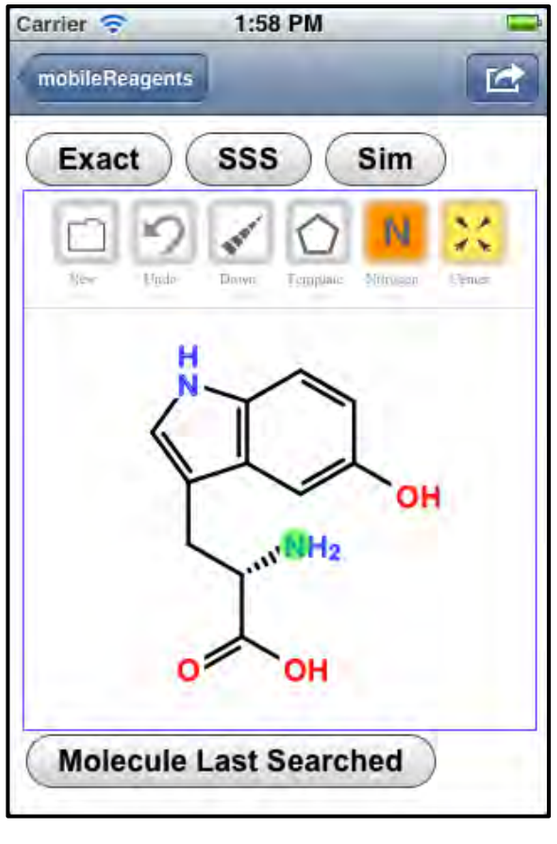


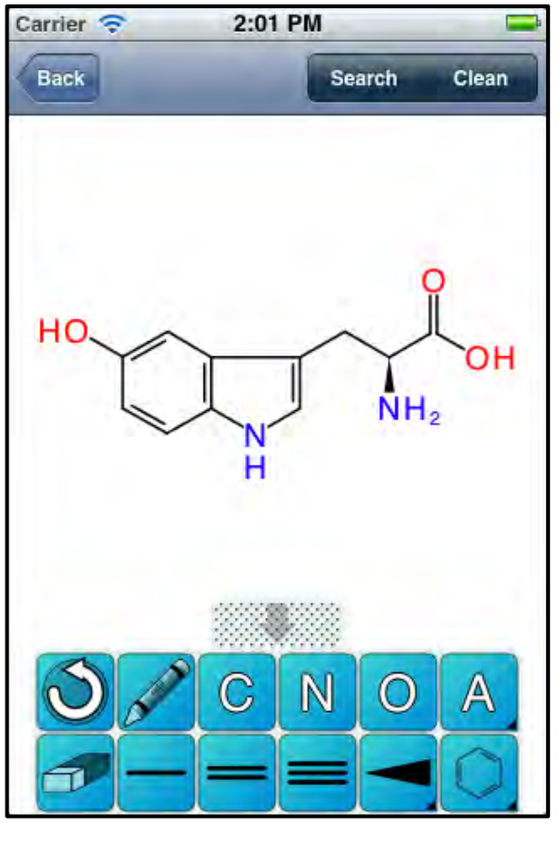
Mobile Reagents - iOS, Android, and....



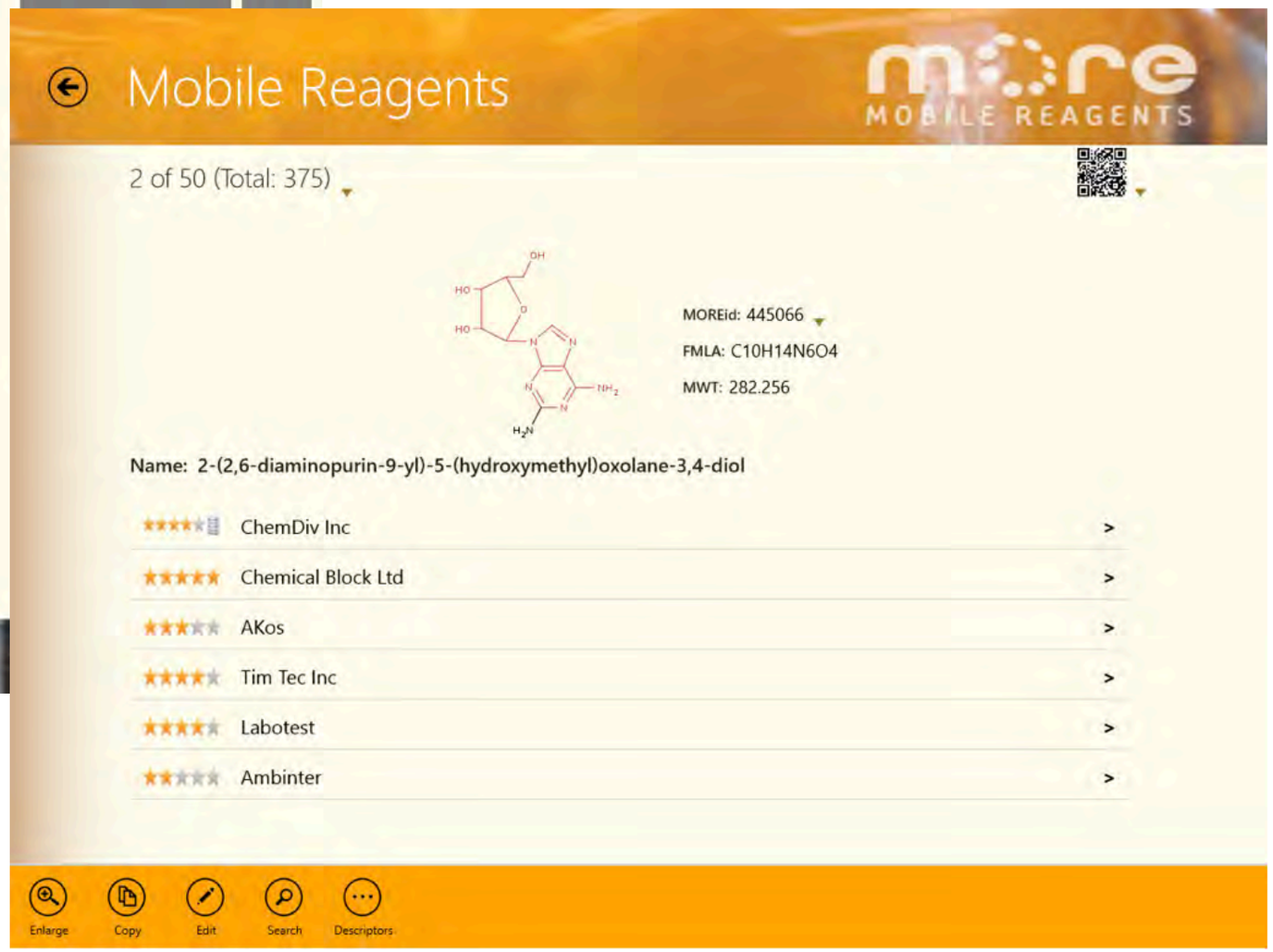






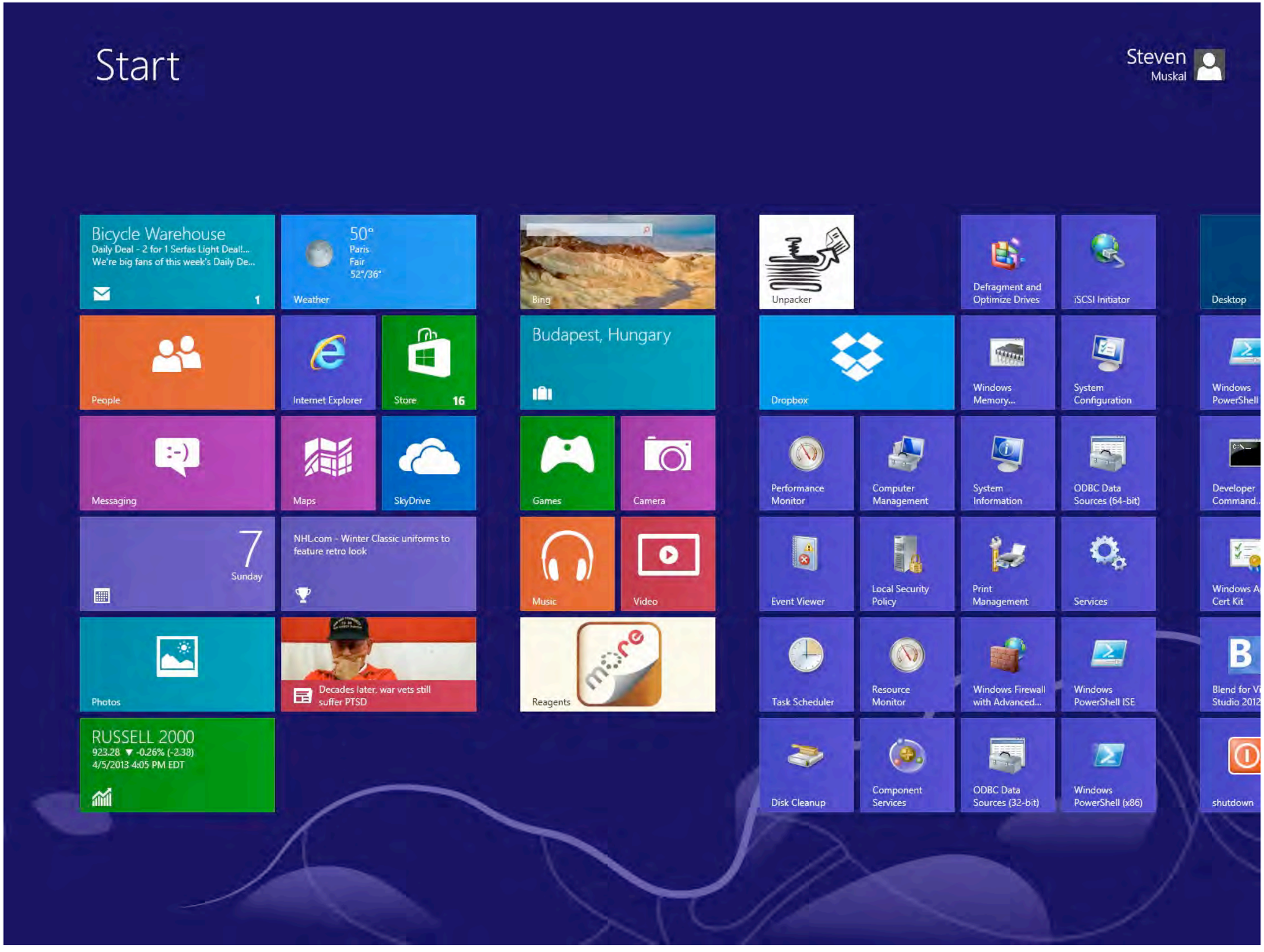


Coming Soon: Mobile Reagents for Win8



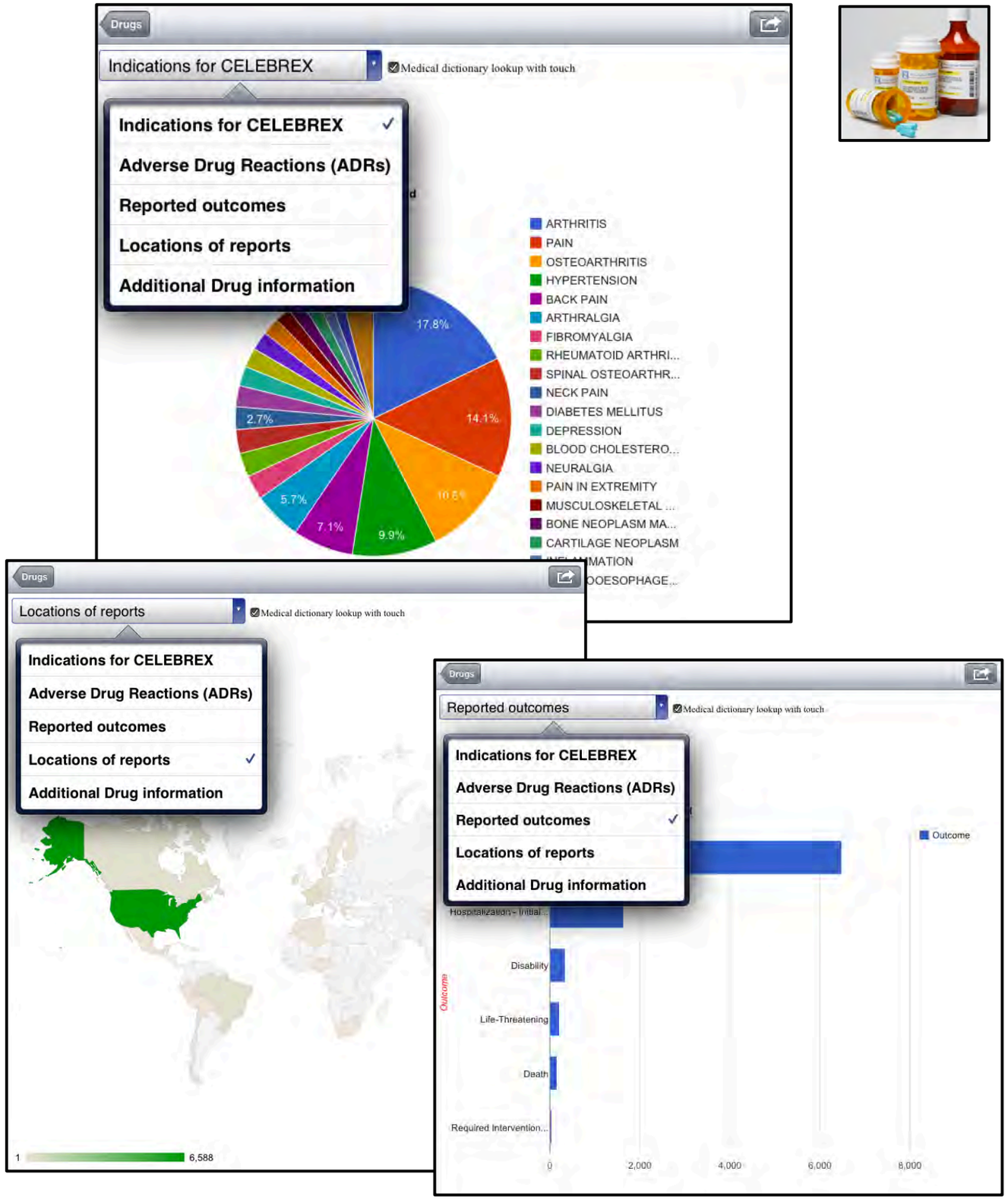
In partnership with Intel

Coming Soon: Mobile Reagents for Win8 (DEMO)

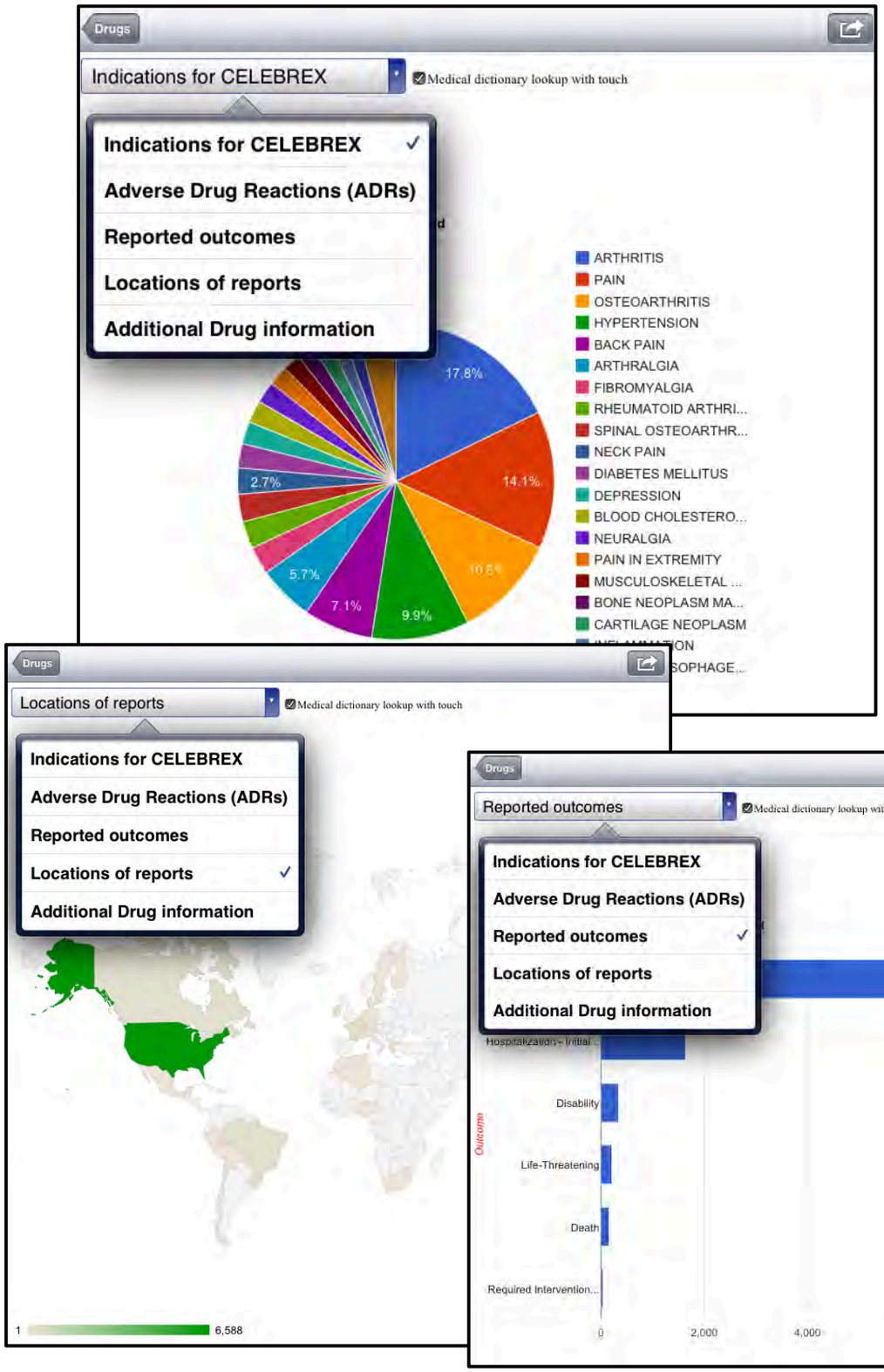


One More Thing....

New App coming Soon: mobileDrugReports



New App coming Soon: mobileDrugReports (DEMO)



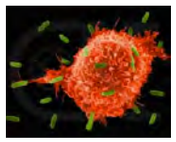
Summary

- Massive changes in our marketplace: many new opportunities
- Post-PC revolution is here - Go Mobile!
- Mobile and cloud computing pair well
- Apps support real workflows (not just phenomenal marketing vehicles)
- Try to support as many platforms as is feasible
- Patience is important…**Don’t** expect a field of dreams - i.e. “Build it and they will come…”

Acknowledgements

- Dr. Rajan Sharma and Prof. Stephan Schurer
  - 

iKinase 

iKinasePro 
iOncology
- Dr. Maurizio Bronzetti
  - Mobile Reagents Reaction101 SPRESImobile
- Dr. Alex Clark
  - MMDSLib: Mobile Reagents iProtein
  - Reaction101 Yield101 SPRESImobile
- Dr. Tony Yuan
  - JSDraw: 

iKinasePro Mobile Reagents iProtein
- Dr. Peter Löw, Dr. Josef Eiblmaier, et al.
  - SPRESImobile
- Dr. David Brown, Yury Rozenman
  - 
mobileDrugReports