

# Expanding the Reach of ChemInformatics through Mobile Computing

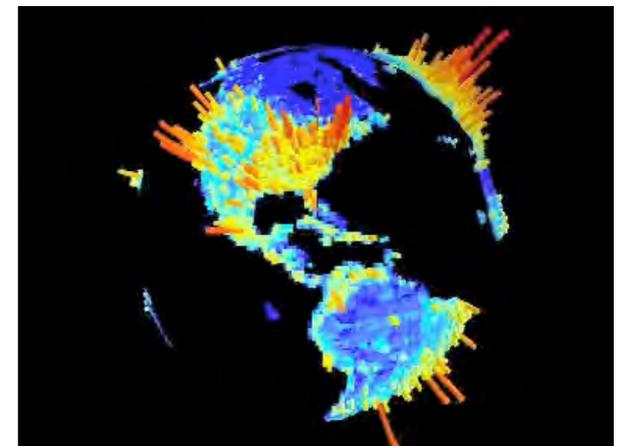
Dr. Steven Muskal

Chief Executive Officer

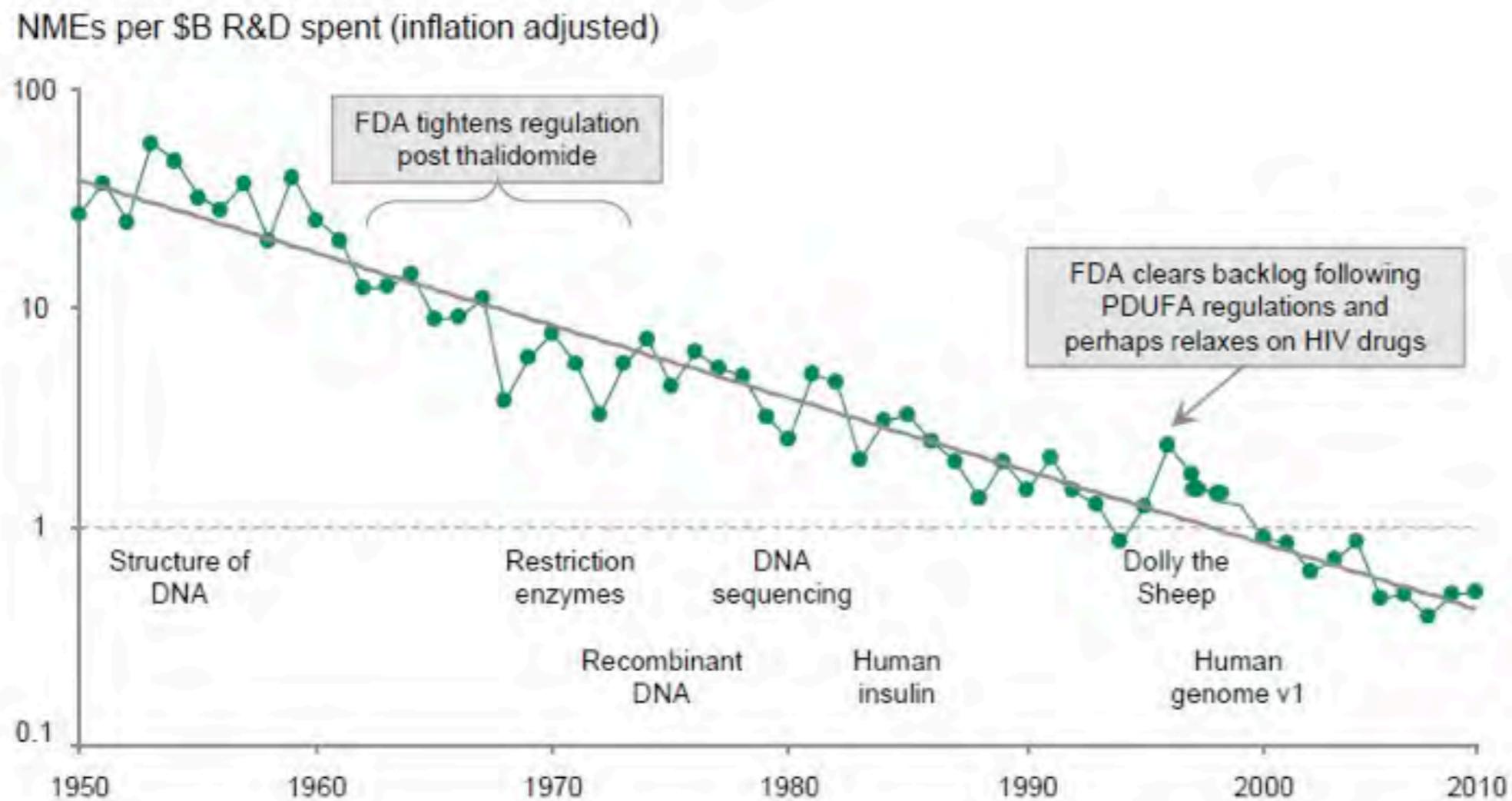
Eidogen-Sertanty, Inc

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

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



# 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!

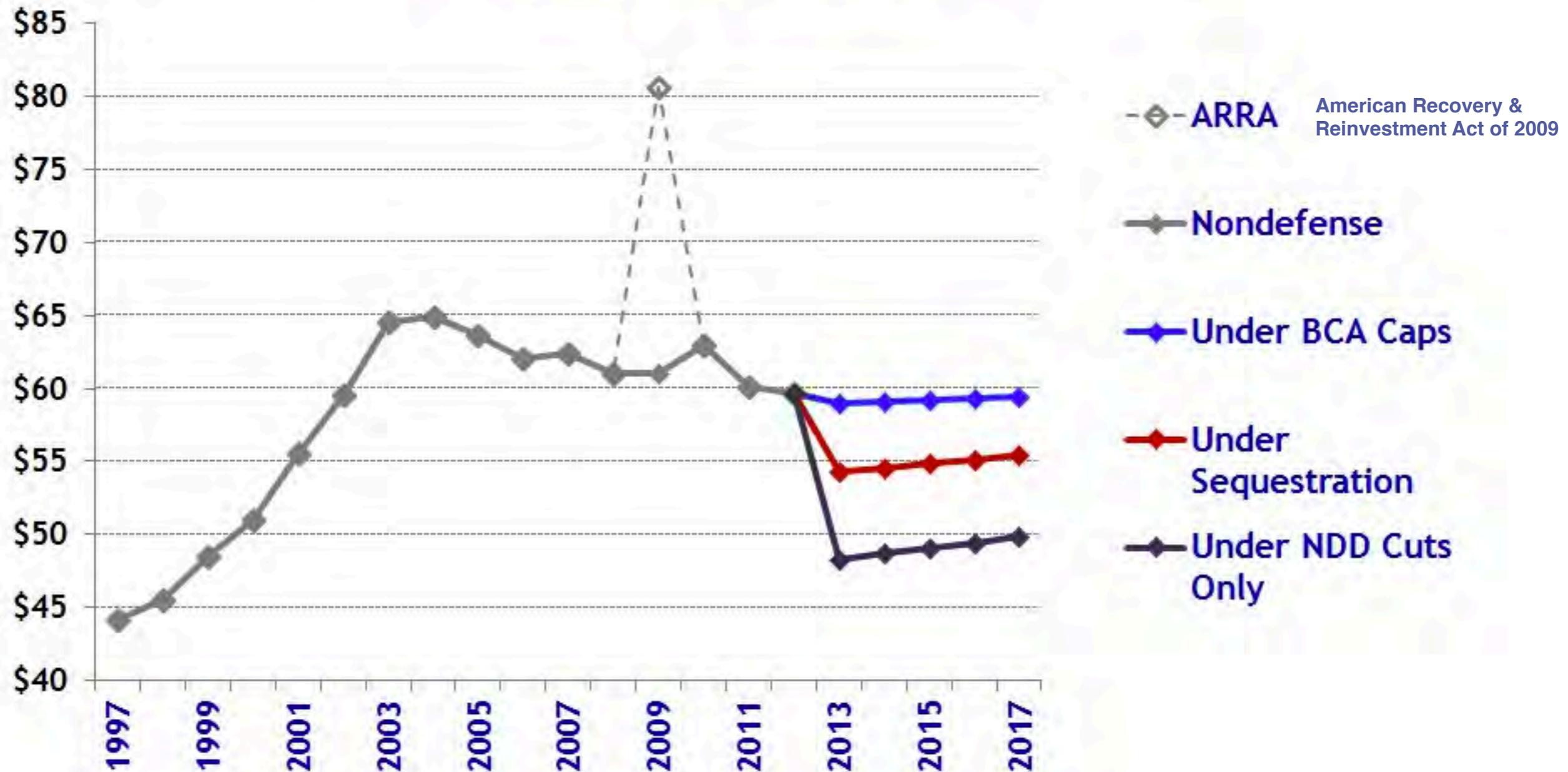
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<b>A Decade In Drug Industry Layoffs</b>	
<b>Year</b>	<b>Number of jobs cut</b>
2000	2,453
2001	4,736
2002	11,488
2003	28,519
2004	15,640
2005	26,300
2006	15,638
2007	31,732
2008	43,014
2009	61,109
2010	53,636
2011 (First three months)	3,385
<b>TOTAL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

Source: Challenger, Gray & Christmas, Inc. ©

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

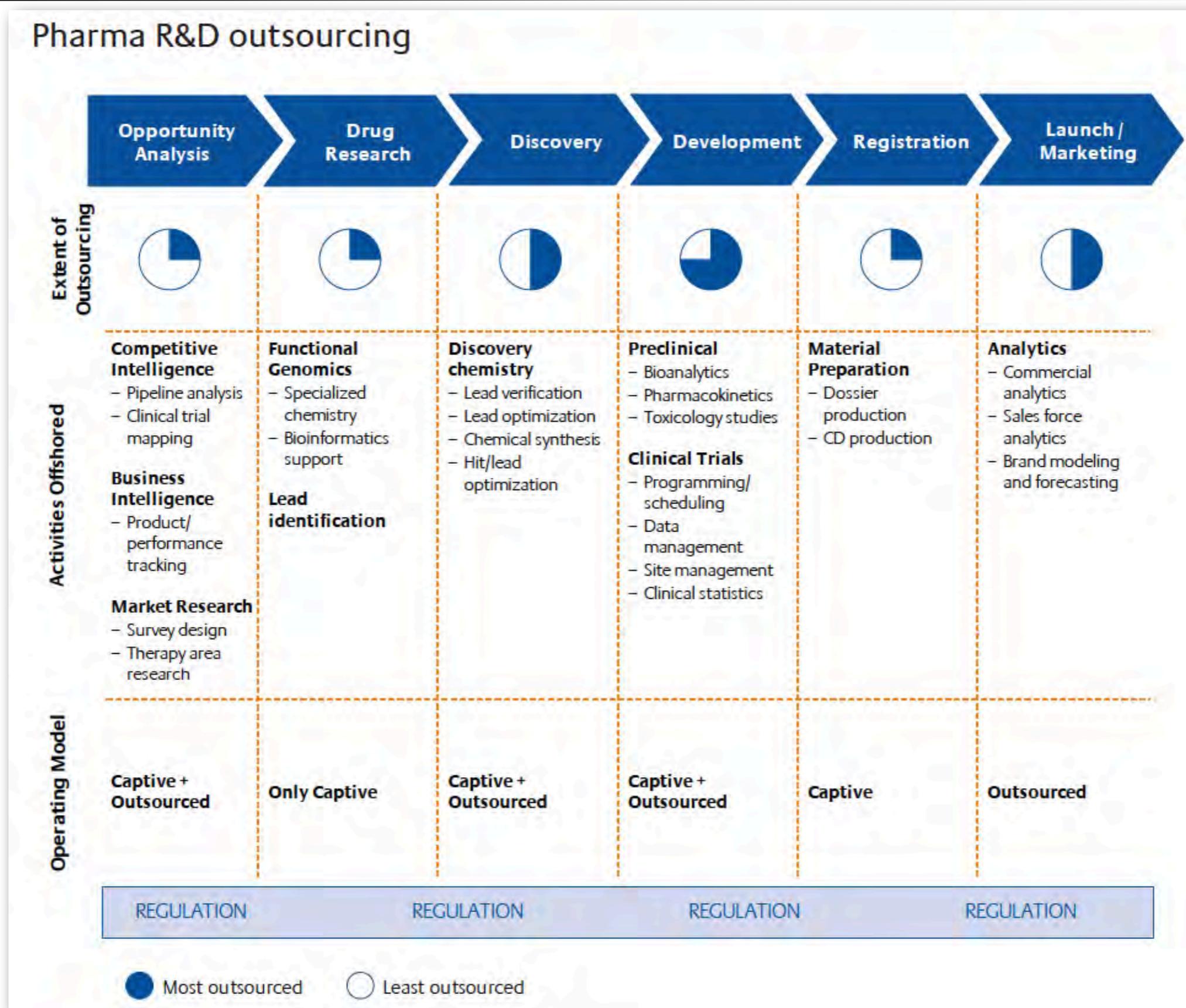
in billions of constant FY 2012 dollars

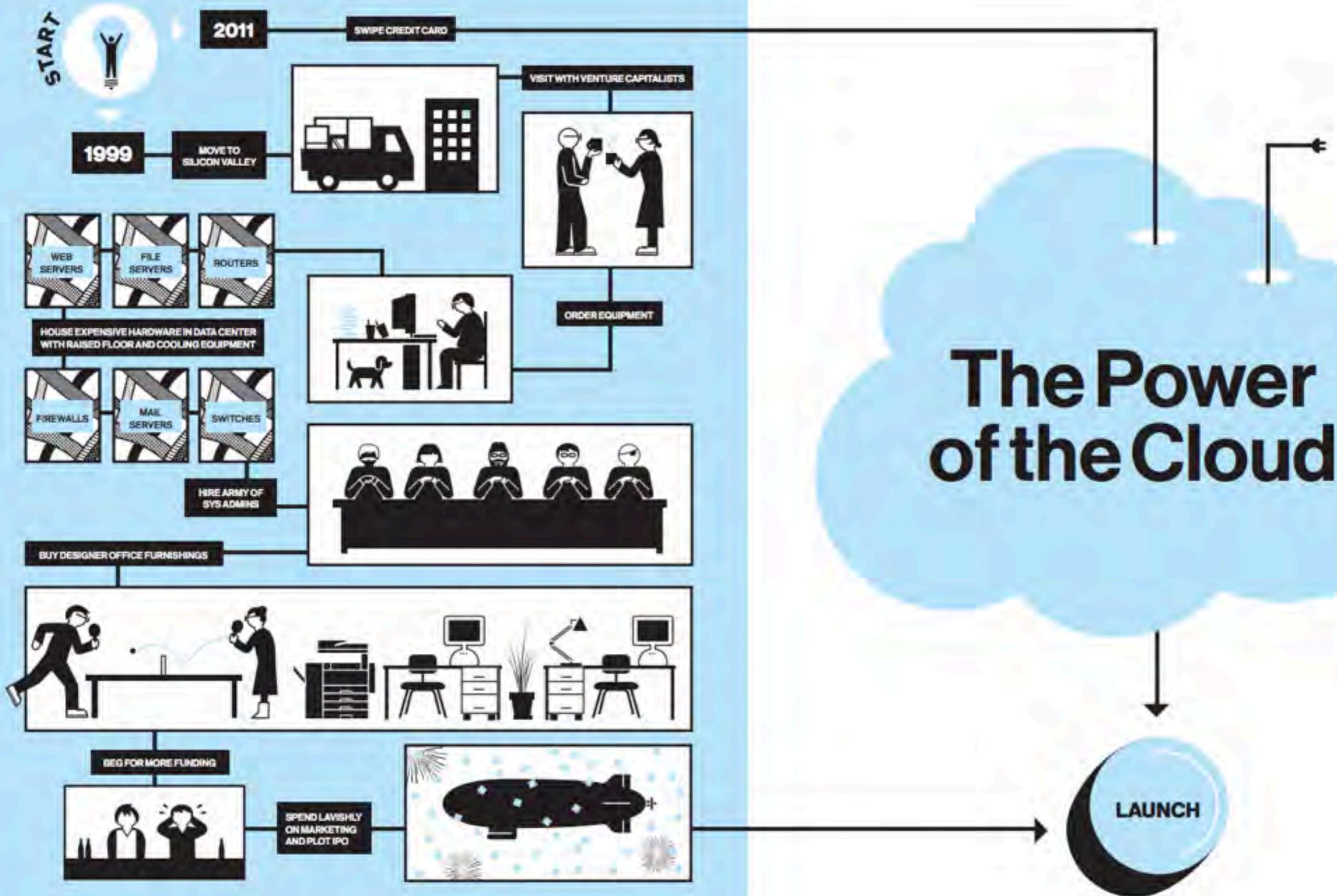


Source: Based on AAAS estimates of R&D funding and the FY 2013 budget, and CBO analyses of the Budget Control Act. <http://www.aaas.org/spp/rd/fy2013/SeqBrief.pdf>

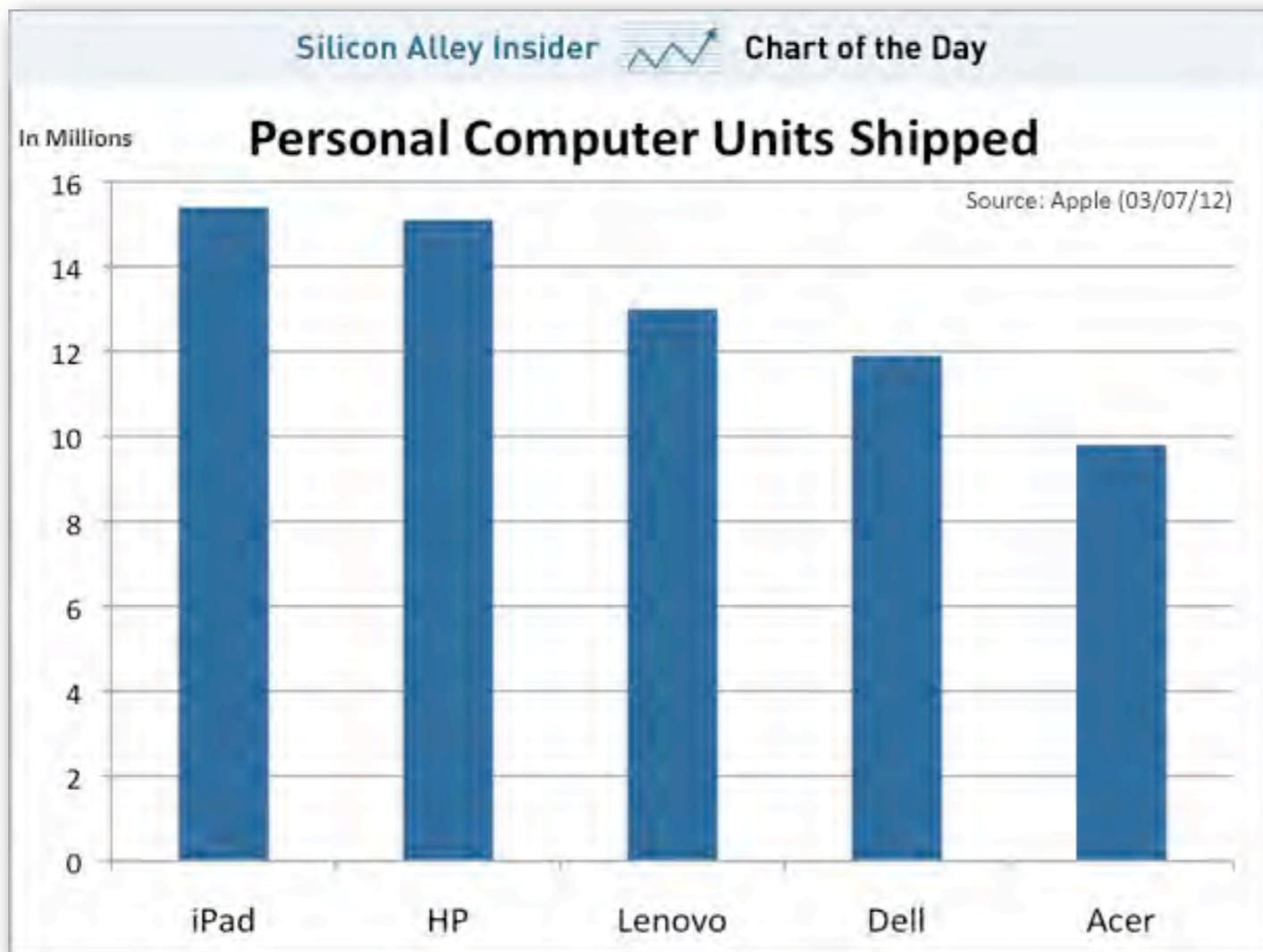
# Outsourcing Trends

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





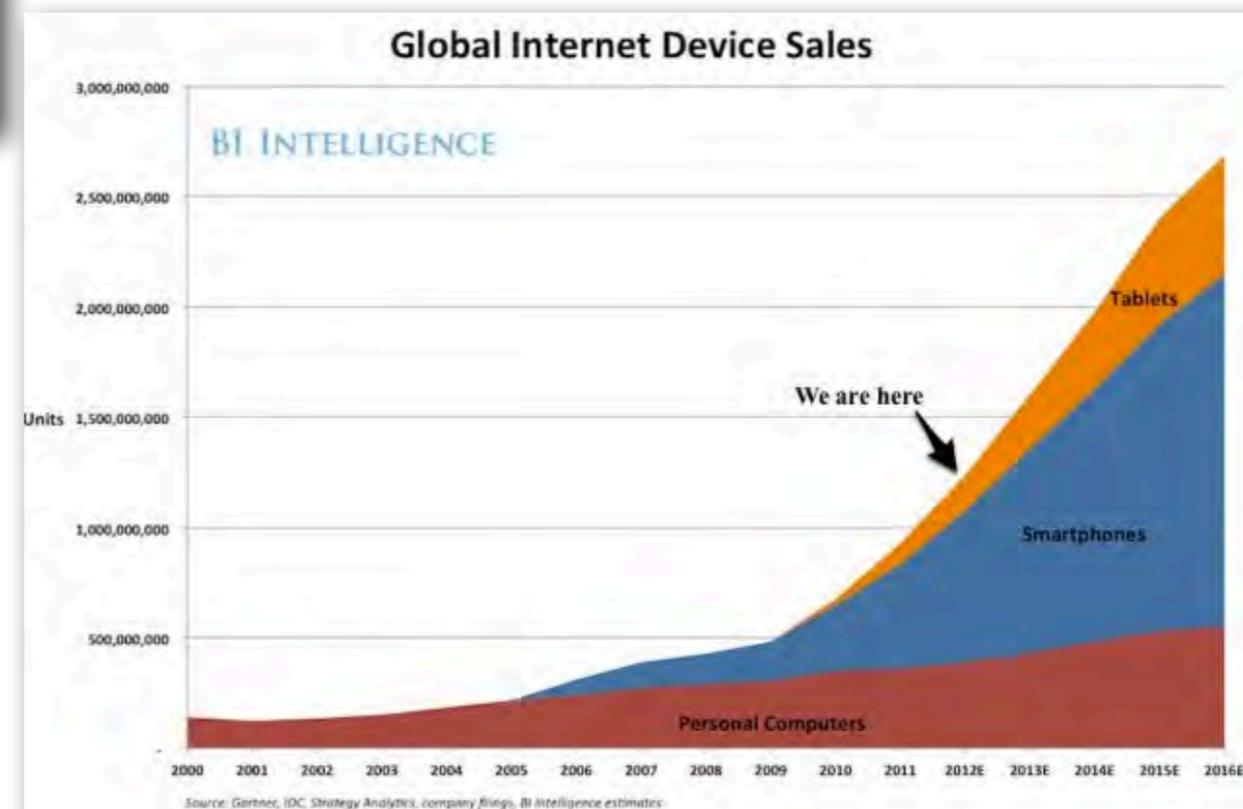
# The Post-PC Revolution Is Here...



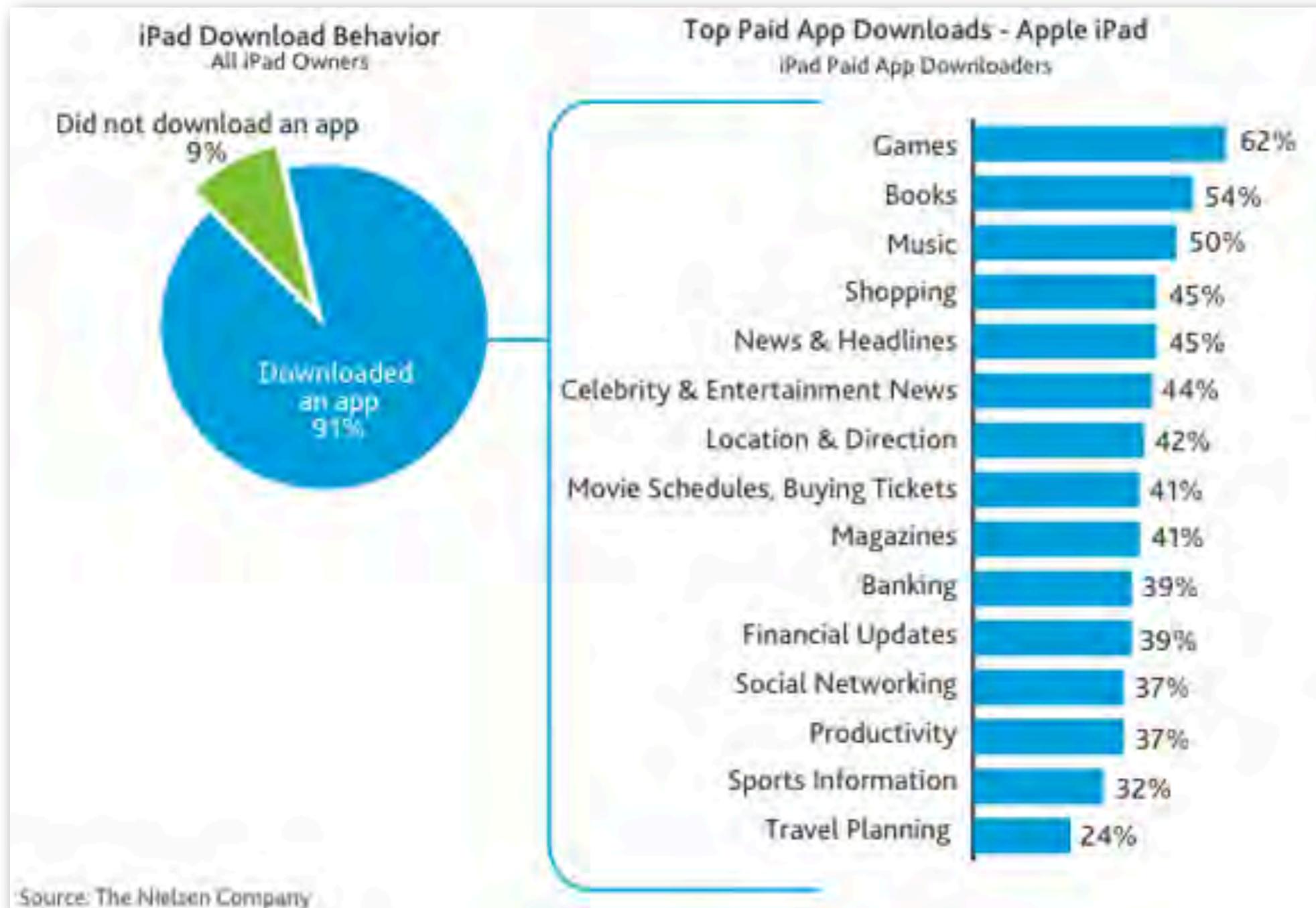
Apple Sold More iPads In Q411 Than Any Single Manufacturer Sold PC Devices

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



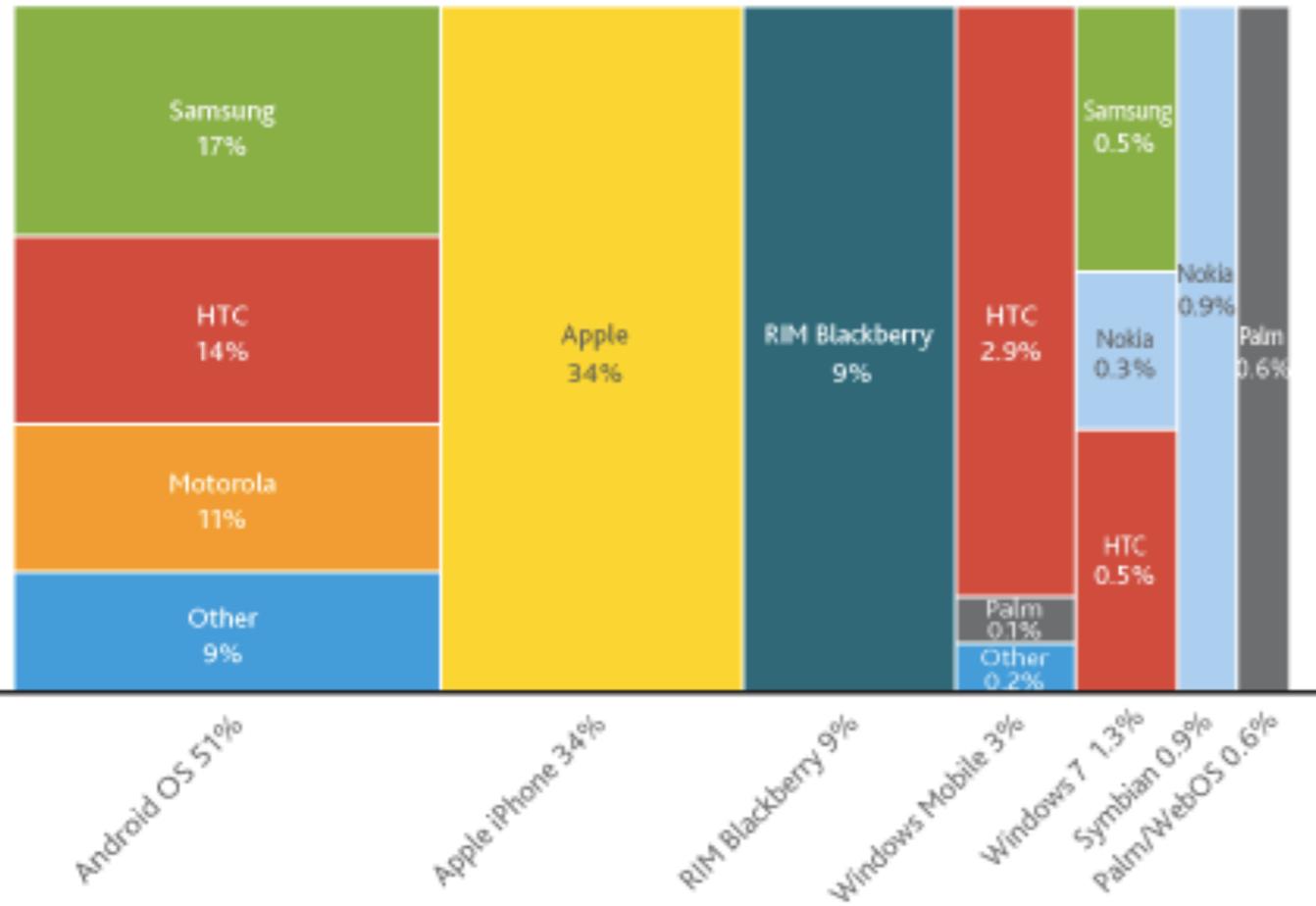
# Almost All Tablet Owners Download Apps



# Top Smartphone Platforms

## Smartphone manufacturer share by operating system

Q2 2012, US mobile subscribers



Source: Nielsen



### 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](http://www.comscore.com/Insights/Press_Releases/2013/4/comScore_Reports_February_2013_U.S._Smartphone_Subscriber_Market_Share)

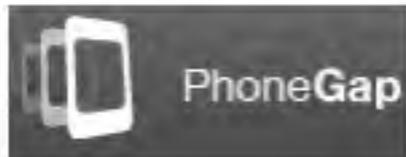
# Many Cross Platform Development “Choices”



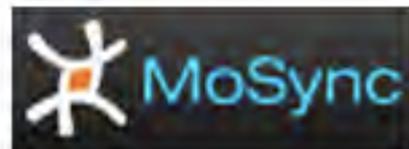
Xamarin



appMobi{!}



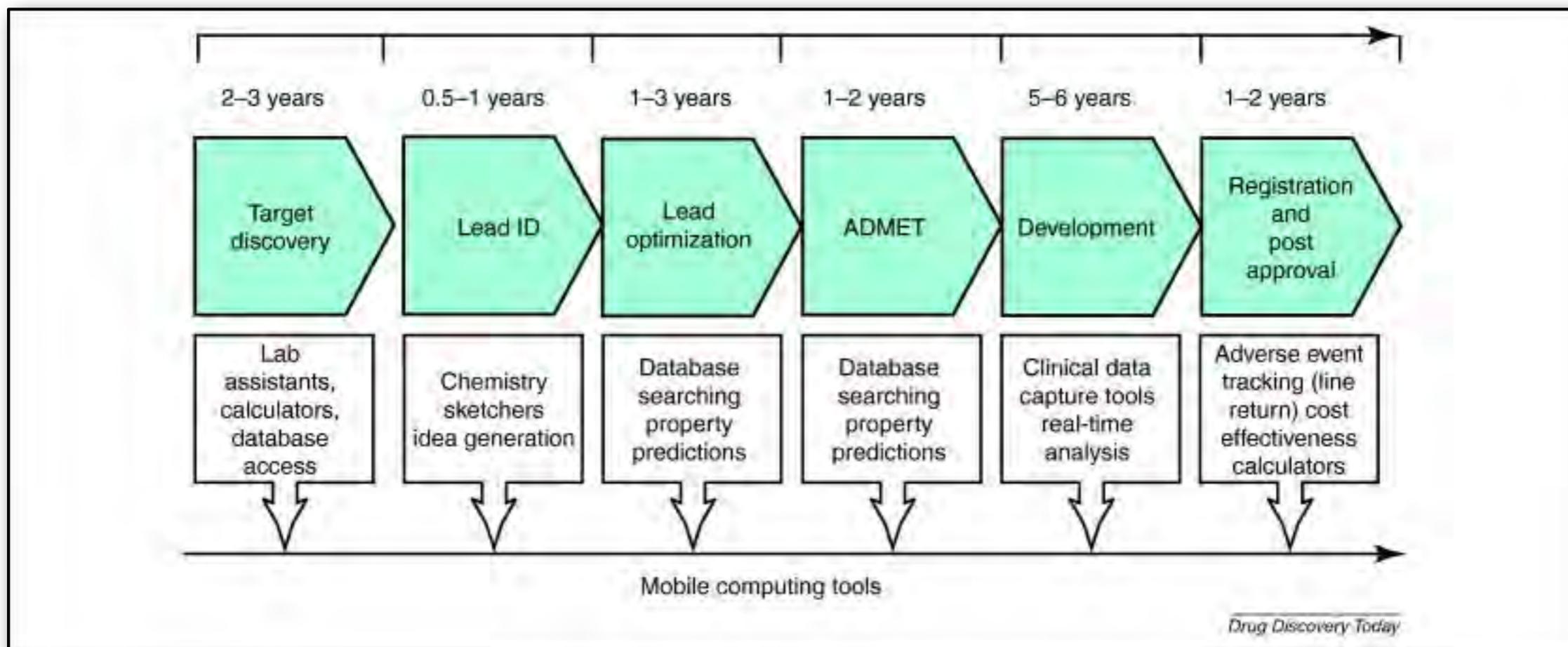
widgetpad.com



a appcelerator®



# Mobile Computing Opportunities in “Our Space”



# 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)

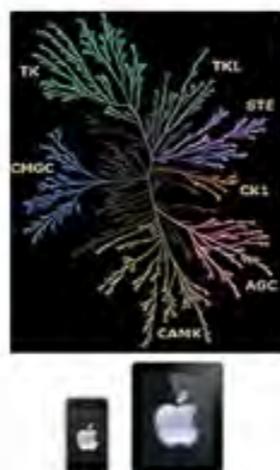


# Eidogen's iOS, Android, and Win8\* apps

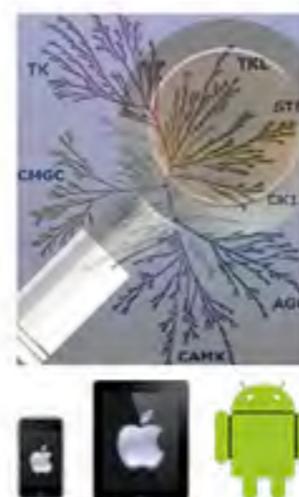
iProtein



iKinase



iKinasePro



iOncology



Mobile Reagents



Reaction101



Yield101



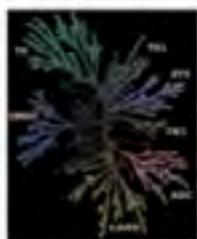
SPRESImobile



\* In partnership with Intel

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

# MobileApps: Worldwide Access



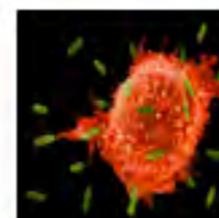
iKinase

iKinase



iKinasePro

iKinasePro



iOncology



iProtein



Mobile Reagents



Reaction101



Yield101



SPRESImobile

~ 30,000 People Use Eidogen Mobile Apps

# MobileApps Support Real Scientific Workflows

KKBid: 2087

Edit SAR SSS Sim Super MORE

Total DataPoints: 1271

**PDGFRA [Cell-Based Assay] ID: 2087**  
Assessment of Cytotoxicity in EOL-1 Cells  
IC50 0.0002 uM (pval: 9.699)

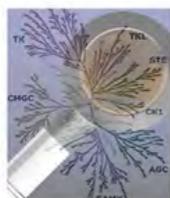
**DDR1 [Enzyme Assay]**  
Assessment of DDR1 Kinase Activity  
Kd 0.7 nM (pval: 9.155)

**DDR1 [Enzyme Assay]**  
Inhibition of DDR1 Kinase Activity  
Kd 0.7 nM (pval: 9.155)

**ABL1 [Enzyme Assay]**  
Assessment of ABL1 (Nonphosphorylated) Kinase Activity  
Kd 1.1 nM (pval: 8.959)

**ABL1 [Enzyme Assay]**  
Assessment of ABL1 (Q252H) (Nonphosphorylated) Kinase Activity  
Kd 1.8 nM (pval: 8.745)

**ABL1 [Enzyme Assay]**  
Assessment of Binding Affinity of ABL1 Kinase Inhibitors



Bioactivity searching (e.g. kinase SAR)

SSSearch results

Reaction101 Draw and balance chemical reactions

Copy Edit Search Descriptors Open In...

C1=CC=C(C=C1)C(=O)Nc2cnc3c2cnc3

MOREid: 5085865  
FMLA: C29H31N7O  
MWT: 493.6027

Name: imatinib

- ★★★★★ ChemDiv Inc
- ★★★★★ AKos
- ★★★★★ Key Organics Limited



Commercial availability

Home Structure Molecules Reactions

1 of 2

C1=CC=C(C=C1)C(=O)Nc2cnc3c2cnc3 + C1=CC=C(C=C1)C(=O)Cl → C1=CC=C(C=C1)C(=O)Nc2cnc3c2cnc3

**Calculated Properties**  
Conditions: 15 h, 70 degree, DMF

**Patents**  
Kankan Rajendra Narayanrao, Rao Dharmaraj Ramachandra, "Imatinib preparation and salts" (2005) Patent owner: Cipla Ltd Patent country: GB Patent number: 2398565

Reactant 1	Reactant 2	Product 1
<chem>C1=CC=C(C=C1)C(=O)Nc2cnc3c2cnc3</chem> MW: 277.324 MF: C <sub>16</sub> H <sub>15</sub> N <sub>5</sub>	<chem>C1=CC=C(C=C1)C(=O)Cl</chem> MW: 252.74 MF: C <sub>13</sub> H <sub>17</sub> ClN <sub>2</sub> O	<chem>C1=CC=C(C=C1)C(=O)Nc2cnc3c2cnc3</chem> MW: 493.603 MF: C <sub>29</sub> H <sub>31</sub> N <sub>7</sub> O



Synthesis planning

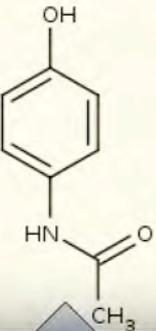
# Examples of Mobile IAC (InterApplicationCommunication)

iPad 3:36 PM 99%

mobileReagents Email

**more**  
MOBILE REAGENTS

Hit(s): 1 of 8



MOREid: 55848  
FMLA: C<sub>8</sub>H<sub>9</sub>NO<sub>2</sub>  
MWT: 151.1626

**Open In...**

- MMDS
- SPRESI
- iProtein
- PyMOL

Name: a

★★★★★

< 50 Ratings

Search Inc

★★★★★ Apin Chemicals

★★★★★ Sigma-Aldrich

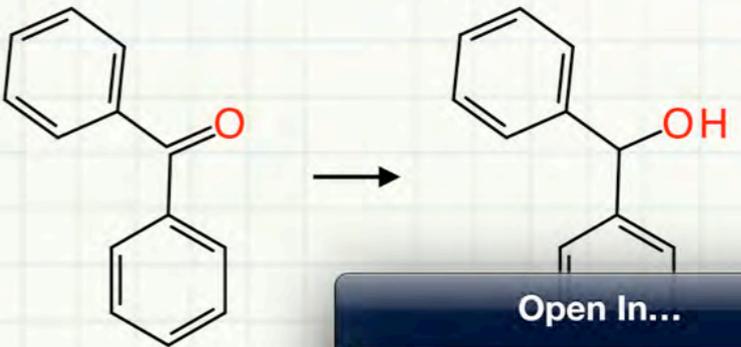
< 50 Ratings

Tocris Bioscience

iPad 3:33 PM 100%

Home Reaction Reactions

1 of 100



**Open In...**

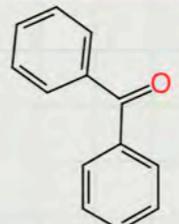
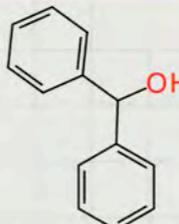
- Reaction101
- Yield101
- MMDS
- MolSync

**Calculated Properties**

**Conditions:** Stage 1: Chlorobenzene, Dichloromethane, hydrogen carbonate I Stage 2: 24 h, 82 °C, NaOH, HKO Potassium hydroxide

**Journal Articles**

Raja Mathiyazhagan Ulaganatha, Ramesh Rengan, Ahn Kyo Han, "Rhodium(III) NCN pincer complexes catalyzed transfer hydrogenation of ketones", Tetrahedron Lett., vol. 50, pp. 7014-7017 (2009)  
<http://dx.doi.org/10.1016/j.tetlet.2009.09.152>

Reactant 1	Product 1
 MW: 182.218 MF: C <sub>13</sub> H <sub>10</sub> O	 MW: 184.234 MF: C <sub>13</sub> H <sub>12</sub> O

1

100

# SPRESImobile - Update: Reaction Searching



## SPRESImobile: 410,000 Chemical Reactions Freely Available

**15 of 100**

**Name & Synonyms (5)**  
2-Methyl-6-methoxyquinoline  
2-Methyl-6-methoxyquinoline  
6-Methoxy-2-methylquinoline  
6-Methoxy-2-methylquinolin

**Journal Articles (29)**  
Wang Xiao-Bing, Zhou Yong-Gui, "Synthesis of Tunable Bisphosphine Ligands and Their Application in Asymmetric Hydrogenation of Quinolines", *J. Org. Chem.*, vol. 73, pp. 5640-5642 (2008)  
<http://dx.doi.org/10.1021/jo800779r>  
Li Zhi-Wei, Wang Tian-Li, He Yan-Mei, Wang Zhi-Jian, Fan Qing-Hua, Pan Jie, Xu Li-Jin, "Air-Stable and Phosphine-Free Iridium Catalysts for Highly Enantioselective Hydrogenation of Quinoline Derivatives+", *Org. Lett.*, vol. 10, pp. 5265-5268 (2008)  
<http://dx.doi.org/10.1021/ol802016w>  
Zhou Haifeng, Li Zhiwei, Wang Zhijian, Wang Tianli, Xu Lijin, He Yanmei, Fan Qing-Hua, Pan Jie, Gu Lianquan, Chan Albert S. C., "Hydrogenation of quinolines using a recyclable phosphine-free chiral cationic ruthenium catalyst: enhancement of catalyst stability and selectivity in an ionic liquid", *Angew. Chem., Int. Ed. Engl.*, vol. 47, pp. 8464-8467 (2008)  
<http://dx.doi.org/10.1002/anie.200802237>

**Information**  
Registration No.: 0006298-800  
Molecular Formula: C<sub>11</sub>H<sub>11</sub>NO  
Molecular Weight: 173.21

**Calculated Properties**  
Calculated Log P: 2.3599999  
Rotatable Bonds: 3  
H-Acceptors: 1  
H-Donors: 0

**Patents (1)**  
Butera John A., Bagli Jehan F., "N-quinolinyl alkyl-substituted 1-aryloxy-2-propanolamine and propylamine derivatives possessing class III antiarrhythmic activity" (1993) Patent owner: American Home Products Corp. Patent country: US Patent number: 5084463

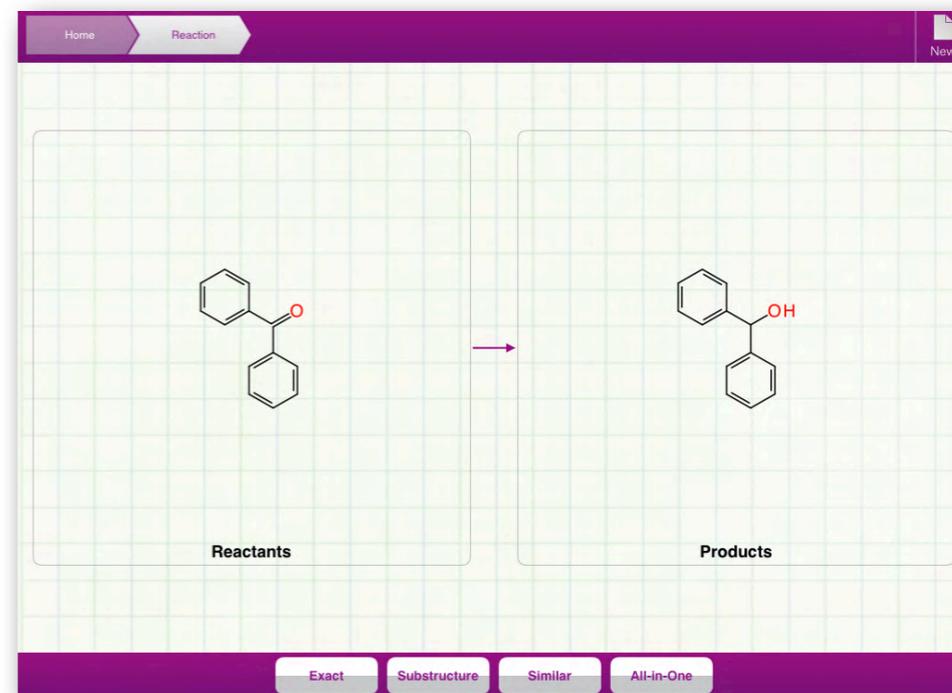
**Commercial Availability (6)**  
Apollo Scientific <http://www.apolloscientific.com>  
Sigma-Aldrich <http://www.sigmaaldrich.com>  
VWR <https://www.vwr.com>

**7 of 21**

**Calculated Properties**  
Yield: 53%

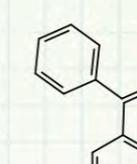
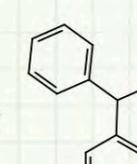
**Journal Articles**  
SHCHUKINA M. N.; VASIL'eva V. F.; ZAGRUDINOVA R. A., "SUBSTITUIERTE 1,2,3,4-TETRAHYDRO-CHINOLINE. 3. 2-(BETA-DIALKYLAMINOETHYL)-DERIVATE.", *KHIM. FARMATSEUT. ZH.*, vol. 9, pp. 24-26 (1975)

Reactant 1	Reactant 2	Product 1
 MW: 173.211 MF: C <sub>11</sub> H <sub>11</sub> NO	 MW: 45.0837 MF: C <sub>1</sub> H <sub>5</sub> N	 MW: 230.306 MF: C <sub>14</sub> H <sub>19</sub> N <sub>2</sub> O



**Home** **Reaction** **Reactions**

**2 of 100**

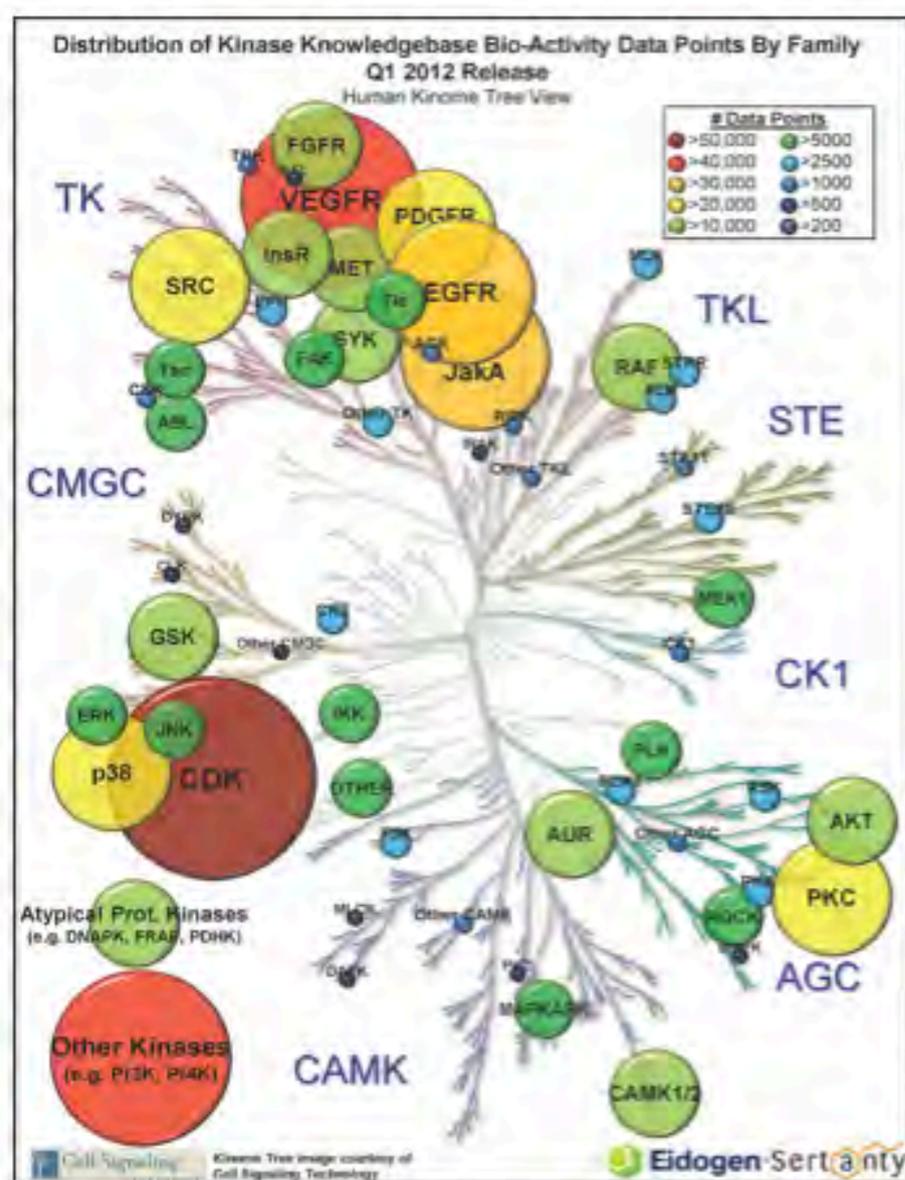
  $\rightarrow$  

**Calculated Properties**  
**Conditions:** Stage 1: Chlorobenzene, Dichloromethane, Water, AsI3 Arsenic(III) iodide, CHNaO3 Sodium-hydrogen carbonate I Stage 2: 24 h, 82 degree, Silver, Methanol, Isopropanol, H3N Ammonia, HKO Potassium hydroxide

**Journal Articles**  
Raja Mathiyazhagan Ulaganatha, Ramesh Rengan, Ahn Kyo Han, "Rhodium(III) NCN pincer complexes catalyzed transfer hydrogenation of ketones", *Tetrahedron Lett.*, vol. 50, pp. 7014-7017 (2009)  
<http://dx.doi.org/10.1016/j.tetlet.2009.09.152>

Reactant 1	Product 1

# iKinasePro: Update: Android Version



Substructure Search

Back to Structure Grid Custom Structure Search

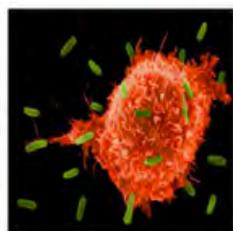
Molecule Last Searched

Chiral

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



OKB ID: 1377

Custom Structure Search Register for e-mail Alert

O=C(O)c1ccc2c(c1)oc3ccccc32N4CCN(C4)c5ccccc5

OKB ID: 1377

Target	Type	Disease	Measure
11 targets	Cell-Based	colorectal carcinoma	IC50
11 targets	Cell-Based	chronic myelogenous leukemia (cml)	IC50
11 targets	Cell-Based	carcinoma	IC50
11 targets	Cell-Free	adenocarcinoma	IC50

Data extracted from the Eidogen-Sertanty Oncology Knowledgebase (OKB) as of Fri May 11 18:53:05 E

OKB ID: 755

Substructure Search

CC(=O)OC12CC3C(C1)OC(=O)C(C2)OC(=O)C3c4ccccc4

Molecule Last Searched

iOncology

**a**

**adenocarcinoma**  
Dp(s) in OKB: 1553 AVG: 6.40 STD: 0.97 Min: 2.00 Max: 9.05

**adenocarcinoma, non-small cell lung cancer**  
Dp(s) in OKB: 24 AVG: 5.55 STD: 0.40 Min: 4.88 Max: 6.37

**b**

**burkitt's lymphoma**  
Dp(s) in OKB: 3 AVG: 5.43 STD: 0.20 Min: 5.20 Max: 5.70

**c**

**carcinoma**  
Dp(s) in OKB: 119 AVG: 5.65 STD: 0.92 Min: 3.00 Max: 8.91

**carcinoma (lung)**  
Dp(s) in OKB: 28 AVG: 6.00 STD: 0.00 Min: 6.00 Max: 6.00

**carcinoma, large cell lung cancer**  
Dp(s) in OKB: 8 AVG: 5.26 STD: 0.92 Min: 4.60 Max: 7.07

**carcinoma, non-small cell lung cancer**  
Dp(s) in OKB: 36 AVG: 6.93 STD: 0.88 Min: 5.00 Max: 8.37

**carcinoma, small cell lung cancer**  
Dp(s) in OKB: 122 AVG: 5.78 STD: 1.01 Min: 3.80 Max: 7.70

**carcinoma/colorectal carcinoma**  
Dp(s) in OKB: 38 AVG: 6.13 STD: 0.00 Min: 6.13 Max: 6.13

**chronic myelogenous leukemia (cml)**  
Dp(s) in OKB: 137 AVG: 5.85 STD: 0.42 Min: 4.30 Max: 6.40

**colorectal adenocarcinoma**  
Dp(s) in OKB: 708 AVG: 5.78 STD: 0.71 Min: 4.00 Max: 7.75

**colorectal carcinoma**  
Dp(s) in OKB: 947 AVG: 6.00 STD: 0.94 Min: 2.00 Max: 9.52

**cutaneous t cell lymphoma**  
Dp(s) in OKB: 9 AVG: 6.54 STD: 0.59 Min: 5.58 Max: 7.35

**cutaneous t cell lymphoma,mycosis fungoides**  
Dp(s) in OKB: 9 AVG: 6.04 STD: 0.64 Min: 5.12 Max: 6.92

**cutaneous t-cell lymphoma, acute myelogenous leukemia, hodgkin's disease,...**  
Dp(s) in OKB: 420 AVG: 6.26 STD: 0.81 Min: 4.00 Max: 8.85

**d**

**ductal carcinoma**  
Dp(s) in OKB: 98 AVG: 5.42 STD: 0.62 Min: 4.00 Max: 7.00

Structure Search

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



Reagents for Organic Synthesis & Screening Compounds

**SEARCH BY**

NAME

FORMULA

STRUCTURE

NARROW DOWN YOUR SEARCH BY

**SUPPLIER**

ABOUT HELP TELL A FRIEND SETTINGS

Carrier 1:59 PM

Back Search results Email

Descriptors Open In...

MOREid: 44843

FMLA: C<sub>11</sub>H<sub>12</sub>N<sub>2</sub>O<sub>3</sub>

MWT: 220.2246

Name: oxitriptan

- ★★★★☆ AKos
- ★★★★☆ Calbiochem
- ★★★★☆ Tim Tec Inc
- ★★★★☆ AcrosOrganics

Carrier 2:00 PM

Search results

Pubmed

Common name: **oxitriptan**

IUPAC name: (2S)-2-amino-3-(5-hydroxy-1H-indol-3-yl)propanoic acid

Synonyms: (2S)-2-amino-3-(5-hydroxy-1H-indol-3-yl)propanoic acid, (2S)-2-amino-3-(5-hydroxy-1H-indol-3-yl)propanoic acid, 4350-09-8, 56570\_FLUKA, Lopac0\_000627, NCGC00091062-01, NCGC00015526-01, L-5-HTP, CHEBI:17780, H9772\_SIGMA, L-2-Amino-3-(5-hydroxyindolyl)propanoic acid, ST048776, EU-0100627, C00643, 107751\_ALDRICH, NCGC00091062-04, Lopac-H-9772

QR Code:

Vendors			
	AMBIWER	Mpja Chemicals	IBS
	Calbiochem	AKos	

Descriptors	Value
ALogP	1.554
Aqueous Solubility [0:Extremely low, 1:Very Low, 2:Low, 3:Good, 4:Optimal, 5:Very High]	4
Blood Brain Barrier Penetration	4

Carrier 1:58 PM

mobileReagents

Exact SSS Sim

New Undo Draw Template Nitrogen Erase

Molecule Last Searched

Carrier 2:01 PM

Back Search Clean

Chemical structure of oxitriptan

Chemical keyboard with buttons for C, N, O, A, and other symbols.

# Coming Soon: Mobile Reagents for Win8



Mobile Reagents

Reagents for Organic Synthesis & Screening Compounds

Search By

- MOREid
- Keyword
- Formula
- Structure

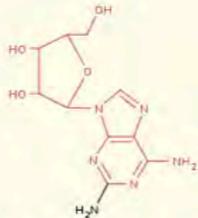
Narrow Down Your Search By

- Supplier
- Name or CAS No.

OSRA

Mobile Reagents

2 of 50 (Total: 375)



MOREid: 445066  
FMLA: C10H14N6O4  
MWT: 282.256

Name: 2-(2,6-diaminopurin-9-yl)-5-(hydroxymethyl)oxolane-3,4-diol

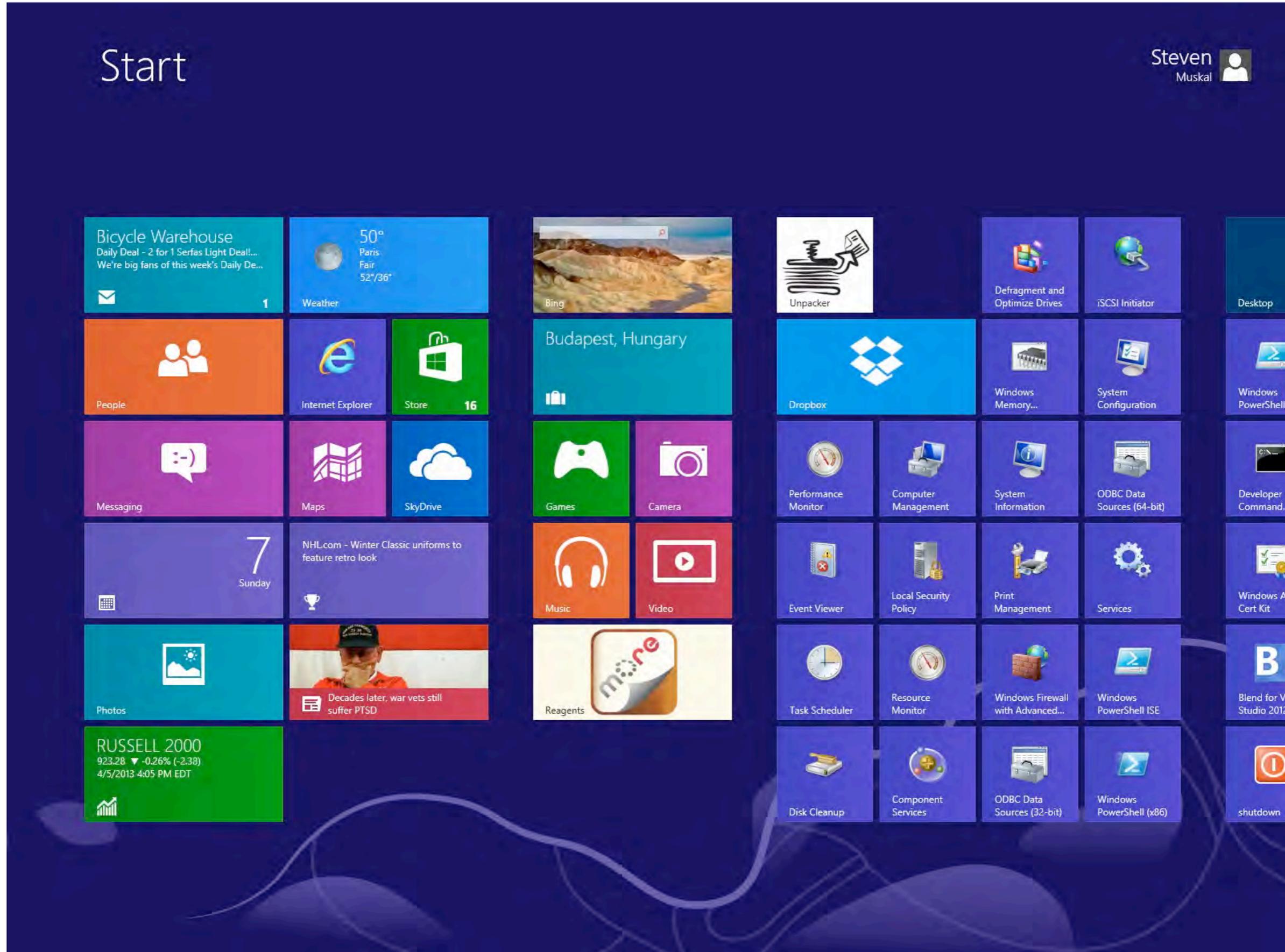
- ★★★★★ ChemDiv Inc
- ★★★★★ Chemical Block Ltd
- ★★★★★ AKos
- ★★★★★ Tim Tec Inc
- ★★★★★ Labotest
- ★★★★★ Ambinter

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In partnership with Intel

# Coming Soon: Mobile Reagents for Win8 (DEMO)



One More Thing....

# New App coming Soon: mobileDrugReports

## United States FDA Adverse Event Data

Last Report Date: 20120501

**Drugs**

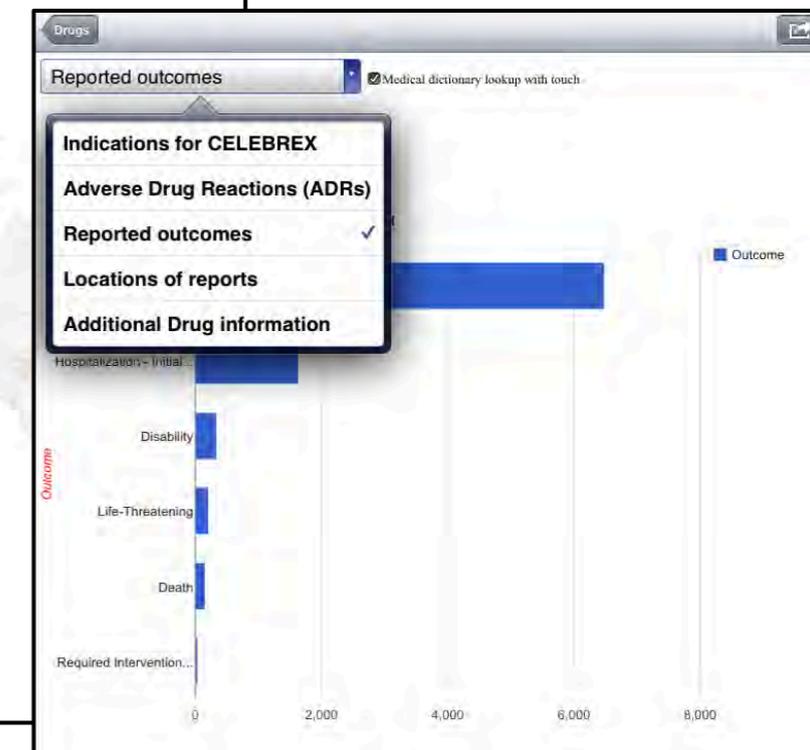
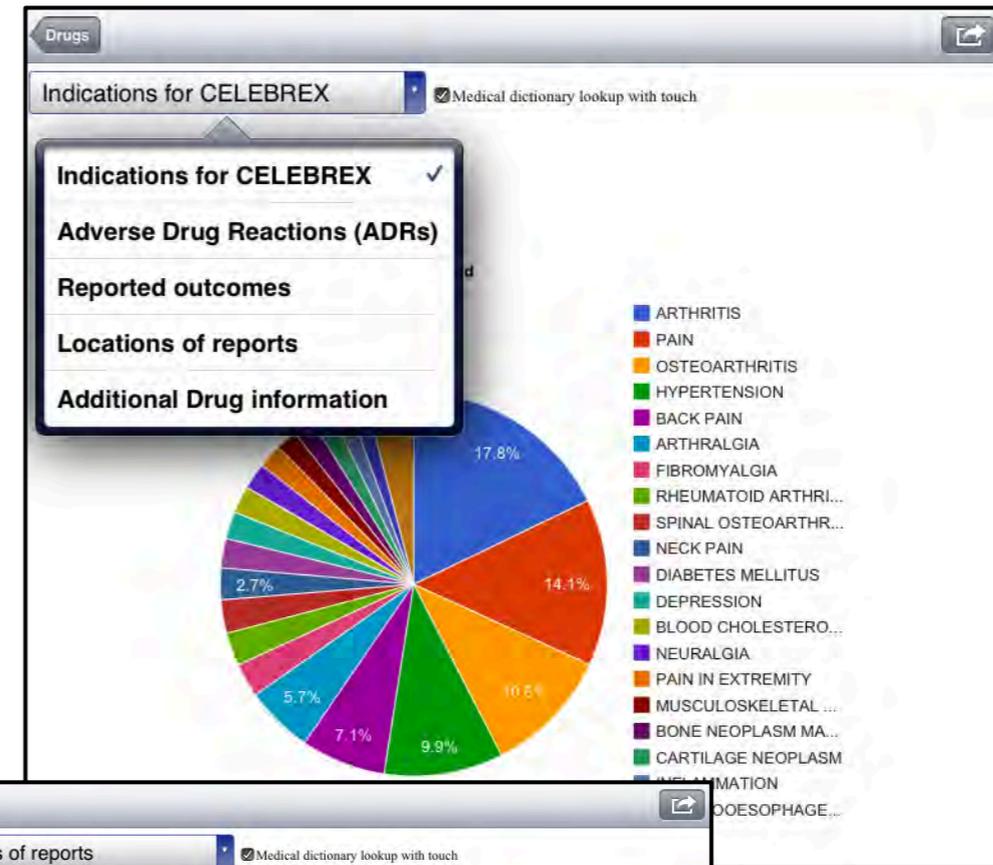
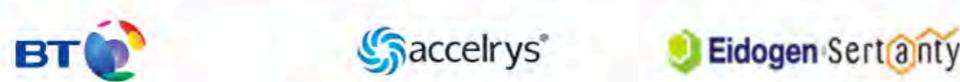
**Indications**

**Adverse Drug Reactions (ADRs)**

**Drug Interactions**

**Drug Manufacturers**

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# New App coming Soon: mobileDrugReports (DEMO)

United States FDA Adverse Event Data  
Last Report Date: 20120501

Drugs

Indications

Adverse Drug Reactions (ADRs)

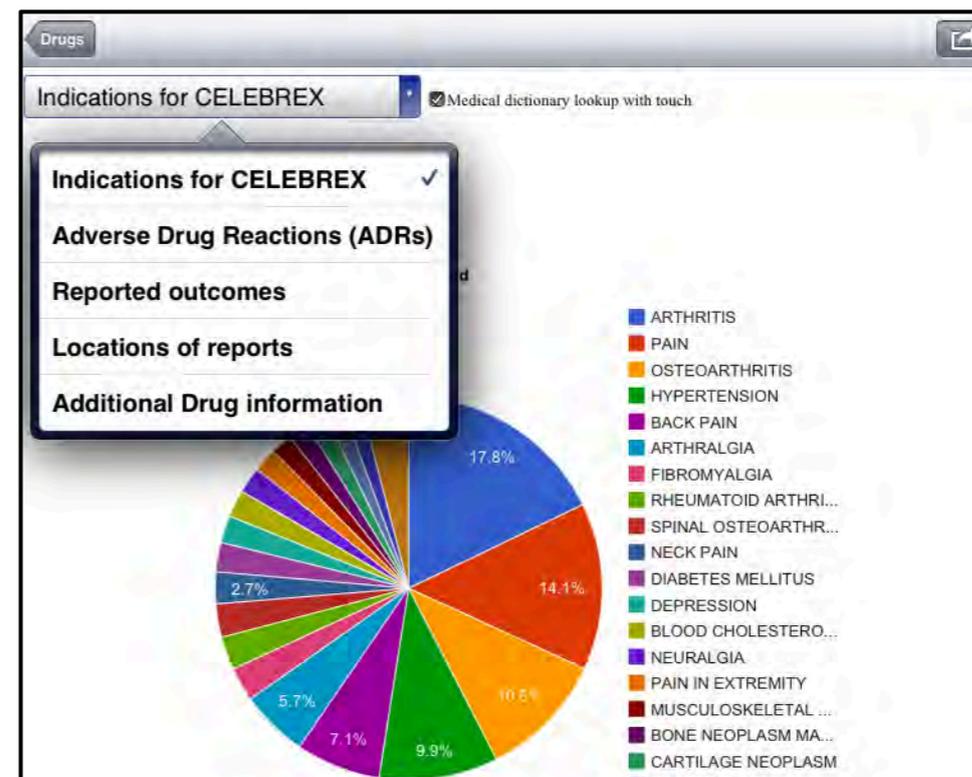
Drug Interactions

Drug Manufacturers

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BT accelrys Eidogen Sertanty

Reaction101 Draw and balance chemical reactions



# 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..."

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- Dr. Rajan Sharma and Prof. Stephan Schurer



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