

# New Strategy to Engage Mobile Computing Users and Developers

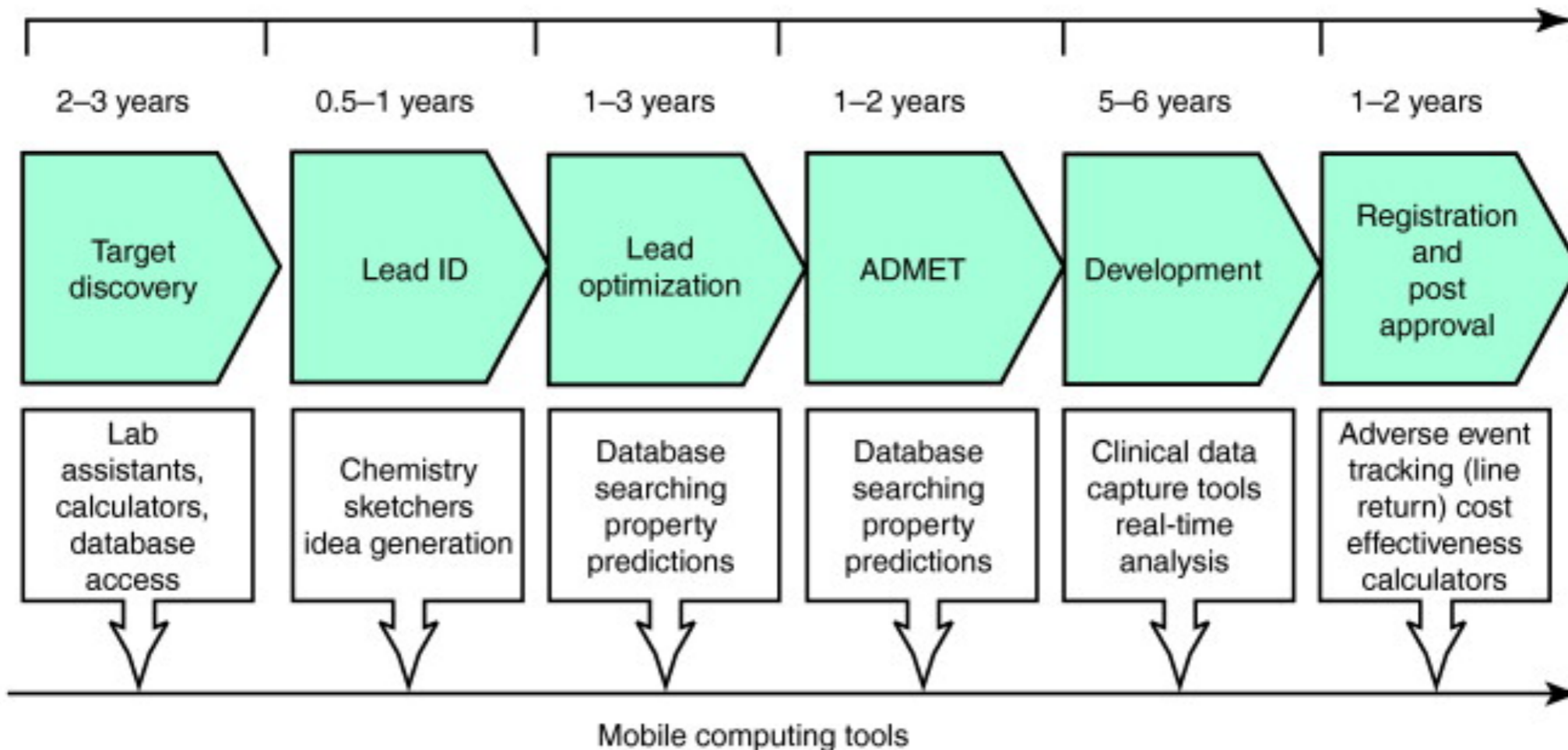
Dr. Steven Muskal

Chief Executive Officer

Eidogen-Sertanty, Inc

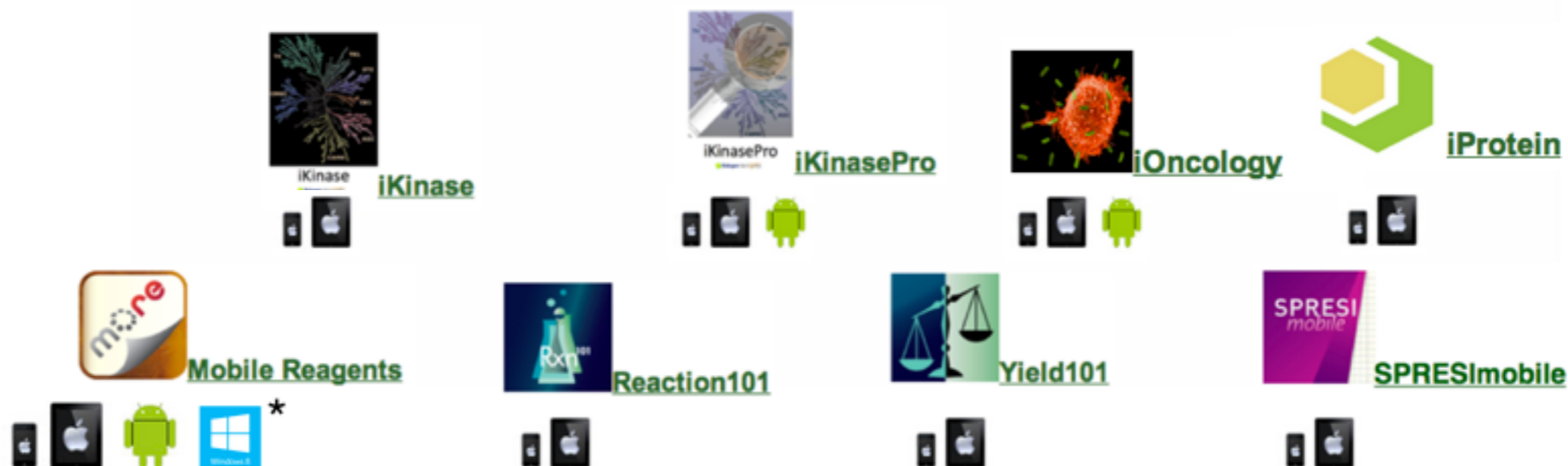
[smuskal@eidogen-sertanty.com](mailto:smuskal@eidogen-sertanty.com)

# Mobile Computing Opportunities in “Our Space”



*Drug Discovery Today*

# Eidogen's Apps: More than 40K Downloads



\* In partnership with Intel

Note: Reaction101, Yield101, and SPRESImobile - Built Collaboratively with Molecular Materials Informatics, Inc.

# MobileApps Support Real Scientific Workflows

KKBid: Gleevec      KKBid: 2087      Email Alert

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)

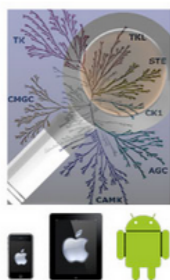
**DDR1 [Enzyme Assay]**  
Assessment of DDR1 Kinase Activity  
Kd 0.7 nM (pval: 9.155)

**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)

Back      SSSearch results      Email

Reaction101 Draw and balance chemical reactions      more MOBILE REAGENTS

Copy Edit Search Descriptors Open In...

MOREid: 5085865  
FMLA: C29H31N7O  
MWT: 493.6027

Name: imatinib

★★★★★ ChemDiv Inc >  
★★★★★ AKos >  
★★★★★ Key Organics Limited >



Commercial availability

Home Structure Molecules Reactions

1 of 2

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
MW: 277.324 MF: C <sub>16</sub> H <sub>15</sub> N <sub>5</sub>	MW: 252.74 MF: C <sub>13</sub> H <sub>17</sub> ClN <sub>2</sub> O	MW: 493.603 MF: C <sub>29</sub> H <sub>31</sub> N <sub>7</sub> O



Synthesis planning

# Science Apps of Today

- Largely Vertical, Point Solutions
- Development Requires Sophisticated Knowledge of Mobile Computing Development Environments
- Development Often Requires Knowledge of Cloud Computing/LAMP environments
- Only Some Enable App Integration (e.g. client-side standard filetype sharing)

# Science Apps of Today

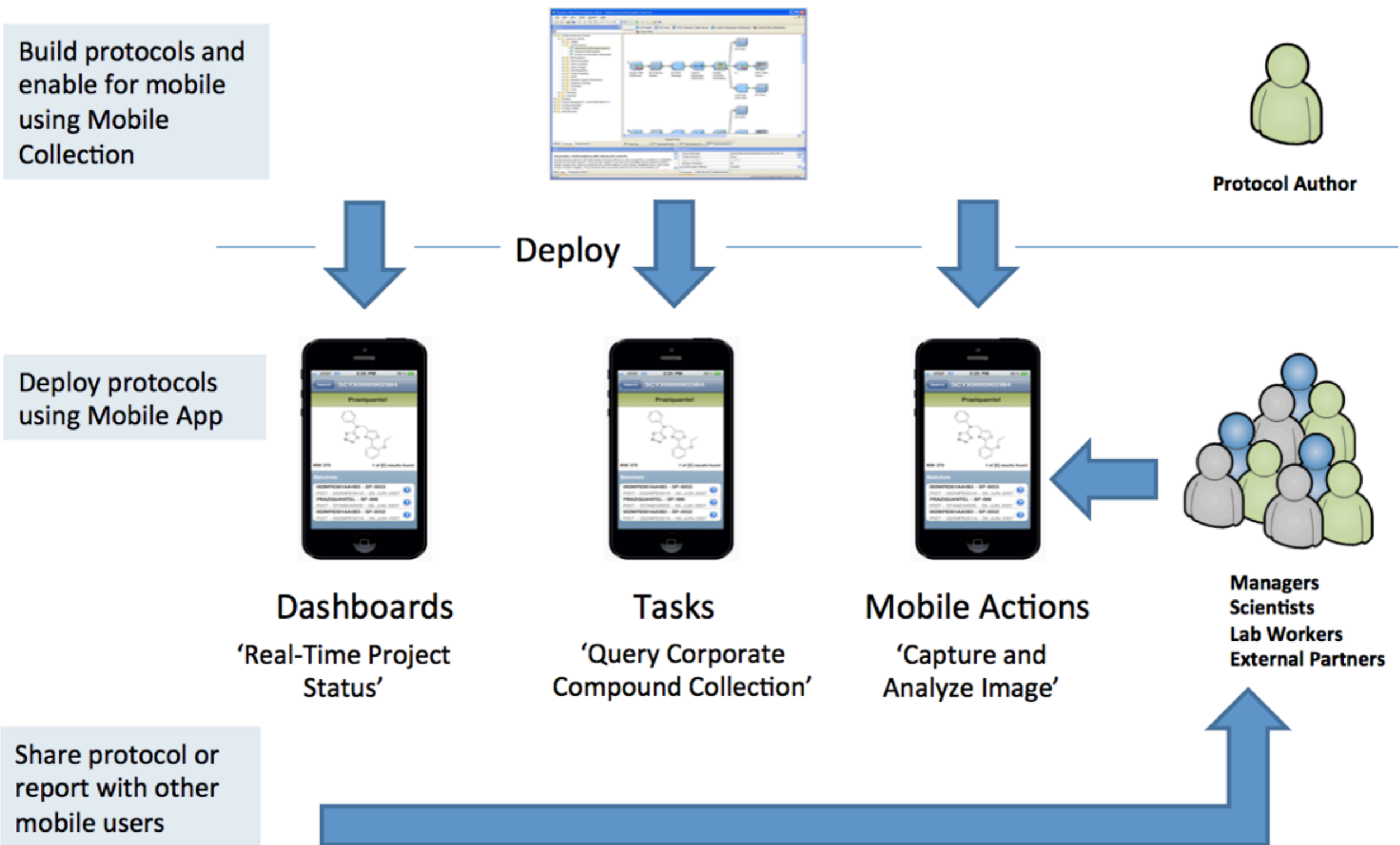
- Largely Vertical, Point Solutions
- Development Requires Sophisticated Knowledge of Mobile Computing Development Environments
- Development Often Requires Knowledge of Cloud Computing/LAMP environments
- Only Some Enable App Integration (e.g. client-side standard filetype sharing)

Things are about to change....

# Introducing PP Mobile / Accelrys Science-Cloud

- What is it?
  - ▶ An iOS application for iPhones and iPads (Android devices in the future)
  - ▶ 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
- Comments, Questions, and Requests to Participate in the testing program:
  - ▶ Ton van Daelen, Product Manager, Accelrys Science Cloud ([tvd@accelrys.com](mailto:tvd@accelrys.com))

# Deploying Protocols on Mobile Devices





# “Mobilize” Sophisticated Pipeline Pilot Protocols

The screenshot displays the Pipeline Pilot Professional Client interface for a 'Site Management Report'. The main workspace shows a complex data pipeline with the following components:

- 1. Set data source and time period** (A:=B)
- 2. JavaScript: For highlighti...**
- 3. Report Title** (Abc..)
- 4. Dates not OK?** (Abc..)
- 5. Previous Period Link** (Abc..) and **Next Period Link** (Abc..)
- 6. SD Reader**
- Is compound registered?**
- Sort Data**
- Pie Chart**
- Group Data by Tag**
- Statistics** (A:=B)
- Sort Data**
- Calculate Color** (A:=B)
- Bar Chart**
- Create Table**
- Tile Horizontal** (multiple instances)
- Tile Vertical**
- Page**
- HTML Report Viewer**

The pipeline flows from left to right, with data from the SD Reader and various processing steps being distributed into multiple tiles (horizontal and vertical) before reaching the final HTML Report Viewer.

**Jobs**

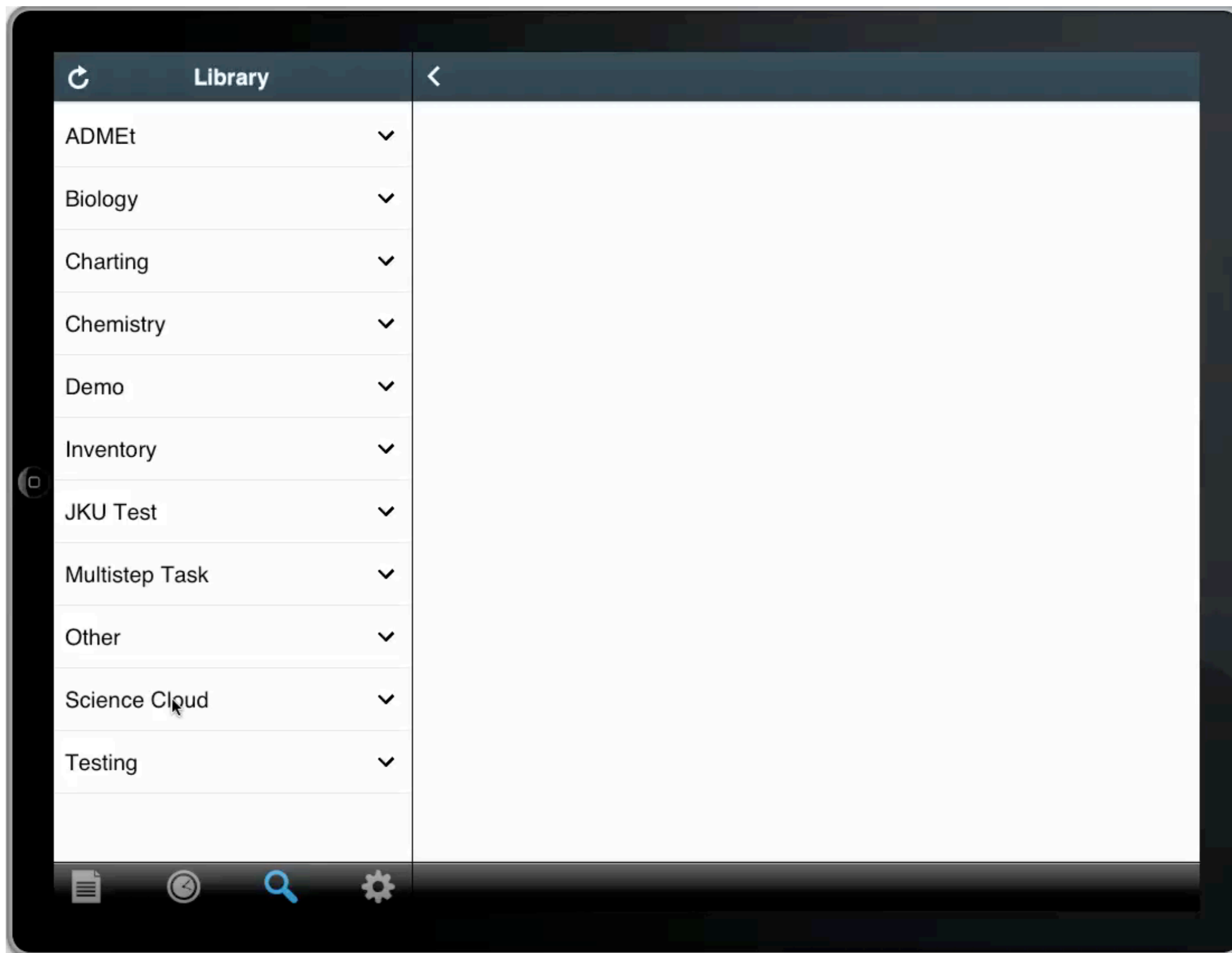
Protocol Name	Status	Start Date
Site Management Report	Not Started	
New ProtocolR	Finished	Tue Sep 03 10:...

**Parameters**

Year	2008
Period	January - June

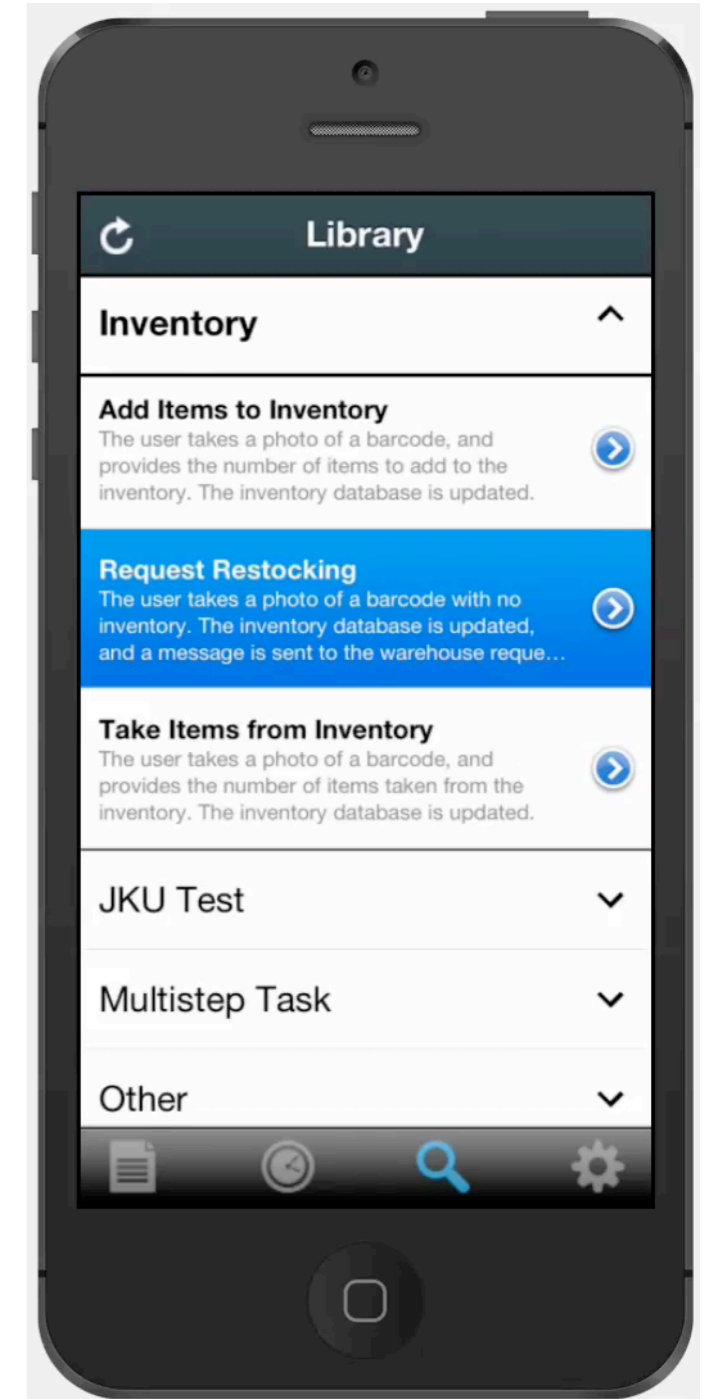
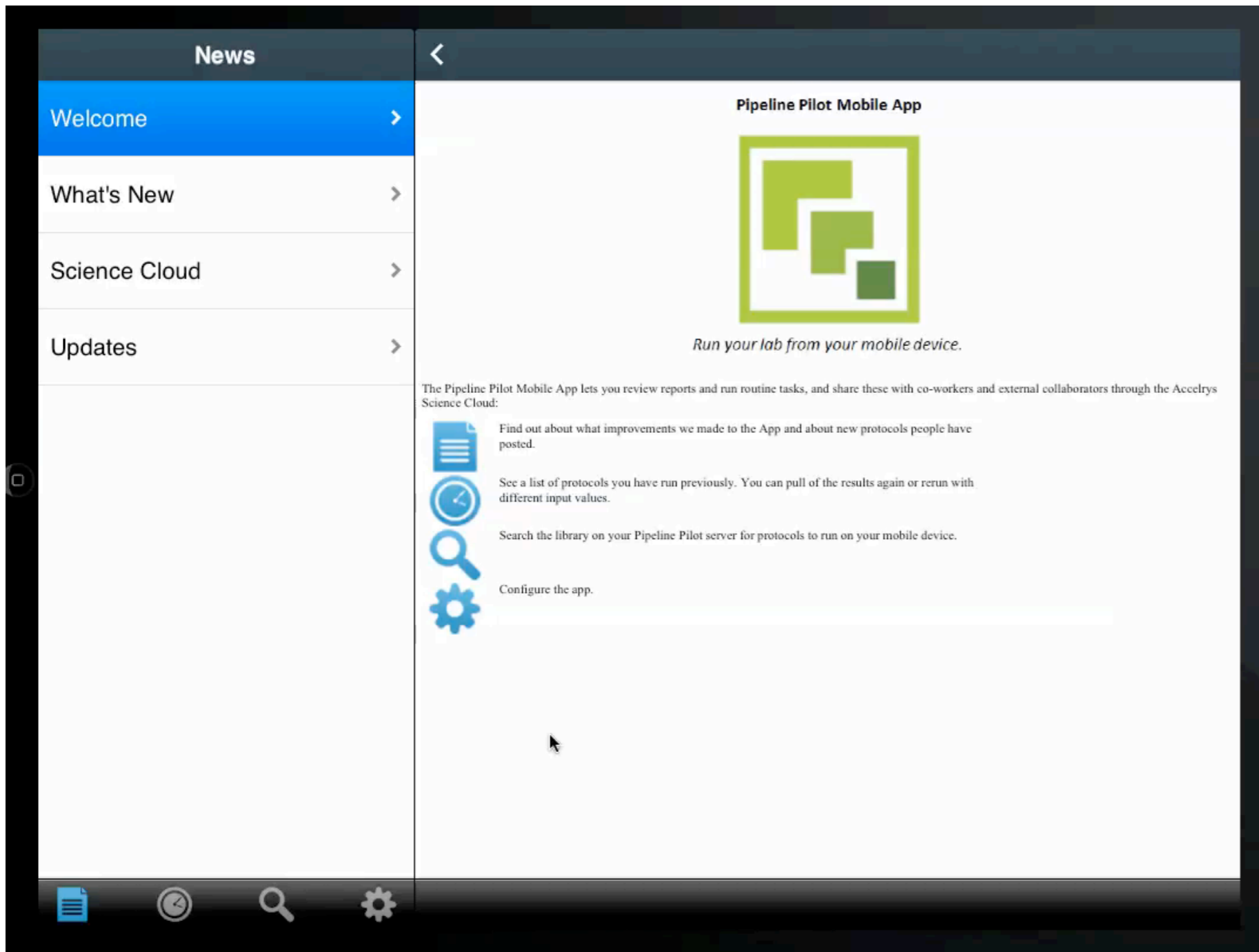
Additional interface elements include a menu bar (File, Edit, View, Tools, Window, Help), a toolbar with various icons, a search bar for the protocol database, and a left-hand navigation pane showing a tree view of protocols such as 'Accelrys Discovery Studio', 'Examples', 'Mobile Services', 'Science Cloud', and 'Web Services'.

# “Mobilize” Sophisticated Pipeline Pilot Protocols

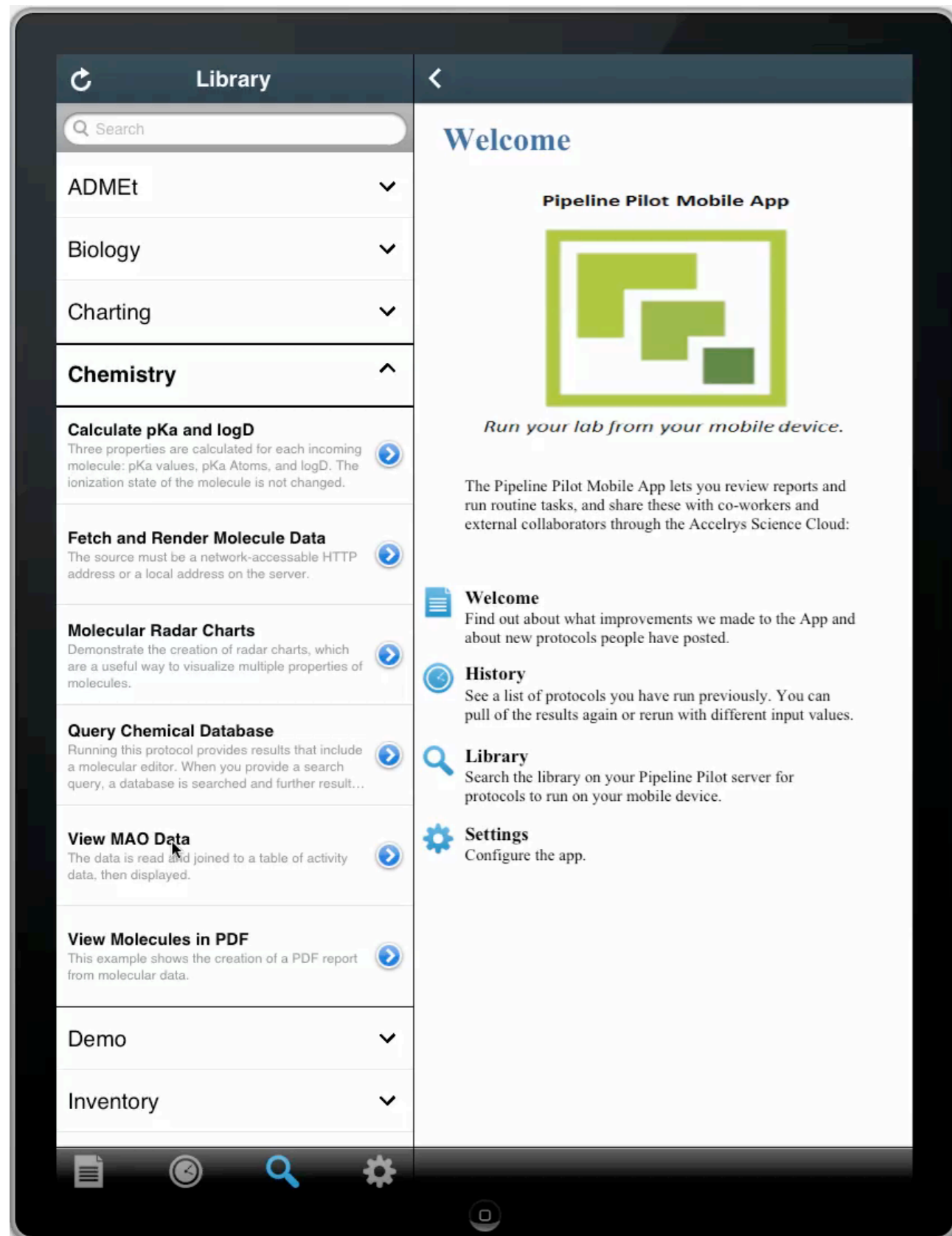


# Leverage Mobile Device Capabilities

- Camera, Audio, GPS, other Peripherals, etc.

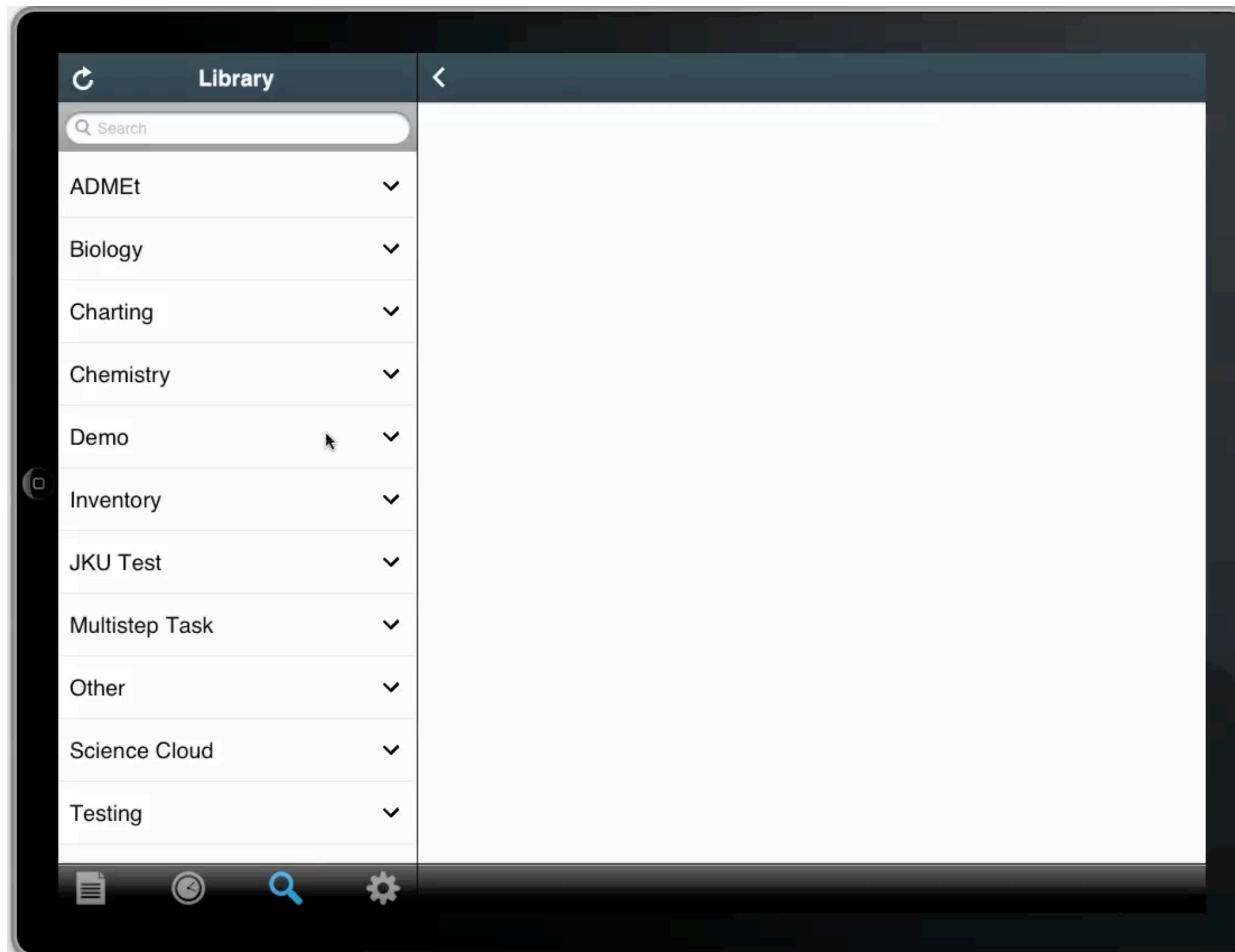


# Embed and Deploy

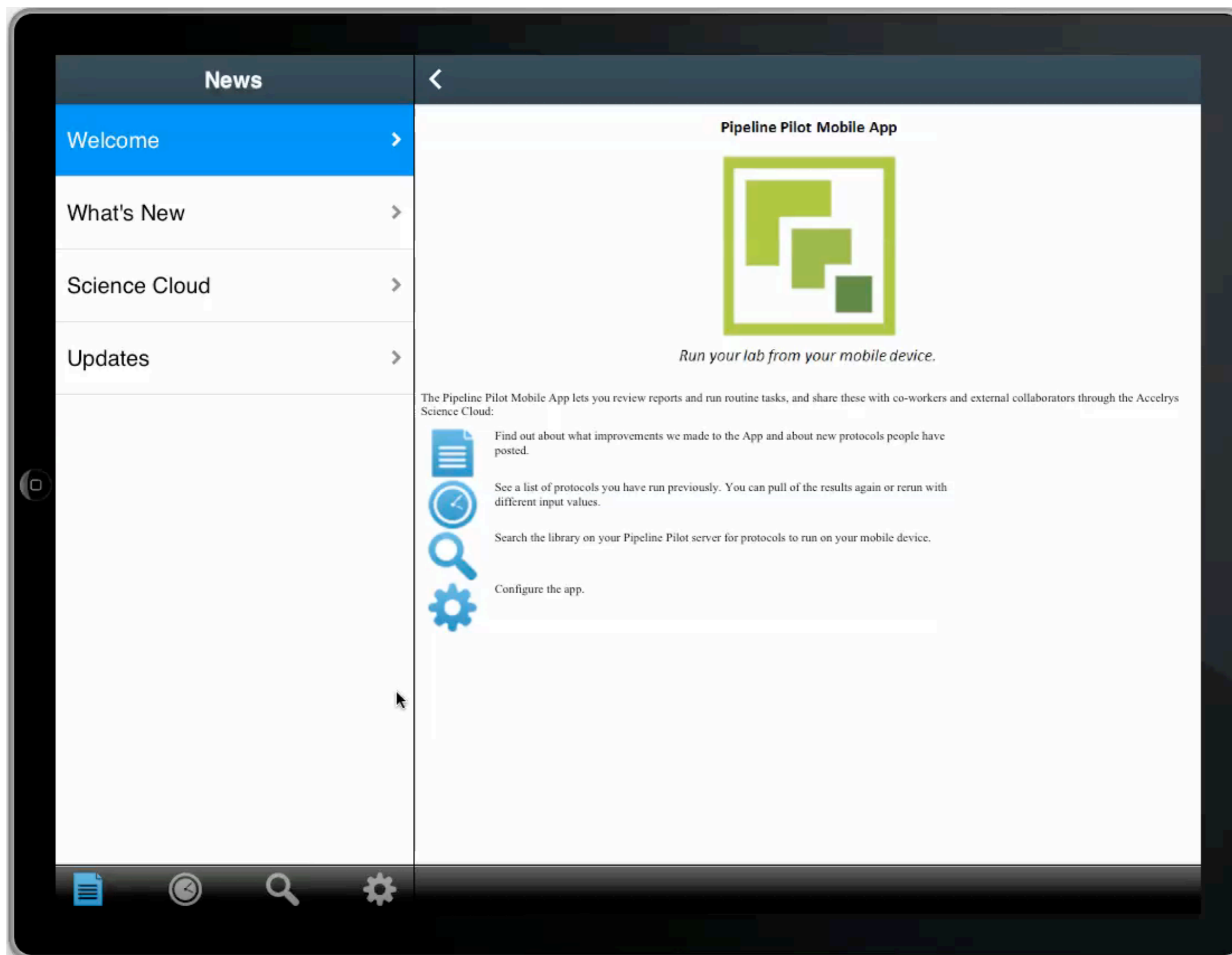


Embed powerful applications within Pipeline Pilot protocols and deploy to mobile users

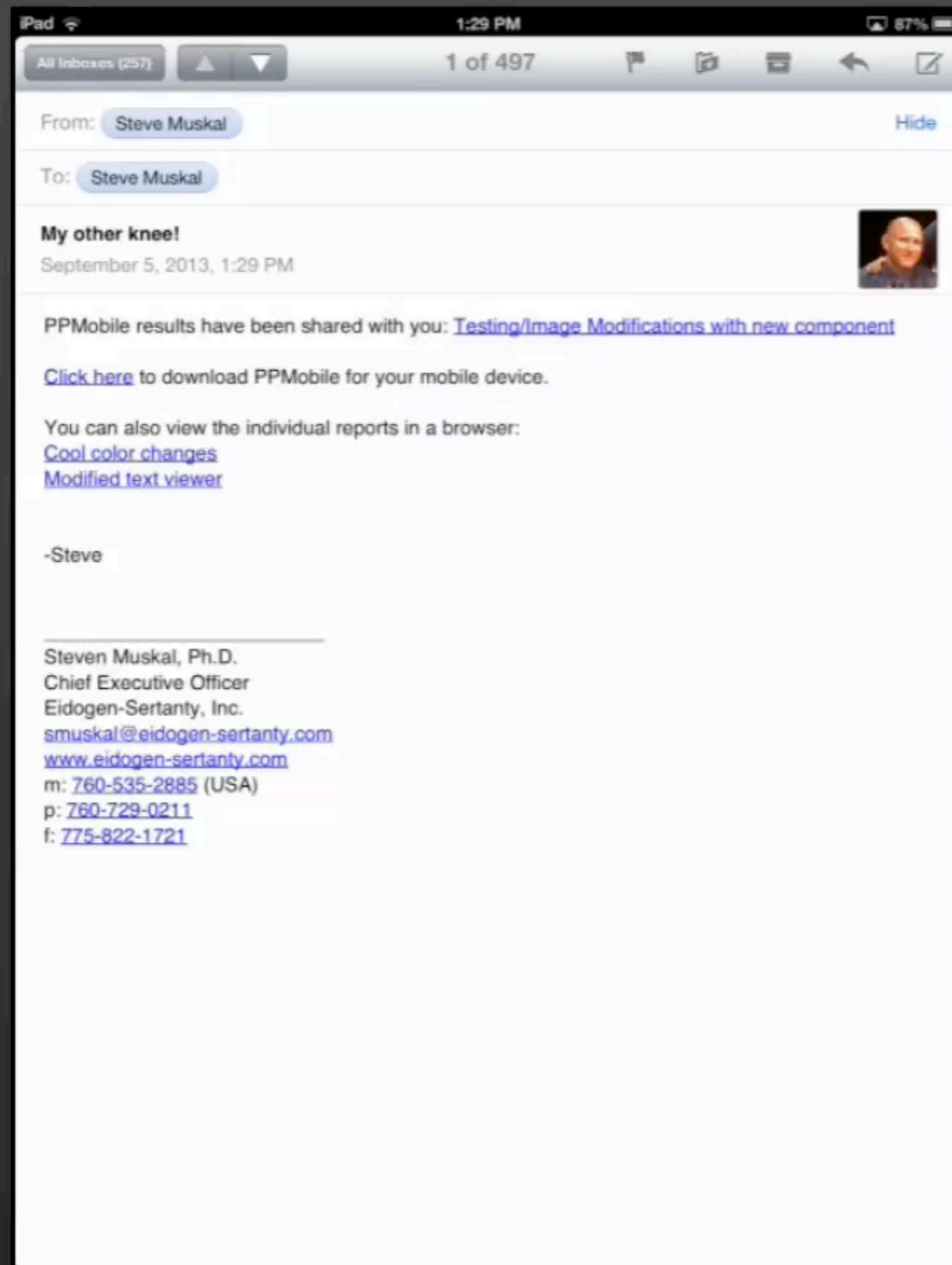
# Utilize Dynamic Graphs and Charts



# Submit Long-Running Protocols “On-the-Go”



# Share Protocol Reports



Results can be shared between mobile devices, from desktop to mobile, and from mobile to desktop

# Initiate Protocols from WebSite URLs



Embed links in websites which will launch and execute protocols through PP Mobile



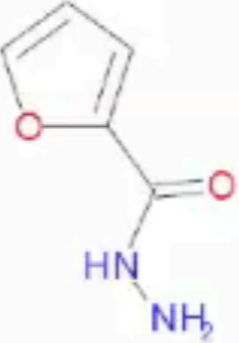
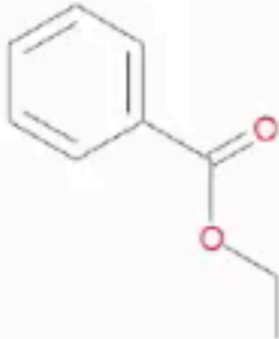
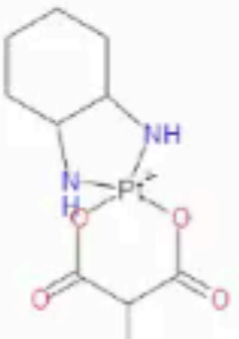
# Export and Share Data with Other Apps

share Cancel

Share molecule data

Results

Display records 1 to 25 of 50 Update <<First <Previous Next>>Last>>

Molecule	Name	cas_m	nci	Molecular_Weight	Molecular_Formula	LogP	activityclass
	Furoic acid, hydrazide	<a href="#">3326-71-4</a>	35574	126.116966434067	C5H6N2O2		
	Benzoic acid, ethyl ester (EC:RC)	93-89-0	6684	150.178967276216	C9H10O2	2.66	
		61914-17-8	266044	423.341993331909	C10H16N2O4P1		

Navigation icons: Home, Back, Search, Settings, Forward, App Drawer

# Engaging Mobile Users and Developers

The screenshot displays the Pipeline Pilot Professional Client interface. The main window shows a workflow diagram with three parallel paths. Each path starts with an 'SD Reader Aminoacids' component (labeled '1') that feeds into an 'Enumerate Ionization States' component. The first path has a value of '20' and connects to an 'HTML Molecular Grouped Viewer' showing '67' unique states. The second path also has a value of '20' and connects to another 'HTML Molecular Grouped Viewer' showing '70' unique states. The third path has a value of '20' and connects to a third 'HTML Molecular Grouped Viewer' showing '108' unique states. Three yellow callout boxes provide details for each path:

- Top Path:** Enumerate Ionization States. Minimum pH = 0, Maximum pH = 14, pH Tolerance = 0. 67 unique states. All pKa sites are treated independently.
- Middle Path:** Enumerate Ionization States. Minimum pH = 0, Maximum pH = 14, pH Tolerance = 2. 70 unique states. pKa sites within 2 pH units of each other are treated as a group for which all charge combinations are enumerated.
- Bottom Path:** Enumerate Ionization States. Minimum pH = 0, Maximum pH = 14, pH Tolerance = 14. 108 unique states. All pKa sites in the 0-14 range are grouped together. All possible charge combinations are enumerated.

The interface includes a 'Protocols' tree on the left, a 'Jobs' table at the bottom, and a 'Parameters' pane on the right. The 'Jobs' table shows the current job as 'Enumerate all Ionization States' with a status of 'Finished' and a start date of 'Thu Sep 05 10:...'.

Protocol Name	Status	Start Date
Enumerate all Ionization States	Finished	Thu Sep 05 10:...
InspectProtocol	Finished	Tue Sep 03 10:...

Parameters: There are no parameters defined. To create parameters, right-click in this pane and select "Edit...".

Ready | smuskal | 75.124.74.42 | 9.0.2

# Summary

- Many Mobile Opportunities Exist in our “Space”
- Until Now, Science Apps Have Been Largely Vertical, Point Solutions
- A New “Game Changing” Mobile Collection / Mobile App Will Greatly Broaden the Scope of Apps in our Space
- Comments, Questions, and Requests to Participate in the Testing Program:
  - ▶ Contact Ton van Daelen, Product Manager, Accelrys Science Cloud (tvd@accelrys.com)

# Acknowledgements

- Accelrys



- ▶ Matt Hahn
- ▶ Dave Rogers
- ▶ Jung Ku
- ▶ Ton van Daelen

- Maurizio Bronzetti
- Alex Clark

- InfoChem



- ▶ Peter Löw
- ▶ Josef Eiblmaier
- ▶ Valentina Eigner-Pito



# SPRESImobile - Update: Reaction Name Searching



## SPRESImobile: 410,000 Chemical Reactions Freely Available

15 of 100

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

**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

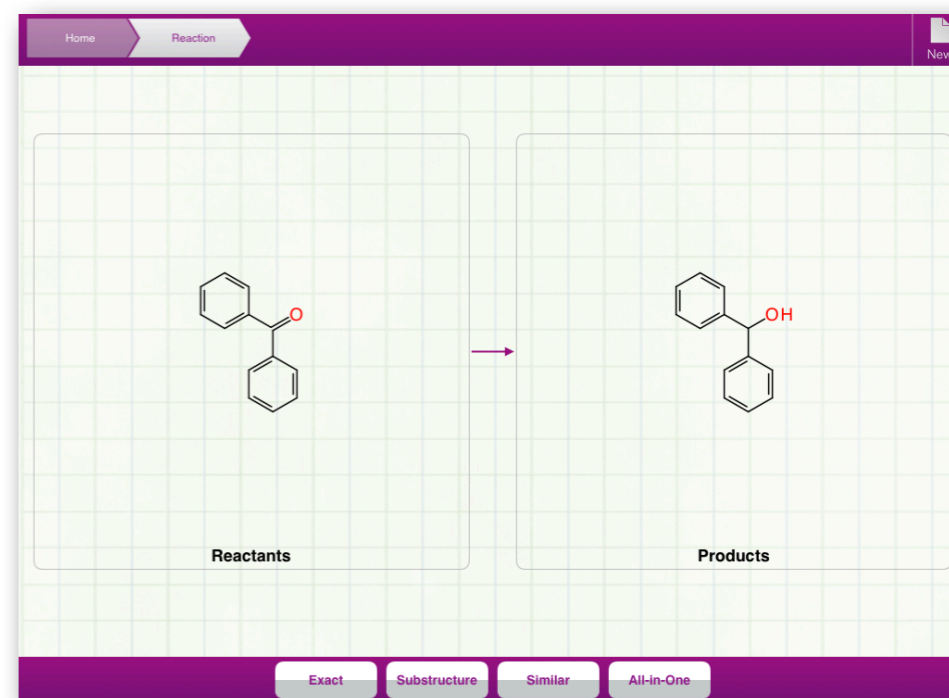
**Commercial Availability (6)**  
Apollo Scientific <http://www.apolloscientific.com>  
Sigma-Aldrich <http://www.sigmaaldrich.com>  
VWR <https://www.vwrsp.com>

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>2</sub> H <sub>7</sub> N	 MW: 230.306 MF: C <sub>13</sub> H <sub>19</sub> N <sub>2</sub> O



Home Reaction Reactions

2 of 100

Reactant 1

Product 1

**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>

