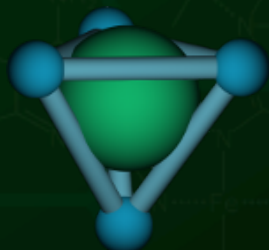


# Building a mobile app ecosystem for chemistry collaboration

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March 2012



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<http://molmatinf.com>

# Mobile apps

- Most action is for iOS
- Chemistry feature set is becoming very powerful: content **consumption** and **creation**
- **Structure** drawing, **reactions**, **datasheets**
- Access to webservices, calculations, graphics, RPC, social networking, cloud storage



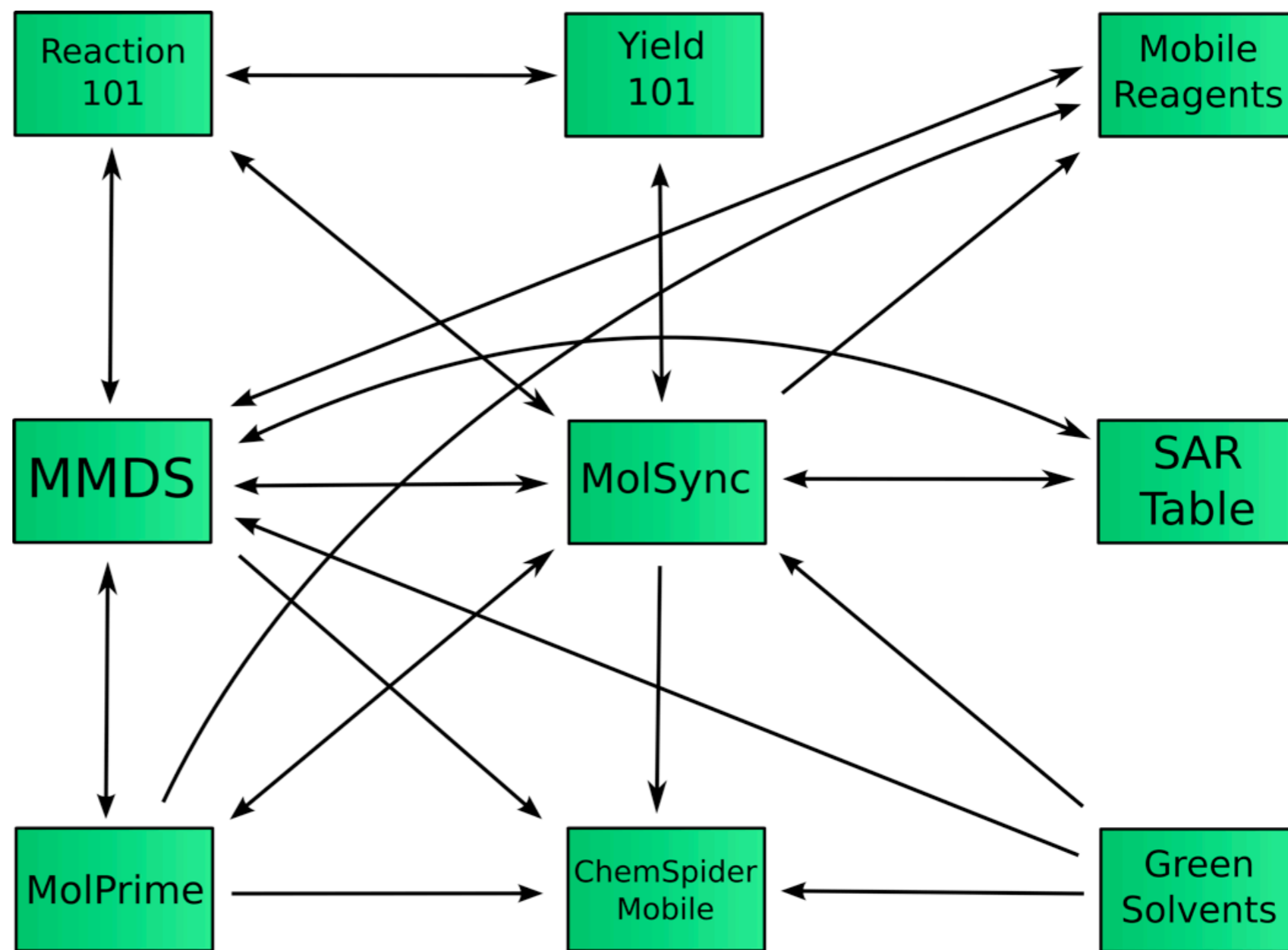
# So many apps



- Should be limited in scope, narrow focus...
- ... combine them and they become a toolchest
- Apps can be a major part of a workflow

# Interprocess comms

- Apps on same device
- Share data:
  - guided
  - unguided
  - clipboard

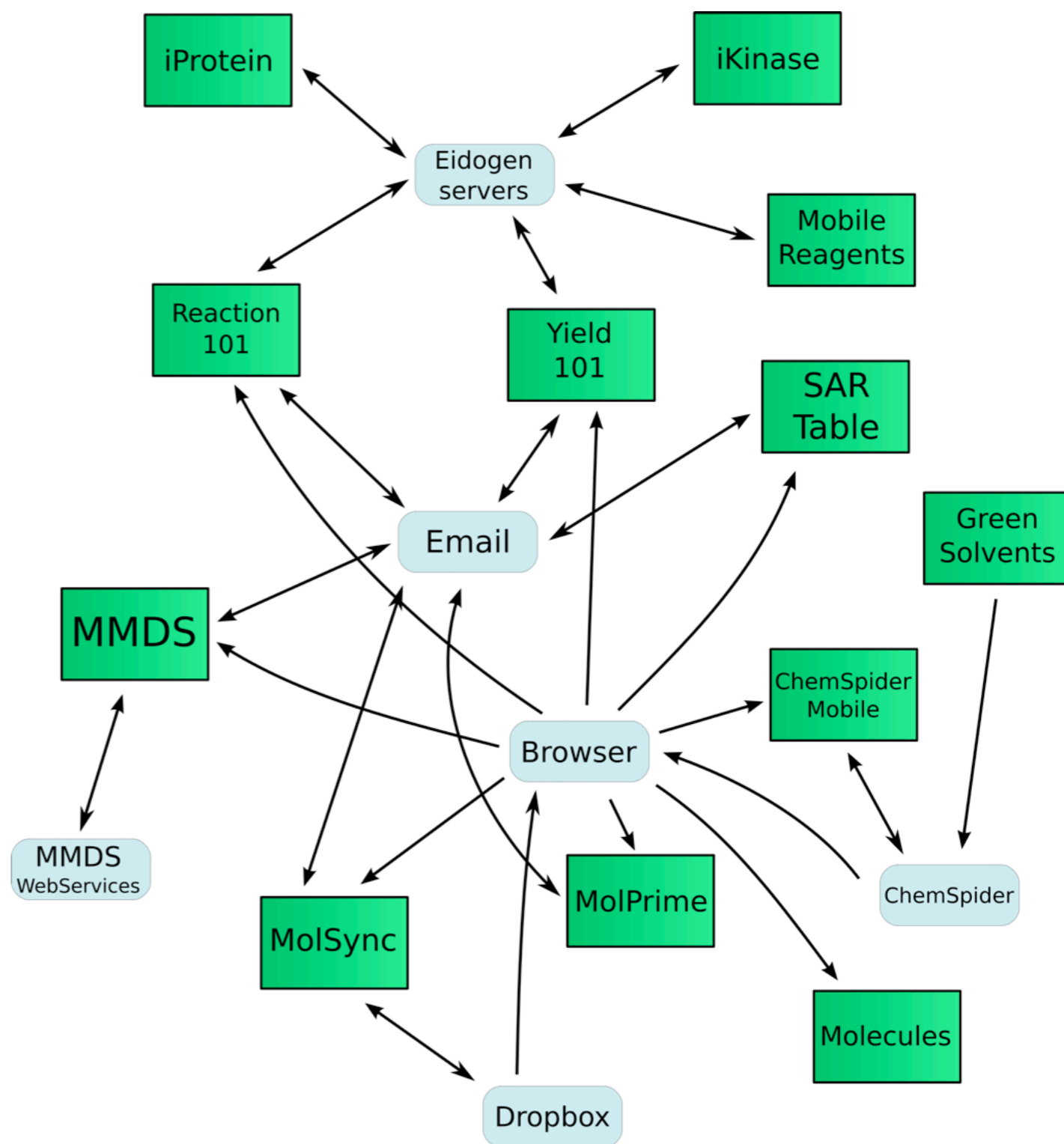


# Network comms

- Many different transport mechanisms

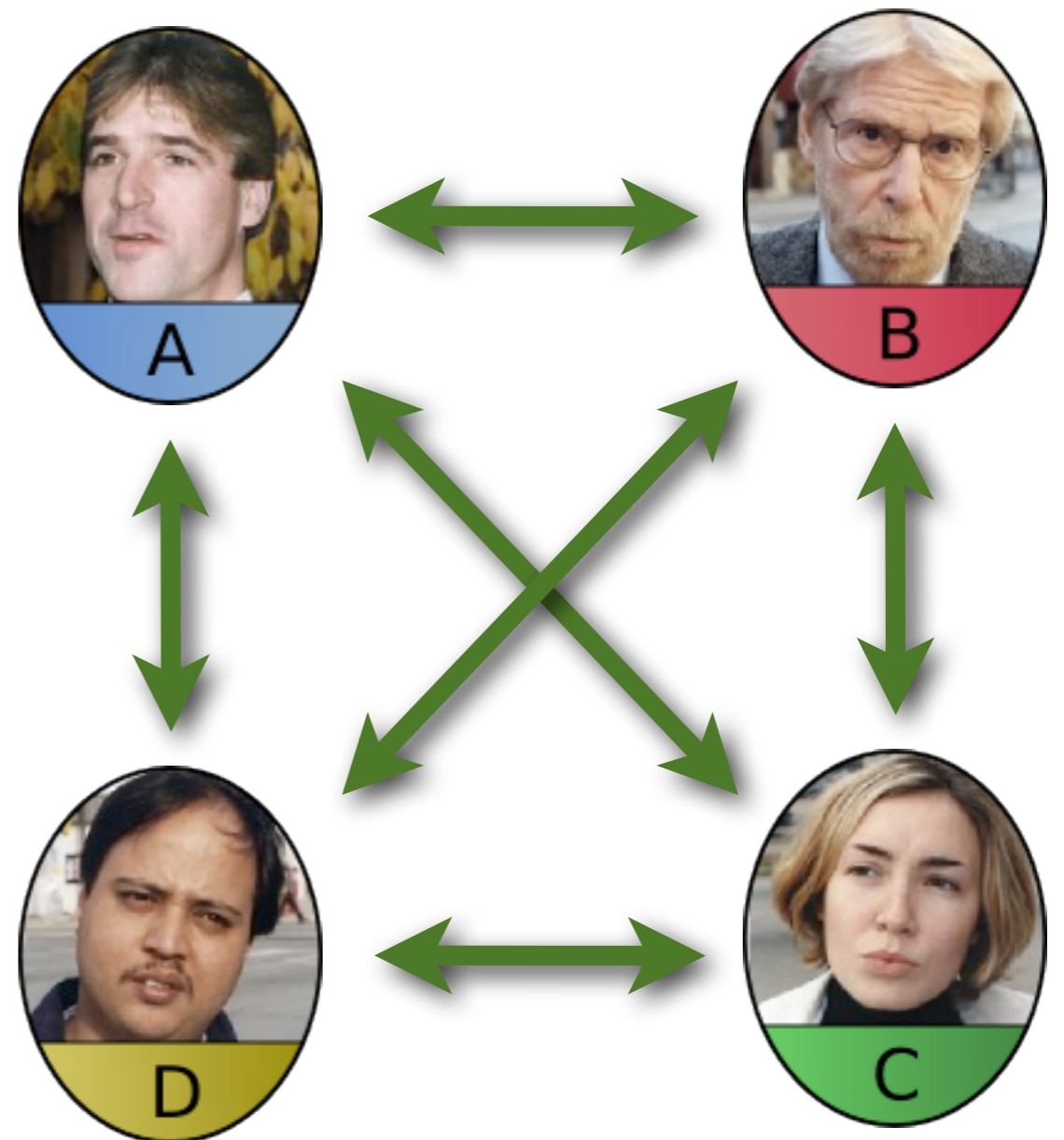
- email
- file export
- web access
- cloud storage
- client-server RPC

- Heterogeneous platforms



# Story

- Illustrating a chemical workflow, involving collaboration between:
  - ▶ 4 chemists...
  - ▶ ... several devices...
  - ▶ ... and lots of apps.





# MolPrime+



Draw publication-quality structure from scratch, using gestures and templates



[bit.ly/GEGonX](http://bit.ly/GEGonX)

Added to molecule collection

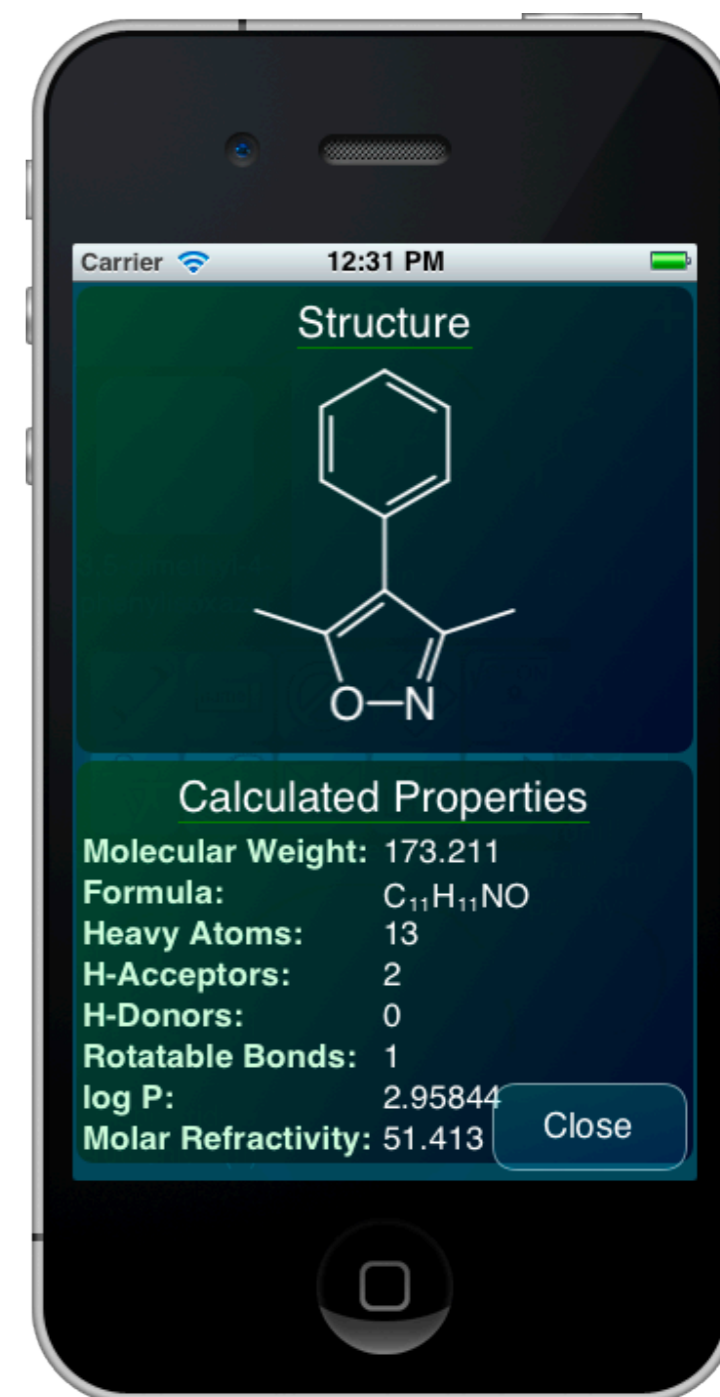




# Calculated Properties



- Access calculated properties
- Simple properties calculated within the app
- Complex properties use **RPC** call to web service (log P, MR)



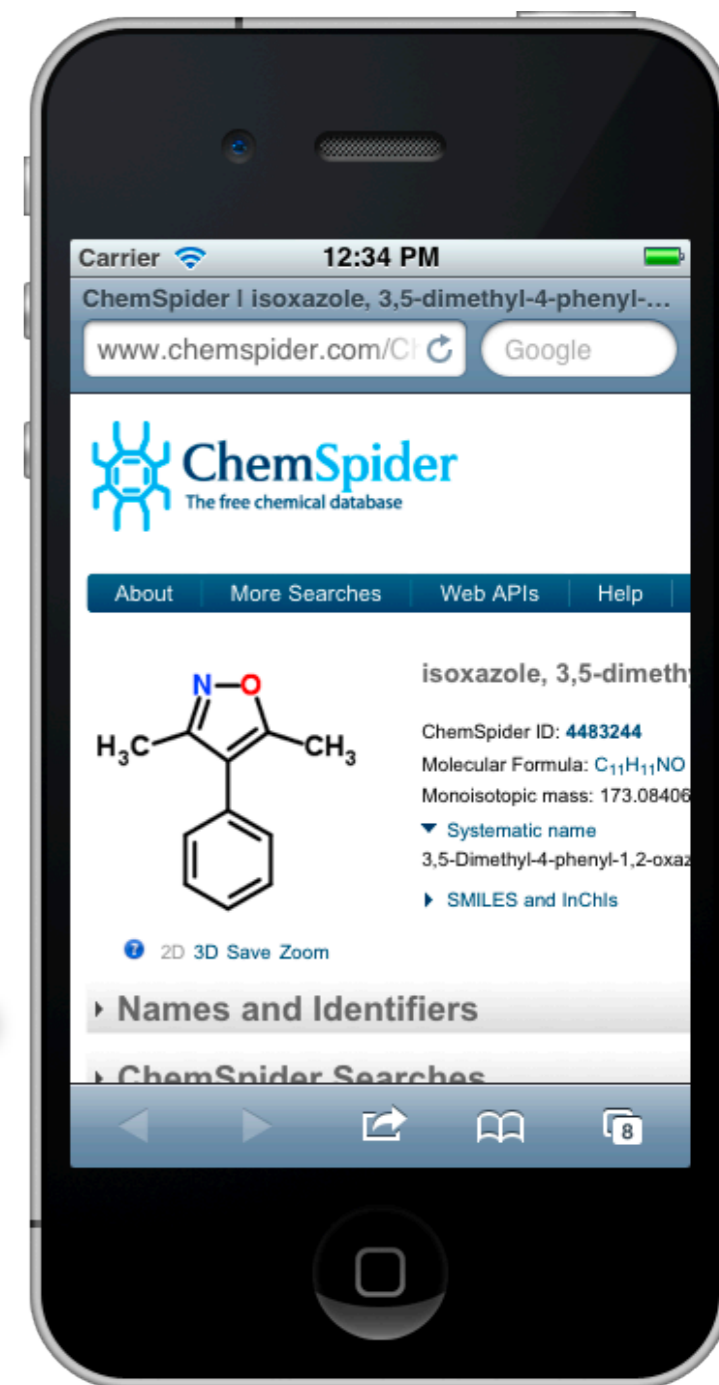


# ChemSpider Mobile



Use **Open With** to  
send the structure  
to the *ChemSpider  
Mobile* app

Search and open  
the web page





# Email



- Prepare an outgoing email
- Includes structure data, and prepared image
- Send to **Person B**

Cancel Molecule: 3,5-dimethyl-4-phenylisoxazol Send

To: person\_B

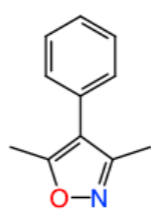
Cc/Bcc:

Subject: Molecule: 3,5-dimethyl-4-phenylisoxazol

Molecule from MolPrime+ for iPhone/iPod/iPad.  
<http://molmatinf.com>  
Molecular Formula: C<sub>11</sub>H<sub>11</sub>NO  
Molecular Weight: 173.2111

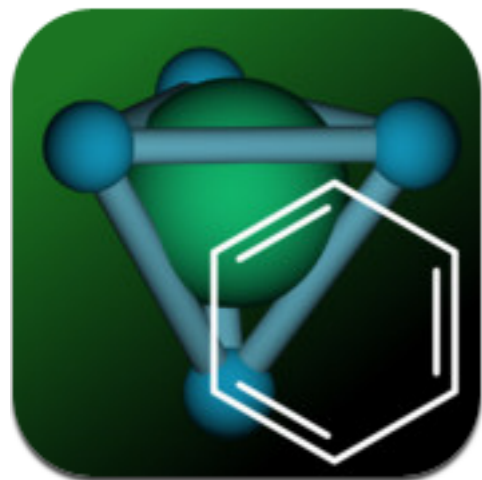
structure.el

structure.mol



Sent from my iPhone

Q W E R T Y U I O P  
A S D F G H J K L return  
Z X C V B N M @ .  
. ? 123 - =



# MMDS



- Email offers a list of apps that can handle each attachment
- Person B is a power user...
- ... opens the structure file with the *Mobile Molecular DataSheet*

From: **Person A**


To: **Person B**


**Molecule: 3,5-dimethyl-4-phenylisoxazole**  
26 February, 2012 1:15 PM

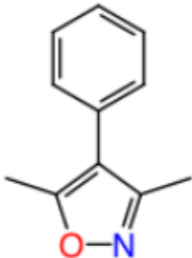
Molecule from MolPrime+ for iPhone/iPod/iPad.  
<http://molmatinf.com>  
Molecular Formula: C<sub>11</sub>H<sub>11</sub>NO  
Molecular Weight: 177.20

**Open In...**

- MMDS
- MolPrime+
- MolPrime
- SPRESI

 **structure.el**  
0.5 KB

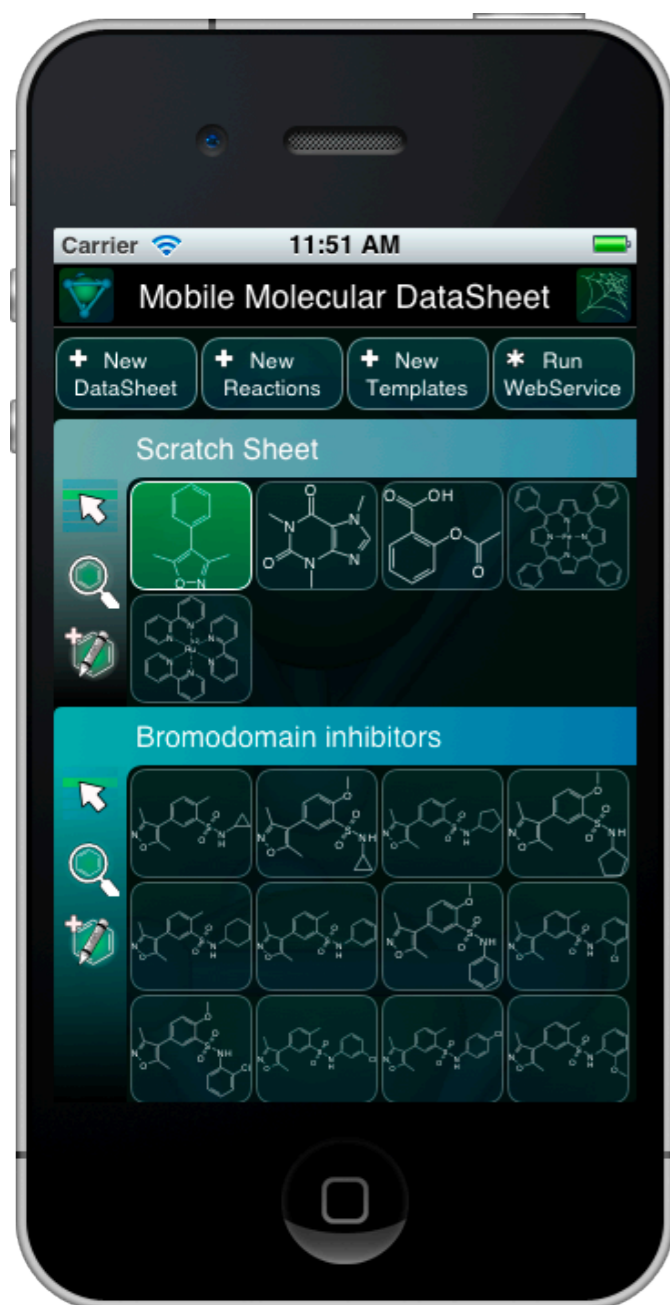
 **structure.mol**  
1.3 KB





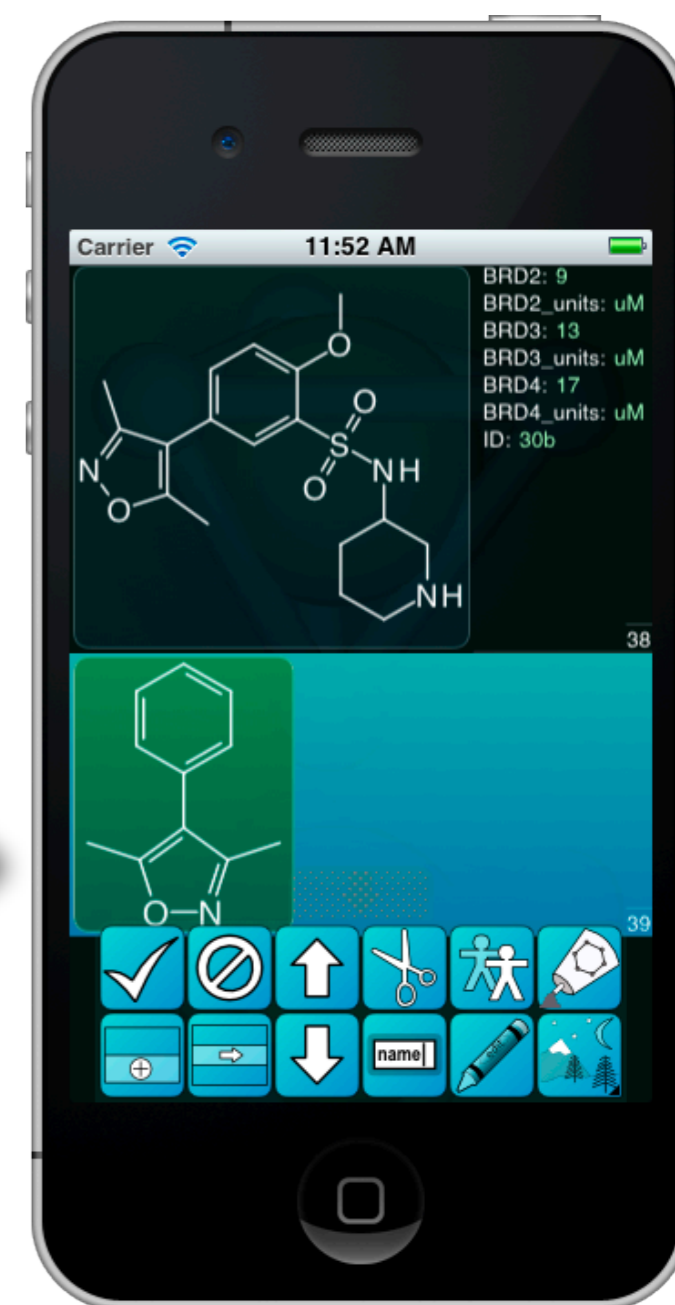
# MMDS

*Mobile Molecular DataSheet*



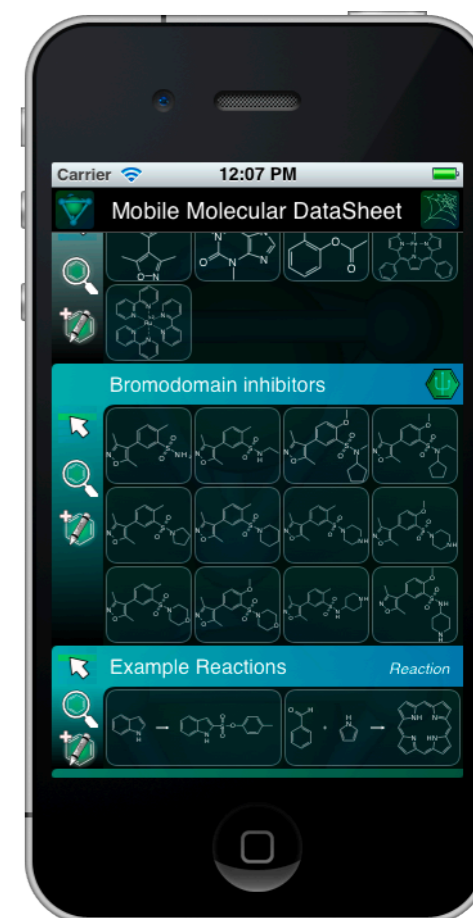
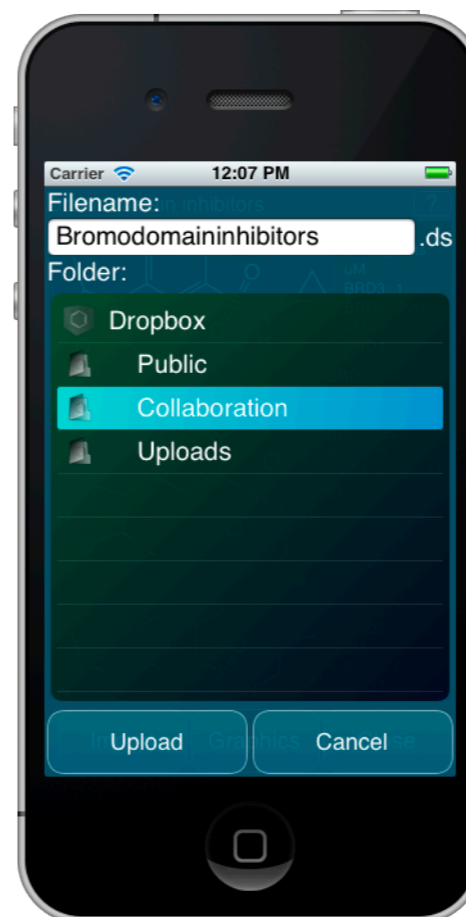
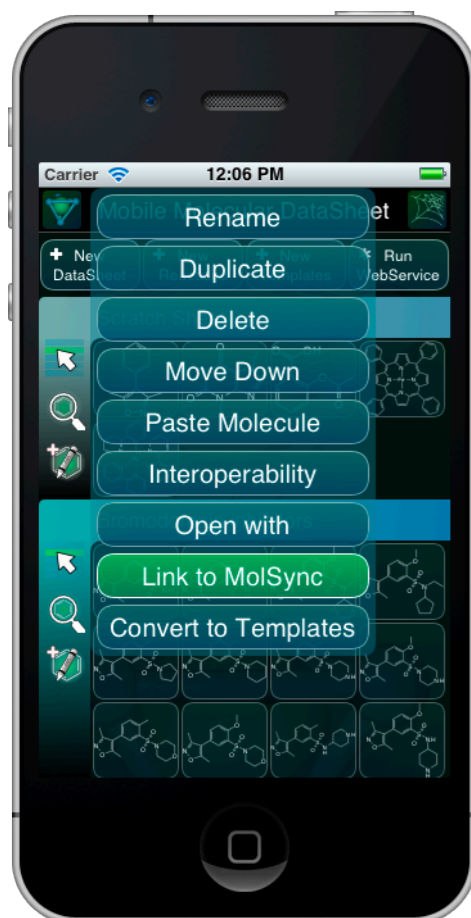
Structure is  
prepended to  
*scratch sheet*

Can copy/paste into  
a datasheet of  
*bromodomain  
inhibitors*





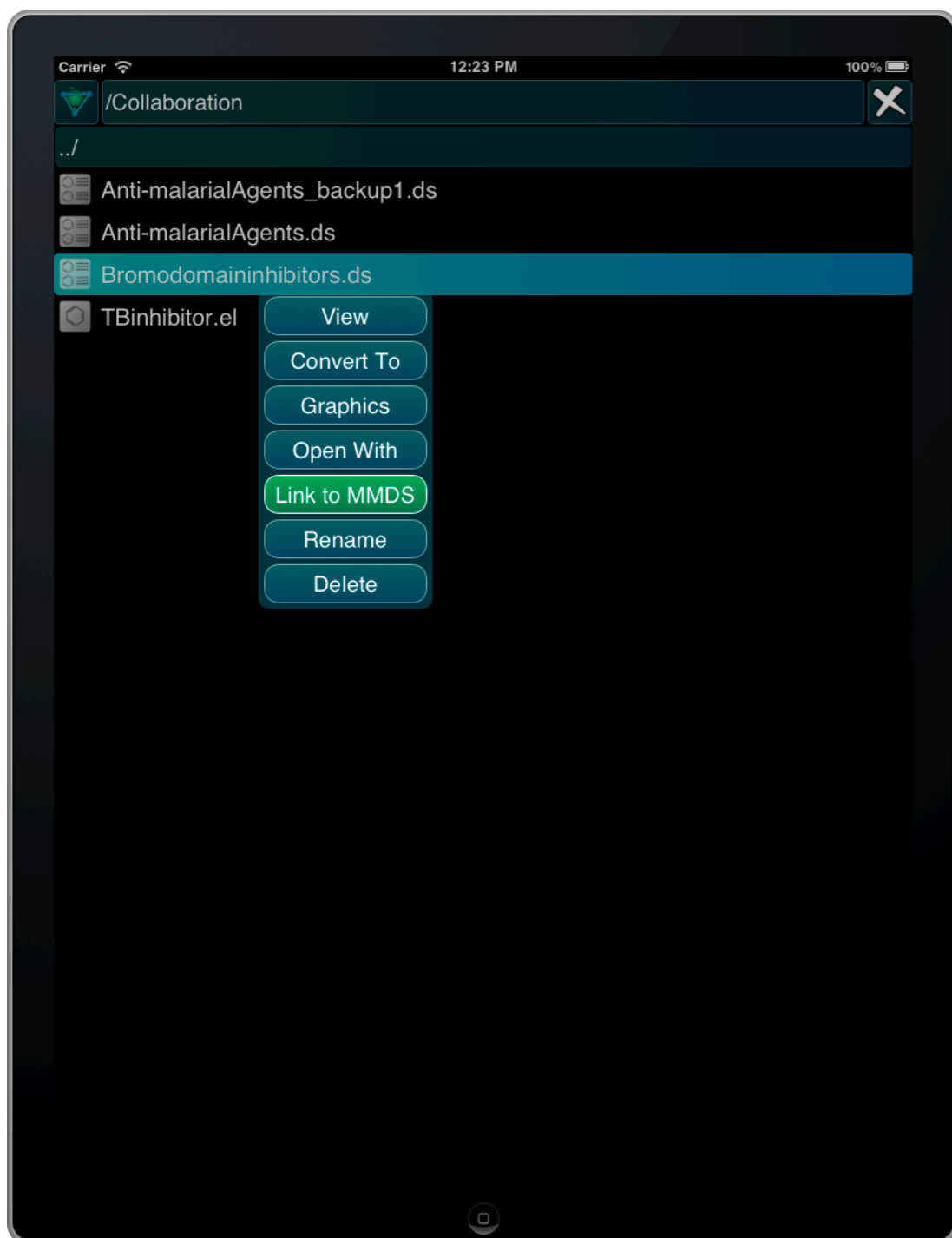
# MolSync



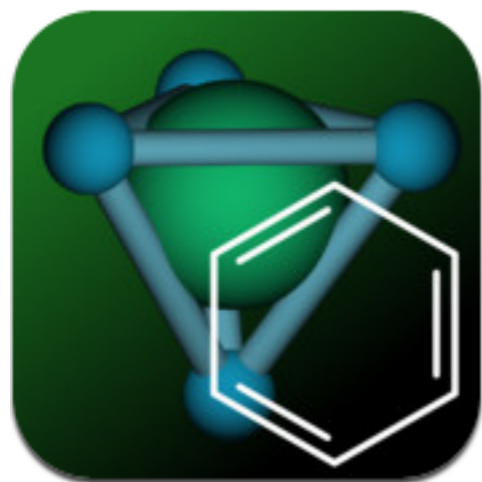
- Communicate with *MolSync*
- *Upload to Dropbox*
- *Create association*



# MolSync



- **Person C**, an experimentalist, accesses shared folder from an iPad
- Opens datasheet with *MMDS*
- Creates shared association



# MMDS



- Runs the experiment, measures the activity values
- Enters the data fields using *MMDS*
- Resyncs the file via *MolSync*...
- ... uploads modified version to *Dropbox* folder

Chemical structure interface showing three molecules and their associated data fields.

**Molecule 1 (Top):** Cc1cc(C2=CC(=O)N2)ccc(S(=O)(=O)N3CCCCC3)c1  
BRD2: 11  
BRD2\_units: uM  
BRD3: 8.4  
BRD3\_units: uM  
BRD4: 10  
BRD4\_units: uM  
ID: 30a

**Molecule 2 (Middle):** COc1cc(C2=CC(=O)N2)ccc(S(=O)(=O)N3CCCCC3)c1  
BRD2: 9  
BRD2\_units: uM  
BRD3: 13  
BRD3\_units: uM  
BRD4: 17  
BRD4\_units: uM  
ID: 30b

**Molecule 3 (Bottom):** Cc1cc(C2=CC(=O)N2)ccc1  
BRD3: 32  
BRD3\_units: %  
BRD4: 32  
BRD4\_units: %  
ID: 3

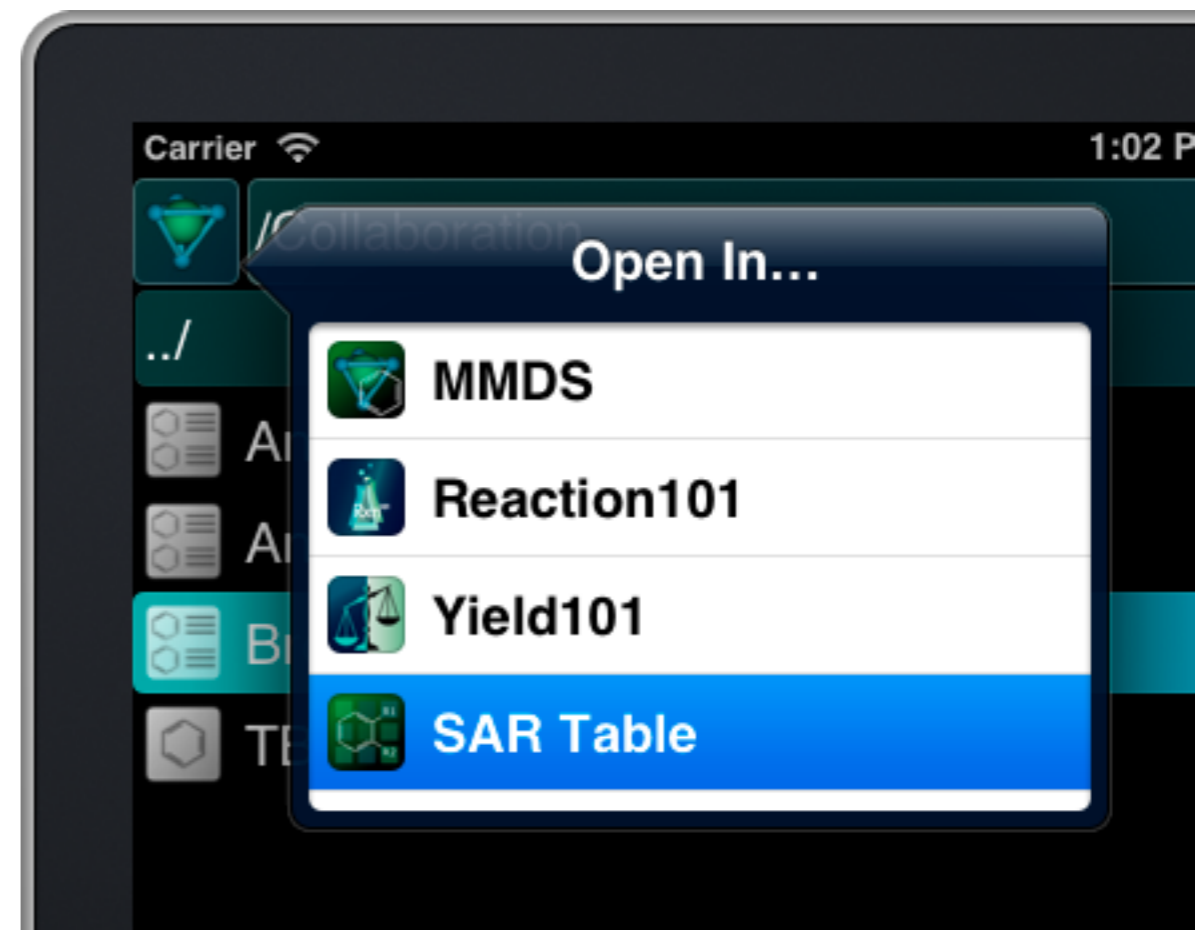
Bottom navigation bar with icons: checkmark, prohibition, up arrow, scissors, plus, right arrow, down arrow, and a text input field labeled "name".



# MolSync



- **Person B** uses *MolSync* to view the datasheet in the shared folder
- Series is complete: open the datasheet with the *SAR Table* app...





# SAR Table



- Imported content has *construct* molecules
- Copy first molecule into *Scaffold* field
- Trim off substituents
- Use the **Match** feature...



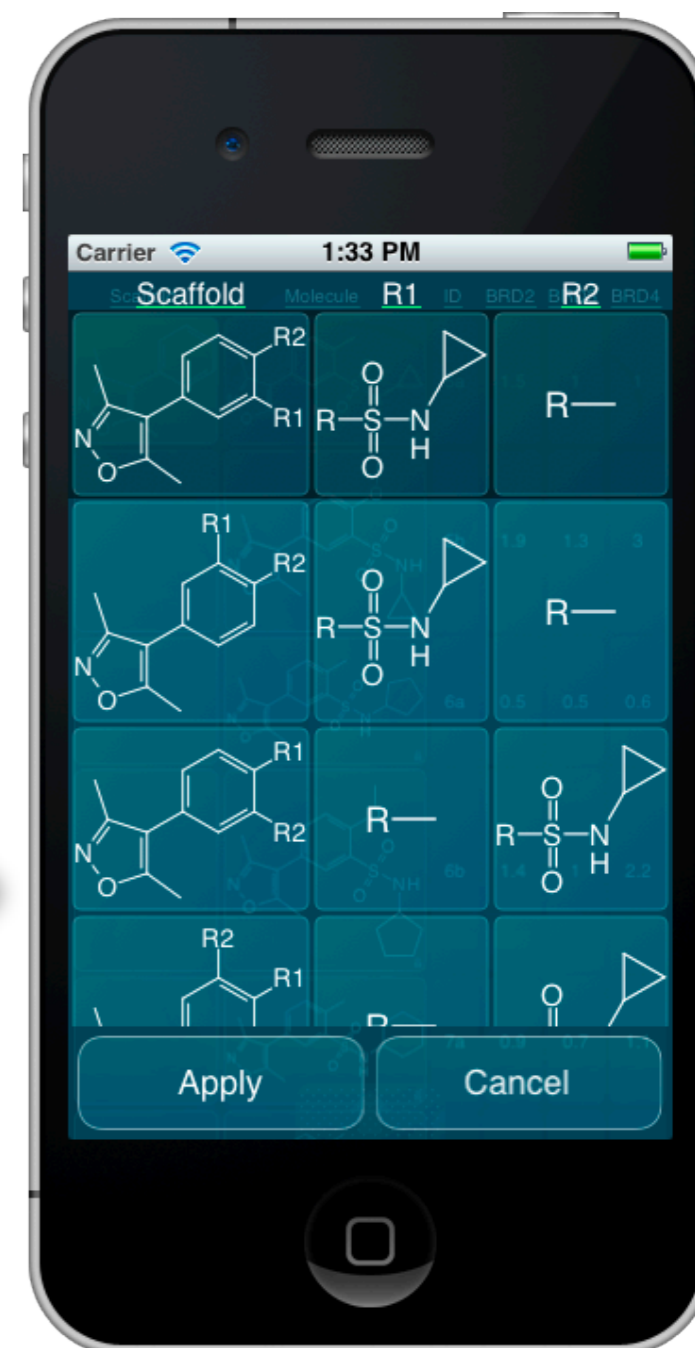
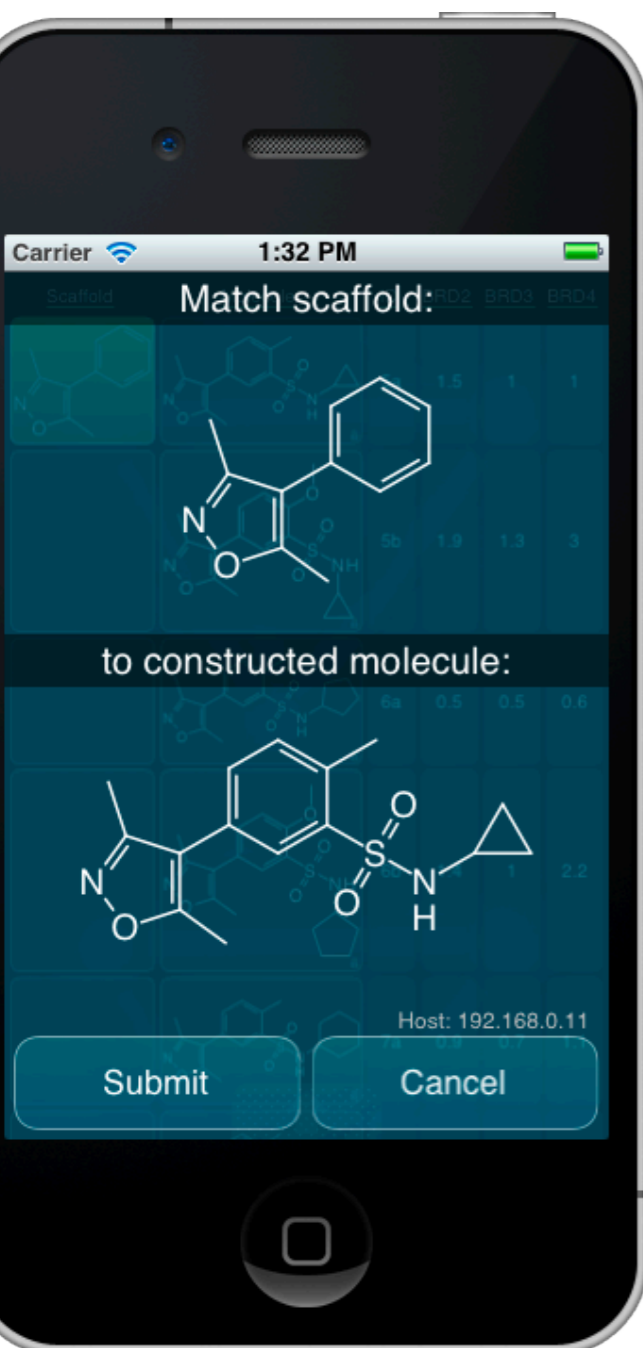


# SAR Table



Initiate the match:  
calculation is done by  
*remote procedure call*

A variety of  
possibilities: select  
the preferred one





# SAR Table



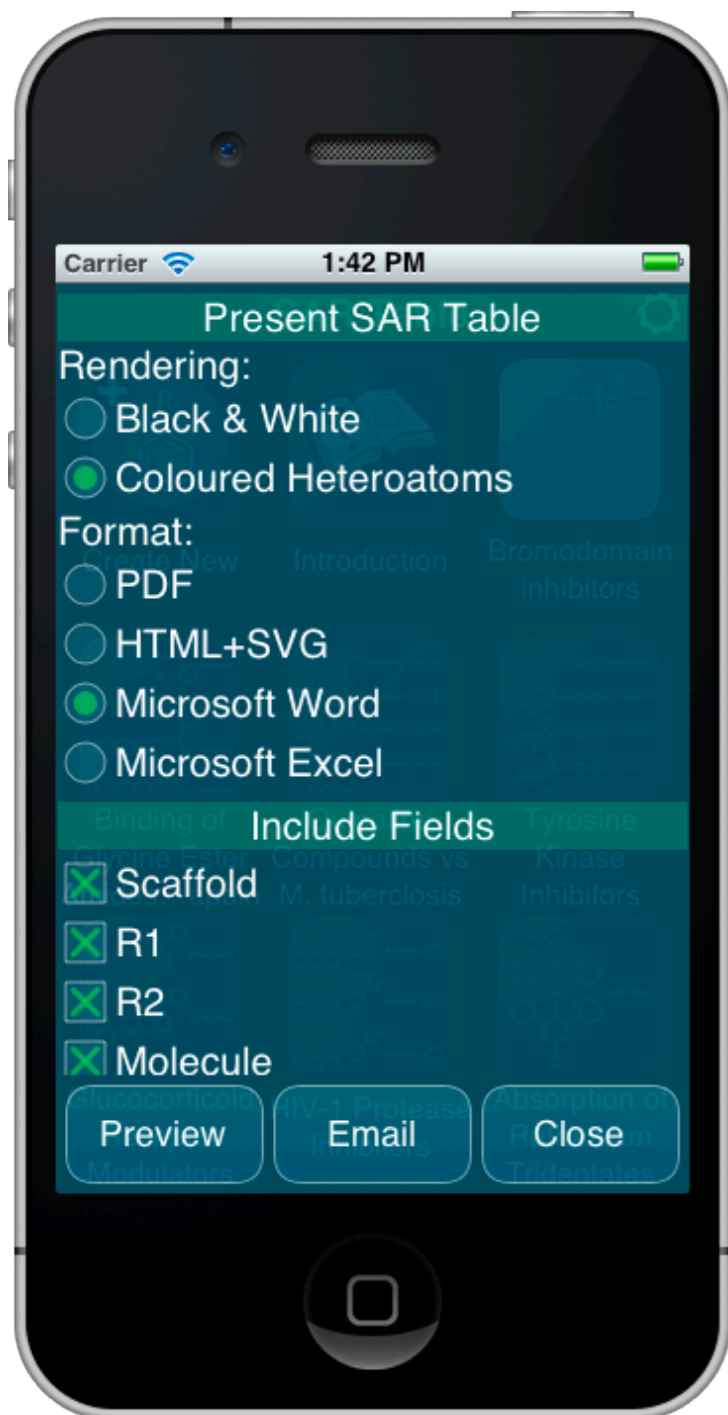
Scaffold	R1	R2	Molecule	ID
				5a
	n/a	n/a		5b
	n/a	n/a		6a
	n/a	n/a		6b
	n/a	n/a		7a

- Scaffold has been decorated
- **R1** and **R2** columns defined
- Rinse and repeat
- Scaffold matching uses previous assignments to influence suggestions



# SAR Table

- Can export the table via email as MS Office documents (.docx, .xlsx)
- Structures use **vector graphics**



Bromodomain inhibitors

*J. Med. Chem.* 55, 587-596 (2012)

Scaffold	R1	R2	Molecule	BRD2	BRD3	BRD4	ID
		R—		1.5	1	1	5a
		R—O—					
		R—		0.5	0.5	0.6	6a
		R—O—					

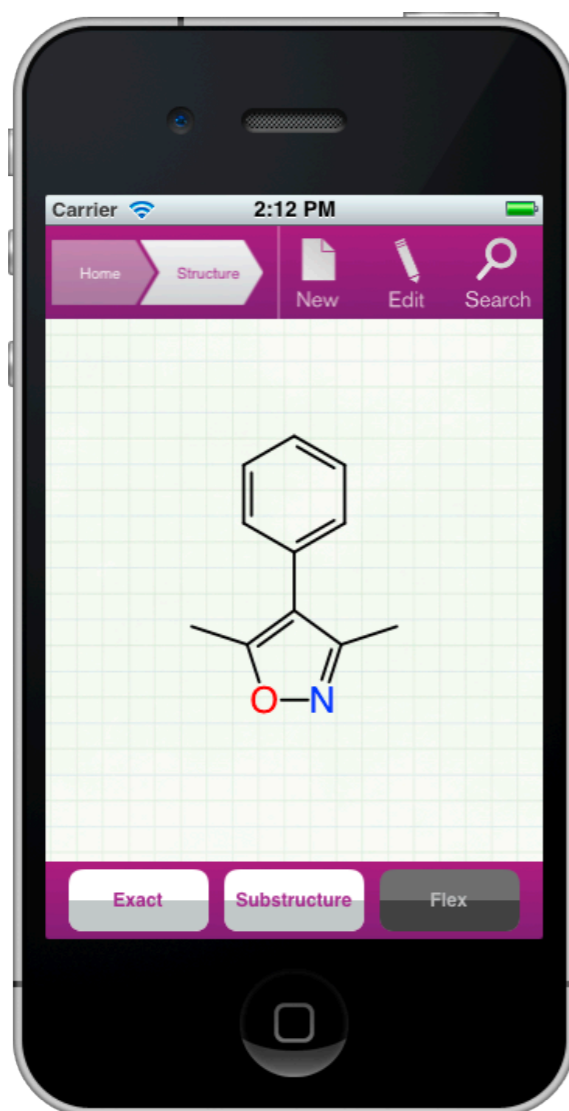


# SPRESImobile

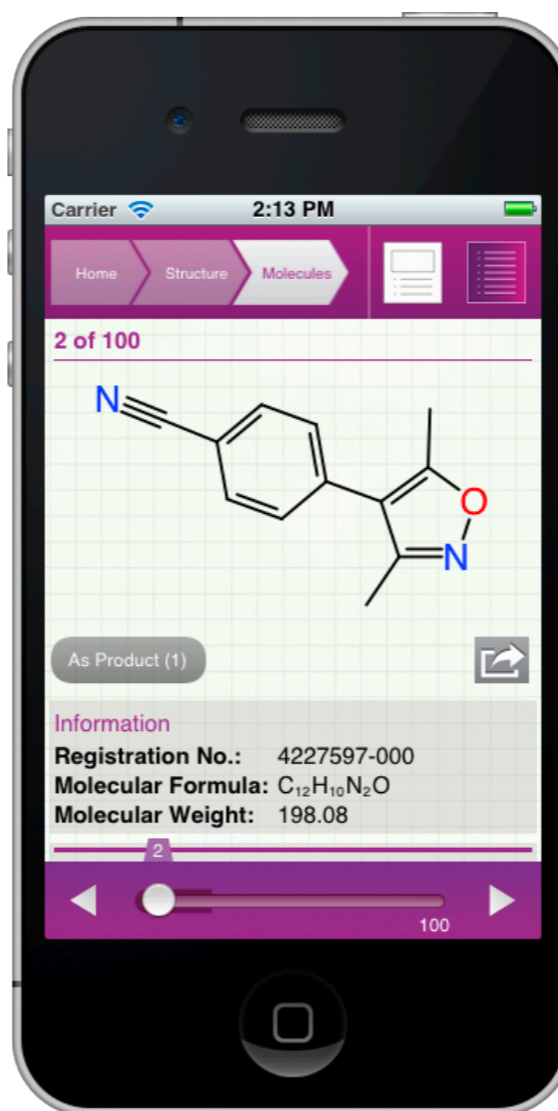


Want to illustrate a representative synthesis: search for the common fragment using SPRESI

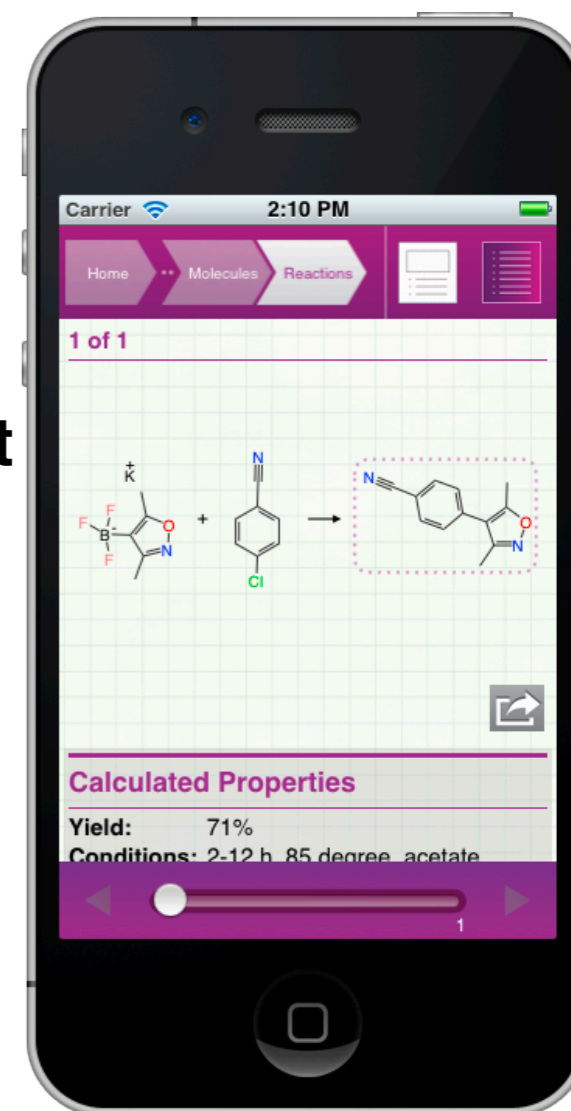
Open With



Search

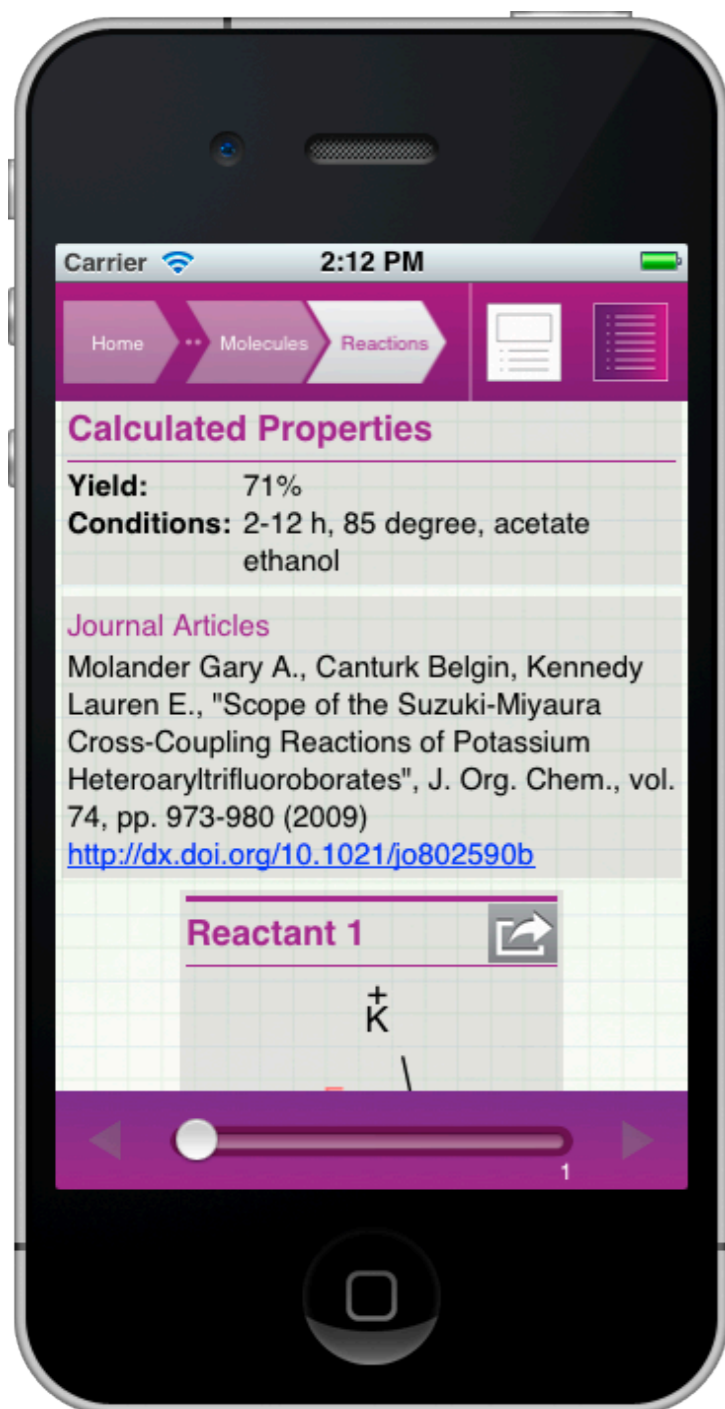


As Product





# SPRESImobile



All content links to  
the scientific  
literature

Can access the  
journal article with  
one tap





# Reaction101



Inbox 1 of 50

To: Person D

SPRESImobile Search Result  
7 March, 2012 9:48 AM

**Information and Properties:**

Registration No.: [4127831](#)  
Yield: 71%  
Conditions: [2-12 h](#), 85 degree, acetate ethanol

**Article Links:**

- [10.1021/jo802590b](#)

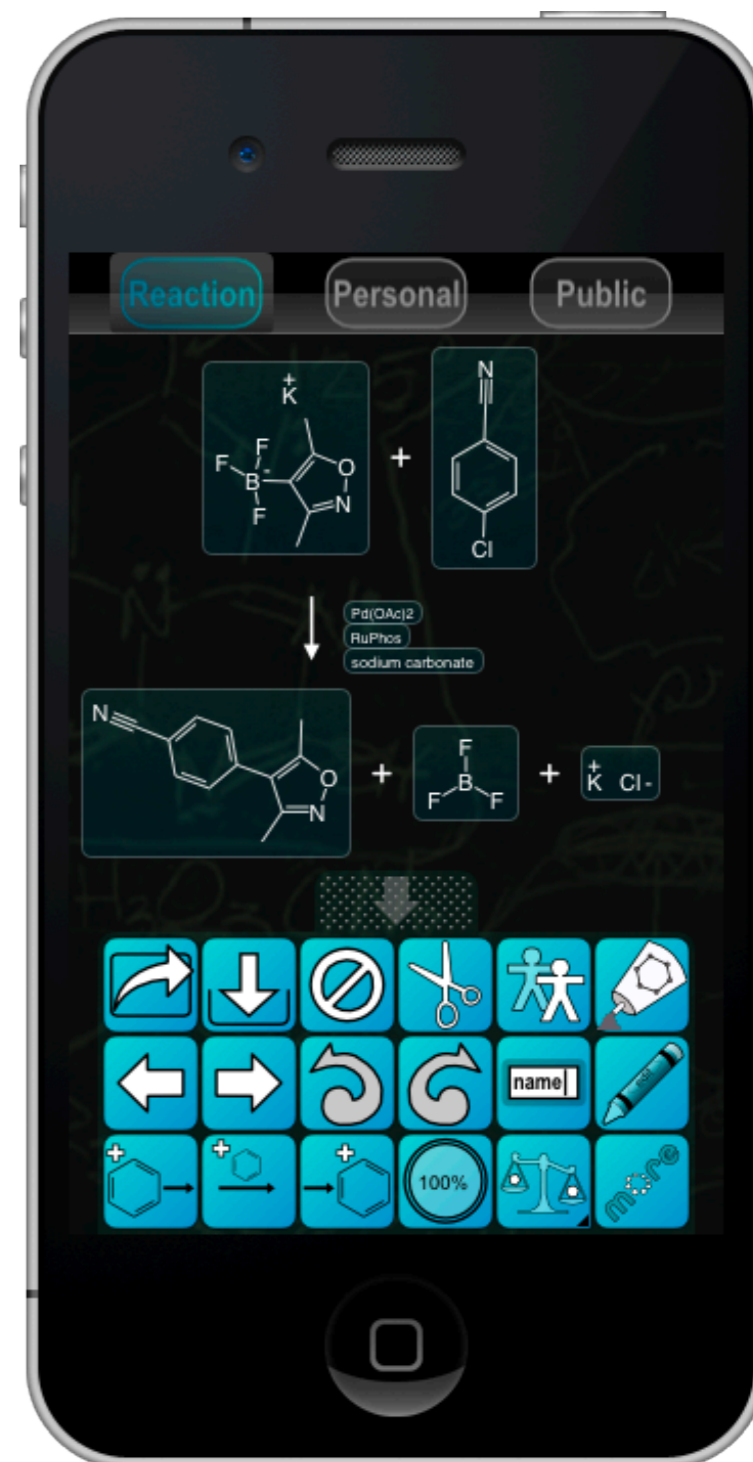
SPRESImobile  
© 2012 [InfoChem](#) GmbH, Munich, Germany

reaction.rxn  
3.7 KB

Open in "Reaction101"

Open In...

- **Person D** opens email with *Reaction101*
- Balance, add reagents, store





# Yield101



- Opens *Yield101* and accesses personal reactions to obtain the balanced reaction template
- Fills in quantities, adds solvent, checks availability with *Mobile Reagents*

The screenshot displays the Yield101 software interface, showing a chemical reaction template with various reagents and their quantities. The interface includes a sidebar with a 'Yield' button and a main area with a grid of reagent cards. Each card shows a chemical structure, name, molecular weight, and input fields for Equiv, Mass, Volume, Moles, Density, Conc, and Primary. The reaction is as follows:

[K+].[B-](F)(F)c1c([N-])nc(C(F)(F)F)c1.[Cl-]C#N + COC(=O)C1OC(=O)C1 + [Na+].[O-]C(=O)C(=O)[O-].[Na+] + C1=CC=C(C=C1)P(C2=CC=CC=C2)(C3=CC=CC=C3)P(C4=CC=CC=C4)(C5=CC=CC=C5)N1 + CCO → C1=CC=C(C=C1)P(C2=CC=CC=C2)(C3=CC=CC=C3)P(C4=CC=CC=C4)(C5=CC=CC=C5)N1 + [K+].[Cl-]

Reagent	Equiv	Mass	Volume	Moles	Density	Conc	Primary
<chem>[K+].[B-](F)(F)c1c([N-])nc(C(F)(F)F)c1</chem>	1	0.0527831 g		0.26 mmol			*
<chem>[Cl-]C#N</chem>	1	0.0343916 g		0.25 mmol			
<chem>COC(=O)C1OC(=O)C1</chem>	0	0.00336762 g		0.015 mmol			
<chem>[Na+].[O-]C(=O)C(=O)[O-].[Na+]</chem>	0	0.0529942 g		0.5 mmol			
<chem>C1=CC=C(C=C1)P(C2=CC=CC=C2)(C3=CC=CC=C3)P(C4=CC=CC=C4)(C5=CC=CC=C5)N1</chem>	0	0.0218604 g		0.03 mmol			
<chem>CCO</chem>	0	1.1046 g	1.4 mL	0.0239774 mol	0.789 g/mL		
<chem>C1=CC=C(C=C1)P(C2=CC=CC=C2)(C3=CC=CC=C3)P(C4=CC=CC=C4)(C5=CC=CC=C5)N1</chem>	1	0.046899 g		0.2366 mmol			
<chem>[K+].[Cl-]</chem>	1						

The bottom of the interface shows a progress bar with a 'Yield' button and a 'Mobile Reagents' button.



# Yield101



- Prepares a printable PDF summary of the reaction
- Takes a hard copy to the lab...
- ... performs the experiment. Enters the yield data, shares the scheme with *MolSync*.

The screenshot displays the Yield101 software interface, which is used for managing chemical reactions and their associated data. The interface includes a top navigation bar with tabs for 'Yield', 'Personal', 'Public', and 'Solvent'. Below this, there are buttons for 'Done' and 'Print'. The main area shows a chemical reaction scheme involving several reactants and products. Below the scheme, the 'Reactants' section lists the following:

Reactant	Molecular Formula	Molecular Weight	Equivalents	Mass	Moles
	$\text{C}_2\text{H}_5\text{BF}_4\text{KNO}$	203.012 g/mol	1	0.0527831 g (calculated)	0.26 mmol
	$\text{C}_7\text{H}_5\text{ClN}$	137.566 g/mol	1	0.0343916 g (calculated)	0.25 mmol
	$\text{C}_{14}\text{H}_{10}\text{O}_2\text{Pd}$	224.508 g/mol	0	0.00336762 g (calculated)	0.015 mmol
	$\text{CNa}_2\text{O}_3$	105.988 g/mol	0	0.0529942 g (calculated)	0.5 mmol
	$\text{C}_{30}\text{H}_{20}\text{ClNO}_3\text{PPd}$	728.679 g/mol	0	0.0218604 g (calculated)	0.03 mmol
	$\text{C}_3\text{H}_8\text{O}$	46.0684 g/mol	0	1.1046 g (calculated)	0.0239774 mol (calculated)

The 'Products' section lists the following:

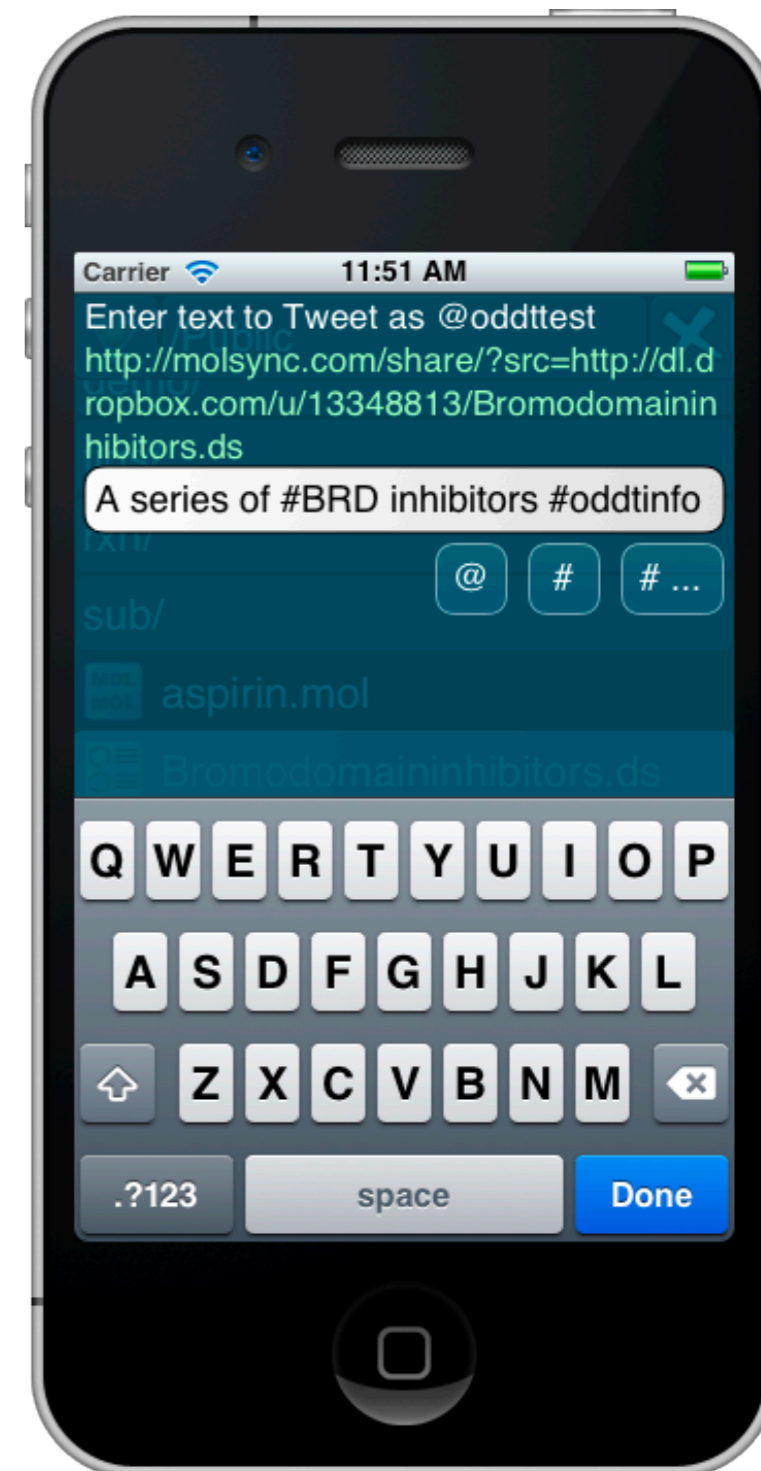
Product	Molecular Formula	Molecular Weight	Equivalents	Mass	Moles	Yield
	$\text{C}_{10}\text{H}_{10}\text{N}_2\text{O}$	198.221 g/mol	1	0.046899 g (calculated)	0.2366 mmol (calculated)	91 %
	$\text{BF}_3$	67.8062 g/mol	1			
	$\text{ClK}$	74.5513 g/mol	1			



# MolSync



- A number of chemical data files have been created and shared on a *Dropbox* account
- Files in the **Public** folder can be shared on the web, or tweeted
- Tweeting certain hash tags has interesting effects



# MolSync web

**MolSync Sharing**

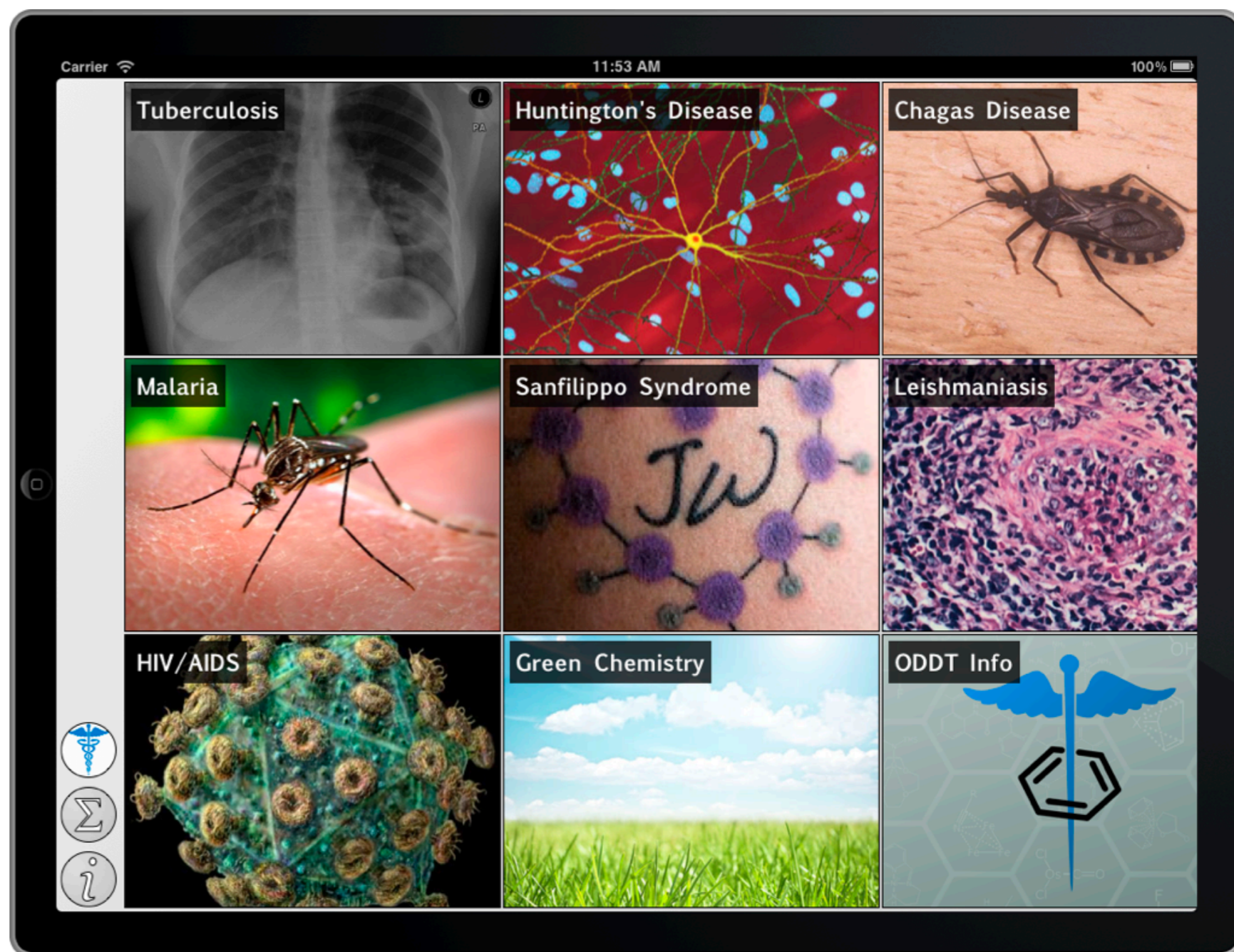
Bromodomain inhibitors  
*J. Med. Chem.* 55, 587-596 (2012)

	Scaffold	R1	R2	Molecule	ID	BRD2	BRD3	BRD4
Row#1 <a href="#">Download</a>		R—			5a	1.5 uM	1.0 uM	1.0 uM
Row#2 <a href="#">Download</a>		R—O—			5b	1.9 uM	1.3 uM	3.0 uM
Row#3 <a href="#">Download</a>		R—			6a	0.5 uM	0.5 uM	0.6 uM
Row#4 <a href="#">Download</a>								

- Raw presentable data wrapped by HTML5 layer: can view, download, render, convert...

# Open Drug Discovery Teams (ODDT)

- Aggregates open data from Twitter
- Crowd-sourced curation
- Flipboard-like app interface
- Free. Current alpha testing



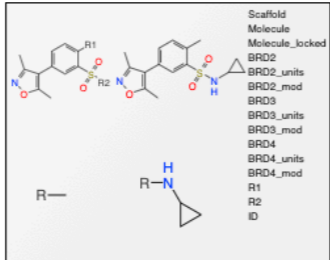
from  
MolSync

# ODDT

Carrier 12:24 PM 100%

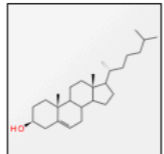
## ODDT Info

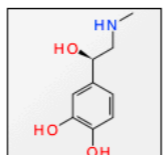
Incoming  
Recent  
Content

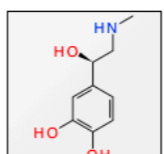


Scaffold  
Molecule\_locked  
BRD2  
BRD2\_units  
BRD2\_mod  
BRD3  
BRD3\_units  
BRD3\_mod  
BRD4  
BRD4\_units  
BRD4\_mod  
R1  
R2  
ID

@oddttest: (link) Series of #BRD inhibitors #oddtinfo  
<http://molsync.com/share/?src=http://dl...>

@oddtinfo: ChemSpider | Cholesterol | C<sub>27</sub>H<sub>46</sub>O: (link) #oddtinfo  
  
<http://www.chemspider.com/Chemical-St...>

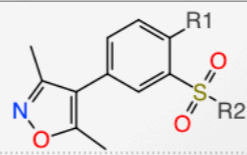
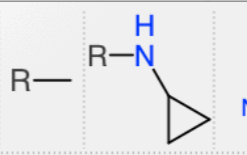
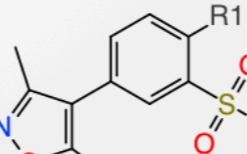
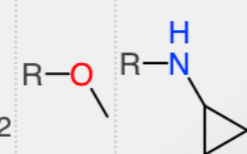
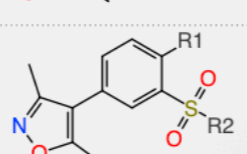
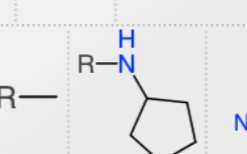
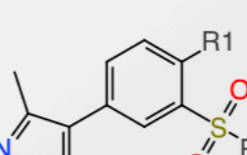
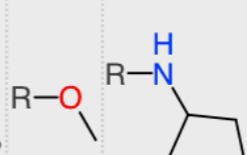
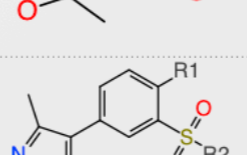
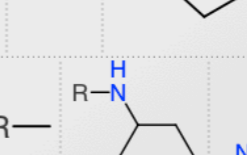
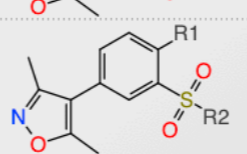
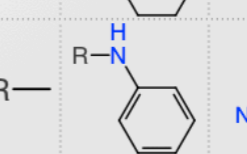
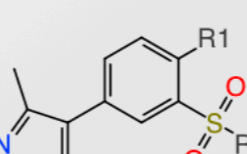
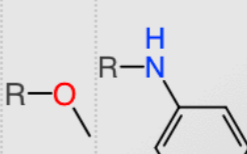
@oddtinfo: (link) #oddtinfo retry  
  
<http://www.chemspider.com/Chemical-St...>

@oddtinfo: (link) #oddtinfo  
  
<http://www.chemspider.com/Chemical-St...>

#oddtinfo



Carrier 12:24 PM 100%

		ID: 5a BRD2: 1.5 uM BRD3: 1 uM BRD4: 1 uM
		ID: 5b BRD2: 1.9 uM BRD3: 1.3 uM BRD4: 3 uM
		ID: 6a BRD2: 0.5 uM BRD3: 0.5 uM BRD4: 0.6 uM
		ID: 6b BRD2: 1.4 uM BRD3: 1 uM BRD4: 2.2 uM
		ID: 7a BRD2: 0.9 uM BRD3: 0.7 uM BRD4: 1.1 uM
		ID: 8a BRD2: 1.1 uM BRD3: 1 uM BRD4: 1.8 uM
		ID: 8b BRD2: 2.4 uM BRD3: 2.2 uM BRD4: 5.6 uM

# Acknowledgments

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