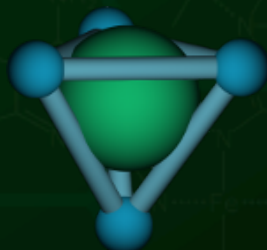


Building a mobile app ecosystem for chemistry collaboration

Dr. Alex M. Clark

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**



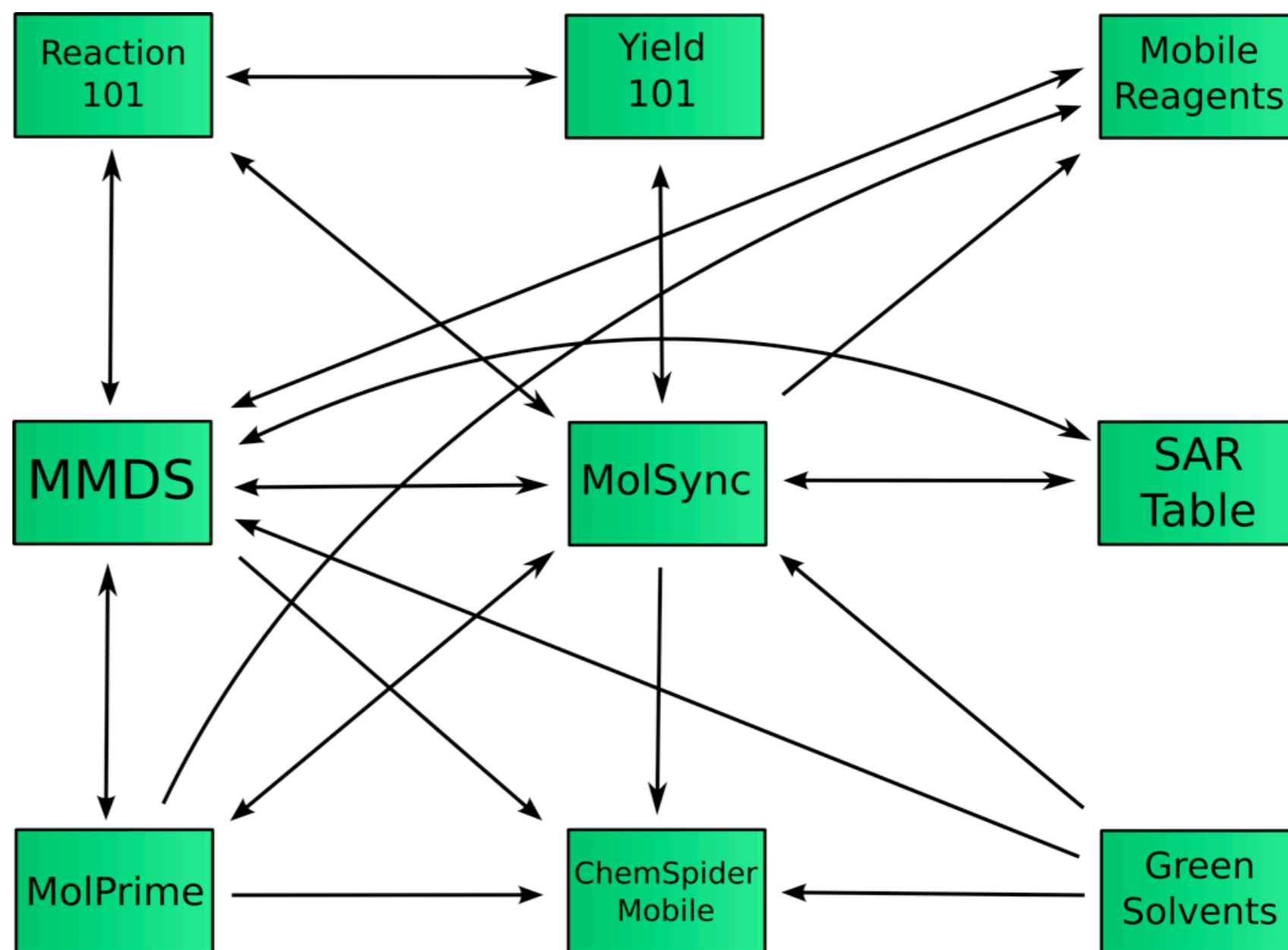
So many apps



- 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

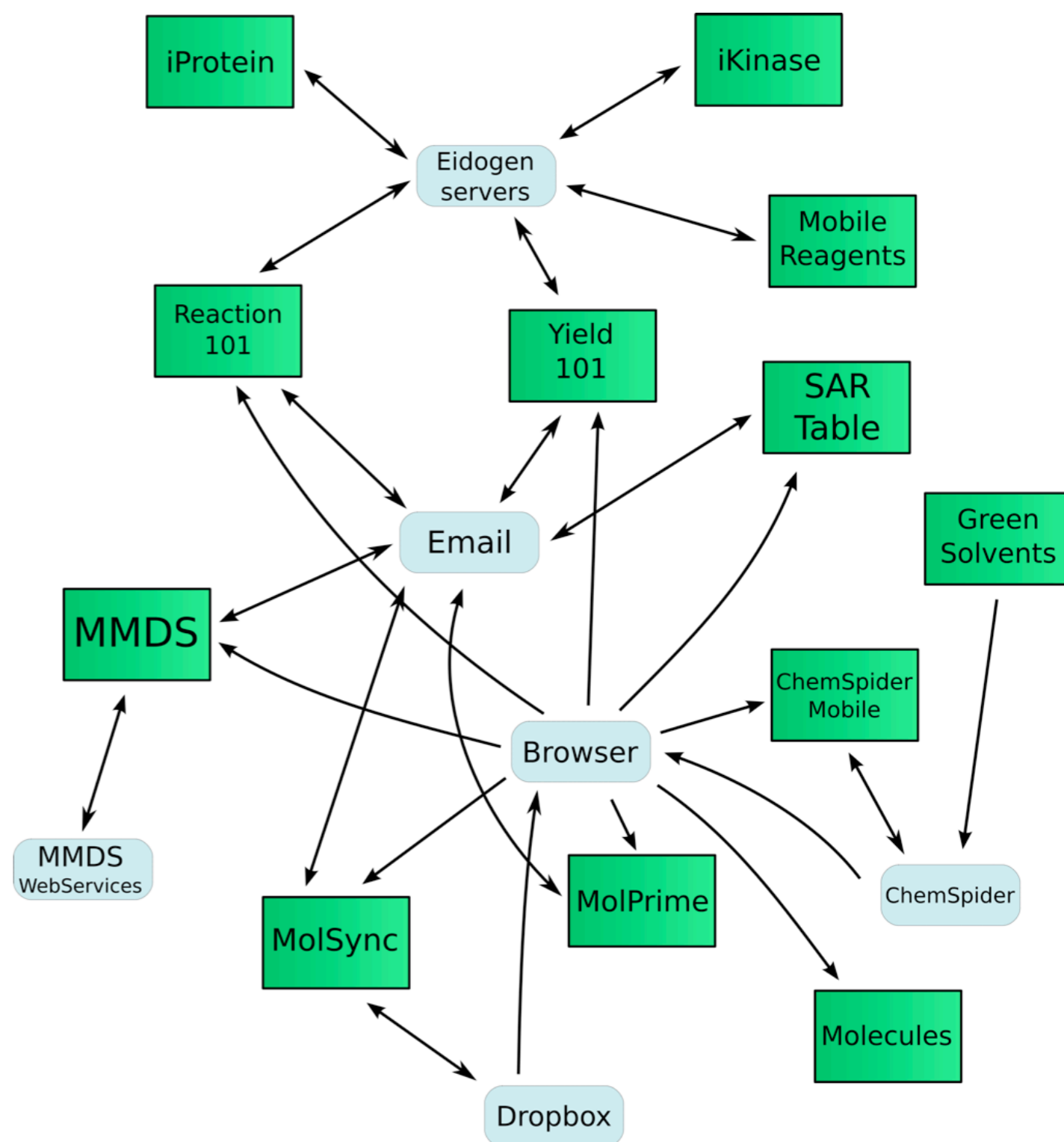


Network comms

- Many different transport mechanisms

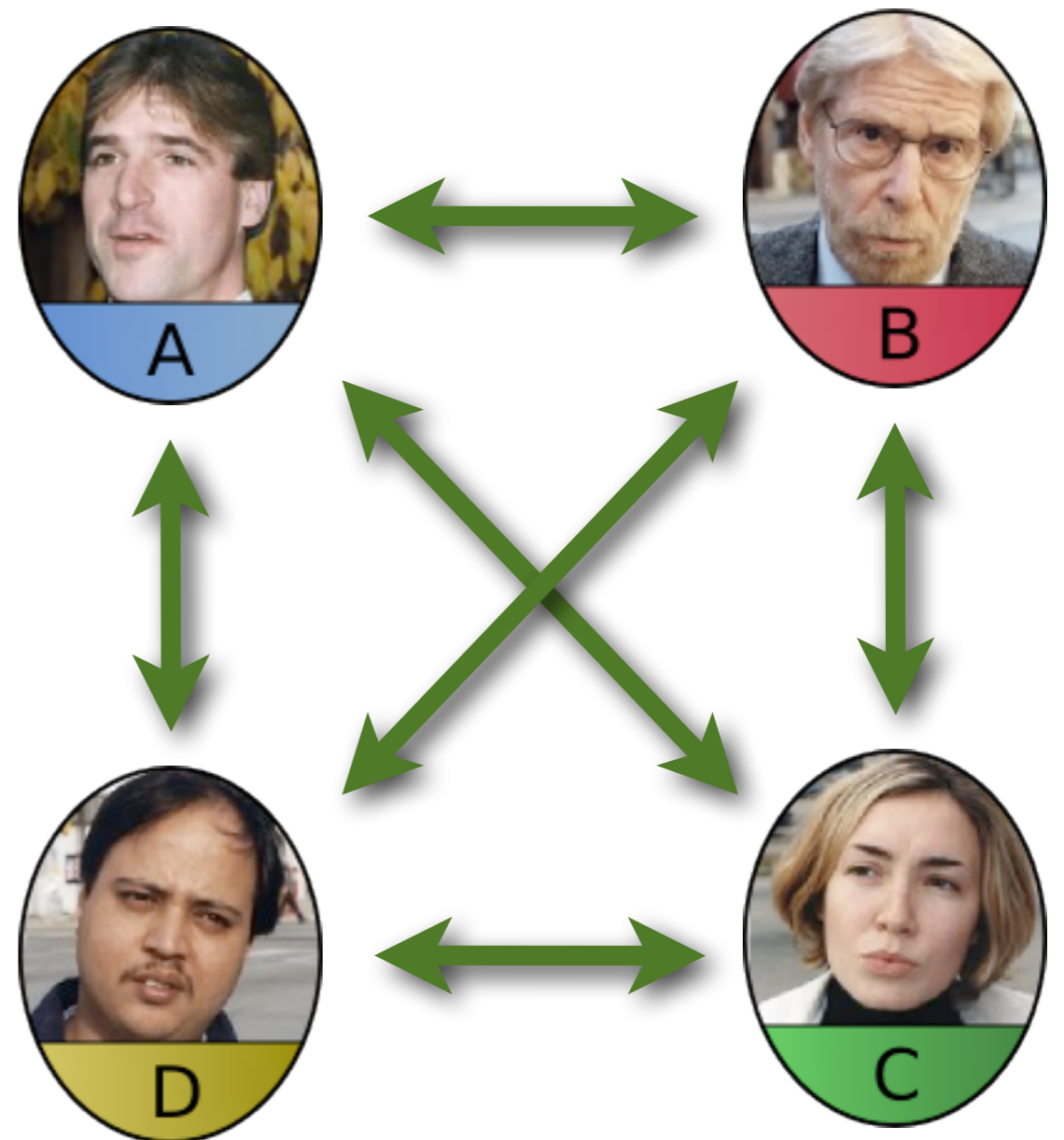
- email
- file export
- web access
- cloud storage
- client-server RPC

- 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

Added to molecule collection

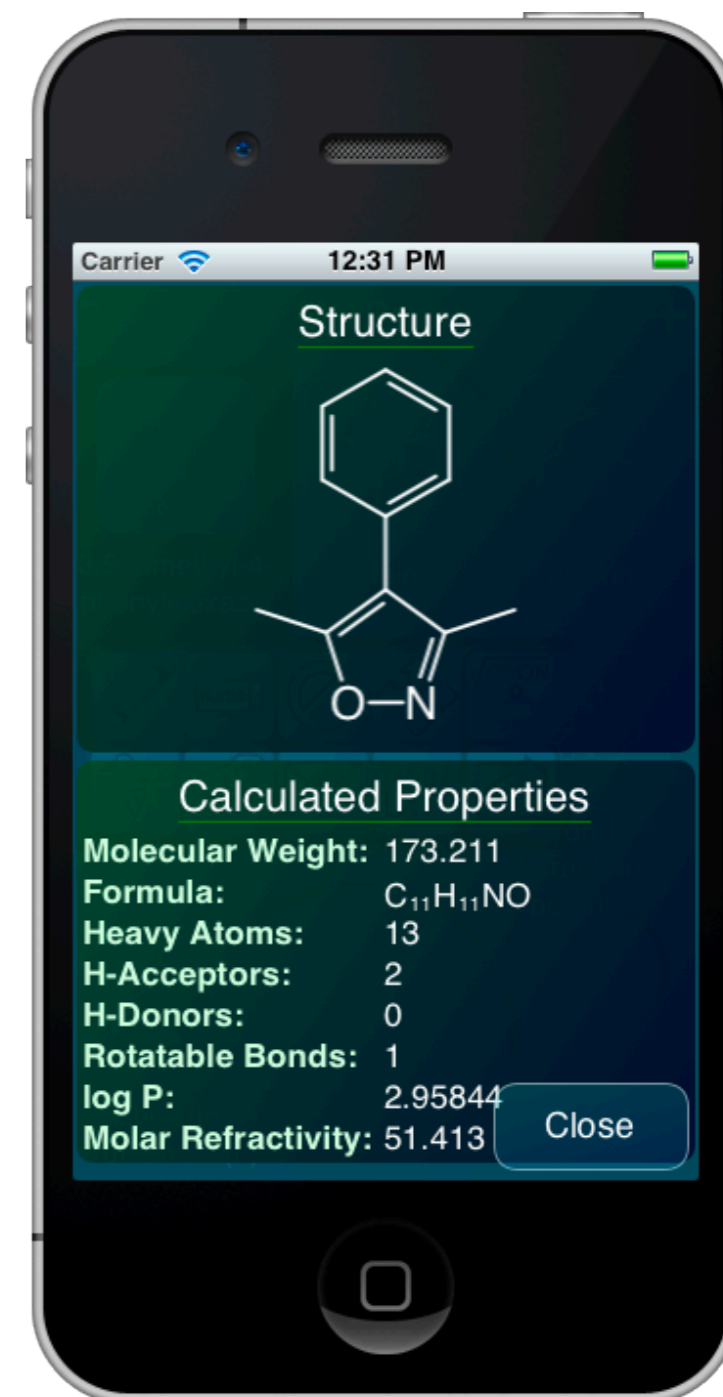




Calculated Properties



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

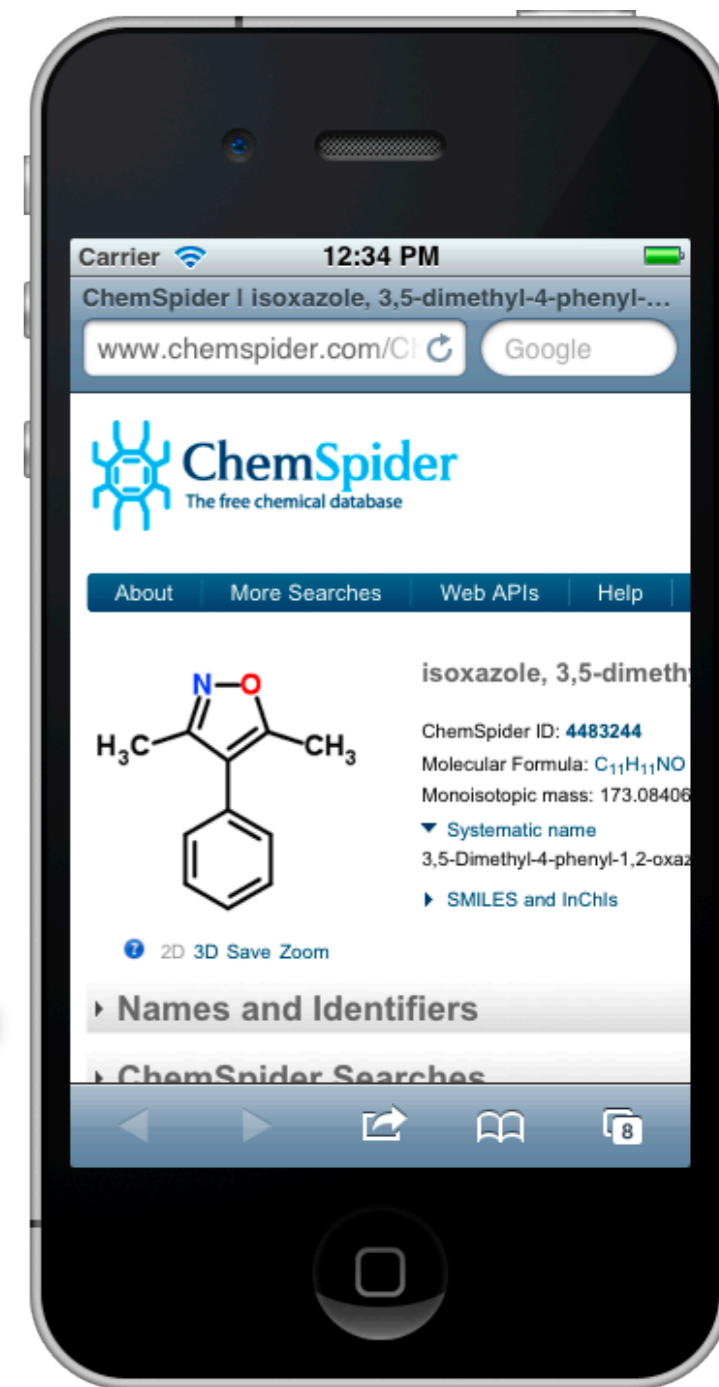


ChemSpider Mobile



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

Search and open the web page

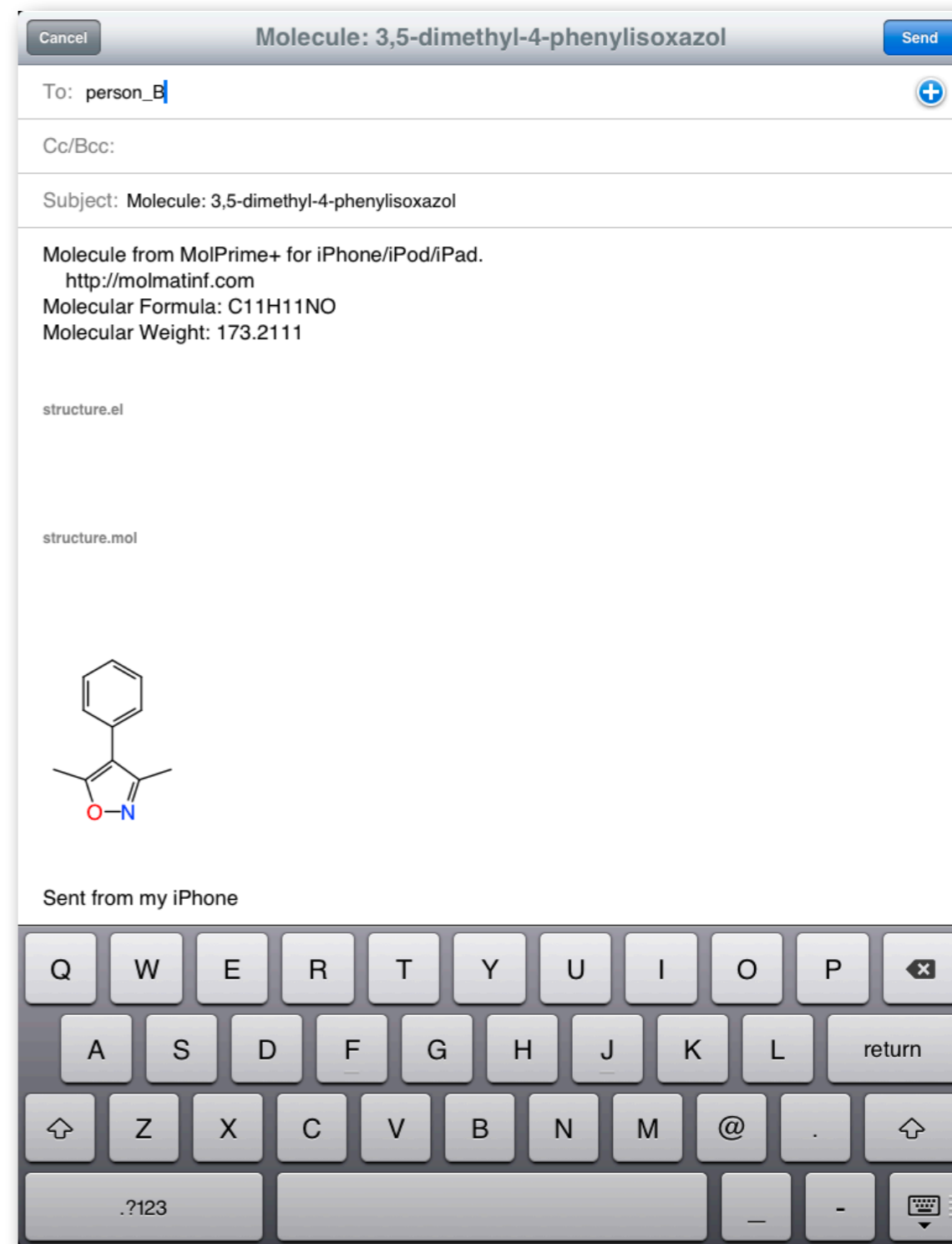


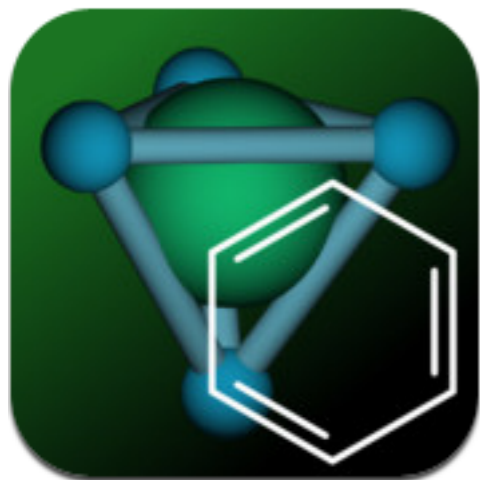


Email



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





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

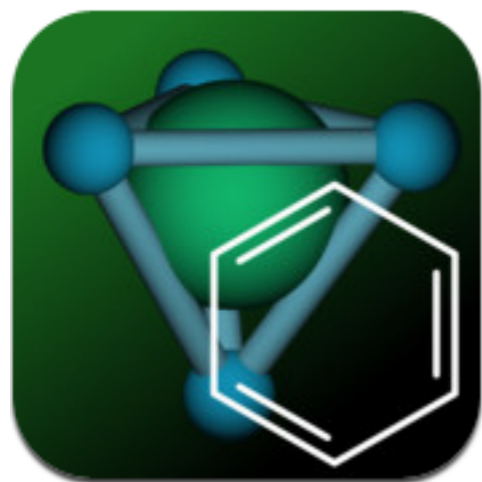
Molecule from MolPrime+ for iPhone/iPod/iPad.
<http://molmatinf.com>
Molecular Formula: C₁₁H₁₁NO
Molecular Weight: 173.21

structure.el
0.5 KB

structure.mol
1.3 KB

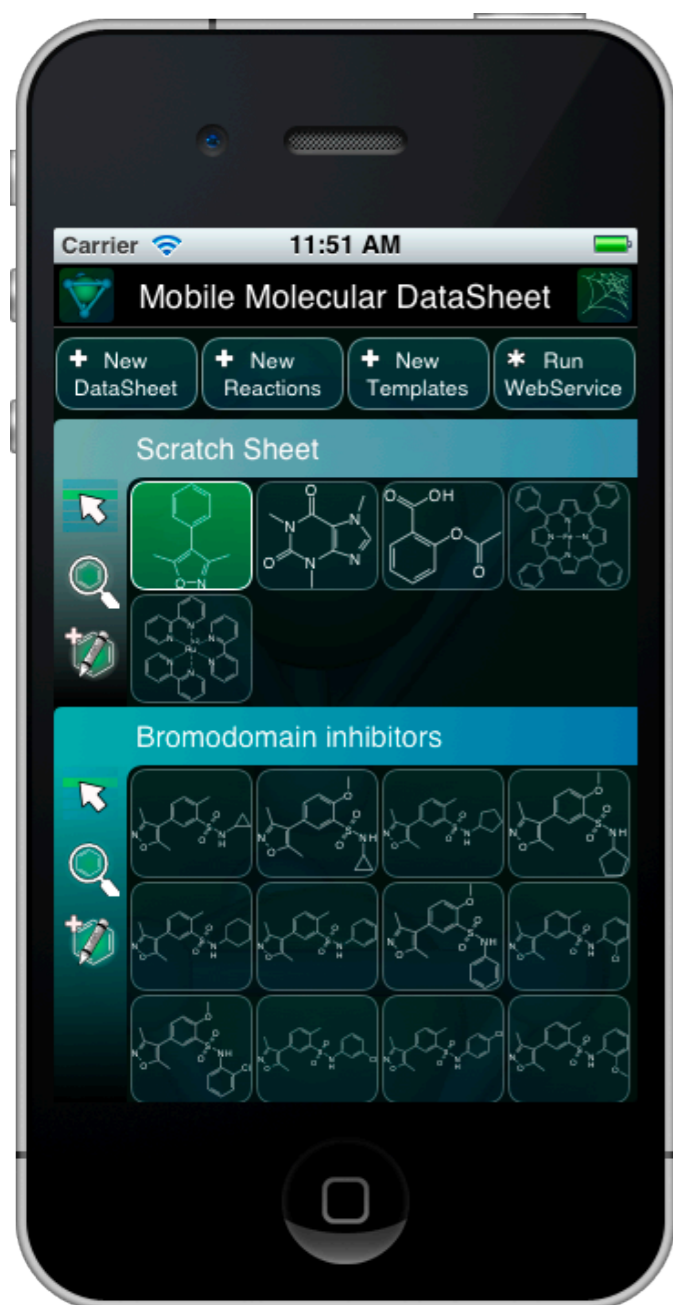
Open In...

- MMDS
- MolPrime+
- MolPrime
- SPRESI



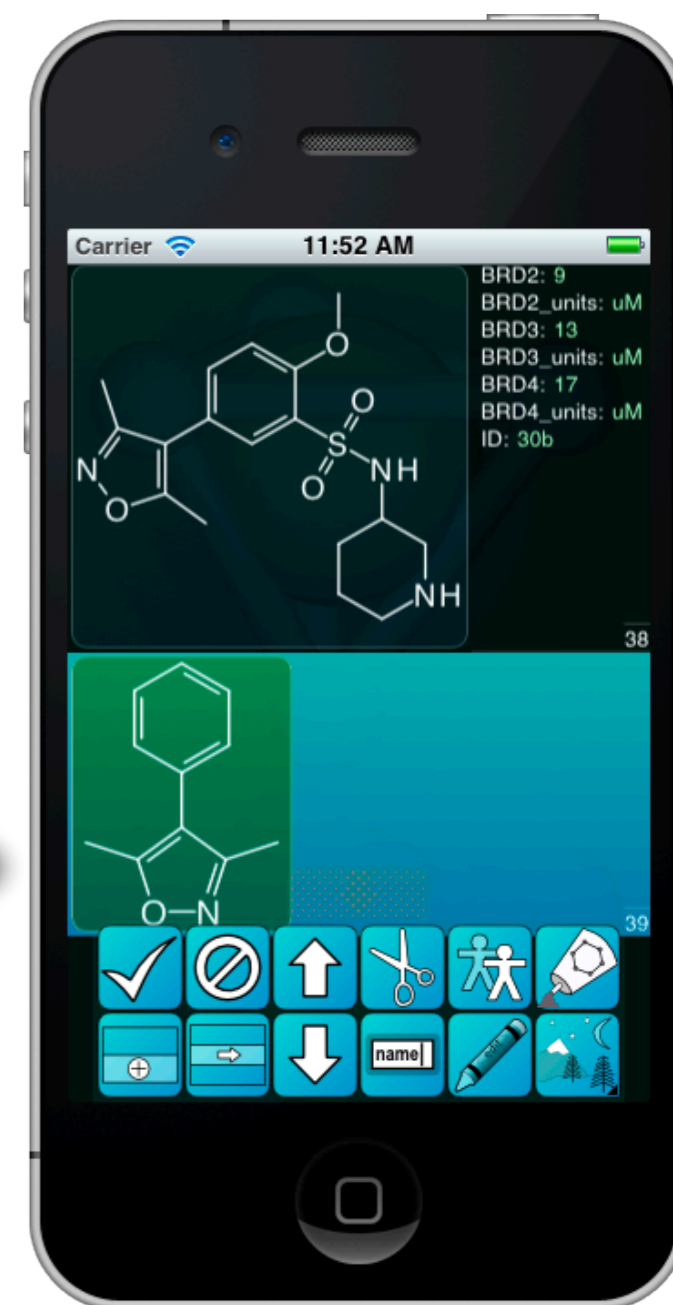
MMDS

Mobile Molecular DataSheet



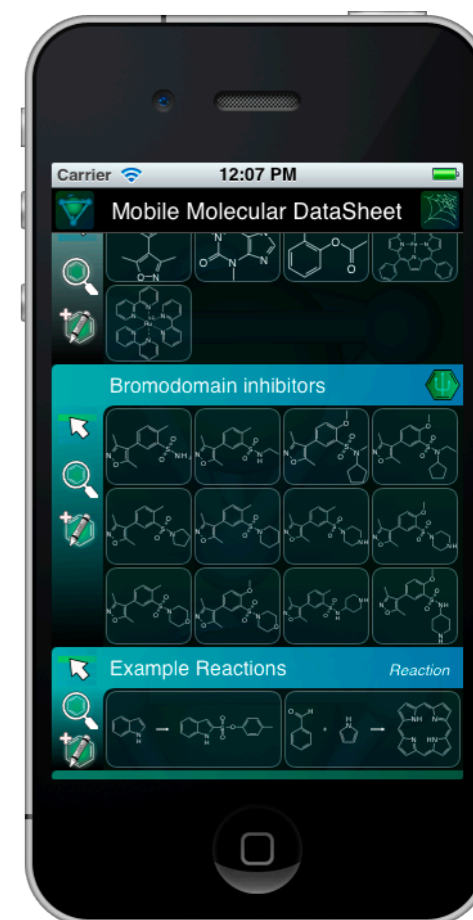
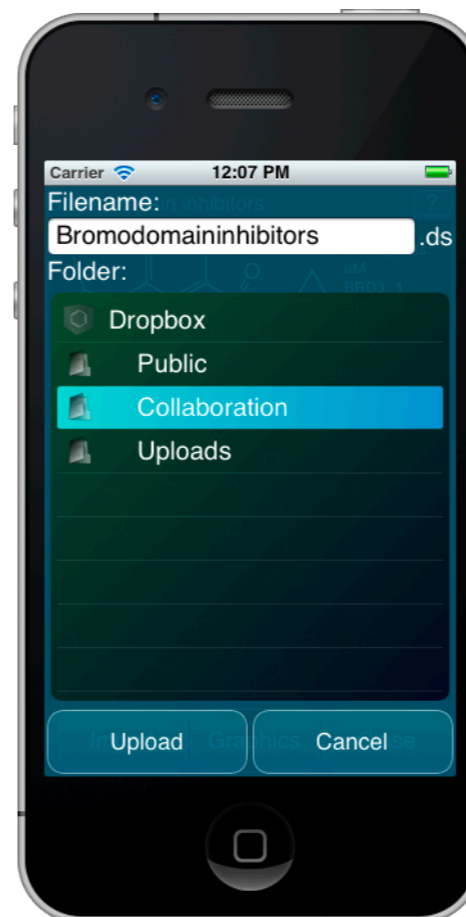
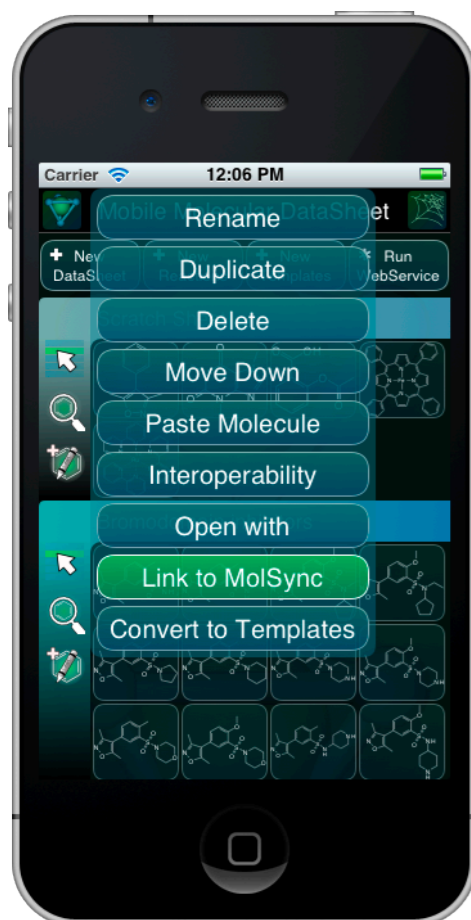
Structure is prepended to *scratch sheet*

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





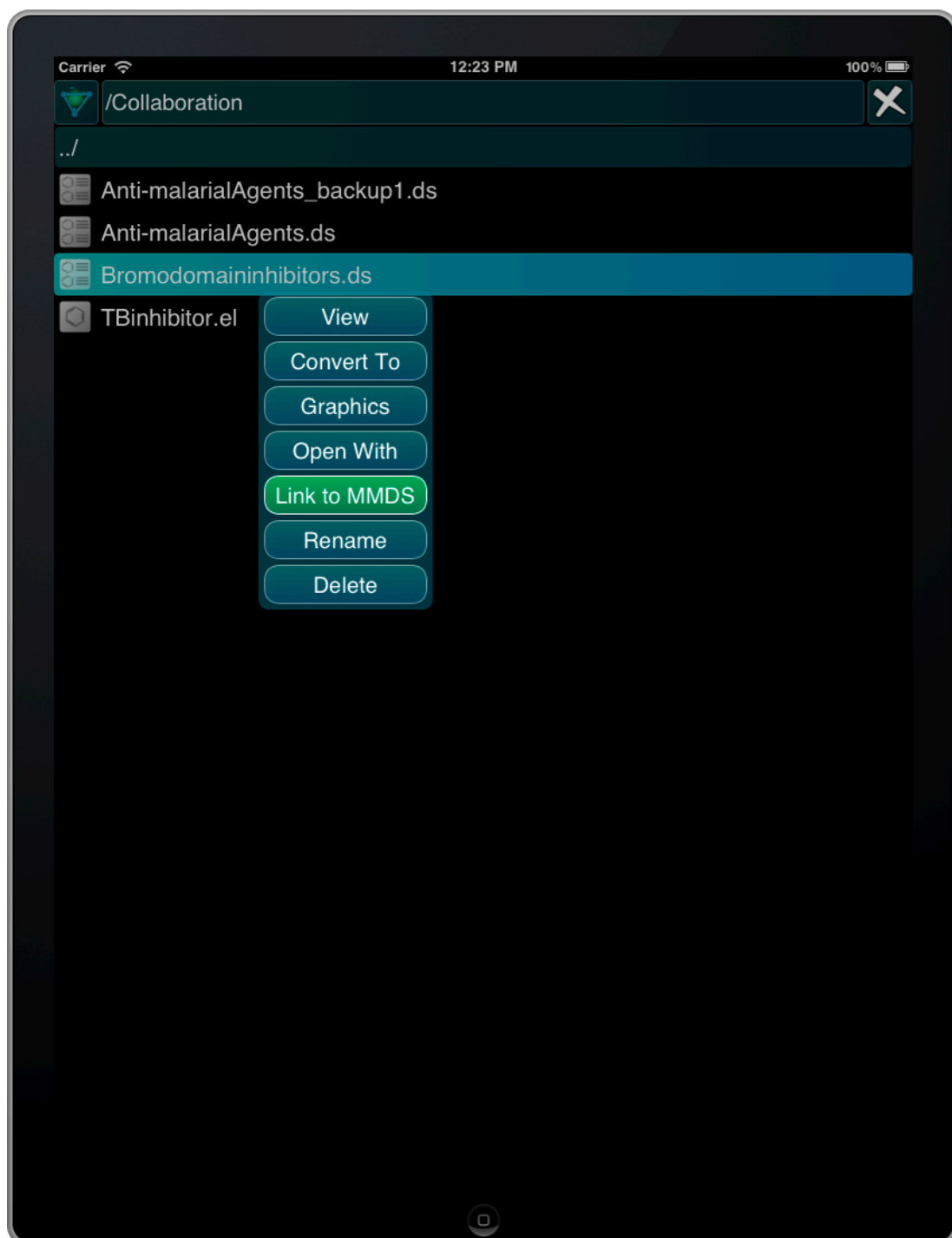
MolSync



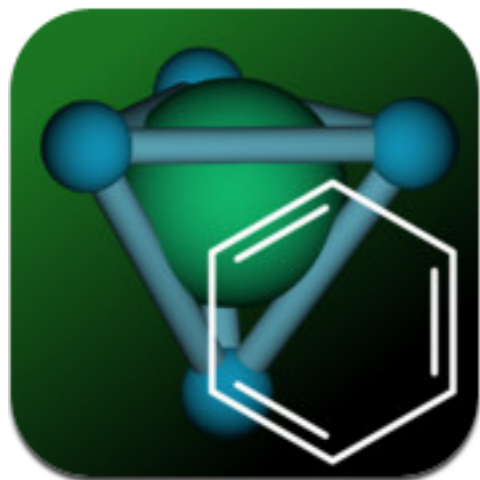
- Communicate with *MolSync*
- *Upload to Dropbox*
- *Create association*



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

The screenshot displays a mobile application interface with a dark background. At the top, there is a header with the letter 'H'. Below this, three chemical structures are shown in separate panels, each with associated data fields:

- Top Panel:** Shows a complex chemical structure. Data fields: BRD2: 11, BRD2_units: uM, BRD3: 8.4, BRD3_units: uM, BRD4: 10, BRD4_units: uM, ID: 30a.
- Middle Panel:** Shows a similar chemical structure with a methoxy group. Data fields: BRD2: 9, BRD2_units: uM, BRD3: 13, BRD3_units: uM, BRD4: 17, BRD4_units: uM, ID: 30b.
- Bottom Panel:** Shows a simpler chemical structure. Data fields: BRD3: 32, BRD3_units: %, BRD4: 32, BRD4_units: %, ID: 3.

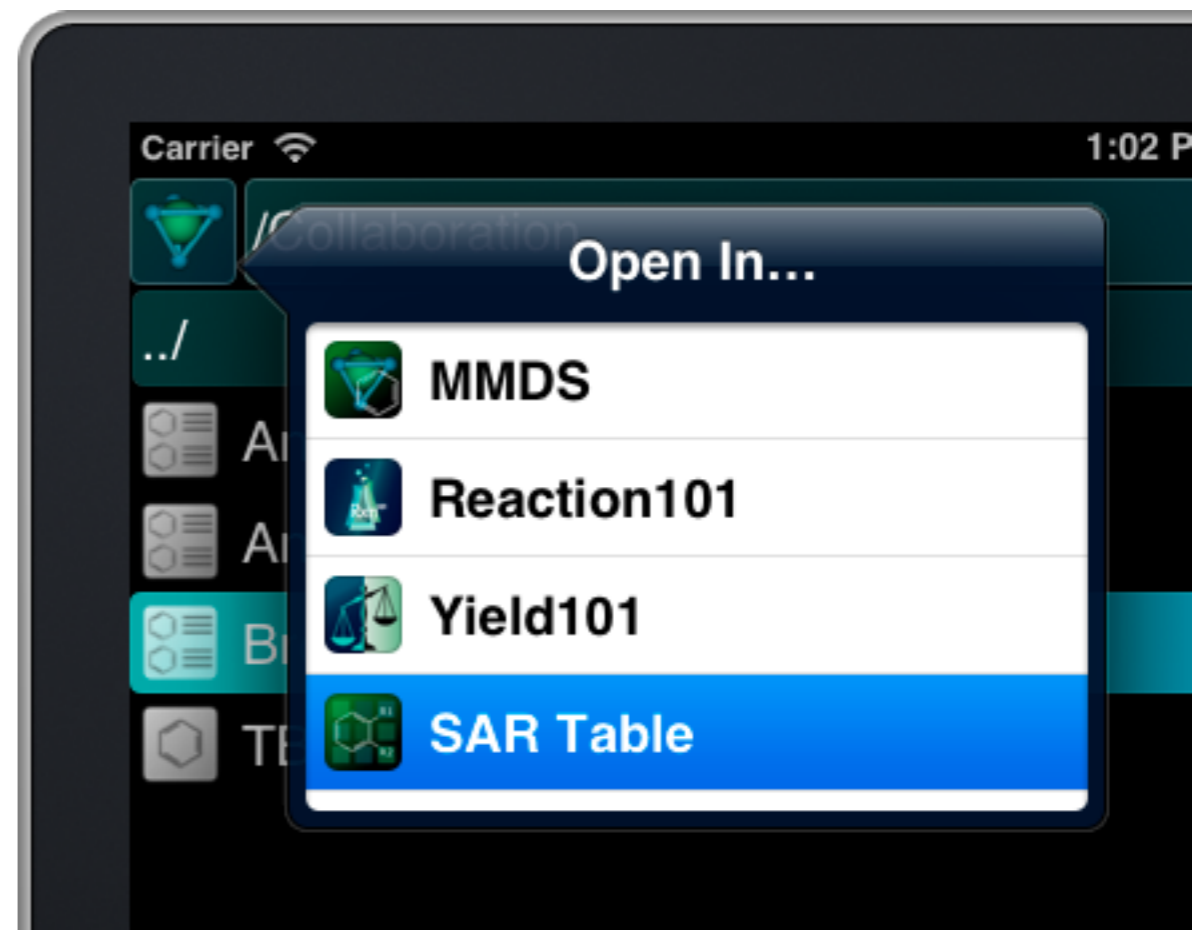
At the bottom of the screen, there is a control panel with several icons: a checkmark, a prohibition sign, an upward arrow, a scissors icon, a plus sign in a box, a right arrow in a box, a downward arrow, and a text input field containing the word 'name'.



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...





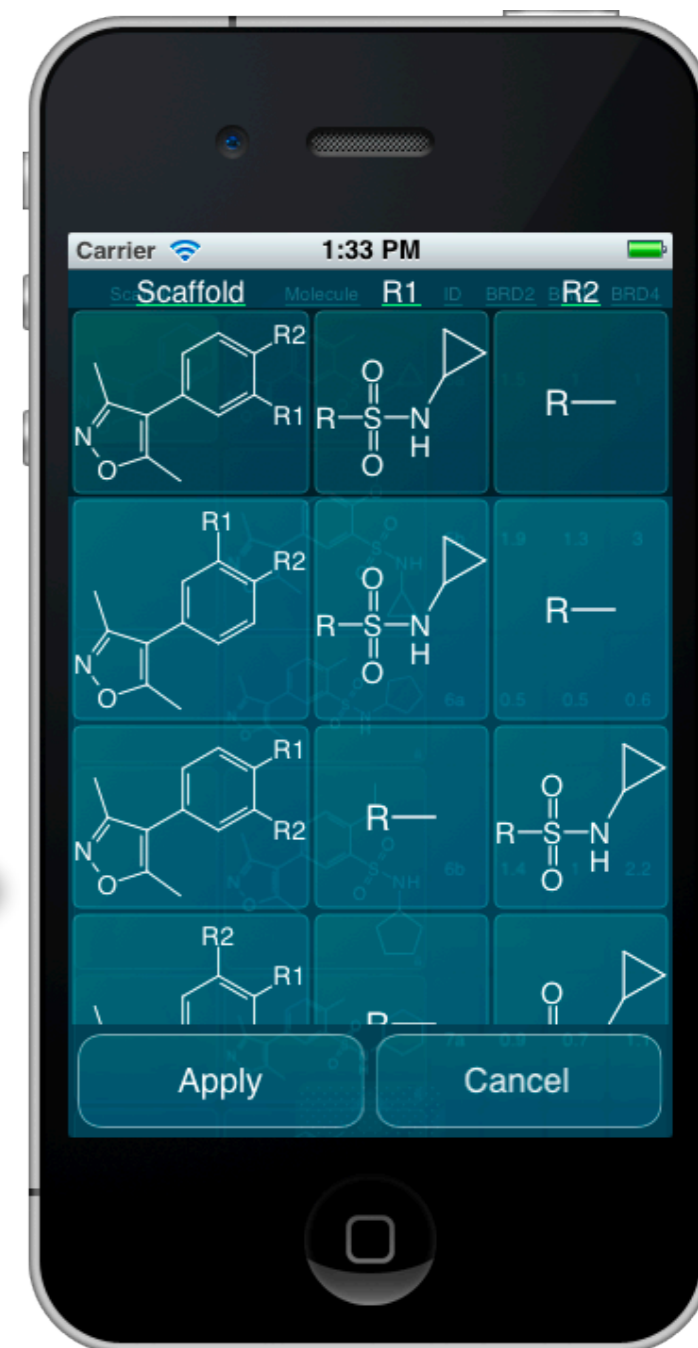
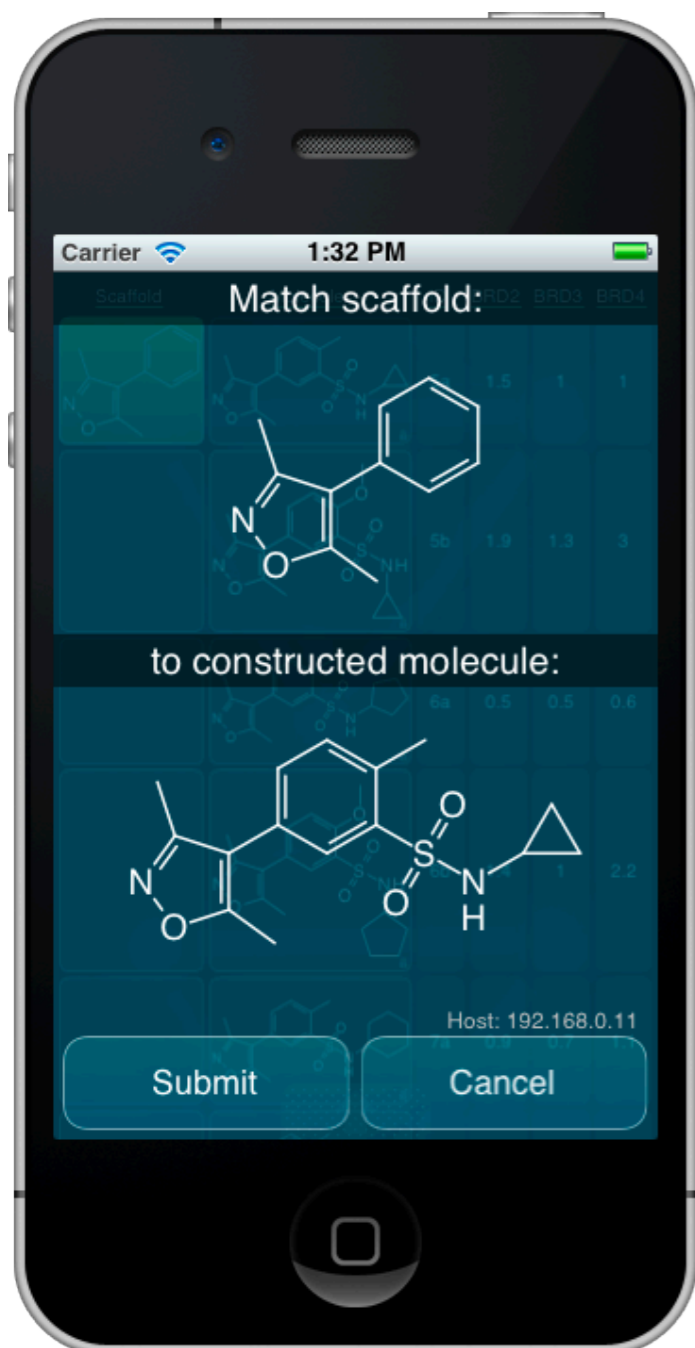
SAR Table



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



A variety of
possibilities: select
the preferred one



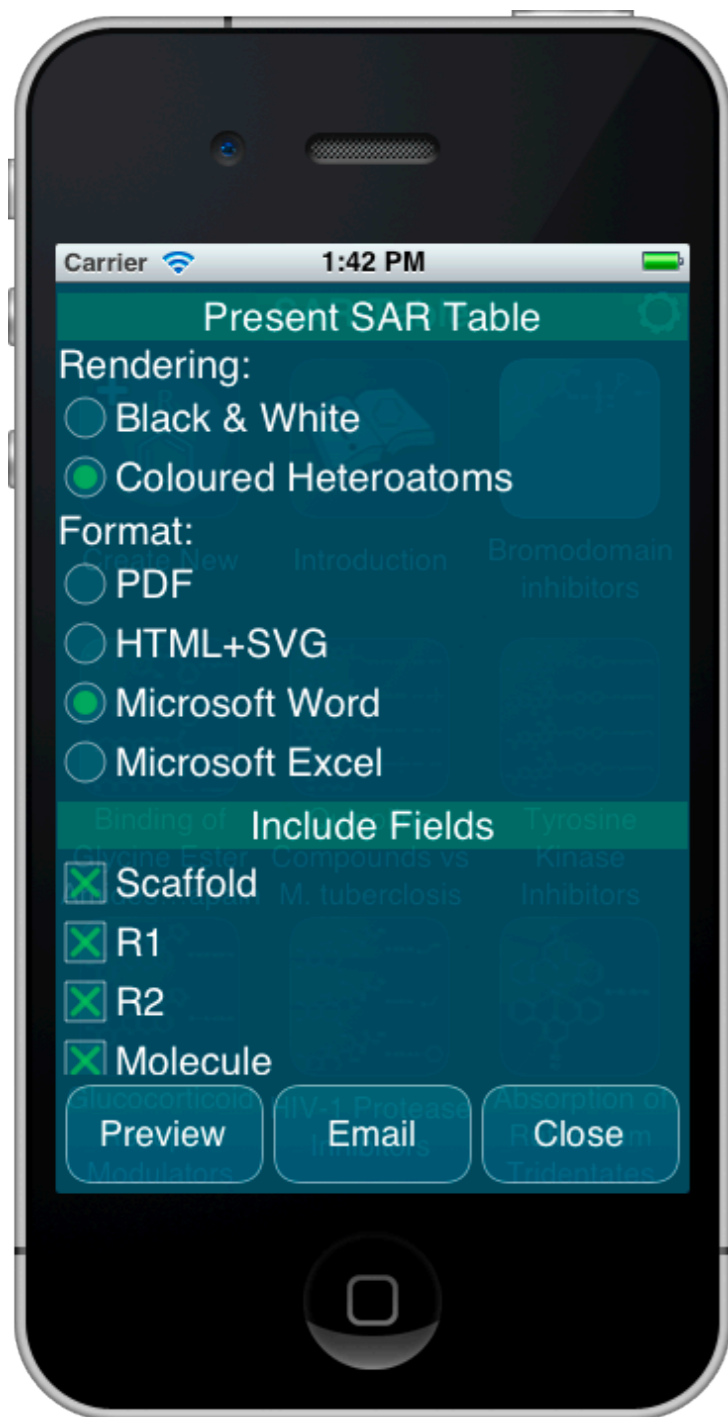


SAR Table



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—					

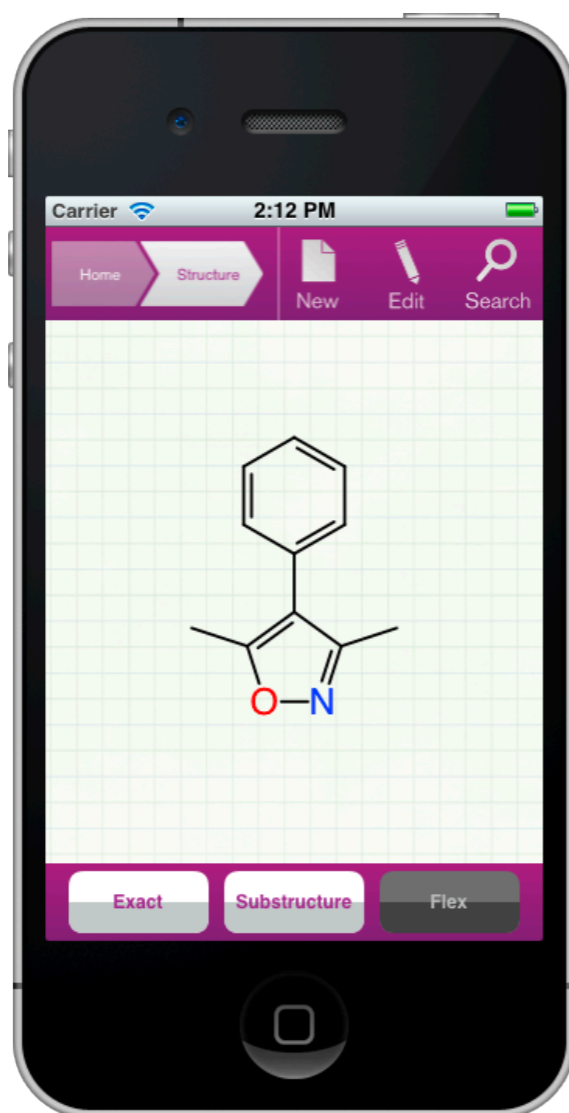


SPRESImobile

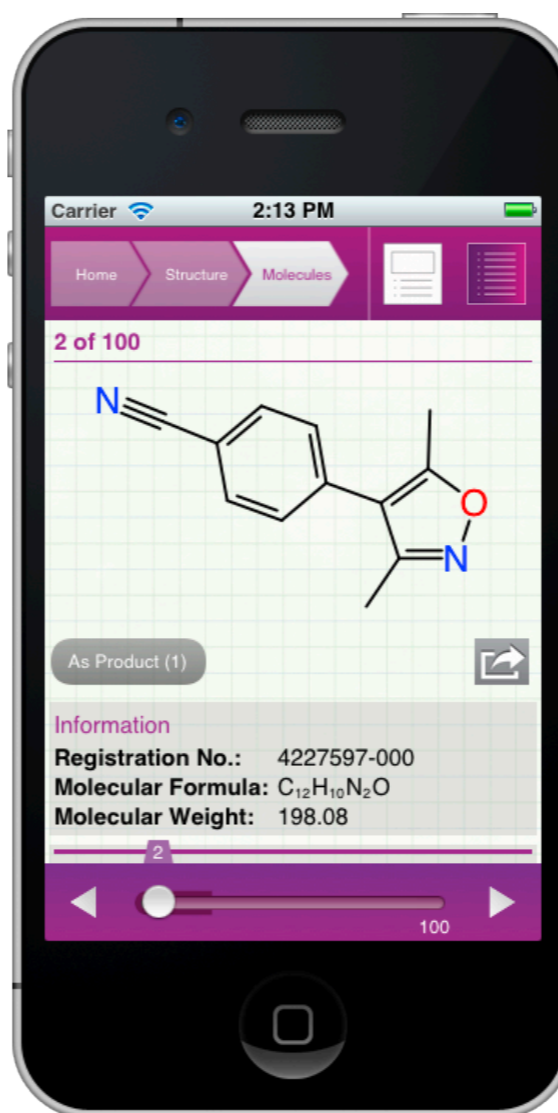


Want to illustrate a representative synthesis: search for the common fragment using SPRESI

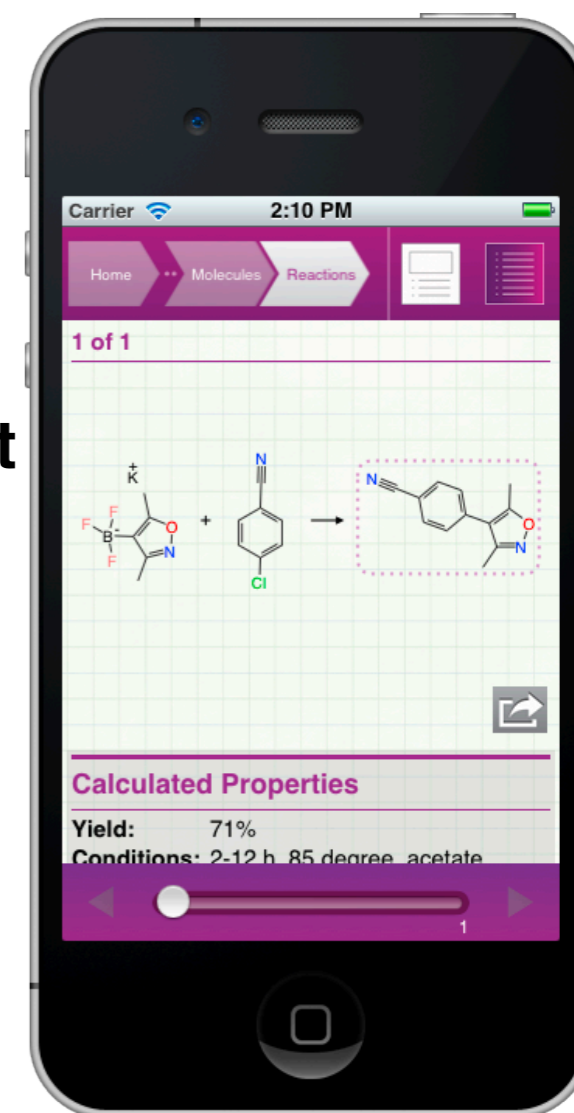
Open With



Search

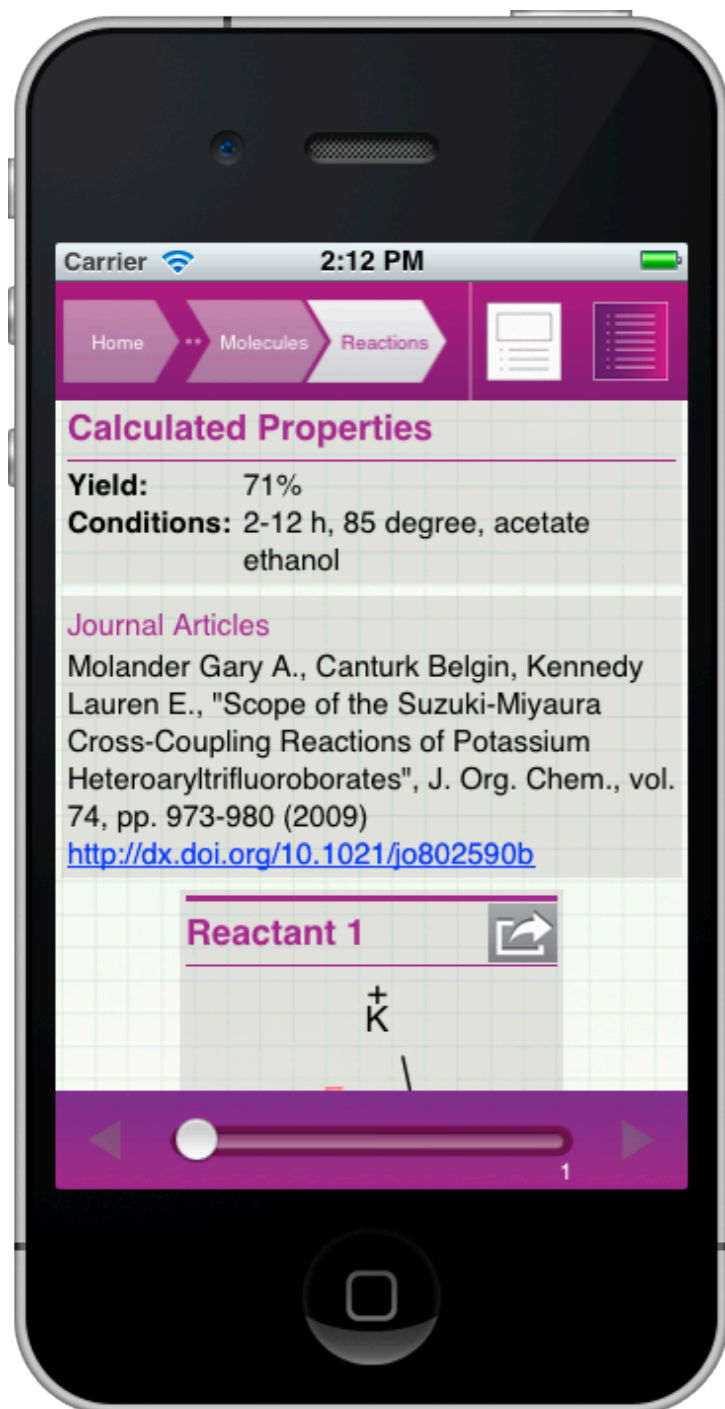


As Product





SPRESImobile



All content links to the scientific literature

Can access the journal article with one tap





Reaction 101



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

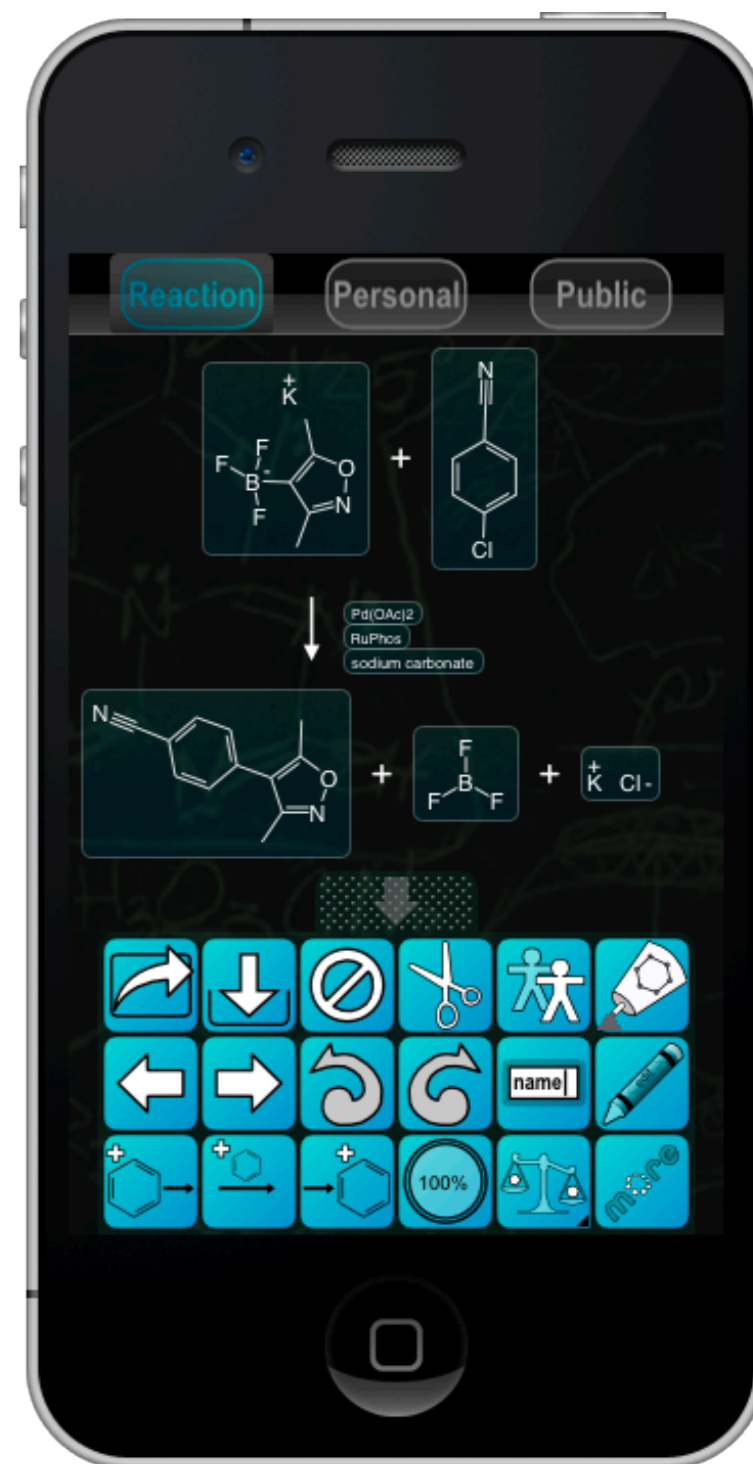
reaction.rxn
3.7 KB

Open in "Reaction101"

Open In...

- **Person D** opens email with *Reaction 101*

- 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 a chemical reaction template in the Yield101 mobile application. The reaction involves the following reagents and products:

Reagent	Chemical Structure	Molar Mass (g/mol)	Equiv.	Mass (g)	Volume (mL)	Moles (mmol)	Density (g/mL)	Conc.	Primary	Yield (%)
1	<chem>[K+].[B-](F)(F)F</chem>	203.01	1	0.0527831		0.26			*	
1	<chem>N#CC1=CC=C(Cl)C=C1</chem>	137.57	1	0.0343916		0.25				
0	<chem>C1OC(=O)Pd(OC1=O)OC1=O</chem>	224.51	0	0.00336762		0.015				
0	<chem>[Na+].[O-]C(=O)C(=O)[O-]</chem>	108.99	0	0.0529942		0.5				
0	<chem>C1=CC=C(C=C1)P(C2=CC=CC=C2)(C3=CC=CC=C3)N4CCCCC4</chem>	728.68	0	0.0218604		0.03				
0	<chem>CCO</chem>	46.07	0	1.1046	1.4	0.0239774	0.789			
1	<chem>C1=CC=C(C=C1)C2=C(C)N(C)C=C2C#N</chem>	198.22	1	0.046899		0.2366				91
1	<chem>F[B-](F)F</chem>	67.81	1							
1	<chem>[K+].[Cl-]</chem>	74.55	1							



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 MolSync software interface. At the top, there are tabs for 'Yield', 'Personal', 'Public', and 'Solvent'. Below the tabs is a 'Done' button on the left and a 'Print' button on the right. The main area shows a chemical reaction scheme with various reactants and products. Below the scheme, there are two sections: 'Reactants' and 'Products'. Each section lists the chemical species with their molecular formulas, molecular weights, equivalents, masses, and moles. The 'Reactants' section includes:

Reactant	Molecular Formula	Molecular Weight	Equivalents	Mass	Moles
	C ₂ H ₂ BF ₃ KNO	203.012 g/mol	1	0.0527831 g (calculated)	0.26 mmol
	C ₇ H ₂ ClN	137.566 g/mol	1	0.0343916 g (calculated)	0.25 mmol
	C ₂₄ H ₂₀ O ₂ Pd	224.508 g/mol	0	0.00336762 g (calculated)	0.015 mmol
	CNa ₂ O ₃	105.988 g/mol	0	0.0529942 g (calculated)	0.5 mmol
	C ₂₈ H ₂₀ ClNO ₂ PPd	728.679 g/mol	0	0.0218604 g (calculated)	0.03 mmol
	C ₂ H ₆ O	46.0684 g/mol	0	1.1046 g (calculated)	1.4 mL

The 'Products' section includes:

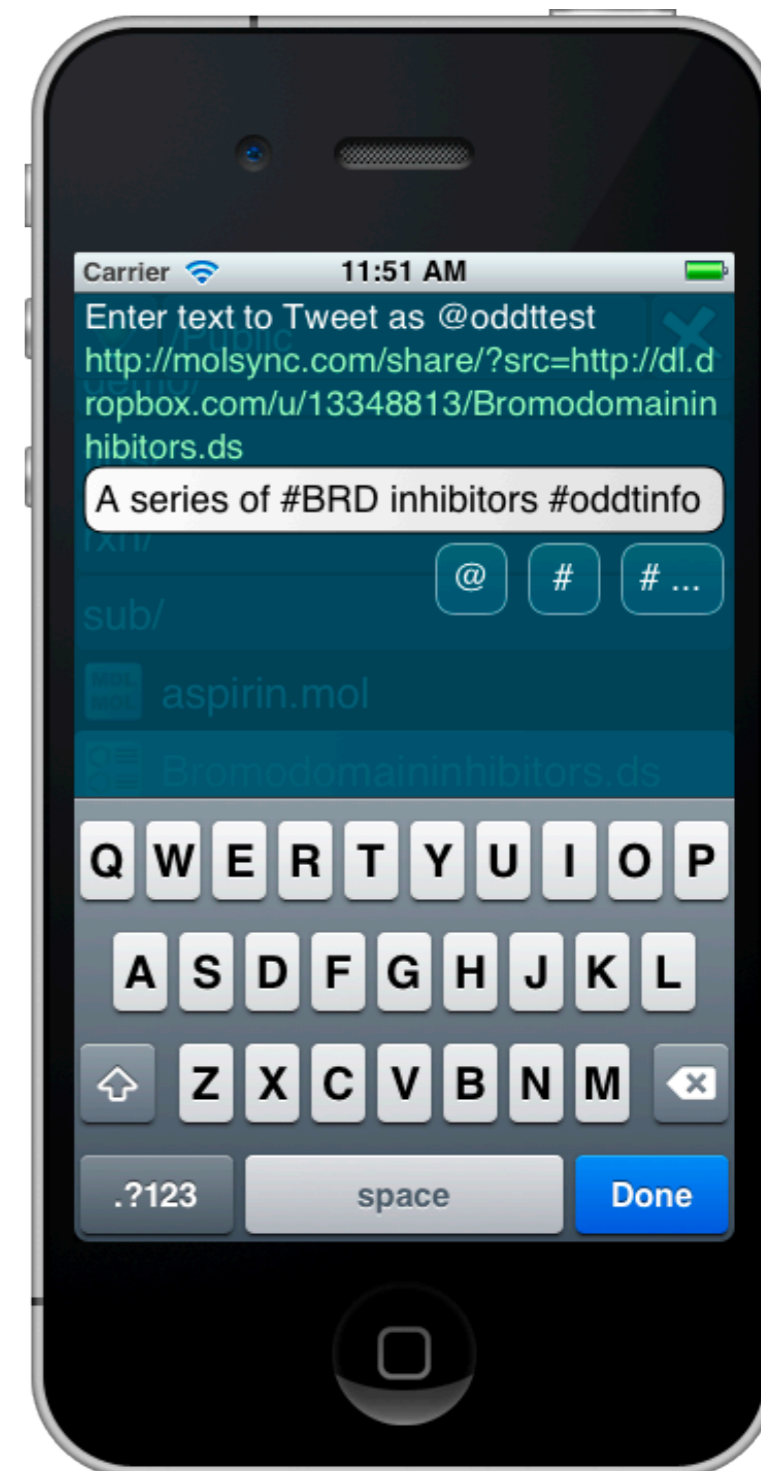
Product	Molecular Formula	Molecular Weight	Equivalents	Mass	Moles	Yield
	C ₁₀ H ₁₀ N ₂ O	198.221 g/mol	1	0.046899 g (calculated)	0.2366 mmol (calculated)	91 %
	BF ₃	67.8062 g/mol	1			
	KCl	74.5513 g/mol	1			



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

2:26 PM 100%

aclarkxyz
[molsync.com/share/?src=htt...](#) Bromodomain inhibitors #SARTable
2/9/12 12:57 PM via iOS

MolSync Sharing

Download DataSheet

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

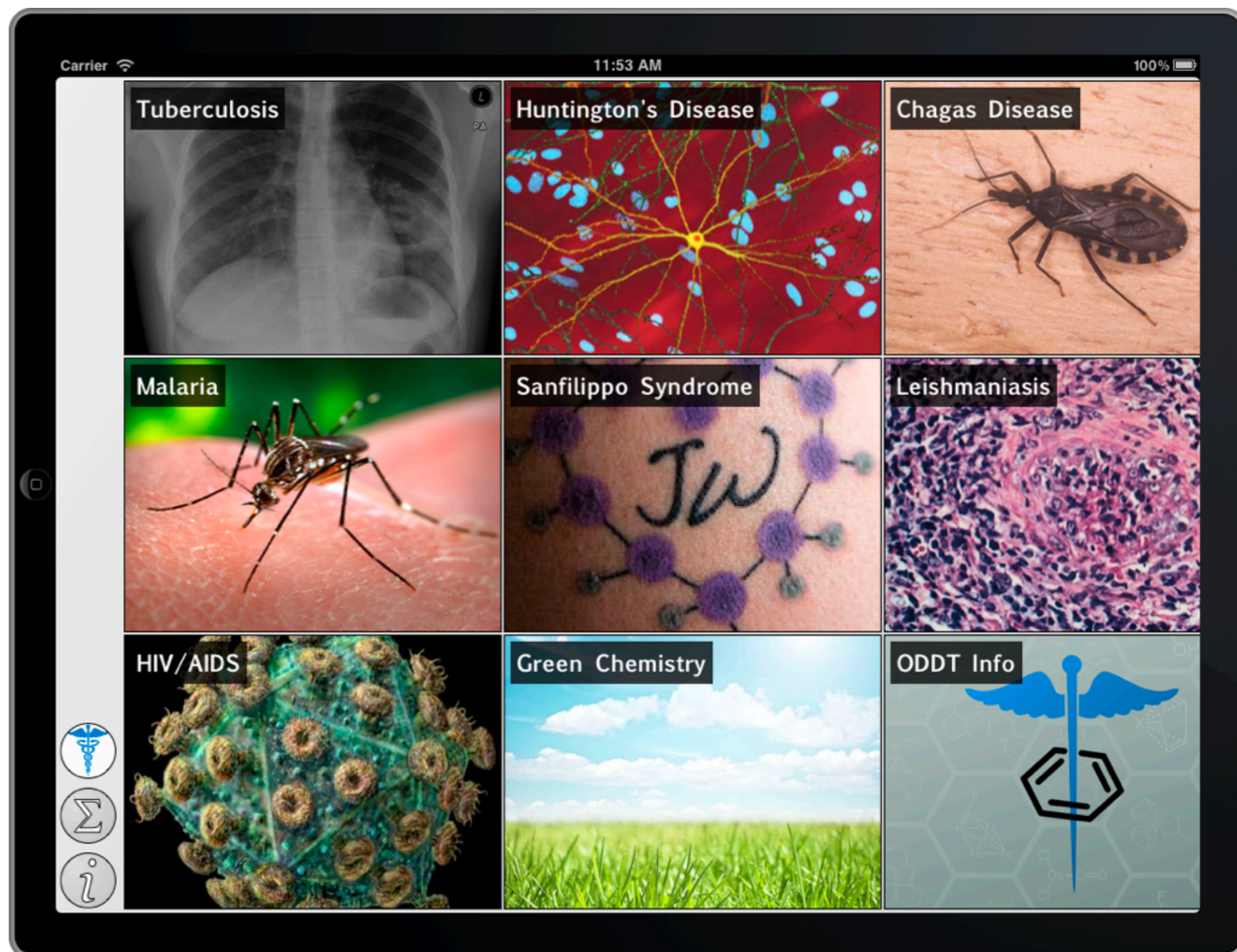
	Scaffold	R1	R2	Molecule	ID	BRD2	BRD3	BRD4
Row#1 Download		R—	R—NH—		5a	1.5 uM	1.0 uM	1.0 uM
Row#2 Download		R—O—	R—NH—		5b	1.9 uM	1.3 uM	3.0 uM
Row#3 Download		R—	R—NH—		6a	0.5 uM	0.5 uM	0.6 uM
Row#4								

MolSync Sharing

- 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
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 | C₂₇H₄₆O: (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

Steve Muskal, Maurizio Bronzetti

Eidogen-Sertanty

Peter Löw, Josef Eiblmaier, and others

InfoChem

Antony Williams

Royal Society of Chemistry

Sean Ekins

Collaborations in Chemistry

<http://molmatinf.com>

<http://molsync.com>

<http://cheminf20.org>

@aclarkxyz

