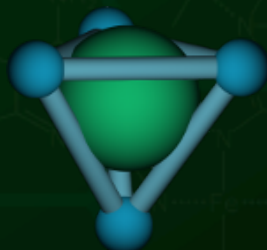


Practical cheminformatics workflows with mobile apps

Dr. Alex M. Clark

October 2012



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<http://molmatinf.com>

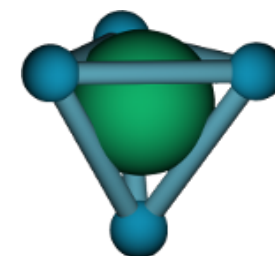
References

- Redefining Cheminformatics with Intuitive Collaborative Mobile Apps, A.M. Clark, S. Ekins, A.J. Williams, *Molecular Informatics*, **31**, 569-584 (2012)
- Mobile apps for chemistry in the world of drug discovery, A.J. Williams, S. Ekins, A.M. Clark, J.J. Jack, R.L. Apodaca, *Drug Discovery Today*, **16**, 928-939 (2011).
- Open Drug Discovery Teams: A Chemistry Mobile App for Collaboration, S. Ekins, A.M. Clark, A.J. Williams, *Molecular Informatics*, **31**, 585-597 (2012)
- Basic primitives for molecular diagram sketching, A.M. Clark, *Journal of Cheminformatics*, **2**:8 (2010).

Introduction

- Mobile apps in chemistry happening real fast: 3 years ago nothing but the most trivial of apps...
- ... now, there's a whole ecosystem. Complex workflows can be executed using just mobile apps & cloud-based infrastructure.
- Three core concepts:
 - **content consumption**
 - **content creation**
 - **communication and sharing**
- *Molecular Materials Informatics* founded with the goal of making mobile + cloud solutions into a viable replacement for cheminformatics infrastructure

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App Functionality

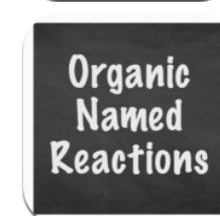
Most chemistry apps concentrate on at least one of:

- 1) Information delivery
- 2) Catalog lookup
- 3) Data visualisation
- 4) Data creation
- 5) Lab notebook
- 6) Collaboration & sharing

For a detailed list, see **www.scimobileapps.com**

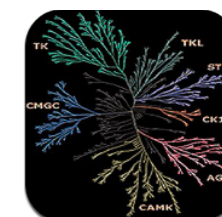
I. Information delivery

- Many apps designed for mainly one-way transmission of information, i.e. *content consumption*
 - **Green Solvents**
 - **Approved Drugs**
 - **The Elements**
 - **ACS Mobile, RSC Mobile**
 - **Reagents, Organic Named Reactions,**
- Typically a very simple user interface: close to zero learning curve
- Many for education, but some are relevant to professionals
- Mobile devices very well suited for these types of apps: quite easy to produce, and can be very useful, despite their limited capacity



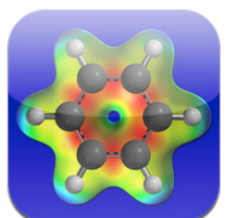
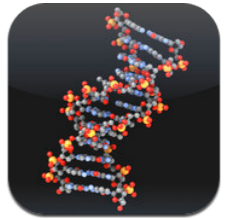
2. Catalog lookup

- Apps designed to input a search query, submit the query to a server, then display and utilise the results
- Examples include:
 - **ChemSpider Mobile**
 - **SPRESImobile**
 - **Mobile Reagents**
 - **iKinase**
 - **iProtein**
- These apps are moderately difficult to produce; most of the action takes place on remote servers, i.e. hosting the data and the search algorithms



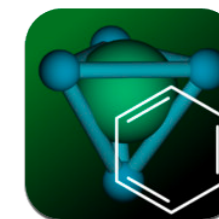
3. Data visualisation

- Apps designed to visualise existing chemical data, e.g. PDB entries, docking results, structure-activity relationships and collections of molecules
- Examples include:
 - **Molecules**
 - **PyMol**
 - **SAR Table**
 - **iMolView**
 - **iSpartan**
 - **iMolecule Builder**



4. Data creation

- Some of the most sophisticated apps provide the ability to assemble chemical data within the app:
 - molecular structures
 - reactions
 - scalar data
 - higher order markup (SAR)
- Data can be created with the app UI, or pieces can be imported from other sources. Examples:
 - **Mobile Molecular DataSheet (MMDS)**
 - **MolPrime**
 - **SAR Table**
 - **Chirys, ChemDoodle Mobile, ChemJuice**



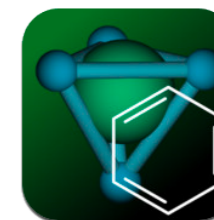
5. Lab notebooks

- Apps designed for entering information about experiments
- Ultimate objective is the paperless laboratory
- Mobile laboratory notebooks are mostly generic rather than chemically aware, i.e. not specifically for synthesis
- Prototypical example is **Yield101** (education focused)
- General purpose scientific lab notebook apps:
 - **LabGuru**
 - **irisnote**
- Many web-based lab notebooks that are vendor-endorsed for iPad use



6. Collaboration and sharing

- Apps have many options for sharing and importing data, e.g.
 - Email (personal, bidirectional)
 - Remote hosting (private, collaborative)
 - Web sharing and tweeting (global, open)
- Examples:
 - **MMDS**
 - **MolSync**
 - **Reaction 101**
 - **ODDT**



Mobile app limitations

- Touchscreen is small, inaccurate, and doubles as a keyboard
- Modern mobile processors are fast (Moore's law), but respecting battery life requires careful conservation of CPU resources
- Limited memory and constricted multi-tasking: an app has a tightly defined lifespan, and is expected to be lightweight, low-state
- Persistent storage is limited and relatively inconvenient to access
- Functionality and making use of data is heavily network dependent
- Limited choice of development environments: *native* or *web*, stark choice of quality vs. portability



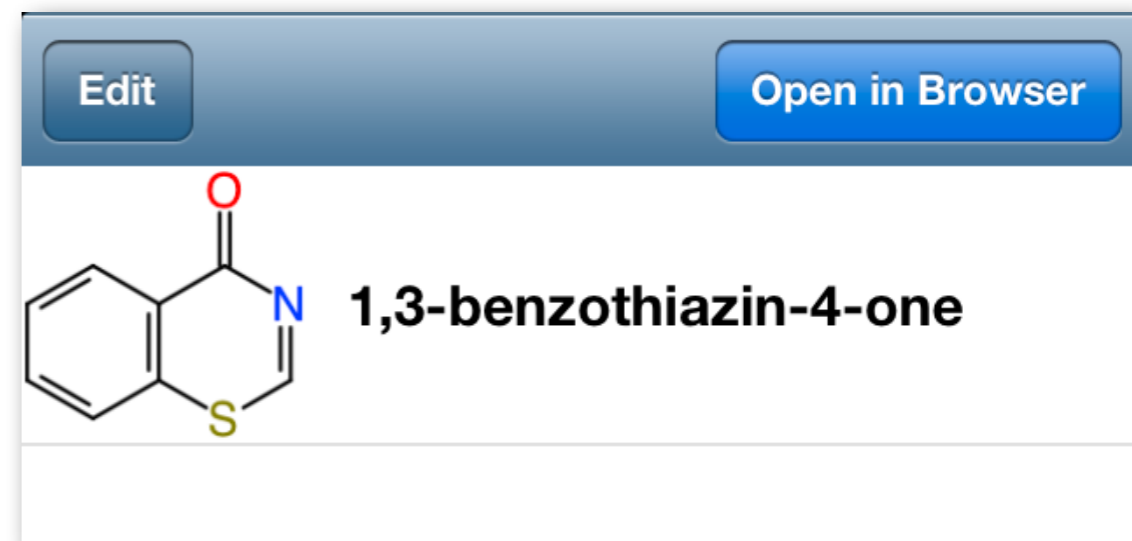
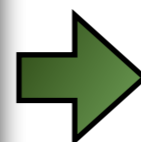
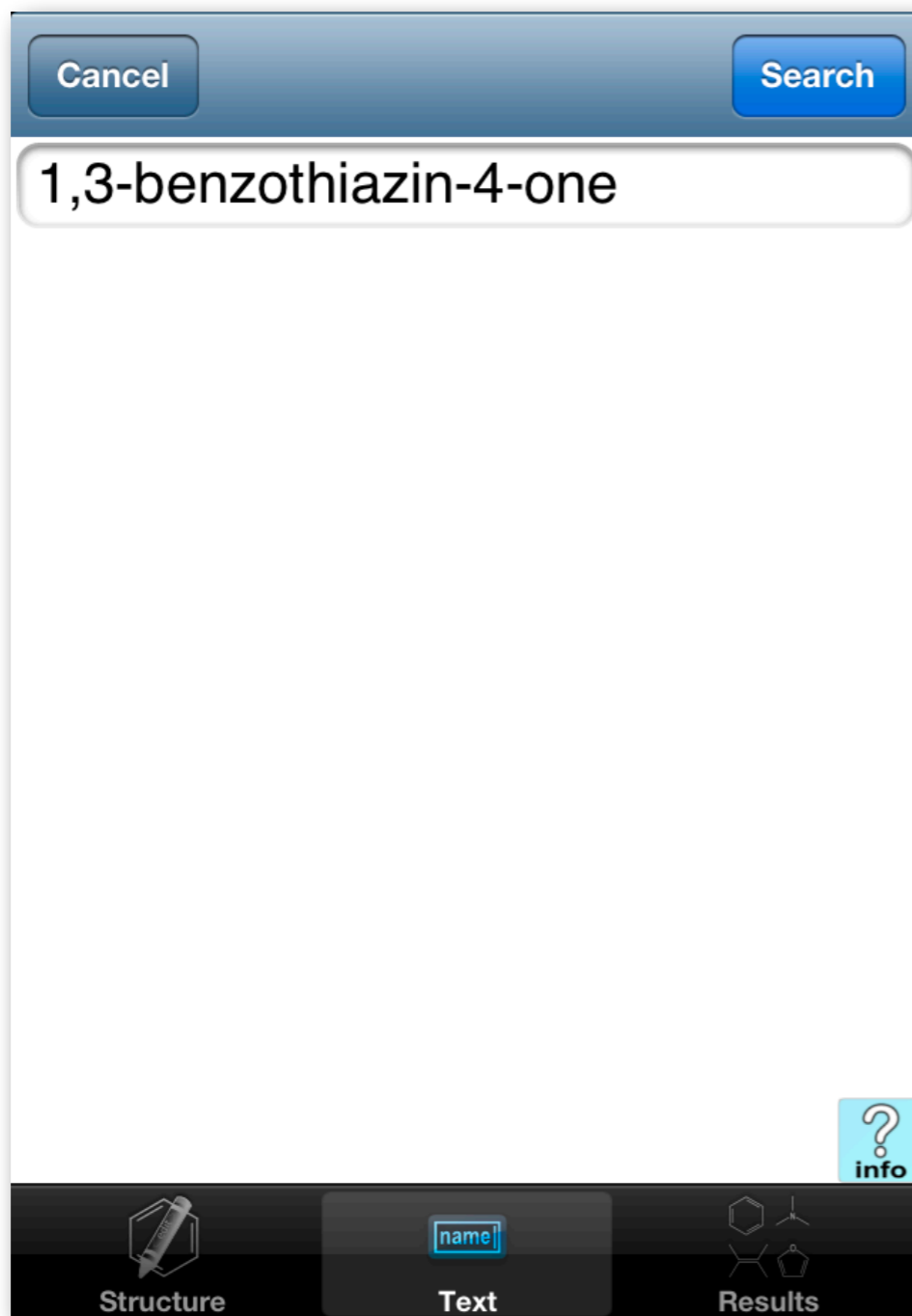
- When these limitations can be overcome, the mobile + cloud combination becomes a *full replacement for desktop computing*

Workflow

- The following slides demonstrate a multipart workflow scenario using:
 - **iOS** apps (Apple iPhone/iPod/iPad)
 - cloud-hosted webservice
- Each step is carried out using technology that is currently available...
- ...and is representative of the state of the art.
- The sequential tasks are based on a medicinal chemistry exploration: investigating new *tuberculosis* drugs
- Any workflow with a similar level of technology is probably either already possible, or could be made possible.

Step 1: Lookup

- Lookup a core scaffold for a series of known *tuberculosis* inhibitors using the *ChemSpider Mobile* app:



ChemSpider

1,3-benzothiazin-4-one | C₈H₅NOS | ChemSpider

www.chemspider.com/C Search

ChemSpider The free chemical database

RSC Advancing the Chemical Sciences

About More Searches Web APIs Help eg. Pyridine Search

1,3-benzothiazin-4-one

ChemSpider ID: 14339264
Molecular Formula: C₈H₅NOS
Average mass: 163.196396 Da
Monoisotopic mass: 163.009186 Da

Systematic name
4H-1,3-Benzothiazin-4-one

SMILES and InChIs
Cite this record

2D 3D Save Zoom

Names and Identifiers
ChemS
Propert
Spectra
CIFs
Articles
Data Sources
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Open in MMDS

Open in ChemSpider

Cancel

- View *ChemSpider* record in mobile browser
- Structure can be downloaded as MDL Molfile
- Mofiles can be opened *directly in apps*
- Select *Mobile Molecular DataSheet (MMDS)*

Step 2: Lookup a datasheet



- Imported molecular structure into the *scratch sheet*

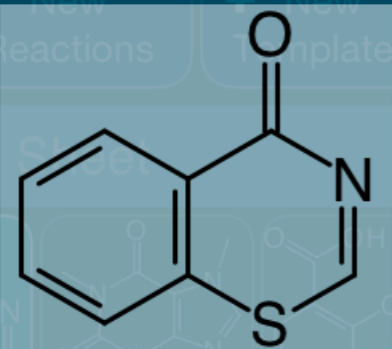


- Open the *Run Webservice* feature...

ChEBI Query

Mobile Molecular DataSheet

Structure:



Paste Select Edit

Search Type:

Exact

Substructure

Similar95%

Similar90%

Similar80%

Similar50%

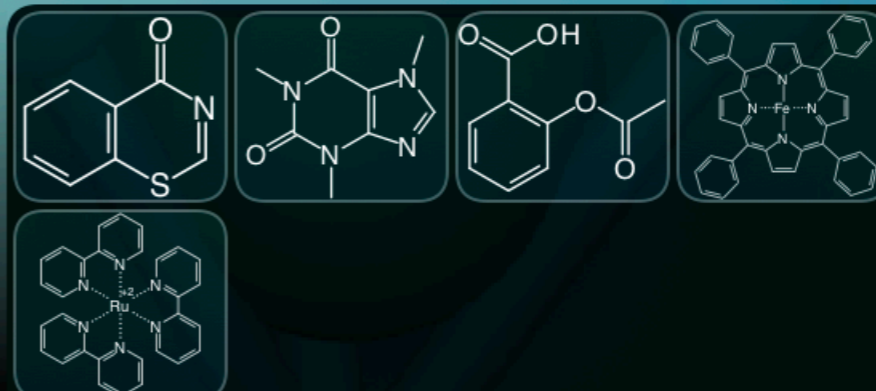
Execute Cancel



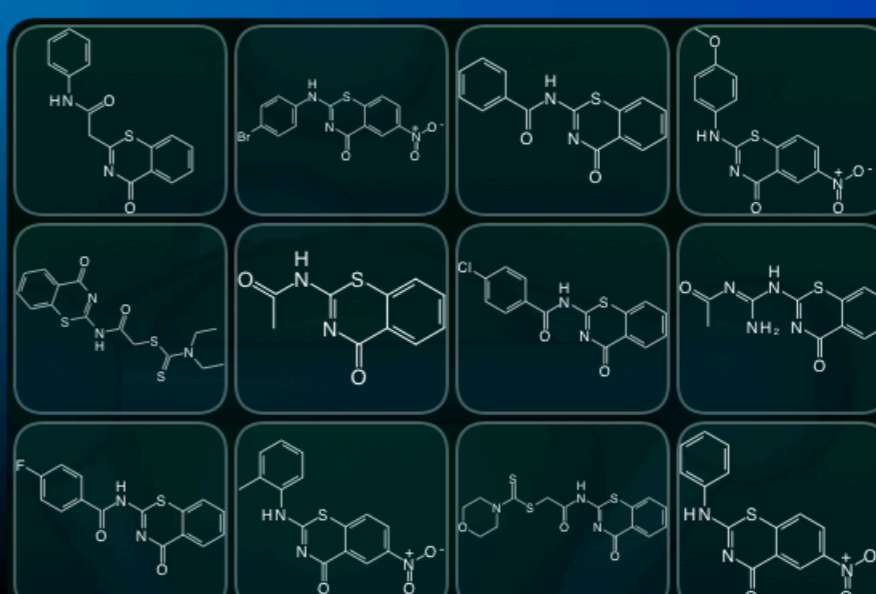
Mobile Molecular DataSheet

+ New DataSheet + New Reactions + New Templates * Run Webservice

Scratch Sheet

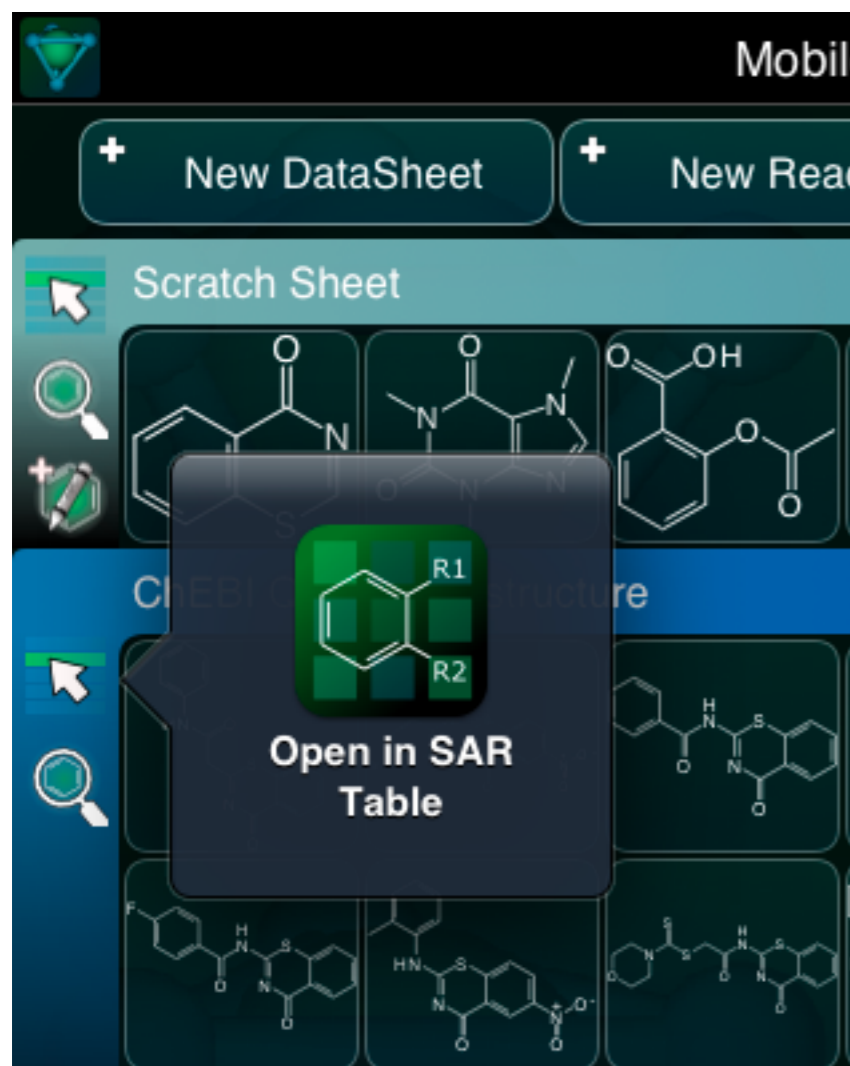


ChEBI Query: Substructure



- Substructure search for the core scaffold produces a new datasheet

Step 3: Assign scaffolds



Scaffold	Molecule	Name	Link
		CHEBI:827437	http://www.ebi.ac.uk/chebi/search.do?chebiid=CHEBI:827437
		CHEBI:860499	http://www.ebi.ac.uk/chebi/search.do?chebiid=CHEBI:860499
		CHEBI:862386	http://www.ebi.ac.uk/chebi/search.do?chebiid=CHEBI:862386
		CHEBI:911375	http://www.ebi.ac.uk/chebi/search.do?chebiid=CHEBI:911375
		CHEBI:912856	http://www.ebi.ac.uk/chebi/search.do?chebiid=CHEBI:912856
		CHEBI:934172	http://www.ebi.ac.uk/chebi/search.do?chebiid=CHEBI:934172

- Open in *SAR Table* app...
- ... which represents a table of compounds as **scaffolds** & **substituents**

1

Scaffold	Molecule	Name	Link
		CHEBI:827437	http://www.ebi.ac.uk/chebi/searchId.do?chebiId=CHEBI:827437
		CHEBI:860499	http://www.ebi.ac.uk/chebi/searchId.do?chebiId=CHEBI:860499



2

Scaffold	R1	R2	R3	Molecule	Name
	?	?	?		CHEBI:827437
	n/a	n/a	n/a		CHEBI:860499



3

Match scaffold:



5

Scaffold	R1	R2	R3	Molecule	Name
		R-H	R-H		CHEBI:827437
	n/a	n/a	n/a		CHEBI:860499



4

R1	R2	Scaffold	Molecule	R1	Name	R2	R3
?	?				CHEBI:827437	R-H	R-H

Scaffolds + Substituents

The screenshot displays a mobile application interface for building chemical structures. The main area is a grid with columns for Scaffold, R1, R2, R3, Molecule, Molecule..., IC50, Name, and Link. The Scaffold column shows a benzothiazine-like core with R1, R2, and R3 substituents. The R1, R2, and R3 columns show various substituent options, such as -NH₂, -NH-C(=O)-R, -NH-C(=O)-C(=O)-R, -NH-C(=O)-C₆H₅, -NH-C(=O)-C₆H₄-F, -NH-C(=O)-C₆H₄-Cl, -NH-C(=O)-C₆H₄-N(CH₂)₂-R, -NH-C₆H₅, -NH-C₆H₄-N(CH₂)₂-R, and -NH-C₆H₄-N(CH₂)₂-R. The Molecule column shows the resulting structure for each combination. The Molecule... column shows the SMILES string for each molecule. The IC50 column is empty. The Name column shows the name of each molecule. The Link column shows the URL for each molecule. At the bottom of the screen, there is a toolbar with various editing tools, including a checkmark, a refresh icon, a zoom icon, a person icon, a pencil icon, an up arrow, a down arrow, a left arrow, a right arrow, a 100% zoom icon, a grid icon, a landscape icon, a cube icon, and a gear icon.

Scaffold	R1	R2	R3	Molecule	Molecule...	IC50	Name	Link
	R-NH ₂	R-H	R-H		CHEBI:1196979			http://www.ebi.ac.uk/chebi/search.do?chebiid=CHEBI:1196979
	R-NH-C(=O)-R	R-H	R-H		CHEBI:934172			http://www.ebi.ac.uk/chebi/search.do?chebiid=CHEBI:934172
	R-NH-C(=O)-C(=O)-R	R-H	R-H		CHEBI:1014377			http://www.ebi.ac.uk/chebi/search.do?chebiid=CHEBI:1014377
	R-NH-C(=O)-C ₆ H ₅	R-H	R-H		CHEBI:862386			http://www.ebi.ac.uk/chebi/search.do?chebiid=CHEBI:862386
	R-NH-C(=O)-C ₆ H ₄ -F	R-H	R-H		CHEBI:1019789			http://www.ebi.ac.uk/chebi/search.do?chebiid=CHEBI:1019789
	R-NH-C(=O)-C ₆ H ₄ -N(CH ₂) ₂ -R	R-H	R-H		CHEBI:827437			http://www.ebi.ac.uk/chebi/search.do?chebiid=CHEBI:827437
	R-NH-C(=O)-C ₆ H ₄ -N(CH ₂) ₂ -R	R-H	R-H		CHEBI:1081605			http://www.ebi.ac.uk/chebi/search.do?chebiid=CHEBI:1081605
	R-NH-C(=O)-C ₆ H ₄ -Cl	R-H	R-H		CHEBI:969320			http://www.ebi.ac.uk/chebi/search.do?chebiid=CHEBI:969320
	R-NH-C(=O)-C ₆ H ₄ -N(CH ₂) ₂ -R	R-H	R-H		CHEBI:912856			http://www.ebi.ac.uk/chebi/search.do?chebiid=CHEBI:912856
	R-NH-C ₆ H ₅	R-H	R-N ⁺		CHEBI:1067881			http://www.ebi.ac.uk/chebi/search.do?chebiid=CHEBI:1067881
	R-NH-C ₆ H ₄ -N(CH ₂) ₂ -R	R-H	R-N ⁺		105663			http://www.ebi.ac.uk/chebi/search.do?chebiid=CHEBI:1105663
	R-NH-C ₆ H ₄ -N(CH ₂) ₂ -R	R-H	R-N ⁺		022502			http://www.ebi.ac.uk/chebi/search.do?chebiid=CHEBI:022502

- Structure-activity relationship is aided by classifying **scaffold** and **substituents**
- Assignment process is partly manual, partly automated
- Structure fragments can be drawn within the app, copied from other cells, or computed by a webservice

Step 4: Merge

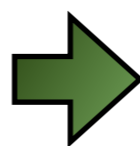
- Have existing table, created from literature data:
 - V. Makarov et al., Benzothiazinones kill Mycobacterium tuberculosis by blocking arabinan synthesis, *Science* **324**, pp. 801-804 (2009)
- Activity values colour-coded by defining a *scheme*
- Append the query data to the end...

Scaffold	R1	R2	R3	Molecule	Molecule Name	IC ₅₀
					10526038	1 μM
					10526043	1 μM
					10526044	1 μM
					10526046	500 μM
					10526045S	500 μM
					10526045R	5000 μM
					10526032	50 μM
					10526035	50 μM

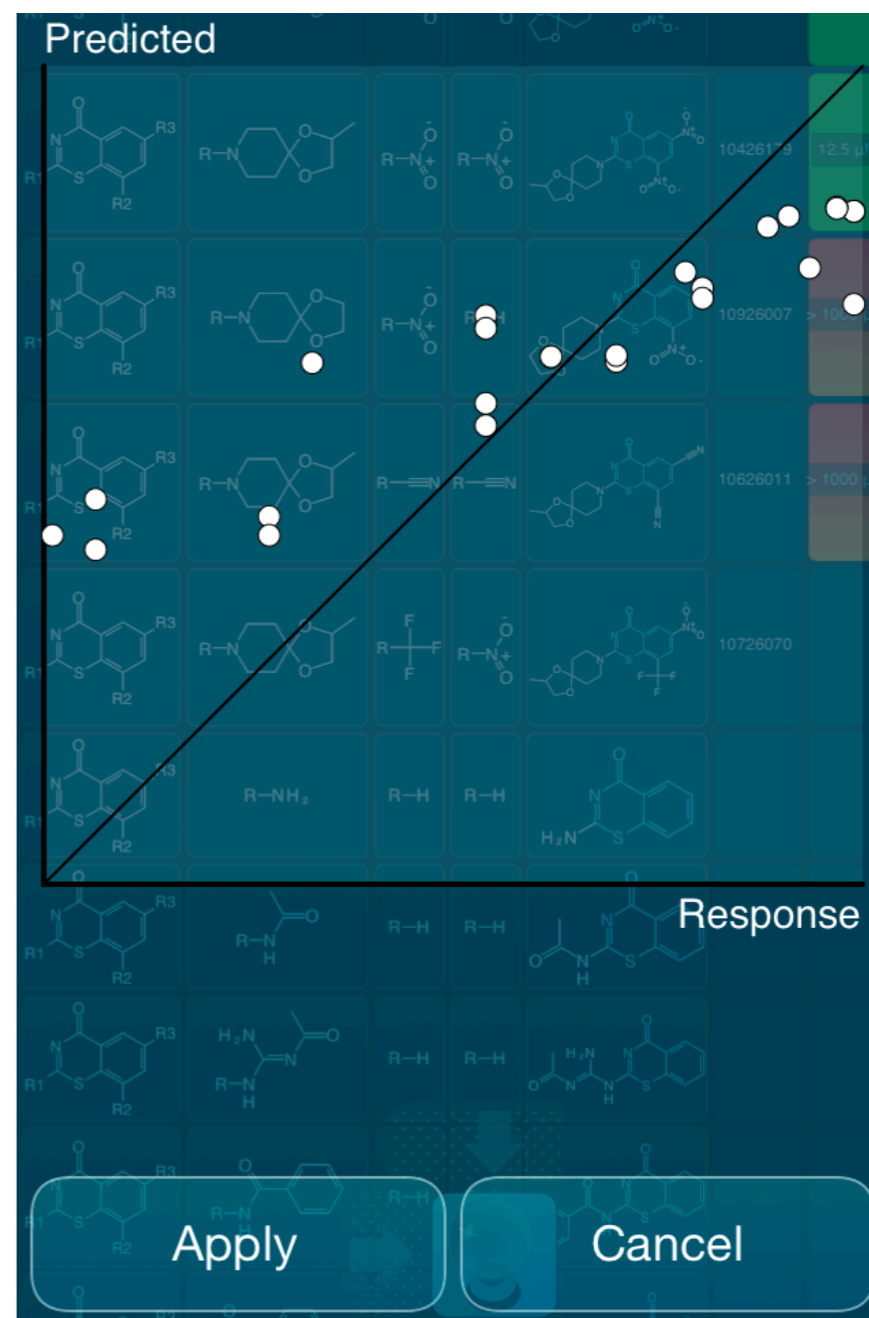
Appended rows

- Webservice builds a model based on existing activity values
- Applies predictions to missing values

Scaffold	R1	R2	R3	Molecule	Molecule Name	IC ₅₀
					10426177	12.5 μM
					10426179	12.5 μM
					10926007	> 1000 μM
					10626011	> 1000 μM
					10726070	



blank activity



Step 5: Examine SAR

Scaffold	R1	R2	R3	Molecule	Molecule Name	IC ₅₀
					10426179	12.5 μM
					10926007	> 1000 μM
					10626011	> 1000 μM
					10726070	

matrix view



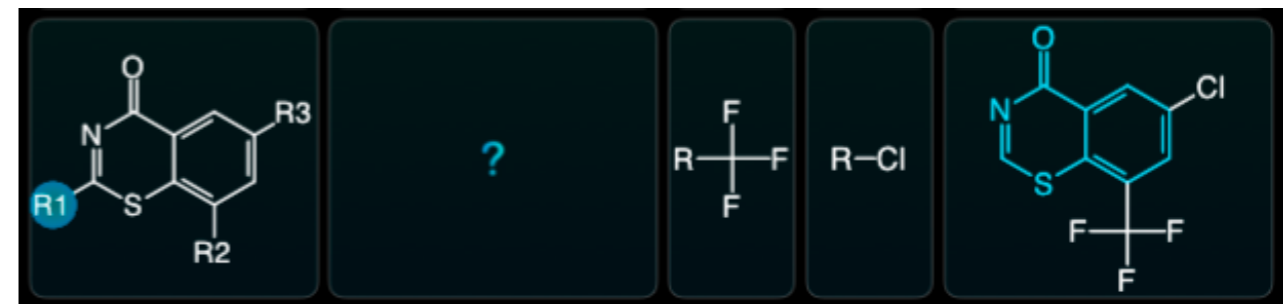
R3					
R2					
	1 μM .. 50 μM	50 μM	1 μM, 25 μM	12.5 μM	> 1000 μM
	500 μM				
	500 μM, 5000 μM				
		> 1000 μM			

- Predicted values suggest some promising **R2** & **R3** substituents, based on known compounds
- These are from ChEBI, so can be looked up

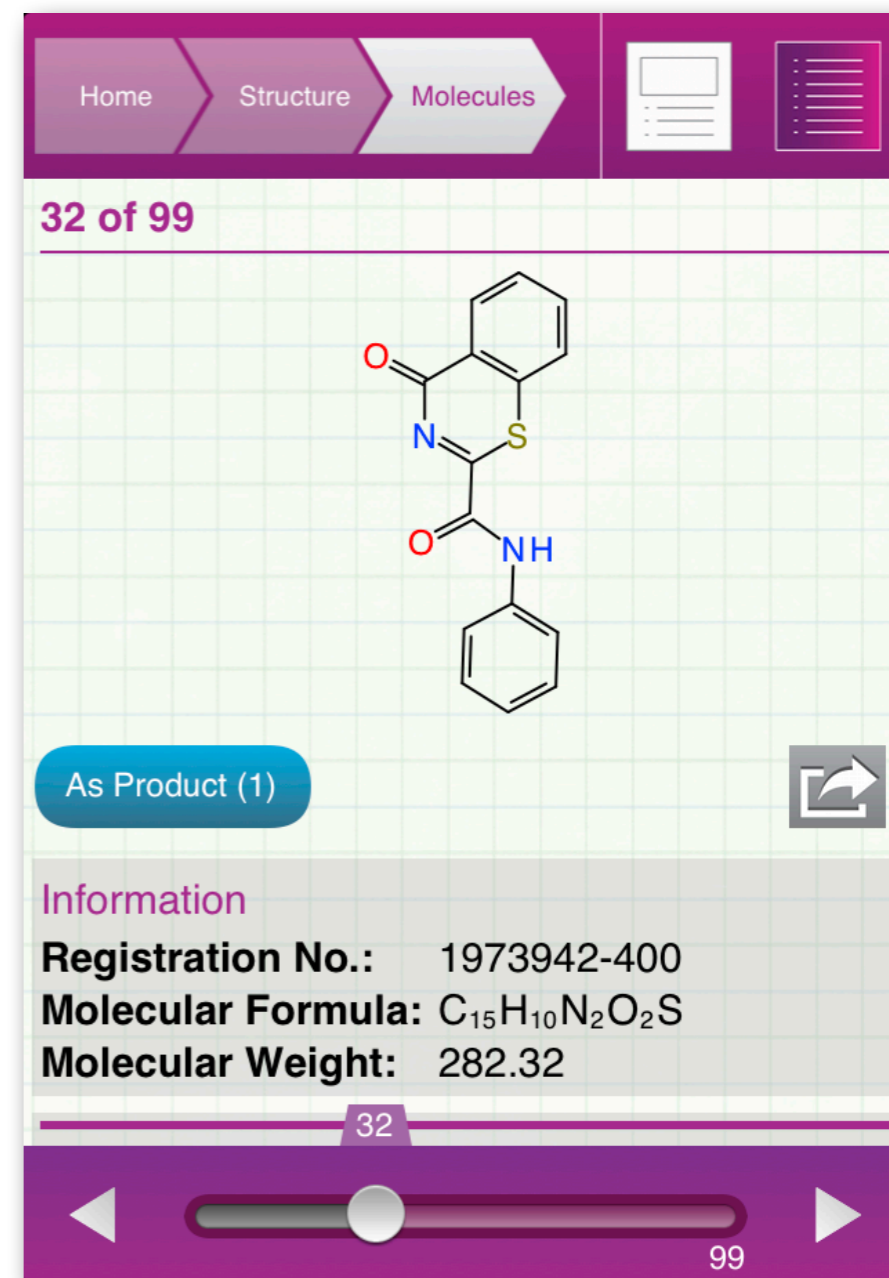
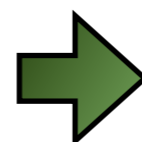
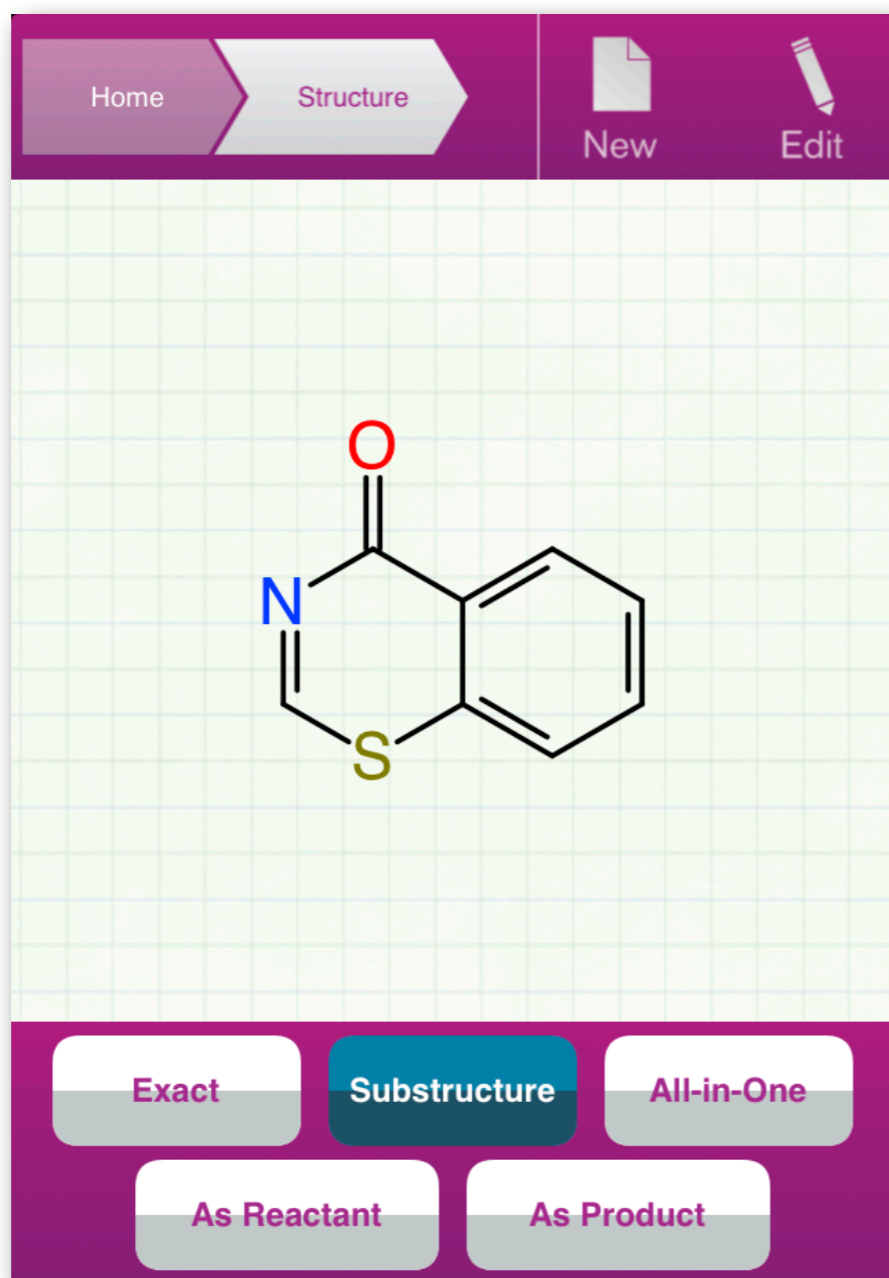
Step 6: Propose new lead

✓ R3	$\text{R}-\text{C}(\text{F})_3$	$\text{R}-\text{C}\equiv\text{N}$	$\text{R}-\text{Cl}$	$\text{R}-\text{N}^+\text{O}^-$	$\text{R}-\text{H}$
R2					
$\text{R}-\text{N}^+\text{O}^-$	1 μM .. 50 μM	50 μM	1 μM , 25 μM	12.5 μM	> 1000 μM
$\text{R}-\text{N}(\text{H})\text{OH}$	500 μM				
$\text{R}-\text{NH}_2$	500 μM , 5000 μM				
$\text{R}-\text{C}\equiv\text{N}$		> 1000 μM			
$\text{R}-\text{C}(\text{F})_3$					
$\text{R}-\text{H}$					

- Identify values for **R2** and **R3** by examining current *structure-activity relationship*
- Create a new row with the proposed substituent moieties:



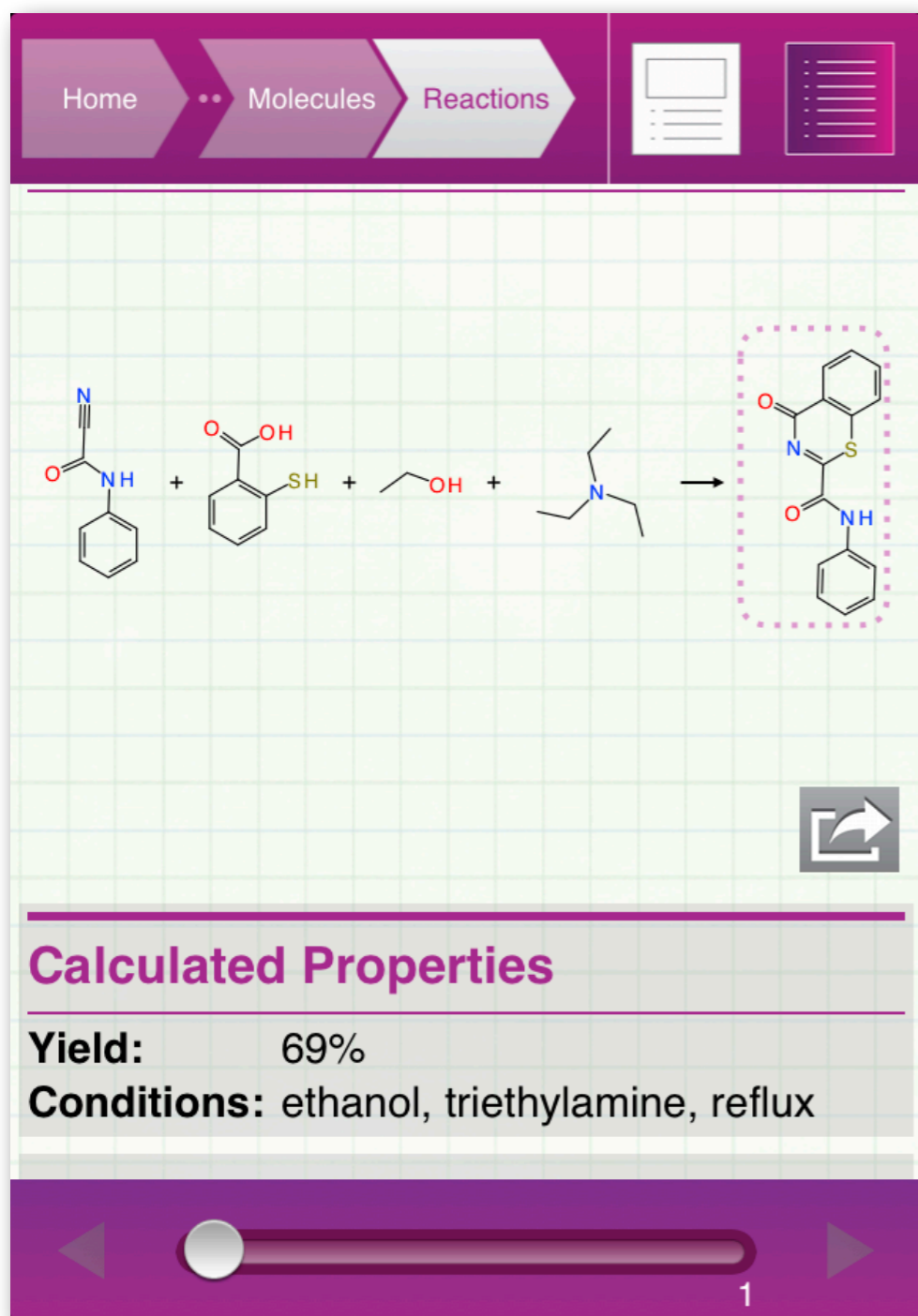
Step 7: Find a recipe



- Open the core structure in *SPRESImobile* app
- Search for similar structures, and search As Product to find a promising synthesis that can be adapted

Find reaction

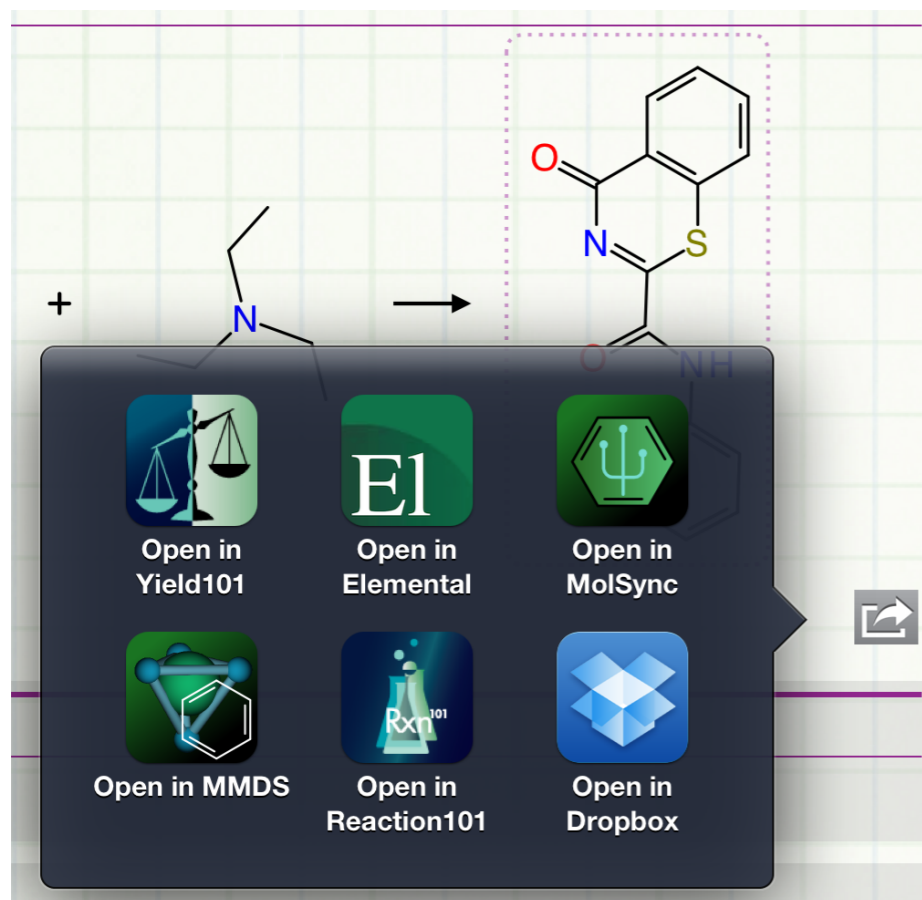
- Found a promising synthesis
- Starting materials suitable for desired functionalisation
- Link to literature provided within the app: can be opened in *Safari Mobile*



Journal Articles

SHERIF, SHERIF MOURAD;MOHAREB, RAFAAT MILAD;ELGEMEIE, GALAL ELDIN H., "NITRILES IN HETEROCYCLIC SYNTHESIS: 1-CYANOFORMANILIDE AS PRECURSOR FOR A VARIETY OF HETEROCYCLIC RING SYSTEMS", Heterocycles, vol. 27, pp. 1579-1583 (1988)
<http://dx.doi.org/10.3987/COM-88-4559>

Step 8: Plan synthesis



Software interface showing a reaction scheme with five components and their associated data fields:

Component	Yield	Personal	Public	Solvent
1	146.45 g/mol	Equiv: 1	Mass: []	0%
2	154.19 g/mol	Equiv: 1	Mass: []	0%
3	46.07 g/mol	Equiv: 1	Mass: []	0%
4	101.19 g/mol	Equiv: 1	Mass: []	0%
5	282.32 g/mol	Equiv: 1	Mass: []	0%

Additional fields for each component: Volume, Moles, Density, Conc, Primary. A 'Process Mass Intensity: unknown / unknown = ?' bar is visible at the bottom.

- Can open the reaction with **Yield101** app: scheme is transferred
- Need to customise the reaction components and add quantities
- Have the literature reference on hand

Adapt synthesis



The screenshot displays a chemical synthesis interface with the following components:

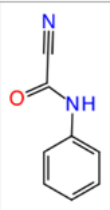
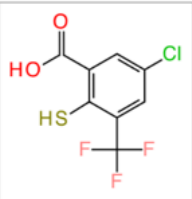
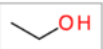
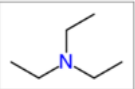
- Reaction Scheme:** A reaction showing four reactants on the left and one product on the right. The reactants are: 1. A benzamide derivative with a cyano group (146.15 g/mol). 2. A thiol derivative with a chlorine and a trifluoromethyl group (256.63 g/mol). 3. Ethanol (46.07 g/mol). 4. Diethylamine (101.19 g/mol). The product is a complex heterocyclic molecule (384.76 g/mol).
- Input Fields:** Below each reactant and the product, there are input fields for Equiv., Mass, Volume, Moles, Density, Conc., and Primary. The values are: Reactant 1 (Equiv: 1, Mass: 5.69483 g, Moles: 0.0389667 mol), Reactant 2 (Equiv: 1, Mass: 10 g, Moles: 0.0389667 mol), Ethanol (Equiv: 0, Mass: 78.9 g, Volume: 100 mL, Density: 0.789 g/mL, Moles: 1.71267 mol), Diethylamine (Equiv: 1.1, Mass: 4.33734 g, Volume: 5.9743 mL, Density: 0.726 g/mL, Moles: 0.0428634 mol), and Product (Equiv: 1, Mass: 10.3451 g, Moles: 0.026887 mol, Yield: 69%).
- Progress Indicators:** At the bottom of each column, there are progress bars with percentages: 6%, 10%, 80%, 4%, and 100%. Each bar has a 'more' button next to it.
- Process Mass Intensity:** A summary bar at the bottom shows: Process Mass Intensity: 98.932 g / 10.345 g = 9.563.

- Edit structure **reactant** and **product** to include functional groups
- Specify known quantities and expected yield: all implied quantities are calculated, as is the *process mass intensity*

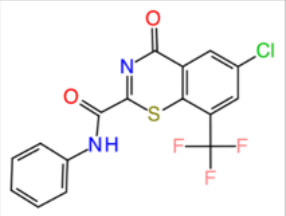
Run the experiment

Done Print

Reactants

	Molecular Formula: $C_8H_6N_2O$ Molecular Weight: 146.146 g/mol Equivalents: 1 Mass: 5.69483 g (calculated) Moles: 0.0389667 mol (calculated)
	Molecular Formula: $C_8H_4ClF_3O_2S$ Molecular Weight: 256.629 g/mol Equivalents: 1 Mass: 10 g Moles: 0.0389667 mol (calculated) (Primary Reactant)
	Molecular Formula: C_2H_6O Molecular Weight: 46.0684 g/mol Equivalents: 0 Mass: 78.9 g (calculated) Volume: 100 mL Moles: 1.71267 mol (calculated) Density: 0.789 g/mL
	Molecular Formula: $C_6H_{15}N$ Molecular Weight: 101.19 g/mol Equivalents: 1.1 Mass: 4.33734 g (calculated) Volume: 5.9743 mL (calculated) Moles: 0.0428634 mol (calculated) Density: 0.726 g/mL

Products

	Molecular Formula: $C_{16}H_8ClF_3N_2O_2S$ Molecular Weight: 384.76 g/mol Equivalents: 1 Mass: 10.3451 g (calculated) Moles: 0.026887 mol (calculated) Yield: 69 %
---	---

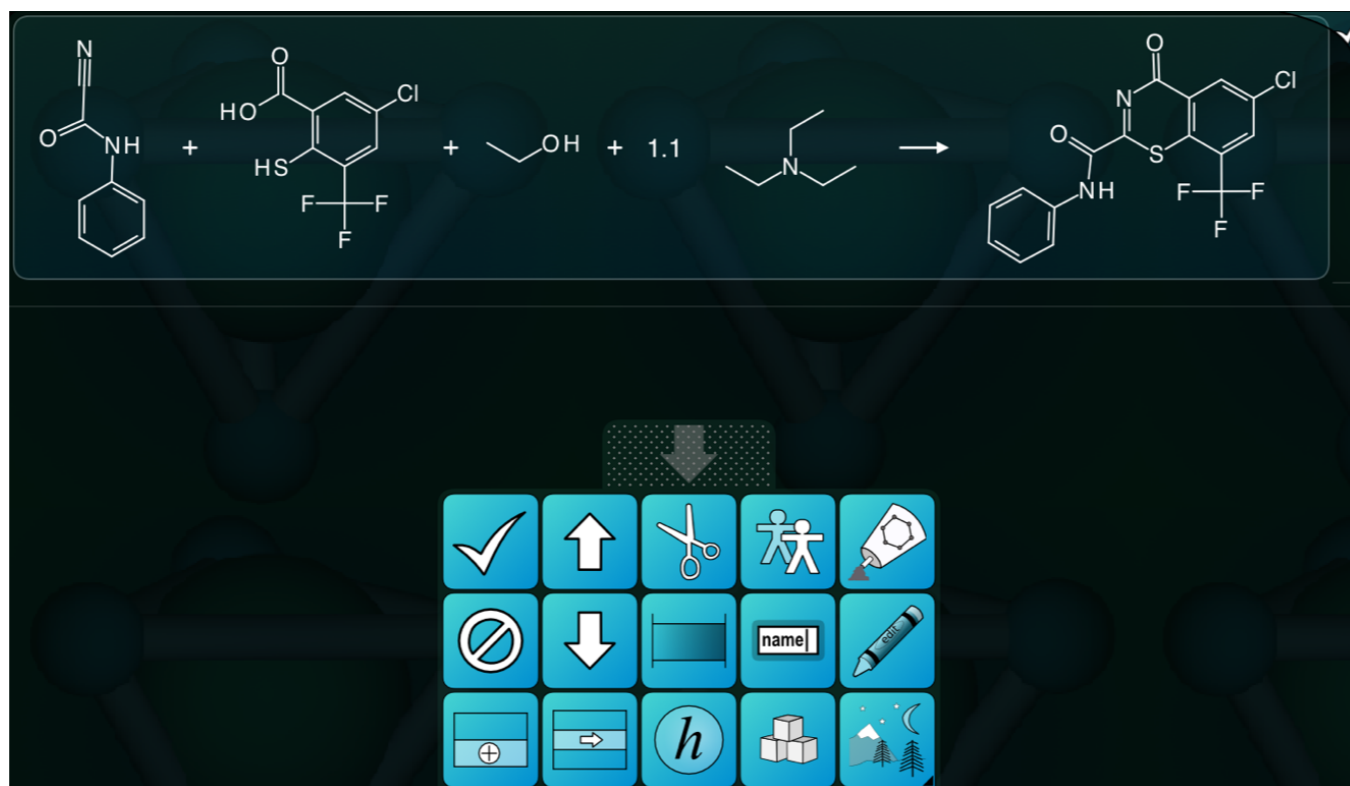
- Can use the mobile device in the lab, and record the results directly

OR:

- Create a PDF document, and print it directly from the device or send the file by email...
- ... then enter the results later.

Step 9: Sharing data

- *Many ways to share data: use Open-With to transfer to MMDS*



- From there, can:
 - send data by email
 - export presentation quality graphics
 - share on web & tweet
 - upload to repositories, e.g. Dropbox

Microsoft Office documents

Cancel Reaction DataSheet Send

To: info@molmatinf.com

Cc/Bcc, From: aclark.xyz@gmail.com

Subject: Reaction DataSheet

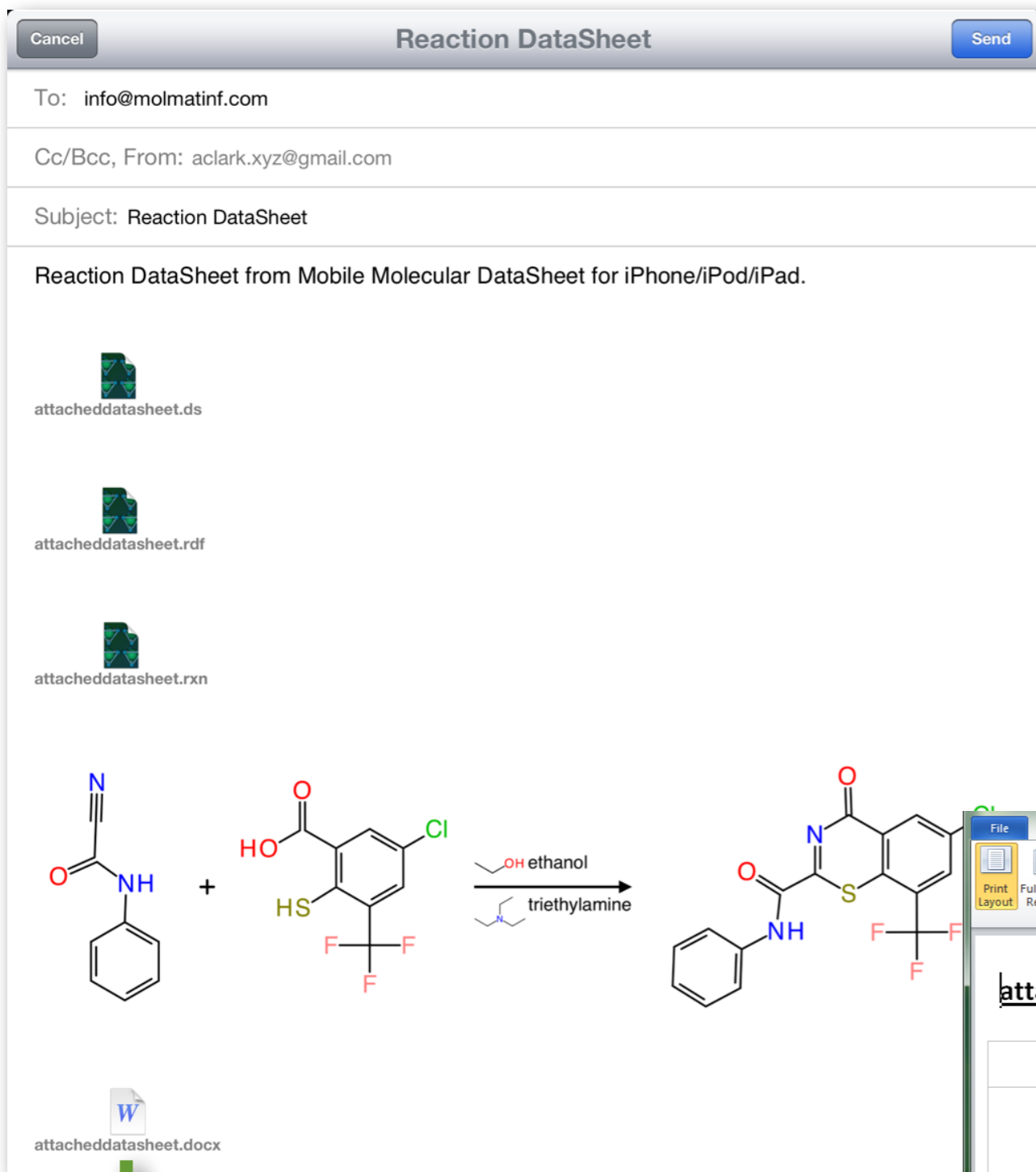
Reaction DataSheet from Mobile Molecular DataSheet for iPhone/iPod/iPad.

attacheddatasheet.ds

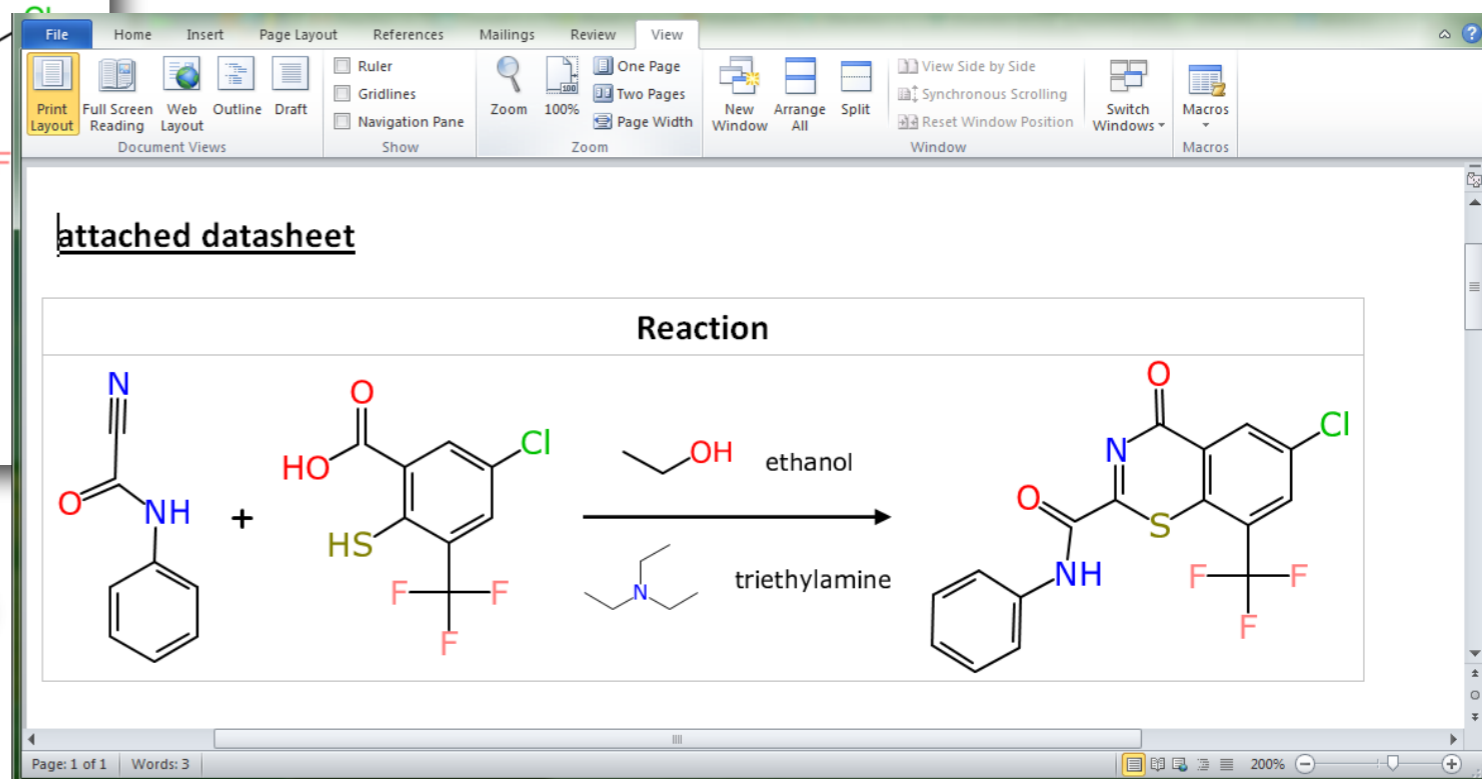
attacheddatasheet.rdf

attacheddatasheet.rxn

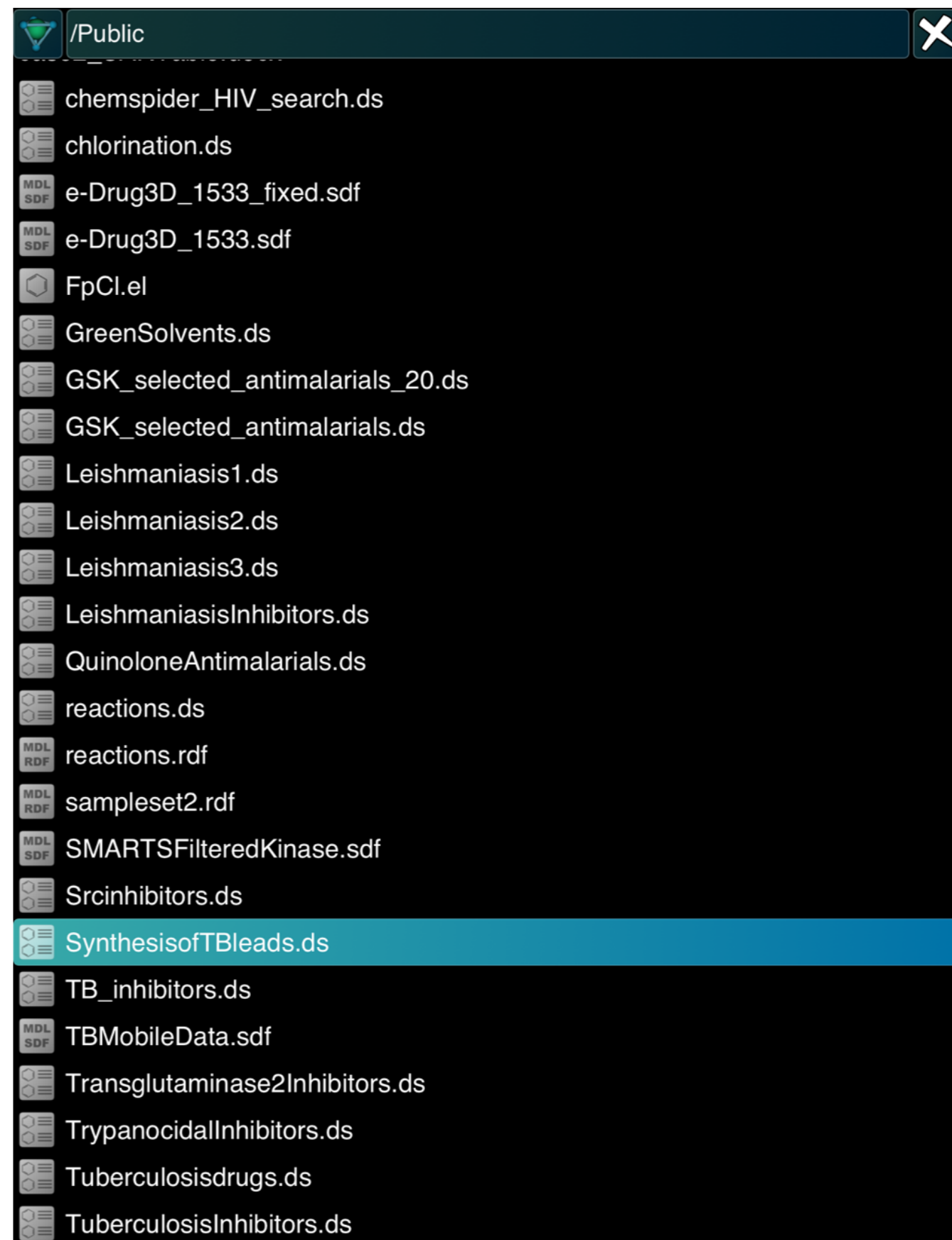
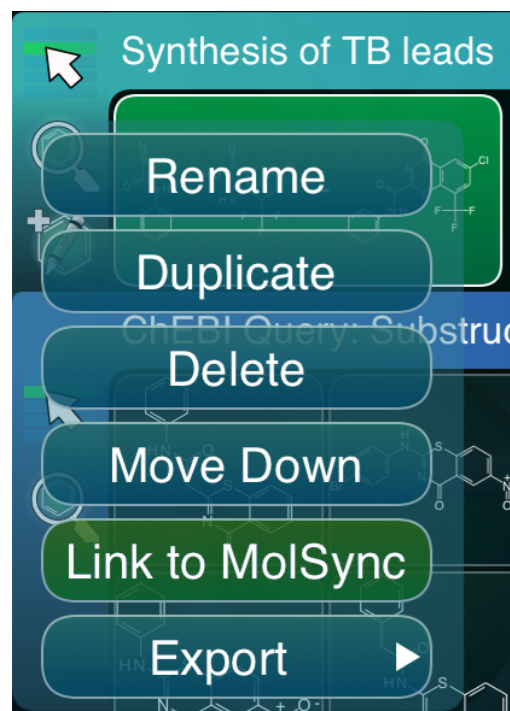
attacheddatasheet.docx



- Outgoing emails can include many attachments:
 - machine-readable data
 - graphics
- Graphics options include MS Word and Excel documents with embedded **vector** graphics



Sharing with Dropbox



- Can link datasheets to *Dropbox* using the *MolSync* app
- Storing data on *Dropbox* opens up an entire landscape of collaboration and sharing options

Step 10: Open sharing

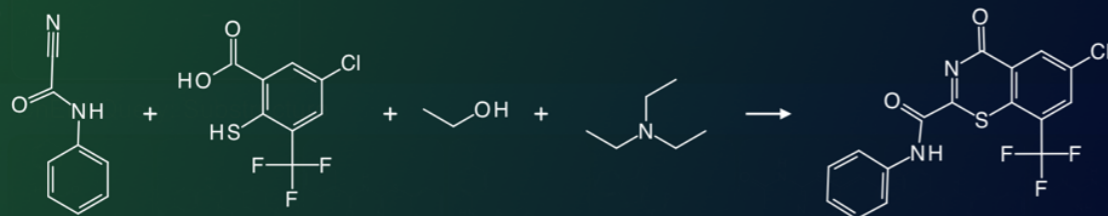
Twitter Account

Confirm the account from which to tweet:

- aclarkxyz
- oddtinfo
- ODDTTest

Content

Prior to tweeting, this data will be uploaded to molsync.com, and made publicly available:



Text

Proposed anti-TB compound

ODDT

Selecting one of the following topics will add hashtags for Open Drug Discovery Teams project:

- None
- #tuberculosis
- #malaria
- #hivaids
- #huntingtons
- #sanfilipposyndrome
- #greenchemistry
- #acsgci
- #chagas
- #leishmaniasis
- #h5n1
- #hhf4gan
- #drugrepurposing
- #rare diseases

Cancel

Tweet

MolSync Sharing

Download DataSheet

attached datasheet

Row#1	Reaction
Download	

Provided by [Molecular Materials Informatics, Inc](#)
Visit the [iTunes AppStore](#) for the mobile *MolSync* app



Alex M. Clark
@aclarkxyz

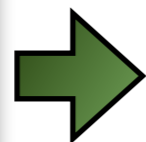
molsync.com/share?ds=36 #tuberculosis #ODDT
Proposed anti-TB compound

2012-09-26 1:11 PM

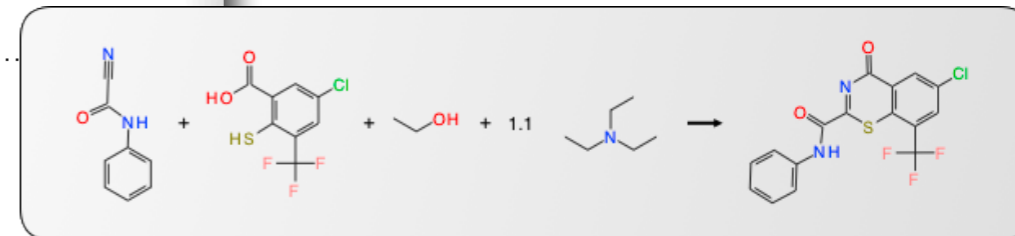


Open Drug Discovery Teams

A screenshot of a social media feed interface. At the top, there are three circular icons: a bird (Twitter), a sigma symbol (mathematics), and an 'i' (information). Below these are six rectangular tiles, each representing a different disease or topic: 'Tuberculosis' (with a chest X-ray), 'Huntington's Disease' (with a neuron diagram), 'Malaria' (with a mosquito), 'Sanfilippo Syndrome' (with a skin lesion), 'HIV/AIDS' (with a microscopic view of cells), and 'Green Chemistry' (with a green field). A red dashed line highlights the 'Tuberculosis' and 'Malaria' tiles. At the bottom, there is a text overlay: 'RT thanks to @joelfrunner Screening for TB intelligently - Learning from the past: <http://t.co/a5Z1EQno> #tuberculosis #ODDT'.



A screenshot of a tweet from @aclarkxyz. The tweet text is: '@aclarkxyz: (link) #tuberculosis #ODDT Proposed anti-TB compound'. Below the text is a chemical structure diagram of a proposed anti-TB compound. To the right of the structure are icons for a thumbs up, a thumbs down, and a share icon. A green arrow points from the tweet to a larger chemical reaction diagram. Below the tweet is a link: <http://molsync.com/share/?ds=36>. Below the link is a section titled 'CORRECTING and REPLACING Coca-Cola and the Global Fund Announce ...'. Below this section is a chemical reaction diagram showing the synthesis of a complex molecule from several starting materials. Below the reaction diagram is a row of small thumbnail images. At the bottom is a link: <http://investing.businessweek.com/resear...>



- Relevant tweets get picked up by the *Open Drug Discovery Teams* project, and made available for browsing with a free app
- Chemical data is parsed and can be accessed with other apps

Conclusion

- Some moderately sophisticated, and quite flexible, workflows are already possible using existing tools
- Workflows involve content creation, content consumption, network sharing and computation
- Native apps are currently quite good for visualisation and data entry, **but**: confined to small data; avoid complex calculations; need network access to offload
- Big data workflows need specialised server and protocols to packetise the data; database querying is a simple example, but more complex schemes are in the works, e.g. *Pistoia Alliance AppStore* infrastructure

Future work

- Evolution from proof-of-concept phase to apps designed to solve specific workflows: expect more customised apps
- Consolidation of platforms and APIs: supporting current platforms requires >5 incompatible codebases... need to pick one
- More integration with cloud services: apps cannot work with big data without back-end support
- *Pistoia Alliance* is currently working on an *AppStore*, which provides
 - an alternative storefront for mobile apps
 - standardised service infrastructure, for big data & calculations
- Gradual replacement of all mainstream chemical information software

Acknowledgments

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- ACS CINF Division
- Inquiries to **info@molmatinf.com**

<http://molmatinf.com>

<http://molsync.com>

<http://cheminf20.org>

@aclarkxyz

