

# ***Building a mobile reaction lab notebook***

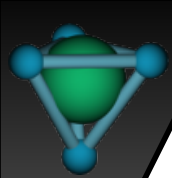
**Alex M. Clark, Ph.D.**

March 2014



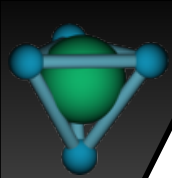
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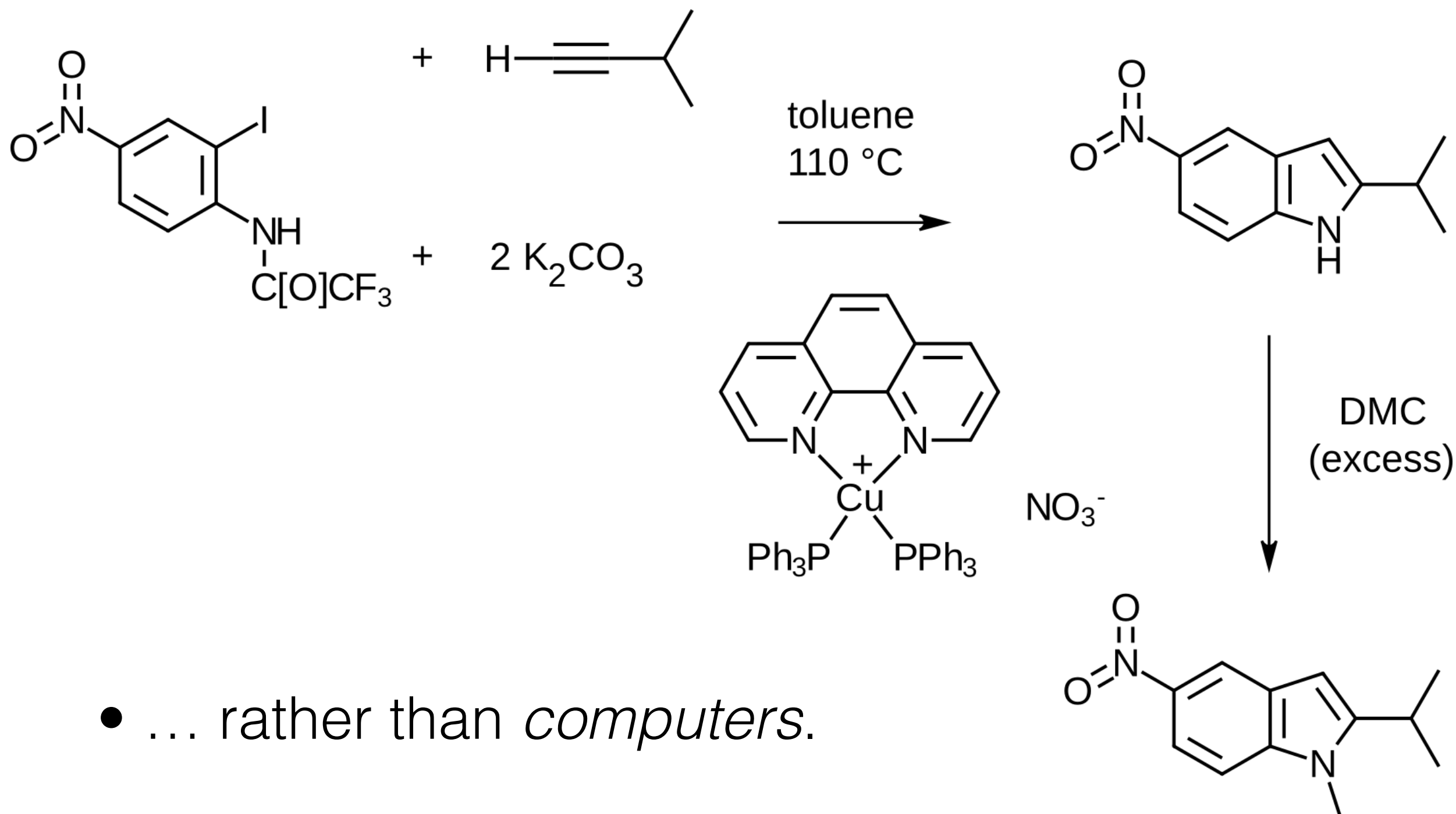
# Electronic Lab Notebooks

- Many shapes & sizes: big, small, hosted, desktop, mobile
- Domains: chemistry, biology, instrumentation
- Many ELNs are generic: functionally equivalent to a Word document
- This talk is about **chemical reactions**

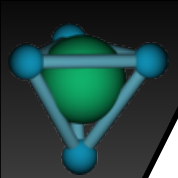


# Data Capture

- Reactions normally drawn for *chemists*...

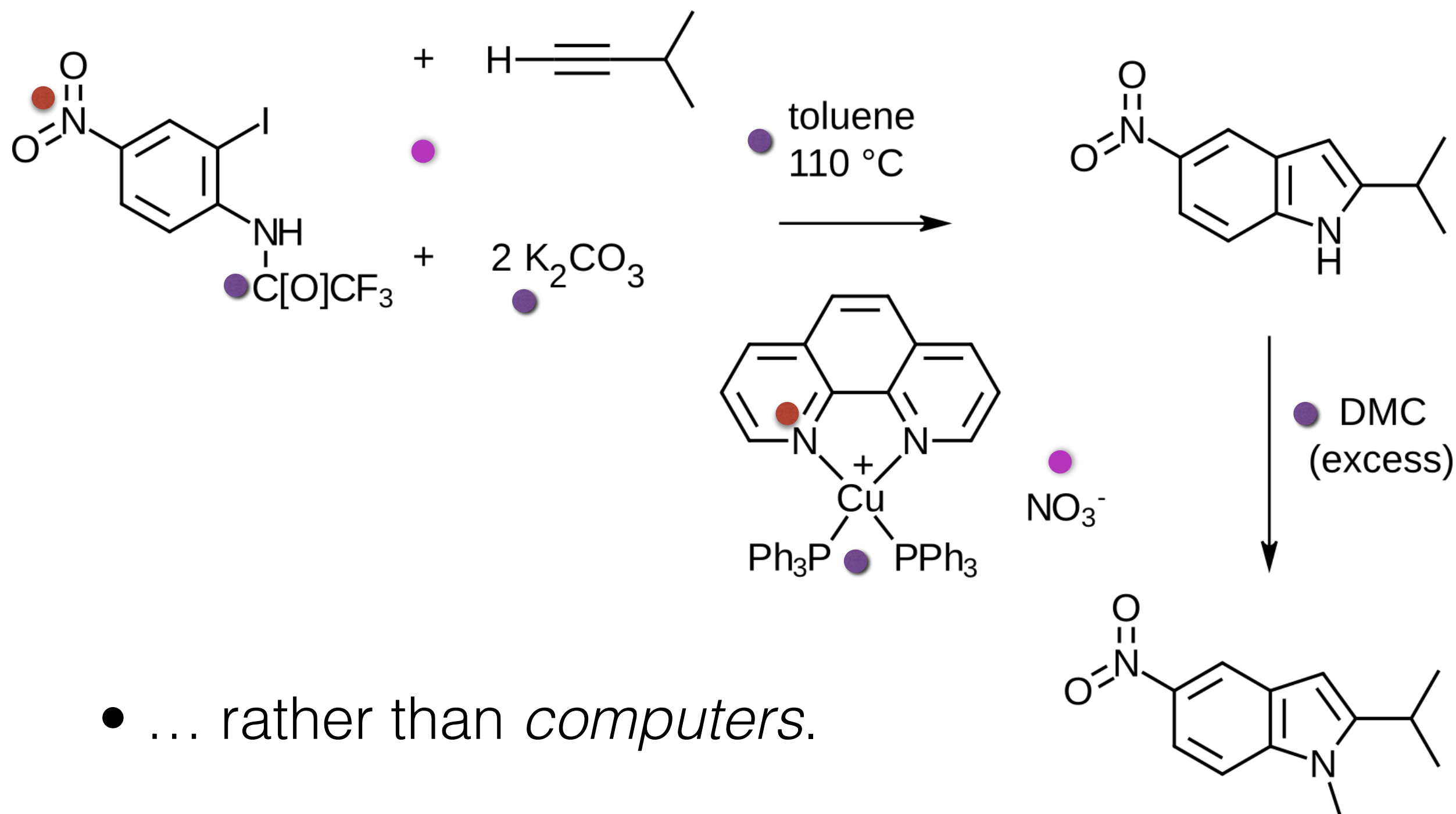


- ... rather than *computers*.



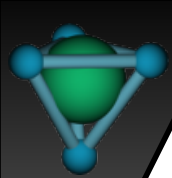
# Data Capture

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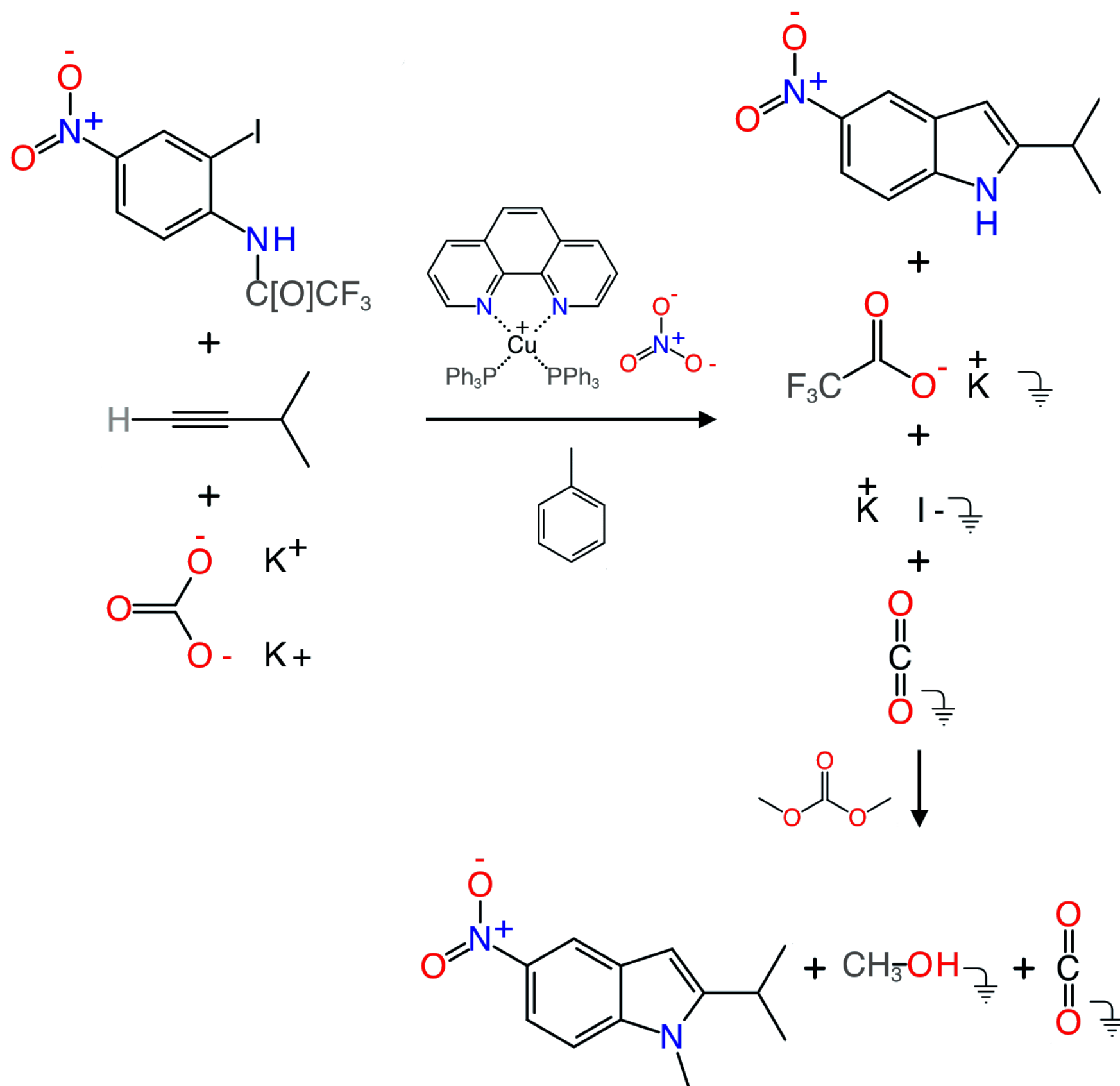


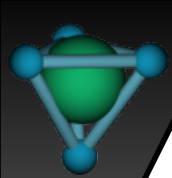
- ... rather than *computers*.



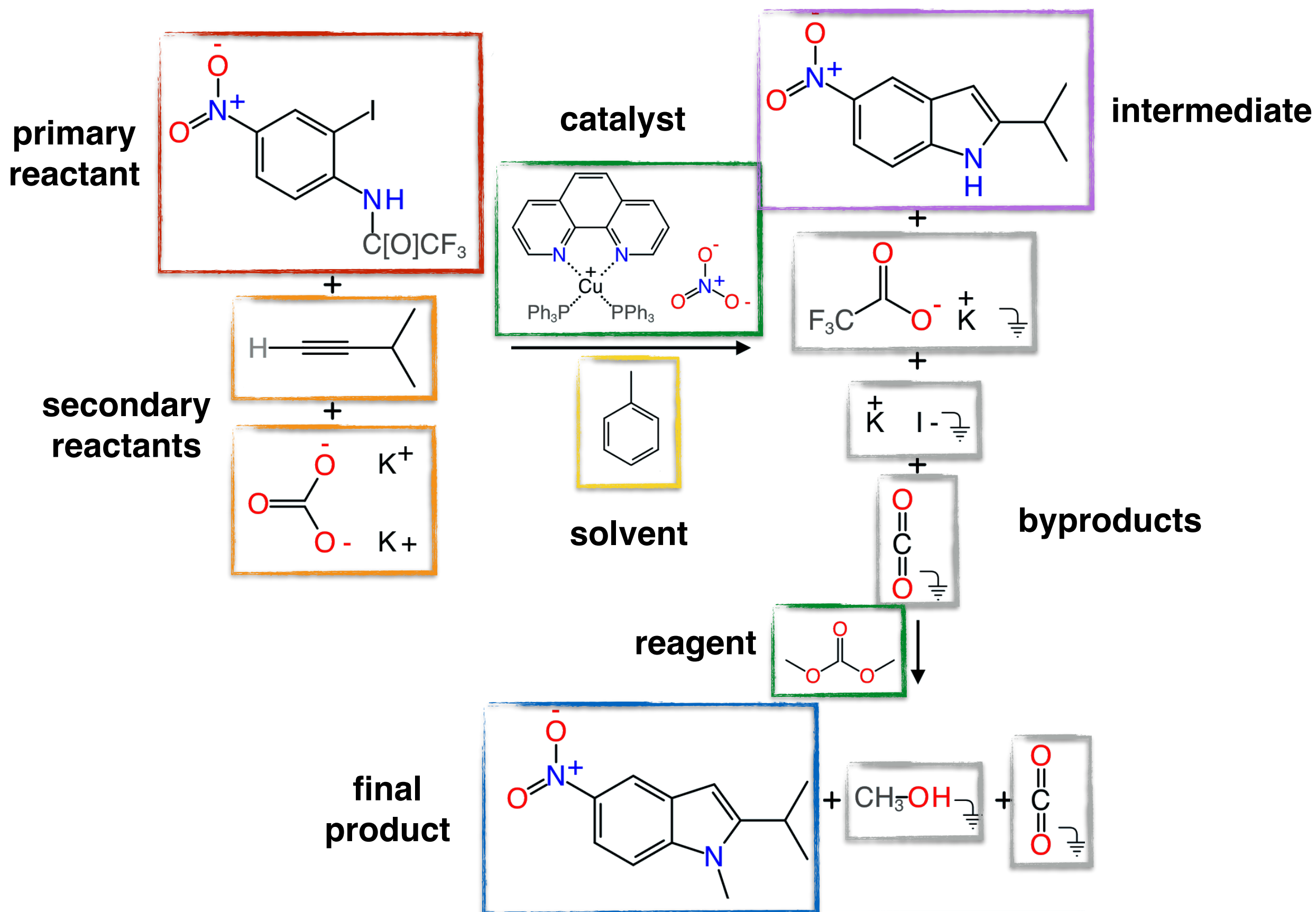


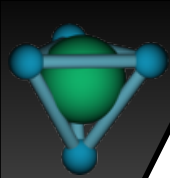
# Digitally Friendly





# Digitally Friendly





# Functionality

- Priorities:
  1. **computer**-friendly datastructures
  2. **human**-friendly workflow
- Because people are flexible! We can do better than the tired paper notebook metaphor

balancing

atom mapping

green metrics

quantity calculation

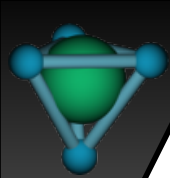
solvent lookup

sustainable feedstocks

byproduct datasheets

reaction transforms

wizards



# Yield101

- Prior art: designed originally for education
- Fancy reaction quantity calculator
- Simple & cheap
- All quantities mapped to structure: stoichiometry, molecular weight, mass, volume, density, concentration, moles, yield

The screenshot displays the Yield101 software interface, which is designed for calculating reaction quantities. It features a central reaction scheme with four components: a reactant (a complex organometallic compound), a reagent (copper(II) nitrate), a solvent (acetic acid), and a product (a complex organometallic compound with two nitro groups). Below the reaction scheme, there are four columns of data, each corresponding to a component. The columns are labeled 'Yield', 'Personal', 'Public', and 'Solvent'. The 'Yield' column shows the calculated yield for each component. The 'Personal' column shows the calculated mass, volume, moles, density, concentration, and primary value for each component. The 'Public' column shows the calculated mass, volume, moles, density, concentration, and primary value for each component. The 'Solvent' column shows the calculated mass, volume, moles, density, concentration, and primary value for each component. At the bottom of the interface, there is a 'Process Mass Intensity' calculation:  $2.838 \text{ g} / 0.095 \text{ g} = 29.876$ . The interface also includes a sidebar with buttons for 'Yield', 'Personal', 'Public', and 'Solvent', and a bottom toolbar with various icons for navigation and editing.

Component	Chemical Structure	MW (g/mol)	Equiv	Mass (g)	Volume (mL)	Moles (mmol)	Density (g/mL)	Conc	Primary	Yield (%)
Reactant 1		982.51	1	0.1		0.10178			*	4%
Reagent 2		187.56	2	0.0381789		0.20356				1%
Solvent 3		102.09	0	2.7	2.5	0.0264476	1.08			95%
Product 4		1072.51	1	0.095		0.0885777				100%


Process Mass Intensity:  $2.838 \text{ g} / 0.095 \text{ g} = 29.876$


# Green Lab Notebook


- Under construction as an iOS app (phones & tablets)
- Superset of **Yield101** core functionality
- General purpose *reaction lab notebook*, with supplementary *green chemistry* features
- Start with experiment drawing...

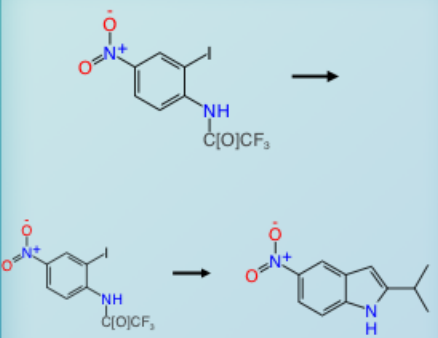
Carrier 12:03 PM


## Green Lab Notebook

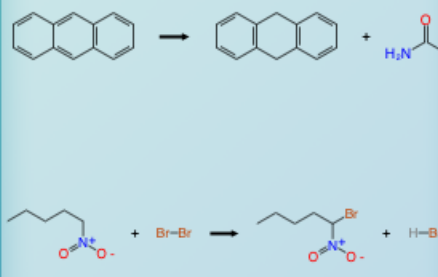
 Tutorial


 New Folder

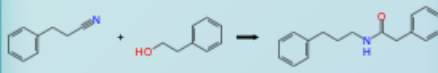
 Experiments #4




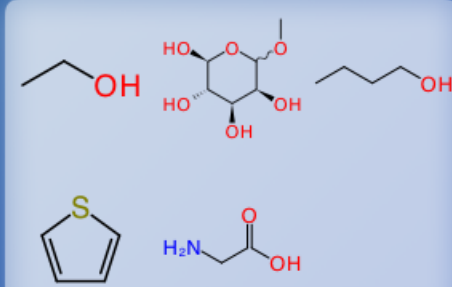
 Experiments #1




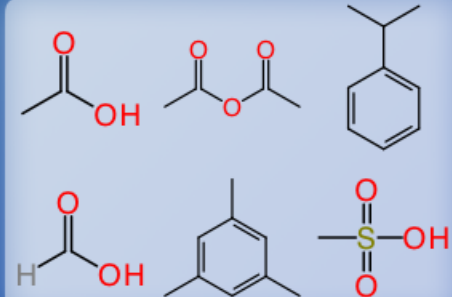
 Experiments #2




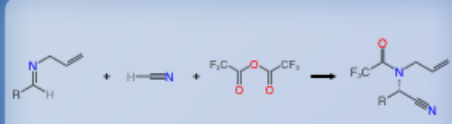
 Feedstocks



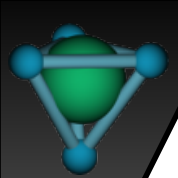
 Solvents



 Transforms

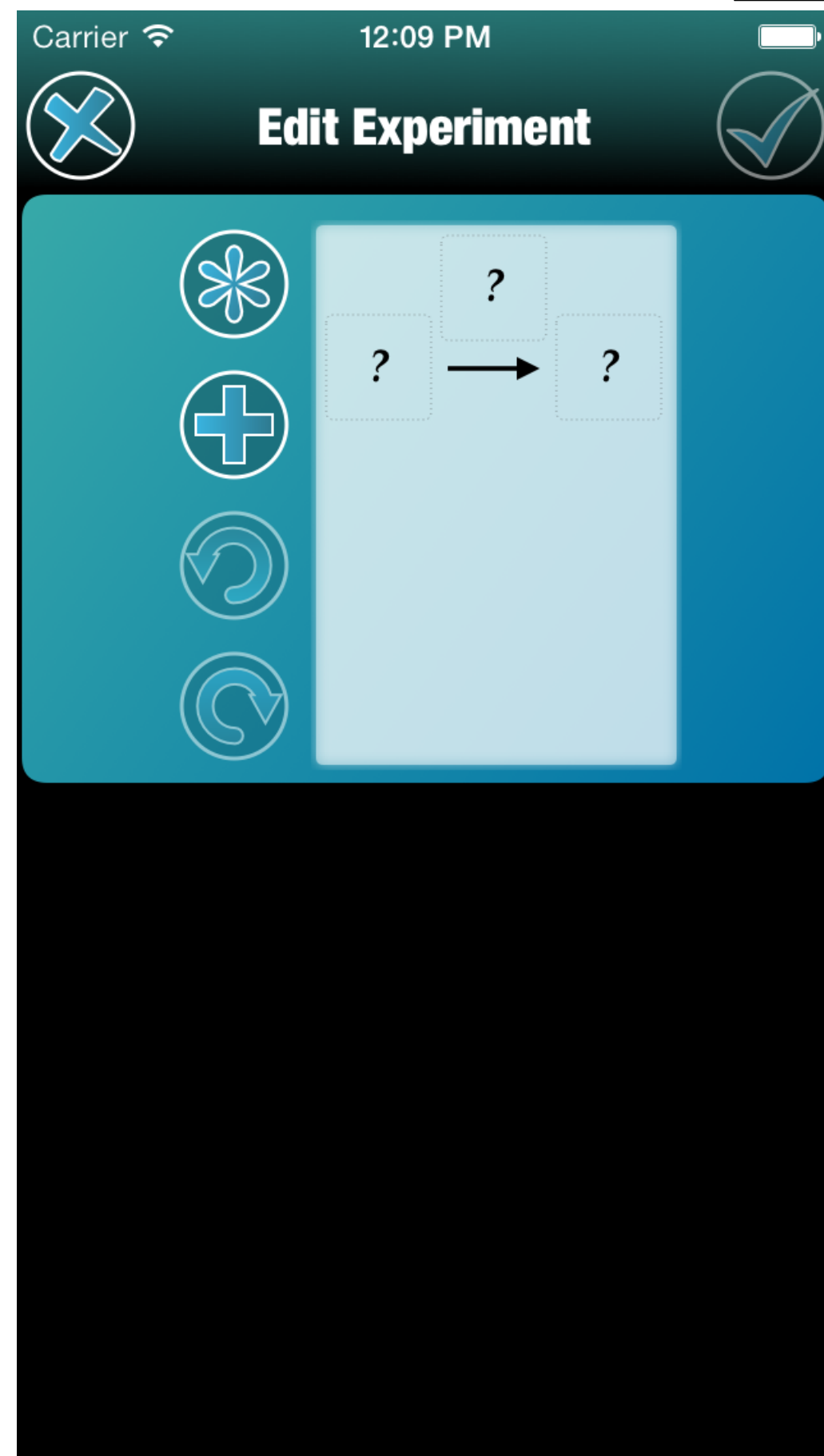


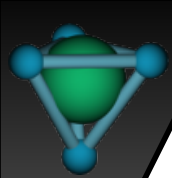




# A New Experiment

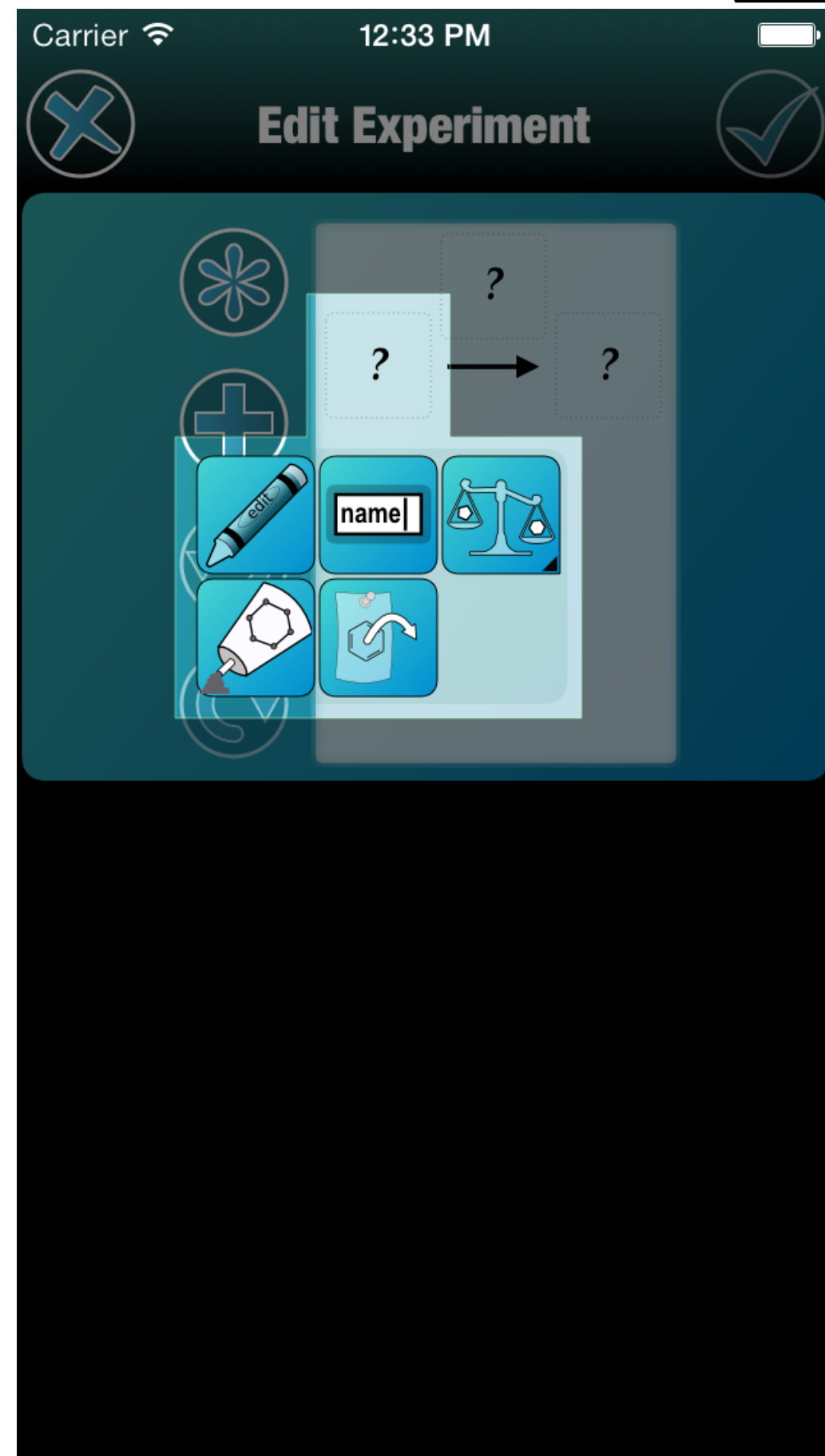
- Start with a fresh slate: select the reactant placeholder
- Select the draw icon
- Sketch the reactant structure
- Apply the change: display shows reaction in progress
- Note molecular formula & molecular weight

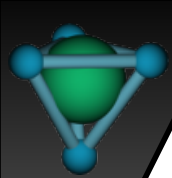




# A New Experiment

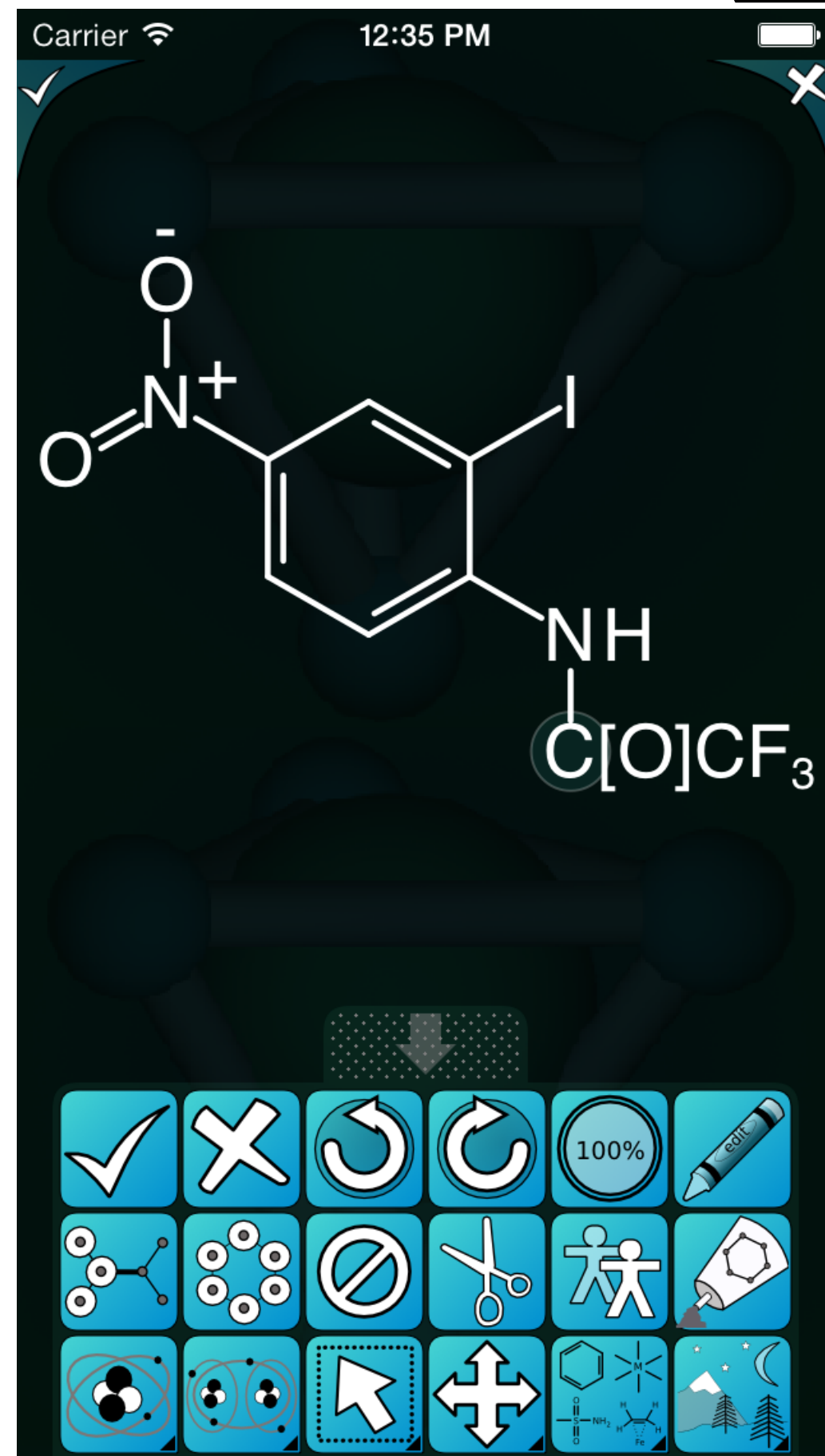
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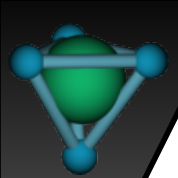




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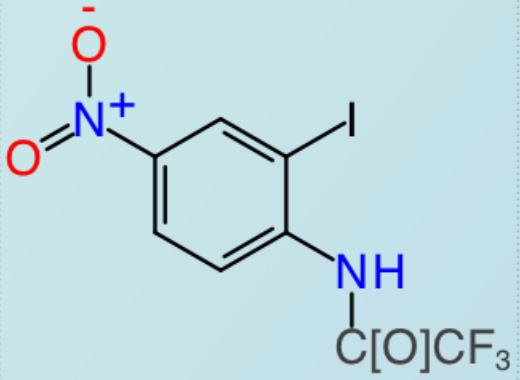


# A New Experiment

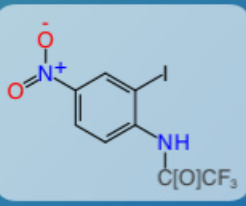
- Start with a fresh slate: select the reactant placeholder
- Select the draw icon
- Sketch the reactant structure
- Apply the change: display shows reaction in progress
- Note molecular formula & molecular weight

Carrier 12:09 PM

**Edit Experiment**



$C_8H_4F_3IN_2O_3 \rightarrow (+C_8H_4F_3IN_2O_3)$



Equiv: 1

MW: 360.029 g/mol

Mass:

Volume:

Moles:

Density:

Conc:

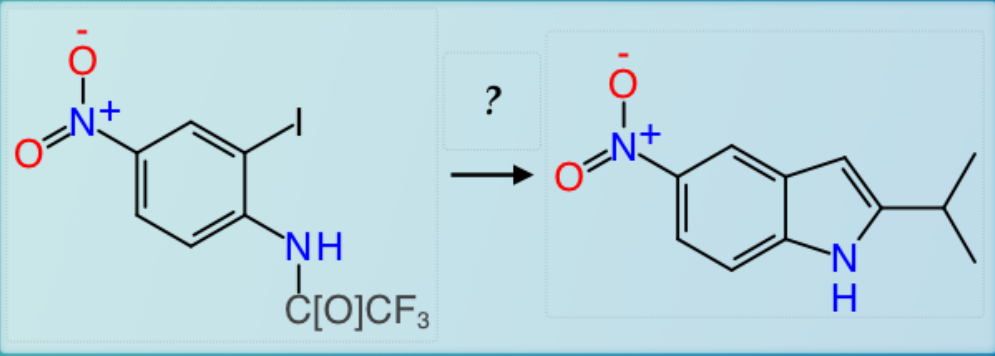
**$\Sigma$  reactants = ? = ?**

# The First Step

- Draw product
- Draw stoichiometric reactants
- Draw reagents
- Balance

Carrier 12:15 PM 100%

Edit Experiment



$C_8H_4F_3IN_2O_3 \rightarrow C_{11}H_{12}N_2O_2$   
(+C<sub>3</sub>H<sub>8</sub>) (+F<sub>3</sub>IO)

	Equiv:	1
MW:	360.029 g/mol	
Mass:		
Volume:		
Moles:		
Density:		
Conc:		

	Equiv:	1
MW:	204.225 g/mol	
Mass:		
Volume:		
Moles:		
Density:		
Conc:		
Yield:		

$\Sigma$  reactants = ? = ?  $\Sigma$  products = ? = ?  $\Sigma$  waste = ? = ?

PMI =  $\frac{?}{?}$  = ?

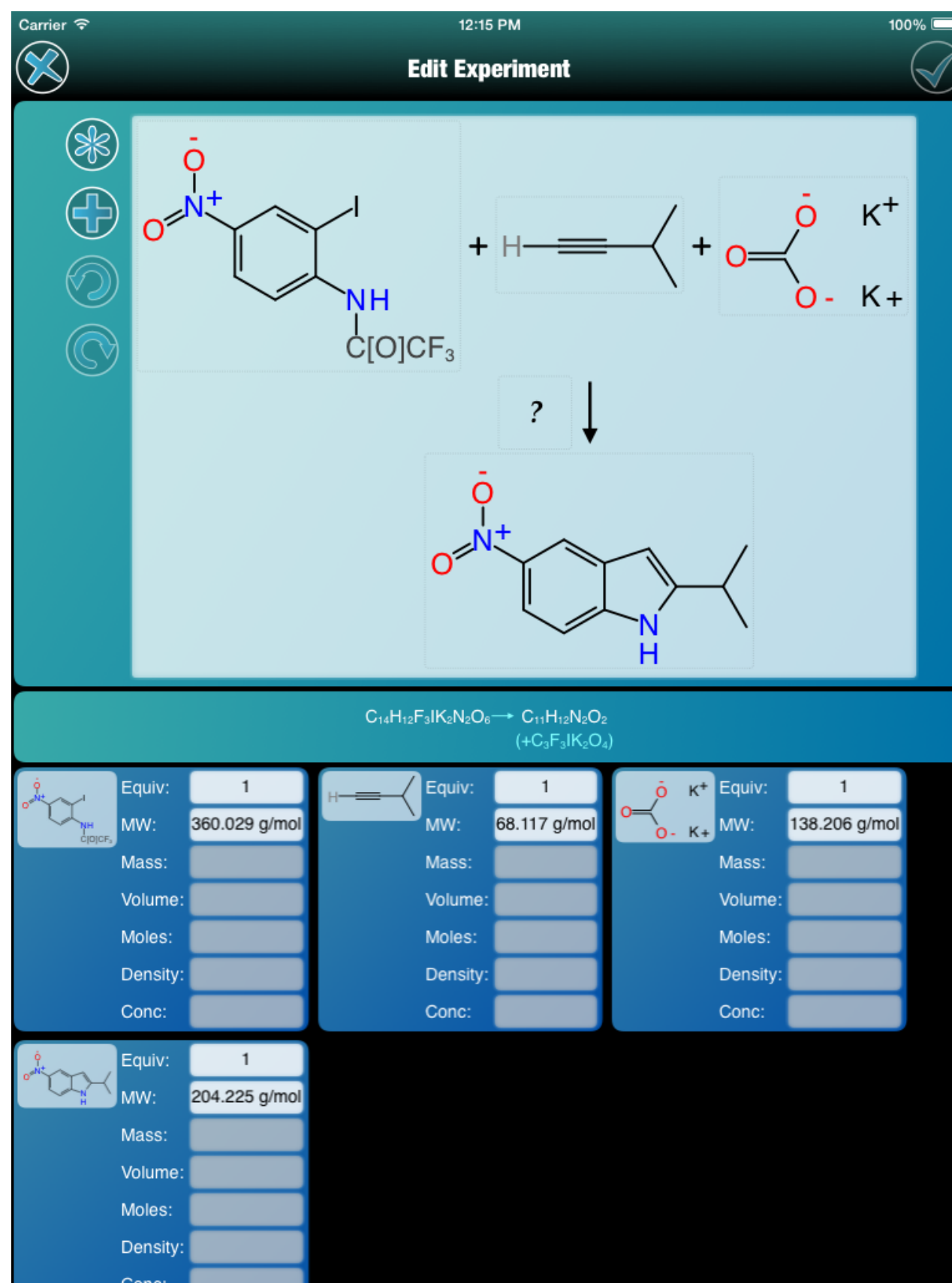
E-factor =  $\frac{?}{?}$  = ?

Atom-E =  $\frac{204.225}{360.029}$  = 56.7247 %



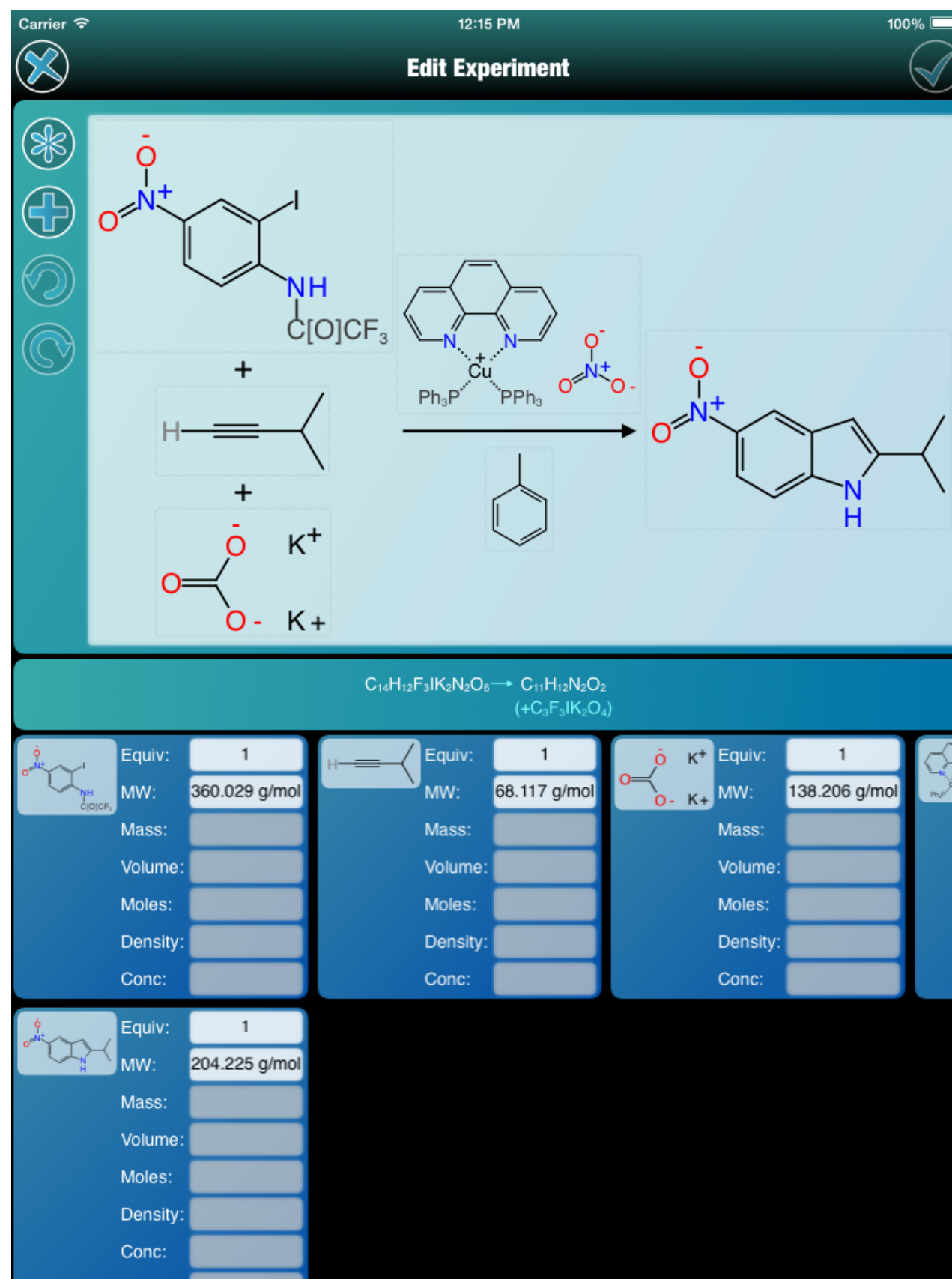
# The First Step

- Draw product
- Draw stoichiometric reactants
- Draw reagents
- Balance



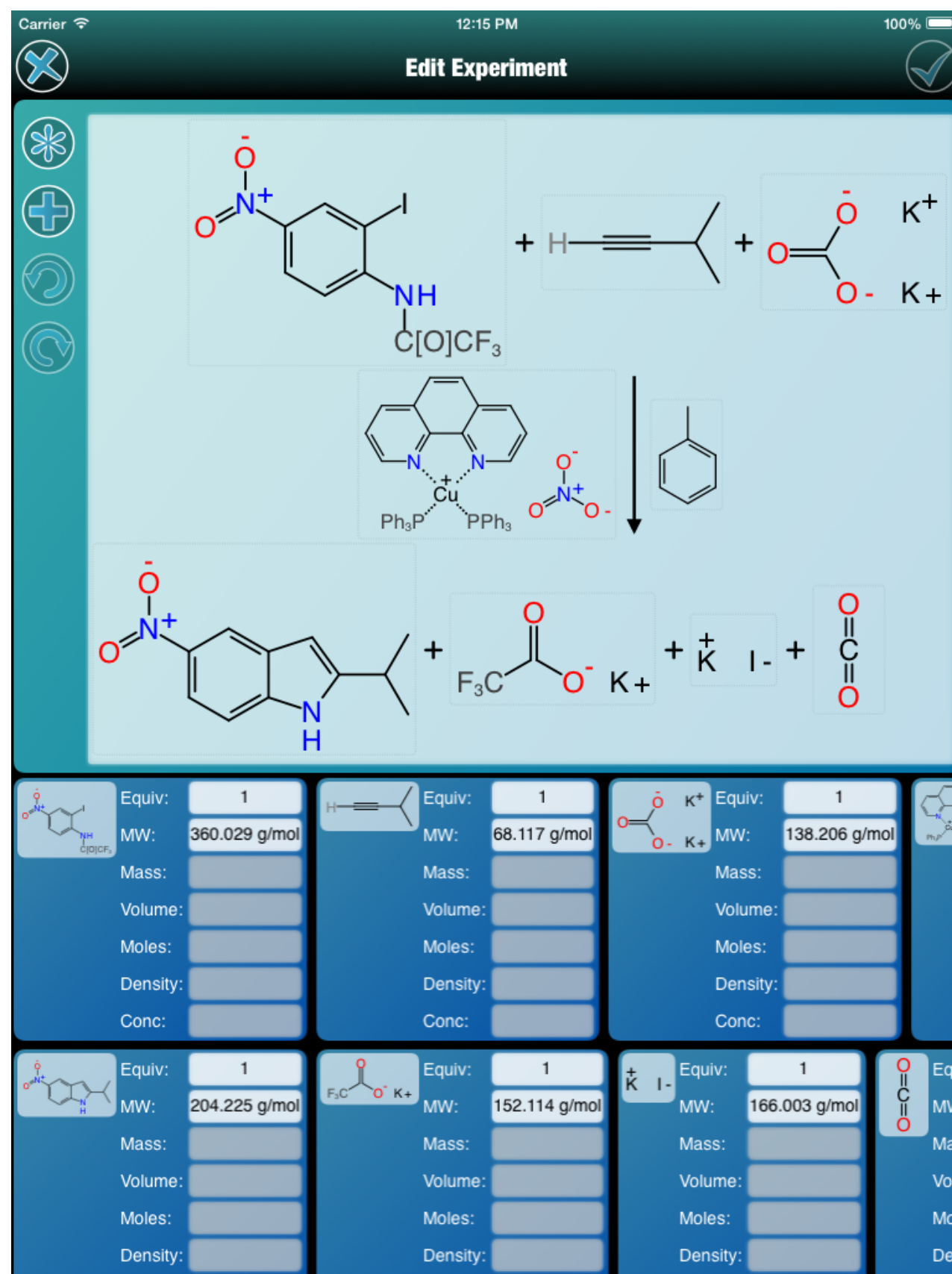
# The First Step

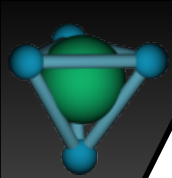
- Draw product
- Draw stoichiometric reactants
- Draw reagents
- Balance



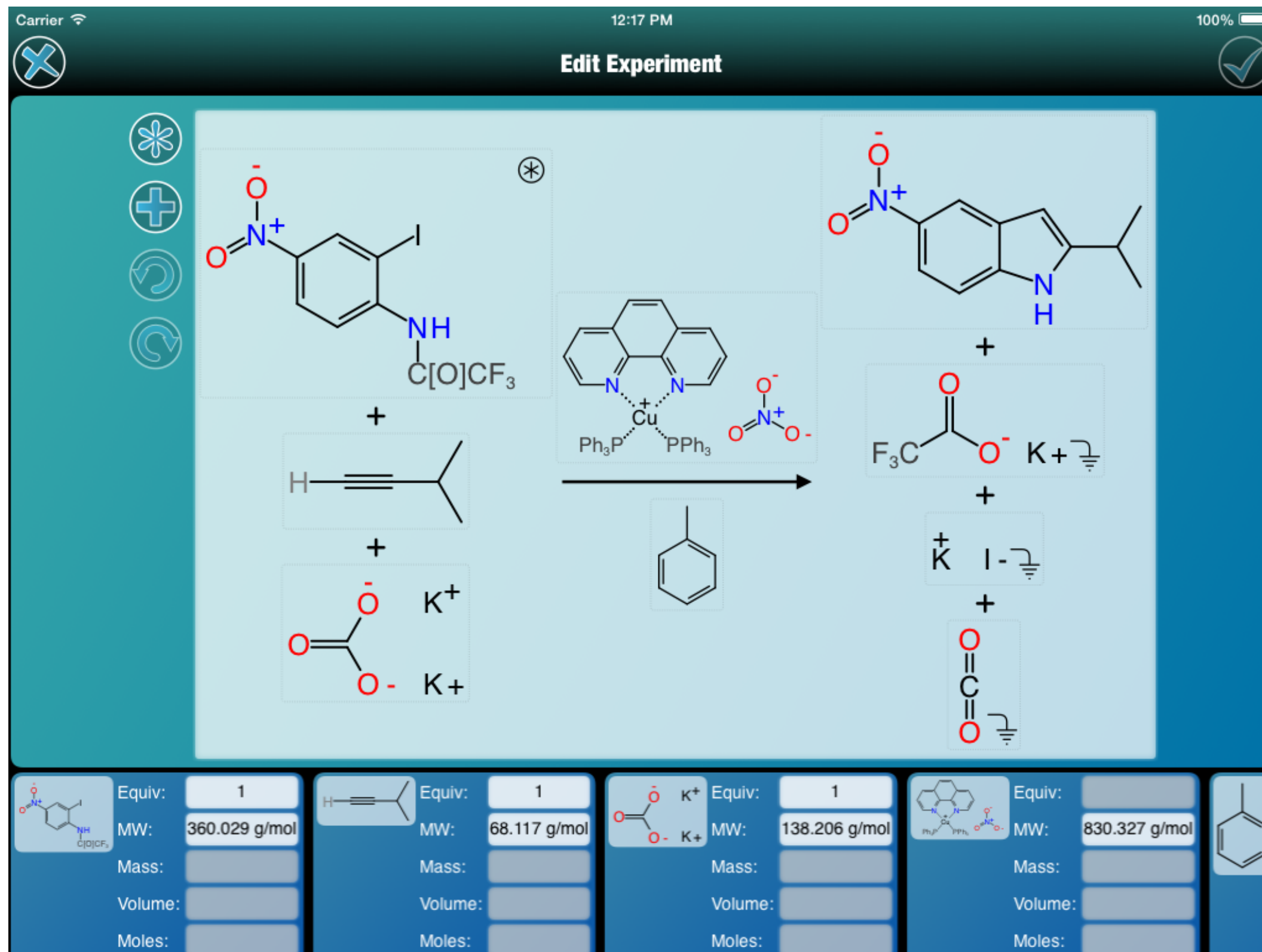
# The First Step

- Draw product
- Draw stoichiometric reactants
- Draw reagents
- Balance

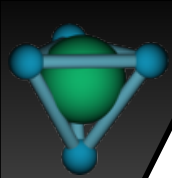




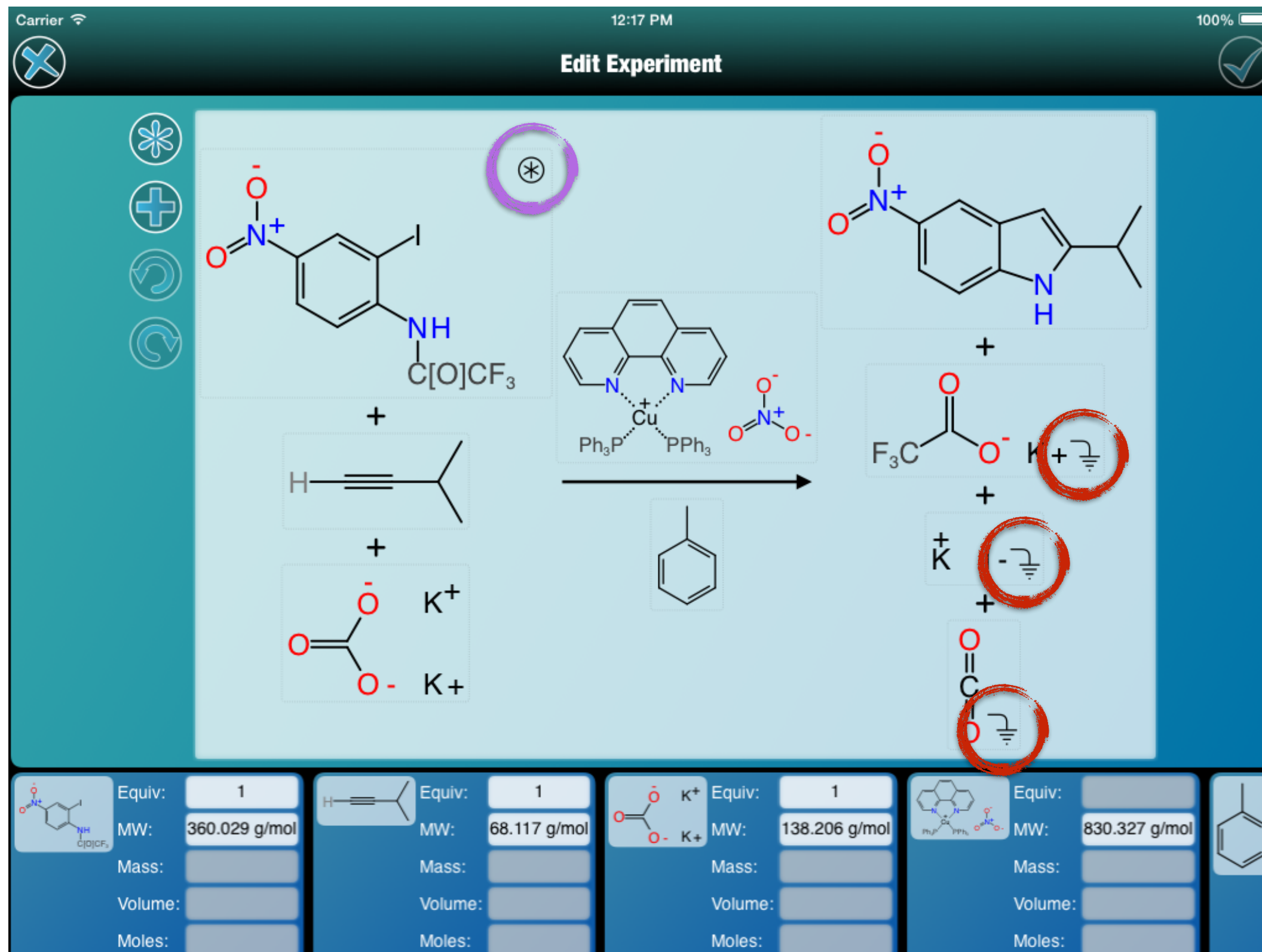
# Quantities



- Classify primary reactants & waste products

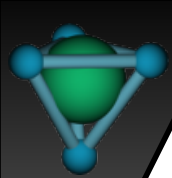


# Quantities



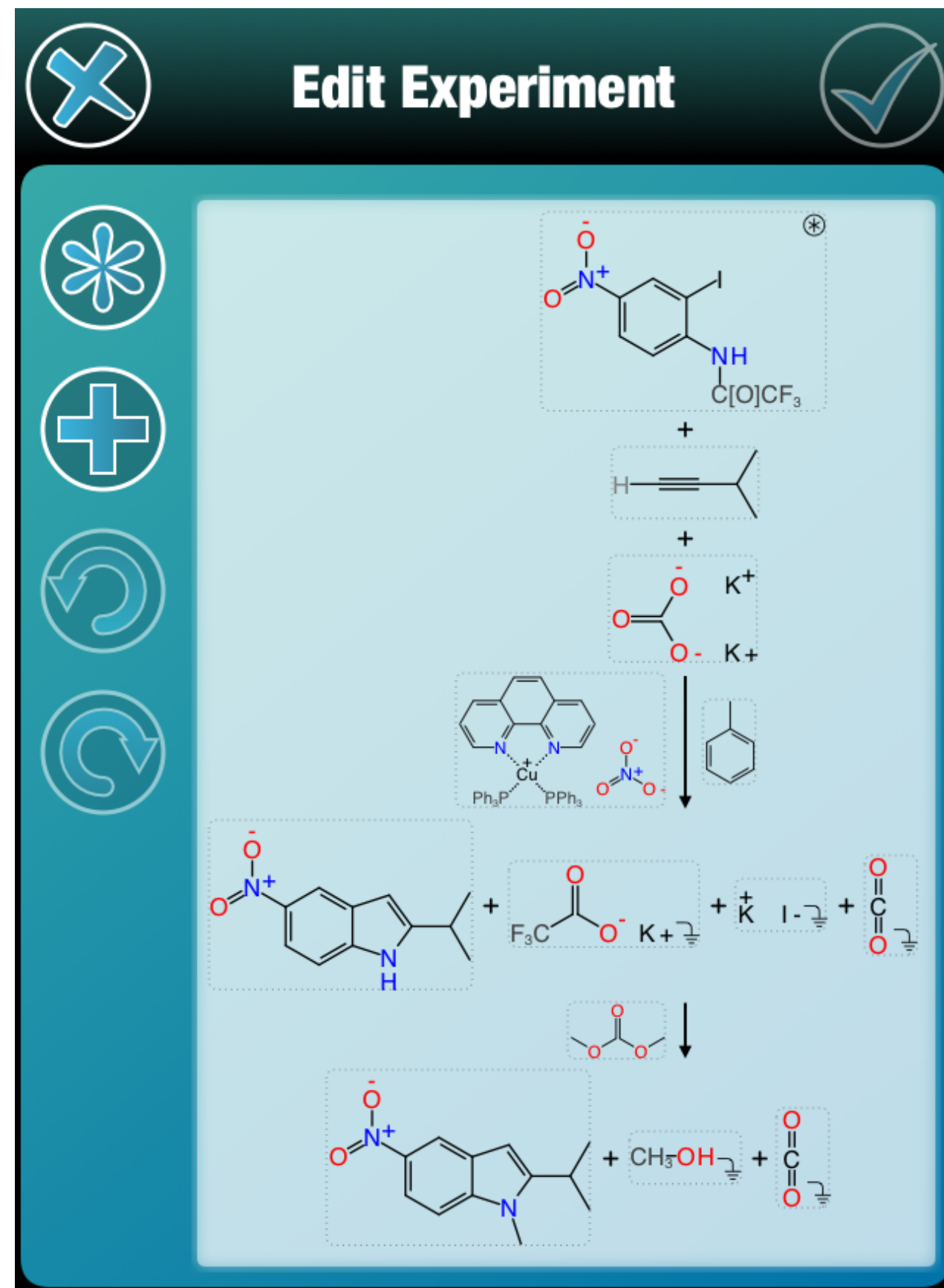
- Classify primary reactants & waste products

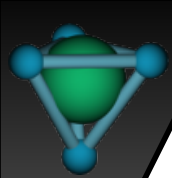




# The Second Step

- Append step
- Draw second product
- Balance: byproducts
- Stoichiometric reagent
- For step 2: any non-waste product from step 1 is a *primary reactant*





# Quantities

- Fill in all available measurements
- All possible mappings auto-calculated
- Cross-fertilised with stoichiometry & molarity
- Molecular weight really matters...

step 1  
reactants  
products  
step 2  
reagents  
products

Carrier 1:53 PM 100%

Edit Experiment

 Equiv: 1 MW: 360.029 g/mol Mass: 1 g Volume: <input type="text"/> Moles: 0.00277756 mol Density: <input type="text"/> Conc: <input type="text"/>	 Equiv: 1 MW: 68.117 g/mol Mass: 0.189199 g Volume: <input type="text"/> Moles: 0.00277756 mol Density: <input type="text"/> Conc: <input type="text"/>	 Equiv: 1 MW: 138.206 g/mol Mass: 0.829233 g Volume: <input type="text"/> Moles: 0.006 mol Density: <input type="text"/> Conc: <input type="text"/>
 Equiv: 1 MW: 204.225 g/mol Mass: 0.567247 g Volume: <input type="text"/> Moles: 0.00277756 mol Density: <input type="text"/> Conc: <input type="text"/> Yield: 100 %	 Equiv: 1 MW: 152.114 g/mol Mass: 0.422504 g Volume: <input type="text"/> Moles: 0.00277756 mol Density: <input type="text"/> Conc: <input type="text"/> Yield: <input type="text"/>	 Equiv: 1 MW: 166.003 g/mol Mass: 0.461082 g Volume: <input type="text"/> Moles: 0.00277756 mol Density: <input type="text"/> Conc: <input type="text"/> Yield: <input type="text"/>
 Equiv: 1.99843 MW: 90.0779 g/mol Mass: 0.5 g Volume: <input type="text"/> Moles: 0.00555075 mol Density: <input type="text"/> Conc: <input type="text"/>		
 Equiv: 1 MW: 218.252 g/mol Mass: 0.606206 g Volume: <input type="text"/> Moles: 0.00277756 mol Density: <input type="text"/> Conc: <input type="text"/> Yield: 100 %	 Equiv: 1 MW: 32.0419 g/mol Mass: 0.0889981 g Volume: <input type="text"/> Moles: 0.00277756 mol Density: <input type="text"/> Conc: <input type="text"/> Yield: <input type="text"/>	 Equiv: 1 MW: 44.0095 g/mol Mass: 0.122239 g Volume: <input type="text"/> Moles: 0.00277756 mol Density: <input type="text"/> Conc: <input type="text"/> Yield: <input type="text"/>

# Quantities

- Fill in all available measurements
- All possible mappings auto-calculated
- Cross-fertilised with stoichiometry & molarity
- Molecular weight really matters...

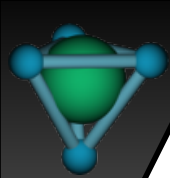
## step 2

## products

## reagents

## products

[illegible]



# Green Metrics

$$\text{Process Mass Intensity (PMI)} = \frac{\text{mass of all reactants}}{\text{mass of products}}$$



$$\text{E-factor} = \frac{\text{mass of waste}}{\text{mass of products}}$$

$$\text{Atom Economy} = \frac{\sum \text{molecular weight products}}{\sum \text{molecular weight reactants}}$$

- Trivial calculations... if the information is available.

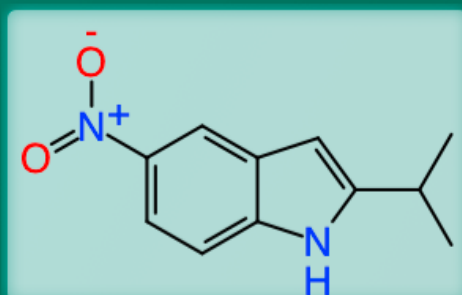


# Green Metrics

$$\Sigma \text{ reactants} = 1 \text{ g} + 0.189199 \text{ g} + 0.829233 \text{ g} + 0.115314 \text{ g} + 17.34 \text{ g} + 0.5 \text{ g} = 19.9737 \text{ g}$$

$$\Sigma \text{ products} = 0.567247 \text{ g} + 0.606206 \text{ g} = 1.17345 \text{ g}$$

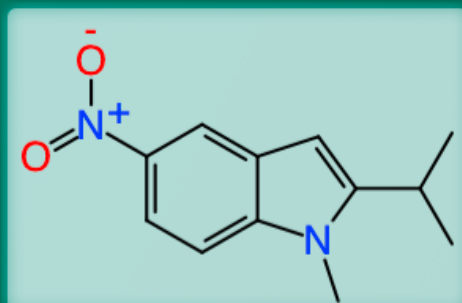
$$\Sigma \text{ waste} = 0.422504 \text{ g} + 0.461082 \text{ g} + 0.122239 \text{ g} + 0.0889981 \text{ g} + 0.122239 \text{ g} = 1.21706 \text{ g}$$



$$\text{PMI} = \frac{1 \text{ g} + 0.189199 \text{ g} + 0.829233 \text{ g} + 0.115314 \text{ g} + 17.34 \text{ g}}{0.567247 \text{ g}} = 34.3303$$

$$\text{E-factor} = \frac{0.422504 \text{ g} + 0.461082 \text{ g} + 0.122239 \text{ g}}{0.567247 \text{ g}} = 1.77317$$

$$\text{Atom-E} = \frac{204.225}{360.029 + 68.117 + 138.206} = 36.0598 \%$$



$$\text{PMI} = \frac{1 \text{ g} + 0.189199 \text{ g} + 0.829233 \text{ g} + 0.115314 \text{ g} + 17.34 \text{ g} + 0.5 \text{ g}}{0.606206 \text{ g}} = 32.9487$$

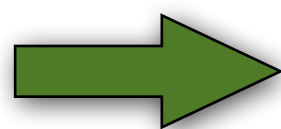
$$\text{E-factor} = \frac{0.422504 \text{ g} + 0.461082 \text{ g} + 0.122239 \text{ g} + 0.0889981 \text{ g} + 0.122239 \text{ g}}{0.606206 \text{ g}} = 2.00767$$

$$\text{Atom-E} = \frac{218.252}{204.225 + 90.0779} = 74.1588 \%$$

- Totals for reactants, products & waste
- For each non-waste product: PMI, E-factor, Atom-E
- Always calculated, always recorded...



# Green Solvents



Carrier 5 33:47 PM

**Solvents**

\* **Formic acid**

OC=O

Class: Acid  
CASRN: 64-18-6  
CSID: 278  
MP: 8 °C  
BP: 101 °C  
Density: 1.22 g/mL

**2** **6**  
**4.5** **7**

\* **Mesitylene**

Cc1cc(C)c(C)cc1

Class: Acid  
CASRN: 108-67-8  
CSID: 7659  
MP: -45 °C  
BP: 165 °C  
Density: 0.864 g/mL

**4** **5**  
**8** **3**  
**1** **4**

\* **Methane sulphonic acid**

CS(=O)(=O)O

Class: Acid  
CASRN: 75-75-2  
CSID: 6155  
MP: 18 °C  
BP: 424 °C  
Density: 1.481 g/mL

**6** **10**

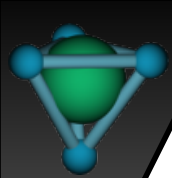
\* **Propionic acid**

CCC(=O)O

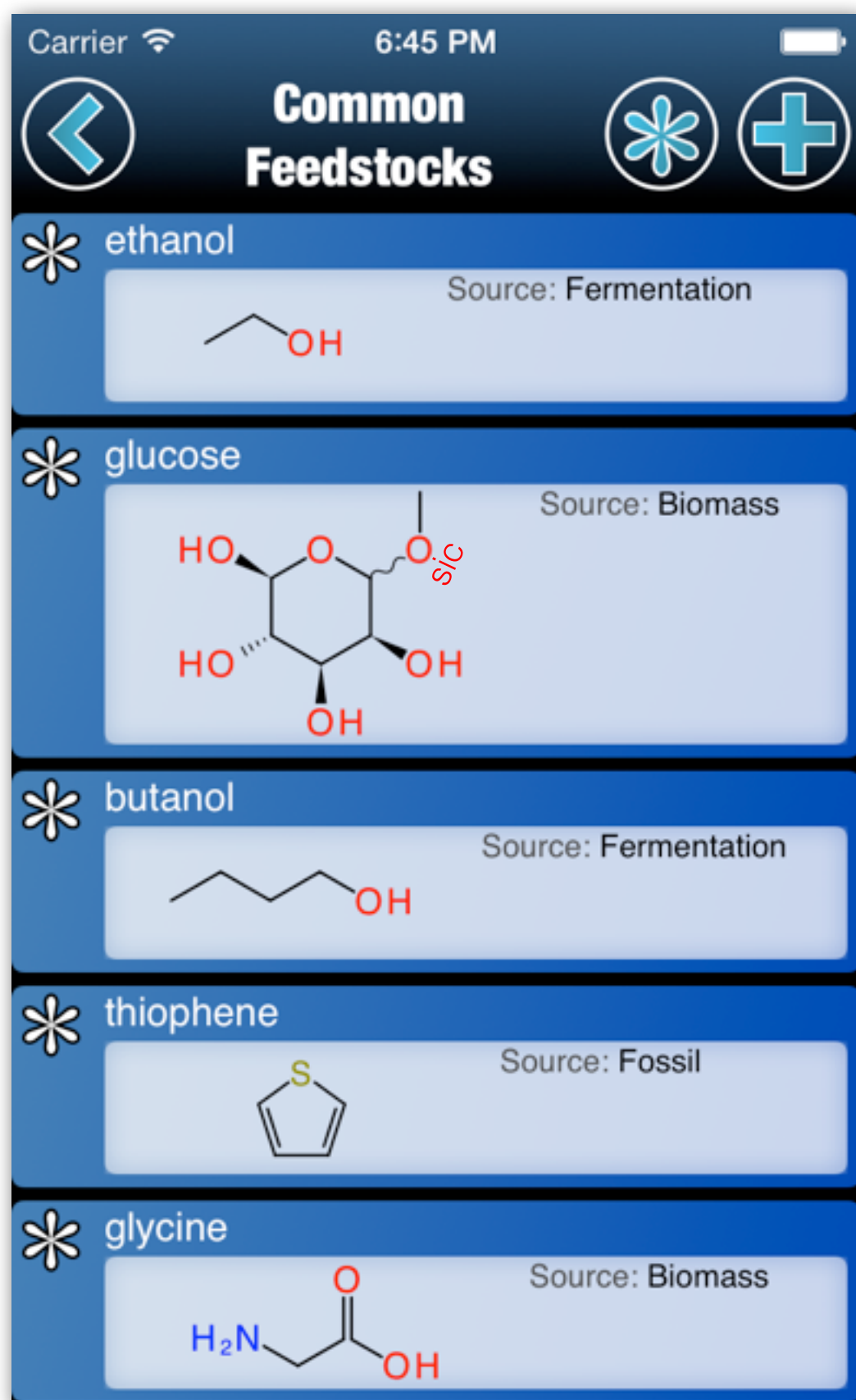
Class: Acid  
CASRN: 79-09-4  
CSID: 1005  
MP: -21 °C  
BP: 141 °C

**2** **5**

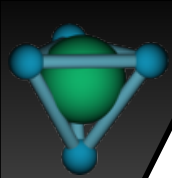
- Environmental data from ACS GCI & GSK



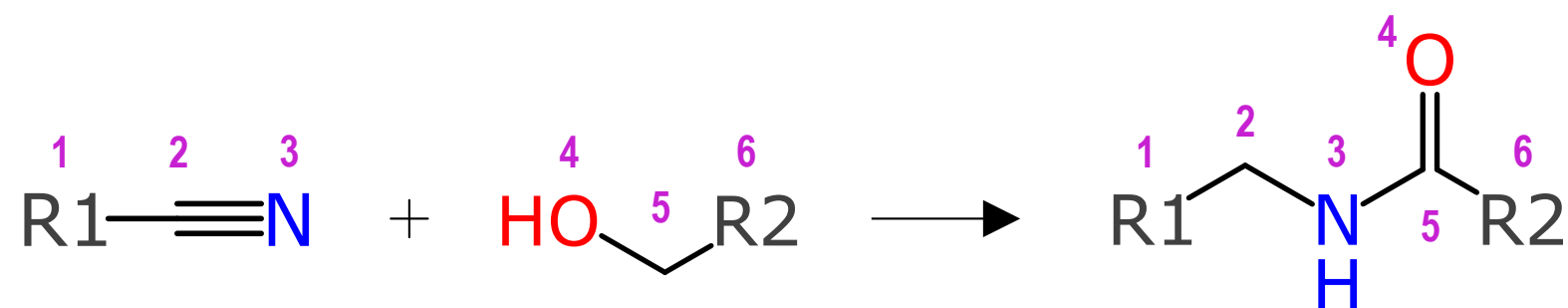
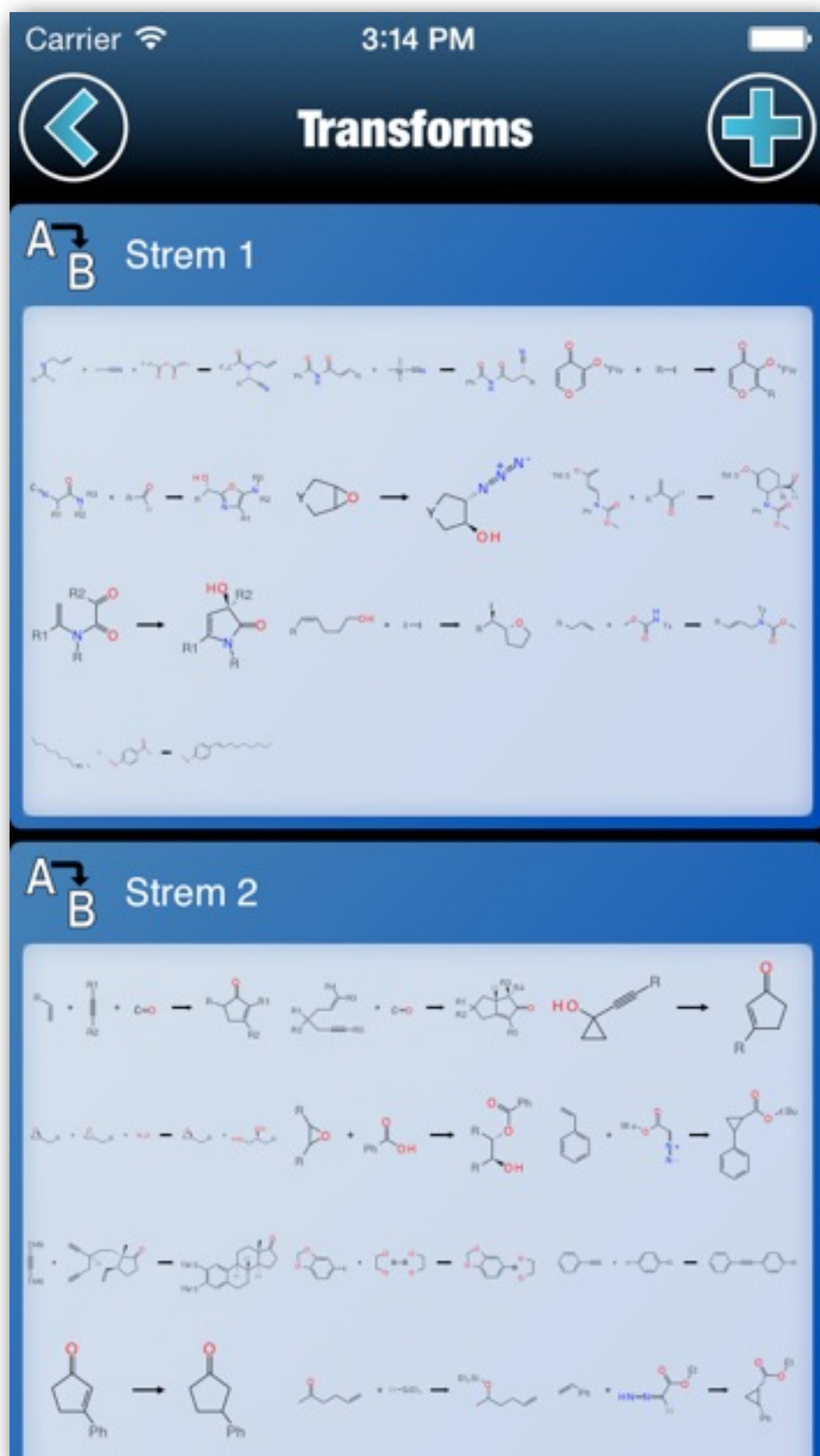
# Feedstocks



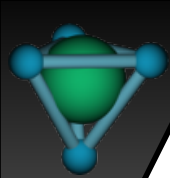
- Reference collection:
  - info about supply chain
  - encourage renewable use
- Link lab-available quantities to experiment records
- Could synchronise with inventory software
- Lookup in vendor catalogs...



# Reaction Transforms



- Provide a pre-curated list of "green" reaction transforms
- Promote user entered experiments into transforms (numbering, clipping)
- Associate with:
  - reagents, catalysts & solvents
  - stoichiometry & quantities
  - yield & experimental conditions
  - literature & green reference data



# Further Work

- Work in progress: minimum viable product is close
- Experiment definition extensions to include preparation details, free text, spectra, references, pictures, etc.
- Synchronisation with centralised databases
- Automated structure lookup of problem-compounds: curation required
- Curation of sustainable feedstocks & green reaction transforms
- Facile promotion of experiment-to-transform: ultra convenient reuse



# Acknowledgments

- Sean Ekins (Green Solvents)
- Eidogen-Sertanty (Yield101)
- Inquiries to **info@molmatinf.com**

**MOLECULAR  
MATERIALS  
INFORMATICS**

<http://molmatinf.com>

<http://molsync.com>

<http://cheminf20.org>

@aclarkxyz

