Building a mobile reaction lab notebook

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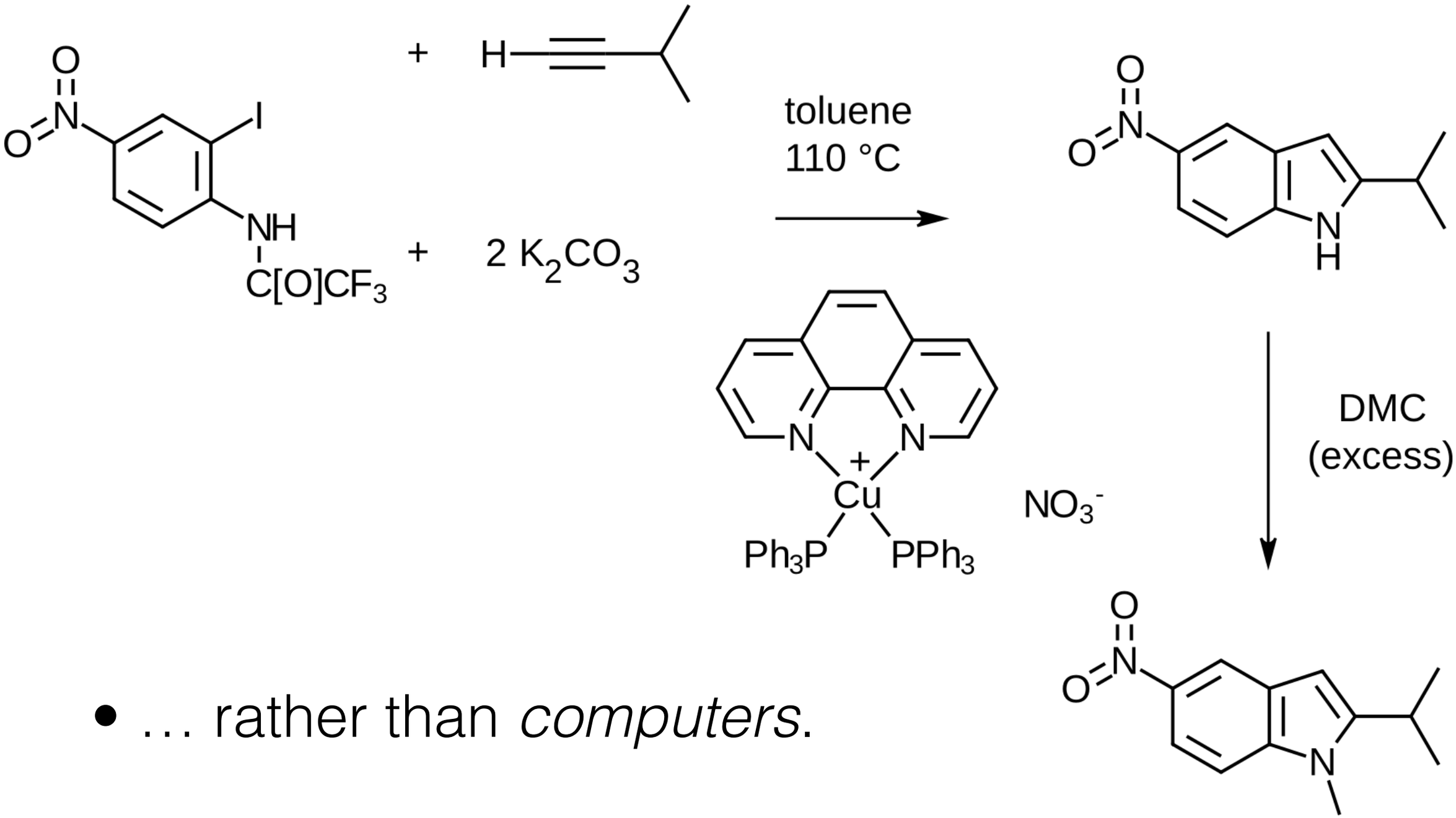
http://molmatinf.com

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*.

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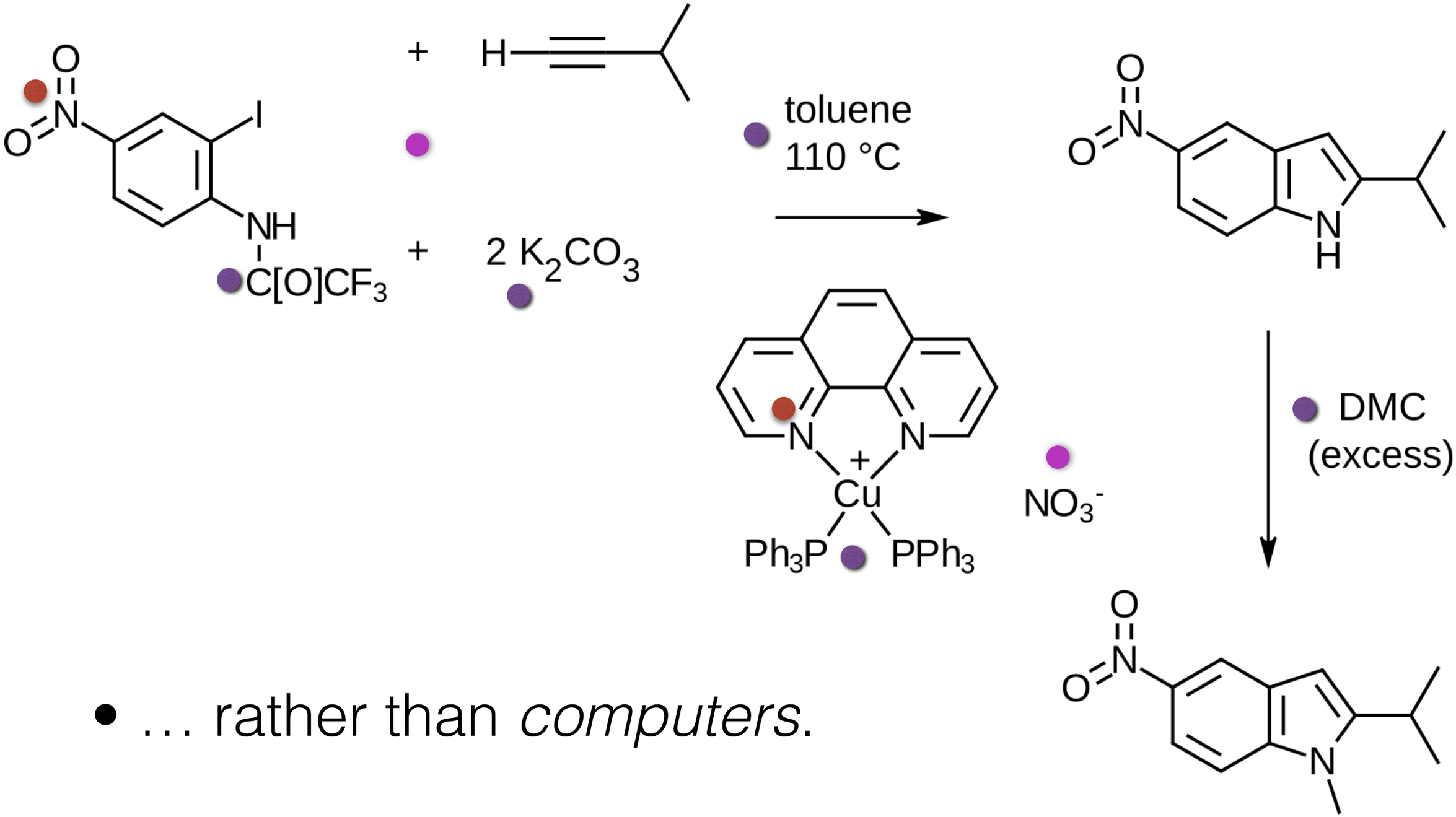

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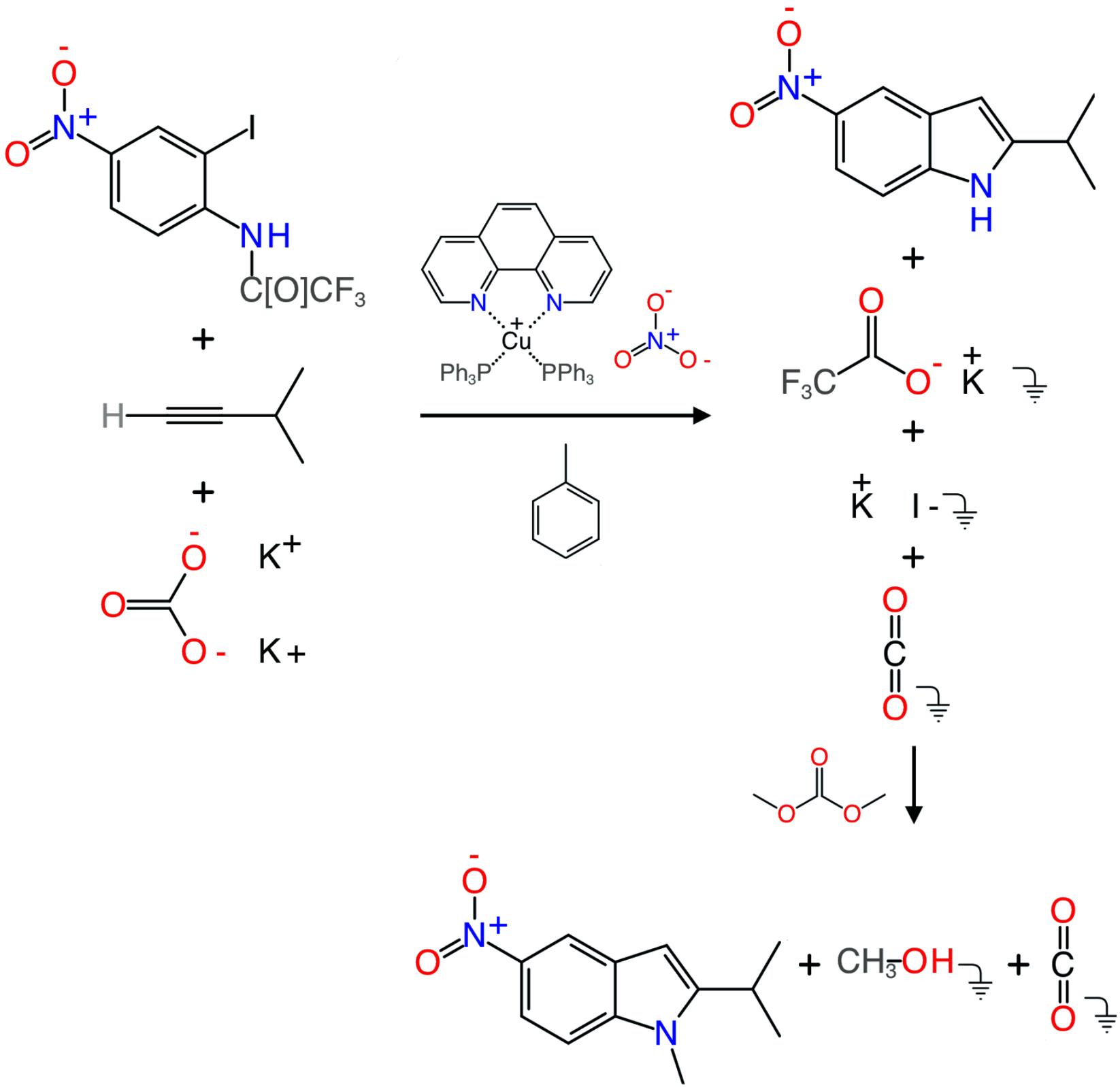
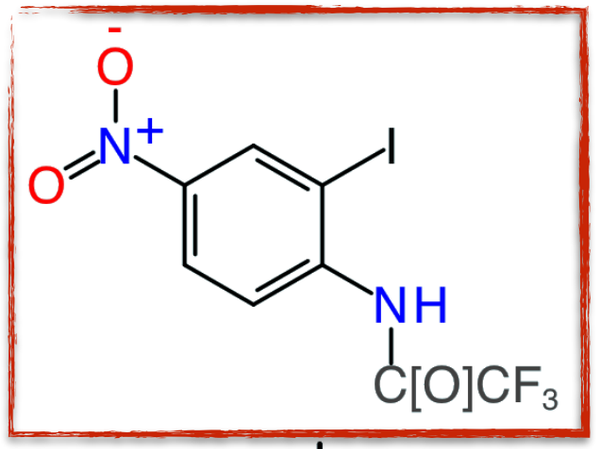
Digitally Friendly



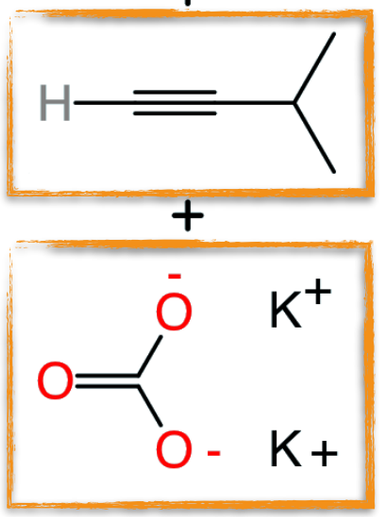
Digitally Friendly

primary reactant

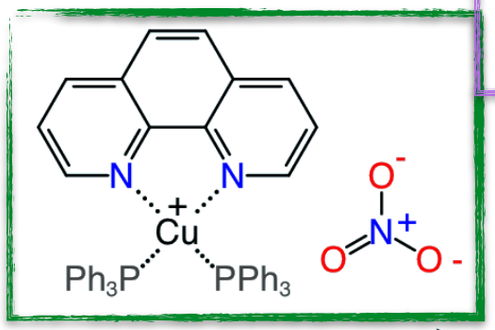


+

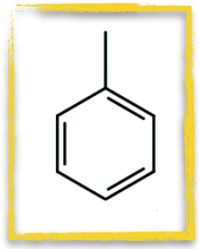
secondary reactants

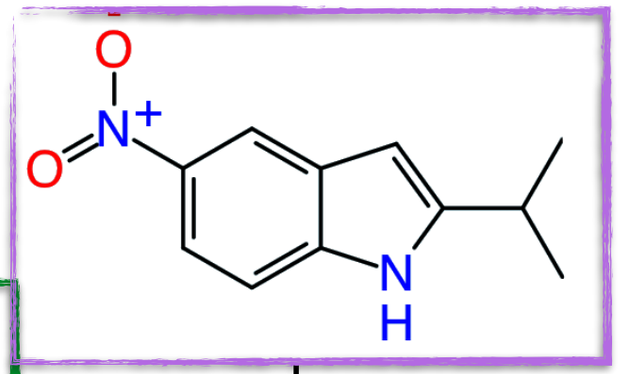


catalyst



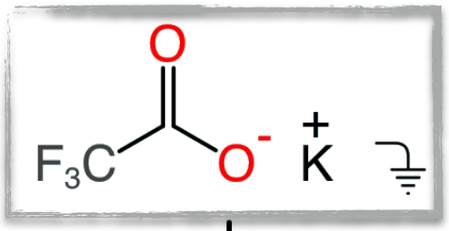
solvent





intermediate

+



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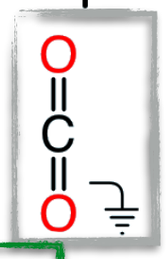
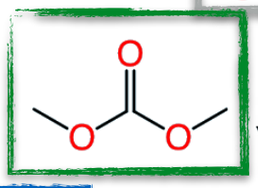
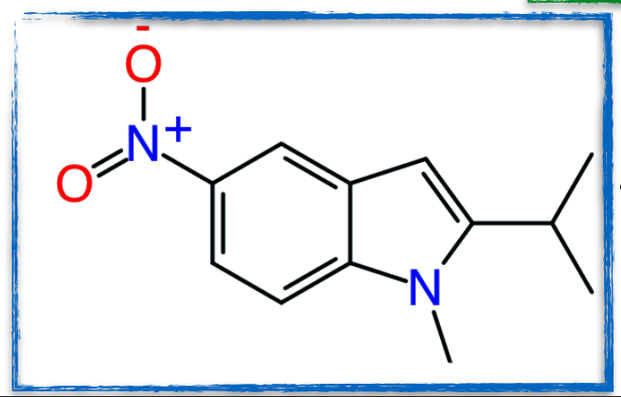


byproducts

reagent



final product



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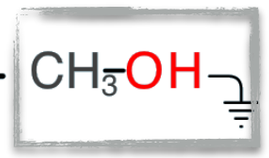

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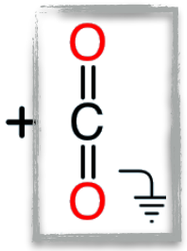


Functionality

- 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

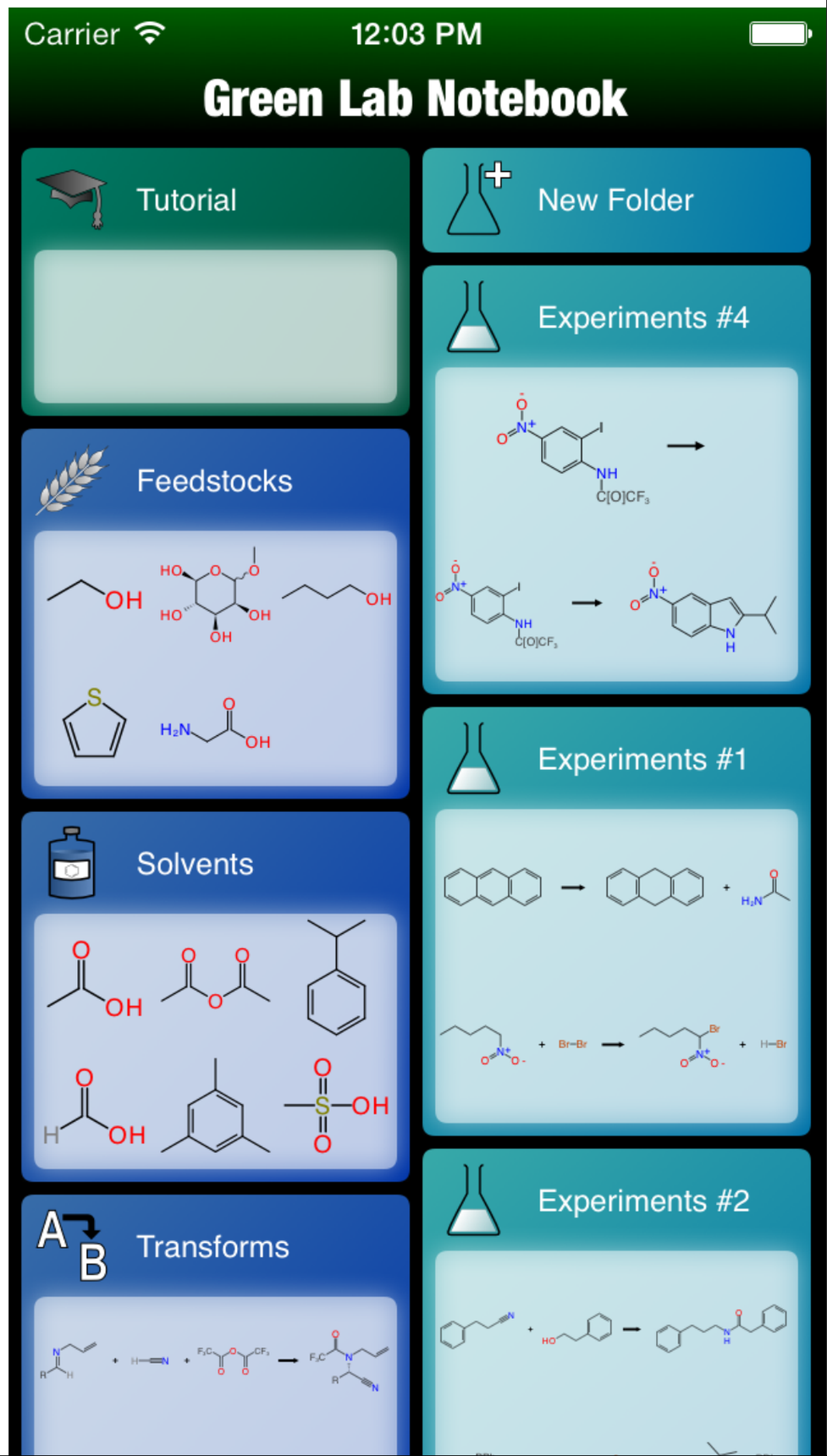
Yield101

- 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

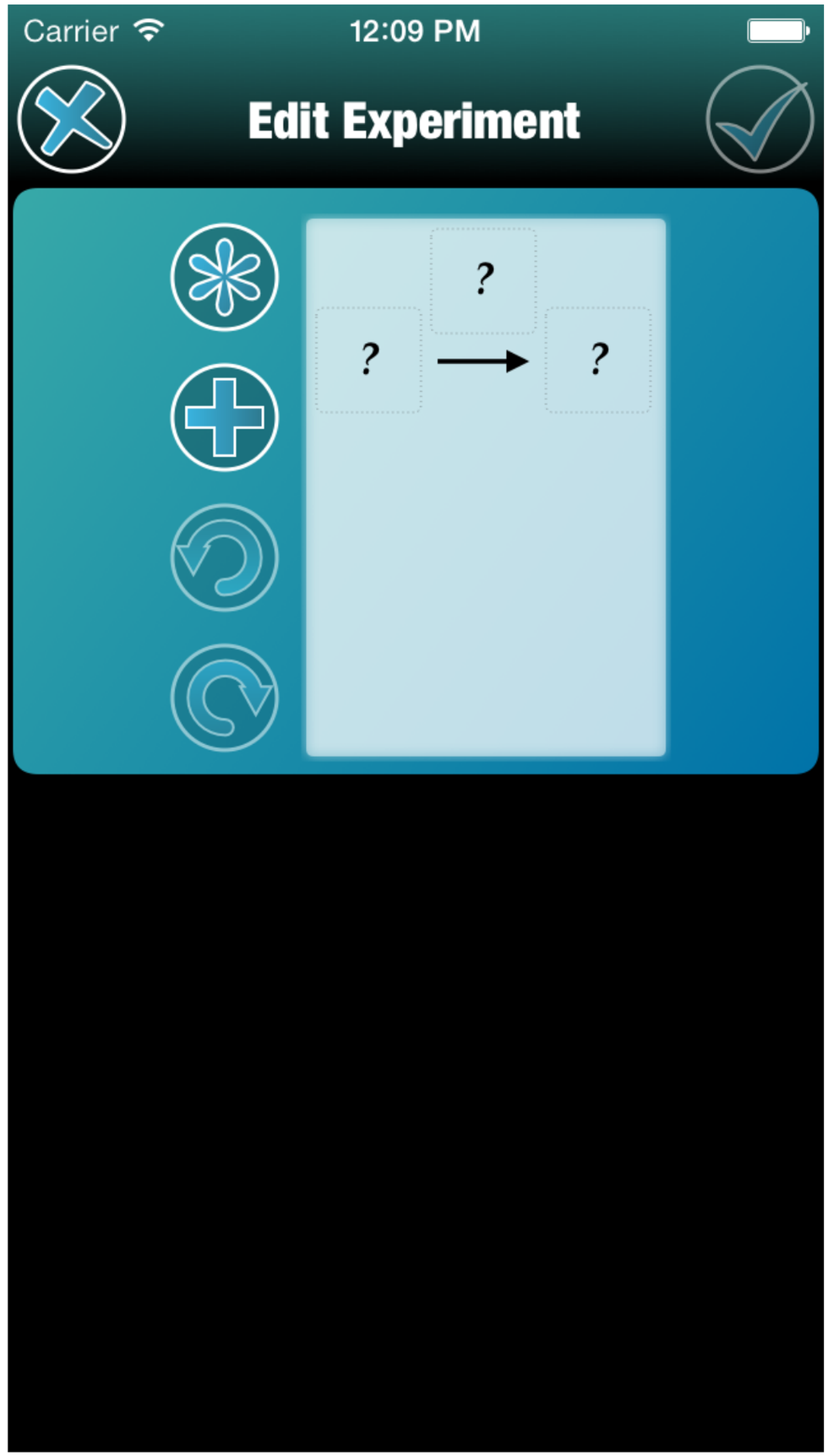
Green Lab Notebook

- 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…



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



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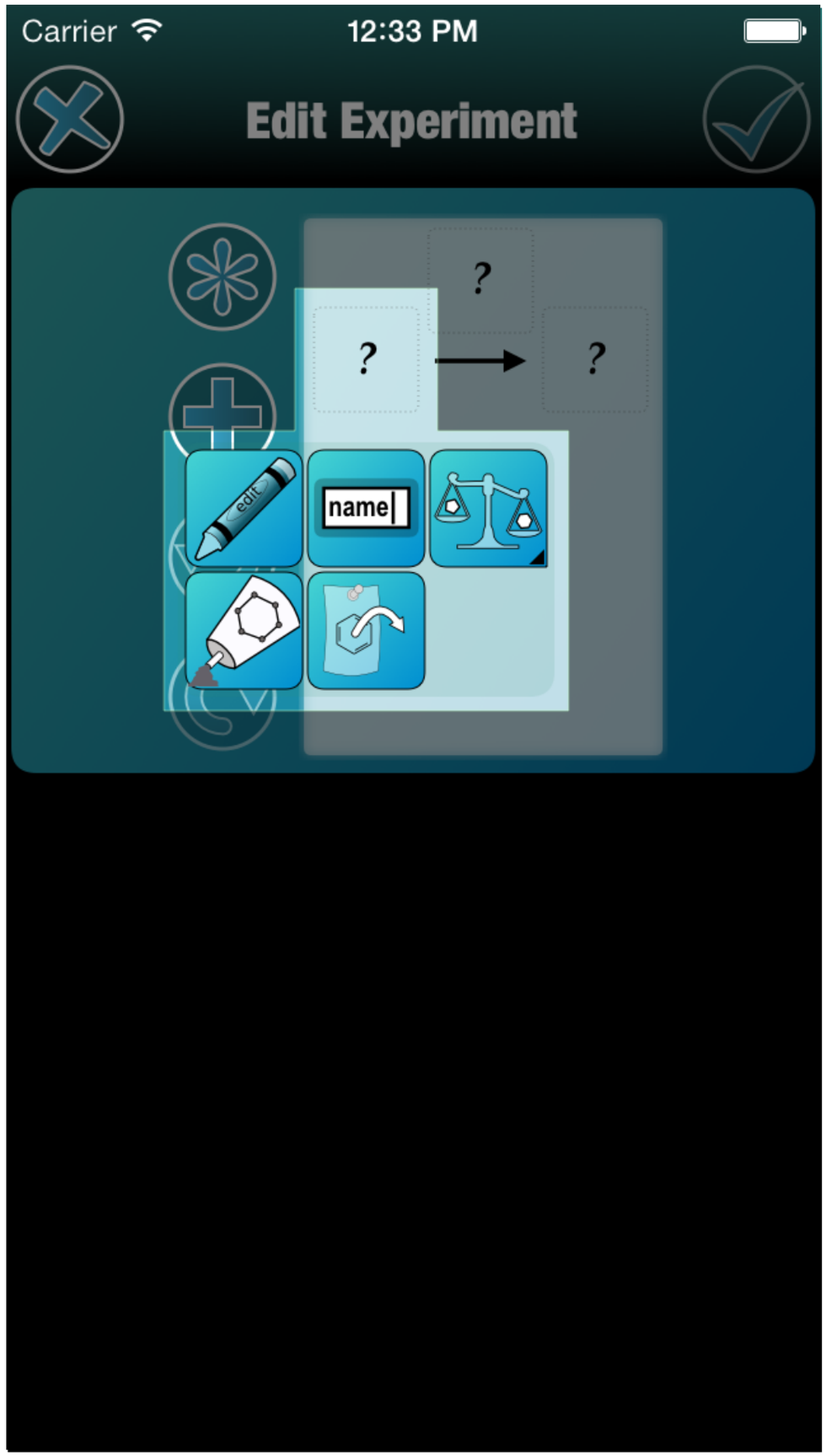

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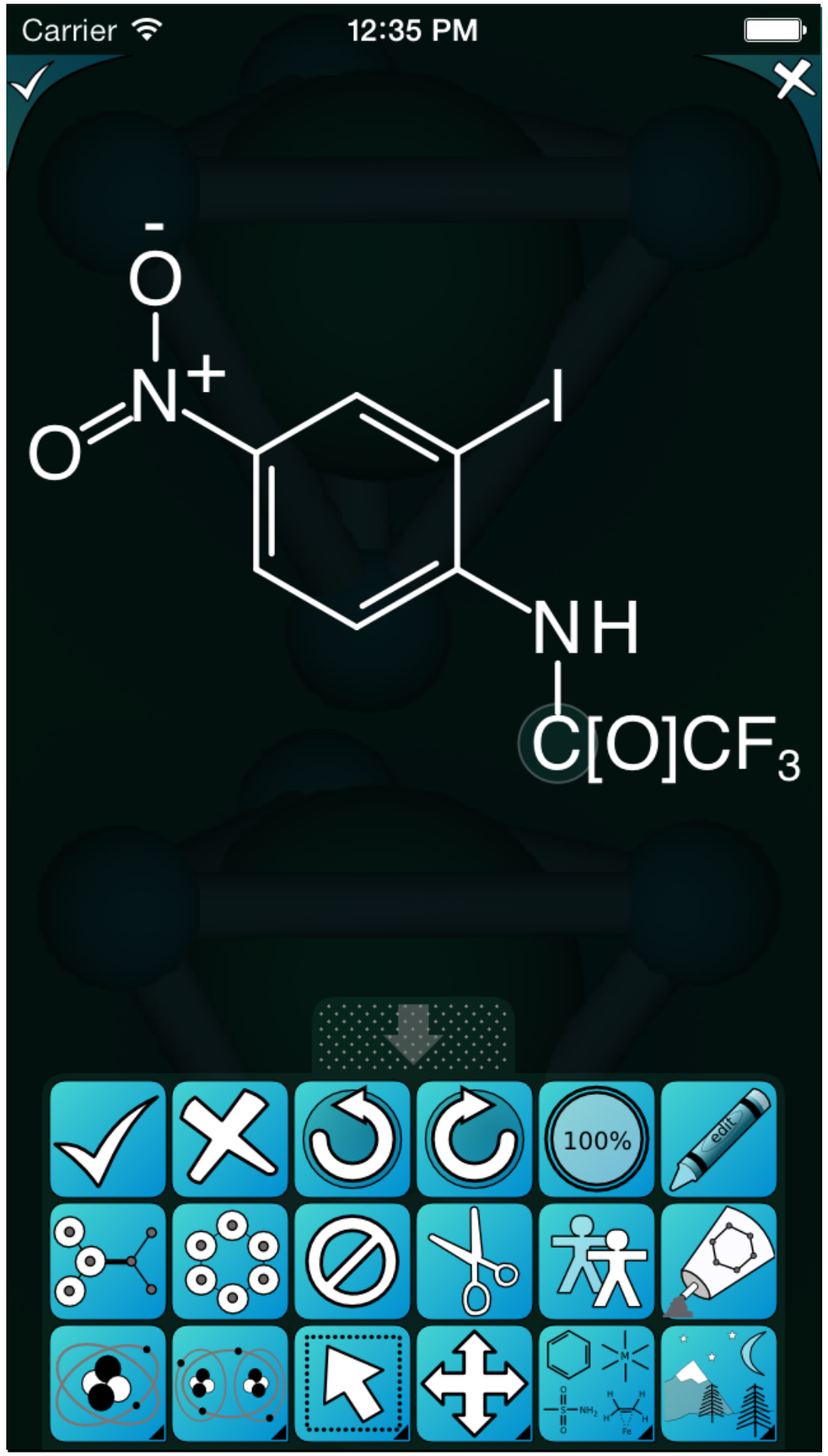

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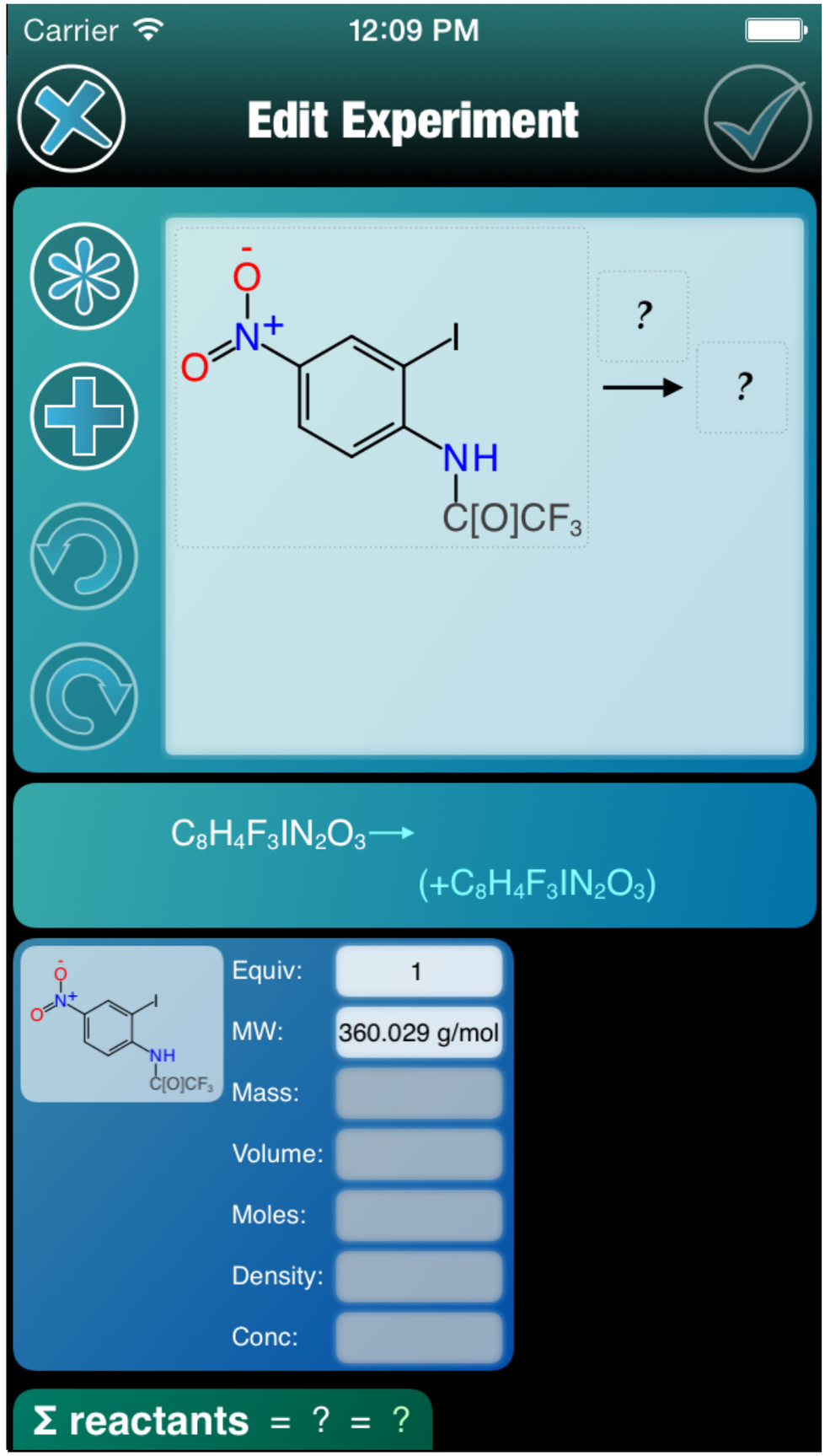
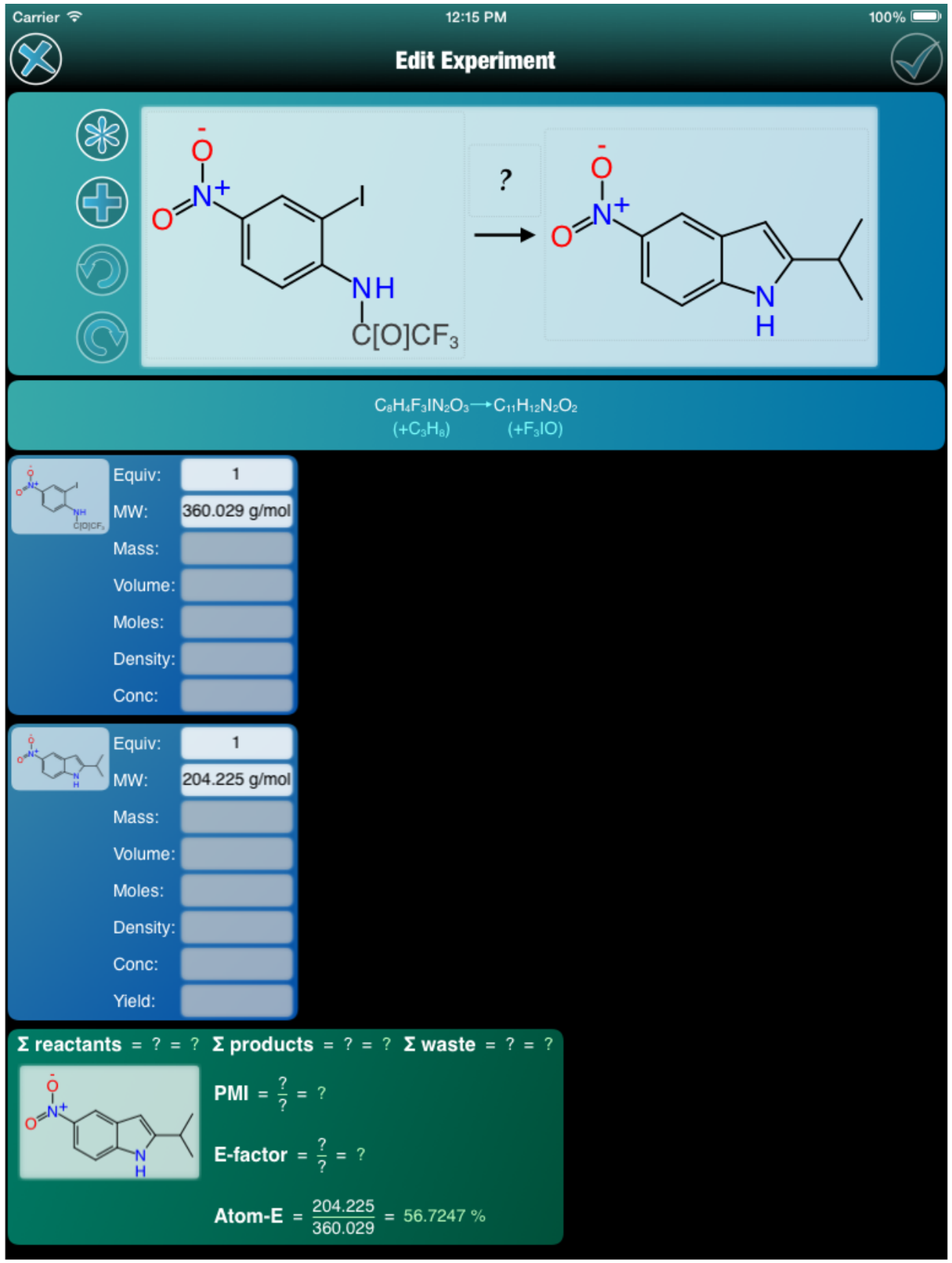


The First Step

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



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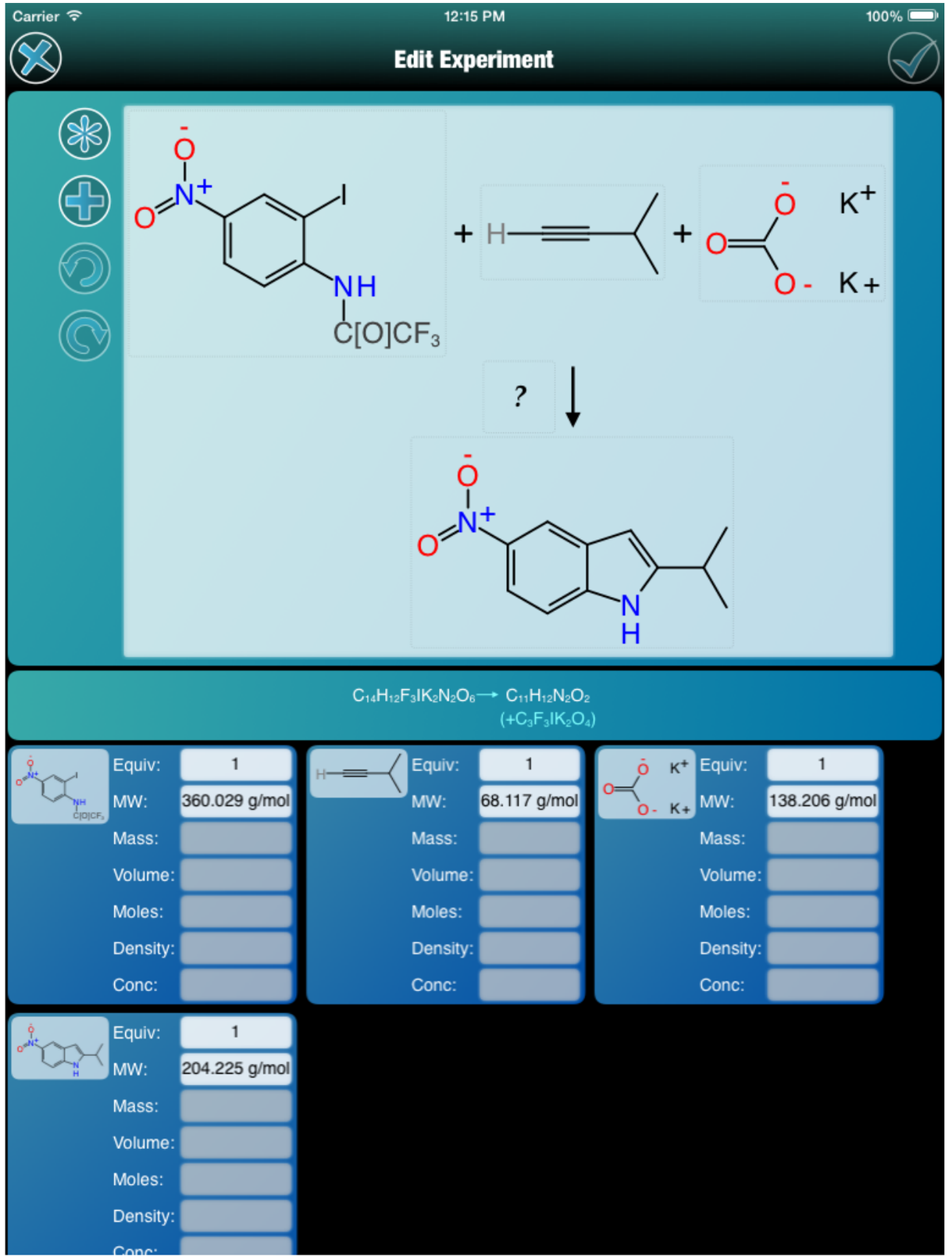

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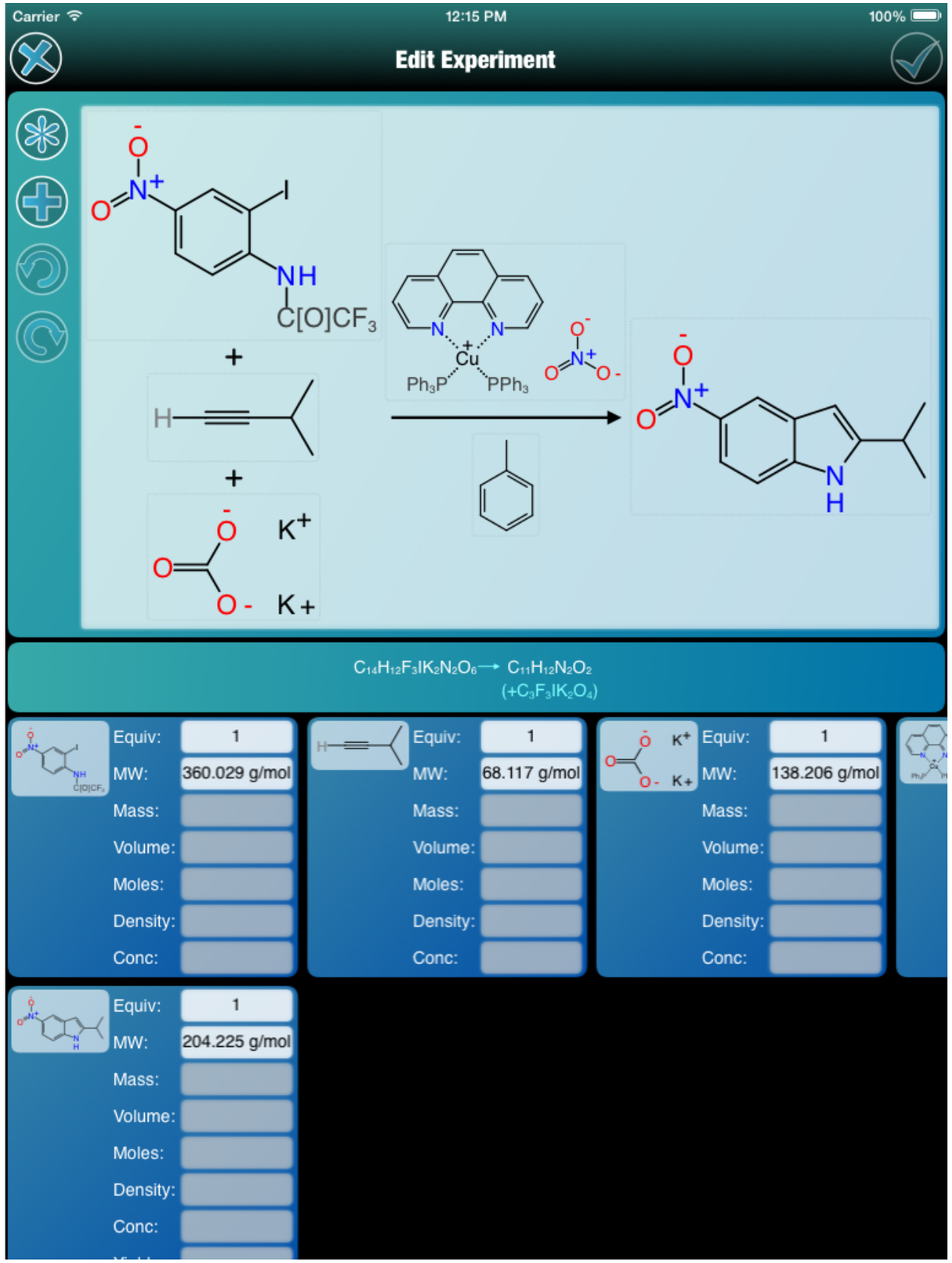

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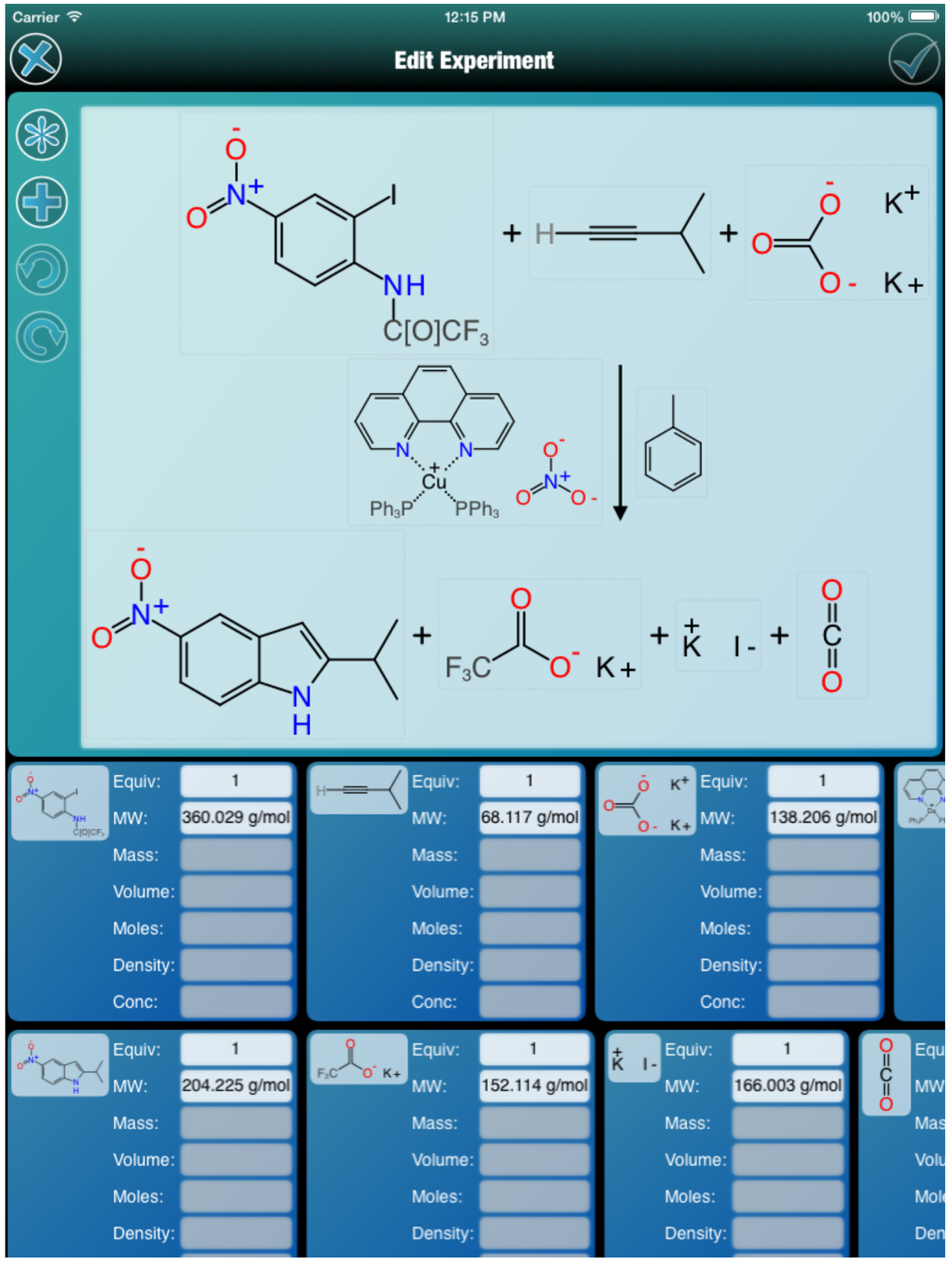
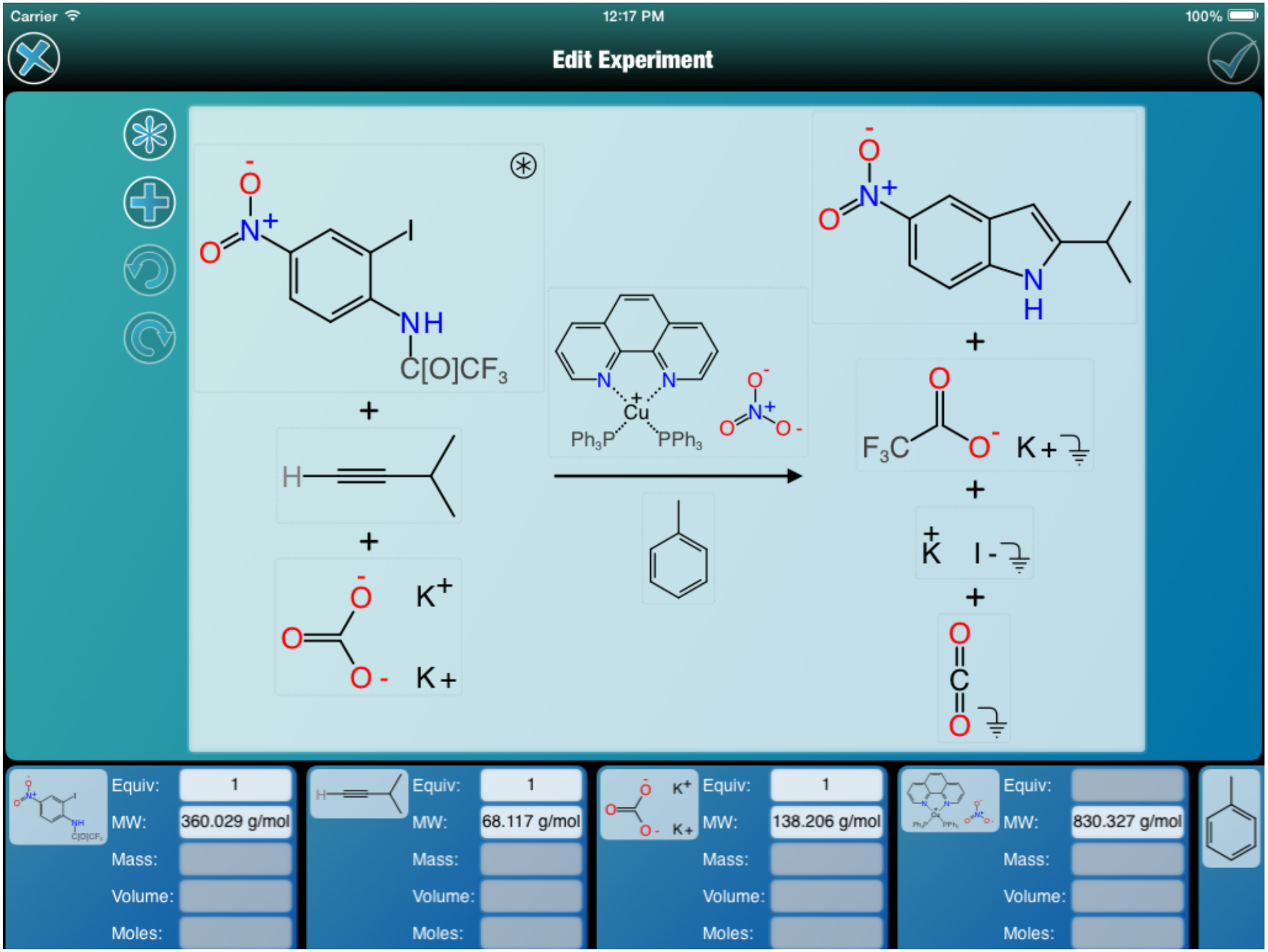


Quantities



- Classify primary reactants & waste products

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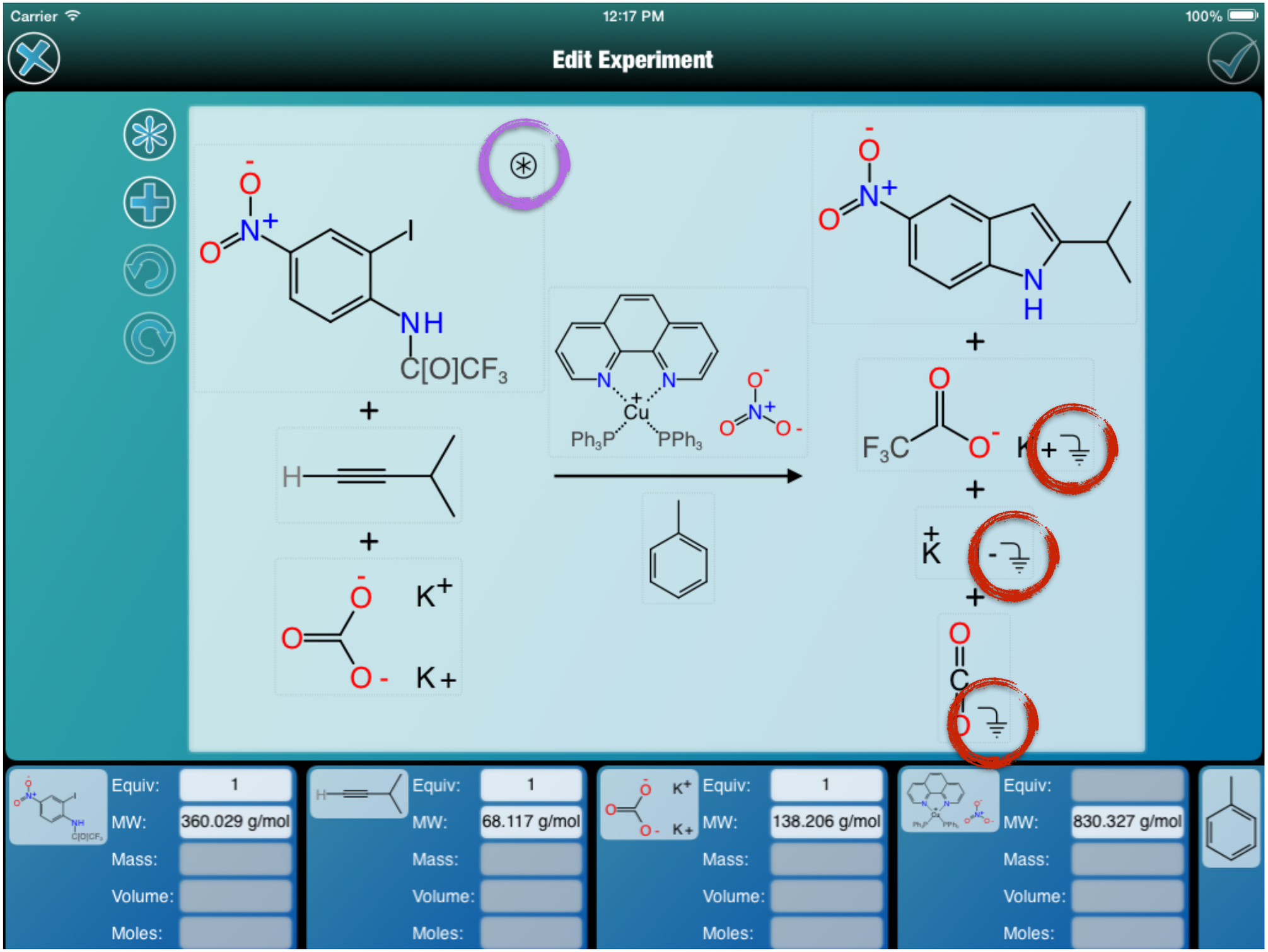
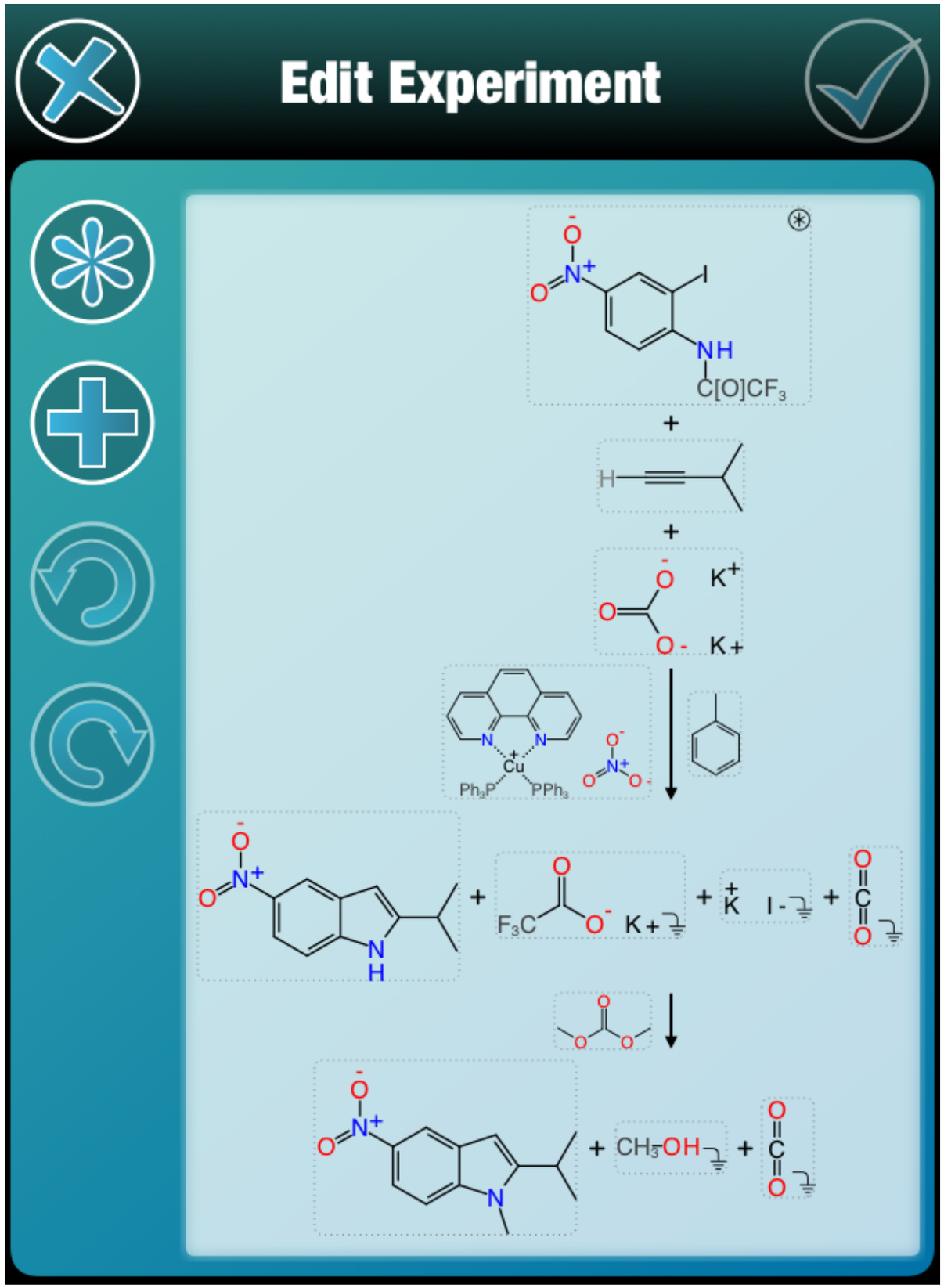


- Classify primary reactants & waste products

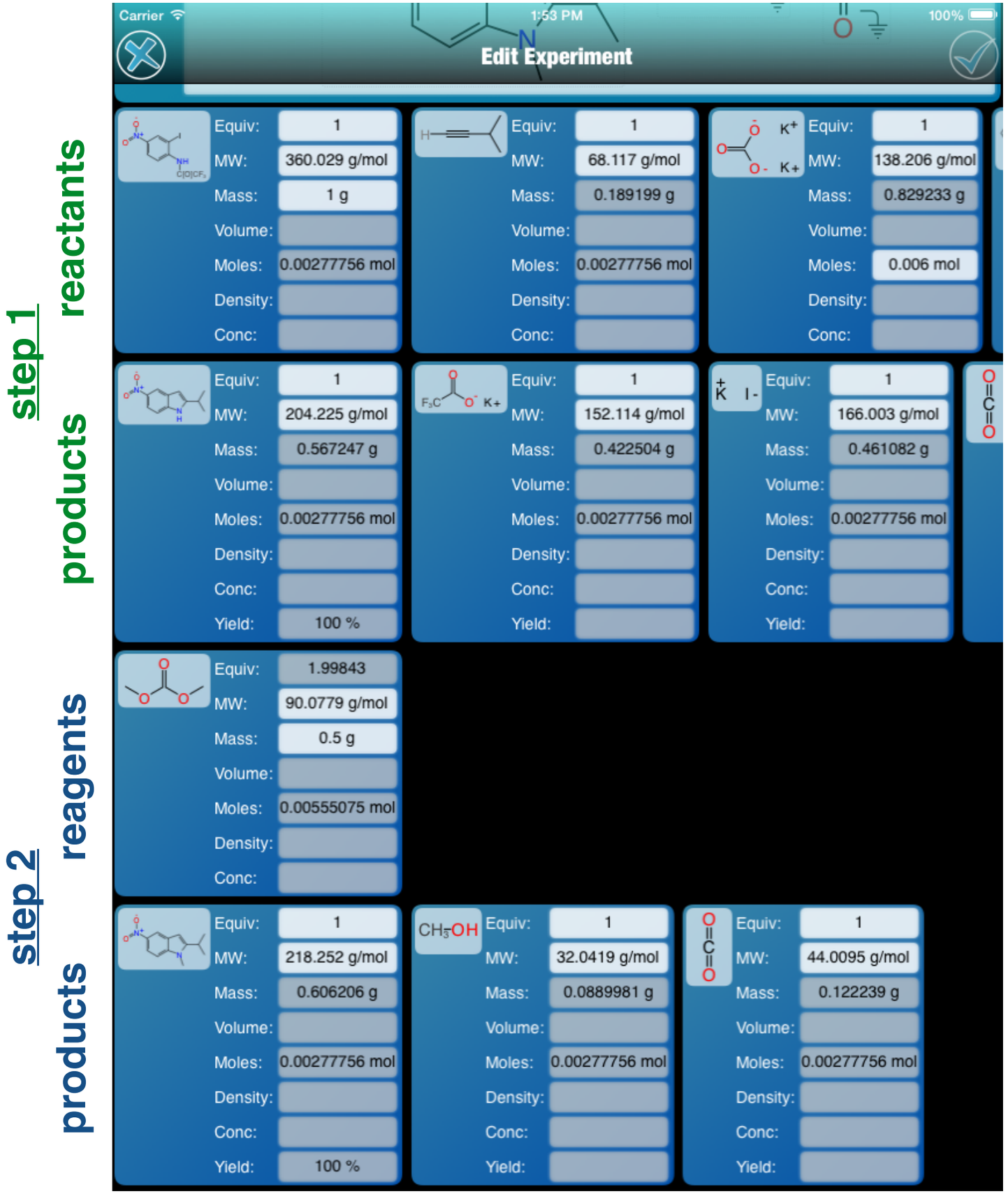
The Second Step

- 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…



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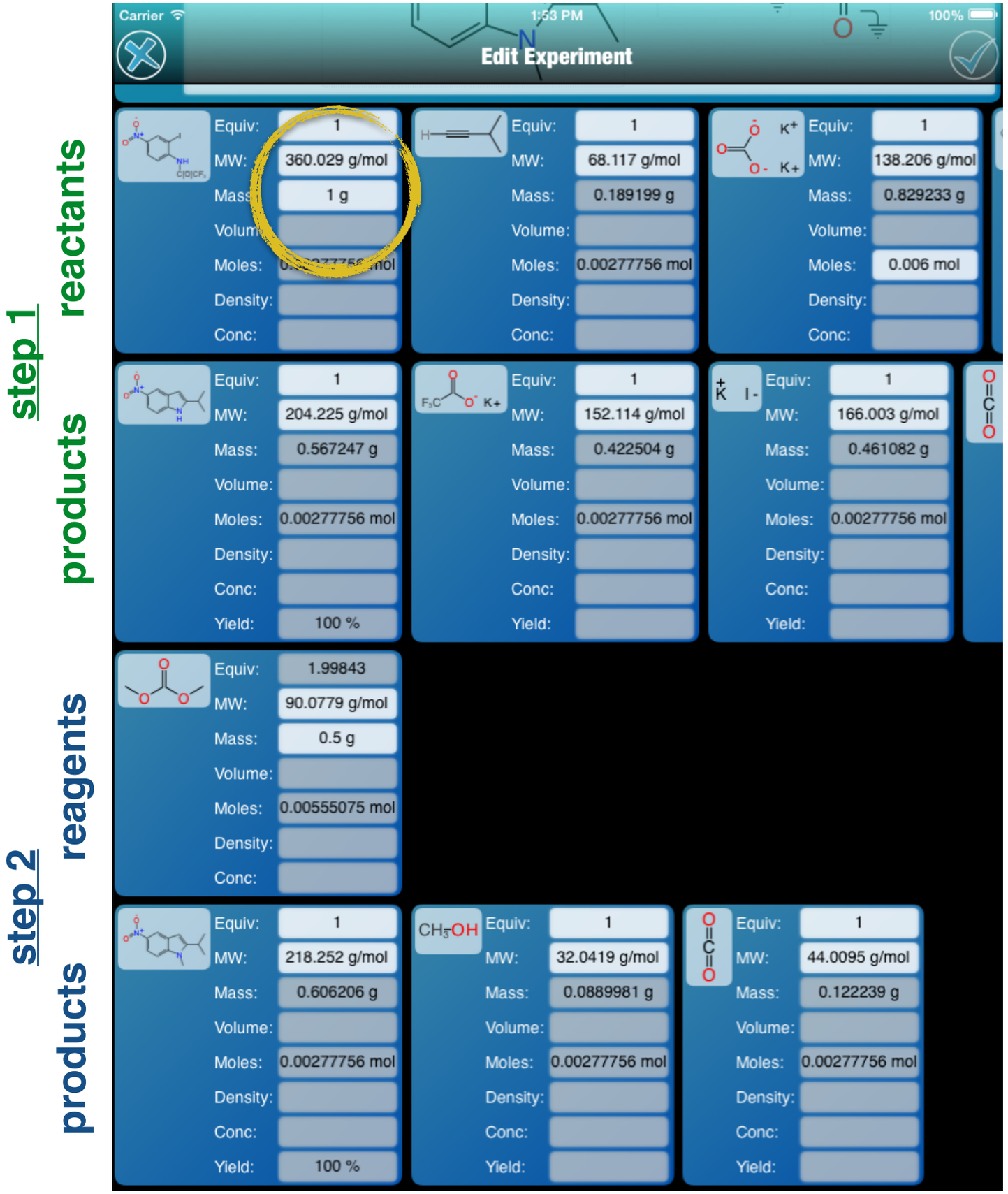


Green Metrics

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

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

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

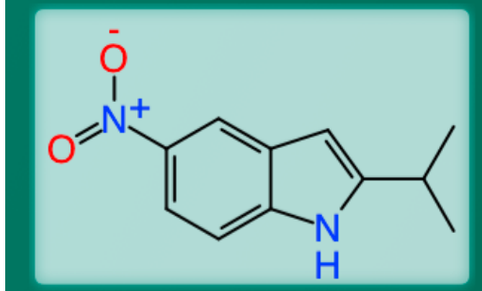
- Trivial calculations… if the information is available.

Green Metrics

Σ reactants = 1 g + 0.189199 g + 0.829233 g + 0.115314 g + 17.34 g + 0.5 g = 19.9737 g

Σ products = 0.567247 g + 0.606206 g = 1.17345 g

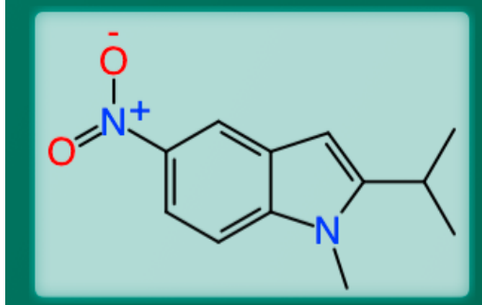
Σ waste = 0.422504 g + 0.461082 g + 0.122239 g + 0.0889981 g + 0.122239 g = 1.21706 g



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

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

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



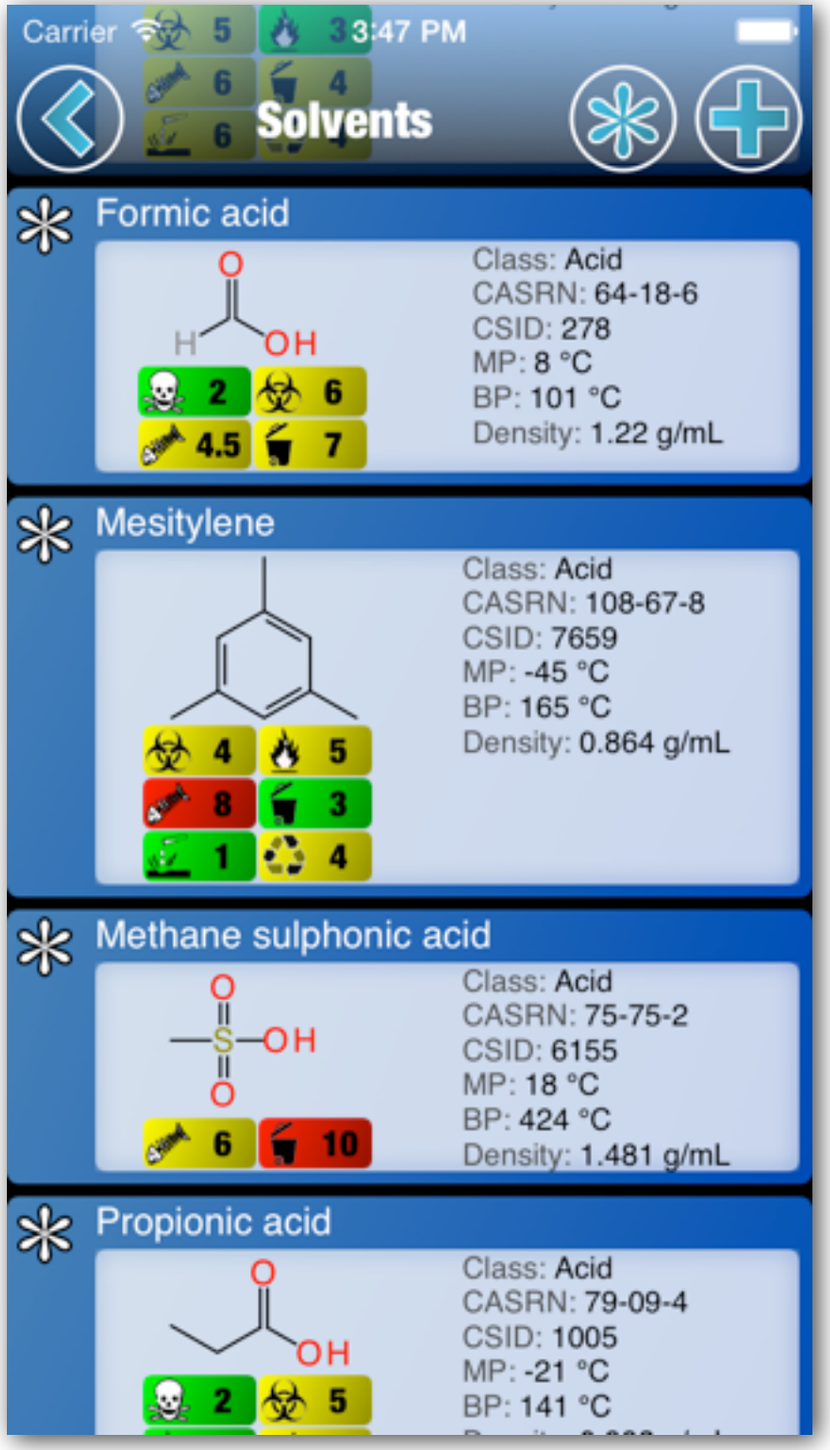
$$\textbf{PMI} = \frac{1\text{ g} + 0.189199\text{ g} + 0.829233\text{ g} + 0.115314\text{ g} + 17.34\text{ g} + 0.5\text{ g}}{0.606206\text{ g}} = 32.9487$$

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

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

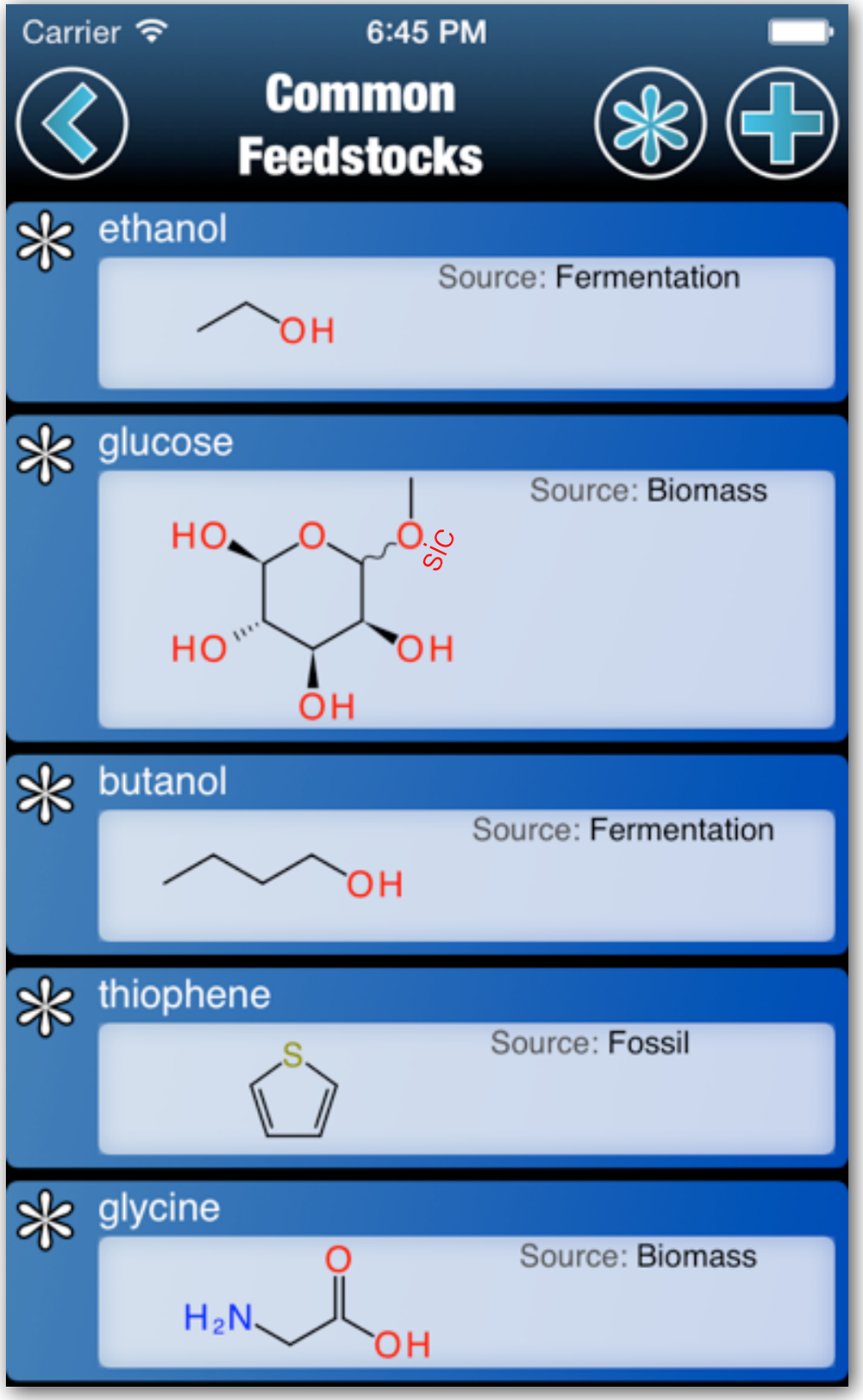
- Totals for reactants, products & waste
- For each non-waste product: PMI, E-factor, Atom-E
- Always calculated, always recorded…

Green Solvents



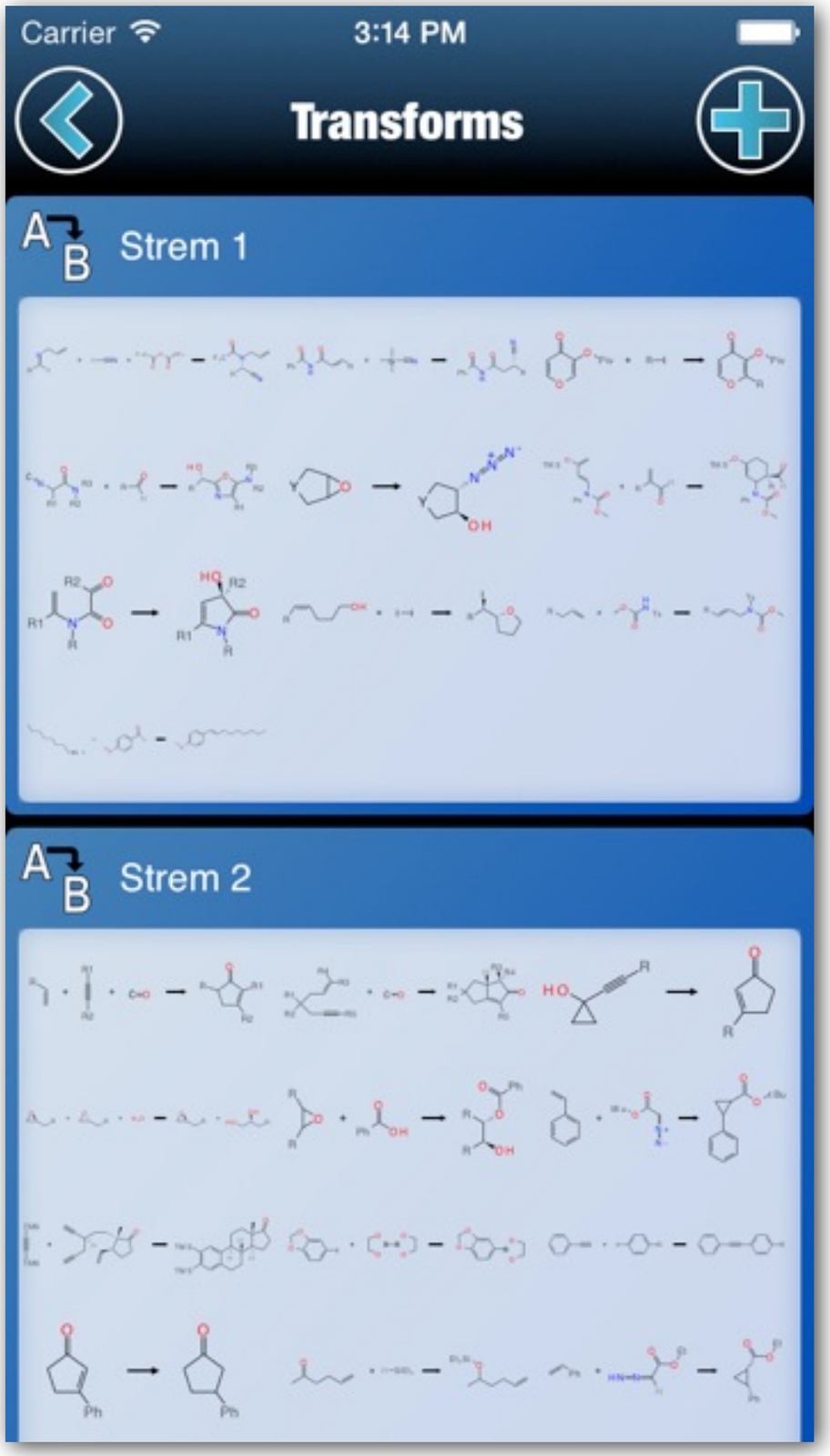
- Environmental data from ACS GCI & GSK

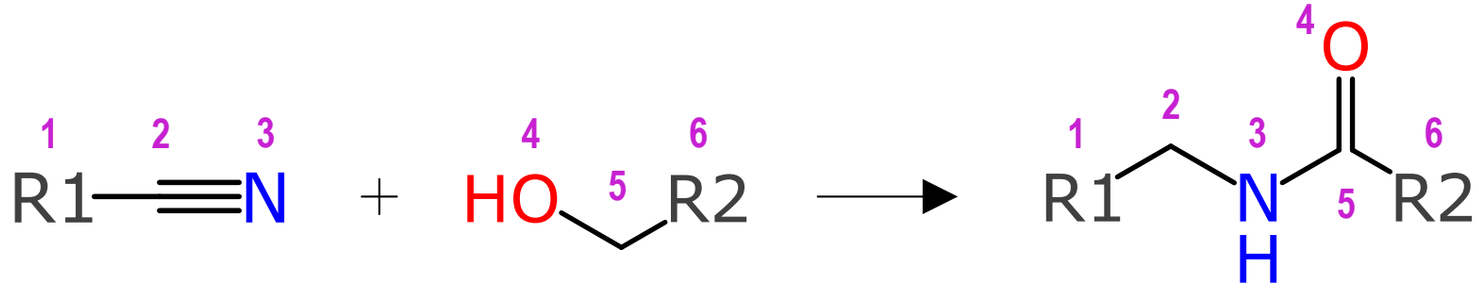
Feedstocks



- 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

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