# Notes from Ami brainstorming session, 7-May-2010

# Solutions identified

## Planning

1. Capture COSHH safety info
2. Access to reaction stoichiometry prediction tools
3. Online access to published literature & internal info
4. Access to reaction prediction tools
5. “Similar expt” in ELN – Failed Expts
6. Online access to department & government safety info

## Discovery/Retrieval

1. Searchable repository
   1. ELN
   2. File stores
   3. Sub-structure search
2. Reasons for failure
   1. Record them
   2. Search them
3. Data store/Repository
   1. “Central” store of publication process
   2. Process <> ELN
4. Access to previous reviewer’s notes
5. Templates for common journals
6. Upcoming events
   1. Deadline for conferences
   2. ELN? Shared lab?
   3. Publication deadlines
7. NMR database 🡪 ?intermediate area? 🡪 ELN/Word/Latex
8. Access to literature or computed properties of chemicals

## Access to experimental results

1. Where’s Jim’s spectral data? (He left 6 months ago…)
2. Tell me what I did 6 months ago
3. If you take an NMR, automatically overlay with known one from databank on your previous expt
4. Intelligent archiving can we group all of my files in one place automatically
5. Information/data to hand (not having to leave fumehood)
6. Access to failed experiments. Don’t repeat mistakes
7. Access to results from similar expts – NMR, crystallography, infrared, etc
8. Repeatability – comparison of repeat expts
9. Who was the Part 3 student who worked on tosylation? Where’s her report?
10. Has the stereochem of our skeleton been confirmed by crystallography

## Write-up as you go

1. ELN input at fumehood
2. Write-up as you go
3. Smart templates for reaction workup
   1. Do extraction
   2. What solvents
   3. How many…
   4. All selectable from the fumehood
4. Write up with dirty hands
   1. Verbal?
   2. Writing in the air?
   3. Dictation to written notes
5. Capture COSHH safety info

## Monitoring

1. If multiple things going on, pull – out Windows for individual experiments
2. Fume hood tracking system (“what do I contain? What is this reaction?”)
3. Making experiment monitoring information available remotely
4. Stream data off equipment
5. Science data from electronic equipment to ELN
6. Fumehood access to ELN
   1. Similar experiments
   2. Group/manage experiments
   3. Compare results
7. Take video
   1. Every 10 minutes when nothing happening
   2. Take more video when something happens
   3. Video of interesting bits
8. Video monitoring of fumehood (visible and infrared)
9. Experiment monitoring tool/apparatus (videoclips, analytical equipment, temperature, pressure)
10. analytical monitoring of reaction and trigger actions I.E. watch the chemistry and then have machines follow program to collect a sample
11. monitor out of bounds behaviour
12. computer watches what you do and “understands” the process, writing it up as you go
13. information on scientists working in this scientific area and do they have this reagent that could be borrowed
14. departmental and group chemical inventory
15. Info on chemical suppliers
16. An equipment management system (model, maintenance, calibration, contracts, people, warranty, price, age, etc)
17. Reagent tracking system (real-time location monitoring – “Where did my bottle of chemicals go?!”)

## Process automation

1. Automatic preparation of samples for analysis
   1. Filter
   2. Dissolve
   3. Appropriate vessel
   4. Label it
2. Remote monitoring and then alert anyone else in the lab to control the reaction
3. Automated service for checking the purity of reagents
4. Safety switch-off
5. Re-prime pump/alert researcher
6. Remote control of apparatus via Bluetooth (stirrers, incubators, etc)

## Supporting the experimentalist

1. Tech as human support rather than replacement
2. Barcode bottles and reagents. Have video monitoring what you do. Verbal confirmation. PC alerts if verbal and bottle different
3. Re-direct incoming calls when at a fumehood
4. Watches what you use. Notes how long it’s left open and reminds you to put lid on
5. (Added later – idea from PMR/Tom) “LabNav” – a satnav type of monitoring helper that prompts/reminds you to do various things at different points of the expt

## Authoring/Publishing

1. Automated analysis tools
   1. E.g. NMR spectra for peaks
   2. Parse data from PDF NMR
2. Standardised programs to process data?
   1. More accessible/easier licensing

## Control – Getting people away from the fumehood

1. Computer display & control at the fumehood
2. Social working/contact info – find colleagues
3. Detect if someone is in the lab or near the fumehood

## Wild Cards

1. Capturing the necessary bureaucracy information for disposals etc
2. Disposing of waste
3. Waste shoots within fume cupboard
4. Glass washing
5. A compact side of fume cupboard glassware washer and dryer
6. What’s the impact factor for current chemistry? Do other Cambridge chemists submit to it

# Original raw ideas

## Planning

* Is cocaine a controlled substance? What do I have to do to get some?
* Access safety data at fumehood
* Recording compliance with safety requirements
* What can I use instead of carbon tetrachloride?
* What’s the boiling point of 1:1 methanol/water
* Boiling point for solvents at non-atmospheric pressure
* Information about the chemicals being used – safety data, availability etc
* How many moles of acetyl chloride is 3 ml? Quick calculator for making up standard solutions

## Access to literature

* Better reaction searching. What have people done before? What didn’t work?
* Intelligent “on the fly” literature searching of chemical reactions
* Searching literature
* Provide a portal to data/methods/reaction conditions at fume hood
* What new methods have been reported in the last six months?
* Access to reference material
* What will benzoic acid dissolve in?
* Be able to ask robot in your fume hood how you work up a common reaction type
* Predict side reactions
* Reduce possibility of reaction failure by route analysis / reaction analysis

## Expt control & monitoring

* Remotely controlled hotplate settings, reagent addition, reaction monitoring
* Programmable reaction start/stop times
* Remote monitoring of a reaction while I’m away from it
* Remote monitoring
* Monitor reaction
* Automatic following of reaction progress based on visual/IR changes just you with normal equipment
* Online monitoring of pumps. Pressure, flow rate, etc
* How is the reaction progressing while I’m not there?
* Reaction status live on desktop
* Continuous reaction monitoring
* Capturing results on my computer
* Capture experimental data as it’s generated
* Voice-controlled retort/clamp movement, open/close
* Video review of reactions (can’t always be there)
* “Replay” the experiment
* Assign destination/end use of product
* Programming machine
* Access to visualising information at the bench or fumehood (i.e. hardware)
* Easy access to information about what the reaction is
* Takes samples to analytical machines
* Continuous monitoring of reaction
* Automate monitoring of long reactions
* Easy ability to keep a log of the expt as it goes along
* Constant LC monitoring of reaction and switch off temp or quench if done
* PDAs to capture experimental procedure as you perform it with ability to automatically convert to an ELN entry
* Haptic devices for remote collaborative lab work
* Haptic devices for virtual lab work
* “Intelligent” robot arms – learn your own movements to ease programming of automated tasks e.g. crystallisation trials
* Manipulate reagent weighing & dissolving
* Handle very toxic things so human does not have to. Get rid of humans wearing gloves. (That one not effective)
* Intelligent monitoring of people at fume cupboards 🡪 towards automated safety warnings etc
* People make decisions, machines do the rest
* Can you look after the reaction over the weekend
* Remote control i.e. check reaction from home
* Remote control reactions
* Remote reaction control (wireless? Or via web?)
* Purify reaction mixtures
* Sourcing parts
* Mark/identify reaction vessels. Write on the labels, RF-tags etc
* Availability of analytical resources
* Safety? Turn off heating when reaction vessel is empty
* Safety. Switch off for reactions. Monitor temperature & pressure
* “Out of spec” alarms
* Text/call when reaction goes out of scope

## Collecting experimental results

* Interpreting data
* Automatic single crystal machine in lab. Crystal in 🡪 Structure out
* Data logging
* Access to my files & PC from the lab fumehood
* Capturing info with “dirty” hands i.e. not using pen or keyboard
* Increase reproducibility. Could “mirror” what is done by experimentalist that way of reducing the number of “capricious reactions”. Get rid of human element
* How did she add the D-ring to our framework
* Send/box up products to collaborator
* Easy capture of non-computerised information (e.g. methods, visual observations)
* Get rough notes directly into ELN
* Data input at workstation/fume hood
* Tool to suggest alternative synthesis methods to make something
* Capture data temperature boiling points etc in context date, who, where, automatically
* Built-in optics for solvent dispensing – no more Winchesters!
* Provide advice to confirm what you’re doing is what you intend to do! “Are you sure you want to do that?”
* Writing on fume hood (black marker pen) transferred into lab book and ideas book
* Voice recognition for experiment write-ups
* Where’s the NMR for compound B234
* Writing results into the ELJN
* Hardware to simply input ELN info in lab environment
* Automated records of protocol
* Voice-activated standard robotic lab procedures
* Automatic distillation (collecting fractions)
* Tell the resol what to write into lab book e.g. press a button and say “Added …, quenched with …, extracted with …” – automatically calculates time
* Dictate write-up as you perform the experiment
* Data organisation – all data for paper grouped together
* Catalogue of spectra to see if what I think I have made matches what else has already done
* Know what reagents I have and where they are, that are analogues for which of things to make
* Automate titration
* Log everything

## Write-up and publication

* When’s the last date for submitting ACS abstracts? Where’s the program?
* NMR data 🡪 paper format for spectrum data
* Write-up. Automatically create spectra reporting sections from spectra
* Convert these spectra into the right form for publication
* Associating supplementary files to paper
* Data straight into papers
* Handling of expt information – pulling the results together for reports/publications
* What problems have reviewers raised with our group’s work?
* Speech-based lab records
* Write reports & presentations
* What do I need to submit for J. Med. Chem?
* Convert my JACS paper to RSC format
* Automatic authoring/ formatting of expt data. Reformatting for different journals

## Inventory

* Where’s the Tosyl Chloride?
* Where is the xxxx? Does anyone have any?
* Source reagents
* Does this chemical exist in the department
* Chemical inventory built into ELN
* Automatic supply of materials based on plans
* Verification of reagents
* Equipment inventory with maintenance history. Does the equipment work?
* Ordering reagents.
* Ordering new chemicals
* Automatic reordering when finishing bottle of common reagent
* Check purity of starting materials

## Social

* Unpaid slave
* Take distracting phone calls & unexpected visitors
* Where’s Jane?
  + GPS systems
  + “Spy” cams
  + Proxy detection. Address issue of why we need to talk to Jane
* What’s Steve’s mobile number? Can I ring him – what time of day is it in Japan?
* Built-in tea lady/man
* Some way to have coffee in lab whilst working (without upsetting safety officer)
* Meet & greet colleagues / collaborators
* Is someone else doing something similar to me?