# Assay Screening Software Tool – Taking Stock – March 2018

Pete H

This the note I promised to send to explain the meeting I’ve scheduled.

The way this has been working is that Chris has been working as a go-between and advising Pete and Prasanna on the problem(s) this software is trying to solve, and the theoretical possibilities of what we could do.

Pete has been doing the thinking about the “art of the possible” from a conceptual point of view, and from a software design and architecture point of view.

Initially Pete was doing experimental development of the “back end” – where the key conceptual logic, and database lives, while Prasanna was developing the front-end – exploring GUI ideas and potential user experiences (UXP), as they became feasible via the back end services. More recently Prasanna has taken on the work on both ends – with Pete’s supervision and support.

Pete has been hesitant to engage with Nicky directly because to communicate effectively between the worlds of software and the world of assay-screening requires really quite expert knowledge of **both** domains, which neither Pete nor Nicky have. We are sufficiently alien to each other (if you’ll forgive the analogy), that communication was too difficult. Hence using Chris as a go-between.

However, in hindsight, we’ve had too many exciting ideas about the “art of the possible” which have led to time-consuming work and dead ends.

We’re on to our third conceptual approach now. Chris is confident this one is better than the previous ones. This meeting is to make sure we explain where we are heading so we can scrutinise it as a group. Hopefully with an early GUI demo that shows the basics. We should then be able to proceed with much tighter and more frequent steering discussions between us, and chase down some real early deliverables.

@Chris please chip in with a commentary if you think it helpful.

**I’ll note below the outline of the approach we’re currently following.**

And we’ll demonstrate as much of this as we can on the day – at a rudimentary stage of evolution.

* Behind the scenes, sits a database that contains information about
  + Reagents, and their stock concentrations
  + Associated information and relationships about Organisms, Strains, and the Primers that have been designed and endorsed by DNAe.
* There is a Web GUI that lets you manage (curate) this data as it evolves over time.
* The database also holds all the experiments that you design and run. This includes the experiment design and the results.
* The core of an experiment design is its set of plates, and the mixtures of liquids you put in each chamber/well, and in some cases, transfers you make between well-to-well.
* The Web GUI lets you design an experiment by specifying what mixture you want in each well, at the **final** required concentration.
* We are working on a user experience (UXP) for this which will let you type in a series of rules to make the specification of the allocations you want, as quick, easy and lucid as we can. (We’ll demo this at the meeting).
* This UXP shows you the allocations of the plates in your experiment at the same time, including transfers. (e.g. preamp product into id plate)
* The UXP will “know” about the reagents that are in the system, and will use this to auto-complete the stuff you have to type in – making it quicker, and harder to get wrong.
* The biggest difference between this suggested process and the current spreadsheets, is that the human being does not have to think about what should be pre-mixed, nor be bothered with dilution factor calculations.
* Instead the intelligence lies inside the system to be able to “discover” what pre-mixes are possible. I.e. it will discover what you could put in a buffermix or mastermix – automatically, and it will “discover” primer pools you have implied.
* It will also take care of the chain of calculations that determine what volumes of each pre-mix is required, and the work-instructions for dispensing sub-volumes into either wells, or intermediate containers.
* The GUI will of course show the premixes, and be capable of formulating mixing work instrutions, and in due course programming the robot to support this.