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C3 Annual Report - 2020

Matters arising from previous reviews

The problem with dusty plates has been fixed by the addition of filter material to the air vents of C3, reducing the particulates in the air of the laboratory.

The Oryx drop size issue has been *partially* resolved by new finer bore tips supplied by vendor.

Things of note from the C3 Huddles:

- Upgraded to Windows 10 throughout C3
    - Needed vendor software updates/dongle updates estimated cost $35K
- Vents cleaned and filters installed in main laboratory
- Phoenix I decommissioned
- New TECAN calibration (dispense weight) spreadsheet
- Loose water inlet water on TECAN fixed
- Multichannel electronic pipette repaired
- New plate protocol (nMC + nMA) for Phoenix II
- QC spreadsheet for Phoenix validation
- 20° Imager repaired (broken board replaced)
- Storage of optimization blocks moved to cold-room to slow down degradation of PEGs
- Storage of standard C3 blocks moved to -20°C freezer
- Nick and Marko both moved on to PhD positions at major universities.
- Phoenix II nanodispenser needle got bent but was straightened out with no ill effects
- Issues (battery and cable) with the camera that images stock lids on TECAN
- Issues with Sypro aspiration and dispensing on Phoenix (valve on tip two loosens over time)
- Some issues with non-continuous barcodes from vendor
    - MC1XXXXX (Pink barcodes)
- Ran out of stability IDs that fit on tube labels
    - Moved to 2D barcodes, and purchased a 2D barcode reader
- New buffer screen, buffer screen 10 (BSX) removes the dangerous chemical piperazine
    - pH 5.5 conditions now using the buffer sodium malonate-malonic acid
- New business rule to only scan out expired plates on Mondays, after accidently confusing an active plate with other expired plates
- New tips for Oryx correct (some of) the persistent different in drop size between subwells
- Densities of stocks measured and stored in DB
- New GHS symbols added to bulk chemicals in Quartzy
- Chris Watkins leaving CSIRO, which will curtail our Machine Learning development
- New user contracts sent out in February 2020 and due back 15th March 2020
    - Major change is inclusion of GST in pricing
- New sample and plate handoff requirements due to the COVID-19 pandemic.
    - C3 closed on COB March 26 until further notice by a decree from the CSIRO executive
- TECAN replacement machine (Hamilton MicroLab Star) has now been installed at CSIRO

    - Waiting for the software tools and training before it can be used in the C3 process.

Software and infrastructure

- iQC workflow is broken
    - difficulty in finding developer to update and maintain
- New column added to DSF content map for ordering of samples in the report
- Added See3 functionality
    - Blocks tab – not yet complete
    - Stocks tab – need to add stock location as well to the table
    - pH curves
    - single condition export
- GPSamplr updates
- Dragonfly recipes available in C6
- New 'Check Stock' function on StockAide
- Hamilton Star ordered and received (not yet functional)
- Block heater/shaker purchased, used to efficiently thaw frozen blocks.

Complaints/Feedback

Issues with LCP plates droplet centering / moving.

Students and Training

- Sebastian Failla (Swinburne Industrial Placement Program)

Significant upgrades or method modifications

- Some updates to SOPs

Development of new tests/methods

N/A

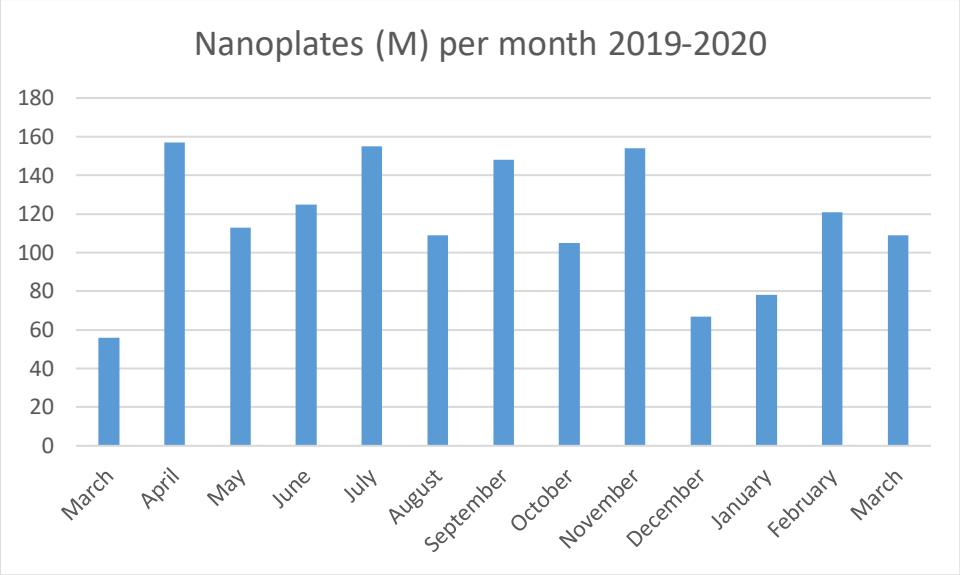
Results of audits

Other items to be raised

- Relocation of C3 to Clayton as per Parkville Relocation Project
    - Significant time investment from C3 staff throughout

Other

- 9 papers acknowledging C3 (We believe that the requirement for acknowledging C3 is not being followed)
- 3 methods papers from C3 work
- 1795 (up from 1371 last year) sitting drop crystallisation plates (MA or MC plates) set up in 2019
- 188 (up from 156 last year) deepwell blocks (Z blocks) dispensed in 2019
- 92 (up from 73 last year) LCP sandwich plates (E0 plates) set up in 2019
- 216 (up from 163 last year) DSF experiments set up in 2019
- 5.06 million images (up from 4.3 million last year) collected last year.



Facility Director's Report

Medium/Long Term Goals:

- Improve autoscoring – online learning
- Develop and implement QC on stock solutions
    - Possibility of using refractometry and osmometry
    - Digitising Stocks notebook and with the aim to coupling in to StockAide
- To continue to develop C3PO optimisation and make it available to users
- Bring DLS and T_{agg} into the C3 as robust analyses
- Datamining using auto-scored images
- Paydirt screen (different precipitants, ionic liquids)
- Streamline stocks
- X-chem
- Continue to remind management that there will be a massive dropoff in C3 usage once the centre is forced to move to Clayton

Funding

- No changes in funding at present
- Seeking partnership opportunities through competitively awarded local and international grants

IT Infrastructure

- All machines now running Win10
- Much of the current IT infrastructure and processes captured on the internal CSIRO confluence page (CCCDM). Active effort to keep this up to date.
- Push to move Oracle database(s) to a single server in Canberra. This would require a move of our Bio21C3 server functionality to Canberra, as known latency issues would devastate our services otherwise. Trials of test databases and servers in Canberra have just started.
- Attempts to set up automatic monitoring of critical infrastructure
- Investigate deployment of a redundant database to reduce server stress and increase speed

Machines

- Incorporate basic mass spec analyses

- Investigate the inclusion of an X-ray generator for *in situ* screening
- Investigate Echo acoustic liquid dispensing technologies
- Commission Hamilton MicroLabStar, include ability to adjust liquid class for each stock using an interative procedure using the in-build balance.

Software

- Re-factor booking software – this was investigated, and no COTS solution exists. Some effort was put into describing what the refactored software would look like, but development was halted due to lack of funding.
- Complete migration from CrystalTrak to See3
- Export C3 software to the greater crystallisation community

Internal Recommendations for Improvements

- Simplify C3 interfaces
- Refine initial screens
- Extend Crystal.csiro.au
- Implement succession planning, including finding long term professional staff for software and labwork.