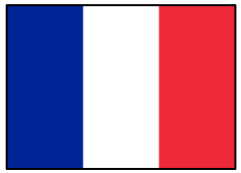



# Status Report DLS

Neil A Smith
31st October 2019

# Contents

- ISPyB Adoption
- ISPyB Developments
  - Life Sciences (MX, EM)
  - Physical Sciences
  - Technical

# Diamond Science Groups

MX

**7 instruments**

Cryo-Imaging

**8 instruments**

Soft Cond. Matter

**4 instruments**

Crystallography

**5 instruments**

Magnetic Materials

**5 instruments**

Spectroscopy

**4 instruments**

Surfaces & structures

**4 instruments**

Imaging and Microscopy

**6 instruments**

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# Diamond Science Groups

## ISPyB Status in 2019

MX

**7 instruments**

Cryo-Imaging

**8 instruments**

Soft Cond. Matter

**4 instruments**

Crystallography

**5 instruments**

Magnetic Materials

**5 instruments**

Spectroscopy

**4 instruments**

Surfaces & structures

**4 instruments**

Imaging and Microscopy

**6 instruments**

**2019: ISPyB integration for physical science beamlines and science groups**
**ISPyB active on 22 beamlines/instruments across DLS**
**>300,000 Data Collections (Jan-Sep)**

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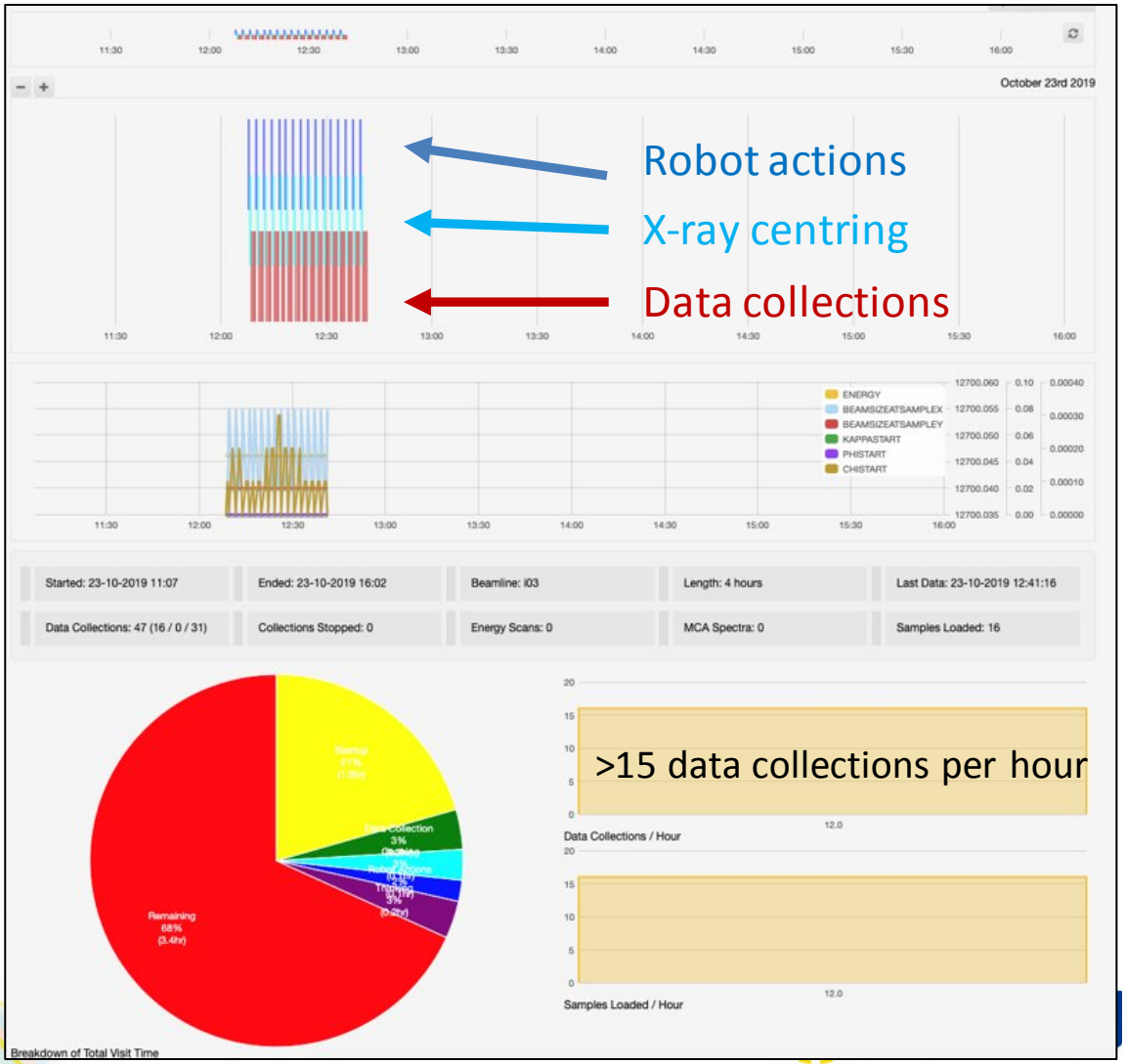
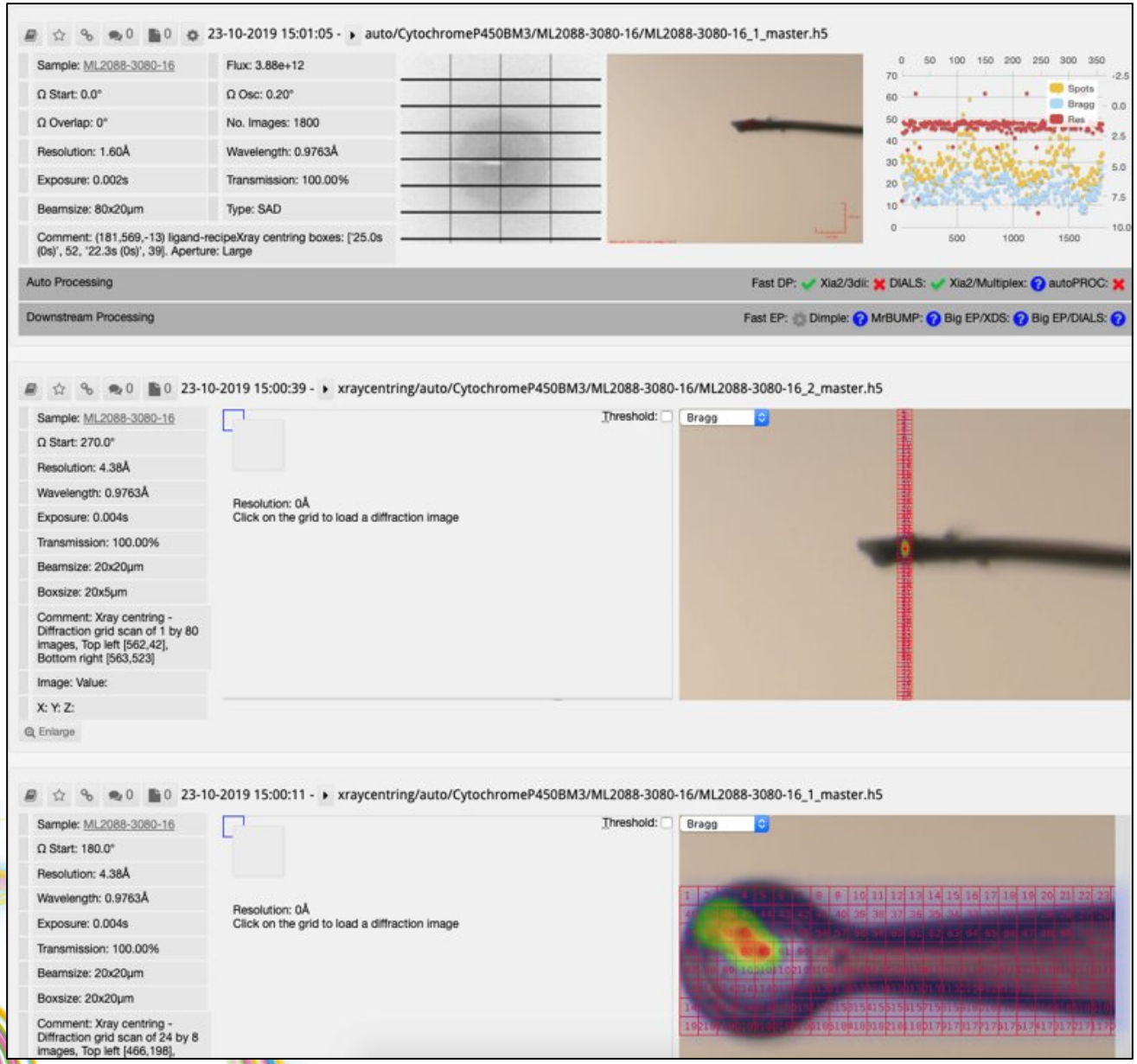
# Developments (MX)

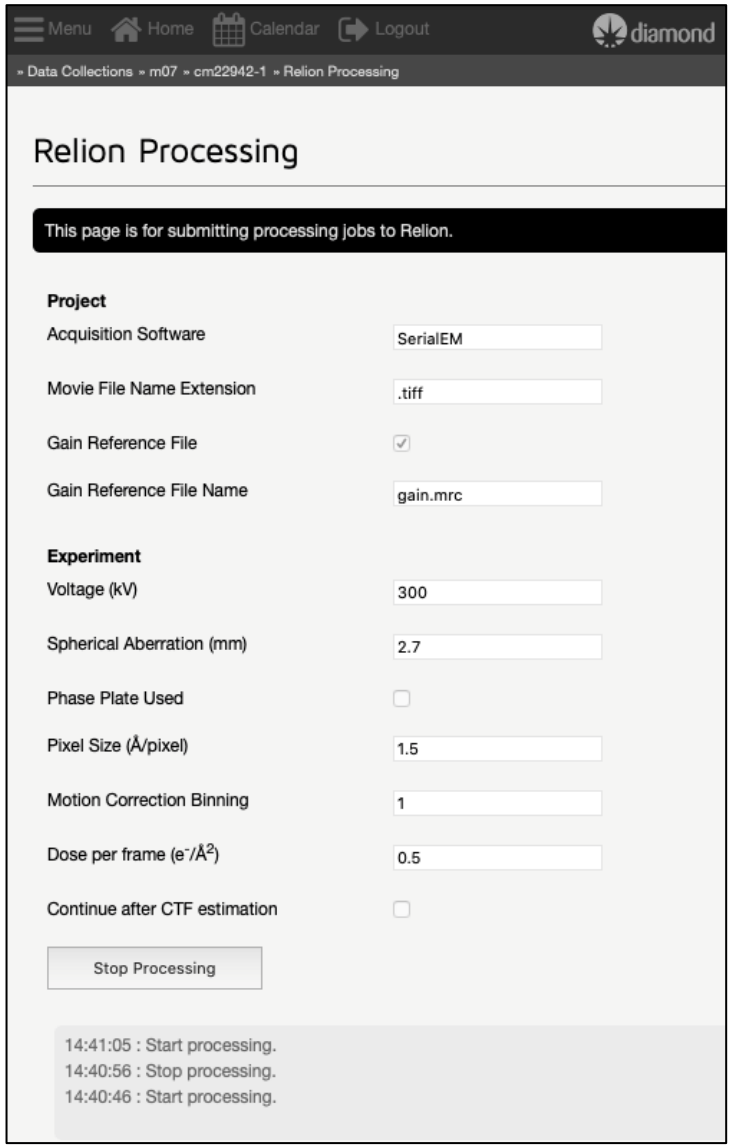
- Streamlining project ongoing – increasing automation on MX beamlines
- Users specify a recipe when shipping samples
- Pucks loaded on beamline between "normal" sessions
- Puck scanning initiates creation of session
- Downstream, acquisition and auto processing

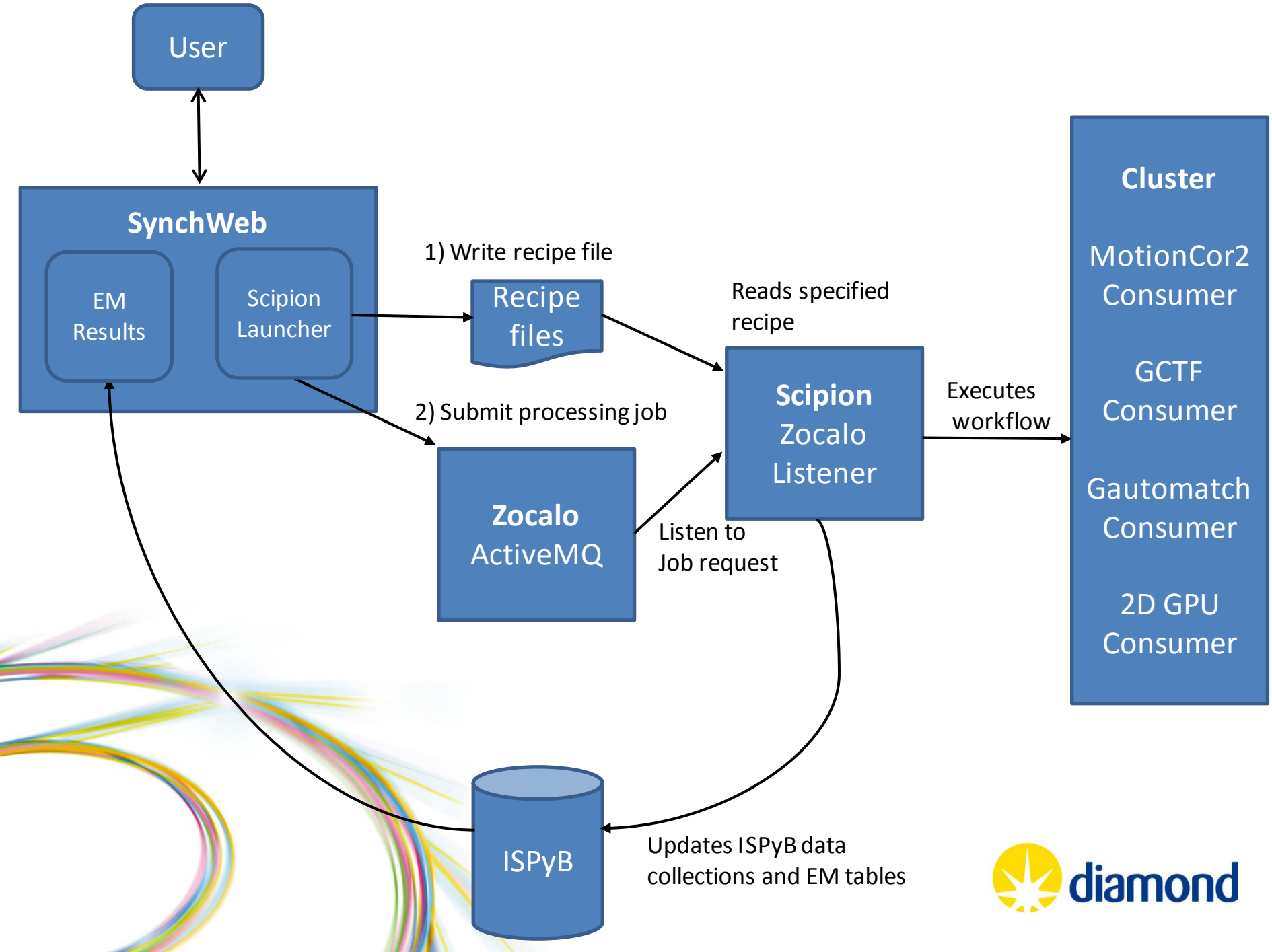



23-10-2019 15:01:05 - auto/CytochromeP450BM3/ML2088-3080-16/ML2088-3080-16_1_master.h5
Sample: ML2088-3080-16
Flux: 3.88e+12
Ω Start: 0.0°
Ω Osc: 0.20°
Ω Overlap: 0°
No. Images: 1800
Resolution: 1.60Å
Wavelength: 0.9763Å
Exposure: 0.002s
Transmission: 100.00%
Beamsize: 80x20µm
Type: SAD
Comment: (181,569,-13) ligand-recipeXray centring boxes: ['25.0s (0s)', 52, '22.3s (0s)', 39]. Aperture: Large
Spots
Bragg
Res
Auto Processing
Fast DP: Xia2/3dii: DIALS: Xia2/Multiplex: autoPROC:
Downstream Processing
Fast EP: Dimple: MrBUMP: Big EP/XDS: Big EP/DIALS:
23-10-2019 15:00:39 - xraycentring/auto/CytochromeP450BM3/ML2088-3080-16/ML2088-3080-16_2_master.h5
Sample: ML2088-3080-16
Ω Start: 270.0°
Resolution: 4.38Å
Wavelength: 0.9763Å
Exposure: 0.004s
Transmission: 100.00%
Beamsize: 20x20µm
Boxsize: 20x5µm
Comment: Xray centring - Diffraction grid scan of 1 by 80 images, Top left [562,42], Bottom right [563,523]
Image: Value:
X: Y: Z:
Enlarge
Threshold:
Bragg
Resolution: 0Å
Click on the grid to load a diffraction image
23-10-2019 15:00:11 - xraycentring/auto/CytochromeP450BM3/ML2088-3080-16/ML2088-3080-16_1_master.h5
Sample: ML2088-3080-16
Ω Start: 180.0°
Resolution: 4.38Å
Wavelength: 0.9763Å
Exposure: 0.004s
Transmission: 100.00%
Beamsize: 20x20µm
Boxsize: 20x20µm
Comment: Xray centring - Diffraction grid scan of 24 by 8 images, Top left [466,198],
Threshold:
Bragg
Resolution: 0Å
Click on the grid to load a diffraction image

# Developments (EM)

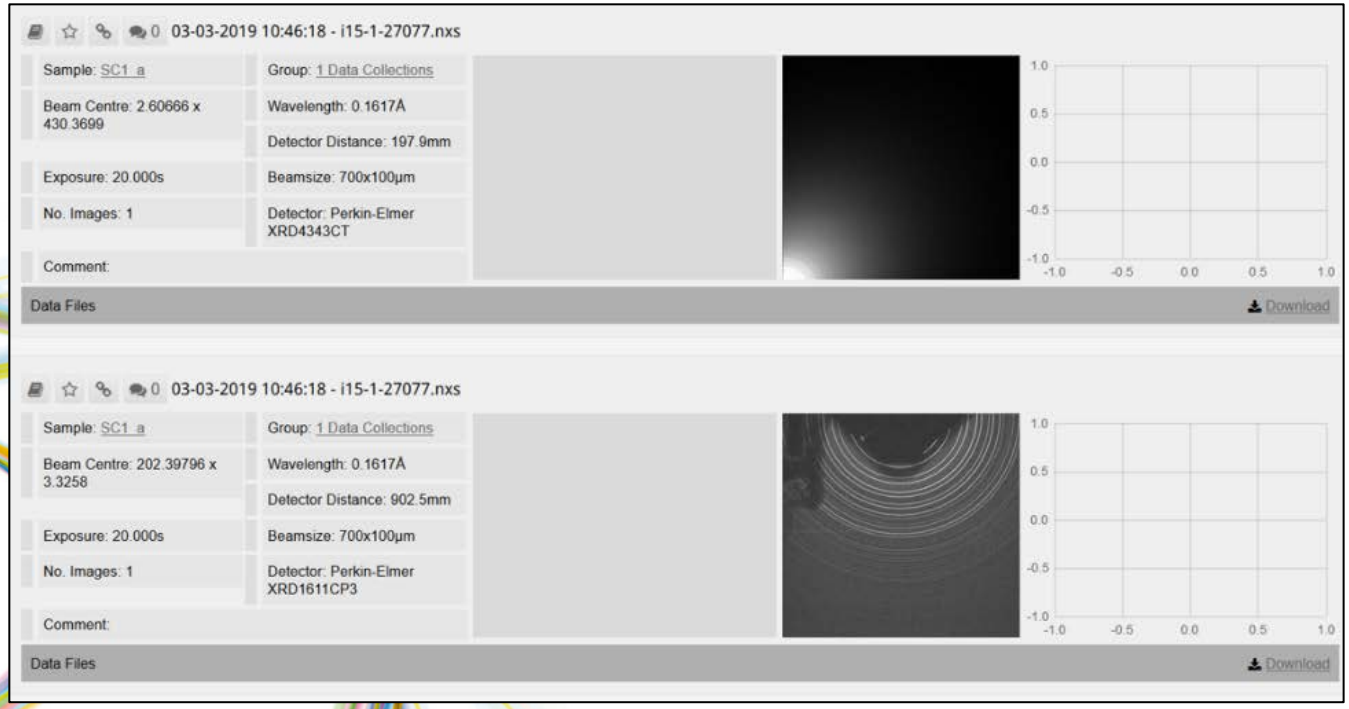
- Processing pipeline integration
  - Scipion launcher was previously migrated to SynchWeb page
  - Allows users to customise Scipion workflow template file and trigger processing through Zocalo/ActiveMQ
- Expanded Processing pipeline integration
  - Relion launcher including in SynchWeb
  - Users customise Relion workflow template and trigger processing through Zocalo
- New Data Collections view planned




User
SynchWeb
EM Results
Scipion Launcher
1) Write recipe file
Recipe files
Reads specified recipe
Scipion Zocalo Listener
Executes workflow
Cluster
MotionCor2 Consumer
GCTF Consumer
Gautomatch Consumer
2D GPU Consumer
2) Submit processing job
Zocalo ActiveMQ
Listen to Job request
ISPyB
Updates ISPyB data collections and EM tables

# Developments (Physical Sciences)

- Active on i15-1, i08, i14 and i18.
- Integration between GDA with ActiveMQ to store data collections entries on scan start and extracting meta data from nexus files to populate ISPyB
- Extended to i11-1, plans to include i12
- Work ongoing to support simple sample creation on i15-1 (hiding container/dewar/shipment restrictions)



# Developments (Technical)

- Updated PHP dependency management to use composer and modern class definitions
  - Allows integration of symfony components (validation, authorization etc.)
- Moved front end build system to use webpack
- Provides single build tool for JS and CSS
  - Also allows use of .vue files (single file components)
  - Potential to include other technologies if required
- General improvements making it less "DLS" specific – removing file scraping and relying on ISPyB

https://vuejs.org

```
<div class=" solid-border columns is-multiline">
  <div class="column is-3" v-for="dewar, rack in rack_locations">
    <div class="box has-background-white-ter" v-on:click="onClearLocation(rack)" v-bind:class="{'has-text-danger'
    dewar.status !== 'dispatch-requested'}">
      <span class="has-text-weight-bold">[[rack]]: </span>
      <span v-if="dewar.barcode" class="content has-text-weight-bold">[[dewar.barcode]]</span>
      <span v-else class="content is-invisible">empty</span>
      <!-- Tags -->
      <div>
        <span v-if="dewar.facilityCode" class="tag is-dark">[[dewar.facilityCode]]</span>
        <span v-if="dewar.status == 'dispatch-requested'" class="tag is-warning">[[dewar.status]]</span>
        <span v-else-if="dewar.needsLN2" class="tag is-danger">needs-refill</span>
      </div>
    </div>
  </div>
</div>

<!-- This pops up to confirm the clear location action -->
<div class="modal" v-bind:class="{ 'is-active' : isRemoveDialogActive }">
  <div class="modal-background"></div>
  <div class="modal-card">
    <header class="modal-card-head">
      <p class="modal-card-title">Confirm Clear</p>
    </header>
    <section class="modal-card-body">
      <p>Confirm removal of dewar from location [[locationToRemove]]?</p>
    </section>
    <footer class="modal-card-foot">
      <button class="button is-success" v-on:click="onConfirmClear(true)">Confirm</button>
      <button class="button" v-on:click="onConfirmClear(false)">Cancel</button>
    </footer>
  </div>
</div>
```

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# Acknowledgements

Jake Filik, Nigel Wilson, Johsua Lobo,
Stu Fisher, Karl Levik, James Hall

Thank you!

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