



C4L meeting
7, 8, 9 October 2019
Barcelona

QCloud Parallel sessions plan

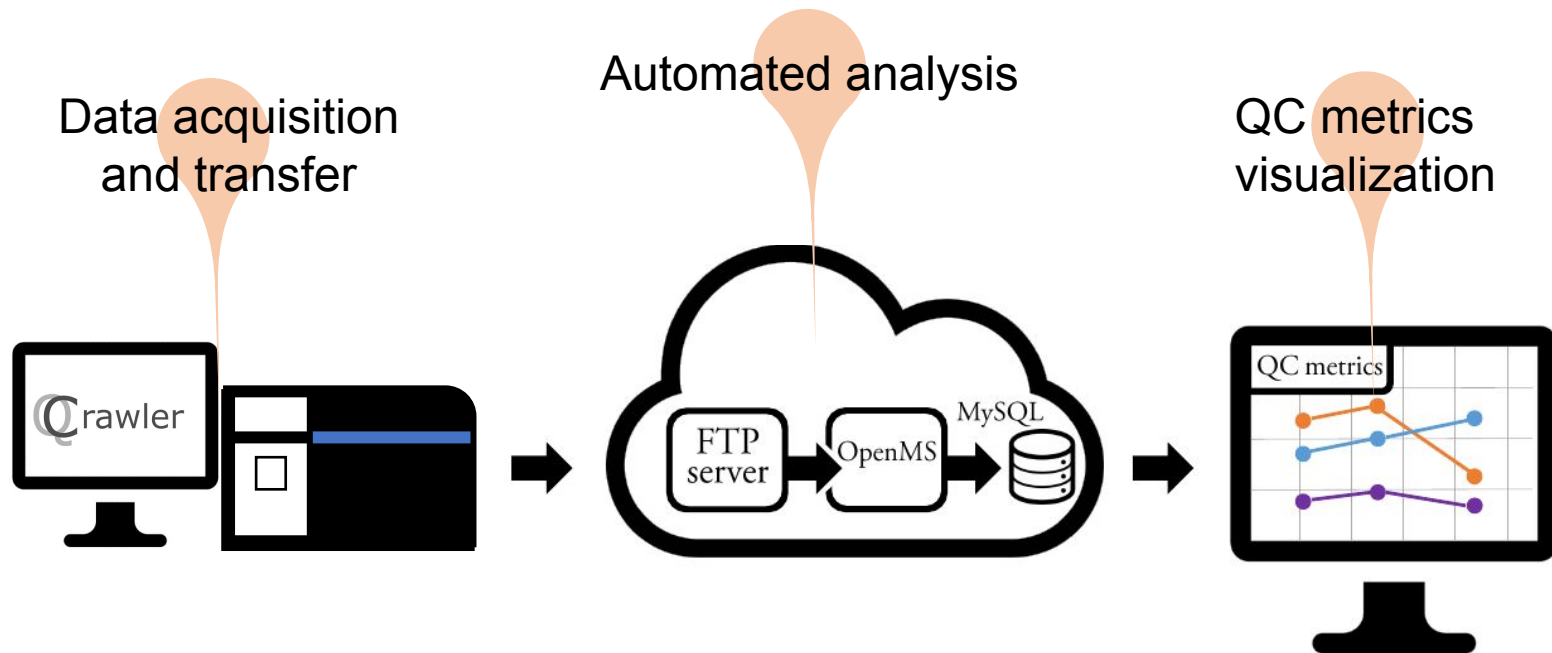
12-13h WG Session 2B: Bioinformatics C4L Parallel Session I ("Barceloneta" Training Room)

- Small update/introduction from each node (5 min).
- Short presentations (10 min aprox.) regarding some specific topics like:
 - QCloud API (@mserret).
 - C4L R package (@cpanse).
 - PDF weekly reports (@anstaes).
- Discussion.

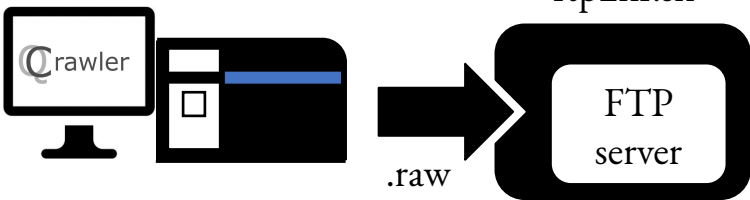
15-17h WG Session 4B: Bioinformatics C4L Parallel Session II ("Barceloneta" Training Room)

- Discussion (follow up).
- Hands on:
 - QCloud API testing.
 - @cpanse @rolivella: hands-on explore a potential integration of [rawDiag](#) within the [QCloud](#).

How the Q_{CLOUD} works?



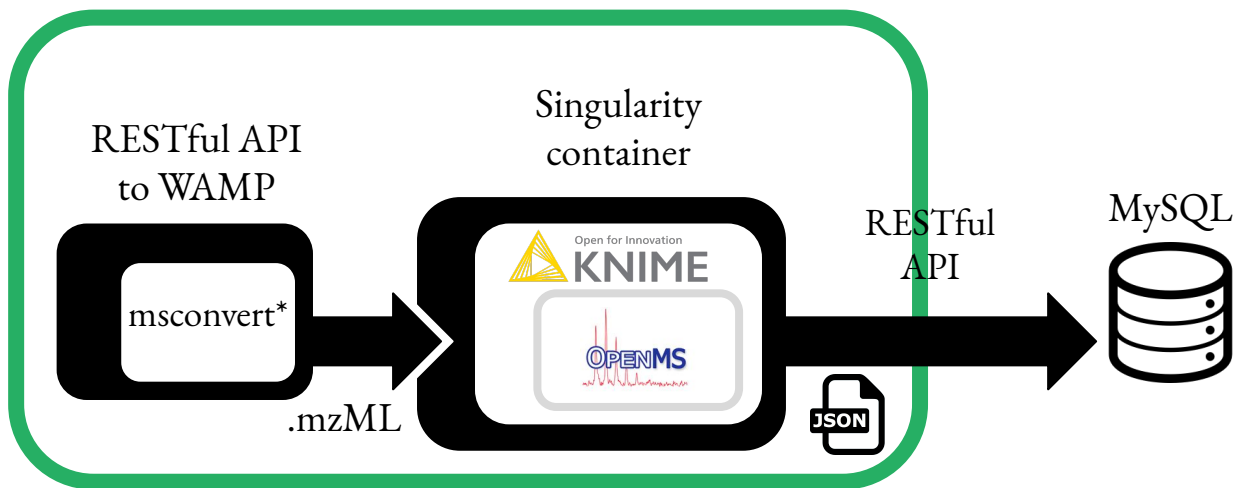
.Net



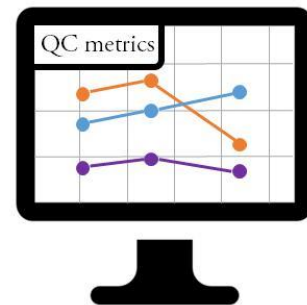
QC1, QC2, QC3



nextflow



Spring boot
Hibernate
Angular 7
Plotly.js



*<https://github.com/compomics/ThermoRawFileParser>

website interface news

- New style (colors, logo, etc.)
- Communication with users:
 - Added “Last file” to instruments tab.
 - Announcements tool.
 - Improved mailing system.
- Annotations:
 - Hide annotations.
 - General annotations.
- Open instrument in a new tab.
- Red cross for processing errors.
- Enable/disable labsystems.
- Added support to new mass spectrometers: Orbitrap Eclipse and Orbitrap Exploris 480.
- Copy filename to clipboard.
- 3 GB: raw file size limit.

QCLOUD speed issue

In general terms, for a profile/profile file QC01, QC02 around 5-10 min and QC03 around 15-20 min. But for instance, a profile/profile QC02 takes around 40 min.

In general depends on:

- File size: **profile/centroid** much faster than **profile/profile**.
- Transfer speed from the external lab.
- Workflow type: **QC01** faster than **QC02** faster than **QC03**.
- Cluster availability. We are now sending our jobs to a shared cluster @CRG.

To improve:

- **msconvert** to **ThermoFileRawParser** (Windows to Linux).
- Optimize nextflow pipeline: send JSON to DB individually for each QC metric.
- Precalculation of some QC metrics (rawDiag). This implies a pipeline reengineering.
- Amazon cluster.