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Delivery of a portal for a cheminformatics pilot database

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Summary

Deliverable report for 4.2.1 and 4.2.2 - the development of a database for project results & reports

Approval

Date	By	Organization	Role
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Distribution list

Name	Organisation	Comments
R. Garbil	EC DG RTD	Through the EC participant portal
All beneficiaries	SACSESS	Through the private online workspace

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1 Deliverable for 4.2.2 & 4.2.1

The plan in Work Package 4.2 was to create a chemoinformatics database and a document database. After discussions with SACSESS partners it was decided to make both of these two components available via one interface for ease of access.

Consultations with SACSESS partners took place in Year 1 to ensure that the database fields captured everything deemed of use by the community that would ultimately be using the database. An initial version of the database was then developed in-house by NNL Software Engineer's and this was presented at the SACSESS meeting in March 2014 for comment. A few improvements were suggested & these were made during the subsequent period of work. This included extending the scope of the project to also include a section for the results from the pyro work. The improved version of the database was then made available for users to test out & feedback received. After a final round of small modifications the database was completed & ready to roll out at the end of 2014.

It has taken a while to sort out & finalise the hosting of the database online as there were questions that needed addressing relating to the location of the database online & related security & access issues. Following the SACSESS meeting in April 2015 it was decided that, for the sustainability of the SACSESS results, and to ensure SACSESS partners have time to input their data after completion of research, that hosting of the database online would be pre-paid and extend for 2 years post the end of SACSESS (i.e. March 2016-March 2018). After this date, the database is frozen & the data collected onto CD & distributed to SACSESS partners.

The backend database is MSSQL Server and it has asp.net MVC application + Lucene index's built on top. The database allows users (once logged in) to add information and search the input information from others across 3 categories : documents, pyro, chemicals.

Once the server has been purchased (due imminently) it should be available within a matter of hours and will then take about 1 -1.5 days to install everything and test. Following which an e-mail will be sent to promote the launch of the database within the SACSESS community.

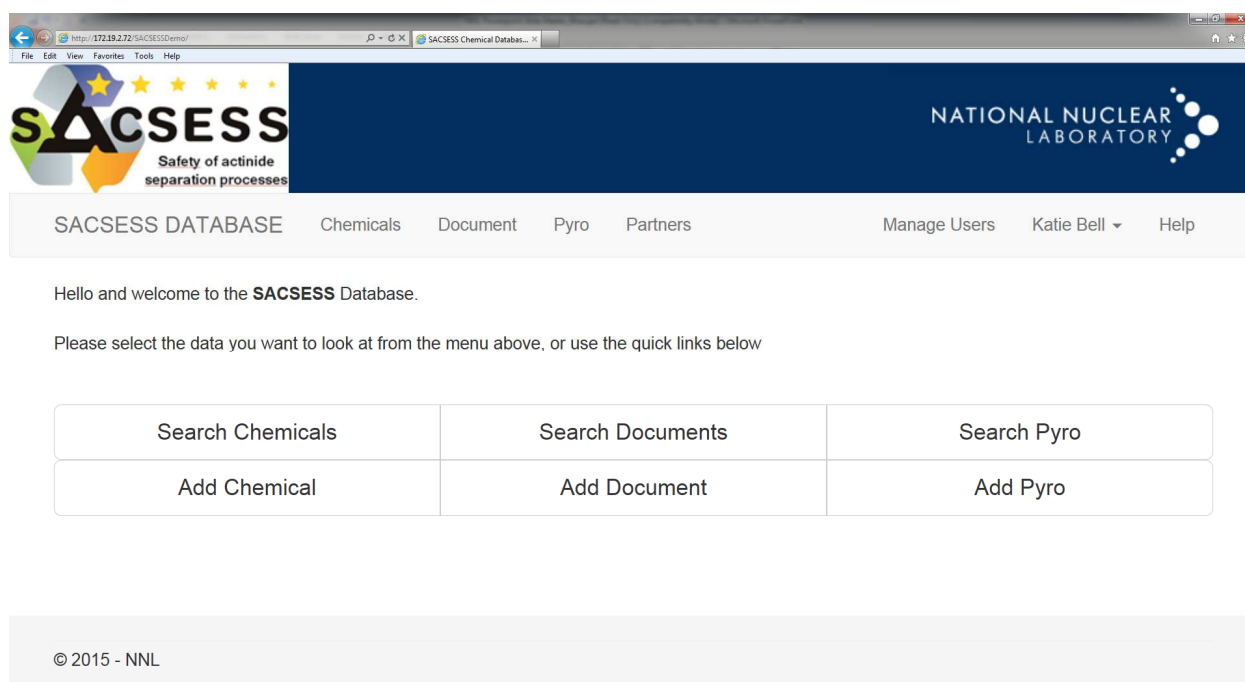


Fig 1: Screenshot of the database homepage