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DOE Collaboratory Enables a Biomedical Research Community

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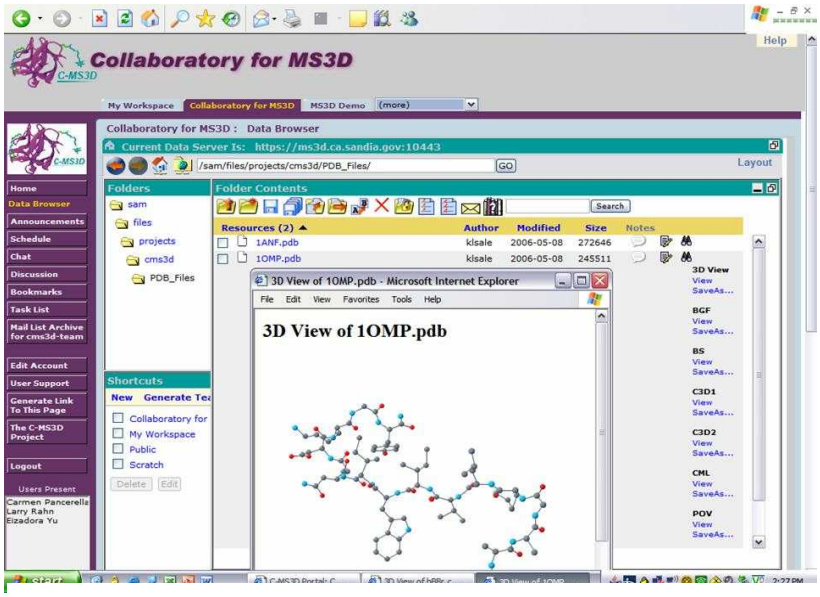
A group of biomedical scientists leading the development of new technique termed 'MS3D' are collaborating with researchers in the Collaboratory for Multi-scale Chemical Science (CMCS) [http://cmcs.org] to build the Collaboratory for MS3D (C-MS3D) [http://ms3d.org] in a multi-institution project funded by the National Institutes of Health. This collaboration has greatly facilitated the new project, enabling deployment of a C-MS3D production portal and a development portal within the first 6 months. MS3D uses chemical crosslinking and mass spectrometry to probe the structure and dynamics of proteins, RNA, and macro-molecular complexes. The objective of this 5-year project is to broadly enable an emerging MS3D collaborative community as it develops new tools, analysis approaches, and data schema to integrate constraint data from chemical crosslinking and mass spectrometry with other information (including that obtained from computation, NMR, EPR, FRET, X-Ray crystallography) to determine otherwise inaccessible macro-molecular structures.



A screen shot of the C-MS3D Portal illustrating the many translations available for a Protein Data Base file.

The more general capabilities developed by CMCS have been made available to others as the Knowledge Environment for Collaborative Science (KnECS). KnECS is an open source portal and data management environment that can be customized with discipline-specific tools, data translators, and data viewers. The KnECS deployment process was revised by the CMCS team to support configuration of the portal for other projects such as C-MS3D. The C-MS3D team branded the portal to reflect the C-MS3D project identity. Using the development library for creating asynchronous web services in KnECS, and the C-MS3D team integrated existing MS3D codes into the portal, making the latest tools accessible across the group. They are using some translators, metadata extractors, and visualization tools developed by CMCS while developing others that are more specific to biology.

This approach is being pursued in other science disciplines as well. "At NCSA, I use CMCS as an example of how cyberinfrastructure can actively support research processes rather than just being a means to provide access to finished, 'text-book' information and services. We've coined the term 'cyberenvironment' to capture the idea of end-to-end support for the research lifecycle that CMCS, with its focus on connecting research at different scales, has pioneered." says Jim Myers, CMCS CTO and AD of Cyberenvironments and Technologies at NCSA/UIUC. At NCSA, the Mid America Earthquake Center's MAEviz Seismic Risk Management cyberenvironment uses SAM, and MAEviz, and our D2K workflow engine are using the DSI interface to SAM built by CMCS.