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Transforming biomedical and structural data into information and knowledge

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The LabDB laboratory information management system (LIMS) tracks, organizes and analyzes data from chemical and solution management, protein production, crystallization, diffraction, structure solution, and in vitro biochemical and biophysical experiments. The system is comprised of multiple modules specialized for different tasks, such as the Xtaldb system for crystallization or the hkldb module of the HKL-3000 suite for diffraction data collection and structure solution. The biochemical/biophysical experiments tracked by LabDB include spectrophotometric binding and kinetics, thermal shift binding, isothermal titration calorimetry (ITC) and protein quantitation. These tools associate functional and structural experiments, for example, for selecting likely substrates for co-crystallization and soaking experiments. Whenever possible, the system harvests data with no or minimal user intervention from laboratory hardware. Devices that may connect to or import data into LabDB include crystal observation (Rigaku Minstrel HT and Formulatrix Rock Imager), liquid handling (Formulatrix Rock Maker and Emerald Opti-Matrix Maker), chromatography (GE Healthcare AKTA), quantitation (Caliper LabChip GX II and Bio-Rad Gel Doc EZ), RT-PCR (Applied Biosystems 7900HT and Bio-Rad C1000/CFX96) and ITC (MicroCal iTC-200) systems. LabDB is used by two high-throughput PSI:Biology centers (MCSG and NYSGRC) as well as other major NIH consortia (the Center for Structural Genomics of Infectious Diseases and the Enzyme Function Initiative), and track millions of experiments on tens of thousands of targets.[1] The system also provides extensive data mining and analysis tools for translating raw experimental data into information and knowledge. We present examples of analyses generated by the system useful in designing new experiments.

***[1]** M.D. Zimmerman, M. Grabowski et al., Meth Mol Biol, 2014, 1140, 1-25*

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