Molecular Libraries Program

Biannual Steering Committee Meeting
Vanderbilt University, Nashville, Tennessee
November 7-8, 2011

The meeting began with NIH Program providing a performance review of the Molecular Libraries (ML) network of centers in year 3 of the program's production phase. The following milestones were met or exceeded in Year 3:

Total assigned projects:	102
Completed primary HTS screens:	119
Number of probe reports filed:	64
Number of network publications:	75

Network Center Driven Projects:
To maintain competition between the network centers, the ML provides limited funds for competitive two year research projects. The specific aims of these center-driven projects are to advance chemical genomics through research on new methods and instrumentation. Center's with a center-driven project provided a progress update to the Steering Committee.

1. Collecting Profiling Data on 30K ML Compounds - The Broad Institute is performing profiling assays (high-throughput gene expression profiling and image-based profiling) to generate a reference database of profiles for compounds found in the ML Small Molecule Repository.
2. Wells to Cells Project – The NIH Chemical Genomics Center is developing new technology that merges high throughput screening with high content screening (imaging) to obtain rich high-resolution data at high speed.
3. Next Generation HTS – The University of Mexico Center is developing instrumentation that will provide high throughput flow cytometry utilizing 1536 well sample plates.
4. Develop Tools for Profiling Nuclear Receptor Modulators – The Scripps Institute Screening Center is developing methods that combine molecular and structural analysis of nuclear receptors with known selectivity profiling of ligands to improve SAR approaches to discovering allosteric modulators.

Next generation database for the Molecular Libraries Program:
The ML network has begun development of a new database to advance the analysis of chemical biology data beyond that currently provided by PubChem. The Molecular Libraries BioAssay Database (MLBD) will enable scientists without specialized training to effectively use Molecular Libraries Program data to answer complex cross-target and cross-compound questions. As the go-to public small-molecule science resource for translational research, the MLBD will inform the entire small-molecule discovery and development process. There was extended discussion by the centers at the meeting on the development of this database.