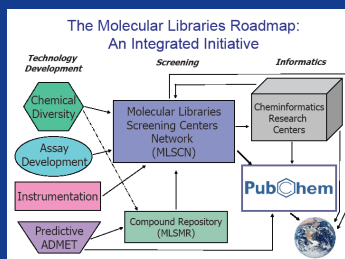


Molecular Library Screening Center Network (MLSCN)

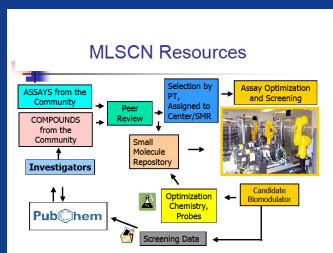
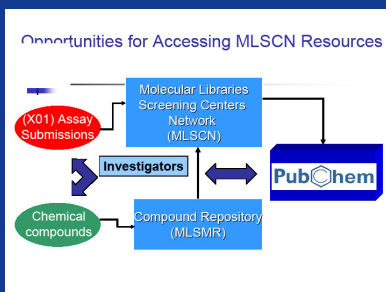
Molecular Libraries Roadmap Components

- Small Molecule Repository (SMR)
- NIH Chemical Genomics Center (NCGC, intramural)
- Extramural Screening Centers
- **Cheminformatics**
- PubChem, Cheminformatics Research Center
- **Technology Development**
- Chemical diversity
- Assay development
- HTS instrumentation
- Predictive ADME/Toxicology



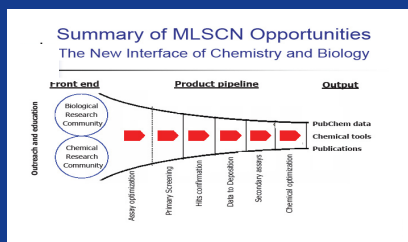
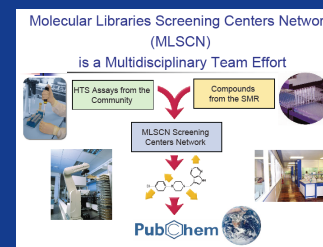
Outreach Mission: Provide the scientists with information on how to access the resources of the MLSCN Network of the screening center through:

- Mentoring for the R21 grants (fast-track)
- How to submit for the X03/R01 grant application



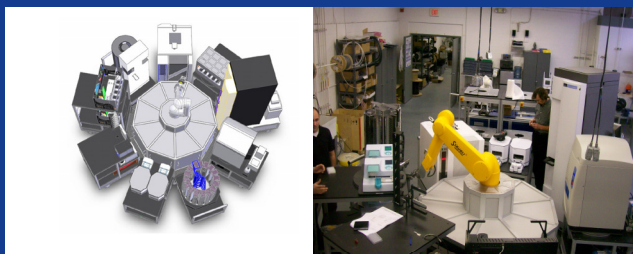
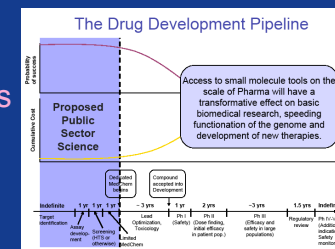
The Molecular Libraries Roadmap Initiative will offer public sector biomedical researchers access to small organic compounds ("small molecules") that can be used as chemical probes to study the functions of genes, cells, and biochemical pathways.

Stimulate collaborations between biologists and chemists: assay providers, compound providers, and the MLSCN centers. Generate scientific publications and new research projects.



Goals of the MLSCN

- Establish a national HTS resource in the academic environment to improve the understanding of biology and disease mechanisms
- Provide HTS approaches for identification of small organic molecules that are active in biological assays
- Synthetic chemistry to improve the utility of small molecules as bioactive probes
- Make HTS data publicly available in PubChem
- Stimulate technology development
- Provide outreach to the (non-) academic community



UltraHTS - This system is operational with a throughput of 96,384, or 1536 well formats using either biochemical or cell-based assays. A theoretical total throughput of over 500,000 compounds per day as of July 1, 2008, and over 2.7 million compounds per day by July 1, 2009 (HighRes Biosolutions MicroStar)

The Burnham Center has successfully deposited 5.7 million screening data-points into PubChem.

- **Entrez links and neighbors:**
- PubMed-PubChem linkage
- Unique chemical structures
- PubChem bioassay links
- ~7,848,000 substance record
- >25 government, academic and commercial organizations
- ~5,270,000 unique chemical structures
- ~200 bioassay data sets deposited

