Resource Summary Report

Generated by kravitz2 on Aug 1, 2026

Molecular Libraries Program

RRID:SCR_008847
Type: Tool

Proper Citation

Molecular Libraries Program (RRID:SCR_008847)

Resource Information

URL: http://mli.nih.gov/mli/

Proper Citation: Molecular Libraries Program (RRID:SCR_008847)

Description: High throughput screening services to identify small molecules that can be optimized as chemical probes to study the functions of genes, cells, and biochemical pathways, along with medicinal chemistry and informatics. This will lead to new ways to explore the functions of genes and signaling pathways in health and disease. The NIH Molecular Libraries Initiative NIH is designed to discover small molecules that interact with biologically important proteins and pathways and to provide open access to the bioassay and chemical data generated by its research centers. This will lead to new ways to explore the functions of genes and signaling pathways in health and disease. As these HTS Technologies were not previously available to the public sector, many investigators may not be familiar with the components and requirements of high throughput screening. A key challenge is to identify small molecules effective at modulating a given biological process or disease state. The Molecular Libraries Roadmap, through one of its components, the Molecular Libraries Probe Production Centers Network (MLPCN), offers biomedical researchers access to the large-scale screening capacity, along with medicinal chemistry and informatics necessary to identify chemical probes to study the functions of genes, cells, and biochemical pathways. This will lead to new ways to explore the functions of genes and signaling pathways in health and disease. There are two kinds of data that are available to the scientific community through a dedicated database: Chemical Compounds and Bioassay Results (NCBI). Various types of data, including informative records on substances, compound structures, and biologically active properties of small molecules are housed respectively within PubChem""'s three primary databases: PCSubstance, PCCompound, and PCBioAssay. To date, PubChem contains over 11 million substance records, details about approximately 5.5 million unique compound structures with links to bioassay descriptions, relevant literature, references, and assay data points and over 250 bioassays, a good percentage of which were contributed by the pilot phase of the MLP. The deposition will continue during the current MLPCN phase. NIH anticipates that these projects will also facilitate the development of new drugs, by providing early stage chemical compounds that will enable researchers in the public and private sectors to

validate new drug targets, which could then move into the drug-development pipeline. This is particularly true for rare diseases, which may not be attractive for development by the private sector. Funding opportunities are available through the site.

Abbreviations: MLP

Synonyms: Molecular Libraries, Molecular Libraries Initiative

Resource Type: data or information resource, portal, service resource, topical portal, material analysis service, production service resource, analysis service resource, organization portal

Keywords: molecule, compound, probe, small molecule, high throughput screening, gene, cell, biochemical pathway, drug development, protein, pathway

Funding: NIH

Resource Name: Molecular Libraries Program

Resource ID: SCR_008847

Alternate IDs: nlx_146246

Record Creation Time: 20220129T080249+0000

Record Last Update: 20260801T190338+0000

Ratings and Alerts

No rating or validation information has been found for Molecular Libraries Program.

No alerts have been found for Molecular Libraries Program.

Data and Source Information

Source: SciCrunch Registry

Usage and Citation Metrics

We found 15 mentions in open access literature.

Listed below are recent publications. The full list is available at kravitz2 .

Dengler DG, et al. (2022) Screening for positive allosteric modulators of cholecystokinin type 1 receptor potentially useful for management of obesity. SLAS discovery : advancing life sciences R & D, 27(7), 384.

He H, et al. (2020) Synthetic high-density lipoproteins loaded with an antiplatelet drug for efficient inhibition of thrombosis in mice. Science advances, 6(49).

Koleti A, et al. (2018) Data Portal for the Library of Integrated Network-based Cellular Signatures (LINCS) program: integrated access to diverse large-scale cellular perturbation response data. Nucleic acids research, 46(D1), D558.

Vladimer GI, et al. (2017) Global survey of the immunomodulatory potential of common drugs. Nature chemical biology, 13(6), 681.

Soufan O, et al. (2016) DRABAL: novel method to mine large high-throughput screening assays using Bayesian active learning. Journal of cheminformatics, 8, 64.

Kim MT, et al. (2016) Mechanism Profiling of Hepatotoxicity Caused by Oxidative Stress Using Antioxidant Response Element Reporter Gene Assay Models and Big Data. Environmental health perspectives, 124(5), 634.

Digles D, et al. (2016) Open PHACTS computational protocols for in silico target validation of cellular phenotypic screens: knowing the knowns. MedChemComm, 7(6), 1237.

van Adrichem AJ, et al. (2015) Discovery of MINC1, a GTPase-activating protein small molecule inhibitor, targeting MgcRacGAP. Combinatorial chemistry & high throughput screening, 18(1), 3.

Zhang J, et al. (2014) Profiling animal toxicants by automatically mining public bioassay data: a big data approach for computational toxicology. PloS one, 9(6), e99863.

McManus OB, et al. (2014) HTS assays for developing the molecular pharmacology of ion channels. Current opinion in pharmacology, 15, 91.

Alonso-Padilla J, et al. (2014) High throughput screening for anti-Trypanosoma cruzi drug discovery. PLoS neglected tropical diseases, 8(12), e3259.

Tice RR, et al. (2013) Improving the human hazard characterization of chemicals: a Tox21 update. Environmental health perspectives, 121(7), 756.

Chung TD, et al. (2010) Assay format as a critical success factor for identification of novel inhibitor chemotypes of tissue-nonspecific alkaline phosphatase from high-throughput screening. Molecules (Basel, Switzerland), 15(5), 3010.

Clifton JD, et al. (2010) Identification of novel inhibitors of dietary lipid absorption using zebrafish. PloS one, 5(8), e12386.

Doghman M, et al. (2010) Identification and characterization of steroidogenic factor-1 inverse agonists. Methods in enzymology, 485, 3.