One-Stop Shop to Enable Early-Stage Drug Discovery

Unique Chemical Collections – No-Thaw Robotic Storage & Retrieval Technology
Ultra-High Throughput Screening & Synergistic Drug Interaction Screening Methods

Technology Readiness Level 9: Actual System Proven in Operational Environment

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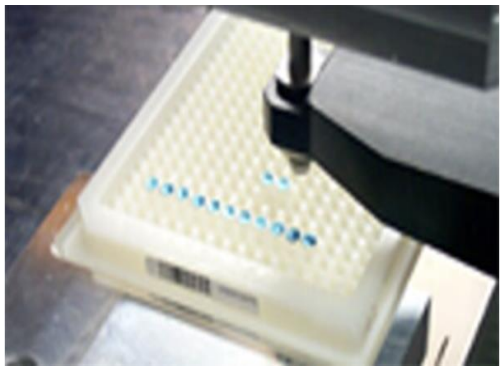
Unmet Need



Chemical collections and methods for rapid storage, retrieval and screening are vital to new drug discovery. The LIMR Chemical Genomics Center (LCGC) owns a large chemical collection that covers a unique structural space not covered by other pharma or commercial libraries. LCGC has developed and validated hardware and software solutions for nonprofit and for-profit laboratories that enable efficient, low-cost drug screens directed to any molecular target of interest. Together these assets offer a complete one-stop acquisition for R&D nonprofit or for-profit organizations seeking complete capabilities for early-stage drug discovery. LIMR seeks to sell some or all of the technology for early-stage drug discovery.

Acquisition Opportunity

Few biomedical R&D organizations have the capability to discover proprietary new drug leads. Intra-institutional collaborations for this purpose are complicated by intellectual property limitations and concerns. Rival methods for preclinical drug discovery (*in silico,* artificial intelligence) are still partially effective at best, posing risks from algorithm bias and requiring intensive time, expertise, and access to data learning sets. LCGC's technologies offer unique tools that, employed together, can enable any R&D organization to engage in early-stage drug discovery.

Key Components

- >100,000 novel fully annotated chemicals covering a unique structural space relative to existing commercial, academic and pharmaceutical chemical collections. Acquired from a large Chem-Ag company that closed its research division, the collection offers a structurally unique library for biomedical drug discovery.
- >150,000 known commercial chemicals including all FDA-approved drugs
- NARS Robotic Storage-And-Retrieval Freezer: A unique 2000 ft^3 robotic freezer to efficiently store, retrieve, and format chemicals for drug screening without freeze-thaw or technician labor to assemble compounds for drug screening. This unique technology has a small footprint yet enables rapid high-integrity management of up to 10,000,000 distinct entities. ***NARS can reduce chemical storage and access costs up to 80%***.
- NARS Storage Plates: Fully addressable 384-well plates with moveable wells that enable assembly of desired compound sets or subsets (see above). Plate technology enables rapid formatting of drug screening plates without freeze-thaw (up to 10,000 picks / day).

Patented Methodologies

- Drug Discovery Software algorithms to fully leverage the NARS-based drug discovery system (see below).
- Orthogonal Pooled Screening to screen multiple small molecule drug candidates in a single well.
- Ultra-High Throughput Screening for Synergy (UHTSS) to discover multi-drug combinations needed to affect a therapeutic target, i.e., a method to identify unknown but useful drug synergies.
- Double-Blinded Drug Discovery (DBD2)® to enable collaboration between non-profit and for-profit entities. DBD2 can blind one organization's enzyme target against another organization's chemical collection, without revealing either organization's propriety information.
- Methods to protect a novel drug target through proof-of-concept drug discovery needed to validate the target. Even if a discovery campaign is not desired, patents for new drug targets are vulnerable to invalidation without a demonstration of proof-of-concept using a small molecule inhibitor or agonist (e.g. U Rochester as patent holder of COX2 inhibitors vs. Merck as COX2 inhibitor developer, due to invalidation of the U Rochester patents which lacked small molecule proof-of-concept)

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Unique Attributes

Chemical Collections: Fully annotated compound collection includes a first-ever proprietary ChemAg library of 104,000 drug-like small molecules, meeting high QC and QA benchmarks. This set encompasses thousands of chemical scaffolds for iteration by medicinal chemistry that are unavailable elsewhere. Additional known chemicals include the following:

- ChemBridge: 100,000 compounds assembled from the 50,000-member DIVERSet™-EXP library, plus the 50,000-compound DIVERSet™-CL library.
- Life Chemicals Inc.: 50,000 compounds selected to complement overall diversity.
- MicroSource Pharmakon: 1,760 drugs, 1,360 (U.S. collection) plus 400 (international collection).
- MicroSource Spectrum: ~1,000 bioactive compounds and natural product analogs.
- NCI-Approved Oncology Set: 166 of the most current FDA-approved anticancer drugs.
- Nutraceuticals: ~150 individual neat powders acquired from Sigma, Cayman and other vendors.
- Miscellaneous: ~8,000 compounds acquired from other vendors, mainly ChemDiv and TimTec.

Unique Automated Chemical Repository: State-of-the-art storage and retrieval to protect and distribute chemical (or biological) assets without freeze-thaw, preserving chemical integrity.

Unprecedented Efficiencies: Up to 80% reduction in storage and retrieval costs. Up to 500% increase in efficiency of high-throughput screening (HTS). Ultra-HTS compression up to 15:1. Provides medicinal chemists just-in-time new chemical scaffolds to assist decision-making on lead and backup drug candidates; opportunity to rapidly screen most approved, generic, or OTC drugs for pharmaceutical repositioning; opportunities for nutraceutical R&D, and other value-add screens.

Intellectual Property

Unique chemical collection is proprietary. Hardware and software technologies are patent-protected.

References Validating Uses of the Technology for Drug Discovery

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