Compound Libraries

Unique and ***Assorted*** Compound (***~83,000***) collections acquired from various resources to fit a ***Diverse*** range of targets and research goals.

Area of Targets: inhibitors, activators, antagonists, and agonists focused on targets in the areas of oncology, infectious diseases, diabetes, epigenetics, ion-channel ligands, GPCRs, proteases, and over 20 signaling pathways such as, PI3K/Akt/mTOR, and MAPK pathways.

Biologically active compounds and Natural products: Potential to speed up drug discovery process by skipping ADME/PK procedures. *Complete set of Selleck Inhibitor collections, NIH Clinical set, Lopac, MicroSource Spectrum, NCI oncology/natural product*.

Kinase set: Custom-assembled compounds with known activity against >100 Kinases. Focused library selected computationally against the protein family (*Chembridge*). *GSK Published Kinase inhibitors (PKIS)*.

Legacy collection: Exclusive collections acquired directly from pharmaceutical companies, non-profit institutes or chemistry collaborators from universities including *UT-Austin, Kansas, Torrey Pines Research Institute*.

Diversity set: Highest potential to identify hits in diverse chemical moieties. *NCI, Chemdiv, Chembridge, Maybridge, Fsp3 Enriched, Natural like.*

Fragment set: Good starting point for lead development or NMR/X-ray crystallography-based screening. *Chembridge, Chemdiv.*

For more compound information visit: http://sites.utexas.edu/ttdddp/technologies/small-molecule-library/

Our Partners

- UT-Austin: Macromolecular Crystallography Facility (MCF) & Drugs Dynamics Institute (DDI)
- Gulf Coast Consortium (GCC)
- Texas Screening Alliance for Cancer Therapeutics (TxSACT; MDAnderson cancer center, Baylor college of medicine, Rice, UTHSCH)
- Torrey Pines Institute for Molecular Studies
- Academic Drug Discovery Consortium (ADDC)
- University of Kansas

New Thinking,

New Competencies,

New Results

Promote an integrated therapeutic development network

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WHAT STARTS HERE CHANGES THE WORLD
THE UNIVERSITY OF TEXAS AT AUSTIN

COLLEGE of PHARMACY

Gulf Coast Consortia for Quantitative Biomedical Sciences

Targeted Therapeutic Drug Discovery & Development Program (TTP)

Advancing Academic Breakthroughs into Therapeutic Functionalization

The Targeted Therapeutic Drug Discovery & Development Program serves our science community to establish a pipeline of potential new treatments for today's most challenging and unmet medical needs by offering access to unique small molecule compounds, high throughput automated technologies, and extensive expertise in the field of drug discovery and development. We engage in active research collaborations with highly respected biomedical research institutions and pharmaceutical industry partners.

CPRIT
CANCER PREVENTION & RESEARCH INSTITUTE OF TEXAS

About Us

Who We Are:

Academic Drug Discovery Hub
Operated in fully Collaborative Strategies.

What we offer: A life science infrastructure to promote scientific interaction where scientists and clinicians can work collaboratively, building upon the existing strengths and the unique resources of the University and the State of Texas for the discovery and development of therapeutic probes. In detail,

Expertise: A team of experienced professionals in biochemistry, chemistry, biology, and informatics with strong expertise in underlying biological mechanisms in diseases and screening of small molecules against individual drug target families with the ultimate goal of identifying novel drugs and druggable targets

Resources: a) Diverse and unique chemical libraries to maSoximize potential in finding breakthrough chemical probes and b) Automated state-of-art instrumentation to fulfill diverse needs among projects and budget

What you can expect:

- Project consultation and education
- Grant/manuscript support
- Staff assisted support or advise on the following areas;

Compound Screening:

* Biochemical/cell-based assay design/optimization
* Small molecule screens & preliminary data analysis
* Follow up screening of primary hits

Medicinal Chemistry:

* Structure-guided synthesis of new analogs
* Scale up synthesize for lead progression

Chemoinformatics & Modeling:

* Preliminary Structure Activity Relationships (SAR) for hit compounds
* Identification of structurally similar commercially available analogs via structure-based docking or pharmacophore searching
* Advanced *in silico* modeling and early prediction of ADMET properties

Lead Characterization:

* Structural biology: X-ray crystal structures of target•inhibitor complexes
* Pharmacokinetics studies: Formulation & evaluation of *in vivo* compound bioavailability

Compound Screening

Detection

Synergy Neo2 & H4 Plate readers: Both filter & monochromator based multimode readers. UV-Vis (230-999nm, 0-4 OD), FI (250-850nm), Lum, FP, TRF, BRET; Plate stacker (20 plates); 2 reagent dispenser, bir-code reader, 20 Plate stacker

Cytation 5 cell imaging Plate reader: Fluorescence (DAPI, YFP, GFP, RFP), brightfield, color brightfield/phase contrast microscopy (4,10, 20, 40x) & multi-mode microplate reading. CO_2/O_2 control, incubation/shaking for live cell assays

EnVision Plate Reader: Filter-based for Abs, FI, FP, TRF, Lance, ultra-Lum, Alphascreen. Dual injector, 50 Plate stacker, bar-code reader

FlexStation 3: Programmable liquid handling specific for fast kinetic studies. Monochromator based & dual optical system for Abs, FI, FP, TRF, Lance, Lum

IncuCyte® ZOOM System: Real-time live cell analysis with a microscope objectives (4x, 10x, 20x) located in a conventional incubator monitoring 2 colors (green/red) simultaneously

J-815 CD spectrometer: Specific for secondary structure analysis of biological molecules. Autosampling (2 x 96 well plates). Temp control (6-110^oC) for thermal melting & 6 cell simultaneous analysis

Cary 4000 UV-Vis: Specific for Thermal melting and high performance UV-Vis. 6x6 pelitier cell, Temp control (-10-100^oC) , 175-900nm.

Liquid Handling

- Echo 550 Acoustic liquid handler
- Janus automated workstation
- Microflo Select bulk liquid dispenser
- EL405lx Plate washer

Tissue Culture

Forma 3110 CO_2 Incubator, Leica DMi1 microscope (4x, 10x, 20x), biosafety hood, centrifuge, water bath

Others

ALSP 3000/PlateLoc Plate Sealers, Centrifuge 5810R, VSpin micro-centrifuge, Bar code printer, 3D bar-code reader. Freezers (-80, -40, -20^oC)

For more Instrument information visit:
http://sites.utexas.edu/ttdddp/technologies/instruments/

Chemoinfomatics and Modeling

Computing facility

Computing cluster (Virtual screening, drug library design, database searching & data file storage), **GPU computing cluster** (Molecular dynamics simulations, lead optimization), **High performance computing cluster** (Molecular modeling & dynamics simulations of protein-ligand binding), **Workstations** (Visualization & manipulation of molecular systems)

Software

CDD: Compound & assay data archive and analysis, mining, clustering
Daylight Reaction Toolkit: De novo ligand design
ROCS, EON, OpenEye: Shape & electrostatic similarity based ligand search
GOLD, GLIDE: Virtual screening, prediction of binding poses & affinity ranking
AMBER, GROAMCS, TINKER, OpenMM: Molecular dynamics simulations of protein-ligand binding, binding affinity/free energy calculation for ligand screening & optimization
Pymol, VMD, Chimera: Visualization & manipulation of protein-ligand systems

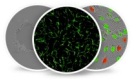
Medicinal Chemistry

- CEM Liberty microwave peptide synthesizer
- MiniBlock synthesizer & Minimapper liquid handler
- Rotavapor RII

Screening Capability

Assay format: 96, 384, or 1536-well/End-point & kinetic measurement
Assay mechanism: Binding, reporter assays, enzymatic, ion channel, membrane potential, cell counting, viability, proliferation, cytotoxicity, cell migration, tumor spheroids

- Homogeneous (mix & read) or heterogeneous (ELISA or bead-based assays)
- Biochemical or cell-based assays



Readout type: Abs, FI, TRF, FRET, BRET, FP, Lum, Lance, Alphascreen, Cellular imaging (DAPI, GFP, RFP, CFP, Texas red; 4x, 10x, 20x, 40x), Thermal melting (Tm), Circular Dichroism (CD), Spectra/well area scan