www.timtec.org

TimTec Screening Collections

Full line of pre-designed collections, starting points for libraries selection, characterized by features:

General Screening Collections

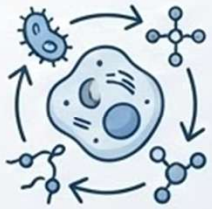
Drug-like and generally diverse selections of different sizes from **1,000 to 100,000+ compounds**.

ActiTarg Series: Targeted Libraries

Kinase, protease, GPCR, HDAC, ion-channel, nuclear receptors modulators, serine proteinase inhibitors.

Nature-Informed Collections

Pure natural material, natural product derivatives, plant extracts.



Activity-Aimed Sets

Specific characteristics: Anti-inflammatory, Anti-Infectives, Privileged Structures, ActiCom, Fragment Based Library.

Custom Collections

Based on customer suggested criteria. Available for **cherry-picking.**

Compound Size & Formatting

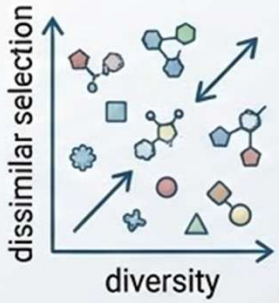
Collections of **2,000 to 100,000+ compounds**. Flexible formatting options.

General Screening Collections

clustering design approach

ActiProbe Series

Access to some of the most diverse chemotypes among distinctly drug-like molecules.
Series includes different in number of compounds stand-alone collections (1K to 25K, up to 50K-100K in ActiGlobe). All share the same clustering design.

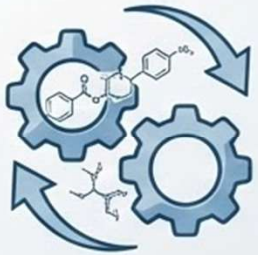


Diversity SET

Leverage discovery with superior collection of dissimilar singletons identified within variety of chemo-types. Designed with diversity in focus in addition to generally drug-like compounds selection gathering 10,000 molecules.

ApexScreen-5040

5,040 compounds representing diversity of TimTec stock in a smaller format.
A perfect starter library and valuable diversity addition. Includes pure natural compounds and natural derivatives.

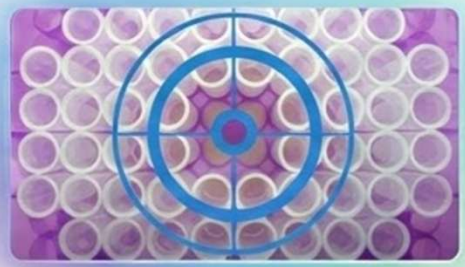


MyriaScreen II

50% updated redesigned version of original MyriaScreen co-developed with Sigma-Aldrich Corporation.
Unites 10,000 compounds, medicinal chemistry guided refined selection from both companies stock.

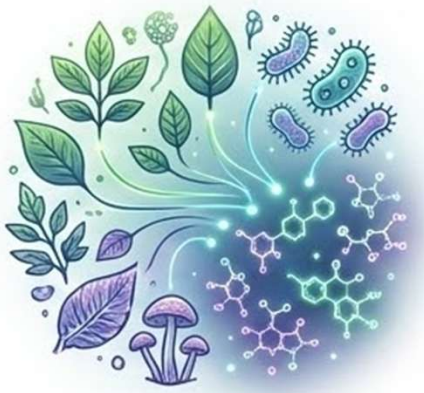
ActiTarg Series – Targeted Libraries

- **ActiTarg-K** Kinase Inhibitors, 6,000 with top diversity selection Actitarg-K 960
- **ActiTarg-G** GPCR ligands, 2,300 compounds
- **ActiTarg-N** Nuclear receptor ligands, 1040 compounds
- **ActiTarg-H** Histone deacetylase (HDAC) inhibitors, 1,700
- **ActiTarg-P** Protease inhibitors, 2,000
- **ActiTarg-S** Serine protease inhibitors, 920
- **ActiTarg-I** Potassium (ion) channel modulators, 800



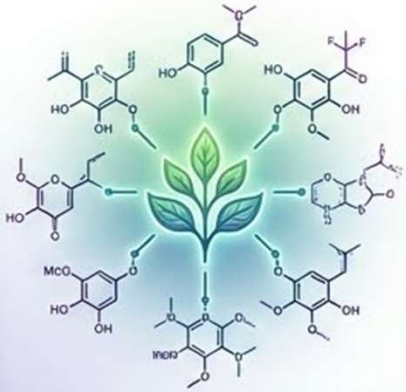
TimTec ActiTarg-Series is designed with the principle of “focused diversity” in mind. It is a common term and desirable strategy for directed screens. The value of ActiTarg Series is in its diversity that is likely to act across targets in each focused category.

Nature-Informed Screening Libraries



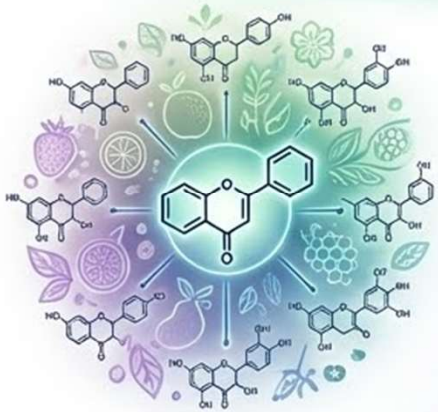
NPL-800

Natural products library of 800 pure individual compounds primarily from plant and also from bacteria, fungi, and animal sources.



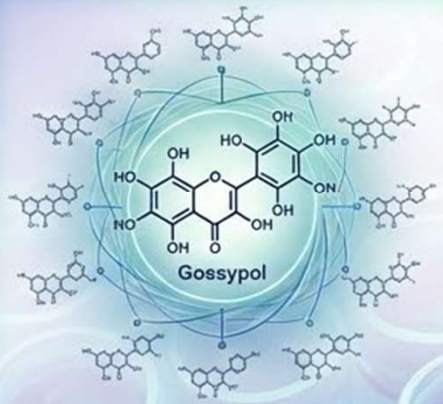
NDL-3000

Natural derivatives library of 3040 chemically diverse compounds that are semi-natural, derived from natural molecules, and synthetic compounds that are natural-compounds-like.



Flavonoids-500

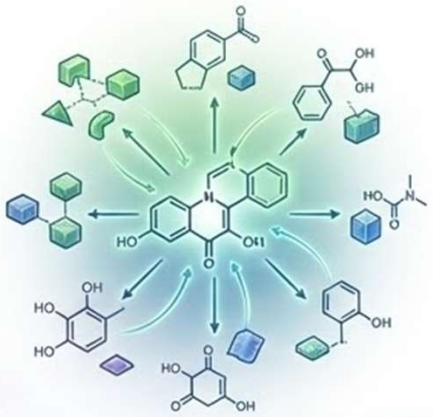
Selection combines natural and synthetic flavonoid derivatives built around 9 core flavonoid scaffolds known for their bioavailability.



Gossypol and Derivatives

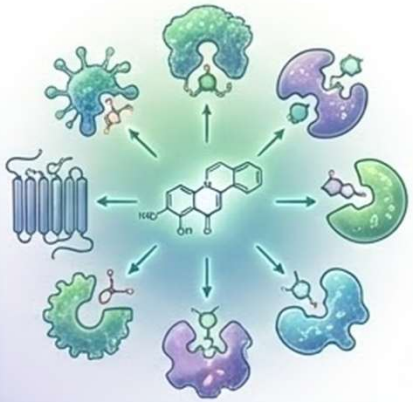
One known active structure focused set of about 80 molecules.

Activity-Aimed Sets



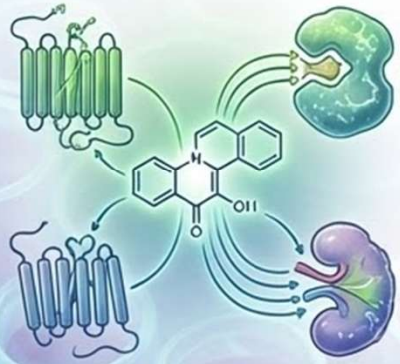
Fragment-Based-Library, FBL-3200

3,200 diverse small molecules pool meets selection criteria for Fragment-Based Drug Discovery, FBDD.



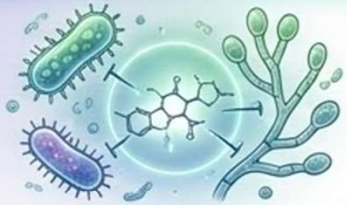
ActiCom - 480

A collection of 480 compounds with known activities or assigned in therapeutic categories.



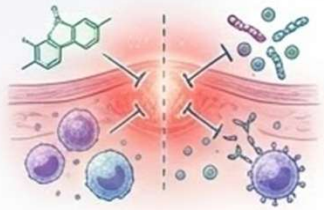
Privileged Structures

Molecular motifs associated with higher biological activity and are given the 'privileged' label when found in compounds that are active at two or more different receptors.



Anti-Infectives

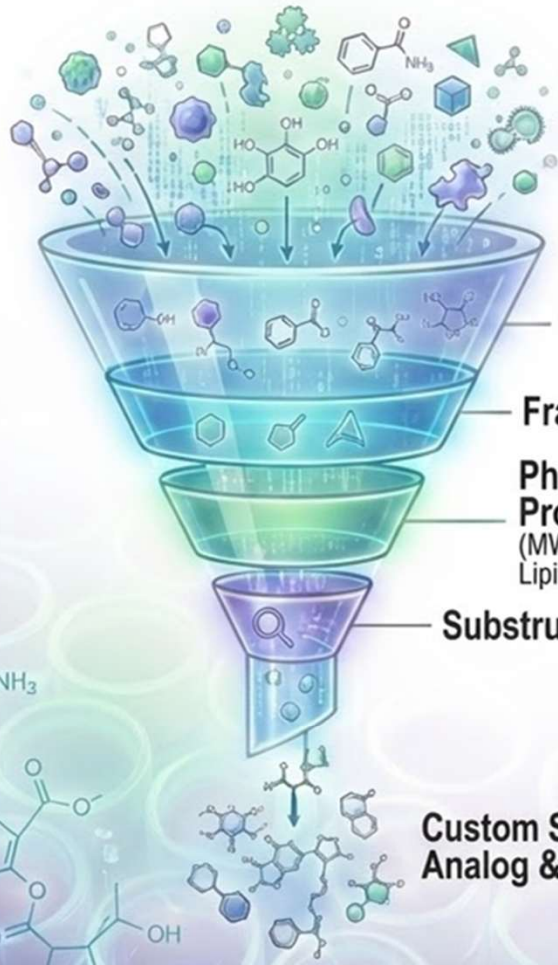
960 low molecular weight, drug-like molecules with scaffolds found in antiseptic agents with anti-bacterial (Gram+ve and Gram-ve), anti-fungoid, anti-microbial activities.



Anti-Inflammatory

1950 low molecular weight drug-like compounds with fragments found in known non-steroidal anti-inflammatory drugs covering variety of targets.

CUSTOM COMPOUND SELECTION



Diverse Compound Pool / Databases

Structure Similarity

Fragment Presence

Physical-Chemical Properties
(MW, cLogP, HBA/HBD, Lipinski Rule of 5, Rule of 3)

Substructure Search

Custom Screening Collection / Analog & Derivative Libraries

Custom Collection Assembly & Analysis

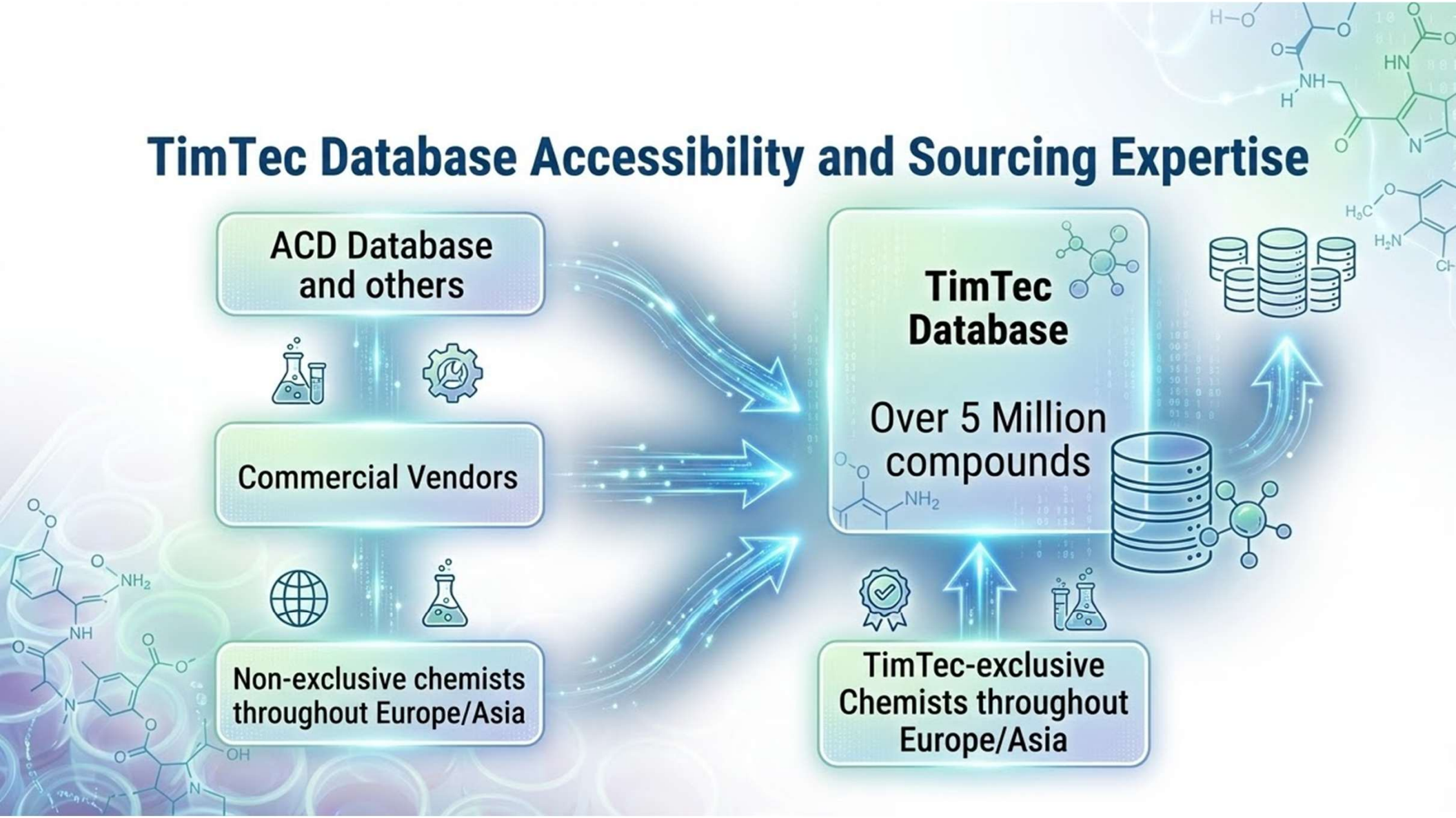
- TimTec assembles screening collections of **any size** using proprietary software based on custom criteria.
- Enables **analog/derivative libraries**, **screens** follow-ups, and **diversity analysis** for existing customer libraries.

CHERRY-PICKING & RESOURCES

Cherry-picking is available across predesigned collections.

DATABASES FOR IN-HOUSE SELECTION

TimTec Database Accessibility and Sourcing Expertise

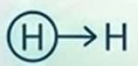


LIPINSKI RULE OF FIVE DISTRIBUTION FOR TIMTEC STOCK

Rule Criteria

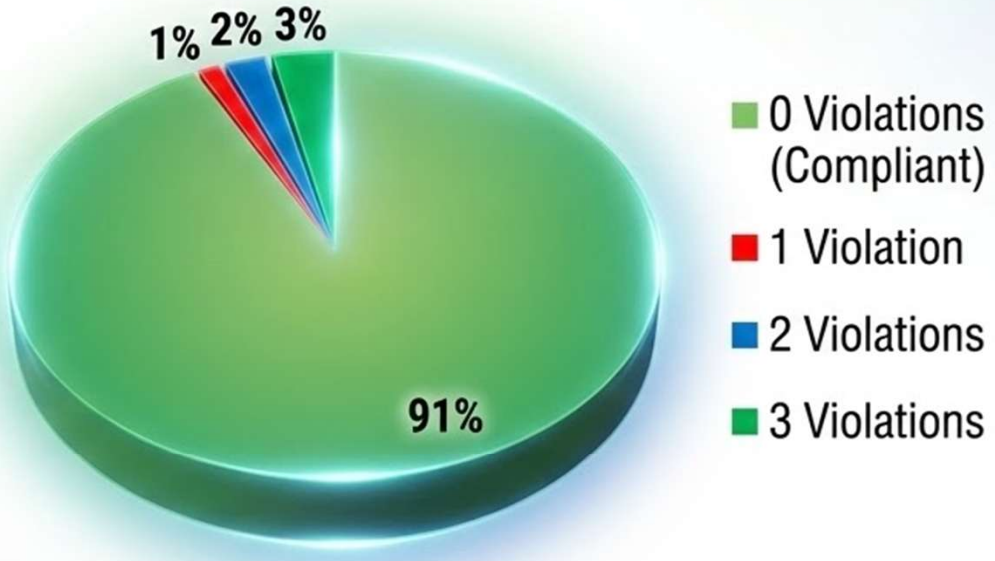
MW ≤ 500
Molecular mass not greater than 500

cLogP ≤ 5
LogP not greater than 5



HBD ≤ 5
No more than 5 hydrogen bond donors

HBA ≤ 10
No more than 10 hydrogen bond acceptors.



TimTec Compounds Characteristics

Individually synthesized

Compounds are crafted individually.

Purity

At least 90%, average 95%.

NMR & LC/MS Analysis

300 MHz or higher; comprehensive characterization.

Drug-like Properties

Adhere to drug discovery standards.

Molecular Weight

Range: 160–600; Average: 280-350.

No Reactive Groups

Chemically stable compounds.

No Heavy Metals

Free from toxic heavy metals.

Flexible Formatting

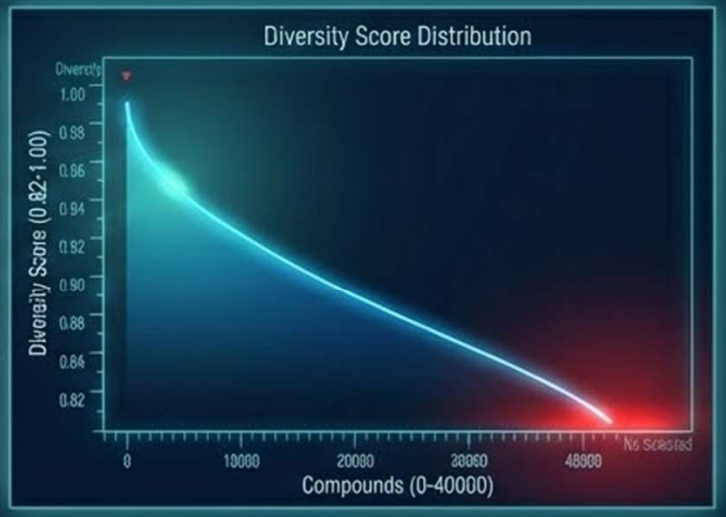
Available in vials, 96/384-well plates, and custom vessels.

Diversity Libraries

A selection of compounds from currently available pool/s of compounds that represents the greatest chemical diversity within a specific library size.

Proprietary software is used to identify “top” diversity screening material.

- ActiProbe Series
- Diversity Set
- ApexScreen 5040
- MyriaScreen II (Sigma-Aldrich)

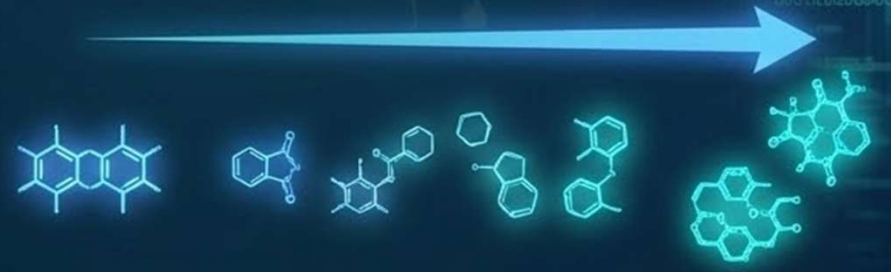


Diversity Assessment

Concept & Calculation

- Diversity characterizes **Similarity** (Cosine coefficient) and **Dissimilarity** of molecules in a dataset.
- Database diversity sorting produces a number from **1** (most structurally dissimilar) to **0.0** (identical compounds).
- Dissimilarity calculation: **D(A,B) = 1 - S(A,B)**, where S is similarity.

Diversity Scale Visualization



S=1, D=0 (Identical) | Intermediate Diversity | S=0, D=1 (Most Dissimilar)

Goal & Application

- Diversity analysis indicates how compounds from one dataset contribute to diversity increase or decrease in another.
- TimTec libraries are designed to **increase diversity** of customer collections.

TimTec Goal: Increase Diversity

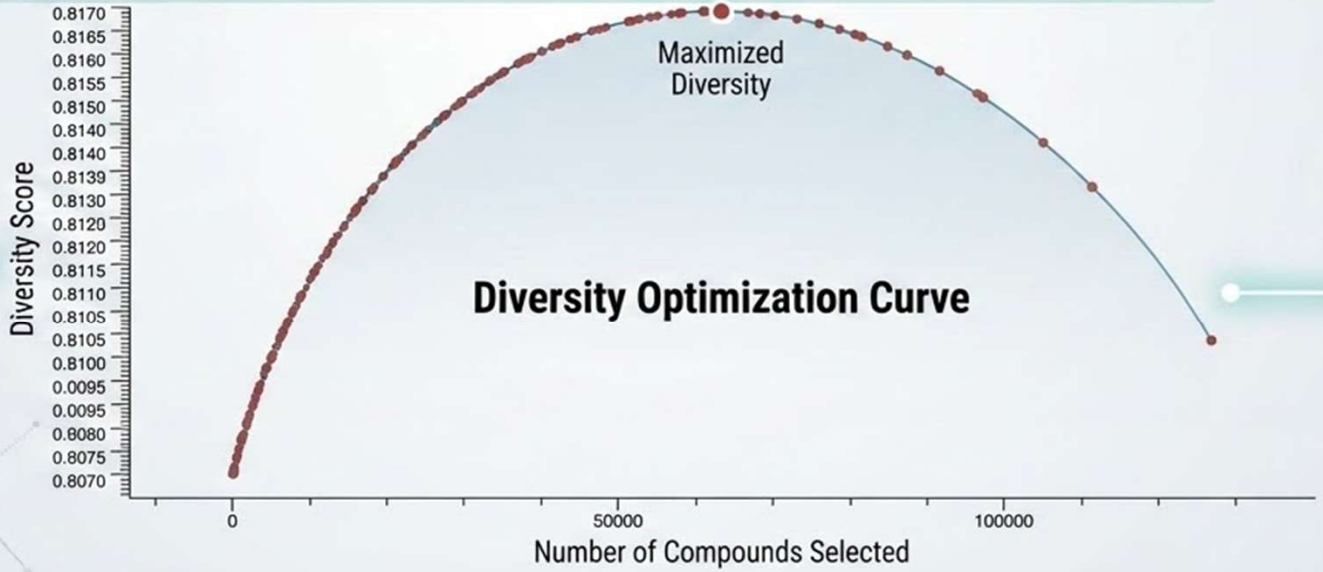
Diversity Analysis of an External Library compared to an In-house Screening Collection Example

- Size of customer's **in-house library**: 561,633 compounds
- Size of TimTec library subset: 133,622 compounds
- Duplicates identified: 6810 compounds
- Number of compounds that will maximize diversity of collection: **~65,000**

TimTec Library Subset

Size: 133,622 compounds

Customer's In-house Library



Diversity Set – Leverage Discovery with Diversity

Understanding the Diversity Set

A superior collection of structurally dissimilar singletons identified within a variety of chemo types a variety of chemo types in TimTec stock. The SET was designed with diversity being in focus in addition to generally drug-like compounds selection.

Diversity is a property of dataset that characterizes Similarity and Dissimilarity* of molecules included in it. Database **diversity sorting** produces a number from 1 (most structurally dissimilar) to 0.0 (identical). Diversity number for **Diversity Set** is **0.88** and is rather high for comparable in size collections.

*Briefly, Dissimilarity (**D**) of the pair of structures **A** and **B** is **D(A,B)=1-S(A,B)**, where **S** is similarity.

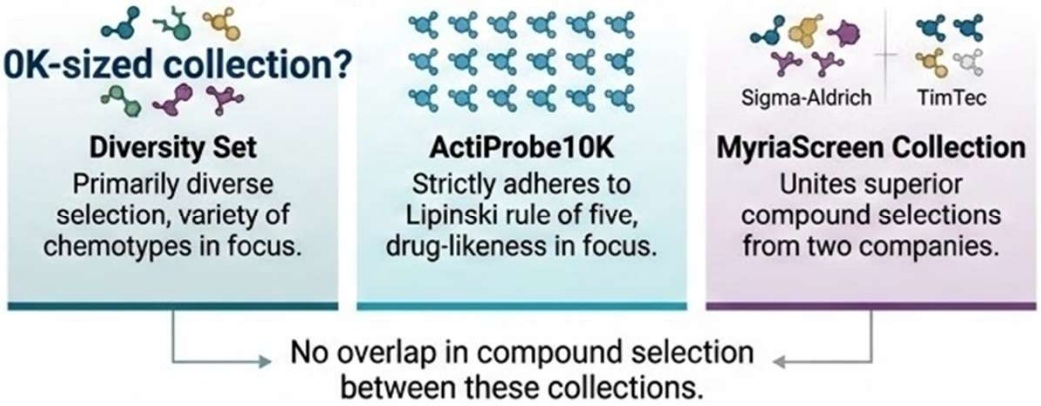
- **How does Diversity Set compares to other 10K-sized collection?**

Diversity Set, ActiProbe10K, and MyriaScreen

Diversity Score: 0.88
(High for comparable size collections)

*Briefly, Dissimilarity (D) of the pair of structures A and B is D(A,B)=1-S(A,B), where S is similarity.

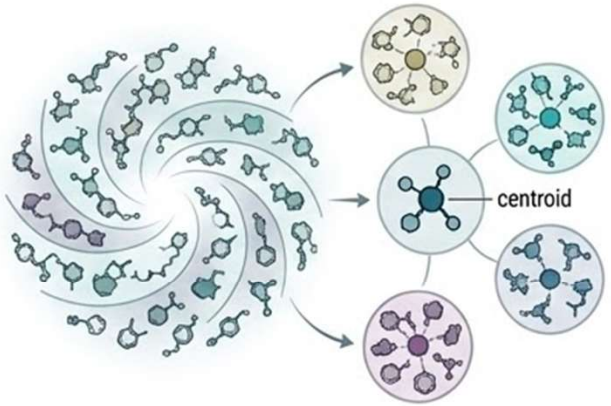
Comparison to Other 10K-sized Collections



ActiProbe Series

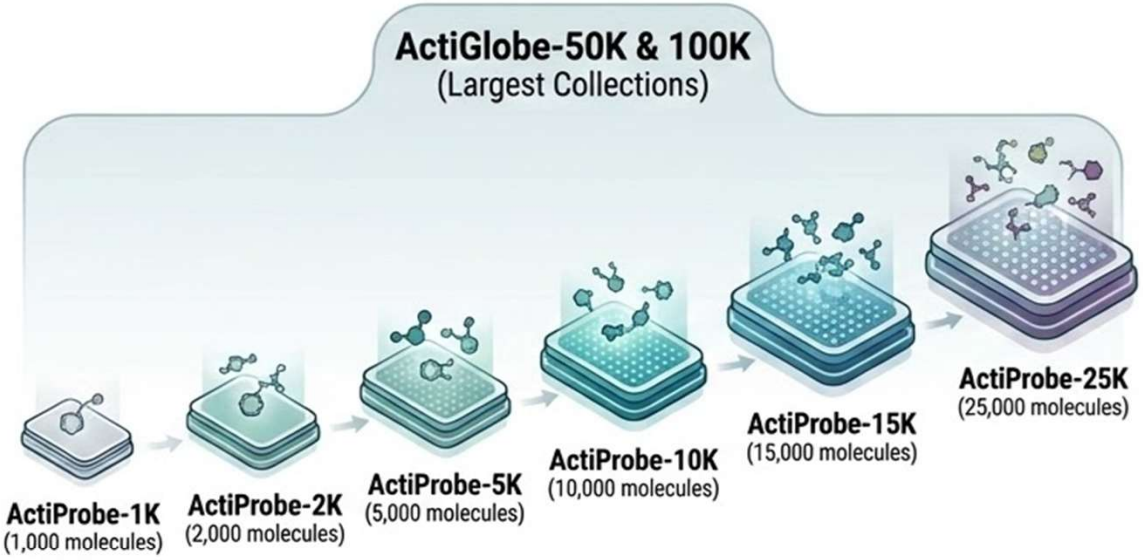
Diverse Chemotypes & Smart Design

Access diverse, drug-like molecules from TimTec's global database. All collections use Jarvis-Patrick clustering for representative sampling from larger pools.



Jarvis-Patrick Clustering

Scalable Collections from ActiGlobe



Tailored to Your Needs

Customize your ActiProbe collection with any number of molecules to match your assay capacity and budget.

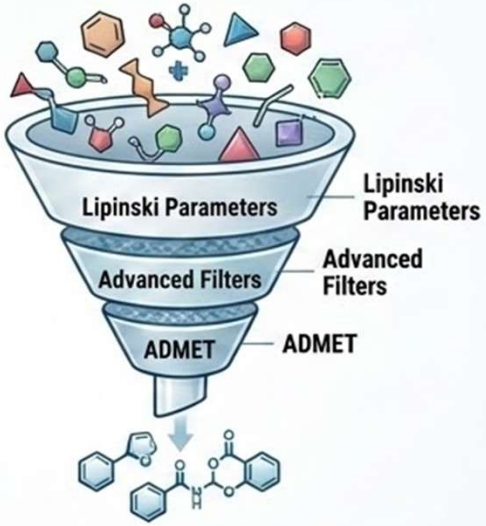
ActiGlobe-50K and 100K

Global Diversity Collection

Compounds Assembled

- From over 2,000,000 candidates worldwide
- Represents chemical diversity from global labs & research centers

Rigorous Filtering & Optimization



Creating High-Quality Starting Points

- Adherence to Lipinski rules
- Eliminates undesirable atoms/fragments
- Optimized for hit and ADMET studies

Access & Request

Due to large file size, database is available on request for download.

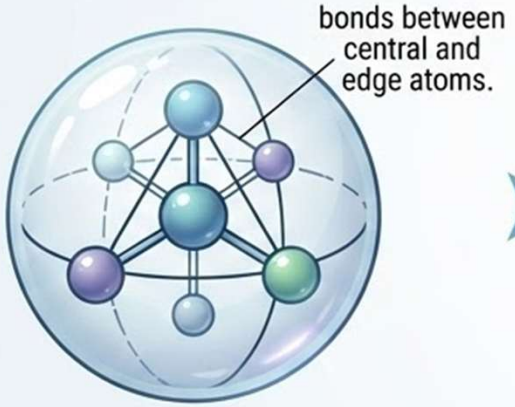
Call:
1 302 292 8500

Email:
timtec@timtec.org

ActiProbe Series: Jarvis-Patrick Clustering

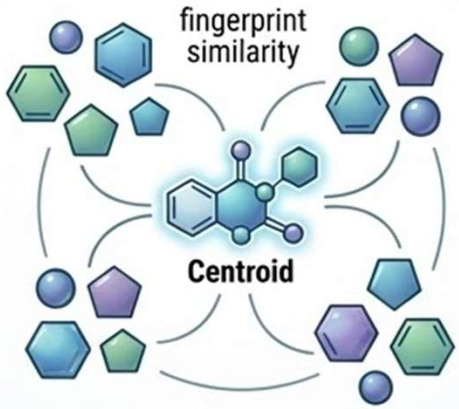
Molecular Characterization & Library Design

1. Molecular Characterization (2D Fragment Descriptors)



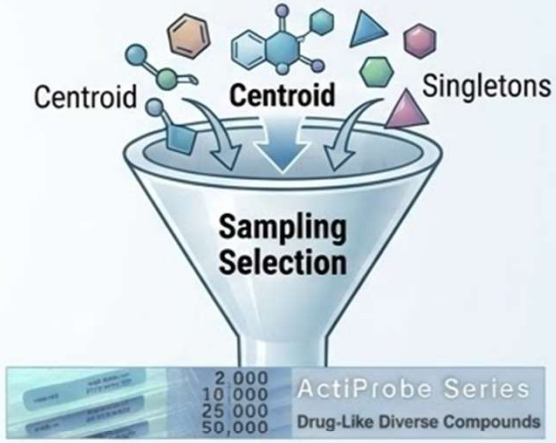
Based on 2D fragment descriptors. Consists of a central atom and neighboring atoms within a predefined sphere size.

2. Grouping & Centroid Identification



Groups based on structural similarity of fingerprints (bit strings). Centroid has highest degree of similarity to other members.

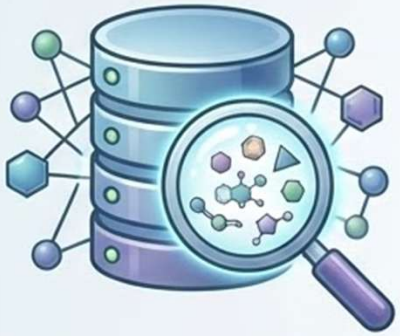
3. Library Sampling & Augmentation



Sampling libraries created from centroid and singleton selection. Augmented with members from the largest groups.

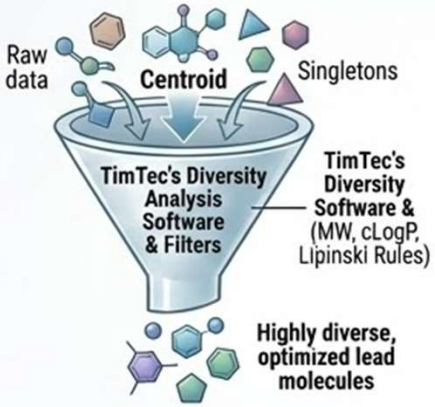
ApexScreen 5040

A Representative Collection



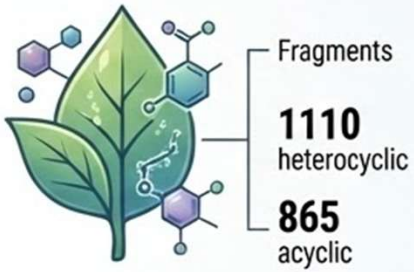
- 5,040 compounds selected to represent the diversity of TimTec stock of over 180,000 compounds
- Smaller format as opposed to larger general screening collections.
- Perfect collection to jump-start any screening project.

Designed for Diversity



- Created with TimTec's Diversity Analysis Software for maximized chemical diversity.
- Further filtered to include molecules within designated MW, cLogP and Lipinski Rule parameters.

Unique Composition & Value



- Includes pure natural compounds from TimTec Natural Product Libraries.
- 2138 unique fragments: 1110 heterocyclic, 865 acyclic.
- A valuable addition to any existing compound library.

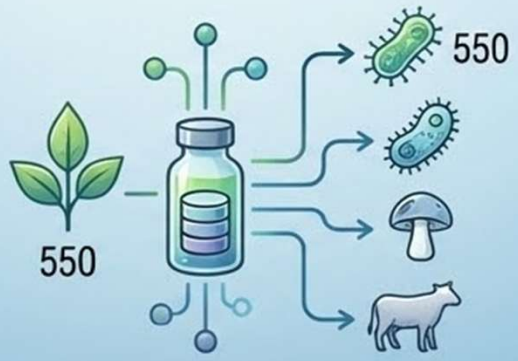
ApexScreen-5040:
Screening collection of 5040 top diversity molecules

NPL – Pure Natural Products Library

Diversity by nature Purity by science Value by design

800 Pure Natural Compounds for Lead Identification

Natural molecules tend to be multi-active across targets being inherently bio-available.



Broad Diversity & Screen-Ready Format

The value is in broad diversity representation. Compounds primarily sourced from plants (550) with remaining samples from bacteria, fungus, and animal sources.

Comprehensive Reference Data Available

Common natural sources and reference information is available for the majority of the samples.

Data on dlcstating aesults and screening moleculest samplet.

Pure Natural Compounds Library NPL
diversity by nature · purity by science · value by design

Screen follow-up results: http://www.timtec.org

NPL – Pure Natural Products Library

Diversity by nature. Purity by science. Value by design.

- **A Collection of 800 Pure Natural Compounds**
  Selected as lead identifying material. Natural molecules tend to be multi-active across targets being inherently bio-available.
- **Broad Diversity & Screen-Ready Format**
  Compounds primarily sourced from plants (550), with remaining samples from bacteria, fungus, and animal sources. Value in diversity representation.
- **Comprehensive Reference Data**
  Common natural sources and reference information is available for the majority of the samples.

Screen follow-up results: http://www.timtec.net/Natural-Compound-Library.html

NDL – Natural Products Derivatives

NDL-3000: Natural & Synthetic Blend

TimTec Natural Product Derivatives Library, NDL-3000, now includes 3040 compounds. These are semi-natural, compounds derived from natural ones, and synthetic compounds that are natural-compound-like. There is no overlap between NPL and NDL.

Broad Structural Diversity & Fragments

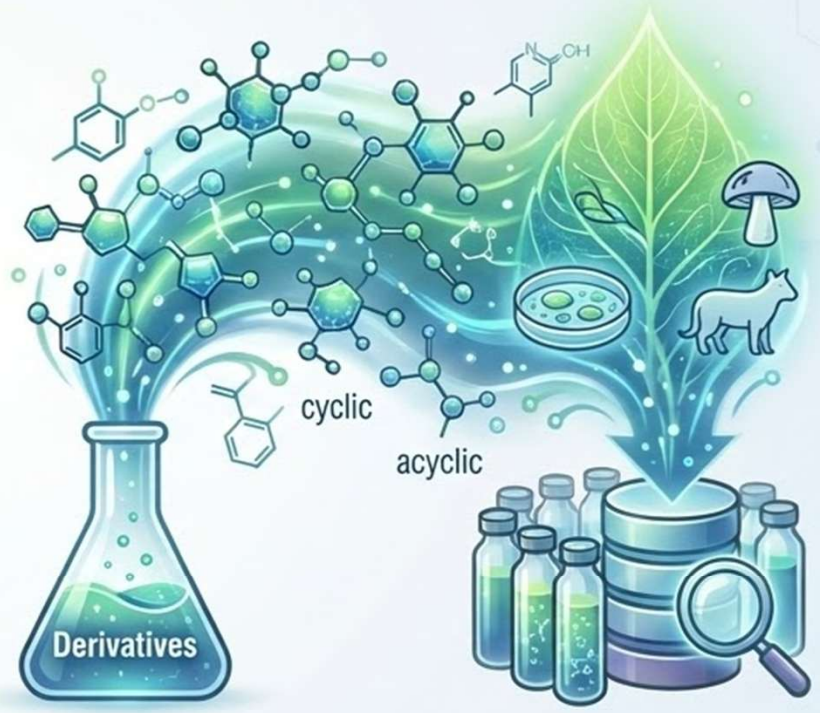
NDL elaborates on structural variety of pure natural compounds. Includes alkaloids, natural phenols, nucleoside analogs, carbohydrates, purines, pyrimidines, flavonoids, steroidal compounds, and natural amino acids. NDL-3000 has 1421 unique fragments: 762 cyclic, 682 heterocyclic, and 659 acyclic fragments.

Distinct Chemical Space & Source Diversity

Natural chemistry occupies chemical space distinct from bioactive and common organic molecules. Natural product structures differ by organism. TimTec NDL includes scaffolds produced by plants, animals, and bacteria.

Design Approach & Reference

Please read more about NDL-3000 design approach, which was described as one of the screening trends in J Med. Chem.



Flavonoid Derivatives

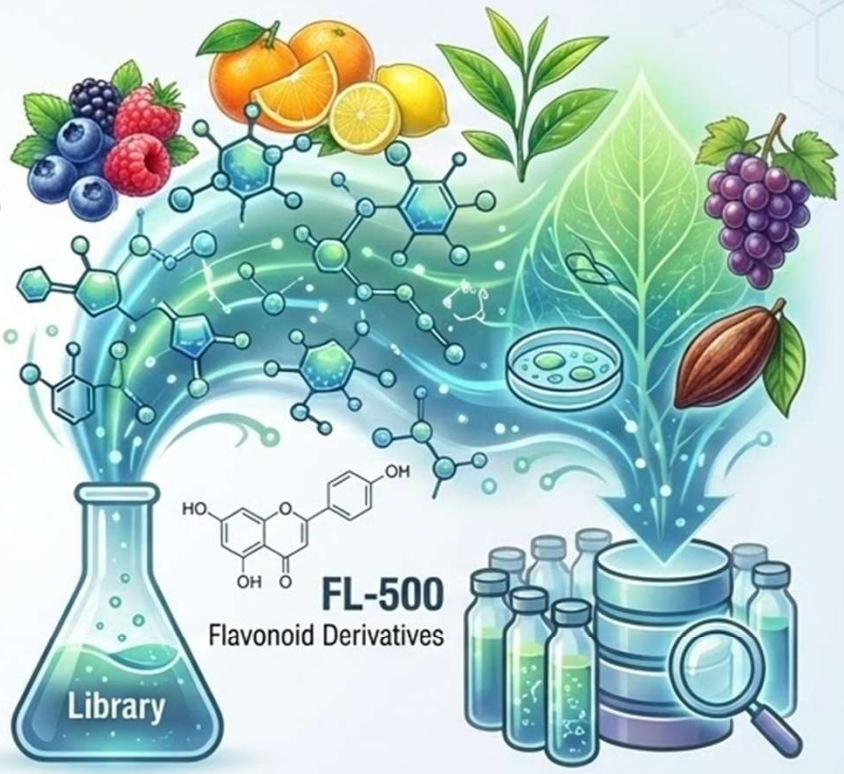
Therapeutic Potential & Natural Fit

Flavonoids are a preferred group of natural chemotypes tested for various biological activities, offering high potency with low toxicity and natural abundance. They are multi-active across a broad spectrum of targets, showing leading performance in anti-inflammatory, anticancer, and anti-oxidant activities.

FL-500 Collection: 9 Core Structures

TimTec's FL-500 collection of 500 Flavonoid Derivatives is assembled using 9 core flavonoid structures:

- -Chalcone
- -Flavanone
- -Flavone
- -Dihydroflavonol
- -Flavonol
- -Flavan
- -Stilbene
- -Isoflavonoid
- -Neoflavonoid



Fragment-Based Library, FBL

TimTec Fragment-Based Library, FBL, gathers structurally diverse 3,200 ligands selected according to the following criteria:

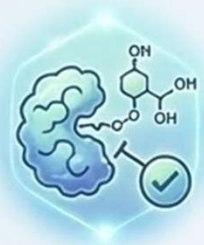
MW:	110-290
ClogP:	≤ 2.5
HBA:	≤ 5
HBD:	≤ 3
Rotatable bond:	≤ 5
Non-hydrogen atoms:	≤ 20
Rings:	1 - 3
Polar Surface Area:	Not defined
LogS calculated:	$>10^{-3}$
Concentration:	1.5mM
Potential IC50's number target:	0.1 to 1.0mM Ki/Kd

*All calculations are performed using TimTec proprietary software ChemDBsoft.

The entire collection, FBL-3,200 compounds, is available in custom formatting in dry form or as a solution.

Activity-Aimed Sets

Active molecules identified after screening TimTec compounds have corresponding collections of structural analogs:



OGT Inhibitors – O-GlcNAc Transferase Inhibitors

AhR Lingands – Aryl Hydrocarbon Receptor Ligands

Activators of Neutrophils – N-Formyl Peptide Receptor Agonists

Anthrax Lethal Factor Inhibitors

TNF-alpha inducers – Potent Tumor Necrosis Factor Alpha Inducers

ST050150, AG-205 – inhibits Pgrmc1 (Progesterone Receptor Membrane Component 1), a heme-1 domain protein that promotes tumorigenesis.

ST50051351, FPSS, interrupts genes control mechanism in foodborne Listeria bacterium.

ST057529, Compound 1, is an inhibitor of ccKDM4C, catalytic core of lysine (K)-specific demethylase 4C.

ST024375, PRT4165, inhibits both Bmi1 (a known oncogene)/Ring1A self-ubiquitination and Top2α ubiquitination in-vitro.

All screening collections - Additional Notes

Price depends on compound selection & sample size.
Custom collections & cherry-picking available.

Custom formatting options for all libraries. See ‘Compound Management’ section.

Prices exclude shipping & consumables charges.

Delivery in vials, 96 or 384 well plates.
Custom storage solutions.

Libraries/databases e-files may exclude recent updates.

All compounds stored dry, freshly prepared in DMSO.

Purity avg ≥ 95% (1H-NMR/MS).
Overall purity ≥ 90%.

Resupply from stock (amount confirmed at order).
Scale up synthesis & re-synthesis services.

TimTec holds no IP rights.
Identified hits are yours for development.

TimTec Services

Sample Management - Comprehensive handling solutions.

Sample Re-formatting/Custom weighing - Precision for any format.

Consolidated Compound Procurement - Multi-source acquisition.

Computational Services - Virtual screening & analysis.

Custom Synthesis - Tailored chemical synthesis.

e-Database management - Data organization & maintenance & maintenance.

Computational Services - Virtual screening & analysis.

Analytical - Advanced characterization.

TimTec - Your trusted partner for scientific solutions.

Sample Management Services

Core Handling & Automation - Dry & liquid handling, small to high throughput, fully automated systems.

Custom Formatting & Precision - Custom organizing, precision weighing & dissolution in various vessels.

Plate Replication & Sets - Preparation of mother/daughter sets, replication of 96 & 384 well plates.

Data & Inventory Management - Electronic records, digital inventory organization, barcoding & labeling.

Specialty Packaging & Logistics - Specialty packaging and dry ice shipments.

TimTec - Your Trusted Partner for Sample Management.

Consolidated Compound Acquisition

Multi-source database mining.

Single point-of-service ordering.

Preparation of appropriately formatted samples and solutions.

Uniform database processing.

Database management.

Possible vendor-to-vendor discounts.

Uniform database processing.

Database management.

Possible vendor-to-vendor discounts.

TimTec

Sample Handling: over 160 inventory storage solutions

Decades of experience, processing thousands of compounds monthly with highest quality standards.

Flexible project sizes, eliminating the need for unutilized specialty equipment.

Intermediary formatting to simplify weighing, plating, labeling, and organizing tasks.

Flexible project sizes, eliminating the need for unutilized specialty equipment.

Uniform, ready-to-use formats with over 160 inventory storage solutions.

Stay In Touch with TimTec

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Schedule consultation on TimTec Compound Library Collections, products, and services.

To receive free updated TimTec libraries and stock database/s, please e-mail your request to orders@timtec.org.
Links for download our catalogs are available at www.timtec.org and www.timtec.net.