2023 Services Catalog

TimTec Screening Collections

Full line of pre-designed collections characterized according to the following features. These are starting points for libraries selection:

1. **General screening** collections include drug-like and generally diverse selections of different sizes from 1,000 to 100,000 compounds.

2. **ActiTarg Series, targeted libraries**: kinase, protease, GPCR, HDAC, ion-channel, nuclear receptors modulators, serine proteinase inhibitors.

3. **Nature Informed**: pure natural material, natural product derivatives, plant extracts.

4. Collections built around **specific compound/s characteristics, Activity-Aimed Sets**: Anti-inflammatory, Anti-Infectives, Privileged Structures, ActiCom (compounds with known activates), Fragment Based Library, specialty sets build around hits.

5. **Custom**: based on customer suggested criteria of selection. Our collections are available for cherry-picking.

6. **Compound collection size and formatting**: There are collections of 2,000cmpds, 5,000cmpds, 10,000cmpds, 25,000cmpds, 50,000cmpd, or even 75-100,000+ cmpds.

General Screening Collections

ActiProbe Series

With ActiProbe Series of screening collections you get access to some of the most diverse chemotypes among distinctly drug-like molecules available from TimTec extended stock. The Series includes different in number of compounds stand-alone collections to suit your assays. All collections share one and the same clustering design approach. Choose any number of compounds from 1,000 to 25,000 as in ActiProbe-1K and 25K, or any number in between, up to 50,000-100,000 in ActiGlobe-50K and 100K.

Diversity SET

Leverage discovery with Diversity SET, a superior collection in terms of the dissimilar selection of singletons identified within variety of chemo types in TimTec stock. The SET was designed with the diversity being in focus in addition to generally drug-like compounds selection gathering 10,000 molecules.

ApexScreen-5040

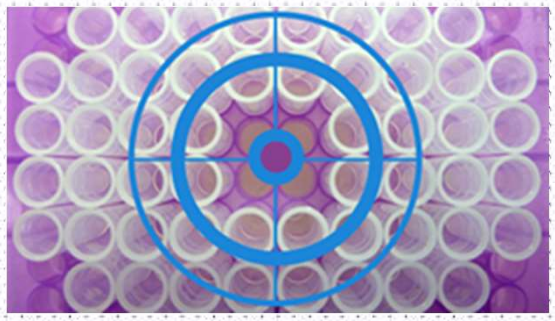
The collection of 5,040 compounds represents the diversity of TimTec stock in a smaller format as opposed to larger screening collections of 10,000 compounds and more. ApexScreen is a perfect starter library and a valuable diversity addition to any existing collection. On top of diverse compound selection ApexScreen includes a number of pure natural compounds and natural derivatives to suit current trends in screening.

MyriaScreen II

It is now 50% updated redesigned version of original MyriaScreen co-developed with Sigma-Aldrich Corporation. The collection unities 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.

These groups of compounds possess structural features and molecular lattices that are representative of agents described in the patent and/or technical literature. Potentially active compound pool is broadened as the combinations of the same fragments from known structures add to newer structural variations. In addition, medicinal chemistry judgment has also been implemented in the selection process to provide libraries that promise lead identification in an expedited manner.

WEB: **http://www.timtec.net/Targeted-Compound-Libraries.html**

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

Plant Extracts

Crude mixtures of compounds, unpurified extracts, covering expansive geo reach and the diversity of plant material. There are over 120 extracts from plants with known traditional or medicinal use.

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

TimTec can use custom designed selection criteria to assemble screening collection of any size.

- Comprising compound collection of different size (from a few to thousands of compounds) utilizing proprietary software based on custom criteria: structure similarity search, presence of a particular fragment/s, defined physical chemical propetes, e.g. MW, clogP, number of HBA and HBD, Lipinski Rule, Rule of 3, etc.
- Analog/derivatives-libraries to compounds with known activities and screens follow-ups. Functional groups, fragments, scaffolds, and substructure searches.
- Compound selection from TimTec databases contributory to the diversity of an existing customer library. Database comparison and diversity analysis.

Cherry-picking is available across predesigned collections.

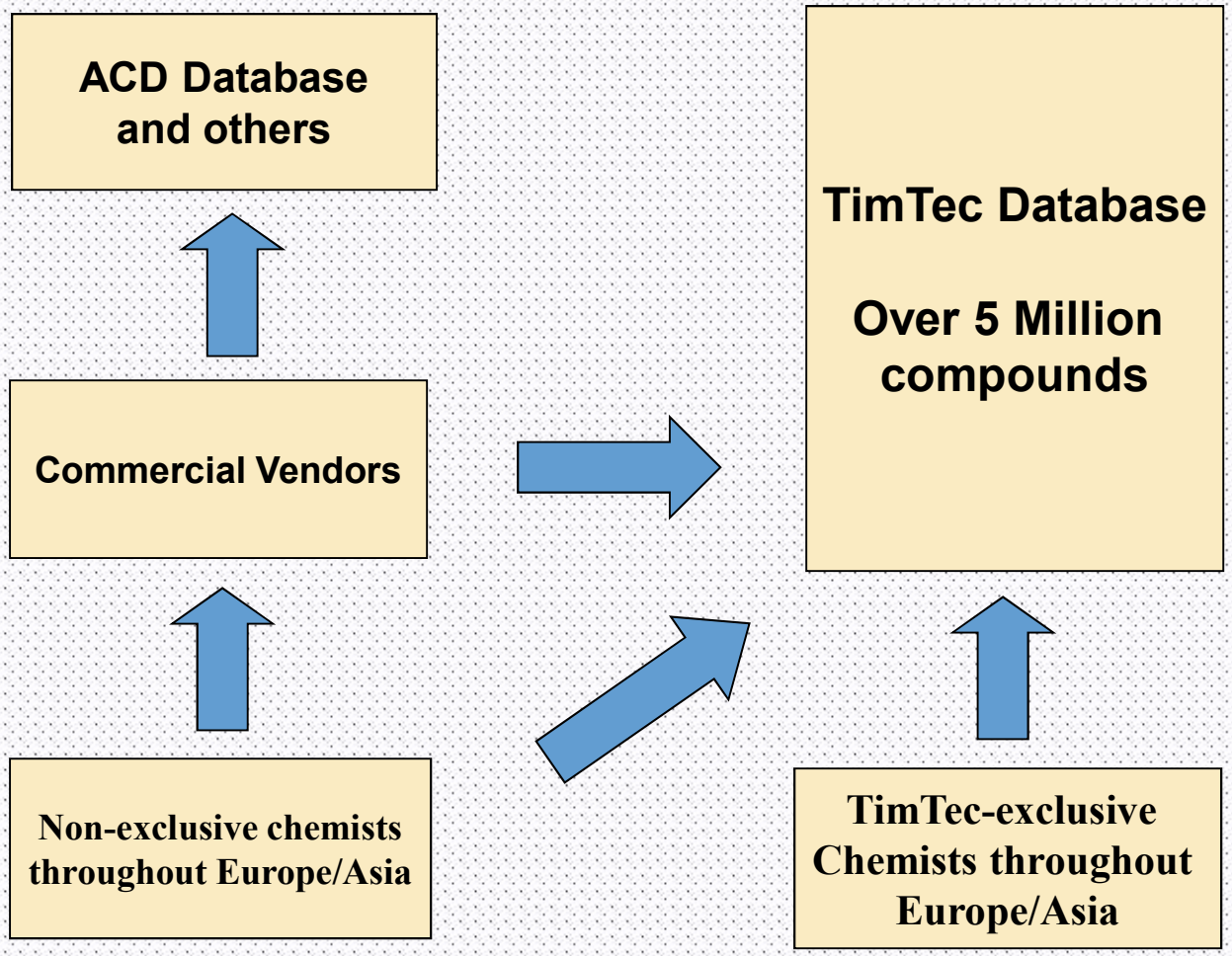
Please use the following databases for any in-house computational selection:

http://www.timtec.net/TT_SDF/ACTIMOL_STOCK.zip
http://www.timtec.net/TT_SDF/TimTec_A.zip 2 weeks
http://www.timtec.net/TT_SDF/TimTec_B.zip 3-4 weeks

Building Blocks:

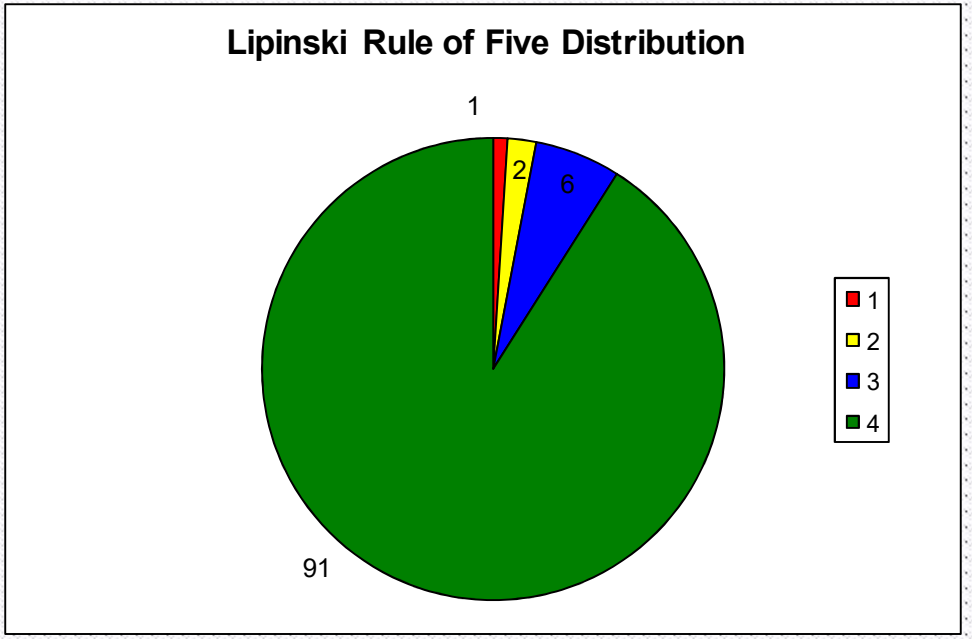
http://www.timtec.net/TT_SDF/TimTec_BB.zip

TimTec Database Accessibility and Sourcing Expertise

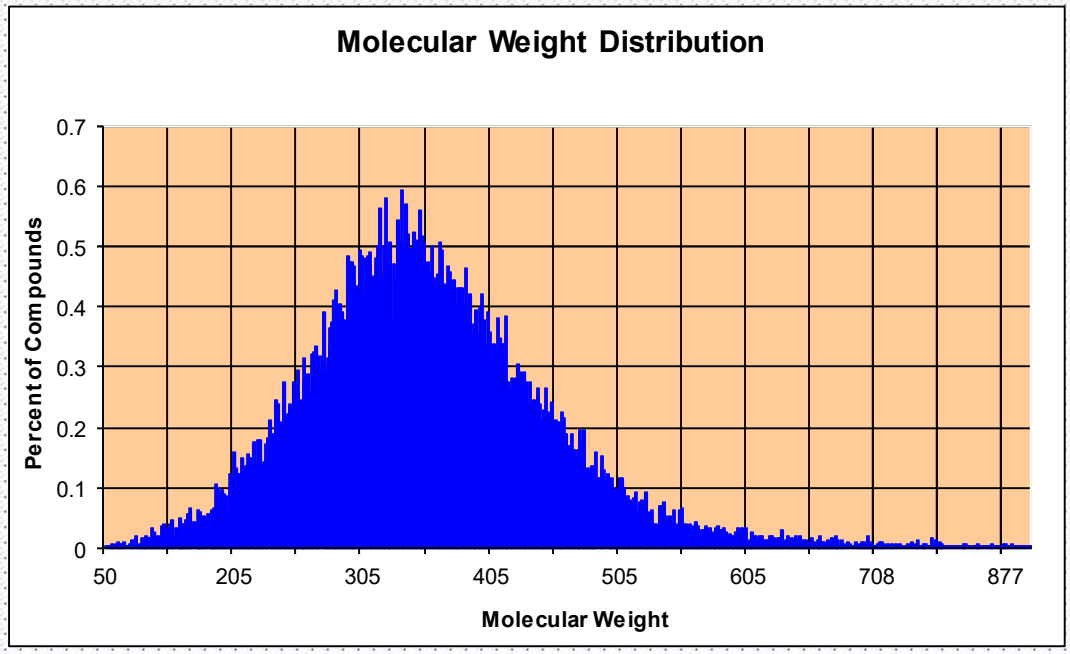


Lipinski Rule of Five Distribution for TimTec stock

- Molecular mass not greater than 500
- LogP not greater than 5
- No more than 5 hydrogen bond donors
- No more than 10 hydrogen bond acceptors



Molecular Weight Distribution of TimTec Compound Stock

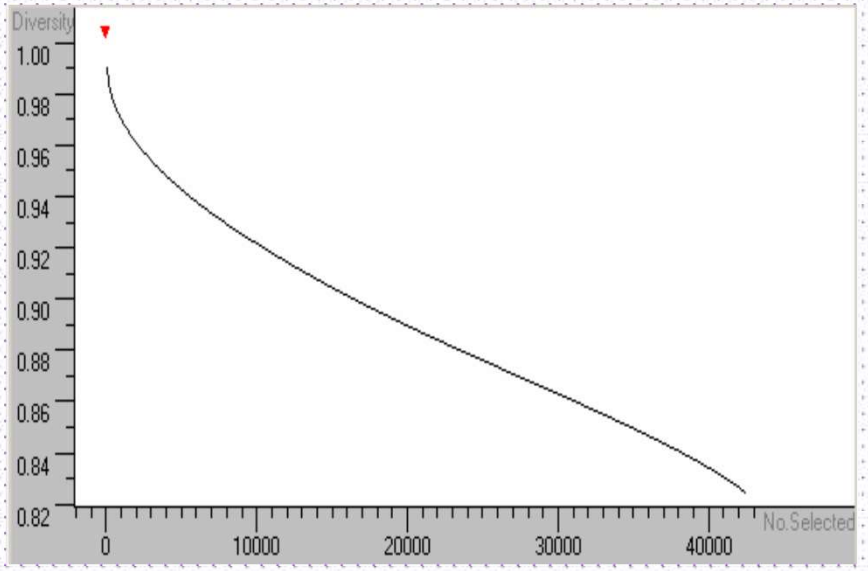


TimTec Compounds Characteristics

- Individually synthesized
- Purity - at least 90%, average 95%
- NMR (300 MHz or higher) and LC/MS
- Possess drug-like properties
- Molecular Weight 160–600, average 280-350
- No reactive groups
- No heavy metals
- Available in vials and/or 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
- Diversity-based screening libraries:
  - ActiProbe Series
  - Diversity Set
  - ApexScreen 5040
  - MyriaScreen II (Sigma-Aldrich)

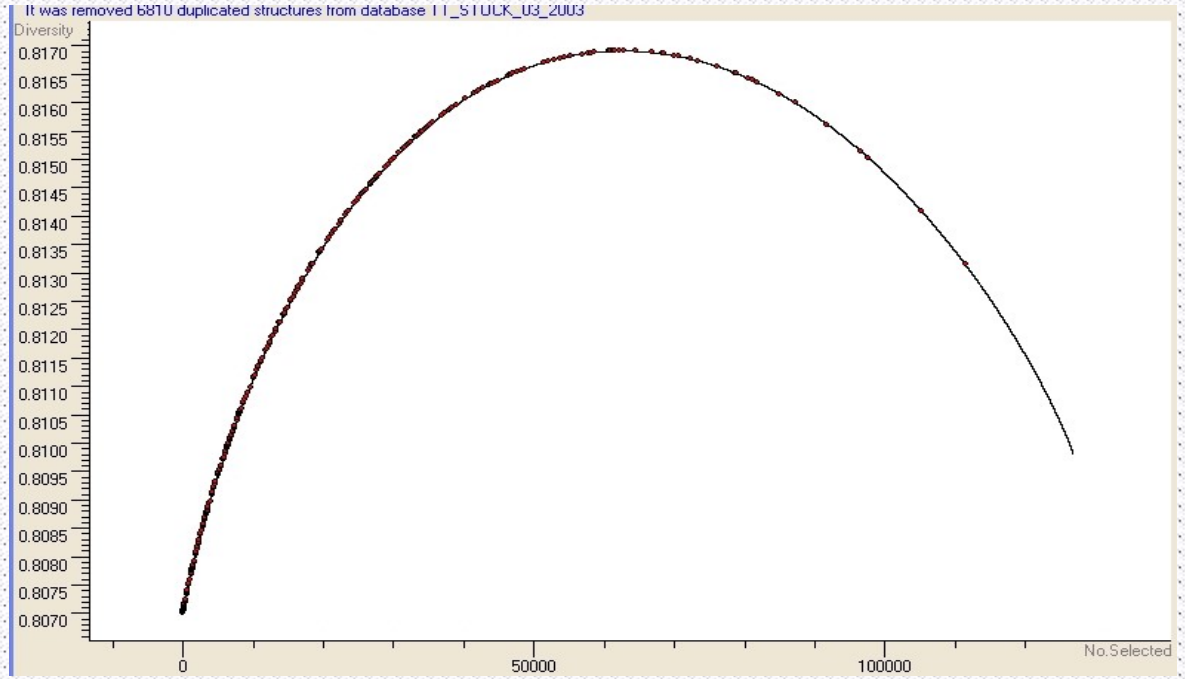


Diversity Assessment

- Diversity is a property of dataset that characterize Similarity (Cosine coefficient is used as a similarity measure) and Dissimilarity of molecules included in it
- Database diversity sorting produces a number from 1, most structurally dissimilar to each other cmpds in a dataset, to 0.0, identical cmpds in a database.
- Briefly, Dissimilarity calculations algorithm for the pair of structures A, B is based on: D(A,B)=1-S(A,B), where S is similarity.
- Diversity analysis can tell how many compounds and which ones from one dataset would contribute towards diversity increase or decrease in another dataset.
- TimTec libraries are designed to increase diversity of current collections of our customers

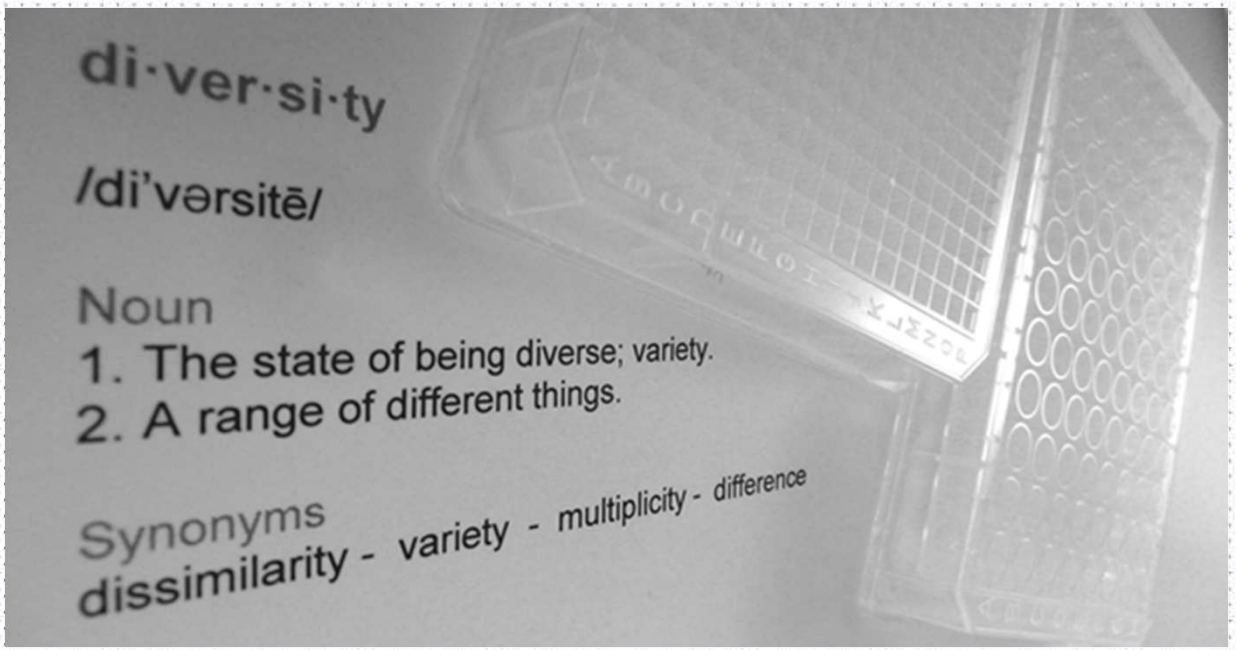
Diversity Analysis of an External Library compared to an In-house Screening Collection Example

- 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



General Screening Collections

The more a researcher understands the underlying molecular and cellular mechanisms concerning a particular therapeutic area, the more specialized and narrow should be the compound selection. A general diversity library is the most appropriate choice when mechanics of interaction and structural characteristics are unknown. Diversity is precursor to discovery.



Diversity Set – Leverage Discovery with Diversity

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

Web: http://www.timtec.net/Diversity-Screening-Set-10K.html

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 collections?**

Diversity Set, ActiProbe10K, and MyriaSreen Collection do not overlap in compound selection. Diversity Set is primarily diverse selection from our stock, variety of chemotypes is above all in focus. ActiProbe10K as entire collection strictly adheres to Lipinski rule of five, drug-likeness is in focus. MyriaScreen unites superior compound selections from two companies: Sigma-Aldrich and TimTec.

ActiProbe Series

- With ActiProbe Series of screening collections you get access to some most diverse chemotypes among distinctly drug-like molecules available from TimTec extended global sourcing database.

- All collections share one and the same design approach: Each smaller collection is assembled from a larger one in the Series through Jarvis-Patrick clustering that permits sampling of large library pools through selection of molecules that are representative of a group (cluster) within this library.

- Largest collection is ActiGlobe-50K, and ActiGlobe-100K, 100,000 compounds
  Smaller stand-alone collections are part of ActiGlobe:

  ActiProbe-1K (1,000 molecules)
  ActiProbe-2K (2,000 molecules)
  ActiProbe-5K (5,000 molecules)
  ActiProbe-10K (10,000 molecules)
  ActiProbe-15K (15,000 molecules)
  ActiProbe-25K (25,000 molecules)

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

ActiGlobe-50K and 100K

The grand diversity collection of 50,000 compounds has been assembled from world wide sources numbering over 2,000,000 compounds-candidates. The collection has molecules representing the chemical diversity of screening samples produced by labs and research centers throughout the world.

In addition to adherence to Lipinski parameters, dozens of advanced filters have eliminated undesirable atoms, functionality and fragments creating a large-sized library that will provide exceptionally good chemical starting points for hit and ADMET optimization.

Due to large file size, ActiGlobe-50K and 100K database is available on request for online download. Please call 1 302 292 8500 or e-mail at timtec@timtec.com

ActiProbe Series Jarvis-Patrick clustering

Molecular characterization is based on 2D fragment descriptors consisting of a central atom and neighboring atoms connected to it within a predefined sphere size -- bonds between central and edge atoms.

Groups of molecules are based on the structural similarity of fingerprints (bit strings of these fragments), and the centroid has the highest degree of similarity to other members of a cluster.

Chemically unique compounds (singletons) with low similarity to other members of the collection are also identified. Sampling libraries are created from centroid and singleton selection along with augmentation with other members from the largest groups.

MyriaScreen-II

- **Superior structural diversity - Distinct drug-like properties**

  MyriaScreen was created by combining medicinal chemistry expertise and decades of experience in compound acquisition from diverse sources. TimTec's proprietary software was used to filter a pool of over 300,000 TimTec and Sigma-Aldrich compounds on the basis of diversity. Additional filters were set to consider MW (>225 and <600), cLogP, H-acceptor, H-donors, and rotatable bonds. Medicinal chemistry specialists refined the selection with great personal attention to remove compounds that were overly represented or not well suited for medicinal chemistry follow-up. MyriaScreen is rich in chemotypes and a valuable source of screening compounds for lead discovery.

- **Ready-to-use format - High purity - Efficient re-supply**

  MyriaScreen is pre-plated for your convenience. The compounds have an average purity > 95% with nothing below 90%. Should you require more material for follow-up, re-supply or re-synthesis is available. Although MyriaScreen is designed for use as a complete set, there are two alternative options to fit your purchasing needs. Compounds can be purchased as individual plates or cherry-picked and plated on a custom basis.

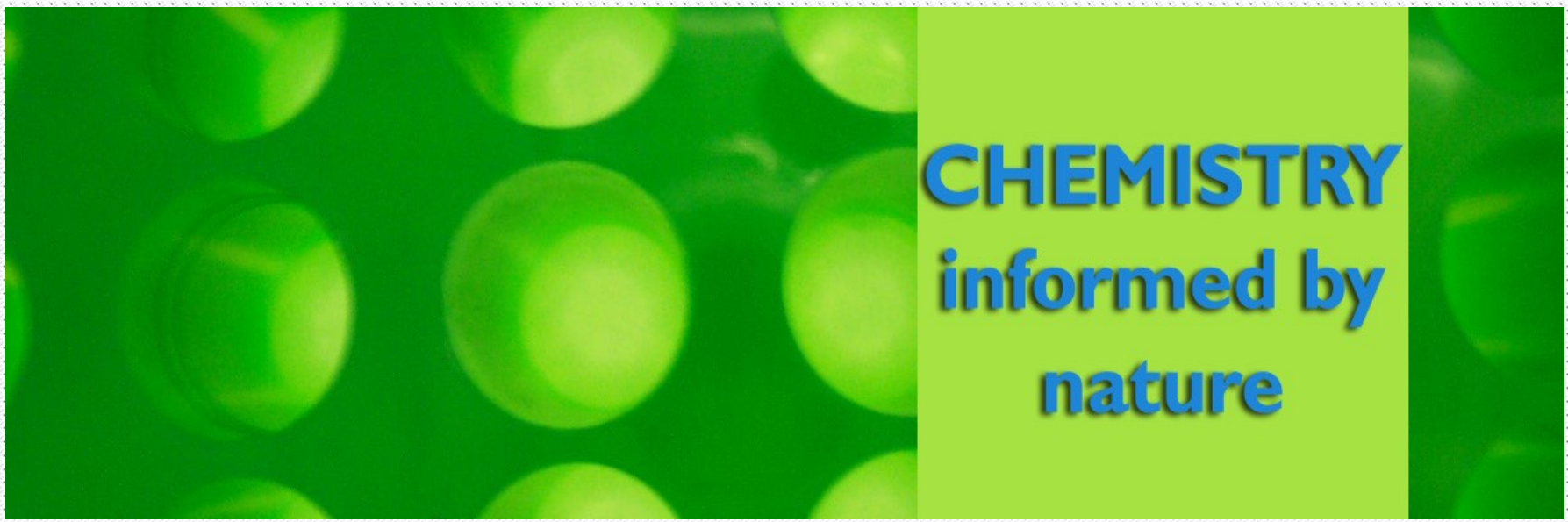
- **Formatting Options Available**

  The collection is available in 10mmol and 1mg/1mL concentration. Solvent is DMSO.

Visit www.myriascreen.com for more information about collection design and for publications.

ApexScreen 5040

- 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.
- ApexScreen in a variety of formatting options tailored to customer requirements is a perfect collection to jump-start any screening project.
- ApexScreen was created with assistance of TimTec's Diversity Analysis Software that allows the assembly of libraries with maximized chemical diversity from databases of compounds that are currently available from TimTec US stock. The diversity selection was further filtered to include molecules that fall within designated MW, cLogP and Lipinski Rule parameters.
- ApexScreen includes a number of pure natural compounds from TimTec Natural Product Libraries to suit current trends in screening.
- 2138 unique fragments including 1110 unique heterocyclic fragments and 865 acyclic fragments
- ApexScreen is a valuable addition to any existing compound library



"There are major teachings in theses natural products that we would do well to consider. They may be reflecting eons of wisdom and refinement. … In fact, one of the most promising approaches in diversity chemistry is to produce diversity-chemistry-derived collections that benefit from partake of the "wisdom" of natural products." *- Samuel J. Danishefsky*

NPL – Pure Natural Products Library

Diversity by nature **Purity by science** **Value by design**

TimTec NPL, Natural Product Library, is composed of 800 pure natural compounds as lead identifying material. Natural molecules tend to be multi-active across targets being inherently bio-available.

The value of the library is in broad diversity representation of selected natural material available in screen-ready format. Compounds are primarily sourced from plants (550) with the remaining samples from bacteria, fungus, and animal sources.

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

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

- NDL elaborates on structural variety of pure natural compounds and includes synthetic and synthetically modified pure natural compounds: alkaloids, natural phenols, nucleoside analogs, carbohydrates, purines, pyrimidines, flavonoids, steroidal compounds, and natural amino acids. The list is not complete. NDL-3000 has 1421 unique fragments. There are 762 cyclic, 682 heterocyclic, and 659 acyclic fragments.

- Please read more about NDL-3000 design approach, which was described as one of the screening trends in J Med. Chem: http://www.timtec.net/ndl-3000-natural-derivatives-library.html

- Natural chemistry does occupy chemical space distinct from bioactive molecules and common organic molecules. What is more, natural product structures differ depending on the organism or natural source they have come from. Based on the presented cheminformatics analysis, TimTec NDL includes the same scaffolds that are produced by plants, animals, and bacteria

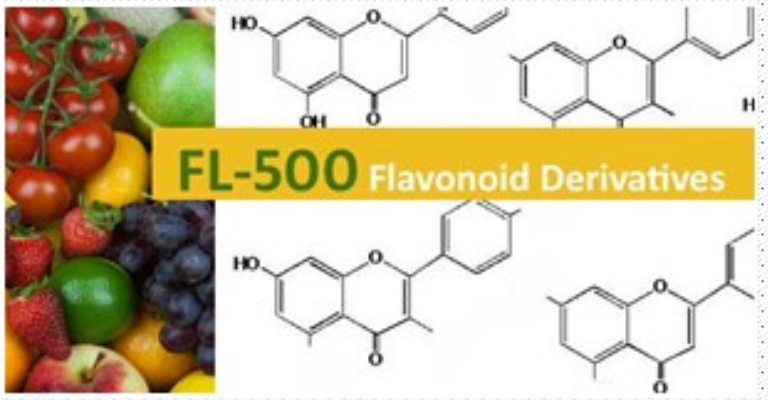
Falvonoid Derivatives

Flavonoids make one of the most preferred groups of natural chemotypes tested for various biological activities. Flavonoids potency is pleasantly complimented with low toxicity and natural abundance.

Flavonoids definitely hold much of therapeutic potential being multiactive across broad spectrum of targets. This group of compounds provides a good example of “natural fit” holding leading performance in anti-inflammatory, anticancer, anti-oxidant activities.

9 core Flavonoid structures are used to assemble TimTec small collection of 500 Flavonoids Derivatives, FL-500:

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



Gossypol and its Derivatives

Gossypol, TimTec catalog number ST065835, is an intriguing compound. It is highly potent and has challenging toxicity, which is yet to be separated from efficacy. Gossypol has history of traditional use and has been studied extensively in modern times. There is no shortage of information about this compound that is still generating research interest.

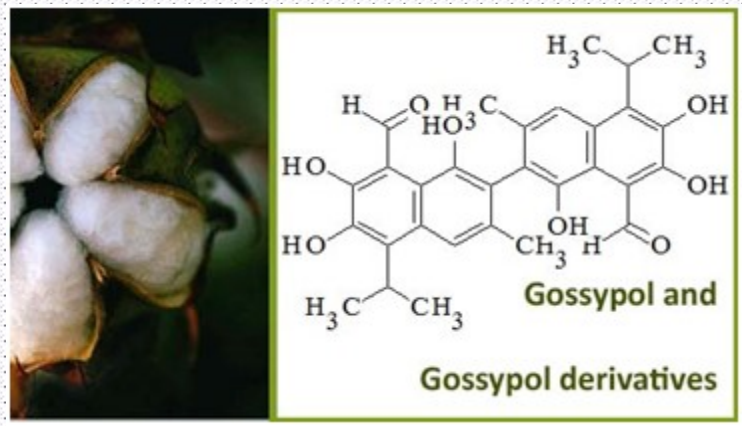
The mechanism of Gossypol activity is rather fascinating making researchers coming back to check with it for more interaction clues. Hence the demand for Gossypol derivatives that assist in probing broader chemical space with the focus on potential activity across targets.

Gossypol and its 80 derivatives are available from TimTec US stock. Gossypol, ST065835.

Gossypol, ST065835, is available in number of package sizes:

50mg/$99.00
100mg/$125.00
500mg/$299.00

1g/$399.00
2g/$499.00
5g/$875.00
10g/$1,500.00



Plant Extracts

About 11,500 cataloged plants from various regions of the former USSR (Eastern Europe and Middle Asia) are available for collection

250 prepared extracts are available in stock. 122 out of 250 are Featured Extracts are fully characterized and have the following information for the majority:

Plant Name
Botanical Info
Geography
Chemical Content
Traditional Medicinal Use and Activity
Images

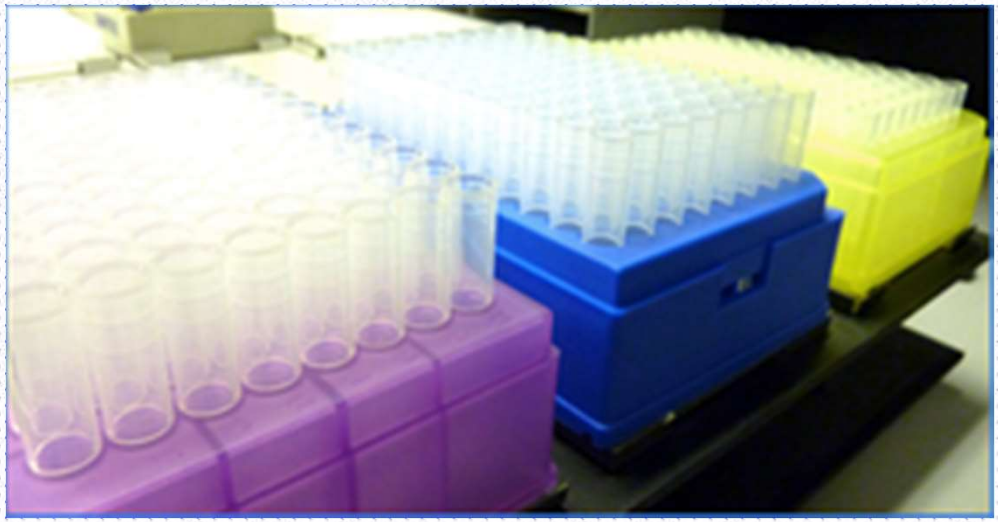
Information is compiled using regional print and online plant registers and reference materials.

Please view the listing of Featured Extracts here:
http://www.naturalcompounds.org/featured-extracts.html

Services:

- Extracts are available on large scale
- Fractionation and active component identification services
- Chemical synthesis and derivatization
- Scaling Up

Activity-Aimed Sets



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.

FBDD complementary benefits to HTS and references: http://www.timtec.net/FBL-Fragment-Based-Library.html

ActiCom – Active Compounds

- 480 compounds, 6 96-well plates
- Classified in general therapeutic categories and/or are assigned reported activities
- Resourceful screening set
- Assay development guide
- Good complement to any of our screening collections.
- Compounds are available individually or in subsets.
- The collection is growing with ongoing addition of new plates

Information available:

Structure, ID, CAS NUMBER

NAME, IUPACNAME, SMILES

Corresponding drug TRADEMARK

THERAPEUTIC CATEGORY and/or VET THERAPEUTIC CATEGORY

ACTIVITY/USE, REFERENCE

Revisiting known active structures is even more momentous now, when investigators are looking for bi-specific therapeutics and when “rediscovery research” is fueling drug repurposing trend.

Privileged Structure Library

- Evaluation of the structures of pharmaceuticals and agents with good pharmacological activity led to identification of molecular substructures frequently associated with a higher level of biological activity.
- Motifs with "privileged" label are found to be present in molecules that were active at two or more different receptors:

  - Aza-(and diaza-)biphenyls
  - Benzhydryl compounds
  - Biphenyls
  - Dihydropyridines
  - Anilino-pyridine, pyrimidine, or triazines
  - Phenylpiperazines

  Please inquire structural data files and quotes

Anti-Infectives

Mechanism	Lattice type
Membrane permeabilizers inhibit bacteria growth	Guanidines
Inhibit cellular respiration and biosynthesis of nucleic acids being acceptors of oxygen	Nitrofurans, Nitroimidazoles
Suppression of bacterial growth by blocking PABA	Sulfonamides
Protein synthesis inhibition in gram-positive microorganisms	Oxazolidinones
Distrupt peptidoglycan layer in the bacterial cell wall	Cephalosporins
Bacteriostatic, IMDH inhibition, anti-PABA, denatures protein while dissolving it	Urea, Diarylurea, Thiourea

Anti-Imflammatory

This activity-aimed set includes low molecular weight drug-like compounds with fragments found in known non-steroidal anti-inflammatory drugs covering variety of targets. About 20 starting drugs fragments are used to assemble the set of 1950 compounds available in 10mmol or 1mg/1mL concentrations and in dry form. Fragmental representation is summarized in the table below. Custom sub-sets can be created to narrow or expand the pre-designed selection.

Lattice type	Lattice Type Occurrence	Drug Example
Aryl acetic acids	353	Acemetacin, Felbinac
Quinolines	300	GSK256066, Compound 35 (Kyowa Hakko Kirin), Compound 19 (BMS)
Amino aryl carboxylic acid	141	Etofenamate, Talniflumate
Aryl carboxylic acid derivatives	705	Clidanac, Tinoridine
Aryl butyric acid derivatives	24	Bumadizon, Fenbufen
Aryl propionic acid derivatives	158	Ibuprofen, Suprofen, Oxaprozin
Pyrazoles	680	Difenamizole, Epirizole
Pyrazolones	586	Propyphenazone, Suxibuzone
Salicylic acid	71	Aspirin, Diflunisal,Parsalmide, Olsalazine
2-hydroxyacetic acid	3	Benzydamine
1,3,5-trihydropyrimidine-2,4,6-trione	26	Bucolome
N-(2-pyridyl)carboxamide	272	Difenpiramide
1,3-oxazole-2-ylamine	4	Ditazol
2-amino-1-phenylethan-1-ol	28	Fepradinol
methanesulfonamide, thiazinecarboxamide	106	Nimesulide, Lexipafant
9-methylenefluorene	3	Paranyline
3,4,5-trihydropyrimidin-2-one	3	Proquazone

Other 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

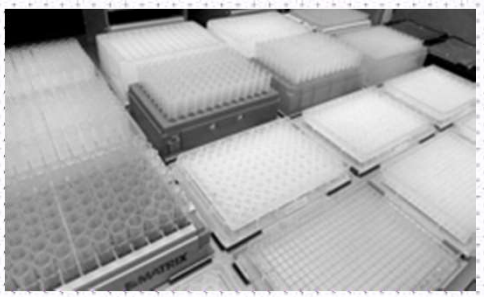
- Price on compound libraries and custom selected collections including cherry-picking would depend on the number of compounds selected and a sample size.
- Custom formatting options are available for all of our libraries. Please refer to the compound management/handling section of this presentation.
- Prices do not include shipping and cost of consumables charge may apply
- Compounds can be delivered in vials, 96 or 384 well plates. We work with custom storage solutions.
- Libraries/databases e-files may exclude most recent updates.
- All compounds we have are stored in dry form and can be freshly prepared in DMSO.
- Purity of compounds in our collections, on average is >/= 95% as determined primarily by high-field 1H-NMR and/or MS. Overall purity is at least 90%.
- Compounds are available for re-supply from stock. Exact amount available for re-supply will be confirmed at the time of re-order.
- Scale up synthesis and re-synthesis services
- TimTec does not hold any IP rights on compounds we sell. Once a hit is identified it is yours for further development.

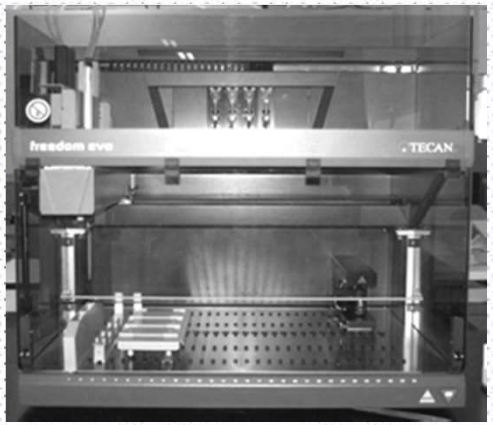
TimTec Services

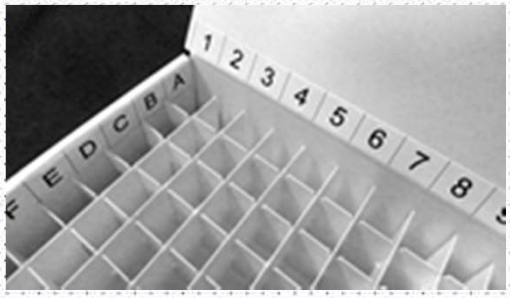
- Sample Management
- Sample Re-formatting/Custom weighing
- Consolidated Compound Procurement
- e-Database management
- Computational Services
- Custom Synthesis
- Analytical

Sample Management Services

- Dry and liquid sample handling
- From small scale to high throughput handling capability
- Fully automated high throughput liquid handling systems
- Organizing and re-formatting of chemical collections according to custom requirements
- Precision weighing and dissolution in fixed or variable solvent volumes in custom vessels
- Preparation of multiple mother and daughter sets
- Replication of 96 and 384 well plates
- Electronic structural records and digital inventory organization
- Barcoding and labeling
- Specialty packaging and dry ice shipments



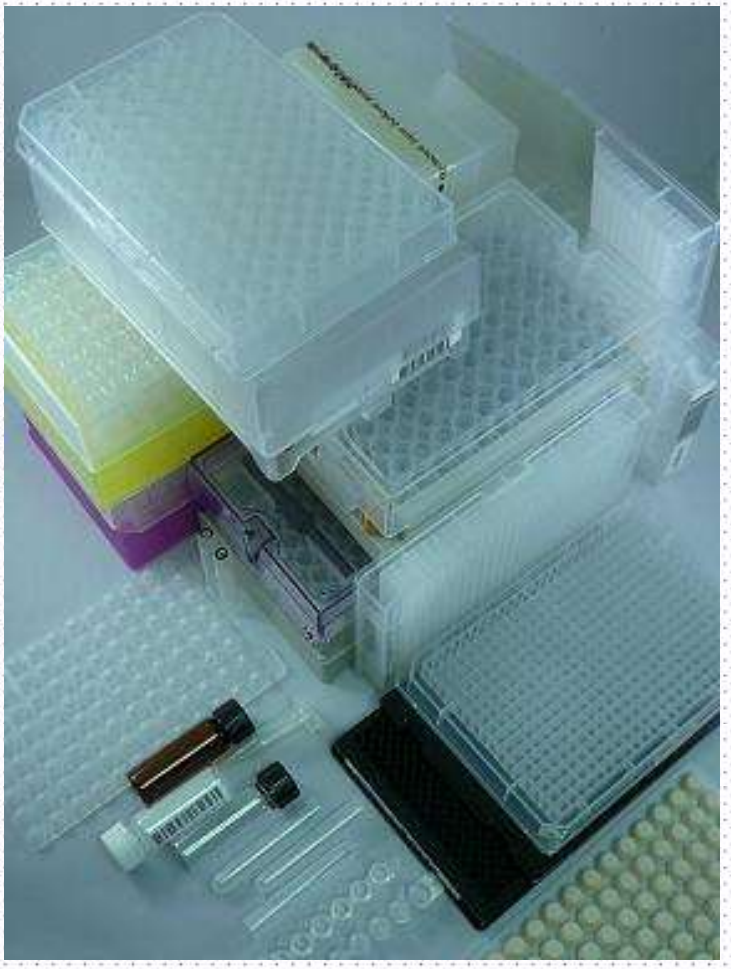




Consolidated Compound Acquisition

- 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

Sample Handling: over 160 inventory storage solutions



TimTec has extensive decades-long experience in compound management being capable of processing thousands of compounds each month while maintaining the highest handling quality standards.

Being a missing formatting intermediary point between you and your collaborators and suppliers we greatly simplify the tedious and time-consuming task of weighing, plating, labeling, and organizing the small and large chemical collections you receive. We take on even the smallest projects freeing you from the need to keep largely unutilized specialty equipment and tools while keeping all your samples in uniform and ready to use format.

Computational Services

- Vendor Database Acquisition and Management (e.g., duplication and availability determination)
- Functional Group and Fragment Filtration
- Lipinski Parameter Assessment
- Library Comparisons (in-house vs. vendor)
- Database Clustering
- Database Comparison and Sorting by Diversity
- Prediction of lipophilicity (LogP and LogD)
- Physical-Chemical prosperities selection and search manipulation

Stay In Touch with TimTec

- For more information please visit our website: www.timtec.net
- Contact: Phone 1-302-292-8500, Fax 1-302-292-8520
- Email: timtec@timtec.net
- You may 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 support@timtec,net or inquire links for download

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