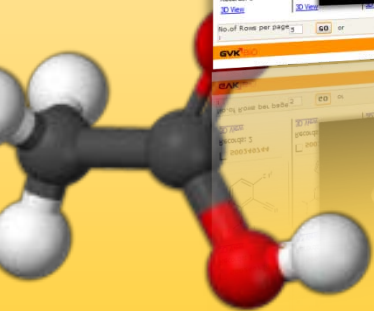


GOSTAR

GVK^{BIO} Online Structure Activity Relationship Database

A Web Based Application with over

- ✓ 5.1 million small molecules
- ✓ 16 million SAR points
- ✓ 6,200 unique targets



Pharmacological
Journals

Patents
(US, WO, EP, GB, JP)

Company web sites,
Conferences

Medicinal Chemistry
Journals



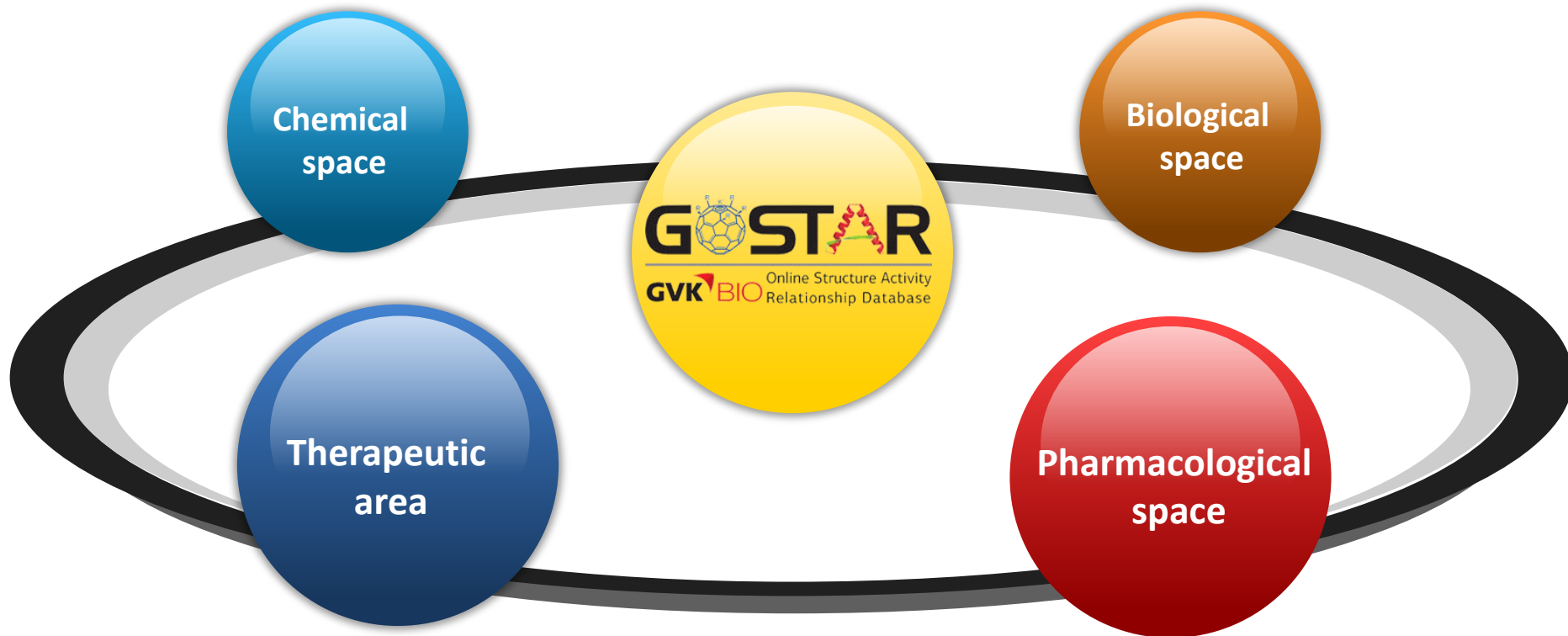
Other web
resources

- ✓ Manual curation with three levels of quality check
- ✓ Standard Ontology for the data fields
- ✓ Regular monthly data updates

More than [15 publications](#), including Drug Discovery Today citing effective utility of [GOSTAR](#) and integrated [databases](#).

Databases Integrated in GOSTAR





- ✓ More than 250 unique data fields
- ✓ Supported by specific reference
- ✓ Links to cross reference- eg. with Pubmed, PDB ID, Entrez ID

Virtual screening
(compound
prioritisation for
screening)

Novelty analysis

Selectivity and
activity
optimisation

Design predictive
models
(QSARs,
pharmacophore
models)



Rapid access to
current
knowledge

Exploration of
chemical &
biological space

Evaluate fast
follower
opportunities
(patent busting)

Avoid redrawing
of
published
structures

GOSTAR Database – User Interface

- User friendly search interface
- Structure and text queries supported
- Try and test queries in every field
- Mine every aspect of the database
- Explore the data with Tree view and other user friendly views
- Search the data using SDF, SMILES or SMARTS.
- Search Bibliography and Advance search using logical operators
- Export the data in formats like SDF, RDF, XML, CSV and Excel

Best Viewed in Internet Explorer version 7.0 and above. [Help](#) [Feedback](#) [Support](#) [Contact Us](#)

GOSTAR
Online Structure Activity
Relationship Database

Search for with value

Welcome, Guest **You are in Search mode** | [Search](#) | [Advanced Search](#) | [My Saved Query](#) | [My Account](#) | [Logout](#) |

Structure ▶

OR Enter SMILES/SMARTS
Compound Name CAS No

Activity ▶

Protein
Source

Activity Type Units Activity Value to:

Bibliography ▶

Patent No PUBMED ID
Keywords Substance
Company name(Reference)

Compound Status ▶

Database Selection ? ▶

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GOSTAR Database – Results Display

Activity Display

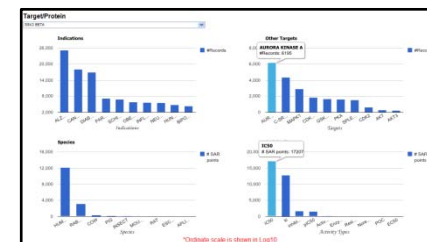
The screenshot shows the GOSTAR Activity Display interface. At the top, it says "Best Viewed in Internet Explorer version 7.0 and above." Below the search bar, it indicates "You are in result mode". The main content is a table of search results. The table has columns for Structure, GVK ID, Protein, Cells, Celline, Organ, Source, Activity Type, and Activity. The first row shows results for GVK ID 2025, with protein PDGFRB and activity > 0.7 uM. The second row shows results for GVK ID 2121, with protein p38 and activity = 2.6 h. The third row shows results for GVK ID 2321, with protein PDGFRB and activity = 0.32 uM. The fourth row shows results for GVK ID 2380, with protein PDGFRB and activity = 0.08 uM. The fifth row shows results for GVK ID 2387, with protein PDGFRB and activity = 0.13 uM. The interface includes navigation options like "Page 1 of 5353" and "Max rows per page: 10".

Structure Display

The screenshot shows the GOSTAR Structure Display interface. At the top, it says "Best Viewed in Internet Explorer version 7.0 and above." Below the search bar, it indicates "You are in result mode". The main content is a grid of chemical structures. Each structure is accompanied by a GVK ID and a "3D View" link. The first row shows structures for GVK IDs 2025, 40, 1380, 1403, 1453, 1454, 1830, and 1892. The second row shows structures for GVK IDs 1993, 6188, 6199, 6204, 6208, 6293, 6294, and 6299. The third row shows structures for GVK IDs 6343, 6381, 6392, 6442, 6447, 6454, 6464, and 6484. The fourth row shows structures for GVK IDs 6507, 6530, 6536, 6552, 6555, 6620, 6628, and 6662. The fifth row shows structures for GVK IDs 6663, 6664, 6667, 6670, 6676, 6686, 6713, and 6735. The interface includes navigation options like "Page 1 of 673" and "No. of Rows per page: 5".

Easy to Explore with

- Customized views
 - ❖ Chemistry
 - ❖ Biology
- List Views
 - ❖ Indication
 - ❖ Target
 - ❖ Assay Method
 - ❖ Reference
- Database Summary
- Result Over view



Analyzer	Utility
Activity Analyzer	Sorting Molecules based on Activity Value(uM)
Heat Map	Understanding the off target Activity
Property Space	Analyze the Physico Chemical Properties and sort based on the properties
Scatter Plots	To find the interesting & Relevant data in the Results
MCSS	To compute the maximum common sub structure with activity range from the Results
LE vs LLE	To identify the molecule to Fragment based drug design and Early hit compound analysis
Molecular Pairs	Helps in identifying the molecular pairs which are similar and different in Activity

Clustering - MCSS

Target List: EGFR Unique Structures: 3656
 Activity Source: HUMAN Please select a level: Level5
 Activity Type: IC50/pIC50
 Activity Profile: Any
 Generate MCSS

MCSS for Level: 5	< 0.1uM	0.1uM to 1uM	1uM to 10uM	10uM to 100uM	100uM to 1000uM	1uM to 10uM	10uM to 100uM	100uM to 1000uM
1.1.1.1.1			1	20	10			
1.1.1.1.2			2	14	11			
1.1.1.1.3			4	15	2			
1.1.1.2.1		1	14	21	1			
1.1.1.2.2		1	3	9	1			
1.1.2.1.1			2	2				
1.1.2.1.2	0	15	9	2				
1.1.2.2.1		1	1					
1.1.2.2.2		1	1					
1.1.2.2.3			1	1				
1.1.2.2.4	2		2					
1.2.1.1.1				2				
1.2.1.1.2				2	3			
1.2.1.2.1								
1.2.1.2.2		3	56	22	4			
1.2.1.2.3				6	8			
1.2.1.3.1	4	5						
1.2.1.3.2	2	2	1					
1.2.1.4.1		1	2	2				
1.2.1.4.2			2	5	19			
1.2.1.4.3	22	116	93	57	36			
1.2.1.4.4				5	1			

Molecular Pairs

Molecular Similarity vs. Activity Difference

Total Unique Molecules for the search criteria: 1000 Total Molecules plotted in the graph: 830
 Minimum -log Activity values: 0.30 Activity Difference: 1.30 Refresh

Molecular Similarity in a Pair vs. Activity Difference (Log Value)

Activity Difference (-Log Value) vs. Molecular Similarity in a Pair

Similarity vs. Activities
 More data values on plot in logarithmic scale

➤ **Marvin Sketch**

- ❖ Drawing & Capturing Chemical Structures

➤ **MolConverter**

- ❖ To convert chemical structure between different chemical formats.
- ❖ To search with SD file

➤ **JChem Cartridge**

- ❖ Structure Search like Sub Structure Search, % Similarity & Exact
- ❖ Tanimoto similarity used in generating **Molecular pairs**

➤ **Library MCS API**

- ❖ To compute the **maximum common sub structure** with activity range from the Results

Few more

Name to Structure, JChem Base, Calculator Plugins, Chemical Workflow Tools, Standardizer

Exploring

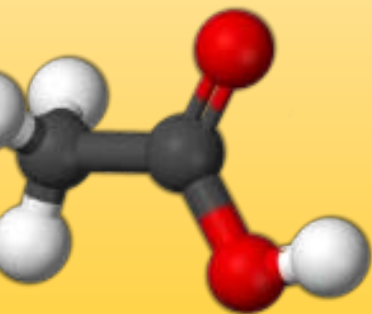
Instant Jchem, JChem Web Services Add-on, Structure Checker, Screen, Reactor, Fragmenter



GVK **BIO** Online Structure Activity
Relationship Database

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