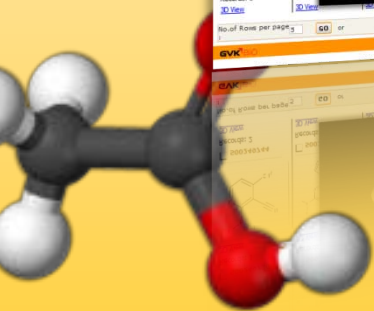


# GOSTAR

GVK<sup>BIO</sup> 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



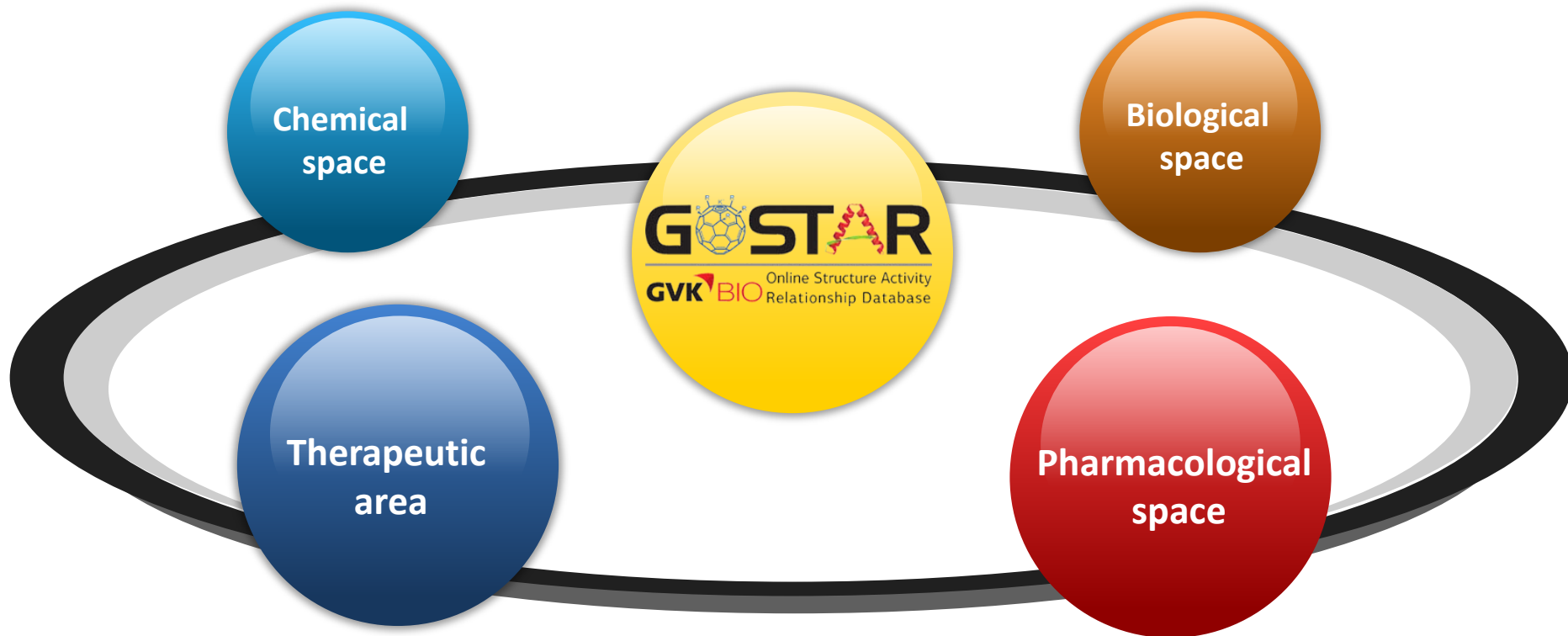
Other web  
resources

- ✓ 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** ? ▶

GVK<sup>1</sup>BIO Terms of Use | Privacy Policy © 2009 GVK Biosciences.



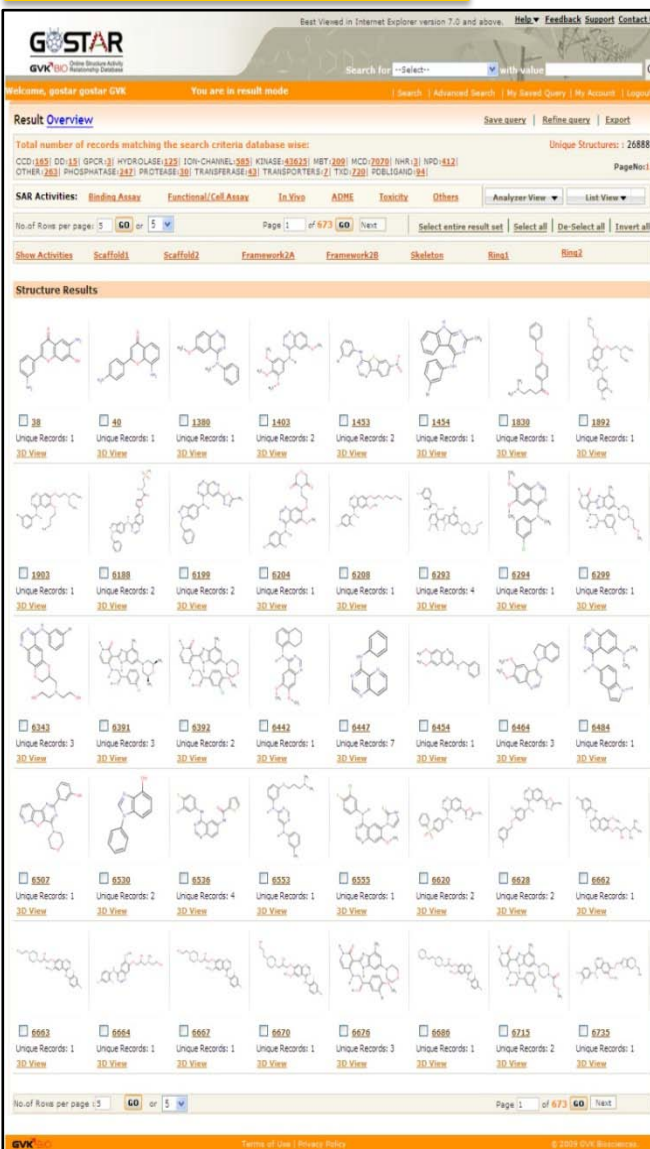
# GOSTAR Database – Results Display

## 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, there are navigation links: "Home, gostar, gostar GVK". The main content area is titled "Result Overview" and shows "Total Unique Records: 46914". Below this, there are filters for SAR Activities: "Binding Assay", "Functional/Cell Assay", "In Vivo", "ADME", "Toxicity", and "Others". The interface includes a table with columns for Structure, GVK ID, Protein, Cells, Cellline, Organ, Source, Activity Type, and Activity. The table is currently displaying results for GVK ID 2025, 2121, 2321, 2380, and 2352. At the bottom, there are pagination controls: "Page 1 of 5353" and "Max rows per page: 10 or 15".

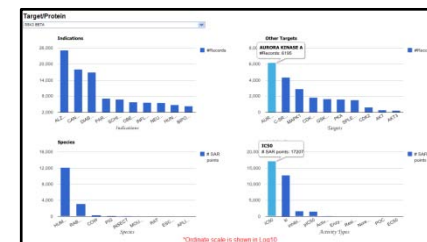
## Structure Display



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, there are navigation links: "Home, gostar, gostar GVK". The main content area is titled "Result Overview" and shows "Total number of records matching the search criteria database wise: Unique Structures: 26888". Below this, there are filters for SAR Activities: "Binding Assay", "Functional/Cell Assay", "In Vivo", "ADME", "Toxicity", and "Others". The interface displays a grid of chemical structures, each with a GVK ID and a "3D View" link. The structures are arranged in rows and columns, with each cell containing a chemical structure and its corresponding GVK ID. At the bottom, there are pagination controls: "Page 1 of 673" and "No. of Rows per page: 5 or 10".

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  
 Activity Source: HUMAN  
 Activity Type: IC50/pIC50  
 Activity Profile: Any  
 Unique Structures: 3656  
 Please select a level: Level 5  
 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	
1.1.1.2.1			1		14		21	
1.1.1.2.2			1		3		9	
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  
 Publish

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

Activity Difference (-Log Value)

Molecular Similarity in a Pair

Similarity vs. Activities  
 More Molecules plotted together: on



## ➤ 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

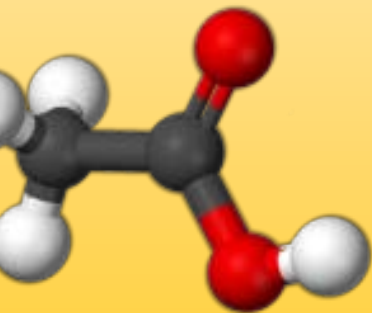
Instant Jchem, JChem Web Services Add-on, Structure Checker, Screen, Reactor, Fragmenter



**GVK** **BIO** Online Structure Activity  
Relationship Database

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