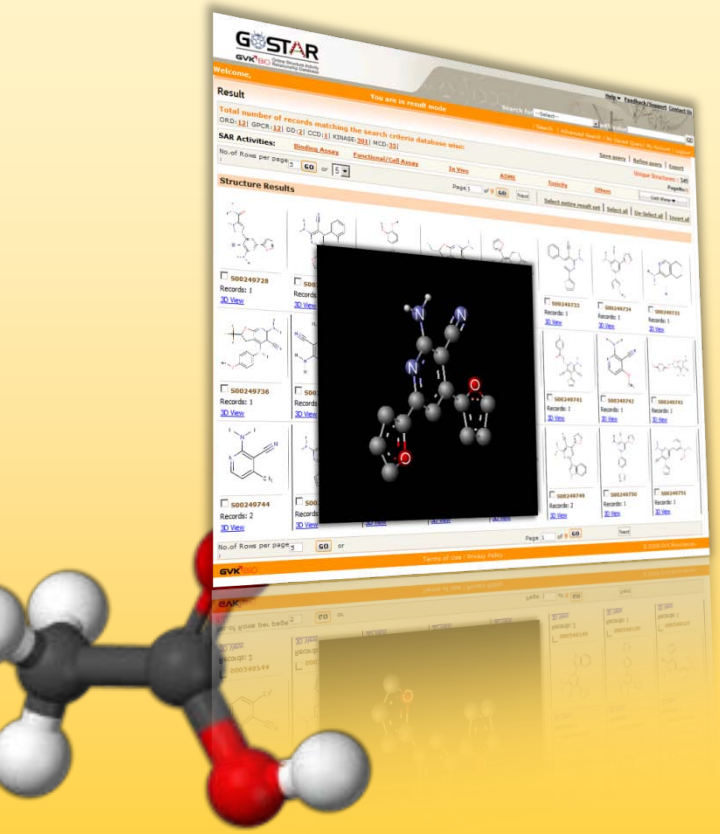


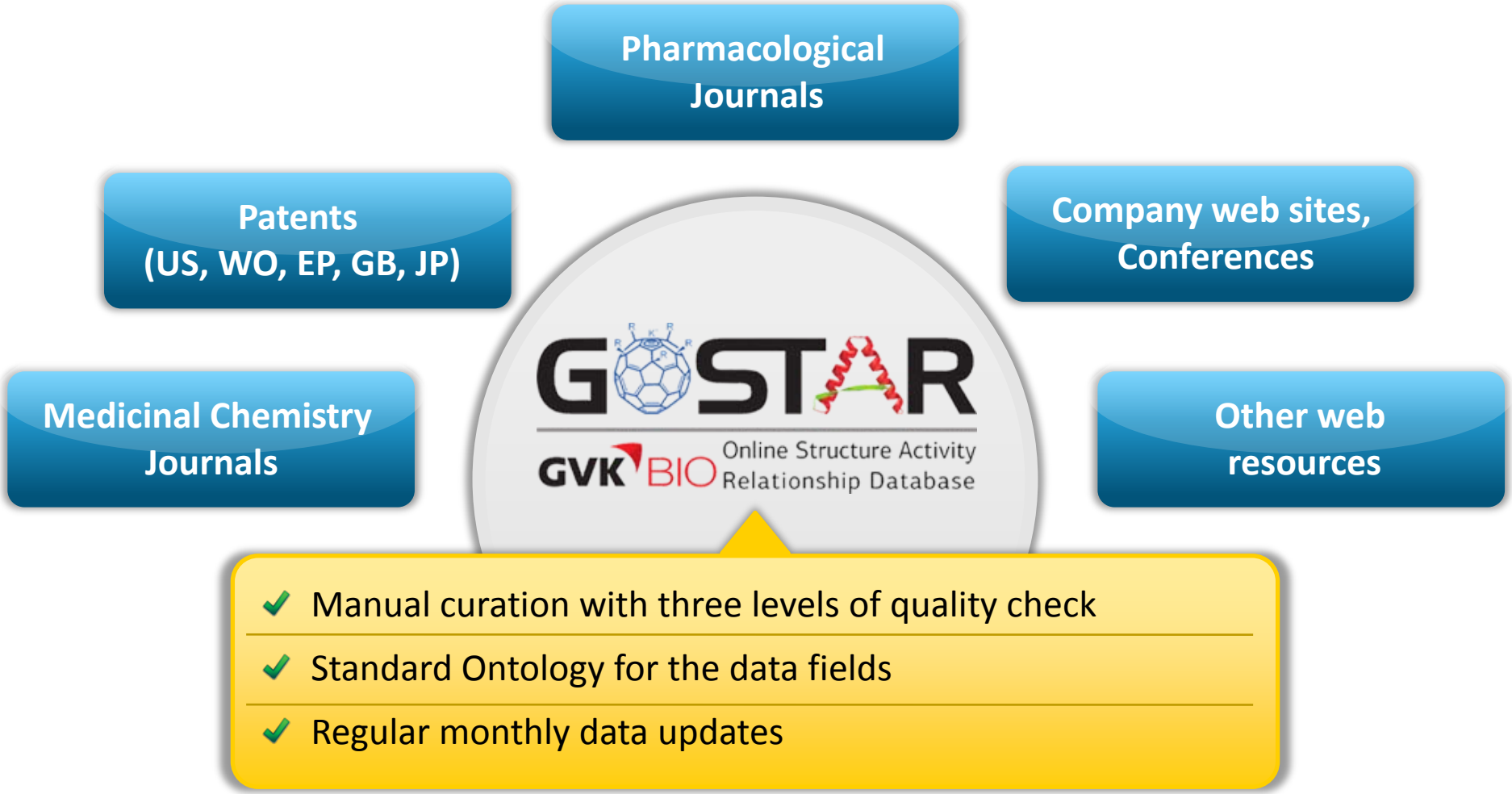
GOSTAR

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

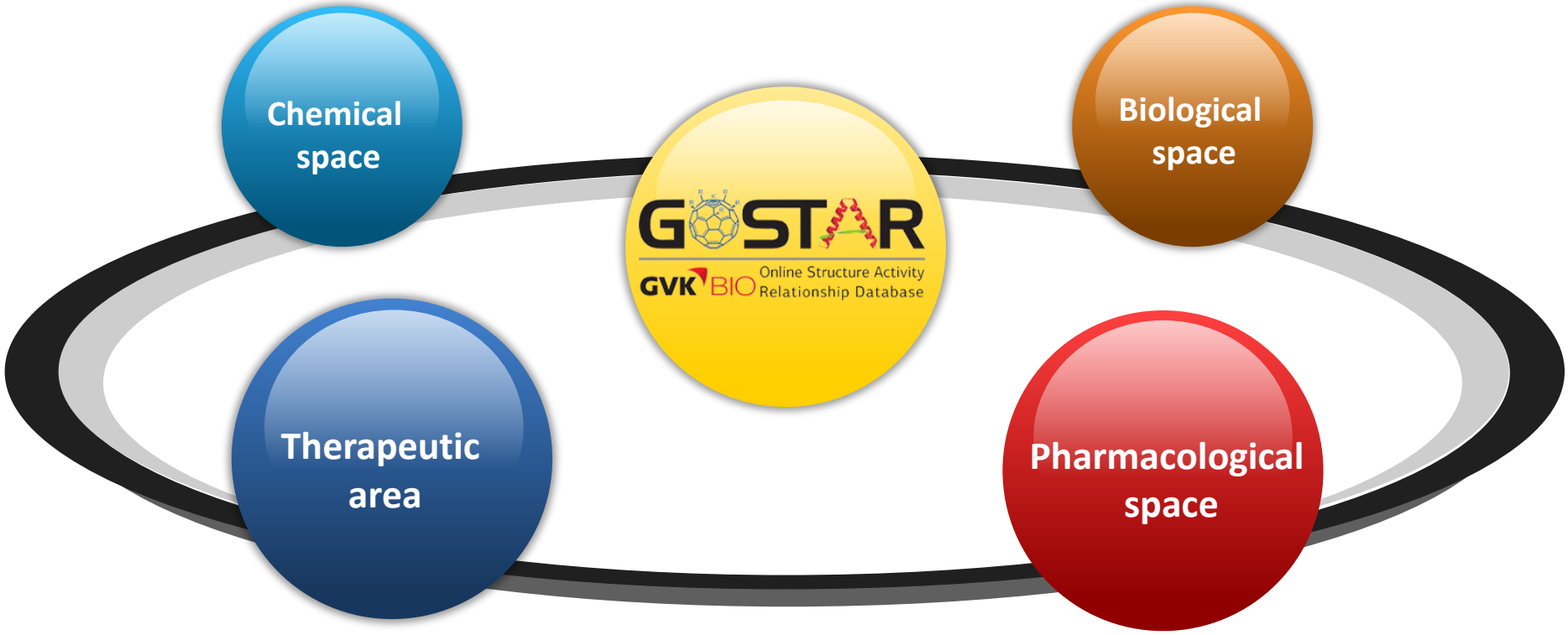
Data Sources



More than 15 publications, including Drug Discovery Today citing effective utility of GOSTAR and integrated databases.

Databases Integrated in GOSTAR

Data Content



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

GOSTAR Database Utility

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

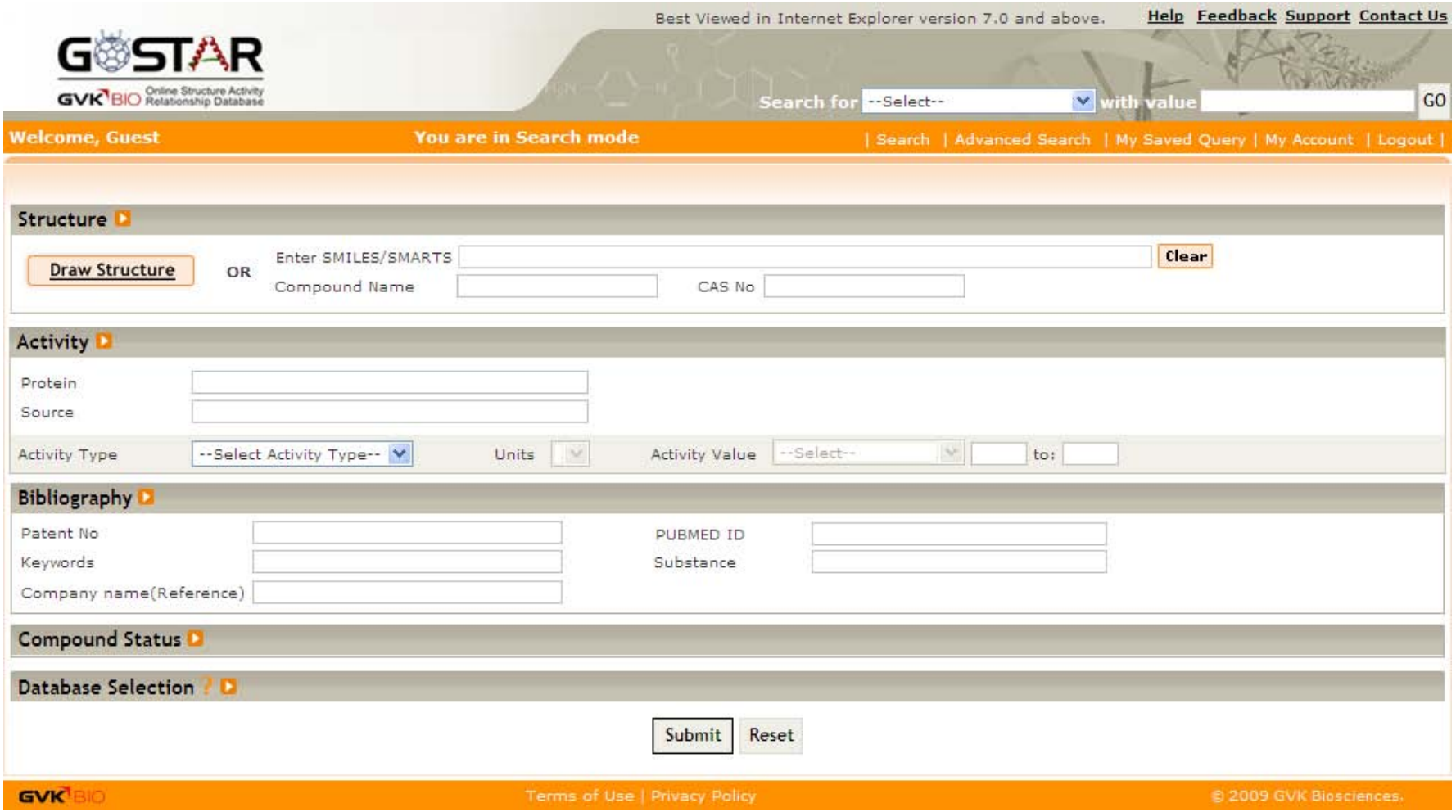
Evaluate fast follower opportunities (patent busting)

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

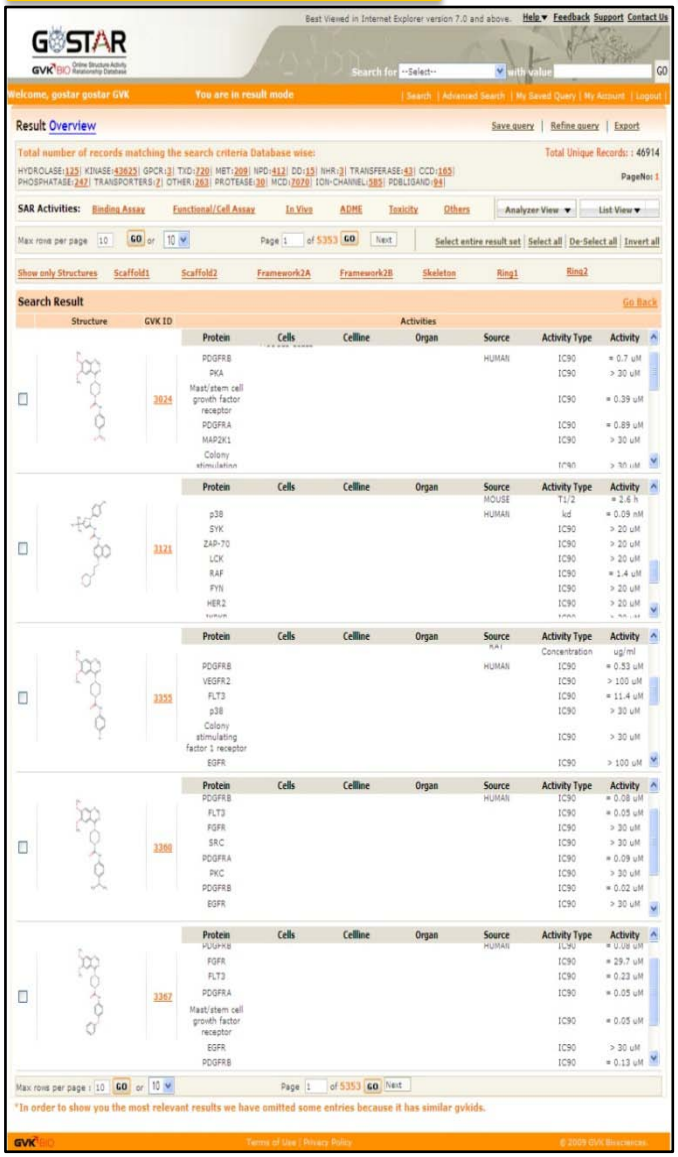
- Explore the data with Tree view and other user friendly views
- Search the data using SDF, SMILES or SMARTS.
- Search Bibliography and Advance search using logical operators
- Export the data in formats like SDF, RDF, XML, CSV and Excel



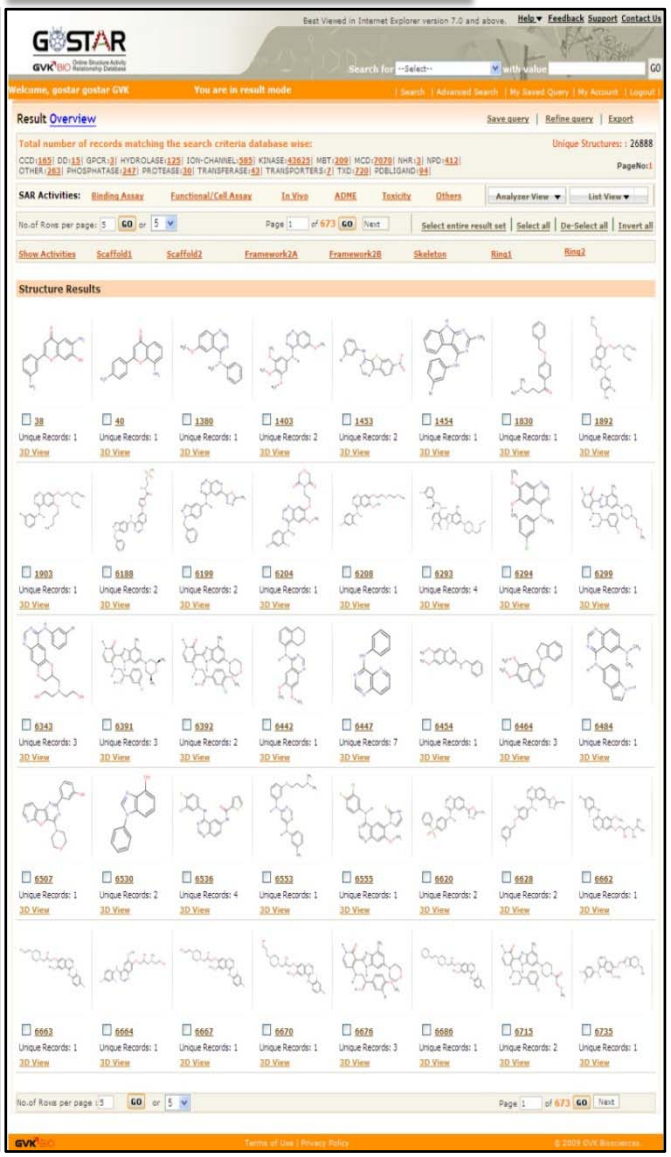
GOSTAR Database – Results Display

GOSTAR Online Structure Activity Relationship Database

Activity Display

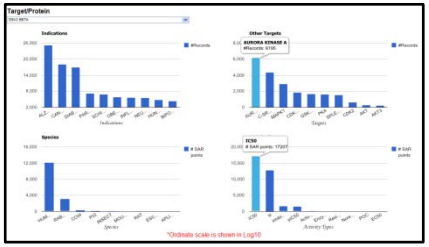


Structure Display



Easy to Explore with

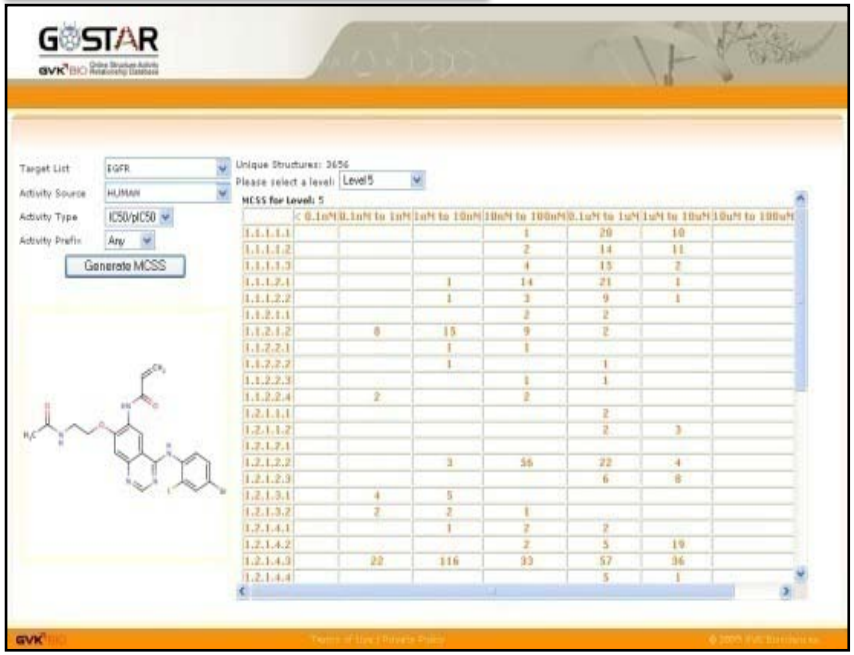
- Customized views
  - Chemistry
  - Biology
- List Views
  - Indication
  - Target
  - Assay Method
  - Reference
- Database Summary
- Result Over view



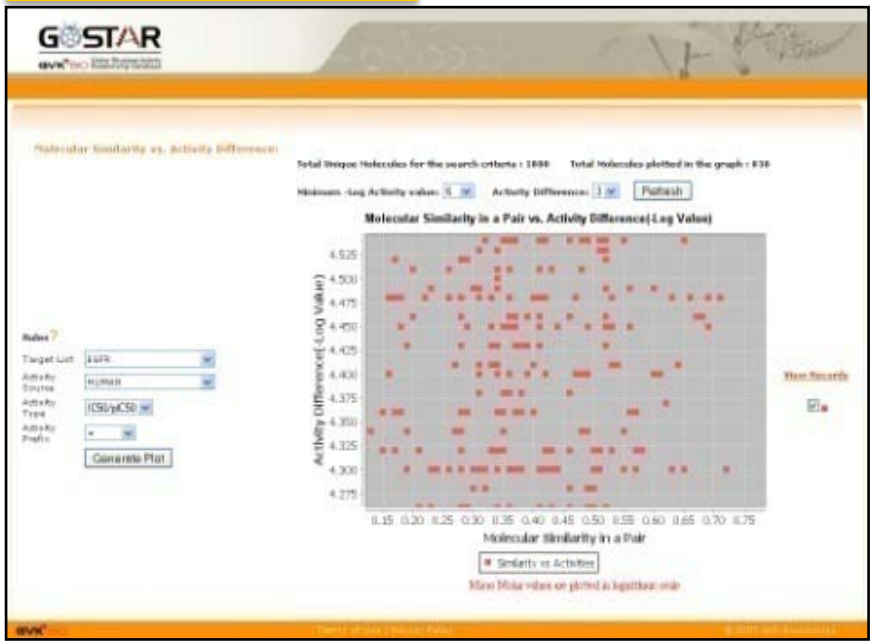
GOSTAR Database – Data Analyzers

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



Molecular Pairs



GOSTAR Database – ChemAxon

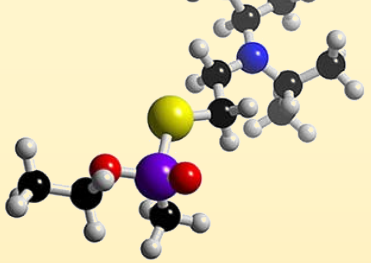
- **Marvin Sketch**
  - Drawing & Capturing Chemical Structures
- **MolConverter**
  - To convert chemical structure between different chemical formats.
  - To search with SD file
- **JChem Cartridge**
  - Structure Search like Sub Structure Search, % Similarity & Exact
  - Tanimoto similarity used in 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

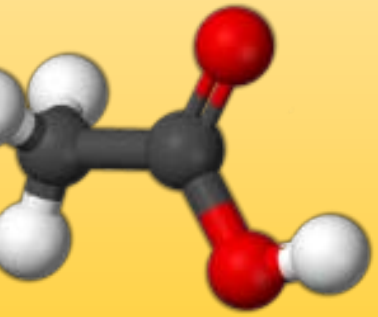


GOSTAR

GVK BIO Online Structure Activity Relationship Database

www.gostardb.com

bdinf@gvkbio.com



Corporate Office - India

GVK Biosciences Private Limited

Plot No. 28 A, IDA Nacharam

Hyderabad – 500076, India

Tel : +91 40 66929999

Mobile: +91 897 860 2727

Fax : +91 40 66929900

US Office

GVK Biosciences Private Limited

5457 Twin Knolls Road, Suite 101

Columbia, MD 21045

Tel: +1 443 838 6260

Fax: (703) 940 4088

www.gvkbio.com