

Make the right decisions
with data you can trust



AURELIS SCIENCES



**Make the right
decisions with data
you can trust**

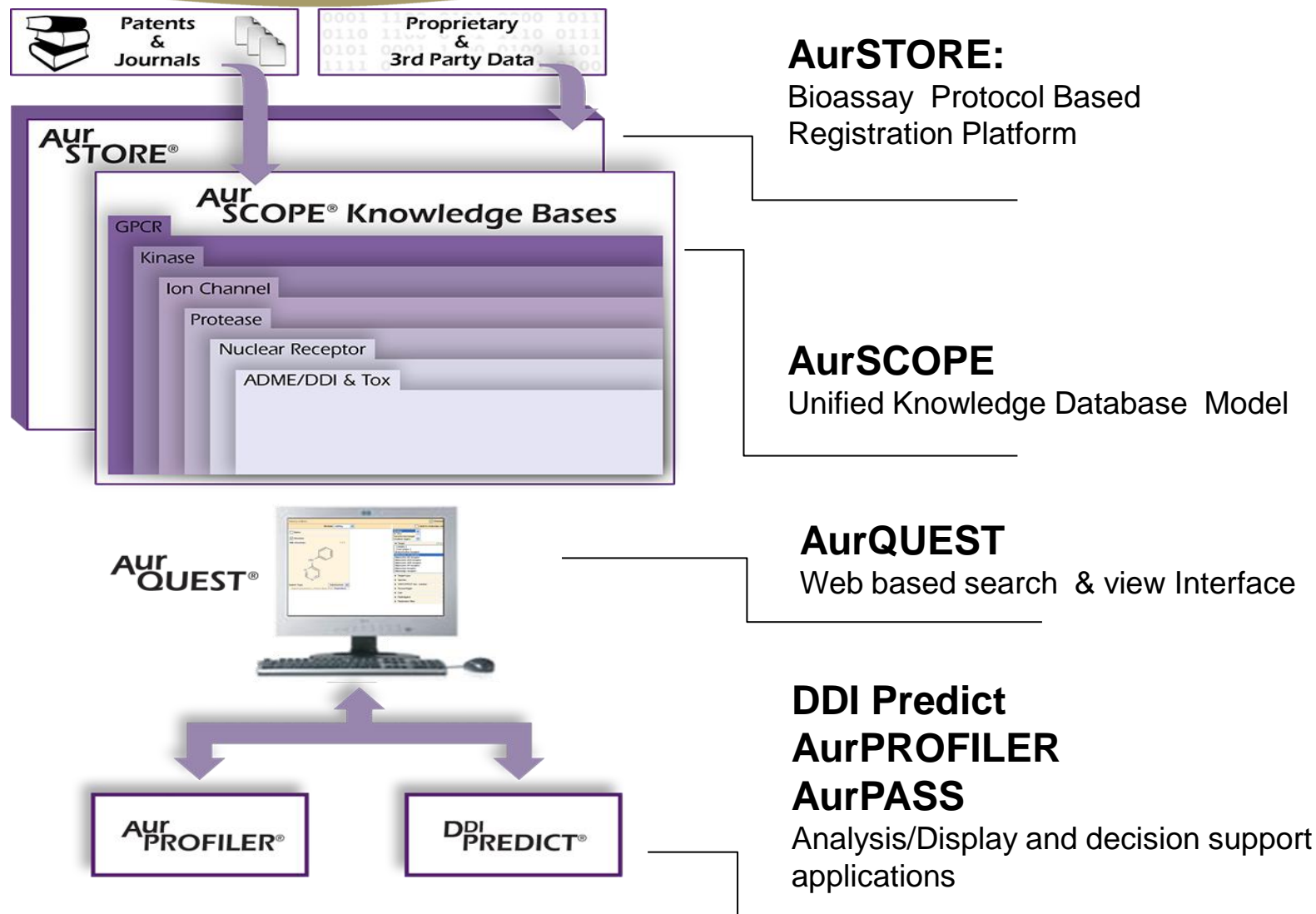


ChemAxon

**Toolkits and desktop
applications for
cheminformatics**

European User Group Meeting
May 16-19, 2011

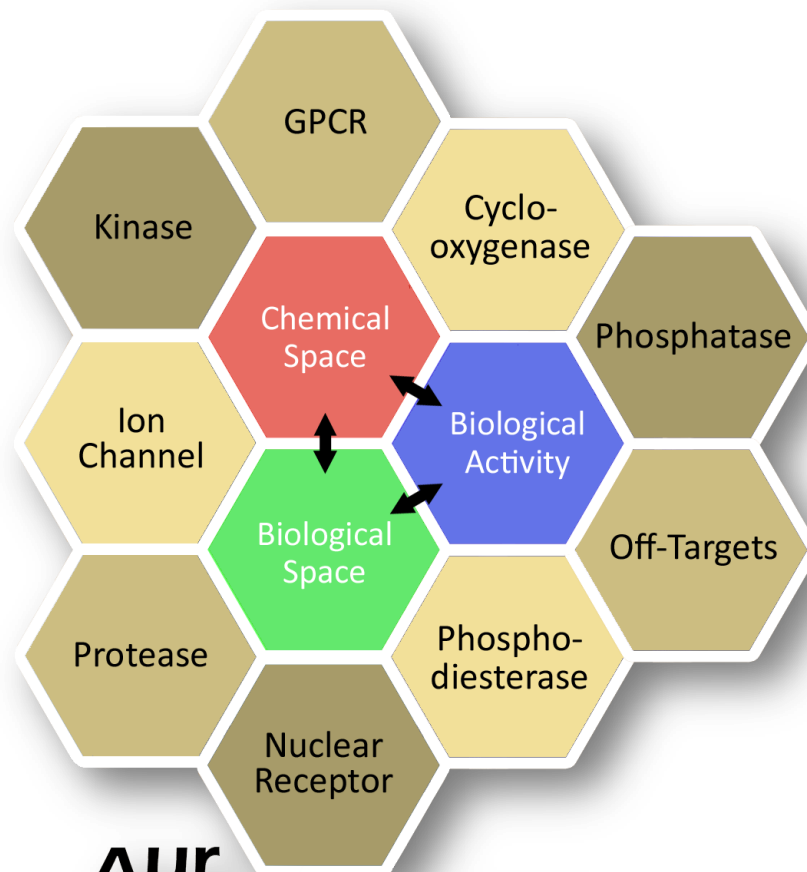
Generating & Organizing Data into Knowledge



10 years Of High Quality Development

Aureus Global Pharmacology Space

| | |
|------------------|------------------------------|
| 63 897 | Publications |
| 3 208 102 | Biological Activities |
| 795 908 | Chemical Ligands |
| 2 248 | Unique Targets |
| 1 626 | Human Targets |
| 115 | Therapeutic Classes |

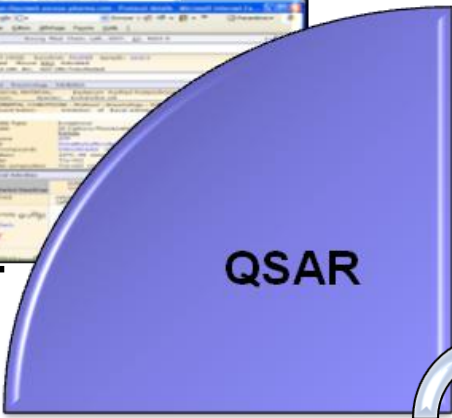


Aur
SCOPE® GPS
Global Pharmacological Space

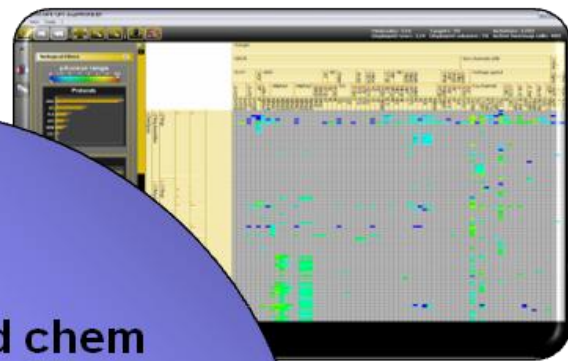
Make The Right Decision With Data You Can Trust



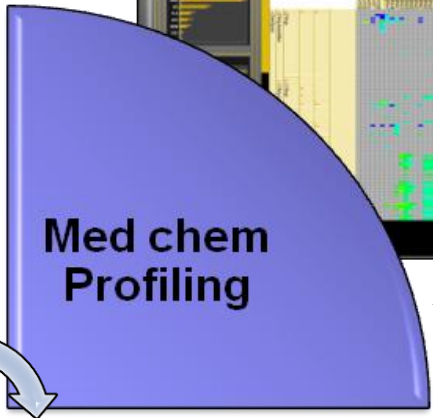
AurQUEST
Data mining



QSAR



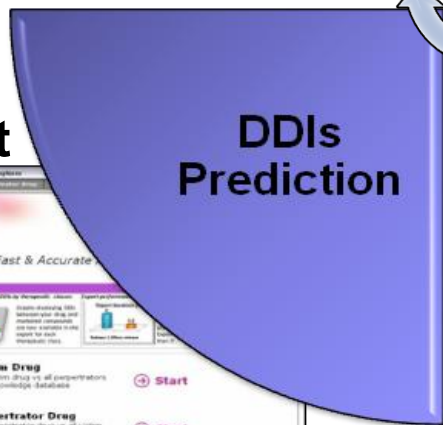
AurPROFILER
Data analysis & Navigation
Medicinal Chemistry Space



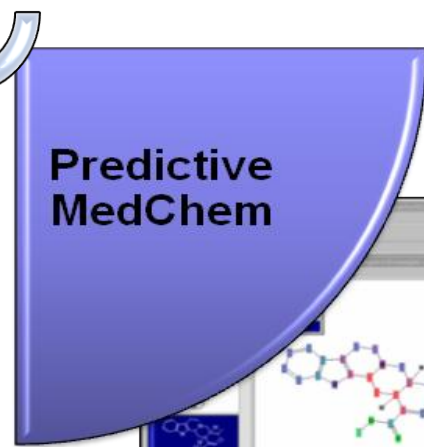
Med chem
Profiling



DDI Predict

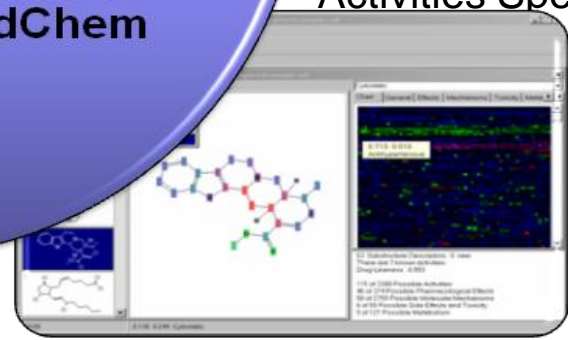


DDIs
Prediction



Predictive
MedChem

AurPASS
Predict Biological
Activities Spectra

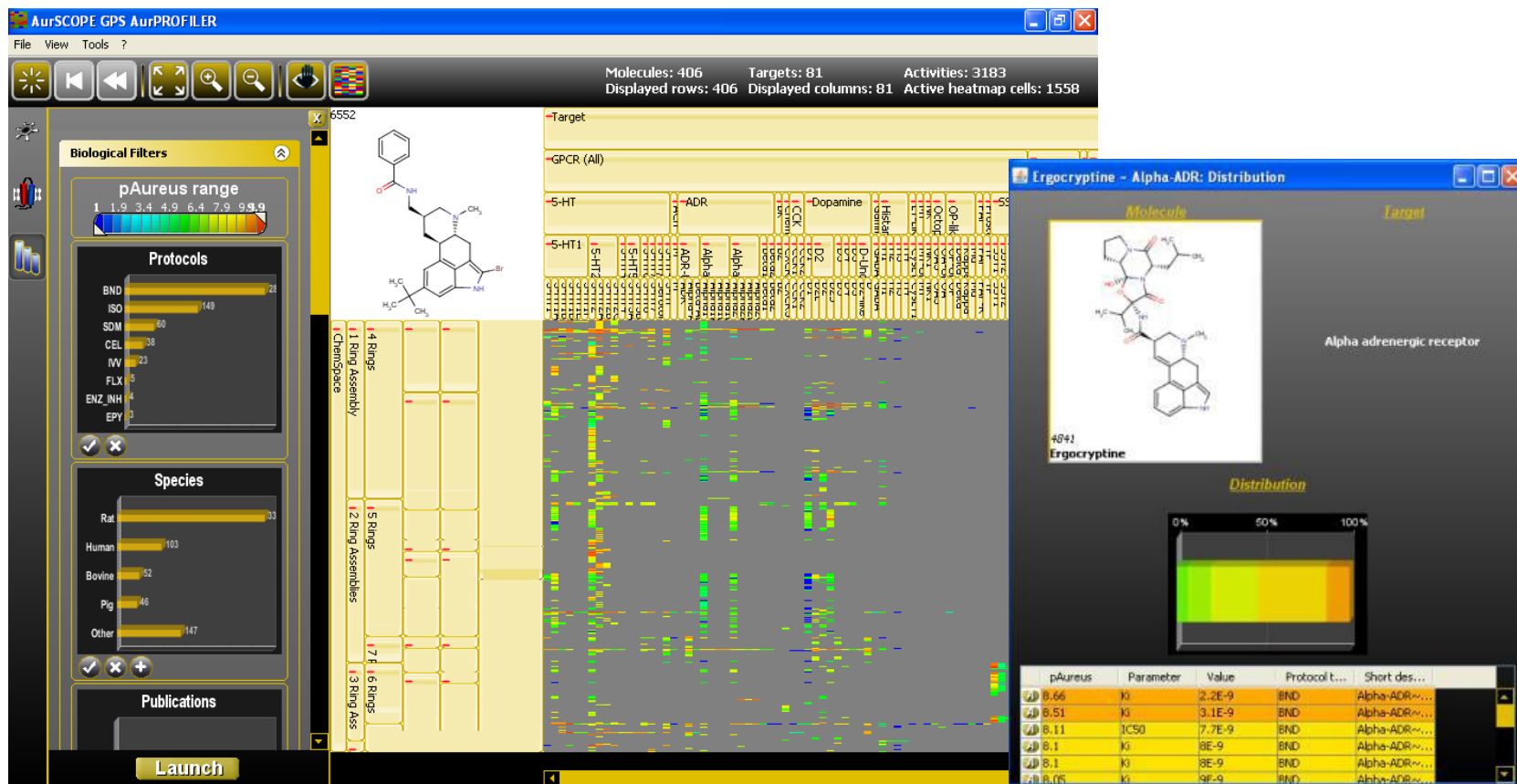




Aureus Products and Solutions

AurPROFILER

- Pharmacological Space Target Profiling & Alerting
 - New insights into target selectivity
 - Learn off-target effects
 - Target associated chemical space



Integrating ChemAxon® Technology in AurPROFILER

- Chemical Similarity
- Pharmacophoric Similarity
- Descriptors Based Similarity



ChemAxon



JChem Base



Calculator



Screen

AurPROFILER – Chemical Similarity Search

Molecules: 196 Targets: 89 Activities: 1368
 Displayed rows: 196 Displayed columns: 89 Active heatmap cells: 423

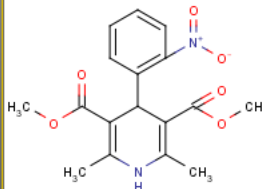


1. INPUT

Name | **Structure** | **Smiles**

nifedipine

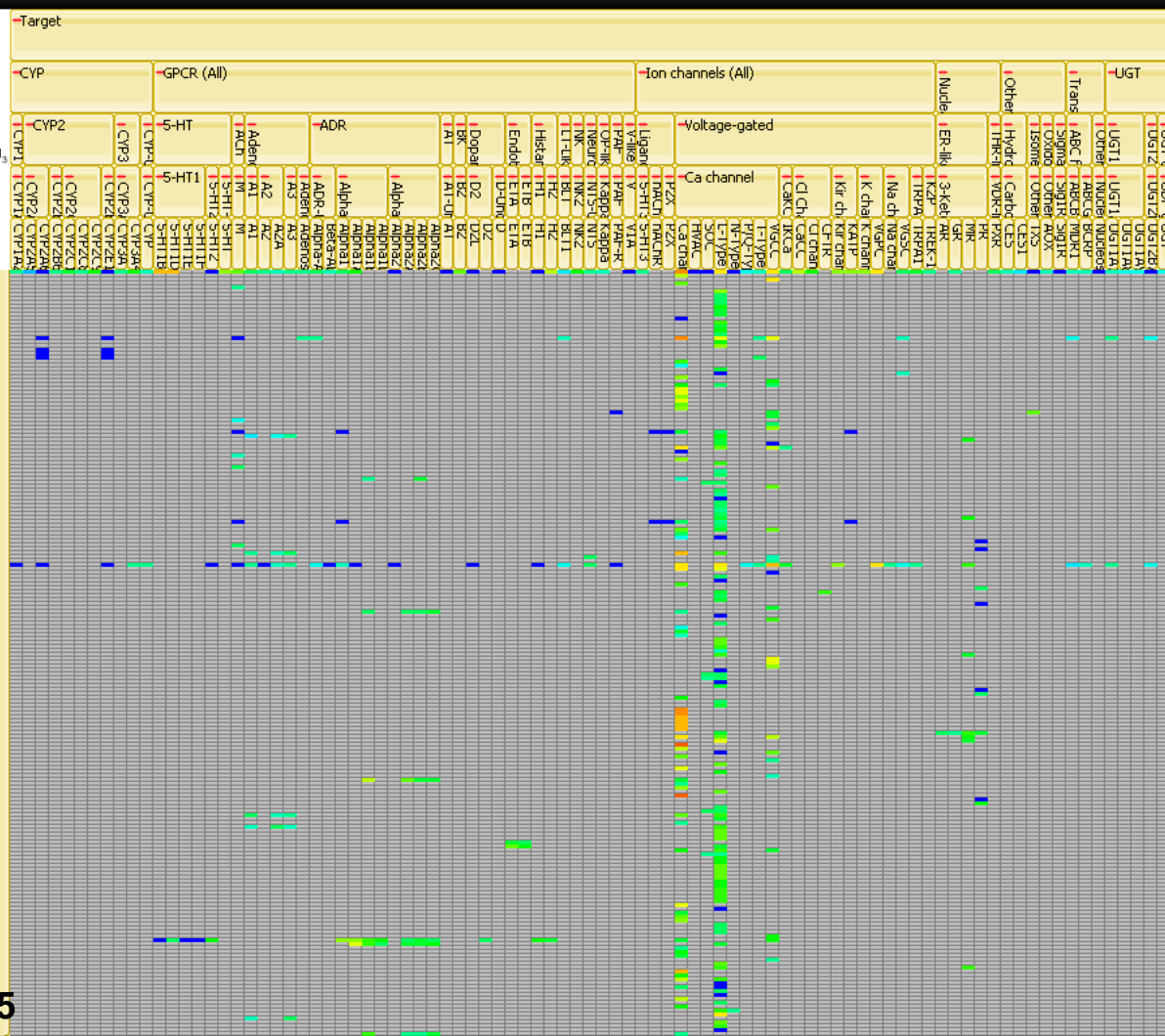
| Name | Synonyms |
|----------------------|----------------------|
| Denitronifedipine | |
| m-Nifedipine | BAY-a 4339 |
| Nifedipine | Niphedipine; Proc... |
| Nifedipine hydroc... | |
| Oxidized Nifedipine | B 4759; BAY-b 4... |



Molecule

SI 1.0

SI 0.75



2. SEARCH METHOD

Powered by ChemAxon's JChem Base

- Substructure
- Exact
- Chemical Similarity
- 2D pharmacophoric Similarity

Similarity threshold:

3. DIMENSION

Target

4. DISPLAYED CHEMSPACE

SI based view

Launch

Aureus Future Directions

- Deliver Additional Knowledge Databases In An Extended Pharmacological Space
- Deliver Additional Drug Safety Databases and Systems
- Develop New Decision Making Applications Improving Access to Data, Profiling and Risk Assessment
- Leverage European Funded Projects Involving our *Partners* and pharma Players

*Thank you for your
attention*



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