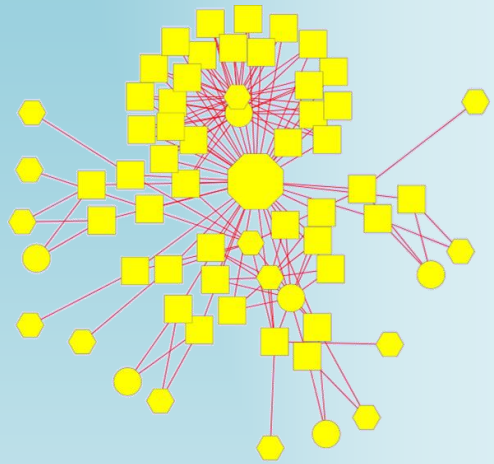
CARLSBAD is a database and knowledge inference system that integrates multiple bioactivity datasets in order to provide researchers with novel capabilities for the mining and exploration of available structure activity relationships (SAR) throughout chemical biology space.



The CARLSBAD platform is offered **FREE** for academic and non-commercial use and will help facilitate researchers performing complex tasks in drug and probe discovery such as:

- Drug Rescue and Repurposing
- Compound Bioactivity Hypotheses
- Mode of Action Identification
- On- and Off-Target Interactions
- And More

To apply for CARLSBAD user group membership and to learn more about this exciting platform, please visit **carlsbad.health.unm.edu.**

The CARLSBAD plugin is available for installation from Cytoscape, which can be downloaded at **www.cytoscape.org**.

To apply for CARLSBAD user group membership, obtain system access, reference the CARLSBAD manual and learn more about UNM's Division of Biocomputing, please visit **carlsbad.health.unm.edu**.

For more questions, please email us at **info-carlsbad@poblano.health.unm.edu**.

CARLSBAD was developed at the UNM's Division of Biocomputing by Tudor Oprea, Cristian Bologa, Stephen Mathias, Oleg Ursu, Jeremy Yang, Gergely Zahoranszky-Kohalmi, Jerome Abear and Jarrett Hines-Kay.

Funded by NIH grant GM095952.

UNM

University of New Mexico School of Medicine
Division of Biocomputing
RIB 170, MSC11 6145
2203 Frontier, Albuquerque, NM, 87131
Phone: 505-272-0238

info-carlsbad@poblano.health.unm.edu

CARLSBAD

The Power to Explore Biological Networks via Chemical Patterns

A new system from the University of New Mexico's Division of Biocomputing

CARLSBAD

Confederated Annotated Research Libraries of Small-molecule Biological Activity Data

Now with 1.4 million bioactivities

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CARLSBAD Platform

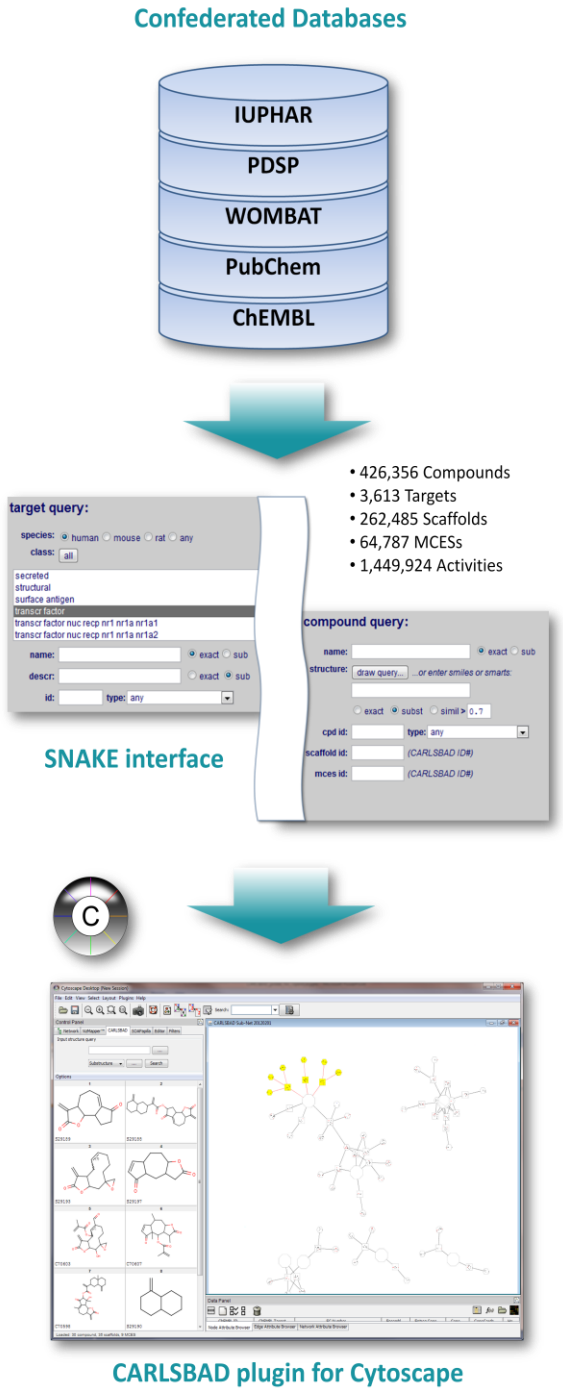
The CARLSBAD platform consists of a web-based extraction tool , **SNAKE**, and a network analysis plugin for Cytoscape, called **CARLSBAD**.

SNAKE

SNAKE (SubNet Application, Kit and Extractor) is a web-based tool that supports target or compound based queries. After performing a query SNAKE delivers target results for the network, an option to view the network with **Cytoscape Web,** as well as the ability to download a network file that can be imported into Cytoscape for advanced network analytics using our customized plugin.

CARLSBAD Plugin

Cytoscape is an open source bioinformatics software platform that CARLSBAD is able to utilize, via the plugin, for powerful network visualization. Combining these capabilities with CARLSBAD's cheminformatics and pattern recognition algorithms, researchers can generate multiple hypotheses concerning the relationship between biological targets, chemical compounds and their common chemical patterns (CCPs).



Features

- Bioactivity networks can be extracted via target-based or ligand-based queries.
- Targets can be queried by common target identifiers (NCBI GI, UniProt, etc.), by target class as defined in ChEMBL, and by species.
- Structures and chemical patterns can be queried by providing SMILES/SMARTS or by using the structure drawing applet.
- Standardized, single bioactivity values are provided for a given compound-target interaction as the negative logarithm of a molar concentration of EC_{50},IC_{50}, K_i, etc.
- CARLSBAD contains common chemical patterns (CCPs), i.e., hierarchical scaffolds (HierS) and maximal common edge subgraphs (MCES), for over 425,000 compounds (substances of interactions translated into unique structures).
- CARLSBAD enables researchers to infer novel chemical-biological associations using biological network visualization tools, as provided in the Cytoscape environment .