

Chem Biography Fact Sheet

Overview

We are pleased to introduce Chem Biography, a full-featured discovery research informatics solution designed for both commercial and academic organizations. If your organization is engaged in research and you have contemplated improving the management of your data in order to facilitate your discovery efforts, Chem Biography represents an ideal solution. We are a particularly attractive option for University labs and biotech startups. Our platform provides four principal components:

- Chemical registry system
- Biological records database
- Web based search and query engine
- Simple to use administrative interface

Chemical Registry

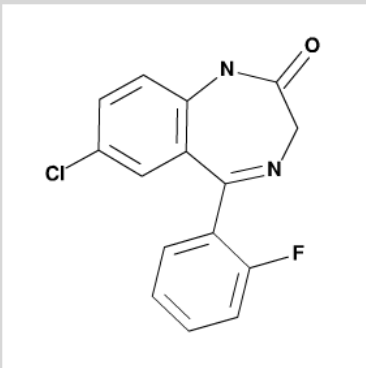
The chemical registry system provided by Chem Biography is designed to be both state of the art and highly customizable to fit the organization's specific needs. Data corresponding to a given molecule are entered via a web based interface (local to computer or organization's intranet) and submitted. The Chem Biography software

automatically calculates molecular weight, formula, chirality, and SMILES string properties and checks the database for existing entries with the same

➤ The ability to easily and rapidly upload associated analytical data (e.g. NMR or LCMS spectra files). Data are uploaded via the web page, stored in the

Chem Biography Chemical Registry

main | search | registry | help | signed in: jmedchem



Registry ID: AB000028-002

date	mol wt	formula	chirality	SMILES
2009-06-16	288.706	Cl ₁ F ₁ O ₁ N ₂ C ₁₅ H ₁₀		Clc1ccc2NC(CN=C(c2c1)c3ccccc3F)=O
origin	chemist	notebook	batch	salt form
Internal synthesis	John Medchem	JM-2009-002	101-202	A: HCL
amount available	program	percent purity	elemental analysis	melting point
200mg	Purine_inhib	95-100	yes	no
NMR data	LC_MS ID	LC_MS purity	comment	
no	no	no	benzodiazepine	

Datafiles: NMR datafile LC_MS ID doc LC_MS purity doc

structure. A new registry ID or version/batch ID is assigned based on the uniqueness of the structure and the configuration specified by the user. Two important features of the chemical registration system are:

➤ A robust yet facile to use java based drawing tool for inputting structures. The tool includes ring templates, chain drawing, and a full range of atom types. It satisfies all the needs of a medicinal chemist.

database for retrieval at any time, and are immediately accessible via hypertext links from the Chem Biography web pages.

Biological Records Management

The Chem Biography biological data records management system allows for consolidation of disparate biological data into a unified and readily searchable database. Data are uploaded directly via Excel XLS or CSV format files; or alternatively, read from a LIMS system output directory. Once biological results are posted for a set of molecules, they are immediately merged with the corresponding chemical data for those molecules. Important aspects of the biological data management tool are:

➤ The database is readily configurable to handle result sets different experiment types - enzyme assays, cellular screens, PK analysis, in vivo data

Chem Biography Main Menu

main | search | registry | help | signed in: gbiologist

Chem Biography Functions	Quick data searches by date	Recently posted data
Database Search	past <input type="text" value="2"/> days: chemical registry	2009-6-18 : bio_ic50 : gbiologist : bRAF_enzyme_20090505.csv
Chemical Registry	past <input type="text" value="2"/> days: cell 1shot	2009-6-16 : cell_1shot : gbiologist : HUVEC_1shots_20090505.csv
Post Biological Results	past <input type="text" value="2"/> days: cell ic50	2009-6-12 : cell_ic50 : gbiologist : pERK_imaging_20090505.csv
Raw Data Links	past <input type="text" value="2"/> days: bio 1shot	2009-6-12 : cell_ic50 : gbiologist : PC3_proliferation_20090505.csv
	past <input type="text" value="2"/> days: bio ic50	2009-6-12 : cell_ic50 : gbiologist : HT29_proliferation_20090505.csv
	past <input type="text" value="2"/> days: PK data	



➤ Associated visual data, e.g. gel images, graphs, FACS analysis, high content screening can be uploaded and linked to the biological results.

➤ The original data file is stored and may be retrieved at any time.

Database Query

The most important result of organizing your data is the ability to learn from it, so called information to knowledge transformation. To accomplish this objective, however, you need to be able to effectively query the data. Chem Biography is particularly skilled in this regard. You may query by multiple means with simple or compound queries:

- Chemical substructure
- Biological or chemical query
- Input of registry ID(s)

Once the query results are returned they are displayed in a web friendly mode and can be further

manipulated via filtering and list logic. One may output results in pdf, csv, or lists of hit registry numbers. Note also that structures render in SVG format for superior display and portability.

Business and Pricing Model

Chem Biography is provided as a preconfigured computer with software installed. The computer

may be used as a standalone workstation (walkup model) or integrated into your network to provide web based *intranet* access to multiple users. All 3rd party software requirements are unencumbered open source. Technically, Chem Biography is built using Apache, PostgreSQL, Python, and compiled C code. It is fully platform independent. We charge an annual license fee for our platform as follows:

- Stand-alone, walkup workstation model
\$4,800 commercial / \$3,600 academic

- Network server model
\$12,400 commercial / \$9,300 academic

We fully guarantee our product and provide a full refund for up to 30 days and pro-rated refund for the current license period at any point afterwards.

Menu Options : views: chem_cb_ic50 edit hits/page: 40 data: all query mol structure: show hide refresh

37 hits total navigation: < < > > pg 1 of 1 filtering: V all clr output: hit list csv pdf query

1. AB000001-001

png pdf mol sub-search

cell ic50: 6 records

registry id	cell line	ic50	std dev	info	file date	file name
AB000001-001	H1975	0.038		Proliferation	2009-01-27	example_cell_ic50.csv
AB000001-001	MV411	0.038		Proliferation	2009-01-27	example_cell_ic50.csv
AB000001-001	pMEK	0.005		Imaging Assay	2009-01-27	example_cell_ic50.csv
AB000001-001	HT-29	0.038		Proliferation	2009-01-27	HT29_proliferation_20090117.csv
AB000001-001	PC-3	0.038		Proliferation	2009-01-26	PC3_proliferation_20090117.csv
AB000001-001	pERK	0.005		Imaging Assay	2009-01-26	pERK_imaging_20090117.csv

bio ic50: 1 record

registry id	assay	ic50	std dev	info	file date	file name
AB000001-001	bRAF	0.015		MEK label	2009-01-26	bRAF_enzyme_20090121.csv

Chem Biography Search admin main registry help signed in: jveal

Menu Options : views: chem_cb_ic50 edit hits/page: 40 data: all query mol structure: show hide search reset

chemical structure

draw mol atom #s clear mol atom-bond wildcard queries

queries data type: field name: operator:

cell ic50: cell line like HT-29; IC50 <= 1.0; and
chemical registry: program like UVW

registry IDs input

AB000003-001
AB000004-001

list management

L1: 0
save L2: 32
add L3: 2
intersect L4: 3
subtract L5: 15
L6: 0

saved searches

all chem ids
inhib1
potent IC50 data:
recent IC50 data:

apply save delete

Learn more:
<http://www.chembiography.com>

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