

ChemCart

...a web-based search and update tool for scientific information

From a web browser, scientists can query and retrieve chemical structures, reactions, data, and images from multiple data sources. The results are displayed in customizable report forms. By using ChemCart update capabilities, scientists can also register information with the same forms.

Project Summary Form

CompID	MR	MF
DS-00001	177.2455	C ₁₀ H ₁₆ N ₂ O

H.Acceptor	H.Donor	LogP
2	0	1.403

LC50 Results

Panel	Cell	HLogP
LNS	NCI-H23	4.05
LNS	NCI-H22	4.06
LNS	AS49ATCC	4.00
LNS	ERYX	4.07
LNS	NCI-H208	4.00
LNS	NCI-H224	4.00
LNS	NCI-H460	4.04
LNS	HDP-42	4.00
LNS	HDP-18	4.08
LNS	HDP-32	4.09
LNS	LFL1-229	4.07
SCL	DM5 114	4.09
SCL	DM5 273	4.00
COL	HT29	4.00
COL	HCC-2998	4.09
COL	HCT-116	4.04
COL	SW620	4.24
COL	COL-205	4.12
COL	DL-1	4.08
COL	NCI-H460	4.06

LC50 Details

Point #	LogConc	% Inh
1	-8	0.52
2	-6	15.26
3	-5	51.26
4	-4.5	65.26
5	-4.25	78.26
6	-4	89.26
7	-3.75	99.26
8	-3.5	98.26
9	-3	101.26
10	-2	100.26

File

File	Details
bio99a.csv	raw data
MS1.pdf	mass spec
Protocol.doc	assay protocol

ChemCart lets scientists search data their way

- Query by Form for chemical structures, reactions, data, documents, files, and images
- Run multiple queries simultaneously with each having different search criteria
- Build customizable forms, or use pre-defined forms to view results
- Draw and display structures and reactions using industry-standard tools
- Full chemical structure and reaction search options – substructure, similarity, exact, and more
- Color results by value
- Generate custom report printouts of search results
- Share forms, lists, queries, reports globally or within a project team
- Extensive result list handling
 - Boolean list operations
 - Save and share
 - Export and import
 - Sort and print
 - Tag items to keep or remove

Register chemical structures and update test result data with ChemCart

- Insert, Update, or Delete data using your customizable forms
- Batch load data from a variety of file types
- Use the Workflow and Business Rule Engines to customize registration

Structure Navigator

CompID: DS-00009

Record 9 of 1388

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Rows: 5

Columns: 5

Structure Navigator eases the task of working with large numbers of structure hits

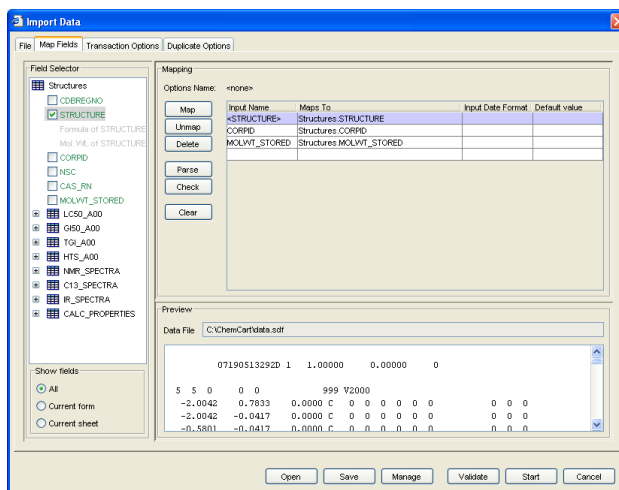
Data Grid View

Comp ID	MW	Avg LC50
DS-000070	408.441	6
DS-000072	348.8116	4.181
DS-000073	234.4885	4.258
DS-000074	38.1521	2.961
DS-000076	172.1768	4
DS-000078	248.207	4
DS-000077	244.2722	4
DS-000078	234.316	4

Analyze structure-activity relationships with Data Grid View

ChemCart benefits developers and IT staff

- Easily design and deploy server based public search/update forms
- Choose the chemical data cartridge that is best for your environment; **ChemCart** is a universal interface
- Deploy from a web browser, no desktop client to load
- Intuitive interface reduces training and support efforts
- Powerful graphical application support module simplifies administration, security, and application building
- Use API to add custom functions to **ChemCart**



Batch load SDFiles and data using the **Import File Mapper**

Structure	Comp ID	MW	MF	Formal Acceptors	Formal Donors	LogP	Molar Refractivity
	DB-000041	215.22	C ₁₉ H ₁₆ N ₂ O	4	2	0.80	58.45
	DB-000070	223.23	C ₁₇ H ₁₆ O ₂	3	8	1.08	35.28
	DB-000541	288.35	C ₁₉ H ₁₆ N ₂ O	3	1	3.78	87.68
	DB-000850	268.22	C ₁₉ H ₁₆ O ₂	5	2	2.24	68.55

Format data in a table layout

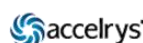
Extend ChemCart capabilities

- Integrate additional data sources with IBM WebSphere Information Integrator
- Access InforSense analysis workflows
- Integrate with SciTegic pipelining tools
- Link to Spotfire visualizations
- Export to chemically aware spreadsheets such as Accelrys Accord for Excel, Symyx ISIS for Excel, InforSense ChemStudio



ChemCart Specifications

- Utilizes Oracle chemistry data cartridge technology such as:
 - Accord Chemistry Cartridge from Accelrys
 - CambridgeSoft Oracle Cartridge
 - JChem Cartridge from ChemAxon
 - DayCart from Daylight
 - Symyx Direct from Symyx
- Supports several popular structure sketchers and renderers
- Supports Windows, Solaris, Linux, and Mac operating systems



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