

# ChemCart ELN

...a web-based electronic laboratory notebook for research scientists

From a web browser, scientists can use ChemCart ELN to record, organize and report their experimental results and conclusions. ChemCart ELN enables sharing and permanent storage of corporate knowledge.

The screenshot displays the ChemCart ELN interface in a web browser. The main window is titled "ChemCart - CHEMCART\_ELN - Windows Internet Explorer". The interface is divided into several sections:

- Title:** Synthesis of Aspirin
- Scientist:** Med Chemist
- Notebook:** D0803
- Expirt:** 1.0
- Date:** 09-Nov-2007
- Continued from:** 1.8

The central part of the interface shows a chemical reaction scheme for the synthesis of aspirin. Below the reaction, there are two tables:

Structure	Name	Lot#	MF	LR	MW	Act MW	Et	Thes Mass	Act Mass	mmol	d	Vol
	acid	1-1	C <sub>7</sub> H <sub>6</sub> O <sub>3</sub>	Y	138.12	138.12	1	138.12	2.50	18.10		
	anhydride	21-3-4	C <sub>4</sub> H <sub>6</sub> O <sub>3</sub>	N	102.09	102.00	1	1.85	1.85	18.10		

Below the reagents table, there is an "Experimental Procedure" section with text describing the synthesis process. At the bottom, there is a "Products" table:

Lot#	ID	Structure	MF	MW	Act MW	Et	Thes Mass	Act Mass	Purity	mmol	% Yield
17-1			C <sub>9</sub> H <sub>8</sub> O <sub>4</sub>	180.15	180.15	1	3.251	3.000	100	16.85	92.0
			C <sub>2</sub> H <sub>4</sub> O <sub>2</sub>	60.05	60.05	1	1.087	0.000			

## ChemCart ELN features that benefit users

- Easy to use, query by form interface
- Use pre-defined forms, modify or build your own form to query, view and update information
- Search by sub-structure and/or any data field through the form, or build more complex queries using AND, OR, NOT logic
- Extensive list handling capabilities – sort, merge, store, retrieve, print, share
- Batch load data from a variety of file types
- Supports several popular chemistry formats, such as Accelrys, CambridgeSoft, ChemAxon, Daylight, Symyx

## Manage experiment data with ChemCart ELN

- Create department specific notebook interfaces with configurable forms
- Record all experiment-related information: reactions, structures, data, images
- Automatically calculate reaction stoichiometry for reactants and products – mass, volume, theoretical yield, % yield
- Duplicate notebook pages for similar reactions & parallel synthesis
- Access reagent inventory information and Material Safety Data Sheets
- Attach files to an experiment (spectra, spreadsheets, documents)
- Register reactions to the corporate reaction repository and products to corporate chemical database
- Search within your own notebook, or search all corporate notebooks
- Audit changes made to notebook entries

The screenshot shows the Structure Navigator interface. It features a search bar at the top with "RXNREGNO: 10" and "Record 7 of 75". Below the search bar is a grid of chemical reactions. The grid is organized into rows and columns, with a navigation pane on the right showing "Page 1 of 5", "Rows 4", and "Columns 4". The reactions in the grid include various organic synthesis reactions, such as the synthesis of aspirin and other pharmaceuticals.

Use the configurable **Structure Navigator** to view and navigate through all reactions stored in a scientist's notebook.

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