

# 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 for a reaction titled "Synthesis of Aspirin". It shows a chemical reaction scheme, a table of reagents (aspirin and acetic anhydride), and a table of products (aspirin and acetic acid). The experimental procedure section describes the synthesis process in detail.

Structure	Name	Lot#	MF	LR	MW	Act MW	ER	Thes Mass	Act Mass	mmol	d	Vol
	aspirin	1-1	C <sub>9</sub> H <sub>8</sub> O <sub>4</sub>	Y	180.12	180.12	1	180.12	2.50	18.10		
	acetic 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		

Lot#	ID	Structure	MF	MW	Act MW	ER	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, which allows users to view and navigate through all reactions stored in a scientist's notebook. It features a search bar, a grid of reaction thumbnails, and navigation controls.

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

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