

ChemTrove: Enabling a generic ELN to support Chemistry by integrating ChemSpider widgets and templates

S.J. Coles ¹, A.E. Day ², J.G. Frey ¹, R. J. Whitby ¹, C.R. Batchelor ².

¹ Chemistry, University of Southampton, UK, ²Royal Society of Chemistry, Cambridge, UK

LabTrove [1] has been developed by the Southampton University since 2005 as a multidisciplinary, open-source electronic (laboratory) notebook for researchers to plan experiments and save and share their results. 'Out of the box' it contains generic tools for researchers from any discipline to upload, display and share data of any file type (either within LabTrove itself or via links), however specific chemistry file types would need to be created and edited outside LabTrove.

Over the last year the Royal Society of Chemistry's ChemSpider [2] has been working with Southampton University in a collaboration guided by the aims of the Dial-a-Molecule Grand Challenge [3] to enhance LabTrove with chemistry-specific functionality and retrieve chemical information from ChemSpider when creating LabTrove entries. We are also working towards a future vision of publishing experimental compound and reaction data from LabTrove to ChemSpider.

So far we have a working prototype of ChemTrove with the added features when editing an entry to:

- Search ChemSpider by name for a compound and retrieve a structure image, name, molecular formula, molecular weight and/or ChemSpider link to add to the entry
- Create or edit a stoichiometry table of the chemicals used and produced in a reaction (with: retrieval of compound properties from ChemSpider; inter-conversion of substance amounts; calculation of product yields; ability to record both planned and actual amounts)
- Draw structures within the LabTrove edit page using JSDraw and render them in a LabTrove post using JSmol lite

The screenshot shows the 'New Post' interface with a search bar for ChemSpider. Below it, a 'ChemSpider' widget displays search options like 'Insert compound information' and 'Insert or edit stoichiometry table'. To the right, the 'Edit Structure' window shows a benzene ring drawn with JSDraw. Below these, a 'New Post' preview shows the rendered output: a benzene structure, its name, formula, and weight, followed by a stoichiometry table for a reaction.

Compound Information	Substance Information	Planned Amounts	Actual Amounts
ChemSpider ID: 971 Name: Phenol Formula: C ₆ H ₆ O MW: 94.1	Role: limiting reactant State: solid Source: Purity (%): 100 Comments:	Ratio: 1.00 Amount (mmol): 53.1 Mass (g): 5.00*	Ratio: 1.00 Amount (mmol): 54.2 Mass (g): 5.10*
Safety Information: ChemSpider ID: 236 Name: Benzene Formula: C ₆ H ₆ MW: 78.1	Role: product State: liquid Source: Purity (%): 100 Density (g/mL): 0.8765 Comments:	Ratio: 0.900* Amount (mmol): 47.8 Mass (g): 3.73 Volume (mL): 4.26	Amount (mmol): 44.9 Mass (g): 3.51 Volume (mL): 4.00* Yield (%): 92.0

This functionality has been added by developing a set of jQuery ChemSpider widgets and TinyMCE editor plugins which add buttons to the "edit" page of LabTrove and load these widgets when clicked. We have demonstrated these widgets in LabTrove but they could in theory be included into any webpage (so could be incorporated into any web-based ELN).

By allowing compound and reaction data to be published from ELNs directly to repositories such as ChemSpider, ChemSpider Synthetic Pages and reaction database (under development) a major enabling step towards making accessible the type of detailed reaction data, of both successful and less successful reactions, required for Dial-a-Molecule will have been realized. Allowing users of ELNs to easily search on and retrieve reactions and characterisations that have previously been performed when planning a new reaction will also aid progress. Towards this aim LabTrove templates have been written to structure entries that contain compound and reaction data so that they will be more understandable when deposited to the ChemSpider repositories than a free-format block of text and files.

The following templates are available:

Compound template for entries that contain compound structures, properties and spectra to be published to ChemSpider

The form includes fields for Title, ChemSpider ID, Name of Compound mol file, Description, Tags, Identifiers (Chemical Name, Common Name, Synonym), and Spectra (Spectrum 1, 2). It also features a table for Properties with columns for Property, Value, Unit, and Comments.

Reaction templates - simple for submission to reaction database (under development) and more detailed for submission to ChemSpider SyntheticPage

The form includes fields for Title, Reaction template, and Text. It features a 'Reaction information' section with fields for Reaction file, Reaction file type, Procedure, Yield (%), Type of Yield, and References. It also has a section for 'For multistep reactions (or their steps)' with fields for Overall reaction, Overall reaction - links to child reaction steps, Step in multistep reaction - link to previous reaction step, and Step in multistep reaction - link to following reaction step. A 'Section' dropdown and 'Metadata' section are also present.

These templates have been tested during a student intern project to digitise thesis data and publish it into 1035 new LabTrove entries (which use these templates) and 208 new compounds and over 600 spectra in ChemSpider.

ChemTrove is being hosted on a cloud server by the company Liberata to undergo a usability trial by selected academics to guide its future development.

1. LabTrove. <http://www.labtrove.org/> (accessed Feb 11, 2014).
2. ChemSpider. <http://www.chemspider.com> (accessed Feb 11, 2014).
3. Dial a Molecule Grand Challenge. <http://www.dial-a-molecule.org> (accessed Feb 11, 2014).

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