

A spider for all molecules...



A new extension to the IDBS's E-WorkBook – the electronic lab notebook (ELN) we use here in the department – makes it easy for chemists to send novel structures to the ChemSpider database.

ChemSpider, which can be found at www.chemspider.com and is owned by the Royal Society of Chemistry, is a free chemical structure database on the internet that provides fast text and structure search access to more than 26 million structures from hundreds of data sources.

Aileen Day at the RSC (who also happens to be married to Graeme Day here in chemistry) has developed a plug-in that allows a user to click on a structure or reaction in the ELN that they wish to make public, and it will automatically send the structures to ChemSpider. The structure can then be found by chemists from all over the world who search the database – a simple and effective way to publicise work.

The new plug-in was developed in collaboration with IDBS, and with additional guidance from Brian Brooks, Tim Dickens, Bobby Glen and Steve Ley in the department.

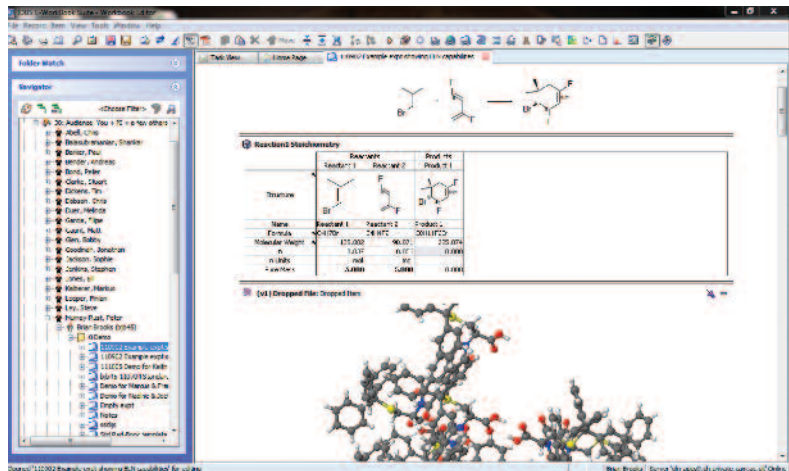
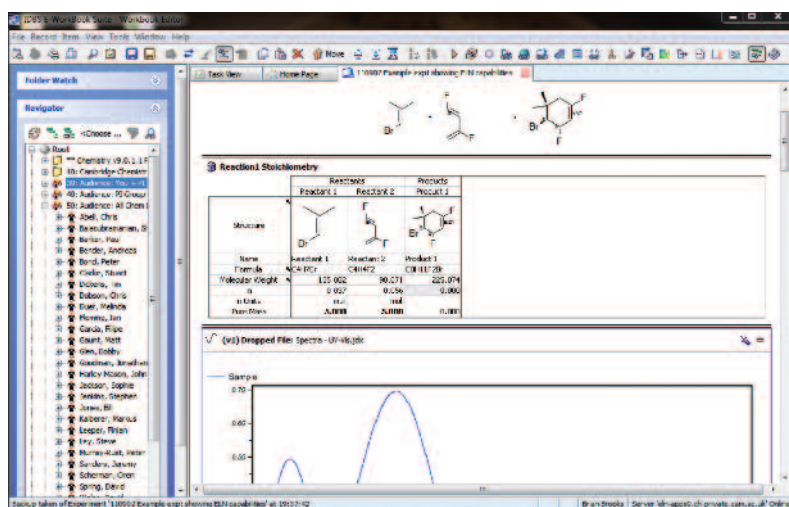
At present, only the chemical structure is passed to ChemSpider. Future versions will allow entire chemical reaction schemes to be published, plus supporting data such as spectra and reaction yields.

The extension also allows searches of ChemSpider to be launched easily from within the ELN. Any structure in the ELN can be used as the search criteria, and the results are returned in an internet browser.

Bobby Glen thinks the plug-in will prove very useful. 'Much of the chemistry that is carried out is lost – it is simply not published and languishes in forgotten lab notebooks,' he says. 'Capturing novel molecules soon after synthesis on a searchable database like ChemSpider is now an effortless process directly from the ELN, which will greatly encourage sharing of compounds, synthetic methods and all the associated data. It's instant messaging for chemists.'

It has also been welcomed by Antony Williams, vice president of strategic development at the RSC. 'The ability to now publish compound data from the IDBS ELN directly to ChemSpider offers

Screenshots of a reaction in the ELN and (bottom) how a molecule appears on ChemSpider



ChemSpider search results for (4aR,8aS)-3,4,4a,5,8,8a-hexahydro-2H-naphthalen-1-one:

ChemSpider ID: 28304821
 Molecular Formula: C₁₀H₁₄O
 Molecular Weight: 150.194 Da
 Solubility: none
 (4aR,8aS)-4,4,4a,5,8,8a-hexahydro-2H-naphthalen-1-one

Data Sources: IDBS E-WorkBook, External (RSC)

a path to direct exposure of novel chemistry as well as the chemist doing the work,' he says. 'This public compound registration capability is the first move towards ultimately exposing synthetic methods and associated experimental data to the community. Our vision is coming to fruition through this collaboration.'

All existing ELN users will be emailed with instructions of how to obtain and use the extension.

Important note: always confirm with your PI if you want to publish a molecule on ChemSpider before it has been published in a journal!