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Interactive articles in *MedChemComm* – connecting readers to a wealth of data and information

Richard Kelly

Chemists and biologists now have access to a staggering array of data and information, and tools to analyse and interpret it. At *MedChemComm* we are making major changes to the HTML versions of articles to connect the research published in the journal directly to chemical and biological data from a range of sources, and to make key research data in manuscripts downloadable in formats that will allow further analysis.

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Have you ever read an article, seen a compound of interest and wondered what the cLogP is? From *MedChemComm* Concise Articles you can now access this and a range of other chemical and biological information direct from the manuscript, simply by clicking on the compound name or number (Fig. 1).

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Open PHACTS. Pharmacological and physicochemical data linking compounds, targets, pathways, diseases and tissues, drawn from several sources including ChEBI, ChEMBL, DrugBank and Swiss-Prot. Note that this option is not shown if there is not yet an Open PHACTS entry for the compound.

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Take a look at an example of the functionality in C4MD00420E.

Downloading and analysing data directly from a manuscript

Later this year we will add the ability to download compounds and tables in Excel or SD format, enabling readers to analyse the data reported in manuscripts themselves. Each table in a manuscript will be available as a separate file, and an additional SD file will contain all of the molecules in the manuscript.

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In this work two hit compounds **14** inhibiting autophagy in ovarian A27 leading to the discovery of another MCF-7 breast cancer cells and the characteristic autophagy vacuole formation was diminished upon the administration of the inhibitors verifying their efficacy. These three compounds can now be developed further with more elaborate experimental/biological testing and by substantially extending the SAR analysis.

COMPOUND LINKS

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high throughput screening developed for hit **14** compounds were tested in

Fig. 1 Sample of text from C4MD00420E showing links from a compound to additional data.



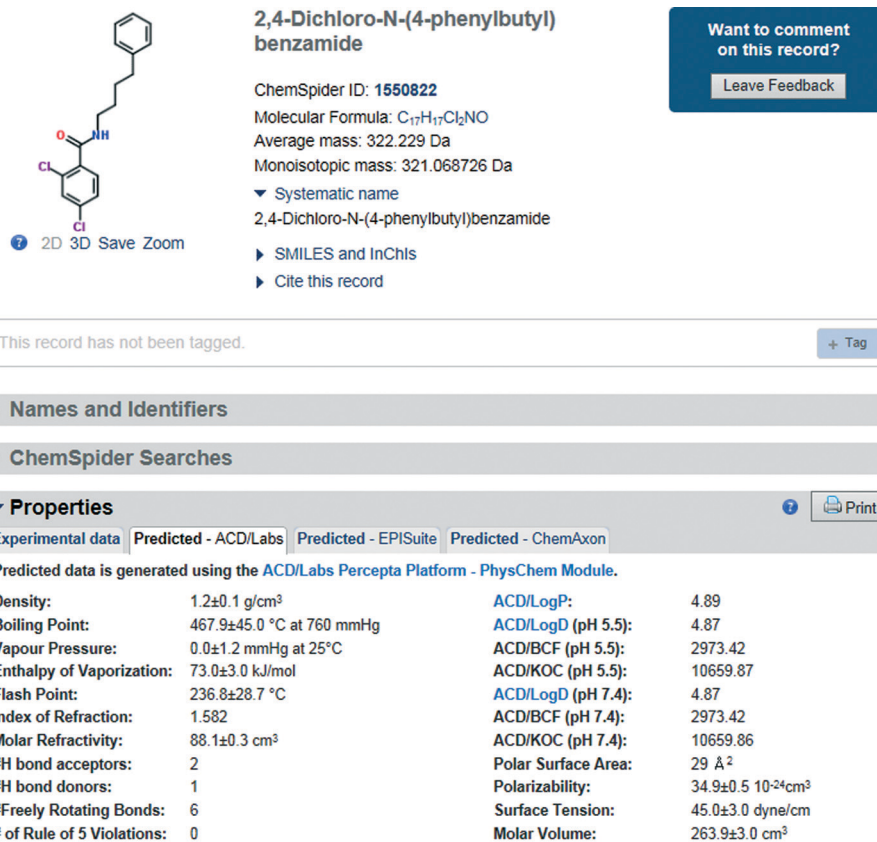


Fig. 2 Sample of ChemSpider data for compound 14 in C4MD00420E.

Both of these enhancements will be available from publication of the electronic issue.

These are just some of the developments we plan to introduce to *MedChemComm* and we are always keen

to hear how we can improve our service to authors and readers. If you have any suggestions please do get in touch.

