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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.

Direct linking to further chemical and biological data

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).

The HTML versions of all 2015 Concise Articles will have links from compounds directly to databases which contain further chemical and biological information about the compound:

ChemSpider. Chemical data and information including predicted properties from ACD Labs such as logP and number of H bond acceptors and donors, published articles and patents for the compound, SMILES and InChIs, and links to external sources such as Google Scholar and Wikipedia. All compounds published in *MedChemComm* are now routinely added to ChemSpider (Fig. 2).

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.

Readers can also download an editable version of the structure as a .mol file directly from the manuscript.

How to use: click on the “Show Compounds” button at the top of an article, hover over any compound name or number highlighted in yellow (on mobile devices just tap) and a bubble containing the links will appear.

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

Downloading and analysing data directly from a manuscript

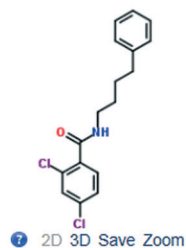
Later this year we will add the ability to download compounds and tables in Excel or SD format, enabling readers to analyse the data reported in manuscripts themselves. Each table in a manuscript will be available as a separate file, and an additional SD file will contain all of the molecules in the 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
[Read more about this on ChemSpider](#)
[Download mol file of compound](#)

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

**2,4-Dichloro-N-(4-phenylbutyl)benzamide**

ChemSpider ID: **1550822**
Molecular Formula: $C_{17}H_{17}Cl_2NO$
Average mass: 322.229 Da
Monoisotopic mass: 321.068726 Da

- ▼ Systematic name
2,4-Dichloro-N-(4-phenylbutyl)benzamide
- SMILES and InChIs
- Cite this record

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▼ Properties

Print

Experimental data Predicted - ACD/Labs Predicted - EPI Suite Predicted - ChemAxon

Predicted data is generated using the ACD/Labs Percepta Platform - PhysChem Module.

Density:	1.2±0.1 g/cm ³	ACD/LogP:	4.89
Boiling Point:	467.9±45.0 °C at 760 mmHg	ACD/LogD (pH 5.5):	4.87
Vapour Pressure:	0.0±1.2 mmHg at 25°C	ACD/BCF (pH 5.5):	2973.42
Enthalpy of Vaporization:	73.0±3.0 kJ/mol	ACD/KOC (pH 5.5):	10659.87
Flash Point:	236.8±28.7 °C	ACD/LogD (pH 7.4):	4.87
Index of Refraction:	1.582	ACD/BCF (pH 7.4):	2973.42
Molar Refractivity:	88.1±0.3 cm ³	ACD/KOC (pH 7.4):	10659.86
#H bond acceptors:	2	Polar Surface Area:	29 Å ²
#H bond donors:	1	Polarizability:	34.9±0.5 10 ⁻²⁴ cm ³
#Freely Rotating Bonds:	6	Surface Tension:	45.0±3.0 dyne/cm
# of Rule of 5 Violations:	0	Molar Volume:	263.9±3.0 cm ³

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.

