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EDITORIAL



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

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

Richard Kelly

analysis

DOI: 10.1039/c5md90014i

www.rsc.org/medchemcomm

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:

Managing Editor, MedChemComm, Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge, CB4 0WF, UK, E-mail: medchemcomm-rsc@rsc.org

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 vellow (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.

COMPOUND LINKS

inhibiting autophagy in ovarian A27 Read more about this on ChemSpider developed for hit 14 leading to the discovery of another a Download mol file of compound

In this work two hit compounds 14

gh throughput screening compounds were tested in

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.

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

\bigcirc	2,4-Dichloro-N-(4-p benzamide	henylbutyl)	Want to comment on this record?
CI CI CI CI Save Zoom	ChemSpider ID: 1550822 Molecular Formula: C ₁₇ H ₁₇ Average mass: 322.229 D Monoisotopic mass: 321.0 ▼ Systematic name 2,4-Dichloro-N-(4-phenylb ▶ SMILES and InChls	Cl₂NO a 68726 Da utyl)benzamide	Leave Feedback
	 Cite this record 		
This record has not been	tagged.		+ Tag
 Names and Identifiers ChemSpider Searches 			
▼ Properties		Producted Observation	😢 🕒 Print
Experimental data Predict	ed - ACD/Labs Predicted - EPISuite	Predicted - ChemAxon	
Predicted data is generated	I using the ACD/Labs Percepta Platfe	orm - PhysChem Module.	
Density: Boiling Point: Vapour Pressure:	1.2±0.1 g/cm ³ 467.9±45.0 °C at 760 mmHg 0.0±1.2 mmHg at 25°C	ACD/LogP: ACD/LogD (pH 5.5): ACD/BCF (pH 5.5):	4.89 4.87 2973.42
Enthalpy of Vaporization: Flash Point:	73.0±3.0 kJ/mol 236.8±28.7 °C	ACD/KOC (pH 5.5): ACD/LogD (pH 7.4):	10659.87 4.87
Index of Refraction: Molar Refractivity:	1.582 88.1±0.3 cm ³	ACD/BCF (pH 7.4): ACD/KOC (pH 7.4):	2973.42 10659.86
#H bond acceptors:	2	Polar Surface Area:	29 Å ²
#H Dond donors: #Ereely Poteting Ponder	6	Surface Tension:	4.5 0±3 0 dyne/cm
#Freely Rotating Bonds: # 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.