

Wikidata now escapes SMILES and CXSMILES!

Egon Willighagen 

Published August 2, 2022

Citation

Willighagen, E. (2022). Wikidata now escapes SMILES and CXSMILES!. In *chem-bla-ics*. chem-bla-ics. <https://doi.org/10.59350/458r6-cmn16>

Keywords

Wikidata, Cxsmiles

Abstract

In the end it was a very simple change today (huge thanks to Nikki!), but Wikidata now escapes SMILES and CXSMILES (P10718) with the formatter URL (P1630)!

Copyright

Copyright © Egon Willighagen 2022. Distributed under the terms of the [Creative Commons Attribution 4.0 International License](#), which permits unrestricted use, distribution, and reproduction in any medium, provided the original author and source are credited.

chem-bla-ics

In the end it was a very [simple change](#) today (huge thanks to [Nikki!](#)), but [Wikidata](#) now escapes SMILES and CXSMILES ([P10718](#)) with the formatter URL ([P1630](#))!

```
112         break;
113     case 233:
114     case 2017:
115     case 8533:
116     case 10718:
117         linkValue = encodeURIComponent( linkValue );
118     break;
119     default:
```

That means that the link to [CDK Depict](#) now also works for SMILES ([P233](#) and [P2017](#)) with a triple bond in it :) And because [Adriano](#) created the so far missing **formatter URL** for CXSMILES, it also works for lipid classes (see [my post yesterday](#)), polymers, etc :)

CXSMILES by Egon Willighagen	<code>[*]SC(=O)CC(=O)CCCCCCC \$_R\$ </code> edit
	▼ 0 references
	+ add reference
	+ add value

CXSMILES for a group of acyl-carrier proteins.

formatter URL by AdrianoRutz	<code>https://www.simolecule.com/cdkdepict/depict/bow/svg?smi=\$1&zoom=2.0&annotate=cip</code> edit
	MIME type <code>image/svg+xml</code>
	▼ 0 references
	+ add reference
	+ add value

The *formatter URL* info added to make the link outs for CXSMILES work. The patch by Nikki ensures that characters like # are escaped before the URL is created.