Wikidata now escapes SMILES and CXSMILES!

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Citation

Keywords

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)!

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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	[*]SC(=O)CC(=O)CCCCCCC |$_R$| edit
	▾ 0 references
	+ add reference
	+ add value

CXSMILES for a group of acyl-carrier proteins.

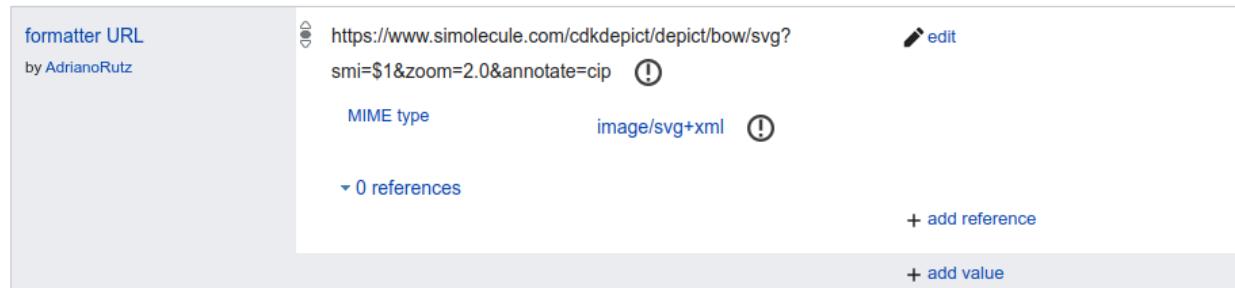| formatter URL by AdrianoRutz	https://www.simolecule.com/cdkdepict/depict/bow/svg? smi=$1&zoom=2.0&annotate=cip (!) edit
	MIME type image/svg+xml (!)
	▾ 0 references
	+ add reference
	+ add value

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.