chem-bla-ics

Biology, ACPs, lipids, cheminformatics, and Dagstuhl

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Published August 1, 2022

Citation

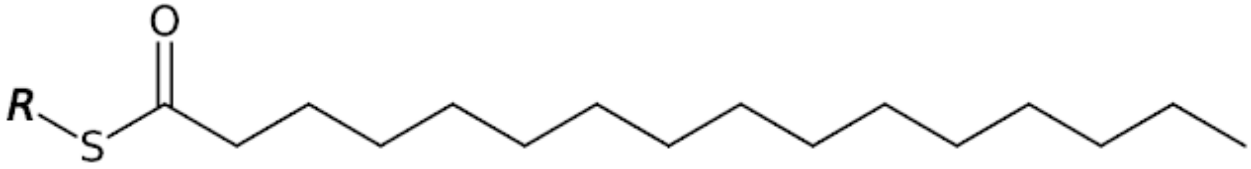
Willighagen, E. (n.d.). In *chem-bla-ics*. chem-bla-ics. https://doi.org/10.59350/ab2rj-qdg37

Keywords

Cdk, Chebi, Dagstuhl, Epilipidnet, Kegg

Already 3 months ago I visited Dagstuhl for the second time. The weather was much better than in the January right before the start of the pandemic. The first I attended the Computational Metabolomics meeting, with the focus From Cheminformatics to Machine Learning, one of the things we concerned ourselves with was how to do computation with compound classes (see Section 3.6 and this online book). We know how to handle SMILES and we know how to the substructure searching with SMARTS, but what if you have compound classes or lipid classes? Biology is a greasy business.

From a WikiPathways there is additional complexity, with modified proteins involved in lipid metabolism, the acyl-carrier proteins. They look like this, and the R group is a protein:



We have quite a few of them in WikiPathway and they also show up in ChEBI (and likely Reactome), LIPID MAPS, and KEGG.

During this years Dagstuhl we used up one session to continue working on it (report pending). Part of the results is that Wikidata (see doi:10.7554/eLife.52614 and doi:10.7554/eLife.70780) now has a property for CXSMILES. CDK 2.0 (doi:10.1186/s13321-017-0220-4) already supported CXSMILES and the above image is actually created with CDK Depict (thx to John!).

So, that means I can now start adding all those ACPs to Wikidata :) Here's hexadecanoyl-[acp] (or this Scholia page):

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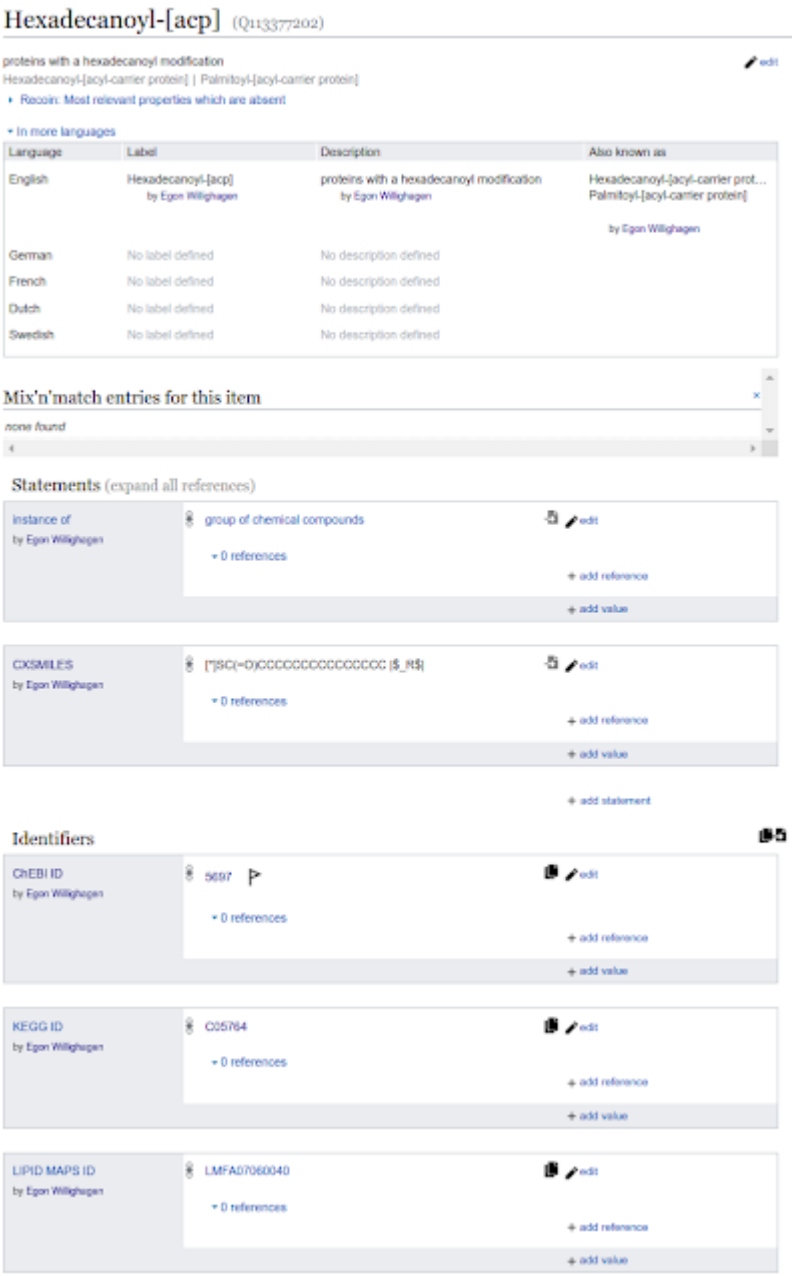
Hexadecanoyl-[acp] (Q113377202)
proteins with a hexadecanoyl modification
Hexadecanoyl-[acyl-carrier protein] | Palmitoyl-[acyl-carrier protein]
Recoin: Most relevant properties which are absent
In more languages
Language
Label
Description
Also known as
English
Hexadecanoyl-[acp]
by Egon Willighagen
proteins with a hexadecanoyl modification
by Egon Willighagen
Hexadecanoyl-[acyl-carrier prot...
Palmitoyl-[acyl-carrier protein]
by Egon Willighagen
German
No label defined
No description defined
French
No label defined
No description defined
Dutch
No label defined
No description defined
Swedish
No label defined
No description defined
Mix'n'match entries for this item
none found
Statements (expand all references)
instance of
by Egon Willighagen
group of chemical compounds
0 references
add reference
add value
CXSMILES
by Egon Willighagen
[*]SC(=O)CCCCCCCCCCCCCCC |$_R$|
0 references
add reference
add value
add statement
Identifiers
ChEBI ID
by Egon Willighagen
5697
0 references
add reference
add value
KEGG ID
by Egon Willighagen
C05764
0 references
add reference
add value
LIPID MAPS ID
by Egon Willighagen
LMFA07060040
0 references
add reference
add value