

Biology, ACPs, lipids, cheminformatics, and Dagstuhl

Egon Willighagen 

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Keywords

Cdk, Chebi, Dagstuhl, Epilipidnet, Kegg

Abstract

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.

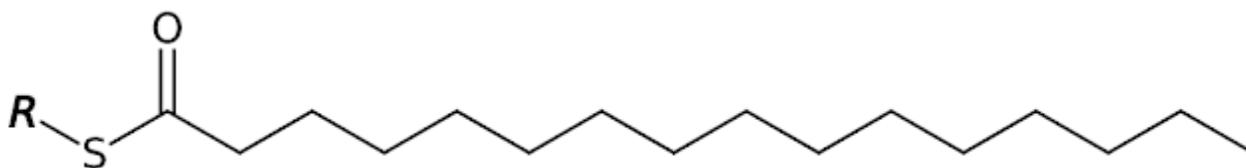
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chem-bla-ics

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](#)):

chem-bla-ics

Hexadecanoyl-[acp] (Q113377202)

proteins with a hexadecanoyl modification

Hexadecanoyl-[acyl-carrier protein] | Palmitoyl-[acyl-carrier protein]

edit

• **Recoil:** 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 edit

- 0 references

+ add reference

+ add value

CXSMILES
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[*]SC(=O)CCCCCCCCCCCCC [\$_R5]

- 0 references

+ add reference

+ add value

+ add statement

Identifiers

ChEBI ID
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5687

- 0 references

+ add reference

+ add value

KEGG ID
by Egon Willighagen

C05764

- 0 references

+ add reference

+ add value

LIPID MAPS ID
by Egon Willighagen

LMFA0706040

- 0 references

+ add reference

+ add value