AllCCS Tutorial

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AllCCS Document

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About AllCCS

AllCCS is a powerful platform to support various applications in Ion Mobility – Mass Spectrometry (IM-MS). It is designed to contain three major parts: **1) Unified CCS database, 2) Machine learning based CCS prediction, and 3) small molecule annotation**. The unified CCS database is one of the most comprehensive CCS databases, covering ~1,700,000 small molecules. It provides a universal platform to contain both experimental CCS values (3,539) and predicted CCS values (over 10,000,000). Machine learning based CCS prediction function supports convenient prediction from SMILES structure to CCS values. This function utilizes the second generation CCS prediction algorithm to generate CCS values and RSS score for novel structures. Small molecule annotation provides an easy-to-use annotation function for various features or compounds. It is supported to search database with measured m/z and CCS for annotation, or in conjunct with any other annotation tools, such as MetFrag, CFM-ID, MS-Finder, and SIRUS etc.

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Citation

If AllCCS is useful in your project, please cite our articles.

- Z. Zhou, Z.-J. Zhu* etc. Advancing CCS database towards metabolite annotation, In preparing

Chapter 1

Introduction of AllCCS

About AllCCS Last edited in Nov. 1, 2019

ABSTRACT AllCCS is a powerful platform to support various applications in Ion Mobility – Mass Spectrometry (IM-MS). It is designed to contain three major parts: 1) Unified CCS database, 2) Machine learning based CCS prediction, and 3) small molecule annotation. The unified CCS database is one of the most comprehensive CCS databases, covering ~1,700,000 small molecules. It provides a universal platform to contain both experimental CCS values (3,539) and predicted CCS values (over 10,000,000). Machine learning based CCS prediction function supports convenient prediction from SMILES structure to CCS values. This function utilizes the second generation CCS prediction algorithm to generate CCS values and RSS score for novel structures. Small molecule annotation provides an easy-to-use annotation function for various features or compounds. It is supported to search database with measured m/z and CCS for annotation, or in conjunct with any other annotation tools, such as MetFrag, CFM-ID, MS-Finder, and SIRUS etc.

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You can label chapter and section titles using `{#label}` after them, e.g., we can reference Chapter 1. If you do not manually label them, there will be automatic labels anyway, e.g., Chapter ??.

Figures and tables with captions will be placed in `figure` and `table` environments, respectively.

```
par(mar = c(4, 4, .1, .1))
plot(pressure, type = 'b', pch = 19)
```

Reference a figure by its code chunk label with the `fig:` prefix, e.g., see Figure 1.1. Similarly, you can reference tables generated from `knitr::kable()`, e.g., see Table 1.1.

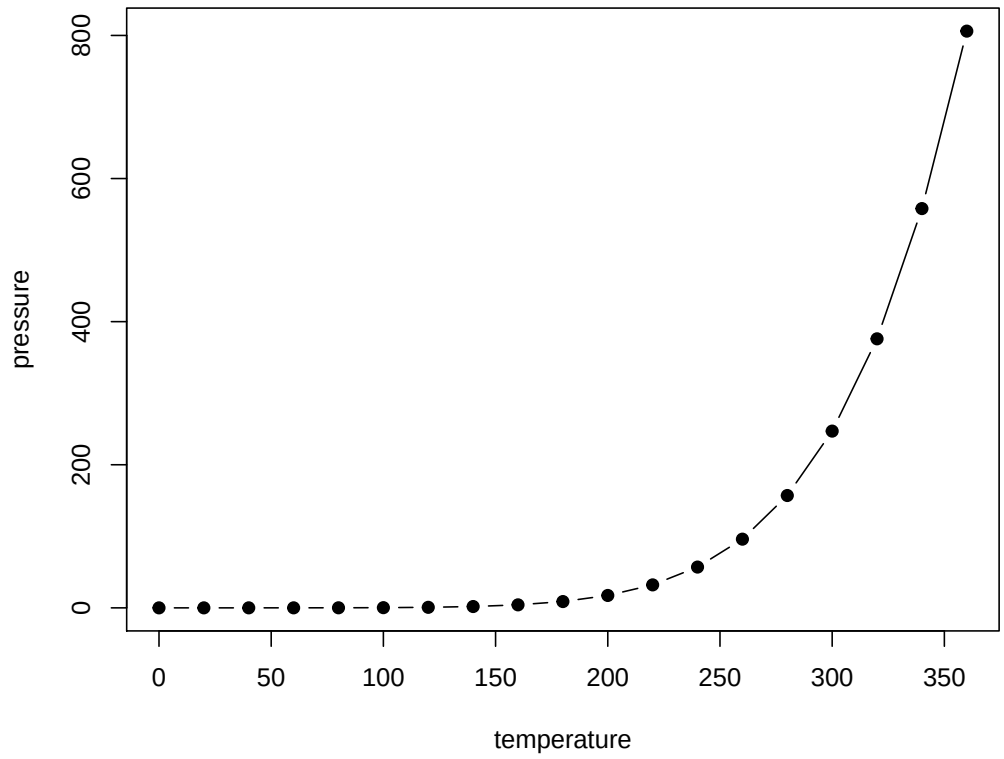

Figure 1.1: Here is a nice figure!

```
knitr::kable(
  head(iris, 20), caption = 'Here is a nice table!',
  booktabs = TRUE
)
```

You can write citations, too. For example, we are using the **bookdown** package (Xie, 2018) in this sample book, which was built on top of R Markdown and **knitr** (Xie, 2015).

Table 1.1: Here is a nice table!

Sepal.Length	Sepal.Width	Petal.Length	Petal.Width	Species
5.1	3.5	1.4	0.2	setosa
4.9	3.0	1.4	0.2	setosa
4.7	3.2	1.3	0.2	setosa
4.6	3.1	1.5	0.2	setosa
5.0	3.6	1.4	0.2	setosa
5.4	3.9	1.7	0.4	setosa
4.6	3.4	1.4	0.3	setosa
5.0	3.4	1.5	0.2	setosa
4.4	2.9	1.4	0.2	setosa
4.9	3.1	1.5	0.1	setosa
5.4	3.7	1.5	0.2	setosa
4.8	3.4	1.6	0.2	setosa
4.8	3.0	1.4	0.1	setosa
4.3	3.0	1.1	0.1	setosa
5.8	4.0	1.2	0.2	setosa
5.7	4.4	1.5	0.4	setosa
5.4	3.9	1.3	0.4	setosa
5.1	3.5	1.4	0.3	setosa
5.7	3.8	1.7	0.3	setosa
5.1	3.8	1.5	0.3	setosa

Chapter 2

Quick Start Guide

Here is a review of existing methods.

Chapter 3

CCS Database

We describe our methods in this chapter.

Chapter 4

CCS Prediction

Some *significant* applications are demonstrated in this chapter.

4.1 Example one

4.2 Example two

Chapter 5

Metabolite Annotation

We have finished a nice book.

Bibliography

Xie, Y. (2015). *Dynamic Documents with R and knitr*. Chapman and Hall/CRC, Boca Raton, Florida, 2nd edition. ISBN 978-1498716963.

Xie, Y. (2018). *bookdown: Authoring Books and Technical Documents with R Markdown*. R package version 0.7.