AllCCS Tutorial V1.00

Zhiwei Zhou

2019-11-01

Contents

List of Tables

List of Figures

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.

Zhiwei Zhou (zhouzw@sioc.ac.cn) Zheng-Jiang Zhu (jiangzhu@sioc.ac.cn) Laboratory for Mass Spectrometry and Metabolomics IRCBC, Shanghai Institute of Organic Chemistry Chinese Academy of Sciences, Shanghai, China

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

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.

Chapter 2

Quick Start Guide

Here is Quick Start Guide

Chapter 3

CCS Database

3.1 Compound Browser

3.2 Compound Card

3.3 Advanced Search

Chapter 4

CCS Prediction

Chapter 5

Metabolite Annotation

We have finished a nice book.