AllCCS Tutorial V1.00

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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

News

November 6, 2019

- Test in web server
- Fix bugs in admin system
- Fix some known bugs
- Update formal database and install AllCCS package V0.1.61
- Correct compound name of drugbank compound

September 22, 2019

- Demo webserver online

Chapter 1

Quick Start Guide

1.1 Create a AllCCS Account

Users need to register AllCCS account to use the webserver. This process is very sample, and **completely private**. To register an account, navigate to the home page. The "Sign up" button is in the upper right corner of the page. Then, you need to fill in your email and verification code which would be sent to your email (Figure 1.1). Finally, input some basic information to complete the registration. You could log in and enjoy all functions in the web server.

1.2 Browser CCS database

You could search you interested compound (name, formula, smiles, inchi, InChIKey etc.) in the search box in navigation bar, or directly browser the all database records in the "browser" page (Figure 1.2).

Then, you can click the link in the column of AllCCS ID to browser detail information of this compound (Figure 1.3). It includes basic meta information, unified CCS values, experimental CCS records, predicted CCS records and other database links etc. Please see section 2 for more details.

1.3 Perform CCS prediction/Annotation

AllCCS also provides CCS prediction function (Section 3) and metabolite annotation functions (Section 4). You could click the link or corresponding item in navigation bar. For CCS prediction function, please input the SMILES list of your compounds in the input panel. The result would be returned on the project panel within several seconds (Figure 1.4).

Figure 1.1: Register AllCCS account

Figure 1.2: Register AllCCS account

Figure 1.3: Register AllCCS account

Figure 1.4: Register AllCCS account

Figure 1.5: Register AllCCS account

For annotation function, you could search experimental feature to search the database with your settings, or filter/rerank candidates to conjunct with MS/MS annotation tools (Figure 1.5).

Chapter 2

CCS Database

2.1 Compound Browser

2.2 Compound Card

2.3 Advanced Search

Chapter 3

CCS Prediction

Chapter 4

Metabolite Annotation

We have finished a nice book.