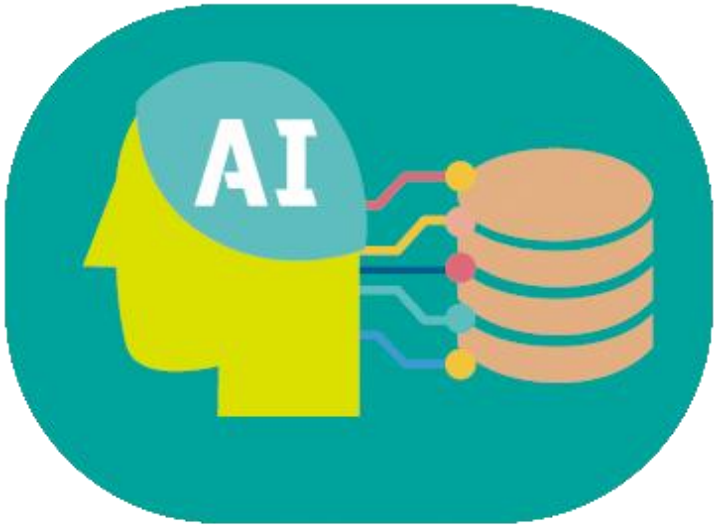


Manual for VirMolAnalyte

Introduction of VirMolAnalyte

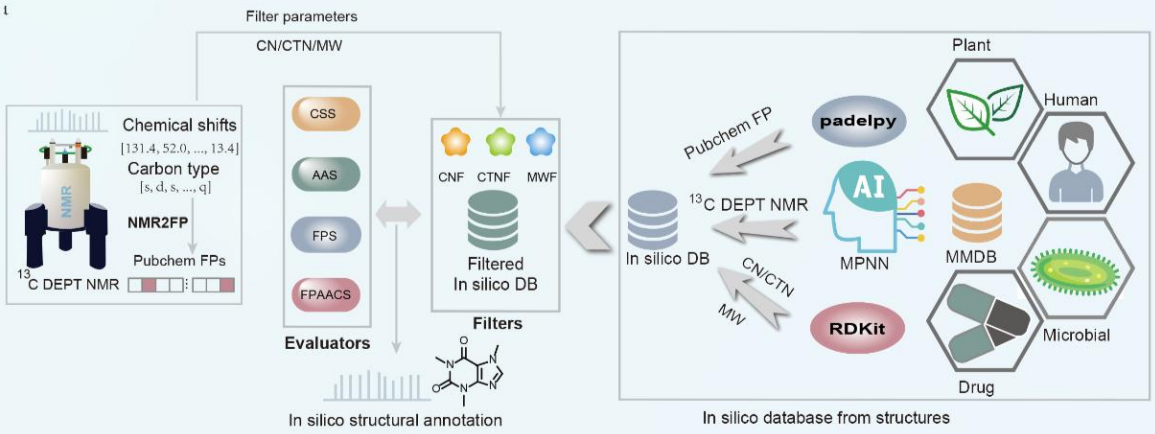
VirMolAnalyte AI-Driven Metabolite Identification Tool

Introduction | Task | Download | Contact Us

VirMolAnalyte: Metabolite Identification Tool

Introduction

VirMolAnalyte is an advanced AI-driven tool designed for identifying metabolites from plant, human, microbial, and drug sources. Based on 13C NMR (Nuclear Magnetic Resonance) data, this tool aims to provide researchers with an efficient and accurate solution for metabolite analysis.

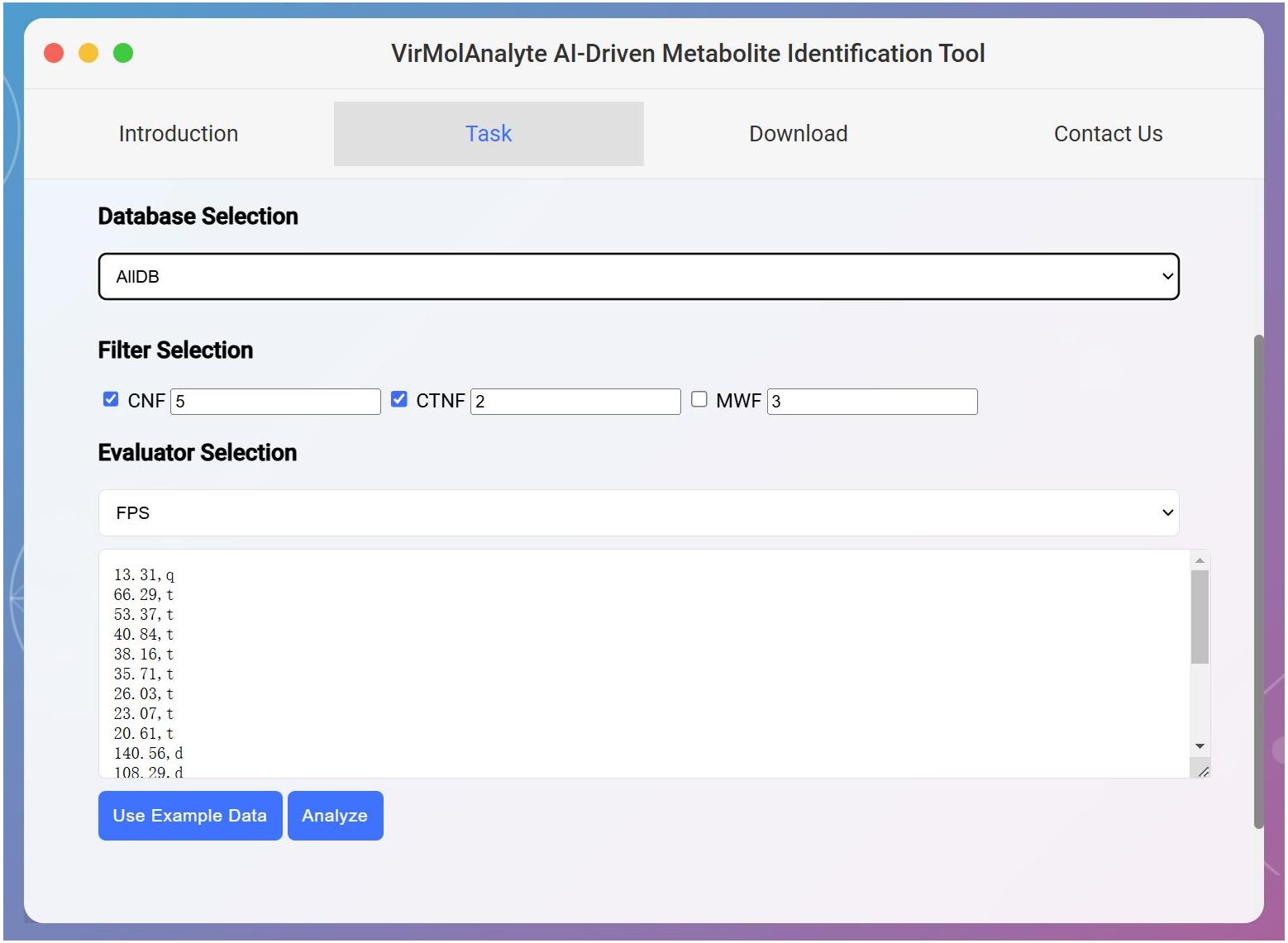


Features

https://www.virmolanalyte.top/

VirMolAnalyte for 13C DEPT NMR analysis

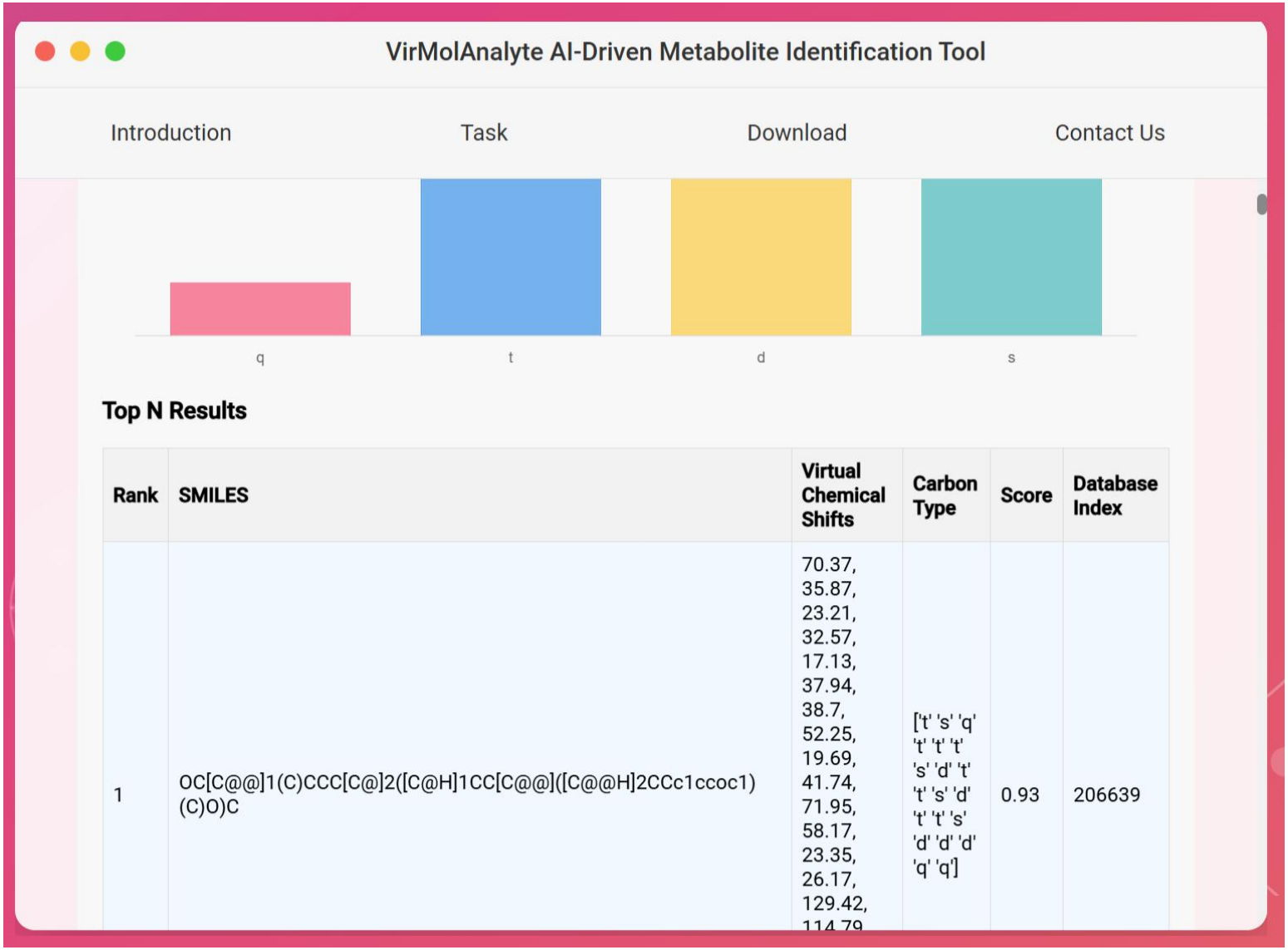
Database selection<Filer selection<Evaluator selection<NMR data input<Analyze



https://www.virmolanalyte.top/

VirMolAnalyte for 13C DEPT NMR analysis

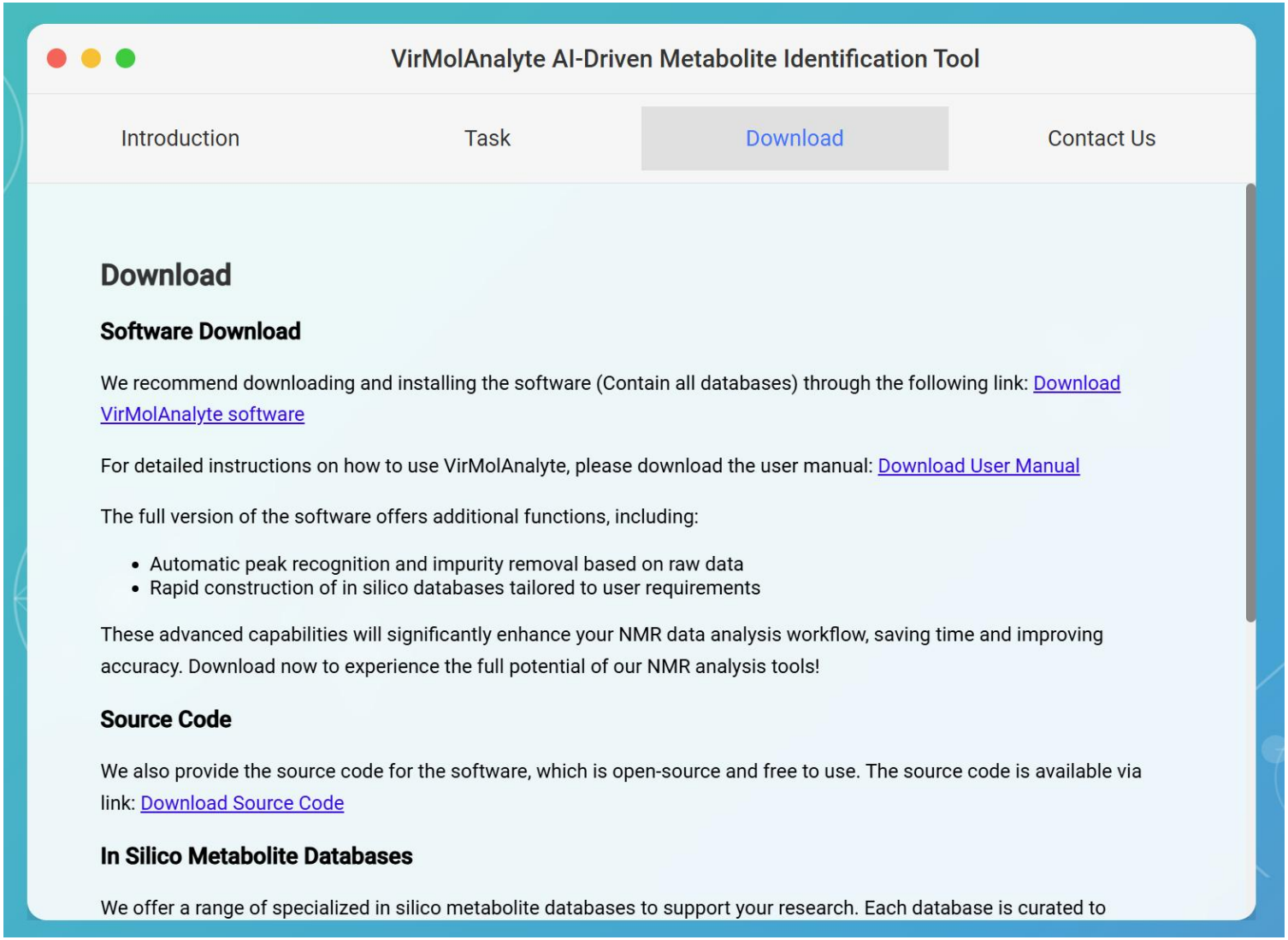
Result analysis



Rank	SMILES	Virtual Chemical Shifts	Carbon Type	Score	Database Index
1	OC[C@@]1(C)CCC[C@]2([C@H]1CC[C@@]([C@@H]2CCc1ccoc1)(C)O)C	70.37, 35.87, 23.21, 32.57, 17.13, 37.94, 38.7, 52.25, 19.69, 41.74, 71.95, 58.17, 23.35, 26.17, 129.42, 114.79	['t' 's' 'q' 't' 't' 't' 's' 'd' 't' 't' 's' 'd' 't' 't' 's' 'd' 'd' 'd' 'q' 'q']	0.93	206639

https://www.virmolanalyte.top/

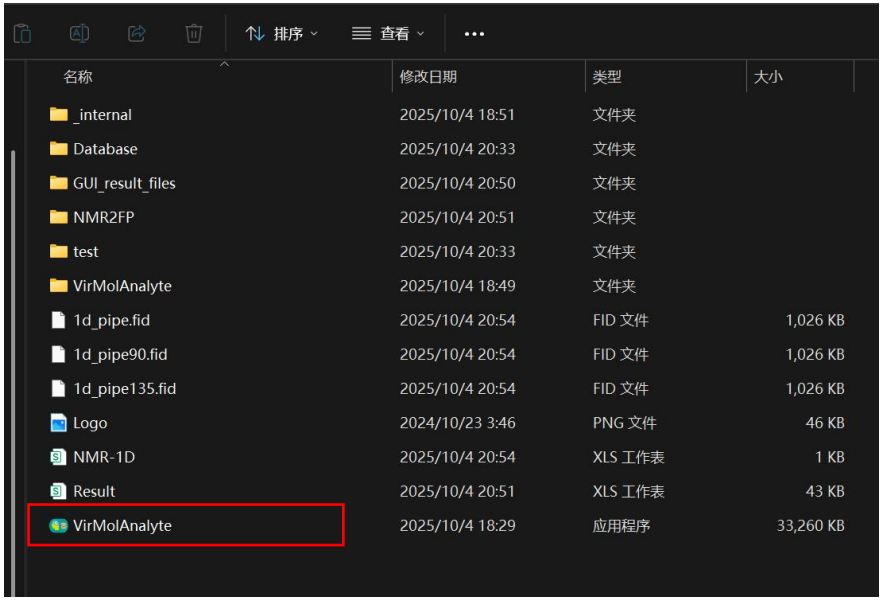
VirMolAnalyte download



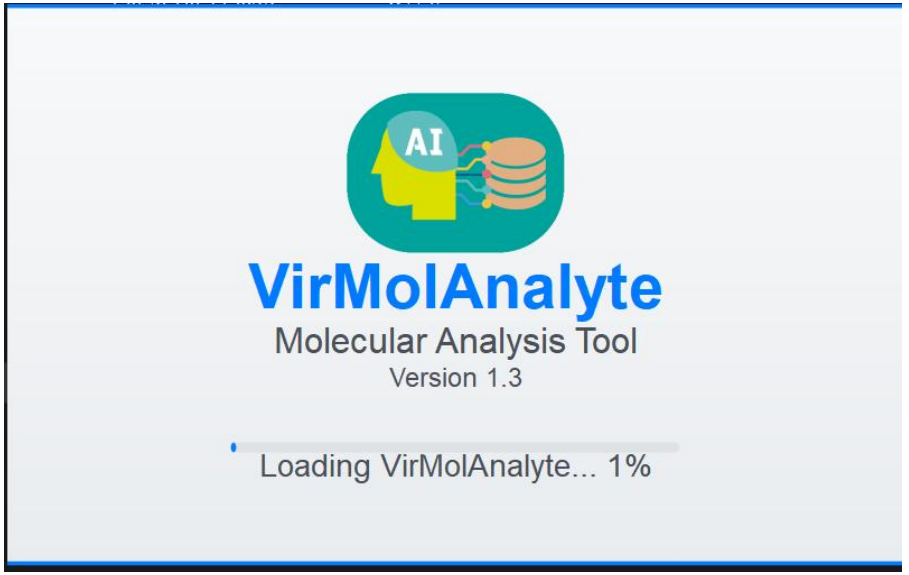
https://www.virmolanalyte.top/

Installation of VirMolAnalyte

1. Extract the installation package.

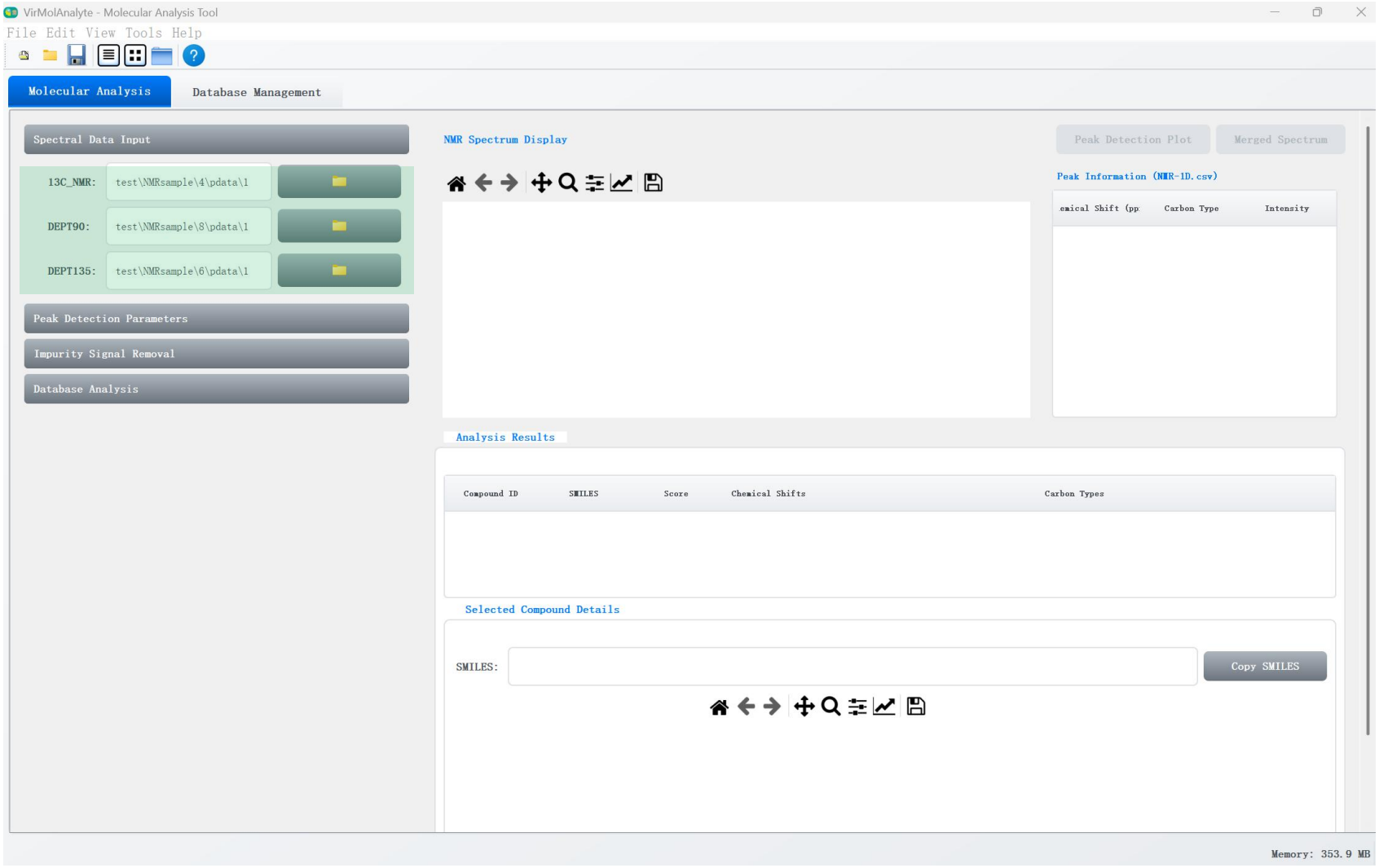


2. Click VirMolAnalyte.exe to run the software



Usage of VirMolAnalyte

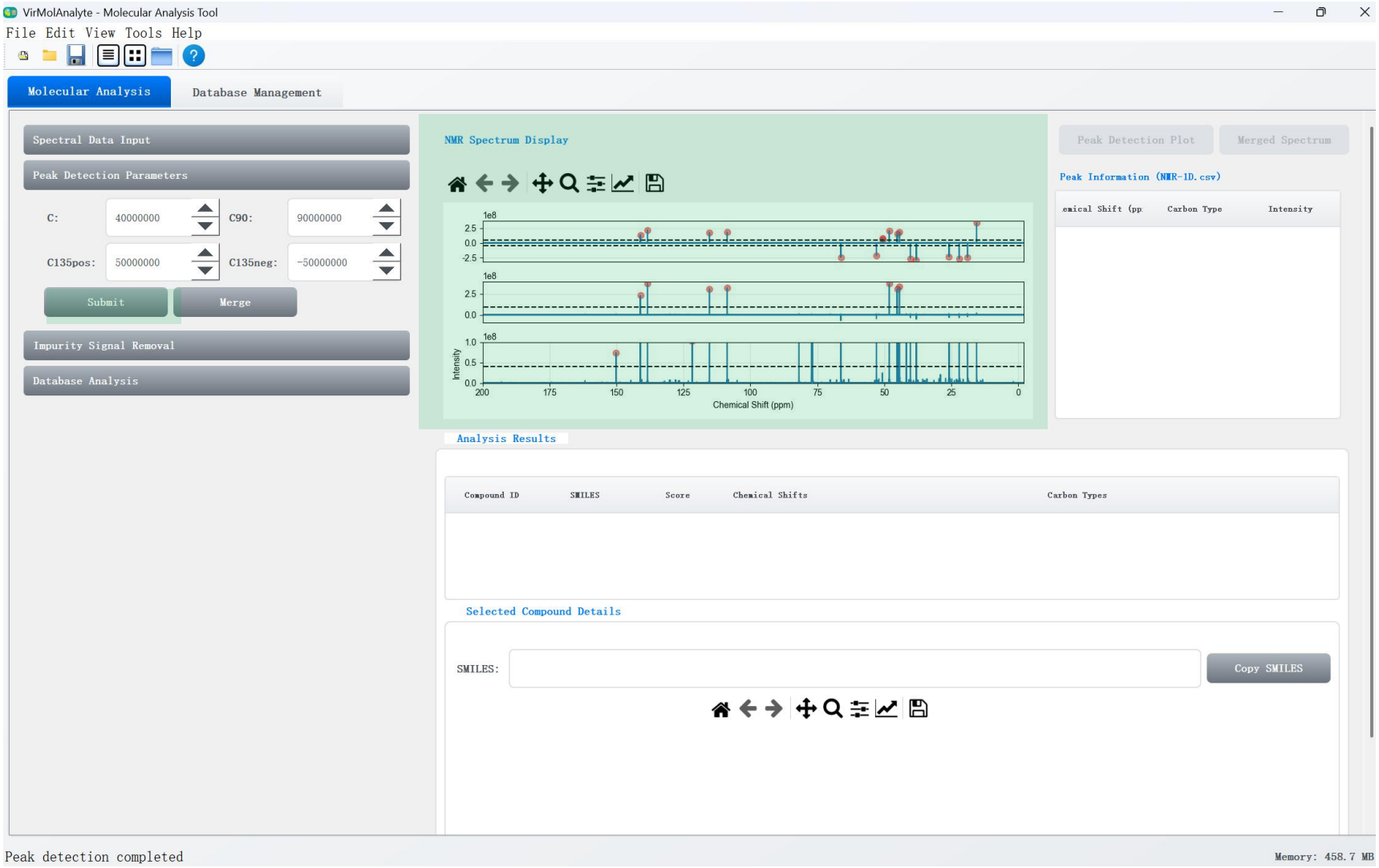
STEP1: Select the path of ^{13}C NMR, DEPT 90, DEPT 135 spectra.



Usage of VirMolAnalyte

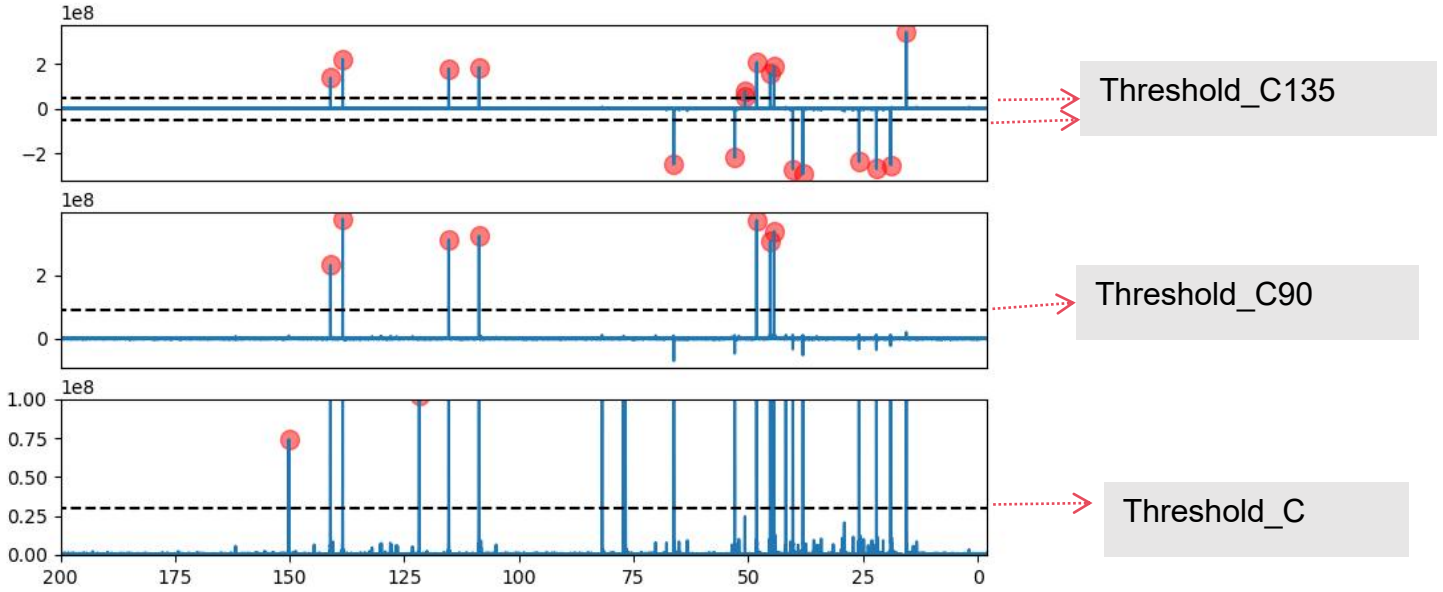
STEP2: Adjust the threshold to extract peaks

Set threshold<Submit



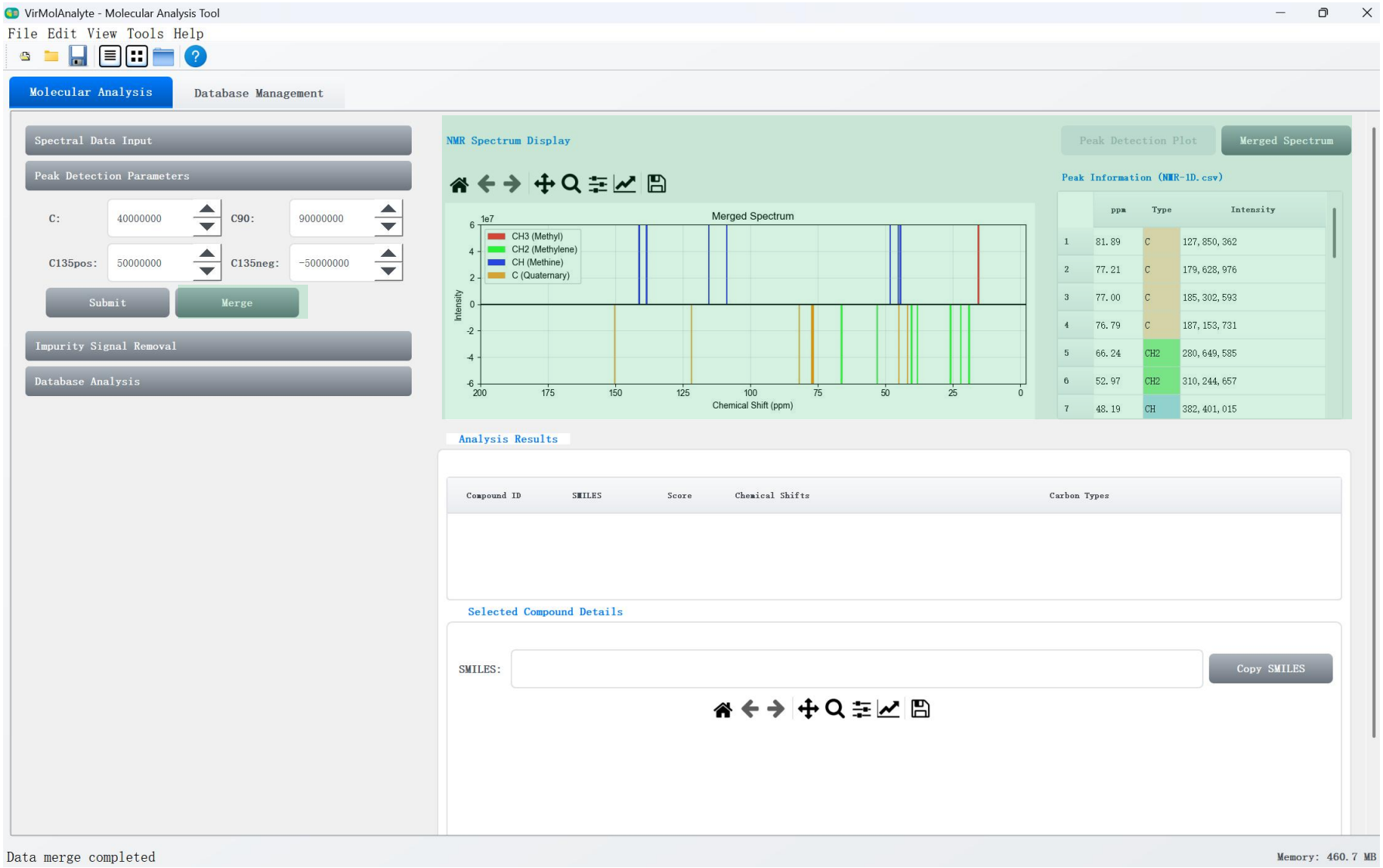
STEP2: Adjust the threshold to extract peaks

After clicking ***submit***, the tool will extract peaks from the raw data and adjust the threshold to ensure reasonable peak extraction



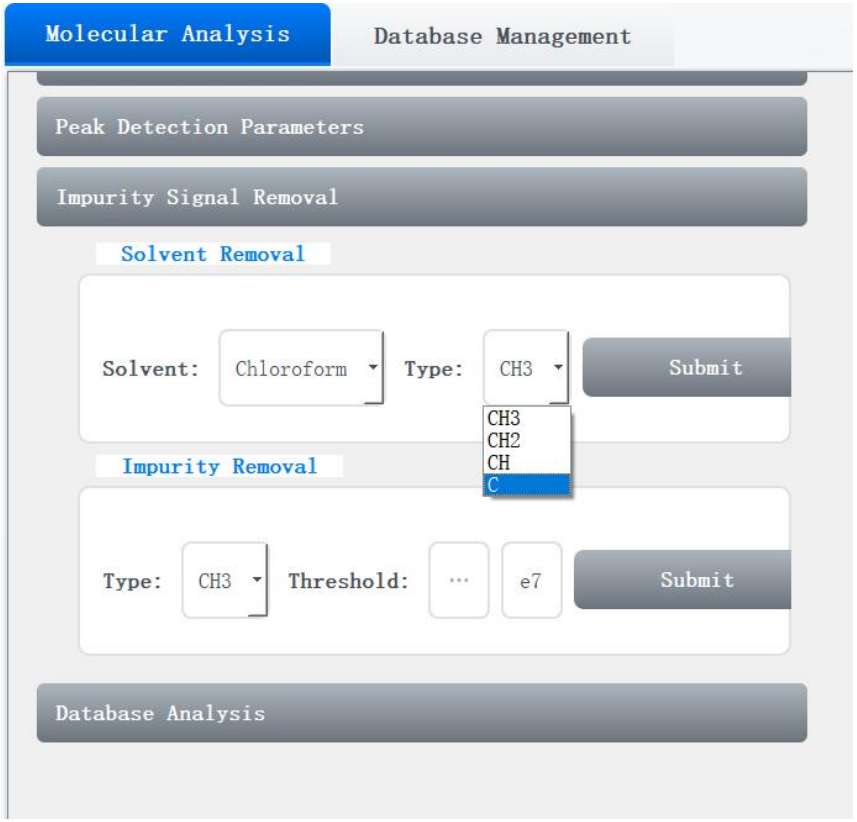
Usage of VirMolAnalyte

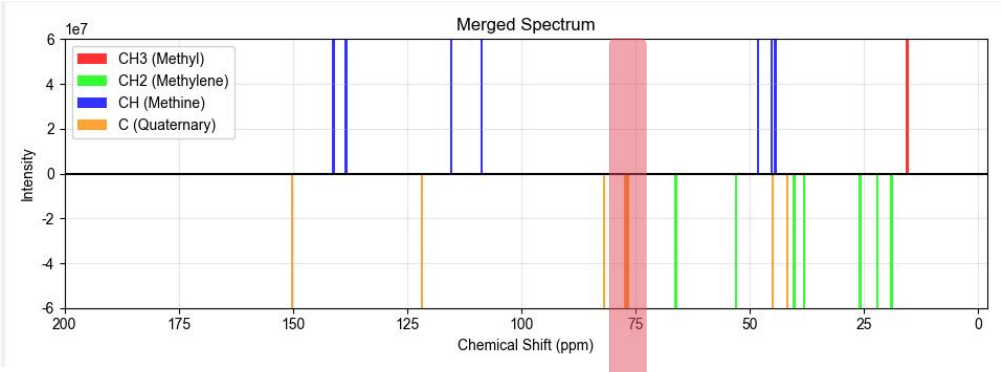
STEP3: Merge spectra to establish ^{13}C DEPT NMR spectra

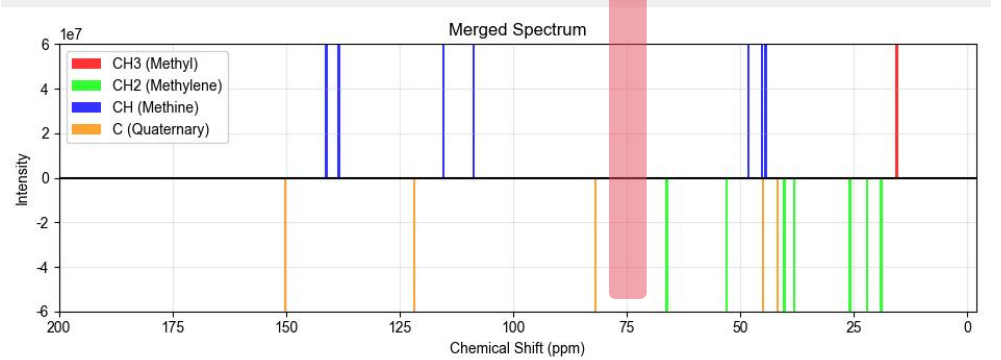


STEP4: Remove the signal peak of the solvent.

Select the solvent to be used in the experiment from the drop-down menu of solvents and choose the carbon signal category to be removed, then ***submit***





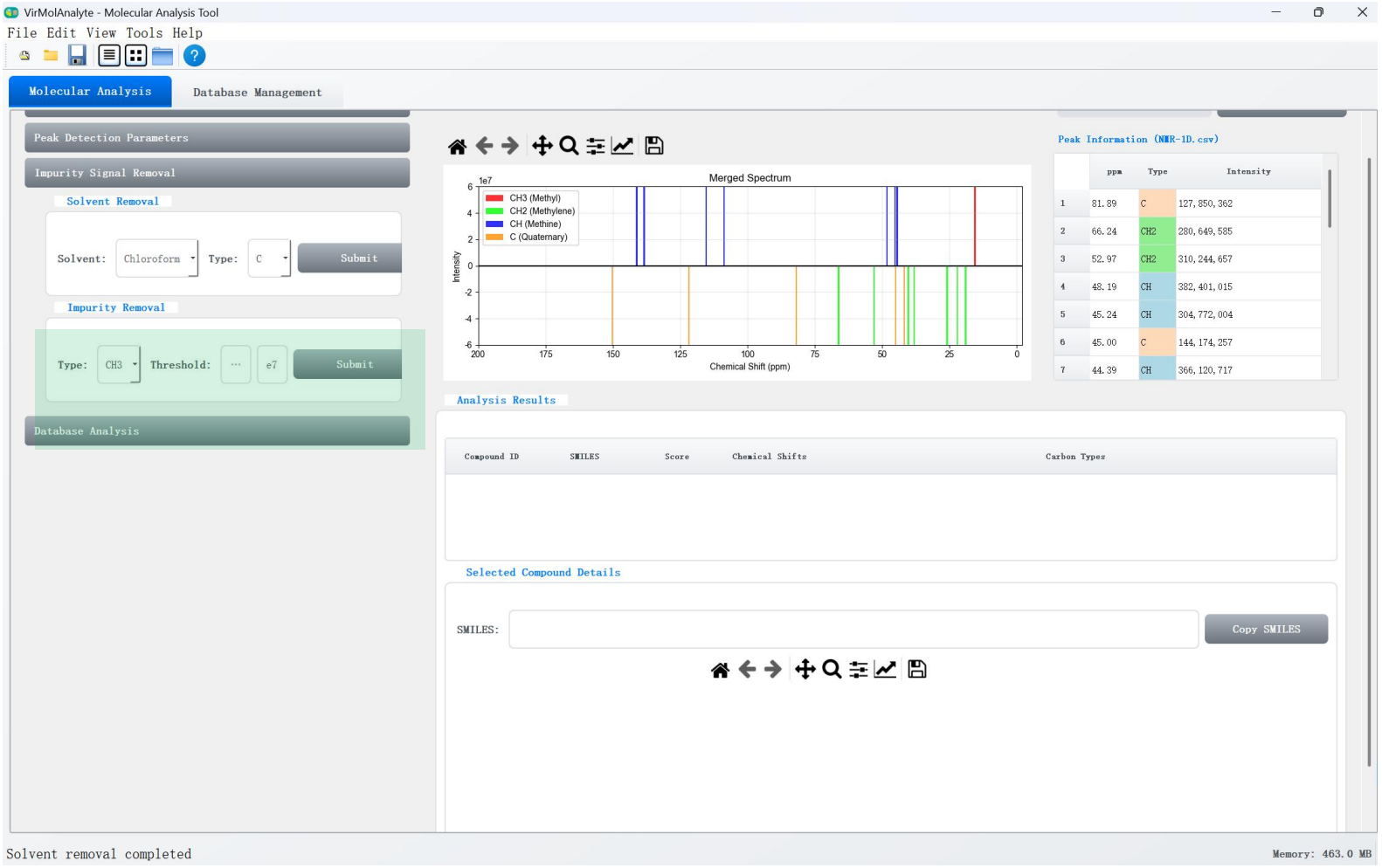


Note:Pay attention to distinguishing the carbon categories of solvent peaks

Usage of VirMolAnalyte

STEP4:Remove impurities

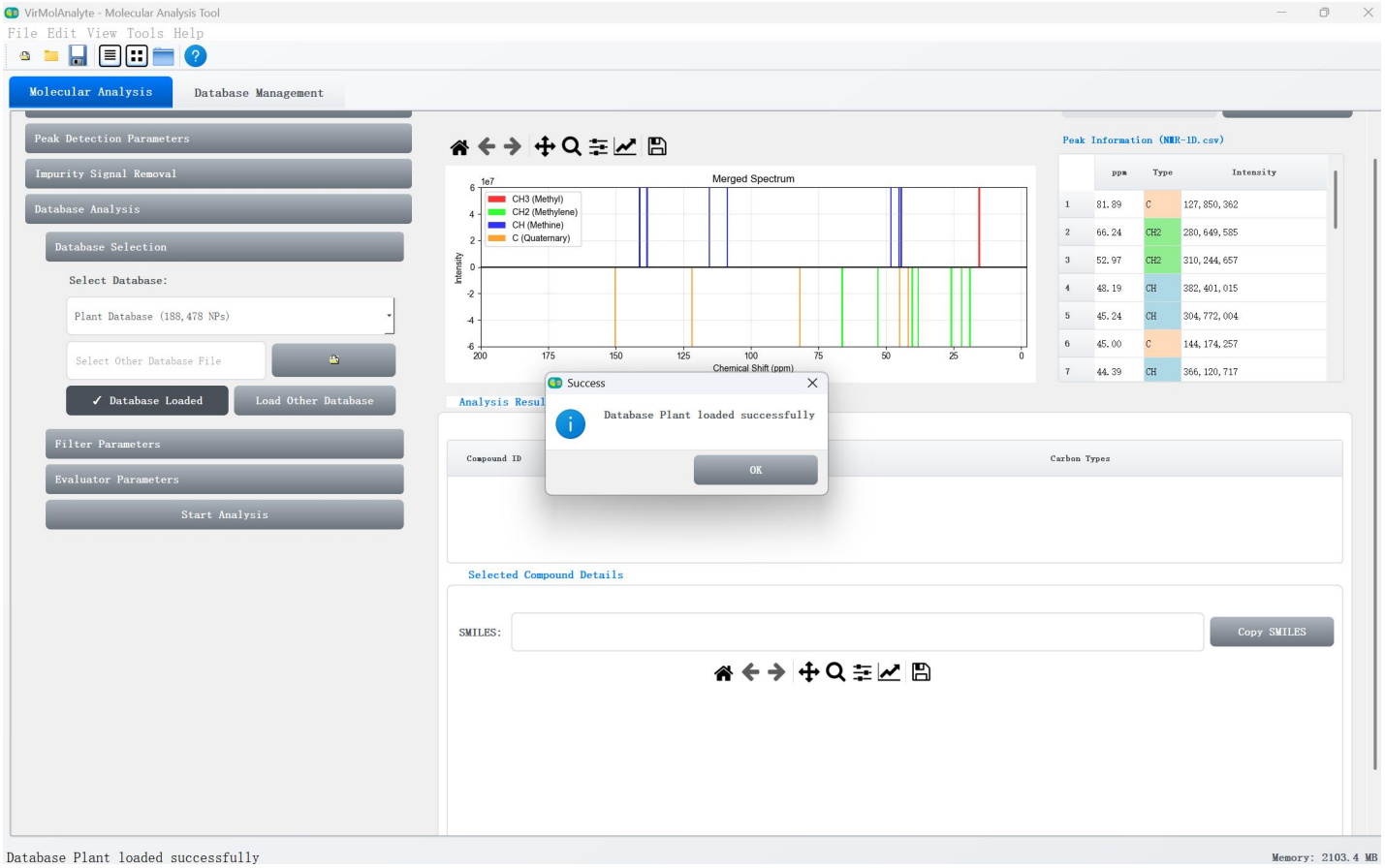
For a mixture where the impurity signal differs from the target compound, impurities can be removed by establishing a carbon-atom-based threshold.



Usage of VirMolAnalyte

STEP5: Load database

Select the appropriate database and click 'load database' to load the database;

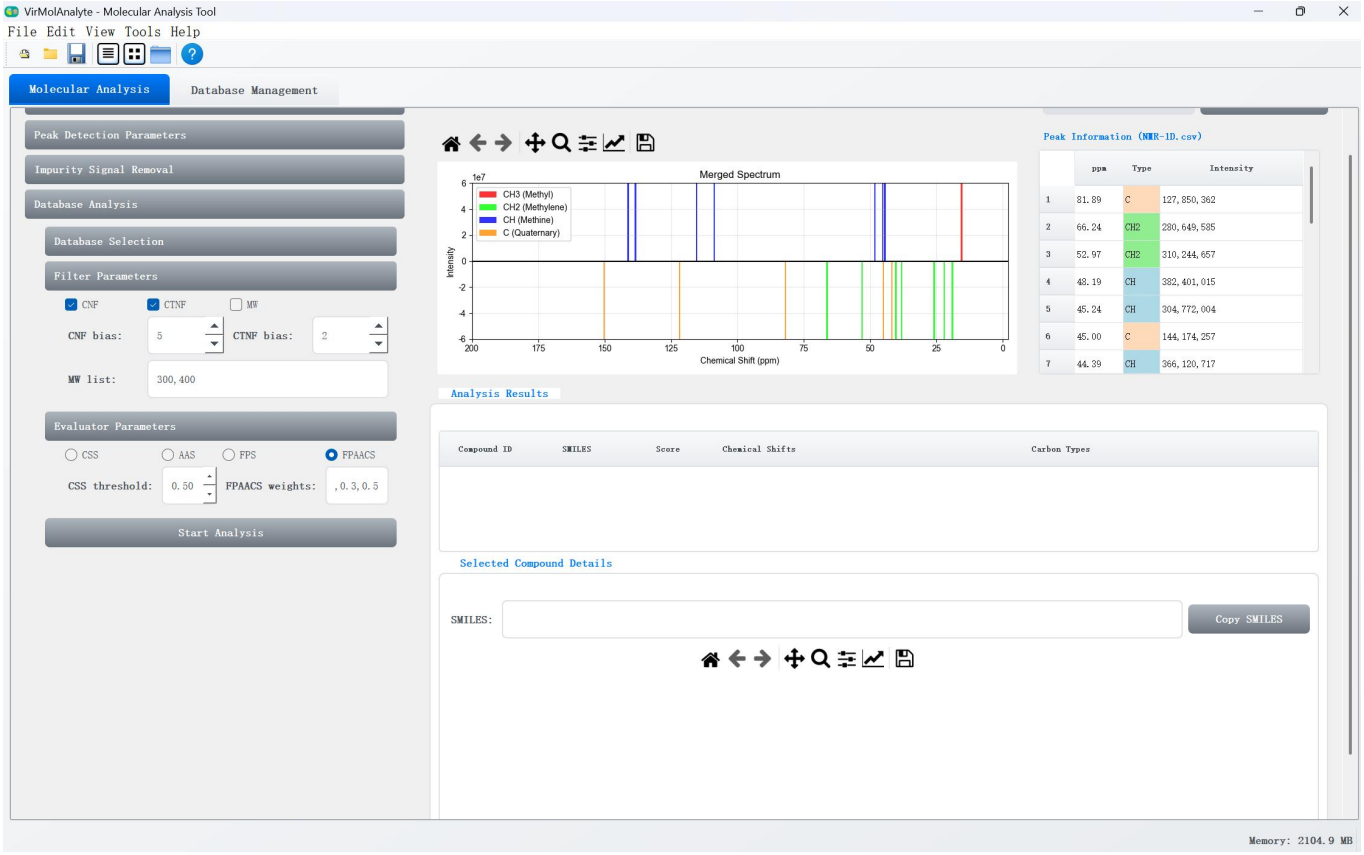


All database:
650,375 metabolites
Plant database:
188,478 metabolites
Human database:
217,347 metabolites
Microorganism:
36,427 metabolites

Note: The database only needs to be loaded during the first use, and subsequent tasks do not require repeated loading

STEP6: Set database search parameters

Select filter (Multiple Choice): By default, CNF (Number of Carbon Filters) and CTNF (Number of Carbon Filter Types) are selected. When the compound has an MS spectrum, MW can be checked and possible molecular weights such as "312, 345, 413" can be entered
Select evaluator (Single Choice): It is recommended to prioritize the FPAACS evaluator. recommended FPAACS_weight: 0.36, 0.16, 0.48



Usage of VirMolAnalyte

STEP7: Perform database search

Click the ***Start Analysis*** button to perform database analysis

STEP8: Analysis of Database Search Results

After clicking on the result entry, you can see the structure and comparison between the experimental ^{13}C DEPT NMR and the virtual ^{13}C DEPT NMR

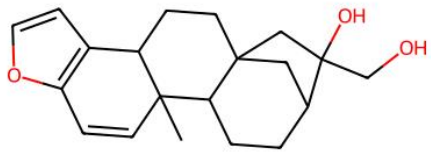
Analysis Results

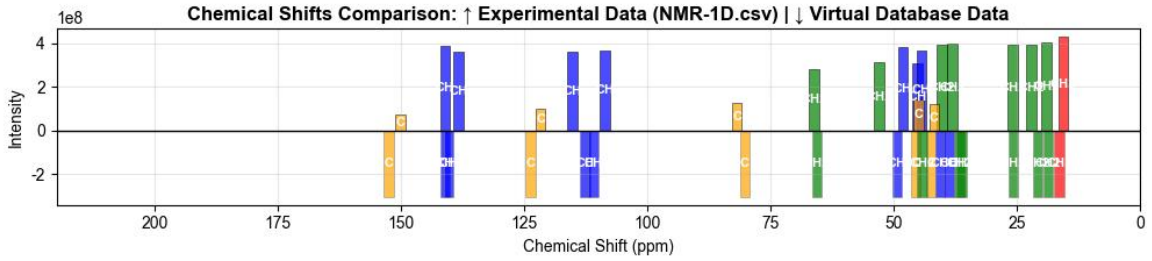
	ompound ID	SMILES	Score	Chemical Shifts (ppm)	Carbon Types
1	4004	CC12C=Cc3occc3C1CCC13CC(CCC12)C(O)(CO)C3	65.002	[16.38527 42.486748 141.12566 112.7092 152.52473 140.4448 110.979485 123.7509 40.602833 20.820316 36.719612 45.52128…	['q' 's' 'd' 'd' 's' 's' 'd' 'd' 's'…
2	165069	CC1=CCCC2C1(C)CC(O)C(C)C2(CO)CCc1ccoc1	62.302	[20.624367 141.7491 121.40474 26.313866 18.379913 43.30023 39.38704 24.387255 44.966553 67.609764 38.62079 12.806296…	['q' 's' 't' 't' 's' 'd' 'd' 's' 'q'…
3	3078	CC12CC=C3C1CCC13CC(CCC12)C(O)(CO)C3	62.046	[16.387362 36.65864 34.748543 18.326387 150.30975 140.08382	['q' 's' 't' 't'

Selected Compound Details

SMILES: CC12C=Cc3occc3C1CCC13CC(CCC12)C(O)(CO)C3

Copy SMILES

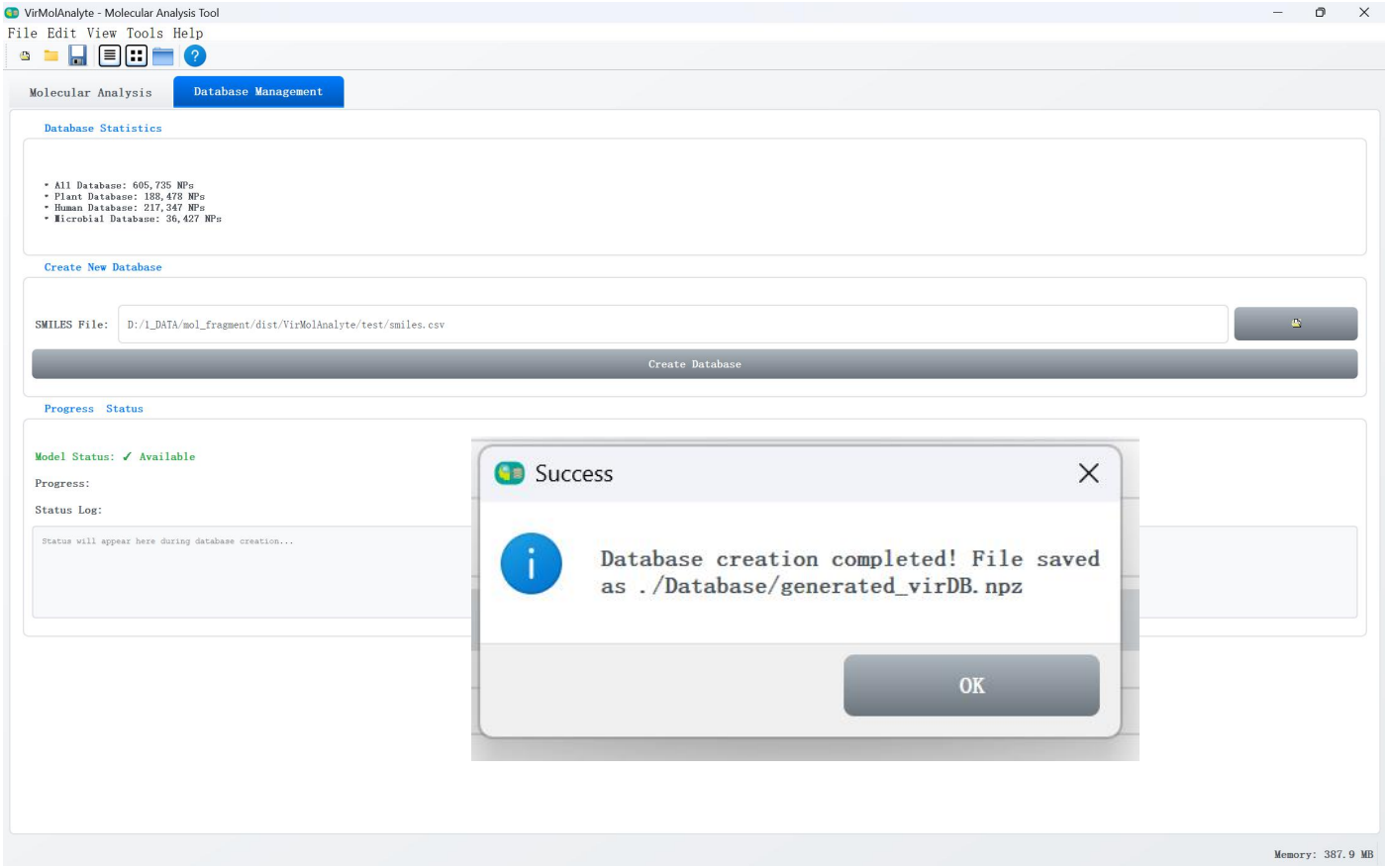




Usage of VirMolAnalyte

Generate your in house database

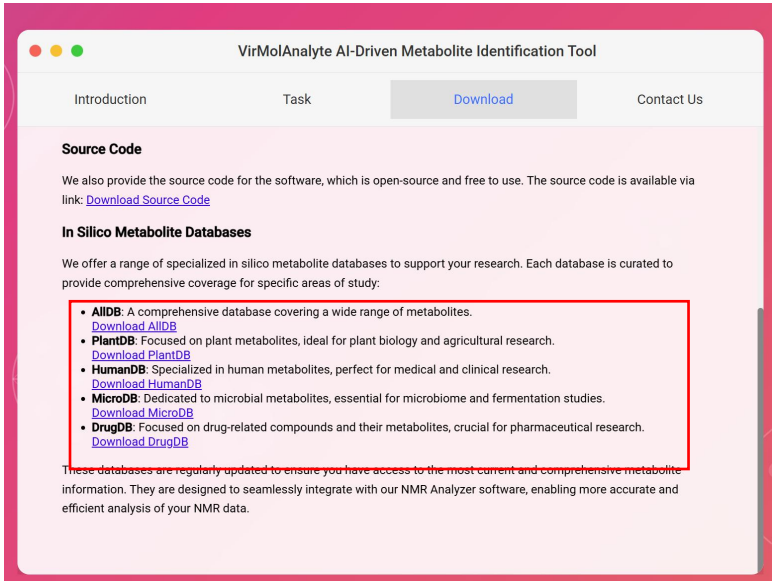
Place the molecular descriptors (smiles) used for database construction in a .csv file, and then run the construction method. *The test file is located at path "./test/smiles.csv"*



Note: In step 5 of the analysis, you can choose your database (Other database<load other database) for NMR analysis;Please ensure that Java is installed on your computer

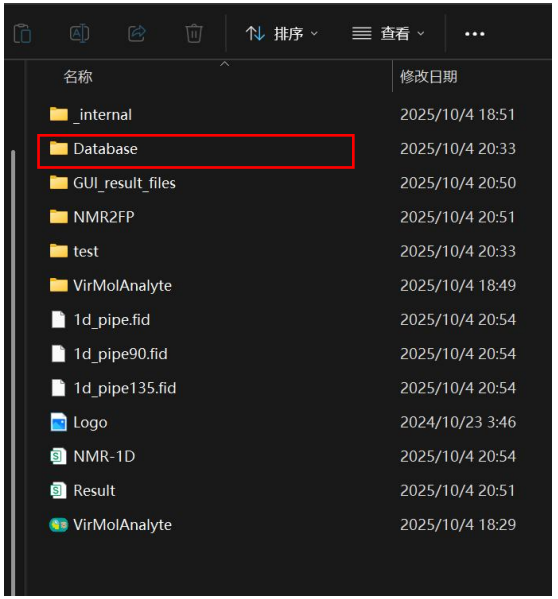
Database installation

1. Download data files from the web page

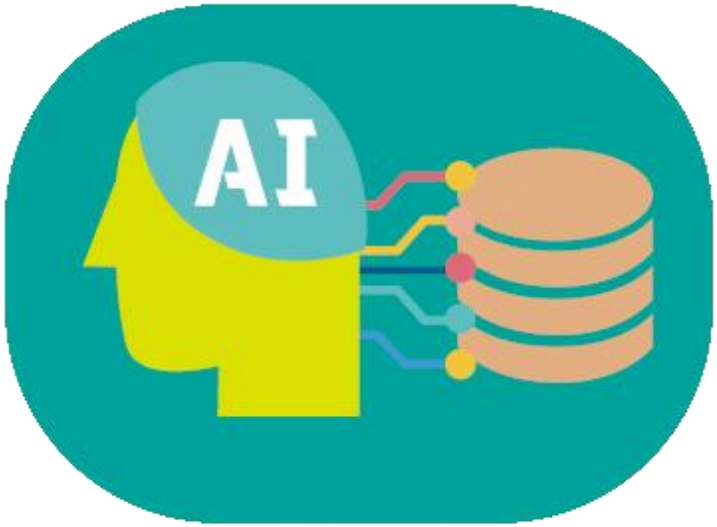


2. Retrieve database file from compressed file

3. Place the decompressed file (. npz) in the ***Database*** folder of the working directory



AllDB: Also known as Metabolites Multidimensional In Silico Database (MMDB), comprising information on 605,735 metabolites.
PlantDB: An in silico database of plant-derived metabolites, containing 188,478 metabolites.
HMDB: An in silico database primarily focused on human-derived metabolites, including 217,347 metabolites.
MicroDB: An in silico database of microbial-derived metabolites, encompassing 36,427 metabolites.
DrugDB: An in silico database focused on drug-related compounds and their metabolites, including 4,280 metabolites.



Thanks