

# ConCISE: Consensus Classifications of In Silico Elucidations

GNPS Task ID ?

Enter your GNPS task ID

CANOPUS summary file ?

Select File

Network info file ?

Select File

Export directory ?

Select Directory

Consensus levels ?

5) Superclass default: 50

6) Class default: 70

7) Subclass default: 70

Build Consensus

conciseBinder.ipynb

File Edit View Run Kernel Tabs Settings Help

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Filter files by name

/ src /

| Name          | Last Modified  |
|---------------|----------------|
| notebookT...  | 16 minutes ago |
| conCISE.py    | 16 minutes ago |
| ConciseAr...  | 16 minutes ago |
| conciseBin... | 16 minutes ago |
| conciseCLI... | 16 minutes ago |
| conciseGui... | 16 minutes ago |
| guiWidgets... | 16 minutes ago |
| testJobIDs... | 16 minutes ago |
| workflowM...  | 16 minutes ago |

Subnetwork consensus annotations from CANOPUS and library ID's

ConCISE takes your library identified compounds and putative annotations exported from CANOPUS in SIRIUS 4 and find consensus annotations at a network level.

Drag and drop your input files in the jupyter lab environment (left panel)

Replace the filenames and library ID number in the function below. If you would like to specify other thresholds for each level replace them as needed. They are ordered as superclass, class, subclass in the function and will default to 50%, 70%, 70%.

The format looks like: python3 conciseCLI.py libraryID canopus\_summary.tsv subnetworkFile.tsv 50 70 70

[ ]: !python3 conciseCLI.py 16616afa8edd490ea7e50cc316a20222 notebookTestFiles/canopus\_summary.tsv notebookTestFiles/Node\_info.tsv 50 70 70

Run the above cell.

Download your putative annotation file (left panel and right click to download).