Data preparation for part 1:

1. In Stats for FBMN web app:
https://fbmn-statsguide.gnps2.org/
    1. Drag and drop metadata and quant table files into data cleaning page
    2. Uncheck “create index automatically” so index will match the nodes of your Cytoscape network
    3. Remove blanks, I change my cutoff to 0.1.
    4. Submit data for statistics and download the filtered feature table as a csv
2. Open csv in excel and delete row ID, row m/z, and row retention time columns
3. Import the csv into the Python notebook and run the part 1 code.

Data preparation for part 2:

1. From GNPS, download Cytoscape data and open in Cytoscape
2. Import Sirius data into the Cytoscape network
    In GNPS/Cytoscape:
        i. SIRIUS will output a bunch of files into your set directory when you export summaries.
        ii. To import this information into your GNPS FBMN cytoscape network:
            1. Open your GNPS graphml cytoscape network.
            2. Click import table.
            3. Import “canopus compound summary”. You can import other tables from SIRIUS, just make sure they have a “featureID column”.
            4. Scroll to the back of this table to find feature ID. This feature id corresponds to the GNPS features.
            5. Click on the header for feature ID and change it to being the “key”. Make sure to be importing this table to the node table.
            6. Click import. This will populate your annotations onto the network.
            7. You can now color by class of compounds, etc. that came from SIRIUS.
3. Import the center scaled peak area csv exported from part 1 into Cytoscape following the same process from step 2, make the metabolite column the key.
4. Remove blank features from the Cytoscape network
    1. Scroll horizontally to the end of the table. There should be columns that correspond to each treatment. Double click the header of one of the columns to sort all of the populated rows together
    2. Any rows that do not have center-scaled peak area data in them were filtered out during blank removal in the stats for FBMN webapp. Shift click to highlight all the rows with peak area data, then right click and choose select nodes from selected rows, then in the toolbar at the top of the page click new network from selection
7. The new network contains only features that were not filtered out during blank removal. Export the Cytoscape table as a csv file

8. Optionally, open the file in numbers or excel and edit the Analog:Compound_Name column so that any library hits are referred to with shorter names. Long labels will mess up the heatmap dimensions and make it harder to read
9. Import the csv into part 2 of the Python notebook and run the code.