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Atmospheric Measurement Techniques
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EGU

Supplement of

UCB-GLOBES: an open-access mass spectral database of identified and unidentified atmospheric organic compounds

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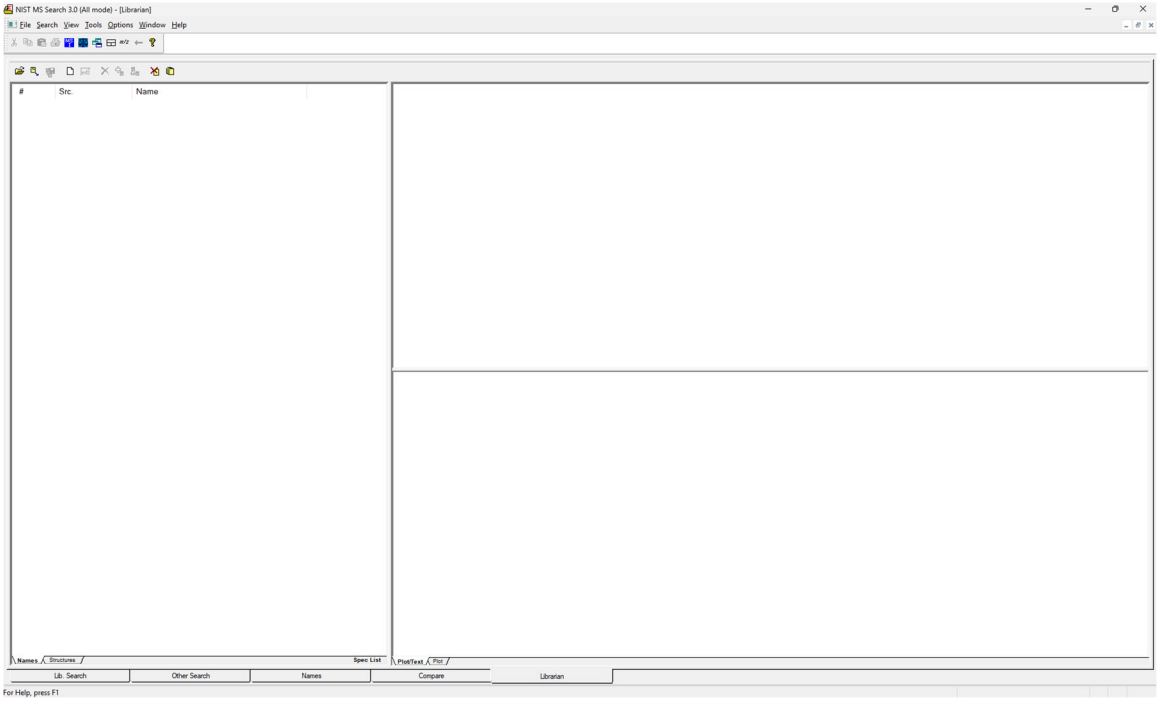
Supplementary Information Contents

S1. Using UCB-GLOBES data within the NIST MS Search Program

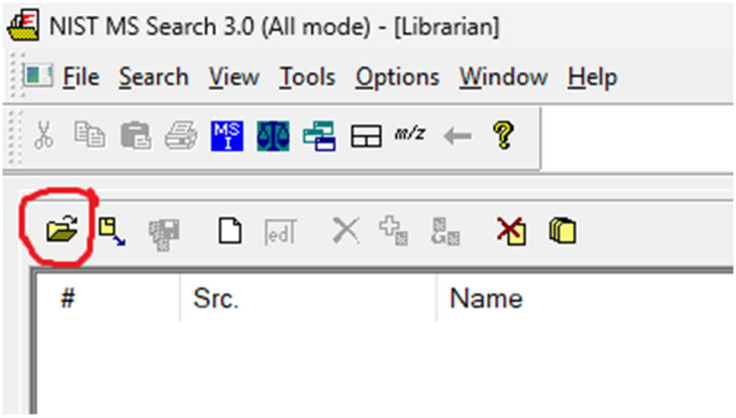
The following instructions are intended as a guide for importing UCB-GLOBES MS libraries into the NIST MS Search program. A free-of-charge version of the NIST MS Search program (NIST MS Demo) is available without the for-purchase NIST main library if the user would like to simply import their own MS and other custom MS libraries such as UCB-GLOBES. These instructions assume that the NIST MS Search/NIST MS Demo program is already installed.

All screenshots shown in this section Steps 1-18. are from NIST MS Search v3.0 program, software created by the NIST Mass Spectrometry Data Center, NIST, Gaithersburg MD, USA (NIST Mass Spectrometry Data Center, 2023).

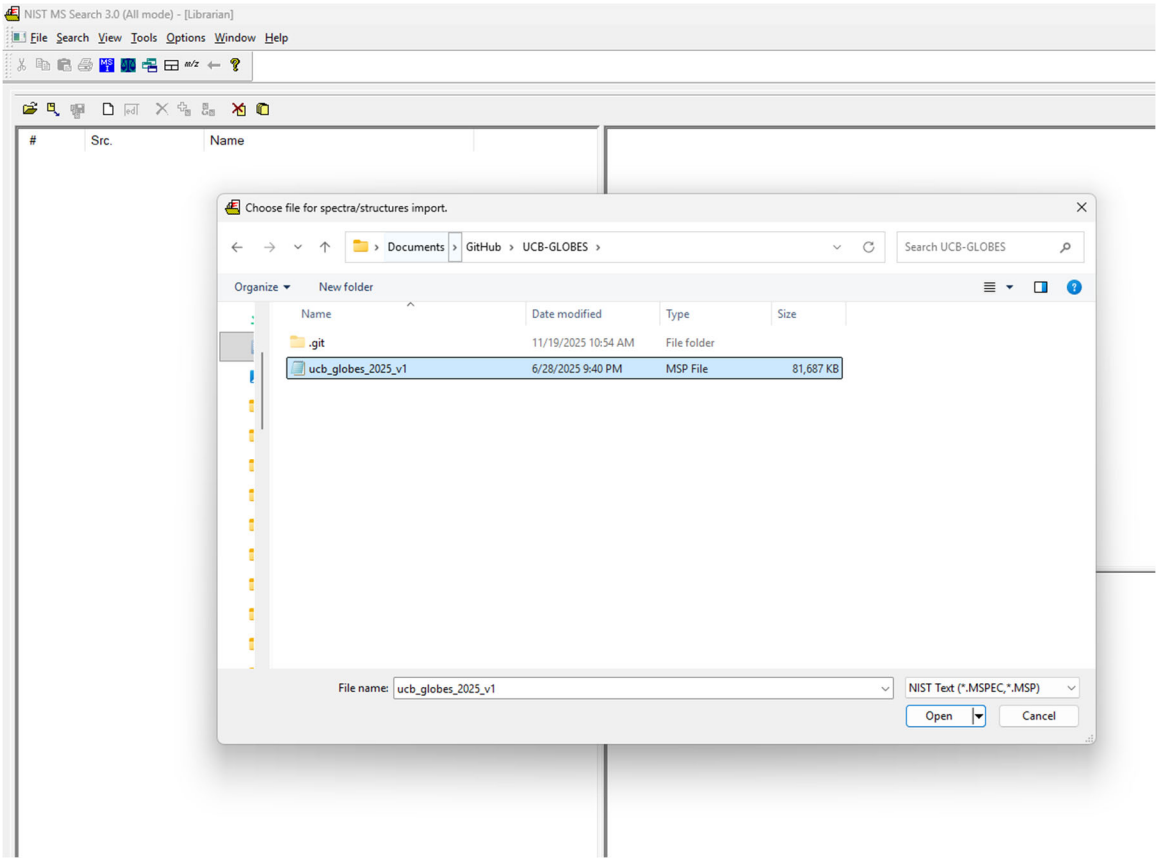
1. Download the desired UCB-GLOBES MS libraries in .MSP file format from https://sites.google.com/berkeley.edu/goldstein-lab/resources
2. The dataset specifically used in this study is also accessible on this webpage as well as through the DOI: 10.5281/zenodo.18176760.
3. Open the NIST MS Search program.
4. Go to the Librarian Tab. If applicable, save/perform any actions with any MS in the SpecList that you would like to do before clearing the list. Then, clear (select CTRL+A and DELETE) any entries in the left SpecList window. Program should look like this:



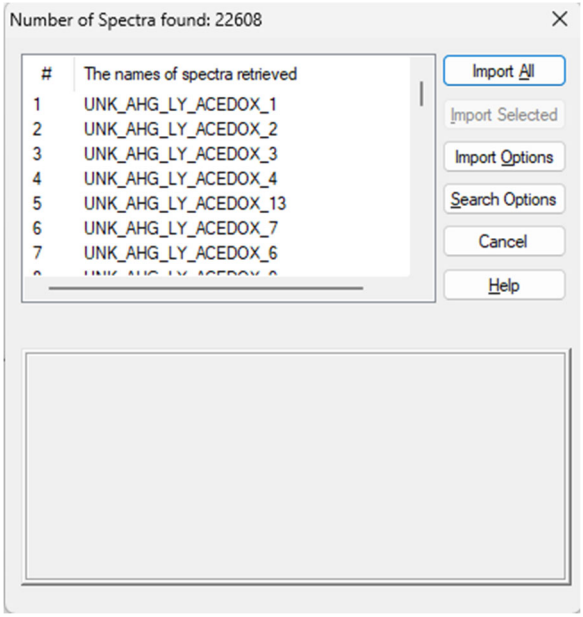
5. Click “Import” in upper left corner:



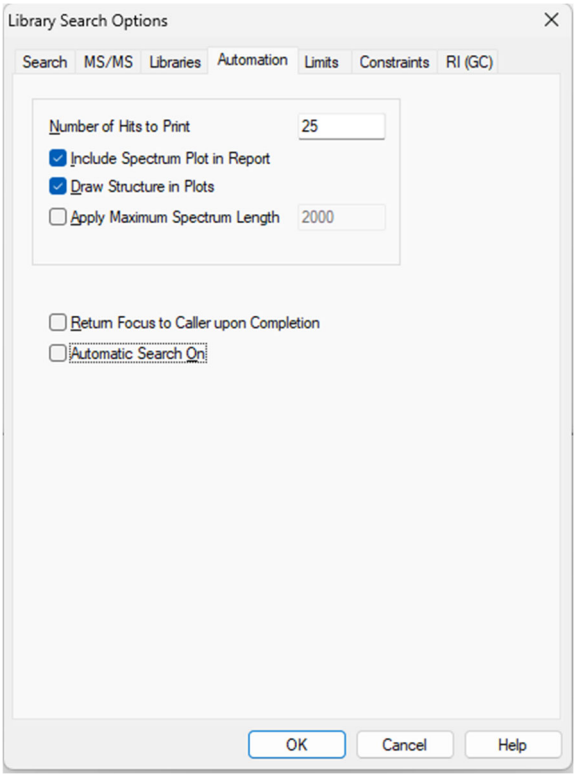
6. Navigate to the location of the downloaded .MSP file that you want to import. Select and click Open.



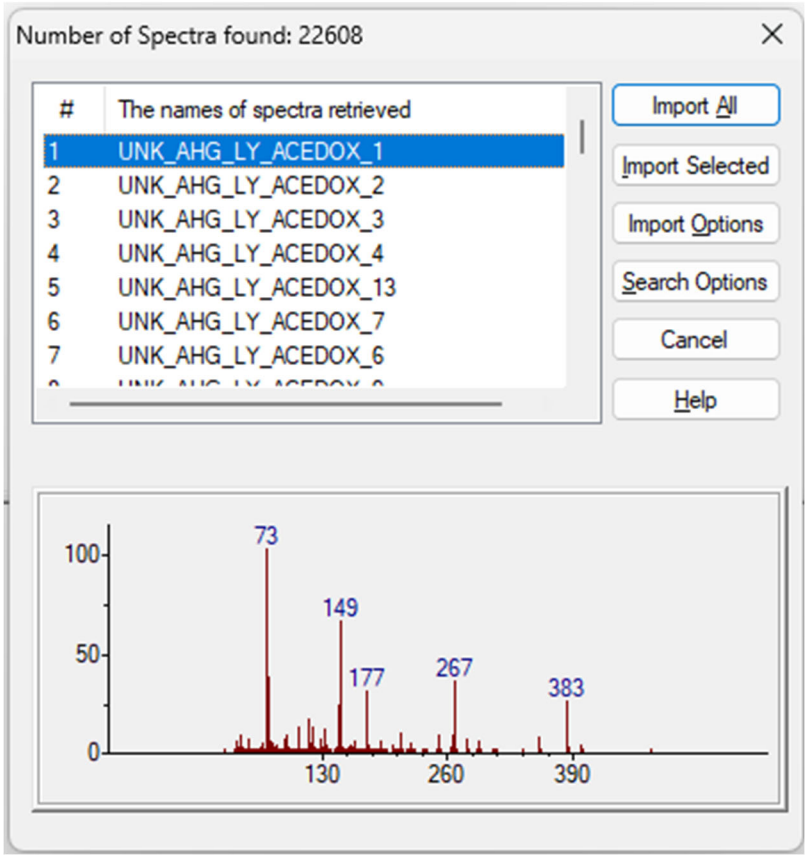
7. A window will open showing the number of spectra found in the .MSP file. Click on “Search Options.”



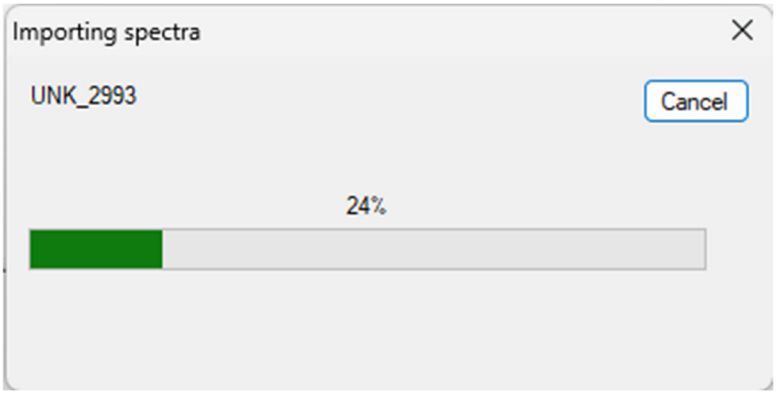
8. To dramatically speed up the import of MS, go to the “Automation” tab, and uncheck the “Automatic Search On” option. Click “OK.”



9. Then choose the spectra from the list that you want to import and select “Import Selected” or “Import All.”

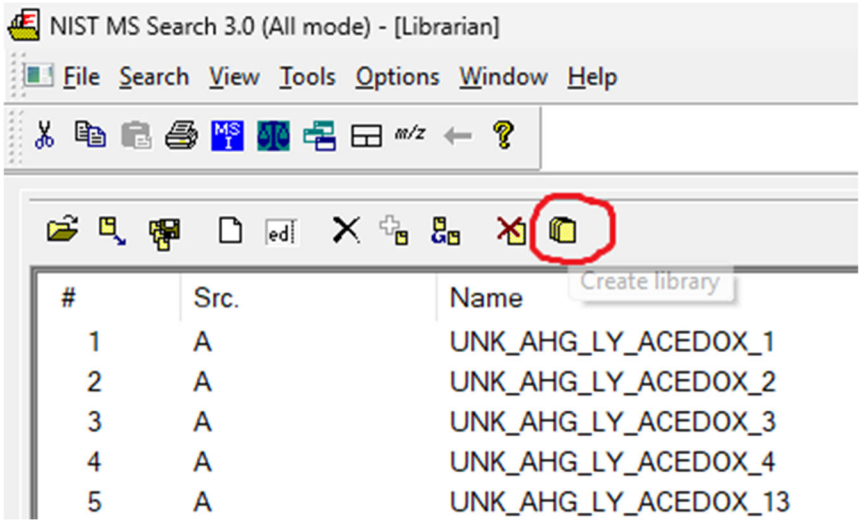


A progress window will show the status of importing mass spectra:

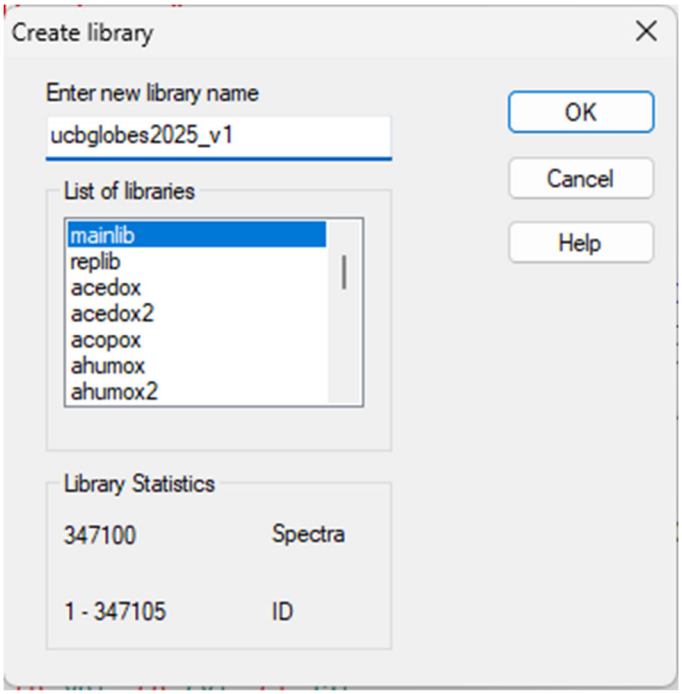


The Librarian tab should now be populated with all the imported spectra.

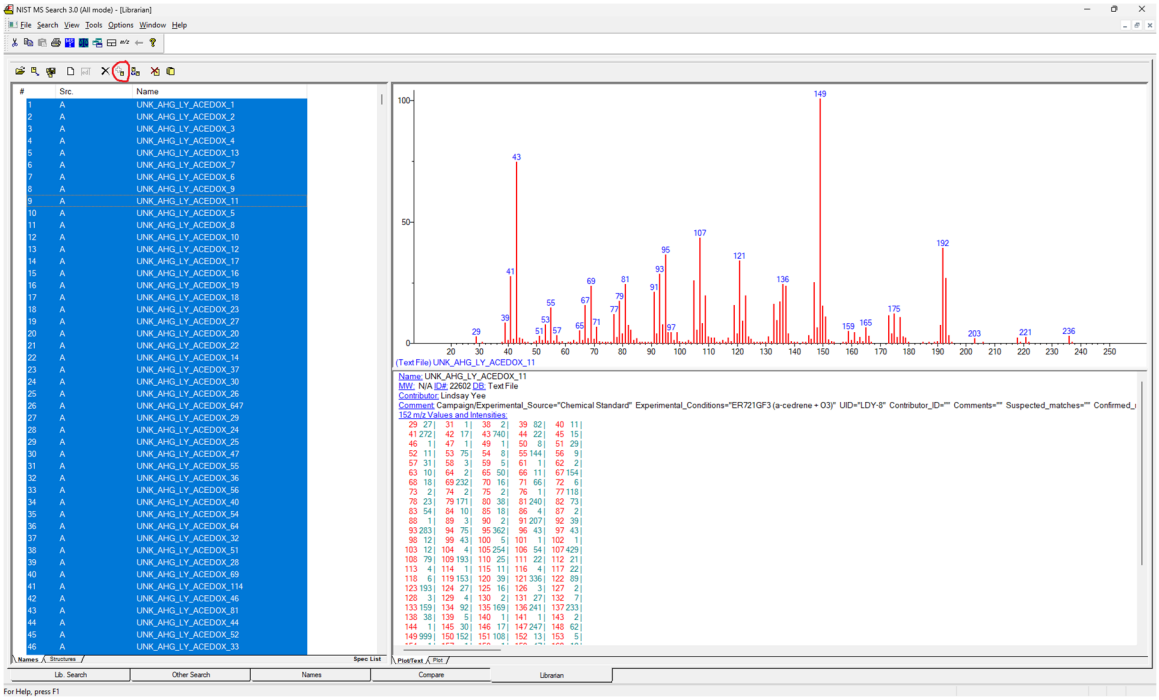
10. Now we will add all the spectra to a user custom library that can be accessible as a library to search against when running MS searches. Click on “Create Library” in the upper left menu bar.



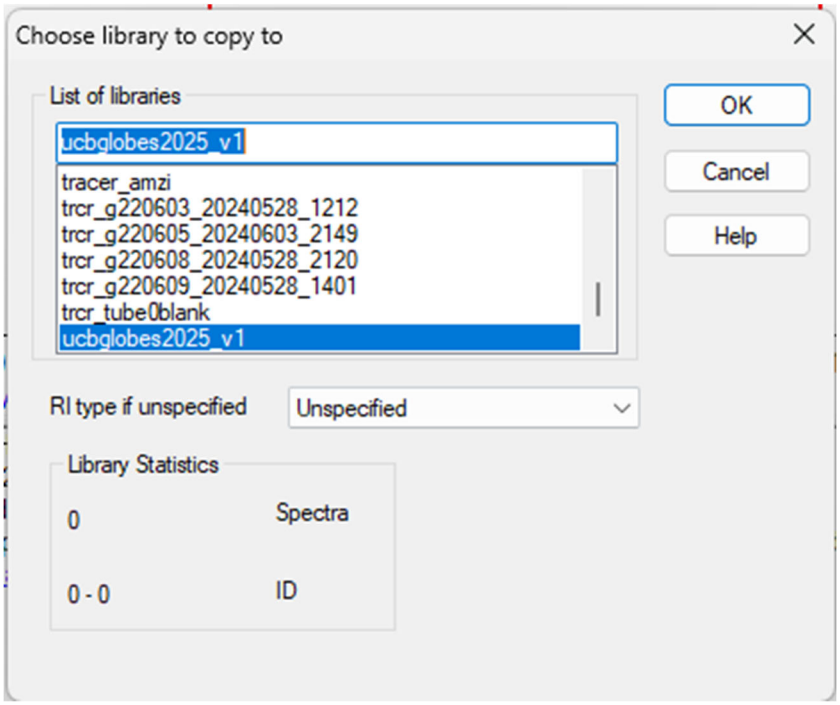
11. Enter a new library name in the prompt and push “OK.”



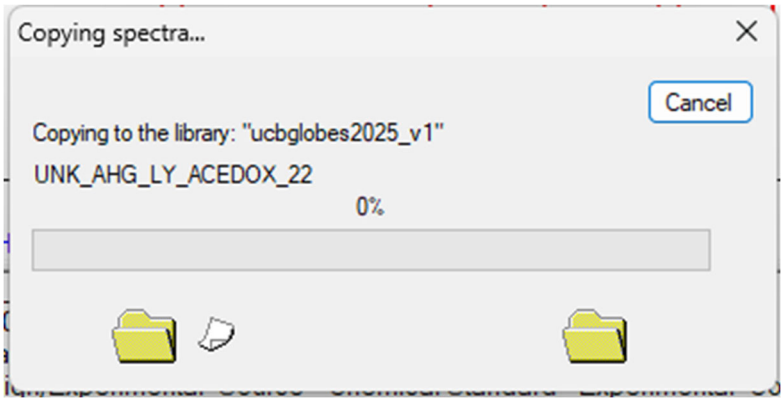
12. Then, select all MS in the librarian tab and click on “Add to Library” in the upper left menu.



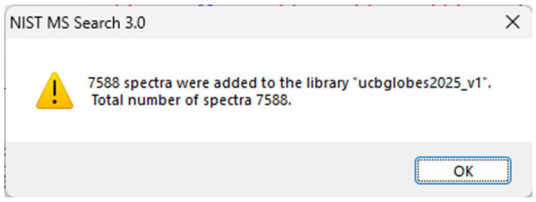
890 13. Choose the library to copy to (the library name you created in step 11). Note that the library currently has 0 spectra in it since you just created it, but have not added spectra to it. Then push “OK.”



It will take some time for the spectra to be copied over to the selected library and you will see a progress bar, example below:

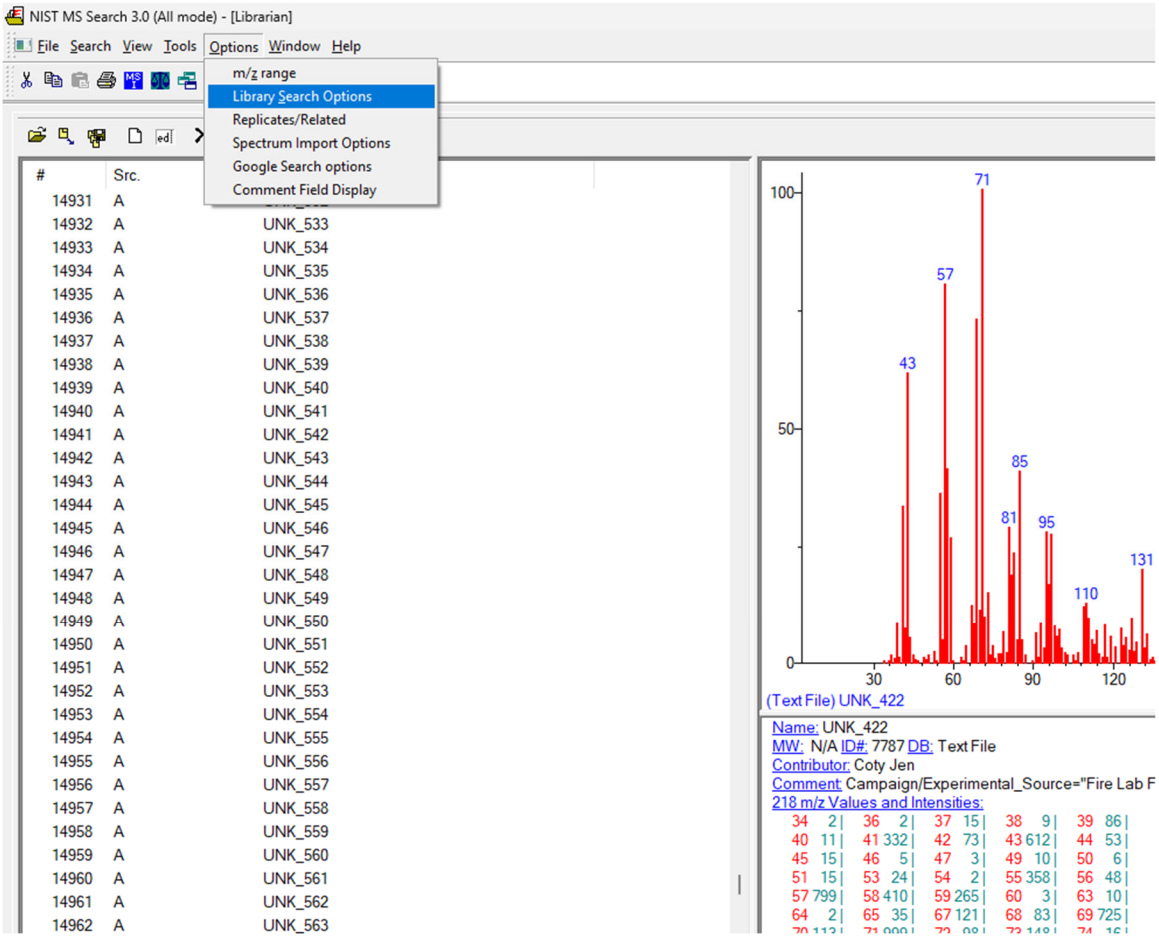


After all spectra are copied over, you should receive a confirmation showing how many spectra have been added to the library (example below):

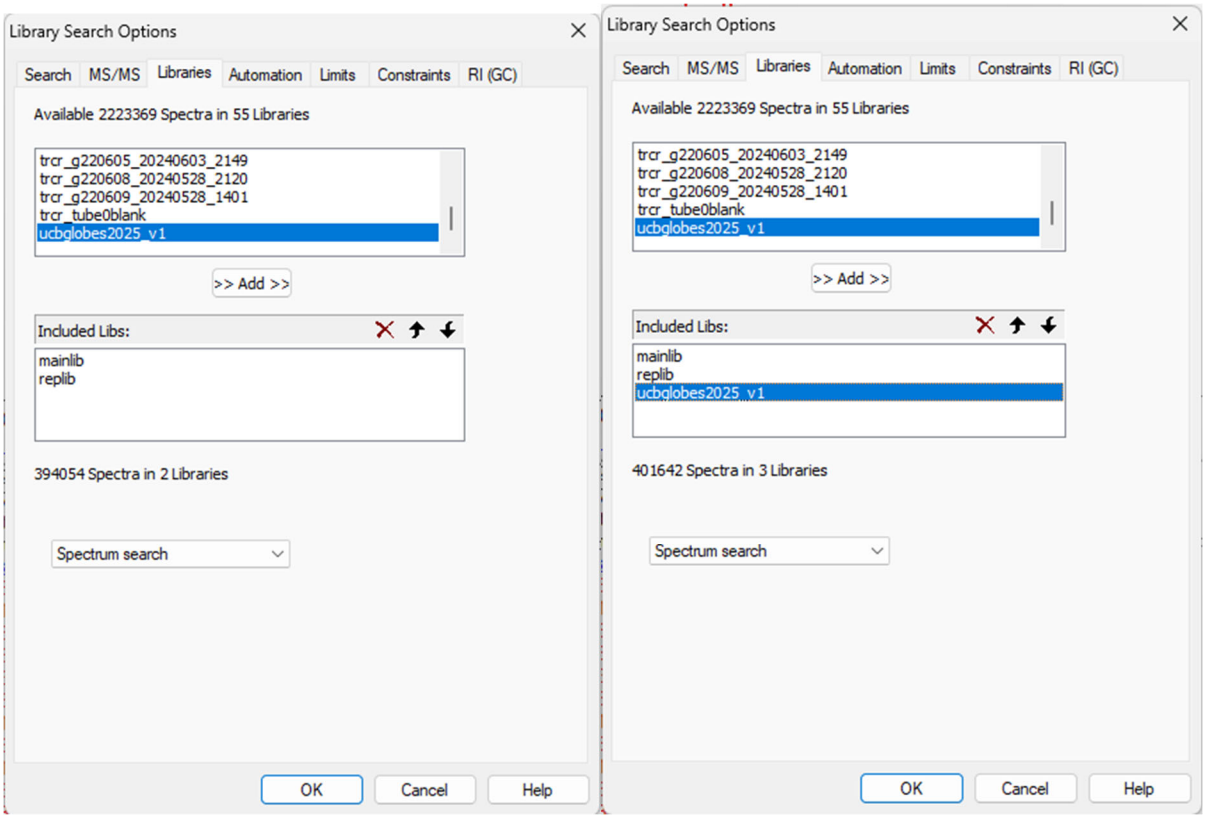


This mass spectral library is now in the NIST MS Search library format and is located in the MSSearch folder of the NIST MS Search program. By default it would be in C:\NISTXX\MSSEARCH with all library files under the library name you created in Step 11.

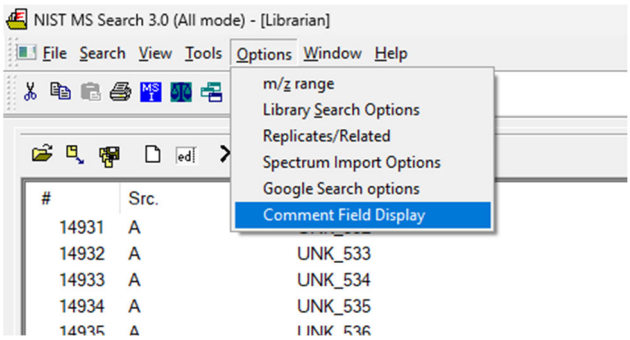
14. Now we need to set NIST MS Search program settings to search against this library and to view the UCB-GLOBES metadata comments in a more readable format. Go to Options > Library Search Options in the upper menu.



15. Under the Libraries Tab, select the library (in this case, ucbglobes2025_v1) in the Available XX Spectra in XX libraries (those that are in the C:\NISTXX\MSSEARCH folder) and click “>>Add>>” so the selected library is now listed under the Included Libs section.



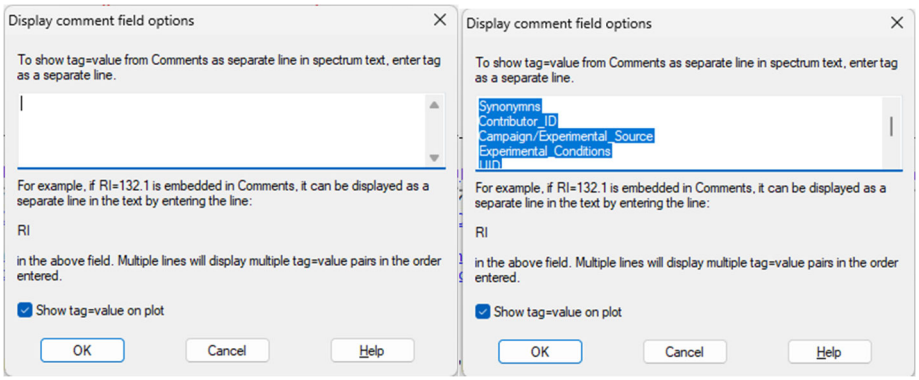
16. Click “OK”.
17. Go to Options > Comment Field Display from the upper left menu.



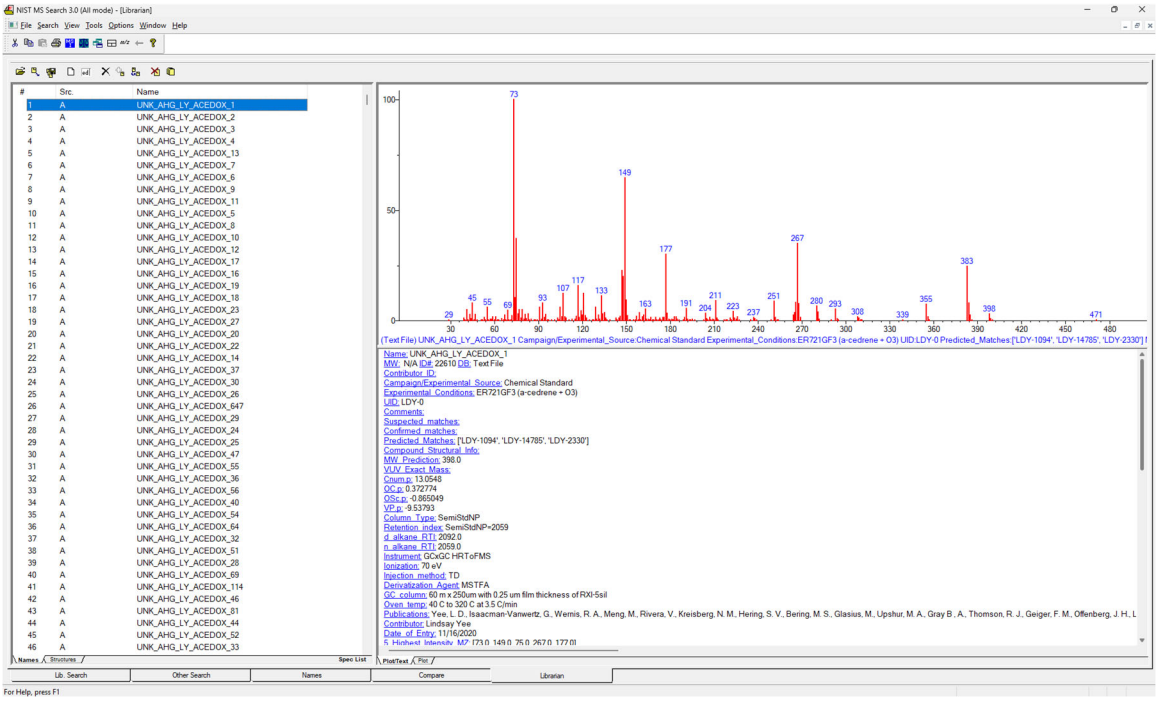
915

18. Copy and paste the following list of "tags" that are used in UCB-GLOBES MS annotations into the Display comment field options dialog.

```
Synonyms
Contributor_ID
Campaign/Experimental_Source
Experimental_Conditions
UID
Comments
Suspected_matches
Confirmed_matches
Predicted_Matches
Compound_Structural_Info
Formula
MW_Prediction
VUV_Exact_Mass
CAS#
Ch3MS-RF_Cnum.p
Ch3MS-RF_OC.p
Ch3MS-RF_OSc.p
Ch3MS-RF_VP.p
Column_Type
Retention_index
d_alkane_RTI
n_alkane_RTI
Instrument
Ionization
Injection_method
Derivatization_Agent
GC_column
Oven_temp
Publications
Contributor
Date_of_Entry
Num Peaks
5_Highest_Intensity_MZ
Base_Peak
```



Click OK. Now, the mass spectral entries are displayed with comment field entries separated into lines based on the comment field "tags" in 18.



960 NIST MS Search is now configured to search amongst the installed UCB-GLOBES libraries when conducting future MS searches and displaying the MS entries in a more accessible format.

S2. UCB-GLOBES MS Data Visualization and Comparison Tools in Jupyter Notebook

The Jupyter Notebook with MS Data Visualization and Comparison Tool is shared online at https://github.com/lyee002/UCB-GLOBES-MS-Data-Visualization-and-Comparison-Tool with DOI: 10.5281/zenodo.18177255 for adaptation and use in analysing MS data from UCB-GLOBES. At the time of publication, this Jupyter Notebook consists of eight cells with screenshots and example cell outputs below. The code/contents of some cells are abbreviated as indicated below.

UCB-GLOBES MS Data Visualization and Comparison Tool

Welcome to the **UCB-GLOBES Mass Spectrometry Data Visualization and Comparison Tool**! This notebook is designed to help you **interactively explore and compare** mass spectra with ease.

What You Can Do with This Tool:

- **Input two mass spectra** and **visually compare** them side-by-side
- **Generate a cosine similarity matrix** from **multiple spectra** of your choice
- Gain insights into **spectral similarity and patterns**

How to Use This Notebook

The following cells will guide you **step-by-step** through the process, including:

1. Uploading or selecting mass spectra
2. Plotting spectra for visual inspection
3. Calculating cosine similarity
4. Interpreting results from the similarity matrix

Feel free to begin at the next cell and follow along — all inputs and actions are clearly explained. Happy analyzing!

Original notebook author Stephanie Xu 7/3/2025, Last modified by Lindsay D. Yee 11/19/2025 as Version_v1

[1]:
```
#Action: Run the cell

#Purpose : Install all the libraries needed for later use
!pip install requests pandas gdown numpy
!pip install ipywidgets
!pip install --upgrade ipywidgets
!pip install plotly
```

```
Requirement already satisfied: requests in c:\anaconda3\lib\site-packages (2.32.3) •••
```

[2]:
```
#Action: Run the cell

#Purpose : Import all the libraries needed for later use

import re
import requests
import pandas as pd
from io import StringIO
import gdown
import plotly.graph_objects as go
import ipywidgets as widgets
from IPython.display import display, clear_output
from math import sqrt
import plotly.io as pio
from datetime import datetime
from IPython.display import HTML
import io
import numpy as np
import plotly.offline as pyo
```

Run Cell 3 to download the latest UCB-GLOBES database as a csv file.

```
[3]: #Action: Run the cell / replace the file_id with new input if necessary
pio.renderers.default = 'notebook'

file_id = '19OqBF98NZEOUX7MnzciliyZC5Vmfe1_Z'
url = f'https://drive.google.com/uc?id={file_id}'
output = 'ucbglobesdatabase.csv'
gdown.download(url, output, quiet=False)

print(f"✅ Data last pulled on data: {datetime.now().strftime('%Y-%m-%d')}")

database = pd.read_csv(output, low_memory=False, on_bad_lines='skip')
database.head()
```

```
Downloading...
From (original): https://drive.google.com/uc?id=19OqBF98NZEOUX7MnzciliyZC5Vmfe1_Z
From (redirected): https://drive.google.com/uc?id=19OqBF98NZEOUX7MnzciliyZC5Vmfe1_Z&confirm=t&uuid=65002136-5afd-4b52-9b37-f6173ffe9c7d
To: C:\Users\Lindsay Yee\Documents\GitHub\UCB-GLOBES-MS-Data-Visualization-and-Comparison-Tool\ucbglobesdatabase.csv
100%|██████████| 117M/117M [00:20<00:00, 5.62MB/s]
✅ Data last pulled on data: 2025-11-19
```

First 5 rows of data will show.

[3]:

	Index	Name	Synon	Campaign/Experimental_Source	Experimental_Conditions	UID	Contributor_ID	Comments	Suspected_matches	Confirmed_ma
0	0	UNK_AHG_LY_ACEDOX_1	NaN	Chemical Standard	ER721GF3 (a-cedrene + O3)	LDY-0	NaN	NaN	NaN	
1	1	UNK_AHG_LY_ACEDOX_2	NaN	Chemical Standard	ER721GF3 (a-cedrene + O3)	LDY-1	NaN	NaN	NaN	
2	2	UNK_AHG_LY_ACEDOX_3	NaN	Chemical Standard	ER721GF3 (a-cedrene + O3)	LDY-2	NaN	NaN	NaN	
3	3	UNK_AHG_LY_ACEDOX_4	NaN	Chemical Standard	ER721GF3 (a-cedrene + O3)	LDY-3	NaN	NaN	NaN	
4	4	UNK_AHG_LY_ACEDOX_13	NaN	Chemical Standard	ER721GF3 (a-cedrene + O3)	LDY-4	NaN	NaN	NaN	

5 rows × 41 columns

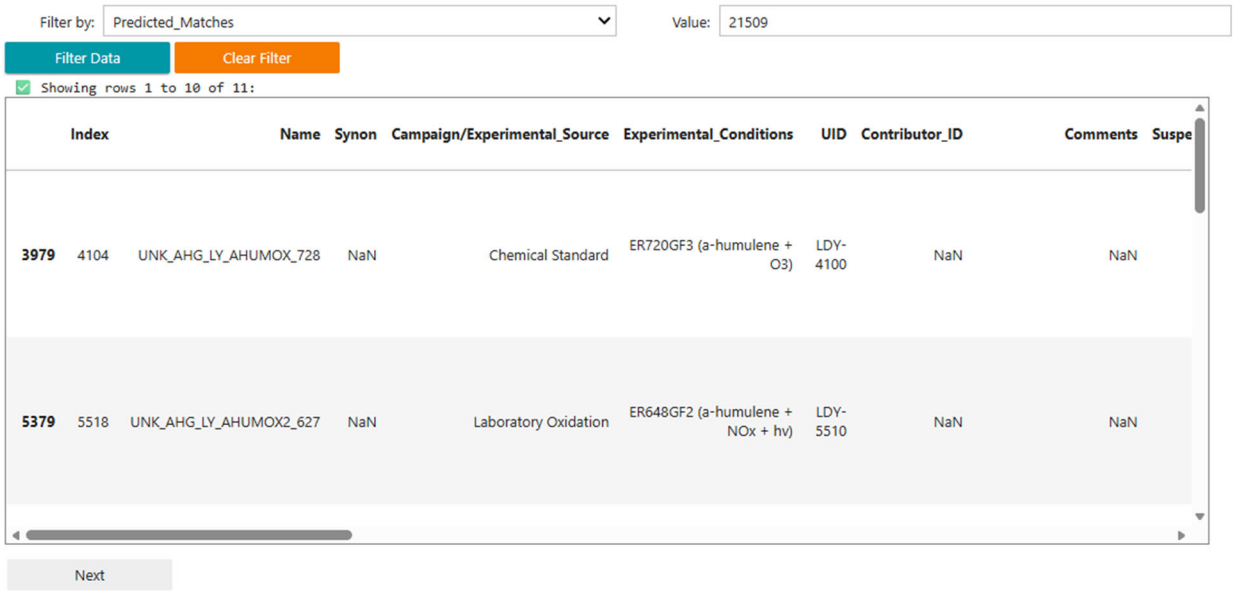
Run the next cell for the widgets to appear prompting for filter criteria.

[4]:
```
ROWS_PER_PAGE = 10



column_dropdown = widgets.Dropdown(
    options=database.columns.tolist(),
    description="Filter by:",
    layout=widgets.Layout(width='50%')
)

filter_text = widgets.Text(
    description="Value:",
    placeholder="Enter value to match (partial OK)",
    layout=widgets.Layout(width='50%')
)

filter_btn = widgets.Button(
    description="Filter Data",
    button_style='info'
)

clear_filter_btn = widgets.Button(
    description="Clear Filter",
    button_style='warning'
)

prev_btn = widgets.Button(description="Previous", button_style='')
next_btn = widgets.Button(description="Next", button_style='')

filter_output = widgets.Output()
pagination_output = widgets.Output()

filtered_df = pd.DataFrame()
current_page = 0

exclude_cols = ["Publications", "MS", "X-Values", "Y-Values"]

def display_page():
    global filtered_df, current_page
    with filter_output:
        clear_output()
        start = current_page * ROWS_PER_PAGE
        end = start + ROWS_PER_PAGE
        if not filtered_df.empty:
            print(f"✅ Showing rows {start + 1} to {min(end, len(filtered_df))} of {len(filtered_df)}:")
            display_df = filtered_df.drop(columns=[c for c in exclude_cols if c in filtered_df.columns])
            html_table = display_df.iloc[start:end].to_html()
            scrollable_html = f'<div style="height:400px; overflow-y:auto; border:1px solid gray;">{html_table}</div>'
            display(HTML(scrollable_html))
        else:
            print("⚠️ No matching rows.")
```

980 ……. Cell content clipped for brevity ……

```
display(widgets.VBox([
    widgets.HBox([column_dropdown, filter_text]),
    widgets.HBox([filter_btn, clear_filter_btn]),
    filter_output,
    pagination_output
]))
```

Filter data by any metadata field and value. In this example, search database for MS that have a predicted MSM with MS entry LDY-21509.



	Index	Name	Synon	Campaign/Experimental_Source	Experimental_Conditions	UID	Contributor_ID	Comments	Suspe
3979	4104	UNK_AHG_LY_AHUMOX_728	NaN	Chemical Standard	ER720GF3 (a-humulene + O3)	LDY-4100	NaN	NaN	
5379	5518	UNK_AHG_LY_AHUMOX2_627	NaN	Laboratory Oxidation	ER648GF2 (a-humulene + NOx + hv)	LDY-5510	NaN	NaN	

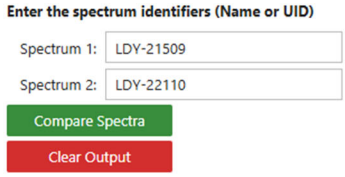
Run next cell for MS data visualization and comparison:

```
[6]: # Action: Run the cell and follow the instruction at the bottom

pio.renderers.default = 'iframe'
pyo.init_notebook_mode(connected=True)

def cosine_similarity(y1, y2):
    dot = sum(a * b for a, b in zip(y1, y2))
    norm1 = sqrt(sum(a ** 2 for a in y1))
    norm2 = sqrt(sum(b ** 2 for b in y2))
    return dot / (norm1 * norm2) if norm1 and norm2 else 0

def align_mass_spectra(x1, y1, x2, y2):
    all_x = sorted(set(x1 + x2))
    y1_aligned = [y1[x1.index(x)] if x in x1 else 0 for x in all_x]
    y2_aligned = [y2[x2.index(x)] if x in x2 else 0 for x in all_x]
    return all_x, y1_aligned, y2_aligned

def plot_mass_spectrum(x, y, name):
    fig = go.Figure()
    fig.add_trace(go.Bar(x=x, y=y, name=name))
    fig.update_layout(title=f"Mass Spectrum for {name}",
                      xaxis_title='m/z',
                      yaxis_title='Relative Abundance')
    fig.show()

def plot_mirrored_spectrum(x1, y1, name1, x2, y2, name2):
    y2_neg = [-v for v in y2]
    fig = go.Figure()

    fig.add_trace(go.Bar(x=x1, y=y1, name=name1, marker_color='blue'))
    fig.add_trace(go.Bar(x=x2, y=y2_neg, name=name2, marker_color='red'))

    fig.update_layout(title=f"Mirrored Plot: {name1} vs {name2}",
                      xaxis_title='m/z',
                      yaxis_title='Relative Abundance',
                      barmode='overlay',
                      bargap=0.1)
    fig.show()

def plot_subtraction(x, y_diff, name1, name2):
    colors = ['blue' if val > 0 else 'red' for val in y_diff]

    fig = go.Figure()
    fig.add_trace(go.Bar(x=x, y=y_diff, marker_color=colors,
                         name=f"{name1} - {name2}"))
```

……. Cell content clipped for brevity ……

```
def get_spectrum_data(identifier):
    filtered = database[database['UID'].astype(str) == identifier.strip()]
    if filtered.empty:
        filtered = database[database['Name'].str.lower() == identifier.lower()]
    if filtered.empty:
        return None, None, None
    row = filtered.iloc[0]
    x = parse_array_string(row['X-Values'])
    y = parse_array_string(row['Y-Values'])
    return row['Name'], x, y
```

Now put in two MS by Name or UID that you want to compare and push “Compare Spectra”



Output is same as in Figure 2 of main text of manuscript.

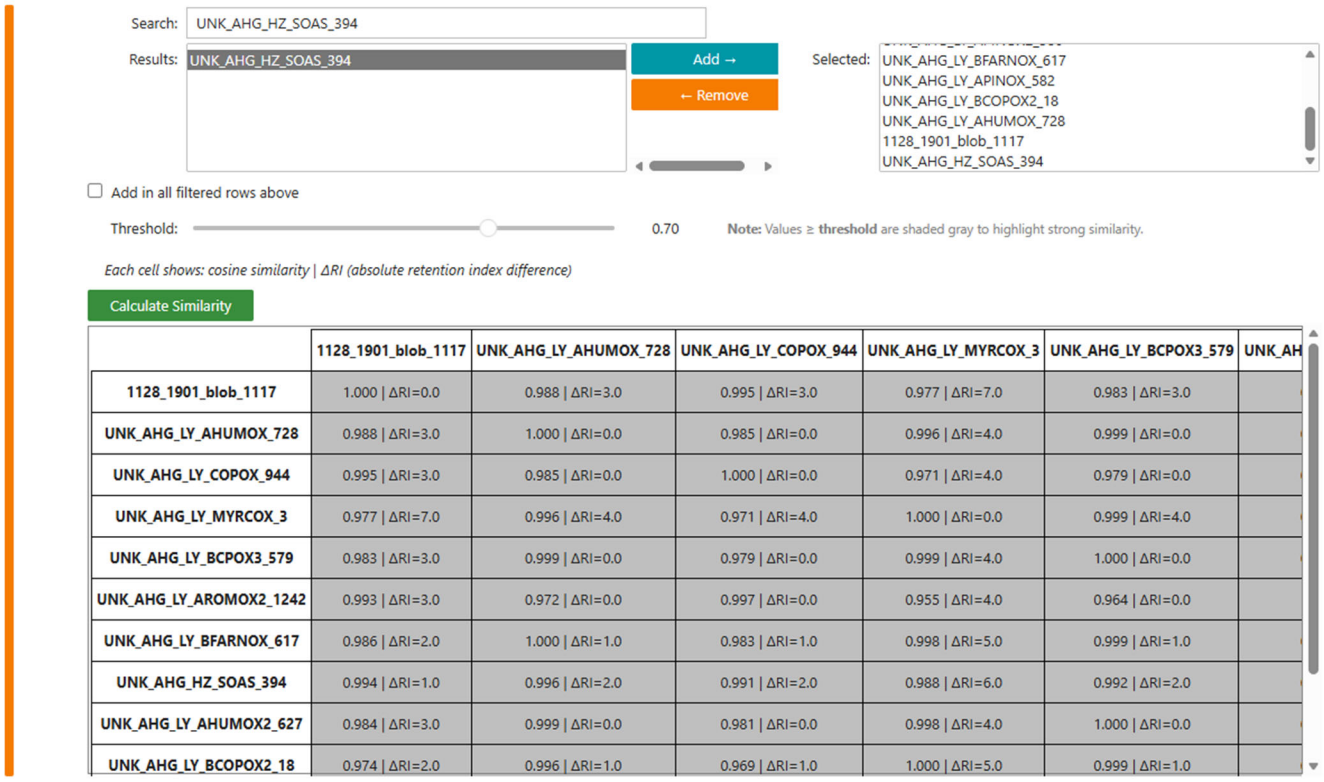
Run Cell 7 to generate user input for cosine angle similarity calculations.

```
•[7]: #Run this cell to initialize widgets for selecting a list of MS that you want to calculate cosine angle similarity values for and their differences in RI

def cosine_similarity(y1, y2):
    dot = sum(a * b for a, b in zip(y1, y2))
    norm1 = sqrt(sum(a ** 2 for a in y1))
    norm2 = sqrt(sum(b ** 2 for b in y2))
    return dot / (norm1 * norm2) if norm1 and norm2 else 0

def get_retention_index(name):
    row = database[database['Name'] == name]
    if row.empty:
        return None
    value = row.iloc[0]['Retention_index']
    if isinstance(value, str) and '=' in value:
        return float(value.split('=')[-1])
```

……. Cell content clipped for brevity ……

```
search_box.observe(update_search_results, names='value')
add_btn.on_click(add_selected)
remove_btn.on_click(remove_selected)
calculate_btn.on_click(calculate_clicked)

button_box = widgets.VBox([add_btn, remove_btn])

display(search_box)
display(widgets.HBox([search_results, button_box, selected_rows]))
threshold_note = widgets.HTML(
    value="""
    <div style="font-size: 90%; color: gray; padding-left: 15px;">
        <b>Note:</b> Values <b>≥ threshold</b> are shaded gray to highlight strong similarity.
    </div>
    """
)

display(use_filtered_checkbox)
display(widgets.HBox([threshold_slider, threshold_note]))
display(widgets.HTML(
    value="<i>Each cell shows: cosine similarity | ΔRI (absolute retention index difference)</i>",
    layout=widgets.Layout(padding="5px 0px 0px 15px")
))
display(calculate_btn)
display(output)
```

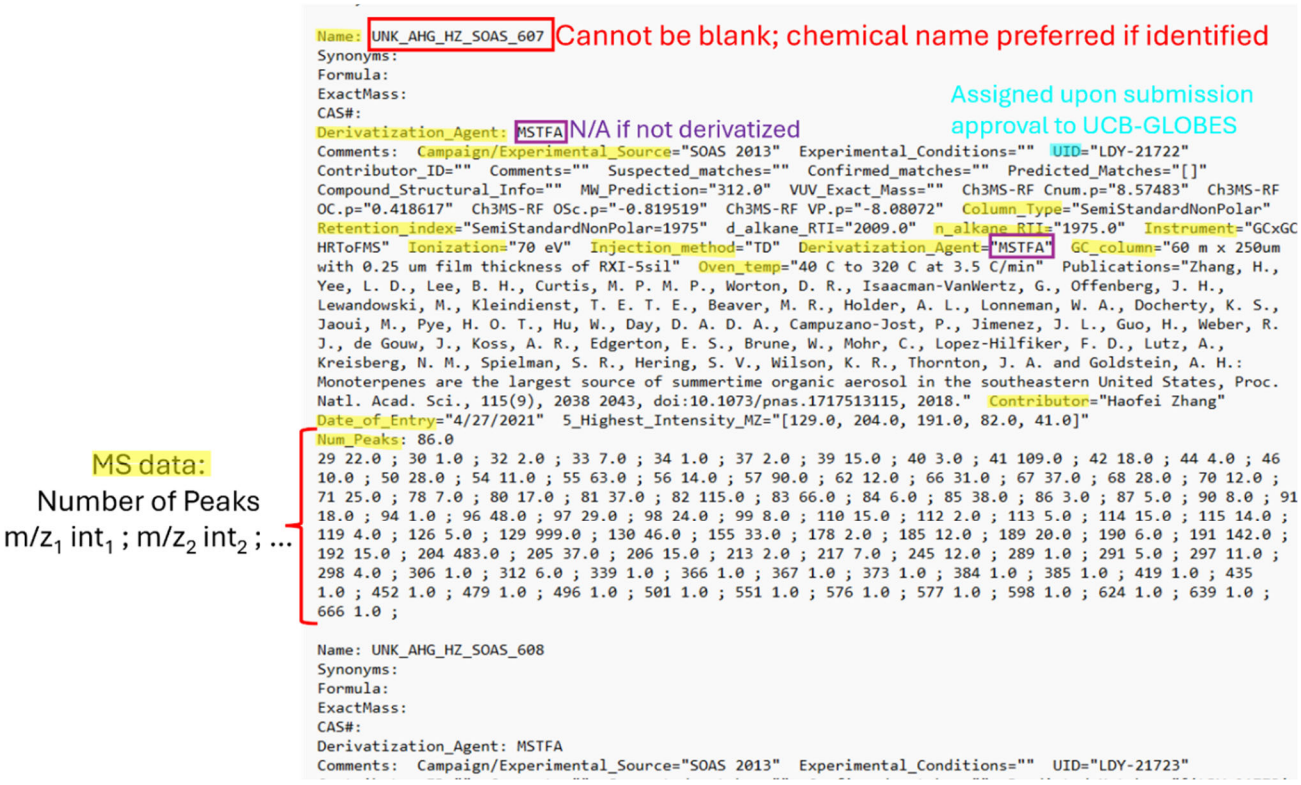
Output widgets allow you to enter as many MS by Name that you want to calculate a cosine angle similarity matrix and differences in retention index for.



	1128_1901_blob_1117	UNK_AHG_LY_AHUMOX_728	UNK_AHG_LY_COPOX_944	UNK_AHG_LY_MYRCOX_3	UNK_AHG_LY_BCPOX3_579	UNK_AH
1128_1901_blob_1117	1.000 | ΔRI=0.0	0.988 | ΔRI=3.0	0.995 | ΔRI=3.0	0.977 | ΔRI=7.0	0.983 | ΔRI=3.0	
UNK_AHG_LY_AHUMOX_728	0.988 | ΔRI=3.0	1.000 | ΔRI=0.0	0.985 | ΔRI=0.0	0.996 | ΔRI=4.0	0.999 | ΔRI=0.0	
UNK_AHG_LY_COPOX_944	0.995 | ΔRI=3.0	0.985 | ΔRI=0.0	1.000 | ΔRI=0.0	0.971 | ΔRI=4.0	0.979 | ΔRI=0.0	
UNK_AHG_LY_MYRCOX_3	0.977 | ΔRI=7.0	0.996 | ΔRI=4.0	0.971 | ΔRI=4.0	1.000 | ΔRI=0.0	0.999 | ΔRI=4.0	
UNK_AHG_LY_BCPOX3_579	0.983 | ΔRI=3.0	0.999 | ΔRI=0.0	0.979 | ΔRI=0.0	0.999 | ΔRI=4.0	1.000 | ΔRI=0.0	
UNK_AHG_LY_AROMOX2_1242	0.993 | ΔRI=3.0	0.972 | ΔRI=0.0	0.997 | ΔRI=0.0	0.955 | ΔRI=4.0	0.964 | ΔRI=0.0	
UNK_AHG_LY_BFARNOX_617	0.986 | ΔRI=2.0	1.000 | ΔRI=1.0	0.983 | ΔRI=1.0	0.998 | ΔRI=5.0	0.999 | ΔRI=1.0	
UNK_AHG_HZ_SOAS_394	0.994 | ΔRI=1.0	0.996 | ΔRI=2.0	0.991 | ΔRI=2.0	0.988 | ΔRI=6.0	0.992 | ΔRI=2.0	
UNK_AHG_LY_AHUMOX2_627	0.984 | ΔRI=3.0	0.999 | ΔRI=0.0	0.981 | ΔRI=0.0	0.998 | ΔRI=4.0	1.000 | ΔRI=0.0	
UNK_AHG_LY_BCOPOX2_18	0.974 | ΔRI=2.0	0.996 | ΔRI=1.0	0.969 | ΔRI=1.0	1.000 | ΔRI=5.0	0.999 | ΔRI=1.0	

S3. How to Contribute MS Data to UCB-GLOBES

UCB-GLOBES is intended to be an open-access fully extensible database of electron ionization mass spectra acquired with GC/EI-MS systems without requirement of known chemical identification. While we have yet to develop an online automated framework for user submissions of MS data, we anticipate all announcements/information on future developments to be posted online at https://sites.google.com/berkeley.edu/goldstein-lab/resources where UCB-GLOBES MS data is presently posted. Meanwhile, please contact the corresponding author for inquiries into MS data submission. To provide the best possible data quality to other users, candidate MS should be derived from chromatographic peaks that are of sufficient signal beyond detection limits and have undergone mass spectral deconvolution to represent a pure compound. As workflows and processing software vary among GC/EI-MS users (particularly in how raw MS data is obtained), we merely provide guidance here for how MS entries should be annotated and formatted to match that of UCB-GLOBES entries. User-submitted MS libraries should follow the same format as in the .MSP/text file formats for ucbglobes2025_v1 where MS entries are annotated with known values (where possible) of metadata fields listed in Table 2. The submitted .MSP/text file can be a running compilation of annotated MS entries as in the example screenshot of an excerpt MS entry in ucbglobes2025_v1 below. The corresponding author can also be contacted for discussion of detailed workflows as used in this work should it be helpful to new contributors, though it is most readily applicable to other users of GCImage software. The minimum required metadata is indicated in highlights below.



S4. SI Tables

Table S1: Matrix of cosine angle similarity values and differences in retention indices (ΔRI) for twelve suspected MS matches. Grey shading indicates values above user selected threshold, in this case, 0.7.

	1128 1901 _blob_1117	UNK AHG LY AHU MOX_728	UNK AHG LY COP OX_944	UNK AHG LY MYR COX_3	UNK AHG LY BCPO X3_579	UNK AHG LY ARO MOX2 124 2	UNK AHG LY BFAR NOX_617	UNK AHG HZ SOAS _394	UNK AHG LY AHU MOX2_627	UNK AHG LY BCOP OX2_18	UNK AHG LY APIN OX2_586	UNK AHG LY APIN OX_582
1128 1901 blob_1117	1.000 | ΔRI=0.0	0.988 | ΔRI=3.0	0.995 | ΔRI=3.0	0.977 | ΔRI=7.0	0.983 | ΔRI=3.0	0.993 | ΔRI=3.0	0.986 | ΔRI=2.0	0.994 | ΔRI=1.0	0.984 | ΔRI=3.0	0.974 | ΔRI=2.0	0.995 | ΔRI=7.0	0.993 | ΔRI=6.0
UNK_AHG LY AHU MOX_728	0.988 | ΔRI=3.0	1.000 | ΔRI=0.0	0.985 | ΔRI=0.0	0.996 | ΔRI=4.0	0.999 | ΔRI=0.0	0.972 | ΔRI=0.0	1.000 | ΔRI=1.0	0.996 | ΔRI=2.0	0.999 | ΔRI=0.0	0.996 | ΔRI=1.0	0.980 | ΔRI=4.0	0.995 | ΔRI=3.0
UNK_AHG _LY_COP OX_944	0.995 | ΔRI=3.0	0.985 | ΔRI=0.0	1.000 | ΔRI=0.0	0.971 | ΔRI=4.0	0.979 | ΔRI=0.0	0.997 | ΔRI=0.0	0.983 | ΔRI=1.0	0.991 | ΔRI=2.0	0.981 | ΔRI=0.0	0.969 | ΔRI=1.0	0.998 | ΔRI=4.0	0.994 | ΔRI=3.0
UNK_AHG _LY_MYR COX_3	0.977 | ΔRI=7.0	0.996 | ΔRI=4.0	0.971 | ΔRI=4.0	1.000 | ΔRI=0.0	0.999 | ΔRI=4.0	0.955 | ΔRI=4.0	0.998 | ΔRI=5.0	0.988 | ΔRI=6.0	0.998 | ΔRI=4.0	1.000 | ΔRI=5.0	0.967 | ΔRI=0.0	0.989 | ΔRI=1.0
UNK_AHG _LY_BCPO X3_579	0.983 | ΔRI=3.0	0.999 | ΔRI=0.0	0.979 | ΔRI=0.0	0.999 | ΔRI=4.0	1.000 | ΔRI=0.0	0.964 | ΔRI=0.0	0.999 | ΔRI=1.0	0.992 | ΔRI=2.0	1.000 | ΔRI=0.0	0.999 | ΔRI=1.0	0.974 | ΔRI=4.0	0.993 | ΔRI=3.0
UNK AHG LY ARO MOX2 124 2	0.993 | ΔRI=3.0	0.972 | ΔRI=0.0	0.997 | ΔRI=0.0	0.955 | ΔRI=4.0	0.964 | ΔRI=0.0	1.000 | ΔRI=0.0	0.969 | ΔRI=1.0	0.983 | ΔRI=2.0	0.967 | ΔRI=0.0	0.952 | ΔRI=1.0	0.997 | ΔRI=4.0	0.986 | ΔRI=3.0
UNK AHG LY BFAR NOX_617	0.986 | ΔRI=2.0	1.000 | ΔRI=1.0	0.983 | ΔRI=1.0	0.998 | ΔRI=5.0	0.999 | ΔRI=1.0	0.969 | ΔRI=1.0	1.000 | ΔRI=0.0	0.994 | ΔRI=1.0	1.000 | ΔRI=1.0	0.997 | ΔRI=0.0	0.978 | ΔRI=5.0	0.994 | ΔRI=4.0
UNK AHG HZ SOAS _394	0.994 | ΔRI=1.0	0.996 | ΔRI=2.0	0.991 | ΔRI=2.0	0.988 | ΔRI=6.0	0.992 | ΔRI=2.0	0.983 | ΔRI=2.0	0.994 | ΔRI=1.0	1.000 | ΔRI=0.0	0.994 | ΔRI=2.0	0.987 | ΔRI=1.0	0.987 | ΔRI=6.0	0.995 | ΔRI=5.0
UNK_AHG LY AHU MOX2_627	0.984 | ΔRI=3.0	0.999 | ΔRI=0.0	0.981 | ΔRI=0.0	0.998 | ΔRI=4.0	1.000 | ΔRI=0.0	0.967 | ΔRI=0.0	1.000 | ΔRI=1.0	0.994 | ΔRI=2.0	1.000 | ΔRI=0.0	0.998 | ΔRI=1.0	0.976 | ΔRI=4.0	0.994 | ΔRI=3.0
UNK_AHG _LY_BCOP OX2_18	0.974 | ΔRI=2.0	0.996 | ΔRI=1.0	0.969 | ΔRI=1.0	1.000 | ΔRI=5.0	0.999 | ΔRI=1.0	0.952 | ΔRI=1.0	0.997 | ΔRI=0.0	0.987 | ΔRI=1.0	0.998 | ΔRI=1.0	1.000 | ΔRI=0.0	0.963 | ΔRI=5.0	0.987 | ΔRI=4.0
UNK_AHG _LY_APIN OX2_586	0.995 | ΔRI=7.0	0.980 | ΔRI=4.0	0.998 | ΔRI=4.0	0.967 | ΔRI=0.0	0.974 | ΔRI=4.0	0.997 | ΔRI=4.0	0.978 | ΔRI=5.0	0.987 | ΔRI=6.0	0.976 | ΔRI=4.0	0.963 | ΔRI=5.0	1.000 | ΔRI=0.0	0.992 | ΔRI=1.0
UNK_AHG _LY_APIN OX_582	0.993 | ΔRI=6.0	0.995 | ΔRI=3.0	0.994 | ΔRI=3.0	0.989 | ΔRI=1.0	0.993 | ΔRI=3.0	0.986 | ΔRI=3.0	0.994 | ΔRI=4.0	0.995 | ΔRI=5.0	0.994 | ΔRI=3.0	0.987 | ΔRI=4.0	0.992 | ΔRI=1.0	1.000 | ΔRI=0.0

Table S2: Updated source categorization using UCB-GLOBES MS and NISTMS20 database for compounds observed during the SOAS field campaign. Table adapted from Zhang et al. (2018) supporting data.

index	Compound Name	Group	Group Determined By	UCB-GLOBES UID	Compound Name Reanalysis	Group Reanalysis	Group Determined By Reanalysis	Group Category Changed 0 = no 1 = yes	MS Confirmed 0 = no 1 = yes
1	pinic acid	MT	MS	LDY-21118	pinic acid, 2 TMS	MT	MS	0	0
2	C16 acid	POAOX	R2	LDY-21119	C16 acid, TMS	POAOX	R2	0	0
3	U1 from Kubatova 2000 AE[f]	MT	MS/Lab Expt	LDY-21120	3-acetylpentanedioic acid, 2 TMS	MT	MS/Lab Expt	0	0
4	3-hydroxyglutaric acid	MT	MS	LDY-21121	2- and 3-hydroxyglutaric acid mixture, 3 TMS	MT	MS	0	0
5	MBTCA	MT	MS	LDY-21122	MBTCA, 3 TMS	MT	MS	0	0
6	hexadecanal	POAOX	R2	LDY-21123	hexadecanal	POAOX	R2	0	0
7	levoglucosan	BBOA	MS	LDY-21124	levoglucosan, 3 TMS	BBOA	MS	0	0
8	pinonic acid isomer	MT	MS	LDY-21125	pinonic acid isomer, 3 TMS	MT	MS	0	0
9	Butanedioic acid, 2-ol	MT	NIST/Lab Expt	LDY-21126	Butanedioic acid, 2-ol, 3 TMS	MT	NIST/Lab Expt	0	0
10	C10H16O4	MT	Lab Expt	LDY-21175	UNK_AHG_HZ_SOAS_60	MT	Lab Expt	0	0
11	MBTCA isomer	MT	MS	LDY-21128	MBTCA isomer, 3 TMS	MT	MS	0	0
12	C8H12O5	MT	Lab Expt	LDY-21129	UNK_AHG_HZ_SOAS_12	MT	Lab Expt	0	0
13	Tricarballylic acid	MT	MS	LDY-21130	Tricarballylic acid, 3 TMS	MT	MS	0	0
14	C8H12O5	MT	MS/Lab Expt	LDY-21129	UNK_AHG_HZ_SOAS_12	MT	MS/Lab Expt	0	0
15	2-methyltetrol_1	ISOP	MS	LDY-21132	2-methyltetrol_1, 4 TMS	ISOP	MS	0	0
16	pinonic acid	MT	MS/R2	LDY-21133	pinonic acid, TMS	MT	MS/R2	0	0
17	d18-nalkane	IStd	MS	LDY-21134	d18-nalkane	IStd	MS	0	0
18	d20-nalkane	IStd	MS	LDY-21135	d20-nalkane	IStd	MS	0	0
19	C9H12O6	MT	Lab Expt/R2	LDY-21136	UNK_AHG_HZ_SOAS_19	MT	Lab Expt/R2	0	0
20	C5H6O6	SQT	Lab Expt	LDY-21137	UNK_AHG_HZ_SOAS_20	SQT	Lab Expt	0	0
21	2,3-erythro-dihydroxyglutaric acid iso1	MT	NIST/R2	#N/A	N/A; MS entry removed through new QA/QC	MT	NIST/R2	0	0
22	C9H12O6	MT	R2	LDY-21136	UNK_AHG_HZ_SOAS_19	MT	R2	0	0

index	Compound Name	Group	Group Determined By	UCB-GLOBES UID	Compound Name Reanalysis	Group Reanalysis	Group Determined By Reanalysis	Group Category Changed 0 = no 1 = yes	MS Confirmed 0 = no 1 = yes
23	2-Pentadecanone, 6,10,14-trimethyl-	POAOX	NIST	LDY-21139	2-Pentadecanone, 6,10,14-trimethyl-	POAOX	NIST	0	0
24	d22-nalkane	IStd	MS	LDY-21140	d22-nalkane	IStd	MS	0	0
25	C8H10O6	MT	Lab Expt/R2	LDY-21181	UNK_AHG_HZ_SOAS_66	MT	Lab Expt/R2	0	0
26	2-MT1, incomplete deriv	ISOP	MS	LDY-21142	2-MT1, incomplete deriv, 4 TMS	ISOP	MS	0	0
27	2,3-threo-dihydroxyglutaric acid iso2	MT	NIST/R2	LDY-21143	2,3-threo-dihydroxyglutaric acid iso2, 4 TMS	MT	NIST/R2	0	0
28	C9H14O6	MTR2	R2	LDY-21144	UNK_AHG_HZ_SOAS_28	MTR2	R2	0	0
29		SQT	Lab Expt	LDY-21145	UNK_AHG_HZ_SOAS_29	SQT	Lab Expt	0	0
30	C8H12O4	MT	MS	LDY-21146	UNK_AHG_HZ_SOAS_30	MT	MS	0	0
31	d24-nalkane	IStd	MS	LDY-21147	d24-nalkane	IStd	MS	0	0
32		MTR2	R2	LDY-21148	UNK_AHG_HZ_SOAS_32	SQT	MS/Lab Expt/Field Expt	1	1
33		BOOA	MS	LDY-21149	UNK_AHG_HZ_SOAS_33	BOOA	MS	0	0
34	C16H30O2	POAOX	NIST	LDY-21150	UNK_AHG_HZ_SOAS_34	POAOX	NIST	0	0
35	Phthalic acid, aged BBOA[g]	ASOA	NIST/Lab Expt	LDY-21151	Phthalic acid, aged BBOA, 2 TMS	ASOA	NIST/Lab Expt	0	0
36		BOOA	R2	LDY-21152	UNK_AHG_HZ_SOAS_36	BOOA	R2	0	0
37	Heptanedioic acid, 4-oxo	MTR2	NIST/R2	LDY-21153	Heptanedioic acid, 4-oxo, 2 TMS	MTR2	NIST/R2	0	0
38	C12 acid	POAOX	MS	LDY-21154	C12 acid, TMS	POAOX	MS	0	0
39		BBOA	Lab Expt/R2	LDY-21155	UNK_AHG_HZ_SOAS_39	BBOA	Lab Expt/R2	0	0
40		MTR2	R2	LDY-21156	UNK_AHG_HZ_SOAS_40	MTR2	R2	0	0
41	C8H12O5	MT	Lab Expt	LDY-21129	UNK_AHG_HZ_SOAS_12	MT	Lab Expt	0	0
42	2-methyltetrol_2	ISOP	MS	LDY-21158	2-methyltetrol_2, 4 TMS	ISOP	MS	0	0
43	C9H14O5	MT	Lab Expt	LDY-21159	UNK_AHG_HZ_SOAS_43	MT	Lab Expt	0	0

index	Compound Name	Group	Group Determined By	UCB-GLOBES UID	Compound Name Reanalysis	Group Reanalysis	Group Determined By Reanalysis	Group Category Changed 0 = no 1 = yes	MS Confirmed 0 = no 1 = yes
44	2-MT2, incomplete deriv	ISOP	MS	LDY-21160	2-MT2, incomplete deriv, 4 TMS	ISOP	MS	0	0
45	Hexanedioic acid, 3-ol	BOOA	NIST	LDY-21161	Hexanedioic acid, 3-ol, 3 TMS	BOOA	NIST	0	0
46	C18 acid	POAOX	R2	LDY-21162	C18 acid, TMS	POAOX	R2	0	0
47	C8H12O4	MT	Lab Expt	LDY-21146	UNK_AHG_HZ_SOAS_30	MT	Lab Expt	0	0
48	tartaric acid 1[h]	BOOA	NIST	LDY-21164	tartaric acid 1, 4 TMS	BOOA	NIST	0	0
49		MT	Lab Expt/R2	#N/A	N/A; MS entry removed through new QA/QC	MT	Lab Expt/R2	0	0
50	d16-nalkane	IStd	MS	LDY-21165	d16-nalkane	IStd	MS	0	0
51		MTR2	R2	LDY-21166	UNK_AHG_HZ_SOAS_51	MTR2	R2	0	0
52	C7H12O4	MT	Lab Expt	LDY-21167	UNK_AHG_HZ_SOAS_52	MT	Lab Expt	0	0
53		SQT	R2	LDY-21168	UNK_AHG_HZ_SOAS_53	SQT	MS/Lab Expt	0	1
54		MTR2	R2	LDY-21169	UNK_AHG_HZ_SOAS_54	MTR2	R2	0	0
55	3-hydroxy-4,4-dimethylglutaric acid	MT	MS/Lab Expt	LDY-21170	3-hydroxy-4,4-dimethylglutaric acid, 3 TMS	MT	MS/Lab Expt	0	0
56		MTR2	R2	LDY-21171	UNK_AHG_HZ_SOAS_56	MTR2	R2	0	0
57		MTR2	R2	LDY-21172	UNK_AHG_HZ_SOAS_57	SQT	MS/Lab Expt/Field Expt	1	1
58		BOOA	MS	LDY-21173	UNK_AHG_HZ_SOAS_58	BOOA	MS	0	0
59	d26-nalkane	IStd	MS	LDY-21174	d26-nalkane	IStd	MS	0	0
60	C10H16O4	MT	Lab Expt	LDY-21175	UNK_AHG_HZ_SOAS_60	MT	Lab Expt	0	0
61	C8H12O5	MTR2	R2	LDY-21129	UNK_AHG_HZ_SOAS_12	MT/SQT	MS/Lab Expt	1	1
62		MTR2	R2	LDY-21177	UNK_AHG_HZ_SOAS_62	MTR2	R2	0	0
63		MTR2	R2	LDY-21178	UNK_AHG_HZ_SOAS_63	MT/SQT	MS/Lab Expt/Field Expt	1	1
64	pinonaldehyde 1	MT	MS	LDY-21179	pinonaldehyde 1	MT	MS	0	0
65	C9H16O3	MT	Lab Expt/R2	LDY-21180	UNK_AHG_HZ_SOAS_65	MT	Lab Expt/R2	0	0
66	C8H10O6	MTR2	R2	LDY-21181	UNK_AHG_HZ_SOAS_66	MTR2	R2	0	0
67	C10H16O5	MT	Lab Expt/R2	LDY-21182	UNK_AHG_HZ_SOAS_67	MT	Lab Expt/R2	0	0

index	Compound Name	Group	Group Determined By	UCB-GLOBES UID	Compound Name Reanalysis	Group Reanalysis	Group Determined By Reanalysis	Group Category Changed 0 = no 1 = yes	MS Confirmed 0 = no 1 = yes
68	C7H10O5	MT	Lab Expt/R2	LDY-21183	UNK_AHG_HZ_SOAS_68	MT	Lab Expt/R2	0	0
69	Azelaic acid	BBOA	R2	LDY-21184	Azelaic acid, 2 TMS	BBOA	R2	0	0
70	C9H14O5	MT	Lab Expt/R2	LDY-21159	UNK_AHG_HZ_SOAS_43	MT	Lab Expt/R2	0	0
71	tartaric acid 2[h]	BOOA	NIST	LDY-21219	tartaric acid 4, 4 TMS	BOOA	NIST	0	0
72	Benzoic acid, 4-ol	BBOA	NIST/R2	LDY-21187	Benzoic acid, 4-ol, 2 TMS	BBOA	NIST/R2	0	0
73		BOOA	MS	LDY-21188	UNK_AHG_HZ_SOAS_73	BOOA	MS	0	0
74	C9H14O5	MT	Lab Expt/R2	LDY-21159	UNK_AHG_HZ_SOAS_43	MT	Lab Expt/R2	0	0
75	C7H12O4	MT	Lab Expt	LDY-21167	UNK_AHG_HZ_SOAS_52	MT	Lab Expt	0	0
76	pentadecanol	POAOX	MS	LDY-21191	pentadecanol, TMS	POAOX	MS	0	0
77		MTR2	R2	LDY-21192	UNK_AHG_HZ_SOAS_77	BBOA	MS/Field Expt	1	1
78	C10H16O3	MTR2	R2	LDY-21193	UNK_AHG_HZ_SOAS_78	MTR2	R2	0	0
79	C8H12O5	MT	Lab Expt/R2	LDY-21129	UNK_AHG_HZ_SOAS_12	MT	Lab Expt/R2	0	0
80	glutaric acid, 2,3-diol	MT	NIST/R2	LDY-21195	glutaric acid, 2,3-diol, 4 TMS	MT	NIST/R2	0	0
81	C5H8O6	MTR2	R2	LDY-21196	UNK_AHG_HZ_SOAS_81	ISOP	MS/Lab Expt/Field Expt	1	1
82	C14 acid	POAOX	MS	LDY-21197	C14 acid, TMS	POAOX	MS	0	0
83	C5alkenetriol 1	ISOP	MS	LDY-21198	C5alkenetriol 1, 3 TMS	ISOP	MS	0	0
84	C10H16O5	MT	Lab Expt/R2	LDY-21182	UNK_AHG_HZ_SOAS_67	MT	Lab Expt/R2	0	0
85	pinonaldehyde 2	MT	MS	LDY-21200	pinonaldehyde 2	MT	MS	0	0
86		Unknown		LDY-21201	UNK_AHG_HZ_SOAS_86	Unknown	0	0	0
87		MTR2	R2	LDY-21202	UNK_AHG_HZ_SOAS_87	SQT	MS/Field Expt	1	1
88	C4H8O5	MTR2	R2	LDY-21203	UNK_AHG_HZ_SOAS_88	MTR2	R2	0	0
89		SQT	R2	LDY-21204	UNK_AHG_HZ_SOAS_89	SQT	MS/Lab Expt	0	1
90	tartaric acid 3[h]	BOOA	MS	LDY-21205	tartaric acid 3, 4 TMS	BOOA	MS	0	0
91	C9H14O3	MT	Lab Expt/R2	LDY-21206	UNK_AHG_HZ_SOAS_91	MT	Lab Expt/R2	0	0

index	Compound Name	Group	Group Determined By	UCB-GLOBES UID	Compound Name Reanalysis	Group Reanalysis	Group Determined By Reanalysis	Group Category Changed 0 = no 1 = yes	MS Confirmed 0 = no 1 = yes
92		BOOA	MS	LDY-21207	UNK_AHG_HZ_SOAS_92	BOOA	MS	0	0
93	C5H8O6	MTR2	R2	LDY-21196	UNK_AHG_HZ_SOAS_81	MT	MS/Field Expt/NIST20	1	1
94	C8H14O5	MTR2	R2	LDY-21209	UNK_AHG_HZ_SOAS_94	MTR2	R2	0	0
95		MTR2	R2	LDY-21210	UNK_AHG_HZ_SOAS_95	MTR2	R2	0	0
96	C9H14O4	MTR2	R2	LDY-21211	UNK_AHG_HZ_SOAS_96	SQT	MS/Lab Expt/Field Expt	1	1
97		MTR2	R2	LDY-21212	UNK_AHG_HZ_SOAS_97	MTR2	R2	0	0
98	beta-nocaryophyllonic acid[i]	SQT	MS	LDY-21213	beta-nocaryophyllonic acid, TMS	SQT	MS	0	0
99	C10H16O4	MT	Lab Expt	LDY-21175	UNK_AHG_HZ_SOAS_60	MT	Lab Expt	0	0
100		MTR2	R2	LDY-21215	UNK_AHG_HZ_SOAS_100	SQT	MS/Lab Expt/Field Expt	1	1
101		BOOA	R2	LDY-21216	Hexadecanolide	BOOA	MS/MANE/ Adams	0	1
102	C7H10O5	MTR2	R2	LDY-21183	UNK_AHG_HZ_SOAS_68	MTR2	R2	0	0
103		MTR2	R2	LDY-21218	UNK_AHG_HZ_SOAS_103	MT	MS/Lab Expt/Field Expt	1	1
104	tartaric acid 4[h]	BOOA	MS	LDY-21219	tartaric acid 4, 4 TMS	BOOA	MS	0	0
105	C7H8O5	SQT	R2	LDY-21220	UNK_AHG_HZ_SOAS_105	MT/SQT	MS/Lab Expt/Field Expt	1	1
106	C7H10O3	BOOA	R2	LDY-21221	UNK_AHG_HZ_SOAS_106	ISOP	MS/Lab Expt/Field Expt	1	1
107	C8H10O4/C12H18O5	SQT	Lab Expt	LDY-21222	UNK_AHG_HZ_SOAS_107	SQT	Lab Expt	0	0
108		MTR2	R2	LDY-21223	UNK_AHG_HZ_SOAS_108	MTR2	R2	0	0
109	C9H12O5	SQT	Lab Expt	LDY-21224	UNK_AHG_HZ_SOAS_109	SQT	Lab Expt	0	0
110	C8H10O5	MT	Lab Expt	LDY-21225	UNK_AHG_HZ_SOAS_110	MT	Lab Expt	0	0
111		BBOA	R2	LDY-21226	UNK_AHG_HZ_SOAS_111	BBOA	R2	0	0
112		MTR2	R2	LDY-21227	UNK_AHG_HZ_SOAS_112	SQT	MS/Lab Expt	1	1
113	C5alkenetriol 2	ISOP	MS	LDY-21228	C5alkenetriol 2, 3 TMS	ISOP	MS	0	0

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114	C9H14O5	MT	Lab Expt	LDY-21159	UNK_AHG_HZ_SOAS_43	MT	Lab Expt	0	0
115		MTR2	R2	LDY-21230	UNK_AHG_HZ_SOAS_115	MTR2	R2	0	0
116		SQT	Lab Expt	LDY-21231	UNK_AHG_HZ_SOAS_116	SQT	Lab Expt	0	0
117	C8H14O4	MT	Lab Expt/R2	LDY-21232	UNK_AHG_HZ_SOAS_117	MT	Lab Expt/R2	0	0
118		BBOA	MS	LDY-21233	UNK_AHG_HZ_SOAS_118	BBOA	MS	0	0
119		MTR2	R2	LDY-21234	UNK_AHG_HZ_SOAS_119	MTR2	R2	0	0
120	C5H6O7	MT	Lab Expt/R2	LDY-21235	UNK_AHG_HZ_SOAS_120	MT	Lab Expt/R2	0	0
121		MTR2	R2	LDY-21236	UNK_AHG_HZ_SOAS_121	MTR2	R2	0	0
122		BOOA	R2	LDY-21237	UNK_AHG_HZ_SOAS_122	MT	MS/Lab Expt/Field Expt	1	1
123		MT	Lab Expt	LDY-21238	UNK_AHG_HZ_SOAS_123	MT	Lab Expt	0	0
124	C8H12O6	MT	MS	LDY-21239	UNK_AHG_HZ_SOAS_124	MT	MS	0	0
125	d28-nalkane	IStd	MS	LDY-21240	d28-nalkane	IStd	MS	0	0
126		BOOA	R2	LDY-21241	UNK_AHG_HZ_SOAS_126	ISOP	MS/Lab Expt/Field Expt	1	1
127		MTR2	R2	LDY-21242	UNK_AHG_HZ_SOAS_127	MTR2	R2	0	0
128		MT	MS	LDY-21243	UNK_AHG_HZ_SOAS_128	MT	MS	0	0
129	C7H10O5	MTR2	R2	LDY-21183	UNK_AHG_HZ_SOAS_68	MT/SQT	MS/Lab Expt/Field Expt	1	1
130	C8H12O5	MT	Lab Expt/R2	LDY-21129	UNK_AHG_HZ_SOAS_12	MT	Lab Expt/R2	0	0
131		SQT	Lab Expt	LDY-21246	UNK_AHG_HZ_SOAS_131	SQT	Lab Expt	0	0
132	C8H6O4	Unknown		LDY-21247	Terephthalic acid, 2 TMS	BBOA/MT	MS/NIST20/ Lab Expt/Field Expt	1	1
133		MTR2	R2	LDY-21248	UNK_AHG_HZ_SOAS_133	MTR2	R2	0	0
134		MTR2	R2	LDY-21249	UNK_AHG_HZ_SOAS_134	MTR2	R2	0	0
135	C6H10O6	SQT	Lab Expt	LDY-21250	UNK_AHG_HZ_SOAS_135	SQT	Lab Expt	0	0
136	C8H12O4	MT	Lab Expt	LDY-21146	UNK_AHG_HZ_SOAS_30	MT	Lab Expt	0	0
137	C9H12O3	MT	Lab Expt	LDY-21252	UNK_AHG_HZ_SOAS_137	MT	Lab Expt	0	0
138		BOOA	R2	LDY-21253	UNK_AHG_HZ_SOAS_138	SQT	MS/Lab Expt/Field Expt	1	1
139	C6H8O4	MTR2	MS	LDY-21254	UNK_AHG_HZ_SOAS_139	MTR2	MS	0	0

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140	C5H6O4	Unknown	MS	LDY-21255	UNK_AHG_HZ_SOAS_140	Unknown	MS	0	0
141	C8H14O5	MT	Lab Expt	LDY-21209	UNK_AHG_HZ_SOAS_94	MT	Lab Expt	0	0
142	Manoyl oxide	POAOX	NIST	LDY-21257	Manoyl oxide	POAOX	NIST	0	0
143	d30-nalkane	IStd	MS	LDY-21258	d30-nalkane	IStd	MS	0	0
144		BBOA	R2	LDY-21259	UNK_AHG_HZ_SOAS_144	BBOA	MS/Lab Expt/Field Expt	0	1
145	Asarone	POAOX	NIST	LDY-21260	Asarone	POAOX	NIST	0	0
146	C6H6O3, aged BBOA	ASOA	Lab Expt	LDY-21261	UNK_AHG_HZ_SOAS_146	ASOA	Lab Expt	0	0
147		MTR2	R2	LDY-21262	UNK_AHG_HZ_SOAS_147	MTR2	R2	0	0
148	C13 acid, co-elution	POAOX	MS	LDY-21263	C13 acid, co-elution, TMS	POAOX	MS	0	0
149		MTR2	R2	LDY-21264	UNK_AHG_HZ_SOAS_149	MTR2	R2	0	0
150	C9H14O6	MTR2	R2	LDY-21144	UNK_AHG_HZ_SOAS_28	MTR2	R2	0	0
151		SQT	Lab Expt	LDY-21266	UNK_AHG_HZ_SOAS_151	SQT	Lab Expt	0	0
152	C7H12O4	MT	Lab Expt	LDY-21167	UNK_AHG_HZ_SOAS_52	MT	Lab Expt	0	0
153	C8H10O4	SQT	Lab Expt	LDY-21268	UNK_AHG_HZ_SOAS_153	SQT	Lab Expt	0	0
154	C7H6O5, aged BBOA	ASOA	Lab Expt	LDY-21269	UNK_AHG_HZ_SOAS_154	ASOA	Lab Expt	0	0
155		MTR2	R2	LDY-21270	UNK_AHG_HZ_SOAS_155	MTR2	R2	0	0
156	C11H10O5	BOOA	MS	LDY-21271	UNK_AHG_HZ_SOAS_156	BOOA	MS	0	0
157		BBOA	R2	LDY-21272	D-Arabino Hexonic acid 3-deoxy-2,5,6-tris-O-(TMS)-lactone	BBOA	MS/Lab Expt	0	1
158		BOOA	MS	LDY-21273	UNK_AHG_HZ_SOAS_158	BOOA	MS	0	0
159		MTR2	R2	LDY-21274	UNK_AHG_HZ_SOAS_159	MTR2	R2	0	0
160	C8H12O6	MTR2	MS	LDY-21239	UNK_AHG_HZ_SOAS_124	MTR2	MS	0	0
161	d32-nalkane	IStd	MS	LDY-21276	d32-nalkane	IStd	MS	0	0
162		SQT	Lab Expt	LDY-21277	UNK_AHG_HZ_SOAS_162	SQT	Lab Expt	0	0
163		MTR2	R2	LDY-21278	UNK_AHG_HZ_SOAS_163	MTR2	R2	0	0
164	C8H14O4	MT	Lab Expt/R2	LDY-21232	UNK_AHG_HZ_SOAS_117	MT	Lab Expt/R2	0	0
165	Threonic acid	ASOA	NIST	LDY-21280	Threonic acid, 4 TMS	ASOA	NIST	0	0

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166		MTR2	R2	LDY-21281	UNK_AHG_HZ_SOAS_166	MTR2	R2	0	0
167		MTR2	R2	LDY-21282	UNK_AHG_HZ_SOAS_167	MTR2	R2	0	0
168	C6H10O6	MT	Lab Expt/R2	LDY-21250	UNK_AHG_HZ_SOAS_135	MT	Lab Expt/R2	0	0
169	C6H8O5	SQT	Lab Expt	LDY-21284	UNK_AHG_HZ_SOAS_169	SQT	Lab Expt	0	0
170		MTR2	R2	LDY-21285	UNK_AHG_HZ_SOAS_170	SQT	MS/Field Expt	1	1
171		MTR2	R2	LDY-21286	UNK_AHG_HZ_SOAS_171	MTR2	R2	0	0
172		Unknown		LDY-21287	UNK_AHG_HZ_SOAS_172	MT	MS/LabExpt /Field Expt	1	1
173	C8H12O4	MTR2	R2	LDY-21146	UNK_AHG_HZ_SOAS_30	MTR2	R2	0	0
174		MT	Lab Expt	LDY-21289	UNK_AHG_HZ_SOAS_174	MT	Lab Expt	0	0
175		MT	MS	LDY-21290	UNK_AHG_HZ_SOAS_175	MT	MS	0	0
176		SQT	Lab Expt	LDY-21291	UNK_AHG_HZ_SOAS_176	SQT	Lab Expt	0	0
177		ASOA	R2	LDY-21292	UNK_AHG_HZ_SOAS_177	ASOA	R2	0	0
178		MTR2	R2	LDY-21293	UNK_AHG_HZ_SOAS_178	MTR2	R2	0	0
179		SQT	Lab Expt	LDY-21294	UNK_AHG_HZ_SOAS_179	SQT	Lab Expt	0	0
180		MT	Lab Expt	LDY-21295	UNK_AHG_HZ_SOAS_180	MT	Lab Expt	0	0
181		MTR2	R2	LDY-21296	UNK_AHG_HZ_SOAS_181	MTR2	R2	0	0
182		MTR2	R2	LDY-21297	UNK_AHG_HZ_SOAS_182	MTR2	R2	0	0
183		MTR2	R2	LDY-21298	UNK_AHG_HZ_SOAS_183	MTR2	R2	0	0
184	C10H14O4	SQT	R2	LDY-21299	UNK_AHG_HZ_SOAS_184	SQT	R2	0	0
185		BBOA	MS	LDY-21300	UNK_AHG_HZ_SOAS_185	BBOA	MS	0	0
186		MTR2	R2	LDY-21301	UNK_AHG_HZ_SOAS_186	MTR2	R2	0	0
187	C6H8O4	Unknown	MS	LDY-21254	UNK_AHG_HZ_SOAS_139	Unknown	MS	0	0
188		BOOA	MS	LDY-21303	UNK_AHG_HZ_SOAS_188	BOOA	MS	0	0
189	Diethyl Phthalate	BBOA	NIST/Lab Expt	LDY-21304	Diethyl Phthalate	BBOA	NIST/Lab Expt	0	0
190		BBOA	R2	LDY-21305	UNK_AHG_HZ_SOAS_190	BBOA	R2	0	0
191		MTR2	R2	LDY-21306	UNK_AHG_HZ_SOAS_191	MTR2	R2	0	0
192	C13H20O5	SQT	Lab Expt	LDY-21307	UNK_AHG_HZ_SOAS_192	SQT	Lab Expt	0	0
193	C13H20O5	SQT	Lab Expt	LDY-21307	UNK_AHG_HZ_SOAS_192	SQT	Lab Expt	0	0
194		POAOX	R2	LDY-21309	UNK_AHG_HZ_SOAS_194	POAOX	R2	0	0
195		MTR2	R2	LDY-21310	UNK_AHG_HZ_SOAS_195	MTR2	R2	0	0
196	C9H16O3	SQT	R2	LDY-21180	UNK_AHG_HZ_SOAS_65	SQT	MS/Lab Expt	0	1
197	C9H14O4	MT	Lab Expt/R2	LDY-21211	UNK_AHG_HZ_SOAS_96	MT	Lab Expt/R2	0	0
198		BOOA	MS	LDY-21313	UNK_AHG_HZ_SOAS_198	BOOA	MS	0	0

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199		BOOA	MS	LDY-21314	UNK_AHG_HZ_SOAS_199	BOOA	MS	0	0
200		BOOA	MS	LDY-21315	UNK_AHG_HZ_SOAS_200	BOOA	MS	0	0
201		BBOA	R2	LDY-21316	UNK_AHG_HZ_SOAS_201	BBOA	R2	0	0
202		BBOA	R2	LDY-21317	3-Deoxy-ribo-hexonic acid 1-4-lactone, 3 TMS	BBOA	MS/Lab Expt	0	1
203	C15 acid	POAOX	R2	LDY-21318	C15 acid, TMS	POAOX	R2	0	0
204	d14-nalkane	IStd	MS	LDY-21319	d14-nalkane	IStd	MS	0	0
205		BBOA	MS	LDY-21320	UNK_AHG_HZ_SOAS_205	BBOA	MS	0	0
206		MTR2	R2	LDY-21321	UNK_AHG_HZ_SOAS_206	MT	MS/Lab Expt	1	1
207		BOOA	MS	LDY-21322	UNK_AHG_HZ_SOAS_207	BOOA	MS	0	0
208		MTR2	R2	LDY-21323	UNK_AHG_HZ_SOAS_208	MTR2	R2	0	0
209		SQT	Lab Expt	LDY-21324	UNK_AHG_HZ_SOAS_209	SQT	Lab Expt	0	0
210		BOOA	MS	LDY-21325	UNK_AHG_HZ_SOAS_210	BOOA	MS	0	0
211		MTR2	R2	LDY-21326	UNK_AHG_HZ_SOAS_211	MTR2	R2	0	0
212	C9H12O5	MTR2	R2	LDY-21224	UNK_AHG_HZ_SOAS_109	MTR2	R2	0	0
213		BOOA	MS	LDY-21328	UNK_AHG_HZ_SOAS_213	BOOA	MS	0	0
214		Unknown		LDY-21329	UNK_AHG_HZ_SOAS_214	MT	MS/LabExpt /Field Expt	1	1
215		Unknown		LDY-21330	UNK_AHG_HZ_SOAS_215	Unknown	0	0	0
216		MT	Lab Expt	LDY-21331	UNK_AHG_HZ_SOAS_216	MT	Lab Expt	0	0
217		MTR2	R2	LDY-21332	UNK_AHG_HZ_SOAS_217	MTR2	R2	0	0
218	C8H12O5	MT	Lab Expt/R2	LDY-21129	UNK_AHG_HZ_SOAS_12	MT	Lab Expt/R2	0	0
219		SQT	Lab Expt	LDY-21334	UNK_AHG_HZ_SOAS_219	SQT	Lab Expt	0	0
220		MTR2	R2	LDY-21335	UNK_AHG_HZ_SOAS_220	MTR2	R2	0	0
221		BBOA	R2	LDY-21336	UNK_AHG_HZ_SOAS_221	BBOA/MT /SQT	MS/Lab Expt/Field Expt	1	1
222	Threonic acid isomer	ASOA	NIST	LDY-21337	Threonic acid isomer, 4 TMS	ASOA	NIST	0	0
223		BOOA	MS	LDY-21338	UNK_AHG_HZ_SOAS_223	BOOA	MS	0	0
224	Adipic acid	MTR2	NIST/R2	LDY-21339	Adipic acid, 2 TMS	MTR2	NIST/R2	0	0
225		MTR2	R2	LDY-21340	UNK_AHG_HZ_SOAS_225	MTR2	R2	0	0
226		SQT	R2	LDY-21341	UNK_AHG_HZ_SOAS_226	SQT	R2	0	0
227		SQT	Lab Expt	LDY-21342	UNK_AHG_HZ_SOAS_227	SQT	Lab Expt	0	0

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228		MTR2	R2	LDY-21343	UNK_AHG_HZ_SOAS_228	MT	MS/Lab Expt	1	1
229		MT	Lab Expt	LDY-21344	UNK_AHG_HZ_SOAS_229	MT	Lab Expt	0	0
230		SQT	Lab Expt	LDY-21345	UNK_AHG_HZ_SOAS_230	SQT	Lab Expt	0	0
231		MTR2	R2	LDY-21346	UNK_AHG_HZ_SOAS_231	MTR2	R2	0	0
232		Unknown		LDY-21347	UNK_AHG_HZ_SOAS_232	Unknown	0	0	0
233	C9H14O4	MT	Lab Expt/R2	LDY-21211	UNK_AHG_HZ_SOAS_96	MT	Lab Expt/R2	0	0
234		POAOX	MS	LDY-21349	UNK_AHG_HZ_SOAS_234	POAOX	MS	0	0
235		BBOA	R2	LDY-21350	UNK_AHG_HZ_SOAS_235	BBOA	R2	0	0
236		MT	Lab Expt/R2	LDY-21351	UNK_AHG_HZ_SOAS_236	MT	Lab Expt/R2	0	0
237	pinic acid isomer	MT	EI	LDY-21352	pinic acid isomer, 2 TMS	MT	EI	0	0
238		SQT	Lab Expt	LDY-21353	UNK_AHG_HZ_SOAS_238	SQT	Lab Expt	0	0
239		BOOA	MS	LDY-21354	UNK_AHG_HZ_SOAS_239	BOOA	MS	0	0
240		MTR2	R2	LDY-21355	UNK_AHG_HZ_SOAS_240	MT	MS/Lab Expt	1	1
241		BOOA	MS	LDY-21356	UNK_AHG_HZ_SOAS_241	BOOA	MS	0	0
242	C9H14O5	MT	Lab Expt	LDY-21159	UNK_AHG_HZ_SOAS_43	MT	Lab Expt	0	0
243	Phthalic acid, butyl isohexyl ester	POAOX	NIST	LDY-21358	Phthalic acid, butyl isohexyl ester	POAOX	NIST	0	0
244	C9H12O5	MTR2	R2	LDY-21224	UNK_AHG_HZ_SOAS_109	MTR2	R2	0	0
245		BOOA	MS	LDY-21360	UNK_AHG_HZ_SOAS_245	BOOA	MS	0	0
246	hexadecanol	POAOX	MS	LDY-21361	hexadecanol, TMS	POAOX	MS	0	0
247		MTR2	R2	LDY-21362	UNK_AHG_HZ_SOAS_247	MTR2	R2	0	0
248		MTR2	R2	LDY-21363	UNK_AHG_HZ_SOAS_248	MTR2	R2	0	0
249		MTR2	R2	LDY-21364	UNK_AHG_HZ_SOAS_249	MTR2	R2	0	0
250		MTR2	R2	LDY-21365	UNK_AHG_HZ_SOAS_250	MT/SQT	MS/Lab Expt/Field Expt	1	1
251		ISOP	R2	LDY-21366	UNK_AHG_HZ_SOAS_251	ISOP	R2	0	0
252		MTR2	R2	LDY-21367	UNK_AHG_HZ_SOAS_252	MTR2	R2	0	0
253		SQT	Lab Expt	LDY-21368	UNK_AHG_HZ_SOAS_253	SQT	Lab Expt	0	0
254		MTR2	R2	LDY-21369	UNK_AHG_HZ_SOAS_254	MTR2	R2	0	0
255		MTR2	R2	LDY-21370	UNK_AHG_HZ_SOAS_255	MTR2	R2	0	0

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256		MTR2	R2	LDY-21371	UNK_AHG_HZ_SOAS_256	Unknown	R2	1	0
257		MTR2	R2	LDY-21372	UNK_AHG_HZ_SOAS_257	MTR2	R2	0	0
258		BOOA	MS	LDY-21373	UNK_AHG_HZ_SOAS_258	BOOA	MS	0	0
259		MTR2	R2	LDY-21374	UNK_AHG_HZ_SOAS_259	MTR2	R2	0	0
260	C5H6O4	MTR2	R2	LDY-21255	UNK_AHG_HZ_SOAS_140	MTR2	R2	0	0
261		SQT	Lab Expt	LDY-21376	UNK_AHG_HZ_SOAS_261	SQT	Lab Expt	0	0
262		Unknown		LDY-21377	UNK_AHG_HZ_SOAS_262	Unknown	0	0	0
263		MTR2	R2	LDY-21378	UNK_AHG_HZ_SOAS_263	MTR2	R2	0	0
264	C4H6O4	BOOA	MS	LDY-21379	UNK_AHG_HZ_SOAS_264	BOOA	MS	0	0
265		BOOA	MS	LDY-21380	UNK_AHG_HZ_SOAS_265	BOOA	MS	0	0
266	Manoyl oxide isomer	POAOX	NIST	LDY-21381	Manoyl oxide isomer	POAOX	NIST	0	0
267	C8H14O4	MTR2	R2	LDY-21232	UNK_AHG_HZ_SOAS_117	MTR2	R2	0	0
268	C7H12O4	SQT	Lab Expt	LDY-21167	UNK_AHG_HZ_SOAS_52	SQT	Lab Expt	0	0
269		BOOA	MS	LDY-21384	UNK_AHG_HZ_SOAS_269	BOOA	MS	0	0
270		MTR2	R2	LDY-21385	UNK_AHG_HZ_SOAS_270	MTR2	R2	0	0
271		MTR2	R2	LDY-21386	UNK_AHG_HZ_SOAS_271	MTR2	R2	0	0
272		MTR2	R2	LDY-21387	UNK_AHG_HZ_SOAS_272	MTR2	R2	0	0
273		MTR2	R2	LDY-21388	UNK_AHG_HZ_SOAS_273	MTR2	R2	0	0
274	Erythritol	BBOA	NIST	LDY-21389	Erythritol, 4 TMS	BBOA	NIST	0	0
275		MTR2	R2	LDY-21390	UNK_AHG_HZ_SOAS_275	MTR2	R2	0	0
276		SQT	Lab Expt	LDY-21391	UNK_AHG_HZ_SOAS_276	SQT	Lab Expt	0	0
277		MTR2	R2	LDY-21392	UNK_AHG_HZ_SOAS_277	MTR2	R2	0	0
278	d34-nalkane	IStd	MS	LDY-21393	d34-nalkane	IStd	MS	0	0
279		MTR2	R2	LDY-21394	UNK_AHG_HZ_SOAS_279	MTR2	R2	0	0
280		SQT	Lab Expt	LDY-21395	UNK_AHG_HZ_SOAS_280	SQT	Lab Expt	0	0
281		BOOA	MS	LDY-21396	UNK_AHG_HZ_SOAS_281	BOOA	MS	0	0
282		POAOX	R2	LDY-21397	UNK_AHG_HZ_SOAS_282	POAOX	R2	0	0
283	C9H12O5	MTR2	R2	LDY-21224	UNK_AHG_HZ_SOAS_109	MTR2	R2	0	0
284		BOOA	MS	LDY-21399	UNK_AHG_HZ_SOAS_284	BOOA	MS	0	0
285		MTR2	R2	LDY-21400	UNK_AHG_HZ_SOAS_285	MTR2	R2	0	0
286		BOOA	MS	LDY-21401	UNK_AHG_HZ_SOAS_286	BOOA	MS	0	0
287		BOOA	MS	LDY-21402	UNK_AHG_HZ_SOAS_287	BOOA	MS	0	0
288		POAOX	R2	LDY-21403	UNK_AHG_HZ_SOAS_288	POAOX	MS/NIST20	0	1
289		BBOA	MS	LDY-21404	UNK_AHG_HZ_SOAS_289	BBOA	MS	0	0
290		SQT	Lab Expt	LDY-21405	UNK_AHG_HZ_SOAS_290	SQT	Lab Expt	0	0

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291		MT	Lab Expt/R2	LDY-21406	UNK_AHG_HZ_SOAS_291	MT	Lab Expt/R2	0	0
292	D7 cMS	ASOA	MS	LDY-21407	D7 cMS	ASOA	MS	0	0
293		MTR2	R2	LDY-21408	UNK_AHG_HZ_SOAS_293	MTR2	R2	0	0
294		BOOA	MS	LDY-21409	UNK_AHG_HZ_SOAS_294	BOOA	MS	0	0
295		Unknown		LDY-21410	UNK_AHG_HZ_SOAS_295	Unknown	0	0	0
296		SQT	Lab Expt	LDY-21411	UNK_AHG_HZ_SOAS_296	SQT	Lab Expt	0	0
297		MTR2	R2	LDY-21412	UNK_AHG_HZ_SOAS_297	SQT	MS/Lab Expt/Field Expt	1	1
298		MTR2	R2	LDY-21413	UNK_AHG_HZ_SOAS_298	MTR2	R2	0	0
299		SQT	Lab Expt	LDY-21414	UNK_AHG_HZ_SOAS_299	SQT	Lab Expt	0	0
300		MTR2	R2	LDY-21415	UNK_AHG_HZ_SOAS_300	MTR2	R2	0	0
301		MTR2	R2	LDY-21416	UNK_AHG_HZ_SOAS_301	MT	MS/Lab Expt/Field Expt	1	1
302	tetradecanol	POAOX	R2	LDY-21417	tetradecanol, TMS	POAOX	R2	0	0
303		BBOA	R2	LDY-21418	UNK_AHG_HZ_SOAS_303	BBOA	R2	0	0
304	1,2,3-butanol	ASOA	NIST	LDY-21419	1,2,3-butanol, 3 TMS	ASOA	NIST	0	0
305		MT	Lab Expt	LDY-21420	UNK_AHG_HZ_SOAS_305	MT	Lab Expt	0	0
306		MTR2	R2	LDY-21421	UNK_AHG_HZ_SOAS_306	MTR2	R2	0	0
307		Unknown		LDY-21422	UNK_AHG_HZ_SOAS_307	Unknown	0	0	0
308		Unknown		LDY-21423	UNK_AHG_HZ_SOAS_308	Unknown	0	0	0
309	hexadecanoic acid, methyl ester	POAOX	R2	LDY-21424	hexadecanoic acid, methyl ester	POAOX	R2	0	0
310		SQT	Lab Expt	LDY-21425	UNK_AHG_HZ_SOAS_310	SQT	Lab Expt	0	0
311		MTR2		LDY-21426	UNK_AHG_HZ_SOAS_311	MTR2	0	0	0
312		MTR2	R2	LDY-21427	UNK_AHG_HZ_SOAS_312	MTR2	R2	0	0
313	C8H10O4	MT	Lab Expt/R2	LDY-21268	UNK_AHG_HZ_SOAS_153	MT	Lab Expt/R2	0	0
314	d36-nalkane	IStd	MS	LDY-21429	d36-nalkane	IStd	MS	0	0
315		MTR2	R2	LDY-21430	UNK_AHG_HZ_SOAS_315	MT/SQT	MS/Lab Expt/Field Expt	1	1
316		Unknown		LDY-21431	UNK_AHG_HZ_SOAS_316	Unknown	0	0	0
317		Unknown		LDY-21432	UNK_AHG_HZ_SOAS_317	Unknown	0	0	0
318		MTR2	R2	LDY-21433	UNK_AHG_HZ_SOAS_318	MTR2	R2	0	0

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319		BOOA	MS	LDY-21434	UNK_AHG_HZ_SOAS_319	BOOA	MS	0	0
320		MTR2	R2	LDY-21435	UNK_AHG_HZ_SOAS_320	MTR2	R2	0	0
321		MTR2	R2	LDY-21436	UNK_AHG_HZ_SOAS_321	MTR2	R2	0	0
322		POAOX	R2	LDY-21437	UNK_AHG_HZ_SOAS_322	MT/SQT	MS/Lab Expt/Field Expt	1	1
323		BBOA	R2	LDY-21864	UNK_AHG_HZ_SOAS_323	BBOA	R2	0	0
324		BOOA	MS	LDY-21439	UNK_AHG_HZ_SOAS_324	BOOA	MS	0	0
325	C7H8O5	SQT	Lab Expt	LDY-21220	UNK_AHG_HZ_SOAS_105	SQT	Lab Expt	0	0
326		ASOA	R2	LDY-21441	UNK_AHG_HZ_SOAS_326	ISOP	MS/Lab Expt/Field Expt	1	1
327		ASOA	R2	LDY-21442	Ribonic acid, 5 TMS	ASOA	MS/Field Expt/NIST20	0	1
328		MTR2	R2	LDY-21443	UNK_AHG_HZ_SOAS_328	MTR2	R2	0	0
329		MTR2	R2	LDY-21444	UNK_AHG_HZ_SOAS_329	MTR2	R2	0	0
330	C10H16O4	MT	Lab Expt/R2	LDY-21175	UNK_AHG_HZ_SOAS_60	MT	Lab Expt/R2	0	0
331		Unknown		LDY-21446	UNK_AHG_HZ_SOAS_331	Unknown	0	0	0
332		Unknown		LDY-21447	UNK_AHG_HZ_SOAS_332	Unknown	0	0	0
333		MT	Lab Expt	LDY-21448	UNK_AHG_HZ_SOAS_333	MT	Lab Expt	0	0
334		MTR2	R2	LDY-21449	UNK_AHG_HZ_SOAS_334	MTR2	R2	0	0
335		MTR2	R2	LDY-21450	UNK_AHG_HZ_SOAS_335	MTR2	R2	0	0
336		MTR2	R2	LDY-21451	UNK_AHG_HZ_SOAS_336	MTR2	R2	0	0
337		MT	Lab Expt	LDY-21452	UNK_AHG_HZ_SOAS_337	MT	Lab Expt	0	0
338		BBOA	R2	LDY-21453	UNK_AHG_HZ_SOAS_338	BBOA	R2	0	0
339		Unknown		LDY-21454	UNK_AHG_HZ_SOAS_339	Unknown	0	0	0
340		ASOA	MS	LDY-21455	UNK_AHG_HZ_SOAS_340	ASOA	MS	0	0
341		MTR2	R2	LDY-21456	UNK_AHG_HZ_SOAS_341	MTR2	R2	0	0
342		POAOX	R2	LDY-21457	UNK_AHG_HZ_SOAS_342	POAOX	MS/Field Expt/NIST20	0	1
343		BOOA	MS	LDY-21458	UNK_AHG_HZ_SOAS_343	BOOA	MS	0	0
344		MTR2	R2	LDY-21459	UNK_AHG_HZ_SOAS_344	MTR2	R2	0	0
345		MT	Lab Expt	LDY-21460	UNK_AHG_HZ_SOAS_345	MT	Lab Expt	0	0
346		MTR2	R2	LDY-21461	UNK_AHG_HZ_SOAS_346	SQT	MS/Lab Expt/Field Expt	1	1

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347		MTR2	R2	LDY-21462	UNK_AHG_HZ_SOAS_347	MTR2	R2	0	0
348		BOOA	MS	LDY-21463	UNK_AHG_HZ_SOAS_348	BOOA	MS	0	0
349		Unknown		LDY-21464	UNK_AHG_HZ_SOAS_349	Unknown	0	0	0
350		MTR2	R2	LDY-21465	UNK_AHG_HZ_SOAS_350	MTR2	R2	0	0
351		MTR2	R2	LDY-21466	UNK_AHG_HZ_SOAS_351	MTR2	R2	0	0
352		MTR2	R2	LDY-21467	UNK_AHG_HZ_SOAS_352	MTR2	R2	0	0
353		SQT	Lab Expt	LDY-21468	UNK_AHG_HZ_SOAS_353	SQT	Lab Expt	0	0
354		MTR2	R2	LDY-21469	UNK_AHG_HZ_SOAS_354	MTR2	R2	0	0
355		SQT	Lab Expt	LDY-21470	UNK_AHG_HZ_SOAS_355	SQT	Lab Expt	0	0
356	C6H10O5	MTR2	R2	LDY-21471	UNK_AHG_HZ_SOAS_356	SQT	MS/Lab Expt/Field Expt	1	1
357		Unknown		LDY-21472	UNK_AHG_HZ_SOAS_357	Unknown	0	0	0
358	C16H32O	POAOX	R2	LDY-21473	UNK_AHG_HZ_SOAS_358	POAOX	R2	0	0
359		MTR2	R2	LDY-21474	UNK_AHG_HZ_SOAS_359	MTR2	R2	0	0
360		MTR2	R2	LDY-21475	UNK_AHG_HZ_SOAS_360	MTR2	R2	0	0
361		MTR2	R2	LDY-21476	UNK_AHG_HZ_SOAS_361	MTR2	R2	0	0
362		BOOA	MS	LDY-21477	UNK_AHG_HZ_SOAS_362	BOOA	MS	0	0
363		MT	Lab Expt	LDY-21478	UNK_AHG_HZ_SOAS_363	MT	Lab Expt	0	0
364	C8H12O6	MTR2	R2	LDY-21239	UNK_AHG_HZ_SOAS_124	MTR2	R2	0	0
365	C9H12O6	SQT	Lab Expt	LDY-21136	UNK_AHG_HZ_SOAS_19	SQT	Lab Expt	0	0
366		BOOA	MS	LDY-21481	UNK_AHG_HZ_SOAS_366	BOOA	MS	0	0
367		MTR2	R2	LDY-21482	UNK_AHG_HZ_SOAS_367	ISOP/MT/SQT	MS/Lab Expt	1	1
368		POAOX	R2	LDY-21483	UNK_AHG_HZ_SOAS_368	POAOX	MS/NIST20	0	1
369	C6H6O3	BBOA	Lab Expt	LDY-21484	UNK_AHG_HZ_SOAS_369	BBOA	Lab Expt	0	0
370		MTR2	R2	LDY-21485	UNK_AHG_HZ_SOAS_370	MTR2	R2	0	0
371		MTR2	R2	LDY-21486	UNK_AHG_HZ_SOAS_371	MTR2	R2	0	0
372	C7H8O4	MT	MS	LDY-21487	UNK_AHG_HZ_SOAS_372	MT	MS	0	0
373		MTR2	R2	LDY-21488	UNK_AHG_HZ_SOAS_373	MTR2	R2	0	0
374		MTR2	R2	LDY-21489	UNK_AHG_HZ_SOAS_374	MTR2	R2	0	0
375		MTR2	R2	LDY-21490	UNK_AHG_HZ_SOAS_375	MTR2	R2	0	0
376		SQT	Lab Expt	LDY-21491	UNK_AHG_HZ_SOAS_376	SQT	Lab Expt	0	0
377	C17 n-alkane	hydrocarbon	MS	LDY-21492	C17 n-alkane	hydrocarbon	MS	0	0
378		Unknown		LDY-21493	UNK_AHG_HZ_SOAS_378	Unknown	0	0	0
379		MTR2	R2	LDY-21494	UNK_AHG_HZ_SOAS_379	MTR2	R2	0	0
380		BOOA	MS	LDY-21495	UNK_AHG_HZ_SOAS_380	BOOA	MS	0	0

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381	D8 cMS	ASOA	MS	LDY-21496	D8 cMS	ASOA	MS	0	0
382		SQT	Lab Expt	LDY-21497	UNK_AHG_HZ_SOAS_382	SQT	Lab Expt	0	0
383	Benzoic acid, 3-ol	ASOA	NIST	LDY-21498	Benzoic acid, 3-ol, 2 TMS	ASOA	NIST	0	0
384		MTR2	R2	LDY-21499	UNK_AHG_HZ_SOAS_384	SQT?	MS/Field Expt	1	1
385		BOOA	MS	LDY-21500	UNK_AHG_HZ_SOAS_385	BOOA	MS	0	0
386		Unknown		LDY-21501	UNK_AHG_HZ_SOAS_386	Unknown	0	0	0
387		MTR2	R2	LDY-21502	UNK_AHG_HZ_SOAS_387	MT	MS/Lab Expt	1	1
388		BOOA	MS	LDY-21503	UNK_AHG_HZ_SOAS_388	BOOA	MS	0	0
389		Unknown		LDY-21504	UNK_AHG_HZ_SOAS_389	Unknown	0	0	0
390		MTR2	R2	LDY-21505	UNK_AHG_HZ_SOAS_390	MTR2	R2	0	0
391		MTR2	R2	LDY-21506	UNK_AHG_HZ_SOAS_391	MTR2	R2	0	0
392	C21 n-alkane	hydrocarbon	MS	LDY-21507	C21 n-alkane	hydrocarbon	MS	0	0
393		MTR2	R2	LDY-21508	UNK_AHG_HZ_SOAS_393	MTR2	R2	0	0
394		MT	MS	LDY-21509	UNK_AHG_HZ_SOAS_394	MT	MS	0	0
395		SQT	Lab Expt	LDY-21510	UNK_AHG_HZ_SOAS_395	SQT	Lab Expt	0	0
396		BOOA	MS	LDY-21511	UNK_AHG_HZ_SOAS_396	BOOA	MS	0	0
397		MTR2	R2	LDY-21512	UNK_AHG_HZ_SOAS_397	SQT?	MS/Field Expt	1	1
398		MTR2	R2	LDY-21513	UNK_AHG_HZ_SOAS_398	MTR2	R2	0	0
399		SQT	Lab Expt	LDY-21514	UNK_AHG_HZ_SOAS_399	SQT	Lab Expt	0	0
400	2,3-dihydroxy-4-oxopentanoic acid	ASOA	MS	LDY-21515	2,3-dihydroxy-4-oxopentanoic acid, 3 TMS	ASOA	MS	0	0
401	C18 n-alkane	hydrocarbon	MS	LDY-21516	C18 n-alkane	hydrocarbon	MS	0	0
402		BOOA	MS	LDY-21517	UNK_AHG_HZ_SOAS_402	BOOA	MS	0	0
403		SQT	Lab Expt	LDY-21518	UNK_AHG_HZ_SOAS_403	SQT	Lab Expt	0	0
404	1,2,3-butanol isomer	ASOA	NIST	LDY-21519	1,2,3-butanol isomer, 3 TMS	ASOA	NIST	0	0
405		MTR2	R2	LDY-21520	UNK_AHG_HZ_SOAS_405	MTR2	R2	0	0
406		MTR2	R2	LDY-21521	UNK_AHG_HZ_SOAS_406	MTR2	R2	0	0
407		MTR2	R2	LDY-21522	UNK_AHG_HZ_SOAS_407	SQT?	MS/Field Expt	1	1
408		MTR2	R2	LDY-21523	UNK_AHG_HZ_SOAS_408	MTR2	R2	0	0

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409		SQT	Lab Expt	LDY-21524	UNK_AHG_HZ_SOAS_409	SQT	Lab Expt	0	0
410		BOOA	MS	LDY-21525	UNK_AHG_HZ_SOAS_410	BOOA	MS	0	0
411		MTR2	R2	LDY-21526	UNK_AHG_HZ_SOAS_411	MTR2	R2	0	0
412		BOOA	MS	LDY-21527	UNK_AHG_HZ_SOAS_412	BOOA	MS	0	0
413		MTR2	R2	LDY-21528	UNK_AHG_HZ_SOAS_413	MTR2	R2	0	0
414		MTR2	R2	LDY-21529	UNK_AHG_HZ_SOAS_414	MTR2	R2	0	0
415		MT	Lab Expt	LDY-21530	UNK_AHG_HZ_SOAS_415	MT	Lab Expt	0	0
416		SQT	Lab Expt	LDY-21531	UNK_AHG_HZ_SOAS_416	SQT	Lab Expt	0	0
417		MTR2	R2	LDY-21532	UNK_AHG_HZ_SOAS_417	MT/SQT	MS/Lab Expt	1	1
418	C10H14O4	SQT	R2	LDY-21299	UNK_AHG_HZ_SOAS_184	SQT	R2	0	0
419		MTR2	R2	LDY-21534	UNK_AHG_HZ_SOAS_419	MTR2	R2	0	0
420		SQT	Lab Expt	LDY-21535	UNK_AHG_HZ_SOAS_420	SQT	Lab Expt	0	0
421		MTR2	R2	LDY-21536	UNK_AHG_HZ_SOAS_421	MT	MS/Lab Expt	1	1
422		POAOX	R2	LDY-21537	Benzenesulfonamide, N-butyl-	POAOX	MS/NIST20	0	1
423		SQT	Lab Expt	LDY-21538	UNK_AHG_HZ_SOAS_423	SQT	Lab Expt	0	0
424		MTR2	R2	LDY-21539	UNK_AHG_HZ_SOAS_424	MT	MS/Lab Expt	1	1
425		MTR2	R2	LDY-21540	UNK_AHG_HZ_SOAS_425	MTR2	R2	0	0
426		BBOA	R2	LDY-21541	UNK_AHG_HZ_SOAS_426	BBOA	R2	0	0
427		SQT	Lab Expt	LDY-21542	UNK_AHG_HZ_SOAS_427	SQT	Lab Expt	0	0
428		MTR2	R2	LDY-21543	UNK_AHG_HZ_SOAS_428	MTR2	R2	0	0
429	C6H8O5	MTR2	R2	LDY-21284	UNK_AHG_HZ_SOAS_169	MTR2	R2	0	0
430		ISOP	R2	LDY-21545	UNK_AHG_HZ_SOAS_430	ISOP	MS/Lab Expt/Field Expt	0	1
431		MTR2	R2	LDY-21546	UNK_AHG_HZ_SOAS_431	MTR2	R2	0	0
432		BBOA	R2	LDY-21547	UNK_AHG_HZ_SOAS_432	BBOA	R2	0	0
433		Unknown		LDY-21548	limone diepoxide	MT	MS/NIST20	1	1
434	C7H8O3	ASOA	R2	LDY-21549	UNK_AHG_HZ_SOAS_434	ASOA	R2	0	0
435		ISOP	R2	LDY-21550	UNK_AHG_HZ_SOAS_435	ISOP	R2	0	0
436		BOOA	MS	LDY-21551	UNK_AHG_HZ_SOAS_436	BOOA	MS	0	0
437		MTR2	R2	LDY-21552	UNK_AHG_HZ_SOAS_437	MTR2	R2	0	0
438		MTR2	R2	LDY-21553	UNK_AHG_HZ_SOAS_438	MTR2	R2	0	0
439		BOOA	MS	LDY-21554	UNK_AHG_HZ_SOAS_439	BOOA	MS	0	0
440		MTR2	R2	LDY-21555	UNK_AHG_HZ_SOAS_440	MTR2	R2	0	0

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441		BOOA	MS	LDY-21556	UNK_AHG_HZ_SOAS_441	BOOA	MS	0	0
442		BOOA	MS	LDY-21557	UNK_AHG_HZ_SOAS_442	BOOA	MS	0	0
443		MT	R2/Lab Expt	LDY-21558	UNK_AHG_HZ_SOAS_443	MT	R2/Lab Expt	0	0
444		Unknown		LDY-21559	UNK_AHG_HZ_SOAS_444	Unknown	0	0	0
445		BBOA	R2	LDY-21560	UNK_AHG_HZ_SOAS_445	BBOA	R2	0	0
446		MTR2	R2	LDY-21561	UNK_AHG_HZ_SOAS_446	MTR2	R2	0	0
447	C6H8O3	MT	Lab Expt	LDY-21562	UNK_AHG_HZ_SOAS_447	MT	Lab Expt	0	0
448		BOOA	MS	LDY-21563	UNK_AHG_HZ_SOAS_448	BOOA	MS	0	0
449		MTR2	R2	LDY-21564	UNK_AHG_HZ_SOAS_449	SQT	MS/Lab Expt/Field Expt	1	1
450		BOOA	MS	LDY-21565	UNK_AHG_HZ_SOAS_450	BOOA	MS	0	0
451		BOOA	MS	LDY-21566	UNK_AHG_HZ_SOAS_451	BOOA	MS	0	0
452		SQT	Lab Expt	LDY-21567	UNK_AHG_HZ_SOAS_452	SQT	Lab Expt	0	0
453		BBOA	R2	LDY-21568	UNK_AHG_HZ_SOAS_453	BBOA	R2	0	0
454		SQT	Lab Expt	LDY-21569	UNK_AHG_HZ_SOAS_454	SQT	Lab Expt	0	0
455		MTR2	R2	LDY-21570	UNK_AHG_HZ_SOAS_455	MT/SQT	MS/Lab Expt	1	1
456		BBOA	R2	LDY-21571	UNK_AHG_HZ_SOAS_456	BBOA	R2	0	0
457		SQT	Lab Expt	LDY-21572	UNK_AHG_HZ_SOAS_457	SQT	Lab Expt	0	0
458	C5 alkenetriols 3	ISOP	MS	LDY-21573	C5 alkenetriols 3, 3 TMS	ISOP	MS	0	0
459		MTR2	R2	LDY-21574	UNK_AHG_HZ_SOAS_459	MTR2	R2	0	0
460		BBOA	R2	LDY-21575	UNK_AHG_HZ_SOAS_460	BBOA	MS/Field Expt	0	1
461		SQT	R2	LDY-21576	UNK_AHG_HZ_SOAS_461	SQT	R2	0	0
462		BOOA	MS	LDY-21577	UNK_AHG_HZ_SOAS_462	BOOA	MS	0	0
463		Unknown		LDY-21578	UNK_AHG_HZ_SOAS_463	Unknown	0	0	0
464		MTR2	R2	LDY-21579	UNK_AHG_HZ_SOAS_464	MTR2	R2	0	0
465		MTR2	R2	LDY-21580	UNK_AHG_HZ_SOAS_465	MTR2	R2	0	0
466		MTR2	R2	LDY-21581	UNK_AHG_HZ_SOAS_466	MTR2	R2	0	0
467		MTR2	R2	LDY-21582	UNK_AHG_HZ_SOAS_467	MTR2	R2	0	0
468		Unknown		LDY-21583	UNK_AHG_HZ_SOAS_468	Unknown	0	0	0
469		BOOA	MS	LDY-21584	UNK_AHG_HZ_SOAS_469	BOOA	MS	0	0
470	d13-nalkane	IStd	MS	LDY-21585	d13-nalkane	IStd	MS	0	0
471		MTR2	R2	LDY-21586	UNK_AHG_HZ_SOAS_471	MTR2	R2	0	0
472		SQT	Lab Expt	LDY-21587	UNK_AHG_HZ_SOAS_472	SQT	Lab Expt	0	0

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473	C5H6O4	MTR2	R2	LDY-21255	UNK_AHG_HZ_SOAS_140	MT	MS/Lab Expt	1	1
474		Unknown		LDY-21589	UNK_AHG_HZ_SOAS_474	Unknown	0	0	0
475	C6H10O3	SQT	Lab Expt	LDY-21590	UNK_AHG_HZ_SOAS_475	SQT	Lab Expt	0	0
476		MTR2	R2	LDY-21591	UNK_AHG_HZ_SOAS_476	MTR2	R2	0	0
477	C6H8O5	MTR2	R2	LDY-21284	UNK_AHG_HZ_SOAS_169	MTR2	R2	0	0
478	2-pentadecanol	POAOX	NIST	LDY-21593	2-pentadecanol, TMS	POAOX	NIST	0	0
479		BOOA	MS	LDY-21594	UNK_AHG_HZ_SOAS_479	BOOA	MS	0	0
480		MTR2	R2	LDY-21595	UNK_AHG_HZ_SOAS_480	MTR2	R2	0	0
481		ISOP	R2	LDY-21596	UNK_AHG_HZ_SOAS_481	ISOP	R2	0	0
482		MTR2	R2	LDY-21597	UNK_AHG_HZ_SOAS_482	MTR2	R2	0	0
483		ISOP	R2	LDY-21598	UNK_AHG_HZ_SOAS_483	ISOP	R2	0	0
484		MTR2	R2	LDY-21599	UNK_AHG_HZ_SOAS_484	MTR2	R2	0	0
485	C8H12O4	MT	Lab Expt	LDY-21146	UNK_AHG_HZ_SOAS_30	MT	Lab Expt	0	0
486		ISOP	R2	LDY-21601	UNK_AHG_HZ_SOAS_486	ISOP	R2	0	0
487		MTR2	R2	LDY-21602	UNK_AHG_HZ_SOAS_487	MTR2	R2	0	0
488	C9H16O5	SQT	Lab Expt	LDY-21603	UNK_AHG_HZ_SOAS_488	SQT	Lab Expt	0	0
489		BOOA	MS	LDY-21604	UNK_AHG_HZ_SOAS_489	BOOA	MS	0	0
490		MTR2	R2	LDY-21605	UNK_AHG_HZ_SOAS_490	MTR2	R2	0	0
491		ISOP	R2	LDY-21606	UNK_AHG_HZ_SOAS_491	ISOP	R2	0	0
492		MTR2	R2	LDY-21607	UNK_AHG_HZ_SOAS_492	MTR2	R2	0	0
493		MTR2	R2	LDY-21608	UNK_AHG_HZ_SOAS_493	MTR2	R2	0	0
494		ASOA	MS	LDY-21609	UNK_AHG_HZ_SOAS_494	ASOA	MS	0	0
495		MTR2	R2	LDY-21610	UNK_AHG_HZ_SOAS_495	MTR2	R2	0	0
496		BOOA	MS	LDY-21611	UNK_AHG_HZ_SOAS_496	BOOA	MS	0	0
497		MTR2	R2	LDY-21612	UNK_AHG_HZ_SOAS_497	MTR2	R2	0	0
498		ASOA	R2	LDY-21613	UNK_AHG_HZ_SOAS_498	ASOA	R2	0	0
499		MTR2	R2	LDY-21614	UNK_AHG_HZ_SOAS_499	MTR2	R2	0	0
500		BOOA	MS	LDY-21615	UNK_AHG_HZ_SOAS_500	BOOA	MS	0	0
501		MTR2	R2	LDY-21616	UNK_AHG_HZ_SOAS_501	MTR2	R2	0	0
502		MTR2	R2	LDY-21617	UNK_AHG_HZ_SOAS_502	MTR2	R2	0	0
503		MTR2	R2	LDY-21618	UNK_AHG_HZ_SOAS_503	MTR2	R2	0	0
504		BOOA	MS	LDY-21619	UNK_AHG_HZ_SOAS_504	BOOA	MS	0	0
505		BOOA	MS	LDY-21620	UNK_AHG_HZ_SOAS_505	BOOA	MS	0	0

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506		MTR2	R2	LDY-21621	UNK_AHG_HZ_SOAS_506	MTR2	R2	0	0
507		MTR2	R2	LDY-21622	UNK_AHG_HZ_SOAS_507	MT	MS/Lab Expt	1	1
508		SQT	Lab Expt	LDY-21623	UNK_AHG_HZ_SOAS_508	SQT	Lab Expt	0	0
509		ISOP	R2	LDY-21624	UNK_AHG_HZ_SOAS_509	ISOP	R2	0	0
510	C10 acid	POAOX	MS	LDY-21625	C10 acid, TMS	POAOX	MS	0	0
511		MTR2	R2	LDY-21626	UNK_AHG_HZ_SOAS_511	MT/SQT	MS/Lab Expt	1	1
512		MTR2	R2	LDY-21627	UNK_AHG_HZ_SOAS_512	BBOA	R2	1	0
513		BBOA	R2	LDY-21628	UNK_AHG_HZ_SOAS_513	BBOA/SQT	MS/Lab Expt/Field Expt	1	1
514		MTR2	R2	LDY-21629	UNK_AHG_HZ_SOAS_514	MTR2	R2	0	0
515		MTR2	R2	LDY-21630	UNK_AHG_HZ_SOAS_515	MTR2	R2	0	0
516		BOOA	MS	LDY-21631	UNK_AHG_HZ_SOAS_516	BOOA	MS	0	0
517		MTR2	R2	LDY-21632	UNK_AHG_HZ_SOAS_517	MTR2	R2	0	0
518		BOOA	MS	LDY-21633	UNK_AHG_HZ_SOAS_518	BOOA	MS	0	0
519		MTR2	R2	LDY-21634	UNK_AHG_HZ_SOAS_519	MTR2	R2	0	0
520	C7H10O4	MT	Lab Expt	LDY-21635	UNK_AHG_HZ_SOAS_520	MT	Lab Expt	0	0
521		Unknown		LDY-21636	UNK_AHG_HZ_SOAS_521	Unknown	0	0	0
522		MTR2	R2	LDY-21637	UNK_AHG_HZ_SOAS_522	MTR2	R2	0	0
523	D9 cMS	ASOA	MS	LDY-21638	D9 cMS	ASOA	MS	0	0
524		BBOA	R2	LDY-21639	UNK_AHG_HZ_SOAS_524	BBOA	R2	0	0
525		MTR2	R2	LDY-21640	UNK_AHG_HZ_SOAS_525	SQT	MS/Lab Expt/Field Expt	1	1
526		BOOA	MS	LDY-21641	UNK_AHG_HZ_SOAS_526	BOOA	MS	0	0
527		MTR2	R2	LDY-21642	UNK_AHG_HZ_SOAS_527	MTR2	R2	0	0
528	C10H16O3	MT	Lab Expt	LDY-21193	UNK_AHG_HZ_SOAS_78	MT	Lab Expt	0	0
529		BOOA	MS	LDY-21644	UNK_AHG_HZ_SOAS_529	BOOA	MS	0	0
530	C6H8O5	MTR2	R2	LDY-21284	UNK_AHG_HZ_SOAS_169	MTR2	R2	0	0
531		BBOA	R2	LDY-21646	UNK_AHG_HZ_SOAS_531	BBOA	R2	0	0
532	Benzamide, N,N-diethyl-4-methyl-	POAOX	NIST	LDY-21647	Benzamide, N,N-diethyl-4-methyl-	POAOX	NIST	0	0
533	C11 acid	POAOX	MS	LDY-21648	C11 acid, TMS	POAOX	MS	0	0
534		BOOA	MS	LDY-21649	UNK_AHG_HZ_SOAS_534	BOOA	MS	0	0
535		MTR2	R2	LDY-21650	UNK_AHG_HZ_SOAS_535	MTR2	R2	0	0
536		BOOA	MS	LDY-21651	UNK_AHG_HZ_SOAS_536	BOOA	MS	0	0

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537		MTR2	R2	LDY-21652	UNK_AHG_HZ_SOAS_537	MTR2	R2	0	0
538		MTR2	R2	LDY-21653	UNK_AHG_HZ_SOAS_538	SQT?	MS/Field Expt	1	1
539		Unknown		LDY-21654	UNK_AHG_HZ_SOAS_539	Unknown	0	0	0
540		POAOX	R2	LDY-21655	UNK_AHG_HZ_SOAS_540	POAOX	R2	0	0
541		BOOA	MS	LDY-21656	UNK_AHG_HZ_SOAS_541	BOOA	MS	0	0
542		BBOA	R2	LDY-21657	UNK_AHG_HZ_SOAS_542	BBOA	MS/Lab Expt	0	1
543		MTR2	R2	LDY-21658	UNK_AHG_HZ_SOAS_543	MTR2	R2	0	0
544	C7H10O4	MTR2	R2	LDY-21635	UNK_AHG_HZ_SOAS_520	MTR2	R2	0	0
545		Unknown		LDY-21660	UNK_AHG_HZ_SOAS_545	Unknown	0	0	0
546		SQT	Lab Expt	LDY-21661	UNK_AHG_HZ_SOAS_546	SQT	Lab Expt	0	0
547		MTR2	R2	LDY-21662	UNK_AHG_HZ_SOAS_547	MTR2	R2	0	0
548		MTR2	R2	LDY-21663	UNK_AHG_HZ_SOAS_548	SQT?	MS/Field Expt	1	1
549		MTR2	R2	LDY-21664	UNK_AHG_HZ_SOAS_549	MT	MS/Lab Expt/Field Expt	1	1
550		MTR2	R2	LDY-21665	UNK_AHG_HZ_SOAS_550	MTR2	R2	0	0
551		ASOA	R2	LDY-21666	UNK_AHG_HZ_SOAS_551	ISOP	MS/Lab Expt/Field Expt	1	1
552		MTR2	R2	LDY-21667	UNK_AHG_HZ_SOAS_552	SQT?	MS/Field Expt	1	1
553		BOOA	MS	LDY-21668	UNK_AHG_HZ_SOAS_553	BOOA	MS	0	0
554	C6H8O5	MTR2	R2	LDY-21284	UNK_AHG_HZ_SOAS_169	MTR2	R2	0	0
555	C9H14O3	MT	Lab Expt/R2	LDY-21206	UNK_AHG_HZ_SOAS_91	MT	Lab Expt/R2	0	0
556		MTR2	R2	LDY-21671	UNK_AHG_HZ_SOAS_556	MTR2	R2	0	0
557		SQT	Lab Expt	LDY-21672	UNK_AHG_HZ_SOAS_557	SQT	Lab Expt	0	0
558		MTR2	R2	LDY-21673	UNK_AHG_HZ_SOAS_558	MTR2	R2	0	0
559		POAOX	R2	LDY-21674	Acetylacetophenone	POAOX	MS/Field Expt/NIST20	0	1
560		MT	Lab Expt	LDY-21675	UNK_AHG_HZ_SOAS_560	MT	Lab Expt	0	0
561		BOOA	MS	LDY-21676	UNK_AHG_HZ_SOAS_561	BOOA	MS	0	0
562		BBOA	R2	LDY-21677	UNK_AHG_HZ_SOAS_562	BBOA	R2	0	0
563		BOOA	MS	LDY-21678	UNK_AHG_HZ_SOAS_563	BOOA	MS	0	0
564		MTR2	R2	LDY-21679	UNK_AHG_HZ_SOAS_564	MTR2	R2	0	0
565		POAOX	R2	LDY-21680	UNK_AHG_HZ_SOAS_565	POAOX	R2	0	0

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566		SQT	R2	LDY-21681	UNK_AHG_HZ_SOAS_566	SQT	R2	0	0
567		SQT	Lab Expt	LDY-21682	UNK_AHG_HZ_SOAS_567	SQT	Lab Expt	0	0
568		BOOA	MS	LDY-21683	UNK_AHG_HZ_SOAS_568	BOOA	MS	0	0
569		SQT	Lab Expt	LDY-21684	UNK_AHG_HZ_SOAS_569	SQT	Lab Expt	0	0
570		MTR2	R2	LDY-21685	UNK_AHG_HZ_SOAS_570	MTR2	R2	0	0
571	beta-caryophyllinic acid	SQT	MS	LDY-21686	beta-caryophyllinic acid, 2 TMS	SQT	MS	0	0
572		MTR2	R2	LDY-21687	UNK_AHG_HZ_SOAS_572	MTR2	R2	0	0
573		ASOA	R2	LDY-21688	UNK_AHG_HZ_SOAS_573	ISOP	MS/Lab Expt	1	1
574		ISOP	R2	LDY-21689	UNK_AHG_HZ_SOAS_574	ISOP	R2	0	0
575		BOOA	MS	LDY-21690	UNK_AHG_HZ_SOAS_575	BOOA	MS	0	0
576		POAOX	R2	LDY-21691	UNK_AHG_HZ_SOAS_576	POAOX	R2	0	0
577		MTR2	R2	LDY-21692	UNK_AHG_HZ_SOAS_577	MTR2	R2	0	0
578		BBOA	R2	LDY-21693	UNK_AHG_HZ_SOAS_578	BBOA	R2	0	0
579		ASOA	R2	LDY-21694	UNK_AHG_HZ_SOAS_579	ASOA	R2	0	0
580		MT	Lab Expt	LDY-21695	UNK_AHG_HZ_SOAS_580	MT	Lab Expt	0	0
581		MTR2	R2	LDY-21696	UNK_AHG_HZ_SOAS_581	SQT?	MS/Field Expt	1	1
582		ASOA	R2	LDY-21697	UNK_AHG_HZ_SOAS_582	BBOA	MS/Lab Expt	1	1
583		BOOA	MS	LDY-21698	UNK_AHG_HZ_SOAS_583	BOOA	MS	0	0
584		MTR2	R2	LDY-21699	UNK_AHG_HZ_SOAS_584	MTR2	R2	0	0
585		BOOA	MS	LDY-21700	UNK_AHG_HZ_SOAS_585	BOOA	MS	0	0
586		MTR2	R2	LDY-21701	UNK_AHG_HZ_SOAS_586	MTR2	R2	0	0
587		ISOP	R2	LDY-21702	UNK_AHG_HZ_SOAS_587	ISOP	R2	0	0
588		BOOA	MS	LDY-21703	UNK_AHG_HZ_SOAS_588	BOOA	MS	0	0
589		MTR2	R2	LDY-21704	UNK_AHG_HZ_SOAS_589	SQT	MS/Lab Expt	1	1
590		ISOP	R2	LDY-21705	UNK_AHG_HZ_SOAS_590	ISOP	MS/Lab Expt/Field Expt	0	1
591		BBOA	R2	LDY-21706	UNK_AHG_HZ_SOAS_591	SQT	MS/Lab Expt/Field Expt	1	1
592	C16 n-alkane	hydrocarbon	MS	LDY-21707	C16 n-alkane	hydrocarbon	MS	0	0
593		MTR2	R2	LDY-21708	UNK_AHG_HZ_SOAS_593	MTR2	R2	0	0
594		POAOX	R2	LDY-21709	UNK_AHG_HZ_SOAS_594	POAOX	R2	0	0
595		Unknown		LDY-21710	UNK_AHG_HZ_SOAS_595	Unknown	0	0	0

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596	C23 n-alkane	hydrocarbon	MS	LDY-21711	C23 n-alkane	hydrocarbon	MS	0	0
597	C9H14O4	MT	Lab Expt	LDY-21211	UNK_AHG_HZ_SOAS_96	MT	Lab Expt	0	0
598		ISOP	R2	LDY-21713	UNK_AHG_HZ_SOAS_598	ISOP	MS/Lab Expt	0	1
599		POAOX	R2	LDY-21714	UNK_AHG_HZ_SOAS_599	POAOX	R2	0	0
600	C5H8O4	MT	Lab Expt/R2	LDY-21715	UNK_AHG_HZ_SOAS_600	MT	Lab Expt/R2	0	0
601		BOOA	MS	LDY-21716	UNK_AHG_HZ_SOAS_601	BOOA	MS	0	0
602		BOOA	MS	LDY-21717	UNK_AHG_HZ_SOAS_602	BOOA	MS	0	0
603		BOOA	MS	LDY-21718	Glycerol, 3 TMS	BOOA	MS	0	0
604		BBOA	R2	LDY-21719	UNK_AHG_HZ_SOAS_604	BBOA	R2	0	0
605		MTR2	R2	LDY-21720	UNK_AHG_HZ_SOAS_605	MTR2	R2	0	0
606		Unknown		LDY-21721	Diethylene glycol, isobutyl ether, trimethylsilyl ether	Unknown	MS/NIST20	0	1
607		POAOX	R2	LDY-21722	UNK_AHG_HZ_SOAS_607	POAOX	R2	0	0
608		ISOP	R2	LDY-21723	UNK_AHG_HZ_SOAS_608	ISOP	MS/Lab Expt	0	1
609		MTR2	R2	LDY-21724	UNK_AHG_HZ_SOAS_609	MTR2	R2	0	0
610		MTR2	R2	LDY-21725	UNK_AHG_HZ_SOAS_610	MTR2	R2	0	0
611		Unknown		LDY-21726	vanillin, TMS	BBOA	MS/NIST20	1	1
612		ISOP	R2	#N/A	UNK_AHG_HZ_SOAS_612	ISOP	MS/Lab Expt	0	1
613		POAOX	R2	LDY-21728	UNK_AHG_HZ_SOAS_613	POAOX	R2	0	0
614		Unknown		LDY-21729	UNK_AHG_HZ_SOAS_614	Unknown	0	0	0
615		MTR2	R2	LDY-21730	UNK_AHG_HZ_SOAS_615	MTR2	R2	0	0
616	tridecanol	POAOX	MS	LDY-21731	tridecanol, TMS	POAOX	MS	0	0
617	C17 acid	POAOX	MS	LDY-21732	C17 acid, TMS	POAOX	MS	0	0
618		POAOX	R2	LDY-21733	UNK_AHG_HZ_SOAS_618	POAOX	R2	0	0
619	C8H14O3	MT	Lab Expt/R2	LDY-21734	UNK_AHG_HZ_SOAS_619	MT	Lab Expt/R2	0	0
620	dodecanol	POAOX	MS	LDY-21735	dodecanol, TMS	POAOX	MS	0	0
621		Unknown		LDY-21736	UNK_AHG_HZ_SOAS_621	Unknown	0	0	0
622	C8H12O5	MTR2	R2	LDY-21129	UNK_AHG_HZ_SOAS_12	MTR2	R2	0	0
623		BOOA	MS	LDY-21738	UNK_AHG_HZ_SOAS_623	BOOA	MS	0	0

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624		MTR2	R2	LDY-21739	UNK_AHG_HZ_SOAS_624	MTR2	R2	0	0
625		BOOA	MS	LDY-21740	UNK_AHG_HZ_SOAS_625	BOOA	MS	0	0
626		Unknown		LDY-21741	UNK_AHG_HZ_SOAS_626	Unknown	0	0	0
627		MTR2	R2	LDY-21742	UNK_AHG_HZ_SOAS_627	MTR2	R2	0	0
628		ISOP	R2	LDY-21743	UNK_AHG_HZ_SOAS_628	ISOP	R2	0	0
629	malonic acid	POAOX	NIST	LDY-21744	malonic acid, 2TMS	POAOX	NIST	0	0
630		MTR2	R2	LDY-21745	UNK_AHG_HZ_SOAS_630	MTR2	R2	0	0
631		MTR2	R2	LDY-21746	UNK_AHG_HZ_SOAS_631	MTR2	R2	0	0
632		MTR2	R2	LDY-21747	UNK_AHG_HZ_SOAS_632	MTR2	R2	0	0
633		BBOA	R2	LDY-21748	UNK_AHG_HZ_SOAS_633	BBOA	R2	0	0
634	Dehydroabietic Acid	BBOA	R2	LDY-21749	Dehydroabietic Acid, TMS	BBOA	R2	0	0
635		BBOA	R2	LDY-21750	Methyl dehydroabietate	BBOA	MS/Lab Expt/Field Expt/NIST20/Adams	0	1
636		MTR2	R2	LDY-21751	UNK_AHG_HZ_SOAS_636	SQT	MS/Lab Expt	1	1
637		BBOA	Lab Expt	LDY-21752	UNK_AHG_HZ_SOAS_637	BBOA	Lab Expt	0	0
638		BOOA	MS	LDY-21753	propanedioic acid, 2 TMS	BOOA	MS	0	0
639		MTR2	R2	LDY-21754	UNK_AHG_HZ_SOAS_639	MT	MS/Lab Expt	1	1
640		MTR2	R2	LDY-21755	UNK_AHG_HZ_SOAS_640	MTR2	R2	0	0
641		MT	Lab Expt/R2	LDY-21756	3,4-dihydroxybutanoic acid, 3 TMS	MT	Lab Expt/R2	0	0
642	C9H14O3	MT	Lab Expt	LDY-21206	UNK_AHG_HZ_SOAS_91	MT	Lab Expt	0	0
643		MTR2	R2	LDY-21758	UNK_AHG_HZ_SOAS_643	MTR2	R2	0	0
644	octadecanol	POAOX	MS	LDY-21759	octadecanol, TMS	POAOX	MS	0	0
645	2-methylglyceric acid	ISOP	MS	LDY-21760	2-methylglyceric acid, 3 TMS	ISOP	MS	0	0
646		BOOA	MS	LDY-21761	UNK_AHG_HZ_SOAS_646	BOOA	MS	0	0
647		Unknown		LDY-21762	UNK_AHG_HZ_SOAS_647	Unknown	0	0	0
648		Unknown		LDY-21763	UNK_AHG_HZ_SOAS_648	Unknown	0	0	0

index	Compound Name	Group	Group Determined By	UCB-GLOBES UID	Compound Name Reanalysis	Group Reanalysis	Group Determined By Reanalysis	Group Category Changed 0 = no 1 = yes	MS Confirmed 0 = no 1 = yes
649		Unknown		LDY-21764	UNK_AHG_HZ_SOAS_649	Unknown	0	0	0
650	C22 n-alkane	hydrocarbon	MS	LDY-21765	C22 n-alkane	hydrocarbon	MS	0	0
651		MTR2	R2	LDY-21766	UNK_AHG_HZ_SOAS_651	MTR2	R2	0	0
652		Unknown		LDY-21767	UNK_AHG_HZ_SOAS_652	Unknown	0	0	0
653		ISOP	R2	LDY-21768	UNK_AHG_HZ_SOAS_653	ISOP	MS/Lab Expt	0	1
654		ASOA	MS	LDY-21769	UNK_AHG_HZ_SOAS_654	ASOA	MS	0	0
655		SQT	Lab Expt	LDY-21770	UNK_AHG_HZ_SOAS_655	SQT	Lab Expt	0	0
656		BOOA	MS	LDY-21771	UNK_AHG_HZ_SOAS_656	BOOA	MS	0	0
657	C19 n-alkane, co-elution	hydrocarbon	MS	LDY-21772	C19 n-alkane, co-elution	hydrocarbon	MS	0	0
658		ASOA	R2	LDY-21773	UNK_AHG_HZ_SOAS_658	ISOP	MS/Lab Expt	1	1
659		MTR2	R2	LDY-21774	UNK_AHG_HZ_SOAS_659	MTR2	R2	0	0
660	C15 n-alkane	hydrocarbon	MS	LDY-21775	C15 n-alkane	hydrocarbon	MS	0	0
661		MTR2	R2	LDY-21776	UNK_AHG_HZ_SOAS_661	MT	MS/Lab Expt	1	1
662		Unknown		LDY-21777	UNK_AHG_HZ_SOAS_662	Unknown	0	0	0
663	d12-nalkane	IStd	MS	LDY-21778	d12-nalkane	IStd	MS	0	0
664		MTR2	R2	LDY-21779	UNK_AHG_HZ_SOAS_664	MTR2	R2	0	0
665	heptadecanol	POAOX	MS	LDY-21780	heptadecanol, TMS	POAOX	MS	0	0
666		ISOP	R2	LDY-21781	UNK_AHG_HZ_SOAS_666	ISOP	R2	0	0
667		BBOA	R2	LDY-21782	UNK_AHG_HZ_SOAS_667	ISOP	MS/Lab Expt/Field Expt	1	1
668		MTR2	R2	LDY-21783	UNK_AHG_HZ_SOAS_668	MTR2	R2	0	0
669		MTR2	R2	LDY-21784	UNK_AHG_HZ_SOAS_669	ISOP/MT	MS/Lab Expt	1	1
670		BOOA	MS	LDY-21785	UNK_AHG_HZ_SOAS_670	BOOA	MS	0	0
671	C16H48O6Si7	ASOA	MS	LDY-21786	UNK_AHG_HZ_SOAS_671	ASOA	MS	0	0
672		ISOP	R2	LDY-21787	UNK_AHG_HZ_SOAS_672	ISOP	MS/Lab Expt/Field Expt	0	1
673		MTR2	R2	LDY-21788	UNK_AHG_HZ_SOAS_673	MTR2	R2	0	0
674		Unknown		LDY-21789	UNK_AHG_HZ_SOAS_674	Unknown	0	0	0
675		ASOA	R2	LDY-21790	UNK_AHG_HZ_SOAS_675	ISOP	MS/Lab Expt/Field Expt	1	1

index	Compound Name	Group	Group Determined By	UCB-GLOBES UID	Compound Name Reanalysis	Group Reanalysis	Group Determined By Reanalysis	Group Category Changed 0 = no 1 = yes	MS Confirmed 0 = no 1 = yes
676		BBOA	R2	LDY-21791	UNK_AHG_HZ_SOAS_676	BBOA	MS/Lab Expt/Field Expt	0	1
677		MT	Lab Expt	LDY-21792	UNK_AHG_HZ_SOAS_677	MT	Lab Expt	0	0
678	hydroquinone	ASOA	NIST	LDY-21793	hydroquinone, 2 TMS	ASOA	NIST	0	0
679		BBOA	R2	LDY-21794	UNK_AHG_HZ_SOAS_679	BBOA	R2	0	0
680		MTR2	R2	LDY-21795	UNK_AHG_HZ_SOAS_680	MTR2	R2	0	0
681	2,6,10-trimethyl tetradecane	hydrocarbon	MS	LDY-21796	2,6,10-trimethyl tetradecane	hydrocarbon	MS	0	0
682		BBOA	R2	LDY-21797	UNK_AHG_HZ_SOAS_682	BBOA	MS/Lab Expt/Field Expt	0	1
683	C9 acid	POAOX	MS	LDY-21798	C9 acid, TMS	POAOX	MS	0	0
684		MT	Lab Expt	LDY-21799	UNK_AHG_HZ_SOAS_684	MT	Lab Expt	0	0
685		ISOP	R2	LDY-21800	UNK_AHG_HZ_SOAS_685	ISOP	R2	0	0
686		POAOX	R2	LDY-21801	UNK_AHG_HZ_SOAS_686	POAOX	R2	0	0
687		BOOA	MS	LDY-21802	UNK_AHG_HZ_SOAS_687	BOOA	MS	0	0
688	pristane	hydrocarbon	MS	LDY-21803	pristane	hydrocarbon	MS	0	0
689		Unknown		LDY-21804	UNK_AHG_HZ_SOAS_689	Unknown	0	0	0
690		MTR2	R2	LDY-21805	UNK_AHG_HZ_SOAS_690	MTR2	R2	0	0
691		MTR2	R2	LDY-21806	UNK_AHG_HZ_SOAS_691	MTR2	R2	0	0
692	D10 cMS	ASOA	MS	LDY-21807	D10 cMS	ASOA	MS	0	0
693		ISOP	R2	LDY-21808	UNK_AHG_HZ_SOAS_693	ISOP	R2	0	0
694	C20 acid	BBOA	R2	LDY-21809	C20 acid, TMS	BBOA	R2	0	0
695	C22 acid	BBOA	R2	LDY-21810	C22 acid, TMS	BBOA	R2	0	0
696	C23 acid	BBOA	R2	LDY-21811	C23 acid, TMS	BBOA	R2	0	0
697	C24 acid	BBOA	R2	LDY-21812	C24 acid, TMS	BBOA	R2	0	0
698	C26 acid	BBOA	R2	LDY-21813	C26 acid, TMS	BBOA	R2	0	0
699	C28 acid	BBOA	R2	LDY-21814	C28 acid, TMS	BBOA	R2	0	0
700	C14 n-alkane	hydrocarbon	MS	LDY-21815	C14 n-alkane	hydrocarbon	MS	0	0
701	C20 n-alkane	hydrocarbon	MS	LDY-21816	C20 n-alkane	hydrocarbon	MS	0	0
702	C24 n-alkane	hydrocarbon	MS	LDY-21817	C24 n-alkane	hydrocarbon	MS	0	0
703	C25 n-alkane	hydrocarbon	MS	LDY-21818	C25 n-alkane	hydrocarbon	MS	0	0

index	Compound Name	Group	Group Determined By	UCB-GLOBES UID	Compound Name Reanalysis	Group Reanalysis	Group Determined By Reanalysis	Group Category Changed 0 = no 1 = yes	MS Confirmed 0 = no 1 = yes
704	C26 n-alkane	hydrocarbon	MS	LDY-21819	C26 n-alkane	hydrocarbon	MS	0	0
705	C27 n-alkane	hydrocarbon	MS	LDY-21820	C27 n-alkane	hydrocarbon	MS	0	0
706	C28 n-alkane	hydrocarbon	MS	LDY-21821	C28 n-alkane	hydrocarbon	MS	0	0
707	C29 n-alkane	hydrocarbon	MS	LDY-21822	C29 n-alkane	hydrocarbon	MS	0	0
708	C31 n-alkane	hydrocarbon	MS	LDY-21823	C31 n-alkane	hydrocarbon	MS	0	0
709		BOOA	MS	LDY-21824	UNK_AHG_HZ_SOAS_709	BOOA	MS	0	0
710		ISOP	R2	LDY-21825	UNK_AHG_HZ_SOAS_710	ISOP	R2	0	0
711	D5 cVMS diol	ASOA	MS	LDY-21826	D5 cVMS diol	ASOA	MS	0	0
712		BOOA	MS	LDY-21827	UNK_AHG_HZ_SOAS_712	BOOA	MS	0	0
713	C9H16O5	SQT	Lab Expt	LDY-21603	UNK_AHG_HZ_SOAS_488	SQT	Lab Expt	0	0
714		Unknown		LDY-21829	UNK_AHG_HZ_SOAS_714	Unknown	0	0	0
715	MBO triol	BOOA	MS	LDY-21830	MBO triol, 3 TMS	BOOA	MS	0	0
716		Unknown		LDY-21831	UNK_AHG_HZ_SOAS_716	Unknown	0	0	0
717		Unknown		LDY-21832	UNK_AHG_HZ_SOAS_717	Unknown	0	0	0
718		BOOA	MS	LDY-21833	UNK_AHG_HZ_SOAS_718	BOOA	MS	0	0
719		Unknown		LDY-21834	UNK_AHG_HZ_SOAS_719	Unknown	0	0	0
720	hexadecanoic acid, butyl ester	POAOX	NIST	LDY-21835	hexadecanoic acid, butyl ester	POAOX	NIST	0	0
721		POAOX	R2	LDY-21836	UNK_AHG_HZ_SOAS_721	POAOX	R2	0	0
722		Unknown		LDY-21837	UNK_AHG_HZ_SOAS_722	Unknown	0	0	0
723		MTR2	R2	LDY-21838	UNK_AHG_HZ_SOAS_723	MTR2	R2	0	0
724		Unknown		LDY-21839	UNK_AHG_HZ_SOAS_724	Unknown	0	0	0
725		POAOX	R2	LDY-21840	UNK_AHG_HZ_SOAS_725	POAOX	R2	0	0
726		MTR2	R2	LDY-21841	UNK_AHG_HZ_SOAS_726	MTR2	R2	0	0
727		MTR2	R2	LDY-21842	UNK_AHG_HZ_SOAS_727	MTR2	R2	0	0
728		BOOA	MS	LDY-21843	UNK_AHG_HZ_SOAS_728	BOOA	MS	0	0
729		BOOA	MS	LDY-21844	UNK_AHG_HZ_SOAS_729	BOOA	MS	0	0
730		BBOA	R2	LDY-21845	UNK_AHG_HZ_SOAS_730	BBOA	R2	0	0
731		BOOA	MS	LDY-21846	UNK_AHG_HZ_SOAS_731	BOOA	MS	0	0
732		MTR2	R2	LDY-21847	UNK_AHG_HZ_SOAS_732	MTR2	R2	0	0
733		SQT	R2	LDY-21848	UNK_AHG_HZ_SOAS_733	SQT	R2	0	0
734		BBOA	R2	LDY-21849	UNK_AHG_HZ_SOAS_734	BBOA	R2	0	0

index	Compound Name	Group	Group Determined By	UCB-GLOBES UID	Compound Name Reanalysis	Group Reanalysis	Group Determined By Reanalysis	Group Category Changed 0 = no 1 = yes	MS Confirmed 0 = no 1 = yes
735		Unknown		LDY-21850	UNK_AHG_HZ_SOAS_735	Unknown	0	0	0
736		BOOA	MS	LDY-21851	UNK_AHG_HZ_SOAS_736	BOOA	MS	0	0
737		Unknown		LDY-21852	UNK_AHG_HZ_SOAS_737	Unknown	0	0	0
738		MTR2	R2	LDY-21853	UNK_AHG_HZ_SOAS_738	MTR2	R2	0	0
739		BOOA	MS	LDY-21854	UNK_AHG_HZ_SOAS_739	BOOA	MS	0	0
740		MTR2	R2	LDY-21855	UNK_AHG_HZ_SOAS_740	MT	MS/Lab Expt	1	1
741		BBOA	R2	LDY-21856	UNK_AHG_HZ_SOAS_741	BBOA	R2	0	0
742		MTR2	R2	LDY-21857	UNK_AHG_HZ_SOAS_742	MTR2	R2	0	0
743		BBOA	R2	LDY-21858	UNK_AHG_HZ_SOAS_743	BBOA	R2	0	0
744	galactosan	BBOA	R2	LDY-21859	galactosan, 3 TMS	BBOA	R2	0	0
745		BBOA	R2	LDY-21860	UNK_AHG_HZ_SOAS_745	BBOA	R2	0	0
746	4-nitrocatechol	BBOA	Lab Expt/R2	LDY-21861	4-nitrocatechol, 2 TMS	BBOA	Lab Expt/R2	0	0
747		BBOA	R2	LDY-21862	UNK_AHG_HZ_SOAS_747	BBOA	R2	0	0
748	vanillic acid	BBOA	R2	LDY-21863	vanillic acid, 2 TMS	BBOA	R2	0	0
749		BBOA	R2	#N/A	UNK_AHG_HZ_SOAS_749	BBOA	R2	0	0
750		BBOA	R2	LDY-21865	UNK_AHG_HZ_SOAS_750	BBOA	R2	0	0
751		BBOA	R2	LDY-21866	UNK_AHG_HZ_SOAS_751	BBOA	R2	0	0
752		BBOA	Lab Expt/R2	LDY-21867	UNK_AHG_HZ_SOAS_752	BBOA	Lab Expt/R2	0	0
753		BBOA	R2	LDY-21868	UNK_AHG_HZ_SOAS_753	BBOA	R2	0	0
754		BBOA	R2	LDY-21869	UNK_AHG_HZ_SOAS_754	MT	MS/Lab Expt/Field Expt	1	1
755		BBOA	R2	LDY-21870	UNK_AHG_HZ_SOAS_755	BBOA	R2	0	0
756		BBOA	R2	LDY-21871	UNK_AHG_HZ_SOAS_756	BBOA	R2	0	0
757		BBOA	R2	LDY-21872	UNK_AHG_HZ_SOAS_757	BBOA	R2	0	0
758		BBOA	R2	LDY-21873	UNK_AHG_HZ_SOAS_758	BBOA	R2	0	0
759		BBOA	Lab Expt/R2	LDY-21874	UNK_AHG_HZ_SOAS_759	BBOA	Lab Expt/R2	0	0
760		BBOA	R2	LDY-21875	UNK_AHG_HZ_SOAS_760	BBOA	R2	0	0
761		BBOA	R2	LDY-21876	UNK_AHG_HZ_SOAS_761	BBOA	R2	0	0
762		Unknown		LDY-21877	UNK_AHG_HZ_SOAS_762	Unknown	0	0	0
763		BBOA	R2	LDY-21878	UNK_AHG_HZ_SOAS_763	BBOA	R2	0	0
764		BBOA	R2	LDY-21879	UNK_AHG_HZ_SOAS_764	BBOA	R2	0	0
765		BBOA	R2	LDY-21880	UNK_AHG_HZ_SOAS_765	BBOA	R2	0	0
766		BBOA	R2	LDY-21881	UNK_AHG_HZ_SOAS_766	BBOA	R2	0	0

index	Compound Name	Group	Group Determined By	UCB-GLOBES UID	Compound Name Reanalysis	Group Reanalysis	Group Determined By Reanalysis	Group Category Changed 0 = no 1 = yes	MS Confirmed 0 = no 1 = yes
767		BBOA	R2	LDY-21882	UNK_AHG_HZ_SOAS_767	BBOA	R2	0	0
768		BBOA	R2	LDY-21883	UNK_AHG_HZ_SOAS_768	BBOA	R2	0	0
769		MTR2	R2	LDY-21884	UNK_AHG_HZ_SOAS_769	MTR2	R2	0	0
770		POAOX	R2	LDY-21885	UNK_AHG_HZ_SOAS_770	POAOX	R2	0	0
771		POAOX	R2	LDY-21886	UNK_AHG_HZ_SOAS_771	POAOX	R2	0	0
772	isopropyl palmitate	BBOA	NIST	LDY-21887	isopropyl palmitate	BBOA	NIST	0	0
773		POAOX	R2	LDY-21888	UNK_AHG_HZ_SOAS_773	POAOX	R2	0	0
774		BBOA	R2	LDY-21889	UNK_AHG_HZ_SOAS_774	BBOA	R2	0	0
775	myristic myristate	BBOA	NIST	LDY-21890	myristic myristate	BBOA	NIST	0	0
776		Unknown		LDY-21891	UNK_AHG_HZ_SOAS_776	Unknown	0	0	0
777		Unknown		LDY-21892	UNK_AHG_HZ_SOAS_777	Unknown	0	0	0
778	C30 n-alkane	hydrocarbon	MS	LDY-21893	C30 n-alkane	hydrocarbon	MS	0	0
779	squalene	hydrocarbon	MS	LDY-21894	squalene	hydrocarbon	MS	0	0
780		POAOX	R2	LDY-21895	UNK_AHG_HZ_SOAS_780	POAOX	R2	0	0
781		Unknown		LDY-21896	UNK_AHG_HZ_SOAS_781	Unknown	0	0	0
782		POAOX	R2	LDY-21897	UNK_AHG_HZ_SOAS_782	POAOX	R2	0	0
783	cholesta-3,4-diene	hydrocarbon	NIST	LDY-21898	cholesta-3,4-diene	hydrocarbon	NIST	0	0
784		BBOA	R2	LDY-21899	UNK_AHG_HZ_SOAS_784	BBOA	R2	0	0
785		Unknown		LDY-21900	UNK_AHG_HZ_SOAS_785	Unknown	0	0	0
786		Unknown		LDY-21901	UNK_AHG_HZ_SOAS_786	Unknown	0	0	0
787		Unknown		LDY-21902	UNK_AHG_HZ_SOAS_787	Unknown	0	0	0
788		Unknown		LDY-21903	UNK_AHG_HZ_SOAS_788	Unknown	0	0	0
789		Unknown		LDY-21904	UNK_AHG_HZ_SOAS_789	Unknown	0	0	0
790		Unknown		LDY-21905	UNK_AHG_HZ_SOAS_790	Unknown	0	0	0
791		POAOX	R2	LDY-21906	UNK_AHG_HZ_SOAS_791	POAOX	R2	0	0
792		POAOX	R2	LDY-21907	UNK_AHG_HZ_SOAS_792	POAOX	R2	0	0
793		POAOX	R2	LDY-21908	UNK_AHG_HZ_SOAS_793	POAOX	R2	0	0
794		POAOX	R2	LDY-21909	UNK_AHG_HZ_SOAS_794	POAOX	R2	0	0
795		POAOX	R2	LDY-21910	UNK_AHG_HZ_SOAS_795	POAOX	R2	0	0
796		POAOX	R2	LDY-21911	UNK_AHG_HZ_SOAS_796	POAOX	R2	0	0
797		POAOX	R2	LDY-21912	UNK_AHG_HZ_SOAS_797	BBOA	MS/Lab Expt/Field Expt/NIST20	1	1

index	Compound Name	Group	Group Determined By	UCB-GLOBES UID	Compound Name Reanalysis	Group Reanalysis	Group Determined By Reanalysis	Group Category Changed 0 = no 1 = yes	MS Confirmed 0 = no 1 = yes
798		POAOX	R2	LDY-21913	UNK_AHG_HZ_SOAS_798	POAOX	R2	0	0
799	isopropyl palmitate	POAOX	R2	LDY-21887	isopropyl palmitate	POAOX	R2	0	0
800	C13H9(OH)	BBOA	R2	LDY-21915	UNK_AHG_HZ_SOAS_800	BBOA	R2	0	0
801		Unknown		LDY-21916	UNK_AHG_HZ_SOAS_801	Unknown	0	0	0
802		Unknown		LDY-21917	isomer of 10-hydroxypinonic acid?	MT/SQT	MS/LabExpt	1	1
803		BOOA	MS	LDY-21918	UNK_AHG_HZ_SOAS_803	BOOA	MS	0	0
804		BBOA	R2	LDY-21919	UNK_AHG_HZ_SOAS_804	BBOA	R2	0	0
805	methyl nitrocatechol isomer	BBOA	Lab Expt/R2	LDY-21920	methyl nitrocatechol isomer, 2 TMS	BBOA	Lab Expt/R2	0	0
806		BBOA	R2	LDY-21921	UNK_AHG_HZ_SOAS_806	BBOA	R2	0	0
807		BBOA	R2	LDY-21922	UNK_AHG_HZ_SOAS_807	BBOA	R2	0	0
808		BBOA	R2	LDY-21923	UNK_AHG_HZ_SOAS_808	BBOA	R2	0	0
809		BBOA	R2	LDY-21924	UNK_AHG_HZ_SOAS_809	BBOA	R2	0	0
810		BBOA	R2	LDY-21925	UNK_AHG_HZ_SOAS_810	BBOA	R2	0	0
811		BBOA	R2	LDY-21926	UNK_AHG_HZ_SOAS_811	BBOA	R2	0	0
812		BBOA	R2	LDY-21927	UNK_AHG_HZ_SOAS_812	BBOA	R2	0	0
813		BBOA	R2	LDY-21928	UNK_AHG_HZ_SOAS_813	BBOA	R2	0	0
814		BBOA	R2	LDY-21929	UNK_AHG_HZ_SOAS_814	SQT?	MS	1	1
815		BBOA	R2	#N/A	UNK_AHG_HZ_SOAS_815	BBOA	MS/Lab Expt/Field Expt	0	1
816		POAOX	R2	LDY-21931	UNK_AHG_HZ_SOAS_816	POAOX	R2	0	0
817		BOOA	MS	LDY-21932	UNK_AHG_HZ_SOAS_817	BOOA	MS	0	0
818		MTR2	R2	LDY-21933	UNK_AHG_HZ_SOAS_818	MTR2	R2	0	0
819		BOOA	MS	LDY-21934	UNK_AHG_HZ_SOAS_819	BOOA	MS	0	0
820		BBOA	R2	LDY-21935	UNK_AHG_HZ_SOAS_820	BBOA	R2	0	0
821		MTR2	R2	LDY-21936	UNK_AHG_HZ_SOAS_821	MTR2	R2	0	0
822		POAOX	R2	LDY-21937	UNK_AHG_HZ_SOAS_822	POAOX	R2	0	0
823		BOOA	MS	LDY-21938	UNK_AHG_HZ_SOAS_823	BOOA	MS	0	0
824		BOOA	MS	LDY-21939	UNK_AHG_HZ_SOAS_824	BOOA	MS	0	0
825		MTR2	R2	LDY-21940	UNK_AHG_HZ_SOAS_825	MTR2	R2	0	0
826		BOOA	MS	LDY-21941	UNK_AHG_HZ_SOAS_826	BOOA	MS	0	0
827		POAOX	R2	LDY-21942	UNK_AHG_HZ_SOAS_827	POAOX	R2	0	0
828		MTR2	R2	LDY-21943	UNK_AHG_HZ_SOAS_828	MTR2	R2	0	0

index	Compound Name	Group	Group Determined By	UCB-GLOBES UID	Compound Name Reanalysis	Group Reanalysis	Group Determined By Reanalysis	Group Category Changed 0 = no 1 = yes	MS Confirmed 0 = no 1 = yes
829		POAOX	R2	#N/A	UNK_AHG_HZ_SOAS_829	POAOX	R2	0	0
830		BOOA	MS	LDY-21945	UNK_AHG_HZ_SOAS_830	BOOA	MS	0	0

S5. SI Figures

Figure S1: Screenshot view of query MS LDY-21509 (UNK_AHG_HZ_SOAS_394) amongst UCB-GLOBES in NIST MS Search 3.0.

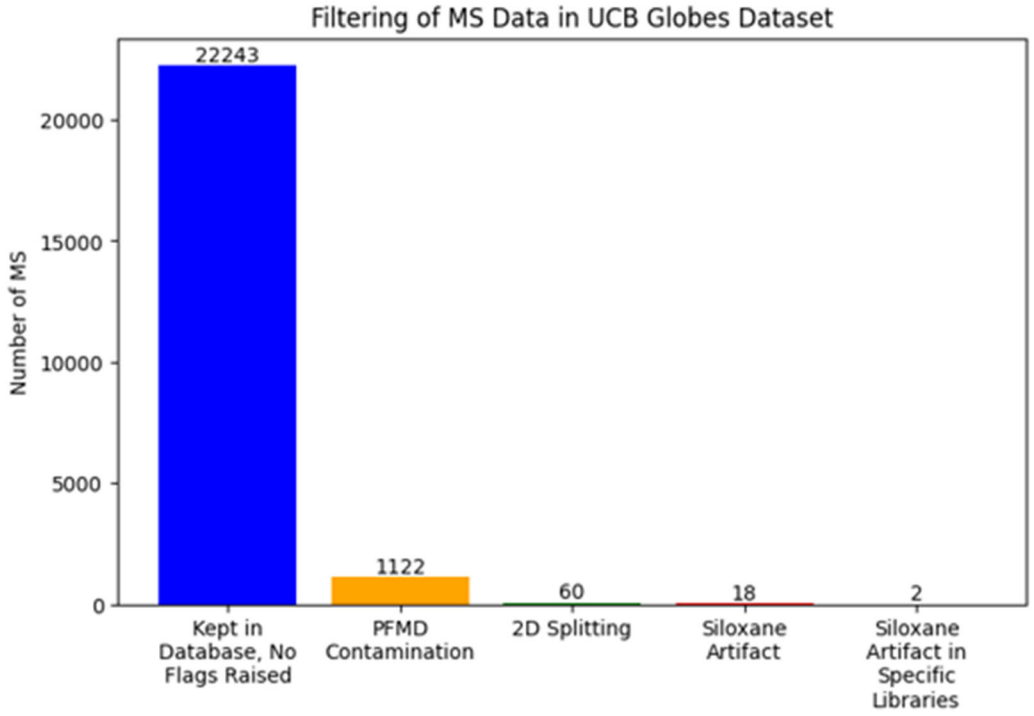

Figure S2: UCB-GLOBES mass spectra were screened for MS contamination from perfluormethyldecalin (PFMD) calibrant, improper 2nd dimension peak splitting, siloxane artifact, and known siloxane artifacts in specific libraries. The majority of MS were kept in UCB-GLOBES database, and the majority of PFMD contaminated MS were found in the FSL_FIREX2016_v2 dataset.

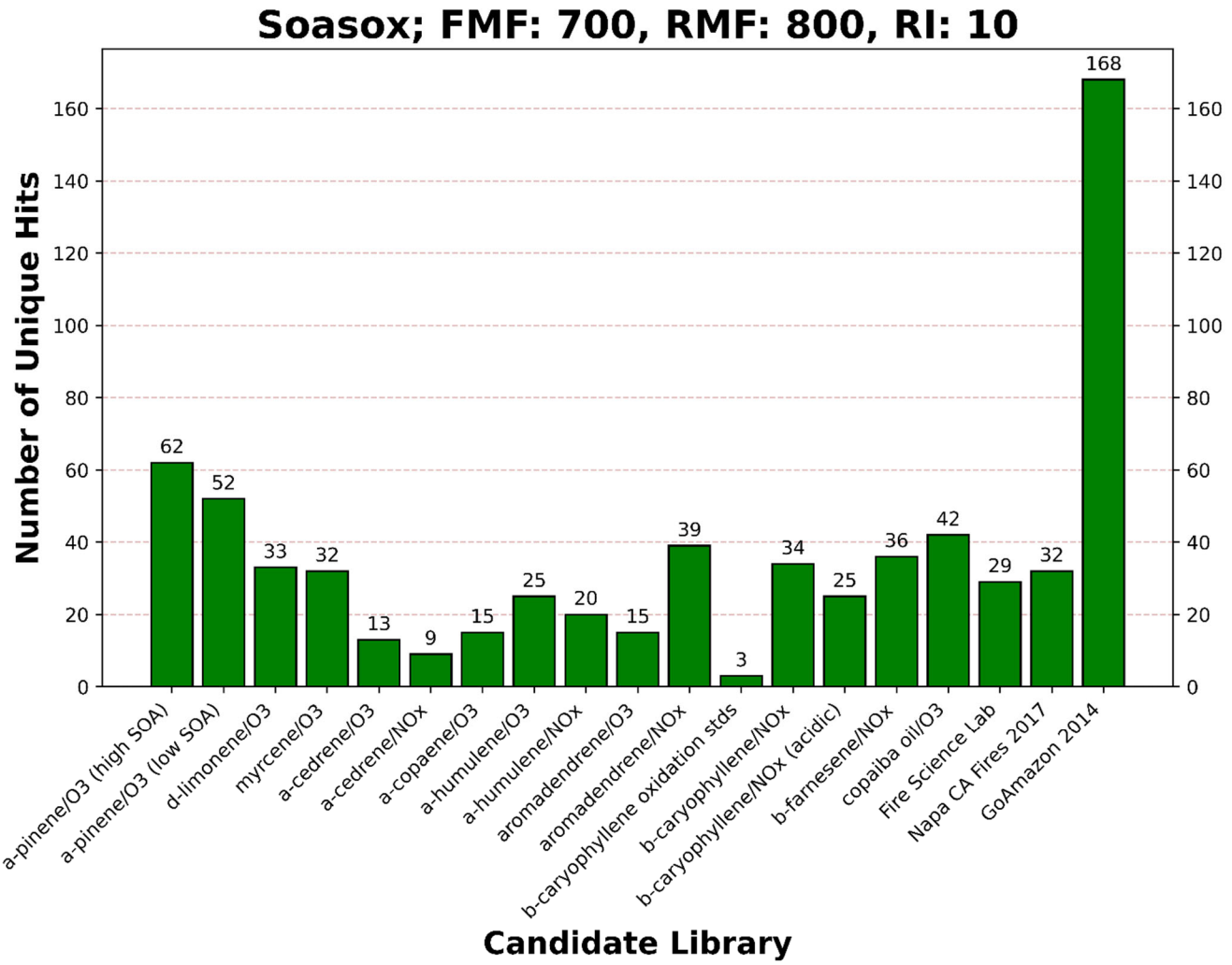

Figure S3: Number of unique MS hits for SOAS MS data by each UCB-GLOBES candidate library dataset. To be considered a hit, forward match factor (FMF) ≥ 700, reverse match factor (RMF) ≥ 800, and retention index (RI) difference ≤ 10 between query MS and hit MS. While a SOAS MS may have multiple hits across multiple libraries, it is constrained to have at most one MS hit from each candidate library to prevent implausible assignment to two different compounds within a candidate library.

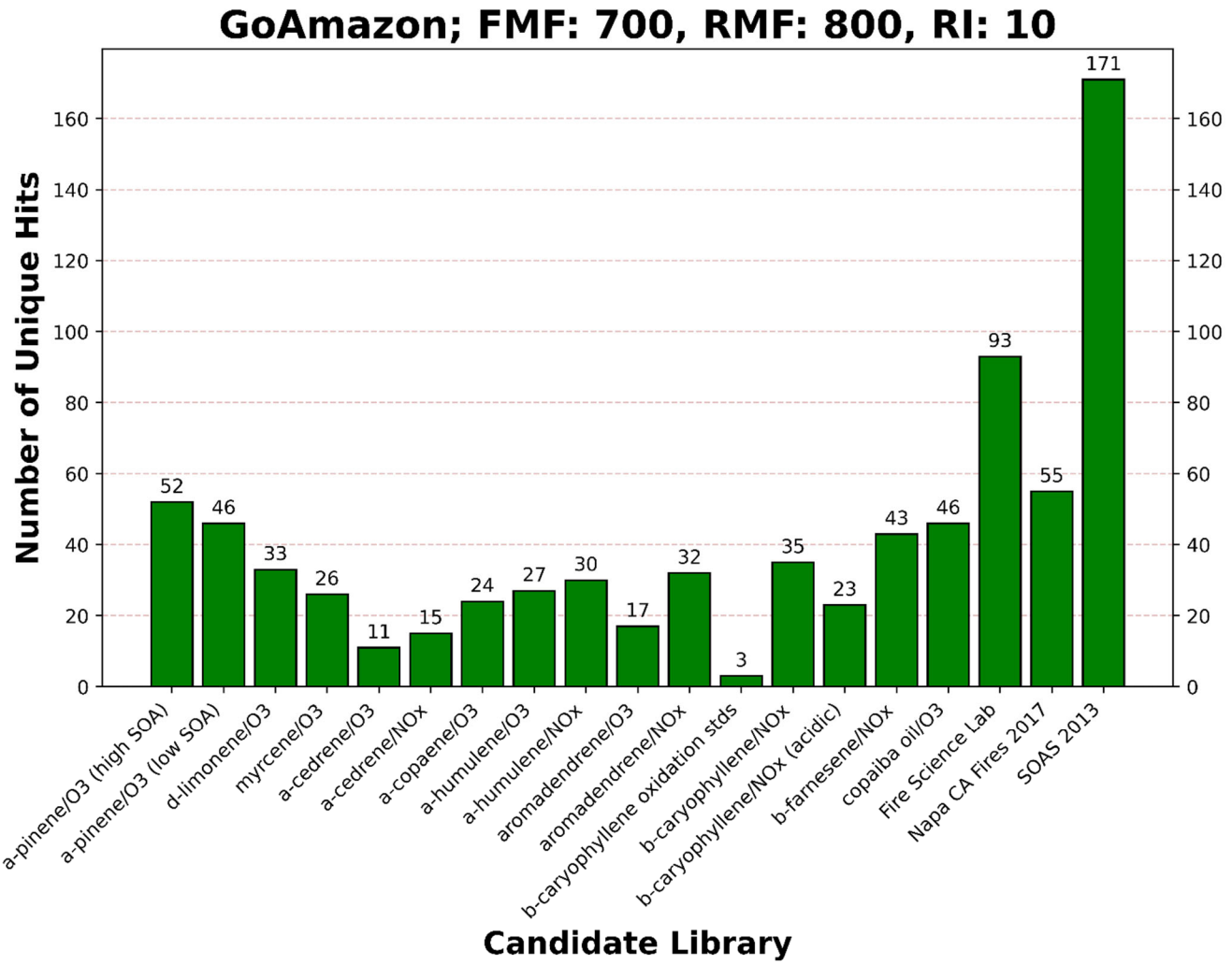

Figure S4: Number of unique MS hits for GoAmazon MS data by each UCB-GLOBES candidate library dataset. To be considered a hit, forward match factor (FMF) ≥ 700, reverse match factor (RMF) ≥ 800, and retention index (RI) difference ≤ 10 between query MS and hit MS. While a GoAmazon MS may have multiple hits across multiple libraries, it is constrained to have at most one MS hit from each candidate library to prevent implausible assignment to two different compounds within a candidate library.

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