

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

Lindsay D. Yee,<sup>1</sup> Emily B. Franklin,<sup>2,a</sup> Robin J. Weber,<sup>1</sup> Jessica Zhao,<sup>3</sup> Tiger Zhang,<sup>4</sup> Stephanie Xu,<sup>4</sup> Isaac Santillan,<sup>4</sup> Fangyuan Li,<sup>5</sup> Coty N. Jen,<sup>1,b</sup> Haoifei Zhang,<sup>1,c</sup> Yutong Liang,<sup>1,d</sup> Gabriel Isaacman Van-Wertz,<sup>1,e</sup> Rebecca A. Wernis,<sup>2</sup> John Offenberg,<sup>6,f</sup> Michael Lewandowski,<sup>6,g</sup> Taekyu Joo,<sup>7,g</sup> Masayuki Takeuchi,<sup>8</sup> Gamze Eris,<sup>8</sup> Weiqi Xu,<sup>9,h</sup> Nga L. Ng,<sup>7,8,9,i</sup> Yuzhi Chen,<sup>10</sup> John E. Shilling,<sup>10</sup> Mary Alice Upshur,<sup>11</sup> Ariana Gray Bé,<sup>11</sup> Regan J. Thomson,<sup>11</sup> Franz M. Geiger,<sup>11</sup> and Allen H. Goldstein<sup>1,2</sup>

<sup>1</sup> Department of Environmental Science, Policy, and Management, University of California, Berkeley, Berkeley, 94720, USA

<sup>2</sup> Department of Civil and Environmental Engineering, University of California, Berkeley, Berkeley, 94720, USA

<sup>3</sup> Department of Industrial Engineering & Operations Research, University of California, Berkeley, Berkeley, 94720, USA

<sup>4</sup> Department of Electrical Engineering & Computer Sciences, University of California, Berkeley, Berkeley, 94720, USA

<sup>5</sup> Department of Statistics, University of California, Berkeley, Berkeley, 94720, USA

<sup>6</sup> Office of Research and Development, Center for Environmental Measurement and Modeling, Atmospheric and

Environmental Systems Modeling Division, US Environmental Protection Agency, Research Triangle Park, 27711, USA

<sup>7</sup> School of Earth and Atmospheric Sciences, Georgia Institute of Technology, Atlanta, 30332, USA

<sup>8</sup> School of Civil and Environmental Engineering, Georgia Institute of Technology, Atlanta, 30332, USA

<sup>9</sup> School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, Atlanta, 30332, USA

<sup>10</sup> Atmospheric, Climate, and Earth Sciences Division, Pacific Northwest National Laboratory, Richland, WA 99352, USA

<sup>11</sup> Department of Chemistry, Northwestern University, Evanston, 60208, USA

<sup>a</sup> Now at CSIRO Environment, Aspendale, Victoria 3195, Australia

<sup>b</sup> Now at Department of Chemical Engineering, Carnegie Mellon University, Pittsburgh, 15213, USA

<sup>c</sup> Now at Department of Chemistry, University of California, Riverside, Riverside, 92507, USA

<sup>d</sup> Now at Thrust of Sustainable Energy and Environment, The Hong Kong University of Science and Technology (Guangzhou), Guangdong, 511453, China

<sup>e</sup> Now at Department of Civil and Environmental Engineering, Virginia Tech, Blacksburg, 24060, USA

<sup>f</sup> Present affiliation: Office of Applied Science and Environmental Solutions, Applied Science and Environmental Methods Division, US Environmental Protection Agency, Research Triangle Park, 27711, USA

<sup>g</sup> Now at Department of Earth and Environmental Sciences, Korea University, Seoul, 02841, South Korea

<sup>h</sup> Now at State Key Laboratory of Atmospheric Boundary Layer Physics and Atmospheric Chemistry, Institute of Atmospheric Physics, Chinese Academy of Sciences, Beijing, 100864, China

<sup>i</sup> Now at Division of Engineering and Applied Science, California Institute of Technology, Pasadena, 91125, USA

\*Retired

Correspondence to: Lindsay D. Yee (lindsay.yee@berkeley.edu)

**Abstract.** Chemical characterization of atmospheric organic aerosols using gas chromatography with 70 eV electron ionization mass spectrometry (GC/EI-MS) has been used for decades in advancing molecular marker detection and identification, though primarily through suspect screening and/or targeted analyses. To advance non-targeted analyses of environmental samples, we have catalogued approximately 27,000 mass spectra (MS) of [the trimethylsilyl derivatives of](#) semi-volatile organic aerosol

(OA) analytes ~~observed in ambient samples from the U.S. and the Central Amazon and/or laboratory simulations of secondary OA (SOA) formation~~ in the open-access University of California Berkeley Goldstein Library of Organic Biogenic Environmental Spectra (UCB-GLOBES). ~~Analytes were observed in ambient samples from the U.S. and the Central Amazon and/or laboratory simulations of secondary OA (SOA) formation.~~ These samples are representative of OA under urban and biomass burning influences as well as SOA derived from biogenic precursors (e.g., isoprene, monoterpenes, sesquiterpenes) and biomass burning intermediates. MS are documented in UCB-GLOBES without regard to known chemical identity, annotated with extensive metadata such as sample source/experimental conditions, any structural information gained from MS analyses, and predicted chemical properties such as average carbon oxidation state and carbon number. UCB-GLOBES MS are compatible for importing into NIST MS Search program, and we have also provided a Jupyter Notebook for MS visualization and comparisons. We demonstrate the utility of UCB-GLOBES through MS reanalyses of prior analytes observed in ambient data, finding a 20% reduction in the number of analytes assigned to OA source categories reliant solely on time series correlation and an overall 11% increase in new MS-based OA source categorization for the Southeast U.S. For 1,513 analytes observed previously in the Central Amazon, we found 375 MS matches using UCB-GLOBES vs. 136 MS matches during prior analyses, representing a 14% gain in newly confirmed or newly categorized OA species. While OA from laboratory oxidation experiments in UCB-GLOBES are highly diverse chemically, on average only 29% of UCB-GLOBES MS have a mass spectral match to another MS entry in UCB-GLOBES and/or in databases of known compounds (the i.e. NIST MS Database, Adams Essential Oil, MANE Flavor and Fragrance Company). This indicates that roughly 70% of UCB-GLOBES MS are unique thus far, not observed more than once among the laboratory oxidation samples and ambient data in UCB-GLOBES MS. Further, only 18% can be positively identified in-using the NIST-MS-these databases or ~~with~~-known authentic standards. This points to a large gap between these laboratory simulations and ambient OA. Overall, the UCB-GLOBES database can be utilized for improving confidence in OA source categorization and/or identification, novel chemical marker discovery, tracking chemical diversity, *de novo* structure and properties prediction, and improving MS search and matching algorithms. This can ultimately inform future research priorities for the chemical characterization of atmospheric organic samples.

## 1 Introduction

Atmospheric organic aerosols are highly complex chemical mixtures, of which most compounds have yet to be chemically identified (Goldstein and Galbally, 2007; Hallquist et al., 2009; Nozière et al., 2015). This is in large part due to the plethora of volatile organic compounds (VOCs) emitted to or formed in the atmosphere that participate in numerous chemical reactions to create many more unique oxidation products (Aumont et al., 2005; C. Ditto et al., 2020; Kanakidou et al., 2005). The multitude of chemicals generated in the gas phase and those that partition into the particle phase, forming secondary organic aerosol (SOA), creates a challenge for probing the chemical makeup of OA. Various analytical techniques have been employed to interrogate the chemical identities of organic compounds within the particle phase with previous

observations finding hundreds to thousands of individual compounds within aerosol samples (Franklin et al., 2023; Hamilton et al., 2004; Isaacman-Vanwertz et al., 2017; Isaacman et al., 2014; Kourtchev et al., 2014; Nizkorodov et al., 2011; Wang et al., 2017; Zhang et al., 2024). Bulk characterization methods through the Aerodyne Aerosol Mass Spectrometer (AMS) can include reporting of elemental ratios (e.g. H:C, O:C) and statistical factor analysis of mass spectra to infer aerosol source-types and origins (Aiken et al., 2007, 2008; Canagaratna et al., 2015; Ulbrich et al., 2009). In addition, resources of characteristic AMS mass spectra available to the community aid in potential chemical classification of OA sources (Jeon et al., 2023). Several molecular-level high-resolution mass spectrometry techniques are employed to obtain molecular formula of analytes (Brophy and Farmer, 2015; Crounse et al., 2006; Lee et al., 2014; Lopez-Hilfiker et al., 2019; Roach et al., 2010a, 2010b), though definitive chemical structure and isomer-specific level identification can only be gained by adaptive configurations and separation (Johnston and Kerecman, 2019; Krechmer et al., 2016; Nozière et al., 2015; Wen et al., 2023). Despite advances in mass spectrometry as well as organic syntheses targeted for atmospheric chemical markers (Gagan et al., 2023), there remains a large fraction of measurable yet chemically unidentified organic compounds in the atmosphere. This problem is chronically plagued by the lack of commercially available standards as well as the extreme difficulty of synthesizing standards of interest. The sheer challenge of measuring (being sensitive to all compound types), much less identifying and quantifying these compounds, typically results in targeted analyses (reporting a specific list of analytes) vs untargeted analyses (reporting all measurable analytes without regard to known identity). Understandably, targeted analyses lessen the burden of increasingly complex data analysis from measurement techniques with increasing capacities. However, this can also lead to a loss in the utilization of available data and unintended potential biases in scientific foci. For example, Franklin et al., (2023) estimated that by restricting analyses to the top hundred analytes by mass observed in the Central Amazon, only ~70% of OA mass associated with either urban influences or biomass burning would be considered with a skew towards biomass burning products.

Discoveries of specific chemical markers in the atmosphere have been born from using gas chromatography with electron ionization mass spectrometry (GC/EI-MS), in which compounds are separated (typically by boiling point) while mass spectra of eluents are also measured to aid in structural identification (Claeys et al., 2004; van Eijck et al., 2013; Lin et al., 2012; Surratt et al., 2007; Szmigielski et al., 2007). In traditional one-dimensional GC, however, separations can be limited by co-elution of compounds with similar properties (e.g., boiling point), leading to convoluted signals and difficulty in acquiring pure compound MS. The application of two-dimensional gas chromatography (GCxGC) has drastically improved the resolving peak capacity compared to that of traditional one-dimensional GC, by performing a second separation (e.g., by polarity) of first-column eluents (Alam et al., 2013; Alam and Harrison, 2016; Goldstein et al., 2008; Hamilton et al., 2006; He et al., 2022; Song et al., 2022; Worton et al., 2012). Additional separation can result in greater chromatographic peak separation and thereby purer MS, allowing for enhanced acquisition of isomer-specific data. For example, Hamilton et al., (2004) isolated over 10,000 individual organic species from a single sample of collected urban aerosol.

Given the wide use of GC/EI-MS for many environmental applications, mass spectral libraries exist for comparing measured spectra to those in open-access and for purchase formats (MassBank, MassBank of North America, Golm

Metabolome Database, Adams Essential Oil, MANE2010 flavor and fragrance mass, Wiley MS Library, NIST/EPA/NIH MS Database) to aid in determination of sample compounds' chemical identities (Stein, 2012). Still, most of these resources only document compounds of known chemical identity or MS generated from authentic standards readily available, with some exceptions of MS data for unidentified compounds in biological samples (Kopka et al., 2005; Mallard et al., 2014). For unidentified compounds or those identified but not provided in state-of-the-art MS databases, it can be challenging for analysts of GC/EI-MS spectra to get a rigorous quantitative comparison such as cosine angle similarity analysis between their query mass spectra and novel mass spectra that are, for example, published as an image in the journal article. An analyst would greatly benefit from having the MS in a data format that allows for automated and computed MS searching in applications like the NIST MS Search program with quantitative calculations that compare the query spectrum against available MS, eliminating the uncertainty in qualitative identification by visual inspection. Qualitative MS comparison can lead to pitfalls in false identification of compounds of similar structure such as isomers or compound families with very similar MS fragmentation patterns (e.g., alkanes), without context of additional data such as Kováts chromatographic retention index, ~~(a proxy for elution time of compounds relative to a standard series such as *n*-alkanes that can be compared across instruments (Kováts, 1958)).~~

Thus, as many atmospheric organic compounds have yet to be identified and limited authentic standards exist, we have established an open-access database of 70 eV electron ionization MS acquired with GCxGC from compounds in ambient atmospheric samples and laboratory oxidation experiments of atmospheric relevance without necessitating that chemical identity be known. Initial datasets included those developed in Worton et al. (2017) and Yee et al. (2018). The growing collection was then formally named the University of California, Berkeley Goldstein Library of Biogenic and Environmental Spectra (UCB-GLOBES) in Jen et al. (2019) with ~4,800 MS and this work extends the database to include a total of ~27,000 MS. UCB-GLOBES includes single instance and replicate MS, multiple instances of MS representing the same compound, that spans a collection of ambient samples analysed over the past decade (e.g., urban, rural, remote, biomass burning influenced) as well as laboratory samples simulating oxidation of isoprene, terpenes, and biomass burning emissions under varied chemical and environmental conditions.

MS data along with useful metadata (e.g., chromatographic retention index, origin of MS sample including field campaign/laboratory source and conditions, predicted chemical properties, inferred structural characteristics, predicted MW/chemical formula) are provided without regard to known chemical identity. The overall goal of UCB-GLOBES is to: 1) advance discovery of novel atmospheric and environmental chemical markers of importance, 2) improve the community's awareness and knowledge of compounds that have been regularly measured but lack identification, 3) encourage more open sharing of annotated MS data across the GC/EI-MS community, 4) increase quantitative confidence in identification by MS matching or narrowing down information about an unknown MS (structural similarity, potential chemical origins), and 5) enable further experimental and modelling studies employing mass spectral data. In this work we describe and expand on the MS datasets in UCB-GLOBES curated and released thus far, demonstrate how they can be used for more efficient analysis of sample MS through reanalysis of past ambient datasets, and conclude with discussions on potential avenues for extending UCB-GLOBES and its use in future studies.

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## 2 UCB-GLOBES dataset description

### 2.1 Method of aerosol samples collection

Pre-baked (550° C for 12 hours) quartz filters were used for collecting various aerosol sample types during several field and laboratory measurement campaigns (Table 1), including the 2013 Southern Oxidant and Aerosol Study (SOAS), the 2014 Green ocean Amazon (GoAmazon) study, western US wildland fuel burns at the U.S. Forest Service Fire Science Laboratory as part of the Fire Influence on Regional and Global Environments Experiment (FIREX2016), and smoke transported to Berkeley, CA during the 2017 Napa, CA wildfires. Additionally, aerosols were also collected from seeded laboratory oxidation experiments of single hydrocarbon precursors including several sesquiterpenes ( $\alpha$ -cedrene,  $\alpha$ -copaene,  $\beta$ -caryophyllene,  $\alpha$ -humulene and  $\alpha$ -farnesene) and an essential oil rich in terpenes (copaiba essential oil, Amazon origin) under varied oxidant conditions ( $H_2O_2$  as OH precursor with added  $NO_x$  or ozonolysis) in the U.S. Environmental Protection Agency National Exposure Research Laboratory as described in previous work (Jaoui et al., 2013; Yee et al., 2018; Zhang et al., 2018). Ozonolysis of monoterpene species such as  $\alpha$ -pinene, d-limonene, and myrcene in the absence of seed aerosol ~~was~~ also tested in an oxidation flow reactor at UC Berkeley (Zhang et al., 2018), while reaction of  $\alpha$ -pinene with nitrate radical ( $NO_3^\bullet$ ) in the presence of seed aerosol was performed in the Georgia Tech Environmental Chamber (GTEC) facility (Walters et al., 2025). Oxidation of furan biomass burning intermediates, 3-methylfuran with OH and furfural with OH (HONO as OH precursor in both cases), ~~was~~ also conducted in GTEC with seed aerosol (Joo et al., 2024). Lastly, isoprene oxidation via reaction with OH radical ( $H_2O_2$  as precursor, in the absence of added  $NO_x$ ) was conducted with seed aerosol in the Pacific Northwest National Laboratory chamber facility according to previous methods (Chen et al., 2023). Of note is that the temperature (T) and relative humidity (RH) conditions tested are varied across the laboratory experiments included here, so experiments and accompanying data should not be considered perfect analogues between hydrocarbon precursor systems. A selection of UCB-GLOBES libraries newly added and/or updated in this work along with the number of records in each is summarized in Figure 1.

Table 1: MS datasets included in UCB-GLOBES with associated publications, number of MS, and brief description

| MS Library (File) Name and Associated/Related Publication(s) | # of MS | Dataset Description                                                                                                                                                                                                                                                                             |
|--------------------------------------------------------------|---------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <u>Field Samples</u>                                         |         |                                                                                                                                                                                                                                                                                                 |
| Worton_VUV_2017.MSP<br><i>Worton et al. (2017)</i>           | 201     | Compounds observed during the Biosphere Effects on AeRosols and Photochemistry Experiment (BEARPEX) 2009, local biogenic emissions from mixed conifer forests dominated by ponderosa pine trees, aged biogenic emissions from oak trees located several hours upwind and urban outflow from the |

| MS Library (File) Name and Associated/Related Publication(s) | # of MS            | Dataset Description                                                                                                                                                                                                                                                                                                                                                                         |
|--------------------------------------------------------------|--------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
|                                                              |                    | Sacramento region; underivatized MS with vacuum ultra violet (VUV) ionization                                                                                                                                                                                                                                                                                                               |
| GoAmazon2014_terpox_v2.MSP<br><i>Yee et al. (2018)</i>       | 70                 | Compounds observed during GoAmazon 2014 wet season confirmed to originate from oxidation of isoprene, a few monoterpenes, and a few sesquiterpenes, "T3" Manacapuru site, AM, Brazil, cleared pasture site located 70 km downwind of urban Manaus and immediately surrounded by secondary forest with clear differentiation between clean conditions versus those with Manaus plume outflow |
| Soasox<br><i>Zhang et al. (2018)</i>                         | 829                | Compounds observed during the Southern Oxidant and Aerosol Study (SOAS) 2013, summertime, Centreville, AL, rural, primarily forested with a mixture of deciduous and coniferous trees with relatively little local influence and occasional urban influence from Tuscaloosa, AL                                                                                                             |
| NAPA_2017_YL<br><i>Liang et al. (2021)</i>                   | 573                | Compounds observed during October-November 2017 at UC Berkeley during period of heavy wildfires in Napa Valley, CA                                                                                                                                                                                                                                                                          |
| Goamz<br><i>Franklin et al. (2023)</i>                       | 1498               | Compounds observed during GoAmazon 2014 wet and dry seasons at "T3" Manacapuru site, AM, Brazil, cleared pasture site located 70 km downwind of urban Manaus and immediately surrounded by secondary forest                                                                                                                                                                                 |
| <u>Laboratory Burns of Biomass</u>                           |                    |                                                                                                                                                                                                                                                                                                                                                                                             |
| FSL_FIREX2016_v2.MSP<br><i>Jen et al. (Jen et al., 2019)</i> | 48 <del>2833</del> | Compounds observed from laboratory burning of common western US wildland fuels at the U.S. Forest Service Fire Science Laboratory as part of the Fire Influence on Regional and Global Environments Experiment (FIREX2016)                                                                                                                                                                  |
| FSL_FIREX2016_v2.2024.MSP<br><i>McGlynn et al. (2025)</i>    | 48 <del>2833</del> | Reanalysis of FSL_FIREX2016_v2 to subtract out PFMD contamination from ~1000 MS as well as new chemical identifications using NIST23.                                                                                                                                                                                                                                                       |
| <u>Surrogate Biomass Burning Laboratory Oxidation</u>        |                    |                                                                                                                                                                                                                                                                                                                                                                                             |
| Mf3ox<br><i>Joo et al. (2024)</i>                            | 353                | 3-methylfuran + OH (HONO as OH source) + (NH <sub>4</sub> ) <sub>2</sub> SO <sub>4</sub> seed, T = 22°C, RH = 50%                                                                                                                                                                                                                                                                           |
| Furfox<br><i>Joo et al. (2024)</i>                           | 233                | furfural + OH (HONO as OH source) + (NH <sub>4</sub> ) <sub>2</sub> SO <sub>4</sub> seed, T = 22°C, RH = 5%                                                                                                                                                                                                                                                                                 |
| <u>Sesquiterpene Laboratory Oxidation</u>                    |                    |                                                                                                                                                                                                                                                                                                                                                                                             |

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| MS Library (File) Name and Associated/Related Publication(s)                                                                                                 | # of MS | Dataset Description                                                                                                                                                                                                                                                |
|--------------------------------------------------------------------------------------------------------------------------------------------------------------|---------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Acopox<br><i>Yee et al. (2018); Experiment conducted under same methodology as in Jaoui et al. (2013) and Offenberger et al. (2017); Zhang et al. (2018)</i> | 1616    | $\alpha$ -copaene + O <sub>3</sub> ; <del>dark</del> , + (NH <sub>4</sub> ) <sub>2</sub> SO <sub>4</sub> seed, T = 22°C, RH = 32%                                                                                                                                  |
| Aromox<br><i>Jaoui et al. (2013); Offenberger et al. (2017); Zhang et al. (2018)</i>                                                                         | 1016    | aromadendrene + O <sub>3</sub> ; <del>dark</del> , + (NH <sub>4</sub> ) <sub>2</sub> SO <sub>4</sub> seed, T = 22°C, RH = 32%                                                                                                                                      |
| Aromox2<br><i>Jaoui et al. (2013); Offenberger et al. (2017); Zhang et al. (2018)</i>                                                                        | 1073    | aromadendrene + NO <sub>x</sub> + hv; + (NH <sub>4</sub> ) <sub>2</sub> SO <sub>4</sub> seed, T = 25°C, RH = 31%                                                                                                                                                   |
| Ahumox<br><i>Jaoui et al. (2013); Offenberger et al. (2017); Zhang et al. (2018)</i>                                                                         | 1554    | $\alpha$ -humulene + O <sub>3</sub> ; + (NH <sub>4</sub> ) <sub>2</sub> SO <sub>4</sub> seed, T = 22°C, RH = 32%                                                                                                                                                   |
| Ahumox2<br><i>Jaoui et al. (2013); Offenberger et al. (2017); Zhang et al. (2018)</i>                                                                        | 1633    | $\alpha$ -humulene + NO <sub>x</sub> + hv; + (NH <sub>4</sub> ) <sub>2</sub> SO <sub>4</sub> seed, T = 24°C, RH = 28%                                                                                                                                              |
| Acedox<br><i>Jaoui et al. (2013); Offenberger et al. (2017); Zhang et al. (2018)</i>                                                                         | 1090    | $\alpha$ -cedrene + O <sub>3</sub> ; + (NH <sub>4</sub> ) <sub>2</sub> SO <sub>4</sub> seed, T = 22°C, RH = 32%                                                                                                                                                    |
| Acedox2<br><i>Jaoui et al. (2013); Offenberger et al. (2017); Zhang et al. (2018)</i>                                                                        | 1019    | $\alpha$ -cedrene + NO <sub>x</sub> + hv + (NH <sub>4</sub> ) <sub>2</sub> SO <sub>4</sub> seed, T = 24°C, RH = 28%                                                                                                                                                |
| Bcpox<br><i>Yee et al. (2018)</i>                                                                                                                            | 5       | $\beta$ -caryophyllene aldehyde, $\beta$ -caryophyllinic acid, $\beta$ -caryophyllonic acid, $\beta$ -nocaryophyllone aldehyde, $\beta$ -nocaryophyllonic acid; synthesized chemical standards by Regan Thomson and Franz Geiger Groups at Northwestern University |
| Bcpox2<br><i>Jaoui et al. (2013); Offenberger et al. (2017); Zhang et al. (2018)</i>                                                                         | 1030    | $\beta$ -caryophyllene + NO <sub>x</sub> + hv + (NH <sub>4</sub> ) <sub>2</sub> SO <sub>4</sub> seed, T = 25°C, RH = 29%                                                                                                                                           |
| Bcpox3<br><i>Jaoui et al. (2013); Offenberger et al. (2017); Yee et al. (2018)</i>                                                                           | 1001    | $\beta$ -caryophyllene + NO <sub>x</sub> + acidic, seed-(NH <sub>4</sub> ) <sub>2</sub> SO <sub>4</sub> and H <sub>2</sub> SSO <sub>4</sub> seed + hv, T = 24°C, RH = 29%                                                                                          |
| Bfarnox<br><i>Jaoui et al. (2013); Offenberger et al. (2017); Yee et al. (2018)</i>                                                                          | 1624    | $\beta$ -farnesene + NO <sub>x</sub> + hv + (NH <sub>4</sub> ) <sub>2</sub> SO <sub>4</sub> seed, T = 25°C, RH = 31%                                                                                                                                               |

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| MS Library (File) Name and Associated/Related Publication(s)                                                                         | # of MS              | Dataset Description                                                                                                                                                                                  |
|--------------------------------------------------------------------------------------------------------------------------------------|----------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Copox<br><i>Yee et al. (2018); Experiment conducted under same methodology as in Jaoui et al. (2013) and Offenberg et al. (2017)</i> | 1356                 | copaiba oil + O <sub>3</sub> + (NH <sub>4</sub> ) <sub>2</sub> SO <sub>4</sub> seed, dynamic, T = 22°C, RH = 32%                                                                                     |
| <u>Monoterpene Laboratory Oxidation</u>                                                                                              |                      |                                                                                                                                                                                                      |
| Apinox<br><i>Zhang et al. (2018)</i>                                                                                                 | 568                  | α-pinene + O <sub>3</sub> (high SOA loading), T = 23°C, RH = 30%                                                                                                                                     |
| Apinox2<br><i>Zhang et al. (2018)</i>                                                                                                | 204                  | α-pinene + O <sub>3</sub> (low SOA loading), T = 23°C, RH = 30%                                                                                                                                      |
| Apinox3<br><i>Experiment conducted under same methodology as in Walters et al. (2025)</i>                                            | <del>2119</del> 1596 | α-pinene + NO <sub>3</sub> + (NH <sub>4</sub> ) <sub>2</sub> SO <sub>4</sub> seed, T = 22°C, RH = 30%                                                                                                |
| Limonox<br><i>Zhang et al. (2018)</i>                                                                                                | 483                  | <del>l</del> imonene + O <sub>3</sub> , T = 23°C, RH = 30%                                                                                                                                           |
| Myrcox<br><i>Zhang et al. (2018)</i>                                                                                                 | 447                  | <del>m</del> Myrcene + O <sub>3</sub> , T = 23°C, RH = 30%                                                                                                                                           |
| <u>Isoprene Laboratory Oxidation</u>                                                                                                 |                      |                                                                                                                                                                                                      |
| Isopox<br><i>Experiment conducted under same methodology as in Chen et al. (2023).</i>                                               | <del>12653</del> 21  | <del>i</del> isoprene + OH (H <sub>2</sub> O <sub>2</sub> as OH source), T = 23°C, RH = 57%, <del>wet</del><br><del>wet -ammonium sulfate</del> (NH <sub>4</sub> ) <sub>2</sub> SO <sub>4</sub> seed |

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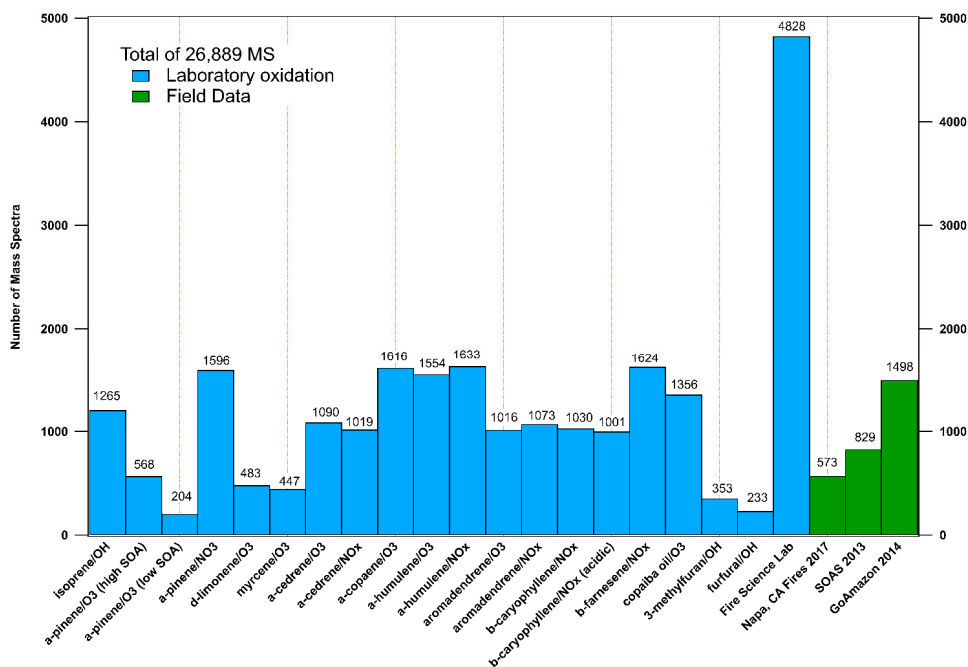


Figure 1: Number of mass spectra (MS) in each library of the UCB-GLOBES database used in this work. Blue bars indicate MS produced from laboratory oxidation experiments and green bars indicate field/ambient datasets.

## 2.2 GCxGC-HR-TOFMS analysis

All samples were analysed offline using two-dimensional Gas Chromatography with High-Resolution Time-Of-Flight Mass Spectrometry (GCxGC-HR-TOFMS) as employed in previous work (Franklin et al., 2023; Jen et al., 2019; Liang et al., 2021; Worton et al., 2017; Yee et al., 2018; Zhang et al., 2018). Briefly, one or multiple aliquots (0.41 cm<sup>2</sup>) of each filter sample were prepared with an applied internal standard. The internal standard is a custom mixture of even carbon number perdeuterated *n*-alkanes spanning C<sub>12</sub>-C<sub>38</sub> (C/D/N Isotopes) and isotopically-labelled compounds with similar structures/functionality of atmospheric compounds previously encountered. Internal standards are used for establishing a basis for normalized chromatographic retention times for comparison across samples as well as for accounting for instrument changes in detector sensitivity and matrix effects during sample desorption.

Field Code Changed

Prepared sample punches were then desorbed into helium using an autosampler (Gerstel TDSA2) and temperature programmed thermal desorption unit (Gerstel TDS3), followed by focusing onto a glass wool liner held at 30 °C in the cooled inlet system (Gerstel CIS4). Contents were then desorbed from the cooled injection system (CIS) with in-situ gas-phase derivatization by MSTFA, *N-methyl-N-trimethylsilyl trifluoroacetamide* (Sigma-Aldrich), before GCxGC separation (Agilent GC 7890). Derivatization converts hydroxyl groups on compounds into trimethylsilyl (TMS) esters, allowing resolution of more polar and oxygenated organics that are not typically GC-amenable. The first GC column is a 60 m × 0.25 mm × 0.25 μm nonpolar capillary column (Restek Rxi-5Sil MS) which leads to separation by volatility. First column effluent is then cryogenically focused on a guard column (1 m × 0.25 mm; Restek Rxi) using a dual-stage thermal modulator (Zoex) and injected every 2.3 s onto the second GC column, 1 m × 0.25 mm × 0.25 μm (Restek Rtx-200MS), which leads to separation by polarity. Helium was used as the carrier gas with a flowrate of 2 mL min<sup>-1</sup> while the GC temperature program comprised of holding at 40 °C for 2 min, followed by ramping 3.5 °C min<sup>-1</sup> until 320 °C is reached, and finally held there for 10 min. The second column was housed within a secondary oven that was maintained at 15 °C above the main oven temperature. Second column effluent was then transferred to the ionization region of a high-resolution ( $m/\Delta m \sim 4000$ ) time-of-flight mass spectrometer (Tofwerk HTOF), where analytes were ionized using 70 eV electron ionization before detection.

### 2.3 Creation of EI MS libraries

Within UCB-GLOBES are several EI MS libraries, each representing MS compiled from a particular field campaign or laboratory oxidation experiment. Following GCxGC-HR-TOFMS analysis, chromatographic and MS data were imported into the GCImage software (GCImage, LLC), in which initial processing steps included automated background subtraction, blob (3-D chromatographic peak) detection, and MS deconvolution. Chromatographic retention indices (RIs) were initially configured based on the perdeuterated alkane series present in the internal standard, and then mathematically translated via linear fit to the more conventional and widely-used *n*-alkanes based Kovats Retention index (Kováts, 1958), using the nearest in time GCxGC run with co-injections of perdeuterated and normal *n*-alkanes. Unit mass resolution MS at the peak of considered blobs were then extracted and searched within the NIST MS Search program v.2.4 (U.S. Department of Commerce) and exported from the Librarian tab to .MSP format or directly saved from GCImage. Unit mass resolution (UMR) spectra were selected for entry into UCB-GLOBES for computational simplification and are more widely useful to the wider GC/EI-MS community that does not necessarily acquire HRMS data. UMR data has not been shown to decrease the fidelity of MS identification through MS searching (Stein, 2012), although HRMS data is better suited for potential molecular formulae assignment of unknowns and determination of MW, which can be useful in hybrid searching to gain additional structural information. Exported peak table information (e.g. retention times, retention index) from GCImage were combined with MS data in the NIST MS Search program generated .MSP file within a Microsoft Excel worksheet with a custom-written macro for data merging. Additional custom metadata entry by analysts were added before reexport of the curated MS library as a .MSP file (to be compatible for reimport as a custom user library in the NIST MS Search program; see Supplementary Information: Using UCB-GLOBES data within NIST MS Search program for further details). Custom metadata entry fields

include those listed and described in Table 2. During import of UCB-GLOBES MS libraries into the NIST MS Search program, the metadata entries will appear in the comments section of MS records with fields formatted and labelled by “Tags” as according to the NIST MS Search program conventions. An example MS entry and its MS search results as viewed in the NIST MS Search program is shown in Figure S1. Further information on how to access UCB-GLOBES MS contents and version control is described under Data Availability. While creation of UCB-GLOBES MS entries here were generated with one specific instrument and method of sample preparation, the database could readily include deconvoluted MS from additional GC/EI-MS instruments with variations in sample prep, column loadings, and GC conditions. The importance of and quality of associated metadata with any MS entry is essential for helping an analyst discern the suitability and confidence in a MS match, just as similar data is included for known identity compounds within the NIST MS Database when available. For example, because analytes were derivatized here with MSTFA and separated on a nonpolar column, other GC/EI-MS analysts searching for MS matches among UCB-GLOBES should take this into account with their sample preparation method, interpretation of analyte MS, and comparison of retention indices. Contributions of new MS to UCB-GLOBES is welcome and further described in detail in Supporting Information.

**Table 2: Metadata entries accompanying each MS entry along with descriptions of each metadata field**

| Metadata field/tag name      | Description                                                                                                                                                                                                                                                                                                                                                                   |
|------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Name                         | Compound name <u>including trimethylsilyl groups if applicable (e.g., levoglucosan, 3TMS); otherwise, a <del>or-givenplaceholder</del> name given by an analyst</u> as an unknown compound (e.g. UNK_AHG_HZ_SOAS_394, following the format: <u>UNKnown_PrincipalInvestigatorInitials_AnalystInitials_Dataset_PeakNumber</u> ) <del>including silyl-groups if applicable</del> |
| Synonyms                     | Synonyms for compound name. Multiple names may be entered in this column, separated by semicolons (;) as delimiter.                                                                                                                                                                                                                                                           |
| Campaign/Experimental Source | Field campaign/laboratory oxidation/standard used                                                                                                                                                                                                                                                                                                                             |
| Experimental_Conditions      | Description of any experimental conditions that may provide scientific insight into the observation of this compound                                                                                                                                                                                                                                                          |
| UID                          | "Universal ID", a unique identifier for the MS within UCB-GLOBES (e.g., LDY-22110, following a format of <u>CuratorInitials-MSNumber</u> )                                                                                                                                                                                                                                    |
| Contributor_ID               | Original compound ID assigned by the contributor.                                                                                                                                                                                                                                                                                                                             |
| Comments                     | Contributor's comments that may aid in interpretation of the compound MS or an unknown compound structure/source; Any comments on MS quality                                                                                                                                                                                                                                  |

| Metadata field/tag name  | Description                                                                                                                               |
|--------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| Suspected_matches        | List of UIDs that are suspected to be potential MS matches, but not necessarily confirmed by an analyzer/additional AI/ML MS match review |
| Confirmed_matches        | List of UIDs that are reasonably confirmed as MS match by an analyst                                                                      |
| Predicted_Matches        | List of UIDs that are predicted to be matched by automated MS review                                                                      |
| Compound_Structural_Info | Contributor's description of compound structure (e.g. sugar, acid, unknown, etc.)                                                         |
| Formula                  | Elemental formula including silyl groups if applicable                                                                                    |
| MW                       | Molecular weight including silyl groups if applicable                                                                                     |
| ExactMass                | Exact molecular weight including silyl groups if applicable                                                                               |
| VUV_Exact_Mass           | VUV measured exact mass if applicable                                                                                                     |
| CAS#                     | IUPAC given CAS# if applicable (identity known)                                                                                           |
| Ch3MS-RF Cnum.p          | Predicted carbon number <i>of underivatized analyte</i>                                                                                   |
| Ch3MS-RF OC.p            | Predicted O:C ratio <i>of underivatized analyte</i>                                                                                       |
| Ch3MS-RF OSc.p           | Predicted average carbon oxidation state <i>of underivatized analyte</i>                                                                  |
| Ch3MS-RF VP.p            | Predicted log(vapor pressure) atm <i>of underivatized analyte</i>                                                                         |
| Column_Type              | Class of GC column: <del>is</del> polar, non-polar, etc.                                                                                  |
| Retention_index          | <i>n</i> -alkane based retention index used in MS searching and RI comparison                                                             |
| d_alkane_RTI             | Deuterated alkane-based retention index                                                                                                   |
| n_alkane_RTI             | <i>n</i> -alkane based retention index                                                                                                    |
| Instrument               | Instrument used to obtain MS                                                                                                              |
| Ionization               | Ionization energy                                                                                                                         |
| Injection_method         | Method used for introducing sample into instrument                                                                                        |
| Derivatization_Agent     | Derivatization agent used if applicable                                                                                                   |
| GC_column                | GC column description                                                                                                                     |
| Oven_temp                | Oven program used                                                                                                                         |
| Publications             | Associated publications that this MS library entry is used in or supporting publications on generation/measurement of this compound       |
| Contributor              | Name of person who made the MS entry                                                                                                      |
| Date_of_Entry            | Date the entry was made                                                                                                                   |
| Num Peaks                | Number of m/z peaks for which MS measured                                                                                                 |
| 5_Highest_Intensity_MZ   | <i>m/z</i> values of the top 5 highest intensity peaks in MS                                                                              |
| Base_Peak                | <i>m/z</i> of the highest intensity peak in MS                                                                                            |
| MS                       | Mass spectrum                                                                                                                             |

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### 2.3.1 Manual/automated MS Quality Checks

Additional manual/automated quality checks were performed in case of compromised MS quality due to potential missed 2<sup>nd</sup> dimension blob co-elutions by the software, filtering out known experimental or system artifacts, noisy MS due to insufficient signal, etc. Additional known contamination~~nts~~ influencing MS quality included convolution of low polarity peaks coinciding with perfluoromethyldecalin (PFMD, an internal pulsed calibrant during chromatographic runs for MS calibration). Figure S2 shows that while the majority of MS were not flagged for failing any of these MS quality checks, a significant portion (~1,000 MS) within the FSL\_FIREX2016\_v2 dataset were found to have systematic PFMD contamination in the MS in those chromatographic runs. MS in FSL\_FIREX2016\_v2 ~~have~~ since been corrected and rereleased as FSL\_FIREX2016\_v2.2024 to subtract out PFMD influence in the MS and include updated identifications using the NIST MS 2024 database (pre-release) and additional analysis methods described in McGlynn et al. (2025).

While considerable effort has been made to identify and correct for any issues that may lead to decreased quality of the MS and its metadata for scientific use (including measures such as complete omission of bad MS entries), it is imperative that any user of UCB-GLOBES data be generally versed in EI-MS interpretation as would be the case in utilizing any MS databases for increasing confidence in identification. Additional training in environmental (atmospheric) chemistry concepts is useful ~~to be able to~~ confidently use the data for scientific purposes (e.g. ascribing query MS matched with UCB-GLOBES entries to the same source/chemical conditions as those under which a UCB-GLOBES MS entry derived from). For example, as is the case for laboratory oxidation experiments, it is very feasible for lingering trace level contaminants to exist between experiments performed for different precursor systems at detectable levels in GCxGC analyses despite minimal/undetected impact on the main chemistry of focus from the perspective of other aerosol analyses. It is also possible for starting precursors though purchased from chemical suppliers to have small amounts of impurities. In these known cases, some MS were completely omitted based on the knowledge that certain compounds should not be generated during oxidation of a particular precursor or notes in the metadata fields of a MS entry highlight the authors' interpretation of a likely contaminant/artifact. It is the intent that should users of UCB-GLOBES database have additional MS interpretations or proposed corrections to the current entries, that the corresponding author be contacted to improve the database quality through informal peer scientific discourse. We expect UCB-GLOBES to be under continuous evolution including deletion/addition of MS records as well as new metadata for existing entries as parallel analyses provide new information (e.g. new annotated MS datasets that inform past MS data, predictive capabilities of compound properties/identification based on MS features evolve).

### 2.3.2 Automated metadata entries from MS featurization: MW prediction, base peak, five highest intensity *m/z* ions

An automated algorithm for picking out the potential molecular ion was generated on the basis that trimethylsilyl derivatives in EI MS tend to have a characteristic  $[M - CH_3]^+$  or  $[M - 15]^+$  ion (Harvey and Vouros, 2020). For each MS, its peaks were first found by simple neighbour comparisons: an ion was considered a peak if its intensity was higher than the

intensities of its left and right neighbours. Then, all pairs of peaks with a 15 amu difference were found; in each pair, the peak with higher  $m/z$  was a candidate for the molecular ion. The candidate with the highest  $m/z$  was selected as the predicted MW ion. If its intensity exceeded the 75th intensity percentile of the MS, it was included in the metadata for that entry under the “MW\_Prediction” metadata field. If no candidates were found or the predicted MW ion had intensity below the enforced percentile, the “MW\_Prediction” metadata field was set as “0” or empty. In contrast, the “MW” metadata field was populated under the following cases: 1) Positive MS identification resulting in known chemical structure, 2) analyst determined MW from examination of isotopic ratios and the molecular ion, and 3) analyst determined molecular ion from complementary analysis of samples using vacuum ultraviolet ionization (also reported under “VUV\_Exact\_Mass” and applicable to only a few datasets in UCB-GLOBES). Custom code was also written to report the base peak ( $m/z$  of the highest intensity peak) and the five highest intensity ions.

## 2.4 MS matching criteria

In the forthcoming analyses presented in Section 3, we leverage the UCB-GLOBES database for improving knowledge about previously observed but unidentified MS in ambient datasets. By searching MS from each dataset against UCB-GLOBES, additional MS matches were found besides those within the NIST20 MS Database, Adams Essential Oil MS Library, and a proprietary MS library from the flavor and fragrance company, MANE. Generally, MS matches (MSM) were considered a potential match as long as the NIST MS Search program forward match factor (FMF)  $\geq 700$ , reverse match factor (RMF)  $\geq 750$ , and the difference in the query and database MS retention indices  $\leq 10$ . Retention index (RI) comparison for library search was not used in match factor calculation since RI tolerances were checked separately. For matches external to UCB-GLOBES, retention time differences  $\leq 30$  were considered a match. The match factor (MF) cutoffs used here are considered to provide “fair” matches (Stein, 1995), which were purposefully lenient in the current analyses to not overattribute MS as unique/unknown by using stricter MF thresholds of 800 or “excellent.” Some were still considered matched per analyst discretion after manual inspection and accounting for spurious MS contaminant peaks and/or consideration of influences from signal to noise that might lower the MF scores.

## 2.5 UCB-GLOBES MS Data Visualization and Comparison Tool

An open-access Python-based tool was developed within Jupyter notebook allowing users to download the latest UCB-GLOBES data, plot MS entries, compare MS, and calculate cosine angle similarity indices between two or more MS as a quantitative indicator for similarity that does not require the NIST MS Search program for match factor calculations. Cosine angle similarity values range from 0 (poor/not a match) to 1 (perfect match). Plots for comparing two user-selected MS are generated following the format developed in Jeon et al. (2023) for comparison of AMS mass spectral data. An example output of the MS data visualization and comparison tool for unidentified MS entries by UCB-GLOBES Universal ID (MS Name) LDY-21509 (UNK\_AHG\_HZ\_SOAS\_394) and LDY-22110 (1128\_1901\_blob\_1117) is shown in Figure 2. Overall, the MS are highly similar (cosine similarity score = 0.994) and close in RI (only differs by one RI unit), indicating that these MS are

likely from the same compound. Furthermore, the MS here are suspected MS matches with 10 additional unidentified MS from other datasets in UCB-GLOBES including LDY-7521, LDY-14099, LDY-10911, LDY-6980, LDY-4100, LDY-11940, LDY-5510, LDY-21509, LDY-20100, LDY-9654, LDY-9794. These MSs are derived from monoterpene laboratory oxidation, sesquiterpene laboratory oxidation, and ambient datasets with majority biogenic OA sources. A cosine angle similarity matrix is generated for evaluating the MS similarity for all twelve of these sample types (Table S1) indicating that there is high MS similarity (cosine similarity scores  $> 0.95$ ) between these compounds which can serve as a potential marker of laboratory and ambient terpene oxidation. Specific information on how to use this Jupyter notebook is discussed in the Supplementary Information.



**Figure 2: Outputs for MS comparison tool as a) MS for UNK\_AHG\_SOAS\_394 (UID LDY-21509), b) MS for 1128\_1901\_blob\_1117 (UID LDY-22110), c) Mirrored comparison plot for both spectra, d) MS subtraction, and e) Correlation plot of relative intensities with calculated cosine angle similarity between MS.**

### 3 Improving knowledge of unknown atmospheric compounds using UCB-GLOBES

#### 3.1 Progression from targeted vs untargeted tracking of measurable compounds

Previous analysis of GCxGC-HR-TOFMS measurement of compounds sampled during the 2013 Southern Oxidant and Aerosol Study (SOAS) was performed through a semi-targeted approach, in which one filter sample was selected as a representative matrix of compounds to trace throughout the whole 6-week campaign (Zhang et al., 2018). A “template” of ~800 chromatographic peaks stored with their retention times and first dimension RI, and ratios of characteristic ions (manually assigned by the analyst after examining all template MS), was utilized for automated template matching within GCImage for over 300 other filter sample runs. As automated template matching primarily performs matches by measured two-dimensional retention times, this method was highly tedious and required manual quality control to check MS matches according to analyser specified ratios of ion abundances for the assigned characteristic ions. To eliminate the need for manual MS constraints to be assigned by an analyst, we adopted a new workflow in which template peaks’ mass spectra along with retention times and first dimension RI are stored in a custom MS library so the peaks within each sample could be searched using their full mass spectra rather than relying on a ratio of two manually chosen characteristic ions as the contingent MS match criteria. This greatly simplified template matching and reduced the time spent in manual quality checks, as MS searches conducted with the NIST MS Search program generate quantitative MS match factors (Stein, 1994) with consideration of retention index matching. We have since generated a custom MS library, Soasox (Table 1), with MS, RI, and metadata entries for the ~800 compounds traced during the SOAS campaign for inclusion in UCB-GLOBES.

By embracing the ability to store full MS data of observed and majority unidentified compounds, we could also generate a consensus template of several compounds viewed over multiple samples during a campaign, rather than select one representative sample that may bias towards time of day/certain chemistry, etc. Such an approach was adopted in Jen et al. (Jen et al., 2019) to generate a dataset with ~4,800 biomass burning marker species spanning over 29 burns featuring varying fuel types burned in a fire laboratory, ~500 species observed in downwind wildfire smoke from Napa, CA (Liang et al., 2021), and ~1,500 species observed during the GoAmazon field campaign (Franklin et al., 2023).

#### 3.2 Improving chemical source category assignment of unknown compounds in ambient data

##### 3.2.1 Source reclassification of compounds observed during SOAS

As an exercise in testing how creation of custom MS libraries can increase the efficiency of classification of unknown compounds to potential sources of chemical origin by MS matching, a MS search was conducted on those of 816 compounds observed during the SOAS 2013 campaign. Previous analysis in Zhang et al. (2018) found 342 MS matches (MSM) among these compounds. Here, we found an additional 91 MS matches (MSM) to UCB-GLOBES entries, and 75 of these were newly classified/reclassified into chemical groups accordingly (Figure 3). This equates to an overall 11% increase in MS match-based confirmations and new information gained about the SOAS dataset. In addition, the number of analytes previously assigned to a chemical source group solely via time series correlation ( $R^2$ ) with other chemical markers of known chemical

origin dropped by 84; this is a 20% reduction in the number of analytes listed as R<sup>2</sup> for the method of source group determination under the “Group Determined By” column in Table S2 compared to the number listed under the “Group Determined By Reanalysis” column.

Using UCB-GLOBES as an additional reference for added MS confirmations helps fortify inferred chemical source assignments based on time series correlation but importantly leads to potential reassignment of some of the compounds on a basis of chemical structure (through MSM or MS similarity) and origin (MS annotated with campaign/experimental source of MS observation). Moreover, many UCB-GLOBES MS are common between multiple libraries, which means that there is potential for measured compounds to originate from more than one precursor (Figure S3 and Figure S4). This is expected as oxidation of VOCs in the atmosphere typically progresses to organic intermediates of increasing average carbon oxidation state and lower carbon number with CO<sub>2</sub> as an eventual endpoint (Kroll et al., 2011). Thus, many oxidation products along fragmentation pathways (i.e. C-C bond cleavage) will be common among various precursor systems. In the case of this SOAS dataset reanalysis, several occurrences of compound MS having several MS matches necessitates new/hybrid chemical source categories to be employed. For example, Zhang et al. (2018) utilizes single precursor class assignments for biogenic organic aerosols as either BOOA = other biogenic organic aerosols, ISOP = isoprene SOA, MTLab = monoterpene SOA observed in literature and lab experiments, MTR2 = monoterpene SOA based on timeline correlation, or SEQT = sesquiterpene SOA. For figure clarity in this study, we have shortened the MTLab and SEQT designations to MT and SQT hereafter. The reanalysis reveals that for 537 compounds previously ascribed to any of these singular biogenic OA categories, 15 of their MS were in fact crossmatched between multiple libraries/multiple precursor systems. This provides evidence of common oxidation products derived from different precursors. As an example, three MS with UIDs LDY-21129, LDY-21220, and LDY-21183 were found to have corresponding chemical formulae of C<sub>8</sub>H<sub>12</sub>O<sub>5</sub>, C<sub>7</sub>H<sub>8</sub>O<sub>5</sub>, and C<sub>7</sub>H<sub>10</sub>O<sub>5</sub>, respectively. LDY-21220 was originally classified as SQT-derived, while the other two were classified as MT based on timeline correlation. Laboratory oxidation MS in UCB-GLOBES shows these MS can all be generated in MT/SQT oxidation, highlighting that these MS can represent compounds as indistinct chemical makers derived from terpene oxidation. There was even a compound with UID LDY-21336 with proposed molecular formula C<sub>4</sub>H<sub>8</sub>O<sub>3</sub> that crossmatched between MT, SQT, and BBOA (biomass burning OA), which is consistent with previous observations of terpenes and their oxidized derivatives being emitted during biomass burning (Hatch et al., 2019). LDY-21336 also matched to other MS among biomass burning UCB-GLOBES datasets including the Napa, CA fires, FSL\_FIREX2016, and laboratory oxidation of biomass burning intermediate 3-methylfuran. Thus additional source group categories reflecting multiple potential sources introduced here include: BBOA/MT/SQT, BBOA/SQT, ISOP/MT/SQT, ISOP/MT, MT, and MT/SQT as shown under the Group Reanalysis column in Table S2 adapted from Dataset S1 (Zhang et al., 2018) and reflected in the Sankey plot (Figure 3). The MS under BBOA/MT/SQT and BBOA/SQT categories could be further interpreted as shared common products derived from terpene oxidation terpene-derived and biomass burning based on Ch3MS-RF predicted carbon numbers <10 and average carbon oxidation states ranging -0.8 to 0 (See Section 3.4 Improving chemical knowledge of unknown UCB-GLOBES compounds through chemical properties prediction). primary organic aerosols. While these hybrid source categories represent an overall small fraction (1.8%) of the

SOAS dataset, > 10% changes in the number of MS assigned to chemical categories in 2018 compared to reassignment through the present reanalysis are non-negligible, with number counts next to each category labelled in Figure 3. Figure 3 shows that the main changes made with 91 new MS match confirmations with UCB-GLOBES data resulted in almost half of those 91 mass spectra getting redistributed from MTR2 to categories like ISOP, MT, MT/SQT, and SQT with MS reanalysis. Changes by percent number of MS within a category include +31% for ISOP, +22% for MT, +34% for SQT, as well as -20% drops each in ASOA (anthropogenic SOA) and in MTR2.

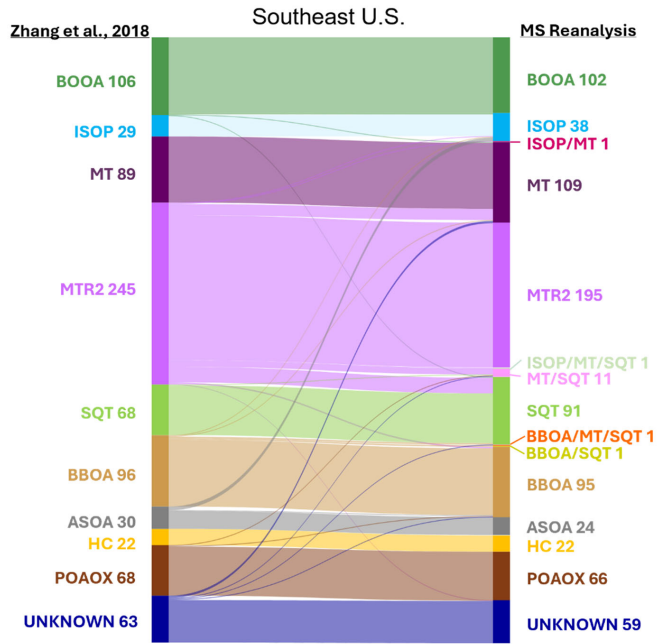


Figure 3: Redistribution of 816 observed compounds during SOAS in the Southeast U.S. by source category based on correlation and mass spectral matching (MSM) performed in Zhang et al., (2018) and reanalysis with MSM utilizing UCB-GLOBES. Reanalysis resulted in 91 new MSM distributed among original and new source categories. Original source categories include other biogenic organic aerosol (BOOA), isoprene-derived organic aerosol (ISOP), monoterpene-derived organic aerosol through MSM (MT), monoterpene-derived organic aerosol inferred by correlation (MTR2), sesquiterpene-derived organic aerosol (SQT), biomass burning organic aerosol (BBOA), anthropogenic SOA (ASOA), hydrocarbon-derived organic aerosol (HC), oxidized primary organic aerosol (POAOX), and unknown. Additional knowledge gained from MSM reanalysis leads to novel hybrid categories from multiple sources including: ISOP/MT, ISOP/MT/SQT, MT/SQT, BBOA/MT/SQT, and BBOA/SQT.

### 3.2.2 Source reclassification of compounds observed during GoAmazon

A similar MS reanalysis was performed for GoAmazon data, in which original source categorization was performed for 1513 compounds observed during the 2014 wet/dry seasons using hierarchical cluster analyses (HCA) and some MS matching using some terpene laboratory oxidation data in UCB-GLOBES and NIST14-databases of known compounds (Franklin et al., 2023). Original HCA resulted in three source categories associated with background biogenic (BKGBIO), biomass burning influence (BB), and urban plume influence (UP). Results of the MS reanalysis are shown in Figure 4a for the wet season and Figure 4b for the dry season. While 136 out of 1513 (9%) of GoAmazon MS were fully identified as originally reported in Franklin et al. (2023), 375 out of 1513 (25%) of the MS in this reanalysis were found to have a MSM when searching among UCB-GLOBES, and NIST20, Adams Essential Oil, and MANE databases. Thus, new chemical knowledge for 16% of the dataset is obtained, resulting in further source confirmation determined through HCA or recategorization as shown in Figure 4. Flow links in the Sankey diagram with darker shades within a category indicate MS with “MSM” and lighter shades for MS with “No MSM.”

Notable findings for the wet season (Figure 4a) include: 1) 92 MSM out of 544 BKGBIO determined by HCA were confirmed while 21 BKGBIO were recategorized into a hybrid category representing BIO/BB influences. For this reanalysis, any MSM with MS entries from laboratory oxidation datasets of isoprene, monoterpene, or sesquiterpenes were categorized as BIO. 2) 16% of the HCA-determined UP category MS (148 out of 390) are further specified as urban plume influence on OA derived from biogenic and/or biomass burning intermediates. These urban plume influence hybrid categories are labelled BIO/UP, BB/UP, and BIO/BB/UP and constitute ~40% of the urban plume category, underscoring the significant influence the urban plume has on the atmospheric fate of biogenic derived VOCs under these conditions. With additional MS data in the future, it might be possible to further specify the remaining 60% of the urban plume-influence category to determine if the organic carbon is likely from anthropogenic or biogenic sources. Biogenic VOC oxidation was found to be particularly sensitive to anthropogenic emissions in this area (Franklin et al., 2023; de Sá et al., 2017, 2018, 2019; Shrivastava et al., 2019). New experiments focusing on Central Amazon conditions: biogenic VOC precursors (e.g., ~10s of ppt, monoterpenes) with varying NO<sub>y</sub> [0-20 ppb<sub>v</sub>] and O<sub>3</sub> [0-40 ppb<sub>v</sub>] levels at high relative humidities (80-93 %) and temperatures (26-28 °C) in the absence and presence of anthropogenic VOC precursors and/or primary anthropogenic OA could provide new MS that help elucidate some of the mechanisms behind the compounds in the urban plume-influence category. However, such high relative humidities and low precursor and oxidant concentrations are typically challenging to achieve in a laboratory setting. 3) Lastly, classification was achieved for 64 of 410 MS that were formerly No Assignment (NA) from HCA, 21 of which were reclassified as BKGBIO, 42 as BB, and 1 as BIO/BB.

In contrast, the dry season (Figure 4b) exhibits more regular biomass burning influence based on the number of MS categorized in BB (196 during wet season, 281 during dry season after MS reanalysis). While 60 MS previously with NA contribute to the increased BKGBIO (+8%) and BB (+1%), a significant portion of UP MS (38%) is further specified into hybrid categories (i.e. BIO/UP, BB/UP, and BIO/BB/UP). This corroborates the significant impact urban plume influence can

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have on SOA formation from biogenic and biomass burning VOCs (Franklin et al., 2023). While modest improvements in MSM (25% of dataset) are achieved, 35% of the dataset remains unclassified from neither HCA nor MSM analyses, underscoring that there is still limited knowledge in reproducing dry season conditions (e.g. exact BBOA sources/BBSOA formation). The MS reanalysis leading to hybrid categories for both wet/dry seasons is not surprising given the multitude of OA sources and conditions sampled during the GoAmazon field campaign. Moreover, there is potential for new chemical markers discovery within these hybrid categories as markers of biogenic OA under urban plume and/or BB influences and processing compared to markers only associated with background conditions.

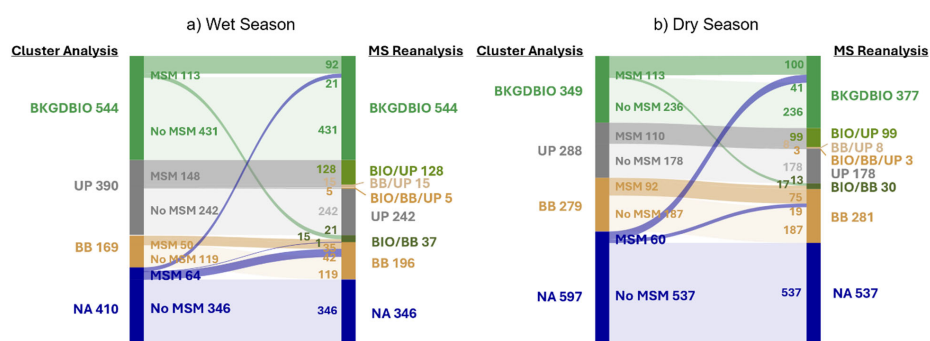


Figure 4: Further specification and source classification of GoAmazon observed compound MS during a) wet season and b) dry season from cluster analyses performed in Franklin et al., (2023) with reanalysis using mass spectral matching (MSM). Source influence categories from cluster analyses include background/biogenic (BKGDBIO), urban plume influence (UP), biomass burning (BB), and no assignment (NA). Additional knowledge gained from MS Reanalysis leads to further specification of urban plume influence on biogenics (BIO/UP), biomass burning (BB/UP), and biogenic/biomass burning (BIO/BB/UP). Additional hybrid category of biogenic/biomass burning (BIO/BB) was also created per MS reanalysis. Darker color links are labelled “MSM” indicating mass spectral match was found; Lighter color links labelled “No MSM” indicate no mass spectral match was found. Outgoing links share the same base color as their cluster analysis source category, while text color of incoming numbers of MS match their destination source category after MS reanalysis.

### 3.3 UCB-GLOBES MS show large mismatch between laboratory and ambient MS data

Despite generous thresholds for considering potential mass spectral matches (i.e. FMF  $\geq 700$ , RMF  $\geq 800$ ), only 29% of all MS in UCB-GLOBES are considered to have a MSM, with the remaining 71% of MS unmatched to other MS within UCB-GLOBES, NIST 20, Adams Essential Oil MS Library, or the MAnEane Fragrance MS Library (Figure 5). On average, 18% of MSs lead to a positive identification for ambient data MS have MSM amongst an authentic standard or the aforementioned libraries of known compounds leading to positive identification, emphasizing the need to better understand the sources and processing of most atmospheric species catalogued here. This also demonstrates that despite the chemical diversity generated in laboratory oxidation experiments using precursors and oxidants that are deemed to be

atmospherically relevant, we have yet to simulate conditions and processes that generate many atmospheric species that have previously been sampled in the Central Amazon, Southern U.S., and Napa Valley wildfires. Given that biomass burning OA observed during Napa, CA fires, 2017 and biogenic SOA observed during SOAS and GoAmazon typically can contribute significant portions of regional OA budgets, this large mismatch between laboratory and ambient data underscores the need to  
450 work towards laboratory simulations that better reveal the sources and origins of ambient OA species. For example, mismatches in simulated relative humidity and OA loadings could be a major source of disconnect (Porter et al., 2021) as well as the relative distribution of RO<sub>2</sub> fate (Kenagy et al., 2024). There are also limited laboratory simulations performed with mixed precursors (Takeuchi et al., 2022) rather than a single precursor, which could allow for cross-system reactions and new SOA products not currently represented in UCB-GLOBES that may better emulate atmospheric chemistry. While UCB-  
455 GLOBES MS represent oxidation of several major biogenic precursors and biomass burning intermediates, we recognize that the laboratory simulations are by no means exhaustive of all ambient SOA precursors and OA types.



used in training were selected to be as representative of the chemical complexity of ambient organic aerosol species as possible with available authentic standards. They span wide-varying volatility, functionality (e.g., alkane, alkene, carboxylic acid, alcohol, aldehyde, ketone, ester, amide), structure (e.g., polyaromatic hydrocarbons, phenol, methoxyphenol, quinone, sugar, sterol), and source types (e.g., known terpene- and isoprene-derived oxidation products). Note that Ch3MS-RF predictions here are inherently limited to compounds amenable to this GC x GC analysis (e.g., organosulfates and organonitrates would be excluded). Franklin et al., (2022) demonstrated Ch3MS-RF to have mean absolute error accuracy of  $\pm 0.25$  for Avg.  $OS_c$  and  $\pm 1.8$  for  $N_c$  when applied to the test case (~130 authentic standards) and the extrapolation case (71 identified GoAmazon compounds). As random forest modelling does not extrapolate and tends to underpredict property extremes of Avg.  $OS_c$  and  $N_c$  space (Franklin et al., 2022), we might expect a wider spread of the true chemical properties' values and higher uncertainty in predictions for any encountered MS with very different MS features from the training and extrapolation datasets.

All UCB-GLOBES entries with predicted Avg  $OS_c$  and  $N_c$  are plotted in Figure 6, demonstrating the variability in these properties by sampled compounds and by source type as previously observed through aerosol mass spectrometry and high resolution mass spectrometry methods (Kroll et al., 2011).

For the experimental conditions and field data represented in Figure 6, we note the following observations by panel: a) despite different oxidation conditions and precursors, there is a similar range of predicted Avg.  $OS_c$  and  $N_c$  for the studied sesquiterpene ( $C_{15}H_{24}$ ) systems, with a good number of predicted  $N_c > 15$  suggesting prevalence of accretion type reactions; b) copaiba oil (an essential oil comprised mainly of sesquiterpenes and some monoterpenes) has a similar spread in Avg.  $OS_c$  and  $N_c$  as the sesquiterpene systems in a) and as the monoterpene ( $C_{10}H_{16}$ ) systems in c) for  $N_c < 20$  in e); c)  $\alpha$ -pinene reaction with  $NO_3$  radical is quite different compared to ozonolysis, leading to much higher  $N_c$  similar to the  $N_c > 15$  range achieved by sesquiterpene oxidation; d) there is a wide variety of chemical properties for compounds sampled during laboratory burns of Western U.S. biomass fuel types during FIREX\_2016, whereas ambient sampling downwind of Napa, CA 2017 wildfires are more disparate across the chemical space like laboratory oxidation of biomass burning intermediates 3-methylfuran and furfural; e) isoprene ( $C_5H_8$ ) oxidation occupies a smaller range in  $N_c$ , such as monoterpene ozonolysis systems, however there is clearly a signature of extensive oligomerization/accretion type reactions with oxidation products of  $N_c > 5$ . While several  $N_c > 5$  oxidation products have been observed from isoprene oxidation in lab/ambient data, the conditions for this experiment (isoprene,  $H_2O_2$ , UV light, wet ammonium sulfate seed, and 57% RH) were intended to simulate SOA formation from isoprene where IEPOX processes are minor, suggesting there are several potential oligomeric species generated from this route under the conditions tested; f) lastly, comparison of ambient datasets from GoAmazon and SOAS show similar occupation of the chemical space for  $N_c < 20$  consistent with biogenic SOA formation from isoprene as in e) and monoterpenes as in c), though GoAmazon has greater numbers of compounds with higher predicted  $N_c > 25$ , which could be consistent with greater prevalence of sesquiterpene oxidation/ $\alpha$ -pinene  $NO_3$  oxidation (Figure 6a/c), and higher avg.  $OS_c > 0.5$  for  $N_c > 12$ , which could be consistent with biomass burning influences as shown in Figure 6d. These potential sources are supported by online measurements of the prevalence of sesquiterpenes and their oxidation products during GoAmazon (Yee et al., 2018) relative

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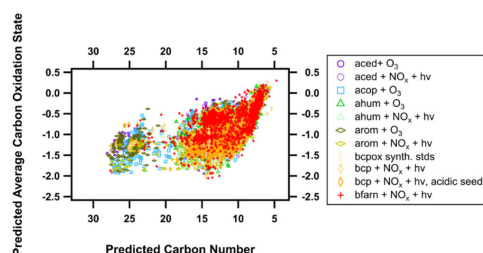
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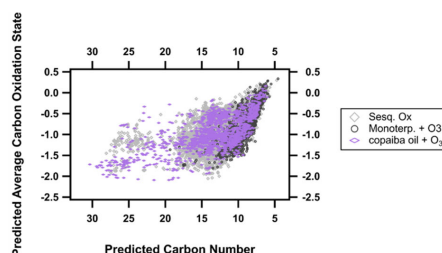
505 to the Southeast U.S. during SOAS and prior characterization of  $OS_c$  and  $N_c$  for biomass burning intermediates and their  
oxidation (Cai et al., 2020; Gilardoni et al., 2016; Sun et al., 2010).

Regardless of the many overlaps of observed compounds in these datasets with the  $OS_c$  and  $N_c$  chemical space, we  
interpret these overlaps as potentially useful indicators of similar chemical processes rather than that of exact  
mechanisms/sources of observed species, as evidenced by the fact that mass spectral matches are not found for many of the  
510 data. Thus, while our predicted  $OS_c$  and  $N_c$  values here are well within the ranges appropriate by sources previously proposed  
and observed in Kroll et al. (2011), exact structure matching (as is only achievable through isomer-specific measurements) is  
still necessary to validate mechanistic hypotheses. UCB-GLOBES thus can serve as an important tool for testing and  
evaluating chemical mechanisms for observed compounds.

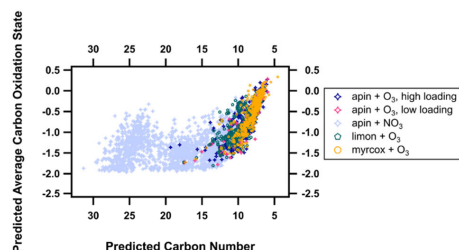
a) Sesquiterpenes ( $C_{15}H_{24}$ ) Laboratory Oxidation



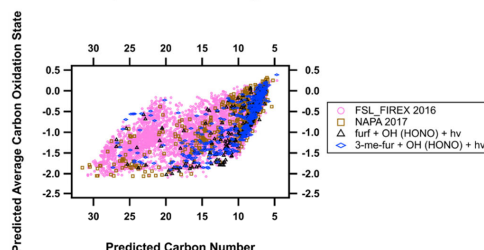
b) Copaiba Oil Laboratory Oxidation



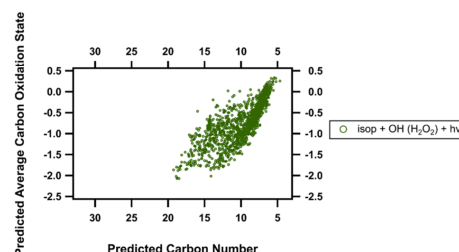
c) Monoterpenes ( $C_{10}H_{16}$ ) Laboratory Oxidation



d) Biomass Burning: Ambient Data, Laboratory Oxidation, and Laboratory Burns



e) Isoprene ( $C_5H_8$ ) Laboratory Oxidation



f) Ambient Datasets Biogenic Oxidation

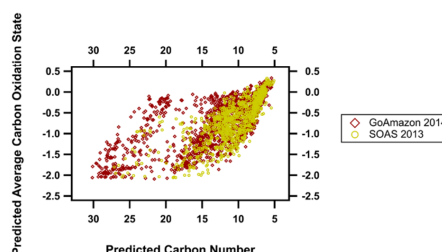


Figure 6: Ch3MS-RF predicted average carbon oxidation state and predicted carbon number for UCB-GLOBES datasets: a) sesquiterpene oxidation systems, b) copaiba oil oxidation, c) monoterpene oxidation systems, d) biomass burning influenced ambient data (NAPA 2017) and laboratory oxidation of biomass burning intermediates (furfural, 3-methylfuran) or Western U.S. fuel types (FSL\_FIREX 2016), e) isoprene oxidation system, f) ambient datasets from Central Amazon, GoAmazon and Southeast U.S., SOAS. Data in panels a) and c) repeated in grey in background of panel b) for comparison since copaiba oil is a complex mixture of terpenes.

## 4 Conclusions

UCB-GLOBES now includes just under 27,000 MS from laboratory and ambient datasets for the purposes of providing: 1) annotated MS data for the wider GC/EI-MS community to use in improving confidence in identification and/or revealing potential origins and sources of organic species in the atmosphere and wider environment, 2) MS data that can be further used in testing and evaluation of MS deconvolution, matching and search algorithms (McGlynn et al., 2025), and *de-novo* chemical structure/properties prediction, 3) development of atmospheric chemical mechanisms and chemical diversity studies, and 4) insights to motivate future research priorities in the identification of novel chemical markers. We provided as examples the utility of UCB-GLOBES in enhancing confidence and accuracy of OA source categorization of real atmospheric species from prior field studies in the Southeast U.S. (SOAS) and the Central Amazon (GoAmazon). One of the most significant advances of using UCB-GLOBES is that for a matched analyte spectrum, there are often several MSMs or closely related MS pointing to the same source(s) (e.g. precursor/s from laboratory oxidation) which strengthens overall confidence in OA source categorizations.

~~In contrast, statistical techniques such as positive matrix factorization (PMF) have been applied to aerosol mass spectrometry data, in which a timeline of composite mass spectra (also with 70 eV ionization) of all non-refractory flash-vaporized aerosol compounds is generated. In other words, “bulk” OA chemical composition is measured, rather than mass spectra of each individual OA analyte. These timelines of composite mass spectral data are separated into statistical factors, each with an average characteristic mass spectrum generated from the weighted signal contributions of the aerosol compounds’ mass spectral fragments assigned to this factor. Thus, a PMF factor mass spectrum will never be a match to any one compound’s mass spectrum. Determination of a “specific” source often relies on factor timeline correlation with known chemical tracers measured by complementary contemporaneous techniques and/or evidence of one or a few enriched characteristic ions within the factor mass spectrum that are also enriched in the MS of an authentic standard or known chemical tracers. In contrast, bulk OA statistical factor techniques (e.g. positive matrix factorization) for aerosol mass spectrometry have been sometimes determined to be “specific” to a source from evidence of one or a few enriched characteristic ions that match to one authentic standard’s MS as the basis for the factor’s chemical categorization.~~ For example, the isoprene epoxydiol-derived SOA (IEPOX-SOA) factor is characterized by enrichment of  $m/z = 82$  from  $C_5H_6O^+$  ion (Robinson et al., 2011), which was later observed in AMS spectra of IEPOX rearrangement products, cis- and trans-3-methyltetrahydrofuran-3,4-diols (Lin et al., 2012). This  $m/z = 82$  ion is also observed in 3-methylfuran oxidation with  $NO_3$  radical, which makes sense given the furan structures in both systems (Joo et al., 2019). Yet, as isoprene is more prevalent in the atmosphere compared to 3-methylfuran, most of the signal associated with  $m/z = 82$  ion tends to be attributed to IEPOX-SOA.

While the majority of UCB-GLOBES data derives from laboratory simulations, we keep in mind that such simulations do not perfectly replicate environmental conditions (e.g., temperature, relative humidity) typical of many regions in the real atmosphere, and additional physicochemical properties (e.g., aerosol phase state, seed chemistry, volume to surface area ratio, etc.) cannot be perfectly controlled/simulated as complexly as in the real atmosphere. Thus, care and general knowledge of

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atmospheric chemistry must be taken in interpreting the applicability of mass spectral matches to real-world conditions. For example, while there are many cases where MS matches can indicate multiple potential sources of an observed compound, all these inferred sources may not be atmospherically relevant and/or there could be yet to be measured systems and conditions that produce the same compound. The precise number of sources that leads to a compound, especially a later-generation structure with little similarity to its parent precursor could be numerous beyond what has been included in the current database.

Future directions for this work include additional MS data to be added to UCB-GLOBES including new field data from anthropogenically influenced areas outside Houston, TX and at the Southern Great Plains, OK as well as additional laboratory oxidation simulating aqueous BBSOA compositions. We encourage others employing GC/EI-MS analyses to consider contributing to UCB-GLOBES (see Supporting Information, III. How to Contribute MS Data to UCB-GLOBES) and/or sharing similarly annotated and formatted MS data to address the growing requests of open-access MS libraries and to move untargeted analyses of environmental samples forward. While the majority of atmospheric SVOC species remain unidentified, our future analyses will include clustering and molecular networking of species by chemical similarity (e.g. chemical families), to gain a greater appreciation for real-world chemical diversity of atmospheric SVOCs, their potential sources, and to identify future targeted research priorities on unidentified species of importance.

From the present analyses of UCB-GLOBES, we recommend a few research priorities going forward to advance understanding of the chemistry and fate of organics in the environment. Firstly, the community would benefit from openly shared quality annotated GC/EI-MS mass spectra of a wide range of environmental and laboratory sample types. Second, we would benefit from technical advancements to conduct and catalogue organic species in atmospheric laboratory simulations that are closer to atmospheric conditions with higher relative humidities (> 75 % RH), lower organic aerosol mass loadings, and lower concentrations of precursors and oxidants. We also recommend new datasets simulating oxidation of a mixture of VOC precursors and their oxidation intermediates, as cross-VOC system reactions as would happen in the atmosphere are not sufficiently represented in UCB-GLOBES yet. Inherent to these recommendations are challenges to technical feasibility, ensuring experiments are at sufficient concentrations for detection, and trade-offs of adding too many variables to the experimental matrix. However, achievements toward these recommendations could provide some of the keys to elucidating the true mechanisms and chemical complexity in ambient observations. Finally, we hope that UCB-GLOBES and other available environmental 70eV EI-MS data will be utilized for comparisons across environmental reservoirs (e.g., lithosphere, hydrosphere, biosphere, and atmosphere), so that the emission, transport, and fate of organic carbon across these sectors can be traced and better quantified through processes such as emission, reaction, and deposition.

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#### Data Availability

All datasets in UCB-GLOBES at time of publication are annotated and formatted according to the above described methods and accessible at <https://sites.google.com/berkeley.edu/goldstein-lab/resources>. Three formatting exceptions include the Worton\_VUV\_2017 (Worton et al., 2017), GoAmazon2014\_terpox\_v2 (Yee et al., 2018), and FSL\_FIREX2016\_v2 (Jen et

al., 2019), which were generated before the full standardization of the methods and curation protocols described in this work. The version of compiled UCB-GLOBES MS data used in this study has the filename ucbglobes2025\_v1 with DOI: 10.5281/zenodo.18176760. Versions are denoted by “\_v#” notation.

### Interactive Computing Environment

590 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. Additional information on using the Jupyter Notebook is provided in the Supporting Information.

### Author Contribution

595 LY and AG designed the experiments. Field samples were collected by LY, GI, RAW, CJ, YL and analysed by LY, EF, HZ, CJ, YL. Laboratory oxidation samples were analysed with GCxGC by LY, EF, HZ, and RJW. GTEC experiments were designed and carried out by NN, TM, TJ, GE, and WX. PNNL chamber experiments were designed and carried out by YZ and JS. Chemical standards were synthesized by MU, AGB, RT, and FG. LY, RJW, JZ, TZ, FL, SX, and IS developed mass spectral analyses codes and spectral data analyses were performed by JZ, TZ, and LY. LY conducted Ch3MS-RF simulations  
600 in consultation with EF. LY prepared the manuscript with contributions from all co-authors.

### Competing interests

The authors declare that they have no conflict of interest.

### Disclaimer

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### Financial support

The UC Berkeley team gratefully acknowledges support from DOE-ASR program (DE-SC0020051) for further analysis of the GoAmazon 2014/15 field campaign dataset and laboratory oxidation samples for addition of MS datasets to the UCB-GLOBES database. Support from DOE-ASR DE-SC0024032 and NSF AGS-2308645 are also gratefully acknowledged for supporting additional method development and analysis of UCB-GLOBES mass spectral data. TJ, MT, GE, and NLN acknowledge support from NSF AGS-1830727 and NOAA NA18OAR4310112. Pacific Northwest National Laboratory (PNNL) authors were supported by U.S. Department of Energy's (DOE) Atmospheric System Research, an Office of Science (SC) Biological and Environmental Research (BER) program. PNNL is operated for the DOE by Battelle Memorial Institute under Contract DE-AC05-76 RL01830. The Northwestern University team was supported by the National Science Foundation (NSF) under grant no. CHE-1607640. Ariana Gray Bé and Mary Alice Upshur gratefully acknowledge support from NSF Graduate Research Fellowships. Mary Alice Upshur also acknowledges an NSF GROW award, National Aeronautics and Space Administration Earth and Space (NASA ESS) Fellowship, and a P. E. O. Scholar Award.

**Commented [LY1]:** Add in acknowledgement of MS match algorithms and MW predictions, unmatched MS/MS filtering to NSF and DOE

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840 **Supporting Information for UCB-GLOBES: An open-access mass  
spectral database of identified and unidentified atmospheric organic  
compounds**

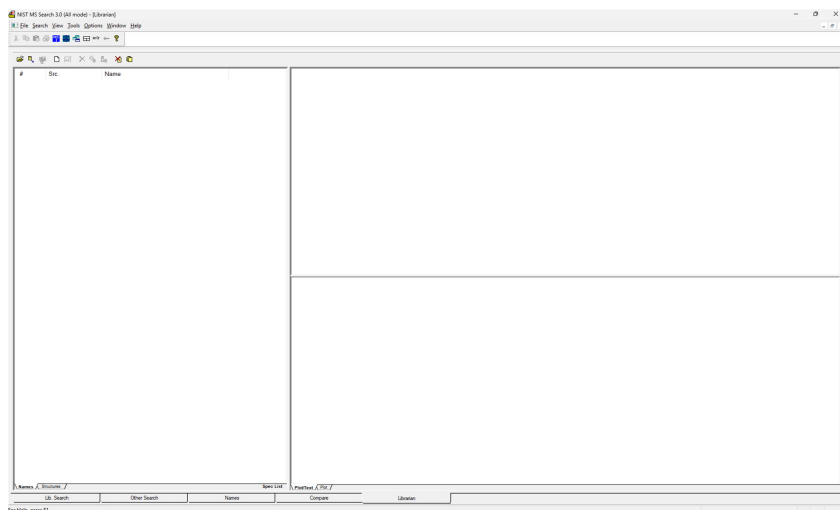
- 845 I. [Using UCB-GLOBES data within the NIST MS Search Program](#)~~Using UCB-GLOBES data within the NIST MS Search  
Program~~
- II. [UCB-GLOBES MS Data Visualization and Comparison Tools in Jupyter Notebook](#)~~UCB-GLOBES MS Data  
Visualization and Comparison Tools in Jupyter Notebook~~
- 850 III. How to Contribute MS Data to UCB-GLOBES
- IV. SI Tables
- V. SI Figures

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

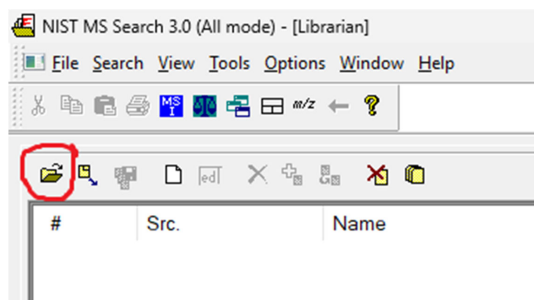
855 The following instructions are intended as a guide for importing UCB-GLOBES MS libraries into the NIST MS Search program. A free-of-charge version of the NIST MS Search program (NIST MS Demo) is available without the for-charge NIST main library if the user would like to simply import their own MS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

860 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).

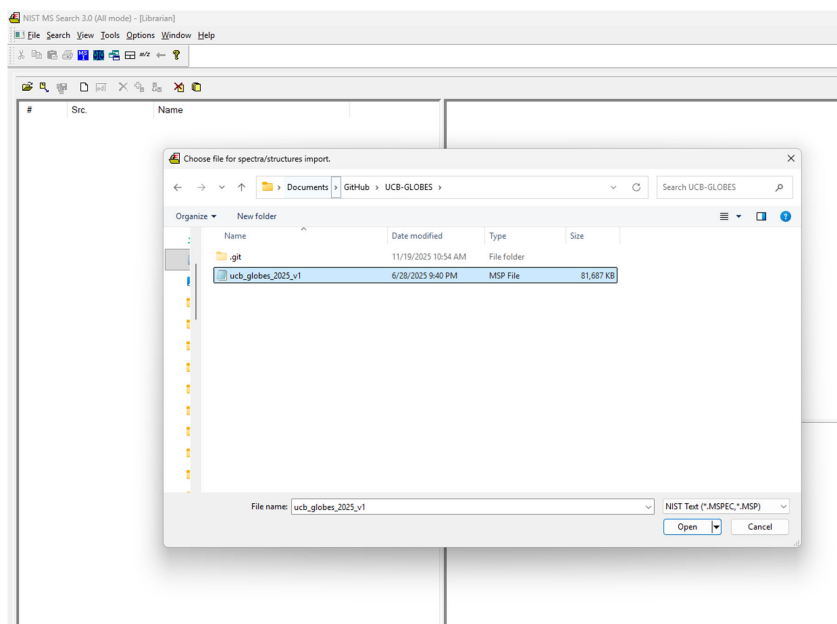
1. Download the desired UCB-GLOBES MS libraries in .MSP file format from <https://sites.google.com/berkeley.edu/goldstein-lab/resources>
- 865 2. The dataset specifically used in this study is also accessible on this webpage as well as through the DOI: [10.5281/zenodo.18176760](https://doi.org/10.5281/zenodo.18176760).
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
- 870 should look like this:



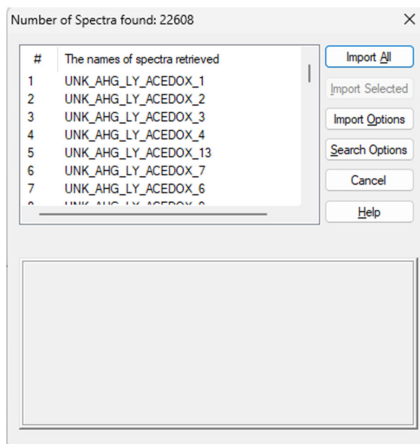
5. Click “Import” in upper left corner:



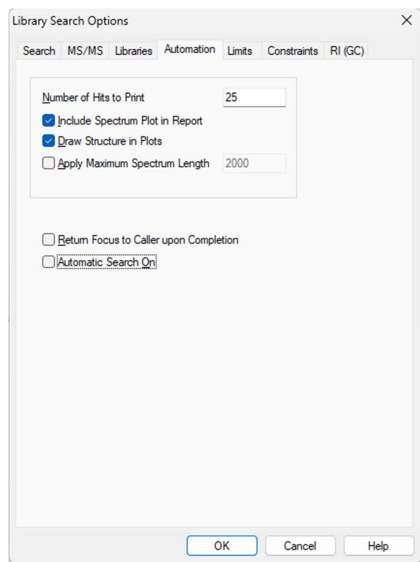
- 875 6. Navigate to the location of the downloaded .MSP file that you want to import. Select and click Open.



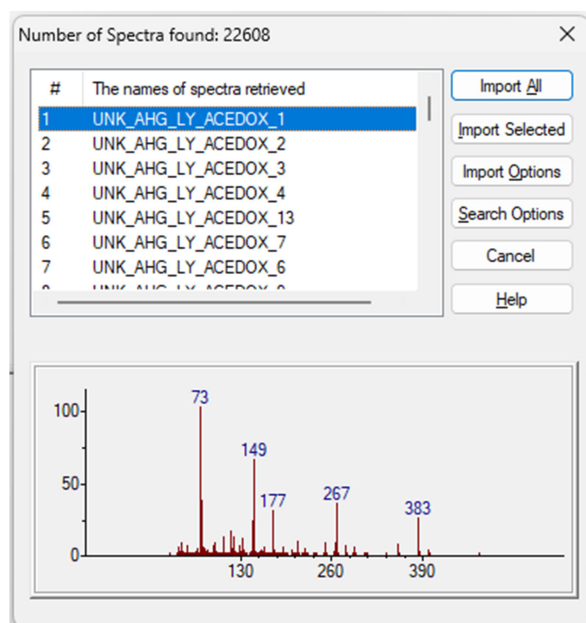
7. A window will open showing the number of spectra found in the .MSP file. Click on “Search Options.”



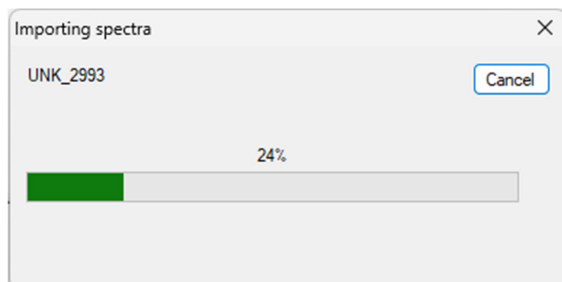
- 880 8. To dramatically speed up the import of MS, go to the “Automation” tab, and uncheck the “Automatic Search On” option. Click “OK.”



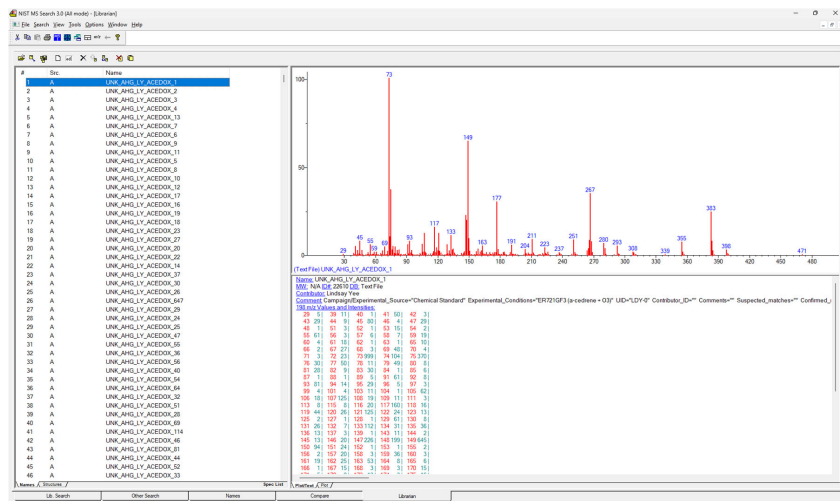
9. Then choose the spectra from the list that you want to import and select “Import Selected” or “Import All.”



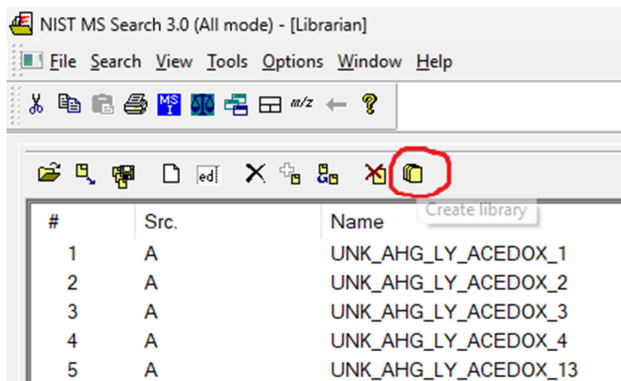
885 A progress window will show the status of importing mass spectra:



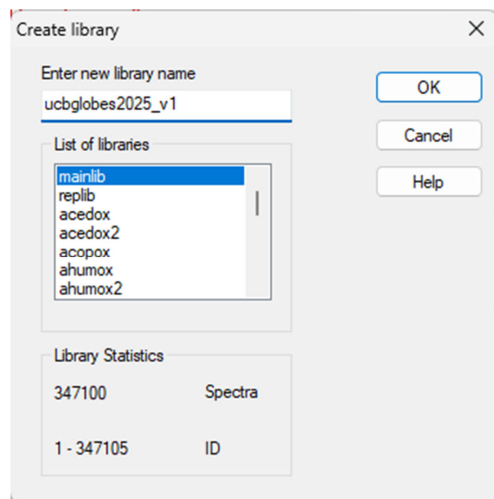
The Librarian tab should now be populated with all the imported spectra.



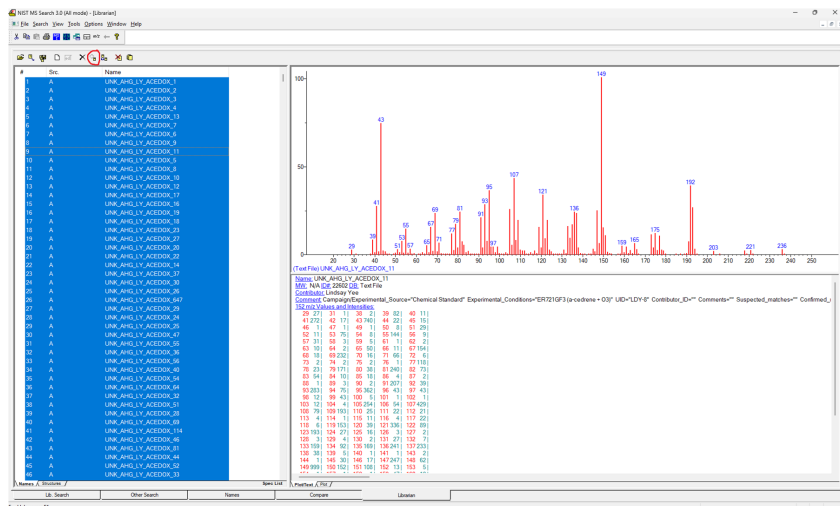
- 890
10. Now we will add all the spectra to a user custom library that can be accessible as a library to search against when running MS searches. Click on “Create Library” in the upper left menu bar.



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

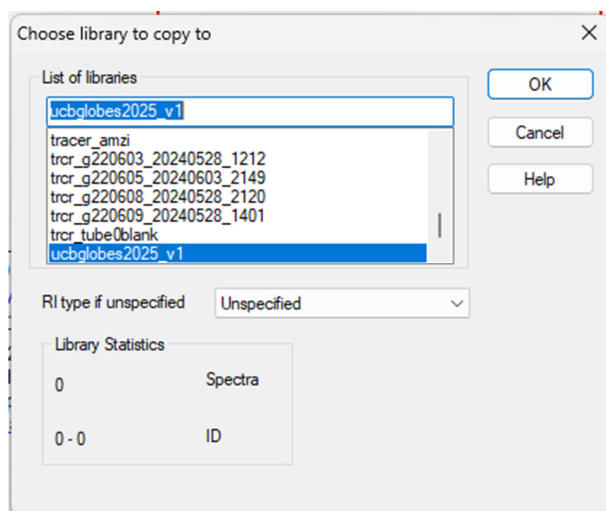


- Then, select all MS in the librarian tab and click on “Add to Library” in the upper left menu.

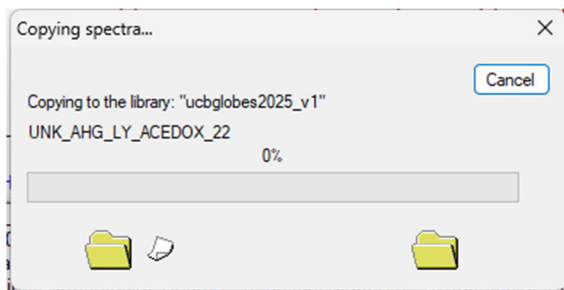


- Choose the library to copy to (the library name you created in step 11). Note that the library currently has 0 spectra in it since you just created it, but have not added spectra to it. Then push “OK.”

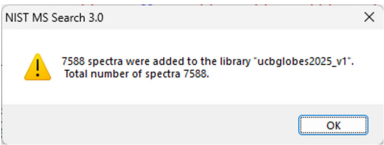
900



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:

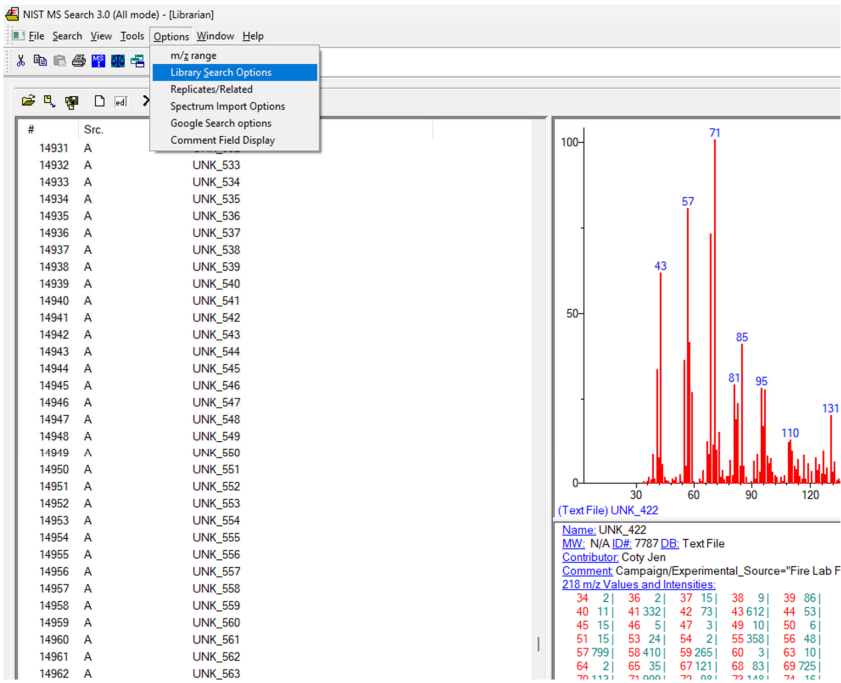


905 After all spectra are copied over, you should receive a confirmation showing how many spectra have been added to the library (example below):

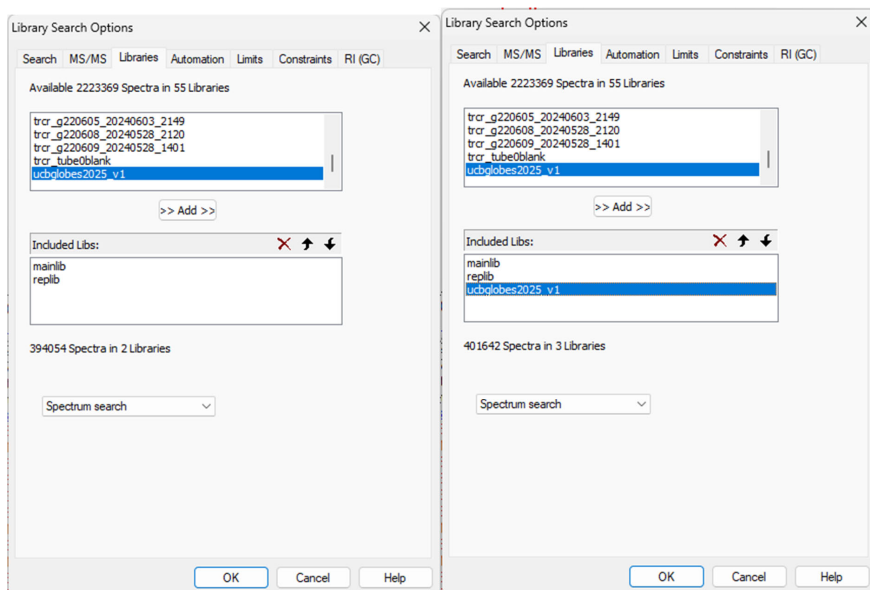


910 This mass spectral library is now in the NIST MS Search library format and is located in the MSSearch folder of the NIST MS Search program. By default it would be in C:\NISTXX\MSSEARCH with all library files under the library name you created in Step 11.

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.



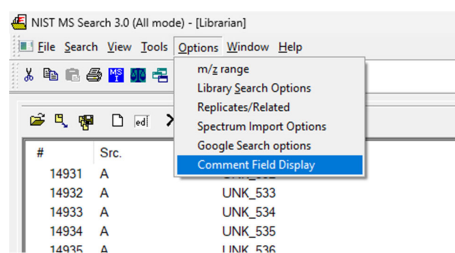
- 915 15. Under the Libraries Tab, select the library (in this case, ucbglobes2025\_v1) in the Available XX Spectra in XX libraries (those that are in the C:\NISTXX\MSSEARCH folder) and click ">>Add>>" so the selected library is now listed under the Included Libs section.



920

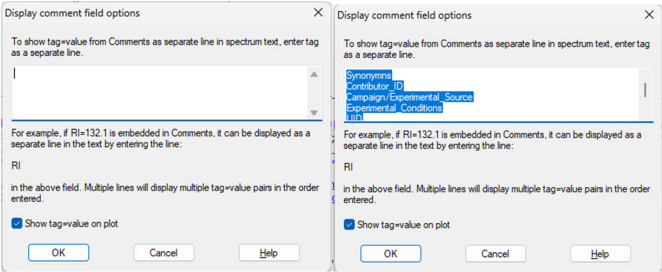
16. Click "OK".

17. Go to Options > Comment Field Display from the upper left menu.

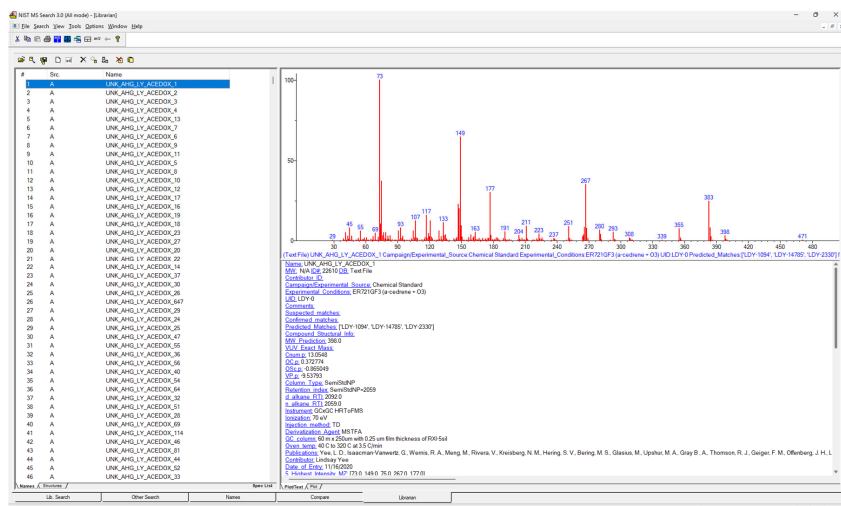


925 18. Copy and paste the following list of “tags” that are used in UCB-GLOBES MS annotations into the Display comment field options dialog.

930       Synonyms  
Contributor\_ID  
Campaign/Experimental\_Source  
Experimental\_Conditions  
935       UID  
Comments  
Suspected\_matches  
Confirmed\_matches  
Predicted\_Matches  
Compound\_Structural\_Info  
Formula  
MW\_Prediction  
940       VUV\_Exact\_Mass  
CAS#  
Ch3MS-RF\_Cnum.p  
Ch3MS-RF\_OC.p  
Ch3MS-RF\_OSc.p  
Ch3MS-RF\_VP.p  
945       Column\_Type  
Retention\_index  
d\_alkane\_RTI  
n\_alkane\_RTI  
Instrument  
950       Ionization  
Injection\_method  
Derivatization\_Agent  
GC\_column  
Oven\_temp  
955       Publications  
Contributor  
Date\_of\_Entry  
Num Peaks  
5\_Highest\_Intensity\_MZ  
960       Base\_Peak



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



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.

II. 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:

- Uploading or selecting mass spectra
- Plotting spectra for visual inspection
- Calculating cosine similarity
- 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

980

13

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 = '190qBF98NZE0UX7HnzcillyZCSVmfel_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=190qBF98NZE0UX7HnzcillyZCSVmfel\\_Z](https://drive.google.com/uc?id=190qBF98NZE0UX7HnzcillyZCSVmfel_Z)  
From (redirected): [https://drive.google.com/uc?id=190qBF98NZE0UX7HnzcillyZCSVmfel\\_Z&confirm=t&usid=65002136-Safd-4b52-9b37-f6173ffe9c7d](https://drive.google.com/uc?id=190qBF98NZE0UX7HnzcillyZCSVmfel_Z&confirm=t&usid=65002136-Safd-4b52-9b37-f6173ffe9c7d)  
To: C:\Users\Lindsay Yee\Documents\GitHub\UCB-GLOBES-HS-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.

|   | Index | Name                 | Synon | Campaign/Experimental_Source | Experimental_Conditions   | UID   | Contributor_ID | Comments | Suspected_matches | Confirmed_ma |
|---|-------|----------------------|-------|------------------------------|---------------------------|-------|----------------|----------|-------------------|--------------|
| 0 | 0     | UNK_AHG_LV_ACEDOX_1  | NaN   | Chemical Standard            | ER721GF3 (a-cedrene + O3) | LDY-0 | NaN            | NaN      | NaN               |              |
| 1 | 1     | UNK_AHG_LV_ACEDOX_2  | NaN   | Chemical Standard            | ER721GF3 (a-cedrene + O3) | LDY-1 | NaN            | NaN      | NaN               |              |
| 2 | 2     | UNK_AHG_LV_ACEDOX_3  | NaN   | Chemical Standard            | ER721GF3 (a-cedrene + O3) | LDY-2 | NaN            | NaN      | NaN               |              |
| 3 | 3     | UNK_AHG_LV_ACEDOX_4  | NaN   | Chemical Standard            | ER721GF3 (a-cedrene + O3) | LDY-3 | NaN            | NaN      | NaN               |              |
| 4 | 4     | UNK_AHG_LV_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.")
```

..... 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.

Filter by: Predicted\_MatchesValue: 21509

Filter DataClear Filter

Showing rows 1 to 10 of 11:

|      | 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      |       |

Next

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',
                       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”

Enter the spectrum identifiers (Name or UID)

Spectrum 1: LDV-21509

Spectrum 2: LDV-22110

Compare Spectra

Clear Output

1000     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)
```

1005

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.

Search: UNK\_AHG\_HZ\_SOAS\_394

Results: UNK\_AHG\_HZ\_SOAS\_394

Add →

← Remove

Selected: UNK\_AHG\_LY\_BFARNOX\_617  
UNK\_AHG\_LY\_APINOX\_582  
UNK\_AHG\_LY\_BCOPOX2\_18  
UNK\_AHG\_LY\_AHUMOX\_728  
1128\_1901\_blob\_1117  
UNK\_AHG\_HZ\_SOAS\_394

☐ Add in all filtered rows above

Threshold: 0.70

Note: Values ≥ threshold are shaded gray to highlight strong similarity.

Each cell shows: cosine similarity | ΔRI (absolute retention index difference)

Calculate Similarity

|                         | 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       |        |

### III. 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 ucgblobes2025\_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 ucgblobes2025\_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.

MS data:  
Number of Peaks  
 $m/z_1$  int<sub>1</sub> ;  $m/z_2$  int<sub>2</sub> ; ...

```
Name: UNK_AHG_HZ_SOAS_607 Cannot be blank; chemical name preferred if identified
Synonyms:
Formula:
ExactMass:
CAS#:
Derivatization_Agent: MSTFA N/A if not derivatized Assigned upon submission
Comments: Campaign/Experimental_Source="SOAS 2013" Experimental_Conditions="" UID="LDY-21722" approval to UCB-GLOBES
Contributor_ID="" Comments="" Suspected_matches="" Confirmed_matches="" Predicted_matches=""
Compound_Structural_Info="" MW_Prediction="312.0" VUV_Exact_Mass="" Ch3MS-RF Cnum.p="8.57483" Ch3MS-RF
OC.p="0.418617" Ch3MS-RF OSC.p="-0.819519" Ch3MS-RF VP.p="-8.08072" Column_Type="SemiStandardNonPolar"
Retention_Index="SemiStandardNonPolar=1975" d_alkane_RTI="2009.0" n_alkane_RTI="1975.0" Instrument="GCxGC
HRTofMS" Ionization="70 eV" Injection_method="TD" Derivatization_Agent="MSTFA" GC_column="60 m x 250um
with 0.25 um film thickness of RXI-5sil" Oven_temp="40 C to 320 C at 3.5 C/min" Publications="Zhang, H.,
Yee, L. D., Lee, B. H., Curtis, M. P. M. P., Worton, D. R., Isaacman-VanWertz, G., Offenberger, J. H.,
Lewandowski, M., Kleindienst, T. E. T. E., Beaver, M. R., Holder, A. L., Lonneman, W. A., Docherty, K. S.,
Jaoui, M., Pye, H. O. T., Hu, W., Day, D. A. D. A., Campuzano-Jost, P., Jimenez, J. L., Guo, H., Weber, R.
J., de Gouw, J., Koss, A. R., Edgerton, E. S., Brune, W., Mohr, C., Lopez-Hilfiker, F. D., Lutz, A.,
Kreissberg, N. M., Spielman, S. R., Hering, S. V., Wilson, K. R., Thornton, J. A. and Goldstein, A. H.:
Monoterpenes are the largest source of summertime organic aerosol in the southeastern United States, Proc.
Natl. Acad. Sci., 115(9), 2038 2043, doi:10.1073/pnas.1717513115, 2018." Contributor="Haofei Zhang"
Date_of_Entry="4/27/2021" S_Highest_Intensity_MZ="[129.0, 204.0, 191.0, 82.0, 41.0]"
Num_Peaks: 86.0
29 22.0 ; 30 1.0 ; 32 2.0 ; 33 7.0 ; 34 1.0 ; 37 2.0 ; 39 15.0 ; 40 3.0 ; 41 109.0 ; 42 18.0 ; 44 4.0 ; 46
10.0 ; 50 28.0 ; 54 11.0 ; 55 63.0 ; 56 14.0 ; 57 90.0 ; 62 12.0 ; 66 31.0 ; 67 37.0 ; 68 28.0 ; 70 12.0 ;
71 25.0 ; 78 7.0 ; 80 17.0 ; 81 37.0 ; 82 115.0 ; 83 66.0 ; 84 6.0 ; 85 38.0 ; 86 3.0 ; 87 5.0 ; 90 8.0 ; 91
18.0 ; 94 1.0 ; 96 48.0 ; 97 29.0 ; 98 24.0 ; 99 8.0 ; 110 15.0 ; 112 7.0 ; 113 5.0 ; 114 15.0 ; 115 14.0 ;
119 4.0 ; 126 5.0 ; 129 999.0 ; 130 46.0 ; 155 33.0 ; 178 2.0 ; 185 12.0 ; 189 20.0 ; 190 6.0 ; 191 142.0 ;
192 15.0 ; 204 483.0 ; 205 37.0 ; 206 15.0 ; 213 2.0 ; 217 7.0 ; 245 12.0 ; 289 1.0 ; 291 5.0 ; 297 11.0 ;
298 4.0 ; 306 1.0 ; 312 6.0 ; 339 1.0 ; 366 1.0 ; 367 1.0 ; 373 1.0 ; 384 1.0 ; 385 1.0 ; 419 1.0 ; 435
1.0 ; 452 1.0 ; 479 1.0 ; 496 1.0 ; 501 1.0 ; 551 1.0 ; 576 1.0 ; 577 1.0 ; 598 1.0 ; 624 1.0 ; 639 1.0 ;
666 1.0 ;

Name: UNK_AHG_HZ_SOAS_608
Synonyms:
Formula:
ExactMass:
CAS#:
Derivatization_Agent: MSTFA
Comments: Campaign/Experimental_Source="SOAS 2013" Experimental_Conditions="" UID="LDY-21723"
```

**IV. SI Tables**

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**Table S1: Matrix of cosine angle similarity values and differences in retention indices ( $\Delta$ RI) 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   $\Delta$ RI=0.0 | 0.988   $\Delta$ RI=3.0 | 0.995   $\Delta$ RI=3.0 | 0.977   $\Delta$ RI=7.0 | 0.983   $\Delta$ RI=3.0 | 0.993   $\Delta$ RI=3.0   | 0.986   $\Delta$ RI=2.0 | 0.994   $\Delta$ RI=1.0 | 0.984   $\Delta$ RI=3.0 | 0.974   $\Delta$ RI=2.0 | 0.995   $\Delta$ RI=7.0 | 0.993   $\Delta$ RI=6.0 |
| UNK_AHG_LY_AHU_MOX_728    | 0.988   $\Delta$ RI=3.0 | 1.000   $\Delta$ RI=0.0 | 0.985   $\Delta$ RI=0.0 | 0.996   $\Delta$ RI=4.0 | 0.999   $\Delta$ RI=0.0 | 0.972   $\Delta$ RI=0.0   | 1.000   $\Delta$ RI=1.0 | 0.996   $\Delta$ RI=2.0 | 0.999   $\Delta$ RI=0.0 | 0.996   $\Delta$ RI=1.0 | 0.980   $\Delta$ RI=4.0 | 0.995   $\Delta$ RI=3.0 |
| UNK_AHG_LY_COP_OX_944     | 0.995   $\Delta$ RI=3.0 | 0.985   $\Delta$ RI=0.0 | 1.000   $\Delta$ RI=0.0 | 0.971   $\Delta$ RI=4.0 | 0.979   $\Delta$ RI=0.0 | 0.997   $\Delta$ RI=0.0   | 0.983   $\Delta$ RI=1.0 | 0.991   $\Delta$ RI=2.0 | 0.981   $\Delta$ RI=0.0 | 0.969   $\Delta$ RI=1.0 | 0.998   $\Delta$ RI=4.0 | 0.994   $\Delta$ RI=3.0 |
| UNK_AHG_LY_MYR_COX_3      | 0.977   $\Delta$ RI=7.0 | 0.996   $\Delta$ RI=4.0 | 0.971   $\Delta$ RI=4.0 | 1.000   $\Delta$ RI=0.0 | 0.999   $\Delta$ RI=4.0 | 0.955   $\Delta$ RI=4.0   | 0.998   $\Delta$ RI=5.0 | 0.988   $\Delta$ RI=6.0 | 0.998   $\Delta$ RI=4.0 | 1.000   $\Delta$ RI=5.0 | 0.967   $\Delta$ RI=0.0 | 0.989   $\Delta$ RI=1.0 |
| UNK_AHG_LY_BCPO_X3_579    | 0.983   $\Delta$ RI=3.0 | 0.999   $\Delta$ RI=0.0 | 0.979   $\Delta$ RI=0.0 | 0.999   $\Delta$ RI=4.0 | 1.000   $\Delta$ RI=0.0 | 0.964   $\Delta$ RI=0.0   | 0.999   $\Delta$ RI=1.0 | 0.992   $\Delta$ RI=2.0 | 1.000   $\Delta$ RI=0.0 | 0.999   $\Delta$ RI=1.0 | 0.974   $\Delta$ RI=4.0 | 0.993   $\Delta$ RI=3.0 |
| UNK_AHG_LY_ARO_MOX2_124_2 | 0.993   $\Delta$ RI=3.0 | 0.972   $\Delta$ RI=0.0 | 0.997   $\Delta$ RI=0.0 | 0.955   $\Delta$ RI=4.0 | 0.964   $\Delta$ RI=0.0 | 1.000   $\Delta$ RI=0.0   | 0.969   $\Delta$ RI=1.0 | 0.983   $\Delta$ RI=2.0 | 0.967   $\Delta$ RI=0.0 | 0.952   $\Delta$ RI=1.0 | 0.997   $\Delta$ RI=4.0 | 0.986   $\Delta$ RI=3.0 |
| UNK_AHG_LY_BFAR_NOX_617   | 0.986   $\Delta$ RI=2.0 | 1.000   $\Delta$ RI=1.0 | 0.983   $\Delta$ RI=1.0 | 0.998   $\Delta$ RI=5.0 | 0.999   $\Delta$ RI=1.0 | 0.969   $\Delta$ RI=1.0   | 1.000   $\Delta$ RI=0.0 | 0.994   $\Delta$ RI=1.0 | 1.000   $\Delta$ RI=1.0 | 0.997   $\Delta$ RI=0.0 | 0.978   $\Delta$ RI=5.0 | 0.994   $\Delta$ RI=4.0 |
| UNK_AHG_HZ_SOAS_394       | 0.994   $\Delta$ RI=1.0 | 0.996   $\Delta$ RI=2.0 | 0.991   $\Delta$ RI=2.0 | 0.988   $\Delta$ RI=6.0 | 0.992   $\Delta$ RI=2.0 | 0.983   $\Delta$ RI=2.0   | 0.994   $\Delta$ RI=1.0 | 1.000   $\Delta$ RI=0.0 | 0.994   $\Delta$ RI=2.0 | 0.987   $\Delta$ RI=1.0 | 0.987   $\Delta$ RI=6.0 | 0.995   $\Delta$ RI=5.0 |
| UNK_AHG_LY_AHU_MOX2_627   | 0.984   $\Delta$ RI=3.0 | 0.999   $\Delta$ RI=0.0 | 0.981   $\Delta$ RI=0.0 | 0.998   $\Delta$ RI=4.0 | 1.000   $\Delta$ RI=0.0 | 0.967   $\Delta$ RI=0.0   | 1.000   $\Delta$ RI=1.0 | 0.994   $\Delta$ RI=2.0 | 1.000   $\Delta$ RI=0.0 | 0.998   $\Delta$ RI=1.0 | 0.976   $\Delta$ RI=4.0 | 0.994   $\Delta$ RI=3.0 |
| UNK_AHG_LY_BCOP_OX2_18    | 0.974   $\Delta$ RI=2.0 | 0.996   $\Delta$ RI=1.0 | 0.969   $\Delta$ RI=1.0 | 1.000   $\Delta$ RI=5.0 | 0.999   $\Delta$ RI=1.0 | 0.952   $\Delta$ RI=1.0   | 0.997   $\Delta$ RI=0.0 | 0.987   $\Delta$ RI=1.0 | 0.998   $\Delta$ RI=1.0 | 1.000   $\Delta$ RI=0.0 | 0.963   $\Delta$ RI=5.0 | 0.987   $\Delta$ RI=4.0 |
| UNK_AHG_LY_APIN_OX2_586   | 0.995   $\Delta$ RI=7.0 | 0.980   $\Delta$ RI=4.0 | 0.998   $\Delta$ RI=4.0 | 0.967   $\Delta$ RI=0.0 | 0.974   $\Delta$ RI=4.0 | 0.997   $\Delta$ RI=4.0   | 0.978   $\Delta$ RI=5.0 | 0.987   $\Delta$ RI=6.0 | 0.976   $\Delta$ RI=4.0 | 0.963   $\Delta$ RI=5.0 | 1.000   $\Delta$ RI=0.0 | 0.992   $\Delta$ RI=1.0 |
| UNK_AHG_LY_APIN_OX_582    | 0.993   $\Delta$ RI=6.0 | 0.995   $\Delta$ RI=3.0 | 0.994   $\Delta$ RI=3.0 | 0.989   $\Delta$ RI=1.0 | 0.993   $\Delta$ RI=3.0 | 0.986   $\Delta$ RI=3.0   | 0.994   $\Delta$ RI=4.0 | 0.995   $\Delta$ RI=5.0 | 0.994   $\Delta$ RI=3.0 | 0.987   $\Delta$ RI=4.0 | 0.992   $\Delta$ RI=1.0 | 1.000   $\Delta$ RI=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<br>0 = no<br>1 = yes | MS Confirmed<br>0 = no<br>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 <sup>f</sup>   | 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    | Tricarballic acid                       | MT    | MS                  | LDY-21130      | Tricarballic 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<br>0 = no<br>1 = yes | MS Confirmed<br>0 = no<br>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 <sup>a</sup> | 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<br>0 = no<br>1 = yes | MS Confirmed<br>0 = no<br>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 <sup>h</sup>        | 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<br>Determined<br>By | UCB-<br>GLOBES<br>UID | Compound Name Reanalysis       | Group<br>Reanalysis | Group<br>Determined<br>By<br>Reanalysis | Group<br>Category<br>Changed<br>0 = no<br>1 = yes | MS<br>Confirmed<br>0 = no<br>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 <sup>h</sup> | 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<br>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<br>Expt/Field<br>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<br>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<br>Expt                          | 0                                                 | 1                                    |
| 90    | tartaric acid 3 <sup>h</sup> | BOOA    | MS                        | LDY-21205             | tartaric acid 3, 4 TMS         | BOOA                | 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<br>0 = no<br>1 = yes | MS Confirmed<br>0 = no<br>1 = yes |
|-------|-----------------------------------------|-------|---------------------|----------------|---------------------------------|------------------|--------------------------------|---------------------------------------------|-----------------------------------|
| 91    | C9H14O3                                 | MT    | Lab Expt/R2         | LDY-21206      | UNK_AHG_HZ_SOAS_91              | MT               | Lab Expt/R2                    | 0                                           | 0                                 |
| 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 <sup>d</sup> | 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 <sup>h</sup>            | 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                                 |

| index | Compound Name   | Group       | Group<br>Determined<br>By | UCB-<br>GLOBES<br>UID | Compound Name Reanalysis | Group<br>Reanalysis | Group<br>Determined<br>By<br>Reanalysis | Group<br>Category<br>Changed<br>0 = no<br>1 = yes | MS<br>Confirmed<br>0 = no<br>1 = yes |
|-------|-----------------|-------------|---------------------------|-----------------------|--------------------------|---------------------|-----------------------------------------|---------------------------------------------------|--------------------------------------|
| 113   | C5alkenetriol 2 | ISOP        | MS                        | LDY-21228             | C5alkenetriol 2, 3 TMS   | ISOP                | MS                                      | 0                                                 | 0                                    |
| 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<br>Expt/Field<br>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<br>Expt/Field<br>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<br>Expt/Field<br>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          | Unknow<br>n |                           | LDY-21247             | Terephthalic acid, 2 TMS | BBOA/MT             | MS/NIST20/<br>Lab<br>Expt/Field<br>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<br>Expt/Field<br>Expt            | 1                                                 | 1                                    |

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|-------|----------------------|---------|---------------------|----------------|-----------------------------------------------------------|------------------|--------------------------------|---------------------------------------------|-----------------------------------|
| 139   | C6H8O4               | MTR2    | MS                  | LDY-21254      | UNK_AHG_HZ_SOAS_139                                       | MTR2             | MS                             | 0                                           | 0                                 |
| 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                                 |

| index | Compound Name     | Group   | Group<br>Determined<br>By | UCB-<br>GLOBES<br>UID | Compound Name Reanalysis | Group<br>Reanalysis | Group<br>Determined<br>By<br>Reanalysis | Group<br>Category<br>Changed<br>0 = no<br>1 = yes | MS<br>Confirmed<br>0 = no<br>1 = yes |
|-------|-------------------|---------|---------------------------|-----------------------|--------------------------|---------------------|-----------------------------------------|---------------------------------------------------|--------------------------------------|
| 165   | Threonic acid     | ASOA    | NIST                      | LDY-21280             | Threonic acid, 4 TMS     | ASOA                | NIST                                    | 0                                                 | 0                                    |
| 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<br>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<br>/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<br>Expt          | LDY-21304             | Diethyl Phthalate        | BBOA                | NIST/Lab<br>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<br>Expt                          | 0                                                 | 1                                    |

| index | Compound Name        | Group   | Group Determined By | UCB-GLOBES UID | Compound Name Reanalysis                     | Group Reanalysis | Group Determined By Reanalysis | Group Category Changed<br>0 = no<br>1 = yes | MS Confirmed<br>0 = no<br>1 = yes |
|-------|----------------------|---------|---------------------|----------------|----------------------------------------------|------------------|--------------------------------|---------------------------------------------|-----------------------------------|
| 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                                 |
| 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                                 |

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|-------|-------------------------------------|---------|---------------------|----------------|-------------------------------------|------------------|--------------------------------|---------------------------------------------|-----------------------------------|
| 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                                 |
| 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                                 |

| index | Compound Name       | Group   | Group Determined By | UCB-GLOBES UID | Compound Name Reanalysis | Group Reanalysis | Group Determined By Reanalysis | Group Category Changed<br>0 = no<br>1 = yes | MS Confirmed<br>0 = no<br>1 = yes |
|-------|---------------------|---------|---------------------|----------------|--------------------------|------------------|--------------------------------|---------------------------------------------|-----------------------------------|
| 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                                 |
| 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                                 |

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|-------|---------------------------------|---------|---------------------|----------------|---------------------------------|------------------|--------------------------------|---------------------------------------------|-----------------------------------|
| 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                                 |
| 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                                 |

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|-------|---------------|---------|---------------------|----------------|--------------------------|------------------|--------------------------------|---------------------------------------------|-----------------------------------|
| 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                                 |
| 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                                 |

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|-------|---------------|---------|---------------------------|-----------------------|--------------------------|---------------------|-----------------------------------------|---------------------------------------------------|--------------------------------------|
| 342   |               | POAOX   | R2                        | LDY-21457             | UNK_AHG_HZ_SOAS_342      | POAOX               | MS/Field<br>Expt/NIST2<br>0             | 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<br>Expt/Field<br>Expt            | 1                                                 | 1                                    |
| 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<br>Expt/Field<br>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/S<br>QT     | MS/Lab<br>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                                    |

| index | Compound Name                     | Group       | Group<br>Determined<br>By | UCB-<br>GLOBES<br>UID | Compound Name Reanalysis                 | Group<br>Reanalysis | Group<br>Determined<br>By<br>Reanalysis | Group<br>Category<br>Changed<br>0 = no<br>1 = yes | MS<br>Confirmed<br>0 = no<br>1 = yes |
|-------|-----------------------------------|-------------|---------------------------|-----------------------|------------------------------------------|---------------------|-----------------------------------------|---------------------------------------------------|--------------------------------------|
| 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                                    |
| 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                                    |

| index | Compound Name        | Group | Group<br>Determined<br>By | UCB-<br>GLOBES<br>UID | Compound Name Reanalysis     | Group<br>Reanalysis | Group<br>Determined<br>By<br>Reanalysis | Group<br>Category<br>Changed<br>0 = no<br>1 = yes | MS<br>Confirmed<br>0 = no<br>1 = yes |
|-------|----------------------|-------|---------------------------|-----------------------|------------------------------|---------------------|-----------------------------------------|---------------------------------------------------|--------------------------------------|
| 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<br>Expt                        | 1                                                 | 1                                    |
| 408   |                      | MTR2  | R2                        | LDY-21523             | UNK_AHG_HZ_SOAS_408          | MTR2                | R2                                      | 0                                                 | 0                                    |
| 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<br>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<br>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<br>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<br>Expt/Field<br>Expt            | 0                                                 | 1                                    |
| 431   |                      | MTR2  | R2                        | LDY-21546             | UNK_AHG_HZ_SOAS_431          | MTR2                | R2                                      | 0                                                 | 0                                    |

| index | Compound Name     | Group   | Group<br>Determined<br>By | UCB-<br>GLOBES<br>UID | Compound Name Reanalysis | Group<br>Reanalysis | Group<br>Determined<br>By<br>Reanalysis | Group<br>Category<br>Changed<br>0 = no<br>1 = yes | MS<br>Confirmed<br>0 = no<br>1 = yes |
|-------|-------------------|---------|---------------------------|-----------------------|--------------------------|---------------------|-----------------------------------------|---------------------------------------------------|--------------------------------------|
| 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                                    |
| 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<br>Expt/Field<br>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<br>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<br>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                                    |

| index | Compound Name  | Group   | Group<br>Determined<br>By | UCB-<br>GLOBES<br>UID | Compound Name Reanalysis | Group<br>Reanalysis | Group<br>Determined<br>By<br>Reanalysis | Group<br>Category<br>Changed<br>0 = no<br>1 = yes | MS<br>Confirmed<br>0 = no<br>1 = yes |
|-------|----------------|---------|---------------------------|-----------------------|--------------------------|---------------------|-----------------------------------------|---------------------------------------------------|--------------------------------------|
| 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                                    |
| 473   | C5H6O4         | MTR2    | R2                        | LDY-21255             | UNK_AHG_HZ_SOAS_140      | MT                  | MS/Lab<br>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                                    |

| index | Compound Name | Group   | Group<br>Determined<br>By | UCB-<br>GLOBES<br>UID | Compound Name Reanalysis | Group<br>Reanalysis | Group<br>Determined<br>By<br>Reanalysis | Group<br>Category<br>Changed<br>0 = no<br>1 = yes | MS<br>Confirmed<br>0 = no<br>1 = yes |
|-------|---------------|---------|---------------------------|-----------------------|--------------------------|---------------------|-----------------------------------------|---------------------------------------------------|--------------------------------------|
| 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                                    |
| 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<br>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<br>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/SQ<br>T        | MS/Lab<br>Expt/Field<br>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<br>Expt/Field<br>Expt            | 1                                                 | 1                                    |
| 526   |               | BOOA    | MS                        | LDY-21641             | UNK_AHG_HZ_SOAS_526      | BOOA                | 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<br>0 = no<br>1 = yes | MS Confirmed<br>0 = no<br>1 = yes |
|-------|----------------------------------|---------|---------------------|----------------|----------------------------------|------------------|--------------------------------|---------------------------------------------|-----------------------------------|
| 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                                 |
| 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                                 |

| index | Compound Name               | Group | Group<br>Determined<br>By | UCB-<br>GLOBES<br>UID | Compound Name Reanalysis        | Group<br>Reanalysis | Group<br>Determined<br>By<br>Reanalysis | Group<br>Category<br>Changed<br>0 = no<br>1 = yes | MS<br>Confirmed<br>0 = no<br>1 = yes |
|-------|-----------------------------|-------|---------------------------|-----------------------|---------------------------------|---------------------|-----------------------------------------|---------------------------------------------------|--------------------------------------|
| 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<br>Expt/NIST2<br>0             | 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                                    |
| 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<br>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<br>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<br>Expt                        | 1                                                 | 1                                    |
| 582   |                             | ASOA  | R2                        | LDY-21697             | UNK_AHG_HZ_SOAS_582             | BBOA                | MS/Lab<br>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                                    |

| index | Compound Name | Group       | Group Determined By | UCB-GLOBES UID | Compound Name Reanalysis                                | Group Reanalysis | Group Determined By Reanalysis | Group Category Changed<br>0 = no<br>1 = yes | MS Confirmed<br>0 = no<br>1 = yes |
|-------|---------------|-------------|---------------------|----------------|---------------------------------------------------------|------------------|--------------------------------|---------------------------------------------|-----------------------------------|
| 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                                 |
| 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                                 |

| index | Compound Name       | Group   | Group Determined By | UCB-GLOBES UID | Compound Name Reanalysis | Group Reanalysis | Group Determined By Reanalysis      | Group Category Changed<br>0 = no<br>1 = yes | MS Confirmed<br>0 = no<br>1 = yes |
|-------|---------------------|---------|---------------------|----------------|--------------------------|------------------|-------------------------------------|---------------------------------------------|-----------------------------------|
| 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                                 |
| 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                                 |

| index | Compound Name            | Group       | Group<br>Determined<br>By | UCB-<br>GLOBES<br>UID | Compound Name Reanalysis             | Group<br>Reanalysis | Group<br>Determined<br>By<br>Reanalysis | Group<br>Category<br>Changed<br>0 = no<br>1 = yes | MS<br>Confirmed<br>0 = no<br>1 = yes |
|-------|--------------------------|-------------|---------------------------|-----------------------|--------------------------------------|---------------------|-----------------------------------------|---------------------------------------------------|--------------------------------------|
| 639   |                          | MTR2        | R2                        | LDY-21754             | UNK_AHG_HZ_SOAS_639                  | MT                  | MS/Lab<br>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<br>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                                    |
| 648   |                          | Unknown     |                           | LDY-21763             | UNK_AHG_HZ_SOAS_648                  | Unknown             |                                         | 0                                                 | 0                                    |
| 649   |                          | Unknown     |                           | LDY-21764             | UNK_AHG_HZ_SOAS_649                  | Unknown             |                                         | 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                                    |
| 653   |                          | ISOP        | R2                        | LDY-21768             | UNK_AHG_HZ_SOAS_653                  | ISOP                | MS/Lab<br>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<br>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<br>Expt                          | 1                                                 | 1                                    |
| 662   |                          | Unknown     |                           | LDY-21777             | UNK_AHG_HZ_SOAS_662                  | Unknown             |                                         | 0                                                 | 0                                    |
| 663   | d12-nalkane              | IStd        | MS                        | LDY-21778             | d12-nalkane                          | IStd                | MS                                      | 0                                                 | 0                                    |

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|-------|------------------------------|-------------|---------------------|----------------|------------------------------|------------------|--------------------------------|---------------------------------------------|-----------------------------------|
| 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                                 |
| 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                                 |

| index | Compound Name | Group       | Group Determined By | UCB-GLOBES UID | Compound Name Reanalysis | Group Reanalysis | Group Determined By Reanalysis | Group Category Changed<br>0 = no<br>1 = yes | MS Confirmed<br>0 = no<br>1 = yes |
|-------|---------------|-------------|---------------------|----------------|--------------------------|------------------|--------------------------------|---------------------------------------------|-----------------------------------|
| 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                                 |
| 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                                 |

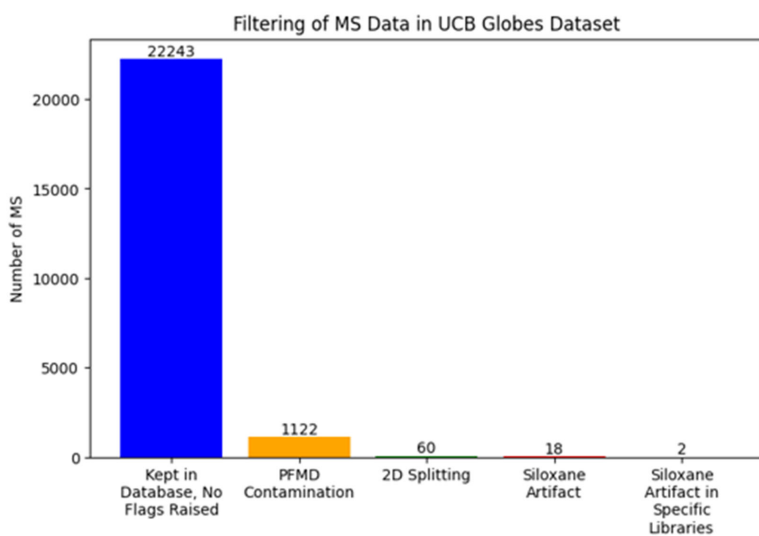
| index | Compound Name                  | Group   | Group Determined By | UCB-GLOBES UID | Compound Name Reanalysis       | Group Reanalysis | Group Determined By Reanalysis | Group Category Changed<br>0 = no<br>1 = yes | MS Confirmed<br>0 = no<br>1 = yes |
|-------|--------------------------------|---------|---------------------|----------------|--------------------------------|------------------|--------------------------------|---------------------------------------------|-----------------------------------|
| 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                                 |
| 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                                 |

| index | Compound Name       | Group   | Group Determined By | UCB-GLOBES UID | Compound Name Reanalysis | Group Reanalysis | Group Determined By Reanalysis | Group Category Changed<br>0 = no<br>1 = yes | MS Confirmed<br>0 = no<br>1 = yes |
|-------|---------------------|---------|---------------------|----------------|--------------------------|------------------|--------------------------------|---------------------------------------------|-----------------------------------|
| 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                                 |
| 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                                 |

| index | Compound Name       | Group       | Group Determined By | UCB-GLOBES UID | Compound Name Reanalysis          | Group Reanalysis | Group Determined By Reanalysis | Group Category Changed<br>0 = no<br>1 = yes | MS Confirmed<br>0 = no<br>1 = yes |
|-------|---------------------|-------------|---------------------|----------------|-----------------------------------|------------------|--------------------------------|---------------------------------------------|-----------------------------------|
| 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                                 |
| 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                                 |

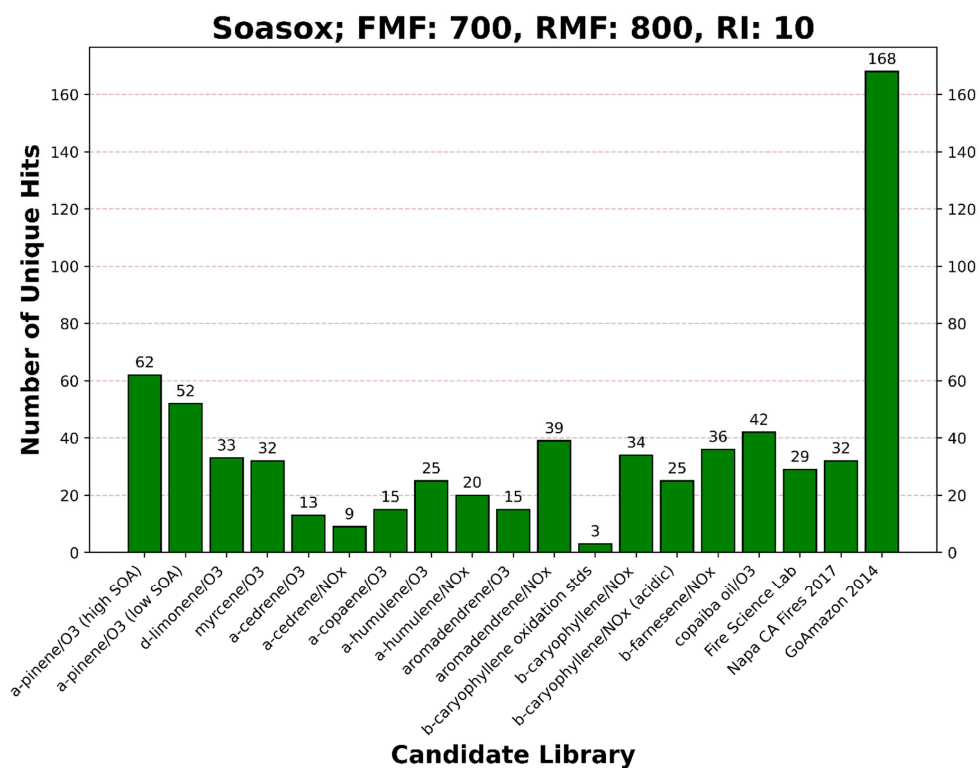
| index | Compound Name                  | Group | Group<br>Determined<br>By | UCB-<br>GLOBES<br>UID | Compound Name Reanalysis              | Group<br>Reanalysis | Group<br>Determined<br>By<br>Reanalysis | Group<br>Category<br>Changed<br>0 = no<br>1 = yes | MS<br>Confirmed<br>0 = no<br>1 = yes |
|-------|--------------------------------|-------|---------------------------|-----------------------|---------------------------------------|---------------------|-----------------------------------------|---------------------------------------------------|--------------------------------------|
| 805   | methyl nitrocatechol<br>isomer | BBOA  | Lab Expt/R2               | LDY-21920             | methyl nitrocatechol isomer, 2<br>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<br>Expt/Field<br>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                                    |
| 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                                    |





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**Figure S2:** UCB-GLOBES mass spectra were screened for MS contamination from perfluoromethyldecalin (PFMD) calibrant, improper 2<sup>nd</sup> 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.



1045 **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)  $\geq 700$ , reverse match factor (RMF)  $\geq 800$ , and retention index (RI) difference  $\leq 10$  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.**

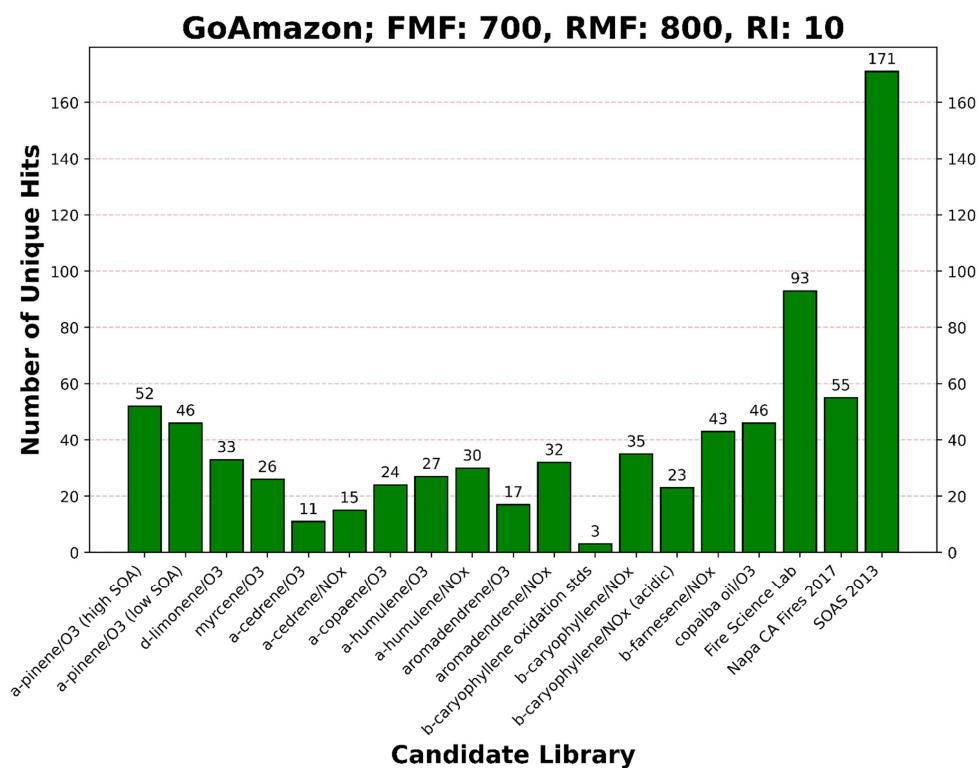


Figure S4: Number of unique MS hits for GoAmazon MS data by each UCB-GLOBES candidate library dataset. To be considered a hit, forward match factor (FMF)  $\geq 700$ , reverse match factor (RMF)  $\geq 800$ , and retention index (RI) difference  $\leq 10$  between query MS and hit MS. While a GoAmazon 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.

## SI References

NIST Mass Spectrometry Data Center: NIST 23 MS Database and MS Search Program v.3.0, 2023.

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