ENVIRONMENTAL CHEMICAL BURDEN IN DIFFERENTIATED THYROID CANCER: SUPPLEMENTARY MATERIAL

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EXPANDED METHODS

High-Resolution Exposomics

Prior to processing samples, several individual reference standards were prepared by spiking pure chemical standards into pooled reference plasma to achieve a common concentration of 0.47 ng/mL. A majority of all chemical standards were purchased from AccuStandard (New Haven, CT, USA), Restek (Bellefonte, PA, USA), MilliporeSigma (Burlington, MA, USA), Santa Cruz Biotechnology (Dallas, TX, USA), Wellington Laboratories (Guelph, ON, Canada), Cambridge Isotope Laboratories (Tewksbury, MA, USA). Plasma reference standards and tissue samples were processed using a modified version of the express liquid extraction (XLE) method.[1] The XLE is optimized for biofluids; however, it was necessary to modify it to ensure analytical consistency across plasma standards and tumor tissue samples, as detailed below.

First, approximately 50 mg of tumor or non-tumor cadaver thyroid tissue was cut and placed into a glass vial (13 $\times$ 100 mm), and exact tissue weights were recorded (mean $\pm$ SD = 52.7 $\pm$ 11.3 mg for tumor tissue, 43.1 $\pm$ 4.5 mg for non-cancer cadaver thyroid tissue). Next, 200 μL of each pooled reference plasma standard (an in-house standard referred to as QStd; see Go et al.[2] for a full description of a previous iteration of this standard) was transferred to glass vials (13 $\times$ 100 mm). For tissues, 500 μL of an extraction buffer comprised of acetone and petroleum ether (1:1 v/v) (MilliporeSigma, Catalog #184519) with 2% internal standard mix, was added to the glass vials containing tissues. For plasma, 200 μL of extraction buffer containing 2% internal standard mix was added to the glass vials containing the pooled reference plasma. 50 μL of formic acid (Emprove® Essential DAC, 98-100% pure, MilliporeSigma, Catalog #1002631000) was then added to tissue and plasma standard vials. To the tissue vials, 20 mg of NaCl was added, and 45 $\pm$ 5 mg of $MgSO_4$ ($\geq$99.99% trace metals basis, Sigma-Aldrich, Catalog #203726) was added to tissue and plasma standard vials.

Tissue samples were then homogenized in this solution using a tissue-tearor, followed by water bath sonication for 30 minutes at room temperature. Plasma samples were shaken vigorously on ice using a multitube vortexer (VWR VX-2500) for 60 min. Following this, both tissue and plasma homogenates were centrifuged at 3000 rpm $\times$ 4 °C $\times$ 10 min. Supernatants were then transferred to new glass vials (13 $\times$ 100 mm) and dried using a vacuum centrifuge for 60 min at 35 °C. Finally, dried samples were reconstituted in 50 μL of isooctane. Reconstituted samples were transferred to autosampler vials with 150 μL vial inserts for analysis. Samples were prepared in batches containing 20 samples along with standard reference material (SRM) samples (NIST 1957, 1958, and several in-house SRMs discussed above). In addition, pooled reference plasma samples, a retention-time batch comparison standard, a method solvent blank that underwent solvent extraction, and a solvent blank were prepared in tandem as part of quality control measures. It should be noted that tumor tissues and non-cancer cadaver thyroid tissues were analyzed at different timepoints and in separate batches, although the same method was used for each tissue. As a result, direct comparison of raw spectral intensities between non-cancer thyroids and tumors was limited; however, quantitative estimates of chemical concentrations in tissues (see the section 'Quantitative Estimates of Chemical Concentrations in Tissues' below) did enable some degree of direct comparison, though these comparisons should be interpreted conservatively and cautiously given the high potential for batch effects.

Following preparation, samples were analyzed in duplicate with a Q Exactive GC hybrid quadrupole Orbitrap mass spectrometer (ThermoScientific), allowing for 25 minutes of data collection on retention times and spectral intensities from m/z 85-850 collected at 60k resolution. Samples were injected at 2 μL and subjected to a capillary DB-5MS column (15 m $\times$ 0.25 mm $\times$ 0.25 μm film thickness) with a gradient as follows: 75 °C for 1 min then 25 °C/min to 180 °C, 6 °C/min to 250 °C, 20 °C/min to 300 °C, with a final 5 min hold. Helium gas flow rate was 1 mL/min. Positive electron ionization was set at 70 eV, the ion source was set at 250 °C, and the transfer line was set at 280 °C.

Data Extraction, Feature Annotation, and Signal Identification

Raw data were extracted on a sample-by-sample basis using MZmine2.[3] Data were interpreted and combined using an in-house algorithm for feature annotation and the identification and quantification of chemicals in GC-MS exposomics data. Briefly, the algorithm utilizes a large library of environmental chemicals (EC) with known concentrations in standards, each of which has been manually quantified to ascertain retention times within the context of the laboratory procedure. In total, 738 unique standards are in the library; however, 28 of these represent chemicals that can be considered largely endogenous and not ECs. The remaining standards can be considered entirely exogenous (700) or both endogenous and exogenous (10) chemicals, resulting in a total of 710 ECs in the library, which can be screened by parallel analysis of standards with samples. This library is compared against sample data to find the best matching signal for ECs if any appropriate candidates exist. Shifts in elution time due to column degradation and the presence of co-occurring isomers pose significant challenges for standard annotation procedures; however, the algorithm addresses this issue by employing time-warping techniques, along with corrective algorithms that mimic manual chemical identification procedures, to overcome these challenges. Chemical identification and accuracy are achieved by leveraging the co-elution and correlation of chemical fragments generated from the same chemical. Standards are run in tandem with samples, which allows not only for the identification and relative quantification of all chemicals in the library of standards but also for the absolute quantification of identified metabolites using the comparative intensity of peak areas. The algorithm specifically assigns "quality fractions" based on the simultaneous detection of multiple fragments of the same chemical. Following the application of the algorithm for annotation, the quality fraction was used to label features as "annotations" (quality fraction of 0) while the remaining signals were labeled "identifications." It is important to note that identification versus annotation status was determined solely in reference to tumor samples and not non-cancer cadaver thyroid samples. Thus, when annotations or identifications are denoted in any figures or tables, these refer to the determination made in the data from thyroid tumors rather than non-cancer cadaver samples. Information on annotation versus identification status in non-cancer cadaver samples can be found in the "primary_data.xlsx" spreadsheet located in the GitHub repository (see below for further details). The algorithm will be published as a Python or R package in the coming 1-2 years. For further details on the algorithm, readers are welcome to contact the corresponding author.

Preprocessing of Exposomics Data

A targeted exposomics feature table (see the associated GitHub repository) was derived from the feature annotation and signal identification process described above. The proportion of missing values (PMV) was then calculated for each feature (total number of missing values/60 total samples). Next, features with PMV $>$ 30% missing values were separated for analysis in "qualitative" mode. The individual spectral intensity values for qualitative features were converted to "1", representing detection, whereas missing values were converted to "0", representing non-detection. Any qualitative features with 100% "0" values (indicating detection in reference standards but complete non-detection in samples) were eliminated and not considered for further analysis. Alternatively, the remaining features with PMV $\leq$ 30% were separated for analysis in "quantitative" mode. The missing values for quantitative features were imputed using the half minimum method (study-wide).[4] Following imputation, all spectral intensity values for quantitative features were $\log_2$-transformed before further analysis. Finally, to determine the total number of unique chemicals annotated per sample, features were consolidated and grouped by their respective Chemical Abstracts Service registry numbers (CAS number), regardless of analytical mode (qualitative versus quantitative), such that the detection of at least one fragment for a given CAS number was considered as detection of that unique chemical. This list of chemicals was then compiled, and chemicals that were mainly endogenous (i.e., carnitines, cholesterol, arachidonic acid metabolites, bile acids, hormones, and hormone precursors) were removed and not considered for exposomics analysis (23 total). Chemicals that had both exogenous and endogenous dispositions (7 total) were retained for exposomics analysis. The number of unique chemicals annotated was then tallied for each sample. The median number of chemicals annotated per variant (prior to imputation) was compared using the Kruskal-Wallis test.

Metadata Annotation of Environmental Chemicals

The name, IUPAC name, CAS number, PubChem Compound Identification (CID), SMILES, InChIKey, InChI, Toxin and Toxin-Target Database[5] ID (when applicable), monoisotopic mass, and formula were obtained for each chemical annotated in at least one sample. For the purposes of data visualization and simplified naming in the manuscript text, a short name or abbreviation was assigned to a large portion of chemicals. The Toxin-Toxin-Targeted Database[5] (T3DB) ID and the International Agency for Research on Cancer (IARC) carcinogen group[6] were assigned to chemicals when applicable and possible (when this information could not be ascertained, the T3DB ID was listed as "NA" and the IARC Group was listed as "Not Classified"). Classification as either a potential endocrine-disrupting chemical (EDC) or non-EDC was assigned to each chemical, per the PARCEDC list.[7] Inclusion on the list resulted in chemicals being marked as potential EDCs; non-inclusion resulted in classification as a non-EDC. The single most common use or best-fit chemical class was identified for each chemical. To facilitate data visualization, broader categories were also assigned to each chemical. For example, if a chemical's common-use class was "Insecticide/Pesticide (Pyrethroid)", this was simplified to "Insecticide/Pesticide" for data display. In the broader categories, metabolites or degradation products of certain chemicals were simply considered as members of the class to which their precursor belonged. For example, aldicarb sulfone, a breakdown product of the carbamate pesticide aldicarb, was classified as an insecticide/pesticide. However, the inclusion of breakdown products is indicated in figures and tables where applicable. ClassyFire[8] was used to designate superclasses, classes, subclasses, direct parents, and molecular frameworks. All chemical metadata are available below in Supplementary Table 1.

Core Statistical Analysis and Data Visualization

All data were compiled and structured using Microsoft Excel (Mac v16.96, Microsoft Corporation, 2025). All code was written and executed using R (v4.3.1)[9] in Visual Studio Code (v1.82.2, Microsoft Corporation, 2025). Source code can be found on the GitHub repository (source_code.R; see below for details). Data visualization was performed using the R package, ggplot2.[10]

Online Code and Data Repository

All source code is available in the accompanying GitHub repository, accessible at the following URL: https://github.com/jdpreston30/thyroid-exposomics-2025.

Manual Validation of Annotations for Select Chemicals

Following initial feature annotation, all putative chemical annotations underwent manual validation to ensure analytical quality. Combined validation plots displaying chromatographic traces for standards and samples were generated and inspected visually. Each chemical was assigned a identification quality score based on systematic criteria. Level 1 identification quality was defined as co-elution of two or more fragments in both standard and sample within a reasonable retention time window. Close co-elution that could be explained by matrix effects was accepted; however, fragments with extreme temporal dispersion were not considered level 1. In select cases where the quantitative fragment (i.e., the fragment which showed statistical differences beetween variants, designated with an asterisk) could not be detected in the standard but was present in the sample, and other fragments co-eluted between standard and sample, level 1 quality was still assigned. Single fragment identifications, even with apparent co-elution in standard and sample, were considered failures and were not considered as level 1 or level 2 identifications. Level 2 identification quality was assigned when co-elution of 2 or more fragments could be detected in the sample but not in the standard, or when standard fragments showed extreme retention time shifts relative to sample fragments. The quantitative fragment used for statistical analysis was evaluated with particular scrutiny: even if it represented a smaller peak among co-eluting fragments, it was required to follow the same general chromatographic trajectory as other fragments from the same chemical. If the quantitative fragment could reasonably be considered noise rather than signal, the identification was designated as a failure. Collectively, this validation process ensured that only high-confidence chemical identifications with appropriate analytical support were retained for downstream statistical analysis and biological interpretation. This process was repeated both for all 63 chemicals that showed statistical differences between variants and for an additional 11 chemicals

which were classified as IARC group 1 (excluding polychlorinated biphenyls, which were difficult to evaluate due to the presence of multiple congeners). IARC group 1 validations were performed for both tumor and non-cancer cadaver thyroids.

Exposome-Wide Association Study

Electron ionization generates multiple fragments for each chemical prior to detection; thus, in many cases, multiple fragments were annotated for the same chemical. In keeping with our exploratory and descriptive approach and to maximize coverage, we treated each fragment as an individual observation during statistical analysis. For qualitative features, Fisher's exact test for count data was employed on the binary exposomics data to determine if any chemical was overrepresented in its detection within any specific variant. Corresponding detection fractions were calculated for each variant (sum of samples with detection of chemical/20 samples per variant). For quantitative features, one-way ANOVA was used to assess differences in mean spectral intensities across variants, with corresponding p-values calculated for each chemical. Post-hoc testing was performed using Tukey's HSD test, which included correction for multiple comparisons. Given the pilot design and exploratory nature of this study, no false discovery rate corrections were applied beyond those used in post-hoc testing. Mean spectral intensities were scaled by converting them to z-scores within each chemical. Chemicals with a $p < 0.05$ from either test were considered significant and were compiled, tabulated, and further classified as described below. Four chemicals had multiple fragments showing significant differences between variants. In these cases, the quantitative fragment was selected if available; otherwise, the fragment with the highest frequency of detection across all samples, irrespective of variant, was selected. Following initial statistical analysis, manual validation of these chemicals (63 total) was performed as described above. Only chemicals that passed manual validation were retained for further analysis (30 total). The top 5 validated quantitative features were visualized via box and whisker plots (of z-scored spectral intensities), and the validated qualitative features via a heatmap (of detection fraction/percent). A balloon plot was constructed based on these results, wherein significant ECs were grouped by usage classes and variants, being counted once each time it was highest, whether by qualitative or quantitative measures in a variant. In cases where the detection percentages were equally high in two variants, a count was assigned to each variant.

Advanced Carcinogenicity Classification of Select Chemicals

To identify any potential carcinogens that have not been evaluated by the IARC, additional research was performed on the chemicals that showed significant differences in presence or concentration between variants (63 in total). To accomplish this, the Global Harmonized System of Classification and Labelling of Chemicals (GHS) statements were screened for any listed H350 ("may cause cancer"), H350i ("may cause cancer by inhalation"), or H351 ("suspected of causing cancer") status (and the corresponding consensus/confidence percentages of data sources as listed on PubChem in section 12.1.1, "GHS Classification"). Systematic logic that considered both the IARC grouping and the GHS carcinogen statement was then applied to categorize chemicals into the groups "Known Carcinogen", "Likely Carcinogen", "Possible Carcinogen", or "Uncertain Risk" (for the function accomplishing this, see the blocks of code under "#+ Carcinogen classification based on GHS and IARC (3E)" in the source_code.R file available in the GitHub repository). Chemicals with no IARC group and GHS statement were not classified. Briefly, the following rules were applied for classification:

- IARC group 1 chemicals were automatically assigned "Known Carcinogen", and group 2A "Likely Carcinogen". These conditions overrode any other considerations.
- If IARC grouping was 2B, 3, or not evaluated, but H350 or H350i 50%, then the chemical was assigned "Likely Carcinogen".
- If IARC grouping was 2B, 3, or not evaluated, but H351 $>$ 0% and/or 0% $<$ H350/H350i $<$ 50%, then the chemical was assigned "Possible Carcinogen".
- IARC group 3 chemicals with no supporting GHS H350, H350i, or H351 statement listed were assigned "Uncertain Risk".
- Chemicals with no IARC evaluation and no supporting GHS H350, H350i, or H351 statement listed were considered "Unclassified" as to their carcinogenicity.

These classifications, along with other relevant chemical metadata, can be found on the GitHub repository (chemical_metadata.xlsx).

Quantitative Estimates of Chemical Concentrations in Tissues

The SRM used for annotation and identification had a concentration of 0.47 ng/mL for each individual EC. Thus, we used the spectral intensities associated with these known concentrations to establish estimates of chemical concentrations within tissues in parts per million (PPM) and parts per billion (PPB). It should be noted that the original data processing pipeline used a nominal concentration of 0.5 ng/mL for calibration calculations; therefore, a correction factor of 0.94 (0.47/0.5) was applied to all concentration estimates prior to PPM and PPB calculations to account for the true SRM concentration. Importantly, we relied on the following experimental features and assumptions:

- Tissues are processed via solvent extraction and subsequent solvent evaporation, followed by reconstitution in 50 μL of isooctane. For the purposes of calculating concentrations in the original samples, we assume 100% extraction efficiency from tissues and plasma, such that the entire amount of the EC present in the sample is recovered in the isooctane.
- A chemical concentration of 0 ng/mL results in an intensity of 0 (i.e., the origin of (0,0)). This is used in combination with the intensity from the known concentration in the SRM (0.47 ng/mL) to establish a two-point standard curve, which assumes linearity.

- While each chemical has a concentration in the SRM of 0.47 ng/mL, the concentration in 50 μL of isooctane is 1.88 ng/mL. This is because 200 μL of SRM plasma is used, and therefore, 0.094 ng of the total EC of interest is extracted. This is dried after extraction and reconstituted in 50 μL of isooctane, resulting in a concentration of 1.88 ng/mL in the injected solution.

Our calculations to estimate tissue concentrations were performed as follows for each individual chemical:

1. A linear model is fit based on the assumptions discussed above, such that:

$$y = \beta x$$

where y is the known concentration of the EC in the SRM (0.47 ng/mL for all ECs analyzed), x is the observed spectral intensity for the given EC, and β is the slope of the calibration curve, defined by the line through the origin (0,0) and the point (x, y).

2. Once the slope (β) for the specific chemical is established, it is then used to estimate concentration (ng/mL) in the sample (C_e) using the following equation:

$$C_e = \beta I$$

where I is the observed spectral intensity for the given EC in the sample. However, to determine the true concentration in the isooctane solvent (C_{es}), we must scale C_e by a factor of 4 to account for the concentration that occurs during extraction. Specifically, the 200 μL of plasma standard extracted contains 0.094 ng total of the EC (0.47 ng/mL). Assuming 100% extraction, this 0.094 ng was then resuspended in 50 μL isooctane (1.88 ng/mL), Therefore, we use a 4$\times$ scaling factor:

$$C_{es} = 4C_e$$

3. Next, the C_{es} is converted from ng/mL to mg/L:

$$C_{es}\ \text{(mg/L)} = C_{es}\ \text{(ng/mL)} \times \frac{10^3\ \text{mL}}{\text{L}} \times \frac{10^{-6}\ \text{mg}}{\text{ng}}$$

$$C_{es}\ \text{(mg/L)} = C_{es}\ \text{(ng/mL)} \times 10^{-3}$$

4. Next, the total mass of the chemical of interest present in 50 μL of isooctane (M_{EC}) is determined:

$$M_{EC}\ \text{(mg)} = C_{es}\ \text{(mg/L)} \times 50\ \mu\text{L solvent} \times \frac{10^{-6}\ \text{L}}{\mu\text{L}}$$

$$M_{EC}\ \text{(mg)} = 5 \times 10^{-5}\ \text{(L)} \times C_{es}\ \text{(mg/L)}$$

5. To derive the mass fraction of the EC in tissue, we divide M_{EC} (mg) by M_T (mg) and scale to PPM or PPB:

$$\text{PPM} = \frac{M_{EC}}{M_T} \times 10^6$$

$$\text{PPB} = \frac{M_{EC}}{M_T} \times 10^9$$

Alternatively, when algorithm outputs are used directly without unit conversions, the following formula can be used, provided C_e is in ng/mL and M_T is in mg:

$$\text{PPM} = \frac{C_e \times 10^2}{M_T}$$

$$\text{PPB} = \frac{C_e \times 10^5}{M_T}$$

Quantitative Comparisons of Tumors and Non-Cancer Cadaver Thyroids

Targeted quantitative feature tables, which were additionally filtered for detection in relevant standards, were generated for tumors and non-cancer cadaver thyroids, and conversion to PPM was performed as described above. Once spectral intensities were converted to PPM, direct comparisons of chemical concentrations were made only for fragments that were detected in both the tumor and non-cancer thyroid tissues. In cases where multiple fragments were annotated for the same chemical in both tumors and non-cancer thyroids, an ideal fragment was first selected based on the highest percentage of detection in tumors, then the highest percentage of detection in non-cancer thyroids, and finally the greatest mean intensity in tumors. For all matching fragments, the mean, maximum, and theoretical minimum (i.e., half the minimum detectable concentration in either the tumors or non-cancer thyroids) were calculated for tumors (all combined) and non-cancer thyroids. These data, along with percentage detection in tumors and non-cancer thyroids, are

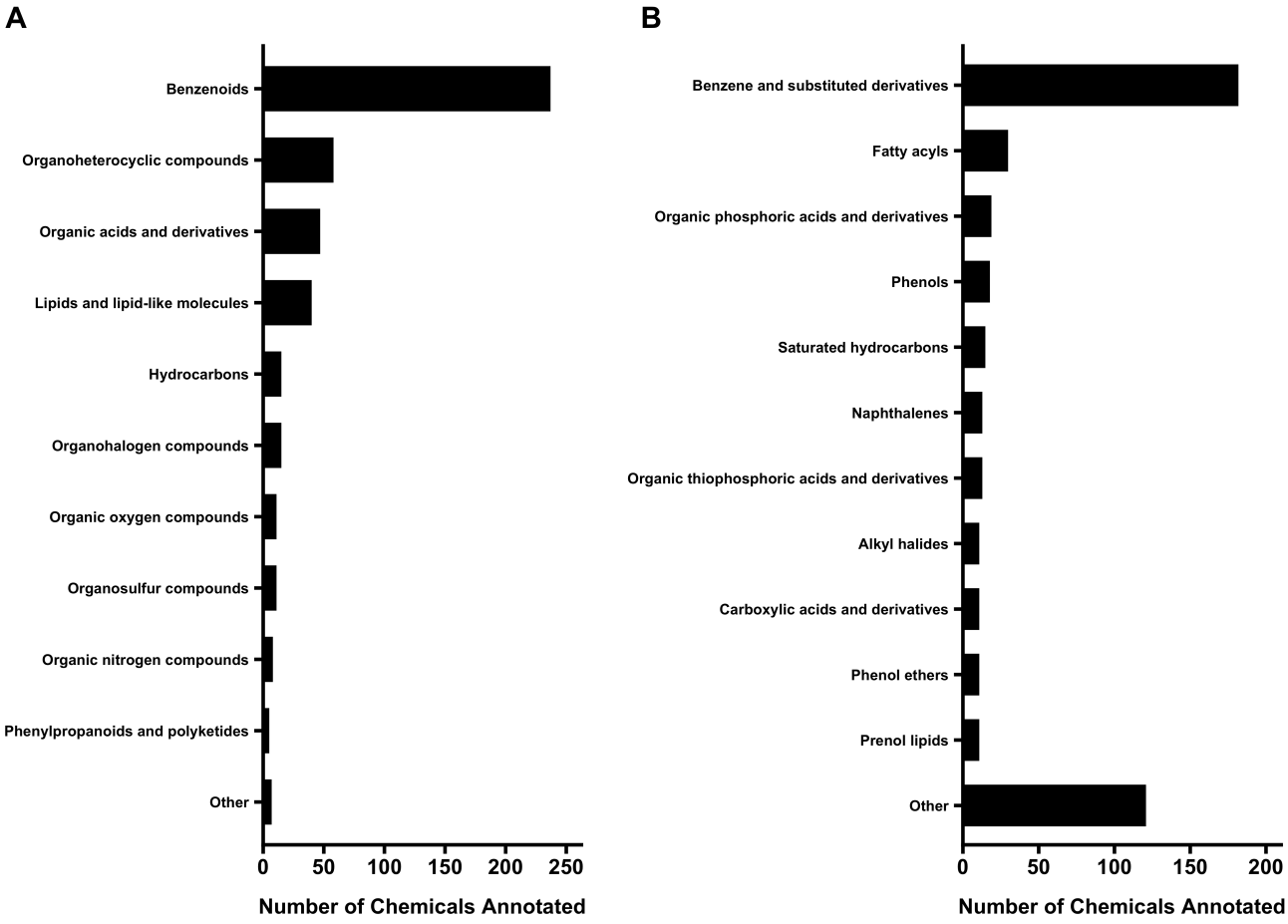
reported as PPB below in Supplementary Table 3. It is important to note that means were calculated using half-minimum imputed data, even if features were detected at 'qualitative' analysis thresholds. Finally, these values were converted to PPM for a direct comparison of tumors to non-cancer thyroids of all detected IARC Group 1 carcinogens (Figure 3E, 3F); however, this comparison was only reported for the two features (4-aminobiphenyl and o-Toluidine) that A) passed manual validation and B) had annotation of the same fragment in both tumor and cadaver (which were run on different batches). Of note, o-Toluidine only had one directly comparable annotated fragment between tumor and thyroid; however, 4-aminobiphenyl had three. For 4-aminobiphenyl, the fragment with the highest annotation frequency across both tumor and cadaver samples was selected for analysis and visualization. T-tests were run on $\log_2$-transformed data to compute p-values for comparing the means between tumors and non-cancer thyroids for these chemicals.

Comparing Observed Concentrations to Literature Values for Select Chemicals

To compare the quantification estimates generated as described above with estimated values in other tissues and matrices, we identified values for select chemicals in the published literature and tabulated our data alongside these reported concentrations (Supplementary Table 2). We prioritized chemicals that were IARC Group 1 carcinogens and polycyclic aromatic hydrocarbon combustion byproducts. For quantitative estimates of 245 individual chemicals, see Supplementary Table 3.

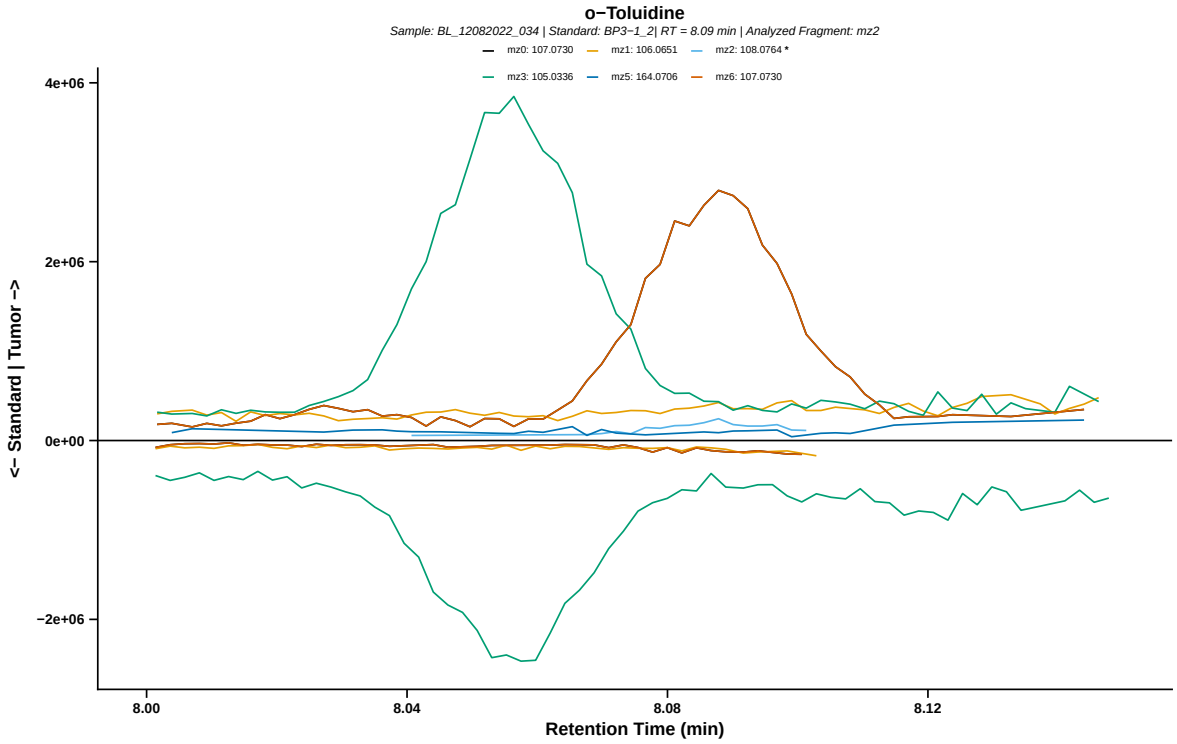
SUPPLEMENTARY FIGURE 1

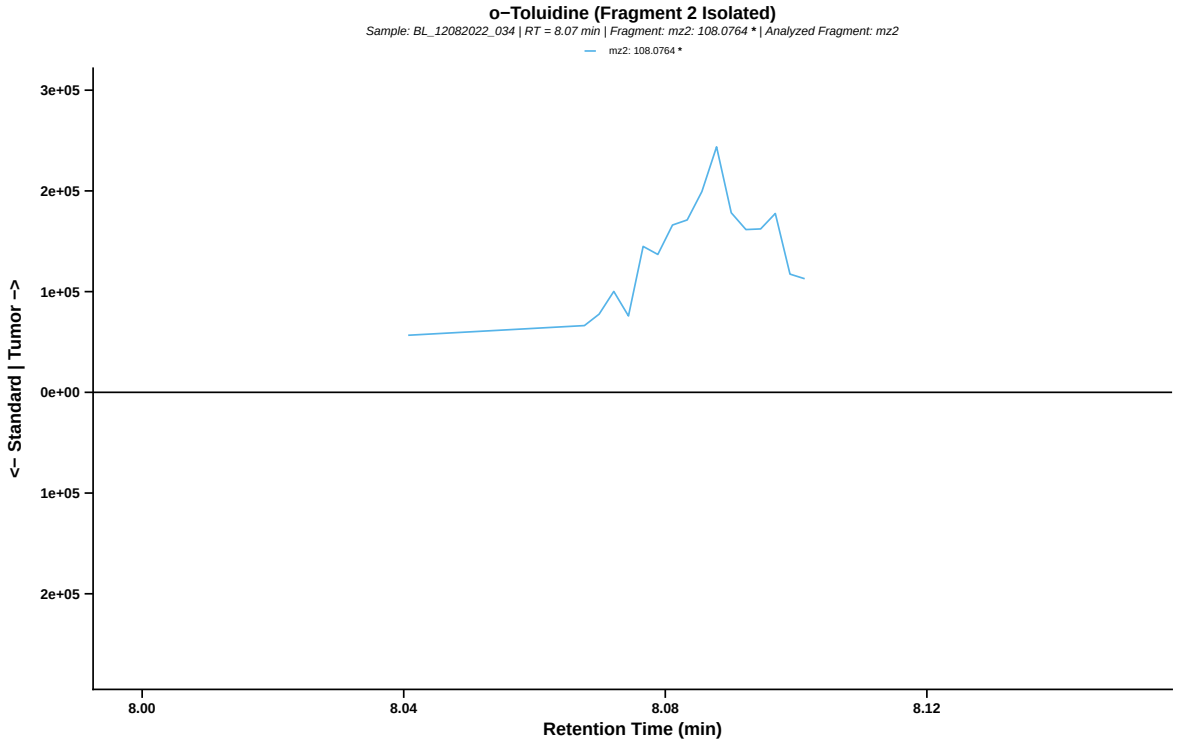
Classification of annotated chemicals. Chemical superclasses (A) and subclasses (B) of all annotated chemicals.



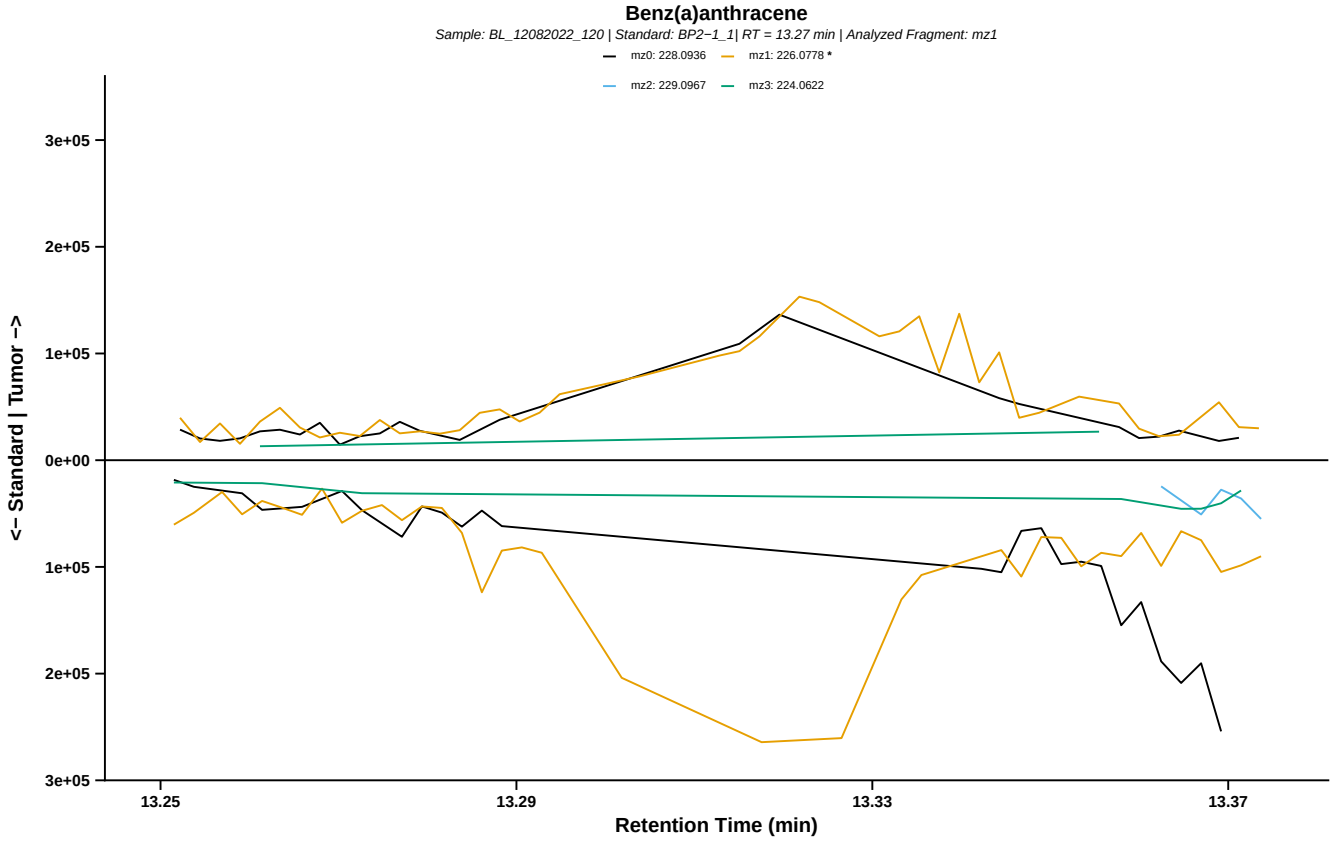
SUPPLEMENTARY FIGURE 2.1

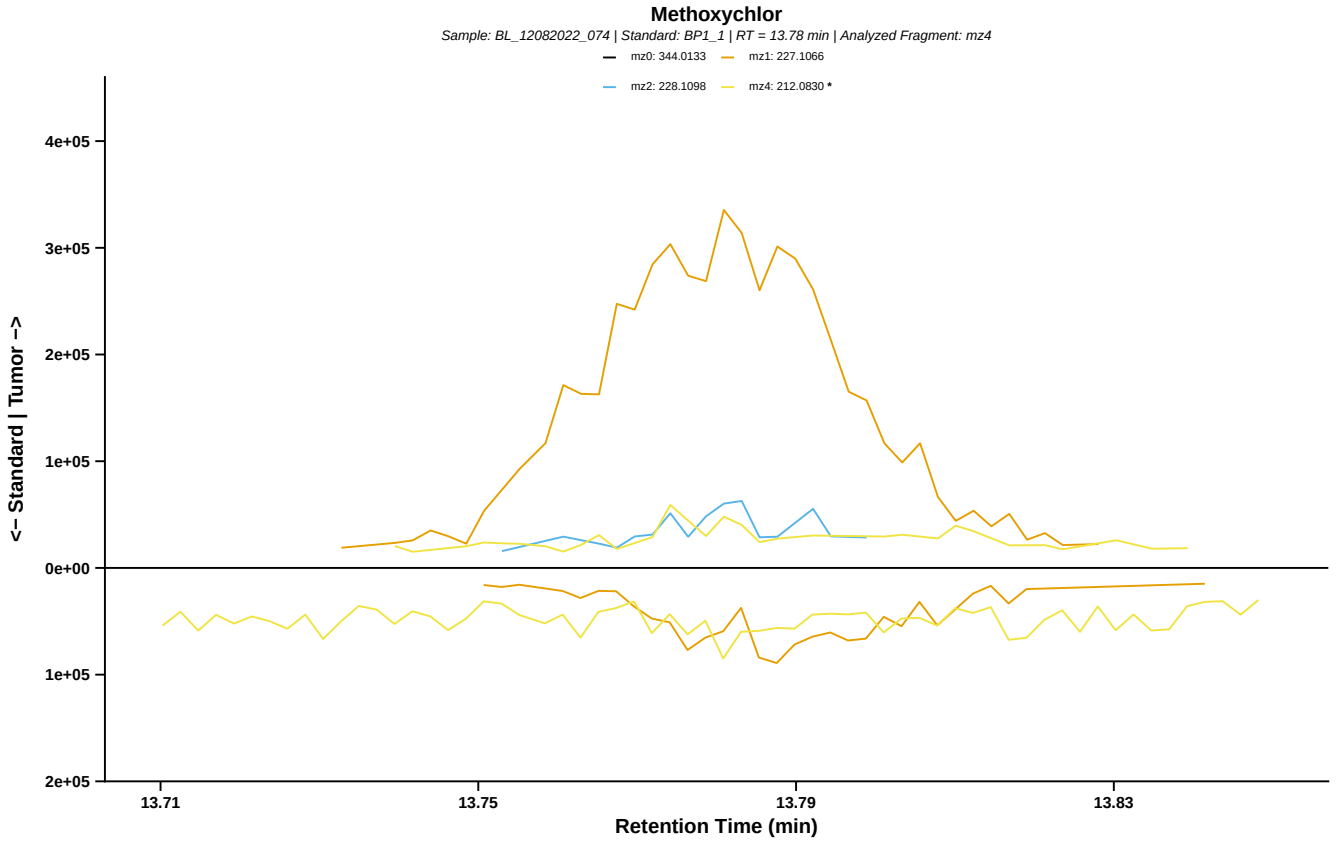
Spectral validation of select chemical identifications in thyroid tumor samples. Sample spectra for all chemicals which showed differences in variants (quantity or presence), displayed either as mirrored plots with reference standard (sample intensity in positive y-axis, standard intensity in negative y-axis) or as non-mirrored plots without standard when reference co-elution was inadequate. Mirrored plots with co-elution of multiple fragments in both standard and sample are considered "Level 1" identifications (2.1, pp. 7-28), while non-mirrored plots where multiple fragments co-elute in the sample but the standard does not show proper co-elution are considered "Level 2" identifications (2.2, pp. 29-31). Asterisks (*) indicate the fragment used for statistical comparison and displayed in Figure 3 and/or Table 3. For select compounds, additional plots display isolated fragments for enhanced visualization clarity.



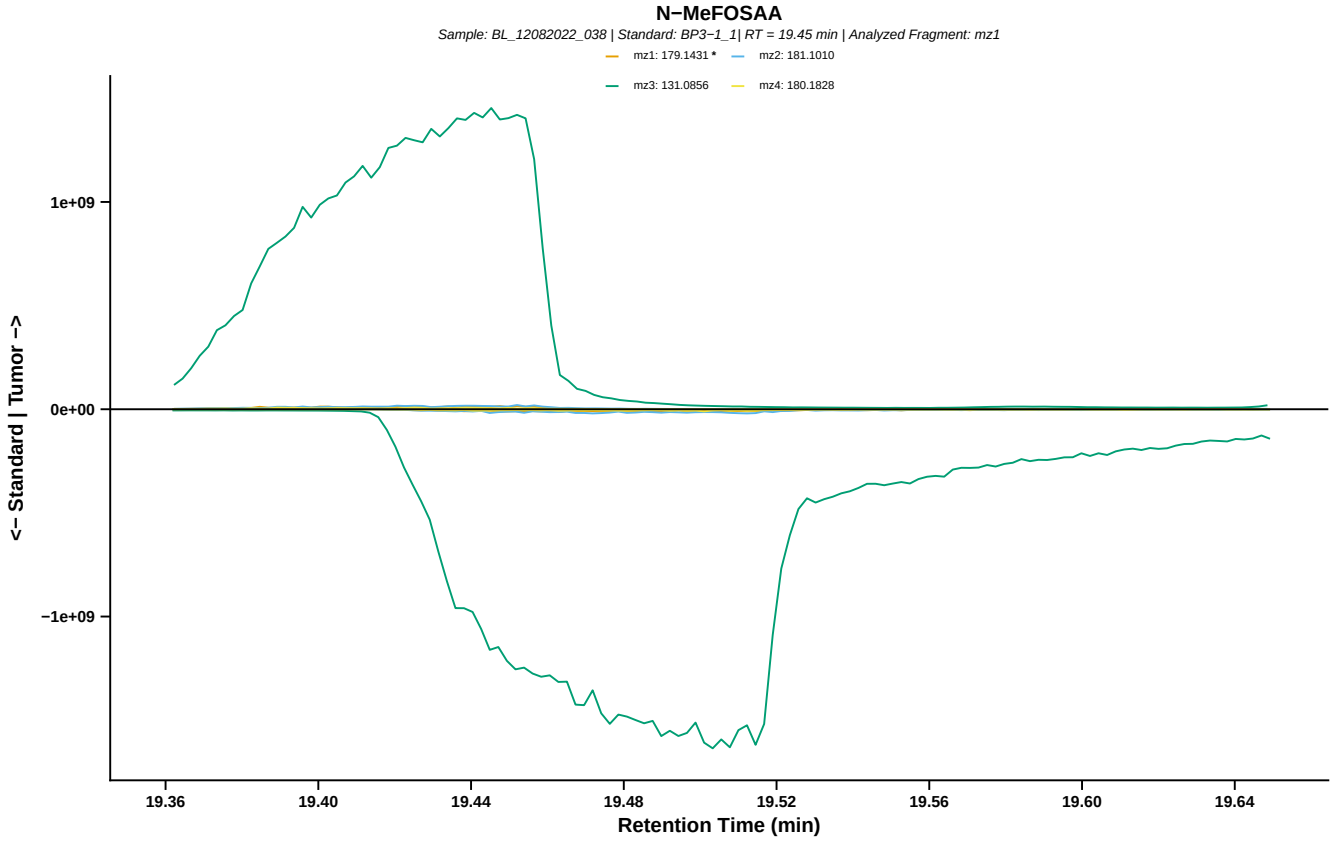


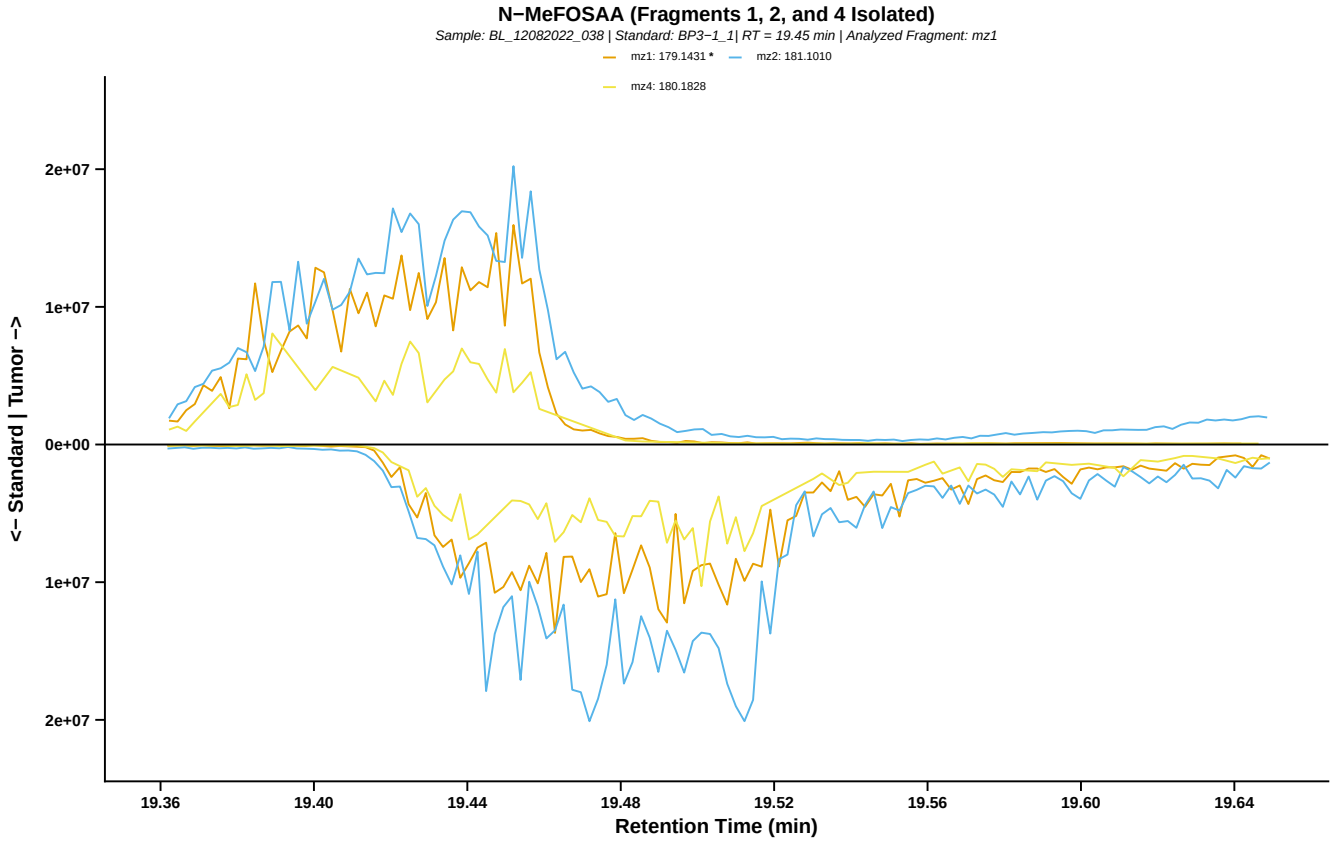
SUPPLEMENTARY FIGURE 2.1 (Continued)



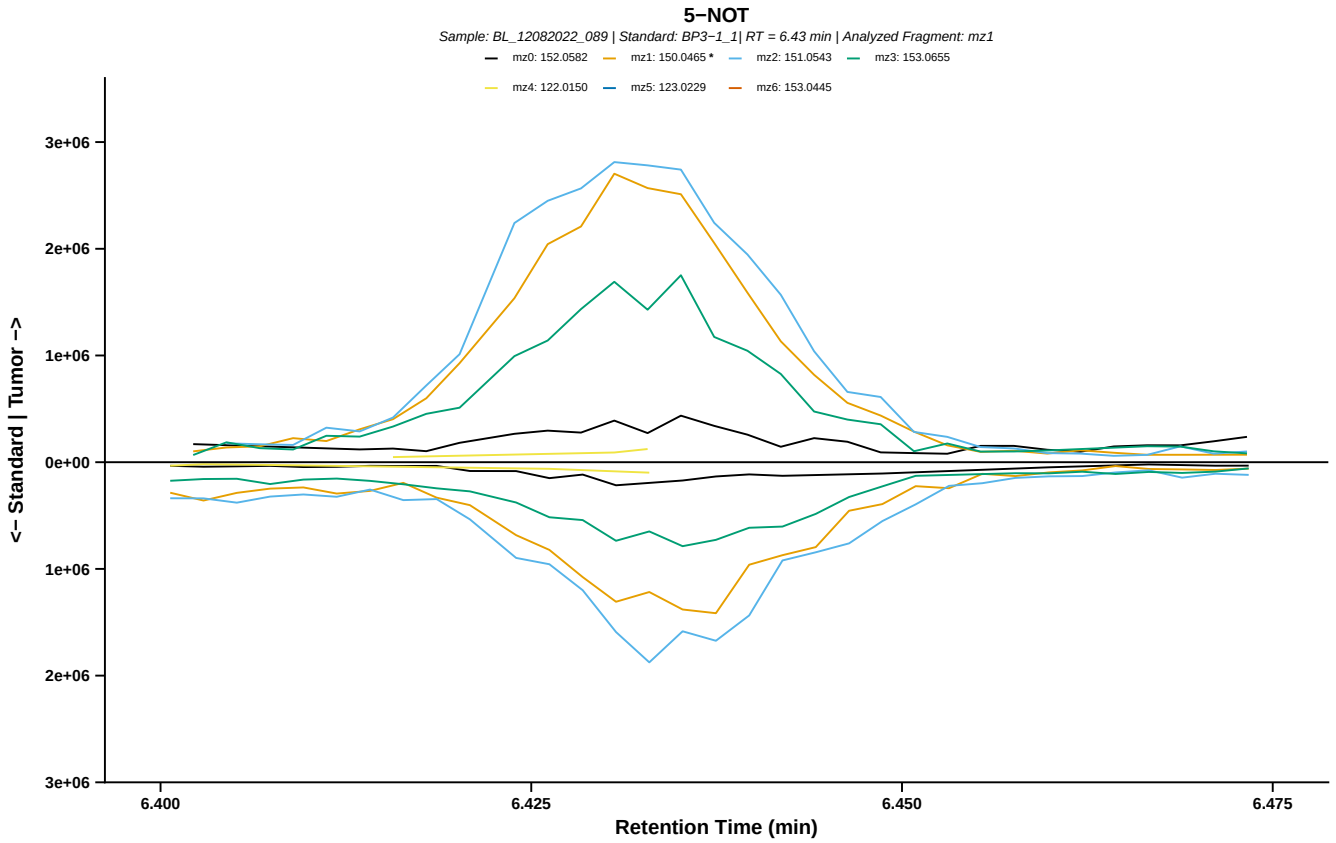


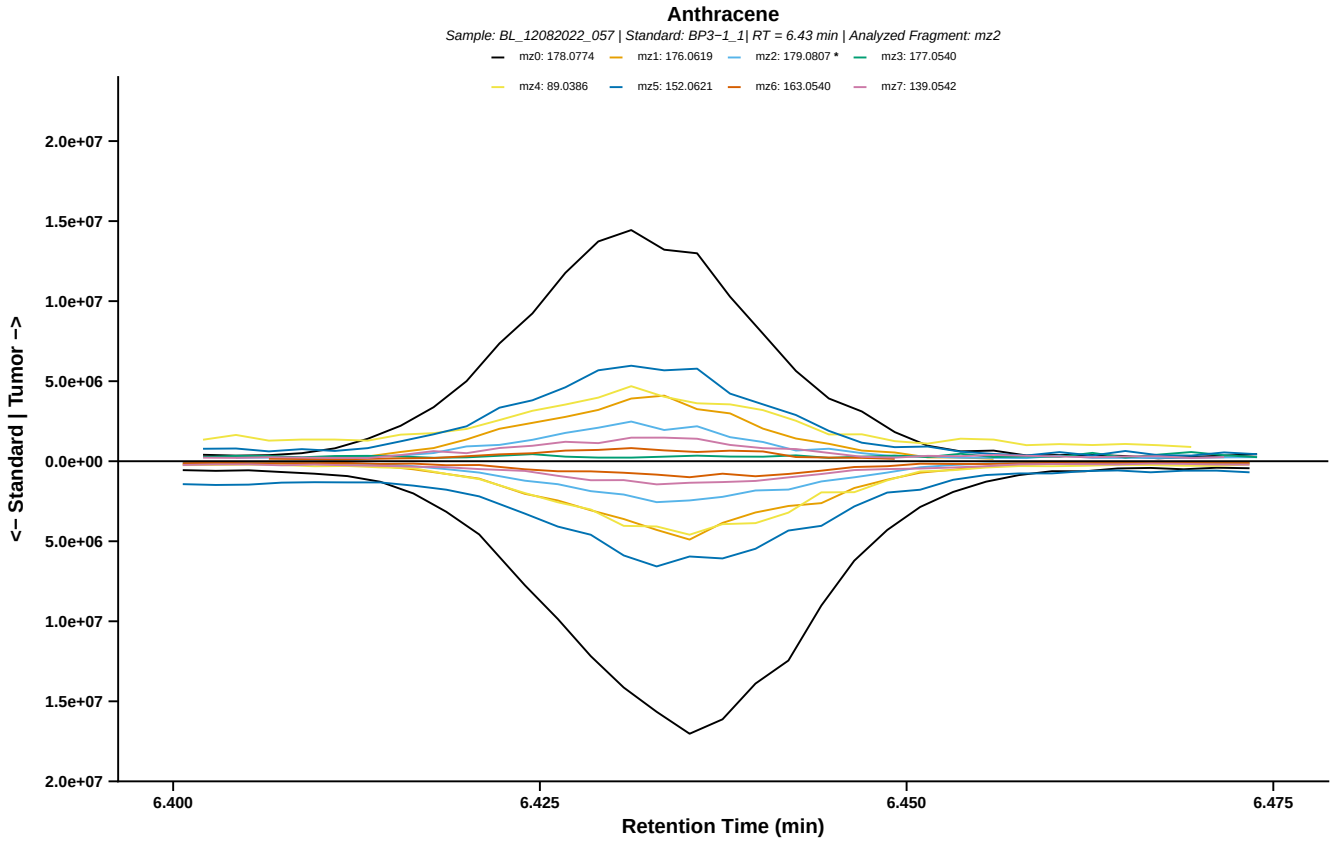
SUPPLEMENTARY FIGURE 2.1 (Continued)



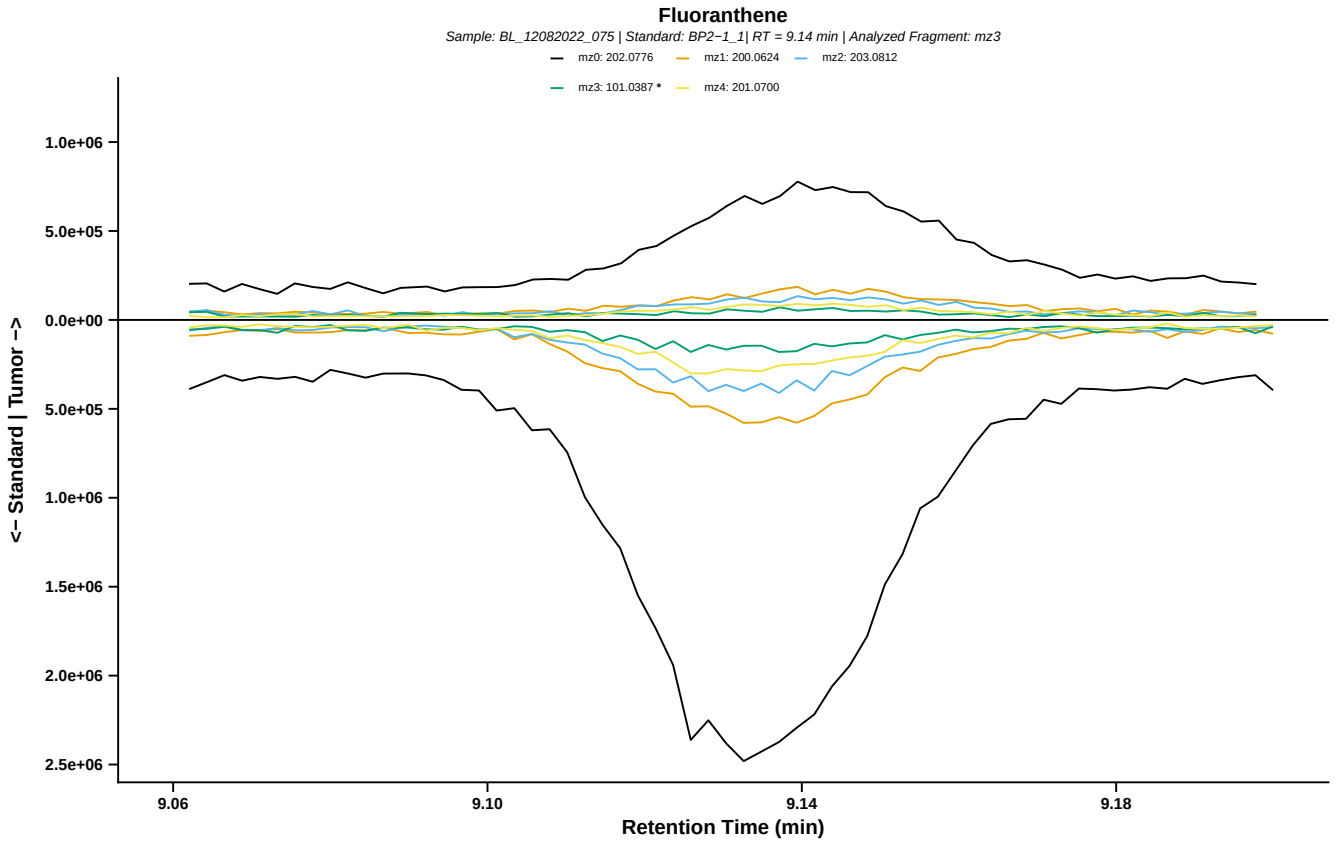


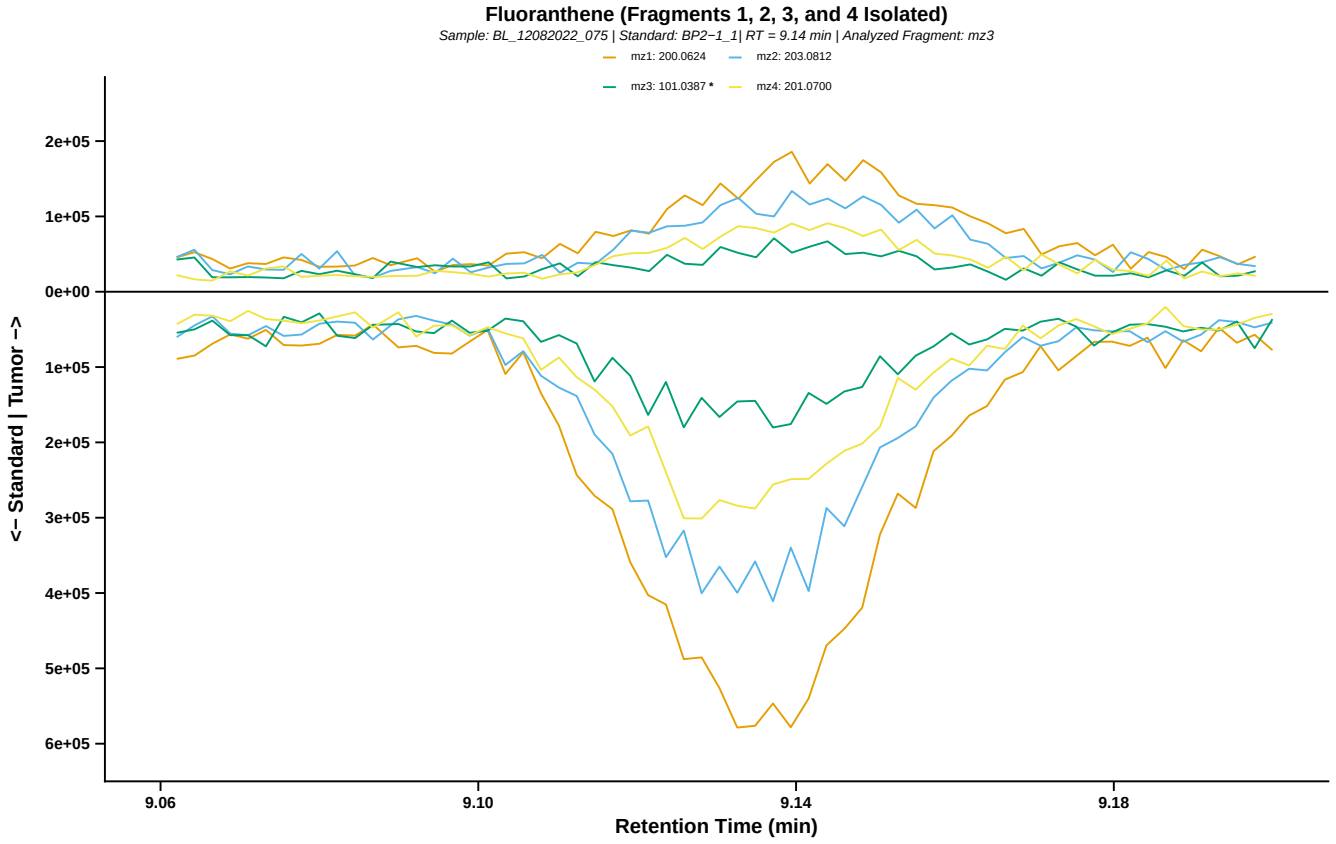
SUPPLEMENTARY FIGURE 2.1 (Continued)



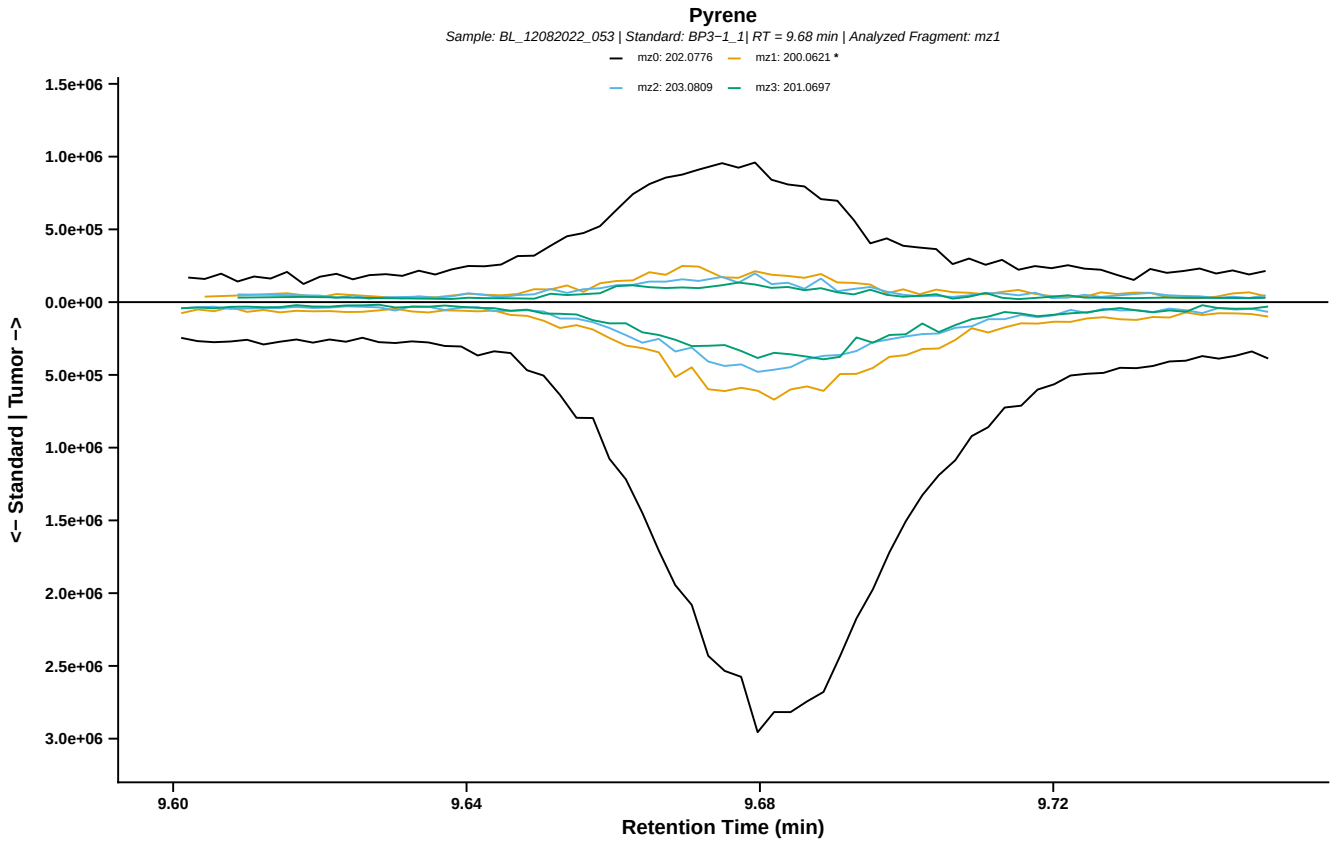


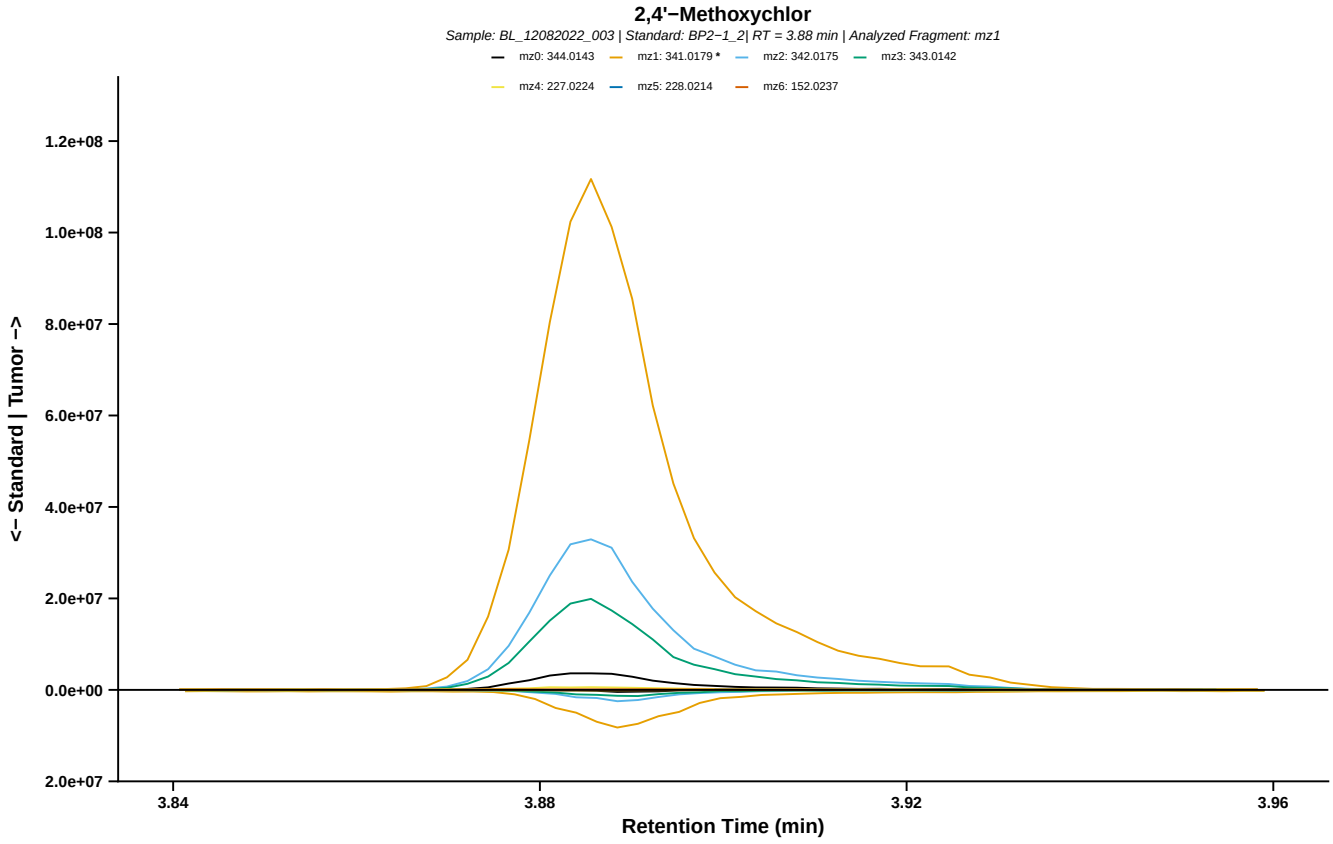
SUPPLEMENTARY FIGURE 2.1 (Continued)



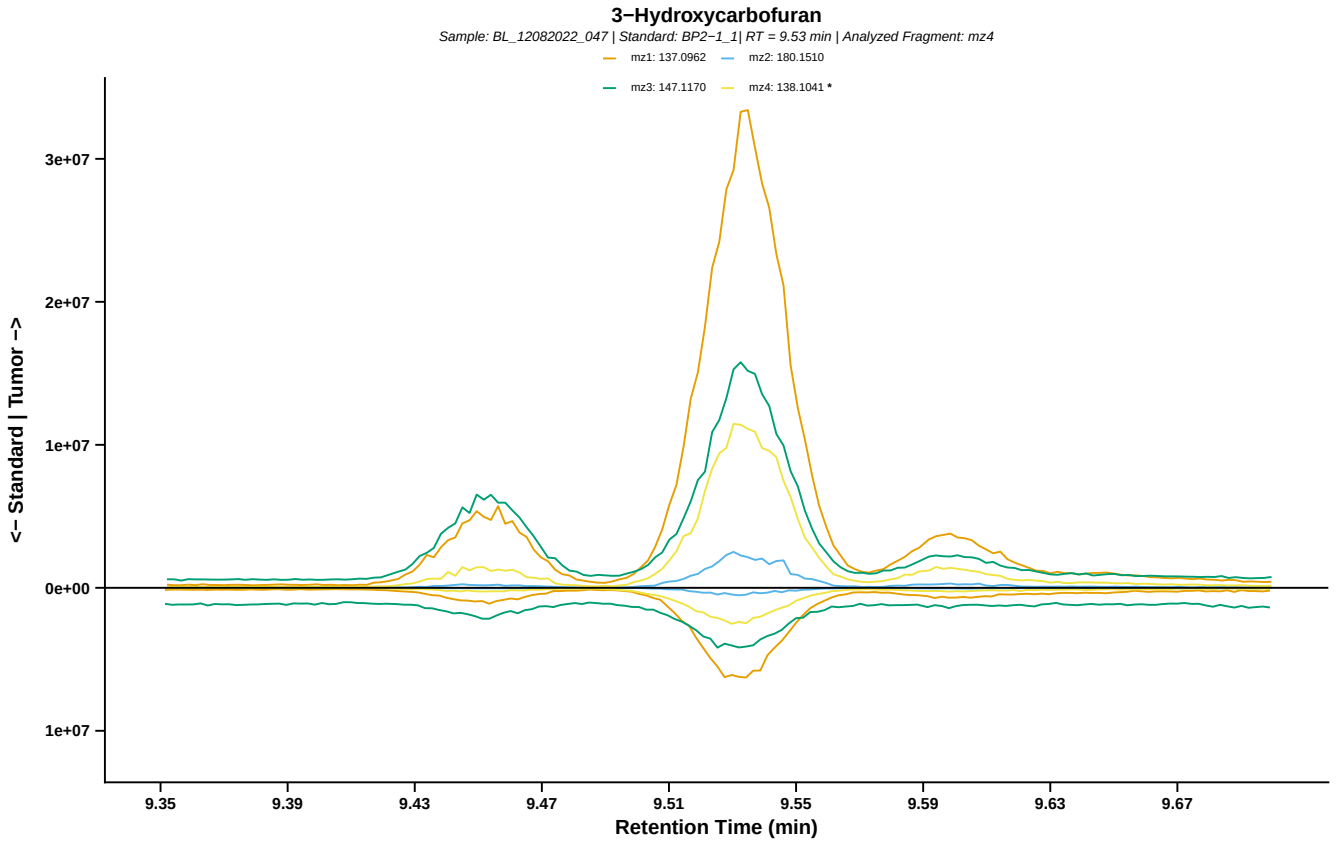


SUPPLEMENTARY FIGURE 2.1 (Continued)

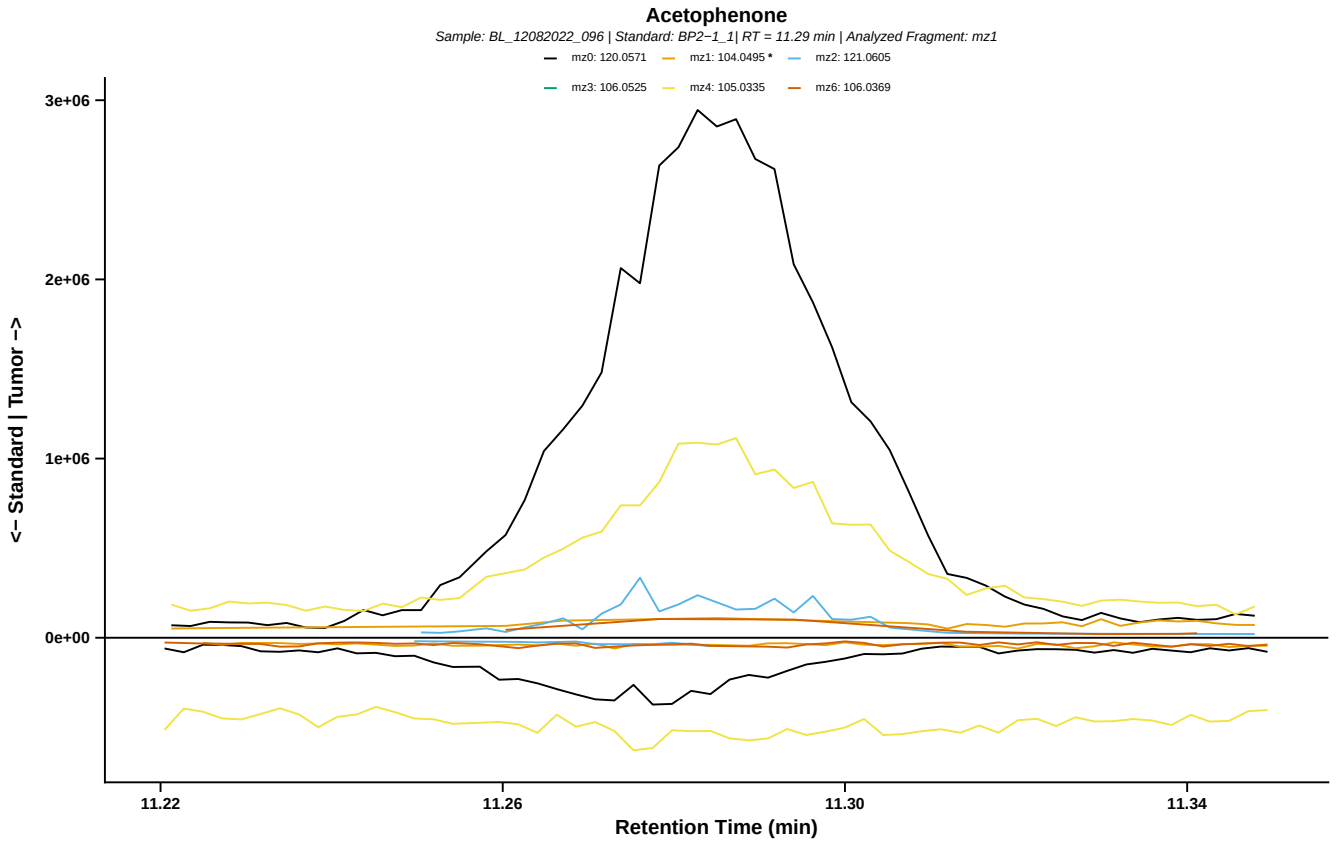


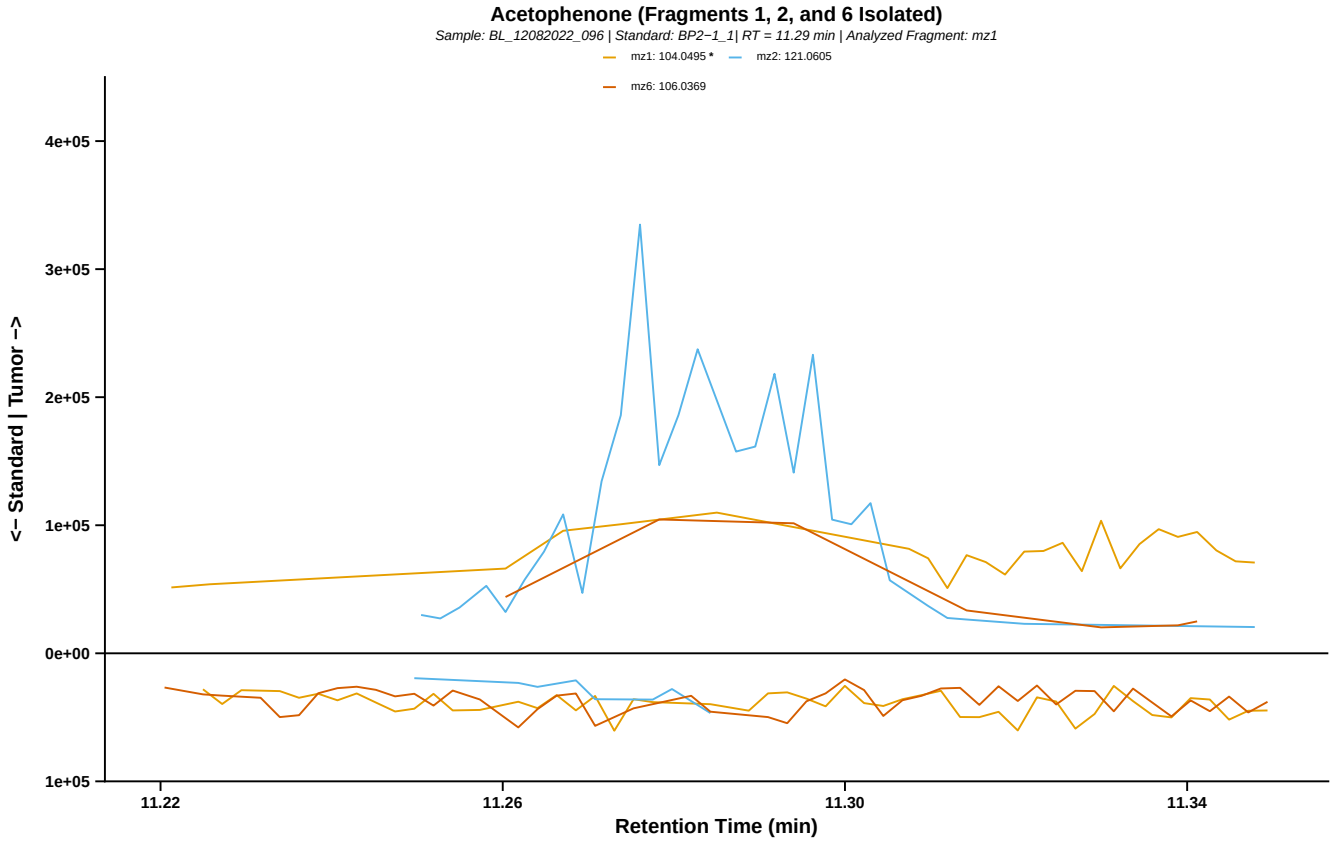


SUPPLEMENTARY FIGURE 2.1 (Continued)

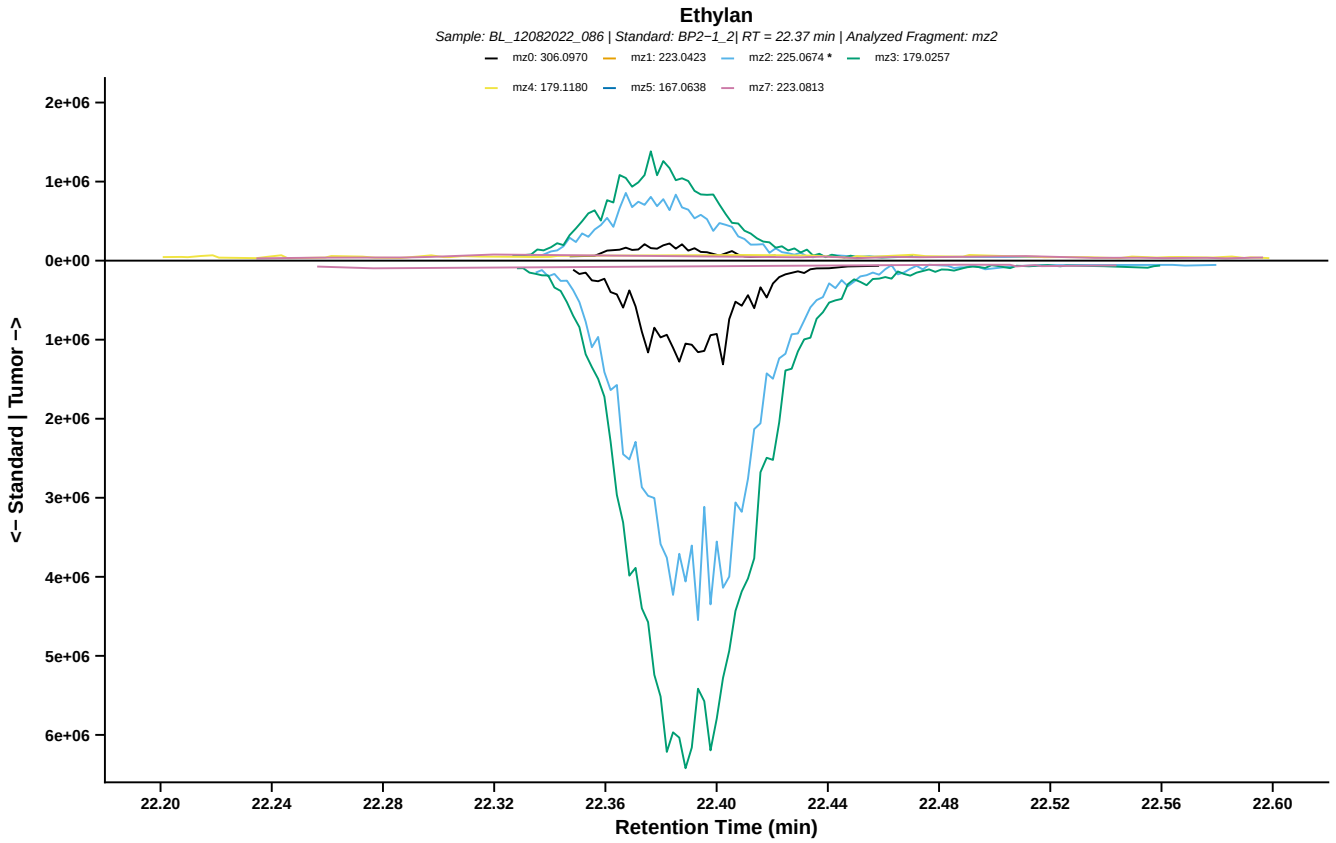


SUPPLEMENTARY FIGURE 2.1 (Continued)

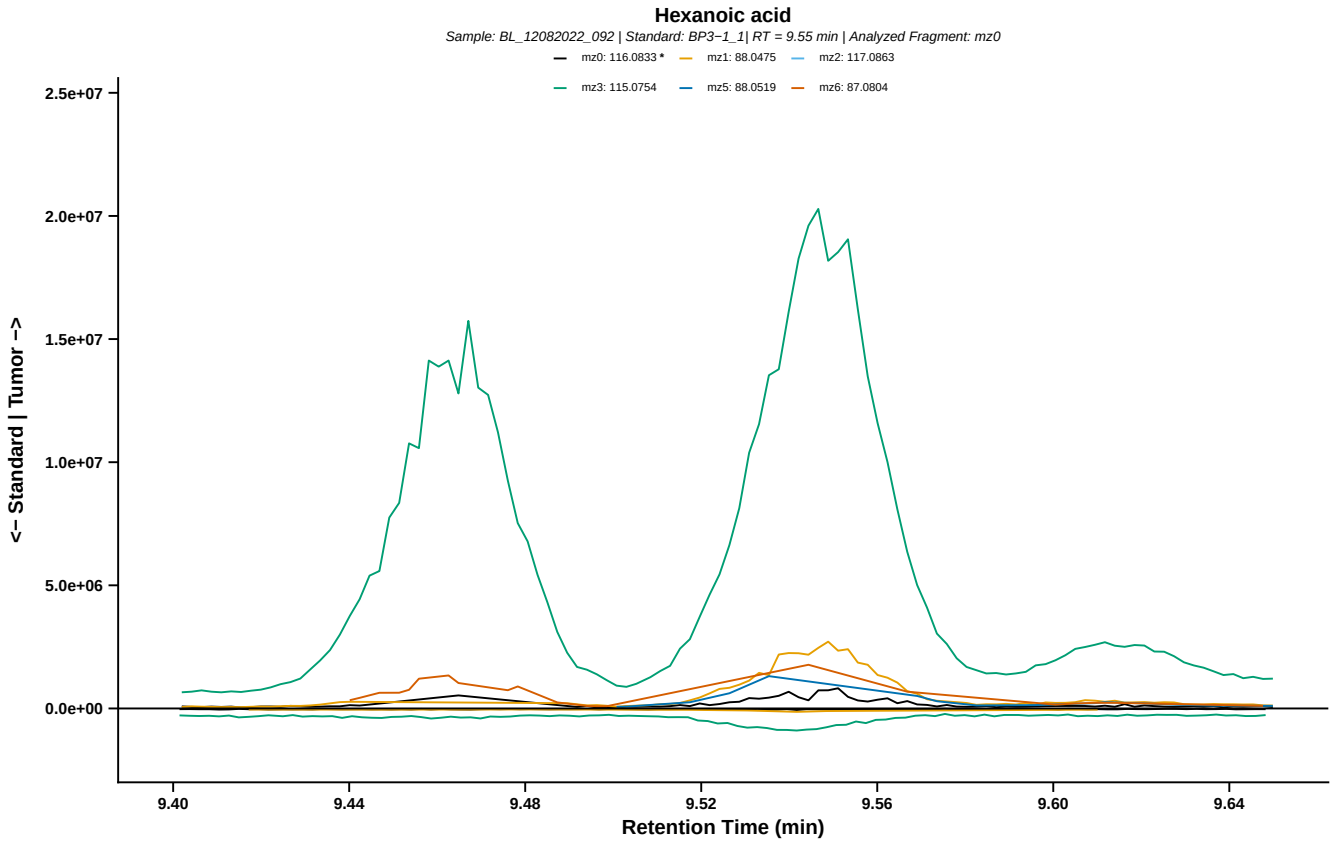


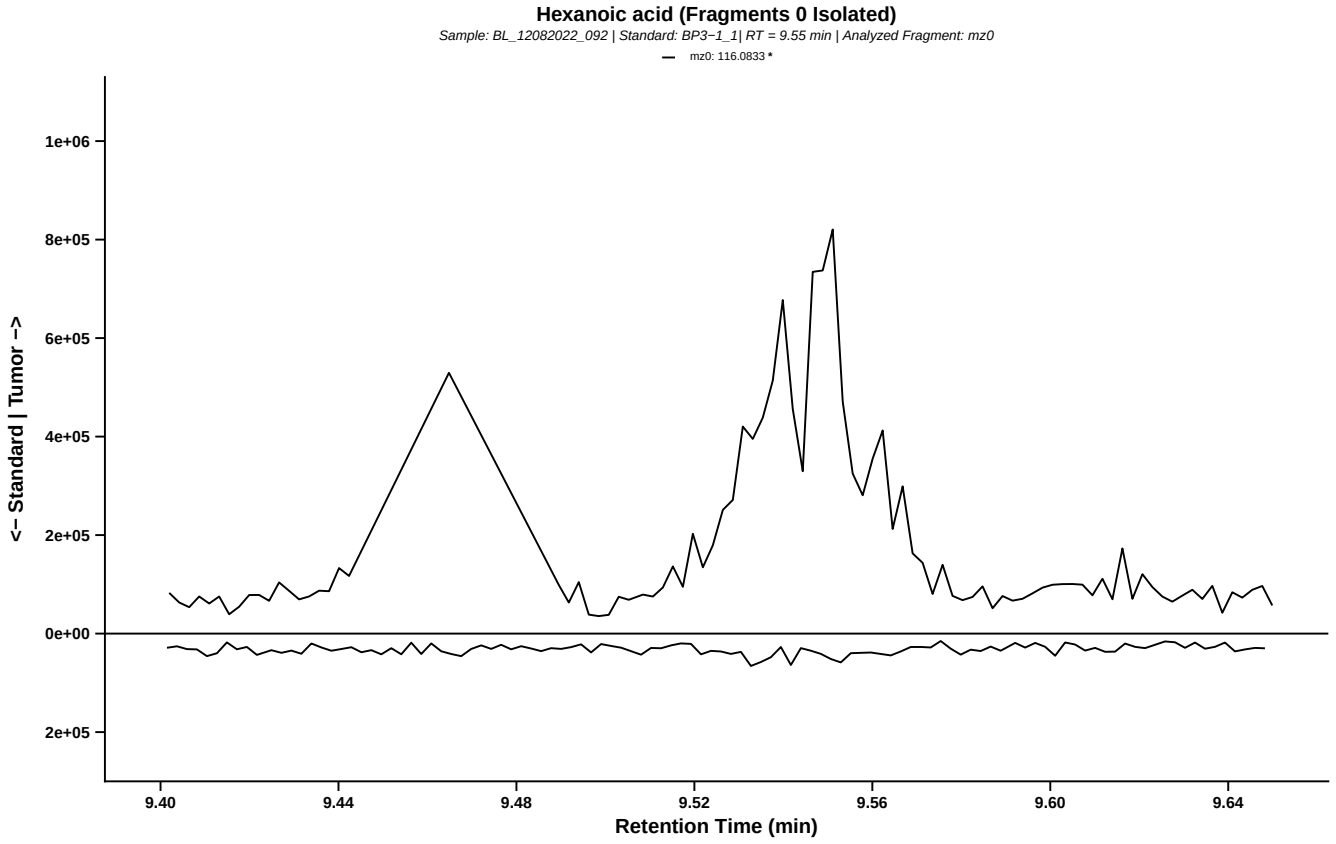


SUPPLEMENTARY FIGURE 2.1 (Continued)

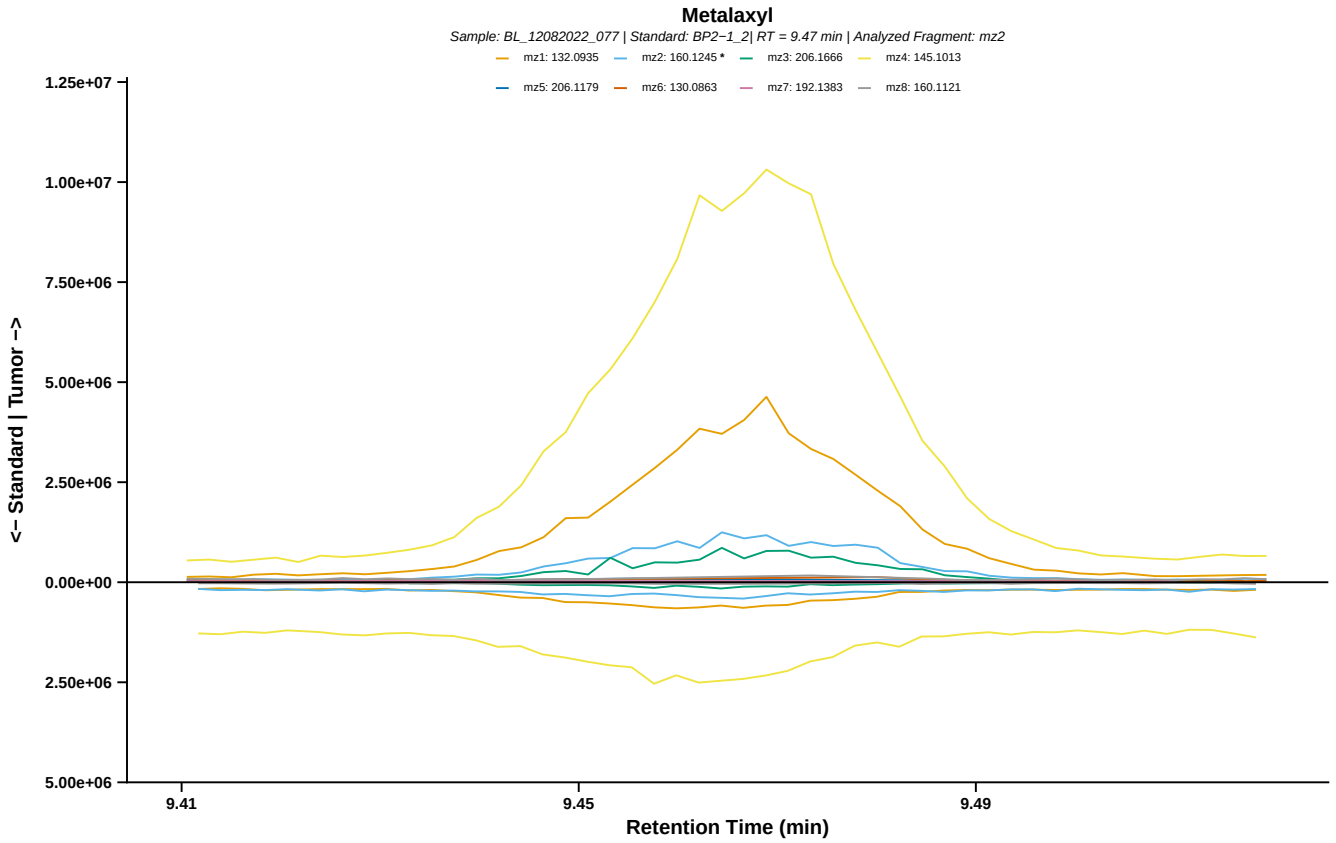


SUPPLEMENTARY FIGURE 2.1 (Continued)

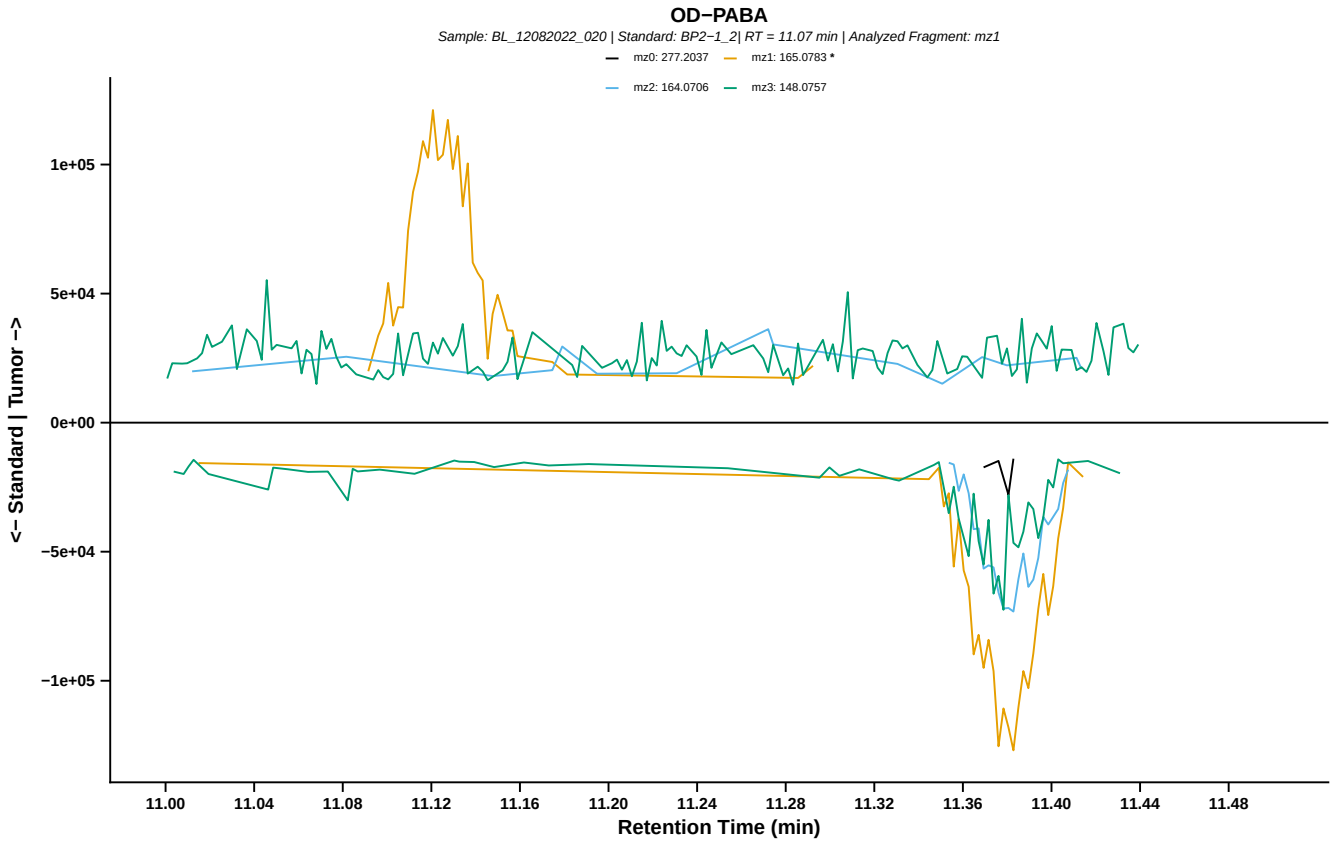




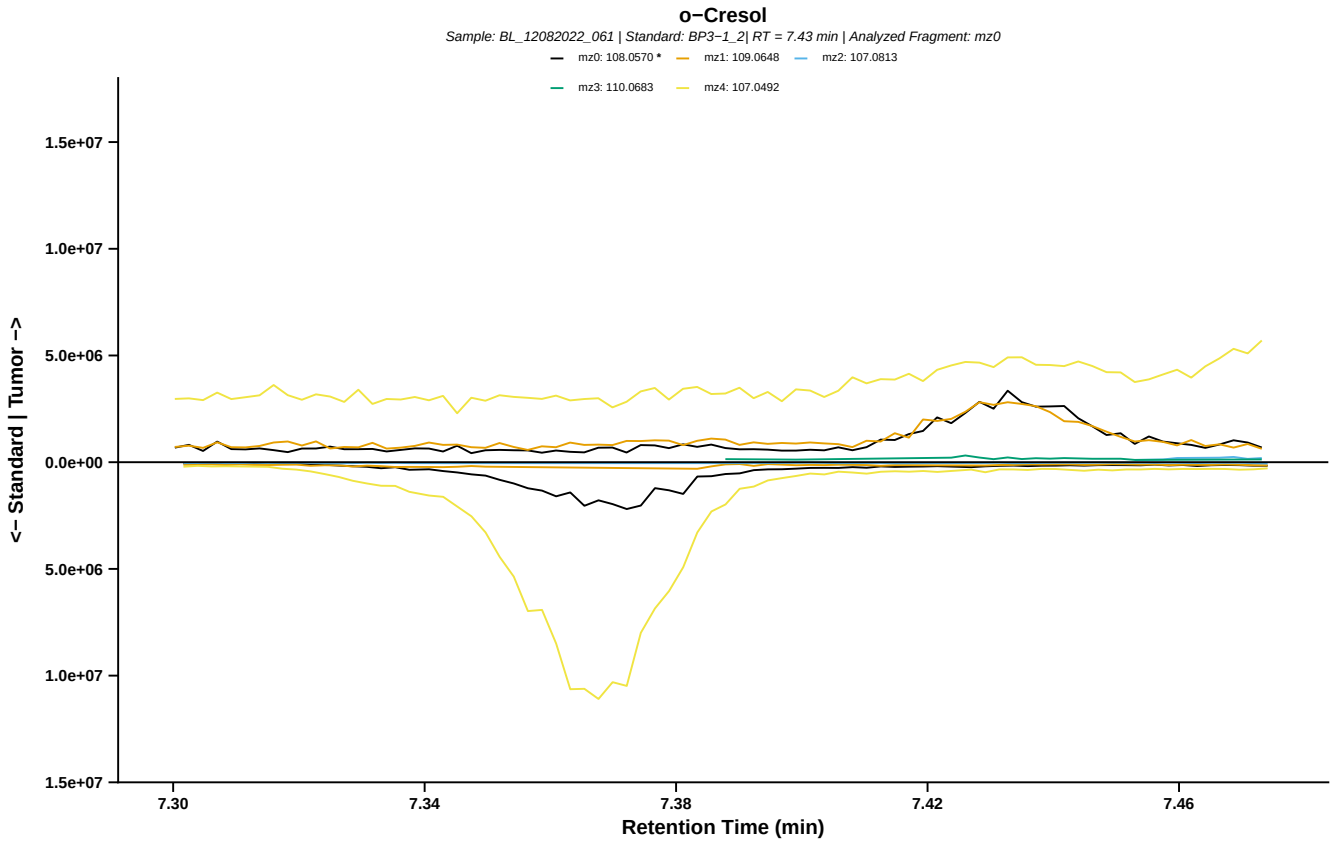
SUPPLEMENTARY FIGURE 2.1 (Continued)

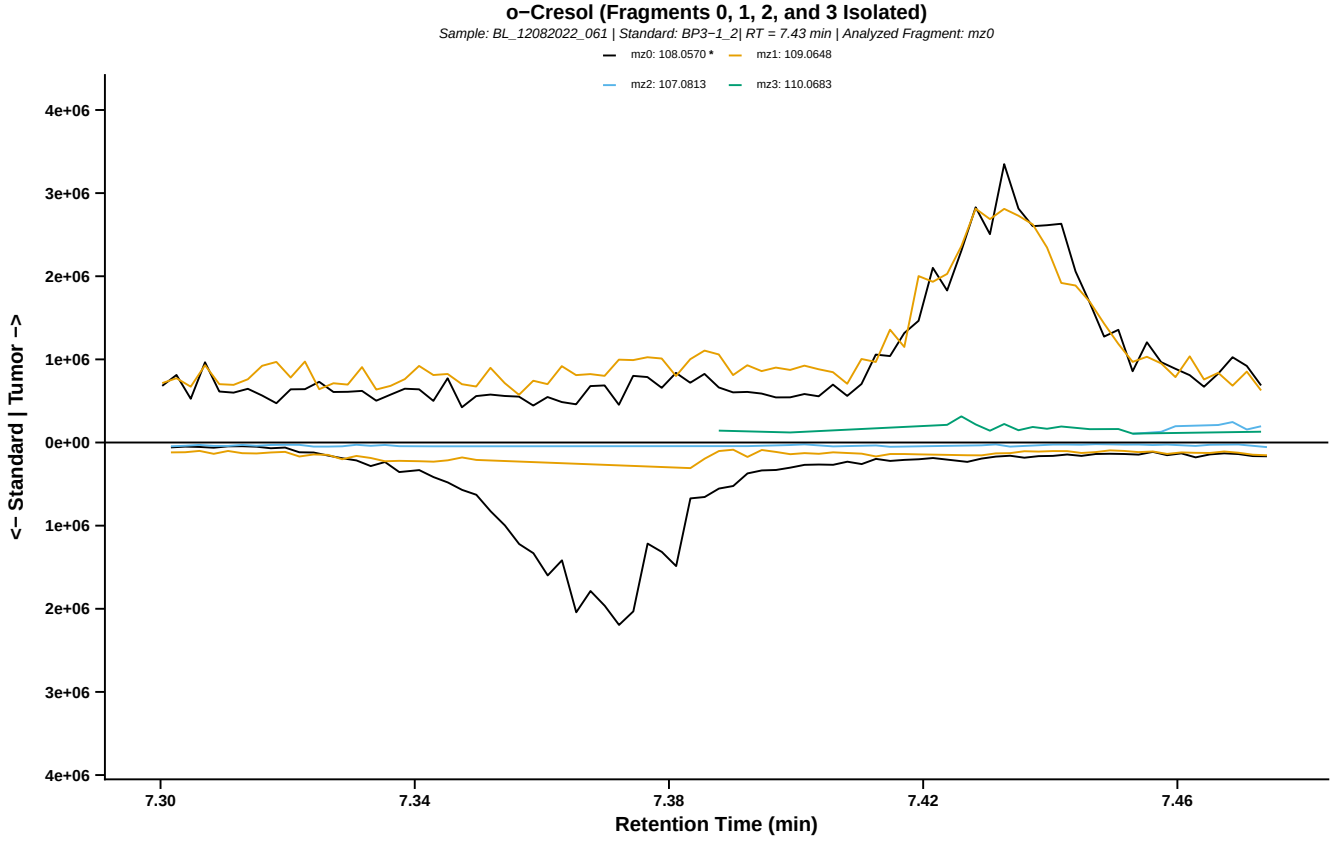


SUPPLEMENTARY FIGURE 2.1 (Continued)

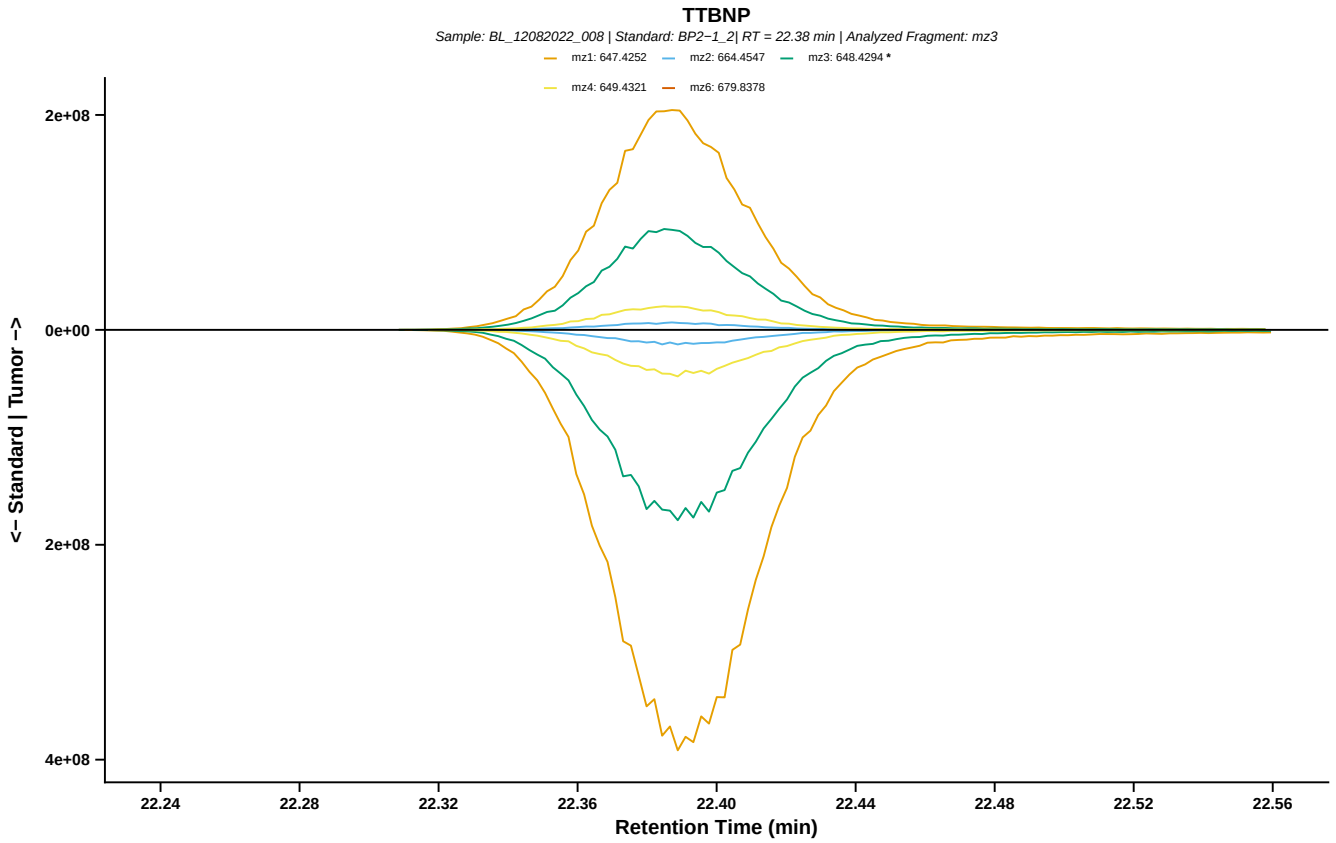


SUPPLEMENTARY FIGURE 2.1 (Continued)

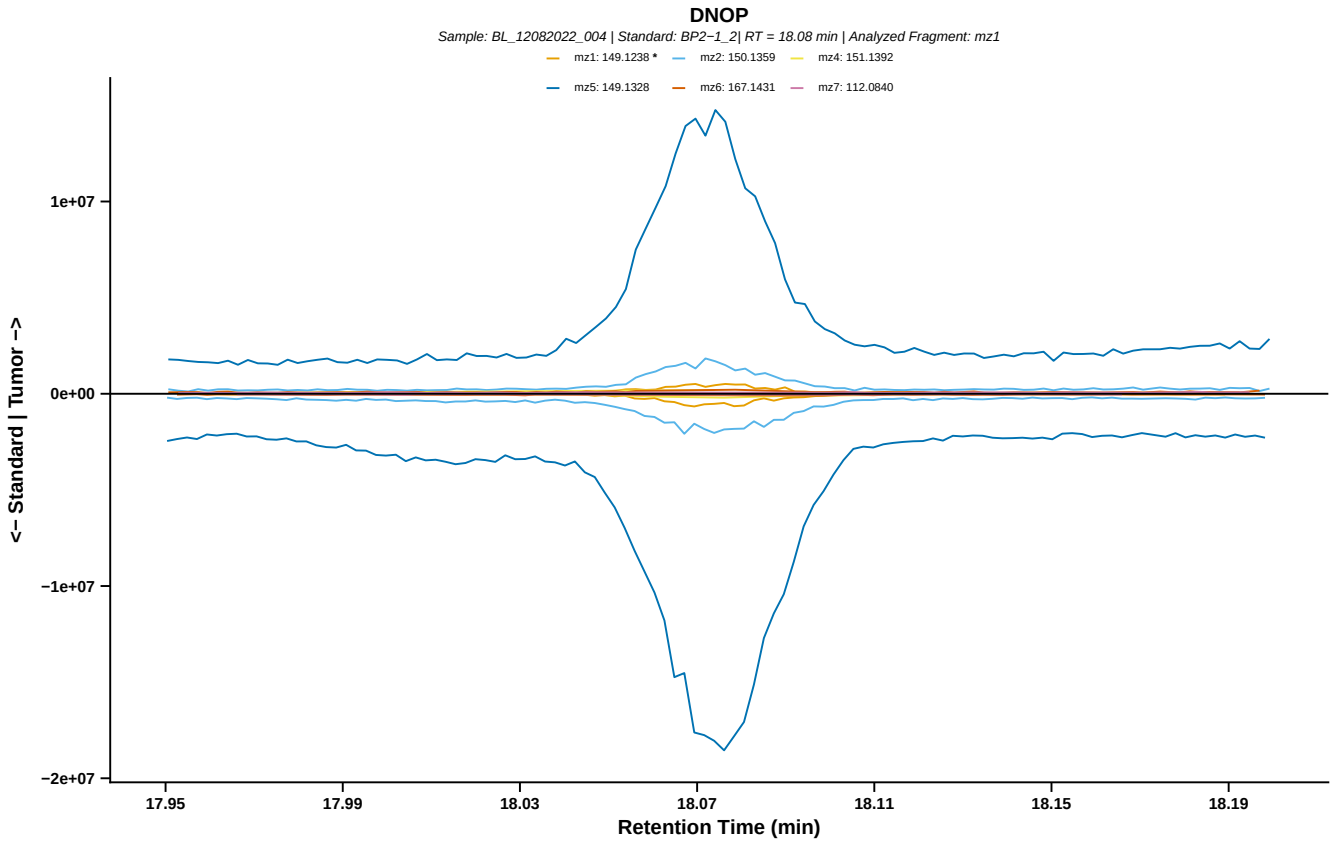


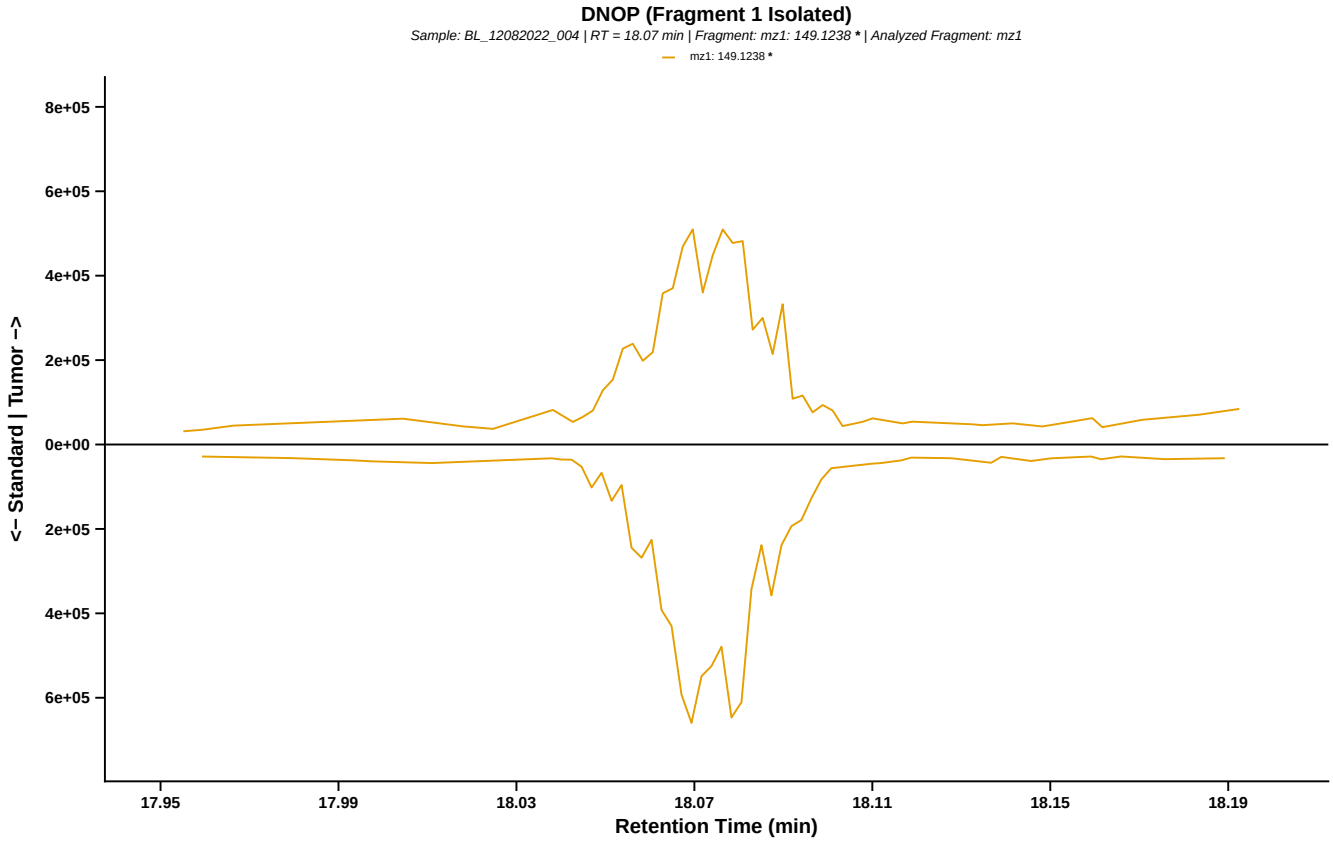


SUPPLEMENTARY FIGURE 2.1 (Continued)

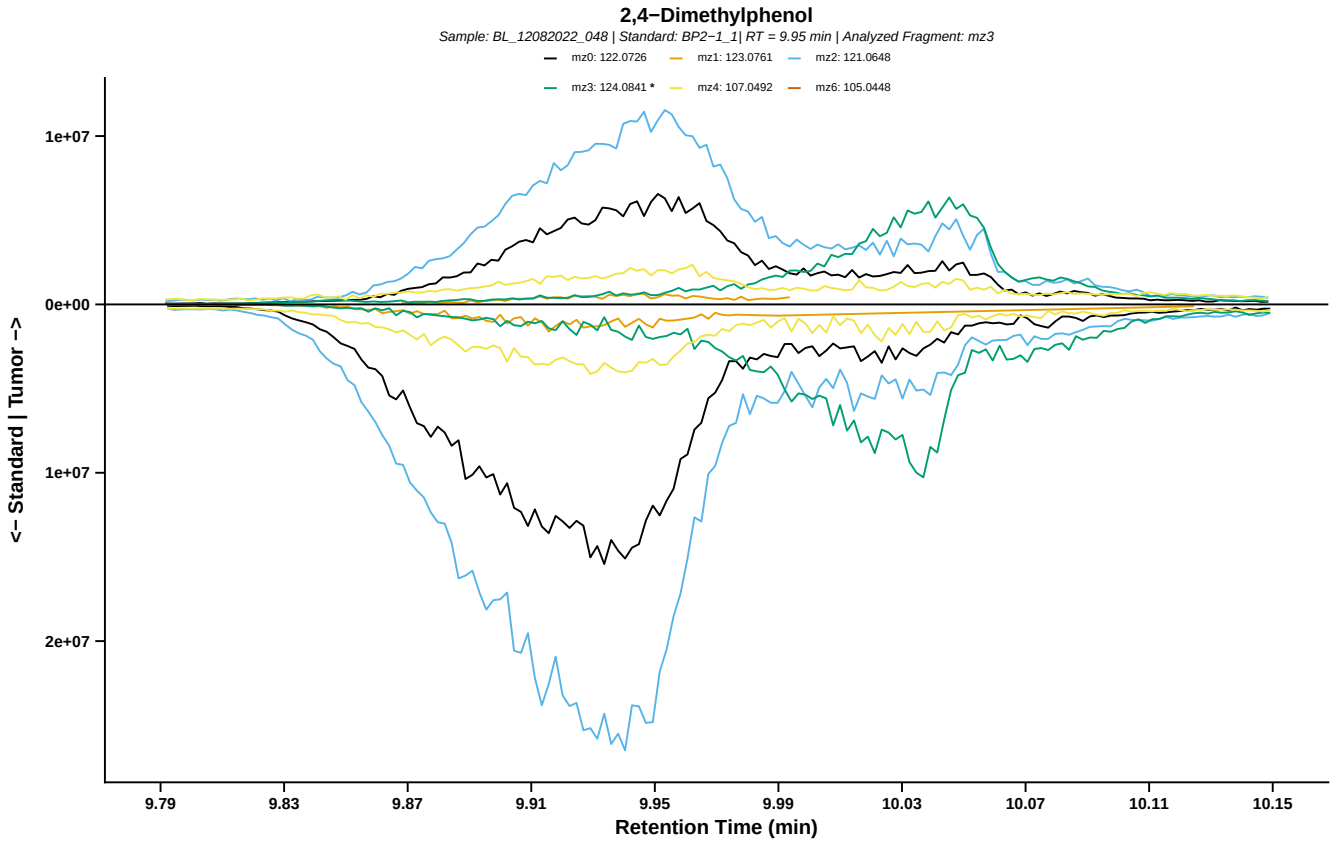


SUPPLEMENTARY FIGURE 2.1 (Continued)

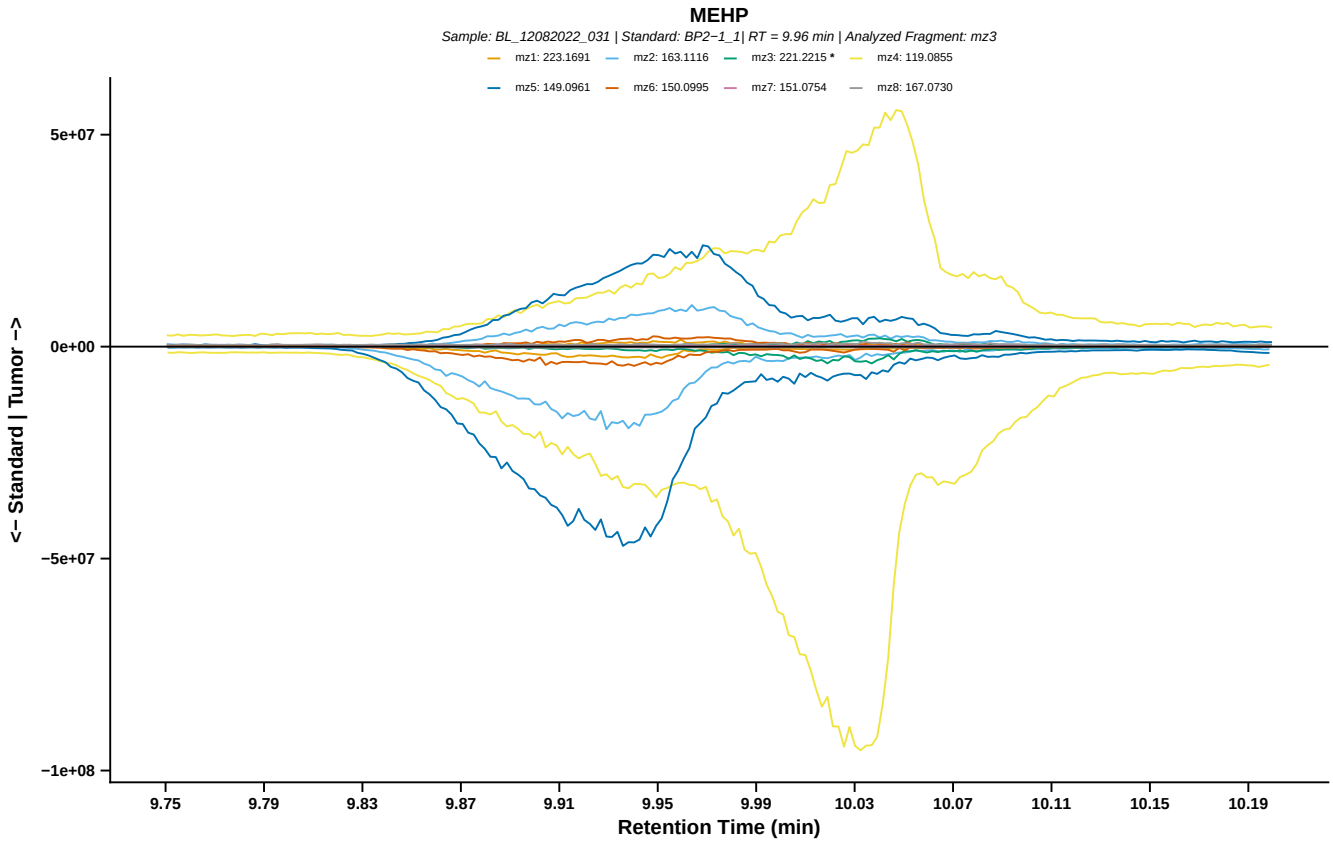


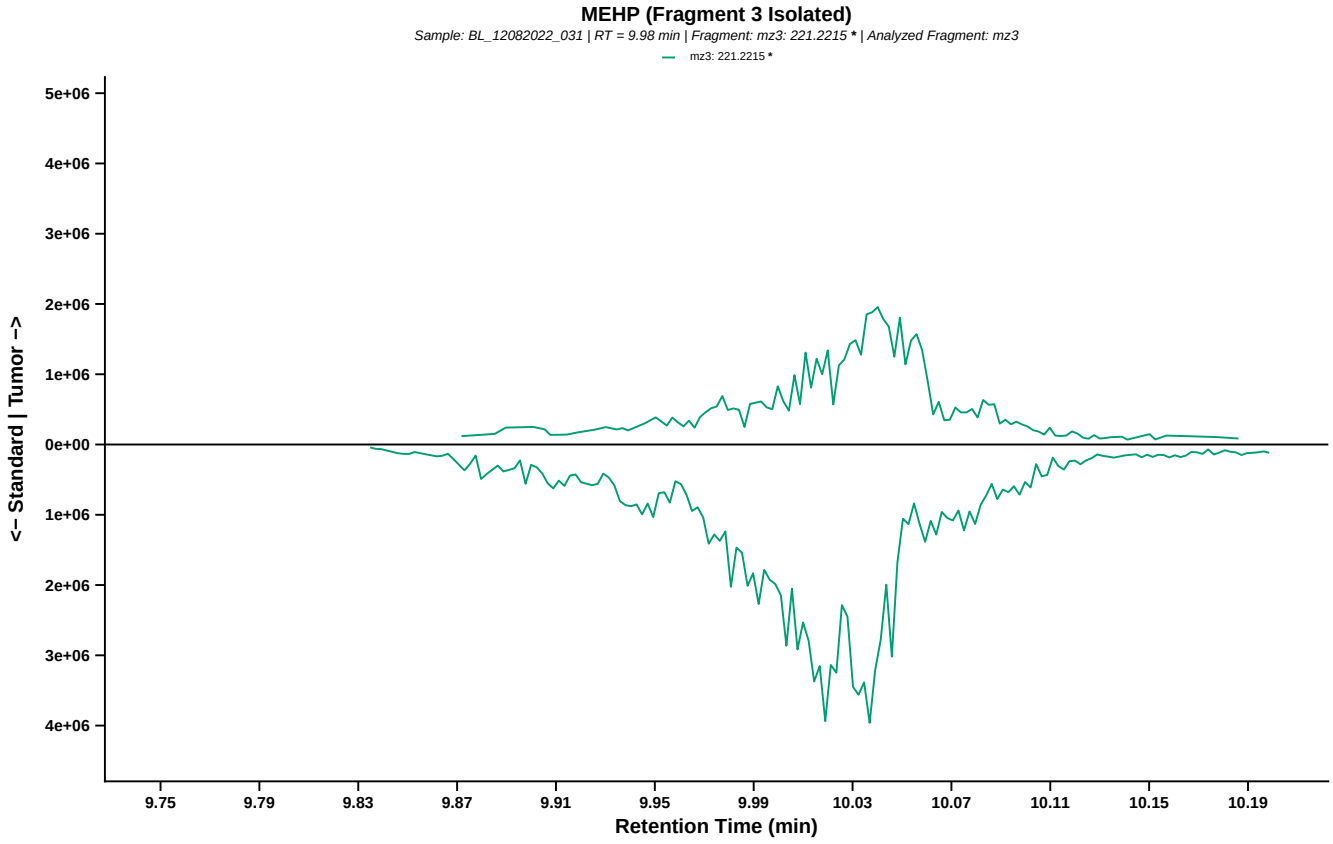


SUPPLEMENTARY FIGURE 2.1 (Continued)

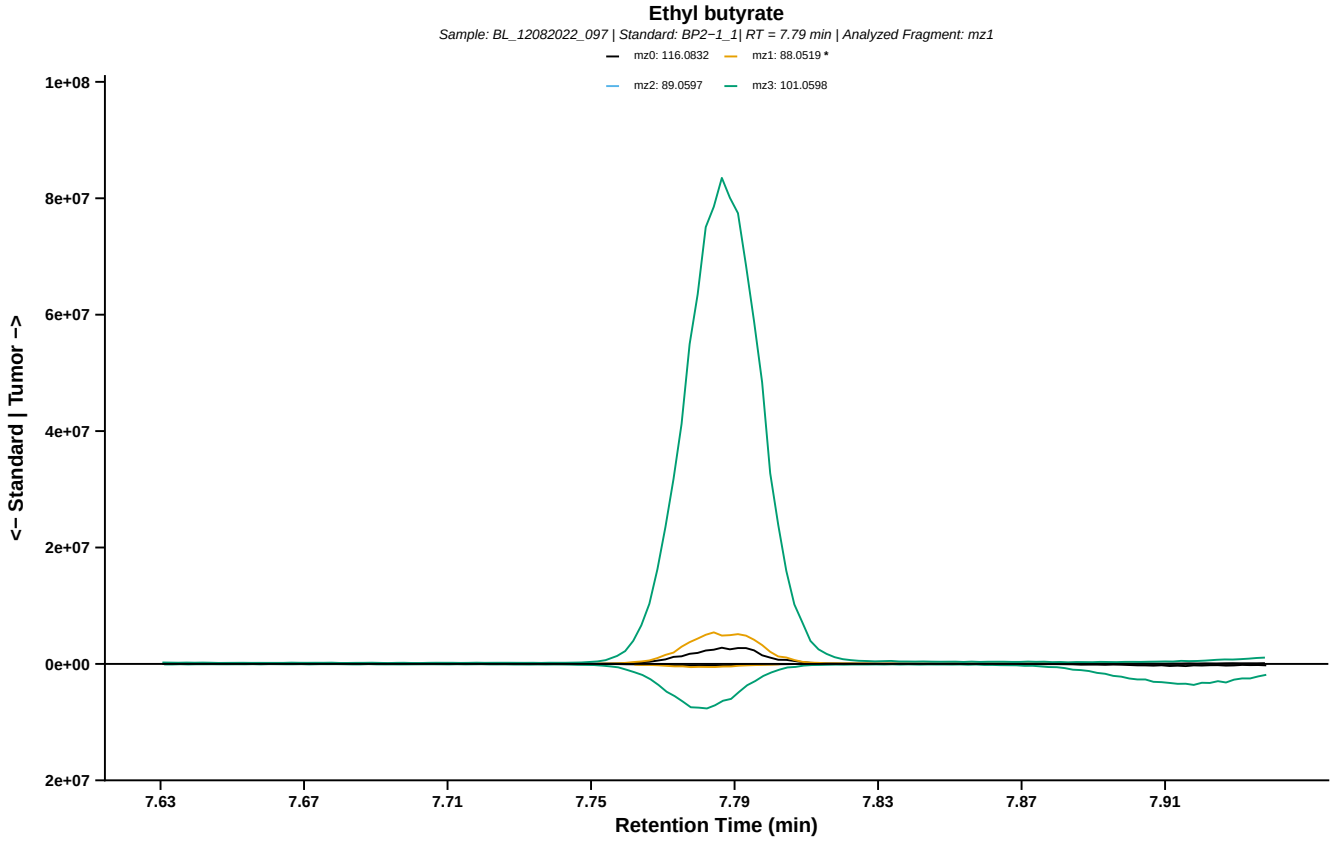


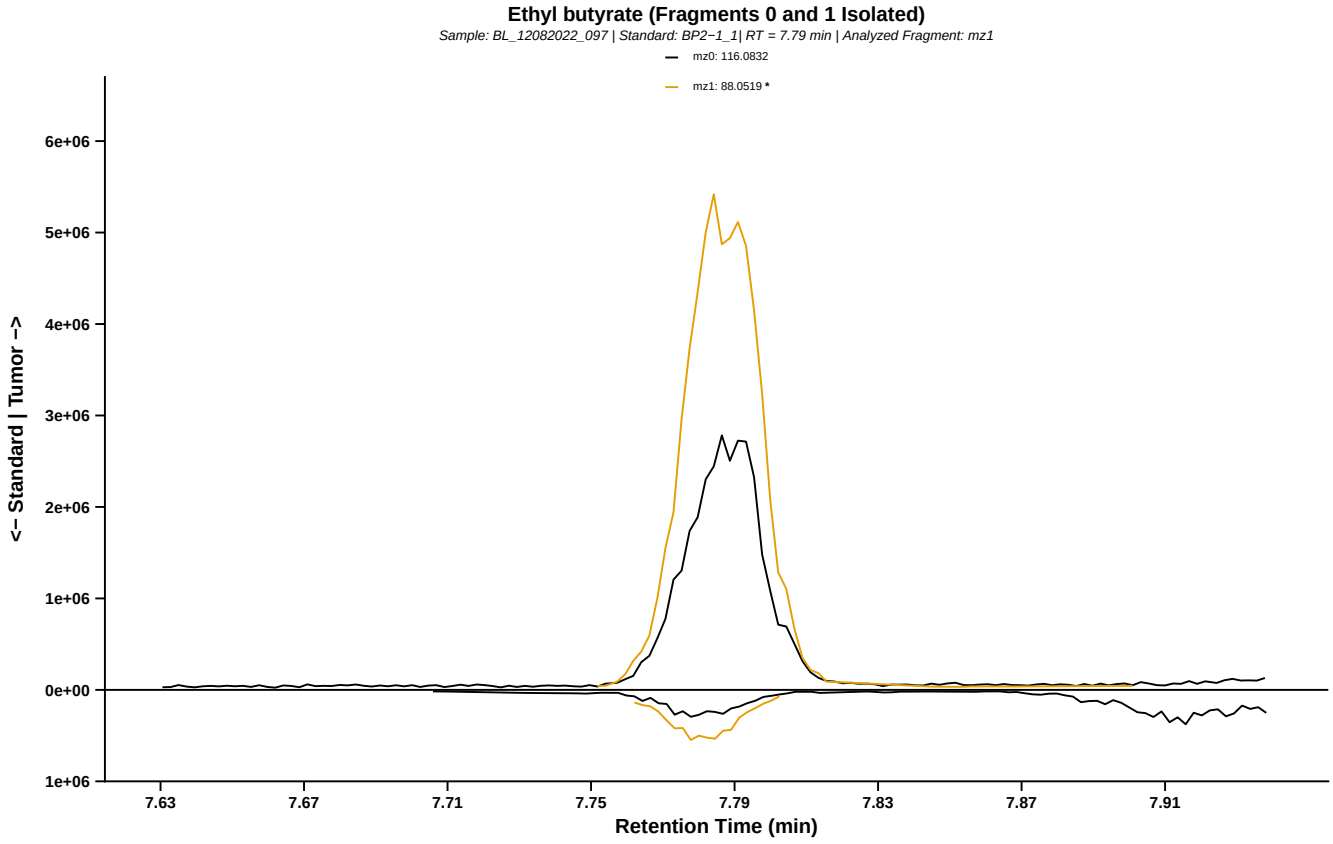
SUPPLEMENTARY FIGURE 2.1 (Continued)



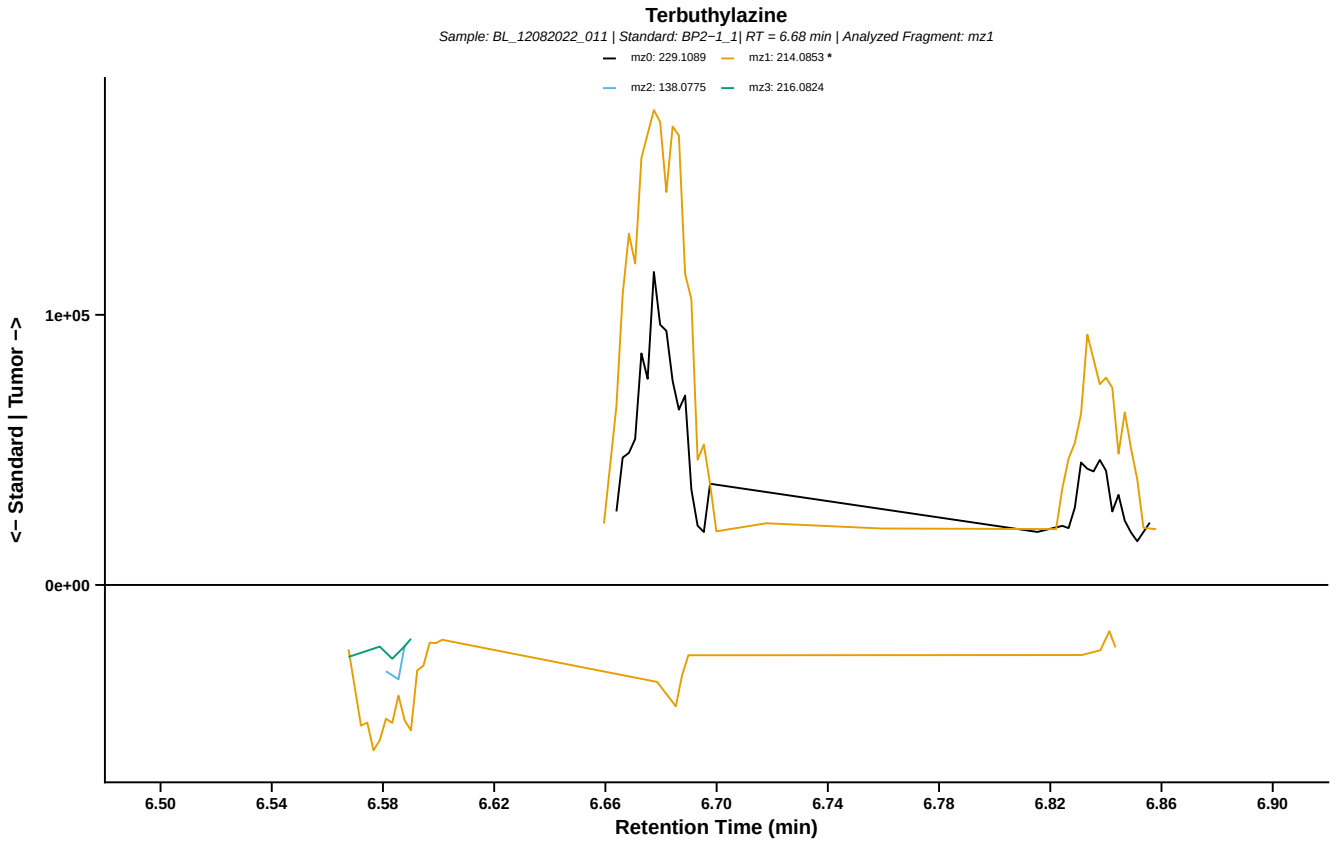


SUPPLEMENTARY FIGURE 2.1 (Continued)

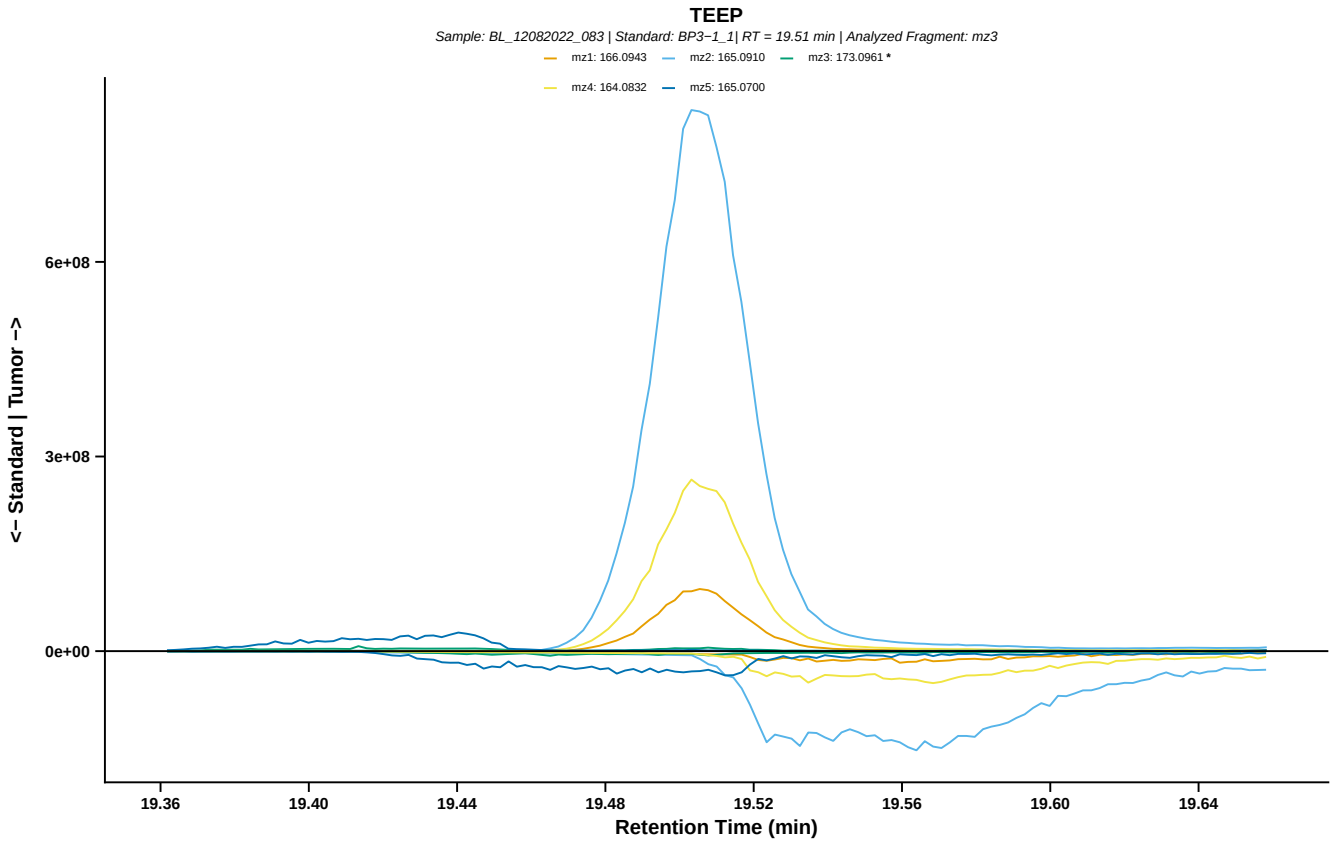


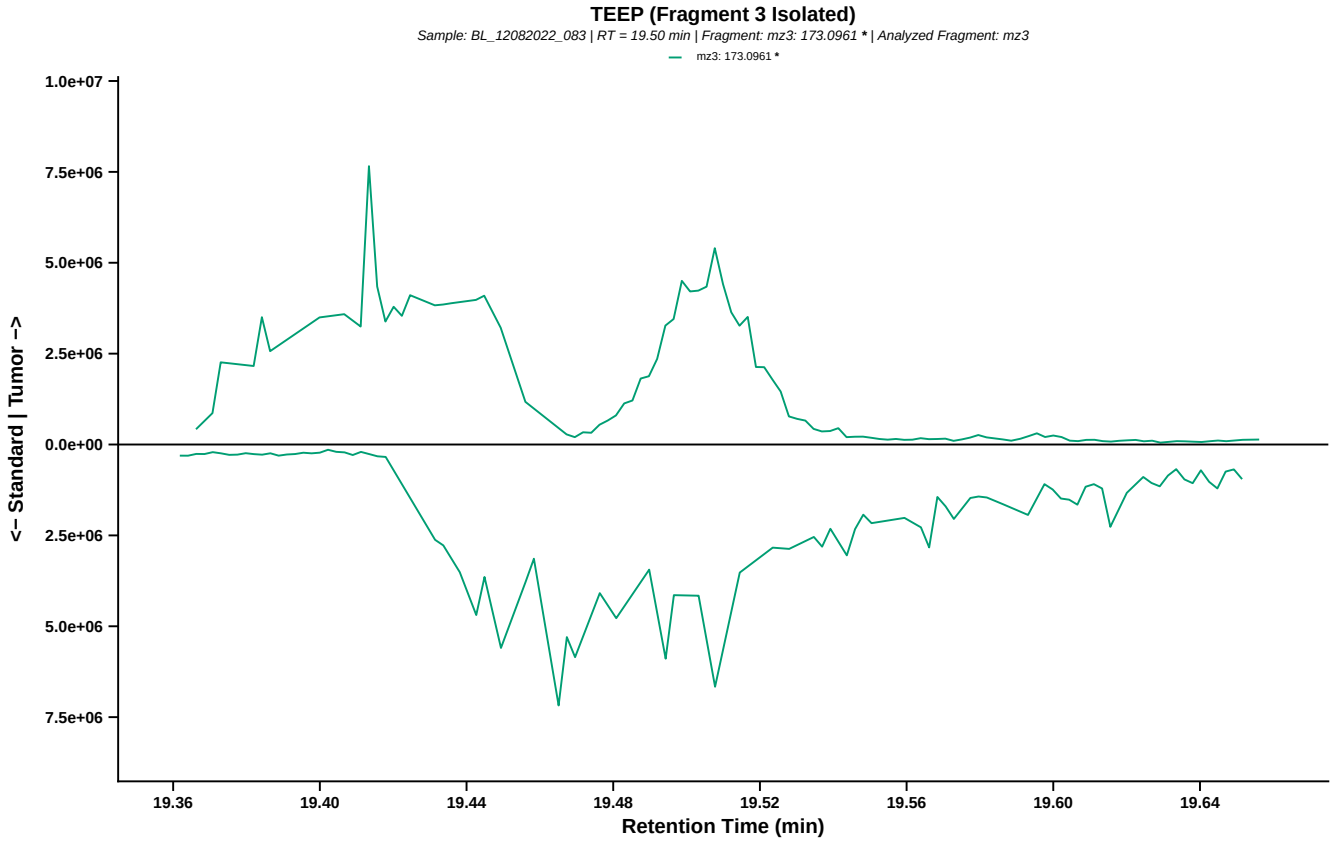


SUPPLEMENTARY FIGURE 2.1 (Continued)

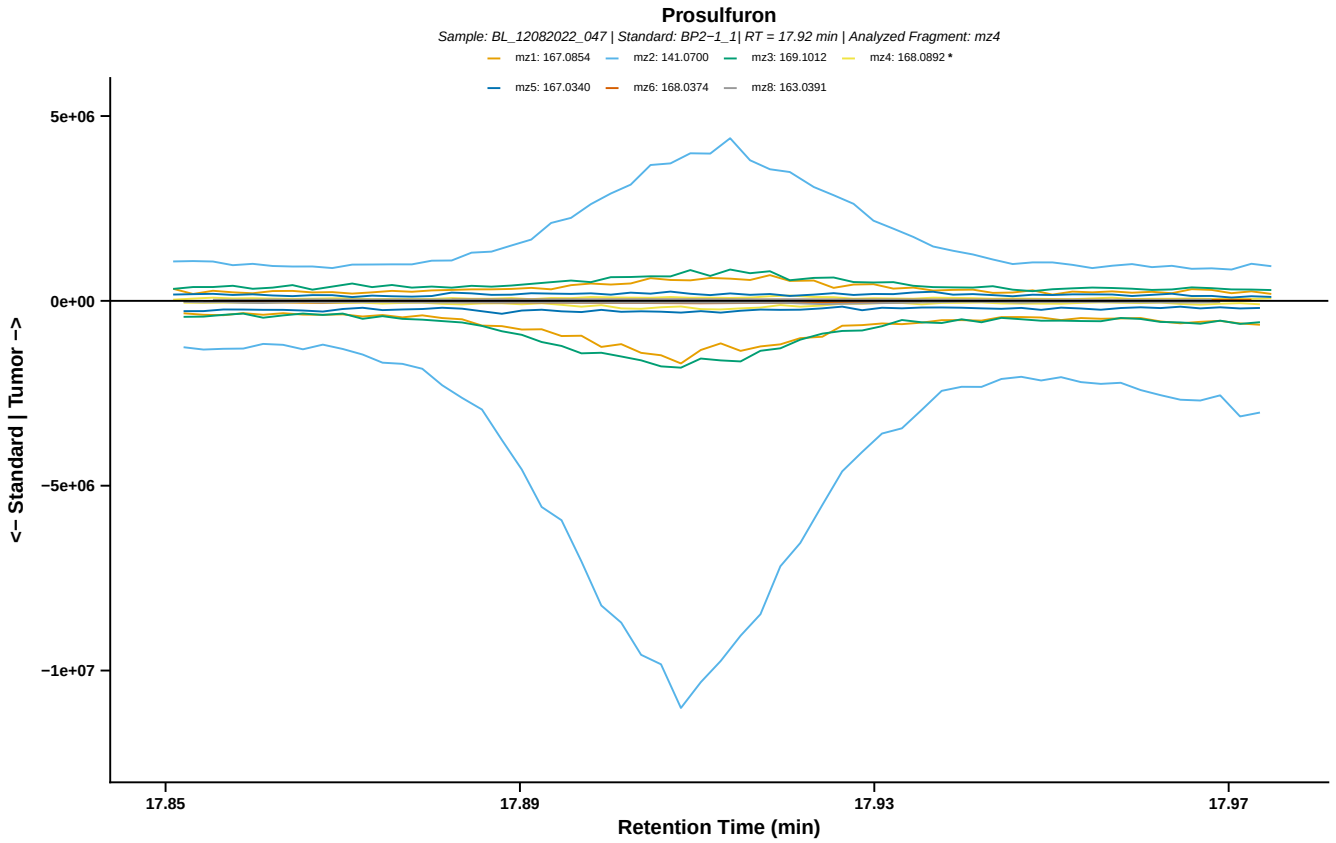


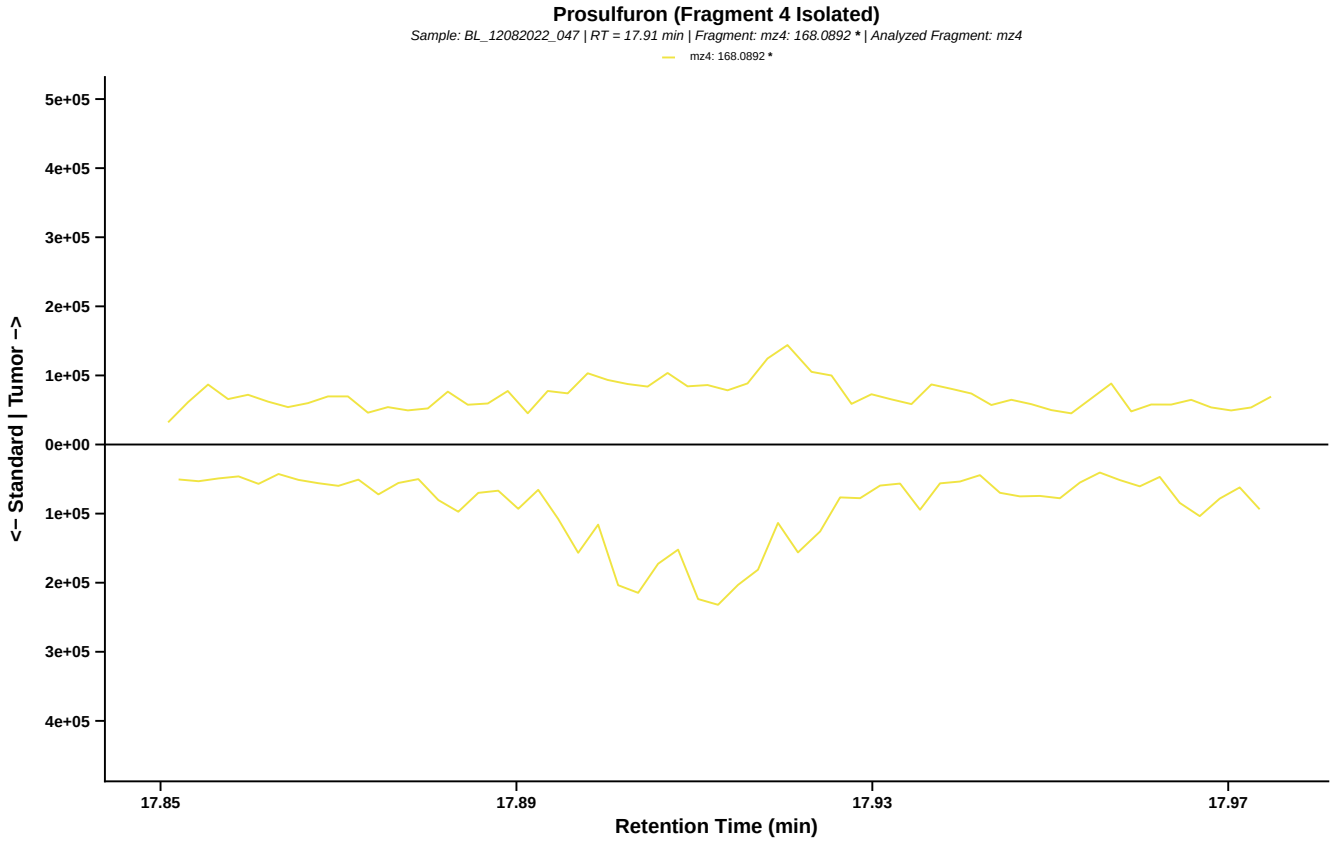
SUPPLEMENTARY FIGURE 2.1 (Continued)



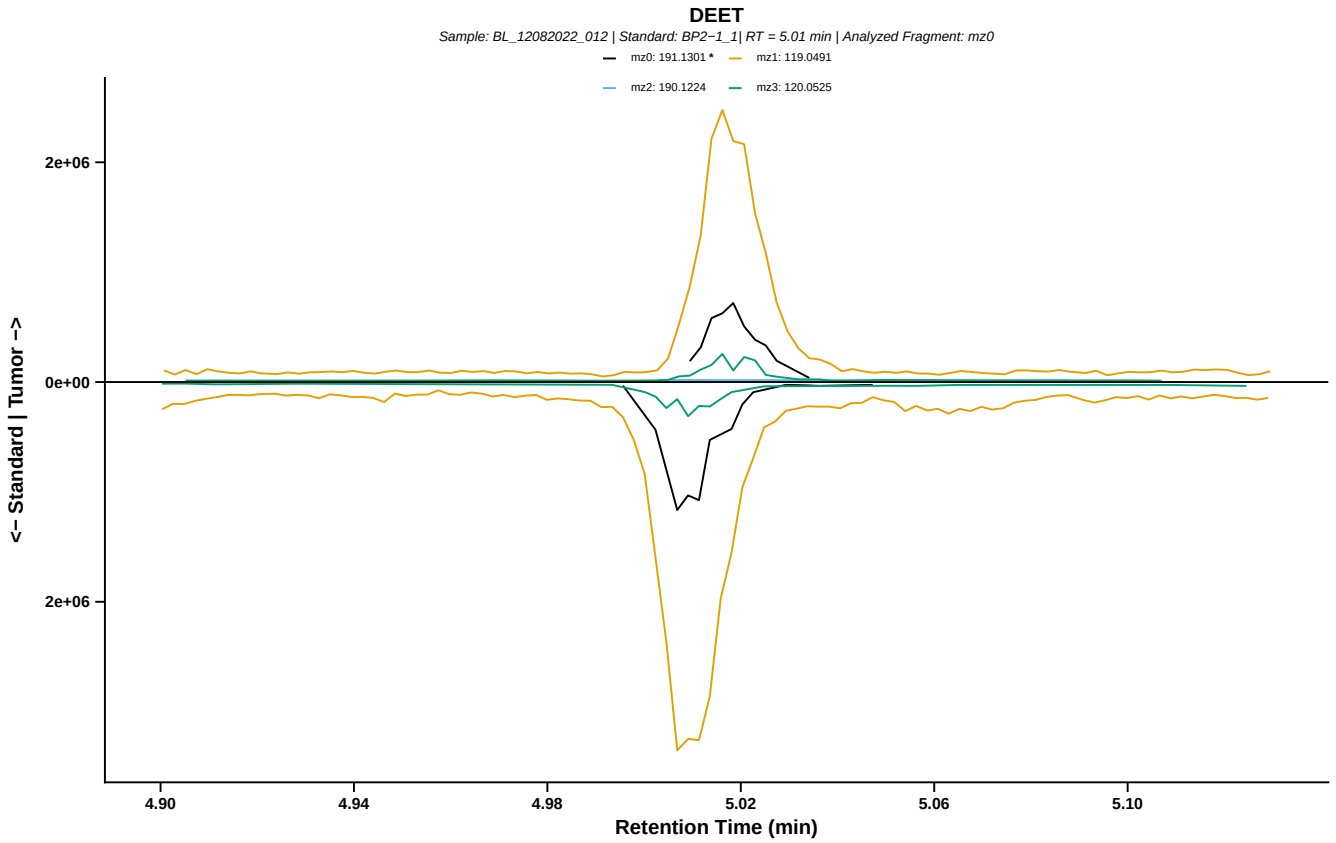


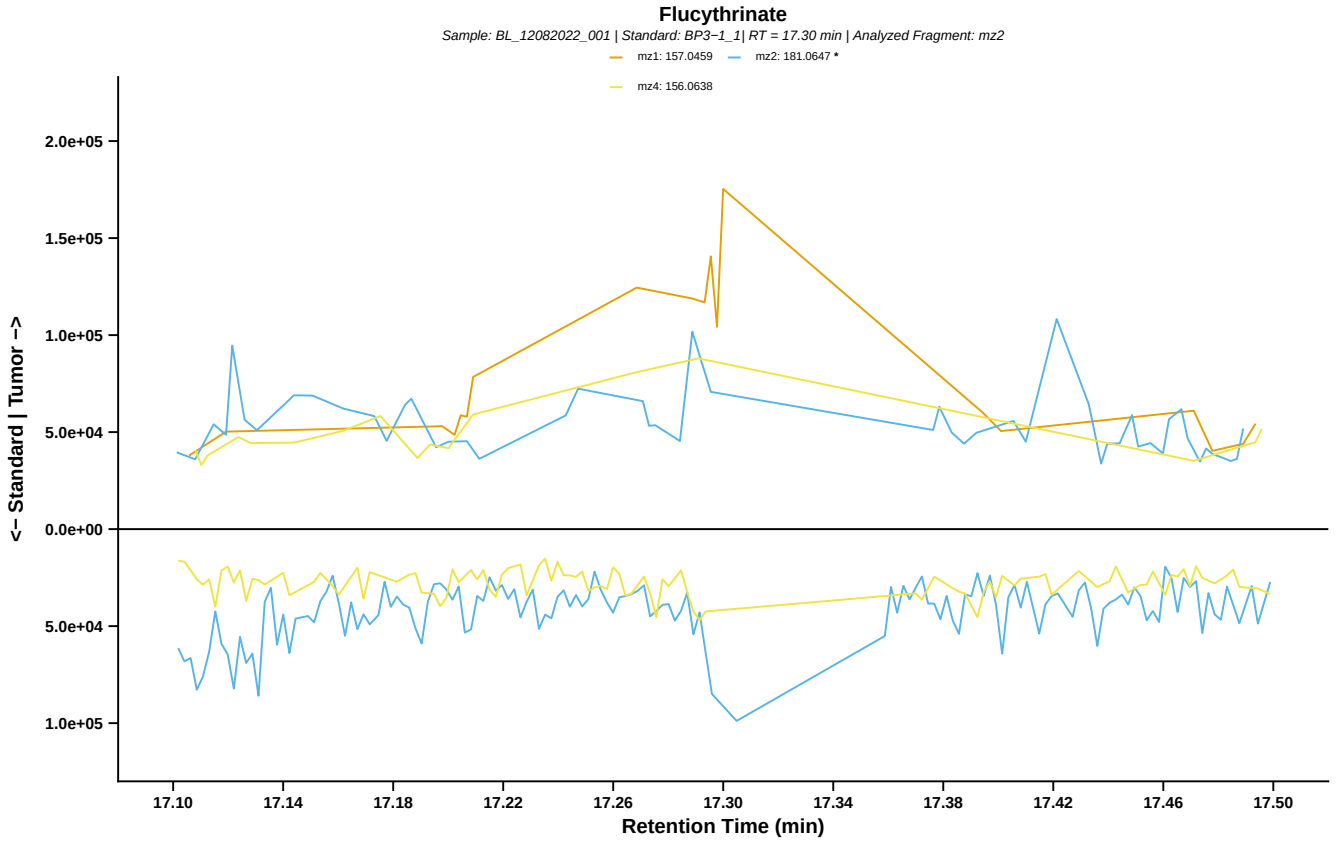
SUPPLEMENTARY FIGURE 2.1 (Continued)



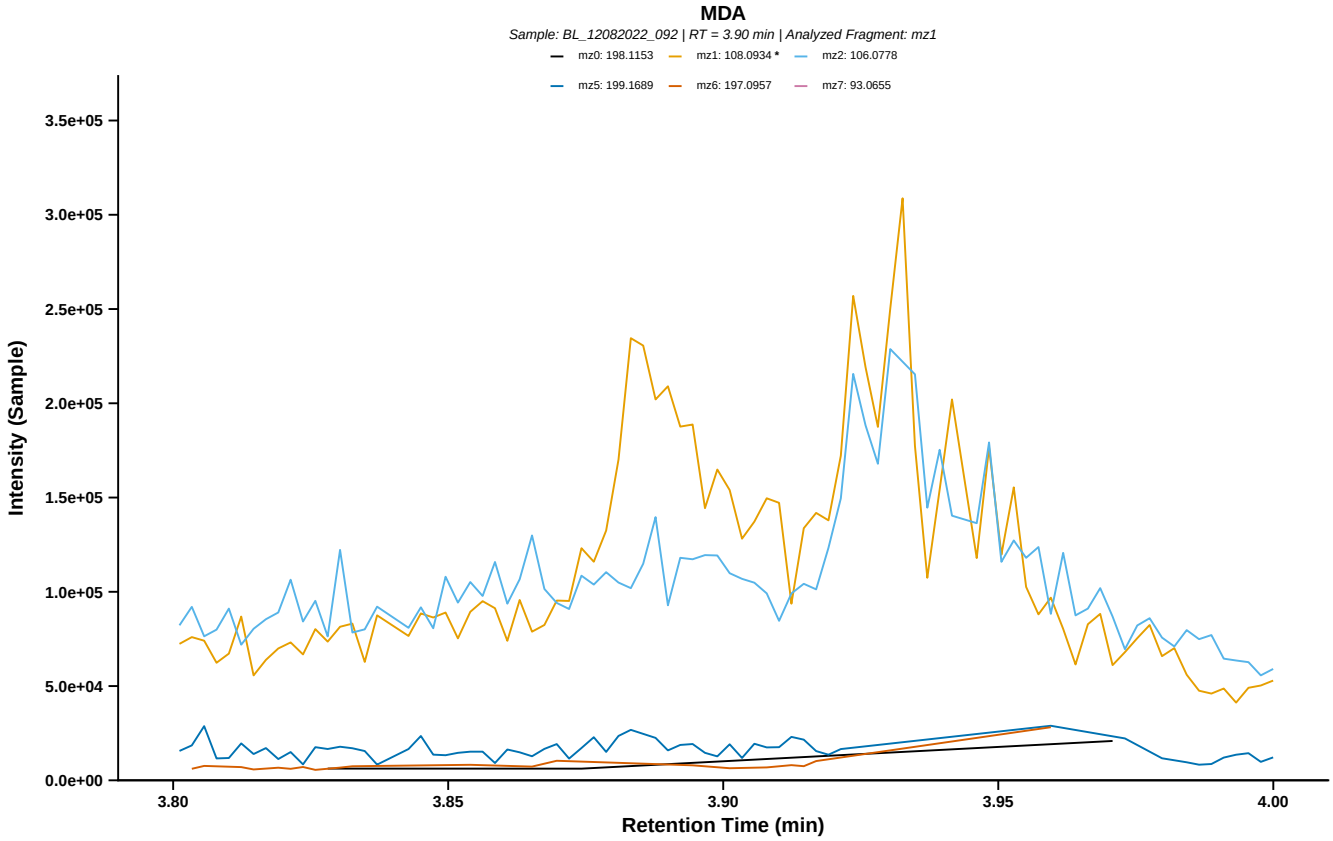


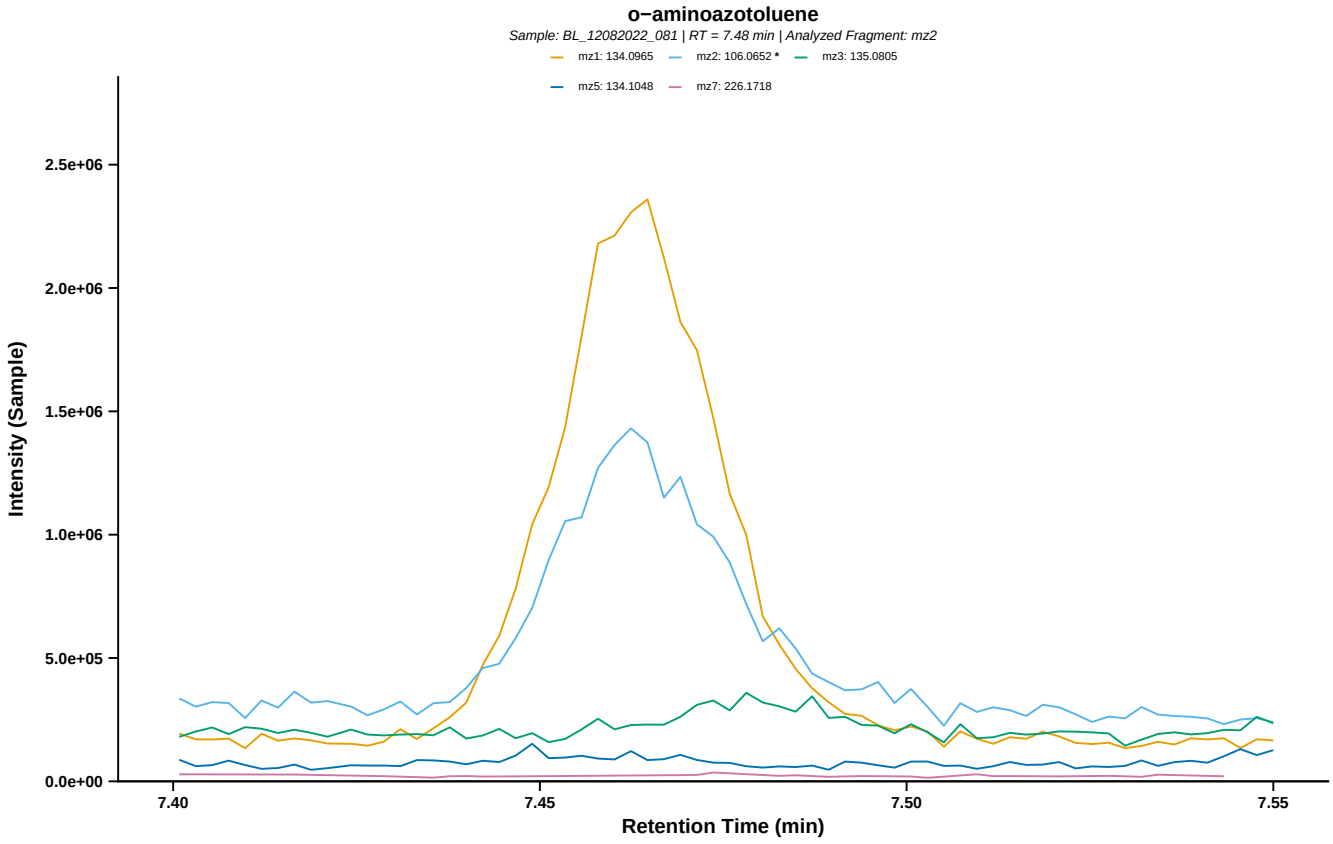
SUPPLEMENTARY FIGURE 2.1 (Continued)



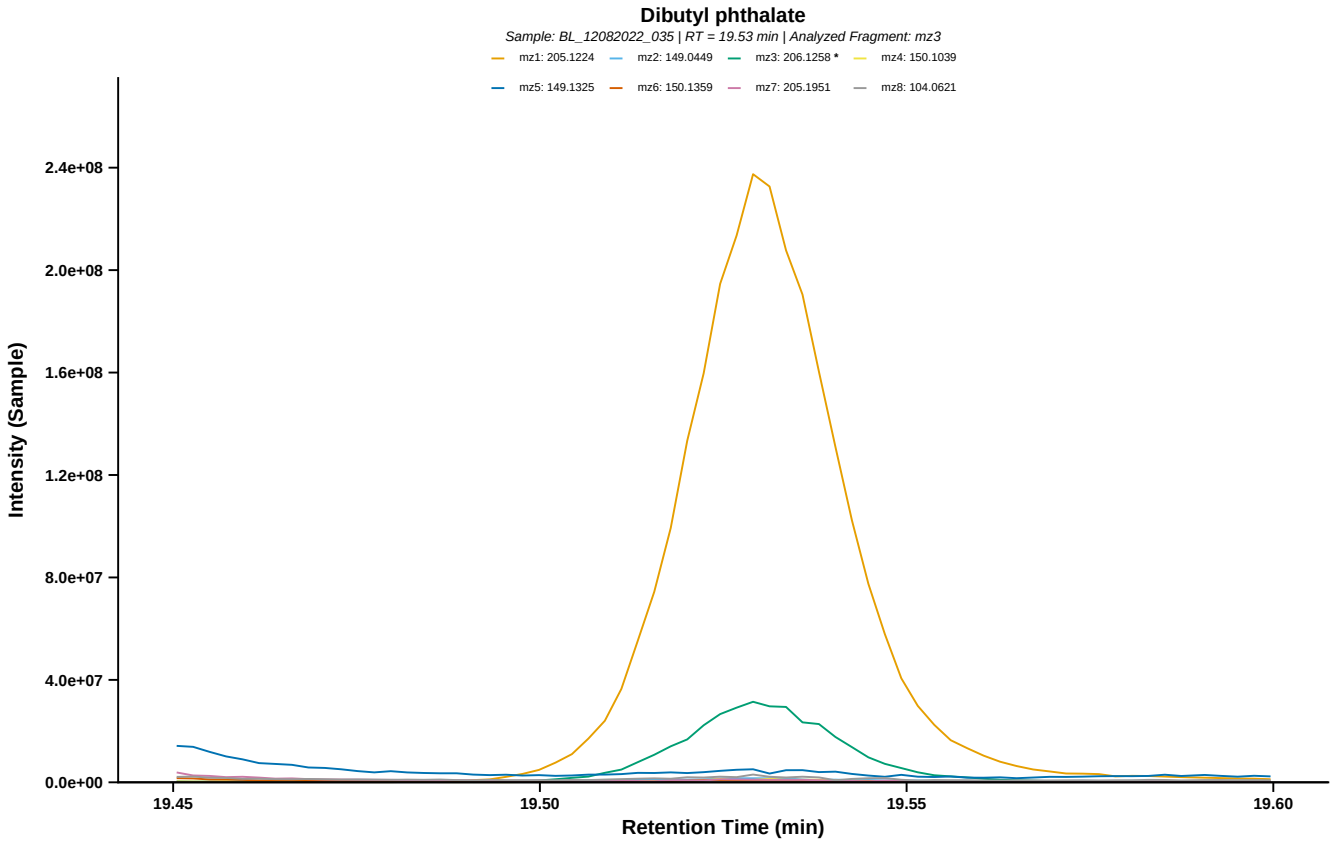


SUPPLEMENTARY FIGURE 2.2

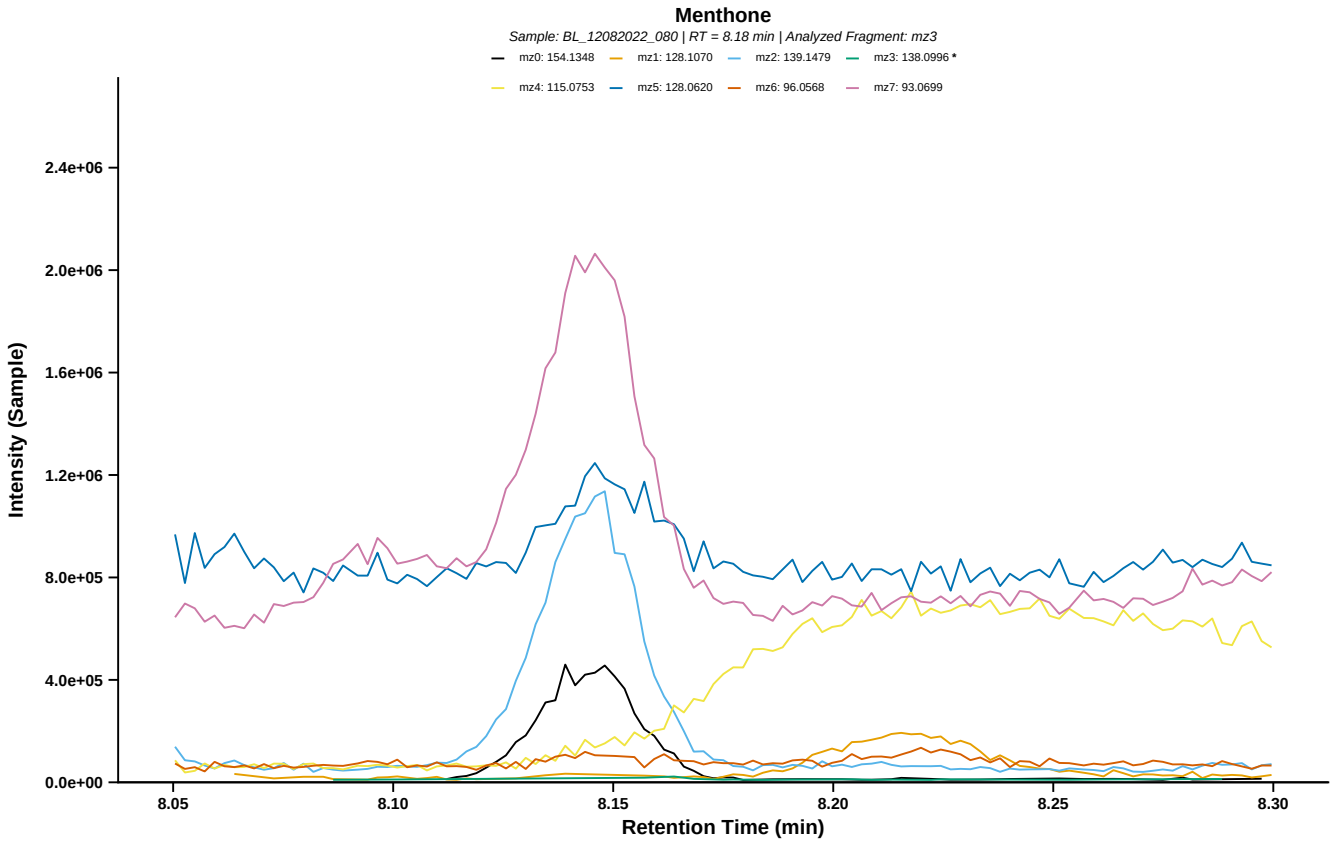


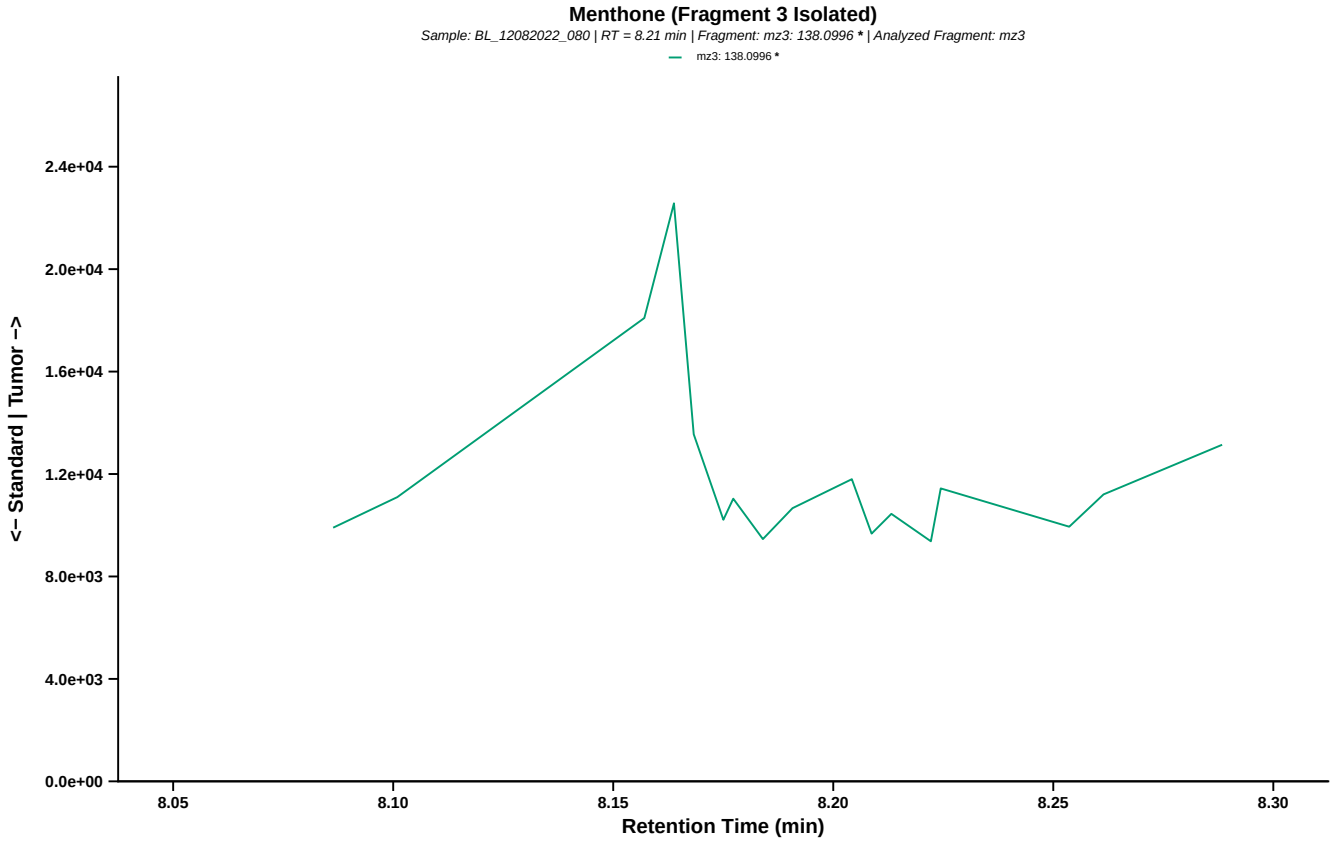


SUPPLEMENTARY FIGURE 2.2



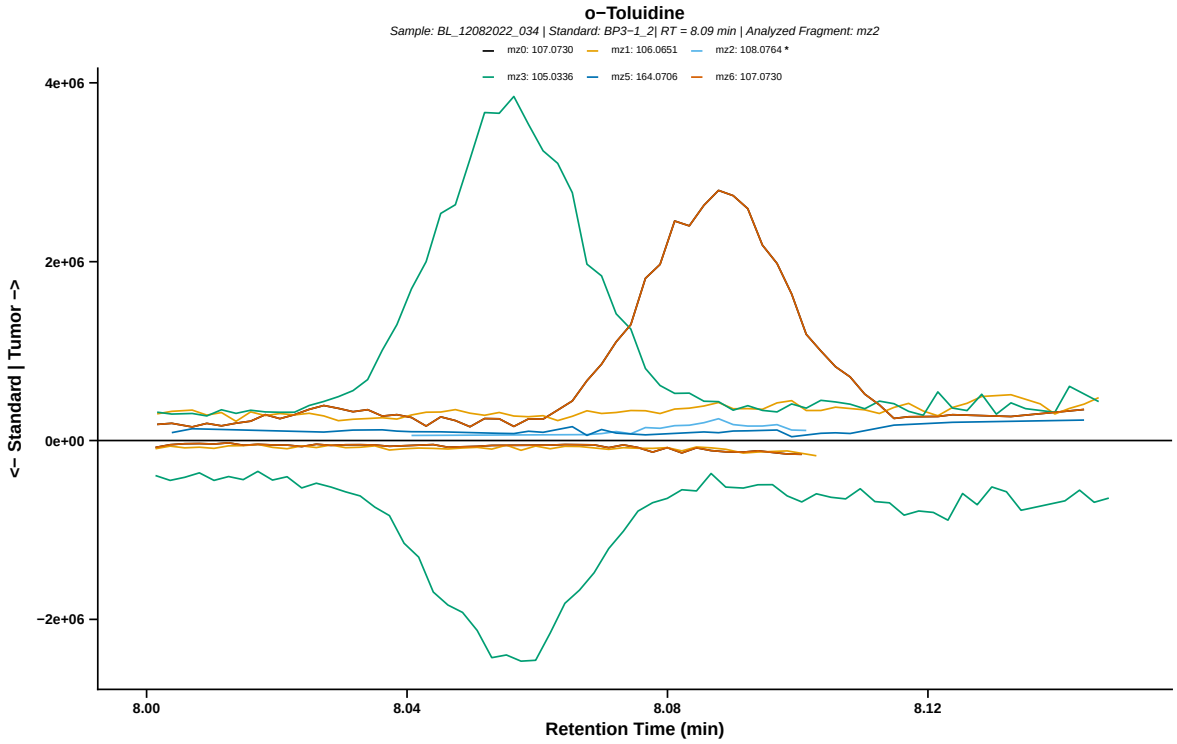
SUPPLEMENTARY FIGURE 2.2 (Continued)

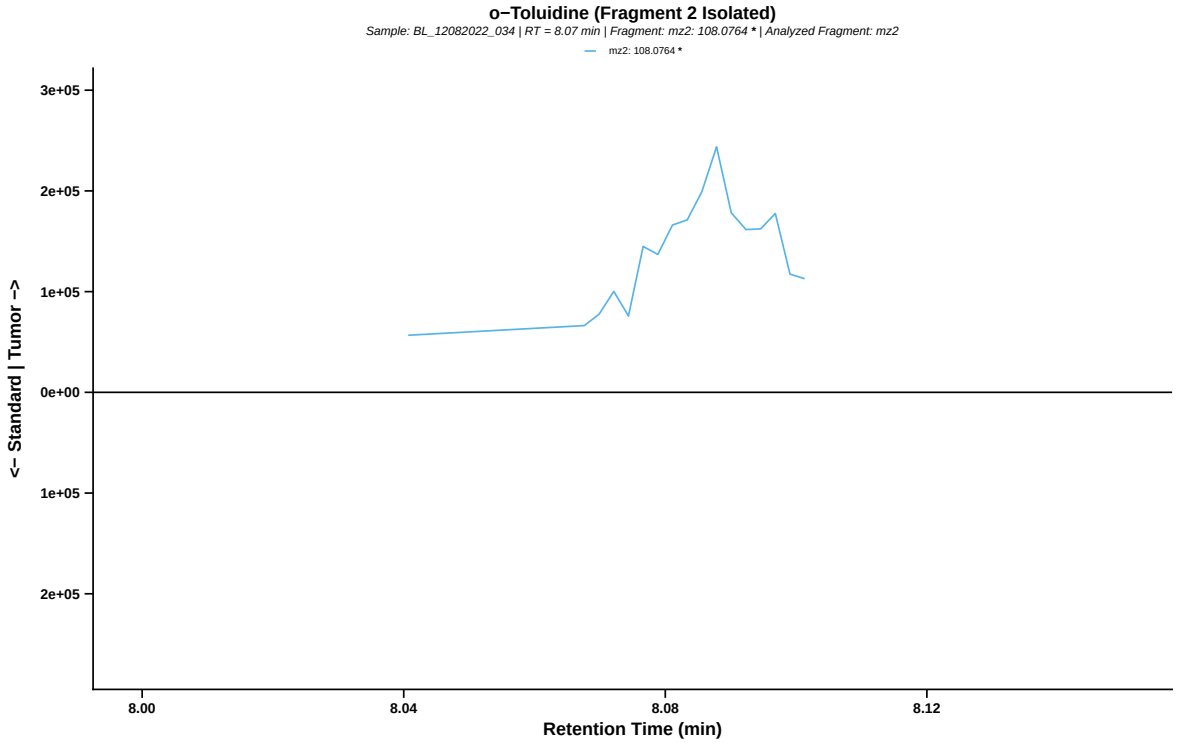




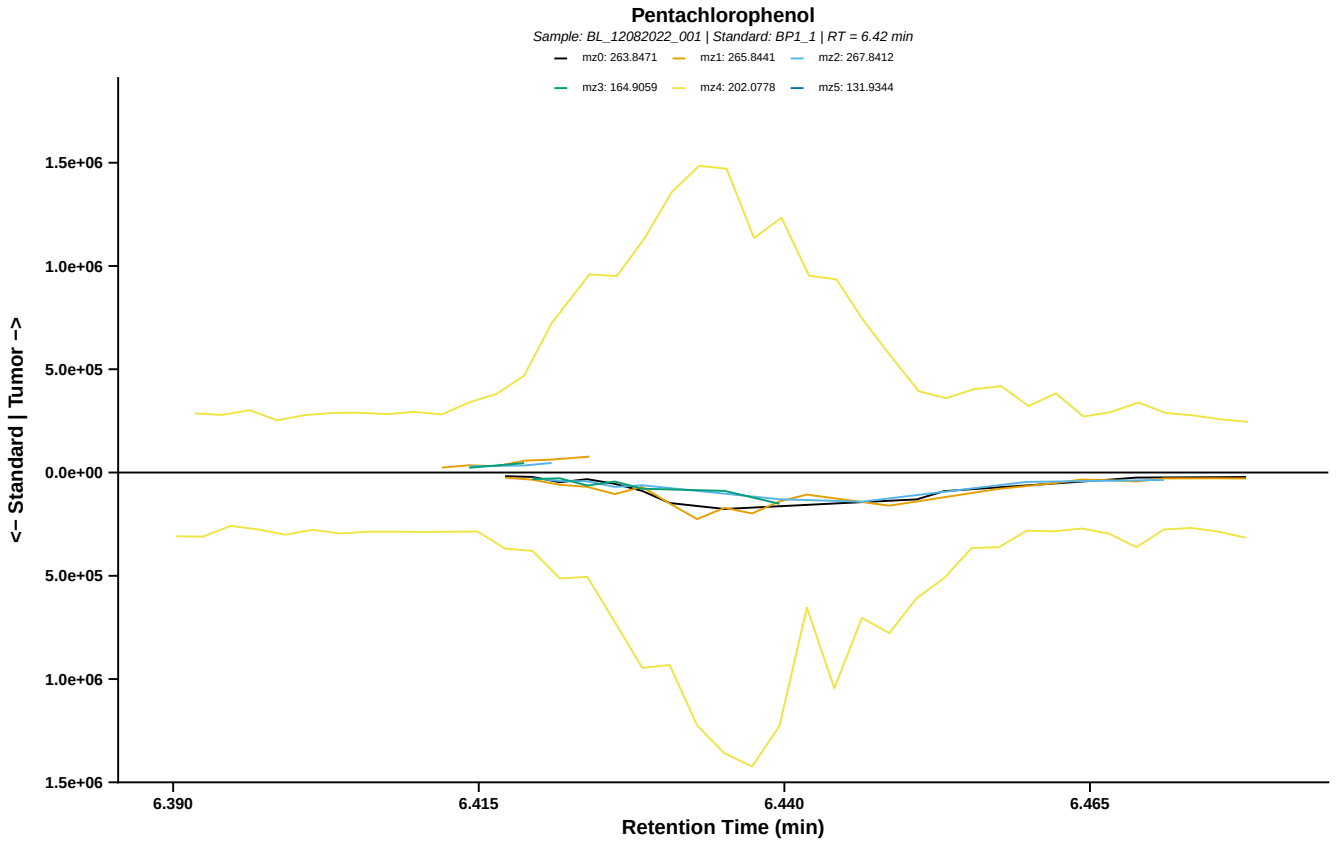
SUPPLEMENTARY FIGURE 3.1

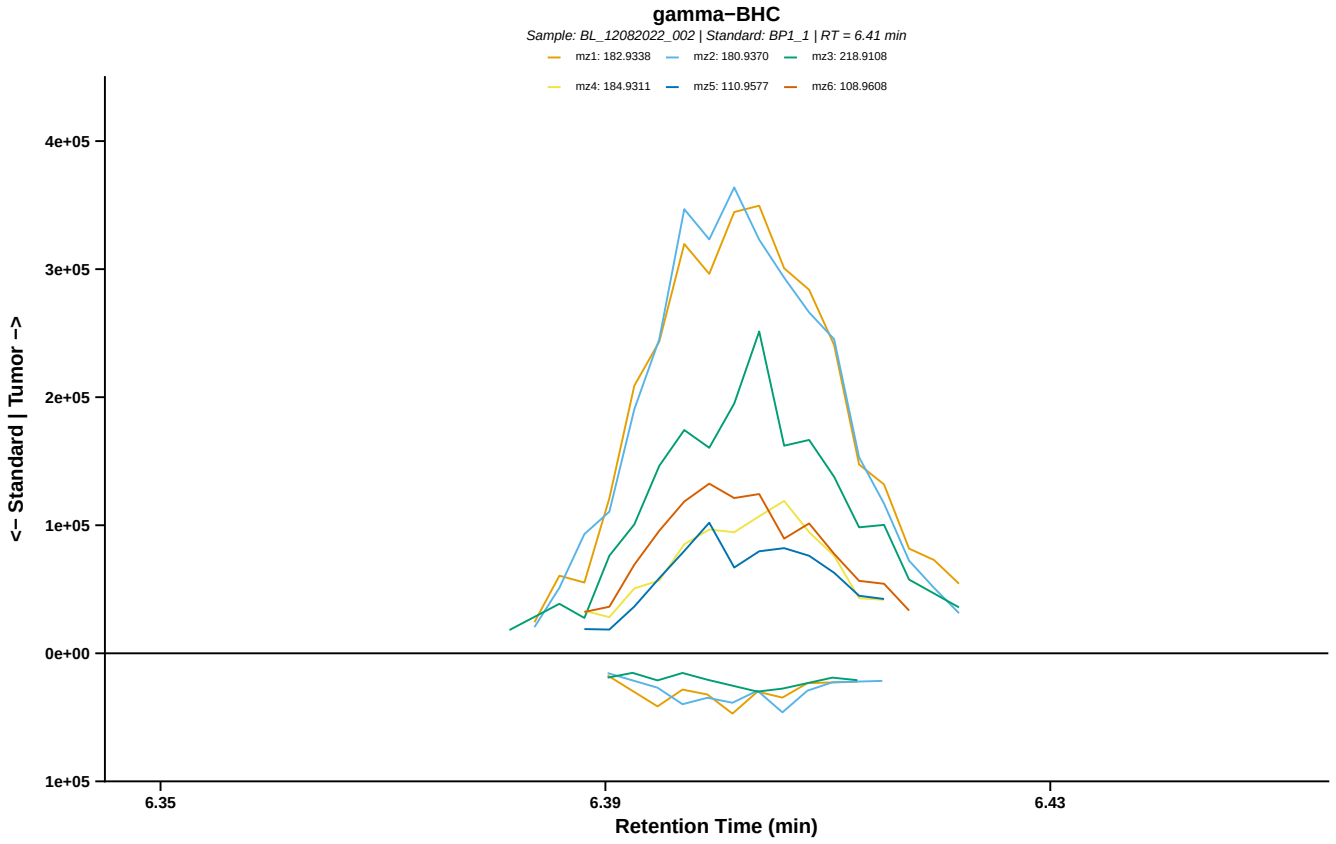
Spectral validation of IARC Group 1 chemicals annotated in tumor samples. Sample spectra for all IARC Group 1 carcinogens annotated in thyroid tumor tissue, displayed either as mirrored plots with reference standard (sample intensity in positive y-axis, standard intensity in negative y-axis) or as non-mirrored plots without standard when reference co-elution was inadequate. Mirrored plots with co-elution of multiple fragments in both standard and sample are considered "Level 1" identifications (3.1, pp. 32-34), while non-mirrored plots where multiple fragments co-elute in the sample but the standard does not show proper co-elution are considered "Level 2" identifications (3.2, pp. 35-36). Asterisks (*) indicate the fragment used for statistical comparison and displayed in Figure 3 and/or Table 3. For select compounds, additional plots display isolated fragments for enhanced visualization clarity.



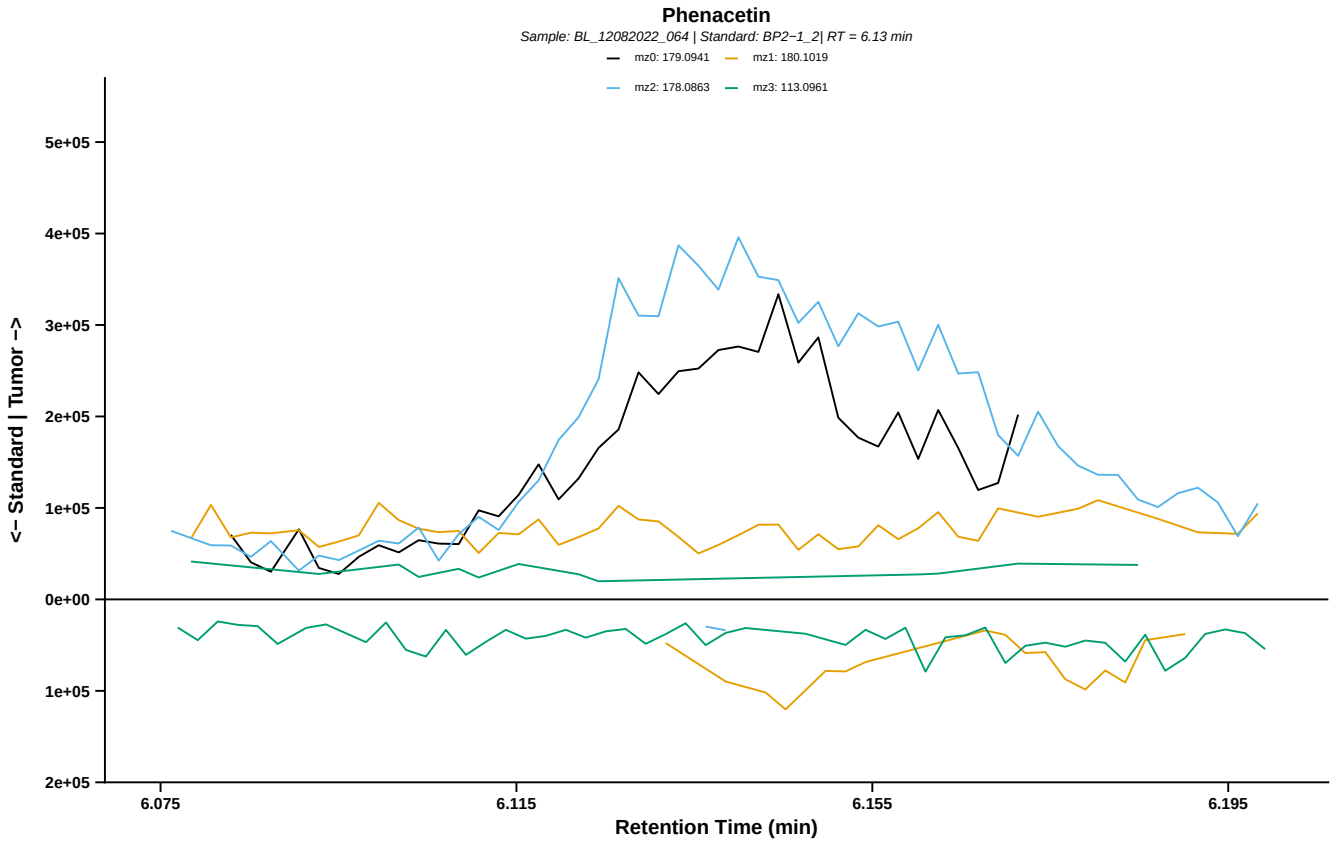


SUPPLEMENTARY FIGURE 3.1 (Continued)

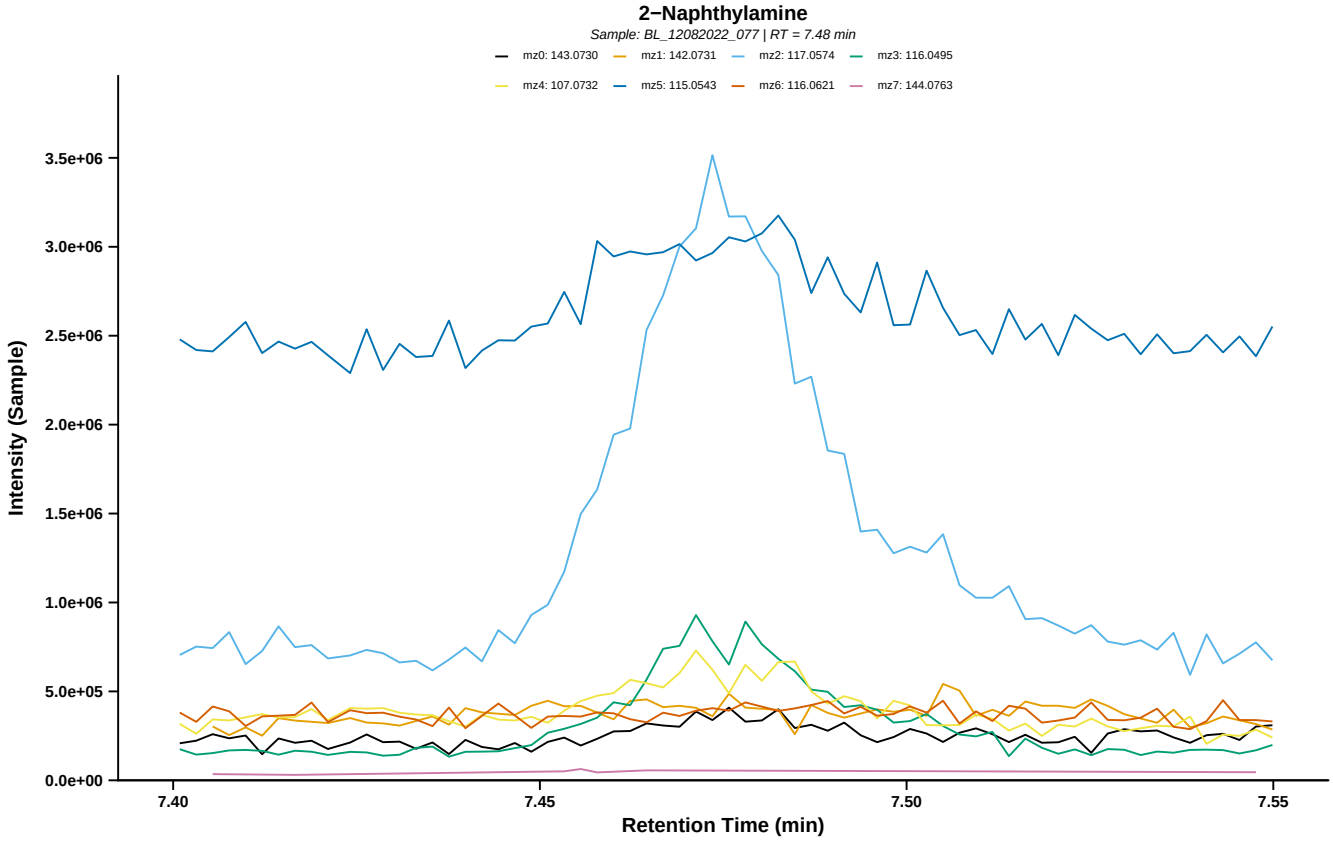


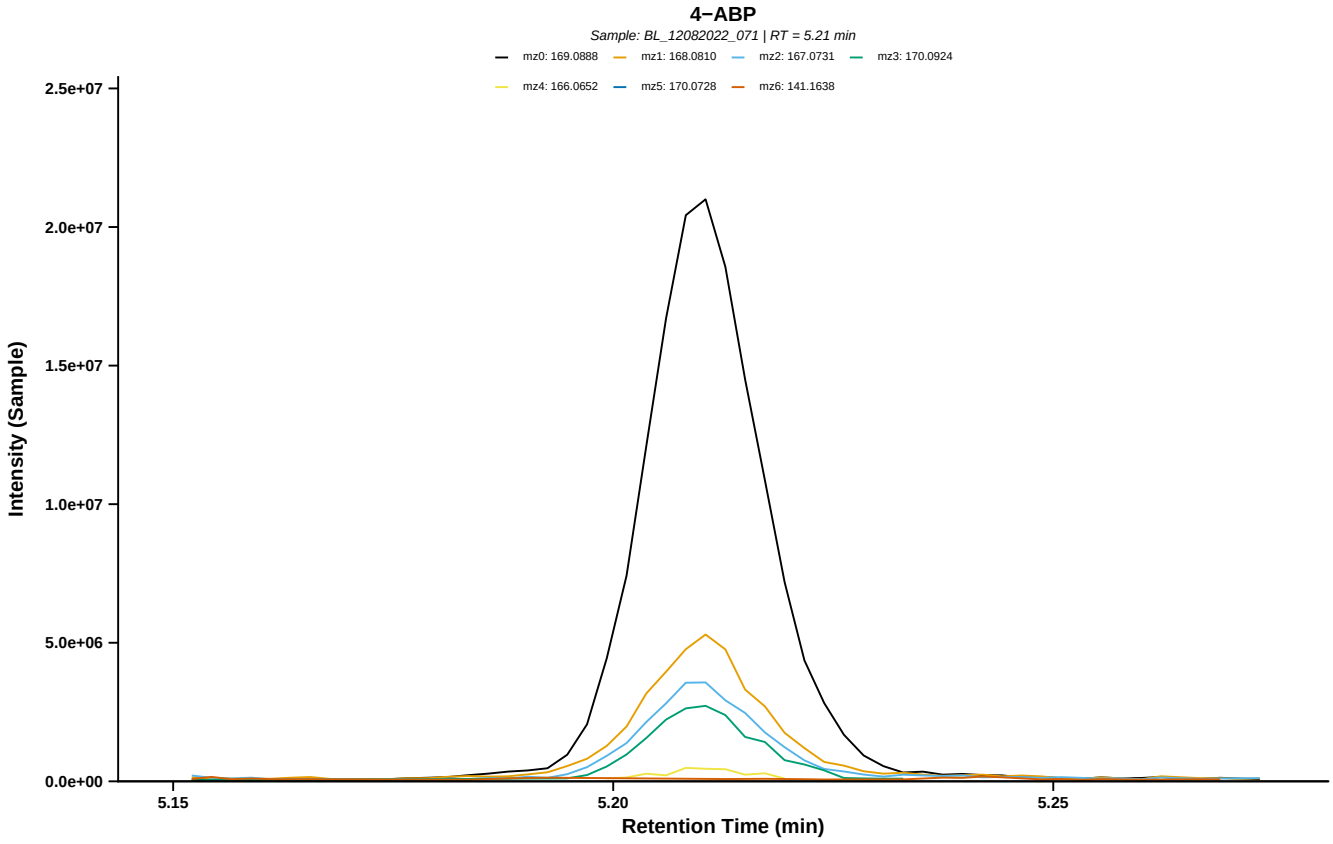


SUPPLEMENTARY FIGURE 3.1 (Continued)

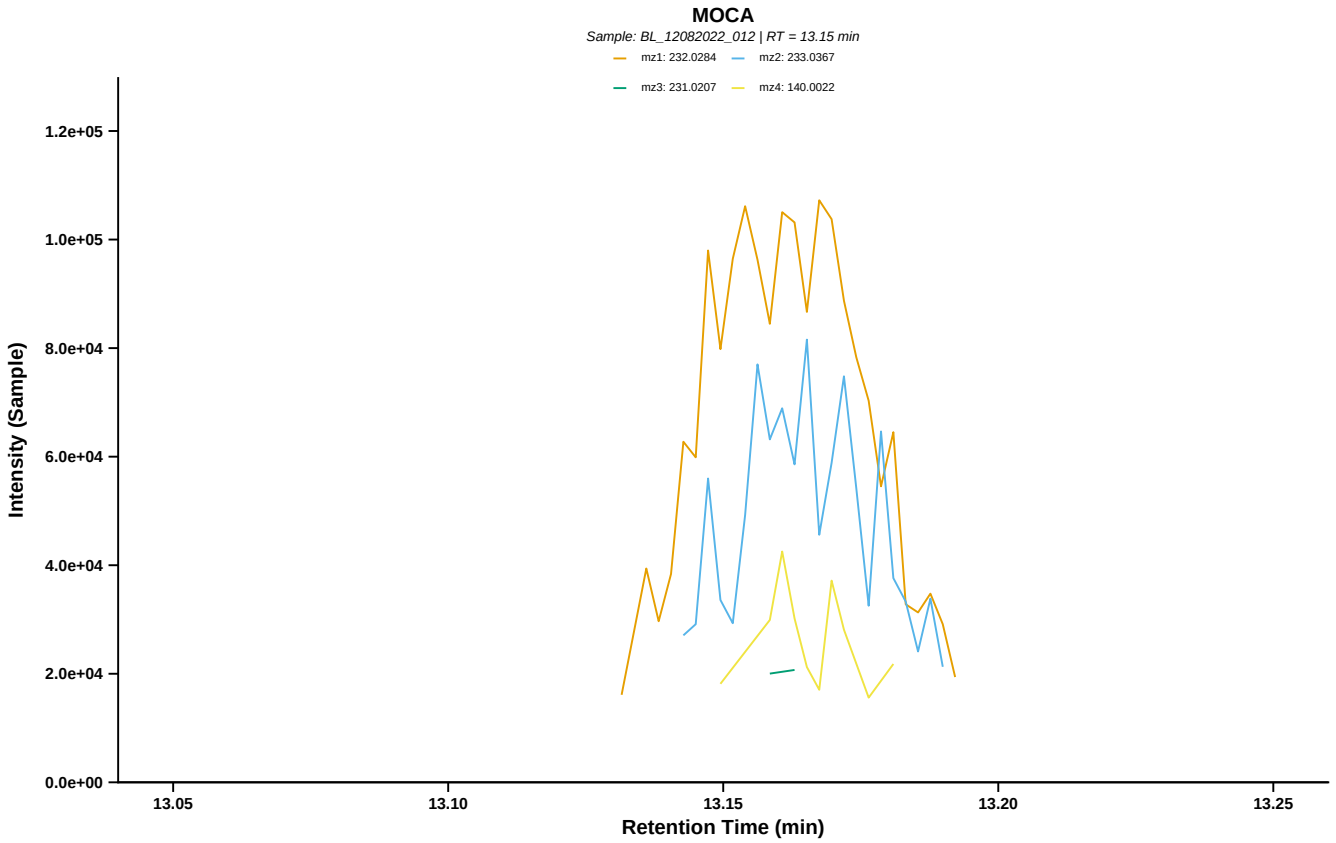


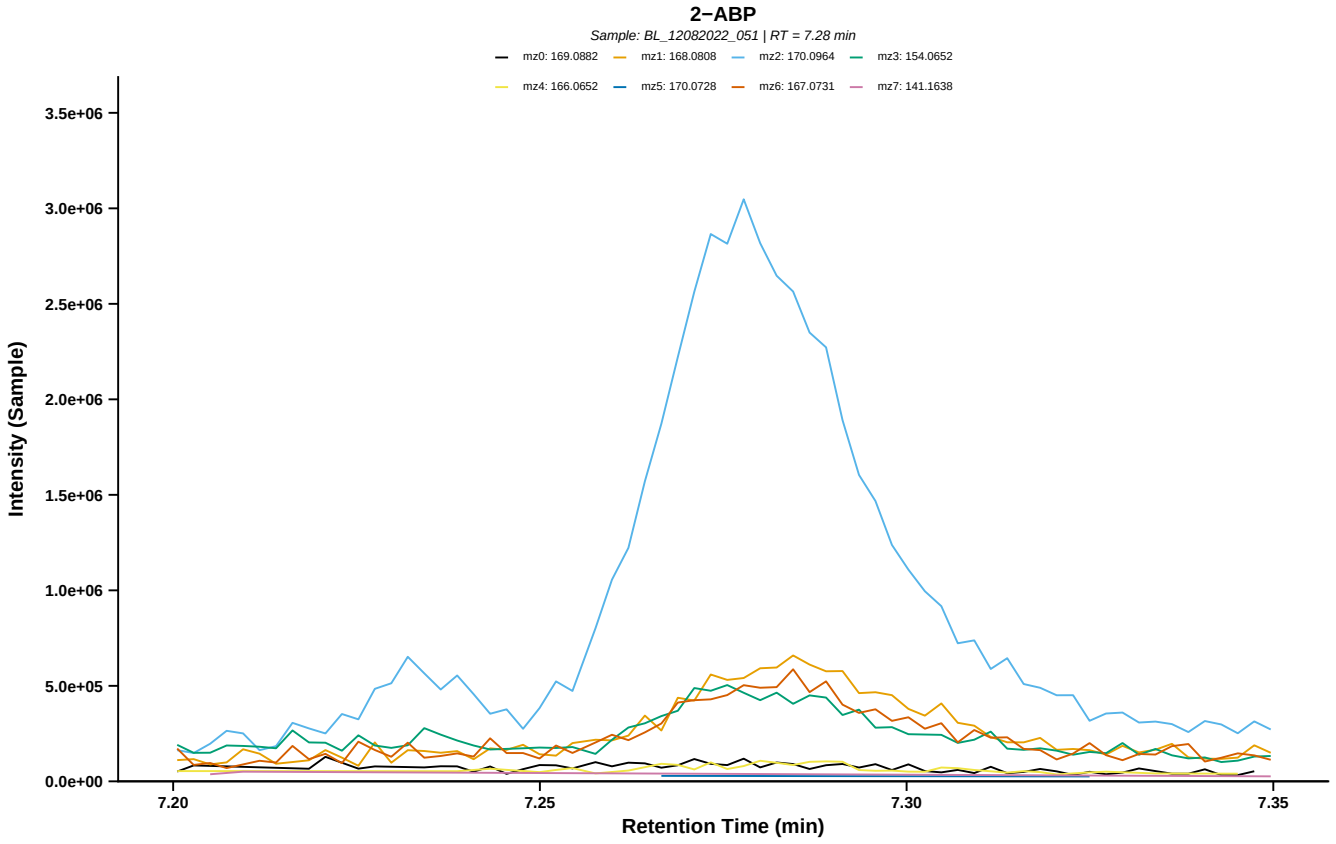
SUPPLEMENTARY FIGURE 3.2





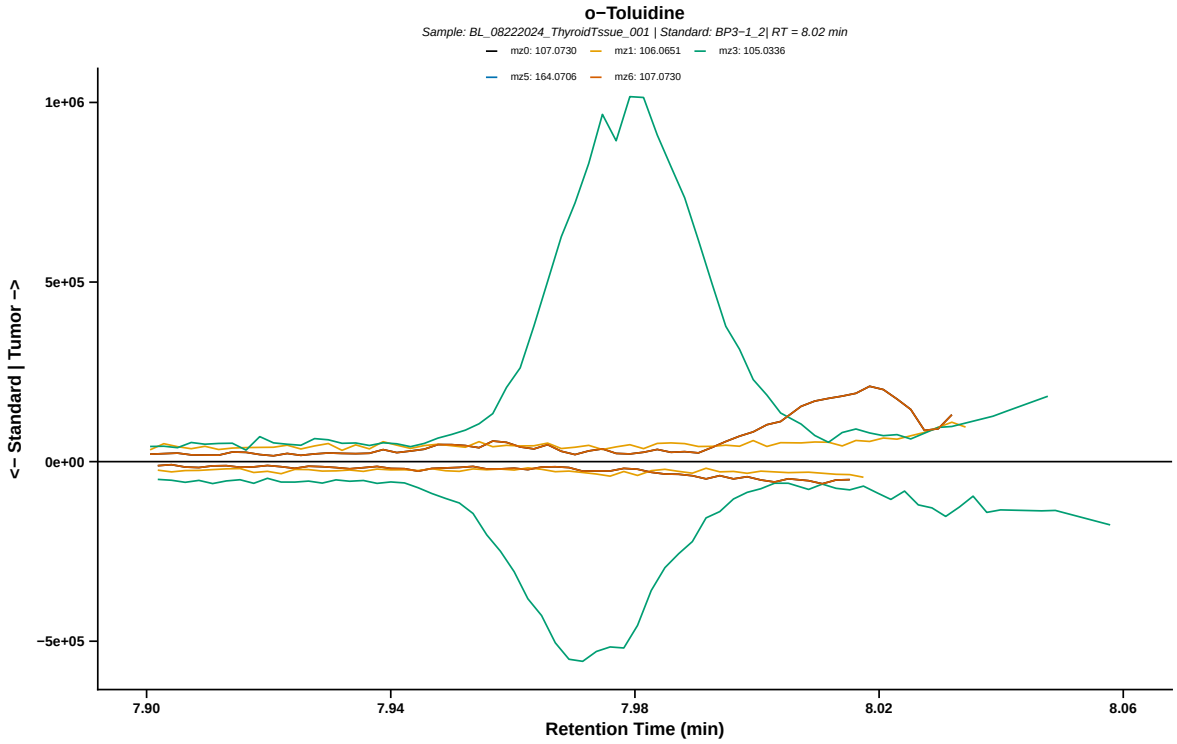
SUPPLEMENTARY FIGURE 3.2

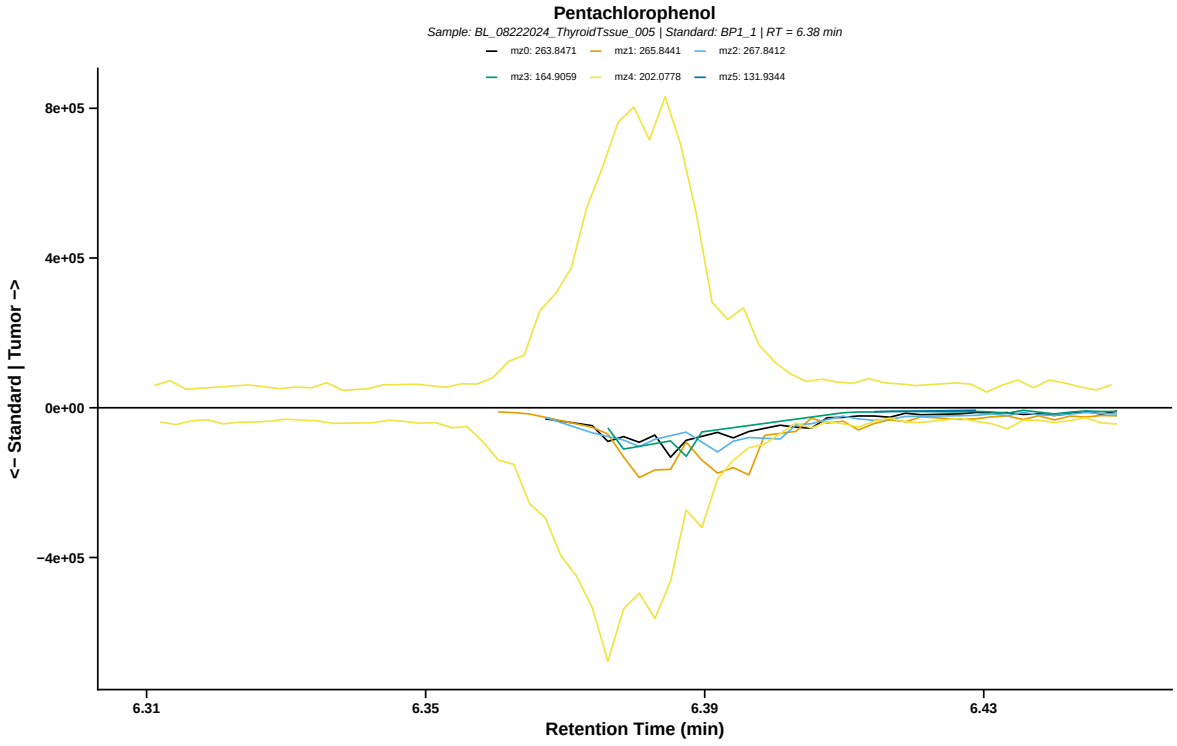




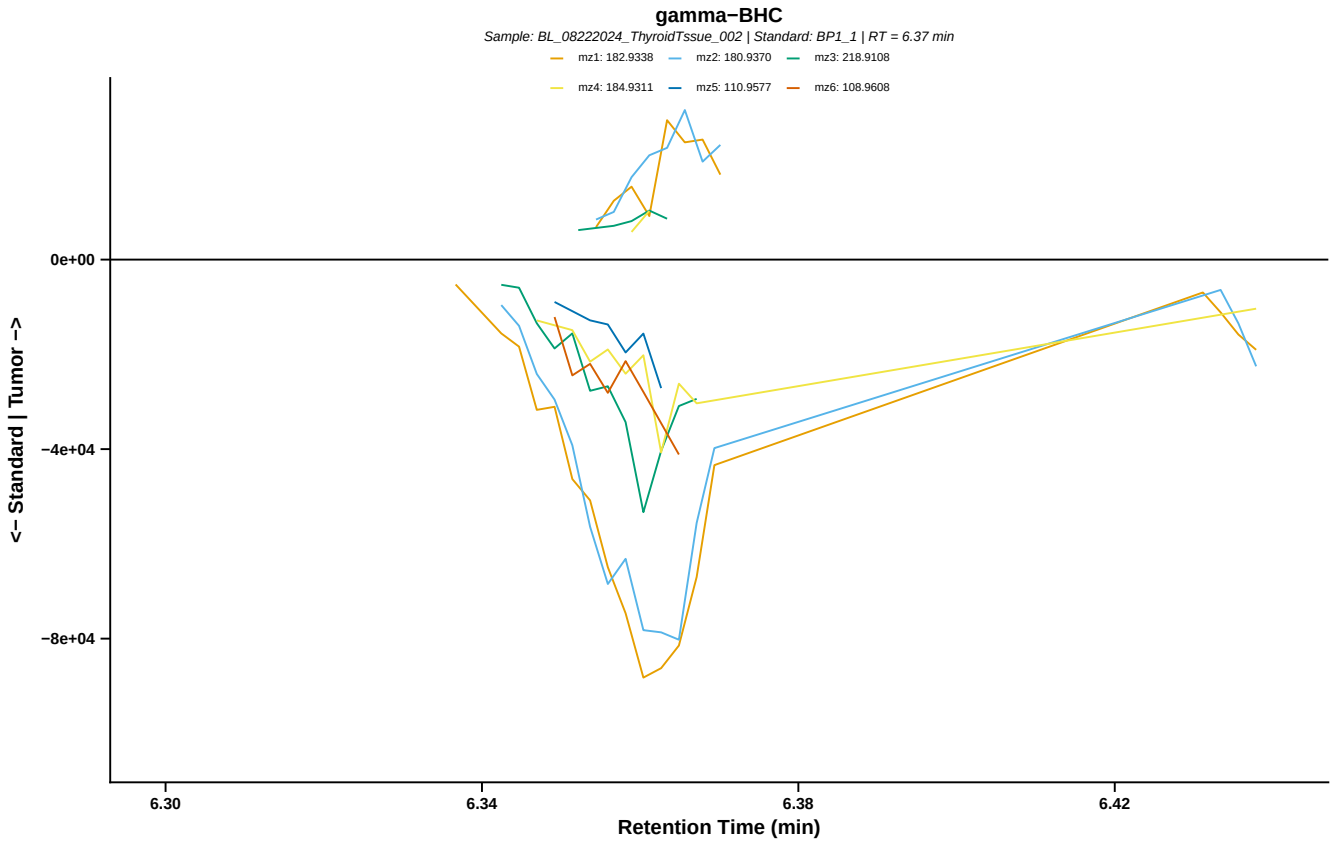
SUPPLEMENTARY FIGURE 4.1

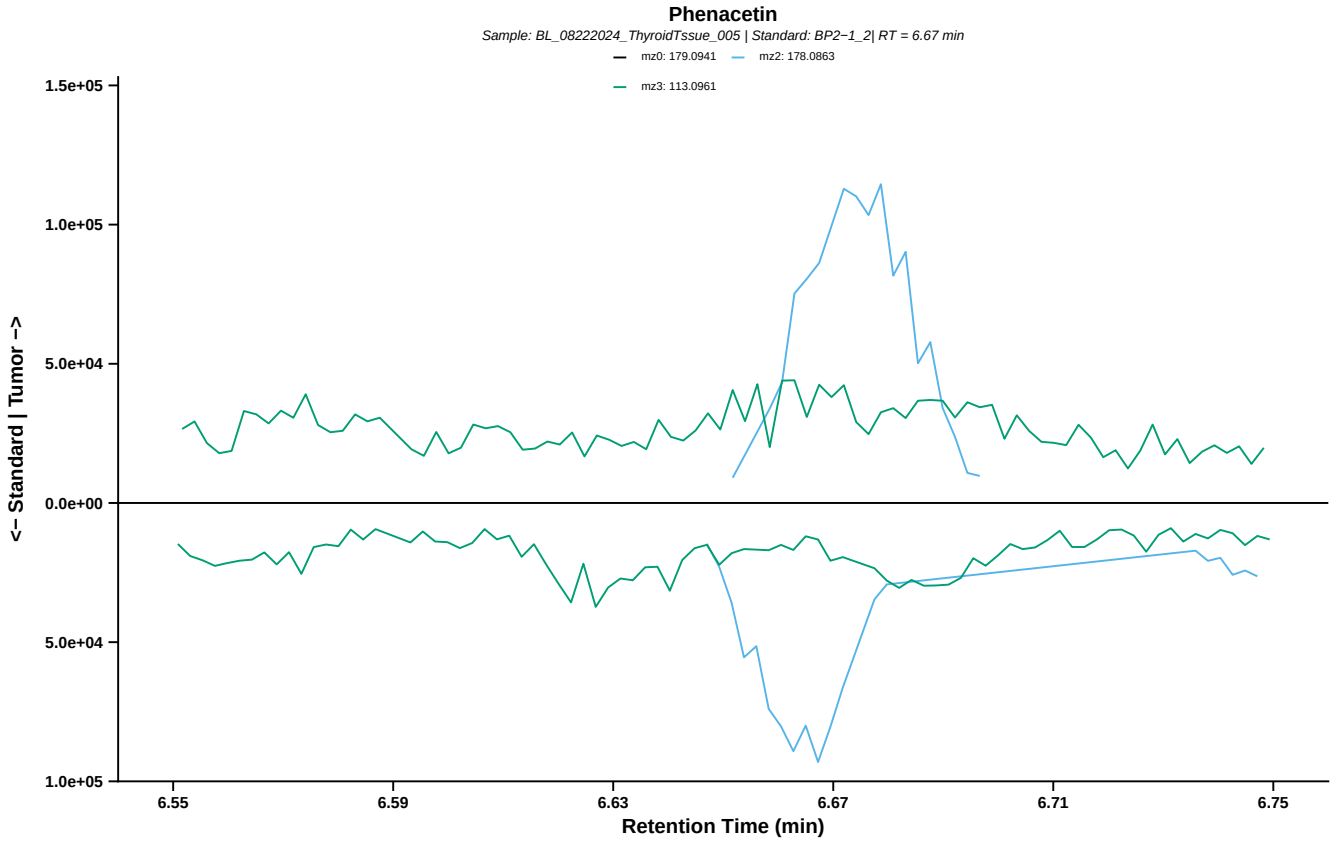
Spectral validation of IARC Group 1 chemicals annotated in cadaver thyroid samples. Sample spectra for all IARC Group 1 carcinogens annotated in non-cancer cadaver thyroid tissue, displayed either as mirrored plots with reference standard (sample intensity in positive y-axis, standard intensity in negative y-axis) or as non-mirrored plots without standard when reference co-elution was inadequate. Mirrored plots with co-elution of multiple fragments in both standard and sample are considered "Level 1" identifications (4.1, pp. 37-39), while non-mirrored plots where multiple fragments co-elute in the sample but the standard does not show proper co-elution are considered "Level 2" identifications (4.2, p. 40). Asterisks (*) indicate the fragment used for statistical comparison and displayed in Figure 3 and/or Table 3. For select compounds, additional plots display isolated fragments for enhanced visualization clarity.



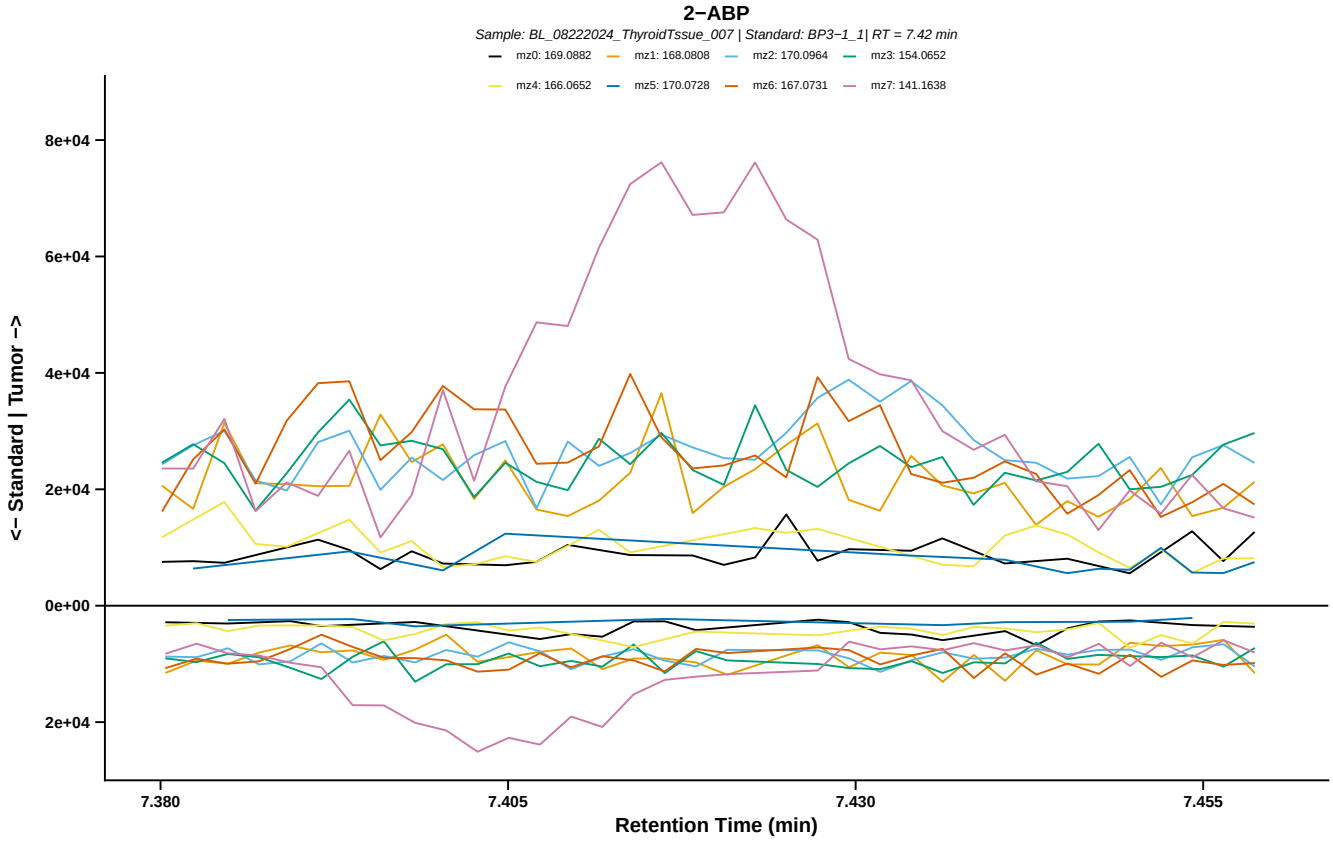


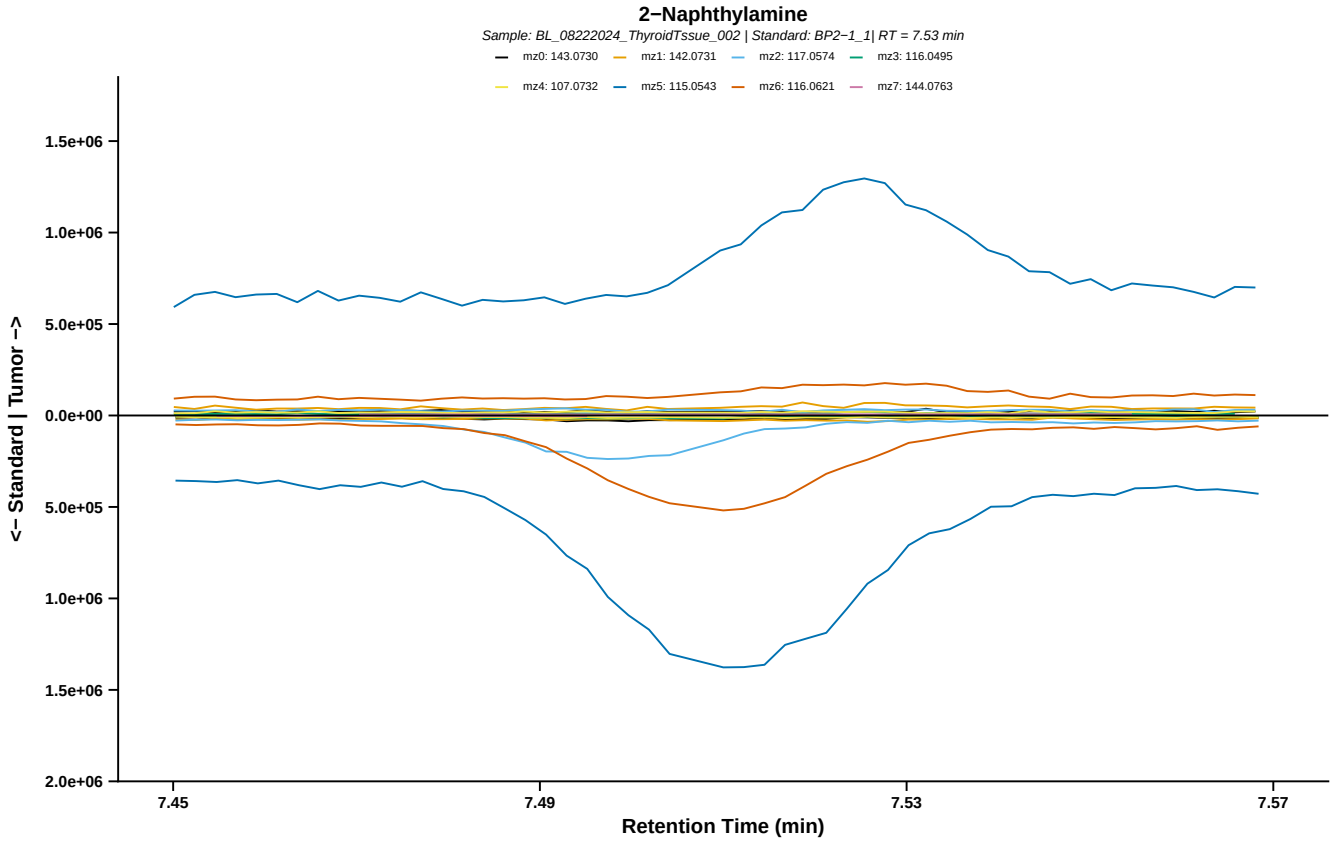
SUPPLEMENTARY FIGURE 4.1 (Continued)



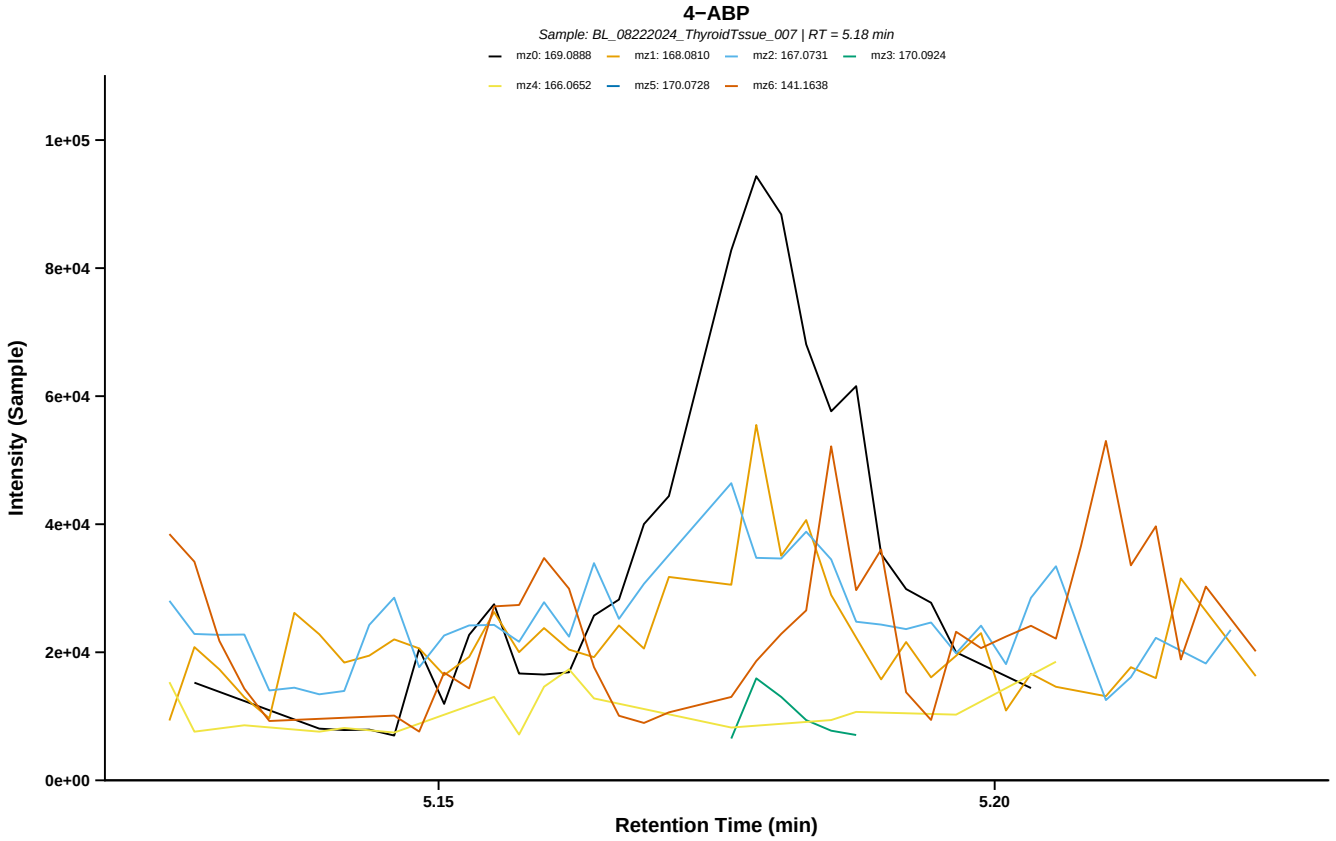


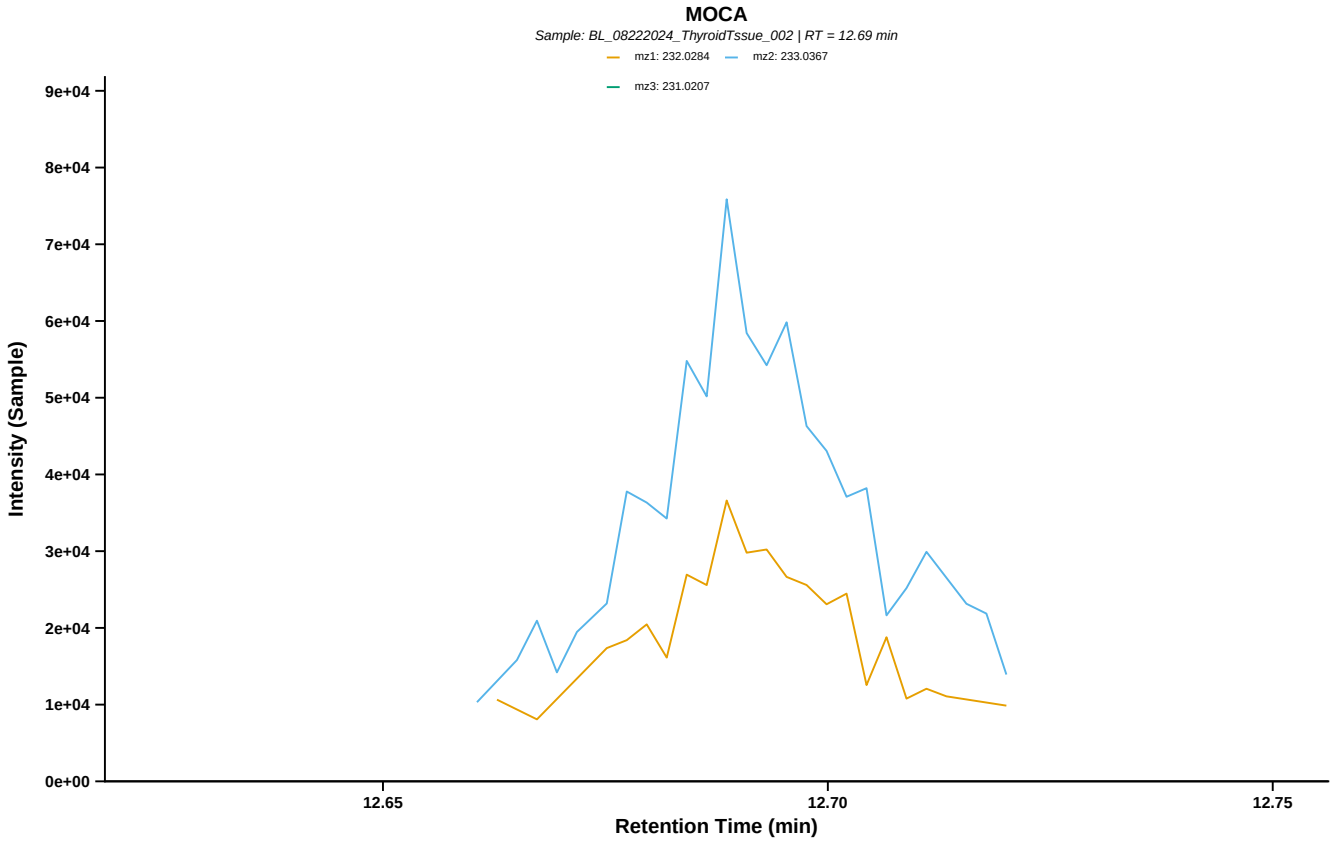
SUPPLEMENTARY FIGURE 4.1 (Continued)





SUPPLEMENTARY FIGURE 4.2 (Continued)





SUPPLEMENTARY TABLE 1

The full library of xenobiotic chemicals employed for chemical annotation and identification. The library of 710 confirmed xenobiotic chemicals employed for chemical identification. All chemicals besides those which were purchased as part of a mixture with variable concentrations were present in pooled reference plasma at a concentration of 0.47 ng/mL. There are 710 total unique chemicals (i.e., unique CAS numbers), but for some chemicals, there are multiple fragments and/or retention times from different standards used for annotation and identification, thus resulting in 892 total rows in the table. The column "Target RT (min.)" refers to the library retention time for the given chemical. The individual mz columns indicate typical fragments observed for the given chemical. [a] *Both an endogenous and exogenous (xenobiotic) chemical;* [b] *Additional fragments used for validation besides those listed in mz0–mz3.*

Index	Library ID	Name	CAS	Monoisotopic Mass	Target RT (min.)	mz0	mz1	mz2	mz3
1	CP3141	(-)-Menthol	2216-51-5	156.1514	4.5056	157.1416	146.0998	188.1103	155.1067
2	CP2286	(3-Methylphenyl) diphenyl phosphate	69500-28-3	340.0864	13.4591	340.0852	339.0783	341.0899	342.0927
3	CP3143	(±)-Nicotine	22083-74-5	162.1157	7.3406	161.1198	132.0808	106.0652	117.0574
4	CP2421	1,1,1,2-Tetrachloroethane	630-20-6	165.8911	5.9580	130.9217	132.9607	94.9683	134.9578
5	CP2421_2	-	-	-	6.3460	130.9217	132.9607	94.9683	134.9578
6	CP2426	1,1,1-Trichloroethane	71-55-6	131.9300	6.3999	96.9133	98.9466	129.9308	130.9386
7	CP2422	1,1,2,2-Tetrachloroethane	79-34-5	165.8911	6.7749	130.9217	132.9607	94.9683	134.9578
8	CP2427	1,1,2-Trichloroethane	79-00-5	131.9300	6.6385	96.9133	98.9466	129.9308	130.9386
9	CP2404	1,1-Dichloroethane	75-34-3	97.9690	5.9827	94.9683	96.9653	95.9342	97.9689
10	CP2406	1,1-Dichloroethene	75-35-4	95.9534	5.9333	95.9528	97.9499	94.9451	96.9421
11	CP2412	1,1-Dichloropropene	563-58-6	109.9690	5.6251	109.9687	95.9529	97.9500	98.9577
12	CP1111	1,2,3,4,6,7,8-HpCDD	35822-46-9	421.7796	17.8154	421.7979	429.6976	423.6484	425.6465
13	CP1112	1,2,3,4,6,7,8-HpCDF	38998-75-3	405.7847	16.0117	405.7845	403.7865	407.7822	401.7887
14	CP1114	1,2,3,4,6,8,9-HpCDF	69698-58-4	405.7847	17.8806	405.7845	403.7865	407.7822	401.7887
15	CP1113	1,2,3,4,7,8,9-HpCDF	55673-89-7	405.7847	16.7717	405.7845	403.7865	407.7822	401.7887
16	CP1107	1,2,3,4,7,8-Hexachlorodibenzofuran	55684-94-1	371.8237	15.8566	373.8213	375.8182	371.8241	377.8151
17	CP1104	1,2,3,4,7,8-HxCDD	39227-28-6	387.8186	16.4444	389.8162	391.8131	387.8190	393.8097
18	CP1105	1,2,3,6,7,8-HXCDD	57653-85-7	387.8186	16.7012	389.8162	391.8131	387.8190	393.8097
19	CP1108	1,2,3,6,7,8-HxCDF	57117-44-9	371.8237	16.2667	373.8213	375.8182	371.8241	377.8151
20	CP1106	1,2,3,7,8,9-HxCDD	19408-74-3	387.8186	16.8191	389.8162	391.8131	387.8190	393.8097
21	CP1109	1,2,3,7,8,9-HxCDF	72918-21-9	371.8237	16.8436	373.8213	375.8182	371.8241	377.8151
22	CP1101	1,2,3,7,8-PeCDD	40321-76-4	353.8576	14.3780	355.8548	353.8577	357.8518	359.8487
23	CP1102	1,2,3,7,8-Pentachlorodibenzofuran	57117-41-6	337.8627	13.6179	335.9045	341.8554	339.8589	337.8628
24	CP2449	1,2,3-Trichloro-4-nitrobenzene	17700-09-3	224.9151	4.5552	224.9147	194.9167	196.9137	198.9108
25	CP2425	1,2,3-Trichlorobenzene	87-61-6	179.9300	3.3022	179.9292	181.9262	183.9233	172.9666
26	CP2429	1,2,3-Trichloropropane	96-18-4	145.9457	5.1355	145.9455	110.9766	109.9732	112.9789
27	CP2429_2	-	-	-	4.5552	145.9455	110.9766	109.9732	112.9789
28	CP2549	1,2,4,5-Tetrachlorobenzene	95-94-3	213.8911	5.7036	213.8906	215.8876	217.8847	219.8817
29	CP2450	1,2,4-Trichloro-5-nitrobenzene	89-69-0	224.9151	4.8997	224.9147	194.9167	196.9137	198.9108
30	CP2202	1,2,4-Trichlorobenzene	120-82-1	179.9300	3.0988	179.9292	181.9262	183.9233	172.9666
31	CP3079	-	-	-	3.0963	179.9295	181.9264	183.9234	172.9666
32	CP2430	1,2,4-Trimethylbenzene	95-63-6	120.0939	7.7169	105.0699	119.0855	91.0542	115.0754
33	CP2307	1,2,5,6-Tetrabromocyclooctane	3194-57-8	423.7670	12.8512	104.7694	186.9950	187.9843	188.9921
34	CP2401	1,2-Dibromo-3-chloropropane	96-12-8	233.8447	13.0490	154.9315	155.9393	156.9427	152.9335
35	CP2402	1,2-Dibromoethane	106-93-4	185.8680	5.9827	106.9358	189.8721	187.8750	108.9329
36	CP2193	1,2-Dichlorobenzene	95-50-1	145.9690	5.9378	145.9687	144.9609	146.9579	132.9608
37	CP2405	1,2-Dichloroethane	107-06-2	97.9690	6.0471	94.9683	96.9653	95.9342	97.9689
38	CP2409	1,2-Dichloropropane	78-87-5	111.9847	3.9986	111.9844	113.9823	110.9811	114.9760
39	CP2431	1,3,5-Trimethylbenzene	108-67-8	120.0939	7.9695	105.0699	119.0855	91.0542	115.0754
40	CP2194	1,3-Dichlorobenzene	541-73-1	145.9690	6.3483	145.9687	144.9609	146.9579	132.9608
41	CP2410	1,3-Dichloropropane	142-28-9	111.9847	4.2322	111.9845	108.9841	110.9811	109.9792
42	CP2195	1,4-Dichlorobenzene	106-46-7	145.9690	6.7838	145.9687	144.9609	146.9579	132.9608
43	CP2513	1,4-Naphthoquinone	130-15-4	158.0368	22.8554	158.0362	102.0631	132.0236	104.0495

Index	Library ID	Name	CAS	Monoisotopic Mass	Target RT (min.)	mz0	mz1	mz2	mz3
44	CP3084	1,8-Cineole	470-82-6	154.1358	9.8262	154.1354	153.1275	125.1237	139.1118
45	CP2435	1-Chloro-2,4-dinitrobenzene	97-00-7	201.9781	5.1905	201.9775	203.9746	109.9918	204.9780
46	CP2437	1-Chloro-2-nitrobenzene	88-73-3	156.9931	3.8227	98.9996	126.9947	110.9997	156.9928
47	CP2436	1-Chloro-3,4-dinitrobenzene	610-40-2	201.9781	5.2444	201.9775	203.9746	109.9918	204.9780
48	CP2438	1-Chloro-4-nitrobenzene	100-00-5	156.9931	3.8666	98.9996	126.9947	110.9997	156.9928
49	CP2510	1-Naphthol	90-15-3	144.0575	7.6213	144.0570	114.0465	115.0541	116.0618
50	CP2534	1-Naphthylamine	134-32-7	143.0735	7.2883	142.0731	117.0574	116.0495	107.0732
51	CP2411	2,2-Dichloropropane	594-20-7	111.9847	4.3454	111.9845	108.9841	110.9811	109.9792
52	CP2322	2,3,4,5-Tetrabromobenzoic acid[b]	27581-13-1	433.6790	17.5398	433.6821	436.5814	419.3524	444.8398
53	CP2448	2,3,4,5-Tetrachloronitrobenzene	879-39-0	258.8761	5.6992	258.8757	202.8794	200.8824	260.8727
54	CP1110	2,3,4,6,7,8-HxCDF	60851-34-5	371.8237	16.9840	373.8213	375.8182	371.8241	377.8151
55	CP1014	2,3,4,6-Tetrabromophenol	14400-94-3	405.6839	7.9939	409.6806	407.6828	411.6786	405.6848
56	CP1013	2,3,4,6-Tetrachlorophenol	58-90-2	229.8860	5.2057	231.8824	229.8855	233.8796	235.8767
57	CP2550	-	-	-	5.2084	229.8855	231.8826	233.8796	235.8793
58	CP1103	2,3,4,7,8-Pentachlorodibenzofuran	57117-31-4	337.8627	13.6583	339.8598	337.8628	341.8568	343.8537
59	CP2469	2,3,4-TCP-4'-NPE	142022-61-5	615.8721	11.2307	235.9799	237.9769	316.9417	286.9430
60	CP2206	2,3,4-Trichlorophenol	25167-82-2	195.9250	12.4501	195.9246	197.9215	96.9840	131.9530
61	CP2074	2,3,5,6-Tetrachloroaniline	3481-20-7	228.9020	5.5363	228.9015	230.8985	232.8955	234.8925
62	CP2074_2	-	-	-	5.7014	228.9015	230.8985	232.8955	234.8925
63	CP2447	2,3,5,6-Tetrachloronitrobenzene	117-18-0	258.8761	5.3319	258.8757	202.8794	200.8824	260.8727
64	CP2466	2,3,5-TCP-4'-NPE	142022-59-1	615.8721	10.4388	282.9797	252.9817	254.9788	284.9767
65	CP2465	2,3,6-TCP-4'-NPE	142022-58-0	615.8721	10.4388	282.9797	252.9817	254.9788	284.9767
66	CP2442	2,3-Dichloronitrobenzene	3209-22-1	190.9541	3.8643	190.9536	191.9569	132.9608	134.9578
67	CP2461	2,3-Dichlorophenyl-4'-nitrophenyl ether	82239-20-1	282.9803	10.5994	282.9796	252.9826	254.9796	284.9777
68	CP1098	2,4'-DDT	789-02-6	351.9147	11.0226	235.0076	237.0046	165.0696	236.0108
69	CP2032	-	-	-	11.0206	235.0076	237.0046	165.0696	236.0108
70	CP3096_2	-	-	-	10.2095	235.0076	165.0697	237.0046	199.0308
71	CP2049	2,4'-Methoxychlor[b]	30667-99-3	344.0138	3.7643	344.0143	341.0179	342.0175	343.0142
72	CP2467	2,4,5-TCP-4'-NPE	22532-68-9	615.8721	10.5994	282.9797	252.9817	254.9788	284.9767
73	CP2371	2,4,5-Trichlorophenol	95-95-4	195.9249	11.6046	195.9246	197.9215	96.9840	131.9530
74	CP3080	-	-	-	4.1333	195.9244	197.9214	96.9839	199.9184
75	CP2280	2,4,5-Trichlorophenoxyacetic acid	93-76-5	253.9304	8.7145	254.8928	216.9374	252.8959	218.9343
76	CP3018	2,4,5-Trimethylaniline	137-17-7	135.1048	5.7984	135.1047	120.0809	134.0965	133.0523
77	CP2464	2,4,6-TCP-4'-NPE	1836-77-7	615.8721	10.1561	282.9797	252.9817	254.9788	284.9767
78	CP2319	2,4,6-Tribromophenol	118-79-6	327.7730	5.6587	329.7717	331.7696	327.7738	333.7675
79	CP2319_2	-	-	-	8.7348	329.7717	331.7696	327.7738	333.7675
80	CP2451	2,4,6-Trichloronitrobenzene	18708-70-8	224.9151	5.1355	224.9147	194.9167	196.9137	198.9108
81	CP2372	2,4,6-Trichlorophenol	88-06-2	195.9249	12.3098	195.9246	197.9215	96.9840	131.9530
82	CP3081	-	-	-	4.2029	195.9244	197.9214	96.9839	199.9184
83	CP3006	2,4-Diaminoanisole (as sulfate hydrate)	615-05-4	138.0793	5.4728	138.0790	123.0554	122.0603	139.0754
84	CP3008	2,4-Diaminotoluene	95-80-7	122.0844	5.0989	122.0838	119.0365	118.0287	120.0398
85	CP3008_2	-	-	-	4.6793	122.0838	119.0365	118.0287	120.0398
86	CP2443	2,4-Dichloronitrobenzene	611-06-3	190.9541	3.9941	190.9536	191.9569	132.9608	134.9578
87	CP2236	2,4-Dichlorophenol	120-83-2	161.9639	9.8509	161.9633	163.9603	97.9919	165.9575
88	CP3048	-	-	-	3.0640	161.9634	179.9293	181.9263	163.9602
89	CP2267	2,4-Dichlorophenoxyacetic acid	94-75-7	219.9694	13.0468	219.9708	247.9655	217.9675	218.9761
90	CP2067	2,4-Dichlorophenyl 4-nitrophenyl ether	1836-75-5	282.9803	10.1561	282.9799	202.0179	284.9771	204.0150
91	CP2237	2,4-Dimethylphenol[b]	105-67-9	122.0731	9.7139	122.0726	123.0761	121.0648	124.0841
92	CP3050	-	-	-	9.7251	122.0722	123.0760	105.0336	106.0369
93	CP2238	2,4-Dinitrophenol	51-28-5	184.0120	8.1974	183.0135	154.0054	155.0184	168.0061
94	CP3052	-	-	-	5.0246	184.0115	185.0148	186.0155	187.0191
95	CP2196	2,4-Dinitrotoluene	121-14-2	182.0328	4.6809	165.0294	119.0367	90.0341	89.0420
96	CP3054	-	-	-	5.0621	182.0321	165.0293	119.0365	108.0205

Index	Library ID	Name	CAS	Monoisotopic Mass	Target RT (min.)	mz0	mz1	mz2	mz3
97	CP2446	2,5-Dichloronitrobenzene	89-61-2	190.9541	4.3477	190.9536	191.9569	132.9608	134.9578
98	CP2348	2,5-Dichlorophenol	583-78-8	161.9639	10.4388	161.9633	163.9603	97.9919	165.9575
99	CP2460	2,5-Dichlorophenyl-4’-nitrophenyl ether	39145-48-7	282.9803	10.9678	279.9937	281.9906	280.9967	296.9962
100	CP2521	2,6-Dichlorophenol	87-65-0	161.9639	11.0835	161.9633	163.9603	97.9919	165.9575
101	CP2458	2,6-Dichlorophenyl-4’-nitrophenyl ether[b]	2093-28-9	282.9803	10.4388	282.9797	139.0545	204.0150	254.9796
102	CP2197	2,6-Dinitrotoluene	606-20-2	182.0328	5.0973	165.0294	119.0367	90.0341	89.0420
103	CP3055	-	-	-	5.4683	182.0321	165.0293	119.0365	108.0205
104	CP2279	2-(2,4-Dichlorophenoxy)butanoic acid	94-82-6	248.0007	12.8399	248.0026	249.9999	231.9926	188.9919
105	CP2517	2-Acetylaminofluorene	53-96-3	223.0997	13.1917	223.0986	106.0701	116.0556	206.0845
106	CP3020	2-Aminobiphenyl[b]	90-41-5	169.0892	7.3406	169.0882	168.0808	170.0964	154.0652
107	CP2264	2-Bromo-4-(2,4,4-trimethylpentan-2-yl)phenol	57835-35-5	284.0780	10.7690	284.0793	282.0735	283.0768	254.0423
108	CP2308	2-Bromoallyl-2,4,6-tribromophenyl ether	99717-56-3	445.7152	8.7258	329.7710	331.7689	300.7682	289.8760
109	CP2308_2	-	-	-	5.6610	329.7710	331.7689	300.7682	289.8760
110	CP2439	2-Chloro-6-nitrotoluene	83-42-1	171.0087	4.1411	171.0081	89.0386	90.0339	154.0055
111	CP2192	2-Chloronaphthalene	91-58-7	162.0240	10.4411	162.0230	164.0200	155.0603	163.0262
112	CP2192_2	-	-	-	10.9633	162.0230	164.0200	155.0603	163.0262
113	CP2192_3	-	-	-	11.2374	162.0230	164.0200	155.0603	163.0262
114	CP3040	-	-	-	4.2915	162.0229	164.0200	155.0603	126.0463
115	CP2235	2-Chlorophenol	95-57-8	128.0029	8.1951	128.0024	129.9994	126.9946	100.0074
116	CP3042	-	-	-	8.1980	128.0025	126.9947	129.0059	129.9995
117	CP2453	2-Chlorophenyl-4’-nitrophenyl ether	2091-61-4	249.0193	8.7527	249.0187	251.0159	250.0222	252.0192
118	CP2398	2-Chlorotoluene	95-49-8	126.0236	3.8666	128.0158	125.0155	124.0077	90.0465
119	CP2287	2-Ethylhexyldiphenylphosphate	1241-94-7	362.1647	12.8040	362.1643	251.0473	249.0318	252.0505
120	CP2373	2-Isopropyl-6-methyl-4-pyrimidinol	2814-20-2	152.0950	6.4956	152.0946	137.0708	124.0631	151.0865
121	CP2239	2-Methyl-4,6-dinitrophenol	534-52-1	198.0277	8.0705	121.0107	169.0139	168.0061	123.0263
122	CP3051	-	-	-	5.4728	198.0271	168.0289	152.0213	199.0300
123	CP2276	2-Methyl-4-chlorophenoxyacetic acid	94-74-6	200.0240	12.6700	200.0252	141.0807	212.0252	211.0411
124	CP2211	2-Methylnaphthalene	91-57-6	142.0783	4.9019	141.0697	142.0772	139.0540	143.0808
125	CP2211_2	-	-	-	3.8340	141.0697	142.0772	139.0540	143.0808
126	CP3065	-	-	-	3.8313	142.0774	141.0698	143.0809	144.0844
127	CP2535	2-Naphthylamine[b]	91-59-8	143.0735	7.3640	142.0731	117.0574	116.0495	107.0732
128	CP3014	-	-	-	7.3405	143.0730	117.0574	118.0652	119.0730
129	CP2212	2-Nitroaniline[b]	88-74-4	138.0429	12.1818	138.0424	108.0444	92.0257	139.0499
130	CP3069	-	-	-	5.4907	138.0424	108.0444	92.0495	139.0458
131	CP2240	2-Nitrophenol	88-75-5	139.0269	5.4475	139.0265	109.0284	110.0318	105.0699
132	CP3073	-	-	-	5.0262	139.0264	109.0283	140.0298	110.0364
133	CP2146	2-Phenylphenol	90-43-7	170.0732	12.8040	170.0722	169.0646	141.0697	115.0541
134	CP2146_2	-	-	-	9.2898	170.0722	169.0646	141.0697	115.0541
135	CP2546	2-Picoline	109-06-8	93.0579	5.4048	93.0573	110.0362	92.0495	94.0607
136	CP2216	3,3’-Dichlorobenzidine	91-94-1	252.0220	13.4816	252.0215	254.0192	256.0163	253.0254
137	CP3009	-	-	-	13.4739	252.0221	255.0764	254.0191	253.0202
138	CP2474	3,3’-Dimethoxybenzidine	119-90-4	244.1212	13.4546	244.1206	229.1136	227.1068	201.0284
139	CP3010	-	-	-	11.4797	201.1274	158.1046	187.1117	229.1587
140	CP3012	3,3’-Dimethyl-4,4’-diaminodiphenylmethane	838-88-0	226.1470	12.2798	211.1483	155.0855	93.0700	135.0805
141	CP2475	3,3’-Dimethylbenzidine[b]	119-93-7	212.1314	7.8819	212.1302	213.1848	211.1691	199.1690
142	CP3011	-	-	-	8.3981	108.0934	211.1300	153.0696	215.0852
143	CP2468	3,4,5-TCP-4’-NPE	142022-60-4	615.8721	10.9678	282.9797	252.9817	254.9788	284.9767
144	CP2060	3,4-Dichloroaniline	95-76-1	160.9799	4.3522	160.9795	161.9686	107.9762	108.9840
145	CP2445	3,4-Dichloronitrobenzene	99-54-7	190.9541	4.2344	190.9536	191.9569	132.9608	134.9578
146	CP2462	3,4-Dichlorophenyl-4’-nitrophenyl ether	22532-80-5	282.9803	11.2307	282.9792	252.9826	254.9796	284.9777
147	CP2275	3,5-Dichlorobenzoic acid	51-36-5	189.9590	3.8599	189.9589	186.9586	188.9556	160.9608
148	CP2444	3,5-Dichloronitrobenzene	618-62-2	190.9541	4.1895	190.9536	191.9569	132.9608	134.9578
149	CP2459	3,5-Dichlorophenyl-4’-nitrophenyl ether	21105-77-1	282.9803	10.4388	282.9795	139.0545	204.0150	254.9796

Index	Library ID	Name	CAS	Monoisotopic Mass	Target RT (min.)	mz0	mz1	mz2	mz3
150	CP2314	3-Bromostyrene	2039-86-3	181.9731	3.0372	181.9725	183.9705	182.9758	184.9740
151	CP3022	3-Chloro-o-toluidine[b]	87-60-5	141.0345	5.1965	141.0343	106.0370	140.0262	105.0294
152	CP2454	3-Chlorophenyl-4'-nitrophenyl ether	2303-23-3	249.0193	8.9414	249.0187	251.0159	250.0222	252.0192
153	CP2506	3-Hydroxycarbofuran[b]	16655-82-6	237.1001	9.8127	137.0962	180.1510	147.1170	138.1041
154	CP2531	3-Methylcholanthrene	56-49-5	268.1252	18.5177	268.1251	267.1170	269.1277	265.1013
155	CP2213	3-Nitroaniline	99-09-2	138.0429	12.4411	138.0424	108.0444	92.0257	139.0499
156	CP3070	-	-	-	5.0262	138.0424	108.0444	92.0495	139.0458
157	CP2328	3-Phenoxybenzoic acid	3739-38-6	214.0630	7.2254	214.0650	215.0573	141.0697	168.0568
158	CP1078	4,4'-DDD	72-54-8	317.9537	11.0226	235.0079	237.0049	165.0697	199.0309
159	CP2029	-	-	-	11.0206	235.0079	237.0049	165.0697	199.0309
160	CP1079	4,4'-DDE	72-55-9	315.9380	10.0335	246.0008	247.9979	317.9357	315.9386
161	CP2031	-	-	-	10.0315	246.0008	247.9979	317.9357	315.9386
162	CP1080	4,4'-DDT	50-29-3	351.9147	11.9275	235.0076	237.0046	165.0696	236.0108
163	CP2033	-	-	-	11.9223	235.0076	237.0046	165.0696	236.0108
164	CP3096	-	-	-	10.6060	235.0075	165.0698	237.0048	199.0311
165	CP3007	4,4'-Diaminodiphenylmethane[b]	101-77-9	198.1157	4.2814	108.0934	106.0778	197.1169	198.1153
166	CP2034	4,4'-Dichlorobenzophenone	90-98-2	249.9952	8.2727	249.9948	138.9945	140.9914	215.0259
167	CP2050	4,4'-Methoxychlor olefin	2132-70-9	308.0371	11.7258	308.0365	238.0991	310.0339	311.0371
168	CP3013	4,4'-Methylenebis(2-chloroaniline)[b]	101-14-4	266.0378	12.8098	232.0284	233.0367	231.0207	140.0022
169	CP3015	4,4'-Oxydianiline[b]	101-80-4	200.0950	7.6448	200.0964	108.0556	171.0572	170.0575
170	CP3016	4,4'-Thiodianiline[b]	139-65-1	216.0721	9.2834	216.0732	184.0882	183.0803	215.0703
171	CP2457	4-(2,4-Dichlorophenoxy)-2-methyl-1-nitrobenzene	42488-57-3	296.9959	11.0902	296.9955	279.9928	281.9898	298.9924
172	CP2518	4-Aminobiphenyl[b]	92-67-1	169.0891	6.6385	169.0884	168.0808	154.0653	141.0699
173	CP3002	-	-	-	5.3660	169.0888	168.0810	167.0731	170.0924
174	CP2452	4-Bromophenyl phenyl ether	101-55-3	247.9837	5.9468	247.9832	249.9810	141.0699	115.0543
175	CP3037	-	-	-	5.9457	247.9831	249.9813	141.0697	115.0541
176	CP2325	4-Bromostyrene	2039-82-9	181.9731	3.0709	181.9725	183.9705	182.9758	184.9740
177	CP2440	4-Chloro-2-nitrotoluene	89-59-8	171.0087	3.8205	154.0055	90.0339	89.0386	171.0081
178	CP2234	4-Chloro-3-methylphenol	59-50-7	142.0185	3.8048	142.0179	107.0491	144.0150	108.0524
179	CP3041	-	-	-	3.7842	142.0179	144.0149	135.0803	145.0183
180	CP2441	4-Chloro-3-nitrotoluene	89-60-1	171.0087	3.8666	154.0055	90.0339	89.0386	171.0081
181	CP3004	4-Chloro-o-toluidine	95-69-2	141.0345	5.2998	141.0342	140.0262	104.0258	142.0581
182	CP2209	4-Chloroaniline	106-47-8	127.0189	5.7014	127.0184	129.0155	92.0495	100.0075
183	CP3039	-	-	-	5.6893	127.0183	129.0155	100.0075	92.0496
184	CP2183	4-Chlorophenyl phenyl ether	7005-72-3	204.0342	5.3914	204.0335	206.0306	141.0182	151.0543
185	CP3043	-	-	-	5.4110	204.0323	206.0292	165.0693	176.0374
186	CP2455	4-Chlorophenyl-4'-nitrophenyl ether	1836-74-4	249.0193	9.1820	249.0187	251.0159	250.0222	252.0192
187	CP2399	4-Chlorotoluene	106-43-4	126.0236	4.1411	126.0232	128.0158	125.0155	124.0077
188	CP2329	4-Fluro-3-phenoxy-benzoic acid	77279-89-1	232.0536	11.0835	215.0259	217.0290	216.0212	209.0470
189	CP3140	4-Hydroxy-2,5-dimethyl-3(2H)-furanone	3658-77-3	128.0473	4.9328	129.0367	111.0262	101.0598	87.0442
190	CP2251	4-Hydroxybenzoic acid	99-96-7	138.0317	7.2680	138.0313	137.0472	136.0394	139.0390
191	CP2251_2	-	-	-	8.7033	138.0313	137.0472	136.0394	139.0390
192	CP2251_3	-	-	-	5.0097	138.0313	137.0472	136.0394	139.0390
193	CP2316	4-Methyl-benzylidene camphor	36861-47-9	254.1671	9.0402	253.1587	255.0215	254.1669	155.2271
194	CP2214	4-Nitroaniline	100-01-6	138.0429	12.3098	138.0424	108.0444	92.0257	139.0499
195	CP3071	-	-	-	4.4295	138.0424	108.0444	92.0495	139.0458
196	CP2463	4-Nitrophenyl phenyl ether	620-88-2	215.0582	7.2254	215.0573	216.0607	217.0630	218.0651
197	CP2514	4-Nitroquinoline-1-oxide[b]	56-57-5	190.0378	11.0880	190.0360	191.0310	192.0107	168.0571
198	CP2351	4-Tert-Octylphenol	140-66-9	206.1671	9.7251	206.1667	135.0806	107.0493	136.0841
199	CP2541	5-Nitro-o-toluidine	99-55-8	152.0586	9.5110	106.0370	92.0258	123.0443	107.0380
200	CP3003	-	-	-	6.5594	152.0582	150.0465	151.0543	153.0655
201	CP2523	7,12-Dimethylbenz(a)anthracene	57-97-6	256.1252	16.7281	256.1247	252.0933	253.0967	250.0779
202	CP3197	9-Chlorohexadecafluoro-3-oxanone-1-sulfonic acid	756426-58-1	531.9029	5.5558	130.9385	182.0837	158.9696	113.9357

Index	Library ID	Name	CAS	Monoisotopic Mass	Target RT (min.)	mz0	mz1	mz2	mz3
203	CP2217	Acenaphthene	83-32-9	154.0783	4.2951	154.0777	153.0699	152.0618	155.0807
204	CP2217_2	-	-	-	4.8570	154.0777	153.0699	152.0618	155.0807
205	CP3023	-	-	-	4.8534	154.0771	153.0697	150.0466	151.0545
206	CP2218	Acenaphthylene	208-96-8	152.0626	4.6877	152.0616	150.0461	151.0539	153.0650
207	CP2218_2	-	-	-	4.8570	152.0616	150.0461	151.0539	153.0650
208	CP2218_3	-	-	-	4.2906	152.0616	150.0461	151.0539	153.0650
209	CP3024	-	-	-	4.6838	152.0620	150.0466	153.0654	149.0388
210	CP2137	Acequinocyl	57960-19-7	384.2301	17.7181	344.2347	343.2226	376.2029	345.2381
211	CP2078	Acetochlor	34256-82-1	269.1183	7.1498	269.1177	146.0962	132.0806	174.0911
212	CP2516	Acetophenone[b]	98-86-2	120.0575	11.4733	120.0571	104.0495	121.0605	106.0525
213	CP2273	Acifluorfen	50594-66-6	360.9965	10.4860	360.9353	363.9406	365.9377	366.9271
214	CP3149	Acrinathrin	101007-06-1	541.1324	15.3145	181.0648	180.0807	178.0653	541.1331
215	CP2079	Alachlor	15972-60-8	269.1183	7.2815	269.1182	160.1118	188.1068	146.0962
216	CP3122	-	-	-	7.3406	269.1176	160.1120	132.0808	130.0652
217	CP2507	Aldicarb[b]	116-06-3	190.0776	10.6667	190.0781	178.0777	105.0699	109.0970
218	CP2503	Aldicarb sulfone	1646-88-4	222.0674	11.7416	222.0677	143.0060	146.0528	86.0152
219	CP2502	Aldicarb sulfoxide	1646-87-3	206.0725	7.2838	206.0732	208.0703	207.0766	209.0735
220	CP1071	Aldrin	309-00-2	361.8757	8.7103	262.8566	264.8536	358.8350	326.8272
221	CP2018	-	-	-	8.5008	361.8751	262.8565	264.8535	260.8595
222	CP2080	Allidochlor	93-71-0	173.0607	18.4436	173.0597	138.0676	174.0674	132.0570
223	CP2305	Allyl 2,4,6-tribromophenyl ether	3278-89-5	367.8050	6.3640	367.8043	209.9670	211.9649	290.8835
224	CP2207	Aniline	62-53-3	93.0580	9.9282	93.0574	94.0607	92.0496	95.0292
225	CP2219	Anthracene	120-12-7	178.0783	6.6655	178.0778	177.0699	176.0621	88.0308
226	CP3025	-	-	-	6.5594	178.0774	176.0619	179.0807	177.0540
227	CP3150	Anthraquinone	84-65-1	208.0524	8.1149	208.0515	152.0618	180.0568	209.0548
228	CP3123	Atraton	1610-17-9	211.1433	6.2533	211.1428	169.1192	215.0933	216.0825
229	CP2106	Atrazine	1912-24-9	215.0938	6.2752	215.0932	200.0695	202.0666	173.0460
230	CP3113	-	-	-	6.2858	215.0932	200.0698	217.0903	216.0966
231	CP2002	Azinphos ethyl[b]	2642-71-9	345.0371	15.1056	132.0445	104.0495	137.0056	133.0477
232	CP2003	Azinphos methyl	86-50-0	317.0058	10.2918	317.0054	105.0697	318.0136	319.0027
233	CP2191	Azobenzene	103-33-3	182.0840	5.5700	182.0840	105.0448	152.0623	153.0702
234	CP3026	-	-	-	5.5603	182.0838	105.0447	152.0620	183.0872
235	CP1118	B8-1413	142534-71-2	409.8291	10.3477	158.9764	340.8800	328.8801	304.9034
236	CP1120	B9-1025	154159-06-5	443.7901	12.4049	158.9763	278.8877	338.8644	374.8410
237	CP1119	B9-1679	66860-80-8	443.7901	10.7912	158.9763	278.8877	338.8644	374.8410
238	CP1064	BDE-100	189084-64-8	559.6260	16.0185	403.7865	419.8223	563.6220	559.6260
239	CP1065	BDE-138	182677-30-1	637.5360	19.4170	483.6946	481.6968	485.6926	643.5317
240	CP1066	BDE-153	68631-49-2	637.5360	18.8022	483.6948	481.6968	485.6925	643.5322
241	CP1067	BDE-154	207122-15-4	637.5360	18.1945	483.6950	481.6969	485.6927	643.5323
242	CP1058	BDE-17	147217-75-2	403.8047	10.4453	403.8047	245.9675	247.9655	405.8021
243	CP1068	BDE-183	207122-16-5	715.4470	20.1229	561.6064	563.6043	559.6085	565.6023
244	CP1094	BDE-206	63387-28-0	871.2678	19.6514	722.4052	718.0084	727.6006	723.5176
245	CP1069	BDE-209	1163-19-5	949.1783	21.4896	822.1349	799.3236	800.1487	819.2586
246	CP1059	BDE-28/33	41318-75-6	403.8047	10.9147	403.8047	245.9677	247.9656	405.8023
247	CP1060	BDE-47	5436-43-1	481.7152	13.7886	325.8760	323.8780	327.8737	485.7104
248	CP1061	BDE-66	189084-61-5	481.7152	14.3254	325.8760	485.7105	483.7125	323.8781
249	CP1062	BDE-71	189084-62-6	481.7152	13.4102	325.8760	485.7105	323.8781	327.8738
250	CP1093	BDE-85	182346-21-0	559.6260	16.7852	403.7863	405.7841	563.6220	565.6200
251	CP1063	BDE-99	60348-60-9	559.6260	17.8042	403.7863	405.7841	563.6220	565.6200
252	CP2357	Bensulfuron-methyl	83055-99-6	410.0896	9.7184	149.0963	150.0997	95.0855	410.0869
253	CP2271	Bentazon	25057-89-0	240.0569	16.9394	240.0569	224.0621	225.0652	198.0464
254	CP2271_2	-	-	-	13.3040	240.0569	224.0621	225.0652	198.0464
255	CP2220	Benz(a)anthracene	56-55-3	228.0939	13.2007	228.0936	226.0778	229.0967	224.0622

Index	Library ID	Name	CAS	Monoisotopic Mass	Target RT (min.)	mz0	mz1	mz2	mz3
256	CP3027	-	-	-	13.1150	228.0935	226.0779	229.0968	113.0385
257	CP2387	Benzene[a]	71-43-2	78.0470	4.3709	144.9607	146.9576	143.9529	145.9499
258	CP2215	Benzidine[b]	92-87-5	184.1000	9.6825	185.0805	183.1334	91.0542	91.0542
259	CP3094	-	-	-	5.6984	184.0996	182.0838	183.0872	181.0761
260	CP2222	Benzo(b)fluoranthene	205-99-2	252.0939	17.7159	252.0942	250.0786	253.0974	248.0629
261	CP3029	-	-	-	16.7092	252.0937	250.0781	253.0969	126.0463
262	CP2223	Benzo(g,h,i)perylene	191-24-2	276.0939	19.7667	276.0938	277.0971	274.0784	272.0627
263	CP3030	-	-	-	19.4792	276.0938	274.0782	277.0969	137.0385
264	CP2224	Benzo(k)fluoranthene	207-08-9	252.0939	17.9076	252.0942	250.0786	253.0974	248.0629
265	CP3031	-	-	-	17.5052	252.0937	250.0781	253.0969	126.0463
266	CP2221	Benzo[a]pyrene	50-32-8	252.0939	16.9112	252.0942	250.0786	253.0974	248.0629
267	CP3028	-	-	-	16.6163	252.0937	250.0781	253.0969	126.0463
268	CP2203	Benzoic acid	65-85-0	122.0368	14.2944	122.0363	105.0335	135.0441	123.0396
269	CP3082	-	-	-	14.3058	122.0363	105.0337	106.0370	123.0398
270	CP3082_2	-	-	-	7.3090	122.0363	105.0337	106.0370	123.0398
271	CP3082_3	-	-	-	3.0348	122.0363	105.0337	106.0370	123.0398
272	CP2470	Benzoylprop ethyl	22212-55-1	365.0585	12.8534	365.0582	295.0292	292.0291	293.0326
273	CP2208	Benzyl alcohol	100-51-6	108.0575	19.2242	108.0572	107.0857	109.0650	105.0701
274	CP3083	Benzyl salicylate	118-58-1	228.0786	7.3045	228.0781	91.0542	92.0576	210.0677
275	CP2257	Benzylparaben	94-18-8	228.0786	10.0809	228.0779	121.0886	227.0725	226.1593
276	CP3151	Bifenthrin	82657-04-3	422.1260	13.3819	181.1011	179.0855	182.1045	180.0932
277	CP3152	Bioallethrin	584-79-2	302.1882	9.5806	135.0805	151.1073	123.1169	303.1949
278	CP2298	Bis(2,3-dibromopropyl) hydrogen phosphate	5412-25-9	493.7130	16.9753	403.7866	405.7848	401.7890	407.7823
279	CP2345	Bisphenol A	80-05-7	228.1150	8.9500	228.1132	133.0886	117.0573	132.0809
280	CP2353	Bisphenol F	620-92-8	200.0837	18.5873	200.0830	191.1021	201.0908	199.0751
281	CP2354	Bisphenol S	80-09-1	250.0300	10.8408	251.0028	252.0060	254.0030	250.0276
282	CP2480	Bromacil	314-40-9	260.0160	7.7035	260.0142	207.1744	203.1798	206.1301
283	CP3124	-	-	-	6.5055	205.0290	204.0210	203.0257	260.0185
284	CP2147	Bromfenvinfos-methyl	13104-21-7	373.8877	14.1012	376.8979	378.8953	377.9014	375.9031
285	CP2148	Bromfenvinphos (E)	33399-00-7	401.9190	10.7779	266.8884	268.9095	270.9056	323.8829
286	CP2388	Bromobenzene	108-86-1	155.9575	5.9535	155.9570	156.9472	157.9505	154.9492
287	CP2389	Bromochloromethane	74-97-5	127.9028	3.2798	129.9047	130.9032	131.9016	132.9004
288	CP2390	Bromodichloromethane[b]	75-27-4	161.8639	9.2336	128.8926	124.9822	85.0285	129.9373
289	CP2391	Bromoform[a]	75-25-2	249.7628	5.9468	172.9419	171.9519	250.9846	249.7641
290	CP2149	Bromophos ethyl	4824-78-6	391.8805	9.2291	358.9087	356.9112	360.9058	242.8611
291	CP2150	Bromophos methyl	2104-96-3	363.8492	8.3751	330.8775	124.9821	329.8830	328.8798
292	CP2138	Bromopropylate	18181-80-1	425.9466	13.2770	340.8994	182.9442	184.9421	338.9016
293	CP2107	Bupirimate[b]	41483-43-6	316.1569	19.8417	208.0731	207.0651	273.0794	316.1539
294	CP2179	Butyl benzyl phthalate	85-68-7	312.1360	19.2399	205.1224	206.1258	150.1040	312.1390
295	CP3032	-	-	-	11.9183	91.0543	205.0859	206.0938	312.1365
296	CP2317	Butyl methoxydibenzoylmethane	70356-09-1	310.1569	17.8470	135.1169	311.2734	136.1203	312.2771
297	CP2484	Butylate	2008-41-5	217.1500	4.5048	217.1496	146.0999	156.1384	188.1104
298	CP3125	-	-	-	4.5058	217.1492	146.0996	156.1382	188.1102
299	CP2256	Butylparaben	94-26-8	194.0943	7.3640	121.0648	139.0753	93.0699	194.0959
300	CP2519	Butylphenoxyisopropyl chloroethyl sulfite	140-57-8	334.1006	16.6237	334.1035	175.1483	135.1171	168.0933
301	CP2471	Caffeine	58-08-2	194.0804	6.9959	194.0794	109.0634	193.0720	167.0728
302	CP2108	Captafol	2425-06-1	346.9108	10.4882	347.9272	348.8922	344.8981	346.9078
303	CP2109	Captan	133-06-2	298.9341	4.6553	298.9344	149.0444	147.0651	150.0440
304	CP2472	Carbaryl	63-25-2	201.0790	7.2254	201.0784	215.0577	185.0595	184.0628
305	CP2233	Carbazole	86-74-8	167.0735	7.0218	167.0727	166.0651	169.0885	168.0760
306	CP2233_2	-	-	-	5.5386	167.0727	166.0651	165.0573	168.0760
307	CP3038	-	-	-	7.0104	167.0728	166.0651	139.0542	168.0761
308	CP2509	Carbofuran	1563-66-2	221.1052	6.1706	164.0831	149.0598	122.0363	221.1072

Index	Library ID	Name	CAS	Monoisotopic Mass	Target RT (min.)	mz0	mz1	mz2	mz3
309	CP2340	Carbofuran phenol	1563-38-8	164.0837	18.4481	164.0831	149.0597	163.0753	165.0876
310	CP2395	Carbon tetrachloride	56-23-5	151.8754	5.3297	116.9061	118.9031	120.9002	122.9688
311	CP2151	Carbophenothion	786-19-6	341.9738	11.6832	341.9733	156.9871	96.9506	295.9855
312	CP2139	Carfentrazone ethyl	128639-02-1	411.0364	11.7213	411.0359	312.0595	310.0196	330.0258
313	CP2266	Chloramben	133-90-4	204.9697	12.7630	204.9692	206.9662	160.9793	162.9764
314	CP2023	Chlorbenside	103-17-3	267.9880	9.2471	267.9874	125.0150	127.0120	126.0183
315	CP2110	Chlorfenapyr	122453-73-0	405.9695	5.9468	247.9832	246.9754	249.9809	250.9843
316	CP2026	Chlorfenson	80-33-1	301.9571	9.7993	301.9567	174.9614	110.9995	176.9583
317	CP2152	Chlorfenvinphos	470-90-6	357.9695	12.3255	266.9662	267.9698	322.9320	268.9632
318	CP2396	Chlorobenzene	108-90-7	112.0080	3.8688	112.0075	114.0047	113.0027	110.0020
319	CP2140	Chlorobenzilate	510-15-6	324.0320	11.4464	324.0334	322.0281	323.0314	325.0273
320	CP2397	Chloroform[a]	67-66-3	117.9144	6.9779	118.9032	119.9763	85.9792	117.9372
321	CP2027	Chloroneb	2675-77-6	205.9901	4.9176	205.9897	190.9662	192.9632	207.9867
322	CP2057	Chlorothalonil	1897-45-6	263.8816	6.3438	263.8465	268.8407	272.8469	269.8375
323	CP2141	Chlorpropham	101-21-3	213.0556	5.6992	213.0550	127.0180	171.0077	129.0150
324	CP3126	-	-	-	5.6893	213.0550	127.0183	171.0081	129.0153
325	CP2004	Chlorpyrifos	2921-88-2	348.9263	7.9717	257.8943	196.9197	198.9167	259.8912
326	CP2005	Chlorpyrifos methyl	5598-13-0	320.8950	12.8309	320.8968	316.9034	318.9005	314.9062
327	CP2143	Chlorthal-dimethyl	1861-32-1	329.9020	8.0526	329.9016	300.8805	298.8835	302.8775
328	CP2153	Chlorthiophos	21923-23-9	359.9577	11.1374	359.9575	268.9264	324.9891	270.9231
329	CP2142	Chlozolinate	84332-86-5	331.0014	8.7898	331.0009	258.9800	185.9869	189.9583
330	CP2225	Chrysene[b]	218-01-9	228.0939	13.2950	228.0936	226.0778	229.0967	224.0622
331	CP3044	-	-	-	13.2160	228.0935	226.0779	229.0968	113.0385
332	CP3086	Cinnamyl acetate	103-54-8	176.0837	4.6089	176.0833	115.0545	133.0652	116.0622
333	CP3087	Cinnamyl alcohol	104-54-1	134.0732	4.7467	134.0726	105.0702	117.0702	135.0763
334	CP2081	Clomazone	81777-89-1	239.0713	12.6995	239.0727	224.0490	176.0833	177.0549
335	CP2154	Coumaphos	56-72-4	362.0145	16.0754	362.0141	96.9508	109.0048	364.0110
336	CP2082	Cycloate	1134-23-2	215.1344	5.5678	215.1338	154.1228	186.0950	155.1260
337	CP3153	Cyfluthrin[b]	68359-37-5	433.0648	8.3914	433.0677	163.0542	165.0699	167.0855
338	CP3158	Cypermethrin[b]	52315-07-8	415.0742	16.8897	163.0075	165.0047	181.0648	180.0806
339	CP3159	-	-	-	17.0683	163.0075	165.0047	181.0648	180.0806
340	CP3160	-	-	-	17.1267	163.0075	165.0047	181.0648	180.0806
341	CP3161	-	-	-	17.2020	163.0075	165.0047	181.0648	180.0806
342	CP2111	Cyprodinil	121552-61-2	225.1266	8.7078	225.1266	224.1183	225.1293	209.0950
343	CP3097	DFTPP	5074-71-5	441.9969	20.6953	198.9064	435.9891	444.7846	436.9484
344	CP3162	Deltamethrin	52918-63-5	502.9731	13.1150	179.0602	185.0384	178.0775	113.0386
345	CP3163	-	-	-	13.2160	179.0602	185.0384	178.0775	113.0386
346	CP2186	Di-n-butyl phthalate	84-74-2	278.1518	4.8997	205.1587	206.1621	149.0836	150.0995
347	CP3047	-	-	-	19.3601	205.1224	149.0449	206.1258	150.1039
348	CP2187	Di-n-octyl phthalate[b]	117-84-0	390.2770	17.8470	149.1238	150.1359	275.1057	151.1392
349	CP3056	-	-	-	14.1913	149.0238	279.1590	150.0302	167.0339
350	CP2083	Diallate-cis	2303-16-4	269.0408	19.2107	207.0327	209.0123	208.0323	87.0442
351	CP2084	-	-	-	19.3073	207.0327	209.0123	208.0323	87.0442
352	CP2006	Diazinon	333-41-5	304.1010	6.4956	304.1008	179.1175	137.0706	199.0627
353	CP2226	Dibenz(a,h)anthracene	53-70-3	278.1096	19.7667	278.1089	276.0939	279.1126	274.0783
354	CP3045	-	-	-	19.5582	278.1094	276.0937	279.1126	281.0514
355	CP2210	Dibenzofuran	132-64-9	168.0575	8.7505	168.0569	139.0543	169.0602	92.0257
356	CP2210_2	-	-	-	8.9437	168.0569	139.0543	169.0602	92.0257
357	CP2210_3	-	-	-	9.1820	168.0569	139.0543	169.0602	92.0257
358	CP3046	-	-	-	5.0284	168.0567	139.0540	165.0294	169.0599
359	CP2400	Dibromochloromethane	124-48-1	205.8134	14.2966	129.0336	92.8103	93.9561	128.0137
360	CP2403	Dibromomethane	74-95-3	171.8523	7.7439	173.9094	175.9064	176.9062	94.9607
361	CP2268	Dicamba	1918-00-9	219.9694	13.0468	175.0155	245.9675	219.9708	172.8420

Index	Library ID	Name	CAS	Monoisotopic Mass	Target RT (min.)	mz0	mz1	mz2	mz3
362	CP2061	Dichlobenil	1194-65-6	170.9643	4.0378	170.9636	172.9607	100.0181	164.0009
363	CP2058	Dichlofluanid	1085-98-9	331.9623	14.2966	123.0442	167.0340	124.0475	168.0373
364	CP2059	Dichloran	99-30-9	205.9650	6.1593	205.9644	175.9664	177.9634	207.9614
365	CP2269	Dichlorprop Acid	120-36-5	233.9850	11.0992	161.9633	163.9603	165.9574	233.9873
366	CP3132	Dichlorvos	62-73-7	219.9459	5.9794	108.9654	219.8630	144.9375	184.9532
367	CP1081	Dieldrin	60-57-1	377.8706	11.1349	342.9009	324.8720	242.9530	146.9998
368	CP2035	-	-	-	9.7656	377.8691	376.8658	260.8548	241.8936
369	CP2283	Diethyl phosphate	598-02-7	154.0395	7.7484	154.0403	125.0421	155.0328	139.0578
370	CP2283_2	-	-	-	8.0660	154.0403	125.0421	155.0328	139.0578
371	CP2184	Diethyl phthalate	84-66-2	222.0890	8.5031	222.0872	177.0659	150.0464	176.0944
372	CP3049	-	-	-	5.3133	149.0596	177.0546	167.0337	222.0893
373	CP2291	Diisopropylphenylphosphate	51496-03-8	258.1021	8.4267	261.0458	260.0618	237.0801	262.0533
374	CP2085	Dimethachlor	50563-36-5	255.1026	16.7281	252.0936	256.1247	253.0968	255.1025
375	CP2281	Dimethyl phosphate	813-78-5	126.0082	11.4329	126.0090	125.0057	94.9950	96.0029
376	CP2281_2	-	-	-	8.1435	126.0090	125.0057	94.9950	96.0029
377	CP2281_3	-	-	-	7.5852	126.0090	125.0057	94.9950	96.0029
378	CP2185	Dimethyl phthalate	131-11-3	194.0580	15.0571	193.0481	138.1426	194.0563	192.0407
379	CP3053	-	-	-	6.7782	194.0576	163.0390	166.0465	116.0621
380	CP2278	Dinoseb	88-85-7	240.0746	5.6138	240.0746	211.0603	212.0681	213.0634
381	CP2086	Diphenamid	957-51-7	239.1310	8.4088	239.1306	167.0853	165.0697	152.0619
382	CP3114	-	-	-	8.4093	239.1306	167.0858	165.0702	168.0892
383	CP2062	Diphenylamine	122-39-4	169.0891	5.5408	169.0885	168.0808	167.0733	170.0921
384	CP2171	Disulfoton	298-04-4	274.0285	6.6363	274.0284	88.0341	89.0419	97.0469
385	CP2476	Diuron	330-54-1	232.0170	10.4276	232.0173	231.0082	233.0052	230.0198
386	CP2007	EPN	2104-64-5	323.0381	13.2276	323.0371	156.9871	141.0099	159.0204
387	CP2155	Edifenphos	17109-49-8	310.0251	11.6854	310.0235	109.0105	108.0026	218.0217
388	CP1082	Endosulfan I	959-98-8	403.8169	10.7845	194.9158	197.9392	106.9314	198.9284
389	CP2036	-	-	-	10.7892	194.9530	337.9201	339.9173	341.9143
390	CP2037	Endosulfan II	33213-65-9	403.8169	9.3920	337.9202	335.9232	339.9169	341.9144
391	CP2038	Endosulfan ether	3369-52-6	339.8550	6.9667	339.8547	240.8956	238.8985	236.8409
392	CP1084	Endosulfan sulfate	1031-07-8	419.8118	11.7143	421.8082	386.8399	271.8101	419.8112
393	CP2039	-	-	-	11.7326	226.8985	228.8957	271.8099	240.8958
394	CP1085	Endrin	72-20-8	377.8706	12.8306	318.9005	316.9033	249.8486	242.9530
395	CP2040	-	-	-	12.4434	316.9410	85.9734	262.9424	249.9824
396	CP1086	Endrin aldehyde	7421-93-4	377.8706	11.1439	344.8982	249.8489	342.9009	316.9032
397	CP2041	-	-	-	11.6023	316.9410	85.9734	344.8986	249.9824
398	CP1087	Endrin ketone	53494-70-5	377.8706	12.8441	317.9066	314.9063	315.9095	249.8486
399	CP2042	-	-	-	12.8467	316.9035	318.9004	314.9065	320.8974
400	CP2063	Ethalfluralin	55283-68-6	333.0936	5.6138	333.0927	276.0590	316.0900	277.0624
401	CP2156	Ethion	563-12-2	383.9876	11.0857	383.9869	230.9736	96.9508	153.0133
402	CP3116	Ethoprop	13194-48-4	242.0564	5.5581	242.0543	240.0573	241.0607	243.0576
403	CP2488	Ethyl acetate	141-78-6	88.0524	3.1707	88.0519	101.0597	89.0597	87.0441
404	CP2490	Ethyl butyrate[b]	105-54-4	116.0837	7.9785	116.0832	88.0519	89.0597	101.0598
405	CP3088	-	-	-	7.9859	116.0833	88.0475	117.0863	115.0754
406	CP2496	Ethyl caprate[a]	110-38-3	200.1776	4.3130	200.1769	131.1068	89.0598	87.0441
407	CP2492	Ethyl caproate	123-66-0	144.1150	7.9807	144.1143	97.1011	98.1044	101.0596
408	CP2492_2	-	-	-	5.3230	144.1143	97.1011	98.1044	101.0596
409	CP2494	Ethyl caprylate	106-32-1	172.1463	3.1662	172.1458	88.0519	87.0440	171.1378
410	CP2494_2	-	-	-	5.3207	172.1458	88.0519	87.0440	171.1378
411	CP2493	Ethyl heptanoate	106-30-9	158.1307	7.9785	158.1298	88.0517	113.0959	101.0596
412	CP2493_2	-	-	-	10.0181	158.1298	88.0517	113.0959	101.0596
413	CP2498	Ethyl laurate	106-33-2	228.2089	5.3207	228.2085	115.0751	87.0439	129.0907
414	CP3145	Ethyl maltol	225-582-5	140.0473	4.4295	140.0469	139.0389	138.0995	97.0285

Index	Library ID	Name	CAS	Monoisotopic Mass	Target RT (min.)	mz0	mz1	mz2	mz3
415	CP2525	Ethyl methacrylate	97-63-2	114.0681	9.8105	99.0440	97.0648	113.0596	96.0570
416	CP2526	Ethyl methanesulfonate	62-50-0	124.0194	5.7328	124.0195	125.0198	126.0151	123.0041
417	CP2526_2	-	-	-	5.7014	124.0195	125.0198	126.0151	123.0041
418	CP2526_3	-	-	-	5.6138	124.0195	125.0198	126.0151	123.0041
419	CP2499	Ethyl myristate	124-06-1	256.2402	7.9785	256.2401	213.1851	199.1694	227.2008
420	CP3183	Ethyl oleate	111-62-6	310.2872	17.0167	311.2948	265.2531	96.0809	263.2371
421	CP2500	Ethyl palmitate	628-97-7	284.2715	10.0248	284.2708	285.2733	87.0441	129.0910
422	CP2175	Ethyl parathion	56-38-2	291.0330	8.1345	291.0325	109.0049	96.9508	291.0332
423	CP2495	Ethyl pelargonate[a]	123-29-5	186.1620	7.9785	186.1613	87.0441	129.0911	115.0754
424	CP2489	Ethyl propionate	105-37-3	102.0681	3.3426	102.0676	103.0710	104.0719	101.0598
425	CP2501	Ethyl stearate[a]	111-61-5	312.3028	10.2963	312.3018	88.0519	129.0913	101.0598
426	CP2497	Ethyl undecanoate[a]	627-90-7	214.1933	4.8291	214.1926	101.0597	115.0753	87.0440
427	CP2491	Ethyl valerate	539-82-2	130.0994	7.9717	130.0987	88.0519	85.1012	101.0598
428	CP2491_2	-	-	-	5.3252	130.0987	88.0519	85.1012	101.0598
429	CP3144	Ethyl vanillin	121-32-4	166.0630	5.0104	166.0623	137.0386	168.0569	138.0676
430	CP2415	Ethylbenzene	100-41-4	106.0783	3.8962	107.0492	135.0805	108.0526	106.0780
431	CP2356	Ethylene thiourea	96-45-7	102.0252	4.0356	100.0182	99.0104	101.0216	102.0216
432	CP2254	Ethylparaben	120-47-8	166.0630	5.0097	166.0625	121.0285	139.0543	138.0464
433	CP2112	Etofenprox	80844-07-1	376.2039	17.8402	163.1116	135.0803	107.0490	376.2034
434	CP2113	Etridiazole	2593-15-9	245.9188	4.3624	245.9185	182.9175	210.9488	184.9145
435	CP2157	Fenamiphos	22224-92-6	303.1058	9.8891	303.1050	154.0445	217.0084	260.0509
436	CP2114	Fenarimol	60168-88-9	330.0327	14.8582	330.0321	138.9944	107.0239	140.9914
437	CP3133	-	-	-	14.8561	138.9946	107.0241	219.0320	221.0291
438	CP2158	Fenchlorphos	299-84-3	319.8997	7.4482	284.9305	286.9274	285.9340	124.9822
439	CP2008	Fenitrothion	122-14-5	277.0174	7.7035	277.0169	260.0142	261.0176	278.0201
440	CP2272	Fenoprop	93-72-1	267.9461	7.7124	97.0605	95.0492	179.1431	178.0942
441	CP2087	Fenpropathrin	39515-41-8	349.1678	13.6194	349.1672	181.0646	265.0737	180.0807
442	CP2044	Fenson	80-38-6	267.9961	8.3639	267.9956	141.0004	98.9995	269.9930
443	CP2159	Fenthion	55-38-9	278.0200	8.0705	278.0197	169.0137	245.0396	124.9822
444	CP3164	Fenvalerate	51630-58-1	419.1288	18.2454	419.1287	125.0152	225.0786	181.0647
445	CP3165	-	-	-	18.4427	419.1285	125.0152	225.0786	181.0647
446	CP2115	Fipronil	120068-37-3	435.9387	8.7808	366.9430	368.9400	367.9465	369.9439
447	CP2144	Fluazifop-p-butyl	79241-46-6	383.1344	10.7667	383.1333	282.0746	254.0432	283.0778
448	CP2064	Fluchloralin	33245-39-5	355.0547	6.5181	306.0697	307.0730	326.0151	327.0182
449	CP3166	Flucythrinate[b]	70124-77-5	451.1595	17.5758	157.0459	181.0647	199.0929	451.1588
450	CP3167	-	-	-	17.8012	157.0459	199.0929	181.0647	451.1588
451	CP2116	Fludioxonil	131341-86-1	248.0397	10.0787	248.0389	127.0416	182.0475	249.0427
452	CP2227	Fluoranthene[b]	206-44-0	202.0783	8.9437	202.0776	200.0624	203.0812	101.0387
453	CP3057	-	-	-	8.9183	202.0776	200.0621	203.0809	201.0697
454	CP2228	Fluorene	86-73-7	166.0783	5.7059	166.0777	165.0699	167.0854	152.0621
455	CP3058	-	-	-	5.3616	165.0699	166.0775	163.0543	164.0620
456	CP2088	Fluquinconazole	136426-54-5	375.0090	18.4863	340.0049	338.9976	342.0006	344.0661
457	CP2117	Fluridone	59756-60-4	329.1028	12.6905	328.0963	329.0987	330.1055	331.1197
458	CP3134	-	-	-	18.0177	328.0943	252.1827	309.1857	329.1016
459	CP2118	Flusilazole	85509-19-9	315.1003	10.2626	315.1003	233.0593	251.0700	206.0543
460	CP2089	Flutolanil	66332-96-5	323.1133	9.8644	323.1129	173.0209	281.0664	145.0259
461	CP2119	Flutriafol	76674-21-0	301.1027	19.2265	123.0806	164.1516	219.2108	204.1829
462	CP2120	Folpet	133-07-3	294.9028	12.8512	260.0241	293.0326	292.0291	104.0495
463	CP2172	Fonofos	944-22-9	246.0302	6.4530	246.0298	108.9870	137.0182	110.0182
464	CP3089	Geraniol	106-24-1	154.1358	5.1393	154.1352	155.1385	121.1012	93.0699
465	CP3147	Glycerin[ab]	56-81-5	92.0473	5.0284	113.0386	168.0568	87.0229	92.0479
466	CP3198	Glyphosate	1071-83-6	169.0140	4.9688	154.0135	107.0128	184.0115	91.0179
467	CP2359	Halosulfuron-methyl	100784-20-1	434.0410	11.0880	182.0601	183.0636	139.9960	184.9733

Index	Library ID	Name	CAS	Monoisotopic Mass	Target RT (min.)	mz0	mz1	mz2	mz3
468	CP1088	Heptachlor	76-44-8	369.8211	7.3681	271.8098	273.8067	370.8289	270.9057
469	CP2045	-	-	-	7.3662	369.8198	271.8101	273.8072	269.8131
470	CP1089	Heptachlor epoxide (isomer B)	1024-57-3	385.8160	8.7148	352.8441	354.8409	350.8469	249.8487
471	CP2046	-	-	-	8.7011	385.8154	352.8441	354.8409	350.8469
472	CP2258	Heptylparaben	1085-12-7	236.1412	13.2254	236.1406	237.1436	235.1346	234.1264
473	CP1009	Hexachlorobenzene	118-74-1	281.8131	5.9841	283.8099	285.8070	281.8129	287.8041
474	CP2047	-	-	-	5.9850	281.8125	283.8099	285.8070	287.8041
475	CP3059	-	-	-	5.9794	281.8125	283.8103	285.8073	287.8043
476	CP2198	Hexachlorobutadiene	87-68-3	257.8131	3.2865	257.8127	224.8409	226.8380	222.8438
477	CP3060	-	-	-	3.2925	257.8127	224.8407	226.8377	222.8436
478	CP2199	Hexachlorocyclopentadiene	77-47-4	269.8131	7.3707	269.8127	236.8408	238.8378	234.8438
479	CP2199_2	-	-	-	14.4076	269.8127	236.8408	238.8378	234.8438
480	CP2199_3	-	-	-	11.7213	269.8127	236.8408	238.8378	234.8438
481	CP3061	-	-	-	14.9190	269.8123	236.8407	234.8437	238.8377
482	CP3061_2	-	-	-	5.6085	269.8123	236.8407	234.8437	238.8377
483	CP3062	Hexachloroethane	67-72-1	233.8131	7.4124	116.9060	200.8826	164.9060	165.9093
484	CP2527	Hexachlorophene	70-30-4	403.8499	5.3319	195.9059	197.9029	193.9088	208.8708
485	CP2528	Hexachloropropene	1888-71-7	245.8131	19.3455	245.8129	213.1125	211.1432	215.1155
486	CP3180	Hexanoic acid[b]	142-62-1	116.0837	10.0404	116.0833	88.0475	117.0863	115.0754
487	CP2481	Hexazinone	51235-04-2	252.1586	19.5229	171.1169	172.1248	169.1012	252.1611
488	CP3127	-	-	-	12.0878	252.1583	171.0874	128.0817	172.0906
489	CP2330	Homosalate	118-56-9	262.1570	17.8447	138.1359	201.1638	109.1012	200.1513
490	CP3090	Hydroxycitronellal	107-75-5	172.1463	9.8284	172.1457	171.1167	175.1481	174.1402
491	CP2229	Indeno(1,2,3-cd)pyrene	193-39-5	276.0939	20.0851	276.0938	277.0971	274.0784	272.0627
492	CP3063	-	-	-	19.8191	276.0938	274.0782	277.0969	137.0385
493	CP2160	Iodofenphos	18181-70-9	411.8353	9.7633	376.8667	378.8654	125.0961	411.8351
494	CP2121	Iprodione	36734-19-7	329.0334	13.1456	314.0097	186.9586	316.0065	188.9557
495	CP2009	Isazophos	42509-80-8	313.0417	6.6498	313.0410	118.9879	119.9957	120.9849
496	CP2260	Isobutylparaben	4247-02-3	194.0940	7.1495	194.0938	121.0649	138.0097	93.0336
497	CP2289	Isodecyl Diphenyl Phosphate	29761-21-5	390.1960	22.7827	392.1253	391.1178	393.1288	250.0989
498	CP2048	Isodrin	465-73-6	361.8760	14.1125	361.8747	376.8981	374.9005	378.8950
499	CP2200	Isophorone	78-59-1	138.1045	3.7643	138.1038	95.0855	129.0909	123.1168
500	CP3064	-	-	-	5.2010	138.1038	137.0961	139.1118	140.1152
501	CP2065	Isopropalin	33820-53-0	309.1689	8.5053	309.1682	238.0828	280.1300	264.1350
502	CP2416	Isopropylbenzene	98-82-8	120.0939	17.2940	120.0934	105.0699	106.0778	119.0857
503	CP2255	Isopropylparaben	4191-73-5	180.0786	8.4425	180.0769	179.0701	178.0650	121.0762
504	CP2529	Isosafrole	120-58-1	162.0681	18.4413	162.0675	161.0597	163.0708	104.0621
505	CP2122	Lenacil	2164-08-1	234.1368	5.6947	152.9976	154.0418	155.0451	234.1385
506	CP2161	Leptophos	21609-90-5	409.8699	14.1057	171.0027	376.8986	374.9009	378.8953
507	CP2090	Linuron	330-55-2	248.0119	7.8190	248.0113	250.0082	251.0112	247.0033
508	CP2090_2	-	-	-	10.4276	248.0113	250.0082	251.0112	247.0033
509	CP2090_3	-	-	-	10.9678	248.0113	250.0082	251.0112	247.0033
510	CP2090_4	-	-	-	10.1561	248.0113	250.0082	251.0112	247.0033
511	CP2162	Malathion	121-75-5	330.0361	7.8235	93.0100	124.9821	127.0390	173.0808
512	CP2339	Malathion diacid	1190-28-9	273.9735	10.4388	282.9799	284.9769	286.9735	287.9776
513	CP2339_2	-	-	-	10.5994	282.9799	284.9769	286.9735	287.9776
514	CP2339_3	-	-	-	11.2307	282.9799	284.9769	286.9735	287.9776
515	CP2339_4	-	-	-	10.1561	282.9799	284.9769	286.9735	287.9776
516	CP3142	Maltol	118-71-8	126.0317	3.3981	126.0313	127.0573	145.0284	109.0398
517	CP2277	Mecoprop	7085-19-0	214.0397	4.9042	107.0492	105.0700	142.0733	214.0399
518	CP3148	Menthone[b]	14073-97-3	154.1358	7.9791	128.1070	139.1479	138.0996	154.1348
519	CP2145	Metalaxyl[b]	57837-19-1	279.1471	9.7251	132.0935	160.1245	206.1666	145.1013
520	CP2091	Metazachlor	67129-08-2	277.0982	19.7667	277.0967	276.0934	274.0775	278.1091

Index	Library ID	Name	CAS	Monoisotopic Mass	Target RT (min.)	mz0	mz1	mz2	mz3
521	CP2091_2	-	-	-	20.0851	277.0967	276.0934	274.0775	278.1091
522	CP2163	Methacrifos	62610-77-9	240.0221	4.8593	240.0217	180.0004	207.9955	124.9818
523	CP2530	Methapyrilene	91-80-5	261.1300	19.2512	97.1012	260.2504	93.0700	261.2584
524	CP2511	Methiocarb	2032-65-7	225.0824	11.7281	168.0010	109.0108	153.0134	226.0944
525	CP2505	Methomyl	16752-77-5	162.0463	5.3689	162.0465	163.0542	161.0387	106.0651
526	CP1090	Methoxychlor[b]	72-43-5	344.0138	13.4529	227.1066	228.1098	152.0618	212.0830
527	CP2092	-	-	-	3.7643	344.0140	341.0177	343.0142	342.0173
528	CP2532	Methyl methacrylate	80-62-6	100.0524	9.8037	100.0519	101.0597	99.0441	87.0441
529	CP2533	Methyl methanesulfonate[b]	66-27-3	110.0037	10.4478	111.0229	111.9889	109.9919	113.0386
530	CP2173	Methyl parathion	298-00-0	263.0017	7.2927	263.0018	127.0154	124.9820	109.0048
531	CP2418	Methylene chloride	75-09-2	83.9534	3.2887	224.8409	222.8438	226.8379	228.8350
532	CP2252	Methylparaben[b]	99-76-3	152.0473	4.3926	152.0468	93.0336	151.0390	121.0525
533	CP2093	Metolachlor	51218-45-2	283.1339	7.2838	162.1277	238.0994	240.0970	163.0627
534	CP2482	Metribuzin	21087-64-9	214.0888	13.4591	196.0882	195.0804	194.0725	198.0629
535	CP2361	Metsulfuron-methyl	74223-64-6	381.0743	7.0757	210.0680	197.0602	199.0572	198.0635
536	CP2174	Mevinphos	7786-34-7	224.0450	10.3031	224.0447	223.0368	226.0238	225.0361
537	CP3117	-	-	-	9.5716	224.0443	127.0157	164.0236	109.0051
538	CP1095	Mirex	2385-85-5	539.6262	14.3029	272.7382	273.8000	274.9293	269.8127
539	CP2051	-	-	-	14.4076	271.8100	269.8129	273.8070	275.8040
540	CP2486	Molinate[b]	2212-67-1	187.1031	5.0950	187.1024	126.0912	98.0964	188.1058
541	CP3128	-	-	-	5.0966	187.1023	126.0916	98.0966	127.0949
542	CP2342	Mono(2-ethyl-5-hydroxyhexyl) phthalate	40321-99-1	294.1467	8.5111	294.1446	280.1293	281.1328	236.1391
543	CP2341	Mono(2-ethyl-5-oxohexyl) phthalate	40321-98-0	292.1311	23.4396	292.1283	293.0511	296.2502	297.2062
544	CP2346	Mono(3-carboxypropyl) phthalate	66851-46-5	252.0634	9.8891	252.0634	243.0241	225.0133	244.0272
545	CP2343	Mono(5-carboxy-2-ethylpentyl) phthalate	40809-41-4	308.1260	18.4481	204.1146	205.1223	199.1118	209.0293
546	CP2382	Mono-2-ethylhexyl phthalate[b]	4376-20-9	278.1518	9.7206	223.1691	163.1116	221.2215	119.0855
547	CP2376	Mono-benzyl phthalate	2528-16-7	256.0735	7.7080	91.0543	109.0648	95.0492	93.0699
548	CP2378	Mono-cyclohexyl phthalate	7517-36-4	248.1049	15.0706	248.1030	149.0582	150.0615	105.0446
549	CP2379	Mono-ethyl phthalate	2306-33-4	194.0579	6.7614	194.0574	149.0597	105.0449	150.0631
550	CP2381	Mono-isobutyl phthalate	30833-53-5	222.0892	17.2693	149.0199	167.0341	104.0257	150.0678
551	CP2383	Mono-isononyl phthalate	106610-61-1	292.1675	8.5111	292.1657	163.0865	164.0945	166.0692
552	CP2384	Mono-methyl phthalate	4376-18-5	180.0423	14.2831	163.0390	179.0340	133.0285	180.8716
553	CP2377	Mono-n-butyl phthalate	131-70-4	222.0892	16.6102	149.0199	167.0341	104.0257	150.0678
554	CP2380	Mono-n-octyl phthalate	5393-19-1	278.1518	4.8291	149.1325	150.1358	167.1430	104.0257
555	CP2477	Monuron	150-68-5	198.0560	7.2231	198.0548	185.0595	156.0570	155.0489
556	CP2124	Myclobutanil	88671-89-0	288.1142	10.2234	288.1139	179.0245	150.0105	152.0386
557	CP2370	N,N-Diethyl-meta-toluamide	134-62-3	191.1310	5.2511	191.1301	119.0491	190.1224	120.0525
558	CP2094	N-(2,4-Dimethylphenyl)formamide	60397-77-5	149.0841	4.8750	149.0836	120.0806	121.0883	106.0649
559	CP2536	N-Nitrosodi-n-butylamine	924-16-3	158.1419	4.5048	156.1384	128.1384	158.1420	115.1309
560	CP2189	N-Nitrosodi-n-propylamine	621-64-7	130.1106	4.1209	130.1114	128.1071	133.0877	132.0844
561	CP2189_2	-	-	-	4.6787	130.1114	128.1071	133.0877	132.0844
562	CP2189_3	-	-	-	4.5946	130.1114	128.1071	133.0877	132.0844
563	CP3075	-	-	-	4.1266	130.1113	128.1070	132.0842	129.1103
564	CP2537	N-Nitrosodiethylamine	55-18-5	102.0793	3.7576	103.0753	101.0597	93.0699	104.0786
565	CP2190	N-Nitrosodiphenylamine	86-30-6	198.0790	8.7505	168.0571	169.0605	157.0761	167.0492
566	CP2538	N-Nitrosoethylmethylamine	10595-95-6	88.0637	4.1209	88.0645	86.0601	104.0529	89.0420
567	CP2539	N-Nitrosomorpholine	59-89-2	116.0586	7.4201	116.0581	99.0227	98.0150	86.0150
568	CP2540	N-Nitrosopyrrolidine	930-55-2	100.0637	11.3160	99.0624	101.0418	87.0261	100.0622
569	CP3184	N-ethylperfluoro-1-octanesulfonamidoacetic acid (linear)	2991-50-6	584.9903	18.1938	585.9483	575.8269	129.9850	534.9703
570	CP3193	N-methylperfluoro-1-octanesulfonamidoacetic acid (linear)[b]	2355-31-9	570.9746	19.2569	179.1431	181.1010	131.0856	180.1828
571	CP2230	Naphthalene	91-20-3	128.0626	3.1617	128.0621	129.0650	126.0462	102.0632
572	CP3068	-	-	-	3.1637	128.0621	127.0544	102.0465	126.0465
573	CP3135	Napropamide[b]	15299-99-7	271.1572	4.1244	128.1070	100.1122	129.1104	130.9451

Index	Library ID	Name	CAS	Monoisotopic Mass	Target RT (min.)	mz0	mz1	mz2	mz3
574	CP2362	Nicosulfuron	111991-09-4	410.1009	13.0580	366.0617	213.0421	182.0602	410.0941
575	CP2066	Nitralin	4726-14-1	345.0995	12.6726	274.0134	316.0602	258.0184	345.0986
576	CP2201	Nitrobenzene	98-95-3	123.0320	8.1390	123.0315	124.0216	122.0236	121.0396
577	CP3072	-	-	-	7.2978	123.0328	121.0285	122.0363	120.0208
578	CP2262	Nonylphenol	104-40-5	220.1827	4.8997	220.1821	135.0805	107.0492	163.1117
579	CP2265	Nonylphenol diethoxylate	9016-45-9	308.2351	19.2489	179.0857	135.0807	107.0493	237.1645
580	CP2263	Nonylphenol monoethoxylate	27986-36-3	264.2089	21.9878	264.2101	179.0257	178.0947	181.0931
581	CP2095	Norflurazon	27314-13-2	303.0386	11.8505	303.0379	302.0304	145.0260	173.0322
582	CP2335	O,O-Diethyl Phosphonate	762-04-9	137.0368	5.5790	137.0363	111.0999	112.1120	139.0155
583	CP2338	O,O-Diethyl dithiophosphate	298-06-6	185.9938	8.1368	185.9934	96.9509	187.9691	106.9951
584	CP2337	O,O-Diethylthiophosphoric Acid	58975-95-4	187.9828	12.8512	187.9843	188.9921	171.9716	190.9893
585	CP2337_2	-	-	-	7.2456	187.9843	188.9921	171.9716	190.9893
586	CP2334	O,O-Dimethyl Thiophosphate	1112-38-5	141.9854	8.1345	141.9849	126.0088	114.9614	113.9536
587	CP2336	O,O-Dimethyl dithiophosphate	756-80-9	157.9625	7.8797	157.9621	142.9927	124.9821	127.9514
588	CP1115	Octachlorodibenzo-p-dioxin	3268-87-9	455.7407	19.0981	458.8721	436.4082	449.7392	431.3833
589	CP1116	Octachlorodibenzofuran	39001-02-0	439.7457	18.9333	444.1823	446.3751	442.7188	439.7500
590	CP1010	Octachlorostyrene	29082-74-4	375.7508	8.5407	307.8099	342.7789	344.7760	309.8070
591	CP2123	Octyl bicycloheptenedicarboximide	113-48-4	275.1885	8.6741	275.1881	164.0704	121.0646	98.0235
592	CP2331	Octyl-dimethyl-p-aminobenzoic acid	21245-02-3	277.2042	11.0655	277.2037	165.0783	164.0706	148.0757
593	CP2096	Oxadiazon	19666-30-9	344.0695	10.1358	344.0688	174.9588	176.9558	258.0320
594	CP2504	Oxamyl	23135-22-0	219.0678	14.9695	219.0678	181.0648	210.0457	220.0758
595	CP2363	Oxasulfuron	144651-06-9	406.0947	5.3207	129.0911	96.0889	97.0649	95.0856
596	CP2315	Oxybenzone	131-57-7	228.0786	8.5717	227.0703	151.0390	105.0448	152.0422
597	CP1012	Oxychlordane	27304-13-8	419.7770	17.7930	114.8006	184.8590	186.6346	338.8635
598	CP2068	Oxyfluorfen	42874-03-3	361.0329	10.2873	361.0315	252.0395	300.0038	317.0064
599	CP1117	PBB-153	59080-40-9	621.5413	18.2124	467.6996	627.5368	546.6187	548.6167
600	CP1031	PCB-101	37680-73-2	323.8834	9.3901	325.8799	253.9452	255.9422	327.8768
601	CP1032	PCB-105	32598-14-4	323.8834	10.7890	325.8799	327.8769	323.8829	253.9452
602	CP1033	PCB-110	38380-03-9	323.8834	10.1468	325.8800	327.8768	323.8828	253.9452
603	CP1034	PCB-118	31508-00-6	323.8834	11.3685	325.8800	327.8770	323.8829	253.9452
604	CP1035	PCB-128	38380-07-3	357.8444	12.5475	359.8409	289.9035	361.8379	287.9064
605	CP1036	PCB-132	38380-05-1	357.8444	11.2935	359.8408	289.9033	361.8378	287.9063
606	CP1037	PCB-138	35065-28-2	357.8444	11.9253	359.8409	361.8379	289.9035	287.9064
607	CP1002	PCB-146	51908-16-8	357.8444	10.6665	359.8407	361.8378	289.9034	287.9064
608	CP1038	PCB-149	38380-04-0	357.8444	10.3926	325.8800	359.8409	327.8770	323.8830
609	CP1039	PCB-151	52663-63-5	357.8444	9.5969	359.8410	289.9034	361.8379	287.9063
610	CP1040	PCB-153	35065-27-1	357.8444	11.1394	359.8407	361.8378	289.9034	357.8437
611	CP1041	PCB-156	38380-08-4	357.8444	13.2047	359.8408	361.8378	357.8438	289.9032
612	CP1003	PCB-157	69782-90-7	357.8444	13.3260	359.8408	361.8378	357.8439	289.9033
613	CP1042	PCB-158	74472-42-7	357.8444	14.3343	359.8408	361.8377	357.8438	289.9033
614	CP1004	PCB-167	52663-72-6	357.8444	12.6688	359.8408	361.8378	393.8018	395.7988
615	CP1043	PCB-169	32774-16-6	391.8055	14.3488	393.8020	395.7989	323.8642	397.7960
616	CP1017	PCB-17	37680-66-3	255.9613	6.4843	186.0231	255.9609	257.9579	220.9920
617	CP1044	PCB-170	35065-30-6	391.8055	14.3735	393.8020	395.7989	323.8642	397.7960
618	CP1045	PCB-171	52663-71-5	391.8055	13.0980	393.8020	395.7989	323.8642	325.8613
619	CP1005	PCB-172	52663-74-8	391.8055	13.4507	393.8020	395.7989	323.8642	325.8612
620	CP1046	PCB-177	52663-70-4	391.8055	12.9710	393.8019	395.7990	323.8644	358.8331
621	CP1018	PCB-18	37680-65-2	255.9613	6.6848	186.0230	255.9609	257.9579	220.9920
622	CP1047	PCB-180	35065-29-3	391.8055	13.6179	393.8021	395.7991	323.8642	397.7961
623	CP1048	PCB-183	52663-69-1	391.8055	12.4228	393.8020	395.7989	323.8642	397.7959
624	CP1049	PCB-187	52663-68-0	391.8055	12.2802	393.8018	395.7988	323.8642	325.8613
625	CP1006	PCB-189	39635-31-9	391.8055	15.1320	393.8017	395.7986	397.7958	323.8642
626	CP1050	PCB-191	74472-50-7	391.8055	13.7359	393.8017	395.7987	323.8643	397.7959

Index	Library ID	Name	CAS	Monoisotopic Mass	Target RT (min.)	mz0	mz1	mz2	mz3
627	CP1051	PCB-194	35694-08-7	425.7665	16.0038	429.7598	427.7628	357.8251	359.8220
628	CP1052	PCB-195	52663-78-2	425.7665	14.7061	429.7601	427.7631	357.8252	359.8221
629	CP1007	PCB-196	42740-50-1	425.7665	14.7016	429.7599	427.7629	357.8252	359.8221
630	CP1053	PCB-199	52663-75-9	425.7665	14.5341	429.7599	427.7629	357.8252	359.8221
631	CP1008	PCB-203	52663-76-0	425.7665	15.4106	429.7599	427.7628	357.8252	431.7568
632	CP1054	PCB-205	74472-53-0	425.7665	16.0903	429.7599	427.7629	431.7569	357.8252
633	CP1055	PCB-206	40186-72-9	459.7275	16.9020	463.7207	461.7240	465.7178	391.7864
634	CP1056	PCB-208	52663-77-1	459.7275	15.3499	463.7207	461.7241	465.7178	391.7863
635	CP1057	PCB-209	2051-24-3	493.6885	17.5608	497.6822	499.6790	495.6852	499.6802
636	CP1019	PCB-28	7012-37-5	255.9613	7.1938	255.9608	257.9578	186.0230	259.9549
637	CP1020	PCB-31	16606-02-3	255.9613	7.1938	255.9609	257.9579	186.0231	259.9550
638	CP1021	PCB-33	38444-86-9	255.9613	8.8240	255.9608	257.9579	186.0230	259.9550
639	CP1022	PCB-44	41464-39-5	289.9224	8.0756	219.9841	291.9189	289.9218	221.9812
640	CP1023	PCB-49	41464-40-8	289.9224	7.8075	291.9189	219.9841	289.9218	221.9812
641	CP1024	PCB-52	35693-99-3	289.9224	7.7459	291.9190	219.9841	289.9219	221.9812
642	CP1001	PCB-66	32598-10-0	289.9224	8.9182	291.9190	289.9220	219.9841	293.9160
643	CP1025	PCB-70	32598-11-1	289.9224	8.7867	219.9841	291.9189	289.9219	221.9811
644	CP1026	PCB-74	32690-93-0	289.9224	8.8778	291.9190	289.9219	219.9841	293.9159
645	CP1027	PCB-82	52663-62-4	323.8834	10.3656	325.8800	253.9452	255.9423	290.9112
646	CP1028	PCB-87	38380-02-8	323.8834	9.9594	325.8799	253.9452	255.9423	327.8769
647	CP1029	PCB-95	38379-99-6	323.8834	8.8868	291.9189	289.9219	325.8799	219.9841
648	CP1030	PCB-99	38380-01-7	323.8834	9.4755	325.8800	253.9452	327.8769	255.9423
649	CP2125	Paclobutrazol	76738-62-0	293.1295	13.2254	236.1405	235.1343	234.1267	238.1481
650	CP2097	Pebulate	1114-71-2	203.1344	4.6764	203.1339	128.1070	132.0843	129.1103
651	CP3136	-	-	-	4.1244	128.1069	132.0841	90.0372	129.1102
652	CP2126	Penconazole	66246-88-6	283.0643	18.4346	159.0805	161.0597	172.0883	160.0840
653	CP2126_2	-	-	-	18.5065	159.0805	161.0597	172.0883	160.0840
654	CP2069	Pendimethalin	40487-42-1	281.1375	8.6189	281.1372	252.0980	162.0784	191.0686
655	CP1015	Pentabromophenol	608-71-9	483.5944	11.6289	487.5915	489.5891	485.5934	491.5875
656	CP2070	Pentachloroaniline	527-20-8	262.8630	6.9779	262.8633	264.8605	266.8575	268.8546
657	CP2054	Pentachloroanisole	1825-21-4	277.8626	6.0471	277.8621	236.8409	264.8362	279.8595
658	CP2542	Pentachlorobenzene	608-93-5	247.8521	4.9859	247.8519	249.8493	251.8464	253.8434
659	CP2071	Pentachlorobenzonitrile	20925-85-3	272.8474	6.3595	272.8469	274.8444	276.8412	278.8383
660	CP2543	Pentachloroethane	76-01-7	199.8521	14.3986	166.9031	116.9061	118.9031	167.9064
661	CP1011	Pentachloronitrobenzene	82-68-8	292.8372	6.2833	236.8408	234.8438	238.8379	199.0450
662	CP2544	-	-	-	6.2841	292.8371	236.8411	238.8382	294.8341
663	CP1016	Pentachlorophenol[b]	87-86-5	263.8470	6.3451	265.8441	267.8412	263.8471	164.9059
664	CP2242	-	-	-	6.3438	263.8466	265.8441	267.8412	164.9059
665	CP3095	-	-	-	6.3172	263.8466	265.8444	267.8403	269.8378
666	CP2055	Pentachlorothioanisole	1825-19-0	293.8398	7.7439	293.8397	295.8367	297.8337	245.8444
667	CP2303	Pentaerythritol tribromide	1522-92-5	321.8200	5.3342	212.8827	214.8791	216.8768	215.8831
668	CP3194	Perfluoro-n-dodecanoic acid	307-55-1	613.9609	5.8761	180.9187	182.9159	179.9296	181.9222
669	CP3187	Perfluoro-n-heptanoic acid	375-85-9	363.9769	18.0788	363.9784	130.9728	180.9515	364.8437
670	CP3189	Perfluoro-n-octanoic acid	335-67-1	413.9737	5.9794	180.9001	130.9315	181.9035	178.9031
671	CP3196	Perfluoro-n-tetradecanoic acid	376-06-7	713.9545	21.9633	647.4247	648.4282	662.4485	131.9121
672	CP3195	Perfluoro-n-tridecanoic acid	72629-94-8	663.9577	19.2905	616.9822	615.9354	666.9864	662.9959
673	CP3188	Perfluorohexanesulfonic acid	355-46-4	399.9439	6.3195	130.9451	181.9087	182.8978	131.9343
674	CP1121	Perfluorohexanoic Acid	307-24-4	313.9801	14.2535	313.9818	131.0494	280.1628	279.1595
675	CP2385	-	-	-	4.6575	268.9787	314.9462	269.9787	270.9754
676	CP3186	-	-	-	9.3844	120.9839	121.9919	267.9825	118.9683
677	CP1122	Perfluorononanoic acid	375-95-1	463.9705	5.9280	130.9218	218.9111	268.7883	132.9607
678	CP2386	-	-	-	13.9451	130.9718	158.9667	160.9637	159.9700
679	CP3191	-	-	-	9.7386	181.1222	130.0777	182.1299	180.1829

Index	Library ID	Name	CAS	Monoisotopic Mass	Target RT (min.)	mz0	mz1	mz2	mz3
680	CP3190	Perfluorooctanesulfonic acid	1763-23-1	499.9375	13.1083	499.9400	497.8907	119.9070	168.8681
681	CP2545	Phenacetin	62-44-2	179.0946	6.3111	180.1019	178.0863	113.0961	179.0941
682	CP2231	Phenanthrene	85-01-8	178.0783	6.5832	178.0778	177.0699	176.0621	88.0308
683	CP3076	-	-	-	6.6390	178.0774	176.0619	179.0807	177.0540
684	CP2243	Phenol[a]	108-95-2	94.0419	3.7778	94.0414	95.0492	92.0577	152.0623
685	CP3077	-	-	-	7.2529	94.0414	95.0491	105.0335	122.0363
686	CP2261	Phenol, 2-octyl-	949-13-3	206.1671	4.9087	206.1667	205.1587	206.1665	191.1430
687	CP3172	Phenothrin, trans	26002-80-2	350.1882	17.8416	123.1169	129.0700	185.1325	187.1481
688	CP3173	-	-	-	17.5488	123.1169	129.0700	185.1325	187.1481
689	CP2176	Phorate	298-02-2	260.0128	7.7035	260.0125	261.0176	262.0102	121.0107
690	CP2010	Phosalone	2310-17-0	366.9868	14.1304	366.9864	182.0001	183.9972	121.0411
691	CP2011	Phosmet	732-11-6	316.9945	13.1232	160.0393	316.0063	161.0427	319.0065
692	CP2270	Picloram	1918-02-1	239.9260	5.7553	239.9241	145.9256	160.9222	111.9202
693	CP2177	Piperonyl butoxide	51-03-6	338.2093	17.8492	176.1560	177.1594	149.1325	178.1673
694	CP2012	Pirimiphos ethyl	23505-41-1	333.1276	8.4267	333.1270	168.0589	318.1041	180.1131
695	CP2013	Pirimiphos methyl	29232-93-7	305.0963	7.6675	305.0957	290.0734	276.0576	180.1133
696	CP2250	Potassium sorbate	24634-61-5	113.0609	6.2931	119.0856	105.0699	133.1012	109.1012
697	CP2098	Pretilachlor	51218-49-6	311.1652	18.4458	162.0676	177.0911	176.0787	238.2292
698	CP2364	Primisulfuron-methyl	86209-51-0	468.0363	22.3722	468.0380	111.9901	117.0548	440.3080
699	CP2099	Prochloraz	67747-09-5	375.0308	4.3881	375.0330	108.0445	376.0337	377.0302
700	CP2127	Procymidone	32809-16-8	283.0167	9.0020	283.0164	96.0567	285.0133	95.0489
701	CP2072	Prodiamine	29091-21-2	350.1202	22.7086	321.1125	349.1076	347.0906	345.0760
702	CP2164	Profenofos	41198-08-7	371.9351	9.9866	371.9343	336.9664	338.9640	268.8859
703	CP2073	Profluralin	26399-36-0	347.1093	6.3483	347.1085	318.0696	330.1061	264.0227
704	CP3118	Prometryne	7287-19-6	241.1361	7.6515	241.1354	184.0656	226.1127	199.0890
705	CP2547	Pronamide	23950-58-5	255.0218	6.4777	255.0224	172.9558	174.9639	239.9979
706	CP3129	-	-	-	6.4920	255.0224	254.0134	256.0105	257.0180
707	CP2100	Propachlor	1918-16-7	211.0764	7.9223	211.0759	162.1275	238.0996	163.1307
708	CP2101	Propanil	709-98-8	217.0061	10.4411	217.0054	175.0124	173.0154	176.0202
709	CP2128	Propargite	2312-35-8	350.1552	12.4568	350.1543	201.0577	351.1578	335.1310
710	CP3119	Propazine	139-40-2	229.1094	6.3329	229.1089	214.0853	172.0383	187.0624
711	CP2102	Propisochlor	86763-47-5	283.1339	7.3640	162.0913	163.0947	164.1070	160.0757
712	CP2349	Propylene thiourea	2122-19-2	116.0410	9.0641	116.0577	113.0386	117.0368	101.0387
713	CP2259	Propylparaben	94-13-3	180.0790	8.1974	180.0769	179.0701	178.0650	122.0602
714	CP2365	Prosulfuron[b]	94125-34-5	419.0875	17.8447	167.0854	141.0700	169.1012	168.0892
715	CP2165	Prothiofos	34643-46-4	343.9628	9.8599	112.9280	266.9467	268.9434	269.6882
716	CP2253	Protocatechuic acid[a]	99-50-3	154.0266	5.4071	109.0285	110.0363	193.0167	104.0495
717	CP2014	Pyraclofos	89784-60-1	360.0464	15.4674	360.0466	194.0242	138.0104	362.0432
718	CP2015	Pyrazophos	13457-18-6	373.0861	15.0571	373.0857	221.0797	232.1084	237.0570
719	CP2232	Pyrene	129-00-0	202.0782	9.4885	202.0776	200.0624	203.0812	201.0700
720	CP3078	-	-	-	9.4481	202.0776	200.0621	203.0809	201.0697
721	CP2103	Pyridaben	96489-71-3	364.1376	16.1080	364.1371	366.1339	365.0147	148.1504
722	CP2016	Pyridaphenthion	119-12-0	340.0647	13.0333	340.0642	199.0865	96.9506	340.0644
723	CP2129	Pyrimethanil	53112-28-0	199.1109	6.6228	199.1102	198.1027	186.1153	197.0950
724	CP2130	Pyriproxyfen	95737-68-1	321.1365	13.7777	321.1371	318.1366	333.1602	320.1336
725	CP2017	Quinalphos	13593-03-8	298.0541	8.9549	298.0533	156.0680	118.0524	157.0757
726	CP3174	Resmethrin	10453-86-8	338.1882	12.7656	338.1877	123.1169	171.0804	128.0621
727	CP2366	Rimsulfuron	122931-48-0	431.0564	14.1057	155.0257	150.0440	167.0553	151.0418
728	CP2478	Rotenone	83-79-4	394.1416	20.4214	394.1411	395.1446	396.1472	379.1178
729	CP2485	S-Ethyl dipropylthiocarbamate	759-94-4	189.1187	4.1187	189.1183	128.1071	132.0844	133.0877
730	CP3115	-	-	-	4.1221	189.1182	128.1072	132.0844	86.0602
731	CP2548	Safrole	94-59-7	162.0681	18.5065	161.0235	147.0445	135.0442	131.0496
732	CP2479	Siduron	1982-49-6	232.1576	9.9282	232.1572	93.0574	92.0496	94.0607

Index	Library ID	Name	CAS	Monoisotopic Mass	Target RT (min.)	mz0	mz1	mz2	mz3
733	CP3137	Simetryn	1014-70-6	213.1048	7.5145	213.1042	155.0387	170.0493	185.0731
734	CP2420	Styrene	100-42-5	104.0626	3.7688	104.0621	105.0656	106.0778	133.0648
735	CP2367	Sulfosulfuron	141776-32-1	470.0678	12.4411	235.9791	173.0153	135.0806	470.0680
736	CP2166	Sulfotepp	3689-24-5	322.0227	5.7553	322.0221	293.9906	145.9250	96.9504
737	CP2167	Sulprofos	35400-43-2	322.0285	11.4464	322.0281	156.0060	140.0289	112.9278
738	CP2131	Tebuconazole	107534-96-3	307.1451	17.8470	125.1327	250.2654	151.1482	165.1638
739	CP2104	Tebufenpyrad	119168-77-3	333.1608	13.7598	333.1602	171.0317	318.1370	276.0900
740	CP3138	Tebuthiuron	34014-18-1	228.1045	6.2611	156.0961	155.0925	154.0849	169.0957
741	CP3175	Tefluthrin	79538-32-2	418.0571	18.9865	418.3715	417.3684	416.3650	413.3410
742	CP2132	Terbacil	5902-51-2	216.0666	7.9874	117.0863	217.0341	216.0683	161.0597
743	CP3139	-	-	-	13.4762	216.0653	213.0464	214.0496	215.0620
744	CP2168	Terbufos	13071-79-9	288.0441	6.4022	288.0438	230.9735	96.9507	174.9106
745	CP2133	Terbuthylazine	5915-41-3	229.1094	6.4395	229.1089	214.0853	138.0775	216.0824
746	CP3120	Terbutryn	886-50-0	241.1361	7.9043	241.1355	170.0498	185.0734	226.1127
747	CP1070	Tetrabromobisphenol A	79-94-7	539.7571	18.8134	528.7294	530.7267	526.7321	543.7524
748	CP2299	-	-	-	18.8497	528.7295	527.4964	530.7244	531.7303
749	CP2300	Tetrabromobisphenol A Bismethyl Ether	37853-61-5	567.7884	18.1273	567.7886	556.7610	558.7590	554.7632
750	CP2311	Tetrabromobisphenol A bis(allyl ether)	25327-89-3	619.8200	8.7482	158.9763	139.0542	338.8268	619.8243
751	CP2310	Tetrabromobisphenol S	39635-79-5	561.6720	13.0670	172.8420	173.9499	174.8400	91.0418
752	CP2309	Tetrabromophthalic Acid	13810-83-8	477.6690	17.5600	463.9313	419.6555	468.2204	465.8980
753	CP2320	Tetrachlorobisphenol A	79-95-8	363.9592	8.7808	350.9481	352.9452	349.9418	347.9442
754	CP2423	Tetrachloroethene	127-18-4	163.8754	3.2932	163.8748	165.8719	167.8690	128.9060
755	CP2169	Tetrachlorvinphos	22248-79-9	363.8993	8.5031	108.9421	328.9033	110.9903	330.9006
756	CP3130	-	-	-	9.3799	240.8958	238.8990	242.8931	106.9451
757	CP2056	Tetradifon	116-29-0	353.8842	13.9473	353.8838	158.9665	228.8858	226.8888
758	CP3182	Tetraethyl ethylenediphosphonate[b]	995-32-4	302.1048	19.3669	166.0943	165.0910	173.0961	164.0832
759	CP2075	Tetrahydrophthalimide[b]	85-40-5	151.0633	4.8862	151.0630	152.0621	150.0464	153.0699
760	CP3176	Tetramethrin	7696-12-0	331.1784	10.0517	164.1516	123.1169	109.1013	151.1118
761	CP2350	Thifensulfuron-methyl	79277-27-3	387.0307	7.7282	141.0259	140.0062	139.0213	138.0374
762	CP3092	Thymol	89-83-8	150.1045	3.7662	150.1038	135.0804	136.0837	151.1071
763	CP2170	Tolclofos-methyl	57018-04-9	299.9544	11.1374	268.9257	270.9224	296.9568	297.9605
764	CP2170_2	-	-	-	10.8229	268.9257	270.9224	296.9568	297.9605
765	CP2424	Toluene	108-88-3	92.0626	5.2848	92.0621	87.0442	88.0520	89.0598
766	CP2076	Tolylfluanid	731-27-1	345.9780	4.6575	345.9761	137.0598	238.9675	239.8740
767	CP3177	Transfluthrin	118712-89-3	370.0150	7.3900	370.0123	163.0154	127.0301	129.0271
768	CP2318	Tri(Chloropropyl) phosphate	1067-98-7	326.0008	8.8414	326.0008	99.0229	156.9607	157.9685
769	CP2306	Tri-M-cresyl phosphate	563-04-2	368.1180	14.5727	368.1182	367.1112	165.0701	261.0684
770	CP2288	Tri-O-cresyl phosphate	78-30-8	368.1177	15.4023	368.1182	367.1112	165.0701	261.0684
771	CP2296	Tri-P-cresyl phosphate	78-32-0	368.1177	16.4743	368.1182	367.1112	165.0701	261.0684
772	CP2483	Triadimefon	43121-43-3	293.0931	9.4953	202.0778	203.0810	207.0325	293.0935
773	CP3121	-	-	-	8.1980	293.0960	208.0276	128.0026	181.0166
774	CP2105	Triallate	2303-17-5	303.0018	10.2918	303.0026	300.0028	304.0154	96.0442
775	CP2368	Triasulfuron	82097-50-5	401.0561	19.4286	401.0529	396.4529	400.0707	398.0725
776	CP2178	Triazophos	24017-47-8	313.0650	11.7191	313.0626	161.0389	162.0464	163.0542
777	CP2285	Tributyl Phosphate	126-73-8	266.1647	19.2489	211.1485	155.0857	152.0622	125.1327
778	CP2428	Trichloroethene	79-01-6	129.9144	5.3342	130.9451	95.9341	93.9372	132.9421
779	CP2347	Triclocarban	101-20-2	313.9780	7.2478	126.9780	160.9794	162.9764	159.9715
780	CP2352	Triclosan	3380-34-5	287.9512	9.3583	287.9511	218.0130	289.9478	288.9539
781	CP2134	Tricyclazole	41814-78-2	189.0361	10.4411	162.0231	161.0153	163.0264	189.0343
782	CP3131	-	-	-	10.0292	189.0354	161.0167	162.0244	180.0351
783	CP2135	Triflumizole	68694-11-1	345.0856	9.1225	345.0854	205.9983	218.0484	178.9872
784	CP2077	Trifluralin	1582-09-8	335.1093	5.7373	335.1082	264.0223	306.0693	248.0274
785	CP2369	Triflusulfuron-methyl	126535-15-7	492.1039	19.0639	492.1051	327.3142	328.2132	325.0566

Index	Library ID	Name	CAS	Monoisotopic Mass	Target RT (min.)	mz0	mz1	mz2	mz3
786	CP2292	Triisopropyl Phosphate	513-02-0	224.1180	8.7190	224.1182	225.1252	208.0870	222.1028
787	CP2282	Trimethyl Phosphate	512-56-1	140.0240	11.4396	140.0251	141.0324	124.0343	123.0206
788	CP2344	Tripentyl Phosphate	2528-38-3	308.2116	19.2512	98.1047	169.1012	239.1794	97.1014
789	CP2284	Tripropyl Phosphate	513-08-6	224.1177	8.7190	224.1182	225.1252	226.1294	222.1027
790	CP2297	Tris(1,3-dichloro-2-propyl) phosphate	13674-87-8	427.8840	11.6113	98.9843	190.9426	208.9532	96.9841
791	CP2295	Tris(1-chloro-2-propyl) phosphate	13674-84-5	326.0008	3.8621	123.9950	124.9921	98.9811	125.9920
792	CP2321	Tris(2-butoxyethyl) phosphate	78-51-3	398.2433	12.7197	124.9998	199.0730	297.1853	197.1724
793	CP2293	Tris(2-chloroethyl) phosphate	115-96-8	283.9539	9.2920	283.9551	245.9996	247.9971	249.0003
794	CP2293_2	-	-	-	10.0270	283.9551	245.9996	247.9971	249.0003
795	CP2304	Tris(2-chloropropyl) phosphate	6145-73-9	326.0008	7.8235	123.9949	124.9921	125.9920	98.9811
796	CP2290	Tris(2-ethylhexyl) phosphate	78-42-2	434.3525	7.9740	99.1168	113.0915	237.2214	129.0909
797	CP2302	Tris(tribromoneopentyl)[b]	21850-44-2	935.4930	21.9653	647.4252	664.4547	648.4294	649.4321
798	CP2313	Tris(tribromoneopentyl) phosphate	19186-97-1	1009.4062	10.0270	255.2318	241.2161	227.2004	228.2038
799	CP3093	Vanillin	121-33-5	152.0473	4.3723	152.0468	151.0391	123.0441	109.0286
800	CP2487	Vernolate[b]	1929-77-7	203.1344	4.6059	203.1338	128.1071	129.1104	86.0604
801	CP2136	Vinclozolin	50471-44-8	284.9959	7.2456	284.9953	212.0027	178.0415	213.9997
802	CP1072	alpha-benzenehexachloride	319-84-6	287.8601	5.9392	182.9338	180.9370	218.9108	184.9311
803	CP2019	-	-	-	5.9401	180.9370	182.9338	218.9108	184.9311
804	CP1073	beta-benzenehexachloride	319-85-7	287.8601	6.2945	182.9338	180.9370	218.9108	184.9311
805	CP2020	-	-	-	6.2999	180.9370	182.9338	218.9108	184.9311
806	CP3210	bis(1,3-Dichloro-2-propyl) phosphate	72236-72-7	427.8839	14.9100	423.8726	425.8694	152.0621	236.8407
807	CP2182	bis(2-Chloro-1-methylethyl)ether	108-60-1	170.0270	6.5001	170.0268	169.0236	121.0341	171.0195
808	CP3035	-	-	-	6.5280	170.0278	121.0203	120.0124	122.0214
809	CP2180	bis(2-Chloroethoxy)methane	111-91-1	172.0060	11.6113	172.0076	173.0155	95.0088	93.0292
810	CP2180_2	-	-	-	12.3187	172.0076	173.0155	95.0088	93.0292
811	CP2180_3	-	-	-	12.4456	172.0076	173.0155	95.0088	93.0292
812	CP3033	-	-	-	5.6893	172.0048	171.0081	173.0051	174.0085
813	CP2181	bis(2-Chloroethyl)ether	111-44-4	141.9952	8.2705	141.9950	138.9948	139.9979	140.9916
814	CP2181_2	-	-	-	10.8341	141.9950	138.9948	139.9979	140.9916
815	CP3034	-	-	-	8.1980	141.9951	138.9947	140.9917	139.9980
816	CP3034_2	-	-	-	5.6713	141.9951	138.9947	140.9917	139.9980
817	CP2188	bis(2-Ethylhexyl)phthalate	117-81-7	390.2770	14.2966	149.0233	167.0340	279.1592	391.2852
818	CP3036	-	-	-	14.2160	394.2938	391.2855	167.0339	150.0265
819	CP2407	cis-1,2-Dichloroethene	156-59-2	95.9534	6.3460	95.9528	97.9499	94.9451	96.9421
820	CP2413	cis-1,3-Dichloropropene	10061-01-5	109.9690	5.3319	106.9685	107.9344	97.9732	110.9612
821	CP2326	cis-3-(2,2-Dichlorovinyl)-2,2-dimethylcylo	59042-49-8	208.0058	6.6475	173.0714	175.0639	207.0325	129.0089
822	CP1076	cis-Chlordane	5103-71-9	405.7978	10.4476	405.8046	407.8003	403.8047	406.8058
823	CP2024	-	-	-	9.2000	405.7969	372.8255	374.8226	376.8197
824	CP1091	cis-Nonachlor	5103-73-1	439.7588	9.5273	408.7842	406.7873	410.7812	404.7901
825	CP2052	-	-	-	9.5334	439.7579	408.7842	406.7873	410.7812
826	CP3170	cis-Permethrin	61949-76-6	390.0789	15.9873	183.0804	168.0570	127.0310	153.0699
827	CP3091	d-Limonene	5989-27-5	136.1252	5.1393	136.1248	93.0701	141.1277	154.1355
828	CP1075	delta-benzenehexachloride	319-86-8	287.8601	6.7829	182.9338	180.9370	218.9108	184.9311
829	CP2022	-	-	-	6.7938	180.9370	182.9338	218.9108	184.9311
830	CP2043	ethyl-DDD[b]	72-56-0	306.0942	21.9653	223.0423	225.0674	179.0257	306.0970
831	CP1074	gamma-benzenehexachloride[b]	58-89-9	287.8601	6.3474	182.9338	180.9370	218.9108	184.9311
832	CP2021	-	-	-	6.3483	180.9370	182.9338	218.9108	184.9311
833	CP3157	lambda-Cyhalothrin	91465-08-6	449.1006	14.8988	449.1007	181.0647	141.0509	197.0340
834	CP2520	m-Cresol	108-39-4	108.0575	5.2848	107.0856	109.0649	105.0700	108.0570
835	CP2524	m-Dinitrobenzene	99-65-0	168.0171	4.6809	168.0166	92.0257	122.0152	121.0161
836	CP2433	m-Xylene	108-38-3	106.0783	17.5465	106.0778	91.0542	105.0699	93.0700
837	CP2392	n-Butylbenzene	104-51-8	134.1096	4.9042	134.1091	119.0854	133.1011	103.0637
838	CP3107	n-Docosane	629-97-0	310.3600	10.0427	85.1012	97.1013	111.1169	125.1325

Index	Library ID	Name	CAS	Monoisotopic Mass	Target RT (min.)	mz0	mz1	mz2	mz3
839	CP3098	n-Dodecane	112-40-3	170.2035	3.2018	170.2045	85.1012	97.1012	111.1169
840	CP3112	n-Dotriacontane	544-85-4	450.5165	20.2748	85.1012	97.1013	111.1169	125.1325
841	CP3106	n-Eicosane	112-95-8	282.3287	7.9881	282.3307	85.1012	97.1013	111.1169
842	CP3103	n-Heptadecane	629-78-7	240.2817	3.2041	240.2806	97.1012	111.1169	125.1326
843	CP3109	n-Hexacosane	630-01-3	366.4226	14.9672	85.1012	97.1013	111.1169	125.1325
844	CP3102	n-Hexadecane	544-76-3	226.2661	5.9008	85.1012	97.1012	111.1169	125.1326
845	CP3105	n-Nonadecane	629-92-5	268.3130	3.2467	268.3120	214.2857	212.1816	272.0948
846	CP3110	n-Octacosane	630-02-4	394.4538	17.2985	85.1012	97.1013	111.1169	125.1325
847	CP3104	n-Octadecane	593-45-3	254.2974	6.5684	85.1012	97.1012	111.1168	125.1325
848	CP3101	n-Pentadecane	629-62-9	212.2504	5.3593	212.2514	85.1012	97.1012	111.1169
849	CP2419	n-Propylbenzene	103-65-1	120.0939	17.5443	120.0934	105.0699	106.0778	119.0857
850	CP3108	n-Tetracosane	646-31-1	338.3913	12.7188	85.1012	97.1013	111.1169	125.1325
851	CP3100	n-Tetradecane	629-59-4	198.2348	4.3476	198.2341	85.1012	97.1012	111.1169
852	CP3111	n-Triacontane	638-68-6	422.4852	19.7877	85.1012	97.1013	111.1169	125.1325
853	CP3099	n-Tridecane	629-50-5	184.2191	4.3521	85.1012	97.1012	111.1169	126.1409
854	CP1096	o,p'-DDD	53-19-0	317.9537	10.1670	235.0079	237.0049	165.0697	199.0309
855	CP2028	-	-	-	10.1695	235.0079	237.0049	165.0697	199.0309
856	CP1097	o,p'-DDE	3424-82-6	315.9380	9.2993	246.0008	247.9979	317.9357	315.9386
857	CP2030	-	-	-	9.2988	246.0008	247.9979	317.9357	315.9386
858	CP3001	o-Aminoazotoluene[b]	97-56-3	225.1266	7.3989	134.0965	106.0652	135.0805	227.0838
859	CP3021	o-Anisidine[b]	90-04-0	123.0684	6.2903	108.0683	125.0472	122.0602	123.0680
860	CP2473	o-Chlorophenyl thiourea	5344-82-1	186.0018	8.9414	185.9997	110.9997	187.9967	186.0000
861	CP2204	o-Cresol	95-48-7	108.0575	4.6787	107.0856	109.0649	105.0700	108.0570
862	CP3066	-	-	-	7.2709	108.0570	109.0648	107.0813	110.0683
863	CP2551	o-Toluidine[b]	95-53-4	107.0735	5.7970	106.0653	107.0730	108.0683	105.0573
864	CP3017	-	-	-	7.8706	107.0730	106.0651	108.0764	105.0336
865	CP2432	o-Xylene	95-47-6	106.0783	17.2962	106.0778	91.0542	105.0699	93.0700
866	CP2332	octyl-Methoxycinnamate	5466-77-3	290.1880	9.8105	150.1405	152.1195	178.1715	179.1429
867	CP3019	p-Aminoazobenzene	60-09-3	197.0953	7.1496	197.0960	198.0499	167.0406	105.0450
868	CP3005	p-Cresidine	120-71-8	137.0841	3.7707	137.0846	121.0647	138.0311	139.0755
869	CP2205	p-Cresol	106-44-5	108.0575	4.8974	107.0856	109.0649	105.0700	108.0570
870	CP3067	-	-	-	9.7341	108.0570	109.0648	122.0683	106.0415
871	CP2522	p-Dimethylaminoazobenzene	60-11-7	225.1266	10.6173	225.1260	120.0809	105.0574	226.1298
872	CP2417	p-Isopropyltoluene	99-87-6	134.1096	6.2886	134.1091	119.0854	133.1011	103.0637
873	CP2241	p-Nitrophenol	100-02-7	139.0269	8.1323	139.0265	109.0284	110.0318	105.0699
874	CP3074	-	-	-	4.4295	139.0265	109.0285	140.0298	110.0364
875	CP2515	p-Phenylenediamine	106-50-3	108.0687	6.4911	108.0684	107.0606	93.0449	109.0650
876	CP2434	p-Xylene	106-42-3	106.0783	17.8470	106.0778	91.0542	105.0699	93.0700
877	CP2508	propoxur	114-26-1	209.1052	19.2489	110.1046	111.0805	152.0832	93.0699
878	CP2393	sec-Butylbenzene	135-98-8	134.1096	7.7169	134.1091	119.0854	133.1011	103.0637
879	CP3168	tau-Fluvalinate	102851-06-9	502.1271	18.4013	502.1266	250.0609	252.0579	181.0647
880	CP3169	-	-	-	18.4853	502.1268	250.0609	252.0578	181.0647
881	CP2394	tert-Butylbenzene	98-06-6	134.1096	7.9785	134.1091	119.0854	133.1011	103.0637
882	CP1099	tetrachlorodibenzo-p-dioxin	1746-01-6	319.8965	12.8329	319.9031	318.9005	320.8976	322.8939
883	CP1100	tetrachlorodibenzofuran	51207-31-9	303.9016	11.7895	305.8986	303.9017	307.8956	306.9017
884	CP2408	trans-1,2-Dichloroethene	156-60-5	95.9534	6.7883	95.9528	97.9499	94.9451	96.9421
885	CP2414	trans-1,3-Dichloropropene	10061-02-6	109.9690	5.7014	106.9685	107.9344	97.9732	110.9612
886	CP2327	trans-3-(2,2-Dichlorovinyl)-2,2-dimethylcylo[b]	59042-50-1	208.0058	6.6745	173.0714	175.0639	207.0325	129.0089
887	CP1077	trans-Chlordane	5103-74-2	405.7978	10.9192	405.8046	407.8003	403.8047	406.8058
888	CP2025	-	-	-	9.4571	405.7969	372.8255	374.8226	376.8197
889	CP3085	trans-Cinnamaldehyde	14371-10-9	132.0575	3.6809	132.0565	131.0495	103.0546	104.0623
890	CP1092	trans-Nonachlor	39765-80-5	439.7588	10.8990	408.7842	406.7873	410.7812	404.7901
891	CP2053	-	-	-	10.8970	439.7580	408.7842	406.7873	410.7812

Index	Library ID	Name	CAS	Monoisotopic Mass	Target RT (min.)	mz0	mz1	mz2	mz3
892	CP3171	trans-Permethrin	61949-77-7	390.0789	16.2041	183.0804	168.0570	127.0310	153.0699

SUPPLEMENTARY TABLE 2

Metadata for all chemicals annotated in samples. [a] *Both an endogenous and exogenous (xenobiotic) chemical.*

GROUP: Class: *Subclass*: Name	CAS	Potential EDC	IARC Group	Superclass: Class
AGROCHEMICALS				
Fungicides				
Anilinopyrimidine				
Cyprodinil	121552-61-2	✓	–	Benzenoids: Benzene and substituted derivatives
Pyrimethanil	53112-28-0	✓	–	Benzenoids: Benzene and substituted derivatives
Azole				
Fluquinconazole	136426-54-5	–	–	Organoheterocyclic compounds: Diazanaphthalenes
Flutriafol	76674-21-0	–	–	Benzenoids: Benzene and substituted derivatives
Penconazole	66246-88-6	✓	–	Benzenoids: Benzene and substituted derivatives
Prochloraz	67747-09-5	✓	–	Benzenoids: Phenol ethers
Tebuconazole	107534-96-3	✓	–	Benzenoids: Benzene and substituted derivatives
Triadimefon	43121-43-3	✓	–	Benzenoids: Phenol ethers
Organochlorine				
Hexachlorobenzene	118-74-1	✓	2B	Benzenoids: Benzene and substituted derivatives
Pentachloronitrobenzene	82-68-8	–	3	Benzenoids: Benzene and substituted derivatives
Phthalimide				
Captan	133-06-2	✓	3	Organoheterocyclic compounds: Isoindoles and derivatives
Folpet	133-07-3	✓	–	Organoheterocyclic compounds: Isoindoles and derivatives
Sulfamide				
Dichlofluanid	1085-98-9	✓	–	Benzenoids: Benzene and substituted derivatives
Tolylfluanid	731-27-1	✓	–	Benzenoids: Benzene and substituted derivatives
Other				
Bupirimate	41483-43-6	✓	–	Organoheterocyclic compounds: Diazines
Fludioxonil	131341-86-1	✓	–	Organoheterocyclic compounds: Benzodioxoles
Metalaxyl	57837-19-1	✓	–	Organic acids and derivatives: Carboxylic acids and derivatives
Procymidone	32809-16-8	✓	–	Organoheterocyclic compounds: Piperidines
Pyrazophos	13457-18-6	–	–	Organic acids and derivatives: Organic thiophosphoric acids and derivatives
Vinclozolin	50471-44-8	✓	–	Benzenoids: Benzene and substituted derivatives
Herbicides				
Amide				
Diphenamid	957-51-7	–	–	Benzenoids: Benzene and substituted derivatives
Napropamide	15299-99-7	✓	–	Benzenoids: Naphthalenes
Pronamide	23950-58-5	✓	–	Benzenoids: Benzene and substituted derivatives
Chloroacetanilide				
Acetochlor	34256-82-1	✓	–	Benzenoids: Benzene and substituted derivatives
Alachlor	15972-60-8	✓	–	Benzenoids: Benzene and substituted derivatives
Allidochlor	93-71-0	–	–	Organic acids and derivatives: Carboxylic acids and derivatives
Dimethachlor	50563-36-5	–	–	Benzenoids: Benzene and substituted derivatives
Metolachlor	51218-45-2	–	–	Benzenoids: Benzene and substituted derivatives
Pretilachlor	51218-49-6	–	–	Benzenoids: Benzene and substituted derivatives
Propachlor	1918-16-7	–	–	Benzenoids: Benzene and substituted derivatives
Propisochlor	86763-47-5	✓	–	Benzenoids: Benzene and substituted derivatives
Dinitroaniline				
Nitralin	4726-14-1	–	–	Benzenoids: Benzene and substituted derivatives
Pendimethalin	40487-42-1	✓	–	Benzenoids: Benzene and substituted derivatives
Dinitrophenol				
2-Methyl-4,6-dinitrophenol	534-52-1	–	–	Benzenoids: Phenols

GROUP: Class: *Subclass*: Name	CAS	Potential EDC	IARC Group	Superclass: Class
Dinoseb	88-85-7	✓	–	Benzenoids: Phenols
Phenoxy				
2-Methyl-4-chlorophenoxyacetic acid	94-74-6	–	2B	Benzenoids: Benzene and substituted derivatives
Fenoprop	93-72-1	–	–	Benzenoids: Benzene and substituted derivatives
Mecoprop	7085-19-0	✓	2B	Benzenoids: Benzene and substituted derivatives
Phenylurea				
Diuron	330-54-1	✓	–	Benzenoids: Benzene and substituted derivatives
Linuron	330-55-2	✓	–	Benzenoids: Benzene and substituted derivatives
Monuron	150-68-5	–	3	Benzenoids: Benzene and substituted derivatives
Siduron	1982-49-6	–	–	Benzenoids: Benzene and substituted derivatives
Tebuthiuron	34014-18-1	–	–	Organoheterocyclic compounds: Azoles
Sulfonylurea				
Bensulfuron-methyl	83055-99-6	–	–	Benzenoids: Benzene and substituted derivatives
Halosulfuron-methyl	100784-20-1	–	–	Organoheterocyclic compounds: Azoles
Metsulfuron-methyl	74223-64-6	–	–	Benzenoids: Benzene and substituted derivatives
Nicosulfuron	111991-09-4	–	–	Organoheterocyclic compounds: Pyridines and derivatives
Oxasulfuron	144651-06-9	✓	–	Organic nitrogen compounds: Organonitrogen compounds
Primisulfuron-methyl	86209-51-0	–	–	Organic nitrogen compounds: Organonitrogen compounds
Prosulfuron	94125-34-5	✓	–	Benzenoids: Benzene and substituted derivatives
Rimsulfuron	122931-48-0	✓	–	Organoheterocyclic compounds: Pyridines and derivatives
Thifensulfuron-methyl	79277-27-3	✓	–	Organoheterocyclic compounds: Thiophenes
Triasulfuron	82097-50-5	–	–	Benzenoids: Benzene and substituted derivatives
Thiocarbamate				
Butylate	2008-41-5	–	–	Organosulfur compounds: Thiocarbonyl compounds
Cycloate	1134-23-2	–	–	Organosulfur compounds: Thiocarbonyl compounds
Diallate-cis	2303-16-4	–	3	Organosulfur compounds: Thiocarbonyl compounds
Molinate	2212-67-1	✓	–	Organoheterocyclic compounds: Azepanes
Pebulate	1114-71-2	–	–	Organosulfur compounds: Thiocarbonyl compounds
S-Ethyl dipropylthiocarbamate	759-94-4	–	–	Organosulfur compounds: Thiocarbonyl compounds
Triallate	2303-17-5	–	–	Organosulfur compounds: Thiocarbonyl compounds
Vernolate	1929-77-7	–	–	Organosulfur compounds: Thiocarbonyl compounds
Triazine				
Atraton	1610-17-9	–	–	Organoheterocyclic compounds: Triazines
Atrazine	1912-24-9	✓	3	Organoheterocyclic compounds: Triazines
Hexazinone	51235-04-2	–	–	Organic nitrogen compounds: Organonitrogen compounds
Metribuzin	21087-64-9	✓	–	Organosulfur compounds: Thioethers
Propazine	139-40-2	✓	–	Organoheterocyclic compounds: Triazines
Simetryn	1014-70-6	–	–	Organoheterocyclic compounds: Triazines
Terbuthylazine	5915-41-3	✓	–	Organoheterocyclic compounds: Triazines
Terbutryn	886-50-0	–	–	Organoheterocyclic compounds: Triazines
Uracil				
Bromacil	314-40-9	–	–	Organoheterocyclic compounds: Diazines
Lenacil	2164-08-1	✓	–	Organoheterocyclic compounds: Diazines
Terbacil	5902-51-2	–	–	Organoheterocyclic compounds: Diazines
Other				
Bentazon	25057-89-0	–	–	Benzenoids: NA
Clomazone	81777-89-1	✓	–	Benzenoids: Benzene and substituted derivatives
Dicamba	1918-00-9	✓	–	Benzenoids: Benzene and substituted derivatives
Fluridone	59756-60-4	–	–	Organoheterocyclic compounds: Pyridines and derivatives
Glyphosate	1071-83-6	✓	2A	Organic acids and derivatives: Carboxylic acids and derivatives
Oxadiazon	19666-30-9	✓	–	Benzenoids: Benzene and substituted derivatives

GROUP: Class: *Subclass*: Name	CAS	Potential EDC	IARC Group	Superclass: Class
Insecticides and Pesticides				
Carbamate				
3-Hydroxycarbofuran	16655-82-6	–	–	Organoheterocyclic compounds: Coumarans
Aldicarb	116-06-3	–	3	Organic acids and derivatives: Carboximidic acids and derivatives
Aldicarb sulfone	1646-88-4	–	–	Organosulfur compounds: Sulfonyls
Aldicarb sulfoxide	1646-87-3	–	–	Organic nitrogen compounds: Organonitrogen compounds
Carbaryl	63-25-2	✓	3	Benzenoids: Naphthalenes
Carbofuran	1563-66-2	✓	–	Organoheterocyclic compounds: Coumarans
Methomyl	16752-77-5	–	–	Organic acids and derivatives: Organic carbonic acids and derivatives
Oxamyl	23135-22-0	✓	–	Organic acids and derivatives: Carboxylic acids and derivatives
propoxur	114-26-1	–	–	Benzenoids: Phenol ethers
Insect Repellents				
N,N-Diethyl-meta-toluamide	134-62-3	–	–	Benzenoids: Benzene and substituted derivatives
Organochlorine				
2,4'-DDT	789-02-6	✓	2B	Benzenoids: Benzene and substituted derivatives
2,4'-Methoxychlor	30667-99-3	–	–	Benzenoids: Benzene and substituted derivatives
4,4'-DDD	72-54-8	✓	–	Benzenoids: Benzene and substituted derivatives
4,4'-DDE	72-55-9	✓	2B	Benzenoids: Benzene and substituted derivatives
4,4'-DDT	50-29-3	✓	2A	Benzenoids: Benzene and substituted derivatives
4,4'-Methoxychlor olefin	2132-70-9	–	–	Benzenoids: Benzene and substituted derivatives
B8-1413	142534-71-2	✓	–	Lipids and lipid-like molecules: Prenol lipids
B9-1025	154159-06-5	–	–	Lipids and lipid-like molecules: Prenol lipids
Butylphenoxyisopropyl chloroethyl sulfite	140-57-8	–	2B	Benzenoids: Benzene and substituted derivatives
Chlorfenson	80-33-1	–	–	Benzenoids: Benzene and substituted derivatives
Endosulfan I	959-98-8	✓	–	Organic oxygen compounds: Organic oxoanionic compounds
Methoxychlor	72-43-5	✓	3	Benzenoids: Benzene and substituted derivatives
alpha-benzenehexachloride	319-84-6	–	2B	Organohalogen compounds: Alkyl halides
beta-benzenehexachloride	319-85-7	✓	2B	Organohalogen compounds: Alkyl halides
cis-Nonachlor	5103-73-1	–	–	Organohalogen compounds: Vinyl halides
ethyl-DDD	72-56-0	–	–	Lipids and lipid-like molecules: Prenol lipids
gamma-benzenehexachloride	58-89-9	✓	1	Organohalogen compounds: Alkyl halides
o,p'-DDD	53-19-0	✓	–	Benzenoids: Benzene and substituted derivatives
Organophosphate				
Azinphos ethyl	2642-71-9	–	–	Organoheterocyclic compounds: Benzo-1,2,3-triazines
Bromfenvinphos (E)	33399-00-7	–	–	Benzenoids: Benzene and substituted derivatives
Chlorpyrifos	2921-88-2	✓	–	Organic acids and derivatives: Organic thiophosphoric acids and derivatives
Chlorthiophos	21923-23-9	–	–	Organic acids and derivatives: Organic thiophosphoric acids and derivatives
Diazinon	333-41-5	✓	2A	Organic acids and derivatives: Organic thiophosphoric acids and derivatives
Diethyl phosphate	598-02-7	–	–	Organic acids and derivatives: Organic phosphoric acids and derivatives
Disulfoton	298-04-4	–	–	Organic acids and derivatives: Organic dithiophosphoric acids and derivatives
Ethyl parathion	56-38-2	✓	2B	Organic acids and derivatives: Organic thiophosphoric acids and derivatives
Fenamiphos	22224-92-6	–	–	Benzenoids: Benzene and substituted derivatives
Fenthion	55-38-9	✓	–	Organic acids and derivatives: Organic thiophosphoric acids and derivatives
Fonofos	944-22-9	–	–	Benzenoids: Benzene and substituted derivatives
Iodofenphos	18181-70-9	–	–	Organic acids and derivatives: Organic thiophosphoric acids and derivatives
Malathion	121-75-5	✓	2A	Lipids and lipid-like molecules: Fatty Acyls
Methyl parathion	298-00-0	✓	3	Organic acids and derivatives: Organic thiophosphoric acids and derivatives
Mevinphos	7786-34-7	–	–	Lipids and lipid-like molecules: Fatty Acyls
O,O-Dimethyl Thiophosphate	1112-38-5	–	–	Organic acids and derivatives: Organic thiophosphoric acids and derivatives
Phorate	298-02-2	–	–	Organic acids and derivatives: Organic dithiophosphoric acids and derivatives
Phosmet	732-11-6	–	–	Organoheterocyclic compounds: Isoindoles and derivatives
Pirimiphos ethyl	23505-41-1	–	–	Organic acids and derivatives: Organic thiophosphoric acids and derivatives
Pirimiphos methyl	29232-93-7	✓	–	Organic acids and derivatives: Organic thiophosphoric acids and derivatives

GROUP: Class: *Subclass*: Name	CAS	Potential EDC	IARC Group	Superclass: Class
Pyraclofos	89784-60-1	–	–	Organoheterocyclic compounds: Azoles
Pyridaphenthion	119-12-0	–	–	Organic acids and derivatives: Organic thiophosphoric acids and derivatives
Quinalphos	13593-03-8	✓	–	Organoheterocyclic compounds: Diazanaphthalenes
Resmethrin	10453-86-8	✓	–	Lipids and lipid-like molecules: Prenol lipids
Sulprofos	35400-43-2	–	–	Benzenoids: Benzene and substituted derivatives
Tetraethyl ethylenediphosphonate	995-32-4	–	–	Organic acids and derivatives: Organic phosphonic acids and derivatives
Triazophos	24017-47-8	–	–	Organoheterocyclic compounds: Azoles
Pyrethroid				
3-Phenoxybenzoic acid	3739-38-6	–	–	Benzenoids: Benzene and substituted derivatives
4-Fluro-3-phenoxy-benzoic acid	77279-89-1	–	–	Benzenoids: Benzene and substituted derivatives
Acrinathrin	101007-06-1	✓	–	Lipids and lipid-like molecules: Fatty Acyls
Bifenthrin	82657-04-3	✓	–	Benzenoids: Benzene and substituted derivatives
Bioallethrin	584-79-2	–	–	Lipids and lipid-like molecules: Fatty Acyls
Cyfluthrin	68359-37-5	✓	–	Lipids and lipid-like molecules: Fatty Acyls
Cypermethrin	52315-07-8	✓	–	Lipids and lipid-like molecules: Fatty Acyls
Deltamethrin	52918-63-5	✓	3	Lipids and lipid-like molecules: Fatty Acyls
Etofenprox	80844-07-1	✓	–	Benzenoids: Benzene and substituted derivatives
Fenpropathrin	39515-41-8	–	–	Benzenoids: Benzene and substituted derivatives
Fenvalerate	51630-58-1	✓	3	Lipids and lipid-like molecules: Fatty Acyls
Flucythrinate	70124-77-5	–	–	Lipids and lipid-like molecules: Fatty Acyls
Phenothrin, trans	26002-80-2	✓	–	Lipids and lipid-like molecules: Fatty Acyls
Tefluthrin	79538-32-2	✓	–	Benzenoids: Benzene and substituted derivatives
Tetramethrin	7696-12-0	✓	–	Organoheterocyclic compounds: Isoindoles and derivatives
Transfluthrin	118712-89-3	–	–	Benzenoids: Benzene and substituted derivatives
cis-3-(2,2-Dichlorovinyl)-2,2-dimethylcylo	59042-49-8	–	–	Organic acids and derivatives: Carboxylic acids and derivatives
cis-Permethrin	61949-76-6	✓	3	Lipids and lipid-like molecules: Fatty Acyls
lambda-Cyhalothrin	91465-08-6	✓	–	Lipids and lipid-like molecules: Fatty Acyls
tau-Fluvalinate	102851-06-9	✓	–	Benzenoids: Benzene and substituted derivatives
trans-3-(2,2-Dichlorovinyl)-2,2-dimethylcylo	59042-50-1	–	–	Organic acids and derivatives: Carboxylic acids and derivatives
trans-Permethrin	61949-77-7	–	3	Lipids and lipid-like molecules: Fatty Acyls
Pyrrole				
Chlorfenapyr	122453-73-0	–	–	Organoheterocyclic compounds: Pyrroles
Synergists				
Octyl bicycloheptenedicarboximide	113-48-4	–	–	Organoheterocyclic compounds: Isoindoles and derivatives
Piperonyl butoxide	51-03-6	–	3	Organoheterocyclic compounds: Benzodioxoles
Plant Growth Regulators				
2,3,4,5-Tetrabromobenzoic acid	27581-13-1	–	–	Benzenoids: Benzene and substituted derivatives
Chlorpropham	101-21-3	✓	3	Benzenoids: Benzene and substituted derivatives
Paclobutrazol	76738-62-0	✓	–	Benzenoids: Benzene and substituted derivatives

GROUP: Class: *Subclass*: Name	CAS	Potential EDC	IARC Group	Superclass: Class
OTHER CHEMICALS				
Antioxidants				
Protocatechuic acid[a]	99-50-3	✓	–	Benzenoids: Benzene and substituted derivatives
Emollients				
Ethyl myristate	124-06-1	–	–	Lipids and lipid-like molecules: Fatty Acyls
Ethyl oleate	111-62-6	–	–	Lipids and lipid-like molecules: Fatty Acyls
Ethyl palmitate	628-97-7	–	–	Lipids and lipid-like molecules: Fatty Acyls
Flavoring or Fragrance Agents				
(-)-Menthol	2216-51-5	–	–	Lipids and lipid-like molecules: Prenol lipids
1,8-Cineole	470-82-6	–	–	Organoheterocyclic compounds: Oxanes
4-Hydroxy-2,5-dimethyl-3(2H)-furanone	3658-77-3	–	–	Organoheterocyclic compounds: Dihydrofurans
Acetophenone	98-86-2	–	–	Organic oxygen compounds: Organooxygen compounds
Benzyl salicylate	118-58-1	✓	–	Benzenoids: Benzene and substituted derivatives
Cinnamyl acetate	103-54-8	–	–	Benzenoids: Benzene and substituted derivatives
Cinnamyl alcohol	104-54-1	✓	–	Phenylpropanoids and polyketides: Cinnamyl alcohols
Ethyl butyrate	105-54-4	–	–	Lipids and lipid-like molecules: Fatty Acyls
Ethyl caprate[a]	110-38-3	–	–	Lipids and lipid-like molecules: Fatty Acyls
Ethyl caproate	123-66-0	–	–	Lipids and lipid-like molecules: Fatty Acyls
Ethyl caprylate	106-32-1	–	–	Lipids and lipid-like molecules: Fatty Acyls
Ethyl heptanoate	106-30-9	–	–	Lipids and lipid-like molecules: Fatty Acyls
Ethyl laurate	106-33-2	–	–	Lipids and lipid-like molecules: Fatty Acyls
Ethyl maltol	225-582-5	–	–	Organoheterocyclic compounds: Pyrans
Ethyl pelargonate[a]	123-29-5	–	–	Lipids and lipid-like molecules: Fatty Acyls
Ethyl propionate	105-37-3	–	–	Organic acids and derivatives: Carboxylic acids and derivatives
Ethyl stearate[a]	111-61-5	–	–	Lipids and lipid-like molecules: Fatty Acyls
Ethyl undecanoate[a]	627-90-7	–	–	Lipids and lipid-like molecules: Fatty Acyls
Ethyl valerate	539-82-2	–	–	Lipids and lipid-like molecules: Fatty Acyls
Ethyl vanillin	121-32-4	–	–	Organic oxygen compounds: Organooxygen compounds
Geraniol	106-24-1	–	–	Lipids and lipid-like molecules: Prenol lipids
Hexanoic acid	142-62-1	–	–	Lipids and lipid-like molecules: Fatty Acyls
Hydroxycitronellal	107-75-5	–	–	Organic oxygen compounds: Organooxygen compounds
Isosafrole	120-58-1	–	3	Organoheterocyclic compounds: Benzodioxoles
Maltol	118-71-8	–	–	Organoheterocyclic compounds: Pyrans
Menthone	14073-97-3	–	–	Lipids and lipid-like molecules: Prenol lipids
Safrole	94-59-7	–	2B	Organoheterocyclic compounds: Benzodioxoles
Thymol	89-83-8	✓	–	Lipids and lipid-like molecules: Prenol lipids
Vanillin	121-33-5	–	–	Benzenoids: Phenols
d-Limonene	5989-27-5	–	3	Lipids and lipid-like molecules: Prenol lipids
trans-Cinnamaldehyde	14371-10-9	✓	–	Phenylpropanoids and polyketides: Cinnamaldehydes
Humectants				
Glycerin[a]	56-81-5	–	–	Organic oxygen compounds: Organooxygen compounds
Organic UV Filters				
Butyl methoxydibenzoylmethane	70356-09-1	–	–	Phenylpropanoids and polyketides: Linear 1,3-diarylpropanoids
Homosalate	118-56-9	✓	–	Benzenoids: Benzene and substituted derivatives
Octyl-dimethyl-p-aminobenzoic acid	21245-02-3	✓	–	Benzenoids: Benzene and substituted derivatives
Oxybenzone	131-57-7	✓	–	Benzenoids: Benzene and substituted derivatives
octyl-Methoxycinnamate	5466-77-3	✓	–	Phenylpropanoids and polyketides: Cinnamic acids and derivatives

GROUP: Class: *Subclass*: Name	**CAS**	**Potential EDC**	**IARC Group**	**Superclass: Class**
Pharmacologic Agents				
(±)-Nicotine	22083-74-5	–	–	Organoheterocyclic compounds: Pyridines and derivatives
Caffeine	58-08-2	✓	3	Organoheterocyclic compounds: Imidazopyrimidines
Methapyrilene	91-80-5	–	–	Organic nitrogen compounds: Organonitrogen compounds
Phenacetin	62-44-2	–	1	Benzenoids: Benzene and substituted derivatives
Preservatives				
Parabens				
Benzylparaben	94-18-8	✓	–	Benzenoids: Benzene and substituted derivatives
Butylparaben	94-26-8	✓	–	Benzenoids: Benzene and substituted derivatives
Ethylparaben	120-47-8	✓	–	Benzenoids: Benzene and substituted derivatives
Heptylparaben	1085-12-7	✓	–	Benzenoids: Benzene and substituted derivatives
Isobutylparaben	4247-02-3	✓	–	Benzenoids: Benzene and substituted derivatives
Isopropylparaben	4191-73-5	✓	–	Benzenoids: Benzene and substituted derivatives
Methylparaben	99-76-3	✓	–	Benzenoids: Benzene and substituted derivatives
Propylparaben	94-13-3	✓	–	Benzenoids: Benzene and substituted derivatives
Other				
4-Chloro-3-methylphenol	59-50-7	✓	–	Benzenoids: Phenols
4-Hydroxybenzoic acid	99-96-7	✓	–	Benzenoids: Benzene and substituted derivatives
Benzoic acid	65-85-0	–	–	Benzenoids: Benzene and substituted derivatives
Benzyl alcohol	100-51-6	–	–	Benzenoids: Benzene and substituted derivatives
Potassium sorbate	24634-61-5	–	–	Lipids and lipid-like molecules: Fatty Acyls
Triclosan	3380-34-5	✓	–	Benzenoids: Benzene and substituted derivatives

GROUP: Class: *Subclass*: Name	CAS	Potential EDC	IARC Group	Superclass: Class
POLLUTANTS AND INDUSTRIAL CHEMICALS				
Carcinogenic Research Chemicals				
2-Acetylaminofluorene	53-96-3	–	–	-: Fluorenes
4-Nitroquinoline-1-oxide	56-57-5	–	–	-: Quinolines and derivatives
Methyl methanesulfonate	66-27-3	–	2A	-: Organic sulfonic acids and derivatives
N-Nitrosodi-n-butylamine	924-16-3	–	2B	-: Organonitrogen compounds
N-Nitrosoethylmethylamine	10595-95-6	–	2B	-: Organonitrogen compounds
N-Nitrosopyrrolidine	930-55-2	–	2B	-: Pyrrolidines
Chemical Synthesis Intermediates				
1,2,3-Trichloro-4-nitrobenzene	17700-09-3	–	–	Benzenoids: Benzene and substituted derivatives
1,3-Dichlorobenzene	541-73-1	✓	3	Benzenoids: Benzene and substituted derivatives
1,4-Naphthoquinone	130-15-4	–	–	Benzenoids: Naphthalenes
2,2-Dichloropropane	594-20-7	–	–	Organohalogen compounds: Organochlorides
2,3-Dichloronitrobenzene	3209-22-1	–	–	Benzenoids: Benzene and substituted derivatives
2,3-Dichlorophenyl-4'-nitrophenyl ether	82239-20-1	–	–	Benzenoids: Benzene and substituted derivatives
2,4,6-Tribromophenol	118-79-6	✓	–	Benzenoids: Phenols
2,4-Dichlorophenol	120-83-2	✓	2B	Benzenoids: Benzene and substituted derivatives
2,4-Dimethylphenol	105-67-9	–	–	Benzenoids: Benzene and substituted derivatives
2,4-Dinitrophenol	51-28-5	–	–	Benzenoids: Phenols
2,6-Dichlorophenyl-4'-nitrophenyl ether	2093-28-9	–	–	Benzenoids: Benzene and substituted derivatives
2-Bromo-4-(2,4,4-trimethylpentan-2-yl)phenol	57835-35-5	–	–	Benzenoids: Benzene and substituted derivatives
2-Chloronaphthalene	91-58-7	–	–	Benzenoids: Naphthalenes
2-Isopropyl-6-methyl-4-pyrimidinol	2814-20-2	–	–	Organoheterocyclic compounds: Diazines
2-Nitrophenol	88-75-5	–	–	Benzenoids: Phenols
3,5-Dichloronitrobenzene	618-62-2	–	–	Benzenoids: Benzene and substituted derivatives
3,5-Dichlorophenyl-4'-nitrophenyl ether	21105-77-1	–	–	Benzenoids: Benzene and substituted derivatives
4,4'-Diaminodiphenylmethane	101-77-9	✓	2B	Benzenoids: Benzene and substituted derivatives
4,4'-Methylenebis(2-chloroaniline)	101-14-4	–	1	Benzenoids: Benzene and substituted derivatives
4,4'-Oxydianiline	101-80-4	–	2B	Benzenoids: Benzene and substituted derivatives
4-Chloro-o-toluidine	95-69-2	–	2A	Benzenoids: Benzene and substituted derivatives
4-Chlorophenyl phenyl ether	7005-72-3	–	–	Benzenoids: Benzene and substituted derivatives
4-Nitrophenyl phenyl ether	620-88-2	–	–	Benzenoids: Benzene and substituted derivatives
Carbofuran phenol	1563-38-8	–	–	Organoheterocyclic compounds: Coumarans
Dibenzofuran	132-64-9	–	–	Organoheterocyclic compounds: Benzofurans
Dimethyl phosphate	813-78-5	–	–	Organic acids and derivatives: Organic phosphoric acids and derivatives
Diphenylamine	122-39-4	–	2B	Benzenoids: Benzene and substituted derivatives
Ethyl methacrylate	97-63-2	–	–	Organic acids and derivatives: Carboxylic acids and derivatives
Ethylene thiourea	96-45-7	✓	3	Organoheterocyclic compounds: Azolidines
Hexachloropropene	1888-71-7	–	–	Organohalogen compounds: Vinyl halides
Isopropylbenzene	98-82-8	–	2B	Benzenoids: Benzene and substituted derivatives
Methyl methacrylate	80-62-6	✓	3	Organic acids and derivatives: Carboxylic acids and derivatives
N-(2,4-Dimethylphenyl)formamide	60397-77-5	–	–	Benzenoids: Benzene and substituted derivatives
N-Nitrosodiethylamine	55-18-5	–	2A	Organic nitrogen compounds: Organonitrogen compounds
N-ethylperfluoro-1-octanesulfonamidoacetic acid (linear)	2991-50-6	–	–	Organohalogen compounds: Alkyl halides
Nitrobenzene	98-95-3	✓	2B	Benzenoids: Benzene and substituted derivatives
O,O-Diethyl Phosphonate	762-04-9	–	–	Organic oxygen compounds: Organooxygen compounds
Phenol, 2-octyl-	949-13-3	✓	–	Benzenoids: Phenols
Phenol[a]	108-95-2	–	3	Benzenoids: Phenols
Propylene thiourea	2122-19-2	–	–	Organoheterocyclic compounds: Azolidines
Styrene	100-42-5	✓	2A	Benzenoids: Benzene and substituted derivatives
Tetrahydrophthalimide	85-40-5	–	–	Organoheterocyclic compounds: Isoindoles and derivatives
Triisopropyl Phosphate	513-02-0	–	–	Organic acids and derivatives: Organic phosphoric acids and derivatives

GROUP: Class: *Subclass*: Name	CAS	Potential EDC	IARC Group	Superclass: Class
Trimethyl Phosphate	512-56-1	–	–	Organic acids and derivatives: Organic phosphoric acids and derivatives
bis(2-Chloroethyl)ether	111-44-4	–	3	Organic oxygen compounds: Organooxygen compounds
m-Cresol	108-39-4	–	–	Benzenoids: Phenols
o-Cresol	95-48-7	–	–	Benzenoids: Phenols
p-Cresol	106-44-5	✓	–	Benzenoids: Phenols
p-Nitrophenol	100-02-7	✓	–	Benzenoids: Phenols
Combustion Byproducts				
Chlorinated				
1,2,3,7,8-Pentachlorodibenzofuran	57117-41-6	✓	3	Organoheterocyclic compounds: Benzofurans
Octachlorodibenzo-p-dioxin	3268-87-9	✓	–	Organoheterocyclic compounds: Benzodioxins
Octachlorodibenzofuran	39001-02-0	✓	3	Organoheterocyclic compounds: Benzofurans
Polycyclic Aromatic Hydrocarbon				
2-Methylnaphthalene	91-57-6	–	–	Benzenoids: Naphthalenes
3-Methylcholanthrene	56-49-5	✓	–	Benzenoids: Phenanthrenes and derivatives
7,12-Dimethylbenz(a)anthracene	57-97-6	✓	–	Benzenoids: Phenanthrenes and derivatives
Acenaphthene	83-32-9	–	3	Benzenoids: Naphthalenes
Acenaphthylene	208-96-8	✓	2A	Benzenoids: Acenaphthylenes
Anthracene	120-12-7	–	2B	Benzenoids: Anthracenes
Benz(a)anthracene	56-55-3	✓	2B	Benzenoids: Phenanthrenes and derivatives
Benzo(b)fluoranthene	205-99-2	✓	2B	Benzenoids: Phenanthrenes and derivatives
Benzo(g,h,i)perylene	191-24-2	–	3	Benzenoids: Pyrenes
Benzo(k)fluoranthene	207-08-9	✓	2B	Benzenoids: Naphthalenes
Benzo[a]pyrene	50-32-8	✓	1	Benzenoids: Pyrenes
Chrysene	218-01-9	–	2B	Benzenoids: Phenanthrenes and derivatives
Dibenz(a,h)anthracene	53-70-3	✓	2A	Benzenoids: Phenanthrenes and derivatives
Fluoranthene	206-44-0	✓	3	Benzenoids: Naphthalenes
Fluorene	86-73-7	–	3	Benzenoids: Fluorenes
Indeno(1,2,3-cd)pyrene	193-39-5	–	2B	Benzenoids: Pyrenes
Naphthalene	91-20-3	–	2B	Benzenoids: Naphthalenes
Phenanthrene	85-01-8	–	3	Benzenoids: Phenanthrenes and derivatives
Pyrene	129-00-0	–	3	Benzenoids: Pyrenes
Disinfectant Breakdown Products				
Bromodichloromethane	75-27-4	✓	2B	Organohalogen compounds: Alkyl halides
Dibromochloromethane	124-48-1	–	3	Organohalogen compounds: Alkyl halides
Dye intermediates				
1-Chloro-2-nitrobenzene	88-73-3	–	2B	Benzenoids: Benzene and substituted derivatives
1-Chloro-4-nitrobenzene	100-00-5	–	2B	Benzenoids: Benzene and substituted derivatives
1-Naphthol	90-15-3	–	–	Benzenoids: Naphthalenes
1-Naphthylamine	134-32-7	–	3	Benzenoids: Naphthalenes
2,4,5-Trimethylaniline	137-17-7	–	3	Benzenoids: Benzene and substituted derivatives
2,4-Diaminoanisole (as sulfate hydrate)	615-05-4	–	2B	Benzenoids: Phenol ethers
2,4-Diaminotoluene	95-80-7	–	2B	Benzenoids: Benzene and substituted derivatives
2-Aminobiphenyl	90-41-5	–	1	Benzenoids: Benzene and substituted derivatives
2-Chloro-6-nitrotoluene	83-42-1	–	–	Benzenoids: Benzene and substituted derivatives
2-Naphthylamine	91-59-8	–	1	Benzenoids: Naphthalenes
2-Nitroaniline	88-74-4	–	–	Benzenoids: Benzene and substituted derivatives
2-Phenylphenol	90-43-7	✓	3	Benzenoids: Benzene and substituted derivatives
3,3'-Dimethoxybenzidine	119-90-4	✓	2B	Benzenoids: Benzene and substituted derivatives
3,3'-Dimethyl-4,4'-diaminodiphenylmethane	838-88-0	–	2B	Benzenoids: Benzene and substituted derivatives
3,3'-Dimethylbenzidine	119-93-7	✓	2B	Benzenoids: Benzene and substituted derivatives

GROUP: Class: *Subclass*: Name	CAS	Potential EDC	IARC Group	Superclass: Class
3,4-Dichloroaniline	95-76-1	✓	–	Benzenoids: Benzene and substituted derivatives
3-Chloro-o-toluidine	87-60-5	–	–	Benzenoids: Benzene and substituted derivatives
3-Nitroaniline	99-09-2	–	–	Benzenoids: Benzene and substituted derivatives
4,4'-Thiodianiline	139-65-1	–	2B	Organosulfur compounds: Thioethers
4-Aminobiphenyl	92-67-1	–	1	Benzenoids: Benzene and substituted derivatives
4-Chloro-2-nitrotoluene	89-59-8	–	–	Benzenoids: Benzene and substituted derivatives
4-Chloro-3-nitrotoluene	89-60-1	–	–	Benzenoids: Benzene and substituted derivatives
4-Chloroaniline	106-47-8	–	2B	Benzenoids: Benzene and substituted derivatives
4-Nitroaniline	100-01-6	–	–	Benzenoids: Benzene and substituted derivatives
5-Nitro-o-toluidine	99-55-8	–	3	Benzenoids: Benzene and substituted derivatives
Aniline	62-53-3	✓	2A	Benzenoids: Benzene and substituted derivatives
Anthraquinone	84-65-1	–	2B	Benzenoids: Anthracenes
Azobenzene	103-33-3	–	3	Organoheterocyclic compounds: Azobenzenes
Benzidine	92-87-5	–	1	Benzenoids: Benzene and substituted derivatives
Carbazole	86-74-8	–	2B	Organoheterocyclic compounds: Indoles and derivatives
o-Aminoazotoluene	97-56-3	✓	2B	Organoheterocyclic compounds: Azobenzenes
o-Anisidine	90-04-0	–	2A	Benzenoids: Phenol ethers
o-Toluidine	95-53-4	–	1	Benzenoids: Benzene and substituted derivatives
p-Aminoazobenzene	60-09-3	–	2B	Organoheterocyclic compounds: Azobenzenes
p-Cresidine	120-71-8	–	2B	Benzenoids: Phenol ethers
p-Dimethylaminoazobenzene	60-11-7	–	2B	Organoheterocyclic compounds: Azobenzenes
p-Phenylenediamine	106-50-3	✓	3	Benzenoids: Benzene and substituted derivatives
Explosive Intermediates				
2,4-Dinitrotoluene	121-14-2	✓	2B	Benzenoids: Benzene and substituted derivatives
2,6-Dinitrotoluene	606-20-2	–	2B	Benzenoids: Benzene and substituted derivatives
m-Dinitrobenzene	99-65-0	–	–	Benzenoids: Benzene and substituted derivatives
Flame Retardants				
Brominated				
2-Bromoallyl-2,4,6-tribromophenyl ether	99717-56-3	✓	–	Benzenoids: Phenol ethers
BDE-100	189084-64-8	–	–	Benzenoids: Benzene and substituted derivatives
BDE-47	5436-43-1	✓	–	Benzenoids: Benzene and substituted derivatives
BDE-66	189084-61-5	–	–	Benzenoids: Benzene and substituted derivatives
Tetrabromobisphenol A	79-94-7	✓	2A	Benzenoids: Benzene and substituted derivatives
Tetrabromobisphenol A bis(allyl ether)	25327-89-3	✓	–	Benzenoids: Benzene and substituted derivatives
Tetrabromobisphenol S	39635-79-5	✓	–	Benzenoids: Benzene and substituted derivatives
Tris(tribromoneopentyl)	21850-44-2	✓	–	Benzenoids: Benzene and substituted derivatives
Tris(tribromoneopentyl) phosphate	19186-97-1	–	–	Organic acids and derivatives: Organic phosphoric acids and derivatives
Chlorinated				
Tri(Chloropropyl) phosphate	1067-98-7	–	–	Organic acids and derivatives: Organic phosphoric acids and derivatives
Tris(1,3-dichloro-2-propyl) phosphate	13674-87-8	✓	–	Organic acids and derivatives: Organic phosphoric acids and derivatives
Tris(1-chloro-2-propyl) phosphate	13674-84-5	✓	–	Organic acids and derivatives: Organic phosphoric acids and derivatives
Tris(2-chloroethyl) phosphate	115-96-8	✓	3	Organic acids and derivatives: Organic phosphoric acids and derivatives
Organophosphate				
(3-Methylphenyl) diphenyl phosphate	69500-28-3	–	–	Organic acids and derivatives: Organic phosphoric acids and derivatives
Tri-M-cresyl phosphate	563-04-2	✓	–	Organic acids and derivatives: Organic phosphoric acids and derivatives
Tri-P-cresyl phosphate	78-32-0	✓	–	Organic acids and derivatives: Organic phosphoric acids and derivatives
Tripropyl Phosphate	513-08-6	–	–	Organic acids and derivatives: Organic phosphoric acids and derivatives
Lubricants				
n-Docosane	629-97-0	–	–	Hydrocarbons: Saturated hydrocarbons
n-Dotriacontane	544-85-4	–	–	Hydrocarbons: Saturated hydrocarbons

GROUP: Class: *Subclass*: Name	CAS	Potential EDC	IARC Group	Superclass: Class
n-Eicosane	112-95-8	–	–	Hydrocarbons: Saturated hydrocarbons
n-Heptadecane	629-78-7	–	–	Hydrocarbons: Saturated hydrocarbons
n-Hexacosane	630-01-3	–	–	Hydrocarbons: Saturated hydrocarbons
n-Octacosane	630-02-4	–	–	Hydrocarbons: Saturated hydrocarbons
n-Tetracosane	646-31-1	–	–	Hydrocarbons: Saturated hydrocarbons
n-Triacontane	638-68-6	–	–	Hydrocarbons: Saturated hydrocarbons
Per- and Polyfluoroalkyl Substances (PFAS)				
9-Chlorohexadecafluoro-3-oxanone-1-sulfonic acid	756426-58-1	–	–	Organic acids and derivatives: Organic sulfonic acids and derivatives
N-methylperfluoro-1-octanesulfonamidoacetic acid (linear)	2355-31-9	–	–	Organohalogen compounds: Alkyl halides
Perfluoro-n-dodecanoic acid	307-55-1	✓	–	Organohalogen compounds: Alkyl halides
Perfluoro-n-tetradecanoic acid	376-06-7	–	–	Lipids and lipid-like molecules: Fatty Acyls
Perfluorohexanoic Acid	307-24-4	–	–	Organohalogen compounds: Alkyl halides
Perfluorononanoic acid	375-95-1	✓	–	Organohalogen compounds: Alkyl halides
Plasticizers and Plastic Additives				
Plastic Additives				
Bisphenol A	80-05-7	✓	–	Benzenoids: Benzene and substituted derivatives
Bisphenol F	620-92-8	✓	–	Benzenoids: Benzene and substituted derivatives
Bisphenol S	80-09-1	✓	–	Benzenoids: Benzene and substituted derivatives
N-Nitrosodiphenylamine	86-30-6	–	3	Benzenoids: Benzene and substituted derivatives
Plasticizer Metabolites				
Mono(2-ethyl-5-hydroxyhexyl) phthalate	40321-99-1	–	–	Benzenoids: Benzene and substituted derivatives
Mono(2-ethyl-5-oxohexyl) phthalate	40321-98-0	–	–	Benzenoids: Benzene and substituted derivatives
Mono(5-carboxy-2-ethylpentyl) phthalate	40809-41-4	–	–	Benzenoids: Benzene and substituted derivatives
Mono-2-ethylhexyl phthalate	4376-20-9	✓	–	Benzenoids: Benzene and substituted derivatives
Mono-benzyl phthalate	2528-16-7	–	–	Benzenoids: Benzene and substituted derivatives
Mono-cyclohexyl phthalate	7517-36-4	–	–	Benzenoids: Benzene and substituted derivatives
Mono-ethyl phthalate	2306-33-4	–	–	Benzenoids: Benzene and substituted derivatives
Mono-isobutyl phthalate	30833-53-5	–	–	Benzenoids: Benzene and substituted derivatives
Mono-isononyl phthalate	106610-61-1	–	–	Benzenoids: Benzene and substituted derivatives
Mono-methyl phthalate	4376-18-5	–	–	Benzenoids: Benzene and substituted derivatives
Mono-n-butyl phthalate	131-70-4	✓	–	Benzenoids: Benzene and substituted derivatives
Mono-n-octyl phthalate	5393-19-1	✓	–	Benzenoids: Benzene and substituted derivatives
Plasticizers				
2-Ethylhexyldiphenylphosphate	1241-94-7	✓	–	Organic acids and derivatives: Organic phosphoric acids and derivatives
Butyl benzyl phthalate	85-68-7	✓	3	Benzenoids: Benzene and substituted derivatives
Di-n-butyl phthalate	84-74-2	✓	–	Benzenoids: Benzene and substituted derivatives
Di-n-octyl phthalate	117-84-0	✓	–	Benzenoids: Benzene and substituted derivatives
Diethyl phthalate	84-66-2	✓	–	Benzenoids: Benzene and substituted derivatives
Dimethyl phthalate	131-11-3	✓	–	Benzenoids: Benzene and substituted derivatives
Tributyl Phosphate	126-73-8	✓	–	Organic acids and derivatives: Organic phosphoric acids and derivatives
Tripentyl Phosphate	2528-38-3	–	–	Organic acids and derivatives: Organic phosphoric acids and derivatives
Tris(2-butoxyethyl) phosphate	78-51-3	✓	–	Organic acids and derivatives: Organic phosphoric acids and derivatives
Tris(2-ethylhexyl) phosphate	78-42-2	–	–	Organic acids and derivatives: Organic phosphoric acids and derivatives
bis(2-Ethylhexyl)phthalate	117-81-7	✓	2B	Benzenoids: Benzene and substituted derivatives
Polychlorinated Biphenyls (PCBs)				
PCB-105	32598-14-4	✓	1	Benzenoids: Benzene and substituted derivatives
PCB-118	31508-00-6	✓	1	Benzenoids: Benzene and substituted derivatives
PCB-132	38380-05-1	✓	1	Benzenoids: Benzene and substituted derivatives
PCB-138	35065-28-2	✓	1	Benzenoids: Benzene and substituted derivatives
PCB-146	51908-16-8	✓	1	Benzenoids: Benzene and substituted derivatives

GROUP: Class: *Subclass*: Name	CAS	Potential EDC	IARC Group	Superclass: Class
PCB-153	35065-27-1	✓	1	Benzenoids: Benzene and substituted derivatives
PCB-172	52663-74-8	✓	1	Benzenoids: Benzene and substituted derivatives
PCB-18	37680-65-2	✓	1	Benzenoids: Benzene and substituted derivatives
PCB-180	35065-29-3	✓	1	Benzenoids: Benzene and substituted derivatives
PCB-187	52663-68-0	✓	1	Benzenoids: Benzene and substituted derivatives
PCB-191	74472-50-7	✓	1	Benzenoids: Benzene and substituted derivatives
PCB-66	32598-10-0	✓	1	Benzenoids: Benzene and substituted derivatives
PCB-70	32598-11-1	–	1	Benzenoids: Benzene and substituted derivatives
Side-Reaction Byproducts				
N-Nitrosodi-n-propylamine	621-64-7	–	2B	Organic nitrogen compounds: Organonitrogen compounds
Solvents				
1,2,4-Trimethylbenzene	95-63-6	–	–	Benzenoids: Benzene and substituted derivatives
1,3-Dichloropropane	142-28-9	–	2B	Organohalogen compounds: Organochlorides
2-Chlorotoluene	95-49-8	–	–	Benzenoids: Benzene and substituted derivatives
2-Picoline	109-06-8	–	3	Organoheterocyclic compounds: Pyridines and derivatives
4-Chlorotoluene	106-43-4	–	–	Benzenoids: Benzene and substituted derivatives
Ethyl acetate	141-78-6	–	–	Organic acids and derivatives: Carboxylic acids and derivatives
Ethylbenzene	100-41-4	✓	2B	Benzenoids: Benzene and substituted derivatives
Isophorone	78-59-1	–	2B	Organic oxygen compounds: Organooxygen compounds
N-Nitrosomorpholine	59-89-2	–	2B	Organoheterocyclic compounds: Oxazinanes
Toluene	108-88-3	✓	3	Benzenoids: Benzene and substituted derivatives
bis(2-Chloro-1-methylethyl)ether	108-60-1	–	3	Organic oxygen compounds: Organooxygen compounds
bis(2-Chloroethoxy)methane	111-91-1	–	–	Organic oxygen compounds: Organooxygen compounds
n-Butylbenzene	104-51-8	–	–	Benzenoids: Benzene and substituted derivatives
n-Dodecane	112-40-3	–	–	Hydrocarbons: Saturated hydrocarbons
n-Hexadecane	544-76-3	–	–	Hydrocarbons: Saturated hydrocarbons
n-Octadecane	593-45-3	–	–	Hydrocarbons: Saturated hydrocarbons
n-Pentadecane	629-62-9	–	–	Hydrocarbons: Saturated hydrocarbons
n-Tetradecane	629-59-4	–	–	Hydrocarbons: Saturated hydrocarbons
n-Tridecane	629-50-5	–	–	Hydrocarbons: Saturated hydrocarbons
o-Xylene	95-47-6	–	3	Benzenoids: Benzene and substituted derivatives
p-Isopropyltoluene	99-87-6	–	–	Lipids and lipid-like molecules: Prenol lipids
sec-Butylbenzene	135-98-8	–	–	Benzenoids: Benzene and substituted derivatives
tert-Butylbenzene	98-06-6	–	–	Benzenoids: Benzene and substituted derivatives
Surfactants or Detergents				
4-Tert-Octylphenol	140-66-9	✓	–	Benzenoids: Benzene and substituted derivatives
Nonylphenol	104-40-5	✓	–	Benzenoids: Phenols
Nonylphenol diethoxylate	9016-45-9	✓	–	Benzenoids: Phenol ethers
Nonylphenol monoethoxylate	27986-36-3	✓	–	Benzenoids: Phenol ethers
Wood Preservatives				
2,4,5-Trichlorophenol	95-95-4	✓	2B	Benzenoids: Phenols
2,4,6-Trichlorophenol	88-06-2	✓	2B	Benzenoids: Phenols
Pentachloroanisole	1825-21-4	–	–	Benzenoids: Phenol ethers
Pentachlorobenzene	608-93-5	✓	–	Benzenoids: Benzene and substituted derivatives
Pentachlorophenol	87-86-5	✓	1	Benzenoids: Phenols

SUPPLEMENTARY TABLE 3

Observed concentrations versus reported literature values. All values originally published as ng/g, µg/L, ng/mL are listed as PPB. Values originally published as pg/mL were converted to ng/mL and then listed as PPB. All values are rounded to the nearest integer or are listed as < 1 PPB when applicable. The corresponding reference from which the comparison value is derived is cited next to the listed concentration. Annotations presented in this table represent estimated concentrations based on algorithmic chemical identification. While specific annotations that failed validation were excluded, many remaining identifications were not manually validated and should be considered preliminary. Annotations detected in fewer than 50% of tumors or non-cancer thyroids were excluded. *[a] The lower bound of the range is the 'theoretical minimum,' which is one half the lowest detected value. This value was used for imputing missing values to determine means; [b] PAH measurements were obtained from a study that analyzed multiple adipose tissue depots across two geographically distinct cohorts[11], while PCB measurements were derived from a separate study that also included two geographically distinct cohorts[16]. Thus, multiple means were listed for various subgroups within these studies. However, for each compound, the highest mean value reported across any cohort or cohort-tissue depot combination is presented; [c] Some urine or plasma values are derived from the CDC's Biomonitoring Data Tables for Environmental Chemicals[14], which is based on data from NHANES cohorts. In the cases where compounds had data listed from multiple cohorts, the maximum geometric mean across any given cohort is listed; [e] Measurements were listed for both smokers and non-smokers. All values listed are derived from smokers, which had the highest values for all these chemicals.*

Name	CAS	IARC Group	Mean Non-Cancer Thyroid Conc. (PPB)	Mean Tumor Conc. (PPB)	Range (PPB)[a]	Adipose Tissue (PPB)[b]	Urine (PPB)[c]	Serum/ Plasma (PPB)[c]
Combustion Byproducts (PAH)								
Acenaphthene	83-32-9	3	1,931	4,967	214- 40,558	10[11]	–	–
Acenaphthylene	208-96-8	2A	1,907	654	16- 3,824	4[11]	–	–
Anthracene	120-12-7	2B	917	83	< 1- 1,726	42[11]	–	–
Benz(a)anthracene	56-55-3	2B	52	1,088	4- 7,250	< 1	–	–
Benzo(b)fluoranthene	205-99-2	2B	6	899	1- 14,794	< 1	–	–
Chrysene	218-01-9	2B	16	132	2- 2,985	< 1	–	–
Dibenz(a,h)anthracene	53-70-3	2A	1,696	13,591	413- 27,924	< 1	–	–
Fluoranthene	206-44-0	3	51	1,030	5- 9,072	49[11]	–	< 1[12]
Naphthalene	91-20-3	2B	679	854	8- 6,714	50[11]	–	< 1[12]
Phenanthrene	85-01-8	3	1,056	92	3- 1,978	139[11]	–	< 1[12]
Pyrene	129-00-0	3	33	379	2- 3,269	28[11]	–	2[12]
Dye Intermediates								
2-Naphthylamine	91-59-8	1	322	35,194	69- 187,964	–	4[e13]	–
4-Aminobiphenyl	92-67-1	1	12	97,538	1- 623,815	–	< 1[e14]	–
o-Toluidine	95-53-4	1	1,413	12,614	100- 82,300	–	< 1[e14]	–
Polychlorinated Biphenyls (PCBs)								
PCB-138	35065-28-2	1	304	16	13- 1,412	3[16]	–	< 1[14]
PCB-153	35065-27-1	1	120	36	14- 553	3[16]	–	< 1[14]
PCB-172	52663-74-8	1	856	42	25- 4,531	–	–	< 1[14]

TABLE ABBREVIATION DICTIONARY

The supplementary tables have a substantial number of abbreviations, largely for chemical names. A full dictionary of abbreviations relevant to all supplementary tables can be found below:

- B8-1413 = 2,3,5,6,8,8,10,10-Octachlorobornane
- B9-1025 = 2,2,5,5,8,9,9,10,10-Nonachlorobornane
- B9-1679 = 2,3,5,6,8,8,9,10,10-Nonachlorobornane
- BDE = Brominated diphenyl ether
- CAS = Chemical Abstracts Service (Number)
- CDC = Centers for Disease Control and Prevention
- DDD = Dichlorodiphenyldichloroethane
- DDE = Dichlorodiphenyldichloroethylene
- DDT = Dichlorodiphenyltrichloroethane
- DFTPP = Decafluorotriphenylphosphine
- EDC = endocrine-disrupting chemical
- EPN = Ethyl p-nitrophenyl phenylphosphorothioate
- HpCDD = Heptachlorodibenzo-p-dioxin
- HpCDF = Heptachlorodibenzofuran
- HxCDD = Hexachlorodibenzo-P-dioxin
- HxCDF = Hexachlorodibenzofuran
- IARC = International Agency for Research on Cancer
- NHANES = National Health and Nutrition Examination Survey
- NPE = Nitrophenyl ether
- PAH = polycyclic aromatic hydrocarbon
- PBB = Polybrominated biphenyl
- PCB = Polychlorinated biphenyl
- PPB = parts per billion
- PeCDD = Pentachlorodibenzo-p-dioxin
- RT = retention time
- TCP = Trichlorophenyl
- min. = minutes
- mz = mass-to-charge ratio

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