

Source Profile Speciation Documentation

Organic Gas Speciation Profiles for Wildfire Emissions

OG1486–OG1491 and OG1497

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Introduction

Wildfires are an important source of reactive organic gases (ROG) and particulate matter in California, and can substantially influence ozone formation, secondary organic aerosol (SOA) formation, visibility, and human exposure to toxic air pollutants. Accurate chemical speciation profiles are needed to represent these emissions in inventories and chemical transport models used for regulatory and planning applications.

The current wildfire-related biomass burning profiles were developed from older biomass burning datasets summarized in Yang (2018) [1]. Those profiles substantially improved the representation of oxygenated compounds relative to earlier hydrocarbon-dominated profiles, but a large fraction of total organic gas (TOG) remained unresolved and the compound list was limited compared with more recent wildfire measurements. As a result, a substantial fraction of total organic gas (TOG) remained unresolved, and many oxygenated volatile organic compounds (OVOCs) and other highly reactive species were either underrepresented or not explicitly included. This limitation is important because oxygenated compounds can contribute significantly to ozone formation and secondary organic aerosol chemistry [1].

The 2019 Fire Influence on Regional to Global Environments and Air Quality (FIREX-AQ) campaign provides substantially broader compound coverage for western U.S. wildfires using complementary aircraft instruments, including proton-transfer-reaction time-of-flight mass spectrometry (PTR-ToF-MS), whole-air sampling, gas chromatography, and chemical-ionization methods [2]. The sampled fires include broad western vegetation classes that occur in, or are reasonably analogous to, California wildland fuels. The observations are therefore used here as vegetation-class proxies for California wildfire emissions rather than as statistically representative measurements of every California wildfire. [2, 3].

This report updates CARB's wildfire TOG speciation using FIREX-AQ wildfire observations reported by Gkatzelis et al. (2024) [2] and related supporting literature. The updated profiles are intended to better represent wildfire emissions in the CARB speciation database by expanding chemical coverage, improving representation of reactive and toxic compounds, and replacing older wildfire assignments with updated profiles. In addition, two supporting profiles were developed to represent generalized flaming and smoldering wildfire conditions and are not proposed for direct inventory assignment at this time. The profiles discussed in this document are:

- OG1486: Wildfire – Grassland
- OG1487: Wildfire – Shrubland
- OG1488: Wildfire – Forest/Woodland
- OG1489: Wildfire – California Statewide Average
- OG1490: Wildfire – Flaming

- OG1491: Wildfire – Smoldering
- OG1497: Wildfire – Savanna

Data Sources and Methods

Reference datasets and measurement basis

Wildfire TOG profiles were developed from compound-specific emission factors reported by Gkatzelis et al. (2024) [2] for nine western U.S. wildfires sampled during FIREX-AQ. The southeastern Blackwater River State Forest fire is not used in the wildfire vegetation profiles because it was identified as prescribed and managed burning by the authors.

Gkatzelis et al. (2024)[2] used the maleic anhydride-to-furan ratio (MA/F) as a chemical-age proxy and selected young plume transects to reduce the influence of atmospheric processing on inferred primary emissions. The retained wildfire transects had a median MA/F ratio of about 0.13 and generally represented smoke sampled within roughly 0.6 to 1.7 hours of emission. These measurements are preferred for source-profile development because the objective is to represent primary emissions before substantial downwind chemical transformation.

Multiple instruments were combined to increase chemical coverage and to resolve compounds that PTR-ToF-MS alone cannot distinguish. Where FIREX-AQ gas-chromatography measurements provided compound-resolved information, those measurements were preferred over generic literature splits. Literature-based allocations were used only for residual unresolved groups and are documented separately.

Fuel selection and development of TOG speciation profiles from emission factors

For each retained transect, measured organic-gas emission factors were compiled and normalized to TOG after species identification and isomer allocation. Repeated transects from the same fire were first averaged to a fire-level profile so that fires with more aircraft transects did not receive disproportionate weight. Fire-level profiles were then averaged within the dominant vegetation classes reported by Gkatzelis et al. (2024).

OG1486 (Grassland) is the equal average of the Ridgetop grassland fire and a Williams Flats grassland fire-level profile formed from transects 0 and 21. OG1487 (Shrubland) is based on the Tucker shrubland fire. OG1488 (Forest/Woodland) is the equal average of six forest-dominated fire-level profiles: Shady, Lick Creek, Horsefly, Williams Flats transect 7, Castle, and Sheridan. OG1497 (Savanna) is based on North Hills and is retained for future use and sensitivity analysis because there is no current savanna-specific wildfire EIC.

Two FIREX-AQ transects used in the revised vegetation grouping, North Hills and Williams Flats transect 7, have methane reported as zero in Supplement Table S3 while other gas measurements and modified combustion efficiency (MCE) are present. Because a literal zero methane value is not physically representative of a wildfire TOG profile, methane for these two observations was estimated from the FIREX-AQ methane emission-factor relationship with MCE using the published slope and an intercept reconstructed from the reported wildfire observations. This targeted imputation is documented as an uncertainty and does not affect the measured non-methane species.

OG1489 is a California statewide vegetation-weighted composite constructed after the four vegetation profiles were developed. The weighting uses 2023 projected inventory TOG emissions by vegetation class: Forest + woodland, Grass/Herbaceous, Shrubland, and Savanna. Forest + woodland uses OG1488; Grass/Herbaceous uses OG1486; Shrubland uses OG1487; and Savanna uses OG1497. For each vegetation class i, a weighting factor w_i was calculated as: The statewide TOG weight for each vegetation class i was calculated as:

$$w_i = \frac{TOG_i}{\sum TOG_i}$$

using the 2023 inventory TOG totals are: Forest + woodland = 22,759.80 tons yr^{-1}, Grass/Herbaceous = 2,400.90 tons yr^{-1}, Shrubland = 15,966.80 tons yr^{-1}, Savanna = 96.50 tons yr^{-1}, and total = 41,224.00 tons yr^{-1}. The resulting weights are 55.21%, 5.82%, 38.73%, and 0.23%, respectively.

The statewide profile is calculated as the weighted sum of the normalized vegetation profiles. The 2023 projection year is used as an inventory reference, not as evidence that 2023 represents an average wildfire year. The weighting should be revisited when the completed 2023 base-year inventory or a future planning inventory becomes available.

$$Profile_{State-wide\ avg.} = \sum(w_i \times Profile_i)$$

where $Profile_i$ represents the vegetation-specific proxy profile derived from the FIREX-AQ measurements for each vegetation class.

Wildfire profiles by combustion phase – flaming and smoldering

Biomass-burning emissions vary with combustion phase. OG1490 and OG1491 are retained as supporting profiles for sensitivity analyses and for potential future inventory applications that explicitly separate flaming and smoldering emissions. They are not combined with the vegetation profiles in the current default assignment.

Modified combustion efficiency (MCE), defined as $\Delta CO_2/(\Delta CO_2+\Delta CO)$, is commonly used as an indicator of combustion efficiency, where higher values correspond to more efficient flaming combustion and lower values indicate smoldering conditions [2].

Following literature recommendations by Kondo et al. (2011) [3] and Gkatzelis et al. (2024) [2], representative combustion conditions were set at MCE = 0.95 for flaming combustion and MCE = 0.80 for smoldering combustion. Regression relationships between emission factors and MCE were then used to estimate species emission factors at these two reference conditions. The regression slopes were directly adopted from the parameterizations reported by Gkatzelis et al. (2024) [2]. These phase-specific emission factors were then normalized to TOG to construct separate speciation profiles representing flaming-dominated and smoldering-dominated burning.

Representing combustion phases separately is important because flaming combustion generally produces larger fractions of small hydrocarbons and high-temperature combustion products, whereas smoldering combustion produces larger fractions of oxygenated and partially oxidized organic compounds. Including phase-specific profiles therefore improves representation of variability in organic gas composition during wildfire events. However, for now the phase-specific profiles provide only a practical way to test the sensitivity of chemical transport modeling to combustion phase. A future phase-resolved inventory could use these profiles directly or motivate development of vegetation-by-phase profiles if sufficient measurements and inventory activity data become available.

Treatment of unresolved masses and isomer assignments

Many of the wildfire measurements used in this study were obtained using PTR-ToF-MS, which reports organic compounds as exact ion masses rather than fully resolved molecular species. As a result, some reported signals represent unresolved mixtures of structural isomers or compound groups with identical masses. To construct chemically explicit TOG speciation profiles suitable for inventory and modeling applications, unresolved PTR-ToF-MS signals were separated into individual species where possible using isomer splits recommended by the authors and supported by complementary measurements such as Trace Organic Gas Analyzer (TOGA), Whole Air Sampler (WAS), or other gas chromatography methods, or by prior literature. Where compound-level attribution was available, the PTR mass signal was apportioned among the corresponding species using the recommended fractions; otherwise, the signal was retained as a grouped species or assigned to an unresolved organic gas category.

Two grouped species were further split based on isomer information reported for similar biomass-burning or wood-combustion emissions. The butenenitrile isomer group was split using biomass-burning measurements reported by Hatch et al. (2015)[4], which identified individual C_4H_5N nitriles in FLAME-4 biomass-burning emissions. The unresolved fraction of $C_6H_6O_2$ group was split among benzene diol isomers using the measured distribution in the residential wood-combustion profile by Schauer et al. (2001)[5], which was used as the closest available biomass-burning analogue. The original grouped mass was conserved during these splits. Additional allocations for the C3H6O2 and C6H8O groups used

information from Koss et al. (2018) [6], as documented in Table A3. Unallocated residual mass was retained as unidentified organic gas.

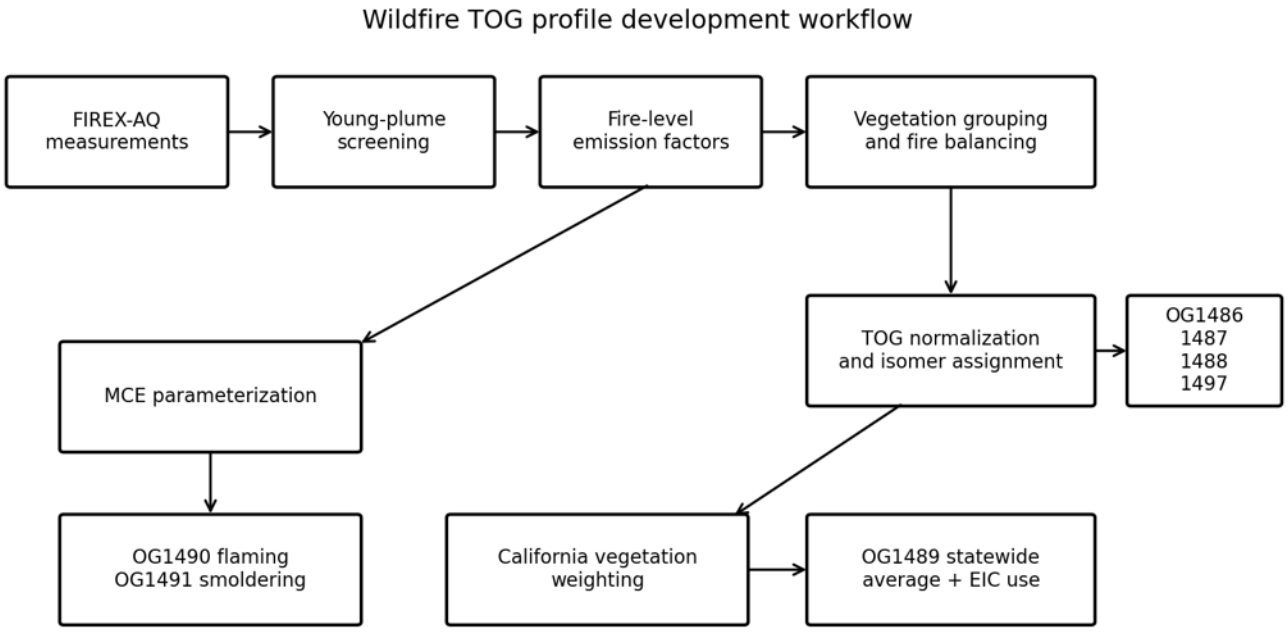


Figure 1. Workflow used to develop vegetation-based wildfire TOG profiles, the California statewide composite, and supporting combustion-phase profiles

Results and Discussion

Table 1. Summary and categorization of newly developed wildfire TOG speciation profiles (OG1486–OG1491 and OG1497). All profiles adopted from Gkatzelis et al. (2024) [2]

Profile Number	Profile Name	Basis / averaging description
OG1486	Wildfire – Grassland	Two fires. Ridgetop plus Williams Flats grassland; Williams Flats transects 0 and 21 are averaged first to one fire-level profile.
OG1487	Wildfire – Shrubland	One fire. Tucker shrubland wildfire.

Profile Number	Profile Name	Basis / averaging description
OG1488	Wildfire – Forest/Woodland	Six fire-level profiles: Shady, Lick Creek, Horsefly, Williams Flats transect 7, Castle, and Sheridan. Repeated transects are averaged within each fire first.
OG1489	Wildfire – California Statewide Average	2023 California vegetation-weighted composite of OG1486, OG1487, OG1488, and OG1497.
OG1490	Wildfire – Flaming	Supporting MCE-based profile at MCE = 0.95; not a current default EIC assignment.
OG1491	Wildfire – Smoldering	Supporting MCE-based profile at MCE = 0.80; extrapolated sensitivity case; not a current default EIC assignment.
OG1497	Wildfire – Savanna	One fire. North Hills savanna; retained for future use and sensitivity analysis; no current savanna-specific EIC.

Differences in Chemical Composition – Old vs New

Across OG1486, OG1487, OG1488, and OG1497, ROG ranges from 67.9% to 76.7% of TOG, methane from 18.5% to 25.0%, non-methane hydrocarbons (NMHC) from 7.1% to 26.5%, and oxygenated volatile organic compounds (OVOC) from 44.8% to 62.2%. The updated profiles contain 76–115 explicitly represented ROG compounds, 25–52 NMHC compounds, and 39–46 OVOC compounds. These ranges are reported descriptively rather than as statistical confidence intervals because the number of contributing wildfire events differs by vegetation class.

The high oxygenated fraction is consistent with recent western U.S. biomass-burning studies. Gkatzelis et al. reported a summed non-methane organic gas emission factor of 26.88 ± 8.5 g kg^{-1}, comparable to WE-CAN and previous temperate-forest estimates. FIREX-AQ emission factors also agreed within a factor of two with most compounds reported by independent laboratory and aircraft studies, although differences remain for individual compounds because of fuel variability, instrumentation, inlet losses, fragmentation, and photochemical processing.

The expanded compound list reflects advances in analytical coverage rather than evidence that every wildfire has the same species distribution. FIREX-AQ combines PTR-ToF-MS with whole-air sampling, gas chromatography, and other compound-specific measurements. The updated profiles therefore provide better compound-level representation while retaining important uncertainty related to fuel type, fire behavior, plume age, and measurement method.

Table 2. Comparison of chemical composition between current CARB wildfire profiles (OG1471, OG1473, OG1477, OG1478) and the revised vegetation-specific wildfire profiles (OG1486, OG1487, OG1488, OG1489, OG1497). New-profile values are descriptive ranges across the four vegetation profiles. Here composition is broadly summarized by Reactive Organic Gases (ROG), methane, Non-Methane Hydrocarbons (NMHC), and Oxygenated Volatile Organic Compounds (OVOC).

Parameter	Current profiles (OG1471, OG1473, OG1477, OG1478)	New Profiles (OG1486–OG1489, and OG1497)
ROG fraction (% of TOG)	83.4 ± 4.25	74.0 ± 3.88
CH4 fraction (% of TOG)	13.6 ± 4.38	20.7 ± 2.92
NMHC fraction (% of TOG)	13.2 ± 0.90	19.5 ± 8.57
OVOC fraction (% of TOG)	11.3 ± 0.45	53.1 ± 7.31
Number of ROG compounds	14–49	76–115
Number of NMHC compounds	6–29	25–52
Number of OVOC compounds	7–11	39–46
Number of toxic species	4–15	40–55

Note: Mean ± standard deviation for the revised composition metrics describes variation among the four vegetation-specific profiles; it is not a confidence interval or a formal

estimate of profile uncertainty. Toxic air contaminant counts use the publicly identified CARB toxic air contaminant designations.

Comparison among new profiles

As seen in **Figure 2**, vegetation profiles differ in ways that are consistent with the broad fuel classifications. OG1487 (Shrubland) is the most oxygenated, with OVOCs at 62.2% of TOG and NMHC at 7.1%. OG1497 (Savanna) has the highest methane (25.0%) and NMHC (26.5%) fractions among the four vegetation profiles. OG1488 (Forest/Woodland), which is supported by the largest number of fires, contains 54.6% OVOC and 73.2% ROG. The California statewide composite OG1489 reflects both OG1488 and OG1487 because forest/woodland and shrubland contribute about 55.2% and 38.7% of the 2023 weighting, respectively. The combustion-phase profiles OG1490 and OG1491 remain supporting phase profiles rather than default inventory assignments. OG1490 (flaming) has lower CH4 and higher ROG and OVOC fractions than OG1491 (smoldering).

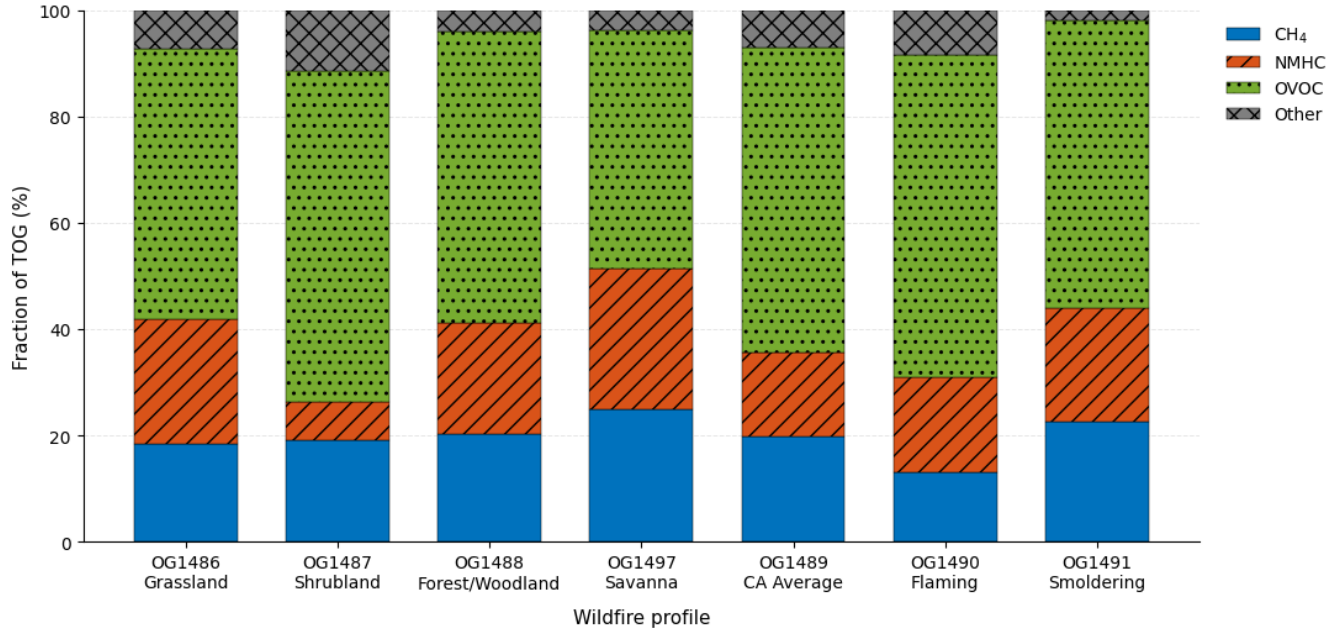


Figure 2. Comparison of chemical composition across newly developed wildfire TOG speciation profiles (OG1486–OG1491,1497), illustrating differences in CH_4, NMHC, OVOC, and other OG fractions by fuel type and combustion phase.

Implications for Emission Inventory and Modeling

Representation of toxic air contaminants

The updated wildfire profiles provide substantially greater compound-level resolution of toxic and reactive organic species than the current CARB wildfire profiles. This improvement reflects the broader chemical coverage of the FIREX-AQ measurements and the explicit resolution of compounds that were previously absent or represented within unresolved organic mass.

Several toxic air contaminants are represented explicitly in the updated profiles, including acrolein, benzene, styrene, naphthalene, propionaldehyde, and other carbonyl compounds. Toxic air contaminant identification follows CARB's publicly identified toxic air contaminant designations, including federal hazardous air pollutants designated as toxic air contaminants under California's air toxics program. Across the four vegetation-specific profiles, 40–55 toxic air contaminants are explicitly represented. Propionaldehyde is introduced through the revised treatment of the C3H6O signal, which is apportioned between acetone and propanal based on compound-resolved FIREX-AQ measurements. The greater number of identified toxic compounds in the updated profiles should therefore be interpreted primarily as an improvement in chemical speciation and measurement coverage, rather than as evidence that wildfire emissions contain a greater toxic fraction than previously assumed.

The updated profiles also contain substantially more oxygenated volatile organic compounds (OVOCs). Across the four vegetation-specific profiles, OVOCs account for approximately 44.8% to 62.2% of TOG, compared with about 11% in the current comparison profiles. This difference reflects the expanded measurement and compound-identification capabilities of the FIREX-AQ dataset, which resolve many oxygenated species that were not explicitly represented in the older CARB wildfire profiles.

Ozone formation potential

The updated profiles also increase the ozone formation potential (OFP) assigned to wildfire emissions in the inventory. OFP was calculated by $OFP = \sum_1^i f_i \times MIR_i$, where f_i is the fractional abundance of species i in TOG and MIR_i is the Maximum Incremental Reactivity (MIR; updated 2010) value for that species. MIR is a reactivity scale used to estimate incremental ozone formation potential under high-NO_X conditions [7]. MIR-based OFP estimates should be interpreted as relative ozone-reactivity metrics rather than direct predictions of ozone formation under all atmospheric conditions. Actual ozone production depends on nitrogen oxides, sunlight, plume dilution, background chemistry, and chemical aging. Therefore, the OFP comparison is most useful for evaluating how the updated chemical speciation changes the relative reactivity assigned to wildfire TOG emissions in the inventory

For a like-for-like statewide screening comparison, the current all-vegetation profile OG1478 has a published OFP of 1.61 g O_3 per g TOG, while the revised California statewide profile OG1489 has an MIR-weighted OFP of approximately 3.39 g O_3 per g TOG. To estimate the potenital ozone formation implied by these profiles, the mean OFP values were multiplied by the corresponding statewide wildfire TOG emissions. Using the 2023 California Emission Projection Analysis Model (CEPAM)'s inventory total of 607.92 tons/day [8], the updated wildfire profiles increase estimated ozone formation from 979 to 2062 tons/day O_3-equivalent, or about 110.7%. This increase is interpreted as a consequence of improved chemical representation. The updated wildfire profiles assign more mass to explicitly resolved reactive compounds, especially oxygenated volatile organic compounds, aldehydes, and other highly reactive species that may contribute strongly to ozone formation.

Table 3. Ozone forming potential of wildfire emission under new profile updates compared to previous.

Metric	Old profiles	New profiles
TOG emissions (tons/day)	607.92	607.92
MIR weighted OFP (g O_3/g TOG)	1.61	3.39
Assigned OFP equivalent (tons/day)	979	2062
Change (tons/day)	–	1083
% change	–	110.7%

Flaming and smoldering wildfire profiles

Two supporting wildfire profiles developed to represent generalized flaming and smoldering combustion conditions show distinct differences in atmospheric reactivity. The flaming profile (OG1490) has a ROG fraction of 81.31% of TOG, an OVOC fraction of 60.61% of TOG, and an OFP of 3.27 g O_3 per g TOG. The smoldering profile (OG1491) has a lower ROG fraction of 71.66% of TOG, an OVOC fraction of 54.09% of TOG, and a higher OFP of 3.78 g O_3 per g TOG. These results indicate that combustion phase can influence both wildfire TOG composition and the ozone formation potential implied by the profiles. Phase-specific profiles are important because they show that a single wildfire profile may not fully represent the variability in emissions across different burning conditions. Flaming and smoldering combustion can differ in the relative abundance of methane, hydrocarbons, oxygenated compounds, and other reactive species, which in turn affects modeled ozone formation and chemical transformation. Although OG1490 and OG1491 are not intended

for direct inventory assignment at this time, they provide a useful framework for sensitivity analyses and for future development of more detailed wildfire speciation approaches. Additionally, introduction of new EICs in future related to flaming and smoldering activities will provide modelers with more refined data when the newly developed profiles are linked with combustion specific EICs.

Uncertainty and limitations

The updated wildfire profiles provide improved chemical representation relative to older wildfire-related biomass-burning profiles; however, several uncertainties remain. The profiles are based on aircraft measurements of young wildfire plumes from FIREX-AQ and may not capture the full variability of wildfire emissions across all California fire conditions. Organic gas composition can vary with vegetation type, fuel moisture, fuel loading, combustion efficiency, combustion phase, plume age, and sampling conditions.

Gkatzelis et al. (2024) reported mean emission factors and standard deviations for individual compounds and unresolved signals. These standard deviations describe variability in the source emission factors and were not propagated into the normalized species fractions. Each species fraction uses the same TOG denominator, and the covariance information needed to determine how the emission factors vary together is unavailable. Quantitative uncertainties are also unavailable for the literature-based isomer assignments, vegetation proxy selections, inventory weights, and some parts of the modified-combustion-efficiency regressions. The proposed profiles provide deterministic, mass-normalized weight fractions for inventory, modeling, and toxic-emissions calculations. Therefore, compound-level uncertainty intervals were not developed as part of this profile update.

PTR-ToF-MS measurements may underrepresent some semi-volatile or low-volatility organic compounds that partition to particles or sampling surfaces during combustion sampling. As a result, the gas-phase TOG profiles may not fully represent all organic vapors relevant to SOA formation.

The vegetation-group profiles represent broad inventory categories. Individual wildfires may include mixed fuels and changing combustion conditions. The California statewide average profile is a generalized, inventory-weighted composite developed using 2023 TOG emissions as the reference year. Because the vegetation mix and emissions assigned to state-wide average can change from year to year, the weighting factors may need to be revisited in future inventory updates. Additionally, the broad vegetation classes do not capture the full diversity of California fuels such as mixed-conifer forest, oak woodland, chaparral, coastal sage scrub, hardwood systems, and mixed fuel complexes. The FIREX-AQ fuel types nevertheless include multiple western forest, woodland, grassland, shrubland, and savanna systems that are useful as broad proxies for California wildfire inventory categories.

The flaming and smoldering profiles were developed from regression relationships based on wildfire plumes with different fuels, locations, and combustion conditions. As a result, these profiles represent generalized flaming- and smoldering-dominated wildfire conditions, not vegetation-specific flaming and smoldering profiles. More detailed phase-specific measurements would be needed to develop separate flaming and smoldering profiles for individual vegetation types. Until such data are available, OG1490 and OG1491 should be treated as generalized profiles and revisited as new information becomes available in literature.

The isomer splits applied to selected grouped species preserve total TOG mass but do not represent plume-specific compound-resolved measurements. These splits are profile-development assumptions based on the best available related literature and may carry uncertainty because the true isomer distribution can vary by fuel type and combustion conditions. However, the expected inventory impact is limited because the affected grouped species are present at low concentrations in the updated profiles. The butenenitrile-isomer group accounts for less than 0.1% of TOG, and the unresolved benzene-diol portion of the $C_6H_6O_2$ group accounts for about 2% of TOG or less after separating 5-methylfurfural. These assumptions should be revisited if future wildfire measurements provide more direct evidence for the relevant isomer distributions.

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Appendix

Table A1. Mapping of Emission Inventory Codes (EICs) to Newly Added Wildfire TOG Speciation Profiles (OG1486, OG1488, OG1489). This table lists the EIC categories and their corresponding updated organic gas speciation profiles used in CARB's wildfire emissions inventory. As of the current inventory structure, OG1487 (Wildfire – Shrubland) is not assigned to any EIC, because no shrubland-specific wildfire EICs exist at this time.

EIC/SCC	Category	Subcategory 1	Subcategory 2	Subcategory 3	New OG Profile ID
93066702000000	WILDFIRES	WILDLAND FIRE USE (WFU)	SOLID FUEL (UNSPECIFIED)	SUB-CATEGORY UNSPECIFIED	OG1489
93093002000000	WILDFIRES	GRASS AND WOODLAND FIRES	SOLID FUEL (UNSPECIFIED)	SUB-CATEGORY UNSPECIFIED	OG1486
93093202000000	WILDFIRES	TIMBER AND BRUSH FIRES	SOLID FUEL (UNSPECIFIED)	SUB-CATEGORY UNSPECIFIED	OG1488
93093402000000	WILDFIRES	ALL VEGETATION	SOLID FUEL (UNSPECIFIED)	SUB-CATEGORY UNSPECIFIED	OG1489

Table A2. Weight Percent of Individual Organic Gas Species Relative to Total Organic Gas (TOG) Across Newly Developed Wildfire Profiles (OG1486–OG1491 and OG1497)

SAROAD	Species	Formula	OG1486 (%)	OG1487 (%)	OG1488 (%)	OG1489 (%)	OG1490 (%)	OG1491 (%)	OG1497 (%)
45208	1,2,4-trimethylbenzene	C9H12	0.0253	0.0369	0.0263	0.0303	0.0578	0.0223	
45207	1,3,5-trimethylbenzene	C9H12	0.0053	0.0088	0.0056	0.0068	0.0039	0.0091	
43222	1,3-butadiyne	C4H2	0.0011	0.0037	0.0019	0.0025	0.0000	0.0035	
43213	1-butene	C4H8	0.5163		0.4294	0.2683	0.6618	0.2730	0.4986
98131	1-butyne	C4H6	0.0165	0.0213	0.0182	0.0193	0.0080	0.0208	
98005	1-heptene	C7H14	0.0561	0.1348	0.0597	0.0886	0.1249	0.0479	0.0526
43245	1-hexene	C6H12	0.0981	0.2507	0.1134	0.1657	0.2298	0.0930	0.1116
47048	1-hydroxy-2-propanone	C3H6O2	0.9274	1.2425	1.2638	1.2355	1.0174	1.4512	1.0824
99915	1-methyl-2-ethylbenzene	C9H12	0.0154	0.0228	0.0148	0.0179	0.0272	0.0148	
99912	1-methyl-3-ethylbenzene	C9H12	0.0244	0.0298	0.0254	0.0270	0.0571	0.0221	

SARO AD	Species	Formula	OG1486 (%)	OG1487 (%)	OG1488 (%)	OG1489 (%)	OG1490 (%)	OG1491 (%)	OG1497 (%)
99914	1-methyl-4-ethylbenzene	C9H12	0.0172	0.0246	0.0179	0.0204	0.0348	0.0167	
43267	1-nonene	C9H18	0.0342	0.0719	0.0354	0.0494	0.0741	0.0250	
43265	1-octene	C8H16	0.0380	0.0885	0.0403	0.0587	0.0734	0.0380	
43224	1-pentene	C5H10	0.2551		0.2106	0.1317	0.3419	0.1227	0.2544
43209	1-propyne	C3H4	0.1635	0.2170	0.1686	0.1870	0.1261	0.1779	0.1272
50842	2(3h)-furanone	C4H4O2	1.5062	1.6557	1.5724	1.6004	1.3445	1.8545	1.3800
47033	2,3-butanedione	C4H6O2	1.0498	1.5707	1.2945	1.3869	1.0726	1.5478	1.1590
43271	2,4-dimethylpentane	C7H16	0.0490		0.0534	0.0325	0.0000	0.0759	0.0636
43330	2,5-dimethylfuran	C6H8O	0.5159	0.6804	0.5399	0.5929	0.4482	0.6283	0.5493
51541	2,6-dimethoxyphenol	C8H10O3	0.1230	0.3618	0.1454	0.2276	0.2089	0.1403	
43552	2-butanone	C4H8O	0.7524	0.8667	0.7243	0.7812	1.3351	0.4259	0.7518
50671	2-butenenitrile	C4H5N	0.0044	0.0090	0.0028	0.0053	0.0061	0.0014	0.0017
47057	2-butyl nitrate	C4H9NO3	0.0000		0.0024	0.0013	0.0476	0.0000	

SARO AD	Species	Formula	OG1486 (%)	OG1487 (%)	OG1488 (%)	OG1489 (%)	OG1490 (%)	OG1491 (%)	OG1497 (%)
98133	2-butyne	C4H6	0.0057	0.0111	0.0060	0.0079	0.0000	0.0155	
43329	2-ethylfuran	C6H8O	0.1172	0.1546	0.1227	0.1347	0.1019	0.1428	0.1248
43225	2-methyl-1-butene	C5H10	0.1439		0.1210	0.0756	0.1743	0.0818	0.1564
43228	2-methyl-2-butene	C5H10	0.1918		0.1584	0.0991	0.2461	0.0993	0.2118
43506	2-methyl-2-propenal	C4H6O	0.5526	0.7019	0.5903	0.6309	0.5901	0.4322	0.4233
43327	2-methylfuran	C5H6O	0.2945	0.3855	0.3871	0.3808	0.6043	0.2090	0.2631
43229	2-methylpentane	C6H14	0.0248		0.0196	0.0123	0.0270	0.0127	0.0207
98036	2-methylpropanal	C4H8O	0.1393	0.1727	0.1492	0.1576	0.1506	0.1370	0.1122
43577	2-oxobutanal	C4H6O2	0.1569	0.2347	0.1934	0.2072	0.1603	0.2313	0.1732
50670	3-butenenitrile	C4H5N	0.0079	0.0161	0.0051	0.0095	0.0110	0.0025	0.0031
50961	3-furaldehyde	C5H4O2	0.0468	0.0593	0.0608	0.0594	0.0509	0.0578	0.0386
43328	3-methylfuran	C5H6O	0.0497	0.0651	0.0653	0.0643	0.0306	0.0690	0.0444
43575	4-methylguaiacol	C8H10O2	1.0480	1.1646	1.4031	1.2903	0.6261	2.0407	1.4947
43363	5-methylfurfural	C6H6O2	1.7052	1.8056	1.7238	1.7550	1.4766	1.9949	1.9771

SAROAD	Species	Formula	OG1486 (%)	OG1487 (%)	OG1488 (%)	OG1489 (%)	OG1490 (%)	OG1491 (%)	OG1497 (%)
43503	acetaldehyde	C2H4O	6.1314	8.0444	5.8559	6.7178	6.5755	5.6565	5.0844
43404	acetic acid	C2H4O2	6.0240	9.2778	5.9111	7.2208	12.1082	2.1687	5.5512
43551	acetone	C3H6O	2.2141	2.4177	2.1779	2.2751	2.2491	1.9860	3.1356
43702	acetonitrile	C2H3N	1.3622	2.0847	0.8760	1.3736	1.2810	0.5856	1.3713
43206	acetylene	C2H2	1.0047		0.7926	0.4992	0.5246	0.8058	1.3246
43505	acrolein	C3H4O	1.8052	2.2983	2.9705	2.6386	3.7821	2.8147	1.4182
43704	acrylonitrile	C3H3N	0.1833	0.2899	0.1105	0.1841	0.2178	0.0486	0.0778
51082	anisole	C7H8O	0.9075	0.9639	0.8380	0.8904	0.7503	0.9592	0.6650
45501	benzaldehyde	C7H6O	0.4646	0.5089	0.4180	0.4561	0.4785	0.4141	0.4861
45201	benzene	C6H6	2.1707	2.6877	2.0730	2.3169	2.6168	1.7391	2.1155
50313	benzofuran	C8H6O	0.2029	0.2204	0.1994	0.2077	0.2306	0.1939	0.1622
51031	benzonitrile	C7H5N	0.3085	0.4388	0.2318	0.3165	0.2850	0.1868	0.2685
43510	butyraldehyde	C4H8O	0.1811	0.2245	0.1940	0.2049	0.2378	0.1582	0.1459
98049	c9 aromatics	C9H12	0.3070	0.2596	0.2601	0.2620	0.5482	0.1419	

SAROAD	Species	Formula	OG1486 (%)	OG1487 (%)	OG1488 (%)	OG1489 (%)	OG1490 (%)	OG1491 (%)	OG1497 (%)
45801	chlorobenzene	C6H5Cl	0.0015		0.0006	0.0004	0.0000	0.0024	
43803	chloroform	CHCl3	0.0012		0.0001	0.0001	0.0021	0.0000	
43217	cis-2-butene	C4H8	0.1382		0.1222	0.0759	0.0749	0.1299	0.1699
43227	cis-2-pentene	C5H10	0.0411		0.0354	0.0221	0.0136	0.0426	0.0504
98156	crotonaldehyde (2-butenal)	C4H6O	0.6754	0.8579	0.7214	0.7711	0.7213	0.7506	0.5174
99278	dimethyl sulfide	C2H6S	0.0055		0.0026	0.0018	0.0000	0.0039	
43202	ethane	C2H6	2.7517		2.8017	1.7130	2.0935	2.7440	2.5381
43302	ethanol	C2H6O	0.0000		0.1194	0.0659	0.0311	0.0522	
43203	ethene	C2H4	4.8713		4.1383	2.5807	3.1730	4.0653	5.2387
50741	ethyl formate	C3H6O2	0.2597	0.3479	0.3539	0.3460	0.2849	0.4063	0.3031
47054	ethyl nitrate	C2H5NO3	0.0022		0.0026	0.0016	0.0031	0.0010	
45203	ethylbenzene	C8H10	0.0461	0.0412	0.0394	0.0405	0.0408	0.0598	0.0512
43502	formaldehyde	CH2O	6.7334	7.4914	6.3841	6.8280	6.8929	6.4784	4.1034
43403	formic acid	CH2O2	2.3441		1.9378	1.2064	2.0254	1.8420	

SAROAD	Species	Formula	OG1486 (%)	OG1487 (%)	OG1488 (%)	OG1489 (%)	OG1490 (%)	OG1491 (%)	OG1497 (%)
99902	furan	C4H4O	0.9517	1.1477	1.2368	1.1845	0.4871	1.3363	0.7469
99312	furfural	C5H4O2	0.4683	0.5927	0.6082	0.5935	1.0788	0.3086	0.3856
47045	glycolaldehyde	C2H4O2	0.3171	0.4883	0.3111	0.3800	0.6373	1.0682	0.2922
90121	glyoxal	C2H2O2	0.4739	0.8775	0.6131	0.7060	0.1476	1.0084	0.0000
43576	guaiacol	C7H8O2	1.7386	1.8889	2.0504	1.9699	1.6529	2.5708	2.1384
43332	hydrogen cyanide	HCN	1.4778	1.8934	0.7887	1.2579	1.4606	0.4151	1.2828
51240	hydroxybenzoquinone	C6H4O3	0.2805	0.3227	0.3428	0.3315	0.1486	0.4809	0.3740
43214	isobutane	C4H10	0.0984		0.0824	0.0515	0.0000	0.1172	0.1123
43215	isobutylene	C4H8	1.2788		1.0091	0.6353	1.6575	0.5159	1.5824
99173	isocyanic acid	HNCO	3.0492	5.5686	1.0981	2.9407	4.0095	0.0000	
98132	isopentane	C5H12	0.0490		0.0408	0.0254	0.0000	0.0714	
43243	isoprene	C5H8	0.3097		0.1698	0.1118	0.1493	0.2689	
43304	isopropanol	C3H8O	0.0209		0.0074	0.0053	0.0722	0.0000	
47056	isopropyl nitrate	C3H7NO3	0.0090		0.0065	0.0041	0.0101	0.0022	

SAROAD	Species	Formula	OG1486 (%)	OG1487 (%)	OG1488 (%)	OG1489 (%)	OG1490 (%)	OG1491 (%)	OG1497 (%)
98043	isopropylbenzene	C9H12	0.0152	0.0140	0.0137	0.0139	0.0136	0.0115	
99024	m & p-xylene	C8H10	0.3820	0.3415	0.3268	0.3359	0.3378	0.4066	0.4246
43568	m-benzenediol	C6H6O2	0.0145	0.0153	0.0147	0.0149	0.0125	0.0169	0.0168
98120	methacrylonitrile	C4H5N	0.0173	0.0351	0.0110	0.0207	0.0240	0.0054	0.0067
43201	methane	CH4	18.4887	19.1589	20.2480	19.7347	12.9983	22.5956	24.9553
43301	methanol	CH4O	3.1189	4.1777	4.6314	4.3673	5.7313	3.9349	4.5305
43432	methyl acetate	C3H6O2	0.6492	0.8697	0.8846	0.8648	0.7122	1.0159	0.7577
99295	methyl formate	C2H4O2	0.0496		0.0764	0.0451	0.0000	0.1148	
47053	methyl nitrate	CH3NO3	0.0105		0.0070	0.0045	0.0093	0.0040	0.0000
47047	methyl vinyl ketone	C4H6O	0.7778	0.9879	0.8307	0.8880	0.8306	1.0918	0.5958
43261	methylcyclohexane	C7H14	0.0165		0.0131	0.0082	0.0000	0.0173	
43262	methylcyclopentane	C6H12	0.0173		0.0142	0.0089	0.0000	0.0308	0.0154
90122	methylglyoxal	C3H4O2	1.1988	3.0324	0.9641	1.7766	0.0000	2.0349	
43123	monoterpenes	C10H16	1.1952	0.3696	1.1346	0.8480	0.0000	1.9916	3.7685

SAROAD	Species	Formula	OG1486 (%)	OG1487 (%)	OG1488 (%)	OG1489 (%)	OG1490 (%)	OG1491 (%)	OG1497 (%)
43212	n-butane	C4H10	0.2759		0.2520	0.1558	0.2906	0.1950	0.2776
43238	n-decane	C10H22	0.0826		0.0701	0.0435	0.0624	0.0696	0.0000
43231	n-hexane	C6H14	0.1033		0.1003	0.0617	0.1759	0.0491	0.1270
43235	n-nonane	C9H20	0.0823		0.0739	0.0458	0.0635	0.0691	0.0878
43220	n-pentane	C5H12	0.1402		0.1348	0.0829	0.1399	0.1165	0.1470
47055	n-propyl nitrate	C3H7NO3	0.0000		0.0010	0.0006	0.0017	0.0001	
45209	n-propylbenzene	C9H12	0.0198	0.0228	0.0129	0.0171	0.0142	0.0116	
98046	naphthalene	C10H8	0.2330	0.3231	0.2330	0.2674	0.4083	0.1555	
99004	nitromethane	CH3NO2	0.2051	0.2100	0.1556	0.1792	0.4219	0.0194	
43569	o-benzenediol	C6H6O2	1.6025	1.6969	1.6200	1.6493	1.3876	1.8747	1.8581
98021	o-cresol (2-methyl-benzenol)	C7H8O	0.9075	0.9639	0.8380	0.8904	0.7503	0.9592	0.6650
45204	o-xylene	C8H10	0.1383	0.1237	0.1183	0.1216	0.1223	0.1375	0.1537
43571	p-benzenediol	C6H6O2	0.0883	0.0935	0.0893	0.0909	0.0765	0.1033	0.1024
90103	pentadiene	C5H8	0.1098		0.0964	0.0600	0.0000	0.1937	0.1669

SAROAD	Species	Formula	OG1486 (%)	OG1487 (%)	OG1488 (%)	OG1489 (%)	OG1490 (%)	OG1491 (%)	OG1497 (%)
45300	phenol	C6H6O	0.5732	0.6217	0.5305	0.5677	0.6214	0.3633	0.2842
43504	propanal	C3H6O	0.6245	0.6819	0.6143	0.6417	0.6344	0.5602	0.8844
43204	propane	C3H8	1.0062		0.9969	0.6115	0.8257	0.9794	1.0589
43205	propene	C3H6	2.5267		2.3213	1.4355	0.8606	2.7169	2.8719
47050	pyrrole	C4H5N	0.0494	0.1004	0.0315	0.0592	0.0677	0.0157	0.0193
45220	styrene	C8H8	0.3550	0.3969	0.2982	0.3400	0.2820	0.3189	0.3946
45202	toluene	C7H8	1.7150	1.5223	1.5233	1.5354	1.1104	1.7676	2.0929
43216	trans-2-butene	C4H8	0.1336		0.0926	0.0593	0.0382	0.1209	0.1627
43226	trans-2-pentene	C5H10	0.0600		0.0478	0.0301	0.0417	0.0495	0.0758
99999	unidentified	-	0.6364	0.8711	0.8312	0.8351	0.61395	0.6899	0.7298
98134	vinylacetylene	C4H4	0.0395	0.0661	0.0408	0.0504	0.0147	0.0514	
	Total		**100.000**	**100.000**	**100.000**	**100.000**	**100.000**	**100.000**	**100.000**

Table A3. Principal unresolved-mass and isomer allocations used in the revised wildfire profiles

Source signal / mixture	Formula	Split set / use	Assigned compound	SAROAD	Allocation (%)	Reference and allocation applied
C3H6O isomers	C3H6O	FIREX-AQ compound-resolved split	Acetone	43551	78	Gkatzelis et al. (2024); FIREX-AQ GC comparison: 78% acetone
C3H6O isomers	C3H6O	FIREX-AQ compound-resolved split	Propanal / propionaldehyde	43504	22	Gkatzelis et al. (2024); FIREX-AQ GC comparison: 22% propanal
C2H4O2 isomers	C2H4O2	Literature-based biomass-burning split	Acetic acid	43404	95	Hatch et al.; 95% of C2H4O2 assigned to acetic acid
C2H4O2 isomers	C2H4O2	Literature-based biomass-burning split	Glycolaldehyde	47045	5	Hatch et al.; 5% of C2H4O2 assigned to glycolaldehyde
Butenenitrile isomers	C4H5N	Literature-based nitrile isomer split	Methacrylonitrile	98120	58.27	Hatch et al. (2015); 58.27% of butenenitrile group

Source signal / mixture	Formula	Split set / use	Assigned compound	SAROAD	Allocation (%)	Reference and allocation applied
Butenenitrile isomers	C4H5N	Literature-based nitrile isomer split	3-Butenenitrile	50670	26.77	Hatch et al. (2015); 26.77% of butenenitrile group
Butenenitrile isomers	C4H5N	Literature-based nitrile isomer split	2-Butenenitrile	50671	14.96	Hatch et al. (2015); 14.96% of butenenitrile group
C4H6O isomers	C4H6O	FIREX-AQ GC-derived isomer split	Methyl vinyl ketone	47047	38	Gkatzelis et al. (2024); 38% methyl vinyl ketone
C4H6O isomers	C4H6O	FIREX-AQ GC-derived isomer split	Methacrolein / 2-methyl-2-propenal	43506	27	Gkatzelis et al. (2024); 27% methacrolein
C4H6O isomers	C4H6O	FIREX-AQ GC-derived isomer split	Crotonaldehyde / 2-butenal	98156	33	Gkatzelis et al. (2024); 33% 2-butenal

Source signal / mixture	Formula	Split set / use	Assigned compound	SAROAD	Allocation (%)	Reference and allocation applied
C4H6O isomers	C4H6O	Residual unresolved fraction	Unidentified	99999	2	Gkatzelis et al. (2024); remaining 2% retained as unidentified
C8H10 isomers	C8H10	FIREX-AQ GC-derived aromatic split	Ethylbenzene	45203	7	Gkatzelis et al. (2024); 7% ethylbenzene
C8H10 isomers	C8H10	FIREX-AQ GC-derived aromatic split	m- & p-Xylene	99024	58	Gkatzelis et al. (2024); 58% m- and p-xylene
C8H10 isomers	C8H10	FIREX-AQ GC-derived aromatic split	o-Xylene	45204	21	Gkatzelis et al. (2024); 21% o-xylene
C8H10 isomers	C8H10	Residual unresolved fraction	Unidentified	99999	14	Gkatzelis et al. (2024); remaining 14% retained as unidentified

Source signal / mixture	Formula	Split set / use	Assigned compound	SAROAD	Allocation (%)	Reference and allocation applied
C6H6O2 isomers	C6H6O2	Primary FIREX-AQ split	5-Methylfurfural	43363	50	Gkatzelis et al. (2024); 50% assigned directly to 5-methylfurfural
C6H6O2 isomers	C6H6O2	50% benzenediol share; Schauer nested split	o-Benzenediol / catechol	43569	46.99	Gkatzelis et al. (2024) + Schauer et al. (2001); 50% × 93.98%
C6H6O2 isomers	C6H6O2	50% benzenediol share; Schauer nested split	m-Benzenediol / resorcinol	43568	0.425	Gkatzelis et al. (2024) + Schauer et al. (2001); 50% × 0.85%
C6H6O2 isomers	C6H6O2	50% benzenediol share; Schauer nested split	p-Benzenediol / hydroquinone	43571	2.59	Gkatzelis et al. (2024) + Schauer et al. (2001); 50% × 5.18%
C3H6O2 isomers	C3H6O2	Koss et al. profile-build allocation	1-Hydroxy-2-propanone / hydroxyacetone	47048	48	Koss et al. (2018); 48% hydroxyacetone

Source signal / mixture	Formula	Split set / use	Assigned compound	SAROAD	Allocation (%)	Reference and allocation applied
C3H6O2 isomers	C3H6O2	Koss et al. profile-build allocation	Methyl acetate	43432	37	Koss et al. (2018); 37% methyl acetate
C3H6O2 isomers	C3H6O2	Koss et al. profile-build allocation	Ethyl formate	50741	14	Koss et al. (2018); 14% ethyl formate
C3H6O2 isomers	C3H6O2	Residual unresolved fraction	Unidentified	99999	1	Koss et al. (2018); remaining 1% retained as unidentified
C6H8O furans	C6H8O	Koss et al. furan allocation	2,5-Dimethylfuran	43330	44	Koss et al. (2018); 44% 2,5-dimethylfuran
C6H8O furans	C6H8O	Koss et al. furan allocation	2-Ethylfuran	43329	10	Koss et al. (2018); 10% 2-ethylfuran
C6H8O furans	C6H8O	Residual unresolved fraction	Unidentified	99999	46	Koss et al. (2018); remaining 46% retained as unidentified

Source signal / mixture	Formula	Split set / use	Assigned compound	SAROAD	Allocation (%)	Reference and allocation applied
C2H6S isomers	C2H6S	FIREX-AQ documented split	Dimethyl sulfide	99278	50	Gkatzelis et al. (2024); 50% assigned to dimethyl sulfide
C2H6S isomers	C2H6S	Residual unresolved fraction	Unidentified	99999	50	Gkatzelis et al. (2024); remaining 50% retained as unidentified