

Air pollution from the Ports of Long Beach and Los Angeles: Volatile Organic Compound Emissions

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S1. Winds at the Ports

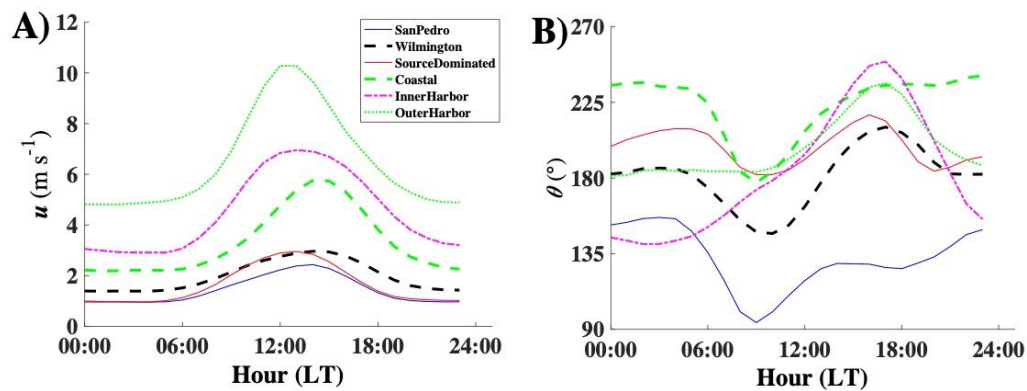


Figure S1. A) wind speed, u , and B) wind direction, θ versus Local Time (LT) for the Ports' air quality sites using wind data 1/2018-9/2022. Data key on panel A. See Fig. 1 for station locations.

Air quality (AQ) station data were downloaded for the five port-area AQ stations, and time-resolved averages were calculated (Fig. S1). AQ data are hourly but spotty, with small to large gaps and other irregularities, including impossible values, such as negative wind speeds and wind directions over 360° . Data gaps and irregularities were replaced with NaNs (Not a Number). Then, NaNs were replaced by the nearest neighbor average if neither was a NaN, i.e., non-persistent data gaps or irregularities.

Winds follow a diurnal cycle, with the weakest winds after midnight. Winds strengthen in the early morning, reaching a maximum at noon for the Harbor sites, at 15:00 for the Coastal site, and in between for other AQ stations (Fig. S1). Winds then decrease to a nocturnal minimum around midnight. Coastal winds (the Inner Harbor, Outer Harbor, and Coastal sites) are stronger than more inland winds.

S2. Standard Instrumentation Suite (SIS)

Table S1. Standard Instrumentation Suite (SIS) analyzers and sensors.

Analyzer Model (-)	Measurement (-)	Rate (Hz)	Typical (Hz)	Specified Precision	SISTER Precision	Manufacturer	Method
Gas Measurements							
Fast Greenhouse Gas Analyzer (911-010)	Carbon Dioxide (CO ₂)	1	1	300	300 ppb	Los Gatos Research	Mid-Infrared Absorption
	Methane (CH ₄)	1	1	1	0.1 ppb		
	Water Vapor (H ₂ O)	10	5	100	100 ppm		
G2210-I Methane Isotope analyzer	dC ¹³ Methane (CH ₄)	1	1	0.05	0.05 ppb	Picarro	Cavity Enhanced Absorption Spectrometry
	Methane (CH ₄)	1	1	0.1	0.1 ppb		
	Ethane (C ₂ H ₆)	1	0.017	1	1 ppb		
	Carbon Dioxide (CO ₂)	1	1	200	200 ppmv		
	Water Vapor (H ₂ O)	10	5		ppm		
Mira CH ₄ ,C ₂ H ₆ , C ₃ H ₈ Analyzer	Methane (CH ₄)	1	1		ppb	Aeris Tech.	Mid-Infrared Absorption
	Ethane (C ₂ H ₆)	1	1		0.050 ppb		
	Propane (C ₃ H ₆)	10	5		0.050 ppb		
	Water Vapor (H ₂ O)	10	5		ppm		
Mira CO, N ₂ O Analyzer	Carbon Monoxide (CO)	1	1	0.5	0.5 ppb	Aeris Tech.	Mid-Infrared Absorption
	Nitrous Oxide (N ₂ O)	1	1	0.5	0.5 ppb		
	Water Vapor (H ₂ O)	10	5		ppm		
42iTL- Trace Analyzer	Nitric Oxide (NO)	0.1	0.1	25	0.025 ppb	ThermoFisher	Fluorescence
	Nitrogen Dioxide (NO ₂)	0.1	0.1	25	0.025 ppb		
42i-Y NO _y Analyzer	Nitrogen oxides (NO _y)	0.1	0.1	0.05	0.05 ppb	ThermoFisher	Fluorescence
49i Ozone Analyzer	Ozone (O ₃)	0.1	0.1	1	0.2 ppb		
Ammonia / Hydrogen Sulfide Analyzer	Ammonia (NH ₃)	1	0.2	1	0.2 ppb	Los Gatos Research	Cavity Enhanced Absorption Spectrometry
	Hydrogen Sulfide (H ₂ S)	1	0.2	15	5 ppb		
450c Trace Analyzer	Sulfur Dioxide (SO ₂)	0.1	0.1	1	0.05 ppb	ThermoFisher	Fluorescence
	Hydrogen Sulfide (H ₂ S)	0.02	0.017	1	0.05 ppb		
5020 SO ₂ analyzer Trace	Sulfur Dioxide (SO ₂)	1	1	0.05	0.05 ppb	ThermoFisher	Fluorescence
Aerosol Measurements							
11-A Aerosol size Spectrometer	0.1-32 μm aerosol size	0.17	0.17		32 channels	Grimm	Optical
31CL Ceilometer	Aerosol optical depth profile	0.02	0.017	10	10 m vertical # srad ⁻¹ km ⁻¹		Lidar
Scanning Mobility Particle Sizer	90-1094 nm	15	15		# cm ⁻³	Grimm, Durag	Venice Electrode
ObservAir	Black Carbon	0.50	0.25	0.10	μg m ⁻³	DS Tech	Optical Absorbtion
Meteorology Measurements							
Anemometer (CSAT)	Wind speed	50	5	0.25	0.3 mm s ⁻¹	Campbell Scientific	Ultrasonic
	Wind direction	50	5	2	2 °		
Anemometer (81000)	Wind speed	4	4	0.3	0.3 m s ⁻¹	RM Young	Ultrasonic
	Wind direction	4	4	2	10 °		
PTU200 Barometer	Pressure	1	1	0.1	0.1 hPA	RM Young	
	Humidity	1	0.08	1	1 %		
	Temperature	1	1	0.2	0.2 °C		
Spectroscopy Measurements							
Pyranometer SP-110	Radiation, (360-1120 nm)	2	1	5%	5% W m ⁻²	Apogee	Thermopile
Pyrgeometer SL-510	Radiation (5-30 μm)	2	1	5%	5% W m ⁻²	Apogee	Thermopile
Spectrometer (HR4000)	Radiation (182-1109 nm, 0.3 nm)	1000	100		300 SNR	Ocean Optics	Grating
Spectrometer (HR4000)	Radiation	1000	100		300 SNR	Ocean Optics	Grating
Spectrometer (HR4000)	Radiation 280-1090	1000	100		300 SNR	Ocean Optics	Grating
Spectrometer (Red Wave)	Radiation (.9-1.7 μm, 0.0016 μm)	1000	1		4000 SNR	Stellarnet	Grating
Radiation Measurements							
Geiger Counter (GCA-04W)	Alpha, Beta Radiation	1	1			ImageSc	GM Tube
Geiger Counter (GCA-04W)	Beta Radiation	1	1			ImageSc	GM Tube

SNR - Signal to noise ratio

Coastal daytime winds are almost entirely west-southwesterlies. Further east and inland (the Source-dominated and Wilmington sites), the onshore daytime flow is more southerly. Nighttime winds are weaker than daytime winds and generally from the northwest to north-northwest for all AQ stations, although the Coastal site also features winds parallel to the coast (easterlies or westerlies). San Pedro winds are distinct from those at other sites with strong east-to-southeast components due to wind forcing by the Palos Verdes Highlands. Inner Harbor wind patterns also differ,

slowly shifting from southeast to south to almost west during the day. Outer Harbor daytime winds slew from south to westerlies during the day.

Surveys used a series of evolving platforms, AMOG Surveyor, SISTER, and SISTER2 (Fig. S2) (Leifer et al., 2016a; Leifer et al., 2016b; Leifer et al., 2018a; Leifer et al., 2018b; Leifer et al., 2019a; Leifer et al., 2019b; Leifer and Melton, 2021; Leifer et al., 2014). Currently, SISTER2 measures meteorology (3D winds, temperature, pressure, humidity), aerosol profiles, and aerosol size spectra (0.1–32 μm , 32 channels, 0.16 Hz). SISTER2 measures trace gases including $\delta^{13}\text{CH}_4$, $\delta^{13}\text{CO}_2$, CH_4 , C_2H_6 , C_3H_8 , CO_2 , CO , H_2O , NH_3 , O_3 , SO_2 , NO , NO_2 , NO_x , NO_y , N_2O , and H_2S) and CO_2 , H_2O at sub-ppm-levels. Current SISTER2 instruments and details are provided in Table S1.

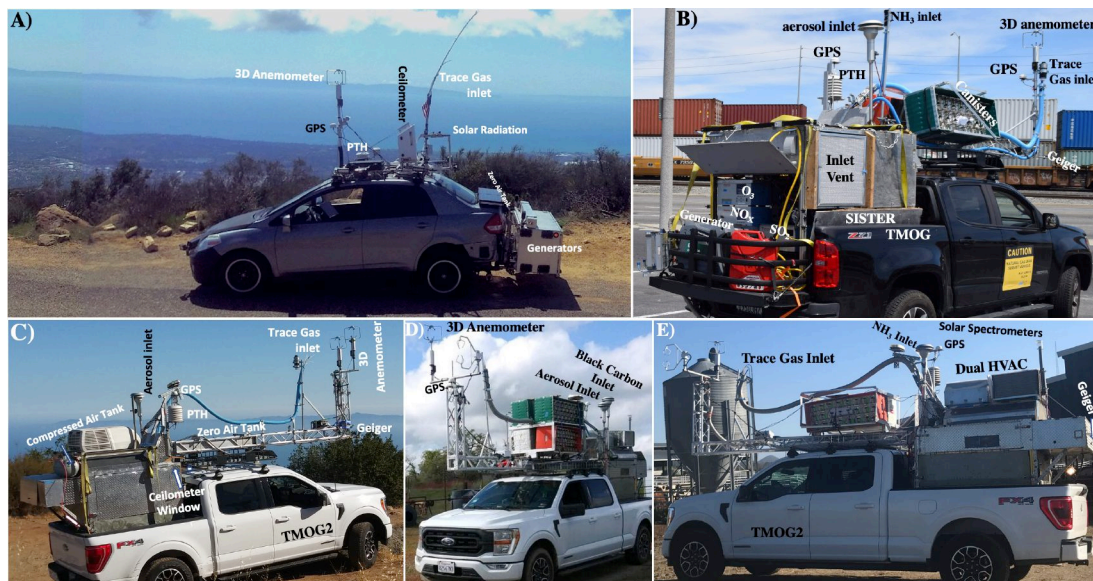


Figure S2. A) AMOG Surveyor on the Santa Ynez Ridge, Santa Barbara County, 29 Mar. 2019, B) SISTER on TMOG at the Port of Long Beach on 28 Apr. 2020, C) SISTER on TMOG2 on the Santa Ynez Ridge on 5 Sept. 2020, D) SISTER2 on TMOG2 at a northern California gas field on 31 March 2023, and E) at the California Polytechnic Research Dairy, San Luis Obispo, CA on 15 February 2023.

AMOG Surveyor was a car-based mobile laboratory designed for satellite validation. This criterion required high accuracy at highway speed to cover multiple satellite pixels within a (3–4 hr.) atmospheric timescale. This timescale necessitates fast analyzers and large vacuum pumps, which are heavy and generate significant heat, requiring substantial electrical power and cooling capacity.

The choice of an automobile was based on avoiding vehicle disturbance of the winds. However, automobile capabilities are limited in terms of power, weight, and are restricted to paved roads. The shift to a larger vehicle (truck) was based on moving the anemometer to a roof-mounted truss to place it outside the vehicle's flow stream. The current SIS, SISTER2, is deployed in a full-size, hybrid pickup truck with a built-in 7.2-kW inverter generator.

Nitrous oxide (N_2O), sulfur dioxide (SO_2), hydrogen sulfide (H_2S), and propane (C_3H_8) detection limits are improved by periodically measuring zero air from an onboard Zero Air Gas generator (737-10, Aadco Inst., OH) or from an aluminum tank filled at the laboratory. Zero air is regulated to 2–3 psi by a low-pressure (0–25 psi) dual-stage regulator (44-226X-A42-010 TESCOM, Emerson, MN).

All sample lines, filter holders, solenoids for zero air switching, and tube fittings are perfluoroalkoxy (PFA) Teflon; filters are polytetrafluoroethylene (PTFE) Teflon. An air suspension frame achieves further signal-to-noise improvements for fluorescence and optical absorption analyzers by reducing vibrations.

All data are integrated in real-time by custom code written in MATLAB, which provides a real-time display in the Google Earth environment to facilitate adaptive surveying. Adaptive surveying is where data visualization allows survey strategy modification to improve science outcomes (Thompson et al., 2015). Real-time data visualization enables targeted air sample collection in the atmospheric context. The real-time display also includes analyzer temperature and cell pressure, and, for some analyzers, flow rates to identify potential problems. Additional SISTER details are provided in the literature cited above.

SISTER2 supports up to 96 1-L evacuated stainless steel canisters for lab analysis for a wide range of trace gases. An air pump pressurizes the air sample canisters with sample air from an inlet adjacent to the inlet of the other analyzers, at 3-m above ground to minimize traffic contamination. Sample canisters are individually and manually filled by slightly opening a bellows valve. Canister collection uses real-time data to collect. Real-time data visualization allows sample collection in the atmosphere's frame of reference, with context provided by continuous SISTER data.

Air samples are analyzed in the laboratory by a three-gas chromatograph analytical system with a range of detectors, including ECD (Electronic Capture Detector), FID (Flame Ion Detector), and MSD (Mass Spectrometry Detector). The system utilizes a state-of-the-art vacuum-line injection system and 6 column/detector combinations. See Colman et al. (2001) and Simpson et al. (2010) for a full description.

S3. Emissions Derivation

In situ emissions are based on filtered absolute winds, which are calculated from relative winds by accounting for vehicle motion and filtering transient wind measurements that may arise from other vehicles (trucks and buses) and near-road obstacles, such as trees, and non-physical jumps in GPS position. Emissions were modeled as a combination of point-source plumes and an area-source plume.

Point source plume emissions are described as a Gaussian plume (Hanna et al., 1982), which relates atmospheric emissions, E_A , to the concentration anomaly, C' , relative to ambient, C , wind speed, u , and the atmospheric turbulence parameters, σ_y and σ_z , defined in a Cartesian coordinate system where x is the downwind, i.e., wind direction, θ , y is the transverse direction, and z is the vertical coordinate,

$$C'(x, y, z) = E_A \frac{\exp\left(\frac{-y^2}{2\sigma_y^2}\right)}{(2\pi u \sigma_z \sigma_y)} \left(\exp\left(\frac{-(z-h)^2}{2\sigma_z^2}\right) + \exp\left(\frac{-(z+h)^2}{2\sigma_z^2}\right) + \exp\left(\frac{-(z-2(BL-h))^2}{2\sigma_z^2}\right) + \exp\left(\frac{-(z+2(BL-h))^2}{2\sigma_z^2}\right) \right), \quad (S1)$$

where h is the release height (after buoyant rise). The second exponential term represents reflection off the surface for a non-sticky molecule, the third term represents reflection off the boundary layer at height BL , and the fourth term represents re-reflection off the surface. C' is relative to the background concentration, C , which is based on the gradient of the concentrations outside the plume's edges.

Parameterization of σ_y and σ_z are:

$$\sigma_y = a(1 + 10^{-4}x)^{-1/2}; \sigma_z = b(1 + cx)^n, \quad (S2)$$

with a , b , and c depending on the stability class (Briggs, 1973). The stability class (Table S2) is based on solar insolation, I , and u (Hanna et al., 1982). These turbulence parameterizations (Eqn. S2) are discrete (Tables S2 and S3), which introduces uncertainty in σ_y and σ_z , particularly at stability class transitions. To remove discretization distortions, a 2nd-order polynomial was fit to the turbulence parameters a , b , and c for each insolation class with respect to u . The polynomial fit then was evaluated for u to determine a , b , and c for all three insolation classes. Weak, moderate, and strong insolation classes were fit for $I = 175$, 500, and 800 W m⁻², respectively. Given the coarse nature of the Pasquill classes, no effort was made to optimize. Instead, the center u for each class was used in the parameterization.

Table S2. Parameters for atmospheric turbulence parameterizations for different stability classes*

Class		a	b	c	n	Class Description
A	<i>open</i>	0.22	0.20	0	-	Extremely unstable
B	<i>open</i>	0.16	0.12	0	-	Moderately unstable
C	<i>open</i>	0.11	0.08	2×10^{-4}	-0.5	Slightly unstable
D	<i>open</i>	0.08	0.06	1.5×10^{-3}	-0.5	Neutral
E	<i>open</i>	0.06	0.03	3×10^{-4}	-1	Slightly stable
F	<i>open</i>	0.04	0.016	3×10^{-4}	-1	Moderately stable

*from Briggs (1973).

Table S3. Conditions defining Pasquill turbulence classes*

u	I_{Strong}	$I_{Moderate}$	I_{Weak}	Night	Night
m s ⁻¹	>700 W m ⁻²	350-700 W m ⁻²	<350 W m ⁻²	>1/2 Clouds	<3/8 Clouds
<2	A	A-B	B	E	F
2	A-B	B	C	E	F
4	B	B-C	C	D	E
6	C	C-D	D	D	D
>6	C	D	D	D	D

*from Hanna et al. (1982). u is wind speed, I is solar insolation.

The Gaussian plume model is for a passive dispersant and assumes negligible along-wind diffusion, that u , σ_y , and σ_z are vertically and horizontally uniform along its trajectory, that u fluctuations are zero, and that u remains parallel to the x -axis (no veering). These assumptions imply an idealized, flat terrain of homogeneous roughness. Violations of these conditions are common in terrestrial settings and can be addressed by model modification, e.g., Briggs (1973); Leifer et al. (2016a), the absence of topography and obstructions at sea implies that marine plumes generally satisfy the Gaussian plume requirements.

The first step in deriving point source emissions is the Gaussian Data Model (GDM), which is applied to C' after removing the background (including gradients) concentration by a first-order, least-squares linear regression analysis

fit to values outside the plume. C' is projected onto a wind-orthogonal plane, and a least-squares linear-regression analysis fits one or more Gaussian functions. The Gaussian Plume Model (GPM) is the least-squares linear regression analysis that fits the GDM.

The area source was modeled as a linear plume, which was allowed to diffuse vertically based on a Gaussian plume model. Lateral dispersion of the linear plume was neglected.

In situ data fall into three classes: fast analyzers, slow analyzers, and discrete sample canisters. Plume structures (i.e., transport) are characterized by fast analyzer data, which allows spatial partitioning of slow analyzer data based on the fast analyzer partitioning (Leifer and Melton, 2021). Key is that both fast and slow gases are co-emitted and that the time of travel from source to SISTER is sufficiently short that chemistry does not alter concentrations significantly. Monte Carlo simulations assess the uncertainty of emissions and location. These MC simulations are based on measured parameter variability. Specifically, normalized distributions of parameters for the plume inversion model (wind speed, u , wind direction, θ , ambient background gas concentration, C) are created with a standard deviation and mean based on *in situ* field measurements during the plume transect. For each Monte Carlo simulation run, plume emissions and source distance are optimized for the maximum correlation coefficient, R^2 , between the measured and modeled concentration anomaly, C' . The parameter distributions then are subsampled randomly as initial conditions for the plume inversion model. A total of 10,000 Monte Carlo simulations are run to calculate distributions of emissions and source distances. Uncertainty in emissions and source distance then is defined based on where each distribution decreases to $1/e$ of its maximum.

S4. Airborne remote sensing by the Mako instrument

Airborne remote sensing was acquired by the thermal infrared (TIR) imaging spectrometer, Mako (Fig. S3). Mako's spectroradiometric performance is described in detail in Buckland et al. (2017) and is summarized in Table S3.

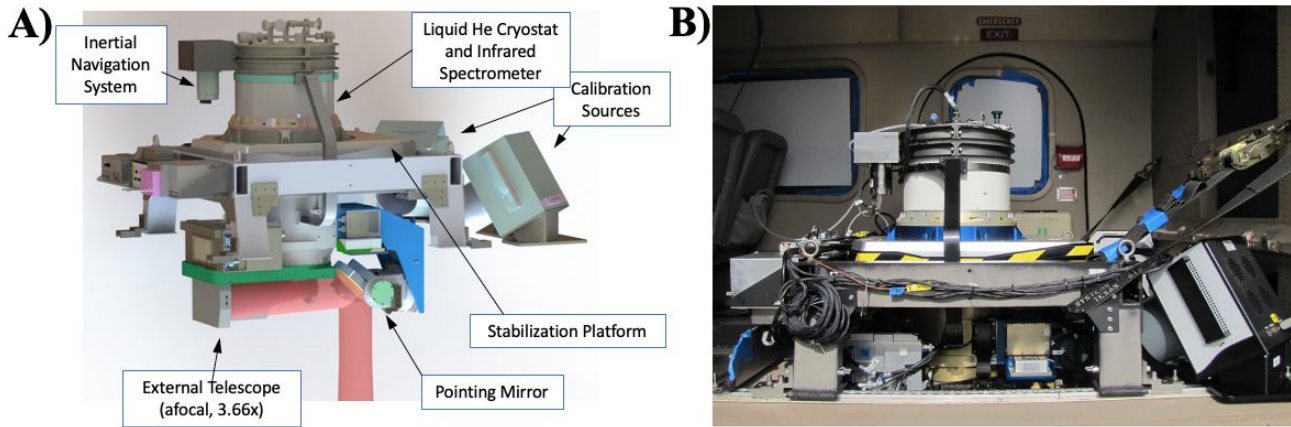


Figure S3. Mako Thermal Infrared Imaging Spectrometer A) Schematic, B) Sensor installed on host aircraft.

Table S3. Mako operating parameters.

Parameter	Specification
Spectral coverage	7.57 – 13.16 μm
Spectral resolution (128 channels)	44 nm
Instantaneous field-of-view, IFOV	0.56 mrad
Along-track FOV (128 pixels per frame)	4.1°

Base frame rate	3255 Hz
Nominal operational frame rate (4 co-adds)	814 Hz
Cross-track pixels (user programmable)	400 – 3600
Cross-track field-of-regard, FOR (relative to nadir)	$\pm 56.4^\circ$ (max.)
Noise-equivalent spectral radiance, NESR (10 μm , 4-frame averages)	$< 0.5 \mu\text{W cm}^{-2} \text{sr}^{-1} \mu\text{m}^{-1}$
Noise-equivalent differential temperature, NEDT (10 μm , 300 K)	0.03 K

S4. Port area sources trace gas profile

The summary, non-normalized, composition profiles of the short-chain hydrocarbons except CH_4 and aromatics are shown in Figure S4 in units of $\mu\text{g m}^{-3}$ which emphasizes larger gases. Trace gas alkane profiles decreased with alkane number as a power law for some sources. In a logarithmic plot, a power law is well described by a linear fit. An example for mean background in Figure 4 is shown in Figure S5.

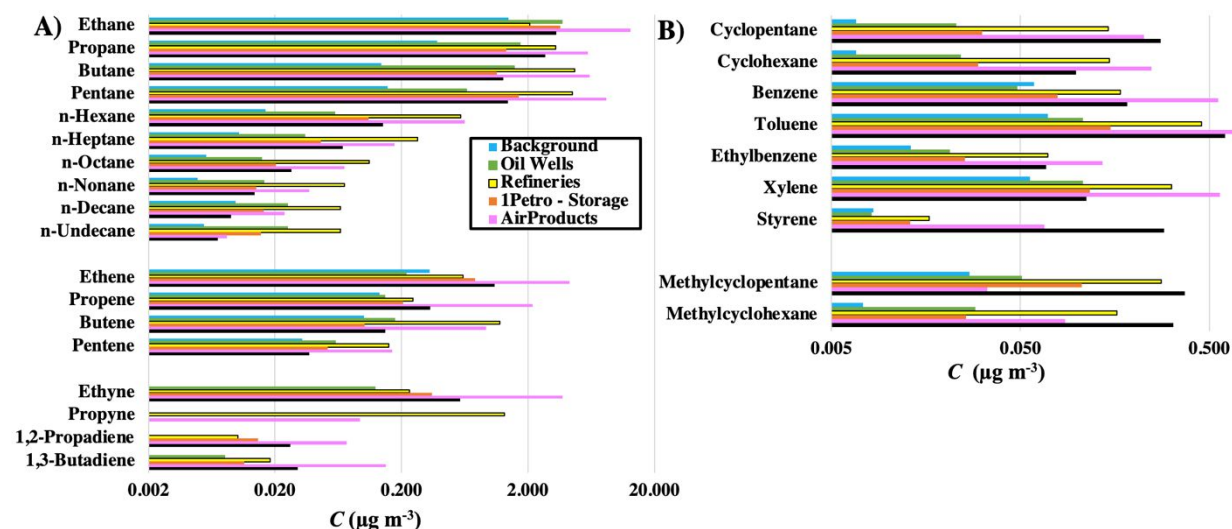


Figure S4. Summary of major port area sources' A) air sample concentrations, $\langle C \rangle$, for short-chain, saturated, and unsaturated non-methane hydrocarbons in units of microgram m^{-3} and B) selected volatile aromatic hydrocarbons. Data key on figure.

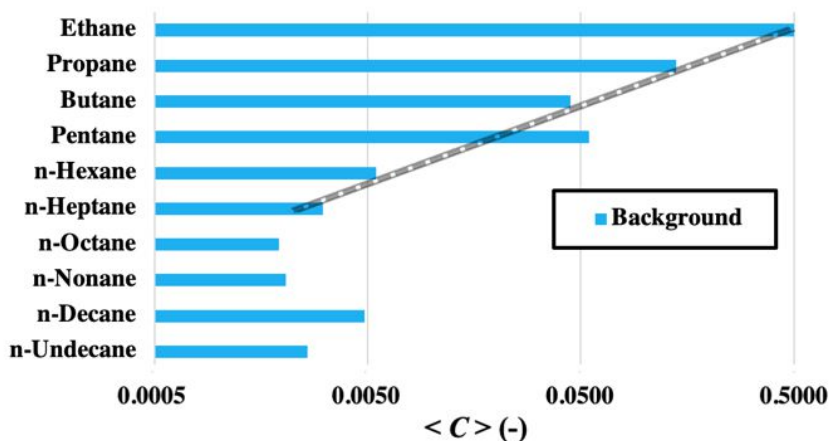


Figure S5. Port-area, normalized, background concentration profile, $\langle C \rangle$. Dashed line illustrates power law for $\text{C}_2\text{-C}_7$.

Samples for each refinery were similar; for example, see Figure S6 for the Valero refinery. Several samples were determined to be outliers; see Figure S7. Specifically, samples #5016 and #5019 were identified as outliers. Sample

#5019 is exceptionally high in toluene, xylene, ethyne, and ethene; sample #5016 was excessively high in hexane and excessively (more than one standard deviation) low in many other species. For Storage (1Petro) samples (Fig. S8), aside from pentane for sample 1309, other species for the three samples were very similar.

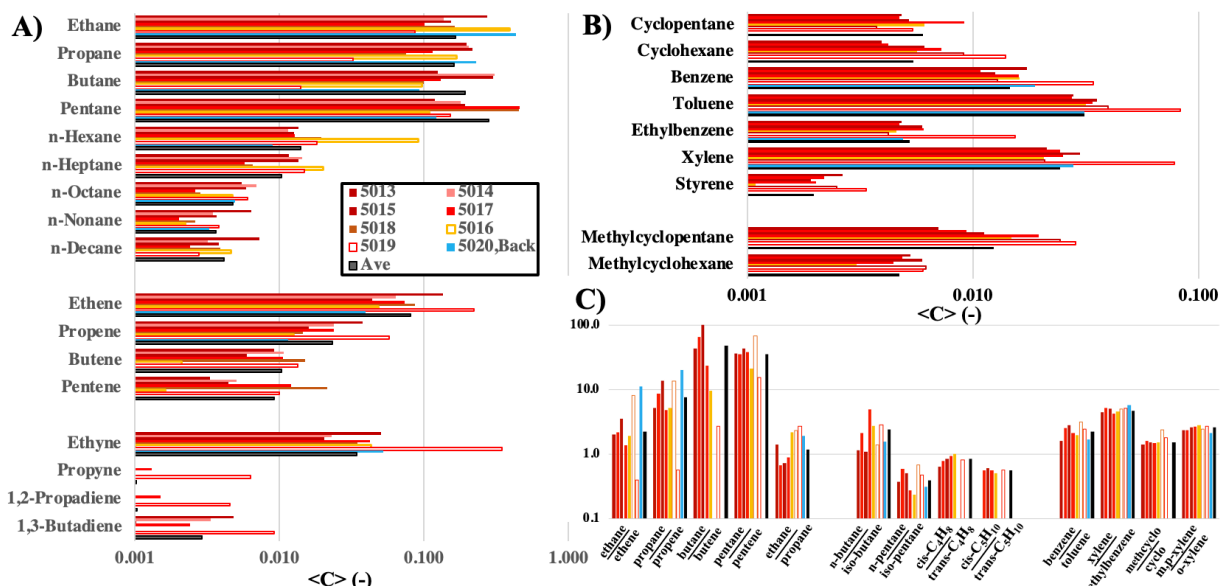


Figure S6. Valero refinery individual air samples, background, and average concentrations, $\langle C \rangle$, for A) short-chain non-methane hydrocarbons, B) selected volatile aromatic hydrocarbons, and C) ratios of alkanes/alkene, isomers of butane, C_4H_{10} , and pentane, C_5H_{12} , butene, C_4H_8 , and pentene, C_5H_{10} , and select aromatics. methylcyclo is methylcyclohexane + methylcyclopentane; cyclo is cyclohexane + cyclopentane. Legend shows sample numbers.

Valero	Ethane/ Ethene	Propane/ Propene	Butane/ Butene	Pentane/ Pentene	Ethane/ Propane		n-Butane/ i-Butane	n-Pentane/ i-Pentane	cis-Butene/ trans-Butene	cis-Pentene/ trans-Pentene		Toluene/ Benzene	Xylene/ Ethylbenzene	Methylcyclo/ Cyclo	m,p-Xylene/ o-Xylene
5013	2.01	5.20	43.5	36.1	1.39		1.14	0.37	0.63			1.61	4.41	1.40	2.34
5014	2.15	8.57	64.7	35.5	0.67		2.10	0.56	0.78	0.553		2.55	5.15	1.59	2.33
5015	3.5	13.6	99.1	43.3	0.71		1.08	0.51	0.85	0.600		2.82	5.00	1.52	2.62
5017	1.38	4.81	23.3	37.9	0.88		4.84	0.27	0.93	0.552		2.11	4.17	1.46	2.68
5018	1.89	5.15	9.60	21.2	2.19		2.69	0.23	1.00	0.500		1.96	4.52	1.52	2.80
5016	6.02	43.45	62.4	2.93			4.99	0.46				3.44	4.64	2.39	2.44
5019	0.30	0.56	2.62	15.3	2.69		2.84	0.42	0.80	0.563		2.43	5.62	4.78	2.62
5020,Back	11.0	20.0			1.89		1.53	0.31				1.65	5.67		2.09
Ave	2.19	7.47	48.0	34.8	1.17		2.369	0.393	0.837	0.551		2.209	4.651	1.496	2.554
Ave+1std	2.99	11.23	83.38	43.01	1.80		3.91	0.54	0.98	0.59		2.69	5.06	1.57	2.76
Ave-1std	1.39	3.71	12.71	26.57	0.53		0.83	0.24	0.69	0.51		1.73	4.24	1.43	2.35

Valero	Ethane	Propane	Butane	Pentane	n-Hexane	n-Heptane	n-Octane	n-Nonane	n-Decane
5013	0.273	0.197	0.124	0.119	0.014	0.012	0.0055	0.0064	0.0073
5014	0.137	0.204	0.309	0.179	0.012	0.014	0.0070	0.0035	0.0032
5015	0.154	0.217	0.303	0.193	0.013	0.014	0.0059	0.0037	0.0038
5017	0.102	0.115	0.131	0.459	0.013	0.006	0.0026	0.0020	0.0024
5018	0.164	0.075	0.100	0.452	0.020	0.007	0.0028	0.0026	0.0039
5016	0.383	0.183	0.062	0.109	0.041	0.020	0.0022	0.0022	0.0046
5019	0.082	0.032	0.054	0.453	0.018	0.015	0.0038	0.0038	0.0028
5020,Back	0.434	0.230	0.094	0.122	0.009		0.0049	0.0033	
Ave	0.166	0.162	0.194	0.280	0.014	0.010	0.0048	0.0036	0.0041
Ave+1std	0.23	0.22	0.30	0.44	0.017	0.014	0.0067	0.0053	0.0060
Ave-1std	0.10	0.10	0.090	0.12	0.011	0.0064	0.0028	0.0020	0.0023

Ethene	Propene	Butene	Pentene	Ethyne	Propyne	1,2-Propadiene	1,3-Butadiene
0.136	0.038	0.0092	0.0033	0.050			0.0048
0.064	0.024	0.0107	0.0051	0.023	0.00088	0.00083	0.0034
0.044	0.016	0.0060	0.0045	0.021	0.00089	0.00076	0.0010
0.074	0.024	0.0106	0.0121	0.042	0.0013	0.0015	0.0024
0.087	0.015	0.0150	0.0214	0.035			
0.049	0.013	0.0024	0.0016	0.043			
0.221	0.058	0.0133	0.0100	0.342	0.0063	0.0045	0.0092
0.039	0.011			0.053			
0.081	0.023	0.010	0.0093	0.6342	0.0010	0.0010	0.0029
0.12	0.03	0.014	0.017	0.047	0.0013	0.0014	0.0045
0.05	0.01	0.0070	0.0017	0.022	0.0008	0.0006	0.0013

i-Butane	n-Butane	i-Pentane	n-Pentane	1-Butene	i-Butene	trans-2-Butene	cis-2-Butene	1-Pentene	trans-2-Pentene	cis-2-Pentene
0.058	0.068	0.087	0.032	0.0064		0.0018	0.0011	0.0022	0.0011	
0.100	0.209	0.114	0.066	0.0059		0.0027	0.0021	0.0022	0.0018	0.0010
0.146	0.157	0.128	0.065	0.0029		0.0017	0.0014	0.0014	0.0019	0.0011
0.022	0.109	0.360	0.098	0.0049		0.0029	0.0027	0.0030	0.0058	0.0032
0.027	0.085		0.085	0.0046		0.0052	0.0052	0.0050	0.0109	0.0054
0.044	0.056	0.065	0.044	0.0021				0.0002	0.0006	
0.004	0.010	0.104	0.049	0.0081		0.0029	0.0023	0.0026	0.0042	0.0026
0.037	0.057	0.093	0.029	0.0041				0.0025		
0.0707	0.1229	0.2111	0.0694	0.0049		0.0028	0.0025	0.0028	0.0043	0.0027
0.12	0.18	0.35	0.0943	0.0063		0.0043	0.0042	0.0041	0.0084	0.0048
0.02	0.06	0.07	0.0444	0.0036		0.0014	0.0009	0.0014	0.0002	0.0006

Valero	Cyclopentane	Cyclohexane	Benzene	Toluene	Ethylbenzene	Xylene	Styrene
5013	0.0048	0.0040	0.017	0.028	0.0048	0.0213	0.0026
5014	0.0047	0.0042	0.011	0.028	0.0047	0.0243	0.0022
5015	0.0052	0.0061	0.013	0.036	0.0060	0.0299	0.0019
5017	0.0092	0.0073	0.016	0.034	0.0061	0.0252	0.0020
5018	0.0061	0.0057	0.016	0.032	0.0046	0.0207	0.0011
5016	0.0037	0.0091	0.013	0.040	0.0042	0.0208	0.0025
5019	0.0054	0.0139	0.034	0.083	0.0154	0.0780	0.0034
5020			0.019	0.031	0.0049	0.0279	
Ave	0.0060	0.0054	0.0146	0.0313	0.0052	0.0243	0.0020
	0.0079	0.0068	0.0173	0.0348	0.0060	0.0281	0.0025
	0.0042	0.0041	0.0118	0.0277	0.0045	0.0205	0.0014

Methylcyclopentane	Methylcyclohexane	m/p-Xylene	o-Xylene
0.0070	0.0053	0.015	0.0064
0.0093	0.0049	0.017	0.0073
0.011	0.0060	0.022	0.0083
0.020	0.0044	0.018	0.0069
0.015	0.0031	0.015	0.0054
0.024	0.0062	0.015	0.0064
0.028	0.0060	0.052	0.021
		0.019	0.0090
0.0124	0.0047	0.0174	0.0069
0.0173	0.0058	0.0202	0.0079
0.0075	0.0036	0.0147	0.0058

Figure S7. Valero refinery individual air samples, background, and average concentrations for short-chain non-methane hydrocarbons and selected volatile aromatic hydrocarbons, and one standard deviation above and below the average. Yellow are outliers. Green are first-pass outliers that became non-outliers once outliers were removed from the averages.

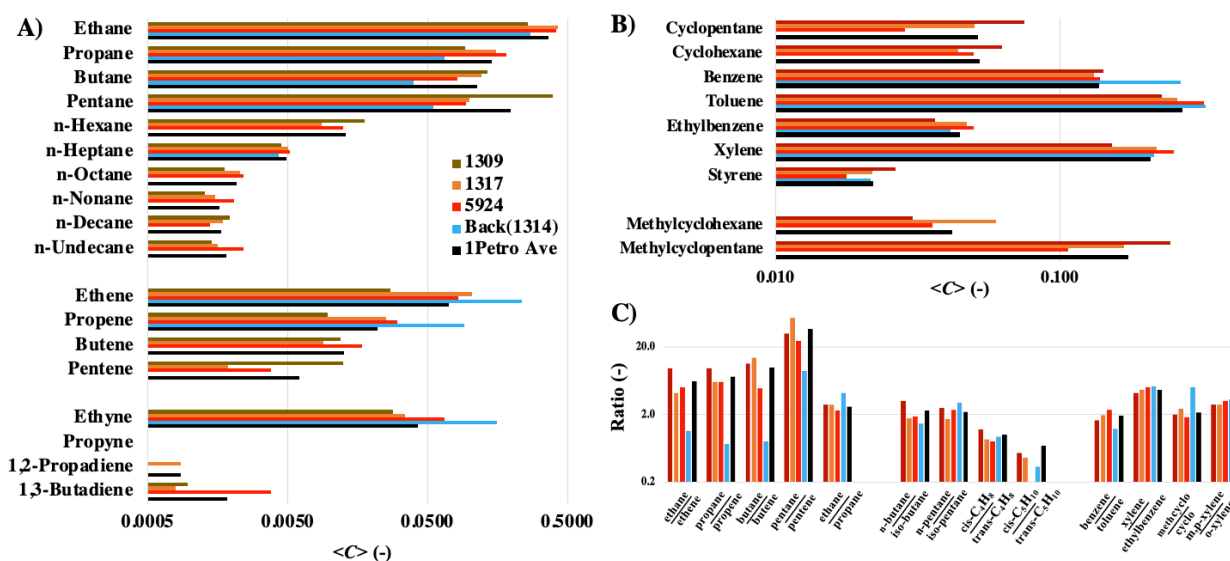


Figure S8. 1Petro (Storage) individual air samples, background, and average concentrations, $<C>$, for A) short-chain non-methane hydrocarbons, B) selected volatile aromatic hydrocarbons, C) Selected gas ratios. Sample #1314 is background. See Fig. S6 caption for data key. Legend shows sample numbers.

Storage light alkanes generally decreased C_2 - C_5 , dropped to C_6 , and were relatively constant for larger alkanes except for sample #5924, which increased for C_{11} but not for the other samples. Sample #1309 did not decrease with n for alkenes, whereas the other two samples decreased, as did the average. Ethyne was comparable to ethene, but propyne was not detected. Storage light alkanes generally decreased C_2 - C_5 except for sample #1309, which had significantly enhanced pentane; however, other trace gas values were similar. Also similar were the ratios. Thus, sample #1309 was not classified as an outlier. Sample #5924 showed cyclohexane was higher than cyclopentane, but decreased for the other two samples. The average showed that these were equal, but this decrease is similar to Port Industry. Only two Wastewater samples were collected, with one having extremely high methylcyclohexane (far higher than toluene), significantly higher than *all* other samples, but no xylene was detected. Hexane and heptane also were elevated in this sample compared to the other sample; however, the light alkanes were very similar, as were the alkenes C_2 - C_4 . One interpretation is that solvent use was captured in one sample; however, it's unknown if this is typical.

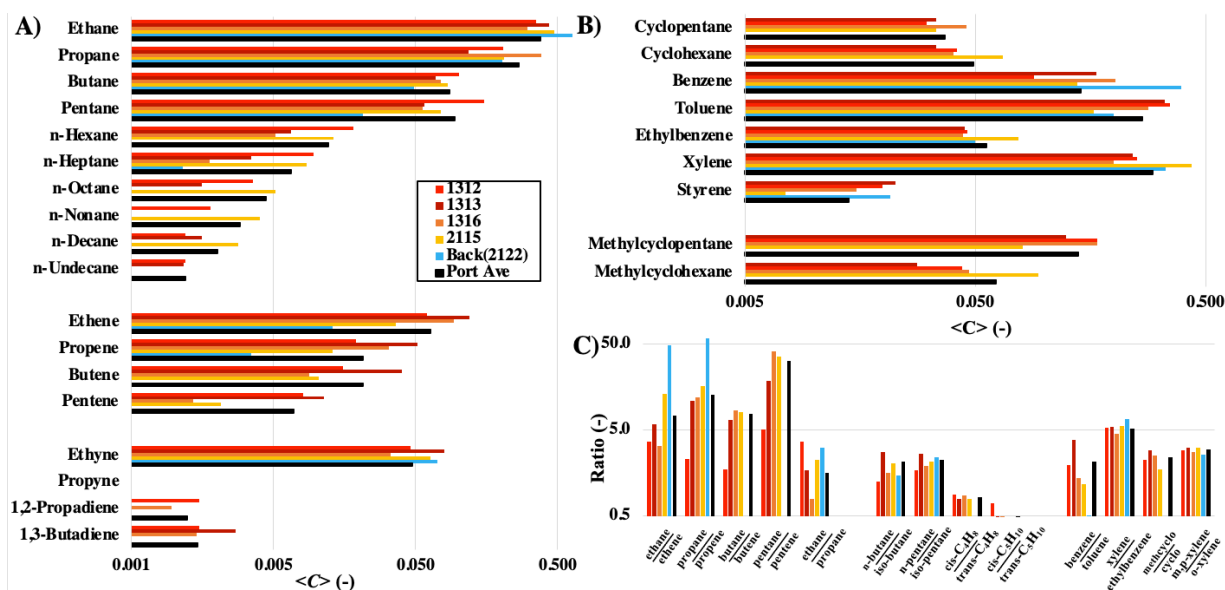


Figure S9. Port's proper individual air samples, background, and average concentrations, $\langle C \rangle$, for A) short-chain non-methane hydrocarbons, B) selected volatile aromatic hydrocarbons, and C) selected gas ratios. Sample 2122 is background. See Figure S6 caption for data key. Legend includes sample canister numbers.

The composition profiles for the Ports' samples generally were highly similar, with some small exceptions (Fig. S9). Sample 1316 featured higher propane than ethane, whereas ethane was higher than propane for the other Ports' samples – perhaps from forklifts. Sample #1312 was enhanced in pentane. Sample #2115 decreased as a relatively weak power law from hexane to decane, whereas the other sample dropped more precipitously from pentane or heptane. Alkenes decreased with increasing n . Toluene was the strongest aromatic hydrocarbon, except for sample #2115, which was stronger than xylene. Sample #2115 also had higher methylcyclohexane than methylcyclopentane; other samples were the reverse. Higher methylcyclohexane than methylcyclopentane was found for Oil Wells and Refineries.

Only two Calciner samples were collected, and were remarkably similar except for cyclopentane, methylcyclohexane, and methylcyclopentane (Fig. S10). As the ratio between the two samples was reversed between cyclopentane and the methylated versions, this could be a case where a process was methylating pentane and hexane, resulting in temporally varying composition.

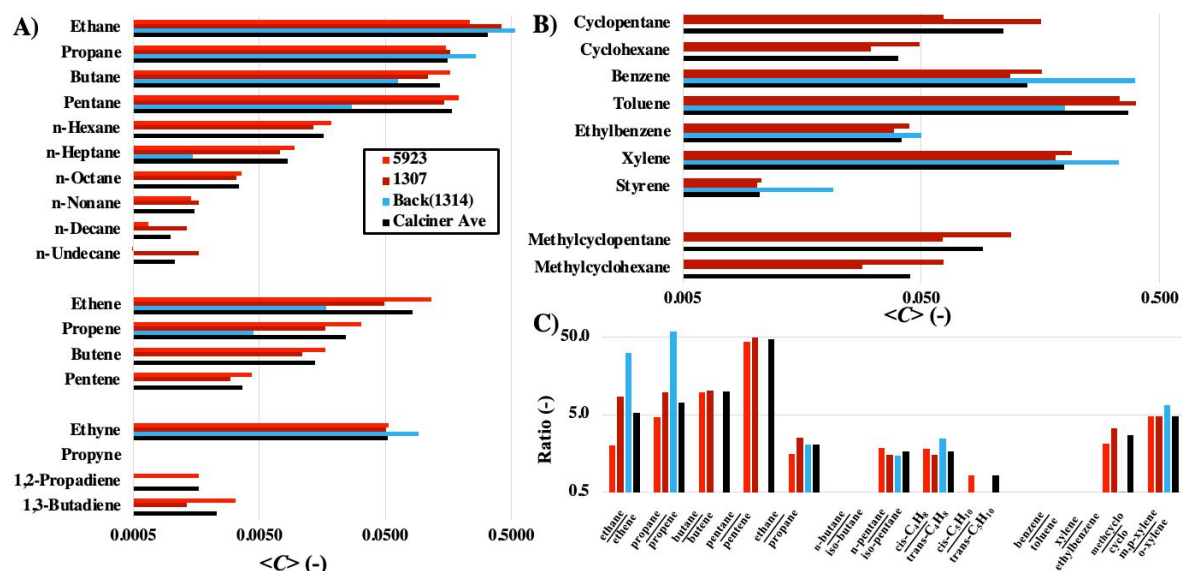


Figure S10. Calciner individual air samples, background, and average concentrations, $\langle C \rangle$, for A) short-chain non-methane hydrocarbons, B) selected volatile aromatic hydrocarbons, and C) selected gas ratios. Sample 1314 is the relevant background. See Fig. S6 caption for data key. Legend includes sample canister numbers.

Overall variability between the Air Products samples was large, making outlier identification difficult (Fig. S11). Still, sample #2108 had too many trace gas concentrations as outliers. There was good agreement between samples for C_2 - C_5 ; however, larger alkanes showed greater variability. Still, most samples smoothly decreased from pentane to decane, i.e., there was no sharp falloff between C_5 and C_6 , as seen for most other sources. High variability also is evident in the alkenes, with all samples decreasing with n , albeit with different concentrations and rates of decrease with n .

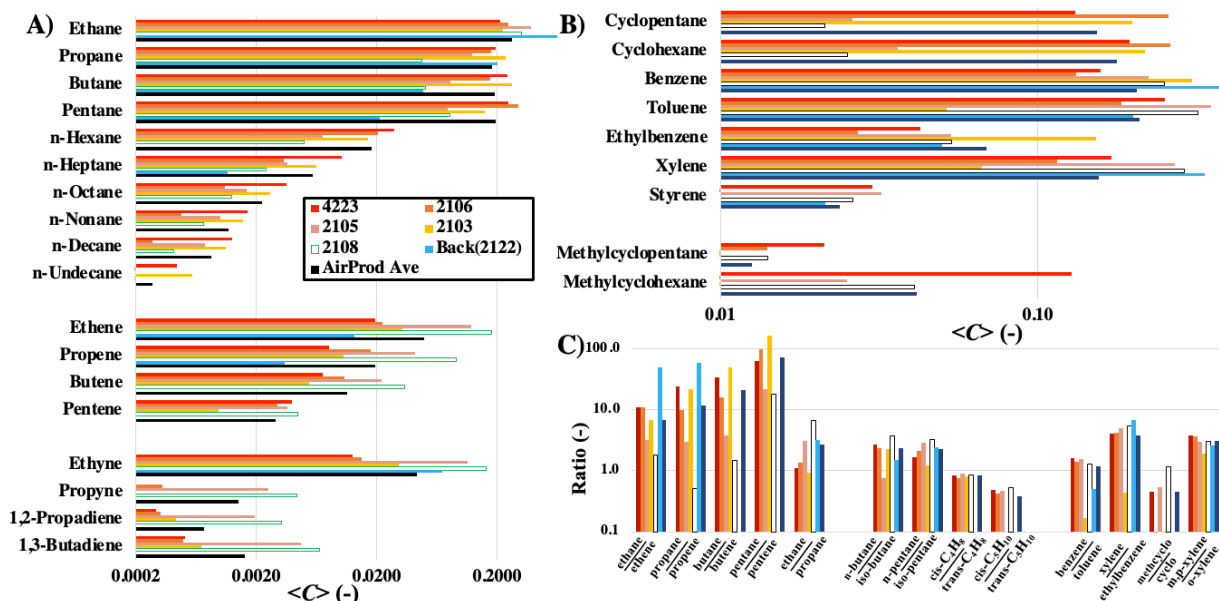


Figure S11. Air Products individual air samples, background, and average concentrations, $\langle C \rangle$, for A) short-chain non-methane hydrocarbons, B) selected volatile aromatic hydrocarbons, C) selected gas ratios. Hollow bars are outliers (sample #2108). Sample #2122 is background. See Figure S6 caption for data key. Legend shows sample number.

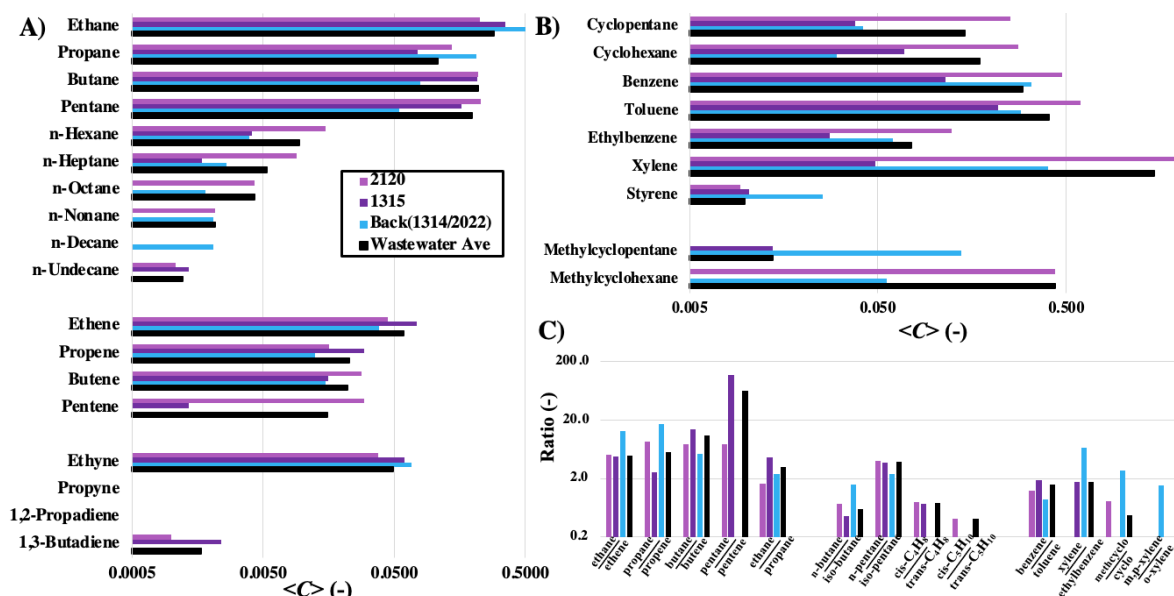


Figure S13. Wastewater treatment individual air samples, background, and average concentrations, $\langle C \rangle$, for A) short-chain non-methane hydrocarbons, B) selected volatile aromatic hydrocarbons, C) selected gas ratios. Background was the average of samples #1314 and #2022. See Figure S6 caption for data key. Legend shows sample number.

Only two Wastewater samples were collected, with one having extremely high methylcyclohexane (far higher than toluene), much higher than *all* other samples from other sources. Additionally, xylene was extremely high, ~3 ppb (Fig. S13). Given the small number of samples, it was not possible to determine which was anomalous, although the background sample concentrations are more elevated in trace gases like methylcyclopentane and xylene than the Wastewater samples. In part, this is due to the normalization of the background sample, but it also suggests heterogeneity in the background (as well as the source), indicating that the single sample poorly characterizes the background. The same sample with elevated methylcyclohexane also had elevated hexane and heptane compared to the other Wastewater sample; however, the light alkanes were very similar between the two samples. There also was good agreement between ethene and butene for the two samples. It's likely that the sample captured solvent use; however, it is unknown if this is typical.

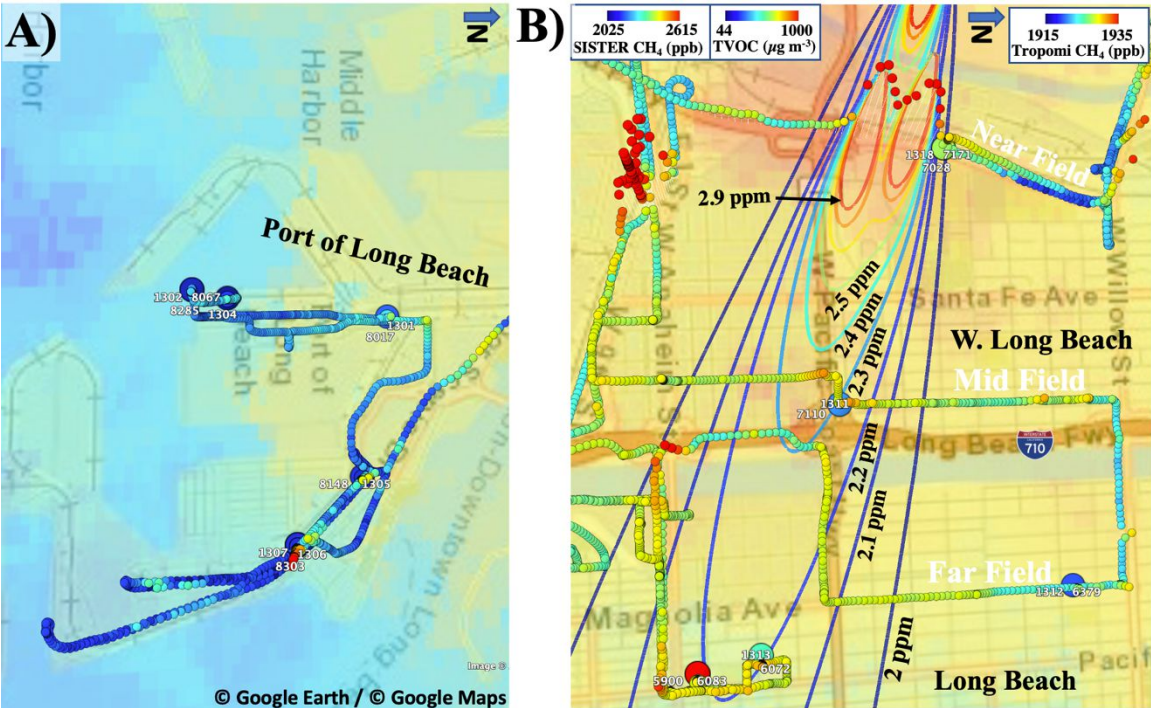
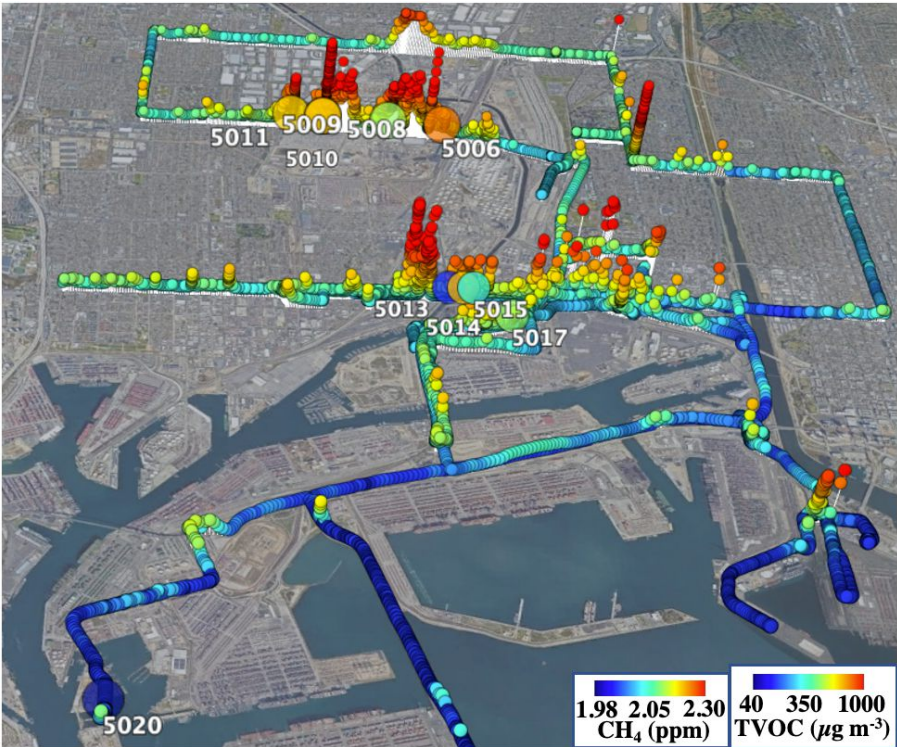


Figure S14. A) Port of Long Beach and B) West Long Beach *in situ* methane, CH₄, and wind speed, *u*, TROPOMI satellite, mean, distance-weighted CH₄, for super-sampling settings: easting and northing grid resolutions, 0.0005°, 0.0002°, respectively, averaging length, 0.016°, cutoff distance, 0.040°, and eccentricity, 1.25. Canister samples shown as big colored circles at collection location. Circle color indicates total volatile organic compounds (TVOC, all organic gases larger than ethane) as in the data key with sample number labeled. Also shown is the Gaussian plume model for CH₄.

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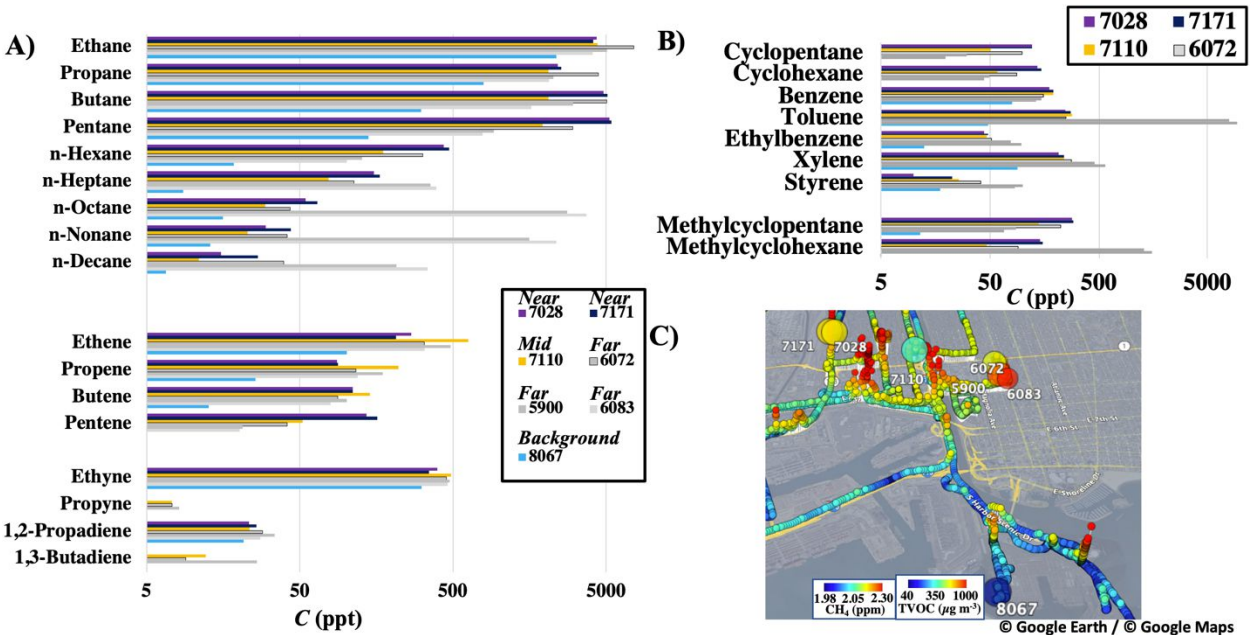
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Figure S15. Sample canister locations and total volatile organic carbon (TVOC, defined as hydrocarbons larger than ethane) and *in situ* methane, CH₄, collected 29 July 2023. Large bubbles are for air samples, sample number labeled, with color showing TVOC. Data key on figure.

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Figure S16. Concentration, C , for selected chain, saturated and unsaturated non-methane hydrocarbons in samples for A) the Long Beach plume and background, and B) for selected aromatic hydrocarbons. C) Location of sample canisters. The color shows sample total volatile organic carbon, TVOC. Also shown is *in situ* methane, CH_4 , acquired 29 July 2023. Data key on panels. Legend shows sample number.

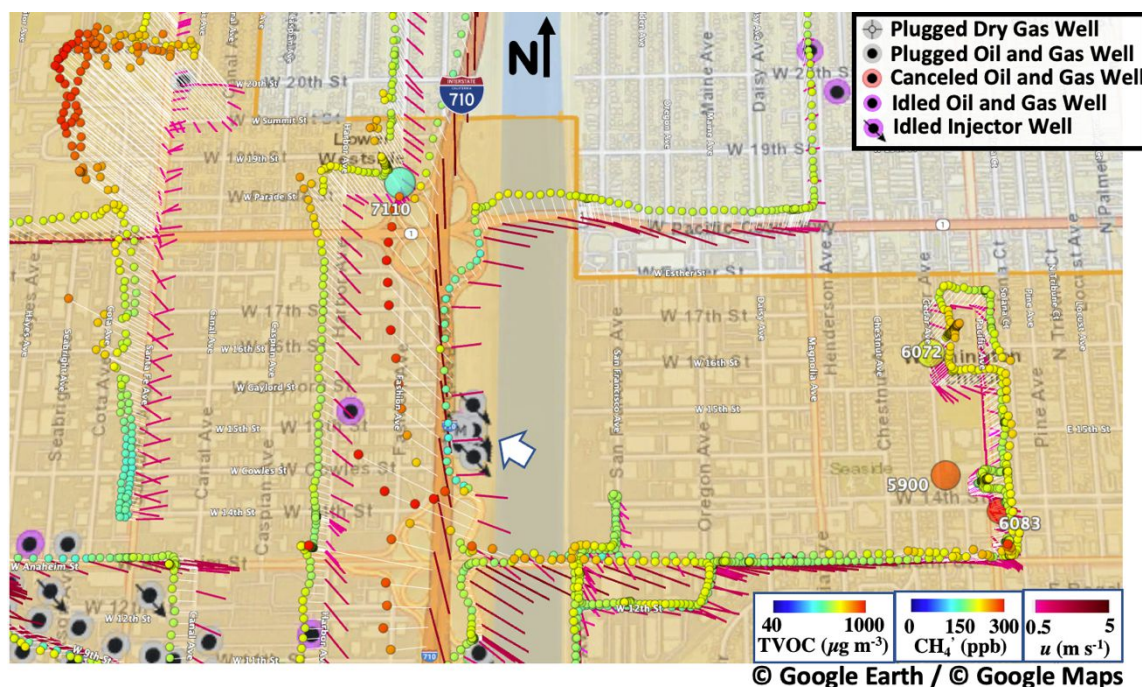


Figure S17. A) Methane, CH_4 , winds, sample locations, and well map (white arrow shows cluster referenced in the text), collection date 8 Mar. 2023. The large color balls show sample total volatile organic compounds, TVOC. Data keys on figure. Sample numbers labeled. Legend shows sample number.

S5. Google Earth Archive

The Google Earth archive, “PortsEmit_Pt3_VOC(10Jan2026).kmz,” contains the data and satellite product presented in this manuscript, version 7 January 2026. Specifically, the archive (Fig. S18) includes the locations of all major industrial sites in the ports and nearby areas and the locations of the six port air quality stations. The archive includes the airborne remote sensing detections (Fig. 2), air sample canister TVOC and location (Fig. 3) used in the analysis, and Long Beach plume *in situ* data (Supp. Fig. S15). The TROPOMI satellite super-sampled data product also is included (Fig. 9).

The Google Earth archive uses where appropriate, time information, which allows the time slider to constrain the visualization to specific surveys.

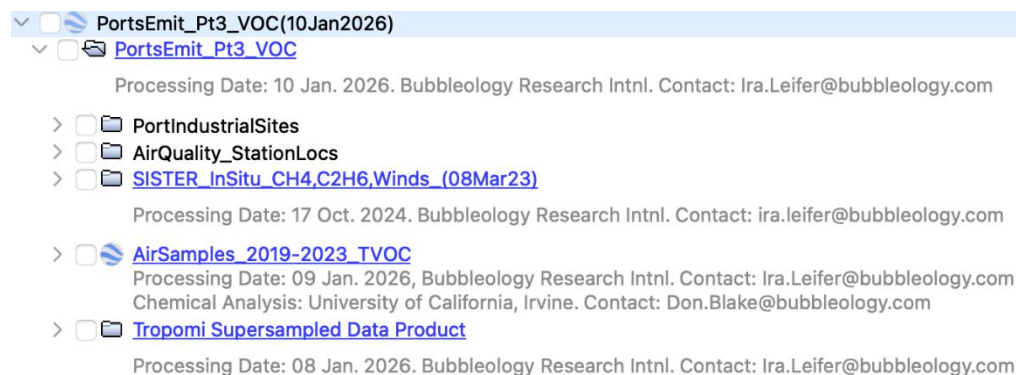


Figure S18. Google Earth archive's Places Panel of main directories of the data used in this study.

The Mako data (Fig. 2) in the archive (Supp. Fig. S19) are labeled by the acquisition date (year – YY, Month – MM, and day – DD), and shows the specific trace gases and their source locations identified.



Figure S19. Google Earth Archive Places Pane of Mako directory.

The *in situ* winds, CH₄, CH₄', and C₂H₆, data are presented in directories for each survey data (year-YYYY, month-MM, day – DD) for each level 1 data product data (Supp. Fig. S20).

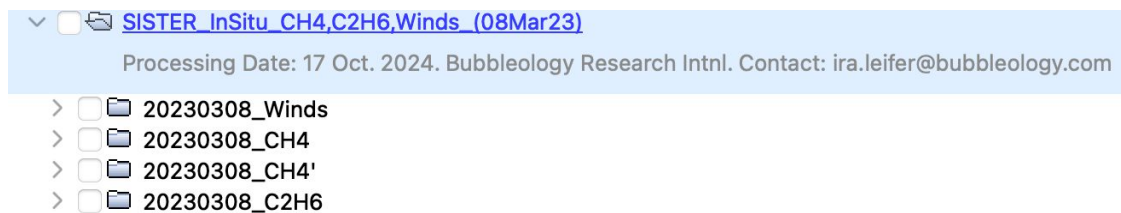


Figure S20. Google Earth archive's Places Pane of *in situ* data directory.



Figure S21. Google Earth archive's Places Pane of air samples and total VOC.

The super-sampled TROPOMI satellite products used in this study were named according to the convention of the Platform (TROPOMI), satellite product (CH₄), region (SCal- Southern California, LA-Los Angeles), longitude, and latitude gridding resolutions, averaging length scale, distance cutoff, and eccentricity, followed by the read (ingestion), gridding, plotting algorithm versions: read version, rv, grid version, gv, plotting version, pv, respectively, and the plotting date. Color scale limits are specified in the note for each data product: The directory for the super sampling shows the gridding latitude and longitude limits and contact information.

The specific data product used was the median. The satellite gridding directory includes the color bar limits used in **Figure 9** and **Figure S14**. Version number is for the google earth algorithms.

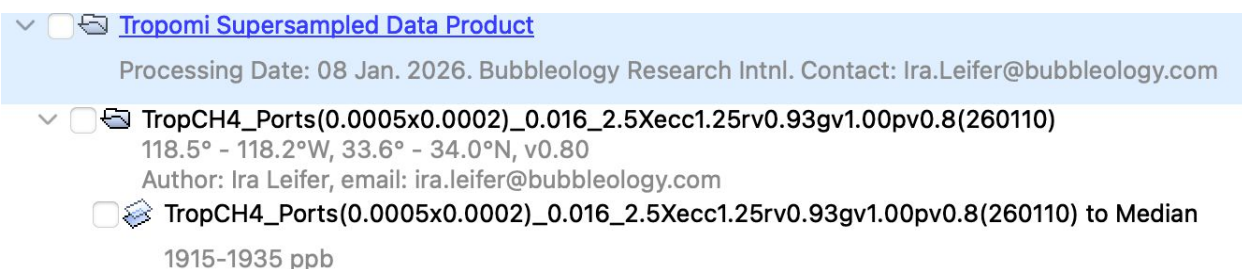


Figure S22. Google Earth Archive Places Pane of TROPOMI satellite super-sampled gridding products and notes.

S6. In situ data archive

The *in situ* data are provided in the file, “SIS_20190711_202601231407_L1_v0.9.zip” as separate ASCII files for each survey date (Fig. S23). Each survey presents the data as Time in UTC, longitude and latitude in degrees, WGS84, altitude in meters, and dry methane, CH₄, in ppm, carbon dioxide, CO₂, in ppm, and water vapor, H₂O, in ppm, followed by meteorology data, temperature in degrees centigrade, wind components northing speed, Wind_u, and easting speed, Wind_v, in meters per second.

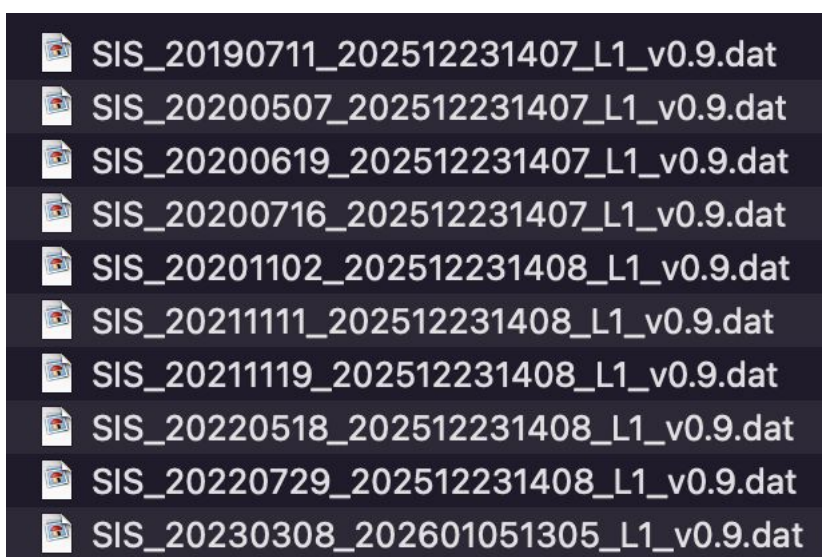


Figure S23. In situ data archives.

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