HEI Energy Franklin Research Report

Assessing Source Contributions to Air Quality and Noise in Unconventional Oil Shale Plays

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Supplementary Appendices A–C

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Although this report was produced with partial funding by the United States Environmental Protection Agency under Contract No. 68HERC19D0010 to the Health Effects Institute, it has not been subjected to the Agency's peer and administrative review and may not reflect the views of the Agency; thus, no official endorsement by the Agency should be inferred. This report also has not been reviewed by private party institutions, including those that support HEI Energy, and may not reflect the views or policies of these parties; thus, no endorsement by them should be inferred.

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Appendix A: Additional Details on Aim 1, Stationary Sampling at Loving, New Mexico

Details of Instrumentation and Sampling Methods

Air Pollutants and Greenhouse Gases

Carbon Dioxide CO_2 was measured with a Picarro G-2301 ring-down spectrometer in air that was sampled from an inlet at 6.1 m height. The sampling line consisted of 11 m length, ¼ inch o.d., 5/32 inch i.d. PFA tubing, equipped with an inlet PFA filter holder that houses a 5 micron Teflon membrane filter. Membrane filters were replaced every 2–4 weeks. The sampling line was shared with the O3 monitor. The Picarro factory-provided calibration variables are used. Side-by-side comparison of our other Picarro analyzers has shown <0.1% deviation between analyzers. Automated calibration checks are run every 49 hours with a breathing air grade ambient air gas mixture from a compressed tank with CO_2 cross-referenced against the NOAA Global Atmospheric Monitoring Laboratory (GML) CO_2 scale; estimated accuracy error of < 3 ppm. Instrument calibration and drift correction were made after the fact, using automated calibration checks. Data from these calibration runs are flagged and do not show up in the air sample data. The readings are plotted in a separate analysis over time to trace the long-term instrument response. Every 6 months, a 10-point linearity check was performed using a Thermo Scientific 146i Multi-gas Calibrator to dilute a 4.9% standard (EPA protocol grade gas, Linde Gas & Equipment Inc.) with Ultra Zero Air grade gas (0, 150, 200, 250, 500, 750, 1000, 1400, 1800, 3000 ppm).

Methane CH_4 was monitored with a Picarro G-2301 cavity ring-down spectrometer in air that was sampled from an inlet at 6.1 m height. The sampling line consisted of 11 m length, ¼ inch o.d., 5/32 inch i.d. PFA tubing, equipped with an inlet PFA filter holder that houses a 5 micron Teflon membrane filter. Membrane filters were replaced every 2–4 weeks. The sampling line was shared with the O3 monitor. The Picarro factory-provided calibration variables were used. Side-by-side comparison of our other Picarro analyzers has shown <0.1% deviation between the two analyzers. A similarly low deviation has been found in the comparison with gas chromatography methane data (Boulder Reservoir station). Automated calibration checks were run every 49 hours with a breathing air grade ambient air gas mixture from a compressed tank with CH4 cross-referenced against the NOAA Global Atmospheric Monitoring Laboratory (GML) CH4 scale; estimated accuracy error of < 2 ppb. Instrument calibration and drift correction were made after the fact, using the automated calibration checks data. Data from the calibration runs were flagged and do not show up in the air sample data. The readings are plotted in a separate analysis over time to trace the long-term instrument response. Every 6 months, a 10-point linearity check was performed using a Thermo Scientific 146i Multi-gas Calibrator to dilute a 497 ppm standard (EPA protocol grade gas, Linde Gas & Equipment Inc.) with Ultra Zero Air grade gas (0, 1.5, 2, 2.5, 5, 7.5, 10, 14, 18, 30 ppm).

Carbon Monoxide CO was measured with a Thermo Scientific model 48CTL. Air was sampled from an inlet at 6 m height. Sampling line is 10 m length, ¼ inch o.d., 1/8 inch i.d. PFA tubing with PFA filter holder with 5 micron Teflon membrane filter. Filters were replaced every 2–4 weeks. The instrument was zeroed every 6 hours for a 10-minute period using its internal zeroing catalyst. Span checks were done using a 2.5 ppm CO primary standard (EPA protocol grade gas, Linde Gas & Equipment Inc.) every 2–4 weeks. The output of the span gas was introduced through the span valve of the instrument. Every 6 months, a 7-level linearity check was performed (0, 500, 1000, 1500, 2000, 2500, 3000 ppb).

Ozone O_3 was measured with a Thermo Environmental Model 49C UV absorption ozone monitor and Thermo Environmental Model 49C PS ozone calibrator. The monitoring and calibration protocol followed the federal regulatory monitoring requirements according to the specifications of '40 Code of Federal Regulations (CFR) Part

58’. The calibration scale was referenced against the EPA Region 8 primary ozone reference standard. Air was sampled from an inlet at approximately 6 m height. The ozone monitor and calibrator were calibrated before field deployment against an EPA-certified Level 2 standard. The calibrator was co-located with the ozone monitor. Each night, the ozone monitor collected both a zero and an 80-ppb span check sample from the ozone calibrator for checking the instrument response. Two hours later, a 50-ppb span check was also performed. Those measurements are flagged and do not show up in the data records. If the instrument failed a zero check (> 1ppb) or a span check (more than 3% deviation around span value), a manual check was performed, and a recalibration was performed if the deviation was confirmed. Every 3 months, a full range linearity check was done at 0, 25, 50, 100, 200, and 400 ppb.

Nitrogen Oxides Nitric oxide (NO) and nitrogen dioxide (NO_2) were analyzed with a commercial Teledyne T200UP analyzer equipped with a photolytic NO_2 converter in air that was pulled at 1100 cc/min from an inlet mounted at 6.1 m height above the surface. The sampling line consisted of 11 m length, ¼ inch o.d., 1/8 inch i.d. PFA tubing equipped with an inlet PFA filter holder that housed a 5 micron Teflon membrane filter. Membrane filters are replaced every 2–4 weeks. The instrument has two operational modes. First NO is measured via NO + O_3 chemiluminescence. In the second mode, NO_2 is measured by redirecting air through the photolytic converter, which selectively causes NO_2 to convert to NO. The measured NO signal in this mode constitutes the sum of NO and NO_2. The NO_2 mixing ratio is then determined by subtracting from the signal the NO result measured in the first measurement mode. Calibrations were performed by dynamic dilution and titration of a 10 ppm NO primary standard (EPA protocol grade gas, Linde Gas & Equipment Inc.) with a Teledyne T700UP Multi-gas Calibrator with Gas Phase Titration system (GPT). An 8-point calibration and linearity test was performed quarterly (0, 25, 50, 75, 100, 200, 300, 450 ppb). Conversion efficiency was tested at 2 levels using the GPT: 350 and 25 ppb NO_2. A linearity check for NO_2 is performed quarterly at 5 levels (25, 50, 80, 200, 350 ppb). A zero and a span check at a level of 180 ppb were run every 3 days. The NO-NO_2 conversion efficiency was tested every 2 weeks with the T700UP as well. If the instrument failed a zero check (> 0.2 ppb) or a span check (more than 5% deviation around the span value), a manual check was performed, and a recalibration was done if the deviation was confirmed. The instrument manufacturer states a 0.05 ppbv detection limit for the analyzer. Any readings below that threshold were replaced in the data record by ½ this value, i.e., with 0.025 ppbv, both for NO and for NO_x.

Hydrogen Sulfide (H2S) was analyzed by gas-phase ultraviolet fluorescence with a Teledyne T101 analyzer in air that was pulled at 615 cc/min from an inlet mounted at 6.1 m height above the surface. The sampling line consisted of 11 m length, ¼ inch o.d., 1/8 inch i.d. PFA tubing equipped with an inlet PFA filter holder that housed a 5 micron Teflon membrane filter. Membrane filters are replaced every 2–4 weeks. Calibrations were performed by dynamic dilution of a 5.36 parts per million (ppm) H2S primary EPA-grade standard (EPA protocol grade gas, Linde Gas & Equipment, certification date 09/26/2022), using a Teledyne T700UP Multi-gas Calibrator. Zero air was generated by running compressed air through a catalyst (platinum on alumina pellets) at 380 °C and then through Sofnofil and Charcoal scrubbers. Every 3 days, calibration checks were performed for zero and a single span value of 200 ppb H2S using the same calibrator connected to the span port of the analyzer, with the zero air sourced via the calibrator into the span port of the analyzer. Quarterly, full calibrations of the H2S analyzer were performed using the output of the calibrator to introduce span gas to the span port of the instrument and zero air through the zero air port of the analyzer. For these calibrations, a zero adjustment was made first, followed by H2S span adjustments using 200 ppb H2S. Every 6 months, a 5-level linearity check was performed (0, 25, 50, 75, 100, 200 ppb). The lower detection limit reported by the manufacturer is 0.4 ppb. Measurements below this value are reported as ½ of the LDL, 0.2 ppb. The ½LDL correction is applied to the original 1-minute data, not to any further averaged data (e.g., 5-minute or hourly).

Sulfur dioxide SO_2 was analyzed by gas-phase ultraviolet fluorescence with the same Teledyne T101 analyzer. Ambient air was pulled at 615 scc/min from an inlet mounted at 6.1 m height above the surface. The sampling line consisted of 11 m length, ¼ inch o.d., 1/8 inch i.d. PFA tubing equipped with an inlet PFA filter holder that housed a 5 micron Teflon membrane filter. Membrane filters are replaced every 2–4 weeks. The monitoring and calibration protocol follows the federal regulatory monitoring requirements according to the specifications of ‘40

Code of Federal Regulations (CFR) Part 58’. Calibrations were performed by dynamic dilution of a 5.08 parts per million (ppm) SO_2 primary EPA-grade standard (EPA protocol grade gas, Linde Gas & Equipment, certification date 08/31/2022), using a Teledyne T700UP Multi-gas Calibrator. Zero air was generated by running compressed air through a catalyst (platinum on alumina pellets) at 380 °C and then through Sofnofil and Charcoal scrubbers. Every 3 days, calibration checks were performed for zero and a single span value of 200 ppb SO_2 using the same calibrator connected to the span port of the analyzer, with the zero air sourced via the calibrator into the span port of the analyzer. Quarterly, full calibrations of the SO_2 analyzer were performed using the output of the calibrator to introduce span gas to the span port of the instrument and zero air through the zero air port of the analyzer. For these calibrations, a zero adjustment was made first, followed by span adjustments using 200 ppb SO_2. Every 6 months, a 5-level linearity check was performed (0, 25, 50, 75, 100, 200 ppb). The lower detection limit reported by the manufacturer is 0.4 ppb. Measurements below this value are reported as ½ of the 5 LDL, 0.2 ppb. The ½LDL correction is applied to the original 1-minute data, not to any further averaged data (e.g., 5-minute or hourly).

Volatile Organic Compounds VOCs were monitored with a custom-made preconcentration system interfaced to an Agilent 6890 gas chromatograph (GC) using a flame ionization detector (FID). Sample air was pulled from an inlet at 6.1 m above the surface on the meteorological tower at a purge rate of 1.5 L/min. The sampling line consisted of 13 m length, ¼ inch o.d., 5/32 inch i.d. PFA tubing, equipped with an inlet PFA filter holder that housed a 5 micron Teflon membrane filter, which was replaced every 2–4 weeks. The sampling line was inside a conduit heated to 40 °C. Hourly, VOCs were extracted over a 10-minute time window at 40 scc/min. Carrier gas was H2 from a Parker H2PEM-160 hydrogen generator or a tank of UHP H2 (Airgas). To preconcentrate VOCs, sample air was directed through a Peltier-cooled water freezeout trap that is held at -45°C. The dried air then flows through an ozone scrubber that contains sodium-thiosulfate-impregnated glass wool, replaced annually. VOCs were then extracted from the downstream air flow on a micro-adsorbent trap (Carboxen 1000 and Carboxen 1016) held at -40°C. VOCs were transferred by rapid heating of the micro-adsorbent trap to 290 °C and purged onto an alumina PLOT GC column (Al2O3/KCl PLOT, 50 m, 0.53 mm i.d., 15 µm film thickness). After temperature-programmed separation, compound identification and quantification were accomplished with the FID using PeakSimple software (SRI Instruments, version 4.94). Within PeakSimple, specifically programmed peak integration was done automatically following each run. The tabulated peak area results were processed by automated scripts using monthly updated calibration carbon response factors (CRF) and effective carbon numbers (ECN) to calculate mixing ratios, which were reported in real time on the program website. Approximately twenty VOCs were traced and quantified routinely. Data represent the 10-minute mean VOC mole fractions over the 10-minute sample collection period, with the recorded time stamp at the middle of that sampling period. A subset of selected VOC tracers (ethane, propane, butane, pentane, hexane, heptane, octane, benzene, toluene, acetylene, ethene, propene, isoprene, cyclopentane, ethyl-benzene, m&p-, o-xylene) were plotted on the web portal (https://www.bouldair.com/loving.htm). The calibration scale was tied to the World Meteorological Organization (WMO) Global Atmospheric Watch (GAW) VOCs scale, using a certified multicomponent 4-ppb primary standard acquired from the U.K. National Physics Laboratory (NPL, calibration date 2/13/2020) – the central calibration laboratory for VOCs recommended by WMO-GAW program. The calibration standard was run approximately every three days. Calibration carbon response factors (CRF) were updated monthly using the averaged result of the NPL standard samples run in the prior month, and are applied to the previous month’s data record retroactively. Real-time data used the CRF values continuing from the prior month. In addition, a 200-ppb NPL standard and a high mole fraction VOC standard dilution curve were run annually to check for the linearity of the instrument response at high levels. The high mole fraction standard (635.4 ppb ethane, 640.6 ppb propane, 532.1 ppb i-butane, 532.1 n-butane, 320.8 ppb i-pentane, 320.8 ppb n-pentane) was diluted to various mixing ratios to create an instrument response curve (ratio of the measured/expected mole fraction vs. measured mole fraction). This same high mole fraction standard was run every 65 runs to monitor the continuity of the instrument response at high levels. A zero air (blank) sample was run every 65 runs (~every three days). Zero air was generated by running compressed air through a catalyst (platinum on alumina pellets) at 380°C. Two xylene isomers, meta-xylene and para-xylene, elute very closely together in the chromatogram and often cannot be separated as individual peaks. The results for these isomers are therefore reported as the sum of both. VOC data are reported in nanomoles per mole by volume (nmol mol^{-1}, i.e., 10^{-9}). The more commonly used unit, ppb (parts-per-billion by volume), is used as a surrogate. VOC lower detection limits (LDL) were calculated from the smallest, reliably identifiable FID peak area and the compound CRFs calculated monthly from the weekly standard runs. Since the calculation of LDL varies with the instrument response calibrated monthly, the lowest values seen in the data vary monthly. VOC species with no detected or quantifiable peak in the GC chromatograms are recorded as ½ of the lower detection limit (which similarly varies monthly).

Radioactivity Airborne radioactivity was measured as alpha radiation, in the gas phase and on a filter collecting particles, with two separate monitors. An AlphaGUARD DF2000 (Bertin Technologies SAS, France) instrument was used to measure alpha radiation emitted from radon gas (Rn-222 and Rn-220). Ambient air was sampled via a 2-m-long sampling line composed of ¼ inch o.d., 5/32 inch i.d. PFA tubing, equipped with a PFA inlet filter holder that housed a 5-micron Teflon membrane filter. Air was sampled at a rate of ~2 L/min from an inlet at 1.5 m height above the surface. The instrument uses a pulse ionization chamber, with a measurement range of 0.05 to 54,000 pCi/L (2 to 2,000,000 Bq/m^3). A second instrument, the AlphaPM radon progeny monitor (Bertin Technologies SAS, France), was used to measure alpha radiation emitted from radon progeny attached to airborne particles. The instrument captures total suspended particulate matter (PM) on a glass fiber filter, and alpha radiation counts are continuously recorded using a sensitive semiconductor (PIPS) detector, with a measurement range of 0.05 to 27,000 pCi/L equilibrium equivalent concentration (EEC) (2 to 1,000,000 Bq/m^3 EEC). The detector is located on the opposite side of the glass fiber filter. The instrument was kept in an airtight, temperature-controlled metal enclosure inside the instrument shelter. The enclosure received outside air adjacent to the AlphaGUARD inlet through a 2-inch diameter 12-inch-long aluminum inlet pipe that protruded horizontally through the shelter wall at 2 m height above the ground. The inlet pipe was heated (temperature-controlled) to 40°C to maintain a constant above-freezing temperature of the sample air reaching the instrument. Air was pulled into the enclosure at a rate of 5–6 L/min using a diaphragm pump, from which the AlphaPM instrument sub-sampled air across the filter with its internal pump at a rate of 1.2 L/min. The AlphaPM sample collection filter was replaced approximately every 2–4 weeks.

Noise was measured with Brüel & Kjær SLM 2250. The hardware comes with two independent frequency-weighted detectors. These were used for RMS/Peak measurements. All time-weighted parameters (using F-weighting) were computed in parallel. The instrument was connected to the stationary platform’s data logger. The effects of sound incidence (frontal or random) were corrected by a built-in filter, and we used a windscreen, thus giving Class 1 precision in all situations. The Sound Level Meter Software allowed us to measure weighted measures LAeq, LCeq, as well as the peak measures LCpeak, LAFmax, and LAFmin. We also collected 1/3 octave band frequencies from LZeq 12.5 Hz to 16 kHz. Measurements can be manually controlled, and we set the time resolution for data collection to 1 minute.

The Brüel & Kjær instrument was installed on the meteorological tower at 3.5 m, away from any hard vertical surface to reduce reflection and sound from the A/C units on the trailer.

Meteorology Meteorological measurements included wind speed, wind direction, temperature, humidity, visible spectrum radiation, and atmospheric pressure. The sensors were mounted onto a standard 10-m triangular meteorological tower adjacent to the station. Factory-calibration functions were used for all meteorological measurements. Data were recorded at 1-minute intervals. Wind conditions, temperature, relative humidity, and barometric pressure were recorded with a Campbell Scientific MetSENS500 instrument, mounted on the tower at 8.7 m height above the surface. Incoming solar radiation was monitored with an Apogee SP-110-SS pyranometer. Ambient air for all analyzers except radioactivity and VOC was pulled through inlet lines housed in a conduit and protected with Teflon membrane particle inlet filters mounted at approximately 6 m height above the surface on the tower. The VOC sampling line was in a separate insulated conduit heated to 40 °C and protected with a Teflon membrane particle inlet filter, colocated with the other inlets.

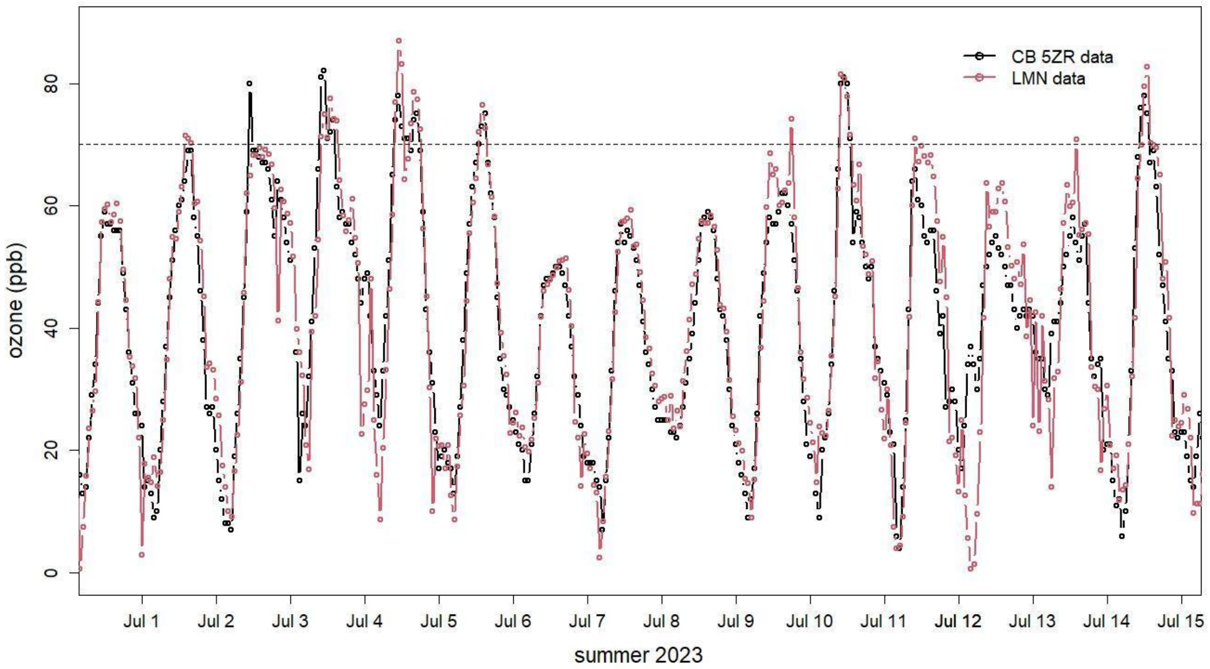


Figure A1. Comparison of ozone at LNM to the New Mexico Environment Department 5ZR site in Carlsbad.

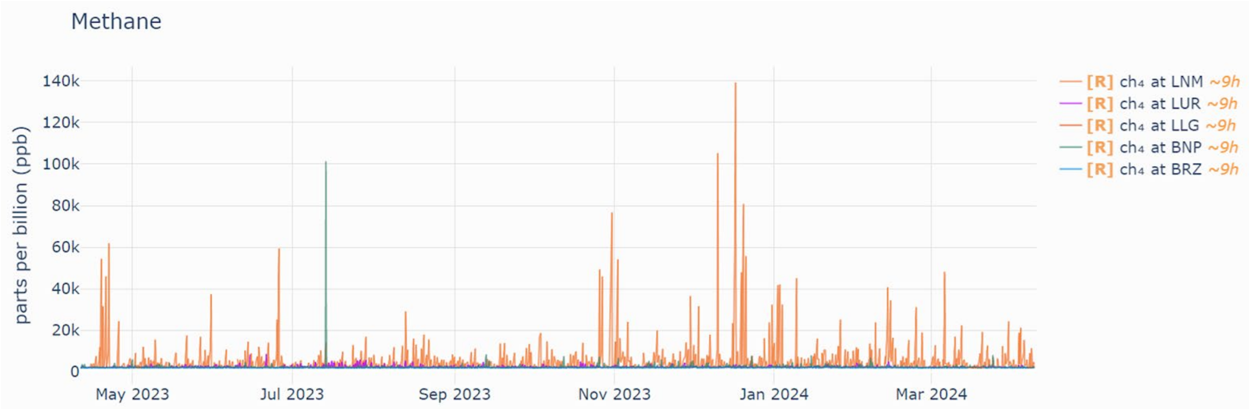


Figure A2. Time series plot showing the full record of methane measurements during the campaign at LNM, along with the concurrent methane records at LUR, LLG, BNP, and BRZ.

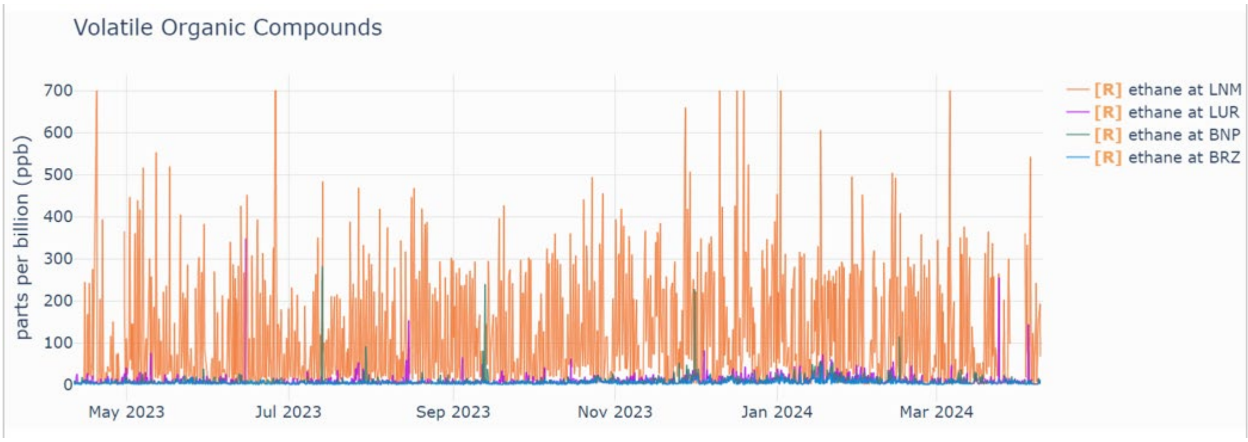


Figure A3. Time series plot showing the full record of ethane measurements during the campaign at LNM, along with the ethane records at LUR, BNP, and BRZ.

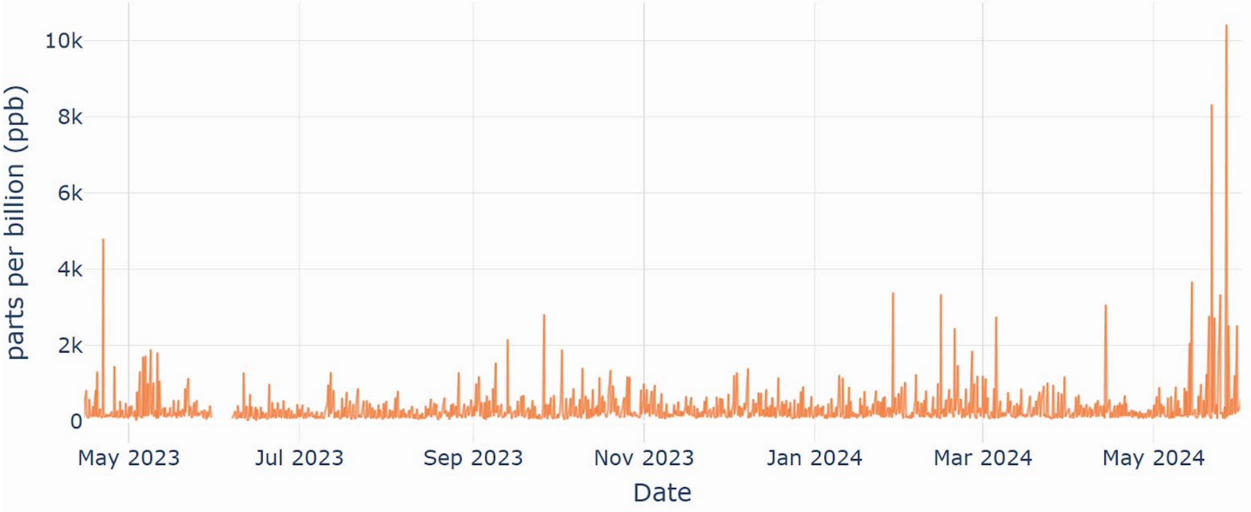


Figure A4. Time series plot showing the full record of carbon monoxide measurements during the campaign at LNM.

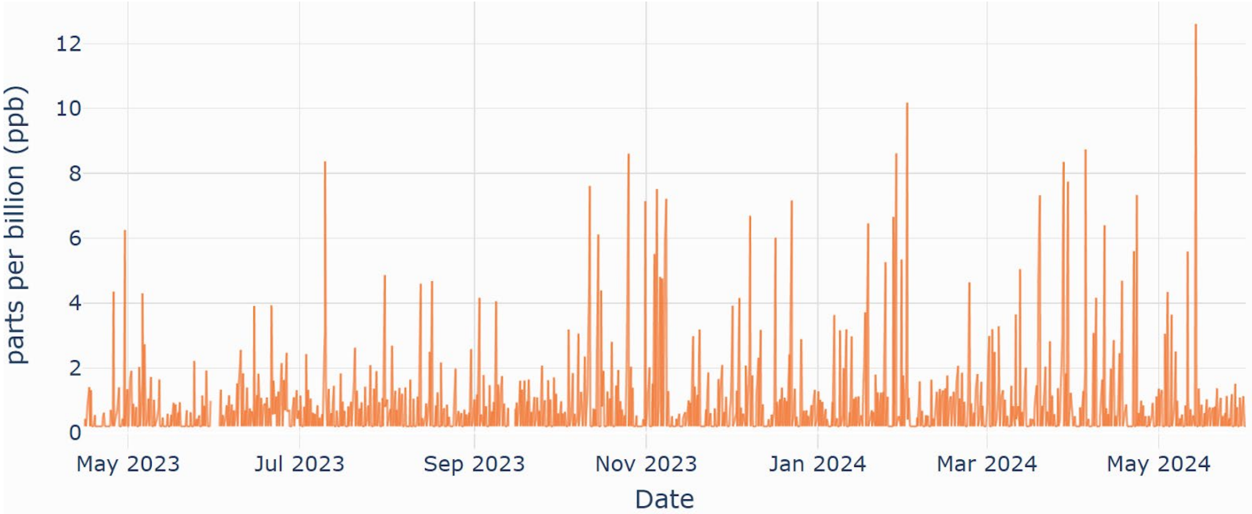


Figure A5. Time series plot showing the full record of sulfur dioxide measurements during the campaign at LNM.

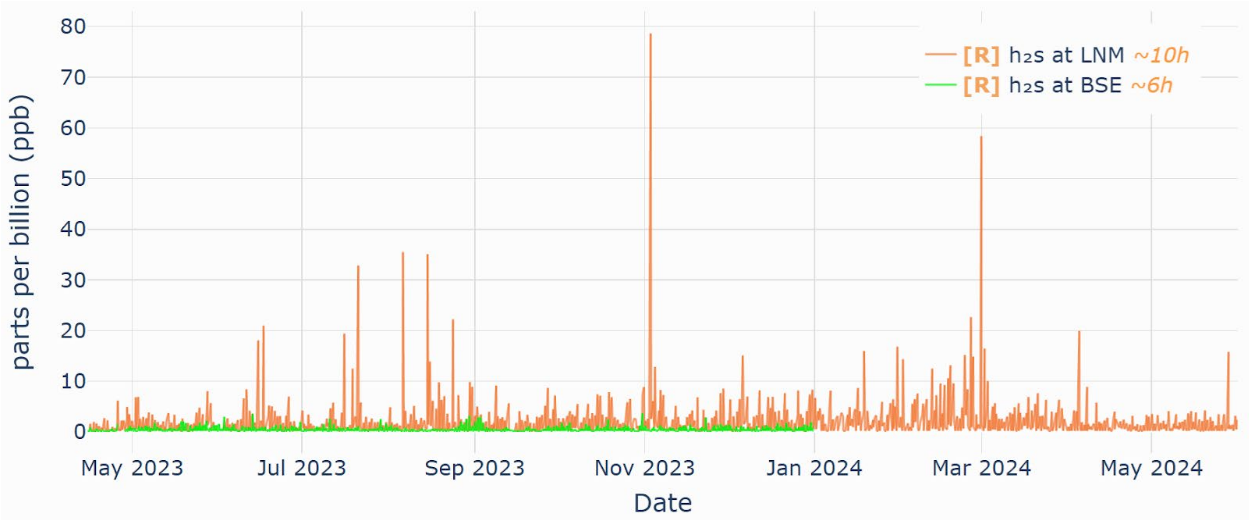
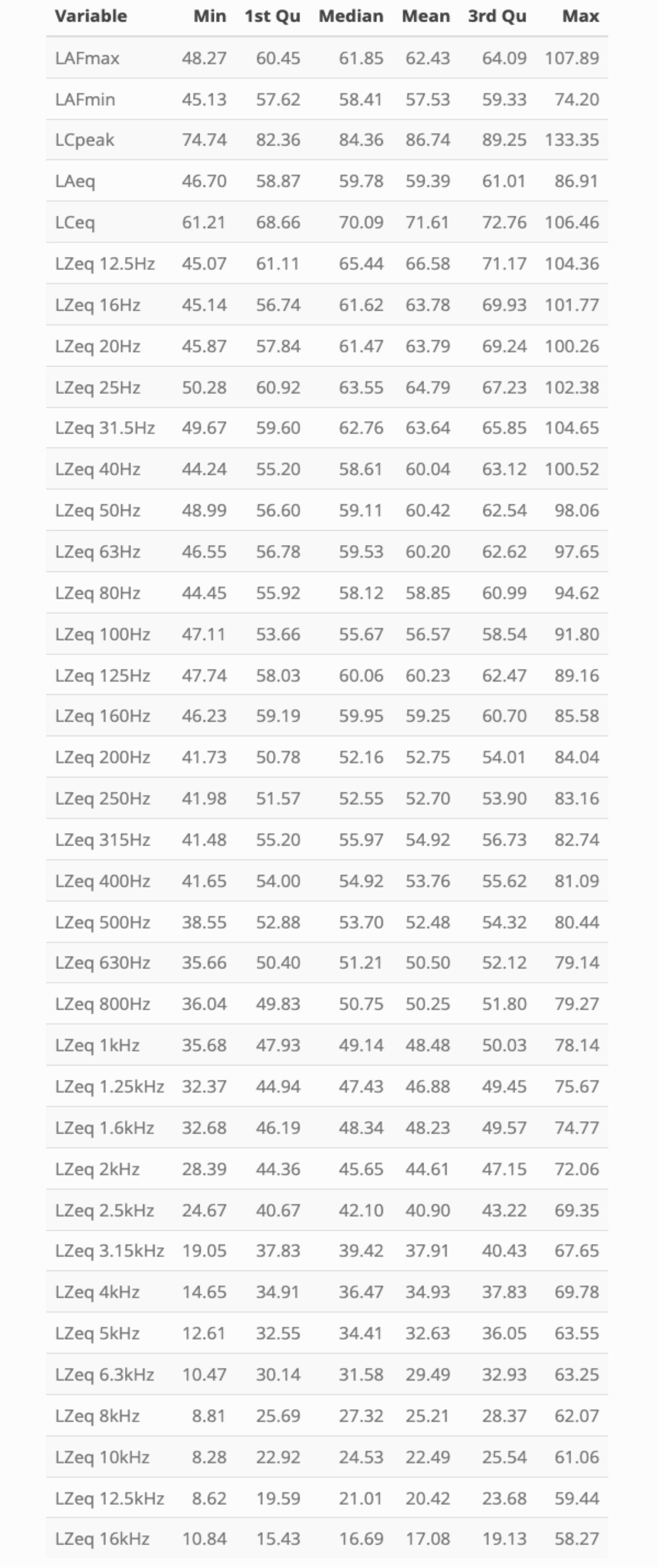


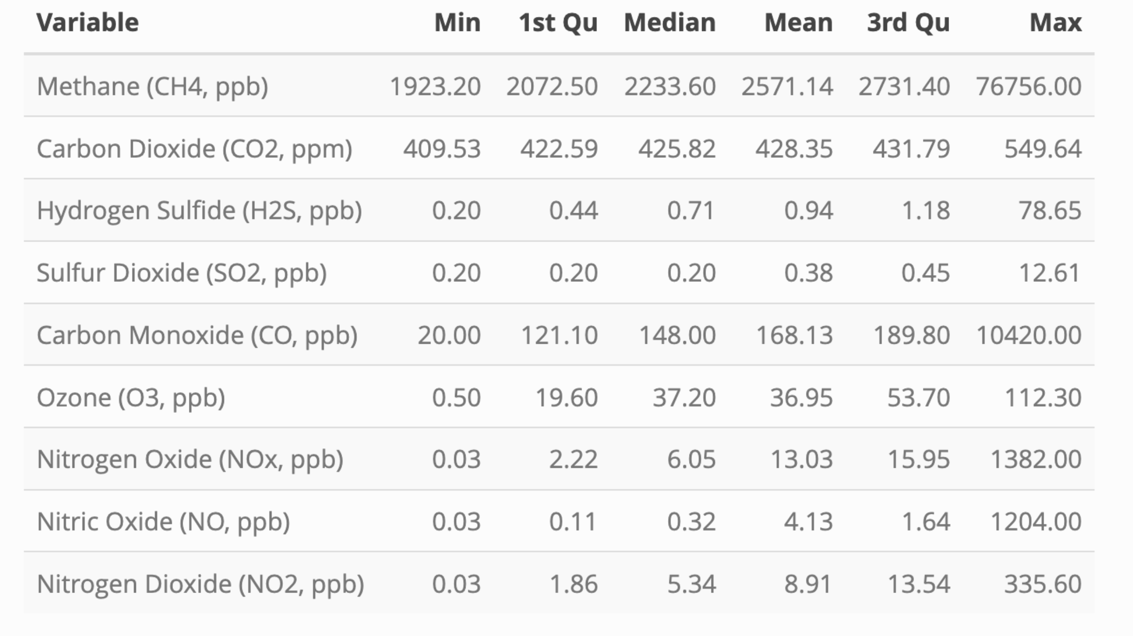
Figure A6. Time series plot showing the full record of hydrogen measurements during the campaign at LNM, compared to overlapping data from BSE.

Table A1. Summary Statistics of Sound Frequencies at 1-Minute Temporal Resolution



Variable	Min	1st Qu	Median	Mean	3rd Qu	Max
LAFmax	48.27	60.45	61.85	62.43	64.09	107.89
LAFmin	45.13	57.62	58.41	57.53	59.33	74.20
LCpeak	74.74	82.36	84.36	86.74	89.25	133.35
LAeq	46.70	58.87	59.78	59.39	61.01	86.91
LCeq	61.21	68.66	70.09	71.61	72.76	106.46
LZeq 12.5Hz	45.07	61.11	65.44	66.58	71.17	104.36
LZeq 16Hz	45.14	56.74	61.62	63.78	69.93	101.77
LZeq 20Hz	45.87	57.84	61.47	63.79	69.24	100.26
LZeq 25Hz	50.28	60.92	63.55	64.79	67.23	102.38
LZeq 31.5Hz	49.67	59.60	62.76	63.64	65.85	104.65
LZeq 40Hz	44.24	55.20	58.61	60.04	63.12	100.52
LZeq 50Hz	48.99	56.60	59.11	60.42	62.54	98.06
LZeq 63Hz	46.55	56.78	59.53	60.20	62.62	97.65
LZeq 80Hz	44.45	55.92	58.12	58.85	60.99	94.62
LZeq 100Hz	47.11	53.66	55.67	56.57	58.54	91.80
LZeq 125Hz	47.74	58.03	60.06	60.23	62.47	89.16
LZeq 160Hz	46.23	59.19	59.95	59.25	60.70	85.58
LZeq 200Hz	41.73	50.78	52.16	52.75	54.01	84.04
LZeq 250Hz	41.98	51.57	52.55	52.70	53.90	83.16
LZeq 315Hz	41.48	55.20	55.97	54.92	56.73	82.74
LZeq 400Hz	41.65	54.00	54.92	53.76	55.62	81.09
LZeq 500Hz	38.55	52.88	53.70	52.48	54.32	80.44
LZeq 630Hz	35.66	50.40	51.21	50.50	52.12	79.14
LZeq 800Hz	36.04	49.83	50.75	50.25	51.80	79.27
LZeq 1kHz	35.68	47.93	49.14	48.48	50.03	78.14
LZeq 1.25kHz	32.37	44.94	47.43	46.88	49.45	75.67
LZeq 1.6kHz	32.68	46.19	48.34	48.23	49.57	74.77
LZeq 2kHz	28.39	44.36	45.65	44.61	47.15	72.06
LZeq 2.5kHz	24.67	40.67	42.10	40.90	43.22	69.35
LZeq 3.15kHz	19.05	37.83	39.42	37.91	40.43	67.65
LZeq 4kHz	14.65	34.91	36.47	34.93	37.83	69.78
LZeq 5kHz	12.61	32.55	34.41	32.63	36.05	63.55
LZeq 6.3kHz	10.47	30.14	31.58	29.49	32.93	63.25
LZeq 8kHz	8.81	25.69	27.32	25.21	28.37	62.07
LZeq 10kHz	8.28	22.92	24.53	22.49	25.54	61.06
LZeq 12.5kHz	8.62	19.59	21.01	20.42	23.68	59.44
LZeq 16kHz	10.84	15.43	16.69	17.08	19.13	58.27

Table A2. Summary Statistics of Pollutants Merged with Sound Frequencies at 1-Minute Temporal Resolution



Variable	Min	1st Qu	Median	Mean	3rd Qu	Max
Methane (CH4, ppb)	1923.20	2072.50	2233.60	2571.14	2731.40	76756.00
Carbon Dioxide (CO2, ppm)	409.53	422.59	425.82	428.35	431.79	549.64
Hydrogen Sulfide (H2S, ppb)	0.20	0.44	0.71	0.94	1.18	78.65
Sulfur Dioxide (SO2, ppb)	0.20	0.20	0.20	0.38	0.45	12.61
Carbon Monoxide (CO, ppb)	20.00	121.10	148.00	168.13	189.80	10420.00
Ozone (O3, ppb)	0.50	19.60	37.20	36.95	53.70	112.30
Nitrogen Oxide (NOx, ppb)	0.03	2.22	6.05	13.03	15.95	1382.00
Nitric Oxide (NO, ppb)	0.03	0.11	0.32	4.13	1.64	1204.00
Nitrogen Dioxide (NO2, ppb)	0.03	1.86	5.34	8.91	13.54	335.60

Table A3. Summary Statistics of Meteorology Merged with Sound and Pollutants at 1-Minute Temporal Resolution

Variable	Min	1st Qu	Median	Mean	3rd Qu	Max
Wind Direction (degrees)	0.00	126.80	171.40	188.19	268.60	360.00
Wind Speed (m/s)	0.03	1.88	3.08	3.53	4.70	19.89
Temperature (F)	29.98	64.76	75.11	74.72	85.71	109.56
Relative Humidity (%)	1.00	18.00	33.00	36.73	53.00	98.00
Solar Radiation (W/m²)	0.00	0.00	34.50	275.45	554.20	1367.00
Pressure (altitude corrected)	998.50	1010.80	1013.40	1013.85	1016.80	1031.50
Rainfall (mm)	0.00	0.00	0.00	0.00	0.00	2.60
Water Vapor Mixing Ratio (g/kg)	0.40	3.80	6.60	6.90	9.70	18.20

Appendix B: Additional Details on Aim 2, Passive Sampling in the Permian Basin and Eagle Ford Shale

Table B1. Passively Sampled Hydrocarbon Statistics in ppb for the Permian Basin Network

Compound	mean	min	lower quartile	median	upper quartile	max	sd	skewness[1]
2-methylpentane	1.46	0.06	0.73	1.11	2.01	5.30	1.08	1.35
3-methylpentane	0.77	0.05	0.38	0.61	1.03	2.79	0.55	1.26
n-hexane	2.38	0.35	1.22	1.95	2.98	9.04	1.62	1.46
2,4-dimethylpentane	0.51	0.04	0.21	0.33	0.73	3.41	0.46	2.19
benzene	0.50	0.05	0.25	0.38	0.63	1.68	0.34	1.22
cyclohexane	0.65	0.09	0.36	0.57	0.86	2.52	0.41	1.55
2-methylhexane	0.51	0.09	0.29	0.45	0.68	1.93	0.31	1.46
n-heptane	0.68	0.09	0.38	0.56	0.86	2.69	0.43	1.69
methyl-cyclohexane	1.00	0.10	0.51	0.83	1.33	3.82	0.70	1.57
toluene	0.67	0.16	0.40	0.61	0.87	1.94	0.35	1.13
n-octane	0.16	0.02	0.09	0.14	0.22	0.51	0.09	0.94
ethyl-benzene	0.08	0.01	0.04	0.06	0.08	0.37	0.06	2.54
m,p-xylene	0.13	0.01	0.07	0.11	0.19	0.53	0.08	1.20
o-xylene	0.08	0.01	0.04	0.06	0.10	0.29	0.05	1.71

[1] Skewness is a (unitless) statistical measure of asymmetry (deviation from a *normal distribution* of skewness = 0); positive values of increasing value signify an increasingly right-skewed/tailed distribution.

Table B2. Passively Sampled Hydrocarbon Statistics in ppb for the Eagle Ford Shale Network

Compound	mean	min	lower quartile	median	upper quartile	max	sd	skewness[1]
2-methylpentane	0.96	0.10	0.46	0.81	1.23	3.70	0.75	1.56
3-methylpentane	0.46	0.04	0.21	0.40	0.59	1.75	0.35	1.53
n-hexane	1.53	0.10	0.72	1.25	2.05	5.73	1.20	1.35
2,4-dimethylpentane	0.17	0.03	0.08	0.14	0.21	0.66	0.12	1.74
benzene	0.23	0.05	0.12	0.20	0.29	0.90	0.15	2.00
cyclohexane	0.39	0.07	0.21	0.33	0.47	1.25	0.26	1.23
2-methylhexane	0.25	0.03	0.14	0.21	0.33	1.06	0.17	1.72
n-heptane	0.27	0.03	0.14	0.22	0.35	0.86	0.20	1.19
methyl-cyclohexane	0.26	0.04	0.15	0.21	0.34	0.90	0.17	1.52
toluene	0.35	0.07	0.19	0.30	0.44	1.28	0.22	1.50
n-octane	0.04	0.01	0.03	0.04	0.05	0.18	0.03	2.06
ethyl-benzene	0.02	0.01	0.01	0.02	0.03	0.14	0.02	2.83
m,p-xylene	0.05	0.01	0.03	0.04	0.06	0.19	0.03	1.79
o-xylene	0.02	0.00	0.01	0.02	0.03	0.10	0.02	1.89

[1] Skewness is a (unitless) statistical measure of asymmetry (deviation from a *normal distribution* of skewness = 0); positive values of increasing value signify an increasingly right-skewed/tailed distribution.

Figure B1. Correlation matrix for Permian basin passive sampler data.

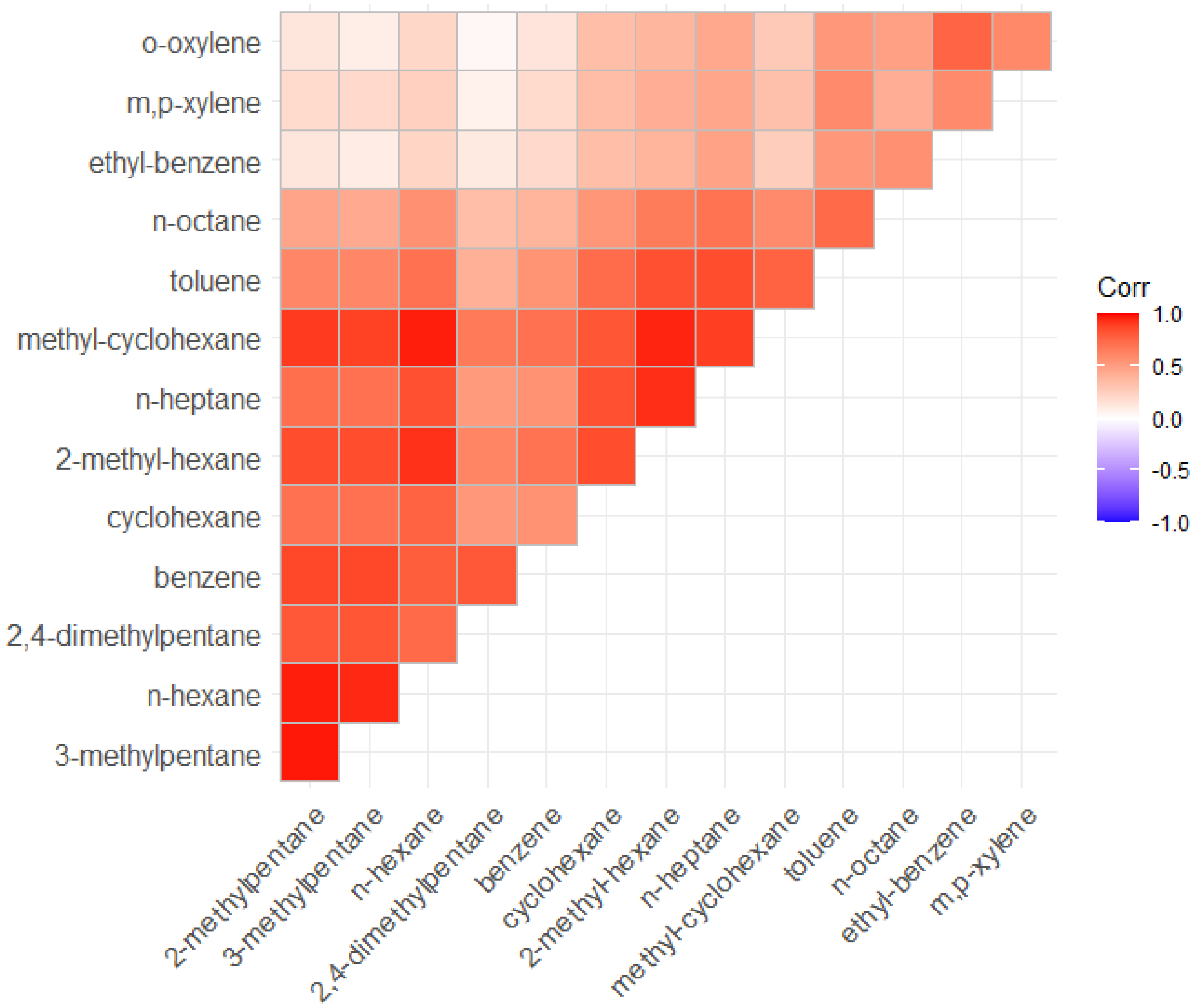


Figure B2. Correlation matrix for Eagle Ford shale passive sampler data.

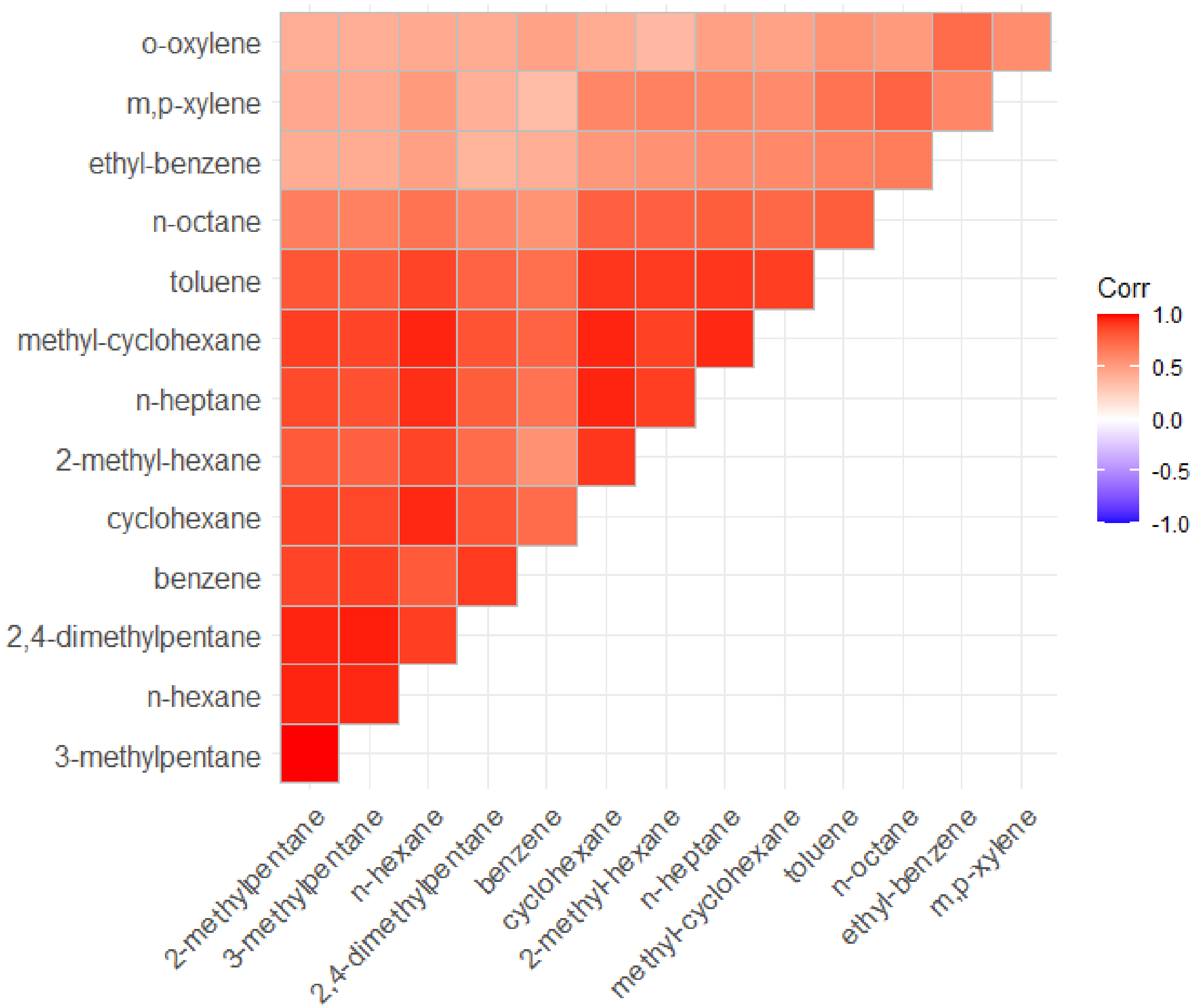


Figure B3. Spatial distributions of select hydrocarbons across the Permian basin network.

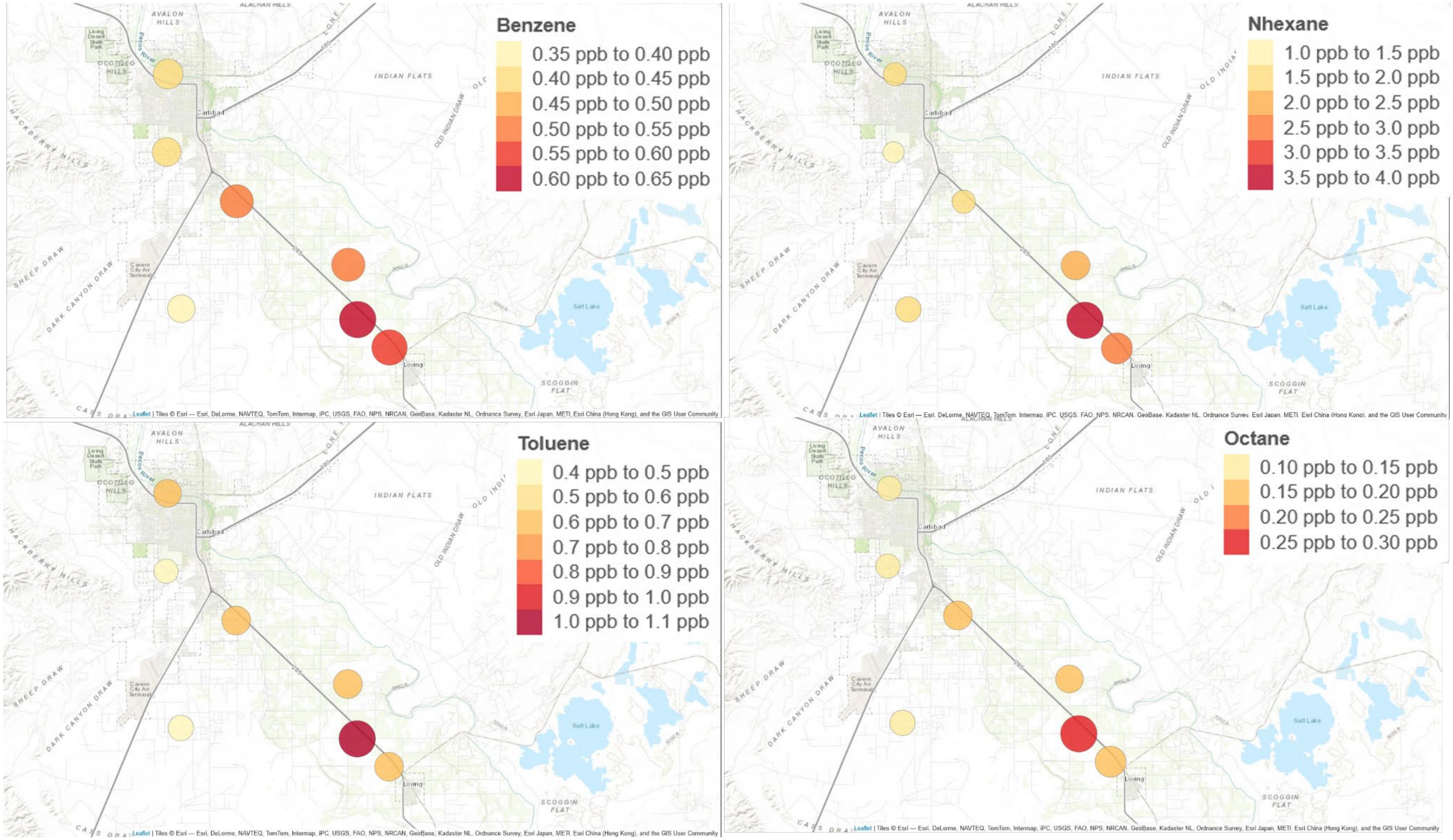


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Figure B4. Correlation matrix between measured hydrocarbons across the five Eagle Ford shale sites and their surrounding well density. (Refer to Figure 45 in the main report for explanation.)

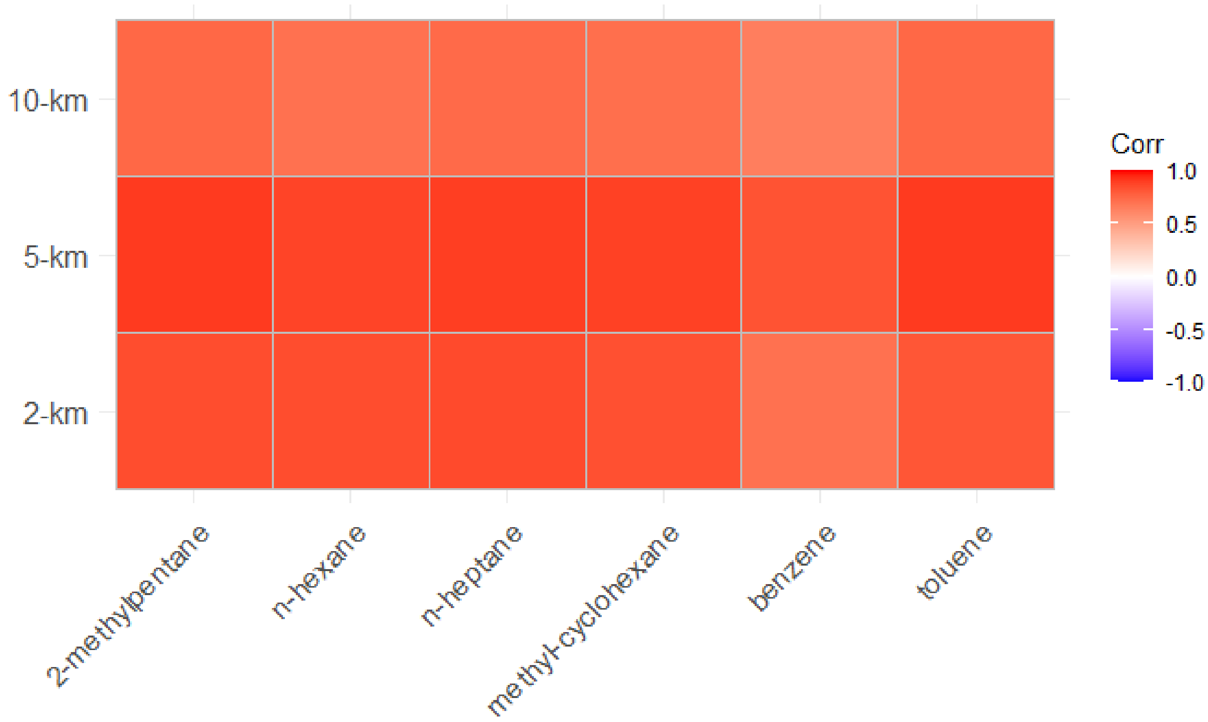
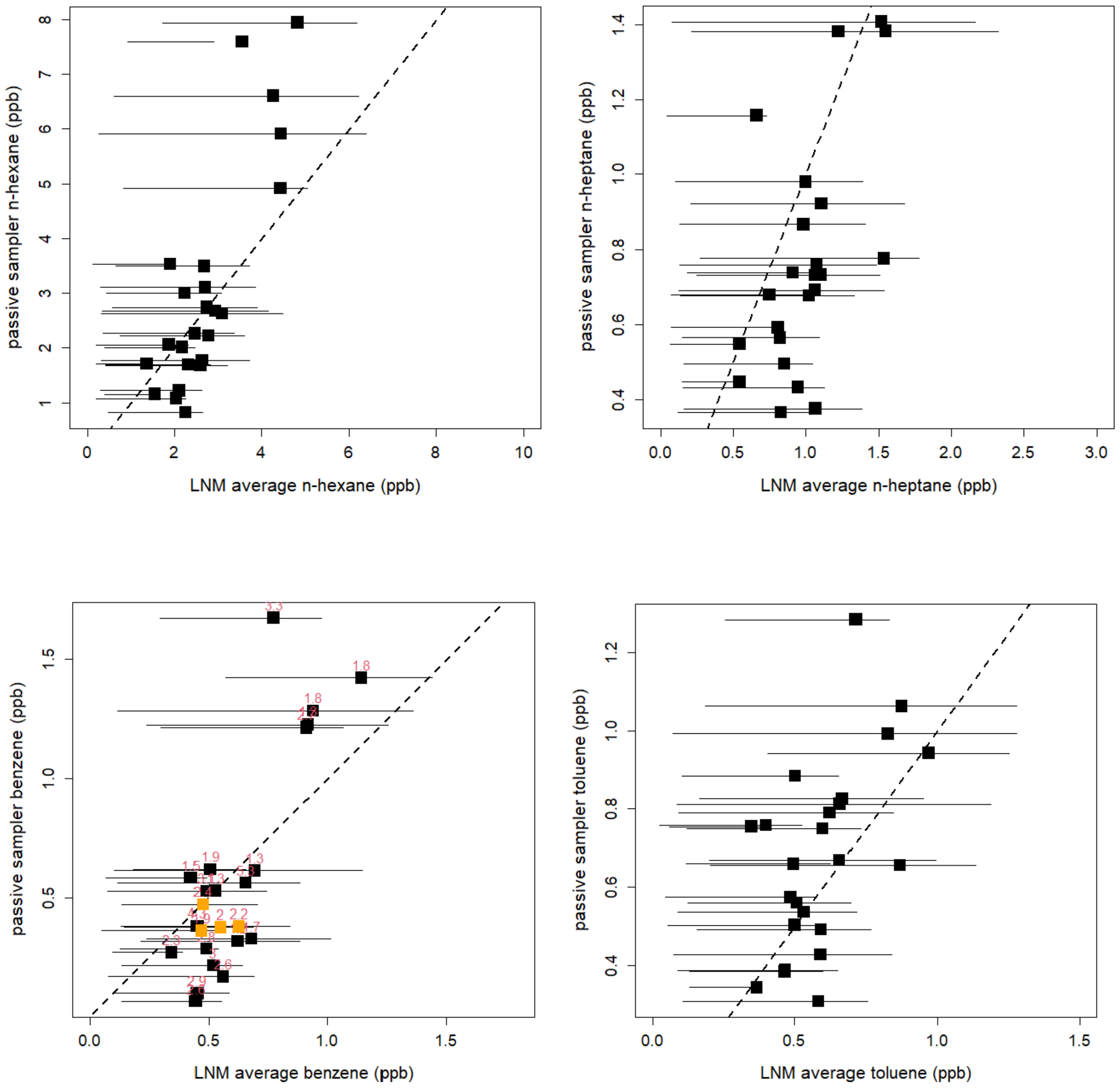
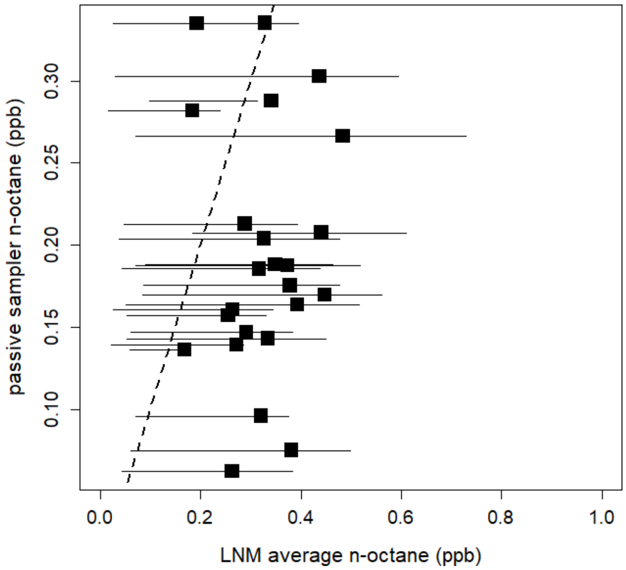
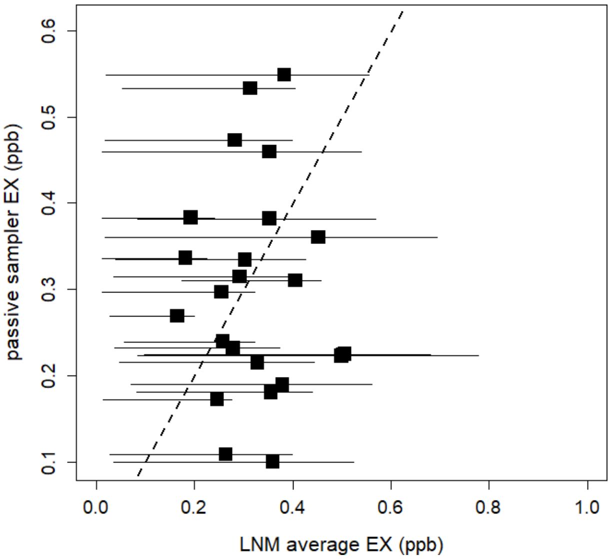


Figure B5. Hydrocarbon measurements comparison plots for the LNM site.

In all plots, the dashed line represents the 1:1 correspondence, while the horizontal lines show the lower to upper quartile (interquartile range, IQR) of the hourly LNM site data during each period of the passive sampler deployment. Note that several data point averages lie outside the IQR due to extreme skewness of the data distribution (the benzene plot additionally shows data points in orange that had larger than 30% replicate differences, and skewness in red font above each data point, for reference). “EX” refers to the sum of ethylbenzene and xylenes.







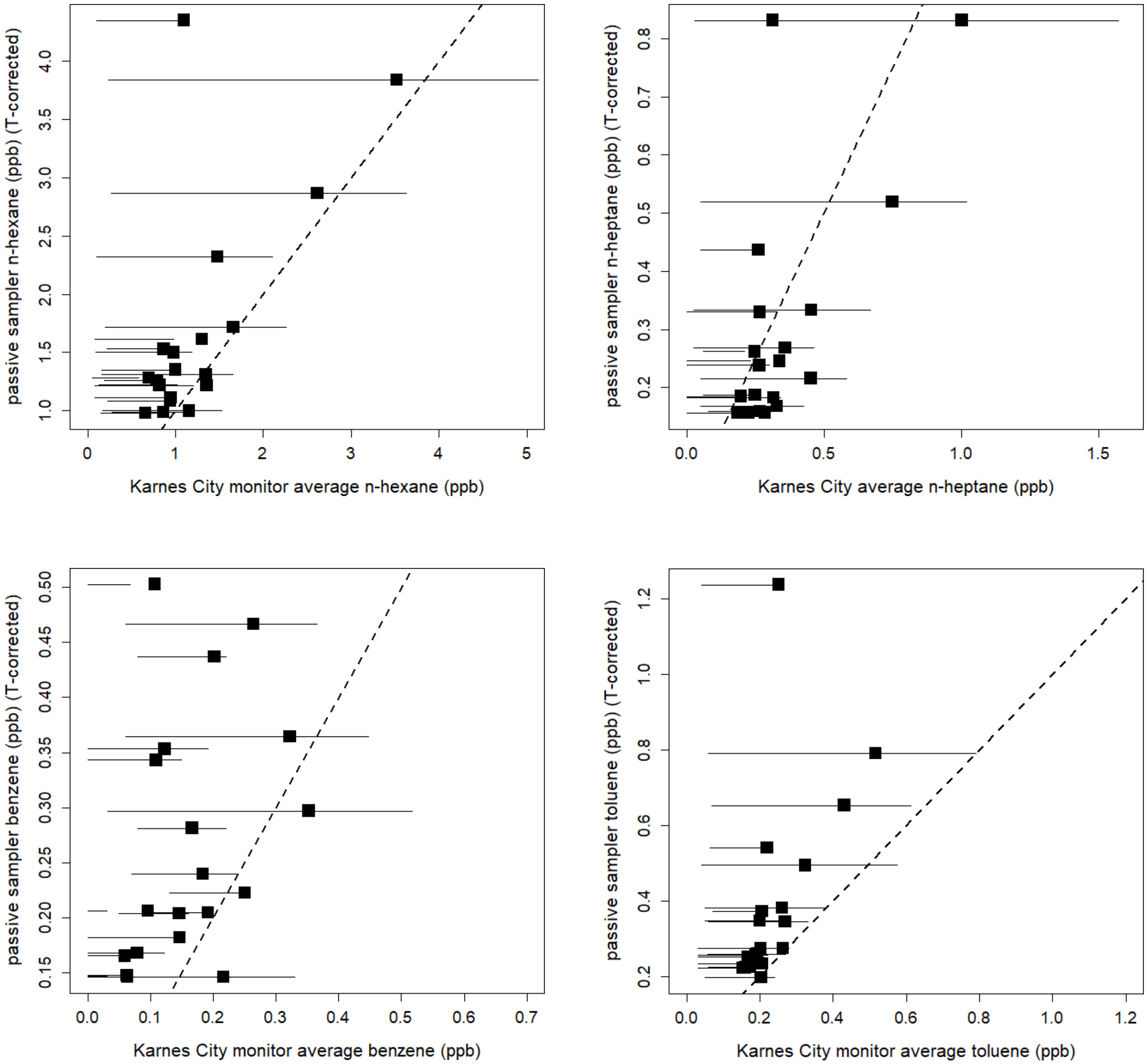
At this site, the physical distance between the passive sampler and the air monitoring site's inlet was approximately 55 m, and the passive sampler was located much closer to the ground (1.5 vs. 6 m agl). In a prior comparison to Boulder A.I.R. stationary platform measurements in Commerce City, CO, slight bias was found between the methodologies (unpublished data).

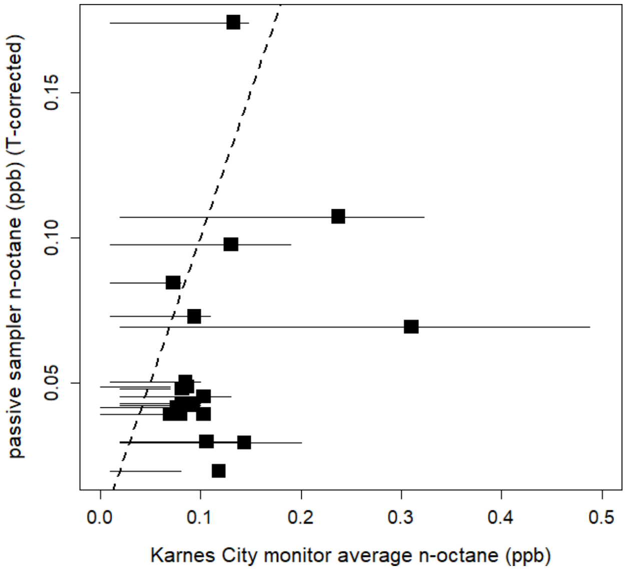
Overall, the compatibility among the two completely independent hydrocarbon measurement methodologies appears to be fair to good. In most cases, the IQR overlaps with the 1:1 line for each compound a comparison was possible (6). In some cases, when ambient concentrations were measured to be higher by the passive sampler (n-hexane, benzene), generally high data skewness was observed. No obvious, strong biases were encountered.

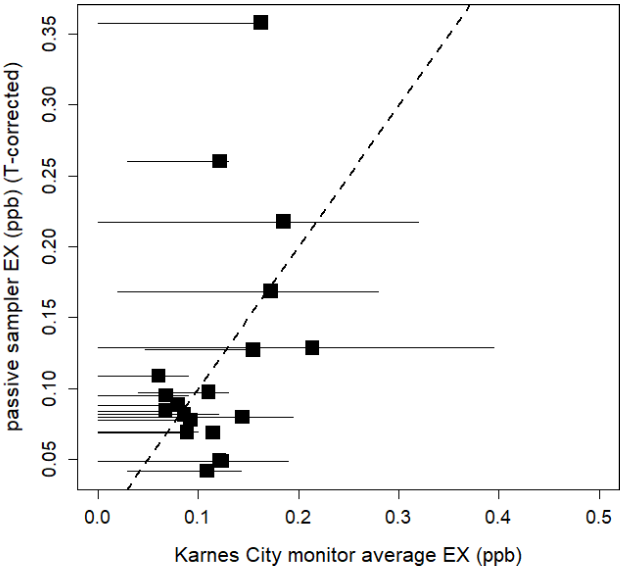
However, the passive sampler generally underestimated n-octane compared to the stationary platform's measurements.

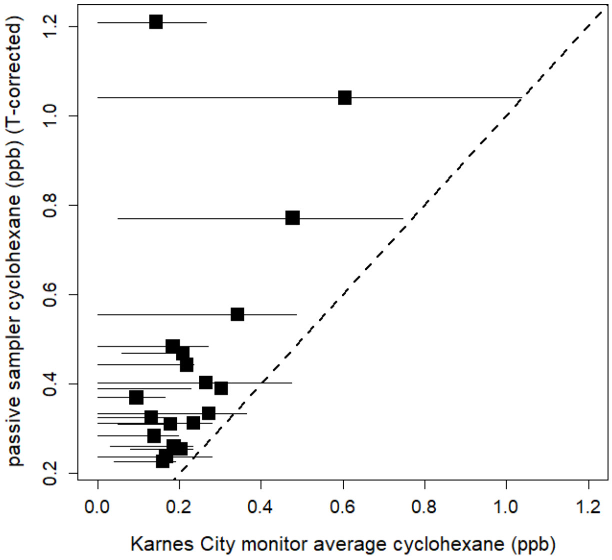
Figure B6. Hydrocarbon measurements comparison plots for the KAC site.

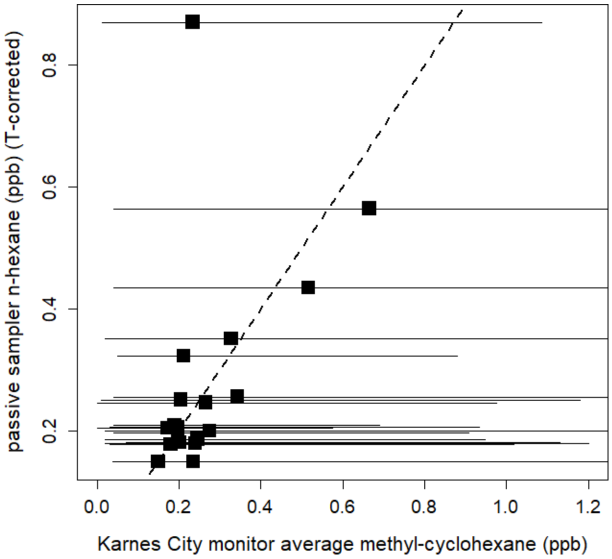
Similar to the Permian site comparisons, in all plots the dashed line represents the 1:1 correspondence, while the horizontal lines show the lower to upper quartile (interquartile range IQR) of the hourly site data from the Karnes City TCEQ air monitor during each period of the passive sampler deployment. Again, several data point averages lay outside the IQR due to extreme skewness of the data distribution (especially in the case of methyl-cyclohexane). “EX” refers to the sum of ethylbenzene and xylenes. Note that in comparison to Figure AB5, a temperature correction was applied to the passive sampling data here, which, however, causes only a <10% change in determined mixing ratios.







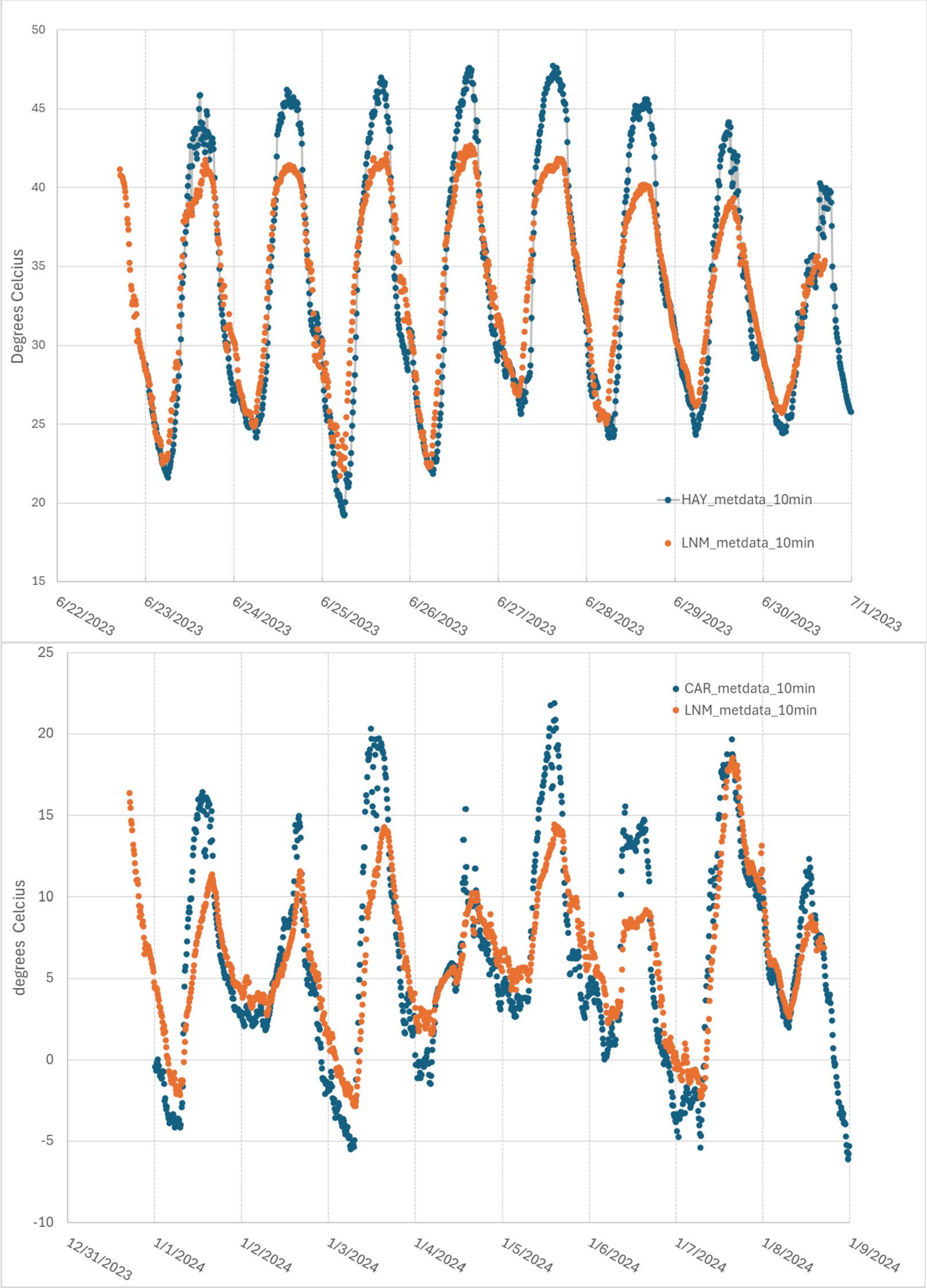




At this site, the physical distance between the passive sampler and the air monitoring site's inlet was approximately 900 m, and again the passive sampler was located closer to the ground (1.5 vs. 4 m agl). In our prior study in the region (Schade and Heienickle 2023), a shorter dataset with a more nearby passive sampling site had shown no obvious biases. However, the larger horizontal distance in this study may have led to biases.

Overall, the compatibility among the two completely independent hydrocarbon measurement methodologies was again fair to good. In most cases, the IQR overlaps with the 1:1 line for each compound a comparison was possible (8). In most cases, the correspondence between the sites was good. However, there were clear differences for benzene, toluene, and cyclohexane, and less so for n-hexane. Since the passive sampler was closer to downtown and near major traffic axes, it makes sense that traffic emissions contributed to these compounds could have enhanced their mixing ratios above those at the TCEQ monitor, which is located at the east edge of the town. Interestingly, the passive sampler again underestimated n-octane levels compared to the stationary platform's measurements, which hints at the possibility that the tabulated sampling rate for n-octane may be biased.

Figure B7. Comparisons between the LNM site and local temperature data.



Examples of two time series of temperature data, one for the HAY site, one for the CAR site, one for summer, and one for winter.

The local HOBO sensors are expected to have experienced some radiation loading from direct solar radiation, similar to the pale yellow diffusion tubes housing the samplers. The shielded temperature sensor at 10 m agl at the

LNM site generally shows lower variability, as expected. In general, the comparisons of these temperature measurements showed agreement between the sensors. However, due to the radiation loading, average temperatures at the shepherd hooks were 1–5 °C higher during summer daytime, and 1–3 °C lower during nights, particularly during strong nighttime inversions at the CAR site. Nevertheless, on average across typical 6–8 day sampling periods, temperatures were only 1–2 °C higher at the two network sites monitored as compared to the LNM site data, and we therefore averaged LNM site measurements to estimate average sampling period cartridge temperatures across the network.

Appendix C: Additional Materials for Aim 3, Analysis of Satellite Flaring

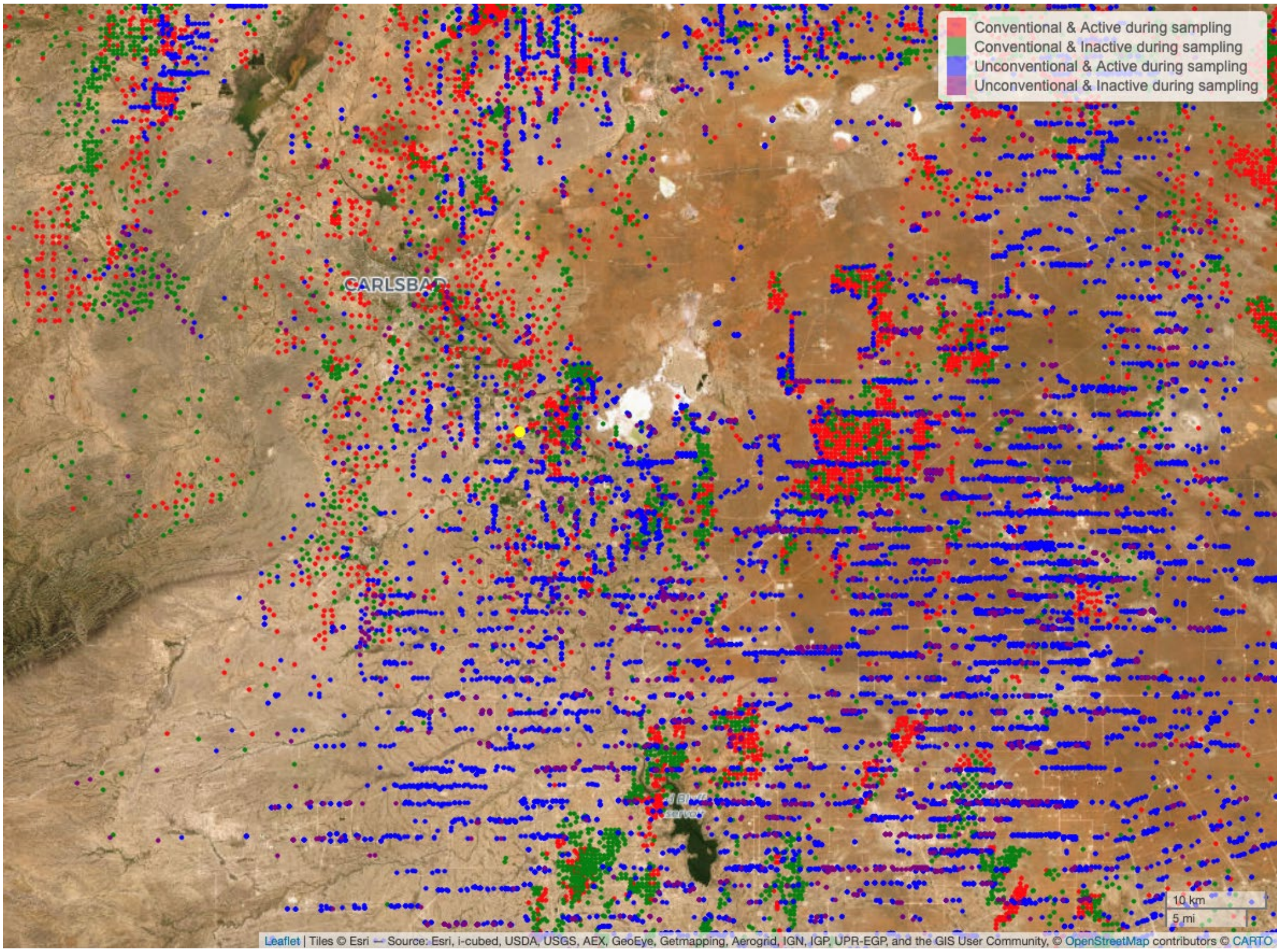


Figure C1. Map of the Carlsbad-Loving, NM region showing locations of active and inactive conventional and unconventional wells. (Data from Enverus.)

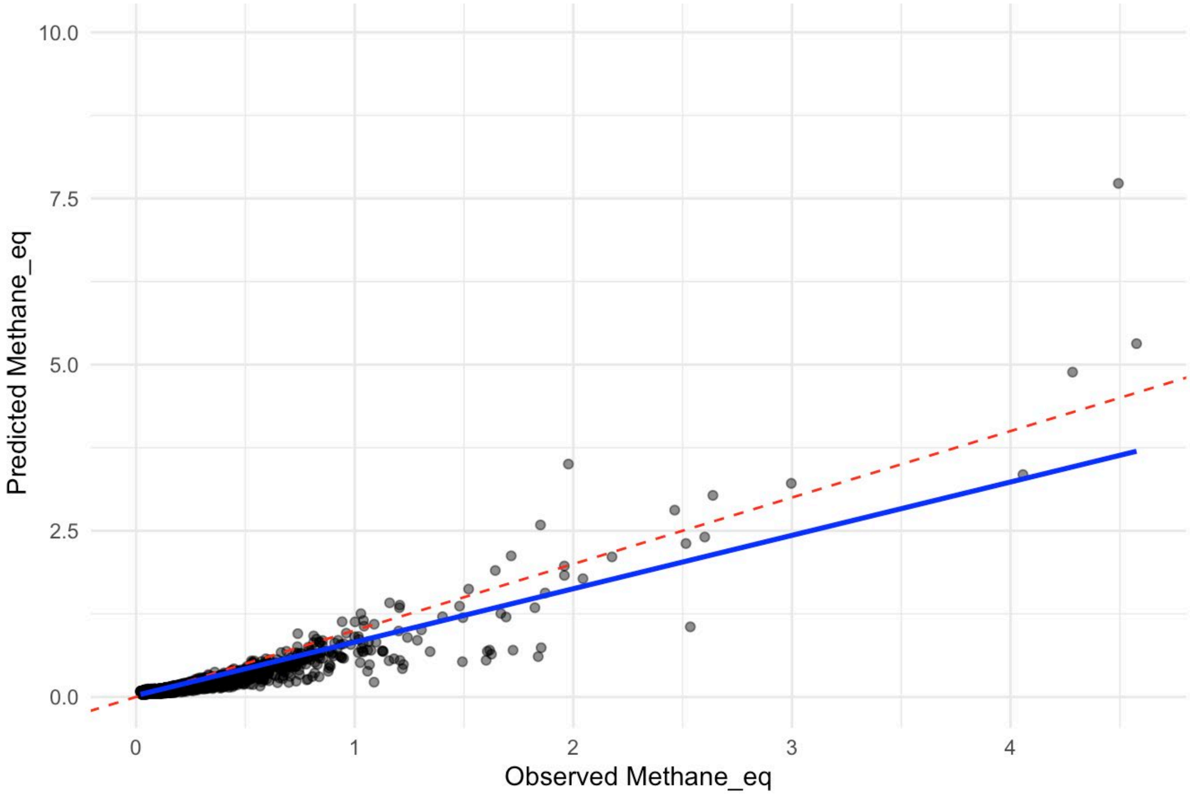


Figure C2. Observed vs. predicted methane equivalents based on the polynomial regression of VIIRS Nightfire temperature and source area.

Table C1. Number of Wells by Type (Conventional or Unconventional) Within 5 km to 50 km Buffer Regions Around the LNM Sampling Site

	Number of Wells					
Well Type	**50 km**	**40 km**	**30 km**	**20 km**	**10 km**	**5 km**
Conventional & Active during sampling	3,212	2,017	1,083	566	213	78
Conventional & Inactive during sampling	2,644	1,596	869	544	174	41
Unconventional & Active during sampling	8,401	5,060	2,890	1,541	546	132
Unconventional & Inactive during sampling	1,873	1,180	644	300	96	29
Total	16,130	9,853	5,486	2,951	1,029	280

Conventional wells were defined by vertical drill type, unconventional wells by horizontal drill type.

Table C2. Oil and Gas Production by Conventional and Unconventional Wells

	Distance from LNM					
Well Type	**50 km**	**40 km**	**30 km**	**20 km**	**10 km**	**5 km**
Conventional Oil Production	2.532 (0.5%)	2.987 (0.9%)	1.207 (0.6%)	0.6979 (0.3%)	0.3454 (0.7%)	0.165 (1.9%)
Conventional Gas Production	14.27 (0.5%)	12.65 (0.7%)	10.76 (1.2%)	7.982 (1.2%)	2.551 (0.8%)	1.467 (2.5%)
Unconventional Oil Production	502.4 (99.5%)	323.2 (99.1%)	190.2 (99.4%)	212.0 (99.7%)	52.47 (99.3%)	8.529 (98.1%)
Unconventional Gas Production	2605.7 (99.5%)	1806.1 (99.3%)	947.4 (98.2%)	670.8 (98.2%)	338.4 (99.2%)	57.64 (97.5%)

Conventional wells were defined by vertical drill type, unconventional wells by horizontal drill type; oil production in million barrels.
Gas production in billion cubic feet.
Data from Enverus.

Table C3. Regression Analyses of Nighttime Averaged Compounds with VIIRS Night Fire Flare Counts in Buffer Regions Around LNM

Compound	Radius	Adj R-sq	Significant_Variables
ch4	5	0.41	wind speed, weighted_monthly_oil
ch4	10	0.41	wind speed, weighted_monthly_oil
ch4	20	0.41	wind speed, weighted_monthly_oil
ch4	30	0.41	wind speed, weighted_monthly_oil
ch4	50	0.42	wind speed, weighted_monthly_oil, n_flare_50
benzene	5	0.39	wind speed, weighted_monthly_oil, n_flare_5
benzene	10	0.39	wind speed, weighted_monthly_oil, n_flare_10
benzene	20	0.38	wind speed, weighted_monthly_oil
benzene	30	0.38	wind speed, weighted_monthly_oil
benzene	50	0.38	wind speed, weighted_monthly_oil, n_flare_50
co	5	0.33	wind direction, wind speed, weighted_monthly_oil, weighted_monthly_gas, n_flare_5
co	10	0.33	wind direction, wind speed, weighted_monthly_oil, weighted_monthly_gas
co	20	0.32	wind direction, wind speed, weighted_monthly_oil, weighted_monthly_gas
co	30	0.32	wind direction, wind speed, weighted_monthly_oil, weighted_monthly_gas
co	50	0.32	wind direction, wind speed, weighted_monthly_oil, weighted_monthly_gas
co2	5	0.32	wind speed
co2	10	0.32	wind speed
co2	20	0.32	wind speed
co2	30	0.32	wind speed
co2	50	0.33	wind speed
nox	5	0.3	wind direction, wind speed, n_flare_5
nox	10	0.3	wind direction, wind speed, n_flare_10
nox	20	0.29	wind speed
nox	30	0.29	wind speed
nox	50	0.3	wind direction, wind speed, n_flare_50
h2s	5	0.09	wind speed, n_flare_5
h2s	10	0.09	wind speed, n_flare_10
h2s	20	0.07	wind speed
h2s	30	0.07	wind speed
h2s	50	0.08	wind speed
so2	5	0.01	(Intercept)
so2	10	0.02	(Intercept)
so2	20	0.01	(Intercept)
so2	30	0.01	(Intercept)
so2	50	0.01	(Intercept)
ethane	5	0.43	wind direction, wind speed, weighted_monthly_oil
ethane	10	0.43	wind direction, wind speed, weighted_monthly_oil, n_flare_10
ethane	20	0.43	wind direction, wind speed, weighted_monthly_oil
ethane	30	0.43	wind direction, wind speed, weighted_monthly_oil
ethane	50	0.44	wind direction, wind speed, weighted_monthly_oil, n_flare_50
ethene	5	0.4	wind direction, wind speed, weighted_monthly_oil, weighted_monthly_gas, n_flare_5
ethene	10	0.39	wind direction, wind speed, weighted_monthly_oil, weighted_monthly_gas
ethene	20	0.38	wind direction, wind speed, weighted_monthly_oil, weighted_monthly_gas
ethene	30	0.38	wind direction, wind speed, weighted_monthly_oil, weighted_monthly_gas
ethene	50	0.38	wind direction, wind speed, weighted_monthly_oil, weighted_monthly_gas
radioactivity	5	0.51	wind direction, wind speed, weighted_monthly_oil
radioactivity	10	0.52	wind direction, wind speed, weighted_monthly_oil
radioactivity	20	0.51	wind direction, wind speed, weighted_monthly_oil
radioactivity	30	0.51	wind direction, wind speed, weighted_monthly_oil
radioactivity	50	0.52	wind direction, wind speed, weighted_monthly_oil, weighted_monthly_gas
Factor1	5	0.35	wind speed, weighted_monthly_gas, n_flare_5
Factor1	10	0.34	wind speed, weighted_monthly_gas
Factor1	20	0.34	wind speed, weighted_monthly_gas
Factor1	30	0.34	wind speed, weighted_monthly_gas
Factor1	50	0.34	wind speed, weighted_monthly_gas
Factor2	5	0.03	wind speed
Factor2	10	0.02	wind speed
Factor2	20	0.03	wind speed
Factor2	30	0.04	wind speed, n_flare_30
Factor2	50	0.03	wind speed, weighted_monthly_gas
Factor3	5	0.22	wind speed, weighted_monthly_oil, n_flare_5
Factor3	10	0.2	wind speed, weighted_monthly_oil
Factor3	20	0.2	wind speed, weighted_monthly_oil
Factor3	30	0.2	wind speed, weighted_monthly_oil
Factor3	50	0.2	wind speed, weighted_monthly_oil
Factor4	5	0.39	wind direction, wind speed
Factor4	10	0.39	wind direction, wind speed
Factor4	20	0.39	wind direction, wind speed
Factor4	30	0.39	wind direction, wind speed
Factor4	50	0.39	wind direction, wind speed
Factor5	5	0.43	wind speed
Factor5	10	0.43	wind speed
Factor5	20	0.42	wind speed, weighted_monthly_oil
Factor5	30	0.43	wind speed, weighted_monthly_oil
Factor5	50	0.42	wind speed, weighted_monthly_oil

Table C4. Regression Analyses of Nighttime Averaged Compounds with VIIRS Night Fire Flared Gas Volume in Buffer Regions Around LNM

Compound	Radius	Adj R-sq	Significant_Variables
ch4	5	0.41	wind speed, weighted_monthly_oil, methane_eq_5
ch4	10	0.41	wind speed, weighted_monthly_oil, methane_eq_10
ch4	20	0.41	wind speed, weighted_monthly_oil, methane_eq_20
ch4	30	0.40	wind speed, weighted_monthly_oil, methane_eq_30
ch4	50	0.40	wind speed, weighted_monthly_oil, methane_eq_50
benzene	5	0.38	wind speed, weighted_monthly_oil, methane_eq_5
benzene	10	0.37	wind speed, weighted_monthly_oil, methane_eq_10
benzene	20	0.37	wind speed, weighted_monthly_oil
benzene	30	0.36	wind speed, weighted_monthly_oil
benzene	50	0.37	wind speed, weighted_monthly_oil, methane_eq_50
co	5	0.30	wind direction, wind speed, weighted_monthly_oil, weighted_monthly_gas, methane_eq_5
co	10	0.29	wind direction, wind speed, weighted_monthly_oil, weighted_monthly_gas
co	20	0.28	wind direction, wind speed, weighted_monthly_oil, weighted_monthly_gas
co	30	0.28	wind direction, wind speed, weighted_monthly_oil, weighted_monthly_gas
co	50	0.28	wind direction, wind speed, weighted_monthly_oil, weighted_monthly_gas
co2	5	0.30	wind speed
co2	10	0.31	wind speed, methane_eq_10
co2	20	0.30	wind speed
co2	30	0.30	wind speed
co2	50	0.30	wind speed
nox	5	0.32	wind direction, wind speed, methane_eq_5
nox	10	0.32	wind direction, wind speed, methane_eq_10
nox	20	0.30	wind speed, methane_eq_20
nox	30	0.30	wind speed
nox	50	0.31	wind speed, methane_eq_50
h2s	5	0.08	wind speed
h2s	10	0.08	wind speed
h2s	20	0.08	wind speed
h2s	30	0.08	wind speed
h2s	50	0.08	wind speed
so2	5	0.05	methane_eq_5
so2	10	0.03	weighted_monthly_oil, methane_eq_10
so2	20	0.01	weighted_monthly_oil
so2	30	0.01	weighted_monthly_oil
so2	50	0.01	weighted_monthly_oil
ethane	5	0.44	wind direction, wind speed, weighted_monthly_oil, methane_eq_5
ethane	10	0.44	wind direction, wind speed, weighted_monthly_oil, methane_eq_10
ethane	20	0.43	wind speed, weighted_monthly_oil, methane_eq_20
ethane	30	0.43	wind direction, wind speed, weighted_monthly_oil, methane_eq_30
ethane	50	0.43	wind direction, wind speed, weighted_monthly_oil, methane_eq_50
ethene	5	0.35	wind direction, wind speed, weighted_monthly_oil, weighted_monthly_gas, methane_eq_5
ethene	10	0.33	wind direction, wind speed, weighted_monthly_oil, weighted_monthly_gas, methane_eq_10
ethene	20	0.32	wind direction, wind speed, weighted_monthly_oil, weighted_monthly_gas
ethene	30	0.32	wind direction, wind speed, weighted_monthly_oil, weighted_monthly_gas
ethene	50	0.32	wind direction, wind speed, weighted_monthly_oil, weighted_monthly_gas
radioactivity	5	0.49	wind direction, wind speed, weighted_monthly_oil
radioactivity	10	0.49	wind direction, wind speed, weighted_monthly_oil
radioactivity	20	0.50	wind direction, wind speed, weighted_monthly_oil, methane_eq_20
radioactivity	30	0.49	wind direction, wind speed, weighted_monthly_oil
radioactivity	50	0.49	wind direction, wind speed, weighted_monthly_oil
Factor1	5	0.36	wind speed, weighted_monthly_gas, methane_eq_5
Factor1	10	0.35	wind speed, weighted_monthly_gas, methane_eq_10
Factor1	20	0.34	wind speed, weighted_monthly_gas
Factor1	30	0.34	wind speed, weighted_monthly_gas
Factor1	50	0.34	wind speed, weighted_monthly_gas
Factor2	5	0.02	weighted_monthly_gas
Factor2	10	0.01	weighted_monthly_gas
Factor2	20	0.02	(Intercept)
Factor2	30	0.03	(Intercept)
Factor2	50	0.01	weighted_monthly_gas
Factor3	5	0.24	wind speed, weighted_monthly_oil, methane_eq_5
Factor3	10	0.21	wind speed, weighted_monthly_oil
Factor3	20	0.21	wind speed, weighted_monthly_oil
Factor3	30	0.21	wind speed, weighted_monthly_oil
Factor3	50	0.21	wind speed, weighted_monthly_oil
Factor4	5	0.40	wind direction, wind speed, methane_eq_5
Factor4	10	0.39	wind direction, wind speed, methane_eq_10
Factor4	20	0.38	wind direction, wind speed
Factor4	30	0.38	wind direction, wind speed
Factor4	50	0.38	wind direction, wind speed
Factor5	5	0.42	wind speed, methane_eq_5
Factor5	10	0.42	wind speed, weighted_monthly_gas
Factor5	20	0.42	wind speed, weighted_monthly_gas
Factor5	30	0.42	wind speed, weighted_monthly_oil
Factor5	50	0.42	wind speed, weighted_monthly_oil