

Supporting Information

Differences between Measured and Reported Volatile Organic Compound Emissions from Oil Sands Facilities in Alberta, Canada

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S1. Summary of Flights during the Aircraft Study over the Surface Mining Facilities in the Alberta Oil Sands Region

Table S1. Summary of flights during the aircraft study over the surface mining facilities in the Alberta Oil Sands Region

Date	Flight	Start Time (LST)	End Time (LST)	Flight Objectives	Facility Studied	Flight Design	Wind Direction
13-Aug-2013	1			Survey	All	Level flight at 350 m agl	southeast
14-Aug-2013	2	11:52	15:23	Emission quantification	SML	Virtual box; virtual screen 150 to 1730 m agl	south southeast
15-Aug-2013	3	12:54	17:42	Emission quantification	SML, SUN, CNRL	Upwind spirals; virtual screens 150 to 1850 m agl	west
16-Aug-2013	4	13:20	18:07	Emission quantification	All	Upwind spirals; virtual screens 150 to 1850 m agl	southwest
17-Aug-2013	5	14:46	17:46	Emission quantification Satellite validation	SUN	Upwind spirals, spirals over satellite pixel; virtual box; 150 to 1800 m agl	southwest
19-Aug-2013	6	10:18	12:34	Emission quantification	SML, SUN	Upwind spirals; virtual screens 150 to 660 m agl	west southwest
19-Aug-2013	7	14:08	19:09	Transformation	All	Virtual screens; spirals 150 to 2800 m agl	west southwest
20-Aug-2013	8	9:58	13:34	Emission quantification	CNRL	Virtual box; spirals 150 to 1500 m agl	west southwest
21-Aug-2013	9	12:59	16:06	Emission quantification	SAJ	Virtual box; spirals 150 to 1700 m agl	west southwest
22-Aug-2013	10	13:26	16:57	Emission quantification	SUN	Virtual box; spirals 150 to 2000 m agl	west southwest
23-Aug-2013	11	10:54	15:50	Survey	All	Level flight at 150 and 350 m agl	southwest
24-Aug-2013	12	10:56	14:21	Emission quantification	SML	Virtual box; spirals 150 to 1730 m agl	southwest
26-Aug-2013	13	15:23	18:14	Emission quantification	CNRL	Virtual box; spirals 150 to 1050 m agl	northeast
28-Aug-2013	14	13:00	16:31	Emission quantification	SUN	Virtual box; spirals 150 to 1800 m agl	west
29-Aug-2013	15	14:03	19:37	Emission quantification	SAJ, SUN, SAU	Virtual boxes; spirals 150 to 1030 m agl	north northeast
31-Aug-2013	16	13:57	17:51	Satellite validation	SUN, SAJ, SAU	Level flight at 350 m agl + spirals 150 to 5860 m agl	west
02-Sep-2013	17	11:10	14:44	Emission quantification	CNRL	Virtual box; spirals 150 to 1630 m agl	north northwest
03-Sep-2013	18	13:27	17:52	Emission quantification Satellite validation	SML	Virtual box; spirals 150 to 5400 m agl	southwest
04-Sep-2013	19	12:54	17:56	Transformation	All	Virtual screens; spirals 150 to 1800 m agl	southwest
05-Sep-2013	20	13:33	18:38	Transformation, Satellite validation	All	Virtual screens; spirals 150 to 4800 m agl	west
06-Sep-2013	21	11:28	16:16	Emission quantification	SAJ, IKL, SAU	Virtual boxes; spirals 150 to 1500 m agl	north
07-Sep-2013	22	12:25	16:02	Satellite validation, Emission quantification	All plus Firebag in situ facility	Level flight at 350 m agl; spirals in satellite pixels 150 to 6000 m agl; virtual box over Firebag	southwest

Note: Short facility names are as follows: SML for Syncrude Mildred Lake; SUN for Suncor Millenium and Steepbank; CNRL for Canadian Natural Resources Ltd Horizon; SAJ for Shell Albian Sands (also known as Muskeg River) and Jackpine; SAU for Syncrude Aurora; IKL for Imperial Kearl Lake. agl – above ground level.

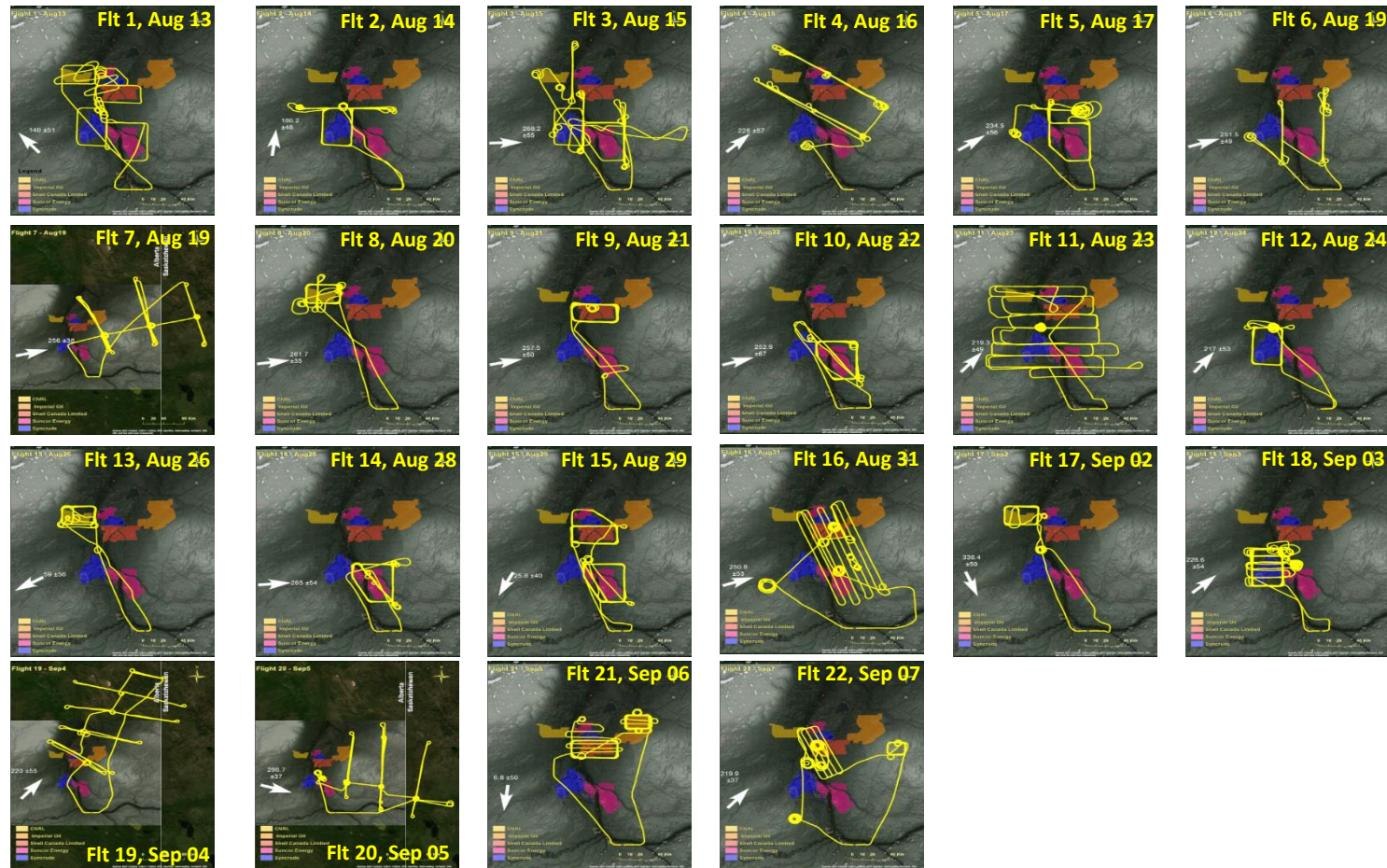


Figure S1. The flight tracks over the surface mining facilities in the Athabasca oil sands region, Alberta during the airborne study in Aug to Sep 2013. The aircraft made 22 flights, with four study objectives (1) emission quantitation and comparison with reported emissions; (2) air pollutant transport and transformation; (3) satellite retrieval validation, and (4) air quality model evaluation. The colors represent the different facilities: blue represents Syncrude Mildred Lake (SML) and Aurora (SAU) facilities; red represents Suncor Millenium/Steepbank (SUN) facility; yellow represents Canadian Natural Resources Ltd Horizon (CNRL) facility; darker orange color represents the Shell Muskeg River/Jackpine (SAJ) facility; and lighter orange color represents the Imperial Kearl Lake (IKL) facility. The white arrow in each plot shows the mean wind direction during the flight.

S2. VOC+OH and VOC+O₃ Reaction Rate Constants

Table S2. Reaction rate constants for VOC+OH and VOC+O₃ measured as reported in Reference 1 or as predicted using a photochemical model in Reference 2. These constants were used in estimation of the oxidative loss correction factors **A** and their uncertainties **ΔA** of the VOCs during transport from sources within a facility to the aircraft interception downwind on the virtual box walls. O₃ mixing ratios of 30-40 ppb were based on observations, whereas OH concentrations of (1-5)×10⁶ molec/cc were taken from a modelling analysis (Ref 34 in main text, repeated here as Ref 3) Empty entries in the facility columns indicate that there were no emission rates determined from this study for those species for the facility (see Table S3, below). The highlighted entries are for species with a correction factor >2.

Compound	Formula	K _{VOC+OH}	Ref	K _{VOC+O₃}	Ref	Correction Factors for Oxidative Loss							
						SML		SUN		CNRL		SAJ	
						A	± ΔA	A	± ΔA	A	± ΔA	A	± ΔA
N-Alkanes													
Ethane	C ₂ H ₆	2.54E-13	(1)			1.00	0.00						
Propane	C ₃ H ₈	1.12E-12	(1)			1.01	0.00	1.01	0.01	1.00	0.00	1.00	0.00
Butane	C ₄ H ₁₀	2.44E-12	(1)			1.02	0.01			1.01	0.01	1.01	0.01
Pentane	C ₅ H ₁₂	4.00E-12	(1)			1.03	0.01	1.04	0.02	1.02	0.01	1.02	0.02
Hexane	C ₆ H ₁₄	5.45E-12	(1)			1.04	0.01	1.05	0.03	1.02	0.01	1.02	0.02
Heptane	C ₇ H ₁₆	7.02E-12	(1)			1.06	0.02	1.07	0.04	1.03	0.02	1.03	0.03
Octane	C ₈ H ₁₈	8.71E-12	(1)			1.07	0.02	1.08	0.05	1.03	0.02	1.04	0.03
Nonane	C ₉ H ₂₀	1.00E-11	(1)			1.08	0.03	1.10	0.06	1.04	0.03	1.04	0.04
Decane	C ₁₀ H ₂₂	1.12E-11	(1)			1.09	0.03	1.11	0.06	1.04	0.03		
Undecane	C ₁₁ H ₂₄	1.29E-11	(1)			1.11	0.04	1.13	0.08	1.05	0.04		
Dodecane	C ₁₂ H ₂₆	1.39E-11	(1)					1.14	0.08				
Branched Alkanes													
Isobutane	C ₄ H ₁₀	2.19E-12	(1)			1.02	0.01			1.01	0.01	1.01	0.01
2-Methylbutane	C ₅ H ₁₂	3.70E-12	(1)			1.03	0.01	1.03	0.02	1.01	0.01	1.02	0.01
2,2-Dimethylpropane	C ₅ H ₁₂	8.50E-13	(1)			1.01	0.00	1.01	0.00	1.00	0.00	1.00	0.00
2-Methylpentane	C ₆ H ₁₄	5.30E-12	(1)			1.04	0.01	1.05	0.03	1.02	0.01	1.02	0.02
3-Methylpentane	C ₆ H ₁₄	5.40E-12	(1)			1.04	0.01	1.05	0.03	1.02	0.01	1.02	0.02
2,2-Dimethylbutane	C ₆ H ₁₄	2.34E-12	(1)			1.02	0.01	1.02	0.01	1.01	0.01	1.01	0.01
2,3-Dimethylbutane	C ₆ H ₁₄	5.78E-12	(1)			1.05	0.02	1.05	0.03	1.02	0.02	1.02	0.02

2-Methylhexane	C7H16	6.69E-12	(1)			1.05	0.02	1.06	0.04	1.03	0.02	1.03	0.03
3-Methylhexane	C7H16	6.30E-12	(1)			1.05	0.02	1.06	0.03	1.02	0.02	1.03	0.02
2,2-Dimethylpentane	C7H16	3.40E-12	(1)			1.03	0.01	1.03	0.02	1.01	0.01	1.01	0.01
2,3-Dimethylpentane	C7H16	1.95E-11	(1)			1.17	0.06	1.20	0.12	1.08	0.06	1.08	0.08
2,4-Dimethylpentane	C7H16	5.00E-12	(1)			1.04	0.01	1.05	0.03	1.02	0.01	1.02	0.02
2,2,3-Trimethylbutane	C7H16	4.24E-12	(1)			1.03	0.01	1.04	0.02	1.02	0.01	1.02	0.02
2-Methylheptane	C8H18	8.82E-12	(1)			1.07	0.02	1.08	0.05	1.03	0.02	1.04	0.03
3-Methylheptane	C8H18	9.24E-12	(1)			1.08	0.03	1.09	0.05	1.04	0.03	1.04	0.04
4-Methylheptane	C8H18	9.24E-12	(1)			1.08	0.03	1.09	0.05	1.04	0.03	1.04	0.04
2,4-Dimethylhexane	C8H18	8.55E-12	(1)			1.07	0.02	1.08	0.05	1.03	0.02	1.04	0.03
2,5-Dimethylhexane	C8H18	7.74E-12	(1)			1.06	0.02	1.07	0.04	1.03	0.02	1.03	0.03
2,3,4-Trimethylpentane	C8H18	7.10E-12	(1)			1.06	0.02	1.07	0.04	1.03	0.02	1.03	0.03
2,2,5-Trimethylhexane	C9H20	4.86E-12	(1)					1.05	0.03	1.02	0.01		
3,6-Dimethyloctane	C10H22	1.23E-11	(1)			1.10	0.04	1.12	0.07				
Cycloalkenes													
Cyclopentane	C5H10	5.02E-12	(1)			1.04	0.01			1.02	0.01	1.02	0.02
Methylcyclopentane	C6H12	6.96E-12	(1)			1.06	0.02	1.07	0.04	1.03	0.02	1.03	0.03
Cyclohexane	C6H12	7.21E-12	(1)			1.06	0.02	1.07	0.04	1.03	0.02	1.03	0.03
Methylcyclohexane	C7H14	1.00E-11	(1)			1.08	0.03	1.10	0.06	1.04	0.03	1.04	0.04
c-1,3-Dimethylcyclohexane	C8H16	1.38E-11	(1)			1.12	0.04	1.14	0.08	1.06	0.04	1.06	0.05
t-1,2-Dimethylcyclohexane	C8H16	1.38E-11	(1)			1.12	0.04	1.14	0.08	1.06	0.04	1.06	0.05
c-1,4/t-1,3-Dimethylcyclohexane	C8H16	1.38E-11	(1)			1.12	0.04	1.14	0.08	1.06	0.04	1.06	0.05
t-1,4-Dimethylcyclohexane	C8H16	1.38E-11	(1)			1.12	0.04	1.14	0.08	1.06	0.04	1.06	0.05
c-1,2-Dimethylcyclohexane	C8H16	1.38E-11	(1)			1.12	0.04	1.14	0.08	1.06	0.04	1.06	0.05
Aromatic Hydrocarbons													
Benzene	C6H6	1.20E-12	(1)			1.01	0.00	1.01	0.01	1.00	0.00	1.00	0.00
Toluene	C7H8	5.63E-12	(1)	4.53E-22	(1)	1.05	0.02	1.05	0.03	1.02	0.02	1.02	0.02
m,p-Xylene	C8H10	1.90E-11	(1)	1.10E-21	(1)	1.16	0.06	1.19	0.12	1.08	0.06	1.08	0.08
o-Xylene	C8H10	1.37E-11	(1)	1.72E-21	(1)	1.11	0.04	1.13	0.08	1.05	0.04	1.06	0.05
Ethylbenzene	C8H10	7.10E-12	(1)			1.06	0.02	1.07	0.04	1.03	0.02	1.03	0.03

1,2,3-Trimethylbenzene	C9H12	3.27E-11	(1)			1.30	0.12	1.37	0.24	1.14	0.10	1.15	0.14
1,2,4-Trimethylbenzene	C9H12	3.25E-11	(1)			1.30	0.12	1.37	0.24			1.15	0.14
1,3,5-Trimethylbenzene	C9H12	5.75E-11	(1)			1.62	0.27	1.78	0.57	1.27	0.21	1.29	0.29
2-Ethyltoluene	C9H12	1.23E-11	(1)			1.10	0.04			1.05	0.03	1.05	0.05
3-Ethyltoluene	C9H12	1.92E-11	(1)			1.17	0.06	1.20	0.12			1.08	0.08
4-Ethyltoluene	C9H12	1.21E-11	(1)			1.10	0.03	1.12	0.07	1.05	0.03	1.05	0.05
n-Propylbenzene	C9H12	6.00E-12	(1)			1.05	0.02	1.06	0.03			1.02	0.02
i-Propylbenzene	C9H12	7.79E-12	(1)			1.06	0.02	1.07	0.04			1.03	0.03
n-Butylbenzene	C10H14	1.31E-11	(1)			1.11	0.04	1.13	0.08	1.05	0.04	1.06	0.05
iso-Butylbenzene	C10H14	1.17E-11	(1)			1.10	0.03	1.11	0.07	1.05	0.03	1.05	0.05
sec-Butylbenzene	C10H14	1.17E-11	(1)			1.10	0.03	1.11	0.07	1.05	0.03	1.05	0.05
tert-Butylbenzene	C10H14	4.60E-12	(1)							1.02	0.01		
1,2-Diethylbenzene	C10H14	1.37E-11	(1)			1.11	0.04	1.13	0.08			1.06	0.05
1,3-Diethylbenzene	C10H14	2.36E-11	(1)			1.21	0.08	1.25	0.16	1.10	0.07	1.10	0.10
1,4-Diethylbenzene	C10H14	1.43E-11	(1)			1.12	0.04	1.14	0.09	1.06	0.04	1.06	0.06
p-Cymene	C10H14	1.50E-11	(1)			1.13	0.04					1.06	0.06
Hexylbenzene	C12H18	1.15E-11	(1)					1.11	0.07				
Styrene	C8H8	5.80E-11	(2)	1.70E-17	(1)	1.70	0.31	1.89	0.66	1.30	0.24	1.32	0.32
Indane (2,3-Dihydroindene)	C9H10	1.90E-11	(1)			1.16	0.06	1.19	0.12	1.08	0.06	1.08	0.08
Naphthalene	C10H8	2.30E-11	(1)	2.01E-19	(1)	1.20	0.07	1.24	0.15				
Straight Chain Alkenes													
Ethene	C2H4	8.52E-12	(1)	1.59E-18	(1)	1.07	0.03					1.04	0.03
Propene	C3H6	2.63E-11	(1)	1.01E-17	(1)	1.3	0.1					1.1	0.1
1-Butene/2-Methylpropene	C4H8	3.14E-11	(1)	1.02E-17	(1)	1.3	0.1					1.2	0.2
c-2-Butene	C4H8	5.64E-11	(1)	1.25E-16	(1)	2.2	0.6					1.5	0.6
t-2-Butene	C4H8	6.40E-11	(1)	1.90E-16	(1)	2.9	1.0			1.7	0.6	1.8	0.8
1-Pentene	C5H10	3.14E-11	(1)	1.00E-17	(1)	1.3	0.1					1.2	0.2
c-2-Pentene	C5H10	6.50E-11	(1)	1.31E-16	(1)							1.6	0.7
t-2-Pentene	C5H10	6.70E-11	(1)	1.60E-16	(1)	2.7	0.9					1.7	0.8
1-Hexene/2-Methyl-1-Pentene	C6H12	3.70E-11	(1)	1.10E-17	(1)	1.4	0.2					1.2	0.2

c-2-Hexene	C6H12	6.00E-11	(1)	1.60E-16	(1)			3.1	1.8				
t-2-Hexene	C6H12	6.00E-11	(1)	1.60E-16	(1)	2.6	0.8			1.6	0.5	1.7	0.7
t-3-Heptene	C7H14	6.76E-11	(2)	2.00E-16	(2)	3.1	1.1	3.9	2.6				
t-2-Heptene	C7H14	6.68E-11	(2)	2.00E-16	(2)	3.0	1.1	3.9	2.6	1.8	0.7	1.8	0.9
1-Octene	C8H16	4.14E-11	(1)	1.20E-17	(2)							1.2	0.2
t-2-Octene	C8H16	6.94E-11	(1)	2.00E-16	(2)					1.8	0.7		
1-Undecene	C11H22	4.79E-11	(1)	1.20E-17	(2)					1.2	0.2		
Branched Alkenes													
2-Methyl-1-Butene	C5H10	6.10E-11	(1)	1.60E-17	(1)	1.7	0.3					1.3	0.3
2-Methyl-2-Butene	C5H10	8.69E-11	(1)	4.03E-16	(1)							2.9	2.2
3-Methyl-1-Butene	C5H10	3.18E-11	(1)	1.10E-17	(1)	1.3	0.1					1.2	0.2
3-Methyl-1-Pentene	C6H12	3.02E-11	(2)	1.20E-17	(2)	1.3	0.1			1.1	0.1	1.2	0.1
4-Methyl-1-Pentene	C6H12	3.02E-11	(2)	1.20E-17	(2)			1.4	0.3			1.2	0.1
c-3-Methyl-2-Pentene	C6H12	8.83E-11	(2)	4.50E-16	(1)							3.2	2.5
t-3-Methyl-2-Pentene	C6H12	8.83E-11	(1)	5.60E-16	(1)							3.9	3.4
t-4-Methyl-2-Pentene	C6H12	6.10E-11	(1)	4.03E-16	(1)					2.4	1.4		
Cyclopentene	C5H8	6.73E-11	(1)	5.70E-16	(1)							3.5	2.9
1-Methylcyclopentene	C6H10	9.38E-11	(1)	6.70E-16	(1)					4.6	4.5	5.0	4.8
Cyclohexene	C6H10	6.77E-11	(1)	8.14E-17	(1)	2.2	0.6	2.6	1.3				
1-Methylcyclohexene	C7H12	9.44E-11	(1)	1.65E-16	(1)	3.6	1.5	4.9	3.7	1.9	0.9		
Alkynes and Diene													
Ethyne	C2H2	8.30E-13	(1)	1.00E-20	(1)	1.01	0.00	1.01	0.00			1.00	0.00
Propyne	C3H4	6.15E-12	(1)	3.00E-20	(2)							1.03	0.02
1-Butyne	C4H6	8.16E-12	(1)	3.00E-20	(2)							1.03	0.03
1,3-Butadiene	C4H6	6.66E-11	(1)	6.30E-18	(1)	1.8	0.4					1.4	0.4
Oxygenated Hydrocarbons													
Methanol	CH4O	9.30E-13	(1)			1.01	0.00			1.00	0.00		
Formaldehyde	CH2O	9.20E-12	(1)			1.08	0.03	1.09	0.05				
Acetaldehyde	C2H4O	1.60E-11	(1)			1.14	0.05					1.07	0.06
Acetone	C3H6O	2.20E-13	(1)			1.00	0.00	1.00	0.00	1.00	0.00	1.00	0.00

Acrolein	C3H4O	2.00E-11	(1)	9.00E-19	(1)	1.18	0.06			1.09	0.08		
MVK+MACR	C4H6O	2.49E-11	(1)	3.75E-18	(1)	1.2	0.1	1.3	0.2	1.1	0.1	1.12	0.11
Butanone	C4H8O	1.50E-12	(1)			1.01	0.00						
Chlorinate Hydrocarbons													
Chloromethane	CH3Cl	1.02E-13	(1)							1.00	0.00		
Dichloromethane	CH2Cl2	1.22E-13	(1)					1.00	0.00				
Chloroform	CHCl3	1.00E-13	(1)					1.00	0.00				
1,1-Dichloroethene	C2H2Cl2	2.60E-13	(1)	3.58E-20	(2)							1.00	0.00
1,2-Dichloroethane	C2H4Cl2	2.20E-13	(1)			1.00	0.00	1.00	0.00	1.00	0.00		
c-1,2-Dichloroethene	C2H2Cl2	1.55E-13	(1)	1.79E-20	(2)							1.00	0.00
Hexachlorobutadiene	C4Cl6	3.00E-14	(2)	7.00E-23	(2)			1.00	0.00			1.00	0.00
Biogenic Hydrocarbons													
Isoprene	C5H8	1.01E-10	(1)	1.28E-17	(1)			3.2	1.9	1.6	0.5	1.6	0.7
a-Pinene	C10H16	5.37E-11	(1)	8.66E-17	(1)			2.3	1.0	1.4	0.3	1.4	0.4
b-Pinene	C10H16	7.89E-11	(1)	1.50E-17	(1)	2.1	0.5	2.4	1.1	1.4	0.4	1.5	0.5
Limonene	C10H16	1.71E-10	(1)	2.00E-16	(1)			5.7	6.7				
Camphene	C10H16	5.30E-11	(1)	9.00E-19	(1)					1.2	0.2	1.3	0.3

S3. Results of Emission Rates of Individual VOC Compounds for Four Oil Sands Surface Mining Facilities

Table S3. The measurement-based top down emission rate (**E**) and its uncertainty (**ΔE**), both in tonnes/day, of each compound for the four oil sands surface mining facilities. VOC compounds that are NPRI Part 1 and Part 5 required reports when the emission rates exceed reporting criteria (*Methods*) are indicated.

Compounds highlighted in gray color indicate that they were matched to the NPRI Part 1 and Part 5 (Ref 4 to 6) Emission Reports of species for chemical profile comparison. Those highlighted in orange color would be reportable under either Part 1 or Part 5 (or both) reporting requirements when the daily rates were upscaled to annual rates after accounting for seasonal changes and subtracting the contributions from mining fleet, which is estimated below (*Section S6*). Those not highlighted are not required for reporting to the NPRI. Empty entries for any of the four facilities indicate that the compounds were quantified but there were no suitable tracers for determining emission rates (in other words, correlation with any tracer was below $R^2 < 0.8$).

				Emission Rates during Aug/Sep (tonnes/day)							
Compound	Formula	NPRI Part 1 Required	NPRI Part 5 Required	SML		SUN		CNRL		SAJ	
				E	±ΔE	E	±ΔE	E	±ΔE	E	±ΔE
N-Alkanes Total				14.9	2.6	20.6	1.7	10.2	1.8	12.1	1.5
Ethane	C2H6	No	No	1.31	0.44						
Propane	C3H8	No	Yes	1.46	0.65	1.69	0.38	1.75	0.66	0.66	0.15
Butane	C4H10	No	Yes	0.25	0.17			1.35	0.51	0.42	0.09
Pentane	C5H12	No	Yes	0.49	0.18	3.34	0.75	0.35	0.51	9.73	1.66
Hexane	C6H14	No	Yes	1.15	0.42	4.32	1.00	0.79	0.30	2.28	0.40
Heptane	C7H16	No	Yes	3.44	1.22	4.22	0.70	3.34	1.30	0.54	0.12
Octane	C8H18	No	Yes	3.81	1.68	2.40	0.41	1.39	0.48	0.13	0.03
Nonane	C9H20	No	Yes	2.40	1.16	1.65	0.36	0.83	0.30	0.08	0.02
Decane	C10H22	No	Yes	0.41	0.22	0.25	0.09	0.36	0.13		
Undecane	C11H24	No	No	0.22	0.12	1.29	0.41	0.058	0.017		
Dodecane	C12H26	No	Yes			1.48	0.47				
Branched Alkanes Total				10.0	2.1	11.0	0.8	31.8	5.2	20.6	2.0
Isobutane	C4H10	No	Yes	0.23	0.12			7.02	2.35	1.12	0.31
2-Methylbutane	C5H12	No	Yes	0.46	0.18	1.70	0.39	12.3	4.3	5.70	1.41
2,2-Dimethylpropane	C5H12	No	Yes	0.15	0.12	0.49	0.11	1.12	0.63	0.04	0.01
2-Methylpentane	C6H14	No	Yes	0.43	0.16	1.58	0.38	0.64	0.23	6.33	1.17
3-Methylpentane	C6H14	No	Yes	0.29	0.10	1.04	0.24	3.58	1.28	3.62	0.66
2,2-Dimethylbutane	C6H14	No	Yes	0.07	0.04	0.13	0.03	0.53	0.16	1.00	0.14
2,3-Dimethylbutane	C6H14	No	Yes	0.20	0.15	0.063	0.024	1.22	0.55	1.27	0.45
2-Methylhexane	C7H16	No	Yes	0.64	0.22	0.94	0.15	0.47	0.16	0.23	0.05
3-Methylhexane	C7H16	No	Yes	1.12	0.36	1.57	0.24	0.76	0.24	0.36	0.08
2,2-Dimethylpentane	C7H16	No	Yes	0.02	0.01	0.01	0.00	0.22	0.07	0.06	0.01
2,3-Dimethylpentane	C7H16	No	Yes	0.43	0.14	0.50	0.08	0.84	0.28	0.20	0.04
2,4-Dimethylpentane	C7H16	No	Yes	0.07	0.03	0.05	0.01	0.17	0.11	0.15	0.03

2,2,3-Trimethylbutane	C7H16	No	Yes	0.13	0.06	0.15	0.03	0.34	0.13	0.30	0.06
2-Methylheptane	C8H18	No	Yes	3.12	1.92	1.55	0.54	0.90	0.32	0.10	0.04
3-Methylheptane	C8H18	No	Yes	1.25	0.48	0.58	0.11	0.60	0.23	0.04	0.01
4-Methylheptane	C8H18	No	Yes	0.81	0.30	0.39	0.08	0.46	0.17	0.05	0.01
2,4-Dimethylhexane	C8H18	No	Yes	0.17	0.14	0.08	0.01	0.33	0.14	0.01	0.00
2,5-Dimethylhexane	C8H18	No	Yes	0.13	0.04	0.08	0.01	0.14	0.04	0.02	0.00
2,3,4-Trimethylpentane	C8H18	No	Yes	0.10	0.04	0.016	0.002	0.13	0.04	0.002	0.001
2,2,5-Trimethylhexane	C9H20	No	Yes			0.005	0.002	0.010	0.003		
3,6-Dimethyloctane	C10H22	No	Yes	0.11	0.11	0.056	0.014				
Cycloalkanes Total				5.8	0.9	4.6	0.4	15.6	3.3	4.9	0.5
Cyclopentane	C5H10	No	Yes	0.01	0.003			1.65	0.61	2.07	0.40
Methylcyclopentane	C6H12	No	Yes	0.82	0.26	1.85	0.40	3.13	1.03	1.33	0.29
Cyclohexane	C6H12	Yes	No	0.54	0.19	0.58	0.13	4.01	1.42	0.64	0.15
Methylcyclohexane	C7H14	No	Yes	2.11	0.67	1.18	0.18	3.01	1.20	0.29	0.07
c-1,3-Dimethylcyclohexane	C8H16	No	Yes	0.77	0.36	0.35	0.05	1.75	1.01	0.11	0.02
t-1,2-Dimethylcyclohexane	C8H16	No	Yes	0.73	0.39	0.32	0.08	1.0	0.3	0.05	0.01
c-1,4/t-1,3-Dimethylcyclohexane	C8H16	No	Yes	0.42	0.16	0.17	0.02	0.41	2.2	0.02	0.00
t-1,4-Dimethylcyclohexane	C8H16	No	Yes	0.16	0.06	0.11	0.02	0.48	0.18	0.04	0.01
c-1,2-Dimethylcyclohexane	C8H16	No	Yes	0.26	0.10	0.065	0.008	0.17	0.21	0.38	0.06
Aromatic Hydrocarbons Total				9.7	1.6	7.7	0.5	2.1	0.3	1.6	0.3
Benzene	C6H6	Yes	Yes	0.24	0.07	0.25	0.04	0.02	0.03	1.20	0.25
Toluene	C7H8	Yes	Yes	2.19	0.71	1.86	0.30	0.64	0.24	0.01	0.00
m,p-Xylene	C8H10	Yes	Yes	2.56	1.01	1.94	0.29	0.36	0.12	0.05	0.01
o-Xylene	C8H10	Yes	Yes	0.98	0.37	0.69	0.09	0.09	0.02	0.03	0.01
Ethylbenzene	C8H10	Yes	Yes	1.68	0.83	0.45	0.06	0.18	0.07	0.03	0.01
1,2,3-Trimethylbenzene	C9H12	No	Yes	0.17	0.06	0.31	0.04	0.23	0.08	0.01	0.00
1,2,4-Trimethylbenzene	C9H12	Yes	Yes	0.34	0.11	0.49	0.07			0.002	0.001
1,3,5-Trimethylbenzene	C9H12	No	Yes	0.15	0.04	0.26	0.03	0.28	0.08	0.02	0.00
2-Ethyltoluene	C9H12	No	No	0.25	0.07			0.045	0.014	0.01	0.00

3-Ethyltoluene	C9H12	No	No	0.32	0.12	0.27	0.04			0.02	0.00
4-Ethyltoluene	C9H12	No	No	0.20	0.06	0.16	0.02	0.058	0.024	0.01	0.00
n-Propylbenzene	C9H12	No	Yes	0.17	0.05	0.22	0.05			0.02	0.01
i-Propylbenzene	C9H12	No	Yes	0.10	0.05	0.02	0.01			0.00	0.00
n-Butylbenzene	C10H14	No	No	0.08	0.03	0.098	0.021	0.021	0.010	0.006	0.001
iso-Butylbenzene	C10H14	No	No	0.009	0.007	0.012	0.003	0.027	0.154	0.009	0.001
sec-Butylbenzene	C10H14	No	No	0.016	0.003	0.092	0.023	0.021	0.021	0.010	0.003
tert-Butylbenzene	C10H14	No	No					0.010	0.003		
1,2-Diethylbenzene	C10H14	No	No	0.02	0.01	0.060	0.016			0.001	0.000
1,3-Diethylbenzene	C10H14	No	No	0.03	0.01	0.072	0.016	0.062	0.068	0.008	0.002
1,4-Diethylbenzene	C10H14	No	No	0.08	0.02	0.038	0.007	0.031	0.055	0.015	0.003
p-Cymene	C10H14	No	No	0.011	0.007					0.055	0.013
Hexylbenzene	C12H18	No	No			0.048	0.014				
Styrene	C8H8	Yes	Yes	0.01	0.00	0.019	0.004	0.027	0.010	0.02	0.00
Indane (2,3-Dihydroindene)	C9H10	No	No	0.09	0.03	0.13	0.01	0.041	0.007	0.010	0.002
Naphthalene	C10H8	Yes	No	0.04	0.04	0.20	0.09				
Straight Chain Alkenes Total				0.71	0.25	0.26	0.03	2.48	0.65	2.23	0.21
Ethene	C2H4	Yes	Yes	0.22	0.22					0.79	0.17
Propene	C3H6	Yes	Yes	0.13	0.10					0.21	0.04
1-Butene/2-Methylpropene	C4H8	No	Yes	0.091	0.044					0.24	0.04
c-2-Butene	C4H8	No	Yes	0.020	0.013					0.005	0.001
t-2-Butene	C4H8	No	Yes	0.032	0.034			0.031	0.010	0.001	0.001
1-Pentene	C5H10	No	Yes	0.042	0.017					0.019	0.003
c-2-Pentene	C5H10	No	Yes							0.031	0.008
t-2-Pentene	C5H10	No	Yes	0.027	0.017					0.38	0.08
1-Hexene/2-Methyl-1-Pentene	C6H12	No	Yes	0.065	0.034					0.092	0.014
c-2-Hexene	C6H12	No	Yes			0.06	0.01				
t-2-Hexene	C6H12	No	Yes	0.021	0.017			0.024	0.007	0.039	0.006
t-3-Heptene	C7H14	No	Yes	0.032	0.034	0.09	0.02				

t-2-Heptene	C7H14	No	Yes	0.025	0.024	0.11	0.02	0.007	0.003	0.006	0.001
1-Octene	C8H16	No	No							0.42	0.09
t-2-Octene	C8H16	No	No					2.13	0.65		
1-Undecene	C11H22	No	No					0.29	0.09		
Branched and Cycloalkenes Total				0.1	0.04	0.4	0.04	0.12	0.07	1.95	0.30
2-Methyl-1-Butene	C5H10	No	Yes	0.025	0.013					0.04	0.01
2-Methyl-2-Butene	C5H10	No	Yes							0.92	0.24
3-Methyl-1-Butene	C5H10	No	Yes	0.011	0.003					0.010	0.002
3-Methyl-1-Pentene	C6H12	No	Yes	0.012	0.013			0.007	0.003	0.007	0.005
4-Methyl-1-Pentene	C6H12	No	Yes			0.06	0.01			0.008	0.005
c-3-Methyl-2-Pentene	C6H12	No	Yes							0.31	0.09
t-3-Methyl-2-Pentene	C6H12	No	Yes							0.016	0.011
t-4-Methyl-2-Pentene	C6H12	No	Yes					0.086	0.038		
Cyclopentene	C5H8	No	No							0.51	0.16
1-Methylcyclopentene	C6H10	No	Yes					0.017	0.055	0.12	0.04
Cyclohexene	C6H10	No	Yes	0.024	0.024	0.06	0.01				
1-Methylcyclohexene	C7H12	No	No	0.075	0.030	0.25	0.04	0.014	0.007		
Alkynes and Dienes Total				0.07	0.02	0.28	0.06	0	0	0.56	0.08
Ethyne	C2H2	No	Yes	0.058	0.024	0.28	0.06			0.560	0.078
Propyne	C3H4	No	No							0.027	0.007
1-Butyne	C4H6	No	No							0.001	0.000
1,3-Butadiene	C4H6	Yes	Yes	0.008	0.007					0.017	0.003
Oxygenated Hydrocarbons Total				8.5	1.3	4.0	0.5	7.05	0.90	0.63	0.67
Methanol	CH4O	No	Yes	2.47	0.85			3.13	0.62		
Formaldehyde	CH2O	Yes	Yes	1.83	0.63	0.68	0.14				
Acetaldehyde	C2H4O	Yes	No	0.90	0.25					0.082	0.087
Acetone	C3H6O	No	No	1.78	0.60	1.11	0.22	1.95	0.29	0.13	0.30
Acrolein	C3H4O	Yes	No	0.05	0.02					0.024	0.13
MVK+MACR	C4H6O	No	No	0.95	0.33	2.18	0.44	1.71	0.60	0.40	0.01

Butanone	C4H8O	No	No	0.56	0.20						
Chlorinated Hydrocarbons Total				0.01	0.00	0.17	0.02	0.27	0.12	0.011	0.003
Chloromethane	CH3Cl	Yes	No					0.24	0.12		
Dichloromethane	CH2Cl2	Yes	No			0.063	0.013				
Chloroform	CHCl3	Yes	No			0.018	0.004				
1,1-Dichloroethene	C2H2Cl2	No	No							0.001	0.000
1,2-Dichloroethane	C2H4Cl2	Yes	Yes	0.01	0.003	0.012	0.003	0.03	0.01		
c-1,2-Dichloroethene	C2H2Cl2	No	No							0.001	0.000
Hexachlorobutadiene	C4Cl6	No	No			0.082	0.014			0.009	0.003
Facility Sum (aE_{voc})				49.9	4.0	49.0	2.1	69.5	6.5	46.4	2.8
Biogenic Hydrocarbons Total				0.17	0.09	6.70	1.46	5.78	1.33	1.47	0.16
Isoprene	C5H8	Yes	No			5.92	1.5	3.57	1.23	0.39	0.10
a-Pinene	C10H16	No	Yes			0.64	0.17	0.47	0.16	0.32	0.06
b-Pinene	C10H16	No	Yes	0.17	0.08	0.12	0.03	1.13	0.42	0.45	0.09
Limonene	C10H16	No	Yes			0.073	0.017				
Camphene	C10H16	No	No					0.60	0.22	0.32	0.06

S4. Regression of Canister VOC compounds with Tracers from PTRMS

A number of VOCs in canister samples in plumes from the oil sands surface mining facilities were tightly correlated with selected PTRMS VOCs. Examples below in Figure S2 show such correlation between 5 VOCs in canister samples with C₇H₈ measured using PTRMS, 5 VOCs in canister samples with C₈H₁₀ measured using PTRMS, and 5 other VOCs in canister samples with C₉H₁₂ from PTRMS for the SML facility. The canisters were collected in downwind plumes of the facility over different days on different flights, and the corresponding PTRMS data were similarly from these different days.

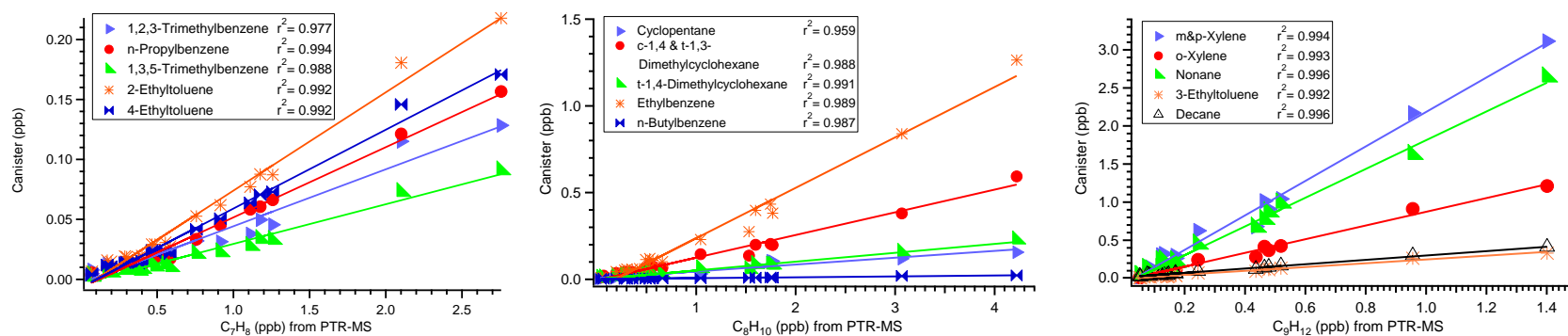


Figure S2. Regressions of 15 VOCs in canister samples to PTRMS C₇H₈ (left), C₈H₁₀ (centre), and C₉H₁₂ (right) in plumes of the SML facility. The slopes of the regression lines in the correlation of these compounds in canister samples with C₇H₈, C₈H₁₀, and C₉H₁₂, respectively, are used to derive emission ratios at sources (*Methods*). Note the correlation coefficients R² are all >0.95. For other compounds, R² drops (see Table S8). A cutoff R² was arbitrarily set at R²=0.80 for calculating the emission ratios.

S5. Estimation of Uncertainties in Mining Fleet Emissions

The VOC emissions from the mining truck fleet (E_{mt}) are not required in the reports to NPRI (Ref 4), but they were part of the aggregate emission rate of VOCs from a facility (aE) as determined from the aircraft measurements. Hence to compare aE with those reported to NPRI, E_{mt} must be subtracted from aE . E_{mt} is reported separately to Alberta Environment and Parks. For the year 2013, it may be estimated using the daily mining truck VOC emissions estimated for 2010 (Ref 39 in main text; repeated here as Ref 7) reported to Alberta Environment and Parks, but scaled to the 2013 volumes of mined oil sands (Ref 40 in main text; repeated here as Ref 8).

Reference 6 reported the mining truck VOC emissions for the year 2010 but did not include estimates of uncertainties and did not present how the emissions were derived. However, it appears that the VOC emissions were determined based on EPA Tier I truck emission factors, judging by the references provided in the report. Hence, it is possible to provide a rough estimate of the uncertainties in these results here by comparing real measurements of NO_x emission factors for these trucks as reported by Watson et al. (Ref 9).

Based on the study conducted by Watson et al. (2013) (Ref 9), these EPA Tier I truck emission factors may have been slightly higher than real emission factors for the oil sands mining fleet. Watson et al. (2013) showed that NO_x emissions from the mining trucks under real operating conditions in the oil sands have a NO_x emission factor lower than the EPA TIER 1 NO_x emission factors by about 10%. This difference may be considered as an indicator of the uncertainties in mining fleet VOC emission estimation used in Reference 7. Assuming that the EPA Tier emission factors used for VOCs emission estimates in Reference 7 were similarly higher by the same margin as was the case for NO_x, then the

actual mining truck VOC emissions would be 10% lower than the values estimated in the paper, and the mining fleet VOC emission E_{mt} subtraction from the aggregate emission rate of VOCs aE would be 10% smaller than presented in the paper. The end results would re-enforce the conclusion that emission reports underestimated the real emissions.

Bitumen production data are closely tracked by the Government of Alberta, as these data form the basis for calculation of royalties, which the facilities must remit to the government. Since no specific uncertainties were reported in Reference 8, the relative uncertainties of the oil sands mined on a daily basis were approximated with the standard errors of the monthly data over a moving window of 3-month period (adjusted for the number of days within a month). It is probable that the standard error in the 3-monthly data on oil sands mined vastly overestimated the relative uncertainties in the daily production data, and as such, the uncertainties in the mining fleet VOC emissions were likely overestimated. However, given the small contributions of E_{mt} to aE , this overestimation of uncertainties had little impact on the comparison between $(aE - E_{mt})$ with the facility total VOC emission reports to NPRI.

S6. Estimation of On-Road Traffic Emissions from the Road Sections Included in the Virtual Flight Boxes over the SML and SUN Facilities.

Highway 63, the main highway through the oil sands surface mining region, runs through the virtual flight boxes over both the SML and SUN facilities with different road lengths included in these boxes. As such, any VOC emissions from the on-road traffic in these boxes need to be subtracted from the aggregate emission rate of VOCs (aE) for comparison with the reported VOC emissions to the NPRI.

For the virtual boxes over the SML and SUN facilities, small stretches (17 km and 13 km, respectively) of Hwy 63 went through the flight virtual boxes. Reference 7 reported that for the road section from Fort Mackay to Ruth Lake (22 km in length, indicated by yellow pins in Figure S3 below) the total VOC emissions were 0.135 t/d (Table S4). Part of this road length, 17 km, was inside the flight box over the SML facility. Thus, the VOC emissions from this section are estimated as $0.135 \times (17/22) = 0.10$ t/d. This emission is about 11% of that emitted from the mining fleet of the facility, which at 0.9 ± 0.1 t/d is a minor fraction of the aggregate aE itself. For completeness, this on-road traffic VOC emission was added to the mining fleet emissions, so that $E_{mt} = 1.0 \pm 0.1$ t/d. This E_{mt} value is subtracted from the aggregated VOC emissions ($aE - E_{mt}$) for the comparison with the reports to NPRI (see main text).

A similar analysis is carried out for the SUN facility, where a section of 13 km of Hwy 63 runs through the virtual flight box. Traffic emissions from this section are similarly estimated as above. The section of Hwy 63 in the box was divided into two parts (Ref 7). The first part, of 5 km length from Ruth Lake to Suncor Turnoff, is entirely within the flight box and has a VOC emission of 0.051 t/d (Table S4). The remaining 8 km part within the virtual flight box, starting from Suncor Turnoff, was part of a larger road section of 26 km from Suncor Turnoff to Fort Murray (indicated by yellow pins in Figure S1 below), for which the VOC emission was reported at 0.362 t/d (Table S4). Hence, the 8-km road part of the section would have a VOC emission of $0.362 \times (8/26) = 0.11$ t/d within the virtual flight box. The total on-road VOC emissions from the two road sections (5 km + 8 km) within the box are then determined to be $0.051 + 0.11 = 0.16$ t/d. Compared to the mining fleet emission (estimated 3.4 ± 0.6 t/d) for SUN, the on-road traffic VOC emissions from Hwy 63 are very small (<5%). More importantly, they are only 0.3% of aE .

Nonetheless, the on-road traffic VOC emissions are added to the mining fleet emissions, so that $E_{mt} = 3.6 \pm 0.6$ t/d, and then subtracted from the aggregate VOC emissions ($aE - E_{mt}$) for comparison with reports to NPRI (see main text).

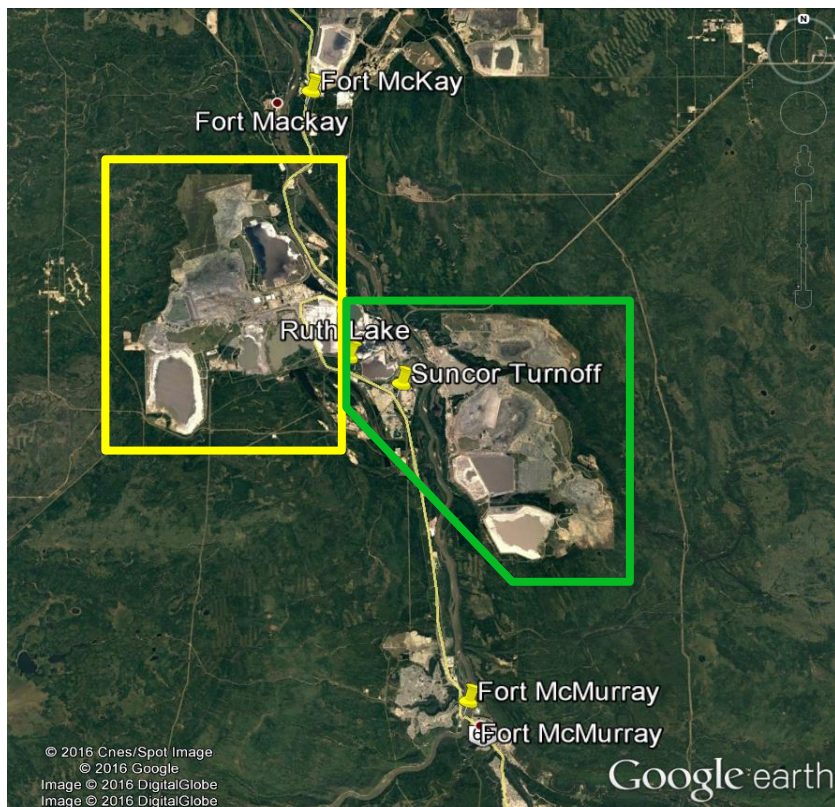


Figure S3. Segments of Highway 63 and virtual flight boxes for SML (yellow) and SUN (green) facilities. Yellow pins are the starting and ending points of each road segment as given in Table S4 below.

Table S4. Segments of Highways 63 entirely or partially within the virtual SML and SUN flight boxes (Ref 7).

Highway 63 Segment	Starting Point		Ending Point		Length (km)	VOC Emission (t/d)
	LAT	LON	LAT	LON		
Fort McKay to Ruth Lake	57.184	-111.637	56.989	-111.551	22	0.135
Ruth Lake to Suncor turnoff	56.989	-111.551	56.969	-111.486	5	0.051

Suncor turnoff to Fort McMurray	56.969	-111.486	56.735	-111.406	26	0.362
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S7. Results of Emission Rates of Individual VOC Compounds for Four Oil Sands Surface Mining Facilities

The percentage contributions from the top 60 VOC compounds to the aggregate emission rate of all VOC compounds **aE** are plotted here for each of the four facilities. The list of compounds is comprised of alkanes, alkenes, and aromatics from the canisters and aromatics and OVOCs from the PTRMS. The canister VOC results are derived from the emission ratios of compounds to tracers from the PTRMS, whereas the emission rates of the OVOCs from the PTRMS are derived from the TERRA algorithm, as shown in *Methods*.

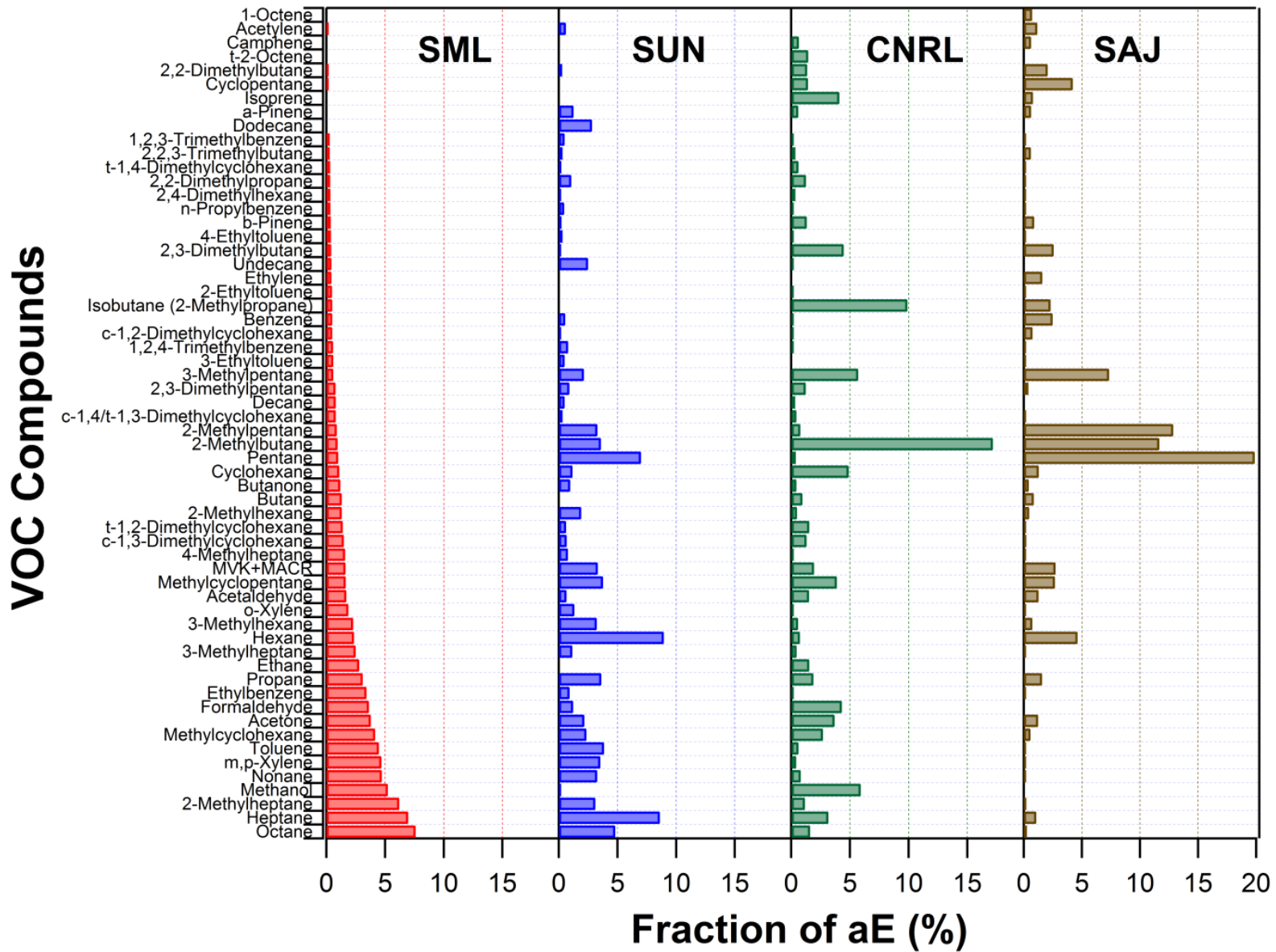


Figure S4. The mass fractions of the top 60 VOC species in aE, accounting for 97%, 96%, 99.5%, and 95% of aE at the four facilities, respectively.

S8. Species Emission Reports to NPRI and Observed Species Emission Rates

Table S5. The reported emission rate of individual species in the NPRI Part 1 (Ref 4) compared to the observed rates derived from upscaling the results in Table S3 after correction for seasonal variations. Note that mining fleet contributions were subtracted from the results in Table S3 by assuming the same fraction of mining fleet contribution as in total VOC emissions. The upscaling also takes into account the seasonal changes. NQ – not quantified. NM – not measured.

NPRI Part 1 Reported Species 2013	Formula	NPRI Species Emission tonnes/year	Observed Species Emission tonnes/year	Observed/ NPRI Report Ratio
SML Reported Part 1 Species				
Isoprene	C5H8	0.2	NQ	
Cumene (i-propylbenzene)	C9H12	8.8	NQ	
Ethene	C2H4	60.9	58.9	1.0
Propene	C3H6	65.6	36.4	0.6
1,3-Butadiene	C4H6	1.3	2.2	1.6
Benzene	C6H6	33.7	64.3	1.9
Cyclohexane	C6H12	91.4	146.6	1.6
n-Hexane	C6H14	121.1	311.6	2.6
Toluene	C7H8	136.4	594.7	4.4
Styrene	C8H8	0.3	2.9	9.0
Xylene isomers 1,2,4-	C8H10	275.3	959	3.5
Trimethylbenzene	C9H12	28.6	93.1	3.3
Ethylbenzene	C8H10	47.6	456.7	9.6
Naphthalene	C10H8	0.3	11.1	42.5
Average Ratio				6.8
Standard Deviation in Ratio				11.6
Median Ratio				2.9
Lower Quartile of Ratios				1.6

Upper Quartile of Ratios				5.5
SUN Reported Part 1 Species				
Ethene	C2H4	81.2	NQ	
Propene	C3H6	6.5	NQ	
Methanol	CH3O	6.1	NQ	
Isopropyl alcohol	C3H8O	0.9	NM	
Benzene	C6H6	13.6	66.4	4.9
Cyclohexane	C6H12	87.0	151.4	1.7
n-Hexane	C6H14	164.0	1135	6.9
Toluene	C7H8	144.0	489.5	3.4
Xylene (all isomers)	C8H10	175.1	810.2	4.6
Ethylbenzene	C8H10	36.4	118.8	3.3
1,2,4-Trimethylbenzene	C9H12	38.8	130.0	3.4
Naphthalene	C10H8	0.6	52.7	93.7
Average Ratio				15.2
Standard Deviation in Ratio				31.8
Median Ratio				4.0
Lower Quartile of Ratios				3.3
Upper Quartile of Ratios				5.4
CNRL Reported Part 1 Species				
Formaldehyde	CH2O	21.2	NQ	
1,2,4-Trimethylbenzene	C9H12	10.1	NQ	
Benzene	C6H6	7.1	5.5	0.8
Cyclohexane	C6H12	223.7	1071.9	4.8
n-Hexane	C6H14	41.7	211.5	5.1
Toluene	C7H8	21.8	170.3	7.8
Xylene isomers	C8H10	40.6	119.0	2.9
Ethylbenzene	C8H10	8.3	47.6	5.7
Average Ratio				4.5
Standard Deviation in Ratio				2.4
Median Ratio				4.9
Lower Quartile of Ratios				3.4
Upper Quartile of Ratios				5.6

SAJ Reported Part 1 Species				
n-Hexane	C6H14	280.8	480.9	1.7
Benzene	C6H6	3.6	253.8	69.9
Average Ratio				35.8

Table S6. The reported emission rate of individual species in the NPRI Part 5 (Ref 4) compared to the observed rates derived from upscaling the results in Table S3 after taking into account seasonal variations. Note that mining fleet contributions were subtracted from the results in Table S3 by assuming the same fraction of mining fleet contribution as in total VOC emissions. The upscaling also takes into account the seasonal changes. NQ – not quantified. NM – not measured.

NPRI Part 5 Reported Species 2013	Formula	NPRI Species Emission tonnes/year	Observed Species Emission tonnes/year	Observed/ NPRI Report Ratio
SML Reported Part 5 Species				
Cyclohexene + isomers	C6H10	0.03	NQ	
Tetrahydrofuran	C4H8O	0.45	NM	
Ethyne	C2H2	1.91	15.6	8.2
Ethene	C2H4	37.03	58.9	1.6
Propene	C3H6	25.11	36.4	1.4
Propane	C3H8	30.26	396.2	13.1
1,3-Butadiene	C4H6	0.49	2.2	4.5
Butene + isomers	C4H8	5.60	38.8	6.9
Butane + isomers	C4H10	27.58	131.1	4.8
Pentene + isomers	C5H10	0.29	23.4	80.5
Pentane + isomers	C5H12	3.25	297.4	91.6
Benzene	C6H6	4.17	64.3	15.4
Hexene + isomers	C6H12	0.08	248.0	3100
n-Hexane	C6H14	0.15	311.6	2023
Hexane isomers	C6H14	0.02	269.5	12251
Toluene	C7H8	1.58	594.7	375
Cycloheptane + isomers	C7H14	0.05	586.2	12744
Heptane + isomers	C7H16	0.06	1590	27891
Styrene	C8H8	0.07	2.9	40.0
Xylene isomers	C8H10	0.73	959	1306
Cyclooctane + isomers	C8H16	0.05	636.4	12728

1,2,4-Trimethylbenzene	C9H12	0.10	93.1	895
Trimethylbenzene isomers	C9H12	0.12	459.7	3863
Nonane + isomers	C9H20	0.07	649.3	9411
Decane and isomers	C10H22	0.03	141.4	5238
Average Ratio				4004
Standard Deviation in Ratio				6846
Median Ratio				375
Lower Quartile of Ratios				11
Upper Quartile of Ratios				4550
SUN Reported Part 5 Species				
Ethene	C2H4	106.5	NQ	
Propene	C3H6	6.5	NQ	
Butene + isomers	C4H8	51.7	NQ	
Butane + isomers	C4H10	332.2	NQ	
Pentene + isomers	C5H10	36.4	NQ	
Methylindan + isomers	C10H12	1.3	NM	
Methanol	CH3O	6.1	NQ	
Methyl isobutyl ketone	C6H12O	2.3	NM	
Ethyne	C2H2	33.4	72.5	2.2
Propane	C3H8	227.2	443.1	2.0
Pentane + isomers	C5H12	231.3	1453	6.3
Benzene	C6H6	13.6	66.4	4.9
Cyclohexene + isomers	C6H10	2.4	15.2	6.3
Hexene + isomers	C6H12	77.1	667.2	8.7
n-Hexane	C6H14	186.6	1135	6.1
Hexane isomers	C6H14	181.1	740.4	4.1
Toluene	C7H8	144.0	489.5	3.4
Cycloheptane + isomers	C7H14	126.3	364.6	2.9
Heptane + isomers	C7H16	335.4	1958	5.8
Xylene isomers	C8H10	175.1	691.4	3.9
Cyclooctane + isomers	C8H16	72.4	267.6	3.7
Octane + isomers	C8H18	254.6	1336	5.2
1,2,4-Trimethylbenzene	C9H12	38.8	130.0	3.4
Trimethylbenzene isomers	C9H12	39.9	456.8	11.4
Nonane + isomers	C9H20	120.7	433.8	3.6

Decane + isomers	C10H22	95.9	81.1	0.8
Dodecane + isomers	C12H26	14.5	389.6	26.8
Formaldehyde	CH2O	6.9	178.6	26.0
Average Ratio				6.9
Standard Deviation in Ratio				7.1
Median Ratio				4.5
Lower Quartile of Ratios				3.4
Upper Quartile of Ratios				6.3
CNRL Reported Part 5 Species				
Propene	C3H6	10.7	NQ	
1,3-Butadiene	C4H6	3.4	NQ	
1,2,4-Trimethylbenzene	C9H12	10.1	NQ	
Formaldehyde	CH2O	30.8	NQ	
Propane	C3H8	156.7	467.8	3.0
Butane + isomers	C4H10	37.3	2237	60.0
Pentane + isomers	C5H12	17.5	4109	234.6
Benzene	C6H6	7.1	5.5	0.8
n-Hexane	C6H14	41.7	211.5	5.1
Hexane isomers	C6H14	19.7	1598	81.0
Toluene	C7H8	21.8	170.3	7.8
Heptane + isomers	C7H16	22.5	1639	72.8
Xylene isomers	C8H10	40.6	119.0	2.9
Octane + isomers	C8H18	16.8	1056	62.8
Average Ratio				58.6
Standard Deviation in Ratio				73.8
Median Ratio				60.0
Lower Quartile of Ratios				5.1
Upper Quartile of Ratios				72.8
SAJ Reported Part 5 Species				
Butene + isomers	C4H8	211.6	52.2	0.3
Pentane + isomers	C5H12	1982.8	3261	1.6
Benzene	C6H6	3.6	253.8	69.9
Cyclohexene + isomers	C6H10	1.2	26.2	22.4
Hexene + isomers	C6H12	3.1	441.6	141.0
n-Hexane	C6H14	280.8	480.9	1.7
Average Ratio				39.5

Standard Deviation in Ratio	56.4
Median Ratio	12.0
Lower Quartile of Ratios	1.7
Upper Quartile of Ratios	58.0

S9. Summary of VOC Measurements Made in Flights over the SML Facility

Measurement statistics for VOC mixing ratios for emission flights over the SML facility as determined from both PTRMS measurements and the canister sampling/GC analysis. Similar results can be obtained from results for flights over the SUN, CNRL, and SAJ facilities but are not tabulated here. Detailed results are published in the Joint Oil Sands Monitoring data portal (<http://jointoilsandsmonitoring.ca/default.asp?lang=En&n=A743E65D-1>).

Table S7. VOC compounds measured with the PTRMS instrument. Air mixing ratio statistics are listed for the SML facility only. Corresponding statistics for air mixing ratio data from the SUN, CNRL, and SAJ facilities can be derived from the original data published in the Joint Oil Sands Monitoring data portal (<http://jointoilsandsmonitoring.ca/default.asp?lang=En&n=A743E65D-1>). The detection limits, precisions, and accuracies for the compounds are the same for the SUN, CNRL, and SAJ facilities. BDL = below detection limit.

Compound Formula	Detection Limit	Precision	Accuracy	SML					
	pptv			%	%	Mean	Max	90th percentile	80th percentile
Response factors determined from calibration standards									
C ₂ H ₃ N	130	3	6	140	680	300	240	140	BDL
CH ₄ O	640	3	8	7700	16000	10400	9700	8400	BDL
C ₂ H ₄ O	500	3	5	660	3500	1340	1070	590	BDL
C ₃ H ₄ O	210	3	5	94	680	280	210	79	BDL
C ₃ H ₆ O	320	3	5	2900	5700	4000	3700	3100	BDL
C ₄ H ₆ O	140	3	6	650	1900	1200	1050	690	BDL
C ₄ H ₈ O	130	3	5	310	1100	560	470	310	BDL
C ₅ H ₈	270	3	5	1200	8300	2900	2200	860	BDL
C ₆ H ₆	84	3	5	83	1700	200	130	51	BDL
C ₇ H ₈	79	3	5	130	3500	325	150	38	BDL

C ₈ H ₁₀	69	3	6	130	5300	310	89	4.7	BDL
C ₁₀ H ₁₆	90	3	5	290	1600	740	560	200	BDL
Response factors determined from proton transfer reaction kinetic rate constants									
C ₆ H ₁₀	96	3	20	220	3400	590	340	90	BDL
C ₆ H ₁₂	55	3	20	31	840	116	67	11	BDL
C ₇ H ₁₄	71	3	20	3.2	200	37	20	BDL	BDL
C ₈ H ₈	130	3	20	25	425	88	59	12	BDL
C ₈ H ₁₆	130	3	20	2.5	130	27	17	BDL	BDL
C ₉ H ₁₀	120	3	20	20	300	79	50	6.9	BDL
C ₉ H ₁₂	72	3	20	67	1900	320	210	BDL	BDL
C ₁₀ H ₁₄	45	3	20	32	610	180	110	1.5	BDL

Table S8. Canister sample VOC compound concentration statistics for the SML facility. Empty entries for species indicate that there were no emission rates determined for those species. NR = not reported, BDL = below detection limit. Reported uncertainties from this method are 30% for concentrations below 0.02 $\mu\text{g m}^{-3}$, 20% for 0.02 $\mu\text{g m}^{-3}$ to 0.2 $\mu\text{g m}^{-3}$, and 10% above 0.2 $\mu\text{g m}^{-3}$ (Ref 10). These detection limits were converted to mixing ratios presented below using the ambient temperature and pressure encountered during the airborne measurements.

For each VOC species determined in the canister samples, correlations with a tracer were investigated, and the tracer with the highest correlation coefficient R^2 was chosen for a particular VOC species in the canisters to determine the regression slope ($b \pm \Delta b$) and further to determine their emission ratios after correction for oxidation losses. Δb is the standard deviation on b , from which the standard error δ_b is calculated for further uncertainty propagation analyses. See main article for the details. In this table, a list of 12 tracers were used for the VOCs species from the canisters, including 10 tracers measured with the PTRMS instrument and CO/CH₄ from a concurrent continuous cavity ring down spectroscopy instrument (Picarro Model G2401) also on board the aircraft (Ref. 11). Empty cells in the correlation table indicate that no emission rates could be determined from this emission ratio approach.

In addition to the listed compounds in this table, laboratory analyses of the canister samples also targeted an additional 72 VOC compounds. These compounds were observed in canisters collected in the plumes from the facility but their concentrations were low. The emission ratio approach was not suitable to determine their emission rates from the facility.

Compound Name	Formula	Detection limit	Precision (n=46)	SML (n = 106)						Correlation with tracers to determine regression slope b			
				Max	90th percentile	80th percentile	Median	Min	Mean	Tracer of Choice	R ²	b	Δb
N-Alkanes													

Ethane	C ₂ H ₆	24	Not Reported	15000	4000	3700	2500	510	2600	C ₆ H ₆	0.924	4.02	0.53
Propane	C ₃ H ₈	50	13%	3300	2600	2300	1800	130	1500	C ₆ H ₆	0.830	3.09	0.66
Butane	C ₄ H ₁₀	11	11%	2700	1200	830	580	42	630	CO	0.915	0.025	0.0004
Pentane	C ₅ H ₁₂	10	11%	680	380	260	190	36	210	C ₆ H ₆	0.893	0.62	0.099
Hexane	C ₆ H ₁₄	12	15%	1500	450	270	88	BDL	190	C ₇ H ₈	0.984	0.56	0.073
Heptane	C ₇ H ₁₆	9.9	19%	4100	960	550	88	BDL	330	C ₇ H ₈	0.988	1.43	0.16
Octane	C ₈ H ₁₈	3.8	20%	5500	840	400	32	BDL	310	C ₈ H ₁₀	0.987	1.22	0.22
Nonane	C ₉ H ₂₀	4.7	23%	2600	450	220	24	BDL	150	C ₉ H ₁₂	0.996	1.89	0.060
Decane	C ₁₀ H ₂₂	4.5	26%	410	130	63	20	BDL	44	C ₉ H ₁₂	0.996	0.29	0.0096
Undecane	C ₁₁ H ₂₄	3.3	25%	180	78	46	18	BDL	31	C ₁₀ H ₁₄	0.973	0.44	0.0096
Dodecane	C ₁₂ H ₂₆	4.1	22%	330	92	65	26	BDL	41				
Branched Alkanes													
Isobutane (2-Methylpropane)	C ₄ H ₁₀	10	8.7%	970	480	360	260	15	250	CO	0.936	0.0095	0.0001
2-Methylbutane	C ₅ H ₁₂	12	8.9%	650	380	320	190	31	210	C ₆ H ₆	0.883	0.58	0.098
2,2-Dimethylpropane	C ₅ H ₁₂	3.7	17%	370	120	78	26	BDL	51	C ₆ H ₁₀	0.869	0.085	0.032
2-Methylpentane	C ₆ H ₁₄	17	15%	560	200	120	59	BDL	90	C ₇ H ₈	0.985	0.21	0.027
3-Methylpentane	C ₆ H ₁₄	11	12%	390	130	78	38	BDL	57	C ₇ H ₈	0.990	0.14	0.015
2,2-Dimethylbutane	C ₆ H ₁₄	13	5.7%	110	48	28	BDL	BDL	19	C ₆ H ₁₀	0.951	0.035	0.0076
2,3-Dimethylbutane	C ₆ H ₁₄	4.3	26%	210	75	48	20	BDL	31	C ₆ H ₁₀	0.965	0.070	0.013
2-Methylhexane	C ₇ H ₁₆	4.4	19%	760	200	110	29	BDL	72	C ₇ H ₈	0.989	0.27	0.029
3-Methylhexane	C ₇ H ₁₆	3.7	16%	1300	350	200	43	BDL	120	C ₇ H ₈	0.990	0.47	0.049
2,2-Dimethylpentane	C ₇ H ₁₆	11	7.8%	25	BDL	BDL	BDL	BDL	BDL	C ₆ H ₁₀	0.954	0.0085	0.0018
2,3-Dimethylpentane	C ₇ H ₁₆	5.9	14%	480	120	77	27	BDL	50	C ₇ H ₈	0.987	0.16	0.019
2,4-Dimethylpentane	C ₇ H ₁₆	4.5	7.5%	82	29	17	8	BDL	12	C ₆ H ₁₂	0.988	0.13	0.003
2,2,3-Trimethylbutane	C ₇ H ₁₆	5.0	17%	120	37	22	7.8	BDL	15	C ₆ H ₁₀	0.975	0.040	0.0062
2-Methylheptane	C ₈ H ₁₈	4.2	29%	3200	540	290	28	BDL	200	C ₇ H ₈	0.991	1.12	0.11
3-Methylheptane	C ₈ H ₁₈	3.6	25%	1300	200	110	9.4	BDL	76	C ₇ H ₈	0.990	0.45	0.048
4-Methylheptane	C ₈ H ₁₈	3.8	23%	820	140	76	12	BDL	54	C ₇ H ₈	0.989	0.29	0.032

2,4-Dimethylhexane	C ₈ H ₁₈	4.2	33%	180	33	19	BDL	BDL	13	C ₇ H ₈	0.988	0.060	0.0073
2,5-Dimethylhexane	C ₈ H ₁₈	3.4	7.6%	130	26	16	3.6	BDL	10	C ₇ H ₈	0.988	0.047	0.0052
2,3,4-Trimethylpentane	C ₈ H ₁₈	3.3	8.7%	110	21	13	3.5	BDL	8.7	C ₆ H ₁₂	0.990	0.17	0.0036
2,2,5-Trimethylhexane	C ₉ H ₂₀	2.3	BDL	10	BDL	BDL	BDL	BDL	BDL				
3,6-Dimethyloctane	C ₁₀ H ₂₂	2.9	14%	56	10	5.4	BDL	BDL	3.4	C ₇ H ₈	0.827	0.018	0.0088
Cycloalkanes													
Cyclopentane	C ₅ H ₁₀	4.1	18%	160	61	32	17	BDL	26	C ₈ H ₁₀	0.959	0.0035	0
Methylcyclopentane	C ₆ H ₁₂	4.7	14%	1100	300	160	53	BDL	110	C ₇ H ₈	0.987	0.40	0.047
Cyclohexane	C ₆ H ₁₂	5.5	13%	760	170	90	27	BDL	66	C ₇ H ₈	0.989	0.27	0.029
Methylcyclohexane	C ₇ H ₁₄	4.2	15%	2500	460	270	43	BDL	180	C ₇ H ₈	0.991	0.87	0.085
c-1,3-Dimethylcyclohexane	C ₈ H ₁₆	3.0	18%	1100	160	90	12	BDL	65				
t-1,2-Dimethylcyclohexane	C ₈ H ₁₆	3.3	17%	770	110	61	9.6	BDL	46				
c-1,4/t-1,3-Dimethylcyclohexane	C ₈ H ₁₆	4.4	19%	590	82	48	6.6	BDL	35	C ₈ H ₁₀	0.988	0.13	0.023
t-1,4-Dimethylcyclohexane	C ₈ H ₁₆	4.2	9.9%	230	37	20	BDL	BDL	15	C ₈ H ₁₀	0.991	0.051	0.0079
c-1,2-Dimethylcyclohexane	C ₈ H ₁₆	5.2	33%	260	30	17	BDL	BDL	13	C ₆ H ₁₂	0.911	0.41	0.027
Aromatic Hydrocarbons													
Benzene	C ₆ H ₆	8.3	8.2%	380	140	90	69	24	79	C ₇ H ₈	0.990	0.13	0.01
Toluene	C ₇ H ₈	25	19%	2800	650	350	89	BDL	230	C ₇ H ₈	0.991	1.0	0.1
m,p-Xylene	C ₈ H ₁₀	14	22%	3100	540	260	34	BDL	190	C ₉ H ₁₂	0.994	2.3	0.09
o-Xylene	C ₈ H ₁₀	8.1	25%	1200	230	120	16	BDL	81	C ₉ H ₁₂	0.993	0.90	0.038
Ethylbenzene	C ₈ H ₁₀	6.6	25%	1300	230	100	14	BDL	75	C ₈ H ₁₀	0.989	0.29	0.049
1,2,3-Trimethylbenzene	C ₉ H ₁₂	6.1	7.2%	130	42	20	7.4	BDL	16	C ₇ H ₈	0.977	0.047	0.0075
1,2,4-Trimethylbenzene	C ₉ H ₁₂	13	8.1%	250	74	35	12	BDL	27	C ₇ H ₈	0.985	0.096	0.012
1,3,5-Trimethylbenzene	C ₉ H ₁₂	6.7	3.0%	91	25	11	BDL	BDL	8.5	C ₇ H ₈	0.988	0.033	0.0039
2-Ethyltoluene	C ₉ H ₁₂	6.7	7.3%	220	51	27	BDL	BDL	19	C ₇ H ₈	0.992	0.082	0.0074
3-Ethyltoluene	C ₉ H ₁₂	7.1	7.9%	330	71	38	8.1	BDL	27	C ₉ H ₁₂	0.992	0.25	0.011
4-Ethyltoluene	C ₉ H ₁₂	5.4	8.4%	170	42	22	BDL	BDL	15	C ₇ H ₈	0.992	0.066	0.0059

n-Propylbenzene	C ₉ H ₁₂	6.4	7.9%	160	35	18	BDL	BDL	13	C ₇ H ₈	0.994	0.059	0.0049
i-Propylbenzene	C ₉ H ₁₂	6.9	27%	300	33	17	BDL	BDL	15	C ₆ H ₁₂	0.733	0.16	0.021
n-Butylbenzene	C ₁₀ H ₁₄	5.5	3.8%	23	7.6	BDL	BDL	BDL	3.0	C ₈ H ₁₀	0.987	0.0051	0.0009
iso-Butylbenzene	C ₁₀ H ₁₄	4.9	BDL	7.9	BDL	BDL	BDL	BDL	BDL	C ₇ H ₈	0.868	0.0027	0.0011
sec-Butylbenzene	C ₁₀ H ₁₄	5.3	2.7%	19	BDL	BDL	BDL	BDL	2.0	C ₈ H ₁₀	0.994	0.0044	0.0005
tert-Butylbenzene	C ₁₀ H ₁₄	6.3	15%	BDL	BDL	BDL	BDL	BDL	BDL				
1,2-Diethylbenzene	C ₁₀ H ₁₄	6.3	BDL	15	BDL	BDL	BDL	BDL	1.7	C ₇ H ₈	0.987	0.0052	0.0006
1,3-Diethylbenzene	C ₁₀ H ₁₄	5.9	2.4%	21	BDL	BDL	BDL	BDL	2.0	C ₇ H ₈	0.988	0.0077	0.0009
1,4-Diethylbenzene	C ₁₀ H ₁₄	8.7	2.0%	57	18	13	BDL	BDL	6.7	C ₇ H ₈	0.982	0.022	0.0030
p-Cymene	C ₁₀ H ₁₄	5.9	23%	190	17	11	BDL	BDL	9.1	CH ₄	0.985	3.1E-5	1.5E-6
Hexylbenzene	C ₁₂ H ₁₈	3.8	BDL	27	8.1	5.1	BDL	BDL	3.3				
Styrene	C ₈ H ₈	8.9	6.6%	15	BDL	BDL	BDL	0.53	BDL	C ₂ H ₄ O	0.959	0.0033	0.0005
Indane (2,3-Dihydroindene)	C ₉ H ₁₀	7.7	2.1%	78	24	12	BDL	BDL	9.0	C ₇ H ₈	0.981	0.030	0.0042
Naphthalene	C ₁₀ H ₈	9.4	35%	37	20	14	BDL	BDL	10	C ₁₀ H ₁₄	0.942	0.092	0.003
Straight Chain Alkenes													
Ethene	C ₂ H ₄	17	NR	1500	640	560	300	69	350	C ₇ H ₈	0.803	0.32	0.17
Propene	C ₃ H ₆	12	8.2%	770	200	170	81	16	110	C ₇ H ₈	0.871	0.11	0.05
1-Butene/2-Methylpropene	C ₄ H ₈	16	9.0%	240	94	80	40	BDL	52	C ₇ H ₈	0.951	0.054	0.013
c-2-Butene	C ₄ H ₈	6.5	8.0%	26	13	8.7	BDL	BDL	5.5	C ₇ H ₈	0.871	0.0067	0.0027
t-2-Butene	C ₄ H ₈	6.0	10%	30	14	9.0	BDL	BDL	5.3	C ₇ H ₈	0.794	0.0085	0.0047
1-Pentene	C ₅ H ₁₀	20	7.3%	61	27	22	BDL	BDL	14	C ₇ H ₈	0.971	0.020	0.0035
c-2-Pentene	C ₅ H ₁₀	6.9	BDL	9.1	BDL	BDL	BDL	BDL	BDL				
t-2-Pentene	C ₅ H ₁₀	4.6	12%	21	8.8	6.1	BDL	BDL	3.5	C ₇ H ₈	0.917	0.0059	0.0019
1-Hexene/2-Methyl-1-Pentene	C ₆ H ₁₂	21	9.7%	64	25	16	BDL	BDL	9.5	C ₇ H ₈	0.937	0.024	0.0065
c-2-Hexene	C ₆ H ₁₂	8.7	BDL	9.1	BDL	BDL	BDL	BDL	BDL				
t-2-Hexene	C ₆ H ₁₂	5.5	6.5%	13	BDL	BDL	BDL	BDL	BDL	C ₇ H ₈	0.863	0.0042	0.0018
t-3-Heptene	C ₇ H ₁₄	6.5	8.0%	7.6	BDL	BDL	BDL	BDL	BDL	C ₇ H ₈	0.811	0.0027	0.0014
t-2-Heptene	C ₇ H ₁₄	5.5	6.1%	11	BDL	BDL	BDL	BDL	BDL	C ₇ H ₈	0.801	0.0036	0.0019

1-Octene	C ₈ H ₁₆	4.4	79%	100	14	7.4	BDL	BDL	5.3				
t-2-Octene	C ₈ H ₁₆	3.7	8.0%	35	BDL	BDL	BDL	BDL	BDL				
1-Undecene	C ₁₁ H ₂₂	3.7	14%	18	BDL	BDL	BDL	BDL	BDL				
Branched and Cycloalkenes													
2-Methyl-1-Butene	C ₅ H ₁₀	6.9	12%	30	12	9.2	BDL	BDL	5.8	C ₇ H ₈	0.920	0.0088	0.0027
2-Methyl-2-Butene	C ₅ H ₁₀	7.3	15%	15	BDL	BDL	BDL	BDL	BDL				
3-Methyl-1-Butene	C ₅ H ₁₀	2.5	13%	17	6.3	5.4	BDL	BDL	3.3	C ₇ H ₈	0.961	0.0053	0.0011
3-Methyl-1-Pentene	C ₆ H ₁₂	6.1	BDL	8.2	BDL	BDL	BDL	BDL	BDL	C ₇ H ₈	0.811	0.0027	0.0014
4-Methyl-1-Pentene	C ₆ H ₁₂	6.8	5.1%	15	BDL	BDL	BDL	BDL	BDL				
c-3-Methyl-2-Pentene	C ₆ H ₁₂	7.4	BDL	7.0	BDL	BDL	BDL	BDL	BDL				
t-3-Methyl-2-Pentene	C ₆ H ₁₂	7.5	BDL	2.7	BDL	BDL	BDL	BDL	BDL				
t-4-Methyl-2-Pentene	C ₆ H ₁₂	8.5	BDL	11	BDL	BDL	BDL	BDL	BDL				
Cyclopentene	C ₅ H ₈	14	BDL	7.6	BDL	BDL	BDL	BDL	BDL				
1-Methylcyclopentene	C ₆ H ₁₀	14	BDL	11	BDL	BDL	BDL	BDL	BDL				
Cyclohexene	C ₆ H ₁₀	8.7	BDL	17	BDL	BDL	BDL	BDL	BDL	C ₇ H ₈	0.798	0.0056	0.003
1-Methylcyclohexene	C ₇ H ₁₄	7.7	BDL	28	8.3	BDL	BDL	BDL	3.1	C ₇ H ₈	0.971	0.0089	0.0016
Alkynes and Dienes													
Ethyne	C ₂ H ₂	9.4	NR	910	380	270	210	60	230	C ₃ H ₄ O	0.862	2.53	0.085
Propyne	C ₃ H ₄	11	27%	25	20	16	BDL	BDL	9.3				
1-Butyne	C ₄ H ₆	6.4	BDL	1.1	BDL	BDL	BDL	BDL	BDL				
1,3-Butadiene	C ₄ H ₆	6.8	6.9%	21	8.1	6.2	BDL	BDL	3.9	C ₈ H ₁₀	0.948	0.0039	0.0015
Biogenic Hydrocarbons													
Isoprene (2-Methyl-1,3-Butadiene)	C ₅ H ₈	10	6.8%	5000	2300	1300	560	BDL	910				
a-Pinene	C ₁₀ H ₁₆	13	12%	171	91	64	24	BDL	40				
b-Pinene	C ₁₀ H ₁₆	13	13%	370	210	64	14	BDL	55	C ₉ H ₁₂	0.975	0.14	0.0106
Camphene	C ₁₀ H ₁₆	16	9.4%	130	97	69	27	BDL	38				
Limonene	C ₁₀ H ₁₆	21	3.5%	230	26	13	BDL	BDL	12				
Chlorinated Hydrocarbons													
Chloromethane	CH ₃ Cl	8.1	4.5%	730	680	660	630	530	630				

Dichloromethane	CH ₂ Cl ₂	4.2	4.2%	140	73	70	65	56	67				
Chloroform	CHCl ₃	4.5	5.8%	33	25	22	18	12	19				
1,1-Dichloroethene	C ₂ H ₂ Cl ₂	5.6	BDL	BDL	BDL	BDL	BDL	BDL	BDL				
1,2-Dichloroethane	C ₂ H ₄ Cl ₂	3.2	7.3%	23	15	14	12	10	13	C ₇ H ₈	0.893	0.0024	0.0009
c-1,2-Dichloroethene	C ₂ H ₂ Cl ₂	5.0	BDL	BDL	BDL	BDL	BDL	BDL	BDL				
Hexachlorobutadiene	C ₄ Cl ₆	5.2	BDL	BDL	BDL	BDL	BDL	BDL	BDL				

Table S9. Canister sample VOC compound concentration statistics for the SUN facility. Empty entries for species indicate that there were no emission rates determined for those species. The details are similar to those explained for Table S8.

Compound Name	Formula	SUN (n = 130)						Correlation with tracers to determine regression slope b			
		Max	90th percentile	80th percentile	Median	Min	Mean	Tracer of Choice	R ²	b	Δb
N-Alkanes											
Ethane	C ₂ H ₆	2600	2570	2010	1000	620	1300				
Propane	C ₃ H ₈	910	870	650	460	230	510	C ₉ H ₁₂	0.56	3.43	0.20
Butane	C ₄ H ₁₀	500	360	330	240	71	240	C ₉ H ₁₂	0.76	4.04	0.13
Pentane	C ₅ H ₁₂	1400	900	780	660	68	630	C ₆ H ₁₀	0.92	0.19	0.01
Hexane	C ₆ H ₁₄	590	540	330	280	BLD	240				
Heptane	C ₇ H ₁₆	740	580	490	340	BLD	290	C ₉ H ₁₂	0.80	4.32	0.12
Octane	C ₈ H ₁₈	350	310	250	170	BLD	150	C ₇ H ₈	0.96	2.14	0.07
Nonane	C ₉ H ₂₀	240	190	140	110	BLD	92	C ₇ H ₈	0.98	1.05	0.03
Decane	C ₁₀ H ₂₂	140	110	82	65	BLD	58	C ₈ H ₁₀	0.95	0.51	0.02
Undecane	C ₁₁ H ₂₄	75	73	68	45	3.5	40	C ₁₀ H ₂₀	0.92	6.01	0.01
Dodecane	C ₁₂ H ₂₆	100	57	54	35	5.1	39	C ₄ H ₈	0.93	0.087	0.01
Branched Alkanes											
Isobutane (2-Methylpropane)	C ₄ H ₁₀	150	130	100	76	34	82				
2-Methylbutane	C ₅ H ₁₂	960	540	530	430	64	420	C ₉ H ₁₂	0.73	2.07	0.075
2,2-Dimethylpropane	C ₅ H ₁₂	230	77	58	30	15	53	C ₆ H ₁₀	0.97	0.16	0.005
2-Methylpentane	C ₆ H ₁₄	410	260	220	110	BLD	130	C ₉ H ₁₂	0.68	1.59	0.066
3-Methylpentane	C ₆ H ₁₄	220	150	140	67	BLD	78	C ₉ H ₁₂	0.73	1.04	0.037
2,2-Dimethylbutane	C ₆ H ₁₄	75	37	29	15	BLD	20	C ₁₂ H ₁₈	0.96	0.56	0.003
2,3-Dimethylbutane	C ₆ H ₁₄	84	50	34	23	5.1	28	C ₃ H ₄ O	0.93	0.21	0.003
2-Methylhexane	C ₇ H ₁₆	170	140	110	84	BLD	71	C ₇ H ₈	0.95	0.48	0.017
3-Methylhexane	C ₇ H ₁₆	290	230	190	140	3.9	120	C ₇ H ₈	0.96	0.80	0.027
2,2-Dimethylpentane	C ₇ H ₁₆	BLD	BLD	BLD	BLD	BLD	BLD	C ₆ H ₆	0.97	0.02	0.0002

2,3-Dimethylpentane	C ₇ H ₁₆	87	71	59	43	BLD	40	C ₇ H ₈	0.96	0.22	0.007
2,4-Dimethylpentane	C ₇ H ₁₆	14	13	12	8.2	BLD	8.3	C ₇ H ₈	0.91	0.03	0.001
2,2,3-Trimethylbutane	C ₇ H ₁₆	61	17	12	7.7	BLD	13	C ₆ H ₁₀	0.98	0.04	0.001
2-Methylheptane	C ₈ H ₁₈	230	190	170	110	BDL	95	C ₇ H ₈	0.99	0.68	0.076
3-Methylheptane	C ₈ H ₁₈	90	72	64	43	BLD	37	C ₇ H ₈	0.98	0.25	0.006
4-Methylheptane	C ₈ H ₁₈	67	57	49	33	BLD	31	C ₇ H ₈	0.97	0.17	0.019
2,4-Dimethylhexane	C ₈ H ₁₈	15	11	11	7.5	BLD	7	C ₇ H ₈	0.98	0.04	0.001
2,5-Dimethylhexane	C ₈ H ₁₈	13	10	10	6.9	BDL	5.9	C ₇ H ₈	0.98	0.03	0.001
2,3,4-Trimethylpentane	C ₈ H ₁₈	19	4.8	3.9	BLD	BLD	4.5	C ₇ H ₈	0.85	0.007	0.0005
2,2,4-Trimethylpentane	C ₈ H ₁₈	4.8	4.5	2.7	BLD	BDL	BLD				
2,2-Dimethylhexane	C ₈ H ₁₈	BLD	BDL	BDL	BDL	BDL	BLD				
2,2,5-Trimethylhexane	C ₉ H ₂₀	BLD	BDL	BDL	BDL	BDL	BLD	C ₅ H ₈	0.93	0.0005	0.0001
3,6-Dimethyloctane	C ₁₀ H ₂₂	23	8.2	5.9	4.3	BDL	5.5	C ₉ H ₁₀	0.91	0.16	0.001
Cycloalkanes											
Cyclopentane	C ₅ H ₁₀	140	29	44	21	BLD	32				
Methylcyclopentane	C ₆ H ₁₂	260	230	160	130	BLD	110	C ₉ H ₁₂	0.83	1.86	0.048
Cyclohexane	C ₆ H ₁₂	88	78	58	47	BLD	39	C ₉ H ₁₂	0.84	0.58	0.015
Methylcyclohexane	C ₇ H ₁₄	220	170	150	110	BLD	90	C ₇ H ₈	0.98	0.60	0.015
c-1,3-Dimethylcyclohexane	C ₈ H ₁₆	59	52	45	28	BLD	26	C ₇ H ₈	0.95	0.15	0.005
t-1,2-Dimethylcyclohexane	C ₈ H ₁₆	38	36	29	21	BLD	20	C ₉ H ₁₂	0.93	0.23	0.003
c-1,4/t-1,3-Dimethylcyclohexane	C ₈ H ₁₆	29	25	21	15	BLD	14	C ₇ H ₈	0.97	0.07	0.002
t-1,4-Dimethylcyclohexane	C ₈ H ₁₆	13	11	10	6.8	BLD	6.4	C ₉ H ₁₂	0.96	0.08	0.001
c-1,2-Dimethylcyclohexane	C ₈ H ₁₆	15	13	12	7.7	BLD	8	C ₇ H ₈	0.90	0.03	0.001
Aromatic Hydrocarbons											
Benzene	C ₆ H ₆	91	84	60	49	30	52	C ₇ H ₈	0.81	0.17	0.014
Toluene	C ₇ H ₈	400	320	260	180	BLD	170	C ₇ H ₈	0.94	1.04	0.043
m,p-Xylene	C ₈ H ₁₀	300	230	200	120	BLD	110	C ₇ H ₈	0.94	0.83	0.032
o-Xylene	C ₈ H ₁₀	120	94	90	55	BLD	50	C ₇ H ₈	0.96	0.31	0.009
Ethylbenzene	C ₈ H ₁₀	88	70	66	41	BLD	37	C ₇ H ₈	0.95	0.22	0.008
1,2,3-Trimethylbenzene	C ₉ H ₁₂	43	34	32	20	BDL	18	C ₇ H ₈	0.93	0.10	0.005
1,2,4-Trimethylbenzene	C ₉ H ₁₂	69	55	50	31	BLD	29	C ₇ H ₈	0.94	0.16	0.007
1,3,5-Trimethylbenzene	C ₉ H ₁₂	24	19	14	8.5	BLD	9.1	C ₇ H ₈	0.89	0.06	0.004
2-Ethyltoluene	C ₉ H ₁₂	32	28	25	17	BLD	16				
3-Ethyltoluene	C ₉ H ₁₂	50	41	38	24	BLD	22	C ₇ H ₈	0.90	0.10	0.006
4-Ethyltoluene	C ₉ H ₁₂	30	25	22	14	BLD	13	C ₇ H ₈	0.92	0.07	0.003
n-Propylbenzene	C ₉ H ₁₂	18	17	16	10	BLD	9.3	C ₃ H ₄	0.94	0.03	0.001
iso-Propylbenzene	C ₉ H ₁₂	8.8	8	7.6	BLD	BLD	BLD	C ₃ H ₄ O	0.94	0.06	0.001
n-Butylbenzene	C ₁₀ H ₁₄	5.8	BLD	BLD	BLD	BDL	BLD	C ₄ H ₈	0.96	0.01	0.0004
iso-Butylbenzene	C ₁₀ H ₁₄	BLD	BLD	BLD	BLD	BDL	BLD	C ₁₂ H ₁₈	0.93	0.03	0.0002

sec-Butylbenzene	C ₁₀ H ₁₄	5.8	BLD	BLD	BLD	BLD	BLD	C ₄ H ₆ O	0.96	0.03	0.001
tert-Butylbenzene	C ₁₀ H ₁₄	BLD	BDL	BDL	BDL	BDL	BLD	C ₅ H ₈	0.97	0.00	0.0004
1,2-Diethylbenzene	C ₁₀ H ₁₄	BLD	BLD	BLD	BLD	BDL	BLD	C ₄ H ₆ O	0.94	0.02	0.0004
1,3-Diethylbenzene	C ₁₀ H ₁₄	BLD	BLD	BLD	BLD	BDL	BLD	C ₃ H ₄	0.91	0.01	0.0004
1,4-Diethylbenzene	C ₁₀ H ₁₄	15	14	13	BLD	BLD	BLD	C ₃ H ₄ O	0.92	0.08	0.001
p-Cymene	C ₁₀ H ₁₄	12	12	12	11	BLD	9.4				
Hexylbenzene	C ₁₂ H ₁₈	9.9	6.4	4.7	BLD	BLD	4	C ₇ H ₈	0.78	0.07	0.006
Styrene	C ₈ H ₈	BLD	BLD	BLD	BLD	BLD	BLD	C ₉ H ₁₂	0.73	0.01	0.000
Indane (2,3-Dihydroindene)	C ₉ H ₁₀	20	17	16	11	BLD	9	C ₇ H ₈	0.98	0.05	0.001
Naphthalene	C ₁₀ H ₈	23	21	10	BLD	BLD	BLD				
Straight Chain Alkenes											
Ethene	C ₂ H ₄	730	660	430	240	88	310	C ₉ H ₁₂	0.88	10.4	0.1
Propene	C ₃ H ₆	220	190	130	89	36	99	C ₉ H ₁₂	0.88	2.7	0.03
1-Butene/2-Methylpropene	C ₄ H ₈	120	82	54	45	BLD	50				
c-2-Butene	C ₄ H ₈	17	12	6.9	BLD	BDL	BLD				
t-2-Butene	C ₄ H ₈	21	15	8.6	BLD	BDL	6.9				
1-Pentene	C ₅ H ₁₀	25	BLD	BLD	BLD	BLD	BLD				
c-2-Pentene	C ₅ H ₁₀	BLD	BLD	BLD	BLD	BLD	BLD				
t-2-Pentene	C ₅ H ₁₀	14	10	5.3	BLD	BLD	4.8				
1-Hexene/2-Methyl-1-Pentene	C ₆ H ₁₂	23	BLD	BLD	BLD	BLD	BLD				
c-2-Hexene	C ₆ H ₁₂	BLD	BLD	BLD	BLD	BDL	BLD	C ₉ H ₁₂	0.78	0.02	0.001
t-2-Hexene	C ₆ H ₁₂	7.3	BLD	BLD	BLD	BLD	BLD	C ₇ H ₈	0.83	0.02	0.001
t-3-Heptene	C ₇ H ₁₄	BLD	BLD	BLD	BLD	BDL	BLD	C ₉ H ₁₂	0.78	0.02	0.001
t-2-Heptene	C ₇ H ₁₄	5.1	4.8	BLD	BLD	BDL	BLD				
1-Heptene	C ₇ H ₁₄	54	BLD	BLD	BDL	BDL	BLD				
c-2-Heptene	C ₇ H ₁₄	BLD	BLD	BLD	BDL	BDL	BLD				
c-3-Heptene	C ₇ H ₁₄	BDL	BDL	BDL	BDL	BDL	BDL				
1-Octene	C ₈ H ₁₆	46	16	13	BLD	BDL	8.7	C ₉ H ₁₂	0.97	0.37	0.002
t-2-Octene	C ₈ H ₁₆	BDL	BDL	BDL	BDL	BDL	BDL				
1-Nonene	C ₉ H ₁₈	BDL	BDL	BDL	BDL	BDL	BDL				
1-Decene	C ₁₀ H ₂₀	100	52	29	15	7.2	26				
1-Undecene	C ₁₁ H ₂₂	62	BDL	BDL	BDL	BDL	5.1				
Branched and Cycloalkenes											
2-Methyl-1-Butene	C ₅ H ₁₀	14	11	BLD	BLD	BLD	BLD				
2-Methyl-2-Butene	C ₅ H ₁₀	12	9.0	BLD	BLD	BLD	BLD				
3-Methyl-1-Butene	C ₅ H ₁₀	8.0	5.4	3.9	3.1	BLD	3.3				
3-Methyl-1-Pentene	C ₆ H ₁₂	BLD	BLD	BLD	BLD	BDL	BLD				
4-Methyl-1-Pentene	C ₆ H ₁₂	BLD	BLD	BLD	BLD	BDL	BLD	C ₉ H ₁₂	0.74	0.04	0.002
c-3-Methyl-2-Pentene	C ₆ H ₁₂	BLD	BLD	BLD	BLD	BDL	BLD				

t-3-Methyl-2-Pentene	C ₆ H ₁₂	BLD	BLD	BLD	BLD	BDL	BLD				
t-4-Methyl-2-Pentene	C ₆ H ₁₂	BDL	BDL	BDL	BDL	BDL	BDL				
c-4-Methyl-2-Pentene	C ₆ H ₁₂	BLD	BLD	BLD	BLD	BDL	BLD	C ₉ H ₁₂	0.92	0.07	0.0007
2-Ethyl-1-Butene	C ₆ H ₁₂	BDL	BDL	BDL	BDL	BDL	BDL				
Cyclopentene	C ₅ H ₈	BLD	BLD	BLD	BLD	BDL	BLD				
1-Methylcyclopentene	C ₆ H ₁₀	BLD	BLD	BLD	BLD	BDL	BLD				
Cyclohexene	C ₆ H ₁₀	BLD	BLD	BLD	BLD	BDL	BLD	C ₇ H ₈	0.81	0.01	0.001
1-Methylcyclohexene	C ₇ H ₁₄	10	8.2	BLD	BLD	BLD	BLD	C ₇ H ₈	0.81	0.03	0.002
Alkynes and Dienes											
Ethyne	C ₂ H ₂	190	170	140	87	53	100	C ₉ H ₁₂	0.66	0.95	0.04
Propyne	C ₃ H ₄	17	14	BLD	BLD	BLD	BLD	C ₉ H ₁₂	0.96	0.22	0.001
1-Butyne	C ₄ H ₆	BDL	BDL	BDL	BDL	BDL	BDL				
1,3-Butadiene	C ₄ H ₆	13	10	BLD	BLD	BLD	BLD				
Biogenic Hydrocarbons											
Isoprene (2-Methyl-1,3-Butadiene)	C ₅ H ₈	870	730	690	550	250	550				
a-Pinene	C ₁₀ H ₁₆	500	240	58	51	35	100	C ₁₀ H ₁₆	0.99	0.52	0.032
b-Pinene	C ₁₀ H ₁₆	110	63	32	27	20	36	C ₁₀ H ₁₆	0.99	0.09	0.006
Limonene	C ₁₀ H ₁₆	72	45	25	BLD	BDL	22	C ₁₀ H ₁₆	0.99	0.06	0.004
Camphene	C ₁₀ H ₁₆	37	34	32	29	BLD	28	C ₁₀ H ₁₆	0.99	0.20	0.004
Chlorinated Hydrocarbons											
Chloromethane	CH ₃ Cl	690	680	650	630	580	630				
Dichloromethane	CH ₂ Cl ₂	73	72	72	70	64	70	C ₆ H ₁₂	0.90	0.12	2E-03
Chloroform	CHCl ₃	23	22	21	21	19	21	CO	0.94	0.00024	5E-07
1,1-Dichloroethene	C ₂ H ₂ Cl ₂	BDL	BDL	BDL	BDL	BDL	BDL	C ₂ H ₄ O	0.99	0.001	5E-05
1,2-Dichloroethane	C ₂ H ₄ Cl ₂	15	15	14	14	12	14	CO	0.93	0.0002	4E-07
c-1,2-Dichloroethene	C ₂ H ₂ Cl ₂	BDL	BDL	BDL	BDL	BDL	BDL	C ₂ H ₄ O	0.99	0.0007	5E-05
Hexachlorobutadiene	C ₄ Cl ₆	BLD	BLD	BDL	BLD	BLD	BLD	C ₄ H ₆ O	0.91	0.002	8E-05

Table S10. Canister sample VOC compound concentration statistics for the CNRL facility. Empty entries for species indicate that there were no emission rates determined for those species. The details are similar to those explained for Table S8.

Compound Name	Formula	CNRL (n = 104)						Correlation with tracers to determine regression slope b			
		Max	90th percentile	80th percentile	Median	Min	Mean	Tracer of Choice	R ²	b	Δb
N-Alkanes											
Ethane	C ₂ H ₆	4000	2300	1630	1100	BDL	1300				
Propane	C ₃ H ₈	1600	1100	940	580	BDL	620	CH ₄	1.00	0.01	0.0003
Butane	C ₄ H ₁₀	900	530	450	220	BDL	280	C ₁₀ H ₁₄	1.00	6.04	0.01

Pentane	C ₅ H ₁₂	1800	890	800	63	BDL	330				
Hexane	C ₆ H ₁₄	530	270	210	21	BDL	96				
Heptane	C ₇ H ₁₆	1700	380	160	22	BDL	130	C ₄ H ₆ O	0.99	0.31	0.001
Octane	C ₈ H ₁₈	630	150	80	10	BDL	58	C ₄ H ₆ O	1.00	1.14	0.01
Nonane	C ₉ H ₂₀	300	68	39	6.3	BDL	27	C ₄ H ₆ O	1.00	0.51	0.01
Decane	C ₁₀ H ₂₂	99	28	17	BLD	BDL	11	C ₄ H ₆ O	1.00	0.22	0.01
Undecane	C ₁₁ H ₂₄	40	19	14	4.4	BDL	7.7	C ₄ H ₆ O	0.99	0.08	0.004
Dodecane	C ₁₂ H ₂₆	75	35	24	8.4	BDL	14	C ₁₀ H ₁₆	0.97	0.028	0.001
Branched Alkanes											
Isobutane (2-Methylpropane)	C ₄ H ₁₀	6100	1400	1100	230	BDL	570	C ₃ H ₆	0.96	6.15	0.03
2-Methylbutane	C ₅ H ₁₂	8700	2700	1900	470	BDL	1000	C ₃ H ₆	0.96	8.61	0.005
2,2-Dimethylpropane	C ₅ H ₁₂	580	290	220	36	BDL	110	C ₃ H ₆	1.00	0.62	0.007
2-Methylpentane	C ₆ H ₁₄	1100	530	450	25	BDL	190	C ₃ H ₆	0.99	0.32	0.0001
3-Methylpentane	C ₆ H ₁₄	2100	760	590	130	BDL	280	C ₃ H ₆	0.98	2.4	0.00002
2,2-Dimethylbutane	C ₆ H ₁₄	510	270	200	33	BDL	94	C ₃ H ₆	0.96	0.56	0.00003
2,3-Dimethylbutane	C ₆ H ₁₄	1000	490	340	74	BDL	160	C ₃ H ₆	0.99	1.87	0.0001
2-Methylhexane	C ₇ H ₁₆	340	85	46	10	BDL	32	C ₇ H ₈	0.98	0.77	0.001
3-Methylhexane	C ₇ H ₁₆	620	170	98	23	BDL	63	C ₁₀ H ₁₆	0.99	0.41	0.01
2,2-Dimethylpentane	C ₇ H ₁₆	120	48	35	BLD	BDL	16	C ₃ H ₆	0.98	0.11	0.001
2,3-Dimethylpentane	C ₇ H ₁₆	520	240	180	39	BDL	86	C ₃ H ₆	0.96	0.44	0.05
2,4-Dimethylpentane	C ₇ H ₁₆	180	73	55	13	BDL	26	C ₃ H ₆	0.99	0.17	0.0009
2,2,3-Trimethylbutane	C ₇ H ₁₆	140	79	57	12	BDL	28				
2-Methylheptane	C ₈ H ₁₈	550	130	97	15	BDL	55	C ₄ H ₆ O	0.98	0.37	0.002
3-Methylheptane	C ₈ H ₁₈	190	46	22	BLD	BDL	17	C ₄ H ₆ O	1.00	0.14	0.002
4-Methylheptane	C ₈ H ₁₈	150	50	36	4.7	BDL	19	C ₃ H ₆ O	0.98	0.05	0.02
2,4-Dimethylhexane	C ₈ H ₁₈	120	56	39	5.9	BDL	18	C ₅ H ₈	0.99	0.04	0.0006
2,5-Dimethylhexane	C ₈ H ₁₈	37	16	12	BLD	BDL	5.7	C ₉ H ₁₀	0.99	0.62	0.0004
2,3,4-Trimethylpentane	C ₈ H ₁₈	100	51	35	8.1	BDL	18	C ₃ H ₆	0.99	0.09	0.02
2,2,4-Trimethylpentane	C ₈ H ₁₈	97	BLD	BDL	BDL	BDL	2.7				
2,2-Dimethylhexane	C ₈ H ₁₈	25	BDL	BDL	BDL	BDL	BLD				
2,2,5-Trimethylhexane	C ₉ H ₂₀	3.1	BLD	BLD	BDL	BDL	BLD	C ₆ H ₁₂	0.97	0.011	0.0004
3,6-Dimethyloctane	C ₁₀ H ₂₂	43	14.4	7.5	BDL	BDL	4.4				
Cycloalkanes											
Cyclopentane	C ₅ H ₁₀	820	420	300	65	BDL	150	C ₃ H ₆	0.96	0.73	0.0002
Methylcyclopentane	C ₆ H ₁₂	1900	590	450	69	BDL	210	C ₃ H ₆	1.00	1.67	0.05
Cyclohexane	C ₆ H ₁₂	2400	890	610	78	BDL	300	C ₃ H ₆	0.97	2.10	0.002
Methylcyclohexane	C ₇ H ₁₄	1700	460	370	67	BDL	180	C ₃ H ₆	0.96	0.99	0.0002
c-1,3-Dimethylcyclohexane	C ₈ H ₁₆	490	150	13	24	BDL	60	C ₅ H ₈	1.00	0.14	0.009
t-1,2-Dimethylcyclohexane	C ₈ H ₁₆	650	310	190	42	BDL	99	C ₃ H ₆	1.00	0.49	0.004

c-1,4/t-1,3-Dimethylcyclohexane	C ₈ H ₁₆	160	83	63	14	BDL	29				
t-1,4-Dimethylcyclohexane	C ₈ H ₁₆	200	66	50	10	BDL	26	C ₃ H ₆	1.00	0.20	0.004
c-1,2-Dimethylcyclohexane	C ₈ H ₁₆	71	42	31	6.4	BDL	14				
Aromatic Hydrocarbons											
Benzene	C ₆ H ₆	130	87	74	26	BDL	42				
Toluene	C ₇ H ₈	340	120	96	BLD	BDL	52	C ₄ H ₆ O	1.00	0.24	0.001
m,p-Xylene	C ₈ H ₁₀	240	60	46	BLD	BDL	27	C ₄ H ₆ O	0.98	0.14	0.01
o-Xylene	C ₈ H ₁₀	110	34	22	BLD	BDL	13	C ₁₀ H ₁₆	0.99	0.06	0.002
Ethylbenzene	C ₈ H ₁₀	85	24	18	BLD	BDL	10				
1,2,3-Trimethylbenzene	C ₉ H ₁₂	43	20	13	BLD	BDL	6.8	C ₆ H ₈	0.99	0.03	0.001
1,2,4-Trimethylbenzene	C ₉ H ₁₂	57	23	15	BLD	BDL	BLD				
1,3,5-Trimethylbenzene	C ₉ H ₁₂	34	20	13	BLD	BDL	BLD	C ₉ H ₁₀	1.00	0.91	0.001
2-Ethyltoluene	C ₉ H ₁₂	30	11	8	BLD	BDL	BLD	C ₁₀ H ₁₆	1.00	0.03	0.0001
3-Ethyltoluene	C ₉ H ₁₂	46	15	11	BLD	BDL	BLD				
4-Ethyltoluene	C ₉ H ₁₂	23	7	BLD	BLD	BDL	BLD				
n-Propylbenzene	C ₉ H ₁₂	19	9	BLD	BLD	BDL	BLD				
iso-Propylbenzene	C ₉ H ₁₂	110	10	BLD	BLD	BDL	BLD	C ₆ H ₈	1.00	0.004	0.001
n-Butylbenzene	C ₁₀ H ₁₄	BLD	BLD	BLD	BDL	BDL	BLD				
iso-Butylbenzene	C ₁₀ H ₁₄	11	BLD	BLD	BLD	BDL	BLD				
sec-Butylbenzene	C ₁₀ H ₁₄	6.9	BLD	BLD	BLD	BDL	BLD				
tert-Butylbenzene	C ₁₀ H ₁₄	BLD	BLD	BDL	BDL	BDL	BLD	C ₆ H ₈	0.97	0.002	0.0002
1,2-Diethylbenzene	C ₁₀ H ₁₄	7.4	BLD	BLD	BLD	BDL	BLD				
1,3-Diethylbenzene	C ₁₀ H ₁₄	13	BLD	BLD	BLD	BDL	BLD				
1,4-Diethylbenzene	C ₁₀ H ₁₄	9.9	BLD	BLD	BDL	BDL	BLD				
p-Cymene	C ₁₀ H ₁₄	16	11	10	7.4	BDL	7.1				
Hexylbenzene	C ₁₂ H ₁₈	9	4.5	BLD	BLD	BDL	BLD				
Styrene	C ₈ H ₈	BLD	BLD	BLD	BLD	BDL	BLD	C ₄ H ₆ O	0.97	0.008	0.0004
Indane (2,3-Dihydroindene)	C ₉ H ₁₀	14	BLD	BLD	BLD	BDL	BLD	C ₆ H ₆	0.99	0.10	0.004
Naphthalene	C ₁₀ H ₈	12	BLD	BLD	BLD	BDL	BLD				
Straight Chain Alkenes											
Ethene	C ₂ H ₄	1200	480	380	180	BDL	260				
Propene	C ₃ H ₆	340	140	100	54	BDL	73				
1-Butene/2-Methylpropene	C ₄ H ₈	110	53	45	27	BDL	31				
c-2-Butene	C ₄ H ₈	12	BLD	BLD	BLD	BDL	BLD				
t-2-Butene	C ₄ H ₈	8.8	BLD	BLD	BDL	BDL	BLD				
1-Pentene	C ₅ H ₁₀	26	BLD	BLD	BLD	BDL	BLD				
c-2-Pentene	C ₅ H ₁₀	BLD	BLD	BLD	BDL	BDL	BLD				
t-2-Pentene	C ₅ H ₁₀	7.9	BLD	BLD	BLD	BDL	BLD				
1-Hexene/2-Methyl-1-Pentene	C ₆ H ₁₂	22	BLD	BLD	BLD	BDL	BLD				

c-2-Hexene	C ₆ H ₁₂	BLD	BLD	BLD	BDL	BDL	BLD				
t-2-Hexene	C ₆ H ₁₂	BLD	BLD	BLD	BDL	BDL	BLD	C ₄ H ₆ O	1.00	0.006	0.002
t-3-Heptene	C ₇ H ₁₄	BLD	BDL	BDL	BDL	BDL	BLD				
t-2-Heptene	C ₇ H ₁₄	BLD	BLD	BDL	BDL	BDL	BLD	C ₄ H ₆ O	1.00	0.002	0.0006
1-Heptene	C ₇ H ₁₄	BLD	BDL	BDL	BDL	BDL	BLD				
c-2-Heptene	C ₇ H ₁₄	BLD	BDL	BDL	BDL	BDL	BLD				
c-3-Heptene	C ₇ H ₁₄	BLD	BDL	BDL	BDL	BDL	BLD				
1-Octene	C ₈ H ₁₆	390	110	41	BDL	BDL	32				
t-2-Octene	C ₈ H ₁₆	420	86	22	BDL	BDL	27	C ₈ H ₁₆	0.99	23.9	0.0003
1-Nonene	C ₉ H ₁₈	360	BLD	BDL	BDL	BDL	8.3				
1-Decene	C ₁₀ H ₂₀	250	100	59	7	BDL	34				
1-Undecene	C ₁₁ H ₂₂	49	BLD	BDL	BDL	BDL	BLD	C ₄ H ₆ O	1.00	0.076	0.005
Branched and Cycloalkenes											
2-Methyl-1-Butene	C ₅ H ₁₀	11	7	BLD	BLD	BDL	BLD				
2-Methyl-2-Butene	C ₅ H ₁₀	BLD	BLD	BLD	BLD	BDL	BLD				
3-Methyl-1-Butene	C ₅ H ₁₀	6.1	3.9	2.7	BLD	BDL	BLD				
3-Methyl-1-Pentene	C ₆ H ₁₂	BLD	BLD	BLD	BDL	BDL	BLD				
4-Methyl-1-Pentene	C ₆ H ₁₂	BLD	BDL	BDL	BDL	BDL	BLD				
c-3-Methyl-2-Pentene	C ₆ H ₁₂	BLD	BDL	BDL	BDL	BDL	BLD				
t-3-Methyl-2-Pentene	C ₆ H ₁₂	BLD	BDL	BDL	BDL	BDL	BLD				
t-4-Methyl-2-Pentene	C ₆ H ₁₂	16	10	BLD	BDL	BDL	BLD	C ₈ H ₁₆	0.96	0.94	0.001
c-4-Methyl-2-Pentene	C ₆ H ₁₂	BLD	BLD	BDL	BDL	BDL	BLD				
2-Ethyl-1-Butene	C ₆ H ₁₂	BLD	BDL	BDL	BDL	BDL	BLD				
Cyclopentene	C ₅ H ₈	BLD	BLD	BLD	BLD	BDL	BLD				
1-Methylcyclopentene	C ₆ H ₁₀	BLD	BLD	BLD	BLD	BDL	BLD				
Cyclohexene	C ₆ H ₁₀	BLD	BLD	BLD	BDL	BDL	BLD				
1-Methylcyclohexene	C ₇ H ₁₄	BLD	BLD	BLD	BLD	BDL	BLD				
Alkynes and Dienes											
Ethyne	C ₂ H ₂	1000	210	160	78	BDL	130				
Propyne	C ₃ H ₄	61	17	13	BLD	BDL	BLD				
1-Butyne	C ₄ H ₆	BLD	BDL	BDL	BDL	BDL	BLD				
1,3-Butadiene	C ₄ H ₆	26	10	7	BLD	BDL	BLD				
Biogenic Hydrocarbons											
Isoprene (2-Methyl-1,3-Butadiene)	C ₅ H ₈	1500	1100	930	610	BDL	680	C ₄ H ₆ O	0.98	2.17	0.001
a-Pinene	C ₁₀ H ₁₆	230	86	67	43	BDL	51				
b-Pinene	C ₁₀ H ₁₆	160	100	65	46	BDL	55	C ₄ H ₆ O	0.99	0.35	0.002
Limonene	C ₁₀ H ₁₆	81	BLD	BLD	BDL	BDL	BLD				
Camphene	C ₁₀ H ₁₆	88	64	46	38	BDL	40	C ₄ H ₆ O	0.97	0.17	0.01
Chlorinated Hydrocarbons											

Chloromethane	CH ₃ Cl	810	700	690	650	BDL	630	CO	0.95	0.008	0.002
Dichloromethane	CH ₂ Cl ₂	81	77	75	68	BDL	68				
Chloroform	CHCl ₃	25	21	20	16	BDL	17				
1,1-Dichloroethene	C ₂ H ₂ Cl ₂	BLD	BDL	BDL	BDL	BDL	BLD				
1,2-Dichloroethane	C ₂ H ₄ Cl ₂	25	17	15	14	BDL	14	C ₃ H ₆	0.98	0.01	0.0004
c-1,2-Dichloroethene	C ₂ H ₂ Cl ₂	BLD	BDL	BDL	BDL	BDL	BLD				
Hexachlorobutadiene	C ₄ Cl ₆	BLD	BDL	BDL	BDL	BDL	BLD				

Table S11. Canister sample VOC compound concentration statistics for the SAJ facility. Empty entries for species indicate that there were no emission rates determined for those species. The details are similar to those explained for Table S8.

Compound Name	Formula	SAJ (n = 76)						Correlation with tracers to determine regression slope b			
		Max	90th percentile	80th percentile	Median	Min	Mean	Tracer of Choice	R ²	b	Δb
N-Alkanes											
Ethane	C ₂ H ₆	2500	1200	1100	910	560	940				
Propane	C ₃ H ₈	790	370	330	200	110	230	C ₉ H ₁₀	0.97	4.18	0.031
Butane	C ₄ H ₁₀	400	110	85	59	16	68	C ₅ H ₁₀	0.96	0.61	0.012
Pentane	C ₅ H ₁₂	13000	2400	1500	67	BLD	1100				
Hexane	C ₆ H ₁₄	2700	460	270	BLD	BLD	210	C ₆ H ₆	0.97	30.7	0.9
Heptane	C ₇ H ₁₆	810	54	24	BLD	BDL	25	C ₆ H ₆	0.98	6.00	0.14
Octane	C ₈ H ₁₈	650	18	11	BLD	BDL	14	C ₉ H ₁₀	0.99	1.26	0.006
Nonane	C ₉ H ₂₀	260	10	7	BLD	BDL	7	C ₈ H ₁₆	0.99	1.38	0.002
Decane	C ₁₀ H ₂₂	92	6	5	BLD	BDL	5.3	C ₈ H ₁₆	0.97	0.77	0.002
Undecane	C ₁₁ H ₂₄	52	9	8	3.6	BDL	6				
Dodecane	C ₁₂ H ₂₆	68	21	15	6.5	BDL	10				
Branched Alkanes											
Isobutane (2-Methylpropane)	C ₄ H ₁₀	540	140	63	24	BLD	51	C ₄ H ₆ O	0.99	1.02	0.018
2-Methylbutane	C ₅ H ₁₂	8600	1500	990	88	BLD	710	C ₆ H ₆	0.99	18.0	0.3
2,2-Dimethylpropane	C ₅ H ₁₂	160	110	66	25	BDL	39	C ₈ H ₁₀	0.95	0.86	0.01
2-Methylpentane	C ₆ H ₁₄	7900	1400	770	BLD	BDL	610	C ₆ H ₆	0.98	16.6	0.4
3-Methylpentane	C ₆ H ₁₄	4200	760	400	12	BDL	340	C ₆ H ₆	0.98	9.50	0.2
2,2-Dimethylbutane	C ₆ H ₁₄	1400	250	130	BLD	BDL	110	C ₆ H ₆	0.98	2.66	0.07
2,3-Dimethylbutane	C ₆ H ₁₄	1500	280	150	16	BDL	130	C ₆ H ₆	0.98	3.32	0.09
2-Methylhexane	C ₇ H ₁₆	160	20	11	BLD	BDL	7.5	C ₅ H ₁₀	0.98	0.19	0.002
3-Methylhexane	C ₇ H ₁₆	300	28	16	BLD	BDL	12	C ₅ H ₁₀	0.97	0.30	0.006
2,2-Dimethylpentane	C ₇ H ₁₆	12	BLD	BLD	BLD	BDL	BLD	C ₉ H ₁₀	0.95	0.14	0.001

2,3-Dimethylpentane	C ₇ H ₁₆	170	40	22	BLD	BDL	15	C ₁₀ H ₁₆	0.96	0.16	0.006
2,4-Dimethylpentane	C ₇ H ₁₆	52	16	9	BLD	BDL	5.6	C ₅ H ₁₀	0.97	0.12	0.002
2,2,3-Trimethylbutane	C ₇ H ₁₆	94	34	20	7	BDL	13	C ₆ H ₁₀	0.99	0.07	0.002
2-Methylheptane	C ₈ H ₁₈	430	15	7	BLD	BDL	9.6	C ₈ H ₁₆	0.97	1.08	0.002
3-Methylheptane	C ₈ H ₁₈	160	5	BLD	BDL	BDL	BLD	C ₈ H ₁₆	1.00	0.47	0.0002
4-Methylheptane	C ₈ H ₁₈	130	10	6	BLD	BDL	4.6	C ₆ H ₁₂	0.96	0.067	0.004
2,4-Dimethylhexane	C ₈ H ₁₈	26	6	BLD	BDL	BDL	BLD	CH ₄	0.98	0.00019	0.000001
2,5-Dimethylhexane	C ₈ H ₁₈	20	BLD	BLD	BDL	BDL	BLD	C ₁₀ H ₁₆	0.99	0.013	0.0002
2,3,4-Trimethylpentane	C ₈ H ₁₈	25	11.0	7.2	BLD	BDL	4.3	C ₇ H ₈	0.98	0.048	0.0006
2,2,4-Trimethylpentane	C ₈ H ₁₈	150	BLD	BLD	BDL	BDL	BLD				
2,2-Dimethylhexane	C ₈ H ₁₈	BLD	BLD	BLD	BDL	BDL	BLD				
2,2,5-Trimethylhexane	C ₉ H ₂₀	2.6	BLD	BLD	BDL	BDL	BLD				
3,6-Dimethyloctane	C ₁₀ H ₂₂	22	13.8	5.8	BDL	BDL	3.5				
Cycloalkanes											
Cyclopentane	C ₅ H ₁₀	3000	460	260	7.7	BDL	220	C ₆ H ₆	0.98	6.71	0.2
Methylcyclopentane	C ₆ H ₁₂	450	140	64	BLD	BDL	45	C ₃ H ₄	0.99	0.30	0.02
Cyclohexane	C ₆ H ₁₂	170	89	25	BLD	BDL	22	C ₉ H ₁₀	0.96	1.78	0.01
Methylcyclohexane	C ₇ H ₁₄	370	45	20	BLD	BDL	17	C ₈ H ₁₆	0.98	3.52	0.01
c-1,3-Dimethylcyclohexane	C ₈ H ₁₆	130	11	4	BLD	BDL	4.9	C ₈ H ₁₆	0.98	1.15	0.002
t-1,2-Dimethylcyclohexane	C ₈ H ₁₆	93	30	19	5.1	BDL	11	CH ₄	0.96	0.0006	0.000004
c-1,4/t-1,3-Dimethylcyclohexane	C ₈ H ₁₆	63	9	7	BLD	BDL	BLD	CH ₄	0.98	0.0002	0.000001
t-1,4-Dimethylcyclohexane	C ₈ H ₁₆	29	7	BLD	BLD	BDL	BLD	C ₈ H ₁₆	0.96	0.43	0.001
c-1,2-Dimethylcyclohexane	C ₈ H ₁₆	29	10	5	BLD	BDL	BLD	C ₇ H ₁₅	0.95	2.20	0.002
Aromatic Hydrocarbons											
Benzene	C ₆ H ₆	370	100	68	39	19	58	C ₅ H ₁₀	1.00	1.31	0.01
Toluene	C ₇ H ₈	420	39	31	BLD	BLD	BLD	C ₇ H ₈	0.98	0.32	0.00
m,p-Xylene	C ₈ H ₁₀	290	BLD	BLD	BLD	BLD	BLD	C ₈ H ₁₆	1.00	0.58	0.0005
o-Xylene	C ₈ H ₁₀	210	BLD	BLD	BLD	BDL	8.6	C ₈ H ₁₆	0.98	0.31	0.0005
Ethylbenzene	C ₈ H ₁₀	120	BLD	BLD	BLD	BDL	BLD	C ₈ H ₁₆	0.99	0.30	0.0005
1,2,3-Trimethylbenzene	C ₉ H ₁₂	21	BLD	BLD	BLD	BDL	BLD	C ₃ H ₆ O	0.98	0.008	0.0003
1,2,4-Trimethylbenzene	C ₉ H ₁₂	36	BLD	BLD	BLD	BDL	BLD	C ₇ H ₈	0.99	0.040	0.0004
1,3,5-Trimethylbenzene	C ₉ H ₁₂	9.9	BLD	BLD	BLD	BDL	BLD	C ₁₀ H ₁₆	0.96	0.012	0.0005
2-Ethyltoluene	C ₉ H ₁₂	29	BLD	BLD	BLD	BDL	BLD	C ₁₀ H ₁₆	0.97	0.008	0.0003
3-Ethyltoluene	C ₉ H ₁₂	38	BLD	BLD	BLD	BDL	BLD	C ₁₀ H ₁₆	0.99	0.015	0.0003
4-Ethyltoluene	C ₉ H ₁₂	23	BLD	BLD	BLD	BDL	BLD	C ₁₀ H ₁₆	0.98	0.009	0.0002
n-Propylbenzene	C ₉ H ₁₂	20	BLD	BLD	BLD	BDL	BLD	C ₁₀ H ₁₆	0.92	0.018	0.0010
iso-Propylbenzene	C ₉ H ₁₂	10	BLD	BLD	BLD	BDL	BLD	C ₁₁ H ₂₂	0.90	0.14	0.0002
n-Butylbenzene	C ₁₀ H ₁₄	BLD	BLD	BLD	BDL	BDL	BLD	C ₁₀ H ₁₆	0.92	0.003	0.0002
iso-Butylbenzene	C ₁₀ H ₁₄	BLD	BLD	BLD	BDL	BDL	BLD	C ₃ H ₄ O	0.86	0.025	0.0006

sec-Butylbenzene	C ₁₀ H ₁₄	BLD	BLD	BLD	BDL	BDL	BLD	C ₄ H ₆ O	0.91	0.004	0.0002
tert-Butylbenzene	C ₁₀ H ₁₄	BLD	BLD	BLD	BDL	BDL	BLD				
1,2-Diethylbenzene	C ₁₀ H ₁₄	BLD	BLD	BLD	BDL	BDL	BLD	C ₂ H ₄ O	0.99	0.00049	0.00004
1,3-Diethylbenzene	C ₁₀ H ₁₄	BLD	BLD	BLD	BDL	BDL	BLD	C ₁₀ H ₁₆	0.86	0.005	0.0004
1,4-Diethylbenzene	C ₁₀ H ₁₄	13	BLD	BLD	BDL	BDL	BLD	C ₁₀ H ₁₆	0.92	0.010	0.0005
p-Cymene	C ₁₀ H ₁₄	34	10	9	BLD	BLD	BLD	C ₈ H ₁₆	0.96	0.48	0.0012
Hexylbenzene	C ₁₂ H ₁₈	9.4	3.9	BLD	BDL	BDL	BLD				
Styrene	C ₈ H ₈	35	BLD	BLD	BLD	BLD	BLD	C ₁₀ H ₁₆	0.99	0.013	0.0002
Indane (2,3-Dihydroindene)	C ₉ H ₁₀	14	BLD	BLD	BLD	BDL	BLD	C ₉ H ₁₀	0.99	0.020	0.0001
Naphthalene	C ₁₀ H ₈	11	BLD	BLD	BLD	BLD	BLD				
Straight Chain Alkenes											
Ethene	C ₂ H ₄	520	280	210	120	41	140	C ₆ H ₁₀	0.95	0.6	0.04
Propene	C ₃ H ₆	120	68	58	32	BLD	40	C ₅ H ₁₀	0.95	0.37	0.01
1-Butene/2-Methylpropene	C ₄ H ₈	69	33	28	BLD	BLD	21	C ₇ H ₁₅	0.93	2.54	0.003
c-2-Butene	C ₄ H ₈	BLD	BLD	BLD	BLD	BDL	BLD	C ₄ H ₈ O	0.99	0.019	0.0001
t-2-Butene	C ₄ H ₈	BLD	BLD	BLD	BLD	BDL	BLD	C ₉ H ₁₂	0.99	0.019	0.0002
1-Pentene	C ₅ H ₁₀	31	BLD	BLD	BLD	BDL	BLD	C ₆ H ₆	0.97	0.055	0.002
c-2-Pentene	C ₅ H ₁₀	28	BLD	BLD	BDL	BDL	BLD	C ₆ H ₆	0.98	0.063	0.002
t-2-Pentene	C ₅ H ₁₀	60	11	6.1	BLD	BDL	4.8	C ₄ H ₈	0.98	0.053	0.003
1-Hexene/2-Methyl-1-Pentene	C ₆ H ₁₂	100	BLD	BLD	BLD	BDL	BLD	C ₆ H ₆	0.98	0.21	0.005
c-2-Hexene	C ₆ H ₁₂	14	BLD	BLD	BDL	BDL	BLD				
t-2-Hexene	C ₆ H ₁₂	31	BLD	BLD	BDL	BDL	BLD	C ₆ H ₆	0.97	0.065	0.002
t-3-Heptene	C ₇ H ₁₄	BLD	BLD	BLD	BDL	BDL	BLD				
t-2-Heptene	C ₇ H ₁₄	BLD	BLD	BLD	BDL	BDL	BLD	C ₁₀ H ₁₆	0.98	0.003	0.0001
1-Heptene	C ₇ H ₁₄	9	BLD	BLD	BDL	BDL	BLD				
c-2-Heptene	C ₇ H ₁₄	BLD	BLD	BLD	BDL	BDL	BLD				
c-3-Heptene	C ₇ H ₁₄	BLD	BLD	BLD	BDL	BDL	BLD				
1-Octene	C ₈ H ₁₆	70	30	17	BDL	BDL	9.1	C ₁₀ H ₁₆	1.00	0.27	0.003
t-2-Octene	C ₈ H ₁₆	41	BLD	BLD	BDL	BDL	BLD				
1-Nonene	C ₉ H ₁₈	5.6	BLD	BLD	BDL	BDL	BLD				
1-Decene	C ₁₀ H ₂₀	100	70	47	13	BDL	24				
1-Undecene	C ₁₁ H ₂₂	53	BLD	BLD	BDL	BDL	BLD				
Branched and Cycloalkenes											
2-Methyl-1-Butene	C ₅ H ₁₀	43	9	BLD	BLD	BDL	BLD	C ₆ H ₆	0.98	0.097	0.002
2-Methyl-2-Butene	C ₅ H ₁₀	120	16	11	BLD	BDL	8.5	C ₅ H ₈	0.99	0.074	0.005
3-Methyl-1-Butene	C ₅ H ₁₀	4.6	BLD	BLD	BLD	BDL	BLD	C ₁₀ H ₁₆	0.96	0.011	0.0004
3-Methyl-1-Pentene	C ₆ H ₁₂	20	BLD	BLD	BDL	BDL	BLD	C ₁₀ H ₁₄	1.00	0.12	0.0005
4-Methyl-1-Pentene	C ₆ H ₁₂	21	BLD	BLD	BDL	BDL	BLD	C ₁₀ H ₁₄	1.00	0.13	0.0004
c-3-Methyl-2-Pentene	C ₆ H ₁₂	26	BLD	BLD	BDL	BDL	BLD	C ₅ H ₁₀	0.99	0.099	0.0007

t-3-Methyl-2-Pentene	C ₆ H ₁₂	13	BLD	BLD	BDL	BDL	BLD	C ₁₀ H ₁₄	1.00	0.076	0.0002
t-4-Methyl-2-Pentene	C ₆ H ₁₂	69	16	BLD	BDL	BDL	BLD				
c-4-Methyl-2-Pentene	C ₆ H ₁₂	43	BLD	BLD	BDL	BDL	BLD				
2-Ethyl-1-Butene	C ₆ H ₁₂	BLD	BLD	BLD	BDL	BDL	BLD				
Cyclopentene	C ₅ H ₈	56	BLD	BLD	BLD	BDL	BLD	C ₅ H ₈	0.98	0.035	0.003
1-Methylcyclopentene	C ₆ H ₁₀	BLD	BLD	BLD	BDL	BDL	BLD				
Cyclohexene	C ₆ H ₁₀	BLD	BLD	BLD	BDL	BDL	BLD				
1-Methylcyclohexene	C ₇ H ₁₄	BLD	BLD	BLD	BDL	BDL	BLD	C ₃ H ₄	0.98	0.006	0.0005
Alkynes and Dienes											
Ethyne	C ₂ H ₂	410	140	120	84	53	97	C ₇ H ₁₅	0.96	14.6	0.01
Propyne	C ₃ H ₄	15	BLD	BLD	BLD	BDL	BLD	C ₁₀ H ₁₆	0.99	0.061	0.001
1-Butyne	C ₄ H ₆	BLD	BLD	BLD	BDL	BDL	BLD	C ₂ H ₄ O	0.99	0.001	0.0001
1,3-Butadiene	C ₄ H ₆	7	BLD	BLD	BLD	BDL	BLD	C ₁₀ H ₁₆	0.99	0.020	0.0004
Biogenic Hydrocarbons											
Isoprene (2-Methyl-1,3-Butadiene)	C ₅ H ₈	1000	660	541	270	110	360	CH ₄	1.00	0.009	2E-05
a-Pinene	C ₁₀ H ₁₆	90	74	68	39	20	46	C ₁₀ H ₁₆	0.96	0.20	7E-03
b-Pinene	C ₁₀ H ₁₆	100	74	65	24	BDL	35	C ₁₀ H ₁₆	0.96	0.28	1E-02
Limonene	C ₁₀ H ₁₆	62	21	BLD	BLD	BDL	BLD				
Camphene	C ₁₀ H ₁₆	86	59	53	19	BLD	29				
Chlorinated Hydrocarbons											
Chloromethane	CH ₃ Cl	690	650	620	600	460	600				
Dichloromethane	CH ₂ Cl ₂	230	74	71	67	54	69				
Chloroform	CHCl ₃	30	21	19	17	13	17				
1,1-Dichloroethene	C ₂ H ₂ Cl ₂	BLD	BLD	BLD	BDL	BDL	BLD				
1,2-Dichloroethane	C ₂ H ₄ Cl ₂	17	14	14	13	11	13				
c-1,2-Dichloroethene	C ₂ H ₂ Cl ₂	BLD	BLD	BLD	BDL	BDL	BLD				
Hexachlorobutadiene	C ₄ Cl ₆	BLD	BLD	BLD	BLD	BDL	BLD				

S10. Comparison of Overlapping Aromatic Hydrocarbon Species by PTRMS and Canister Sampling/GC MS Analysis.

Multiple aromatic hydrocarbons were detected using both the proton transfer reaction time-of-flight mass spectrometry (PTRMS) measurements and the canister sampling/GCMS analysis methods. In the comparisons between these two measurement methods, all samples above detection limits of both methods were used. PTR-ToF-MS results were averaged over corresponding canister sampling period (approximately 20 seconds). In the comparison, PTR-ToF-MS C₈H₁₀ = canister o,m+p-xylenes + ethylbenzene, PTR-ToF-MS C₉H₁₂ = canister propyl-benzene + 1,2,3-trimethyl-benzene + 1,2,4-trimethyl-benzene + 1,3,5-trimethyl-benzene + 1-ethyl,3-methyl-benzene + 1-ethyl,4-methyl-benzene + 1-ethyl,2-methyl-benzene + 1-methylethyl-benzene. All these compounds were detected by PTR-ToF-MS as C₈H₁₀ and C₉H₁₂ isomers.

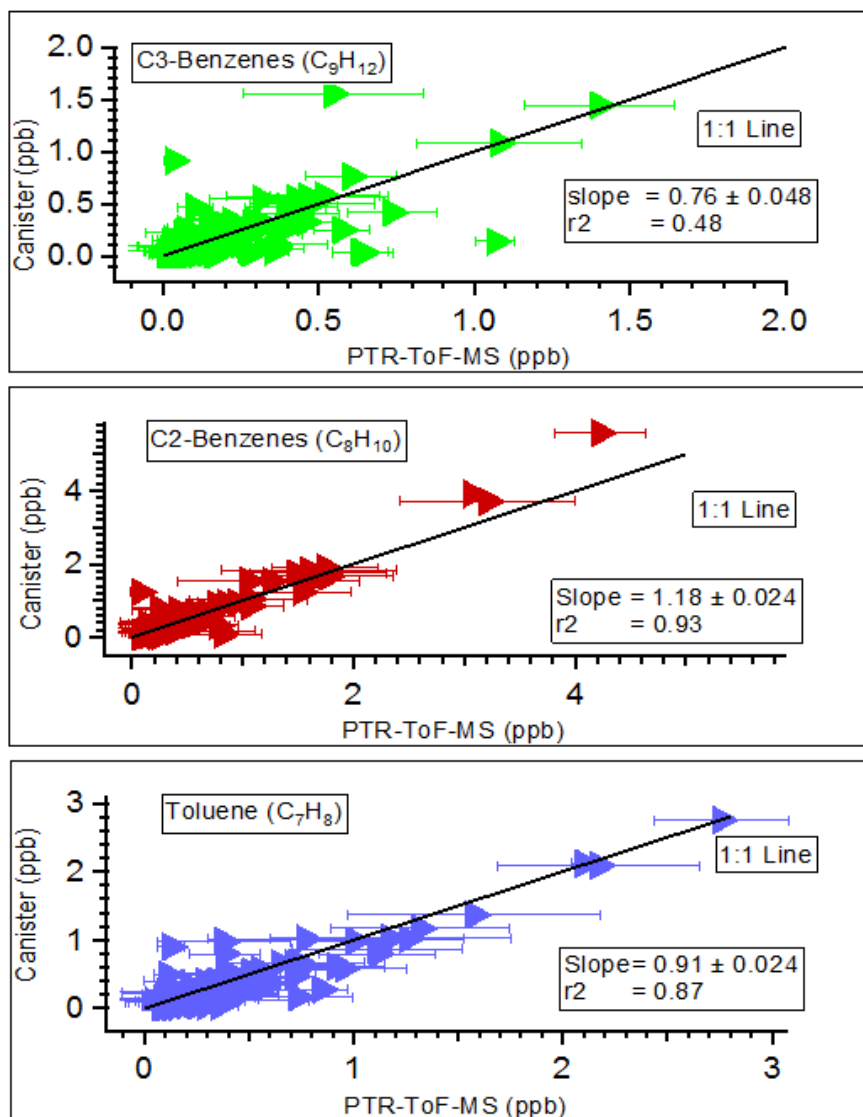


Figure S5. Comparison of three aromatic hydrocarbons measured using the PTRMS and using canister sampling/GCMS analysis. Error bars are 1 standard deviation of the PTRMS concentrations averaged over the corresponding canister sampling times (20 sec duration each sample).

S11. Fractions of Contributions to VOC Emissions from Main Sources

Table S12. The fractions of contributions to VOC emissions by the five main sources in each of the four major oil sands surface mining facilities SML, SUN, CNRL, and SAJ. The results are calculated using the emissions reports for these sources (Ref 7).

Sources	VOC emission fractions (%)			
	SML	SUN	CNRL	SAJ
Stacks - oil sands	2	1	6	0.3
Plant Fugitives	44	52	46	24
Mine Fleet	4	10	5	19
Mine Face	9	9	17	16
Tailings Management Areas	41	28	26	42

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