AirWaterGas

Sustainability Research Network

Leveraging receptor modeling to evaluate oil and gas speciation profiles in the Colorado Front Range

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Drexel UNIVERSITY

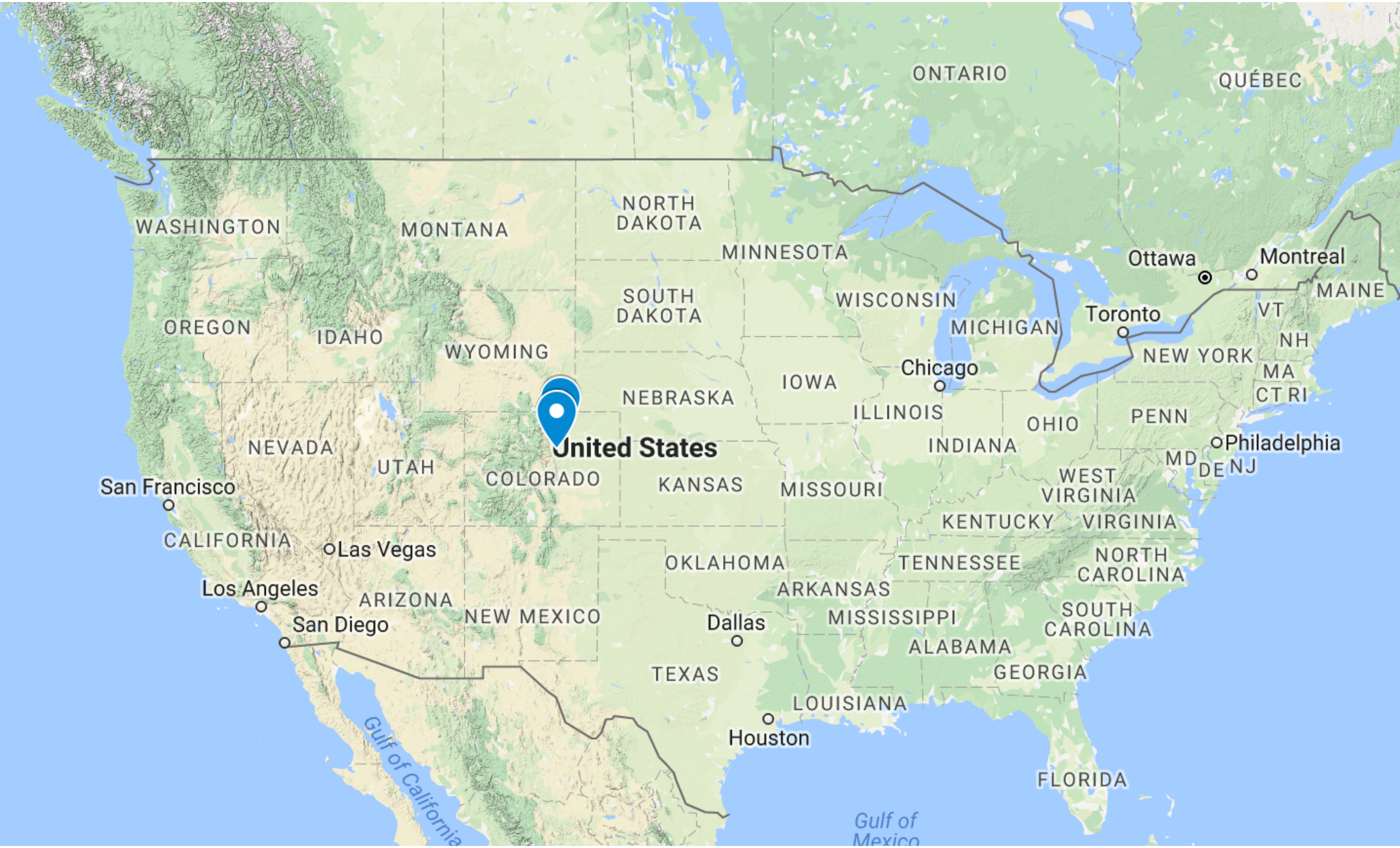
University of Colorado Boulder

Aims

1. Estimate the relative influence of oil & gas emissions and other sources on ozone production and BTEX concentrations

2. Assess the level of agreement between observation-based factors and speciation profiles

Location of Interest



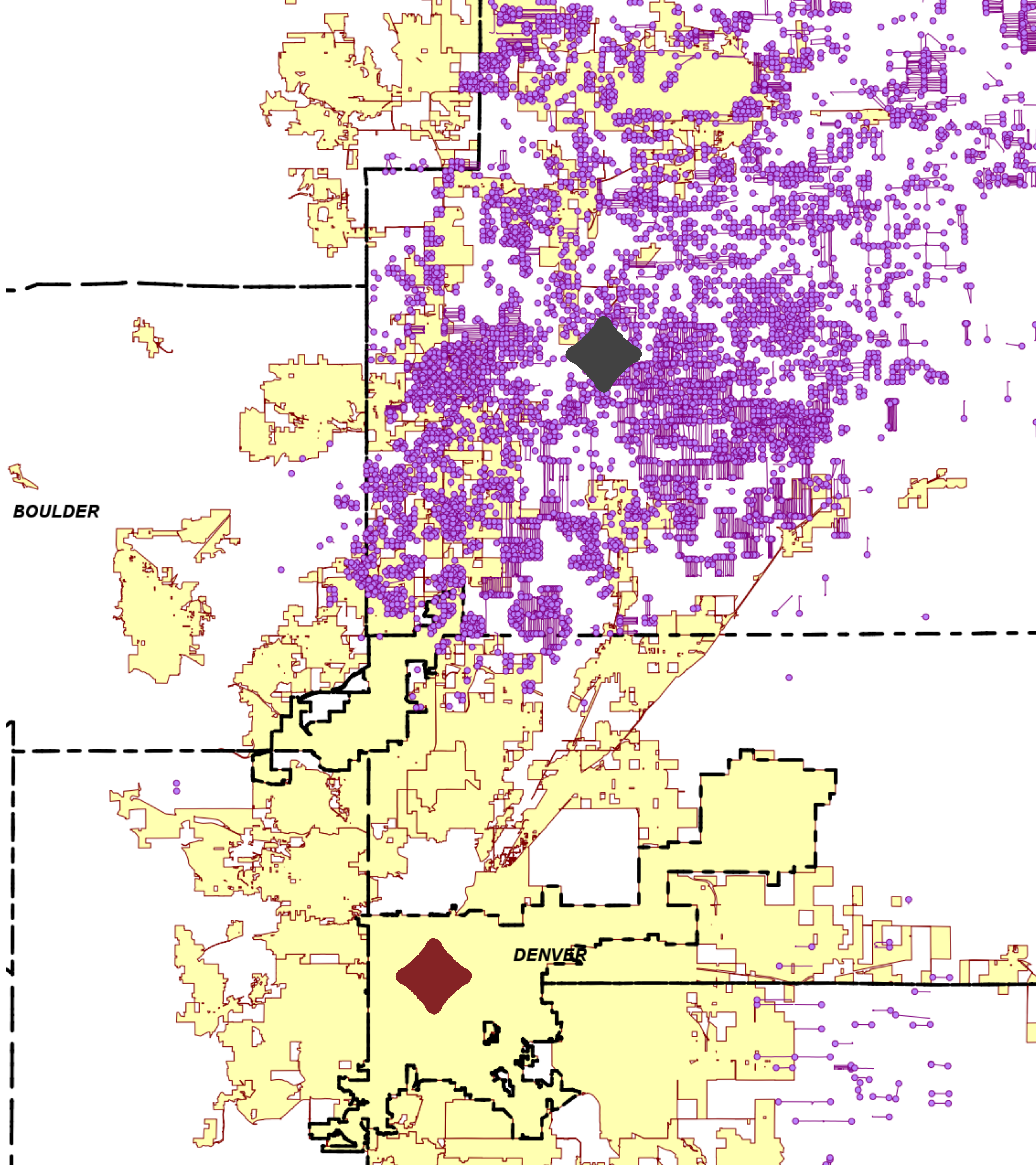
Google Maps

Wells*

Cities

Platteville measurement site

Denver measurement site



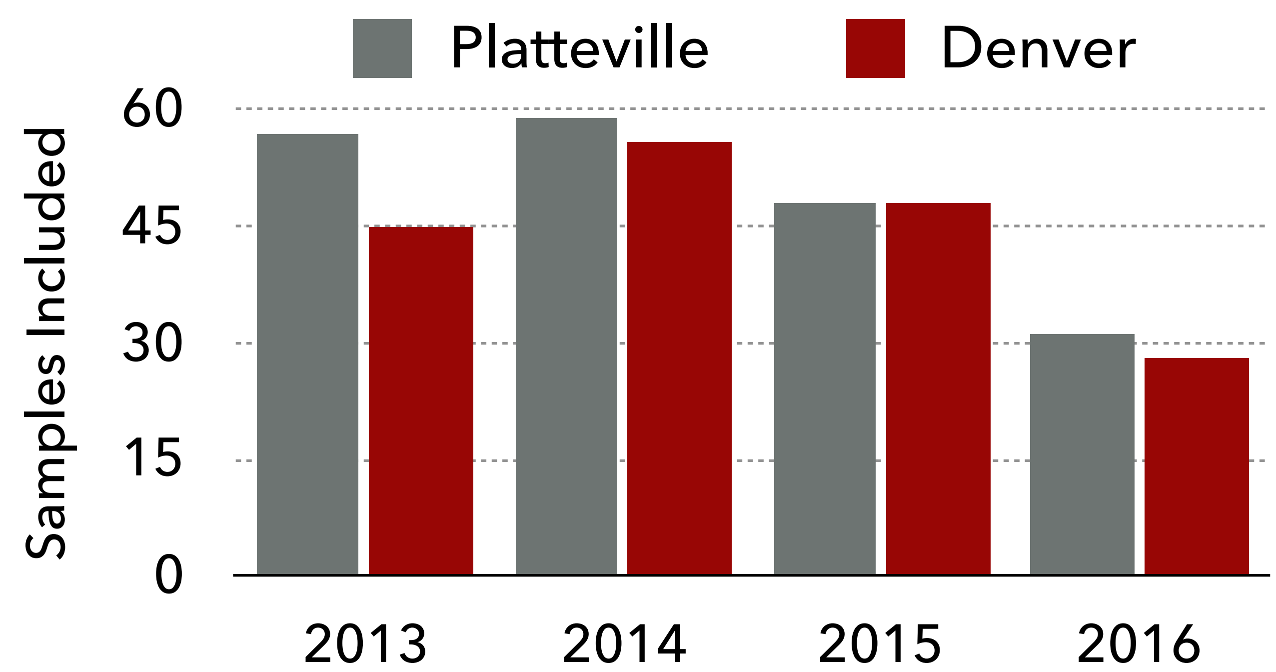
from COGCC Interactive Map (Oct 2016)

*actual directional/horizontal well bottomhole

Measurement Overview

- Conducted by Colorado Department of Public Health & Environment (CDPHE) Air Pollution Control Division Ozone Precursor Study

- 3-hr samples acquired from 6 a.m. to 9 a.m. local time in Summa canisters and analyzed for 79 non-methane organic compounds
    - co-elution of 1-butene and isopentane in sampling led to their exclusion



- methane was also analyzed from the Summa canisters and carbonyls were measured on DNPH cartridges - these species were excluded

- two samples (10 Apr 2013, 16 Feb 2014) at Platteville were excluded due to very high isobutane values

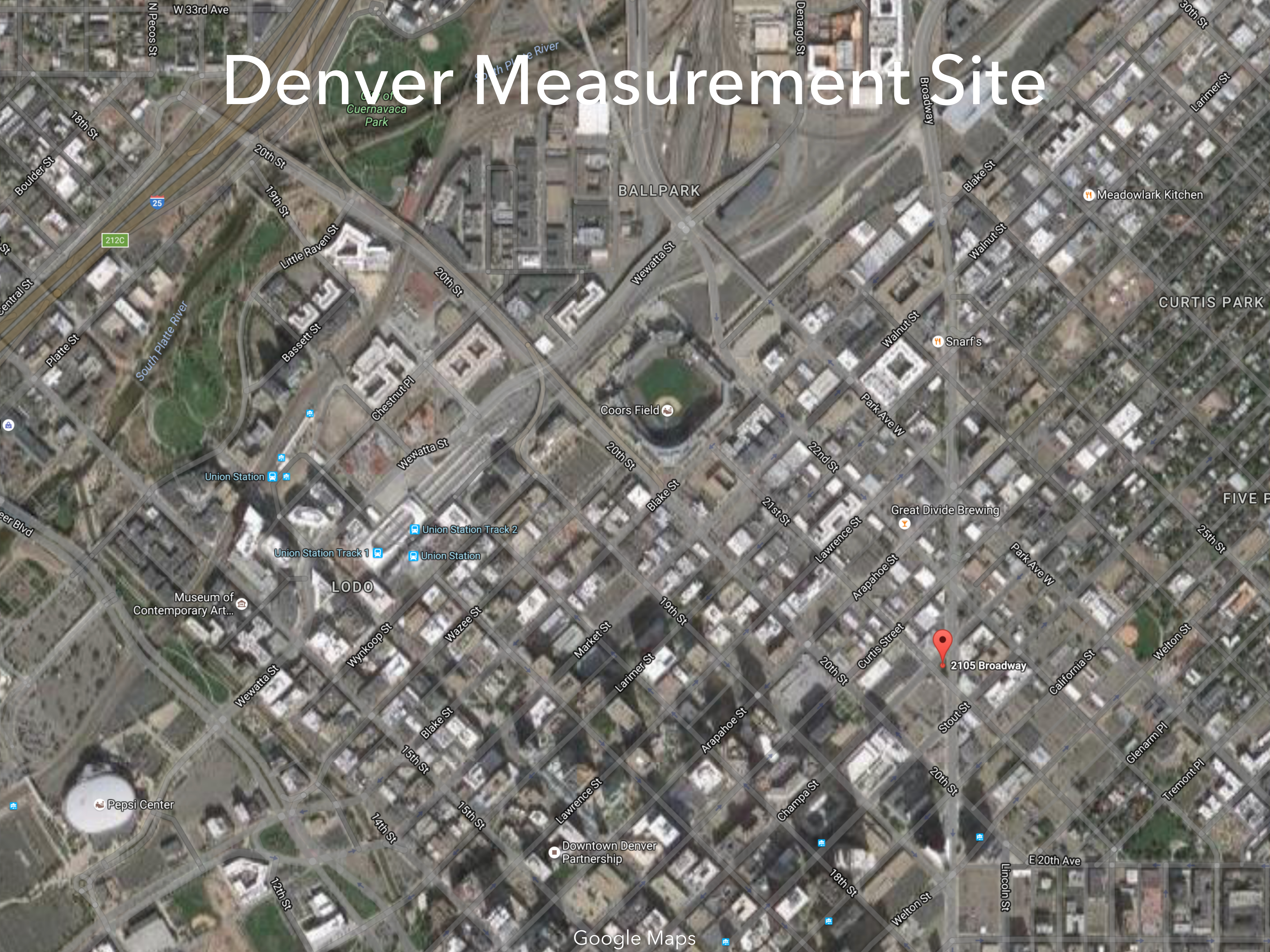
Data courtesy of Gordon Pierce (CDPHE)

Platteville Measurement Site

Google Street View

Platteville Measurement Site

Denver Measurement Site



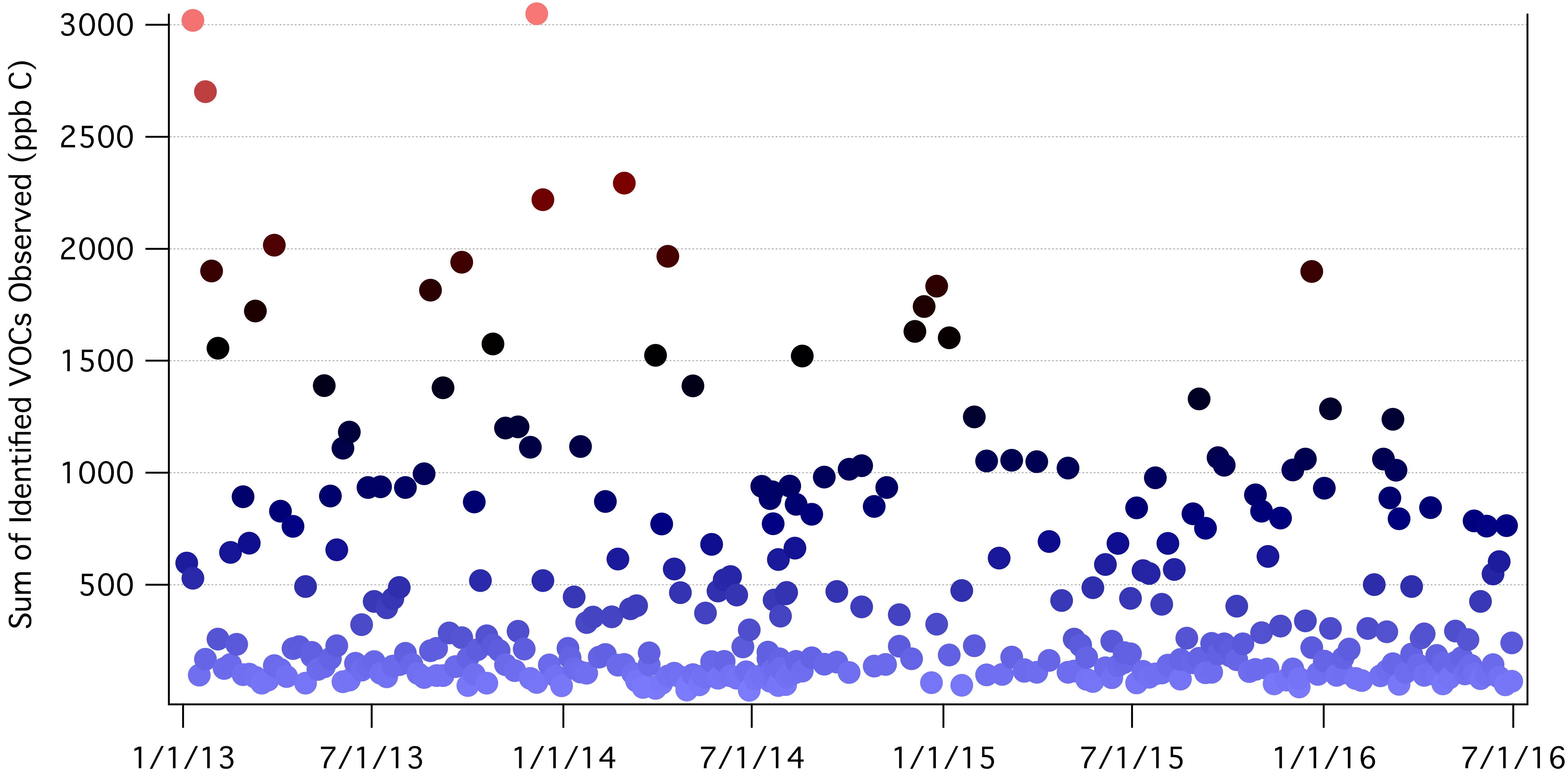
Denver Measurement Site

Google Street View

Aim 1:

Estimate the relative influence
of oil & gas emissions and other sources
on ozone production and
BTEX concentrations

Total Identified VOC Concentration



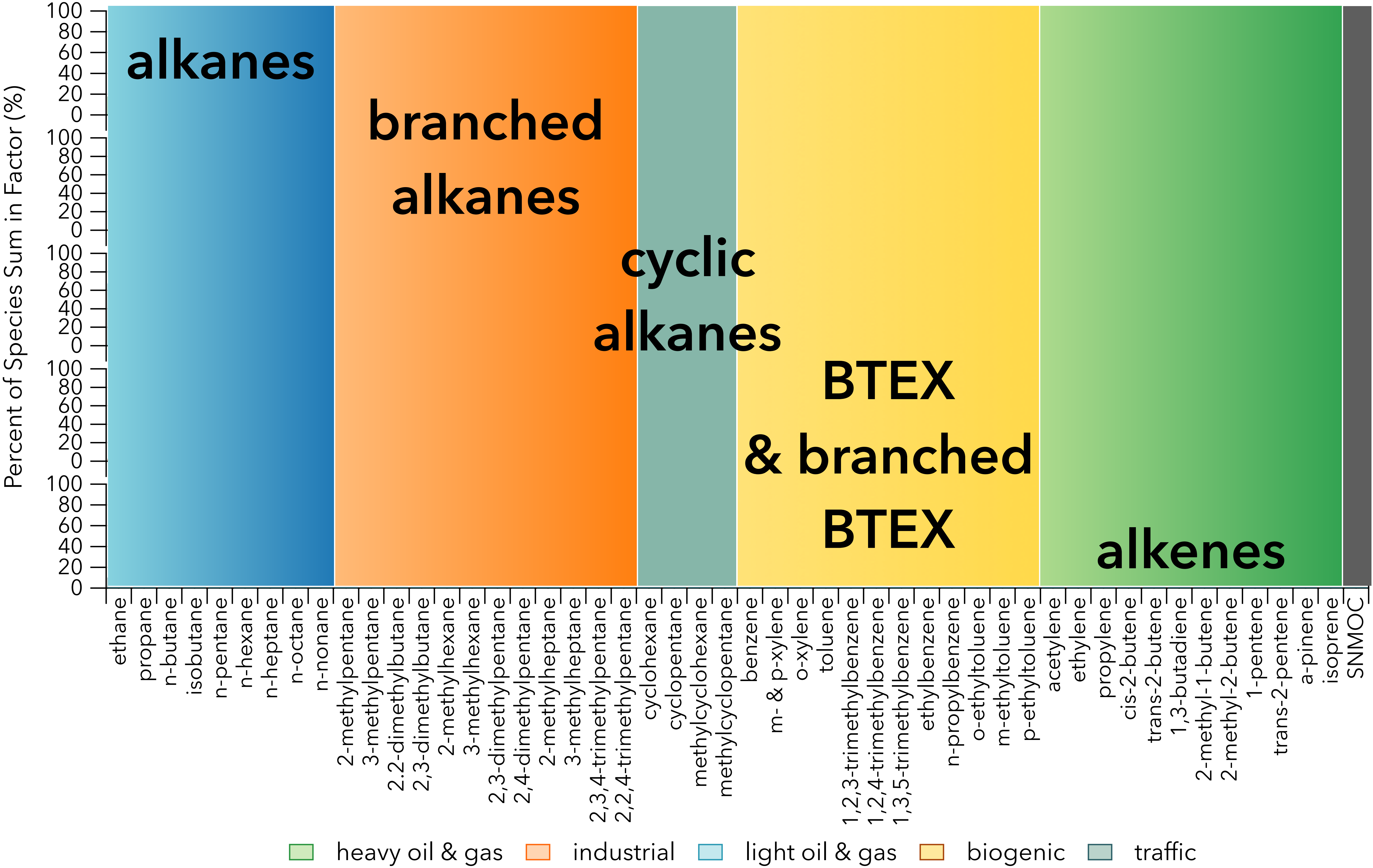
For context, the time series of the
sum of the identified VOCs at each site is shown.

Positive Matrix Factorization (PMF) finds a constrained, weighted least squares solution:

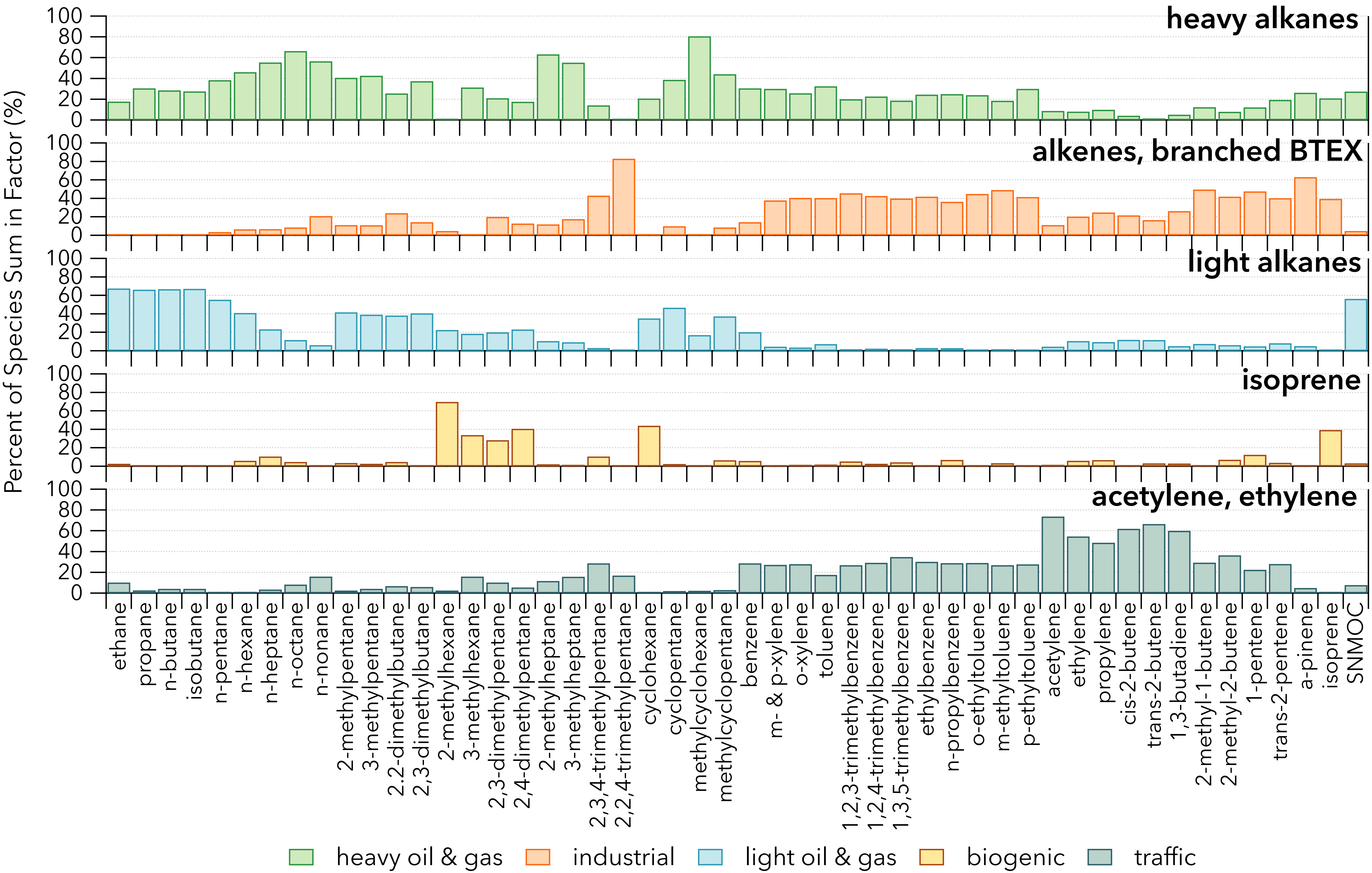
$$E_{ik} = \sum_{j=1}^{p} A_{ij} B_{jk} + \varepsilon_{ik} \qquad i = 1,2,\ldots,m; k = 1,2,\ldots,n$$

- A_{ij}, source profile: loading of compound i on factor j
- B_{jk}, normalized source contribution: j^{th} factor's contribution for the total k^{th} observation
- p, total factors
  - [3-5 evaluated]
- m, compounds observed and attributed
  - [50 NMVOCs]
- n, observations
  - [~46 per site per year]

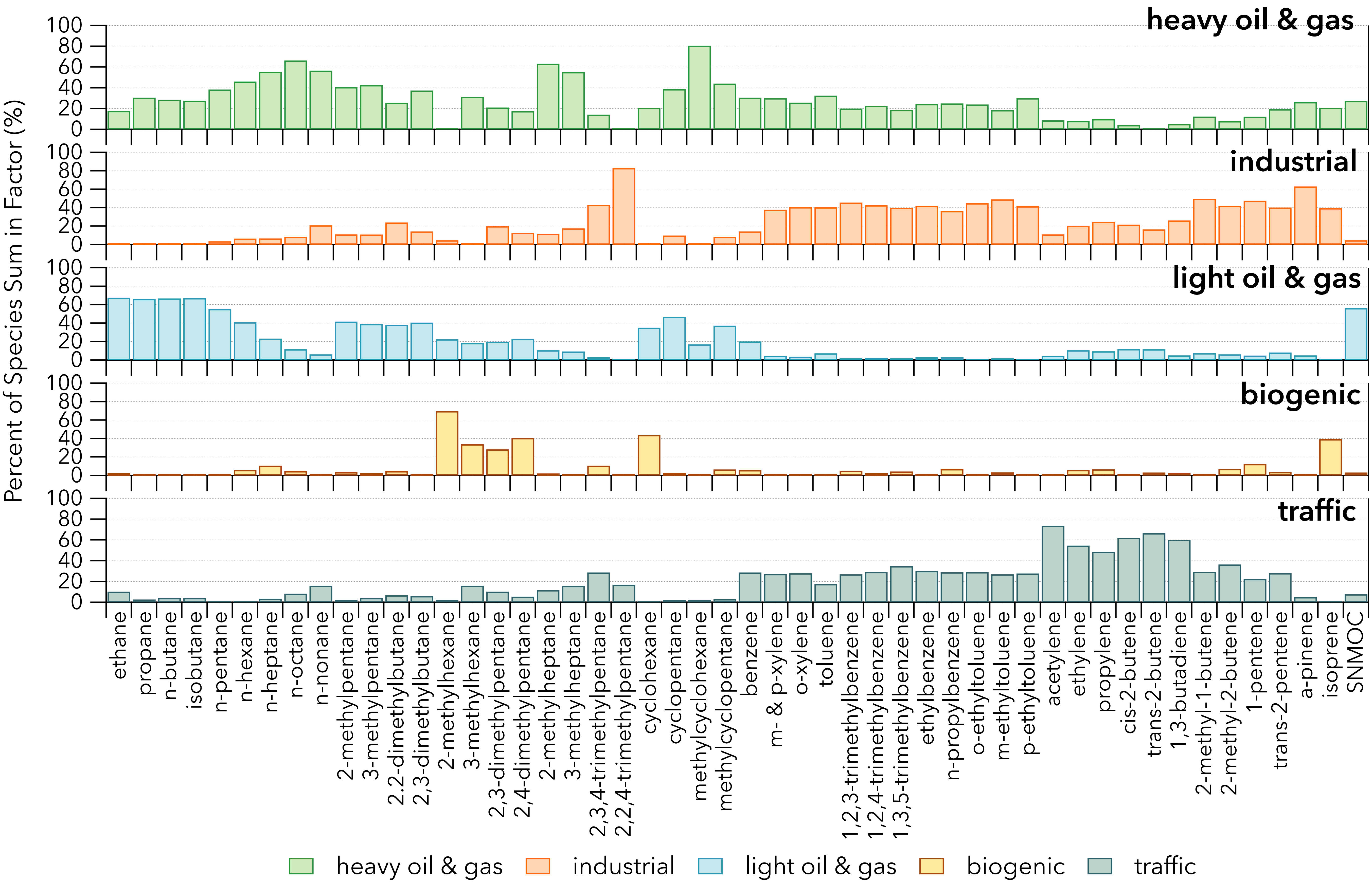
Composition of Factors



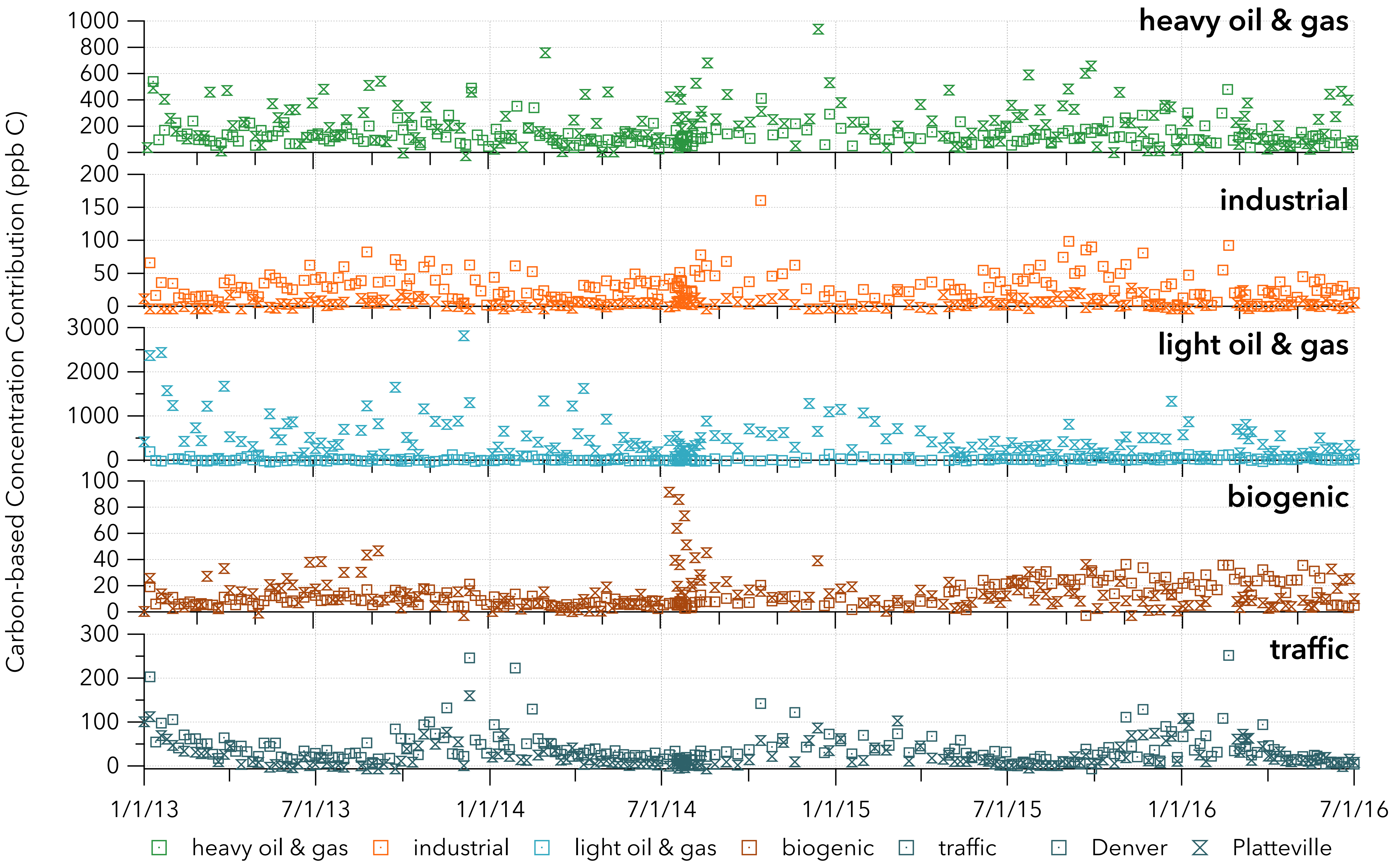
Composition of Factors



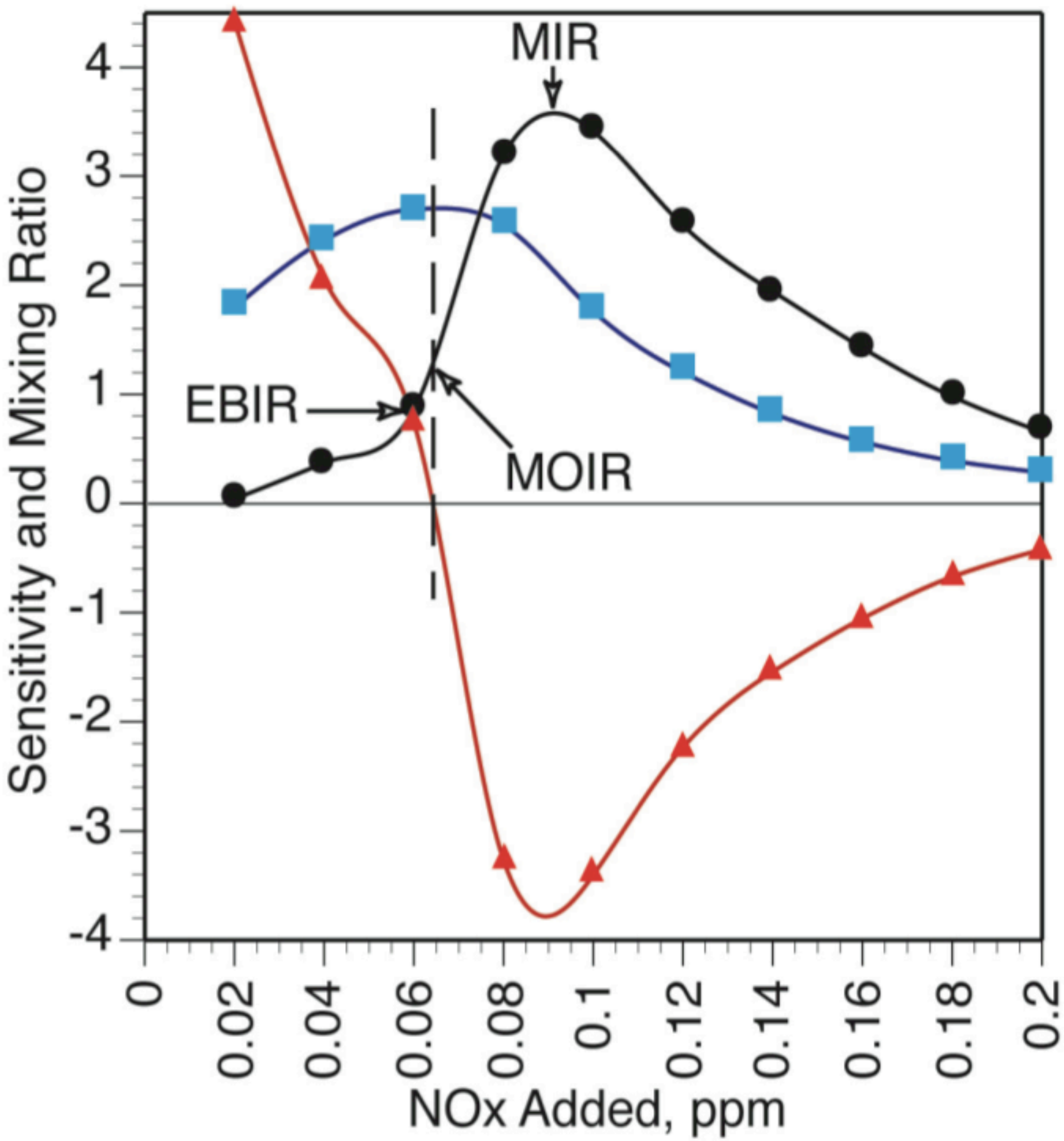
Composition of Factors



Contribution of Factors to VOCs



Estimating Ozone Formation from VOCs



Maximum Incremental Reactivity (MIR)

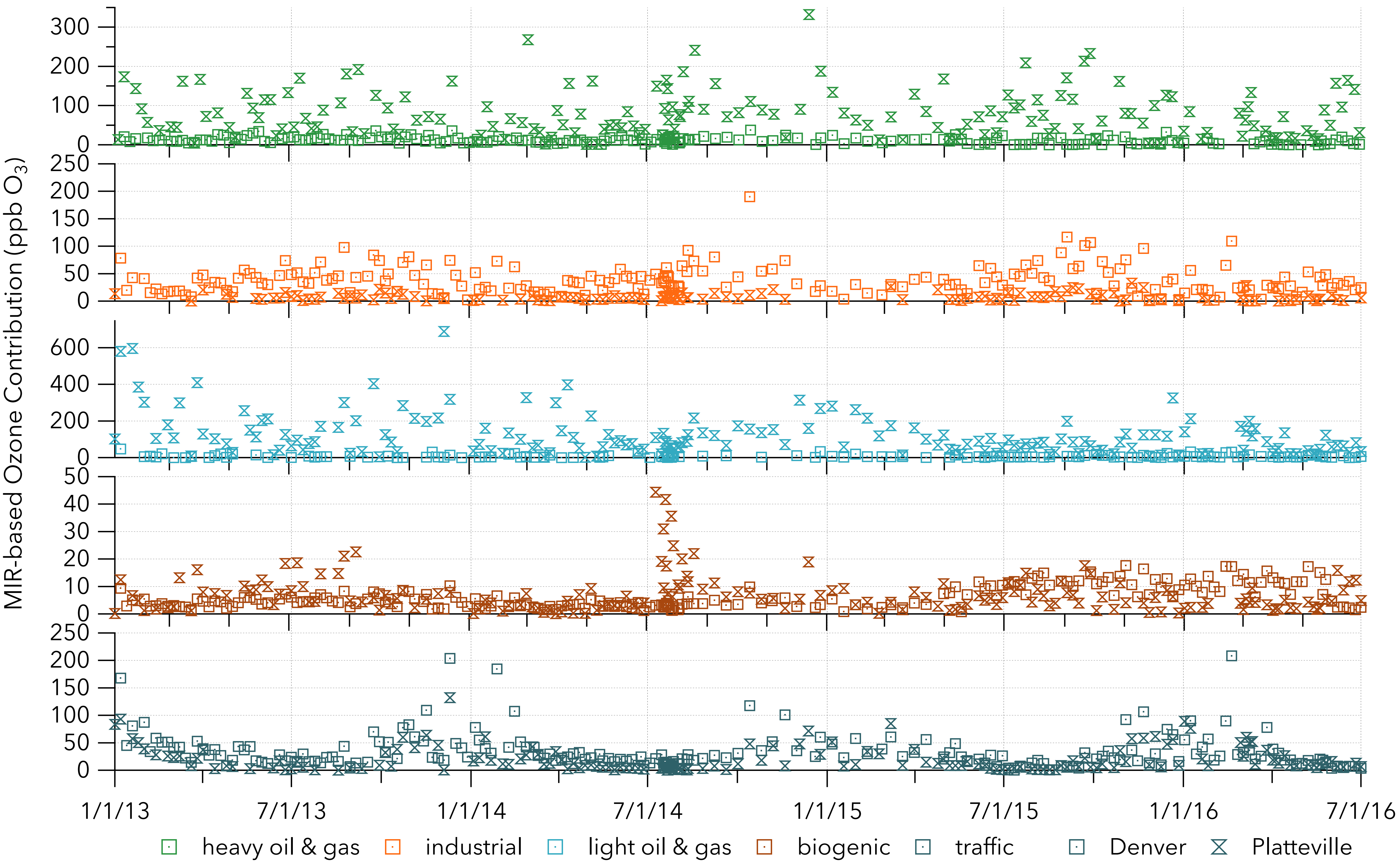
$$MIR_i = \left(\frac{\partial [O_3]}{\partial [VOC_i]} \right) \Bigg|_{\max\left(\frac{\partial [O_3]}{\partial [VOC_{mix}]} \right)}$$

MIR-based Contribution to Ozone

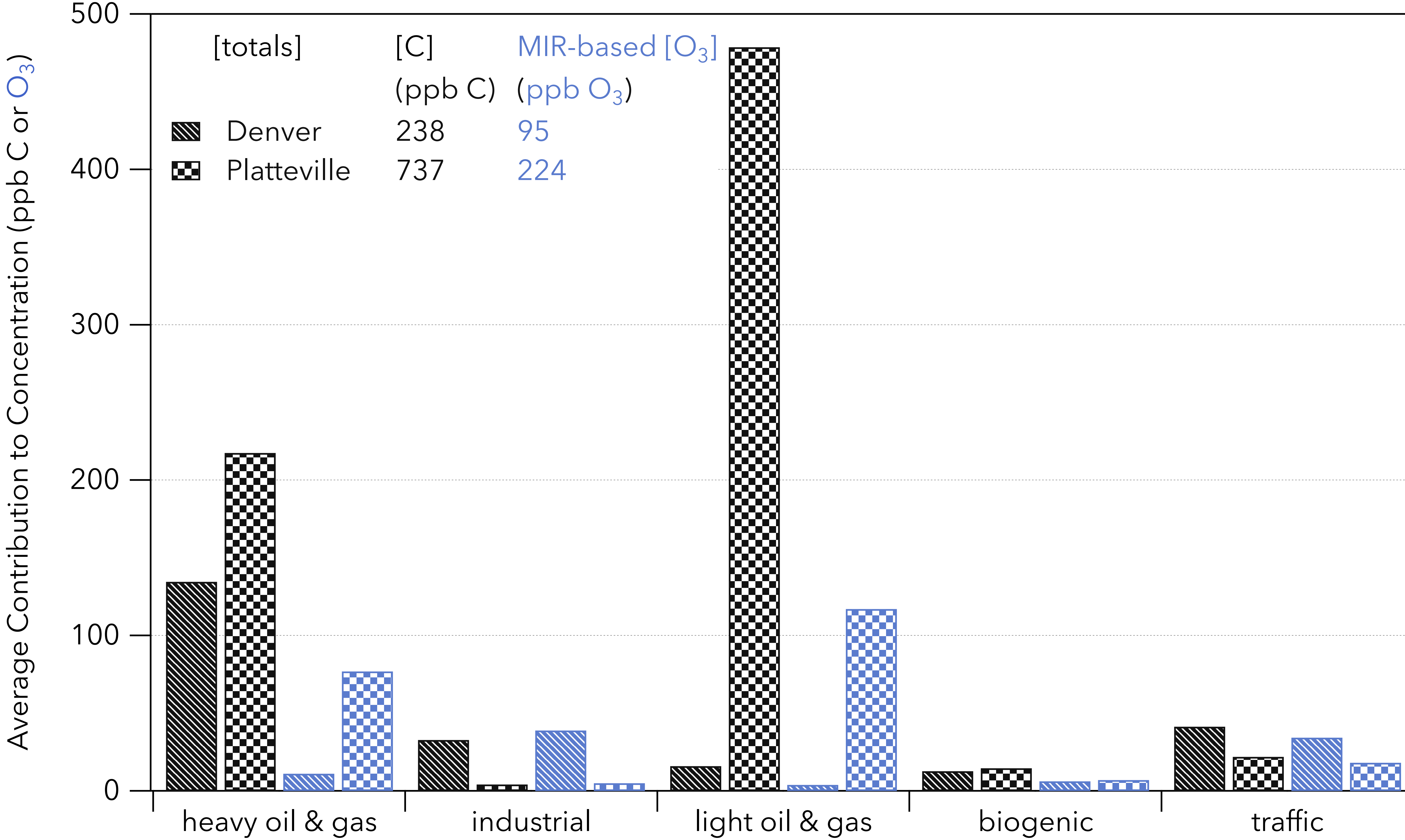
$$\Delta O_{3,i,k} = \frac{\partial O_3}{\partial VOC_i} \Delta VOC_{i,k}$$

Carter (1995) and updates from cert.ucr.edu/carter

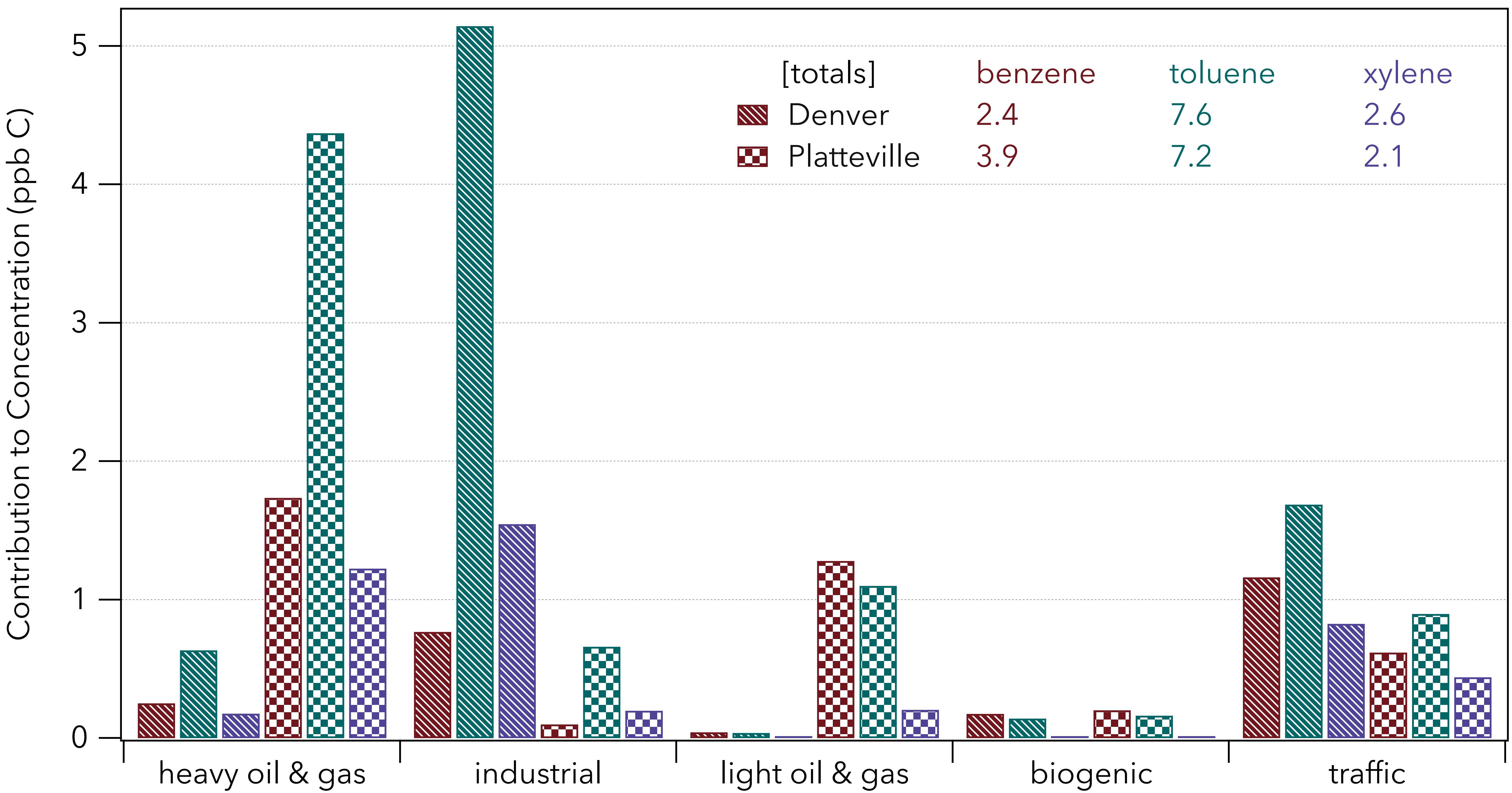
Contribution of Factors to MIR-based O_3



Average Contribution of Factors to C or O_3



Average Contribution of Factors to BTEX



Aim 2:

Assess the level of agreement between observation-based factors and speciation profiles

Comparison of Factors to Emissions Speciation Profiles

- MOVES speciation profiles including *cold start*, *exhaust*, *diurnal evaporation*, and *hot soak*
- Colorado State University (CSU) speciation of emissions from *production*, *fracking*, *liquids load out*, and flowback processes
- Western Regional Air Partnership (WRAP) Phase III Oil & Gas Speciation Profiles from surveys of producers in the Intermountain West basins for *flashed gas* and *produced gas* emissions
- Condensate speciation profiles from Brantley et al. with VOC emissions from oil & natural gas well pads using mobile remote and on-site direct measurements [*averaged of twenty unique profiles*]

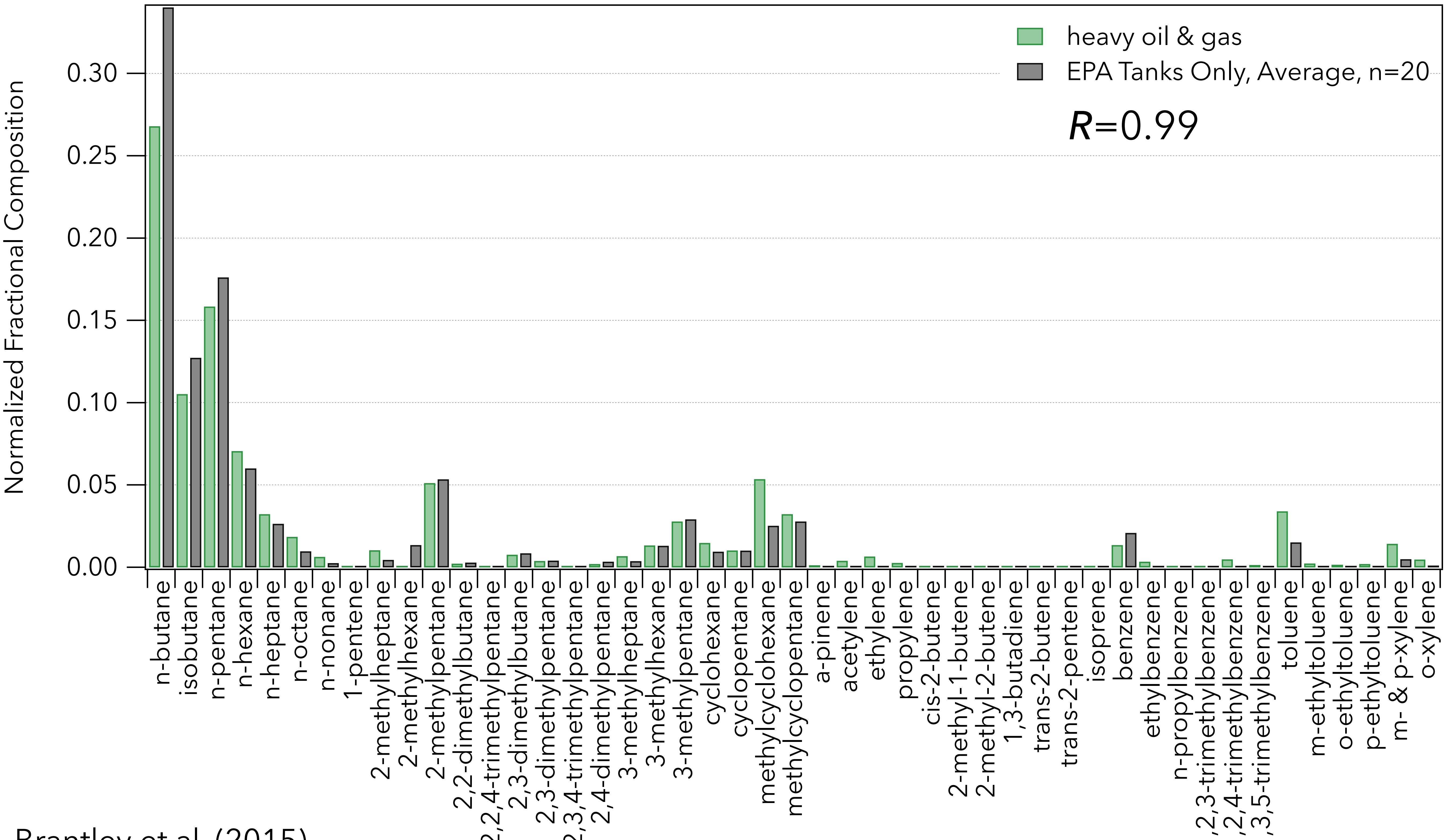
(Shah et al., memo, 2015; Brantley, Thoma & Eisele J. Air & Waste Manage. Assoc. 65(9):1072-1082, 2015)

Comparison to Speciation Profiles

	heavy oil & gas	industrial	light oil & gas	biogenic	traffic
Exhaust Cold Start	0.09	0.45	0.09	0.24	0.64
EXHST1	0.14	0.57	0.11	0.18	0.65
Diurnal RVP7	0.31	0.70	0.17	0.12	0.13
Diurnal RVP10	0.77	0.32	0.76	0.05	0.46
HOTSOK	0.56	0.50	0.55	-0.03	0.39
CSU Production	0.85	0.17	0.88	-0.04	0.56
CSU Fracking	0.04	0.56	0.00	-0.02	0.49
CSU Liquids Load Out	0.94	-0.04	0.99	-0.01	0.52
CSU Flowback	0.86	0.20	0.76	0.09	0.34
WRAP Flash	0.93	-0.04	0.97	-0.01	0.49
WRAP Produced Gas	0.88	0.03	0.87	0.03	0.40
EPA Tanks Only, Average, n = 20	0.99	0.04	0.98	0.03	0.46

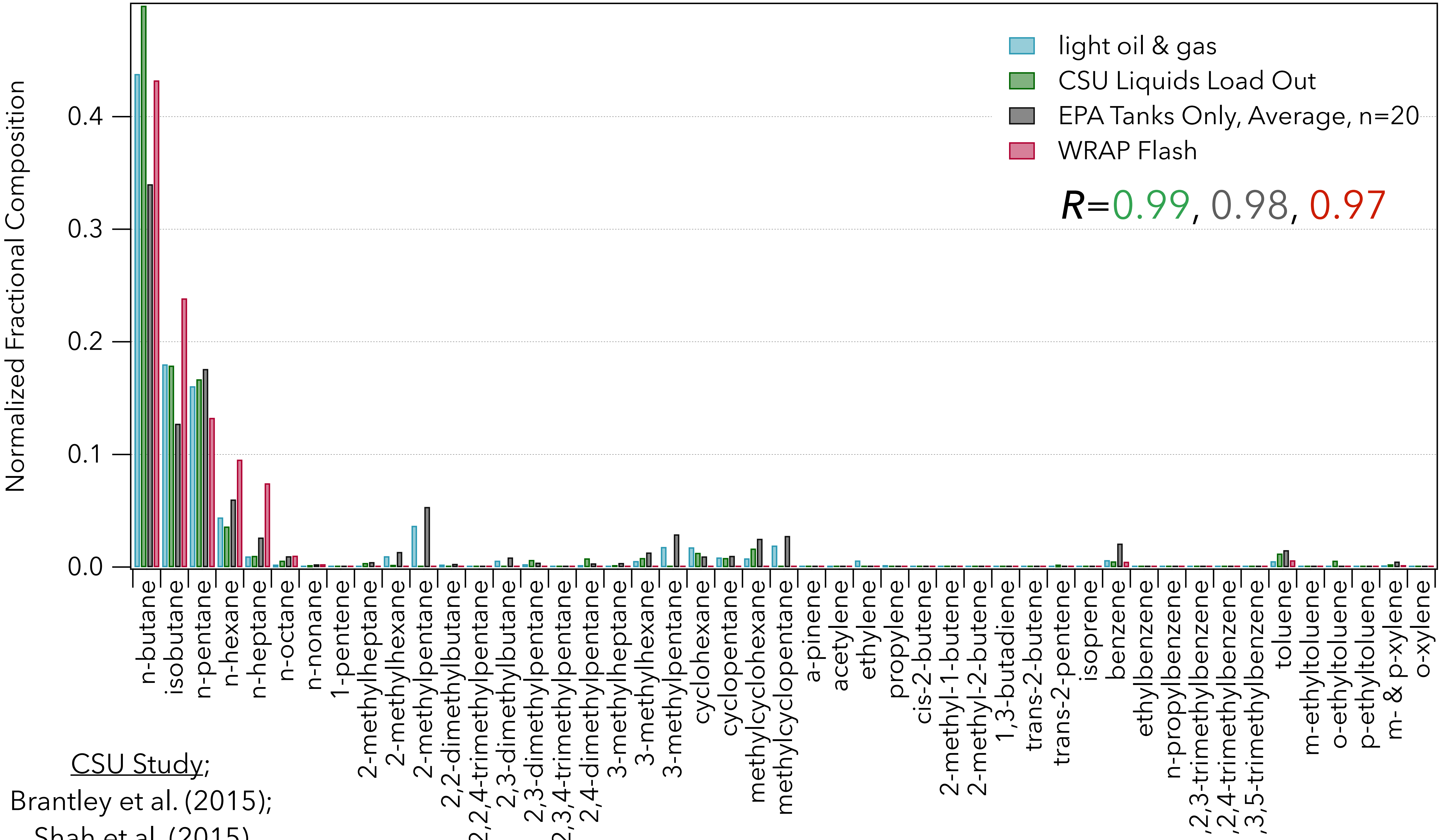
Correlation coefficient (*R*) of carbon-based fraction of factors with speciation profiles neglecting ethane and propane.

Heavy Oil & Gas Well Correlated with EPA Condensate



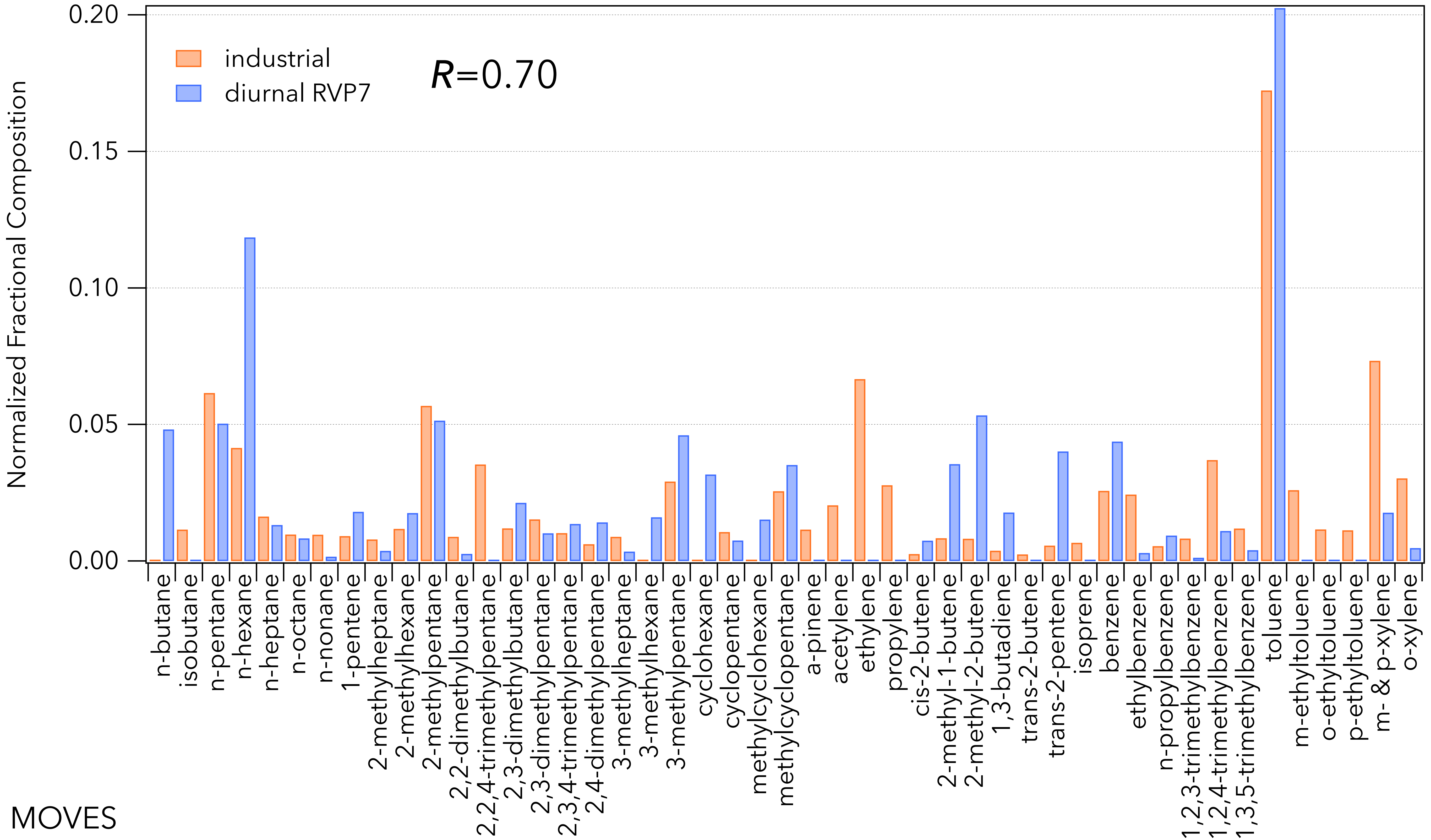
Brantley et al. (2015)

Light Oil & Gas Well Correlated with Multiple Profiles



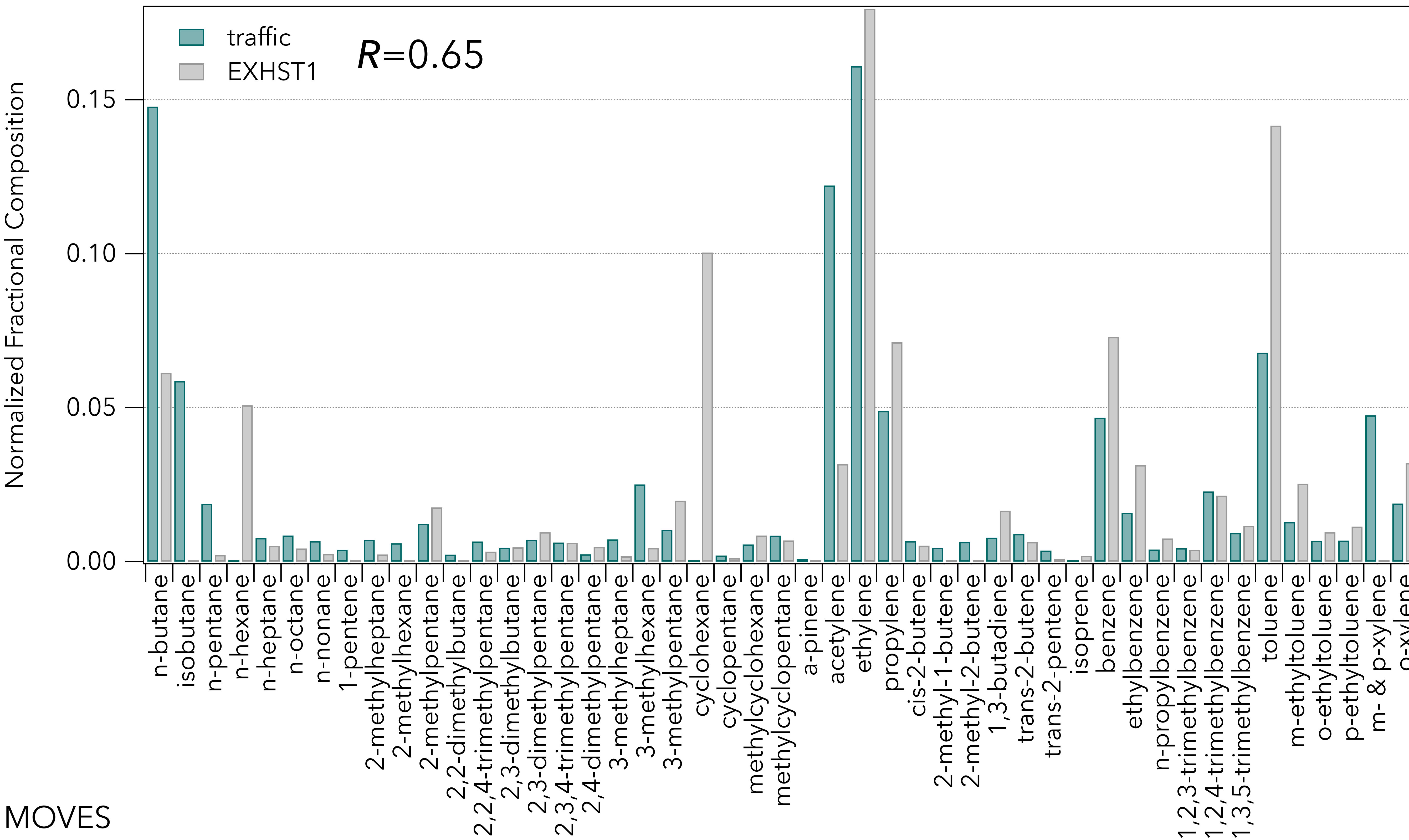
CSU Study;
Brantley et al. (2015);
Shah et al. (2015)

Industrial Best Correlated with Diurnal Evaporative Emissions



MOVES

Traffic Best Correlated with Exhaust Emissions



MOVES

Summary & Conclusions

- 2013-2016 observations of factors composed of VOCs characteristic of oil & gas development were much higher in Platteville than in Denver with the light oil & gas factor declining from 2013 to 2016.
- Though the Platteville oil & gas contributions to total VOC concentrations dominate, MIR reactivity suggests that the ozone impact is not solely from these factors.
- The BTEX contributions are equally significant from the traffic and industrial factors in Denver as heavy oil & gas and traffic factors in Platteville.
- The normalized speciation profiles of the light and heavy oil & gas factors correlated with recent speciation profiles very well, even better than the traffic factor correlated with exhaust emissions.

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Acknowledgements

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