Matrix Factorization of the 2001 Deer Park VOC data for Source Resolution and Apportionment

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Receptor Modeling

$$C_{(ij)} = \sum_{k=1}^{n} \alpha_{(jk)} s_{(ik)} + e_{(ij)}$$

where: i = compounds (1, 2, …)
j = samples (1, 2, …)
k = sources (1, 2, …)

C = concentration of species in ambient samples
α = emission source strengths
s = source profiles
e = difference between ambient concentration and reconstructed source contribution

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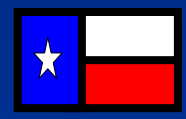
Univariate versus Multivariate

Univariate: Supply known source profiles (Chemical Mass Balancing)

Multivariate: Source profiles and number of sources are unknowns

Positive Matrix Factorization: Use physical limitations on $\alpha_{(jk)}$ and $s_{(ik)}$ to determine number of sources and source profiles



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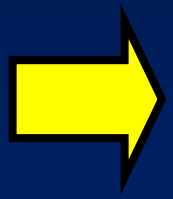
Multivariate Receptor Modeling

More Data  **Resolve More Sources**

Past Applications of PMF have used multiple years of VOC data to resolve upto 15 sources

Our approach is to use only 1 week of hourly data to focus on the 3 or 4 most important sources

(can still analyze a full year of data)

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Dominant Source Profiles

VOC concentrations are dominated by 3 or 4 sources using analyzing hourly data by PMF one week at a time

Using 2001 hourly VOC data from Deer Park, PMF resolves 3 sources in 25% of weekly data and 4 sources in 75% of weeks

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Dominant Source Profiles

Natural Gas:	100% of weeks
Vehicle Exhaust:	98% of weeks
Petrochemical Prod*:	90% of weeks
Refining Operations:	48% of weeks
Gasoline Vapor:	34% of weeks
Biogenic Emissions:	11% of weeks
Methylcyclohexane**:	2% of weeks

* 90% ethylene rich and 10% propylene rich

** one occurrence

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CASE I

Ethane is excluded

(low reactivity and high concentration)

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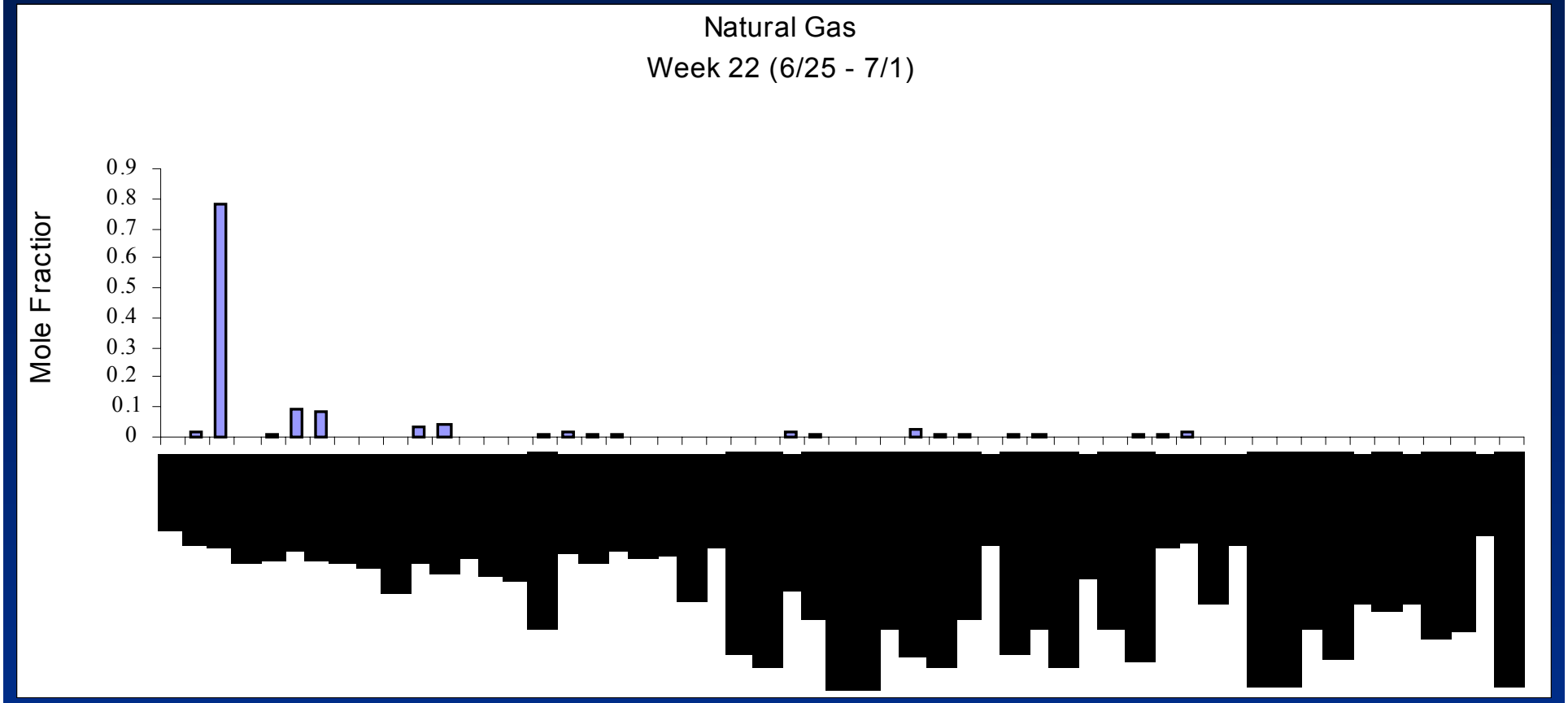
Natural Gas



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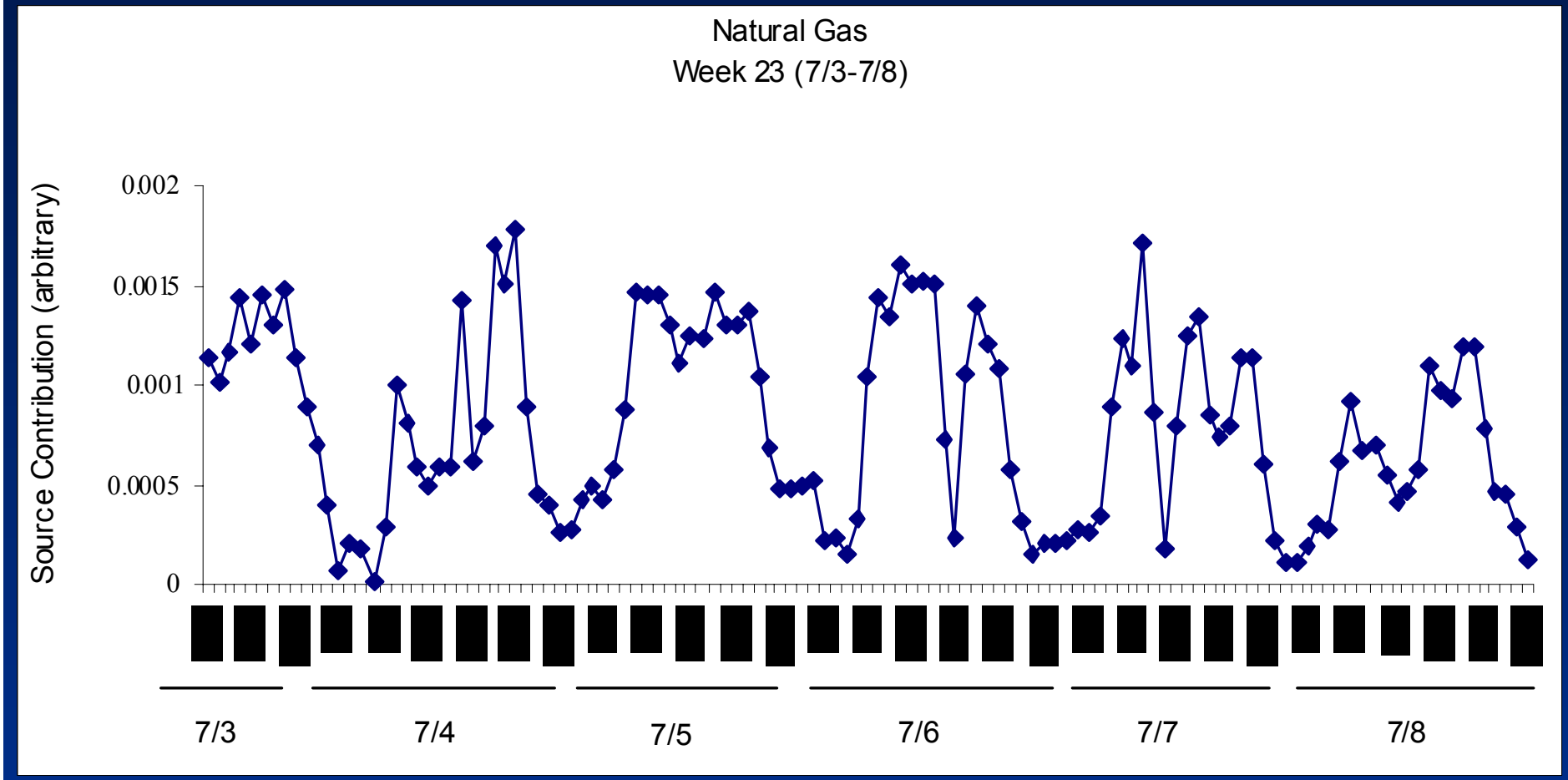
Natural Gas



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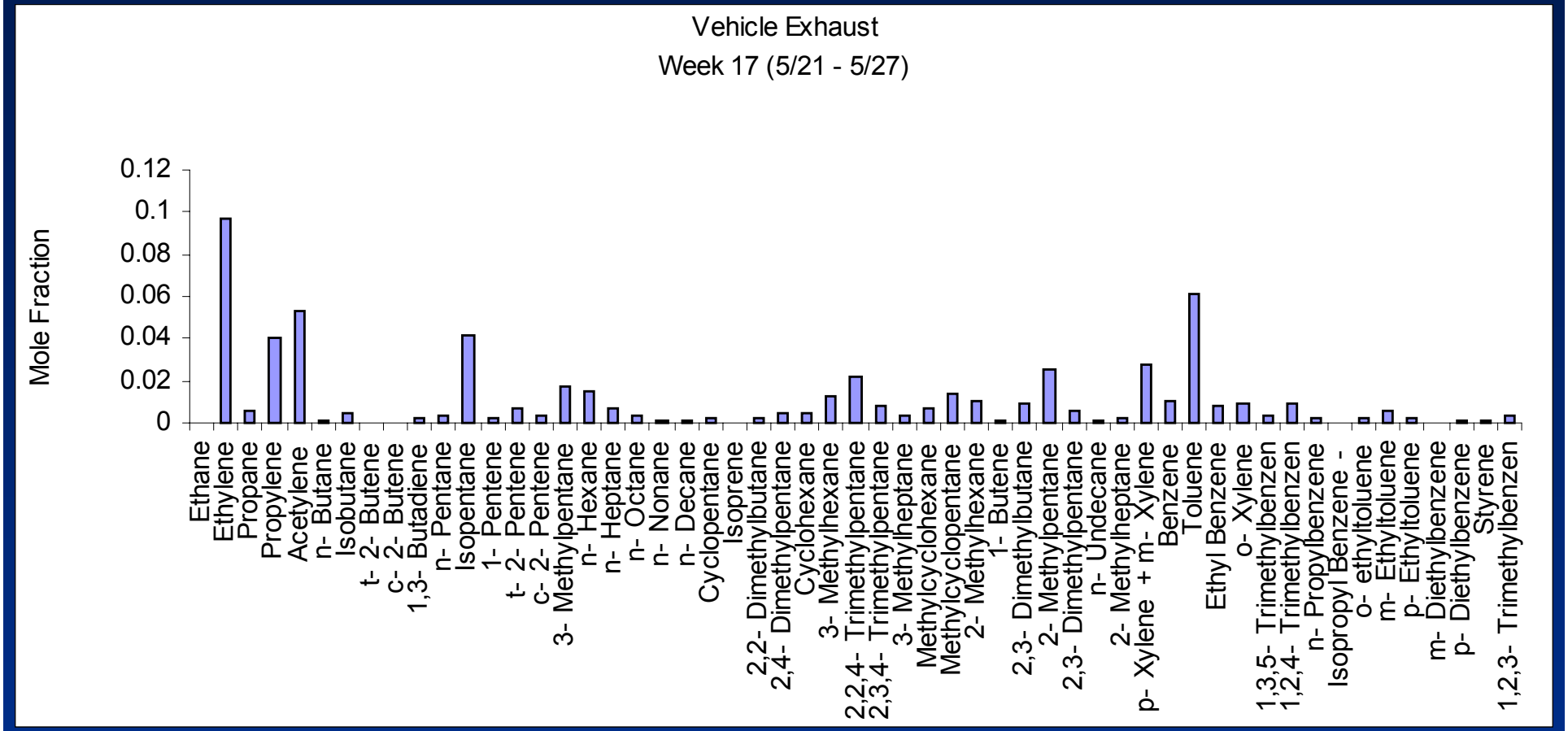
Vehicle Exhaust



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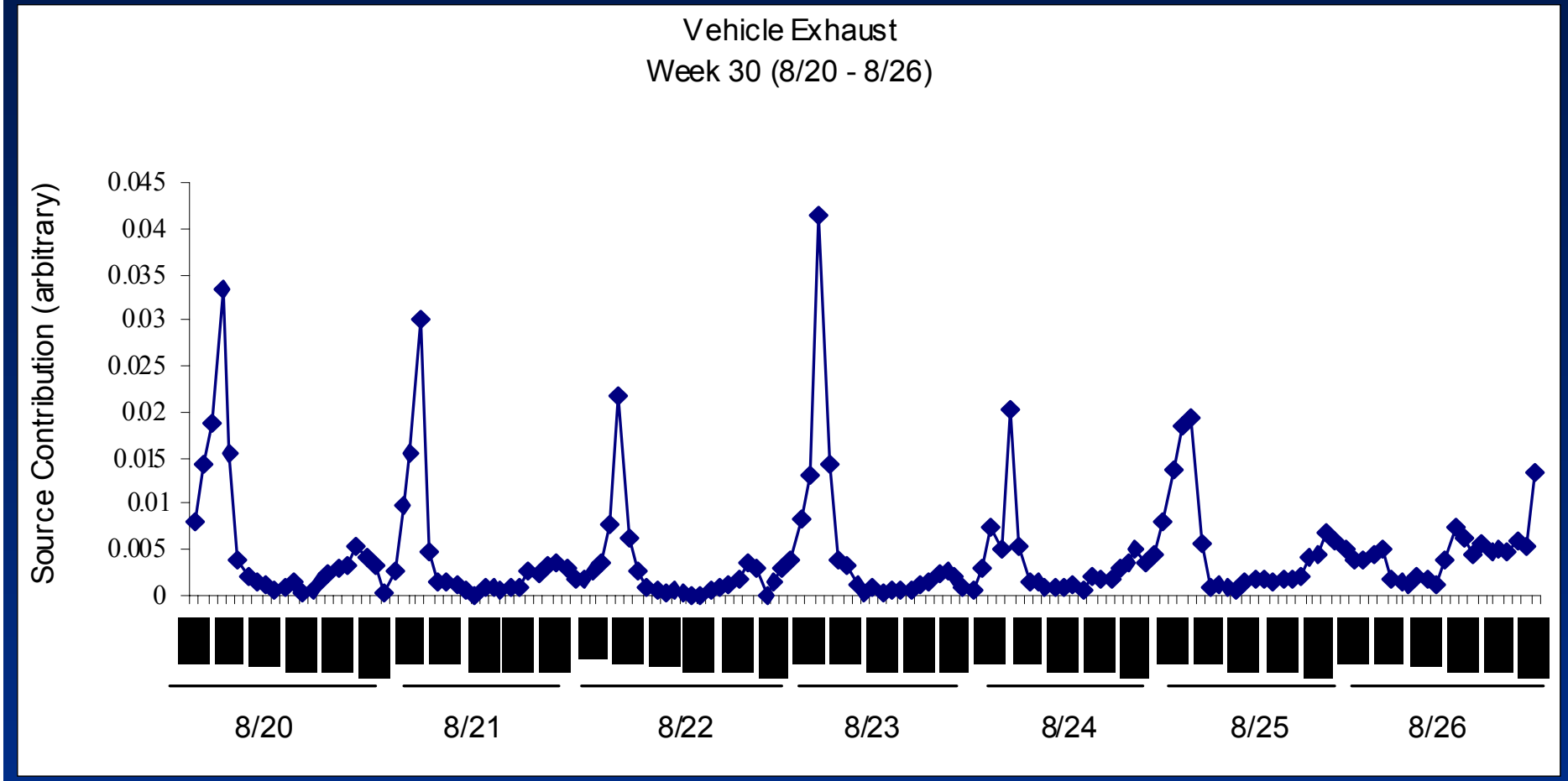

** August 26 was a Sunday (2001)*

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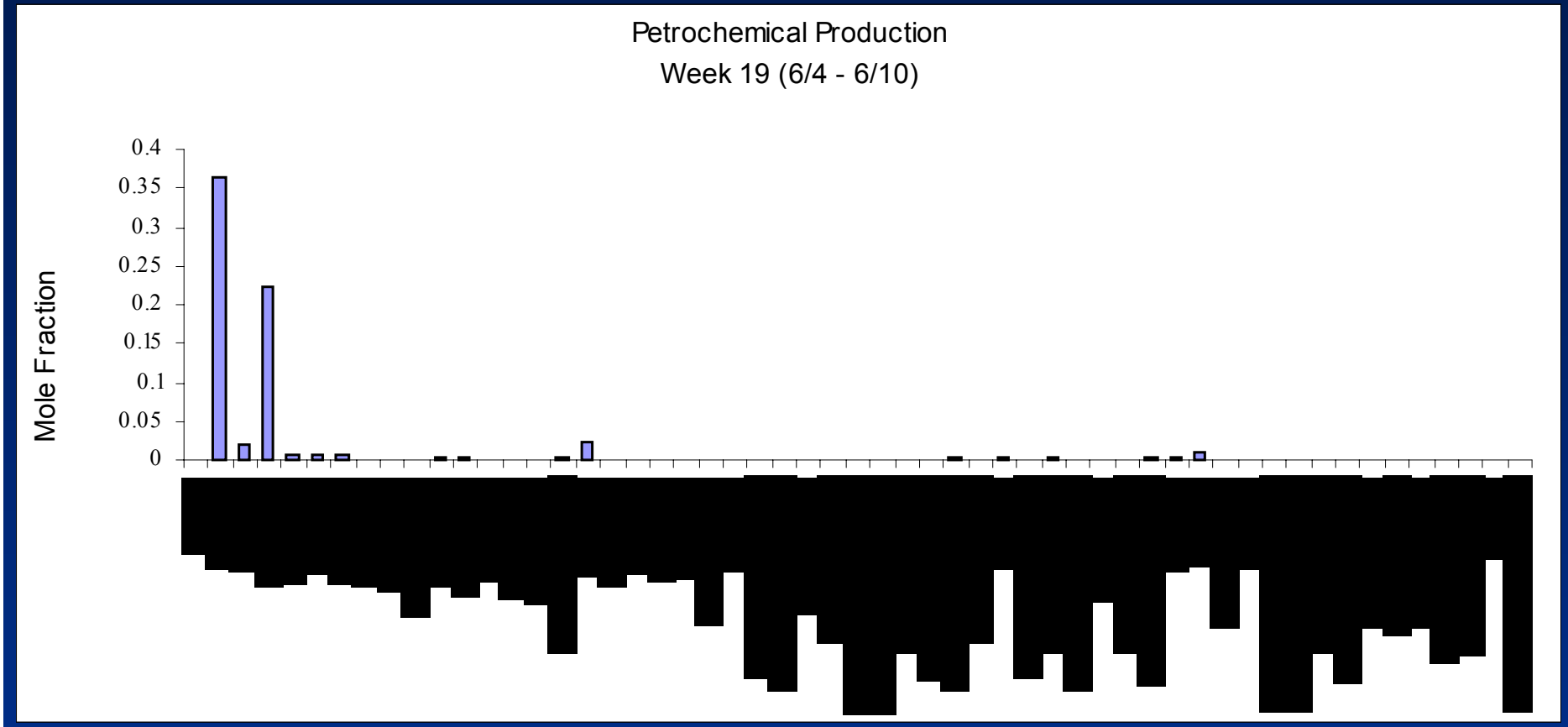
Petrochemical Production



Related source profile with propylene dominant occurs in 10% of the data

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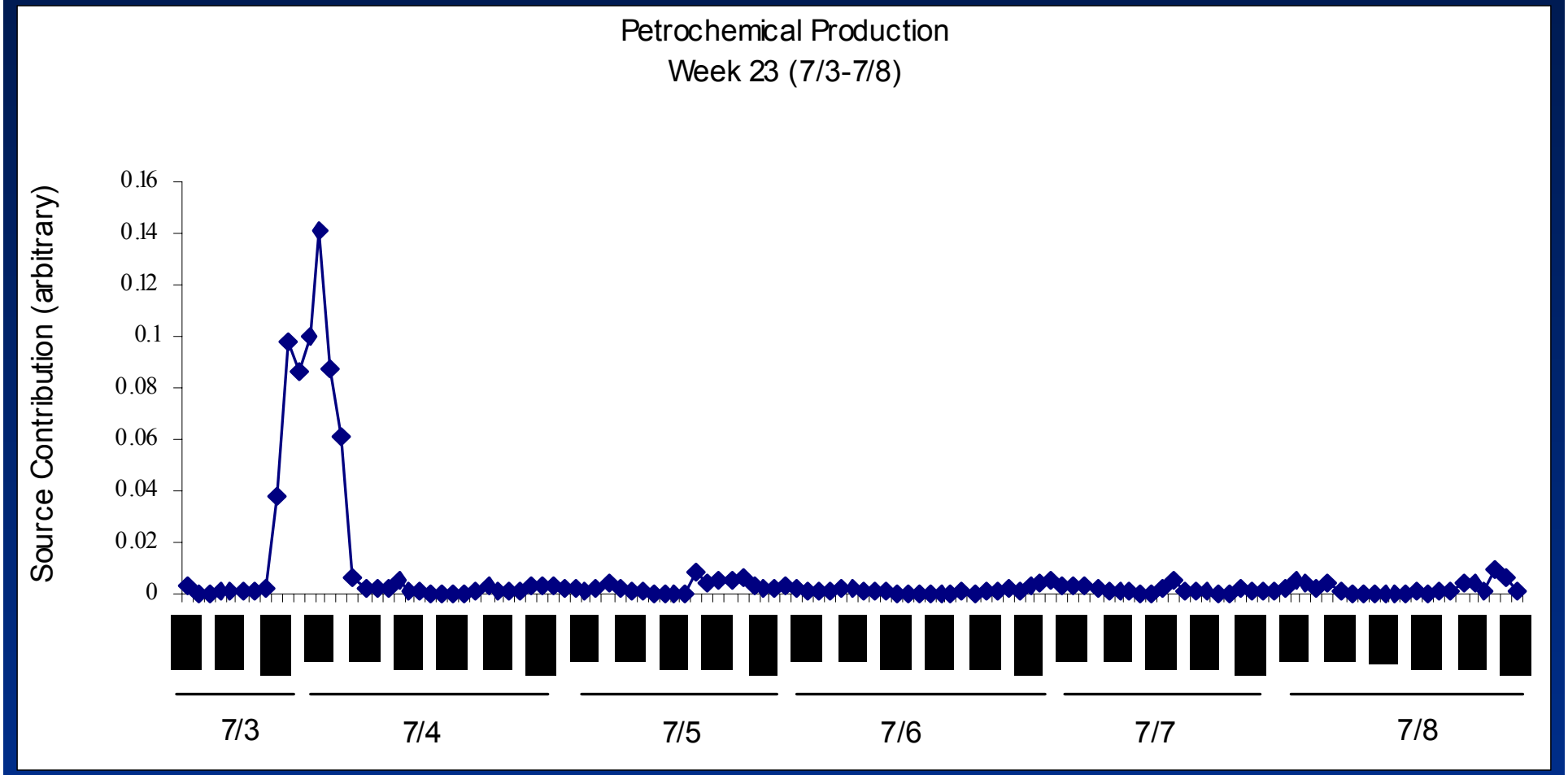
Petrochemical Production



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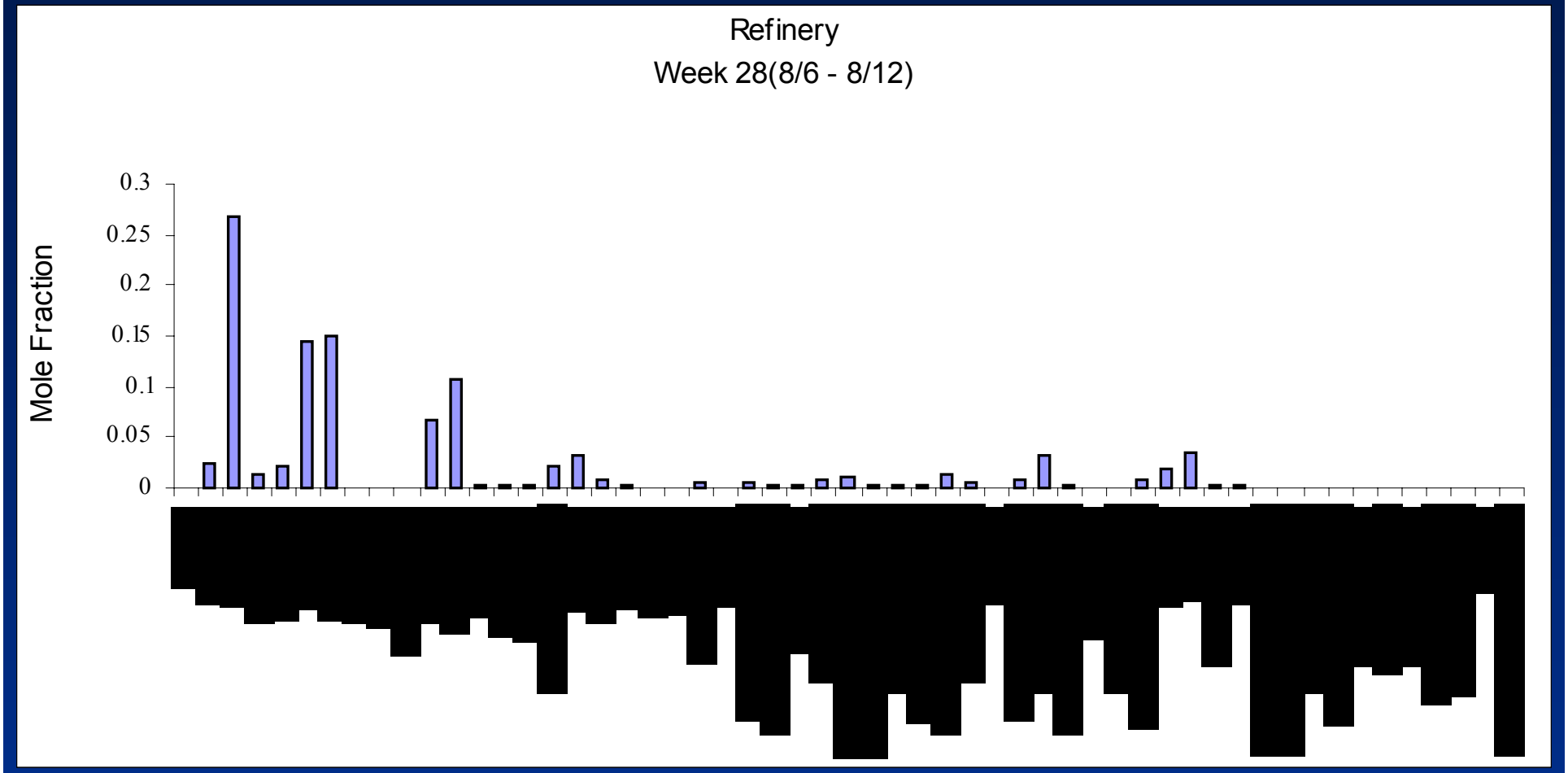
Refining Operations



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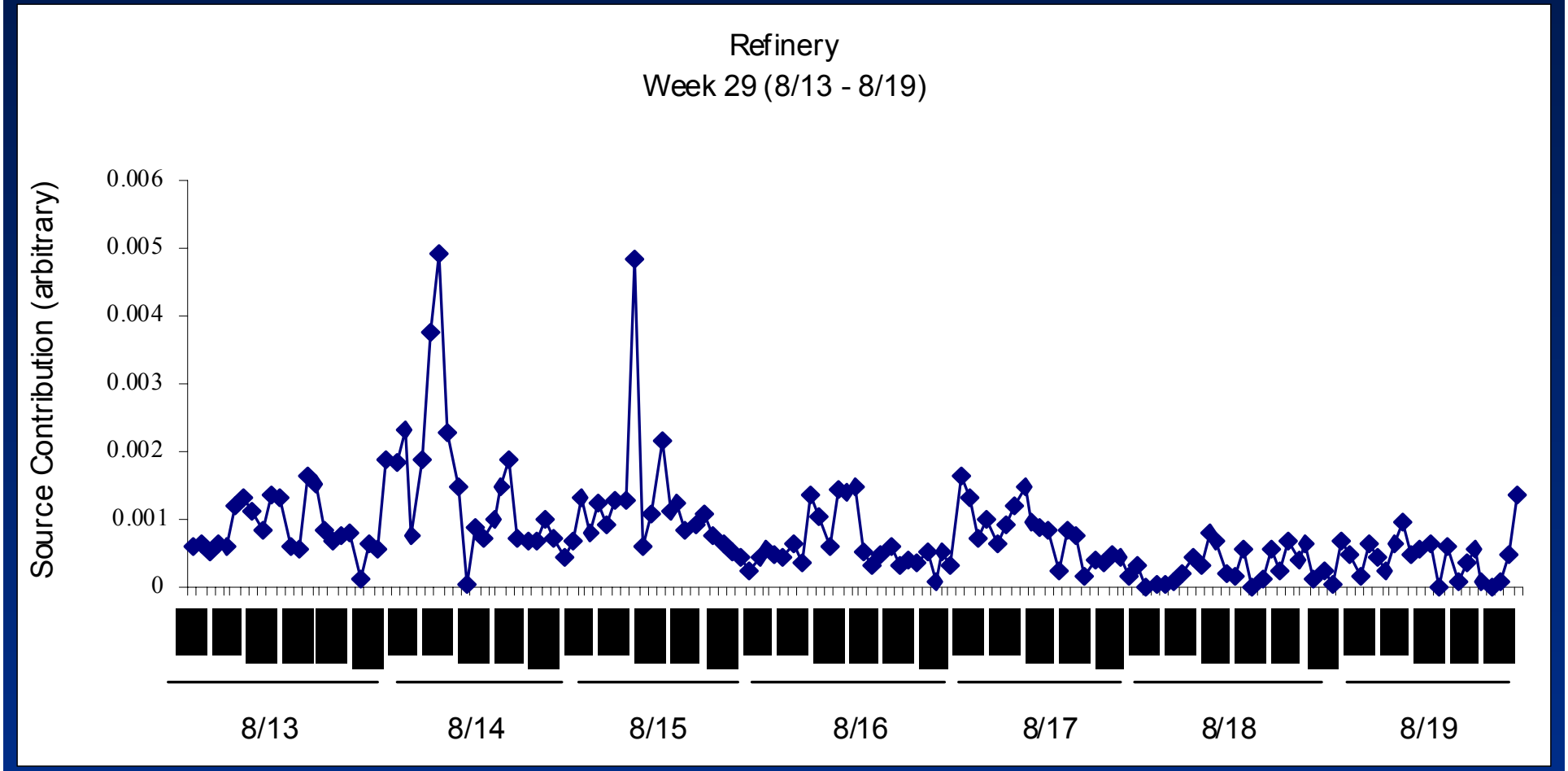
Refining Operations



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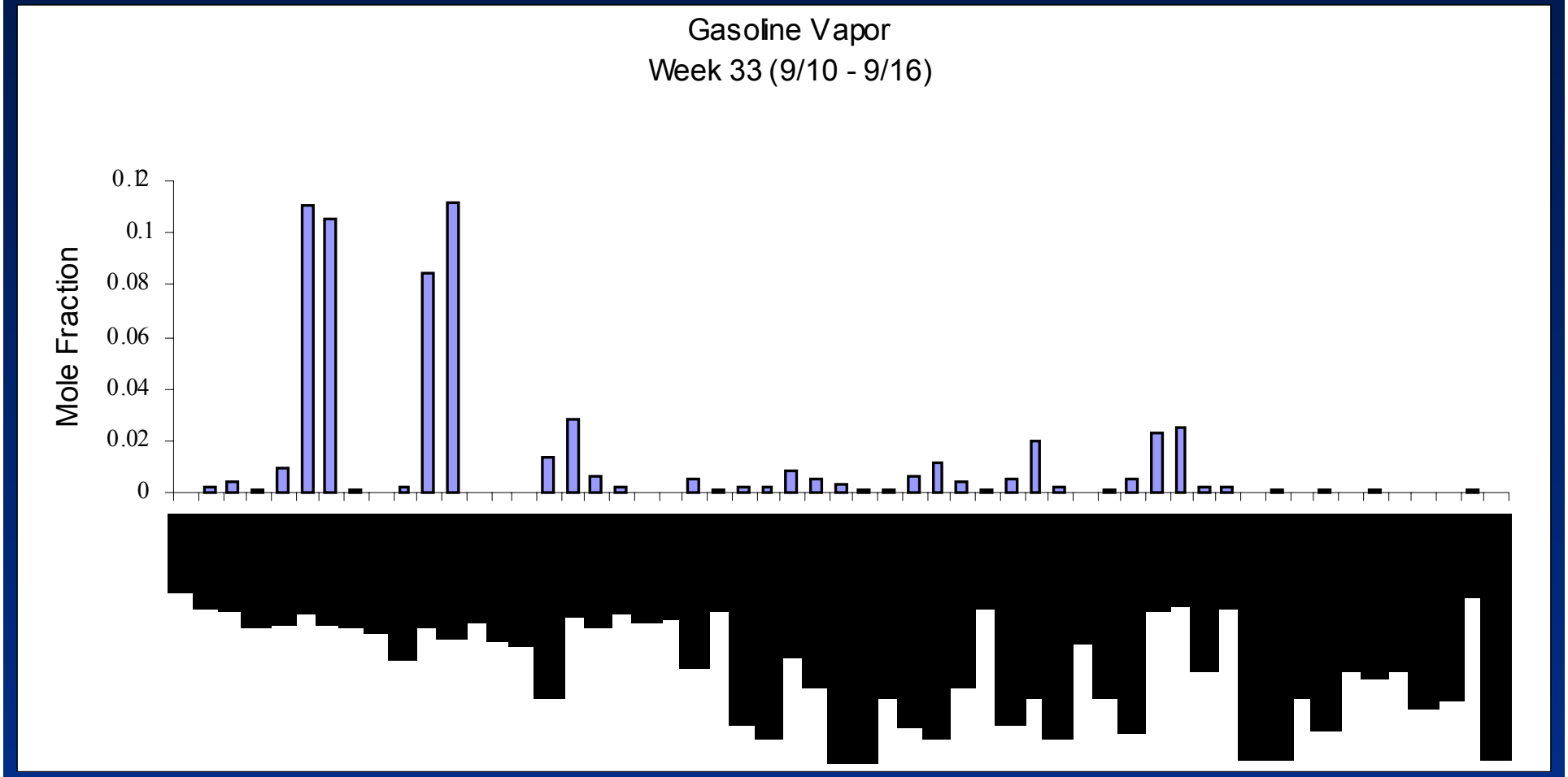
Gasoline Vapor



Does not have acetylene (in vehicle exhaust) or propane (in refining operations)

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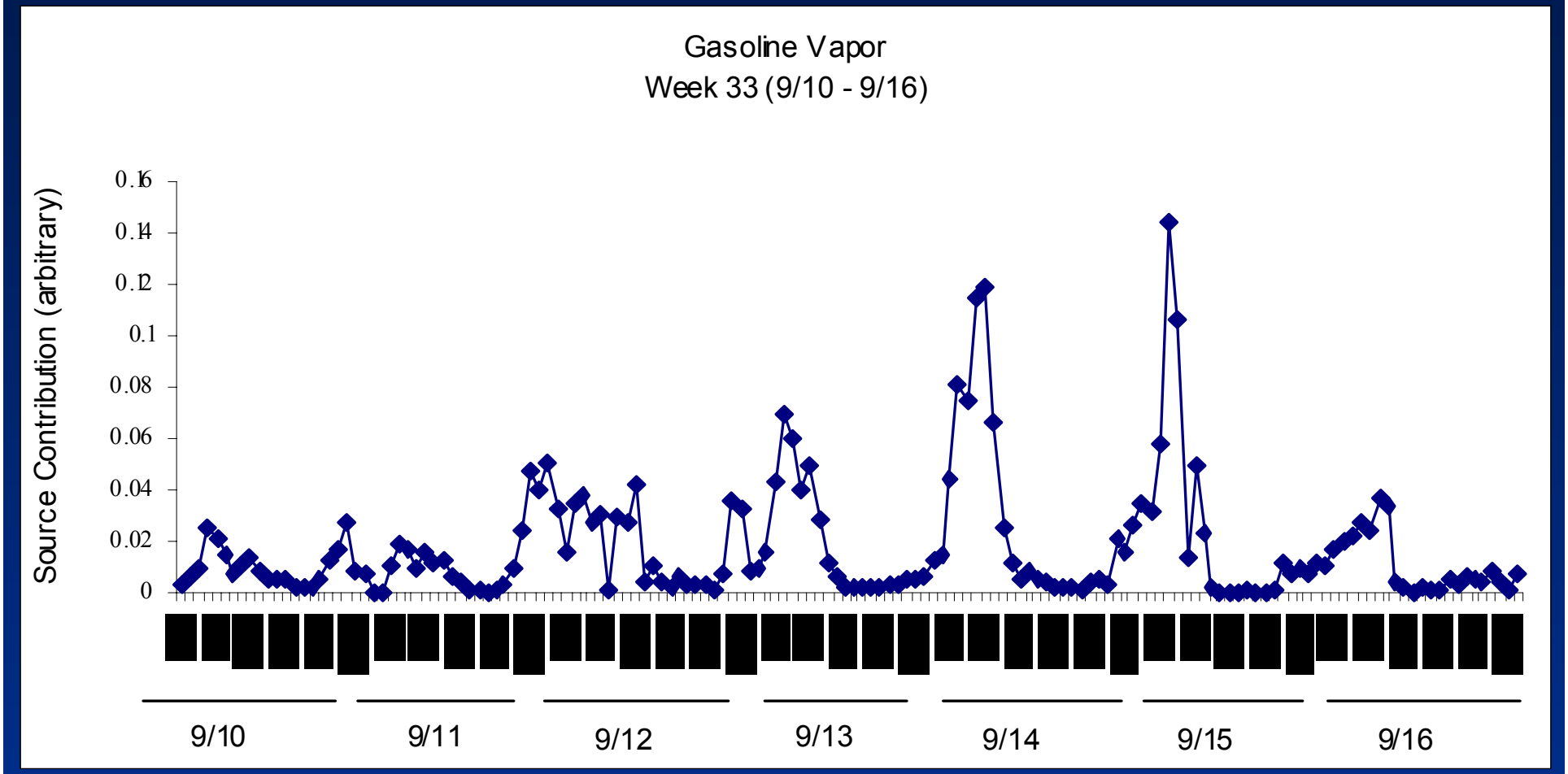
Gasoline Vapor



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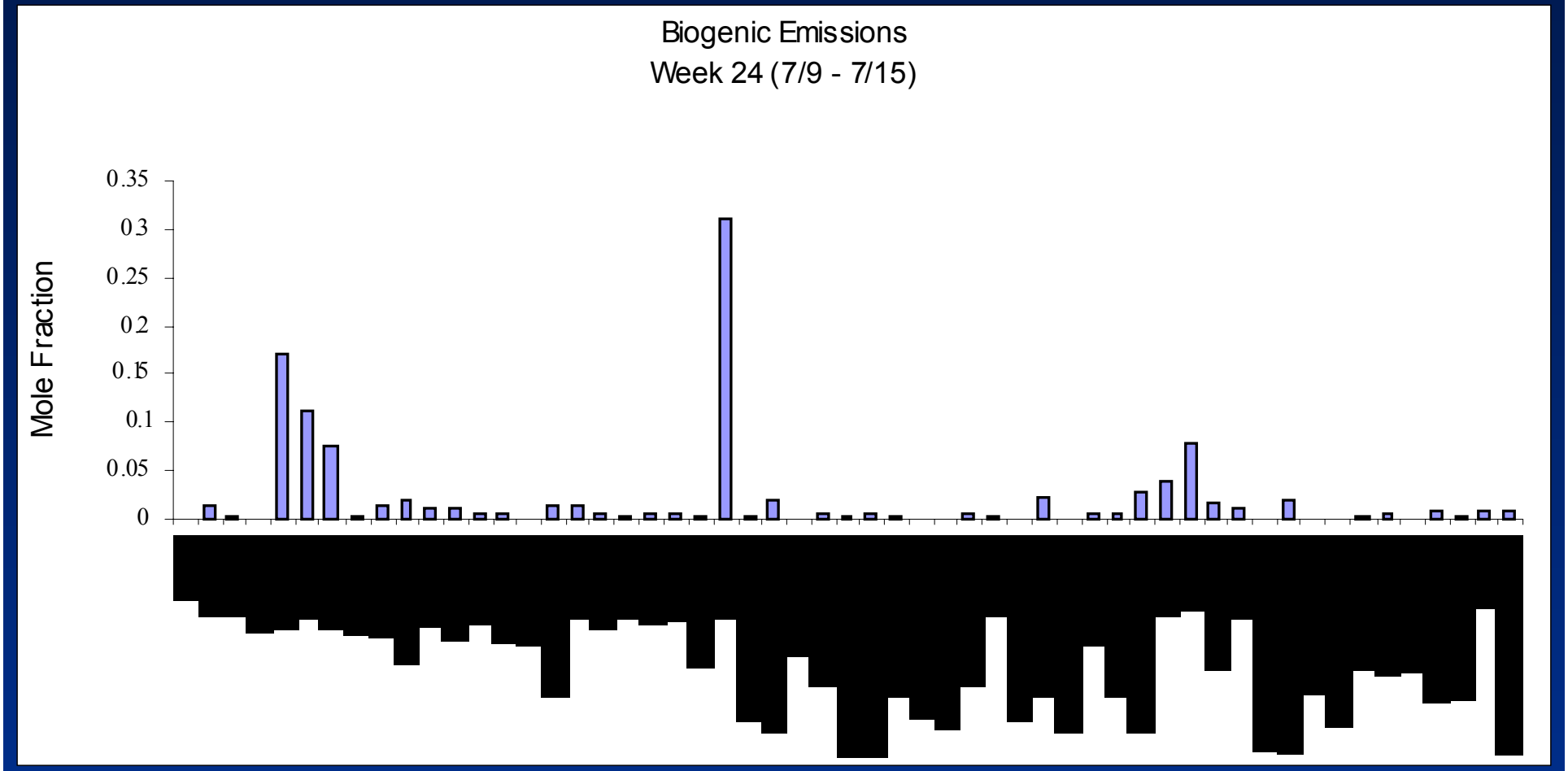
Biogenics



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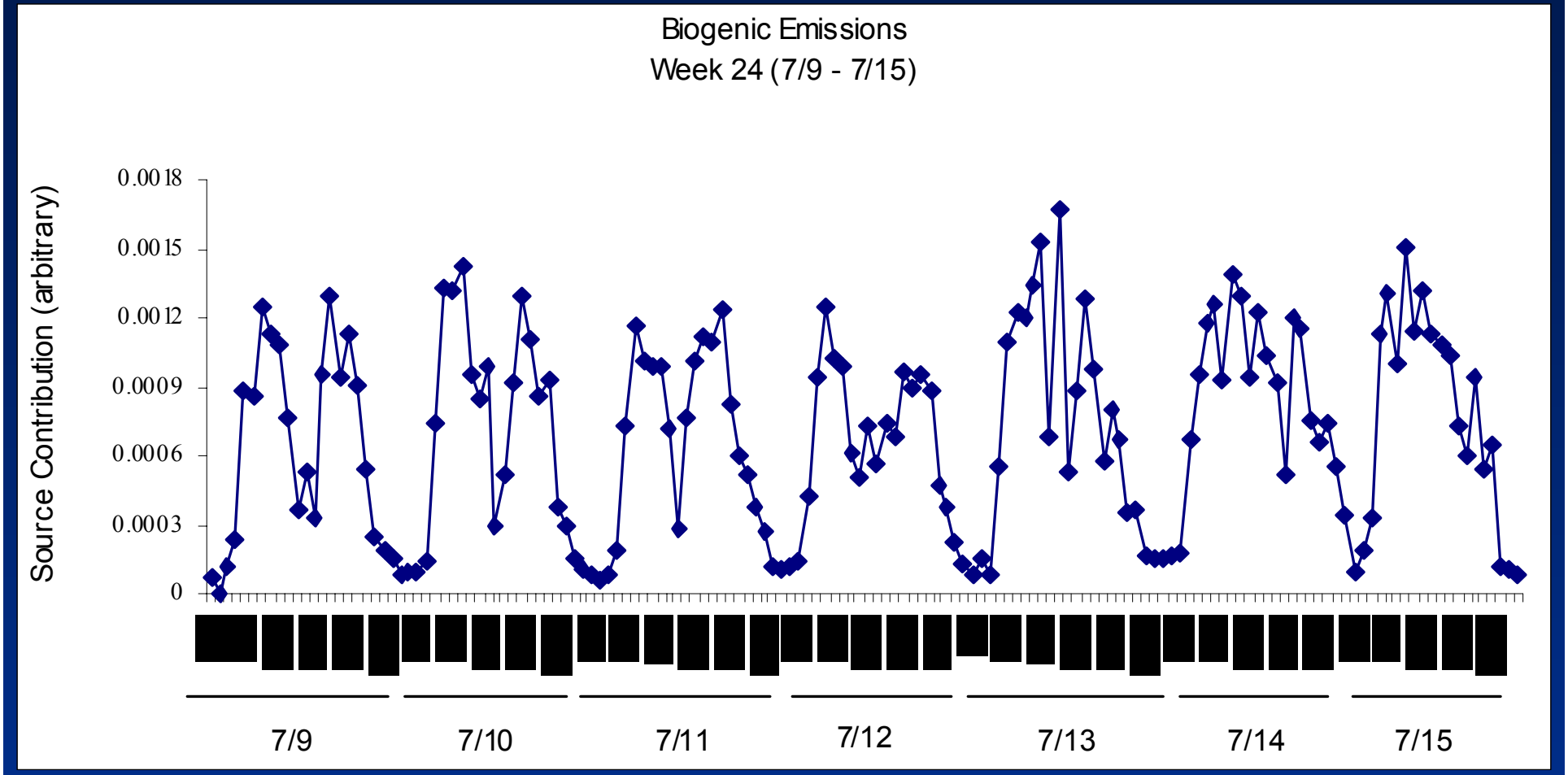

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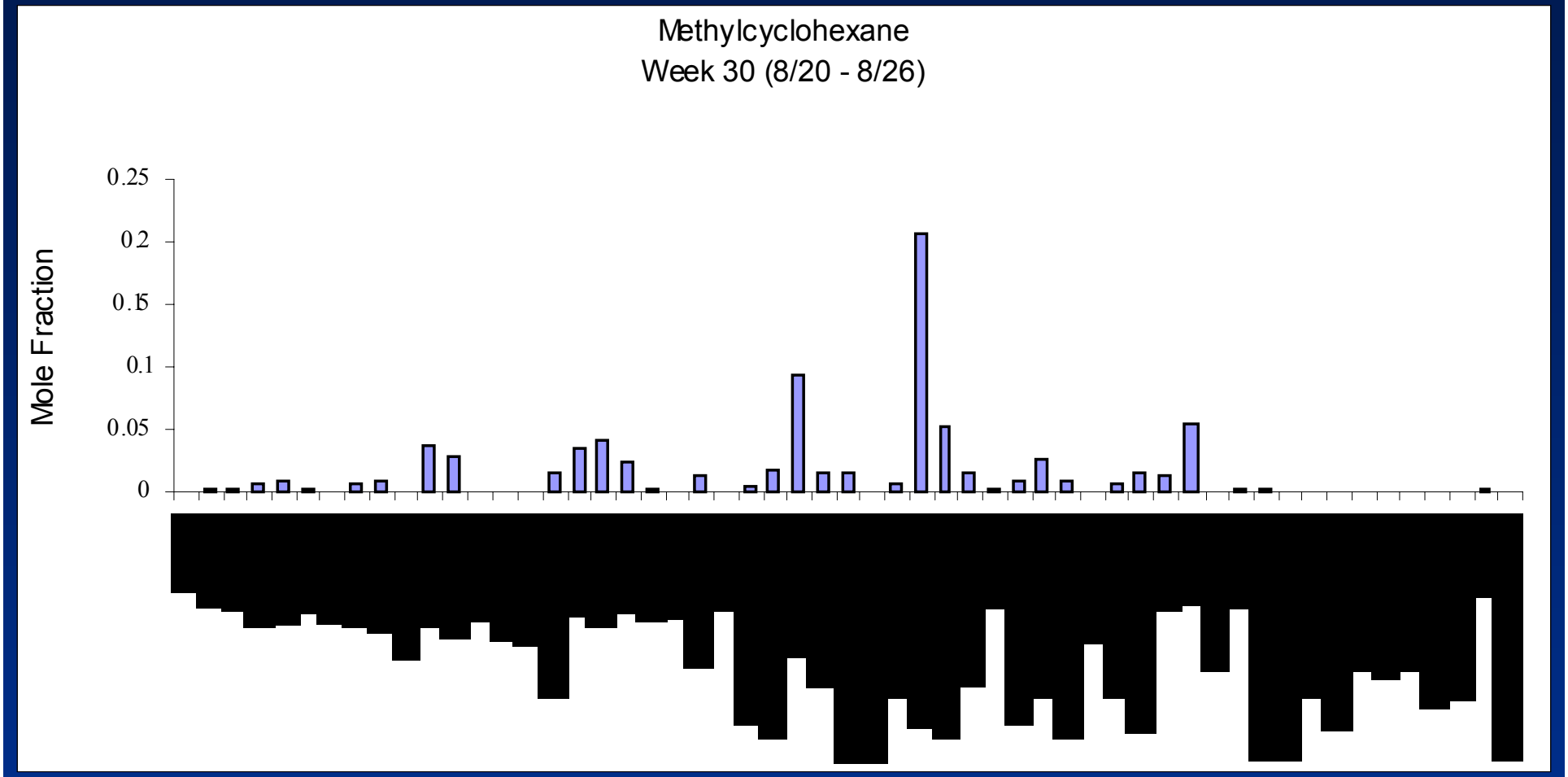
Methylcyclohexane



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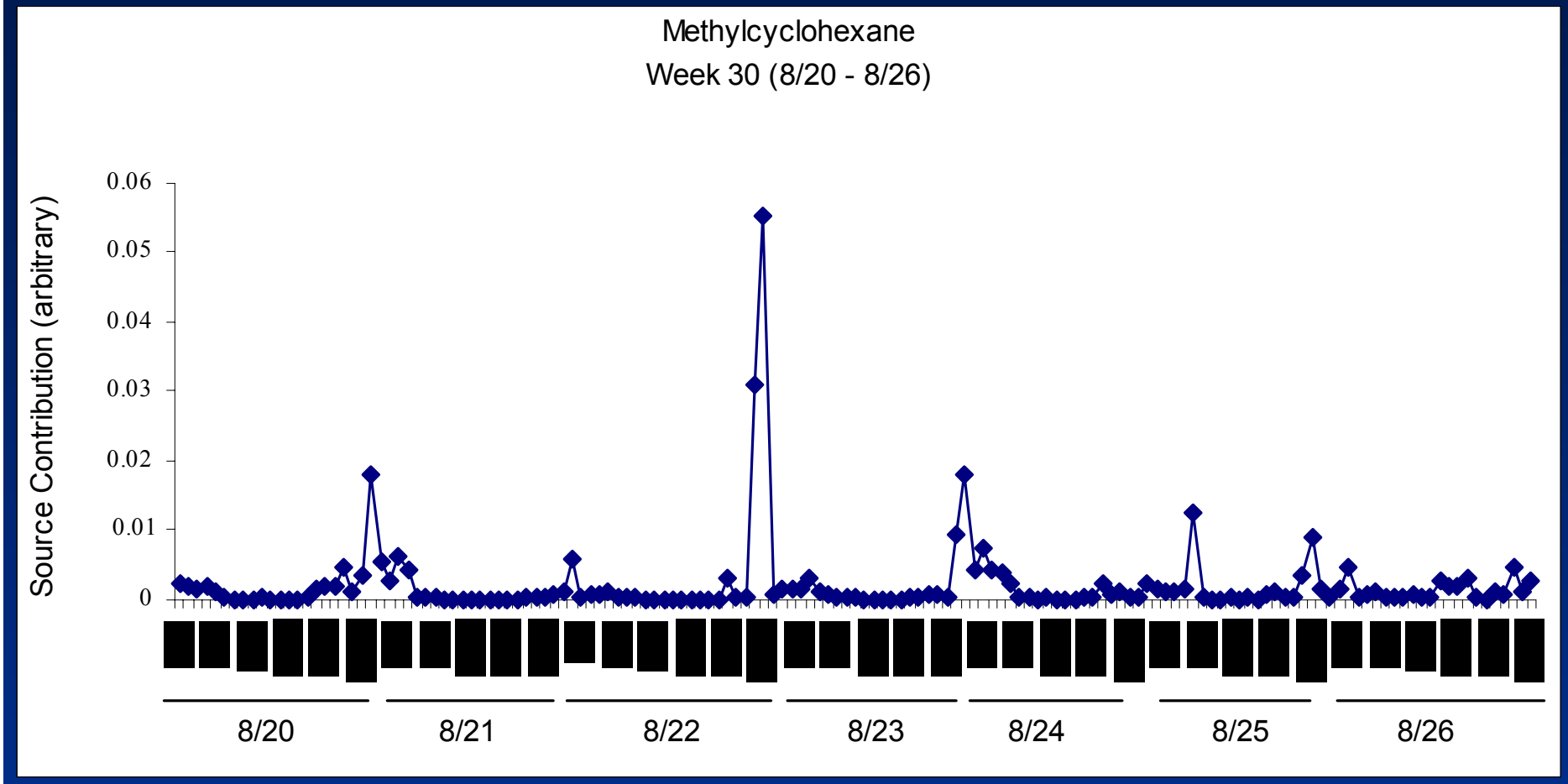

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Source Contributions

Using factorized source contributions from PMF, can perform a multiple linear regression between contribution factor and measured concentration to get overall source contributions

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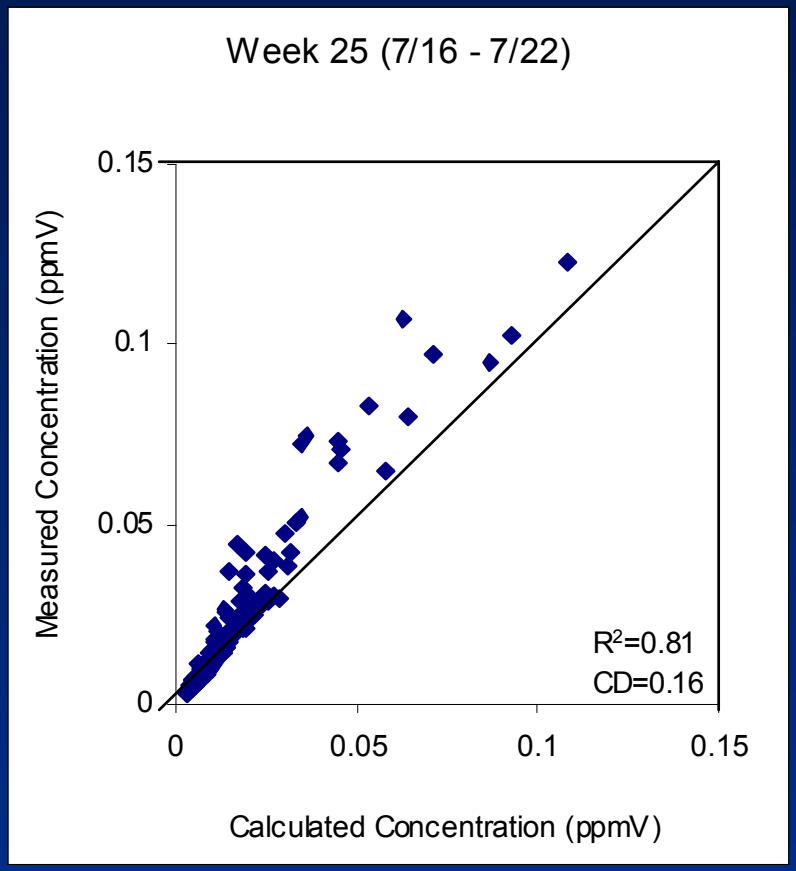
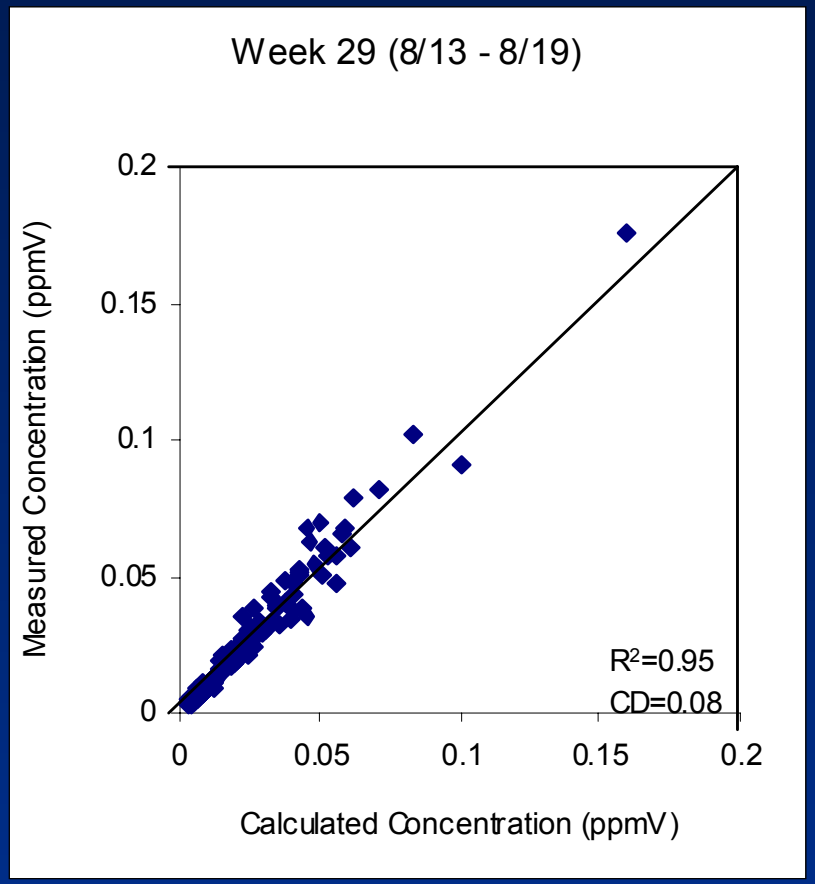
Source Contributions





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CASE II

Ethane is included

Suggested as an important species to differentiate natural gas and refining emissions.

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Dominant Source Profiles

Using 2001 hourly VOC data from Deer Park, PMF resolves 3 sources in 40% of weekly data and 4 sources in 60% of weeks

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Dominant Source Profiles

Natural Gas:	100% of weeks
Vehicle Exhaust:	89% of weeks
Petrochemical Prod*:	79% of weeks
Refining Operations**:	37% of weeks
Gasoline Vapor:	16% of weeks
Biogenic Emissions:	13% of weeks
Methylcyclohexane***:	2% of weeks
Industrial Isoprene***:	2% of weeks

* 90% ethylene rich and 10% propylene rich

** resolve two separate types of refining emissions: fugative and refining feedstock

*** one occurance

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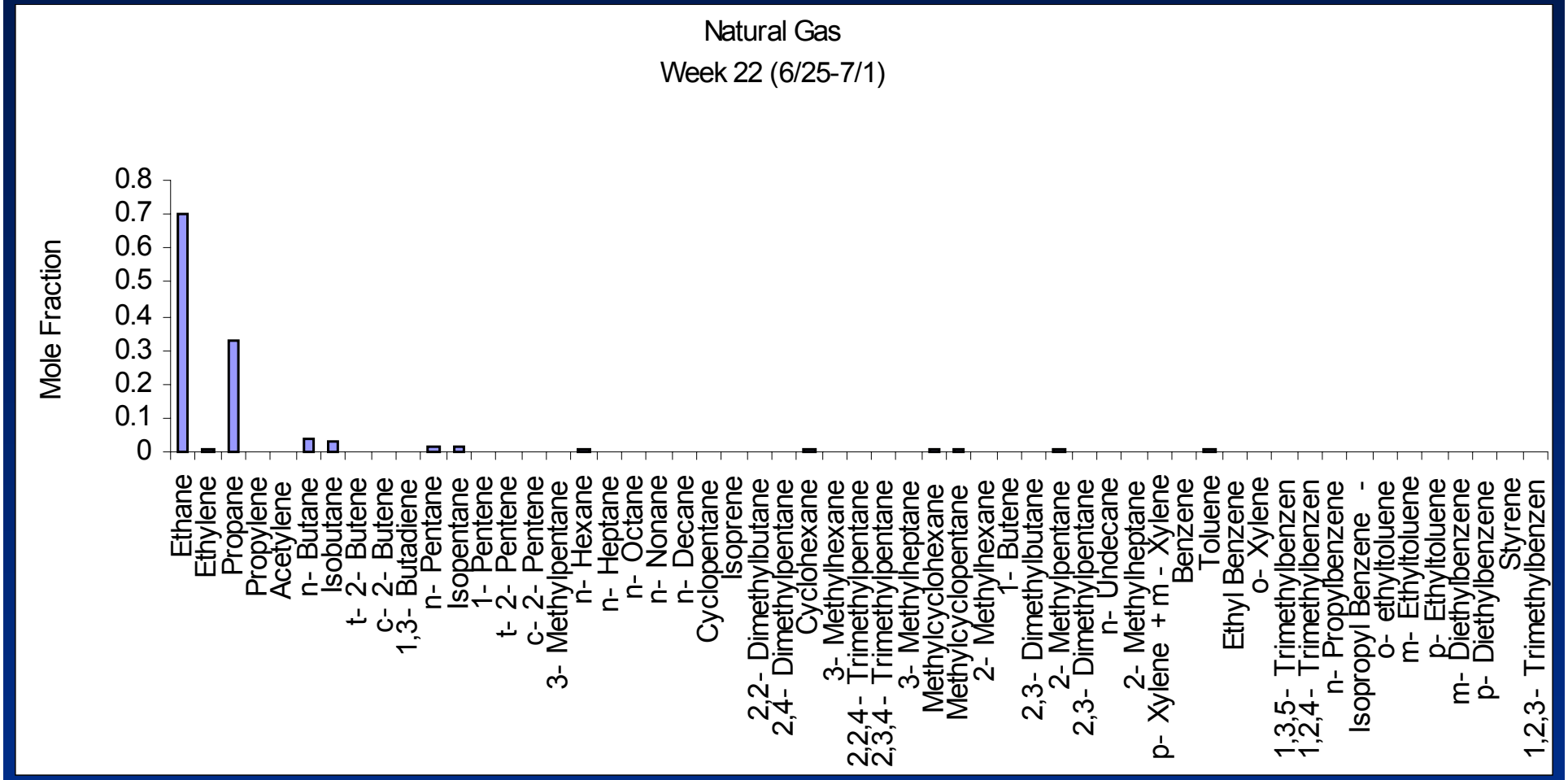
Natural Gas



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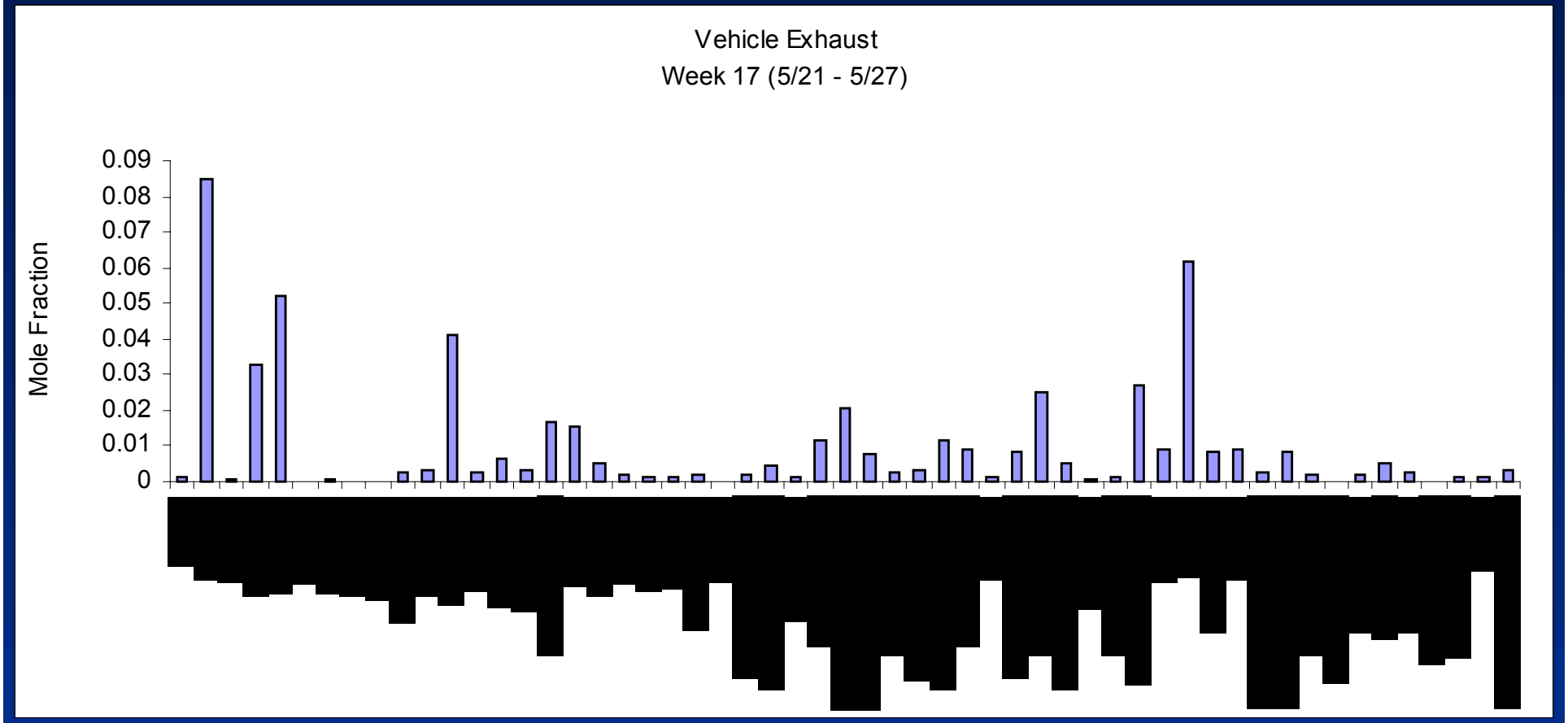
Vehicle Exhaust



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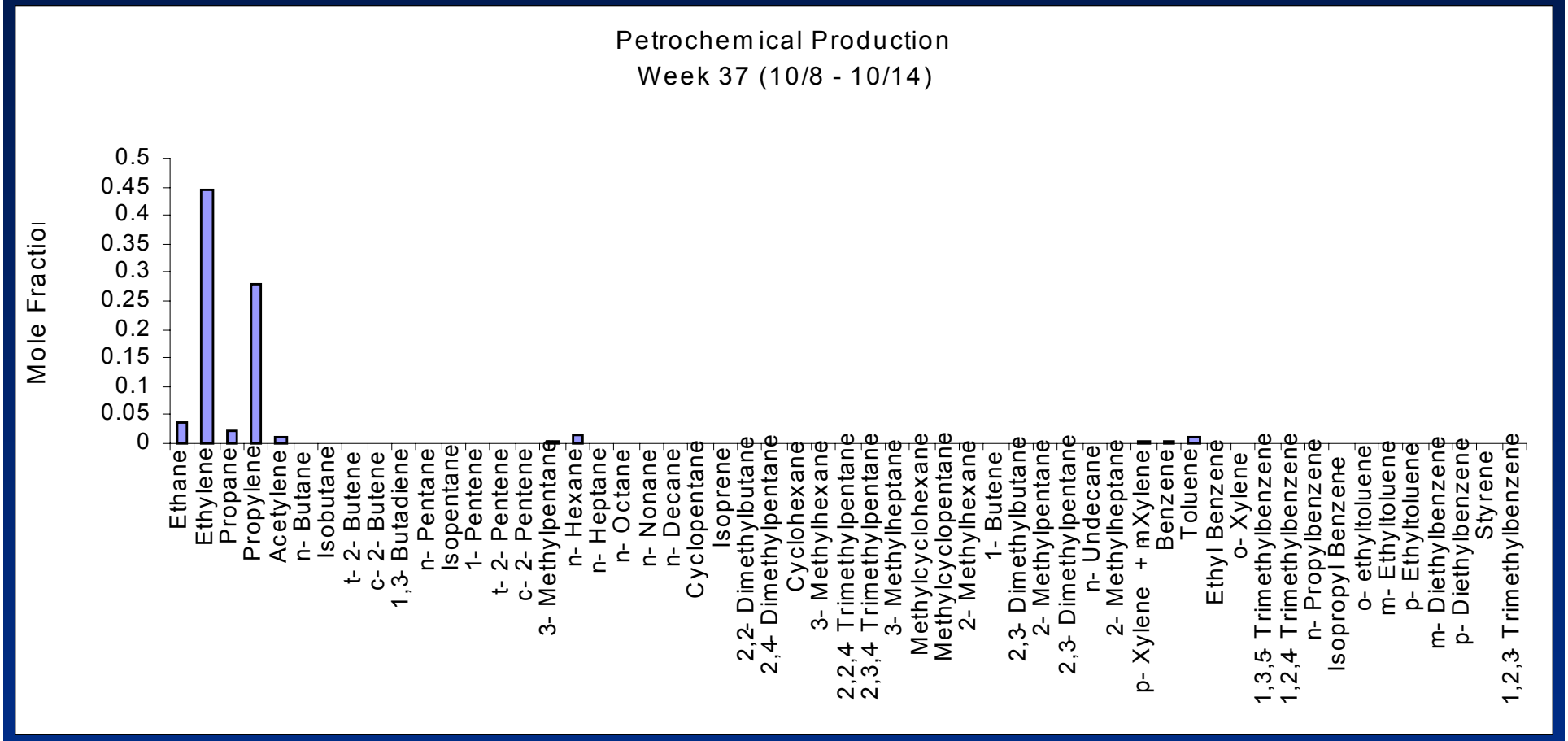
Petrochemical Production



Related source profile with propylene dominant occurs in 10% of the data

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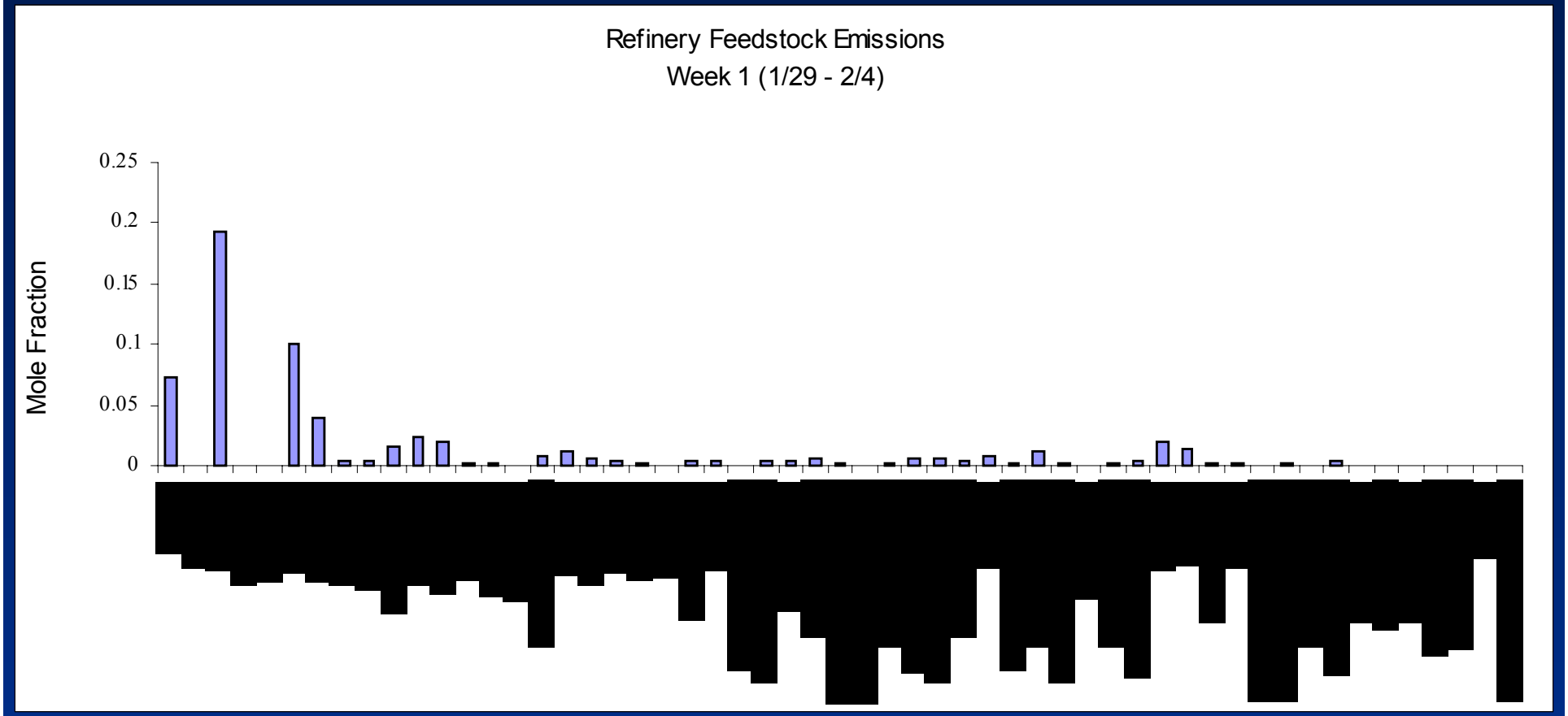
Refining Operations



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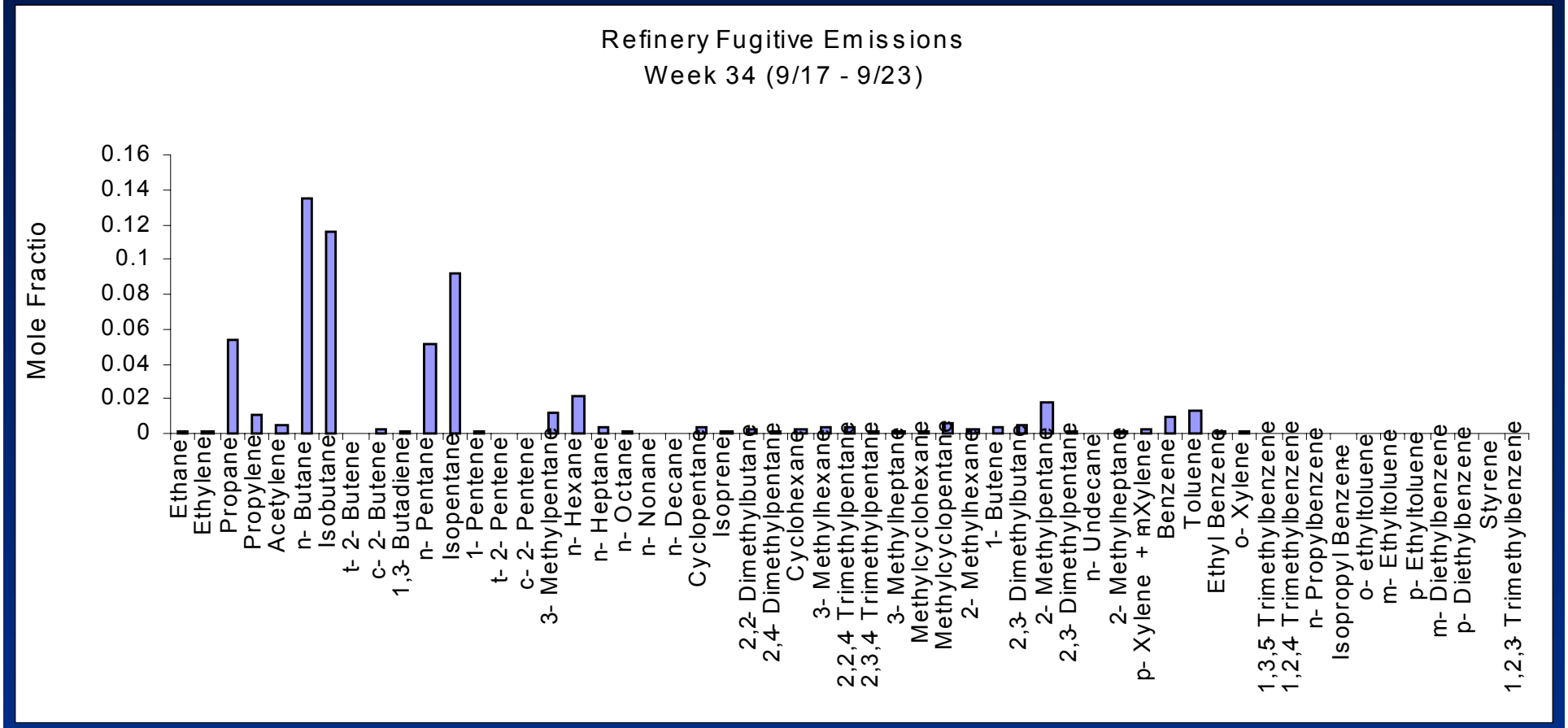
Refining Operations



Fugative refining profile is more prevalent in the data than the feedstock refining emissions profile

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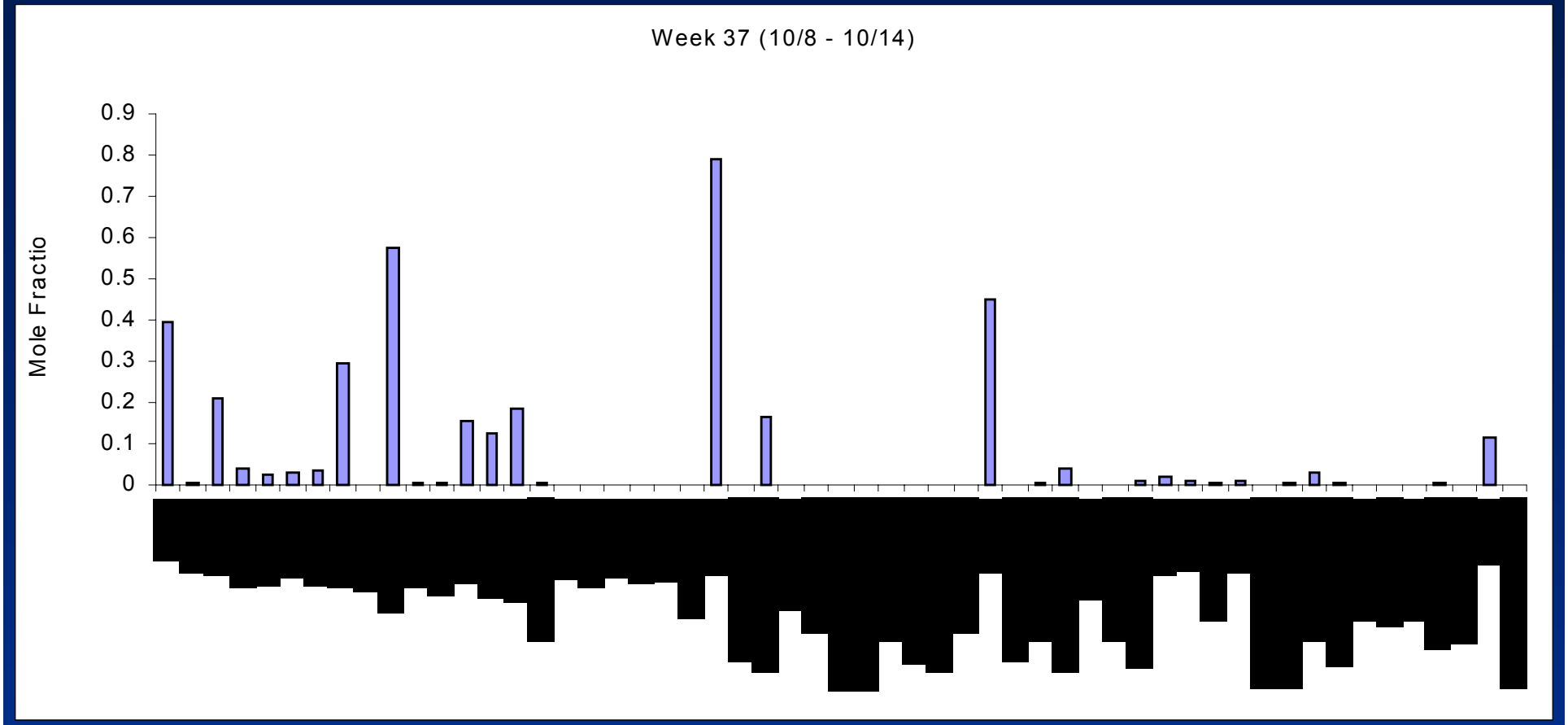
Industrial Isoprene



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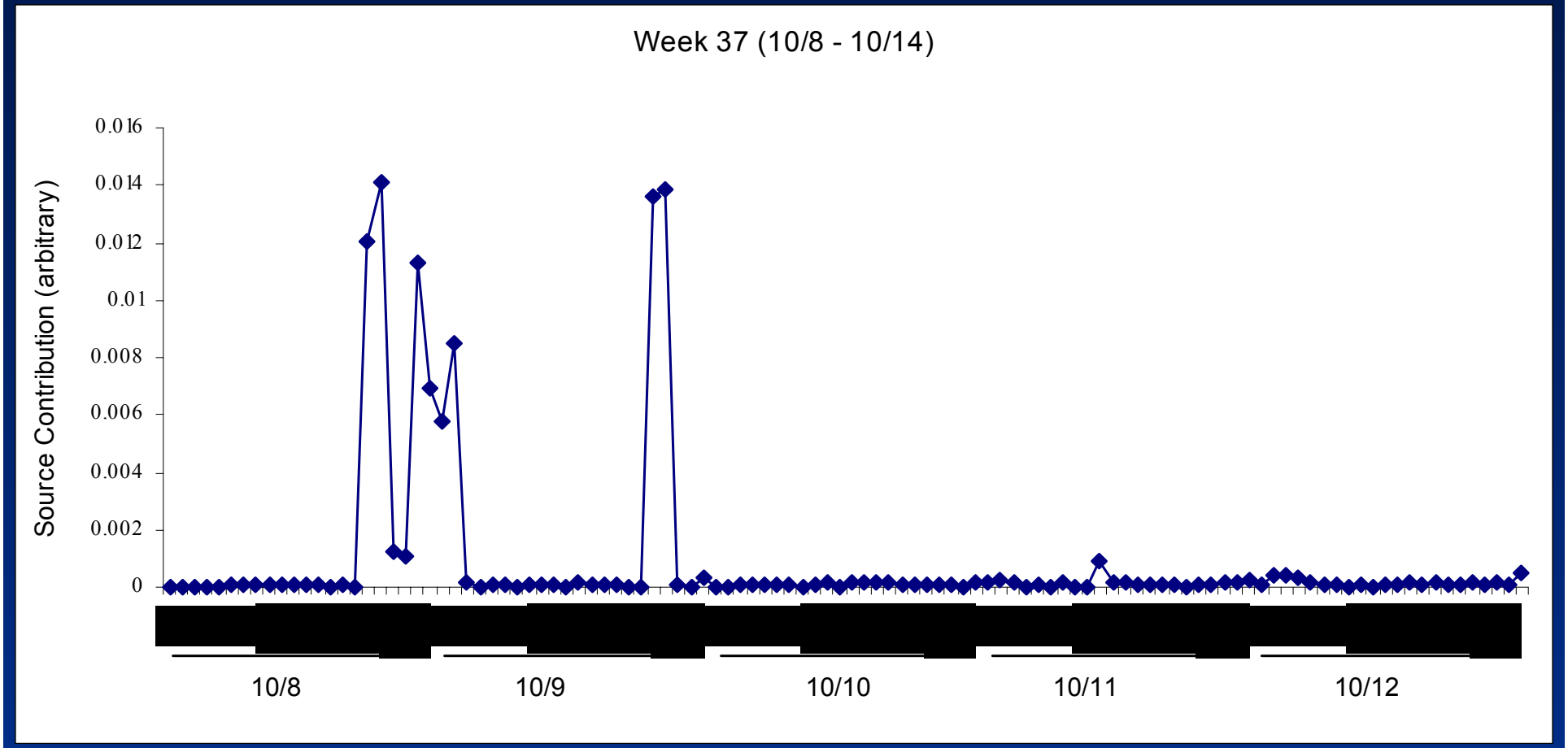
Industrial Isoprene



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Same profiles for the following sources:

Gasoline Vapor

Biogenics

Methylcyclohexane

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On-Going Project:

- Will determine source contributions for rest of the year
- Will determine bias in exclusion of other sources
- Will investigate correlations between source contributions and wind direction, other parameters
- Will compare results to existing inventories

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