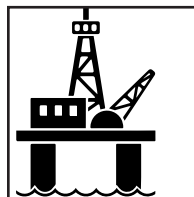
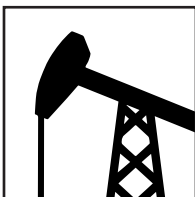
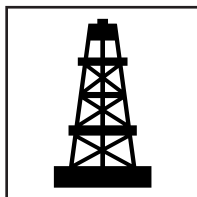


Comprehensive Source of Pattern Recognition Standards for ASTM, EPA, AOAC Total Petroleum Hydrocarbon Methods

by Abdullah Alsamraie and Dr. Jack Hubball
AccuStandard, Inc. 125 Market St. New Haven, CT USA



Background

Analytical chemists have important decisions to make in determining the boiling range and hydrocarbon concentration of a petrochemical product spill. This decision-making process becomes more challenging if the petrochemical product has weathered or multiple products have spilled or leaked at the same site. A common strategy for the identification of a contamination sample is to compare the chromatographic pattern of it with a known petroleum product.

To assist analysts with this identification process, AccuStandard has selected a group of representative petrochemical products typically found when a spill and/or leak assessment site investigation is conducted.

Project plan for the generation of TPH data

Petrochemical reference standards were analyzed using an optimized set of operating conditions for each product boiling range (see operating conditions section). Objectives considered in the methods development included:

- Generation of a uniquely recognizable GC pattern in approximately 30 minutes for each petrochemical product.
- Incorporate a “window defining mix” in the pattern recognition chromatogram that is appropriate for the boiling range of the product.
- Group the pattern recognition standards according to their boiling ranges.

Suggested instructions for use

The “window defining mix” standard is used to determine the beginning and end points of the petrochemical product chromatogram, and establish the boiling range(s) of the contaminant(s). This defined alkane window mix is especially useful when dealing with weathered products or multiple products present in contaminated soil or water samples.

AccuStandard offers three hydrocarbon “window defining mixes” that enable the analyst to more accurately determine the boiling range of the unknown sample.

These mixes aid in the determination of qualitative and semi-quantitative data of the contaminant sample.

The “window defining mixes” are:

C8-C40, **DRH-008S-R2**

C8-C20, **TPH-LOW-01**

C8-C30, **TPH-MID-01**

Single source contamination

By combining a specific petrochemical pattern with a known alkane hydrocarbon standard, the analyst can then calculate a gross hydrocarbon concentration using the petrochemical standard pattern that is the closest match. For lab samples where the spill has recently occurred or is from a single point source this identification and concentration calculation is straight-forward.

Weathered or multiple source contamination

This comparison technique is very useful for weathered or mixed fuel patterns such as gasoline and diesel. By defining the window segment for each fuel in a mixed fuel sample (example gasoline portion/diesel portion) and quantifying the defined segment with the same representative portion from the actual petrochemical standard, better inter-laboratory reproducibility can be achieved. Similarly, the alkane range segment from an actual standard can be used to determine the unknown sample boiling range.

Presentation of the data

The chromatogram for each petrochemical standard with an overlay of the appropriate window defining hydrocarbon mix can be used for the identification of contamination samples.

Pattern recognition between two similar petrochemical products can easily be achieved through the overlay comparison. The comparison provides both the overall pattern as well as the start and end points of the hydrocarbon range.

Contents

Multi-State Hydrocarbon Window Defining Chromatography (C8-C40), (C8-C20), (C8-C30)

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Motor Fuels and Lubricating Oils Chromatograms 1-8

Gasoline, Regular Unleaded	1
Gasoline, Regular Leaded	2
Gasoline, Premium	2
RFA Gasoline (Oxygenate-free)	3
Diesel Fuel	3
#1 Diesel Fuel (Low sulfur)	4
#2 Diesel Fuel (Extra low sulfur)	4
Biodiesel 100 (Consumer grade)	5
Renewable Diesel Fuel #2	5
SAE 30W Motor Oil	6
SAE 40W Motor Oil	6
SAE 50W Motor Oil	7
SAE 5W30 Motor Oil	7
SAE 10W30 Motor Oil	8
SAE 10W40 Motor Oil	8

Heating Fuel Oils Chromatography 9-12

#1 Fuel Oil	9
#2 Fuel Oil	10
#3 Fuel Oil	10
#4 Fuel Oil	11
#6 Fuel Oil	11
Kerosene	12

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Aviation Gasoline (Grade 100-LL)	13
JP-4 Fuel (Weathered)	14
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JP-7 Fuel	15
JP-8 Fuel	15
JP-10 Aviation Fuel	16
JP-TS Aviation Fuel	16
Renewable Aviation Fuel	17
Jet Reference Fuel (Type 1)	17
Turbine (Jet A) Fuel	18
Hydraulic Fluid	18

Household and Industrial Solvents Chromatography 19-21

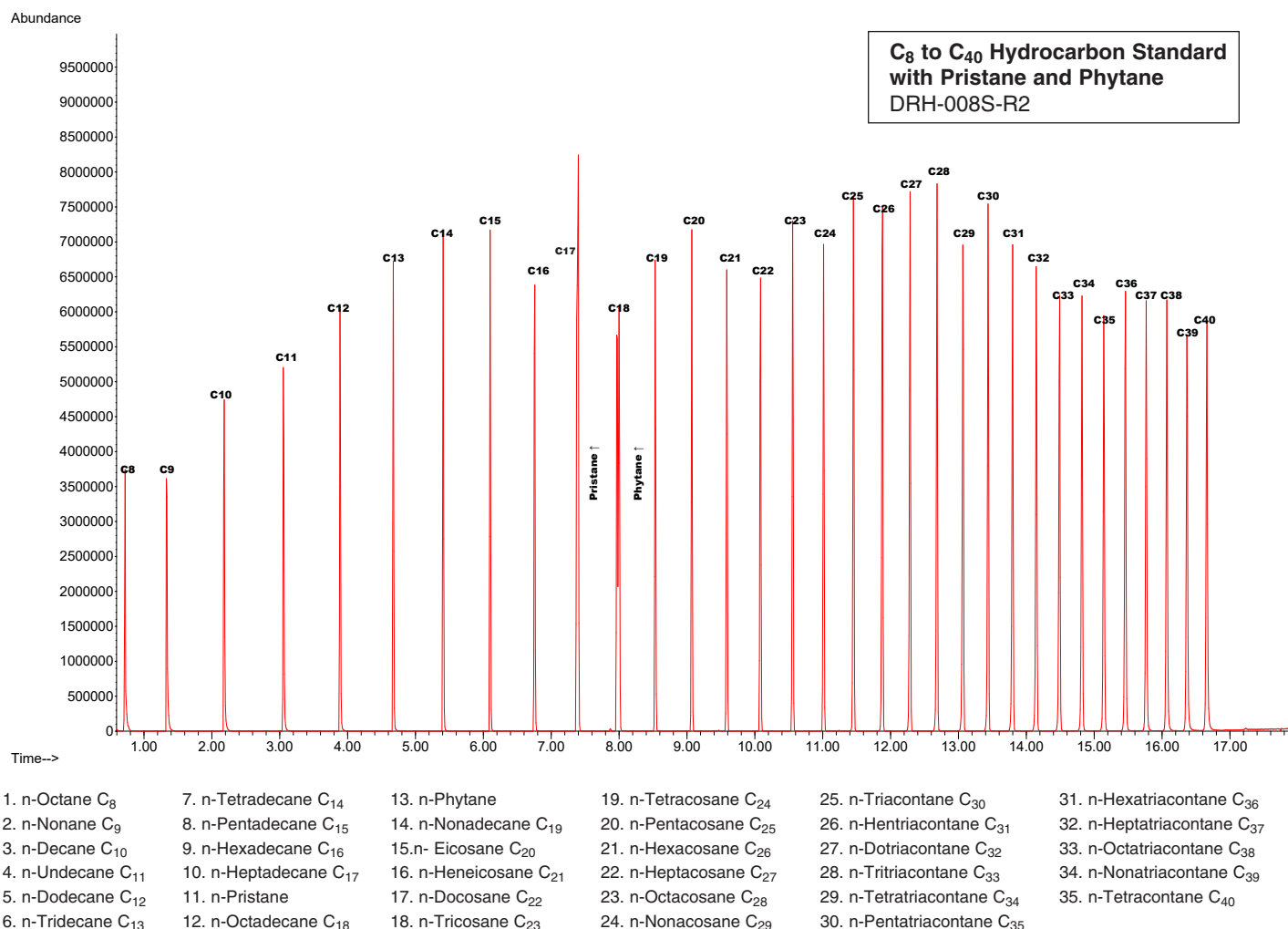
Lacquer Thinner	19
Mineral Spirits	20
Naphtha	20
Turpentine	21
Stoddard Solvent	21

Red Peaks are a n-alkane overlay used as a markers throughout the book.



Multi-State Hydrocarbon Window Defining Standard (C₈-C₄₀)

Hydrocarbon window defining standard with the C₈ to C₄₀ odd and even alkanes, including pristane and phytane in the formulation. Using this single standard measuring the C₁₇ / pristane and C₁₈ / phytane ratio can be used to estimate degradation of fuel oil.



GC/MS operating conditions for TPH

Instrument: Agilent 7890 GC/5975C MSD
 Column: 30M X 0.25 mm id X 0.25 um DB 5-MS
 Column temp. program: 40(2)-250 @ 10/min for low boiling range
 40(2)-300 @ 10/min for mid boiling range
 100-340 @ 20/min for high boiling range (motor oil)
 Inlet temp.: 225 °C for low/mid boiling range samples
 250 °C for high boiling range samples
 Interface temp.: 300 °C
 Injection: 1.0 µl, split 100:1

Hydrocarbon Window Defining Standard (C₈ - C₄₀)

DRH-008S-R2

DRH-008S-R2-PAK

500 µg/mL each in Chloroform

\$ 65 / 1 x 1 mL

5 x 1 mL

35 comps.

n-Octane
n-Nonane
n-Decane
n-Undecane
n-Dodecane
n-Tridecane
n-Tetradecane

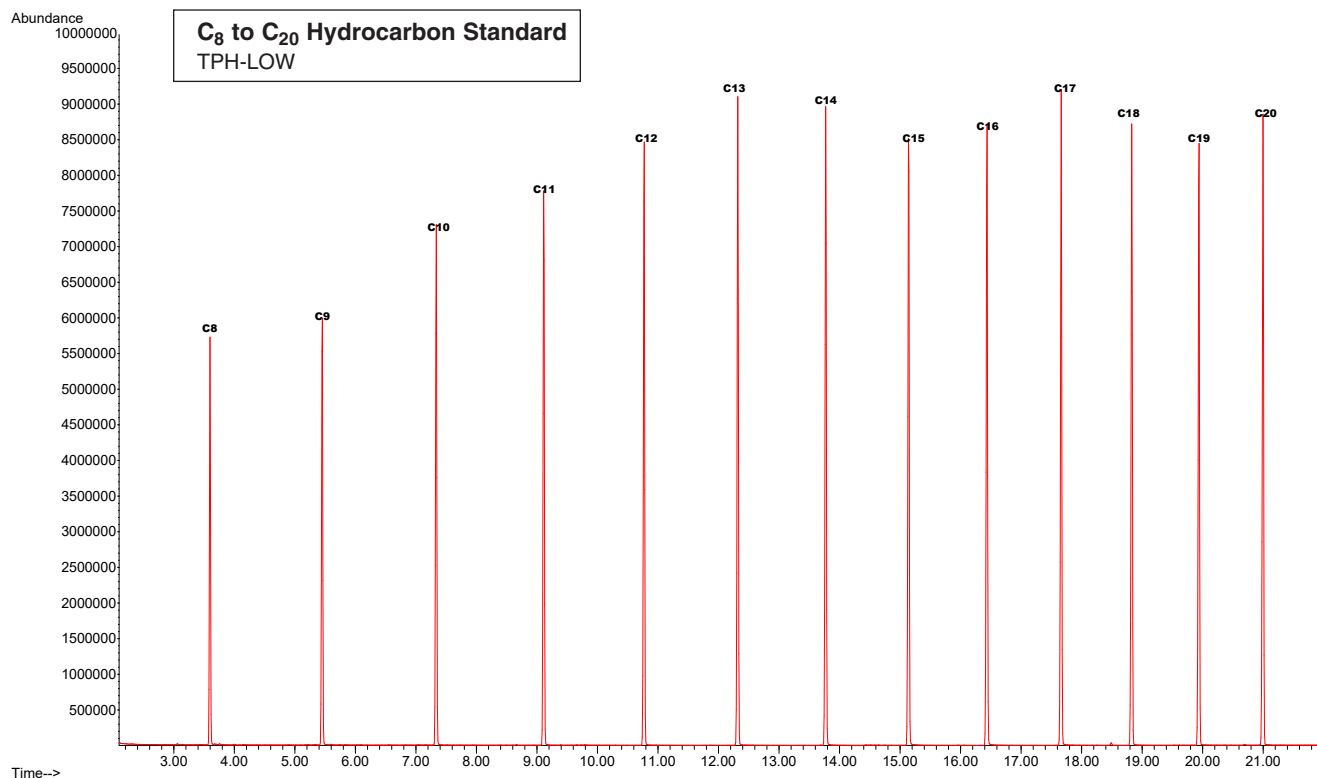
n-Pentadecane
n-Hexadecane
n-Heptadecane
Pristane
n-Octadecane
Phytane
n-Nonadecane

n-Eicosane
n-Heneicosane
n-Docosane
n-Tricosane
n-Tetracosane
n-Pentacosane
n-Hexacosane

n-Heptacosane
n-Octacosane
n-Nonacosane
n-Triacontane
n-Hentriacontane
n-Dotriacontane
n-Tritriacontane

n-Tetraatriacontane
n-Pentatriacontane
n-Hexatriacontane
n-Heptatriacontane
n-Octatriacontane
n-Nonatriacontane
n-Tetracontane

Multi-State Hydrocarbon Window Defining Standard (C8-C20)



GC/MS operating conditions for TPH

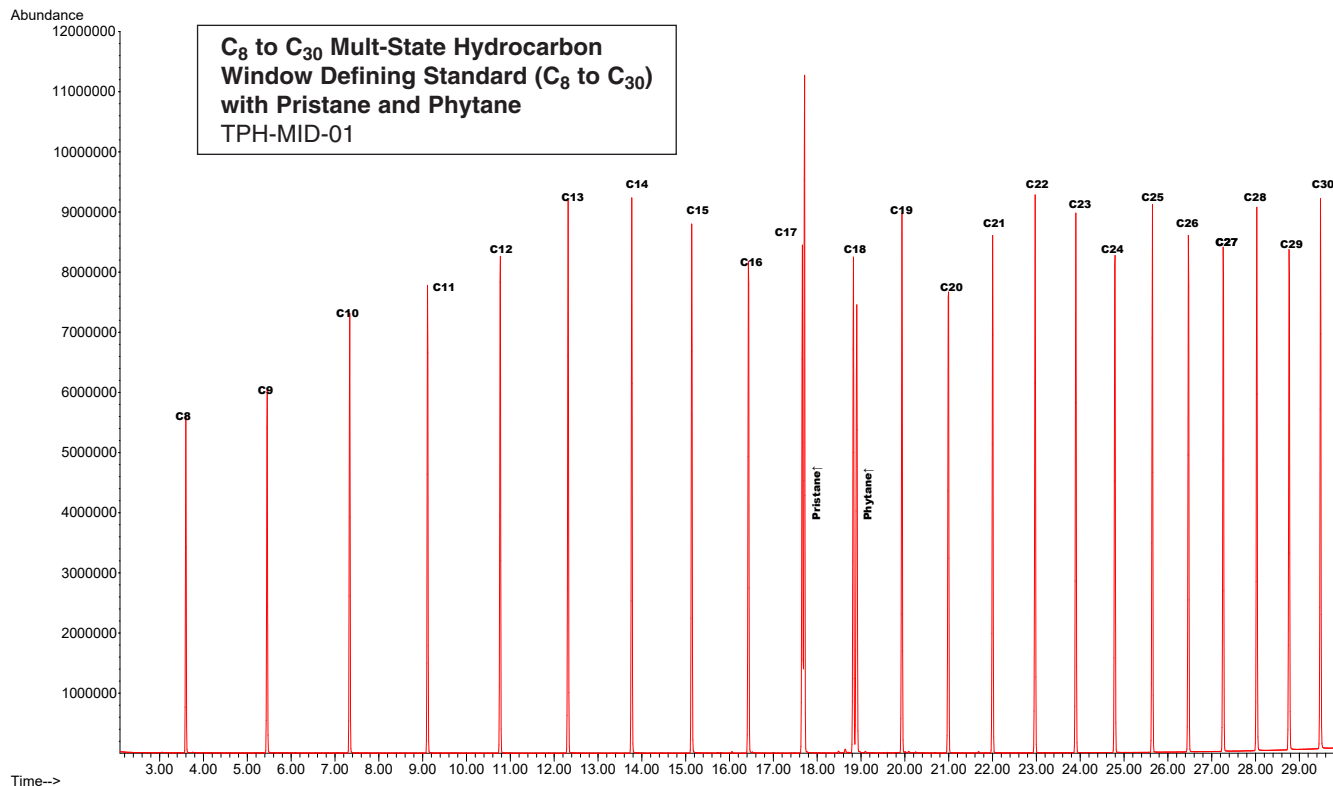
Instrument: Agilent 7890 GC/5975C MSD
 Column: 30M X 0.25 mm id X 0.25 um DB 5-MS
 Column temp. program: 40(2)-250 @ 10/min for low boiling range
 40(2)-300 @ 10/min for mid boiling range
 100-340 @ 20/min for high boiling range (motor oil)
 Inlet temp.: 225 °C for low/mid boiling range samples
 250 °C for high boiling range samples
 Interface temp.: 300 °C
 Injection: 1.0 µl, split 100:1

Total Petroleum Hydrocarbons (C₈ - C₂₀)

TPH-LOW-01 1 x 1 mL
TPH-LOW-01-PAK 5 x 1 mL
 500 µg/mL each in Chloroform 13 comps.

n-Octane	n-Pentadecane
n-Nonane	n-Hexadecane
n-Decane	n-Heptadecane
n-Undecane	n-Octadecane
n-Dodecane	n-Nonadecane
n-Tridecane	n-Eicosane
n-Tetradecane	

Multi-State Hydrocarbon Window Defining Standard (C₈-C₃₀)



GC/MS operating conditions for TPH

Instrument: Agilent 7890 GC/5975C MSD
 Column: 30M X 0.25 mm id X 0.25 um DB 5-MS
 Column temp. program: 40(2)-250 @ 10/min for low boiling range
 40(2)-300 @ 10/min for mid boiling range
 100-340 @ 20/min for high boiling range (motor oil)
 Inlet temp.: 225 °C for low/mid boiling range samples
 250 °C for high boiling range samples
 Interface temp.: 300 °C
 Injection: 1.0 µl, split 100:1

Total Petroleum Hydrocarbons (C₈ - C₃₀)

TPH-MID-01 \$ 65 / 1 x 1 mL
 TPH-MID-01-PAK 5 x 1 mL
 500 µg/mL each in Chloroform 25 comps.

n-Octane	Phytane
n-Nonane	n-Eicosane
n-Decane	n-Heneicosane
n-Undecane	n-Docosane
n-Dodecane	n-Tricosane
n-Tridecane	n-Tetracosane
n-Tetradecane	n-Pentacosane
n-Pentadecane	n-Hexacosane
n-Hexadecane	n-Heptacosane
n-Heptadecane	n-Octacosane
n-Octadecane	n-Nonacosane
Pristane	n-Triacontane
n-Nonadecane	



<https://www.accustandard.com/petrochemical-standards>

Chromatograms of Motor Fuels and Lubrication Oils

Motor Fuels and Lubricating Oils 1-8 Chromatograms

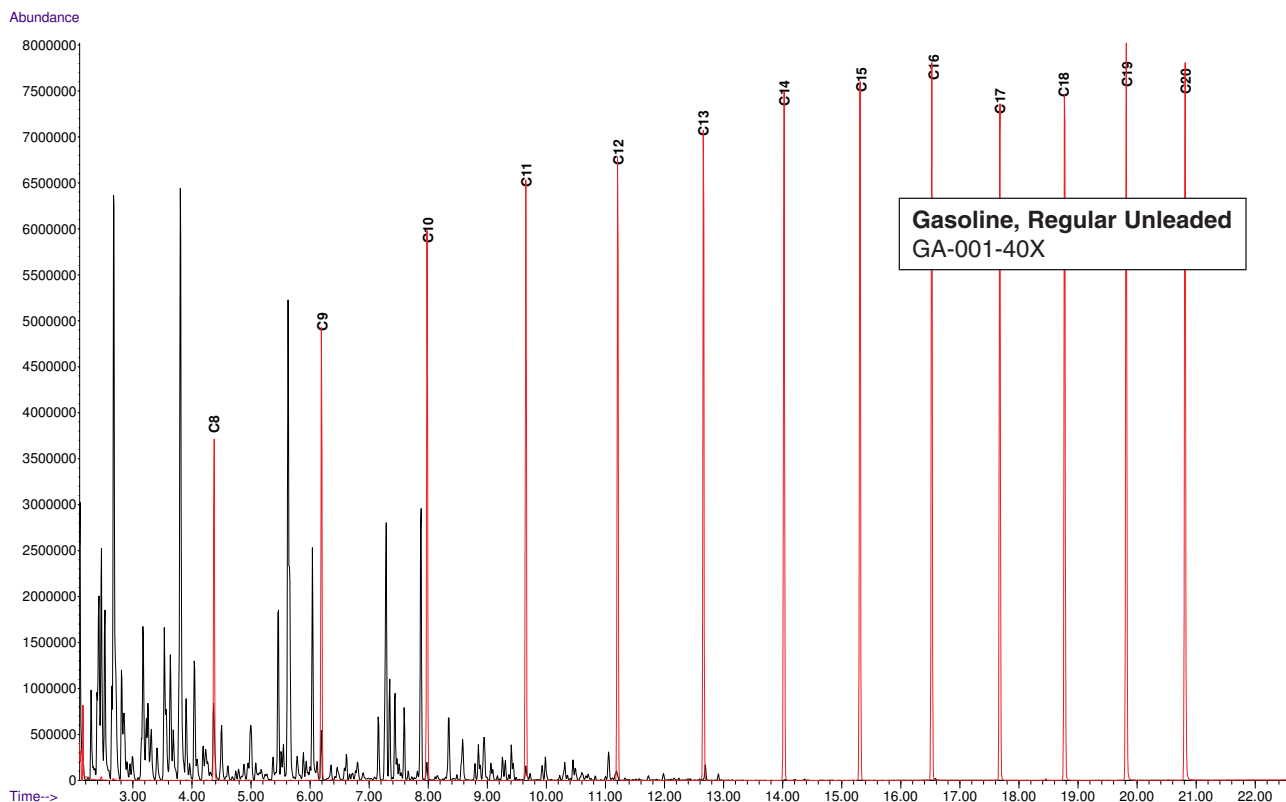
Gasoline, Regular Unleaded	1
Gasoline, Regular Leaded	2
Gasoline, Premium	2
RFA Gasoline (Oxygenate-free)	3
Diesel Fuel	3
#1 Diesel Fuel (Low sulfur)	4
#2 Diesel Fuel (Extra low sulfur)	4
Biodiesel 100 (Consumer grade) *	5
Renewable Diesel Fuel #2	5
SAE 30W Motor Oil	6
SAE 40W Motor Oil	6
SAE 50W Motor Oil	7
SAE 5W30 Motor Oil	7
SAE 10W30 Motor Oil	8
SAE 10W30 Motor Oil	8

Motor Fuels and Lubricating Oils Set TPH-001-R2-SET

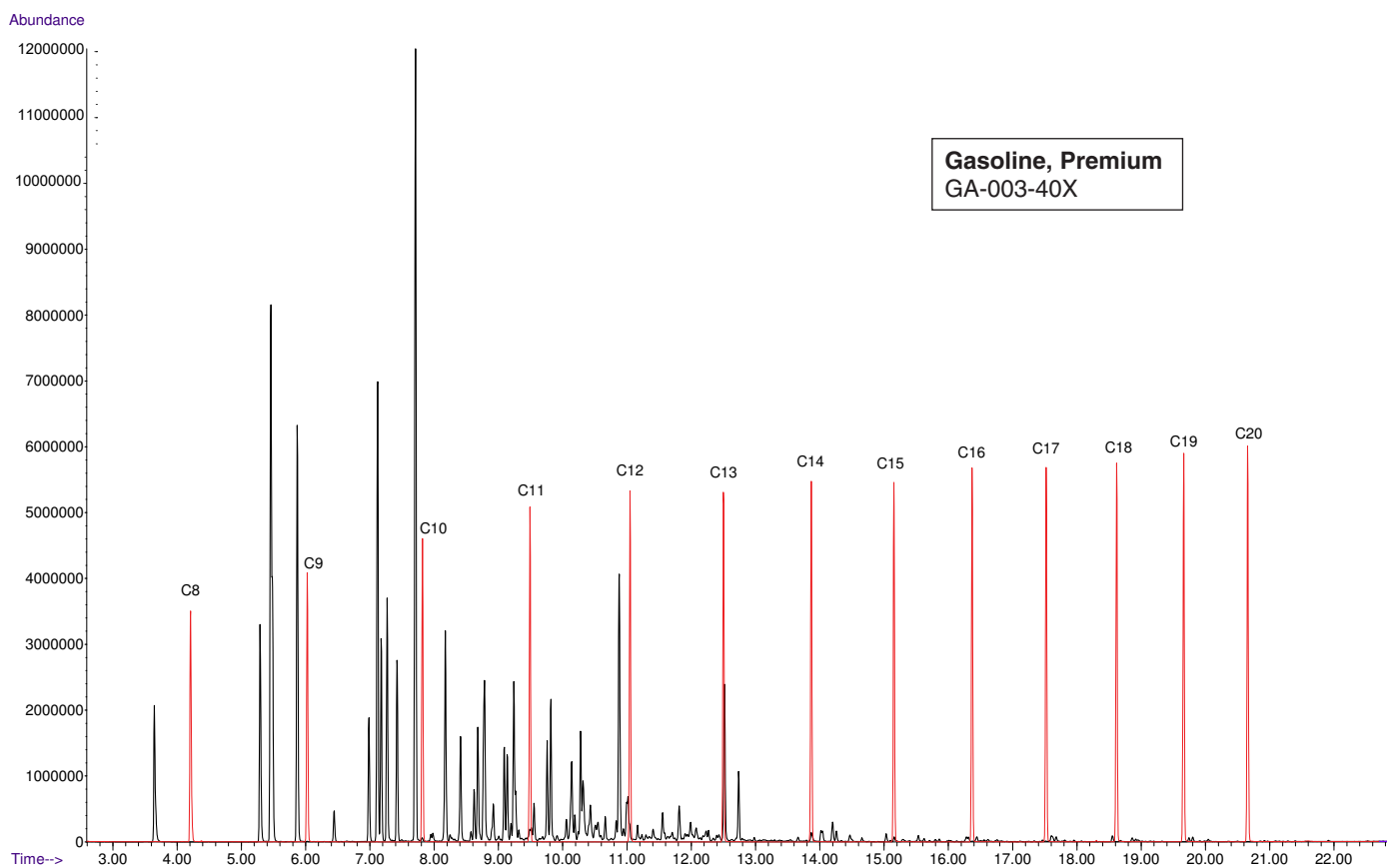
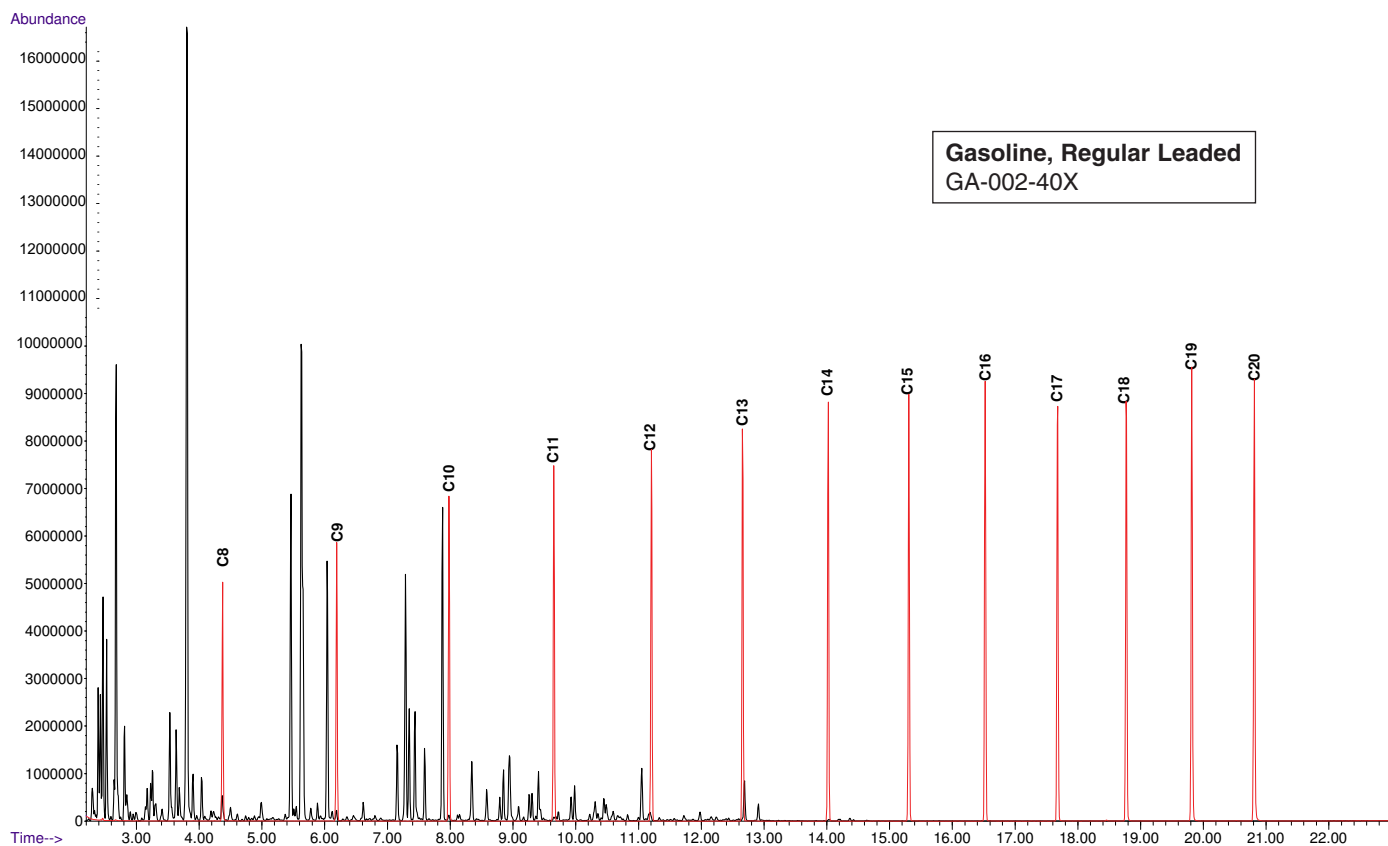
12 x 1 mL

	mg/mL	Solvent	Cat. No.
Gasoline, Regular Unleaded	20	MeOH	GA-001-40X
Gasoline, Regular Leaded	20	MeOH	GA-002-40X
Gasoline, Premium	20	MeOH	GA-003-40X
RFA Gasoline (Oxygenate-free)	20	MeOH	GA-005-40X
Diesel Fuel	20	CH ₂ Cl ₂	FU-009-D-40X
#1 Diesel Fuel (Low sulfur)	20	CH ₂ Cl ₂	FU-013-D-40X
#2 Diesel Fuel (Extra low sulfur)	20	CH ₂ Cl ₂	FU-017-D-40X
Biodiesel 20	20	CH ₂ Cl ₂	FU-030-D-40X
Biodiesel 100 (Consumer grade)	20	CH ₂ Cl ₂	FU-029-D-40X
SAE 30W Motor Oil	20	CH ₂ Cl ₂	FU-018-D-40X
SAE 40W Motor Oil	20	CH ₂ Cl ₂	FU-019-D-40X
SAE 50W Motor Oil	20	CH ₂ Cl ₂	FU-021-D-40X

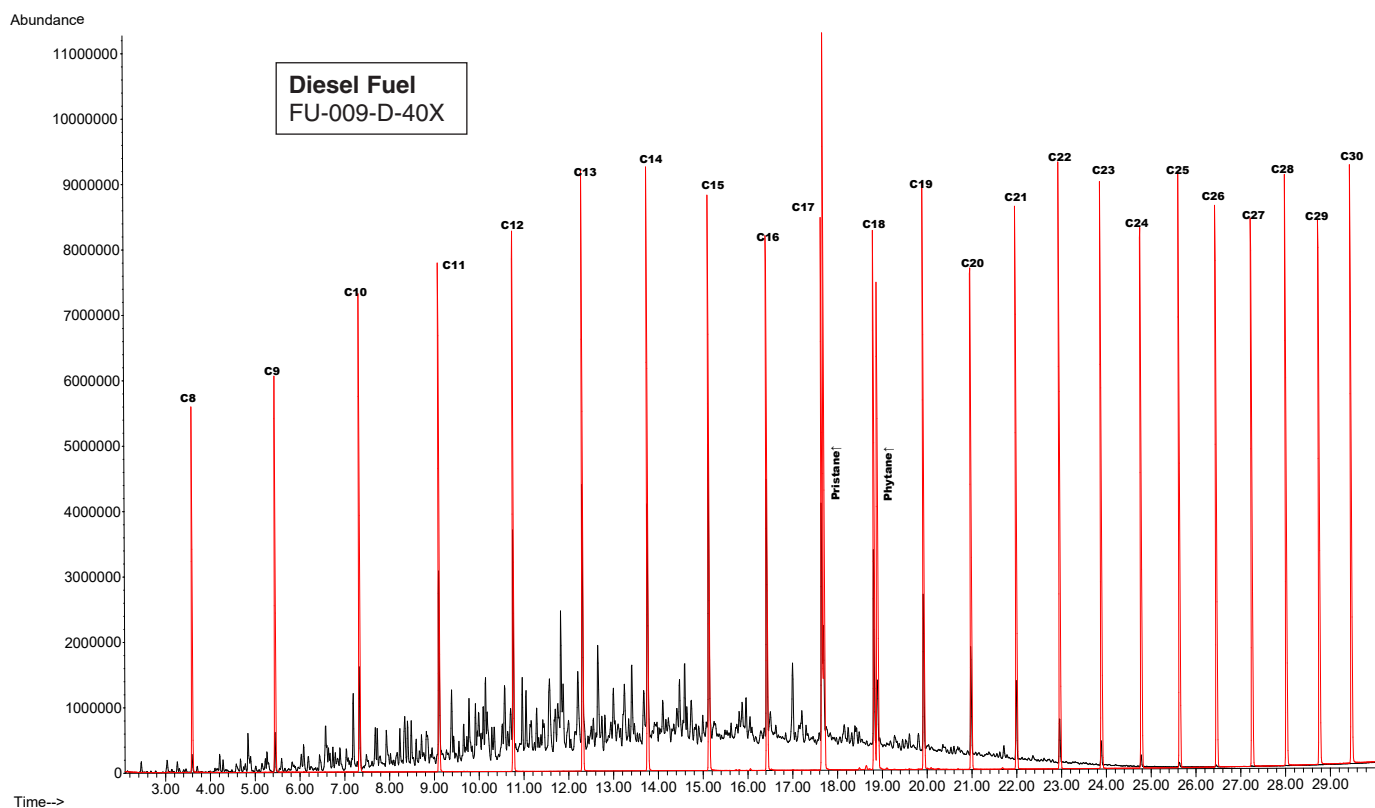
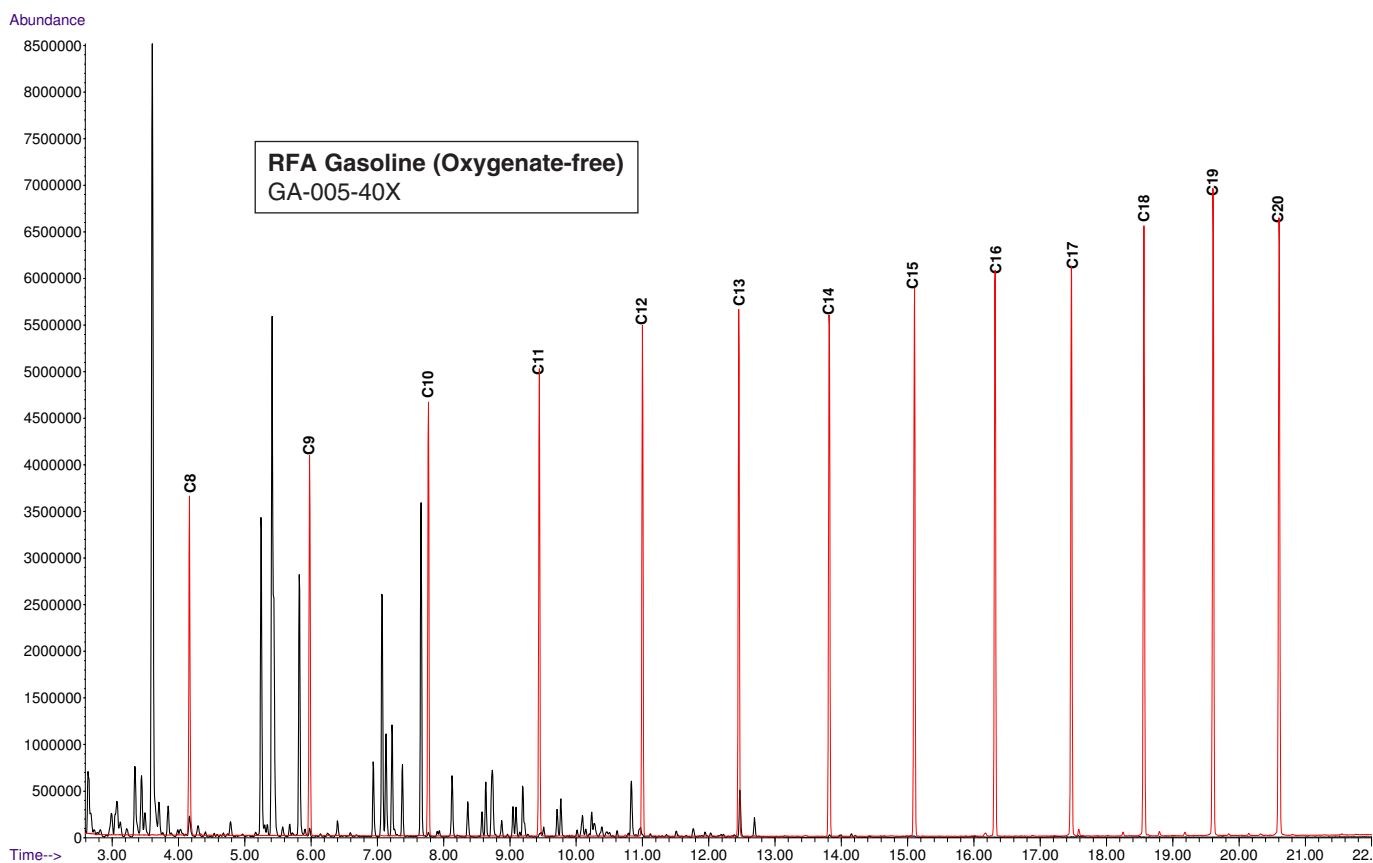
Note: Renewable Diesel Fuel #2, SAE 5W30, 10W30, 10W30 Motor Oil not in set



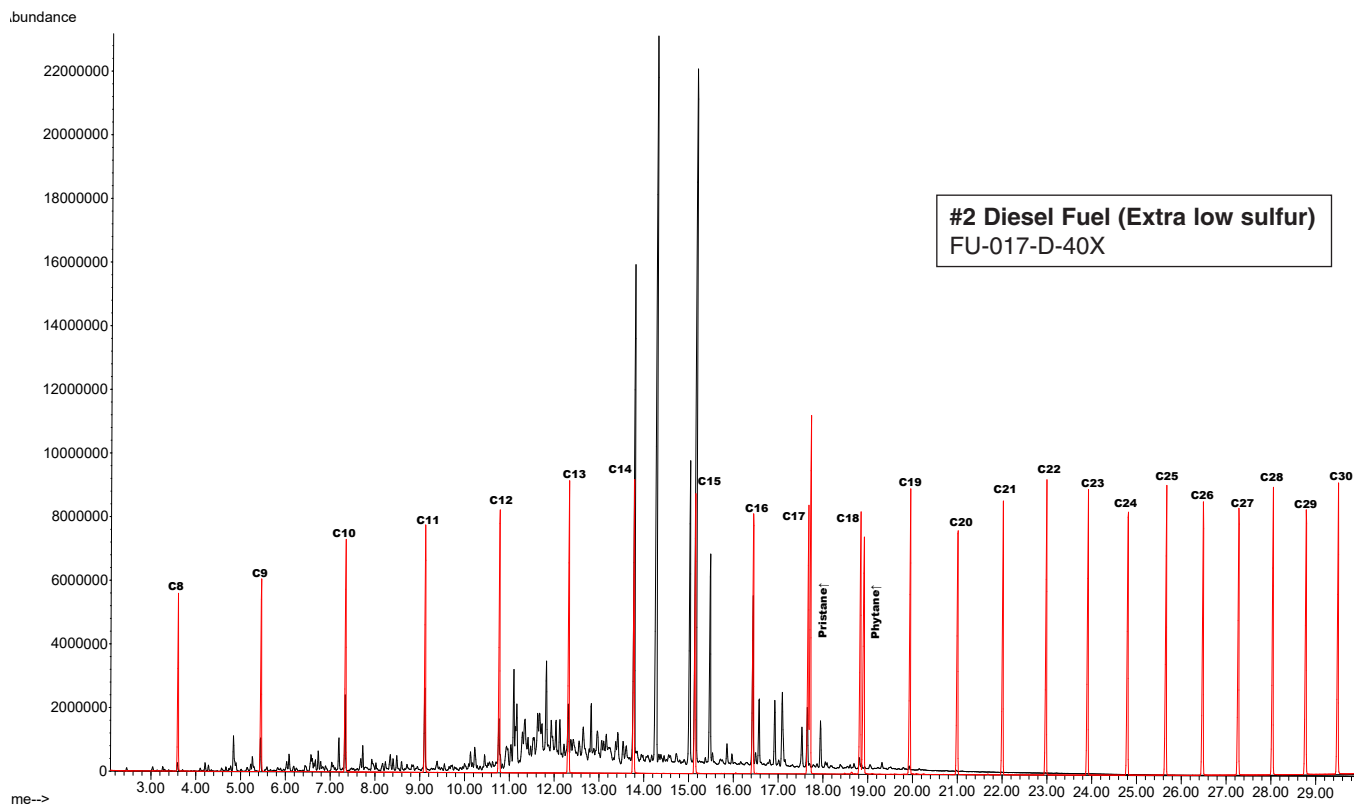
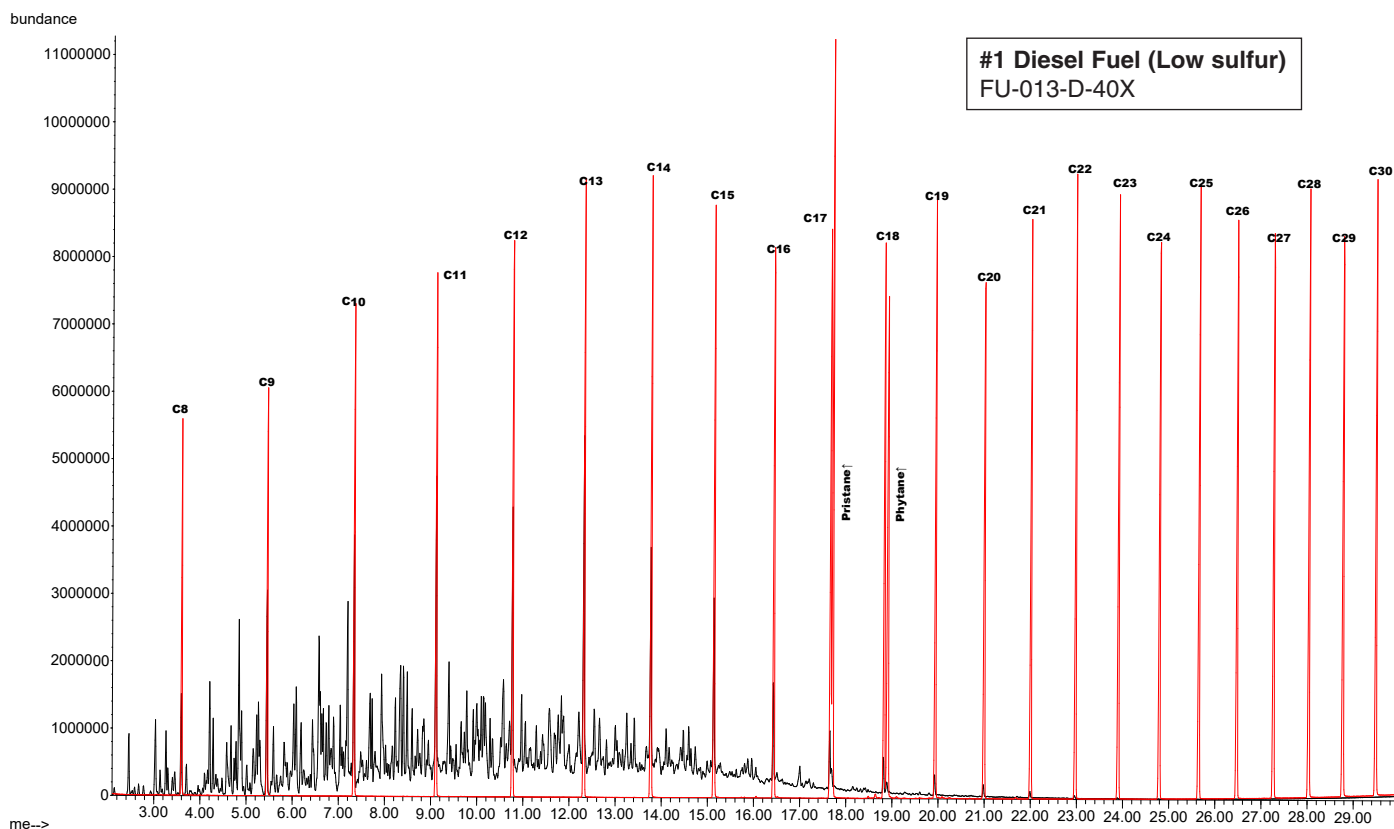
Chromatograms of Motor Fuels and Lubrication Oils (continued)



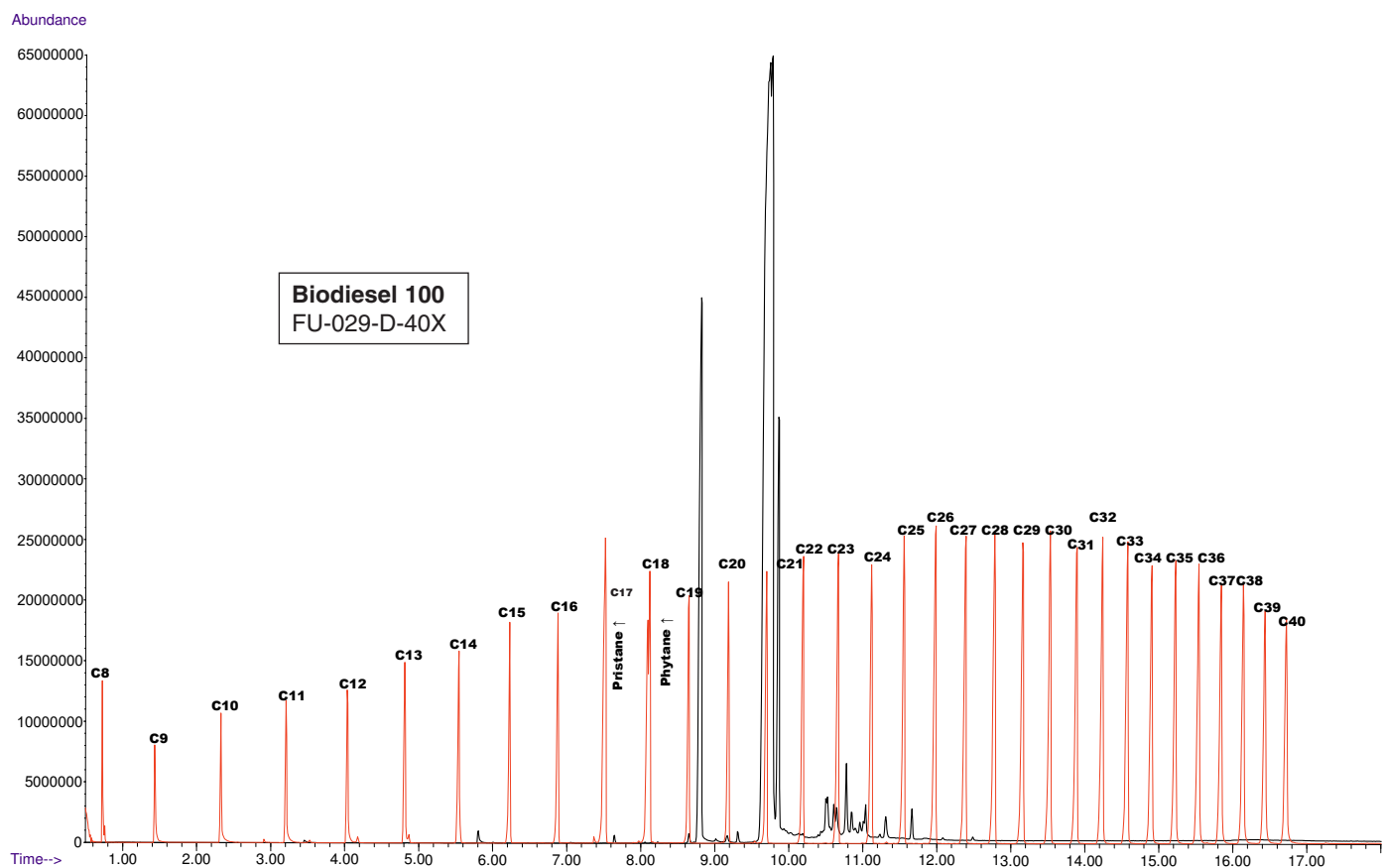
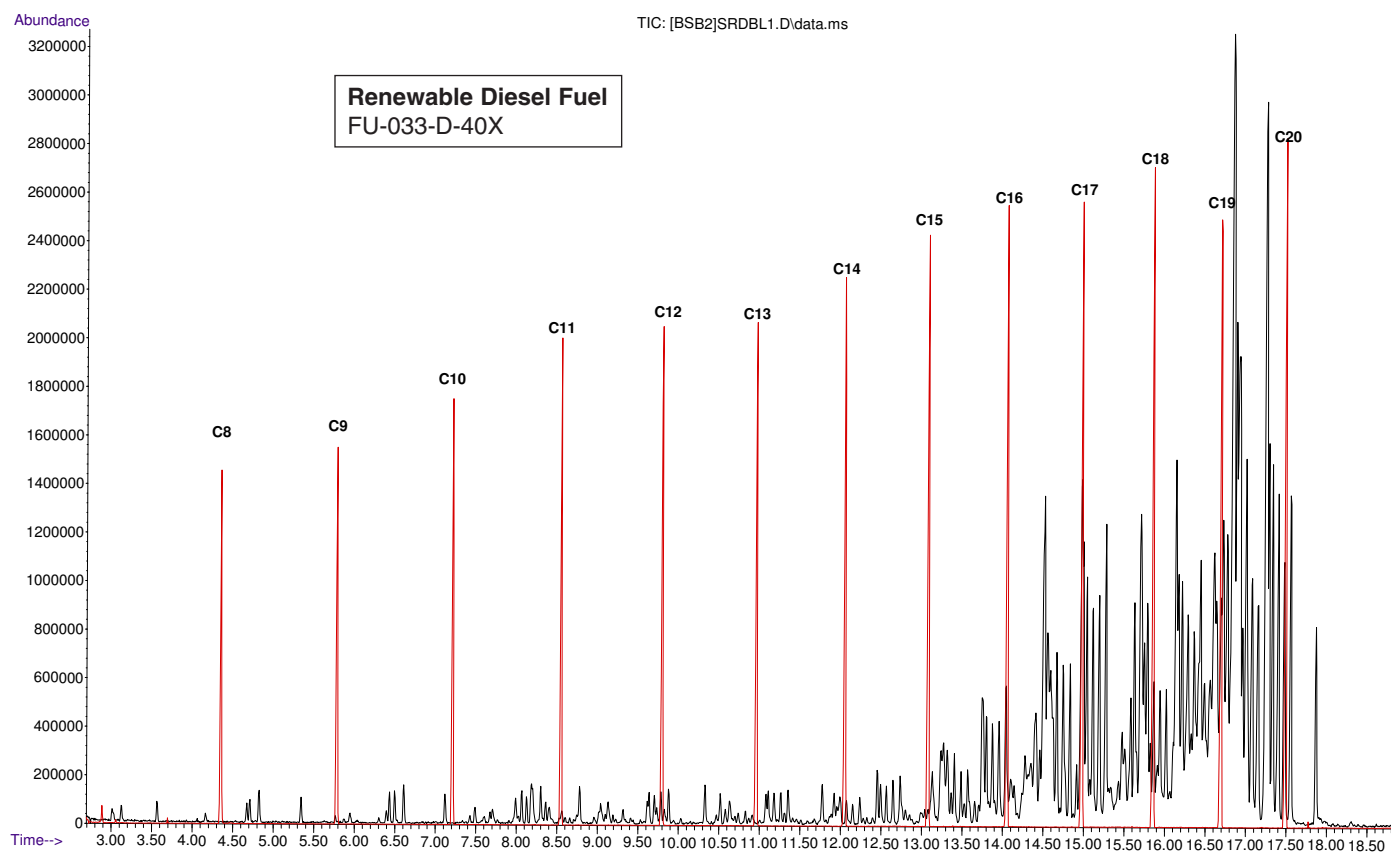
Chromatograms of Motor Fuels and Lubrication Oils (continued)



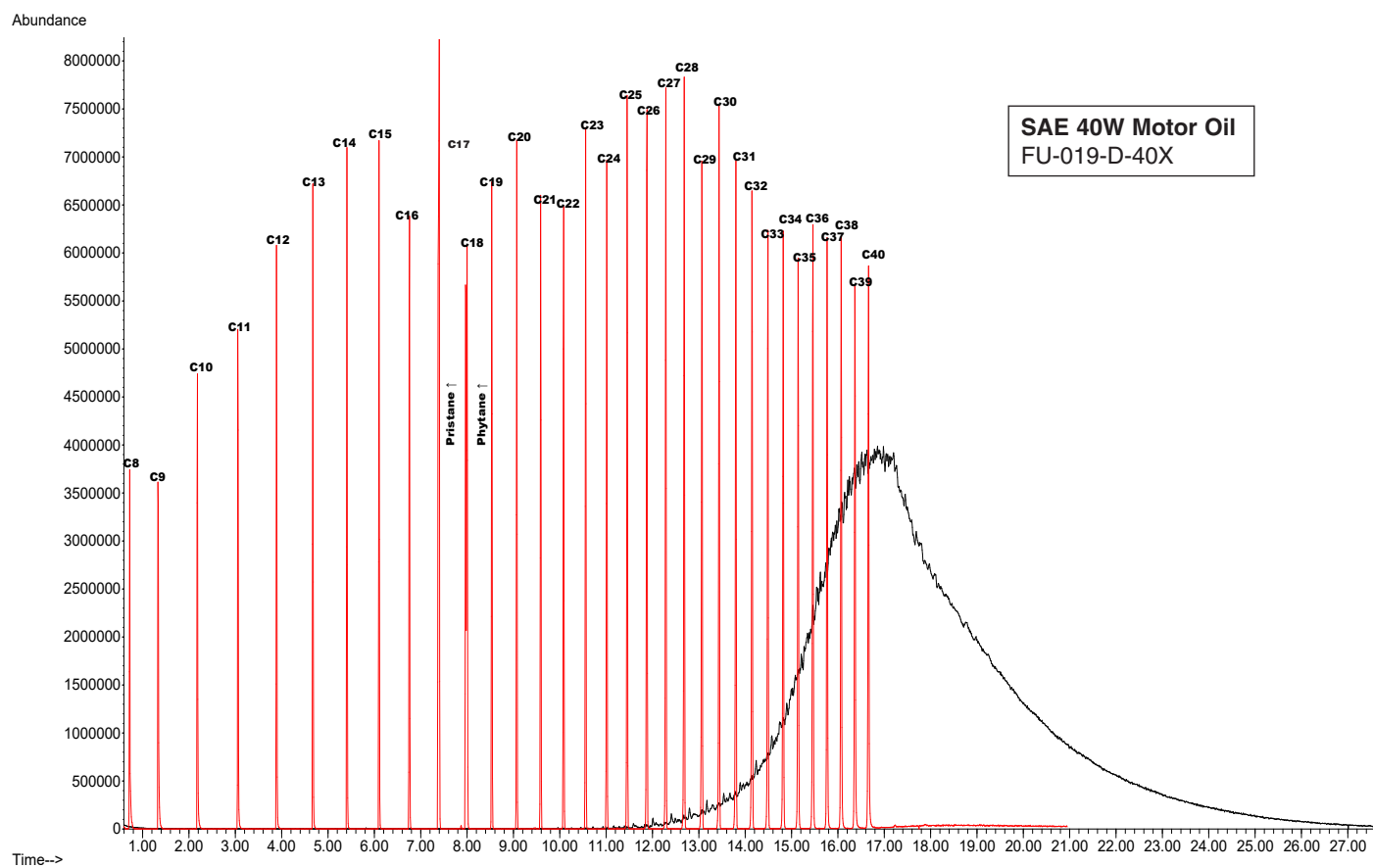
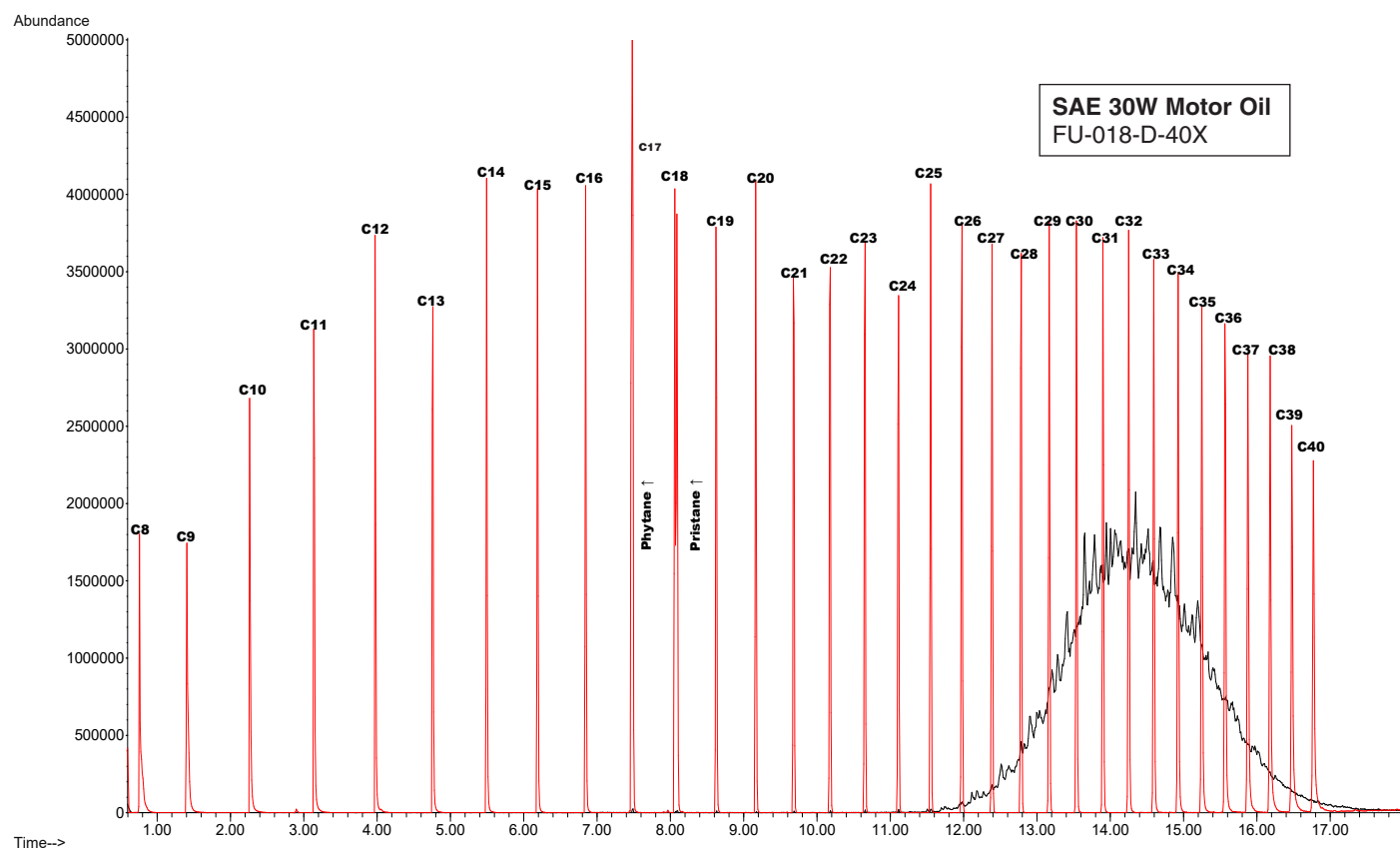
Chromatograms of Motor Fuels and Lubrication Oils (continued)



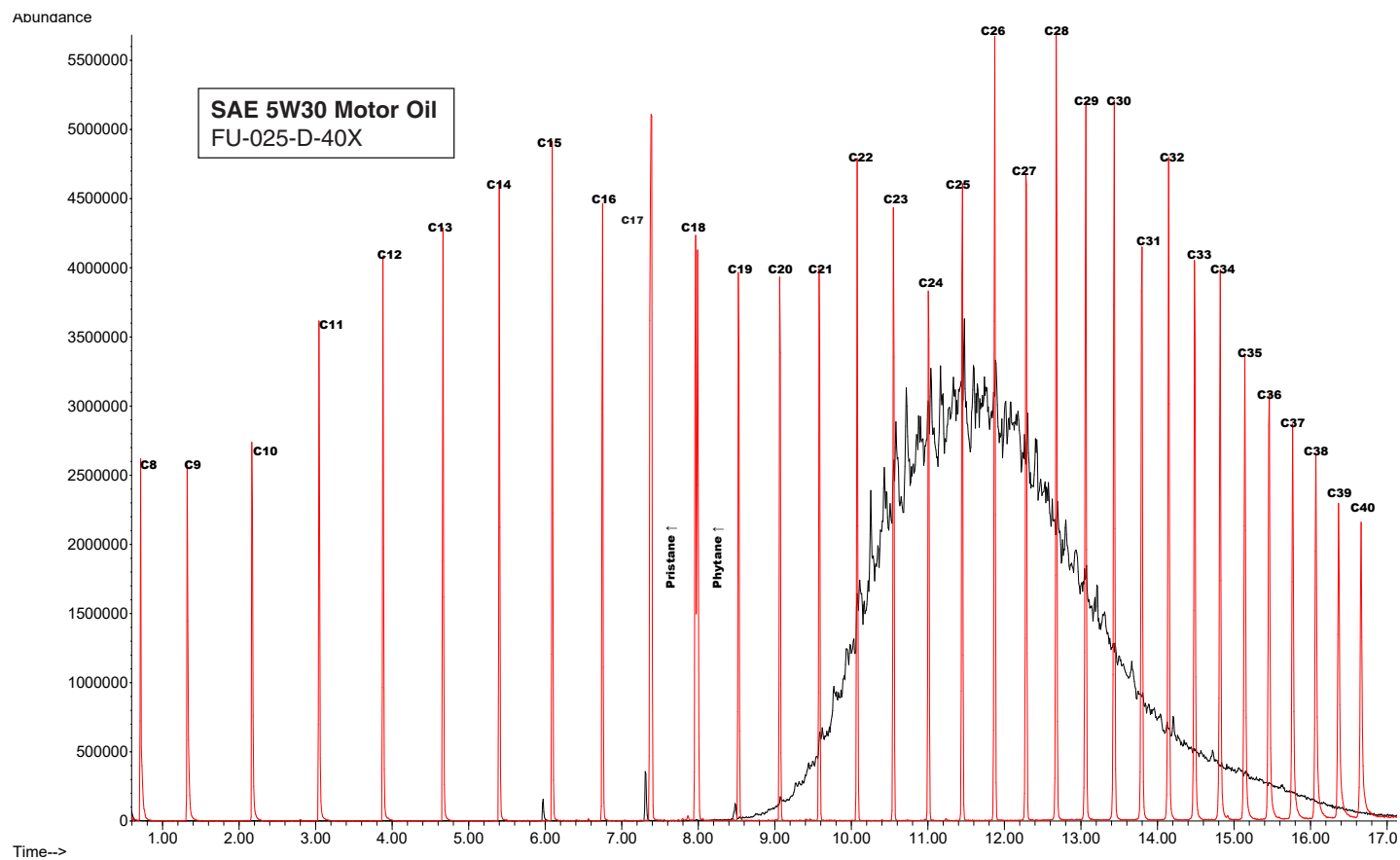
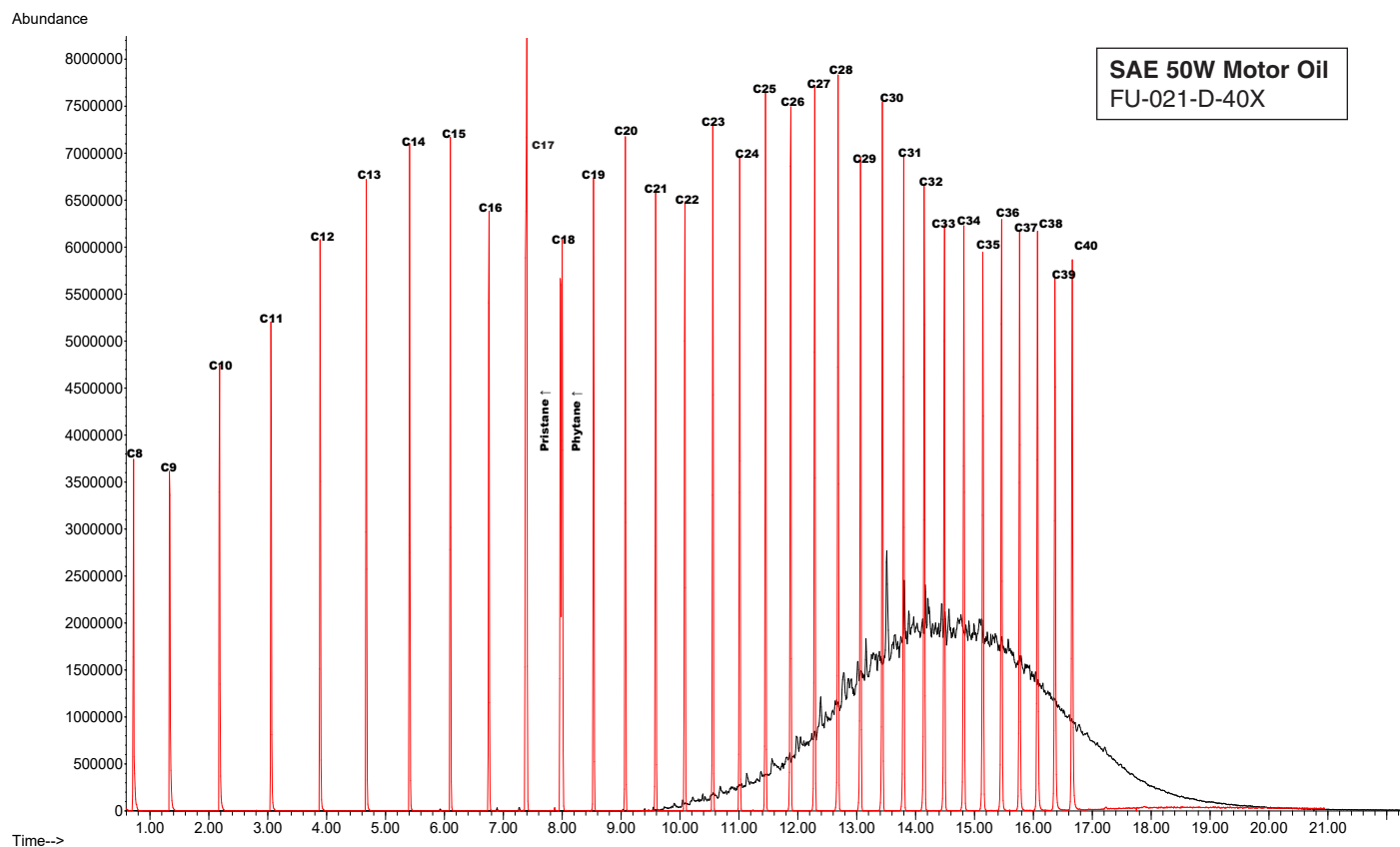
Chromatograms of Motor Fuels and Lubrication Oils (continued)



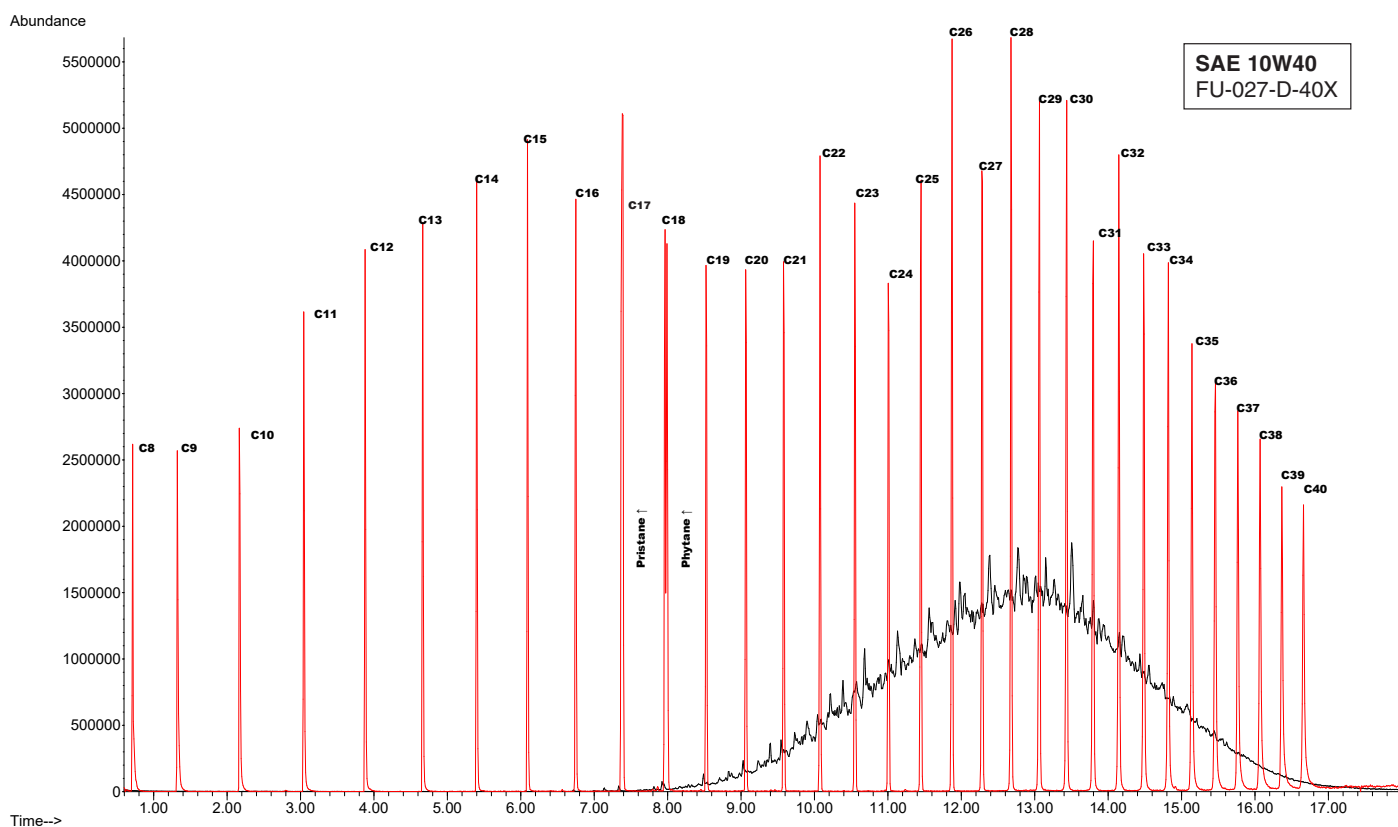
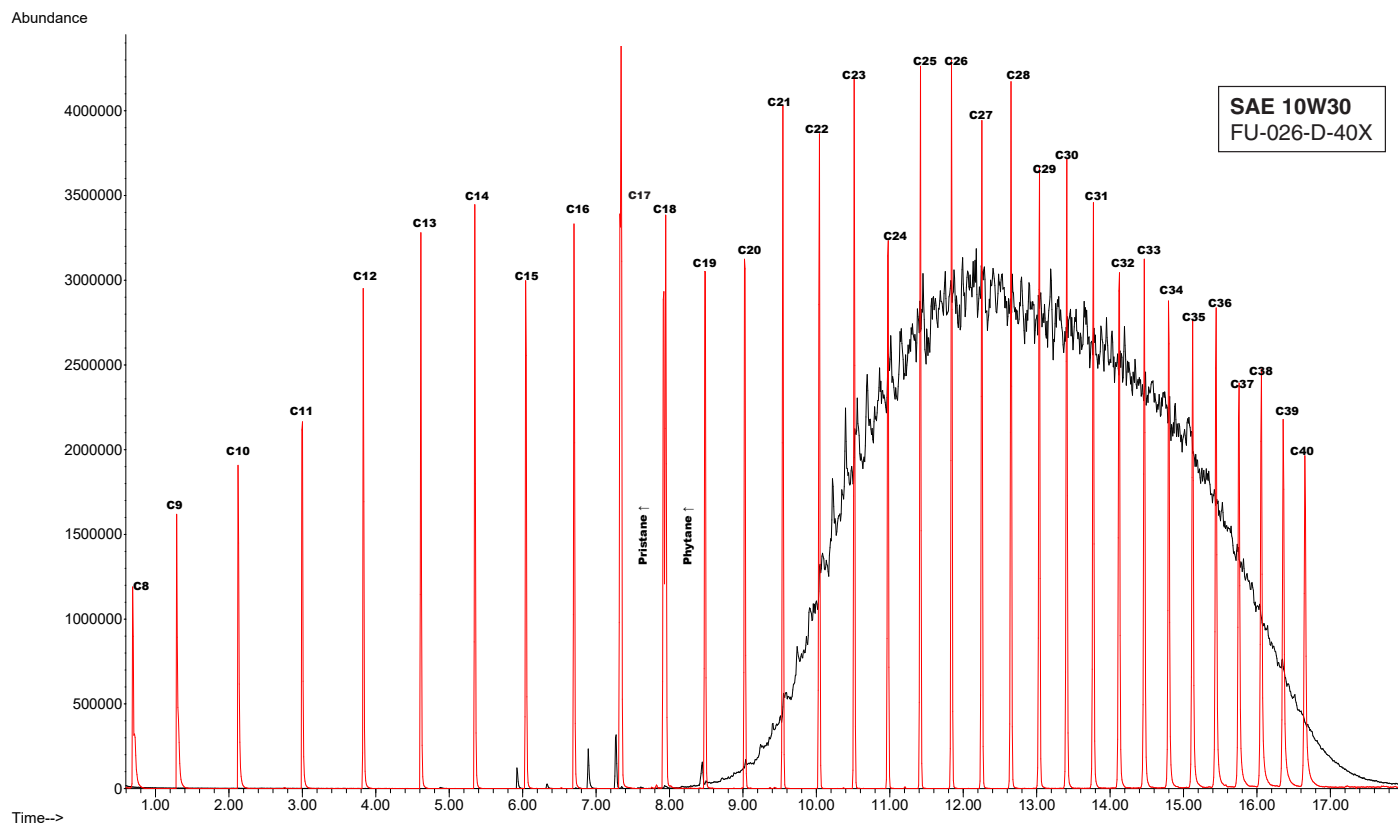
Chromatograms of Motor Fuels and Lubrication Oils (continued)



Chromatograms of Motor Fuels and Lubrication Oils (continued)



Chromatograms of Motor Fuels and Lubrication Oils (continued)



Chromatograms of Heating Fuels Oils

Heating Fuel Oils Chromatography

9-12

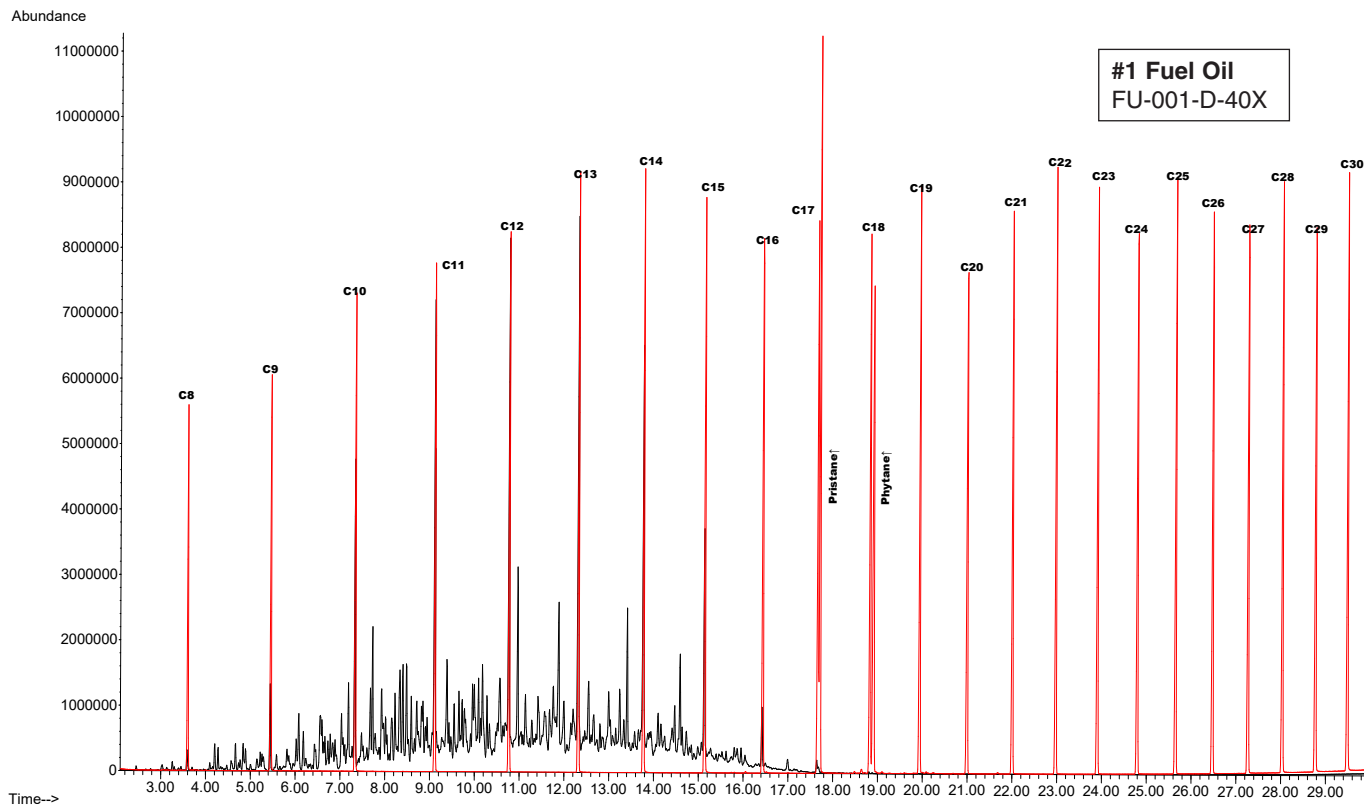
#1 Fuel Oil	9
#2 Fuel Oil	10
#3 Fuel Oil	10
#4 Fuel Oil	11
#6 Fuel Oil	11
Kerosene	12

Heating Fuel Oils Set

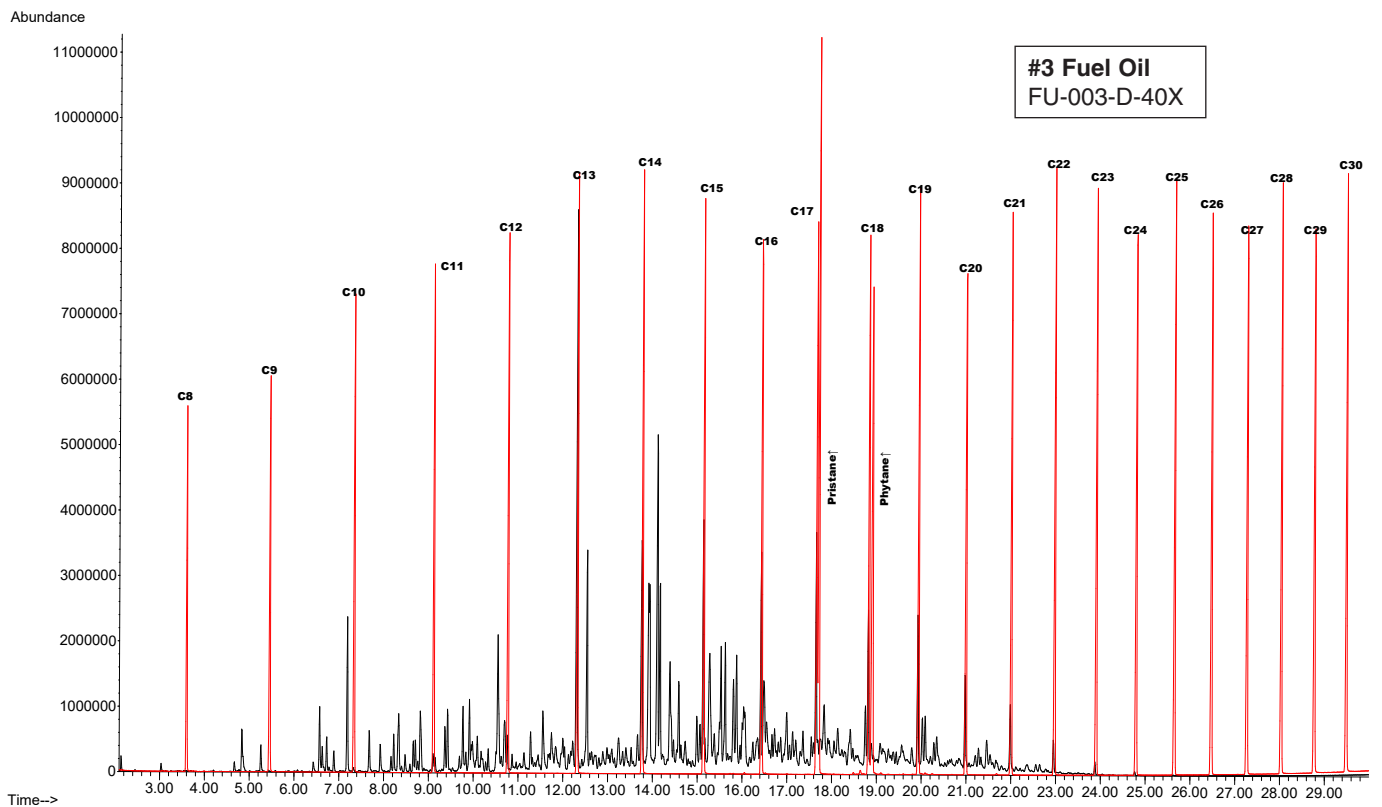
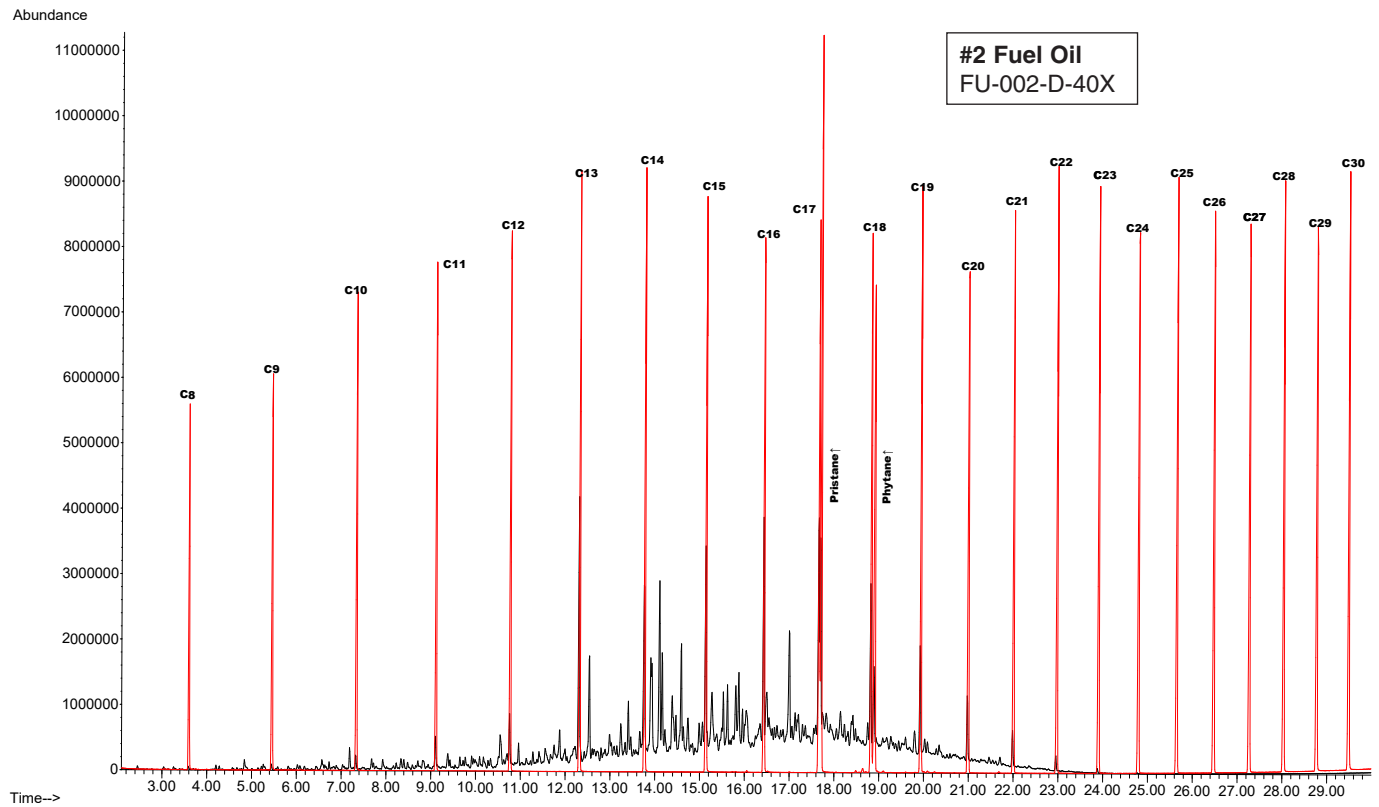
TPH-002-R1-SET

6 x 1 mL

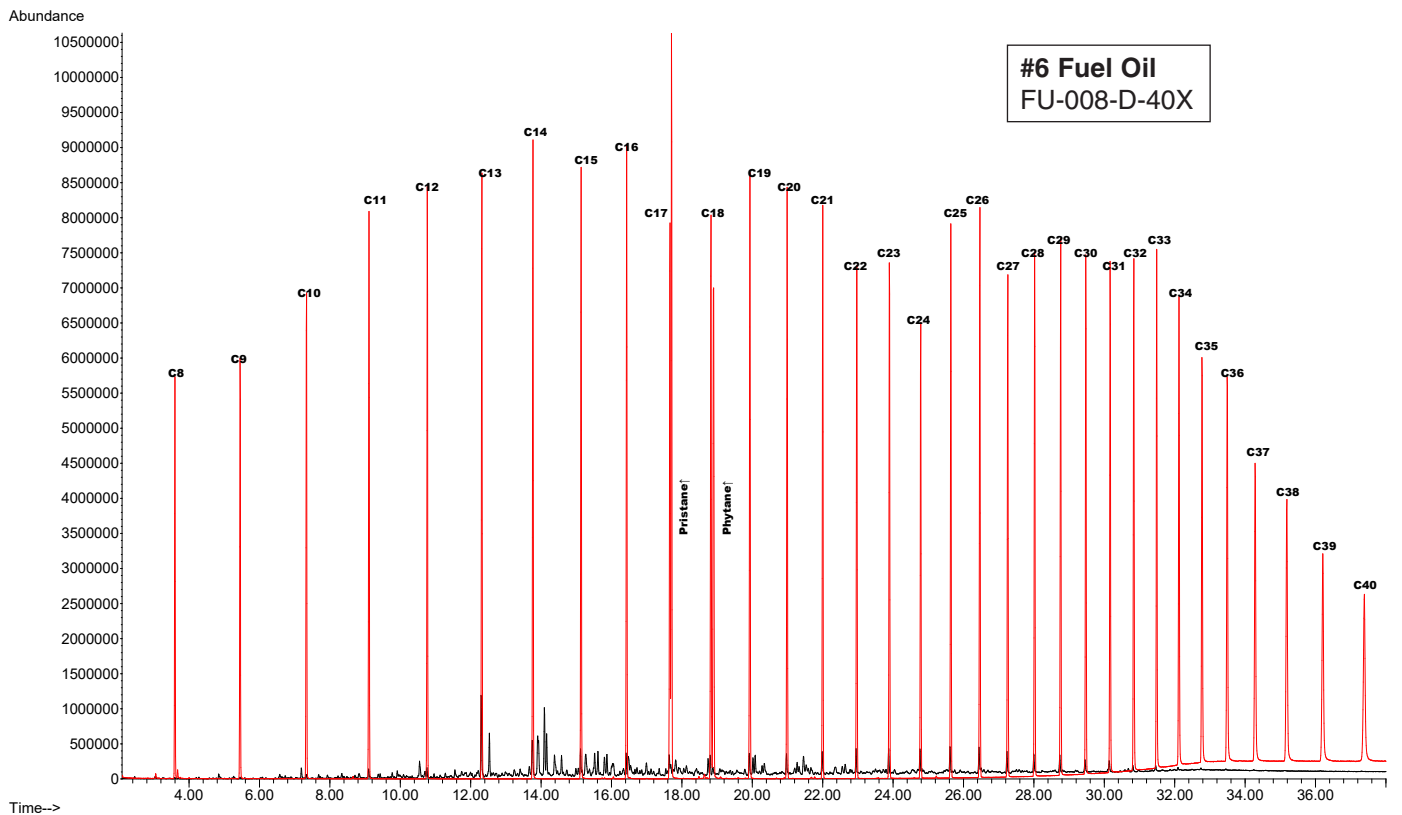
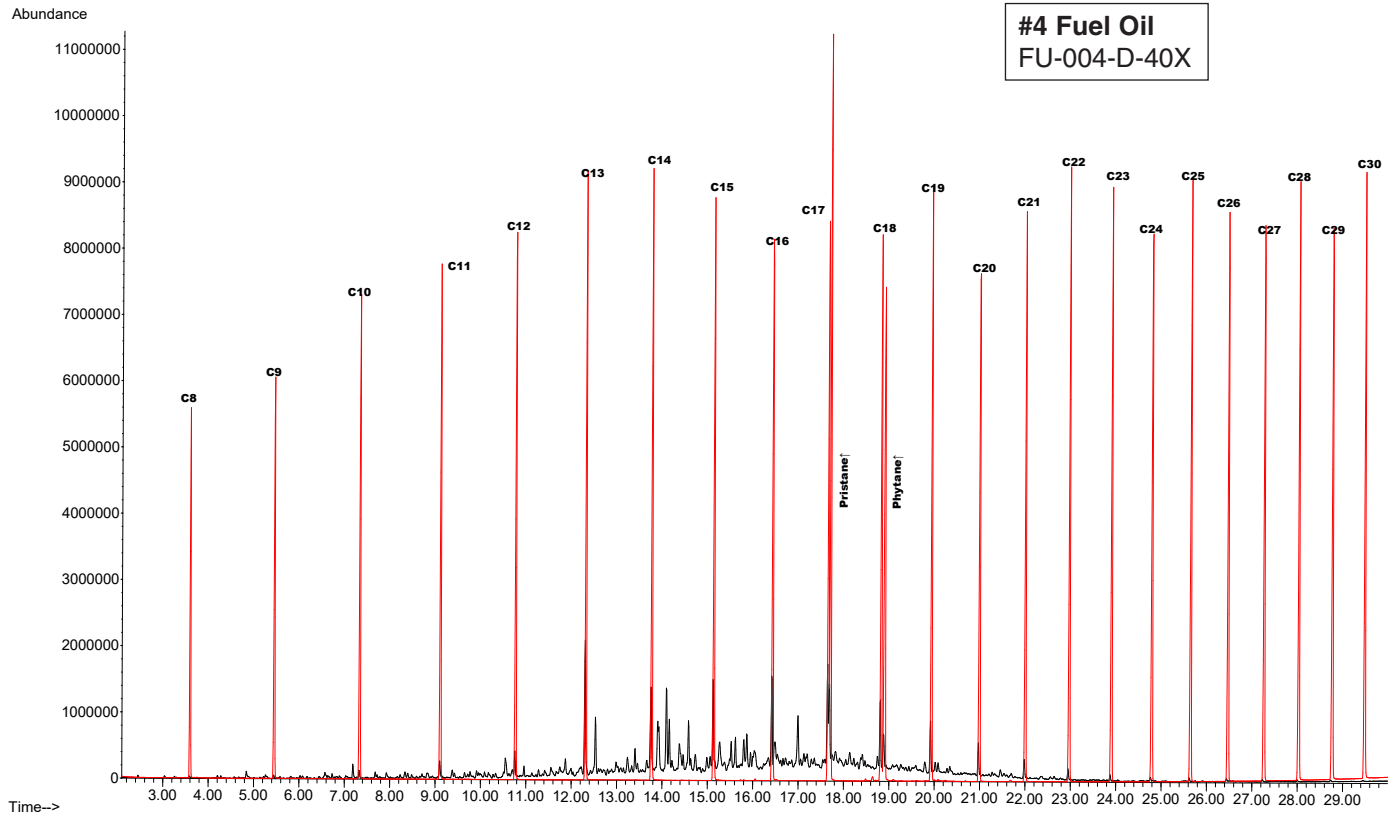
	mg/mL	Solvent	Cat. No.
#1 Fuel Oil	20	CH ₂ Cl ₂	FU-001-D-40X
#2 Fuel Oil	20	CH ₂ Cl ₂	FU-002-D-40X
#3 Fuel Oil	20	CH ₂ Cl ₂	FU-003-D-40X
#4 Fuel Oil	20	CH ₂ Cl ₂	FU-004-D-40X
#6 Fuel Oil	20	CH ₂ Cl ₂	FU-008-D-40X
Kerosene	20	CH ₂ Cl ₂	FU-005-D-40X



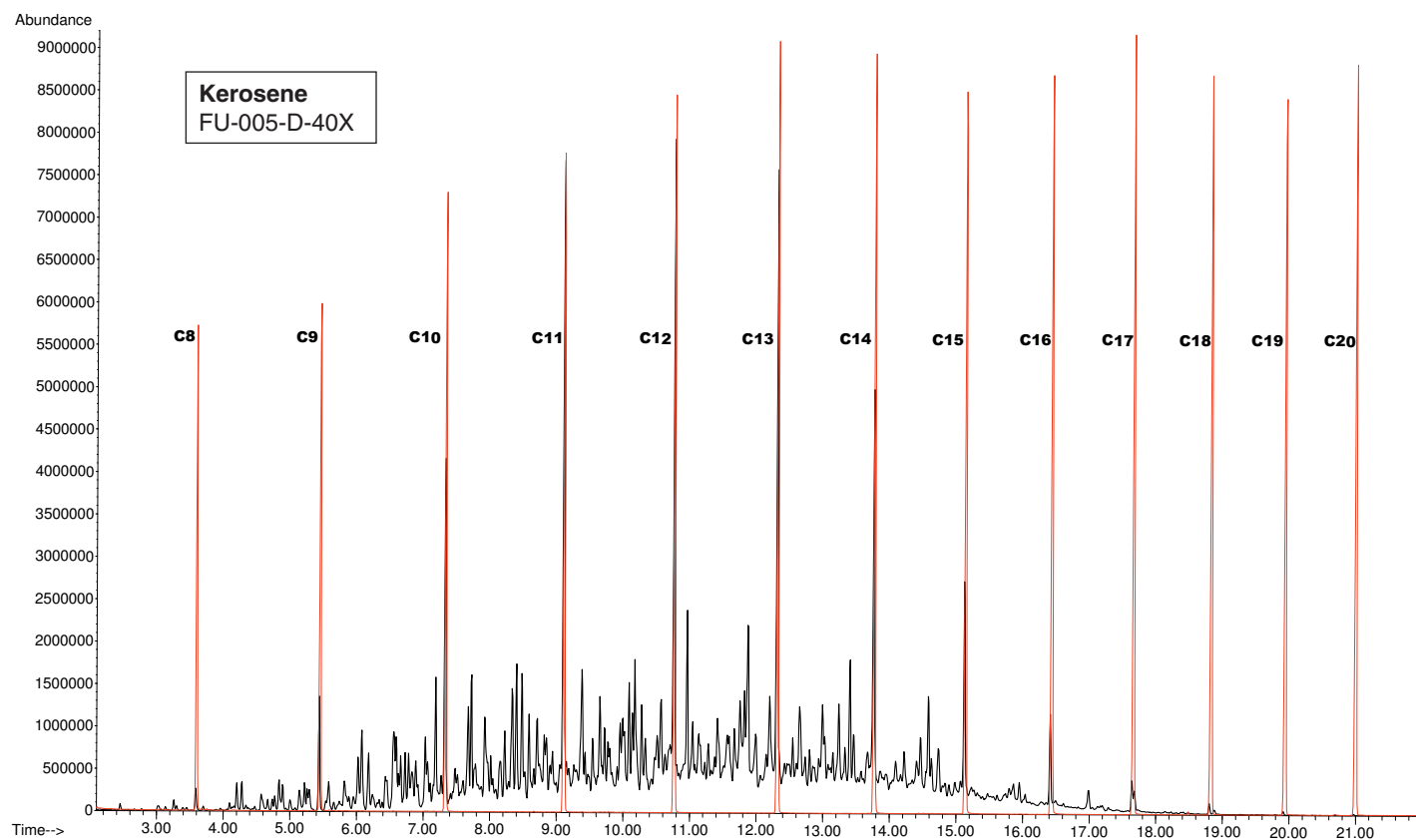
Chromatograms of Heating Fuels Oils (continued)



Chromatograms of Heating Fuels Oils (continued)



Chromatograms of Heating Fuels Oils (continued)

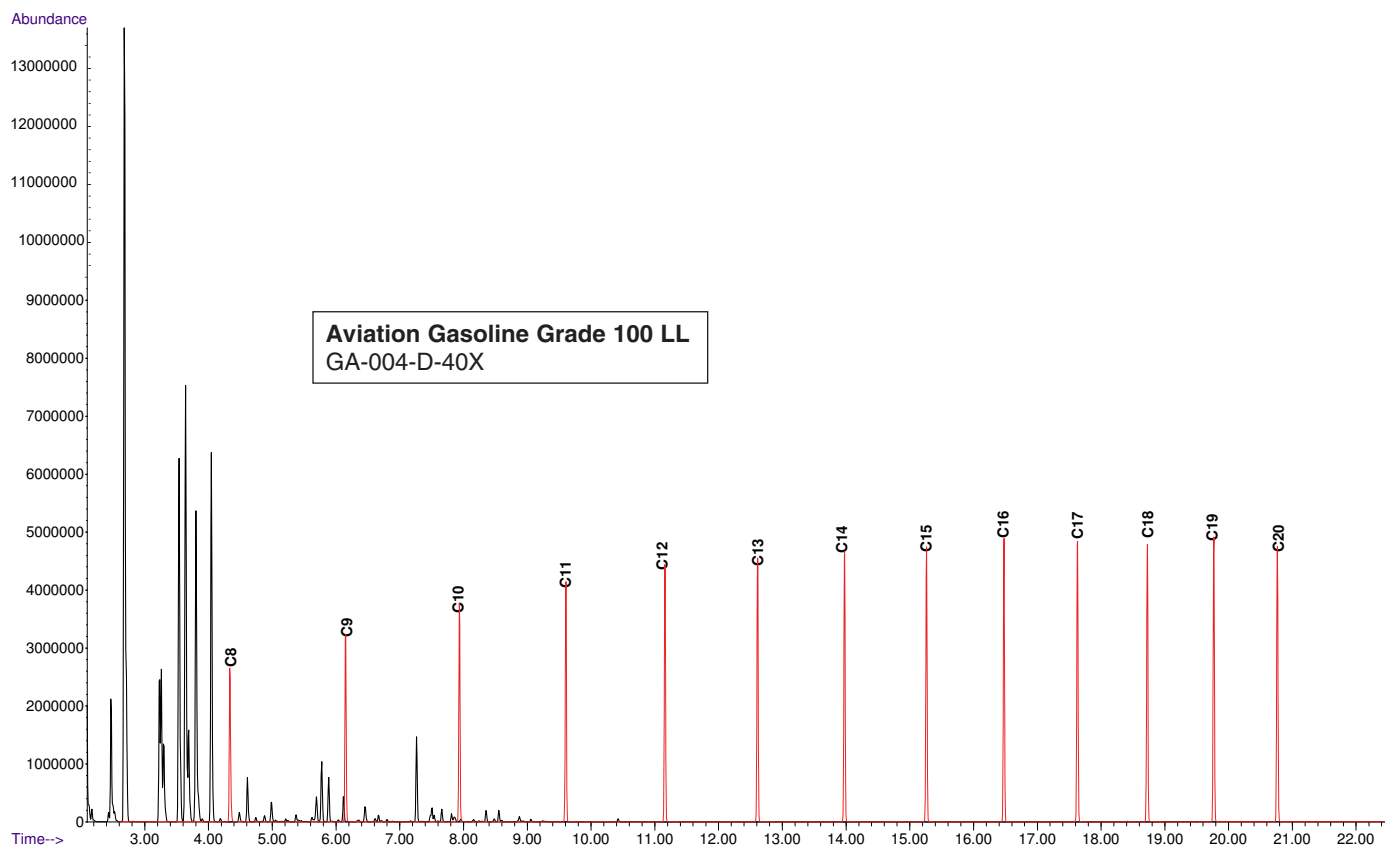


Chromatograms of Aviation Fuels Oils

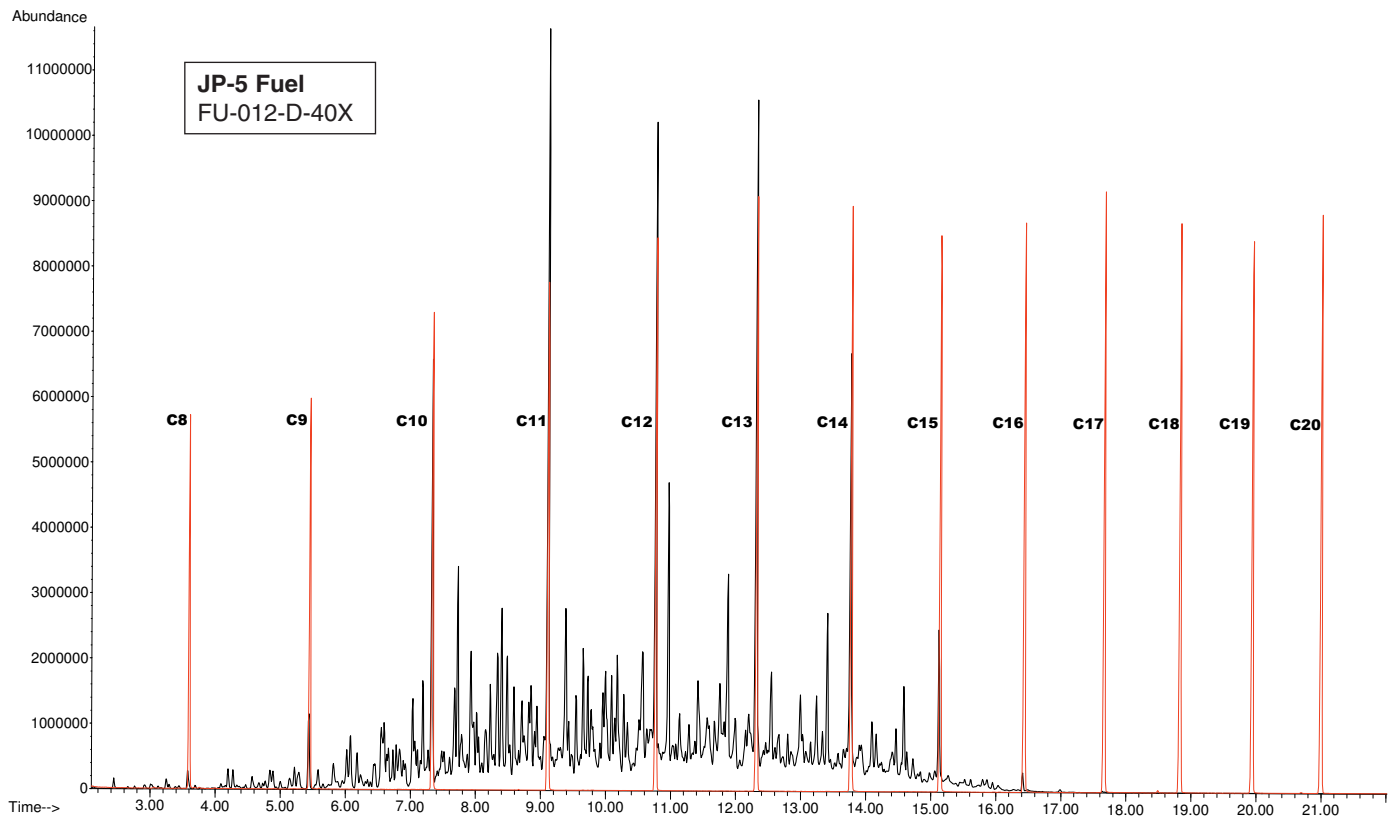
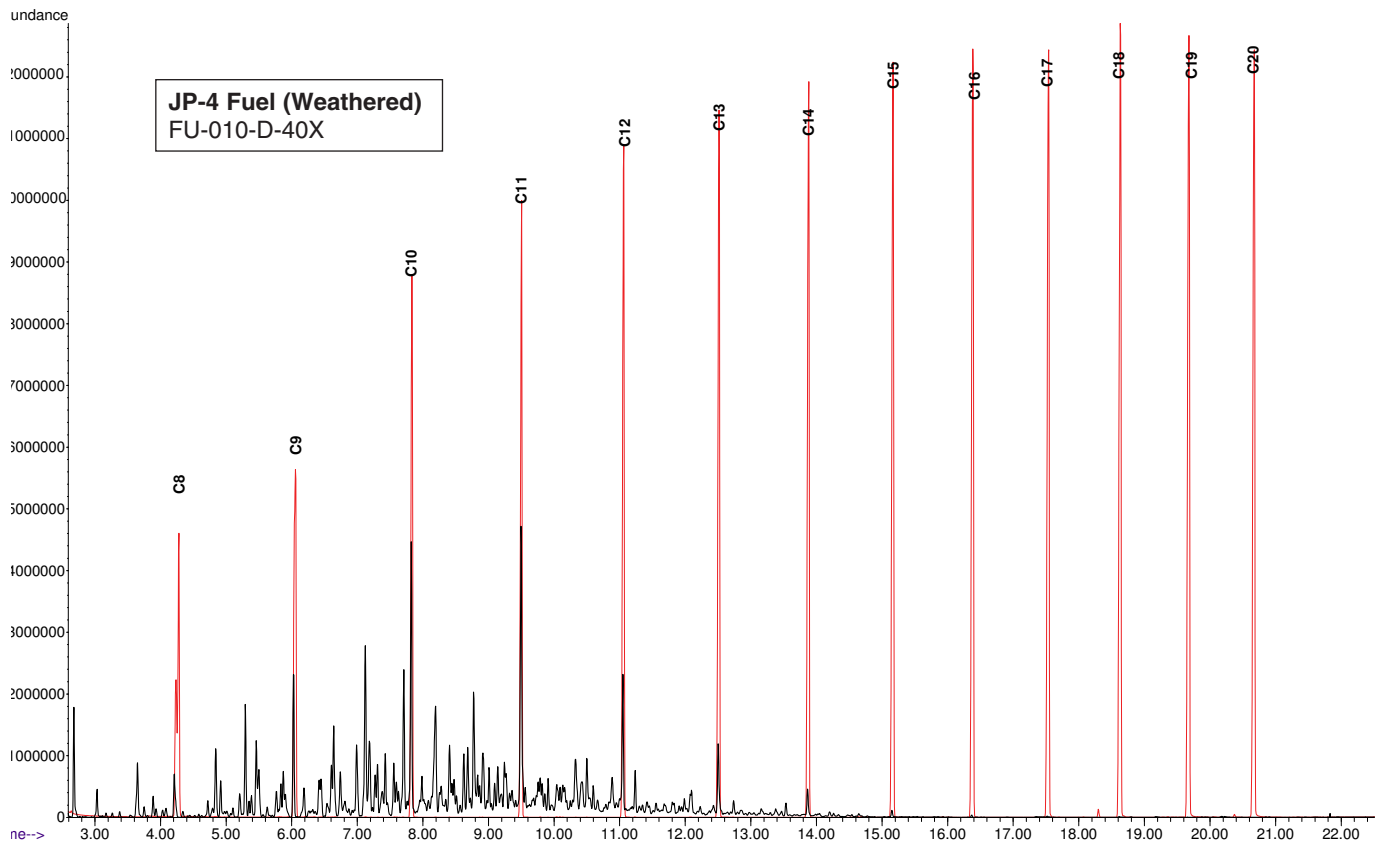
Aviation Fuel Oils Chromatography	13-18
Aviation Gasoline (Grade 100-LL)	13
JP-4 Fuel (Weathered)	14
JP-5 Fuel	14
JP-7 Fuel	15
JP-8 Fuel	15
JP-10 Aviation Fuel	16
JP-TS Aviation Fuel	16
Renewable Aviation Fuel	17
Jet Reference Fuel (Type 1)	17
Turbine (Jet A) Fuel	18
Hydraulic Fluid	18

Aviation Fuels & Oils Set TPH-003-SET	mg/mL	Solvent	10 x 1 mL Cat. No.
Aviation Gasoline (Grade 100-LL)	20	CH ₂ Cl ₂	GA-004-D-40X
JP-4 Fuel (Weathered)	20	CH ₂ Cl ₂	FU-010-D-40X
JP-5 Fuel	20	CH ₂ Cl ₂	FU-012-D-40X
JP-7 Fuel	20	CH ₂ Cl ₂	FU-014-D-40X
JP-8 Fuel	20	CH ₂ Cl ₂	FU-015-D-40X
JP-10 Aviation Fuel	20	CH ₂ Cl ₂	FU-022-D-40X
JP-TS Aviation Fuel	20	CH ₂ Cl ₂	FU-016-D-40X
Jet Fuel (Type 1)	20	CH ₂ Cl ₂	FU-011-D-40X
Turbine (Jet A) Fuel	20	CH ₂ Cl ₂	FU-006-D-40X
Hydraulic Oil	20	CH ₂ Cl ₂	FU-020-D-40X

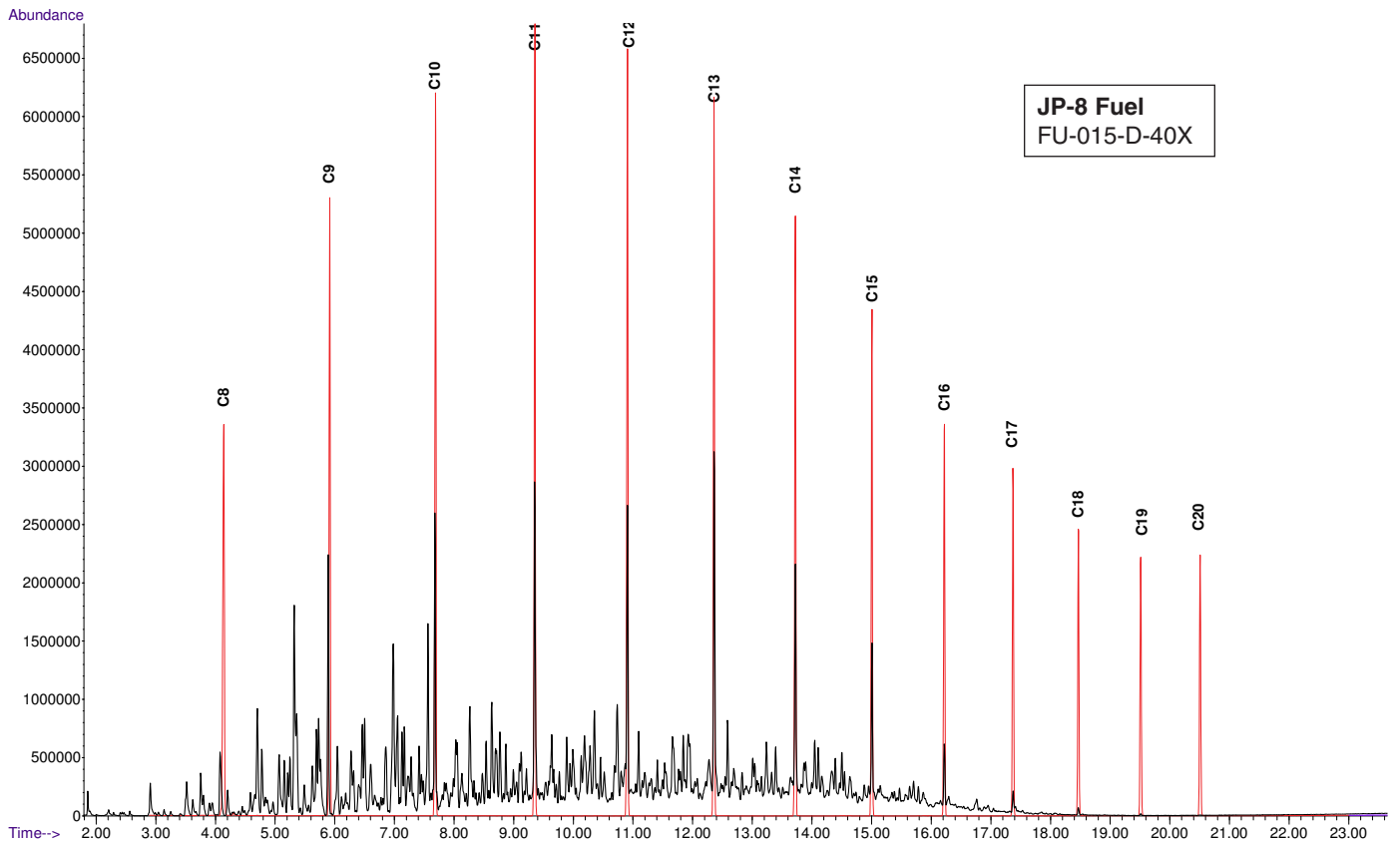
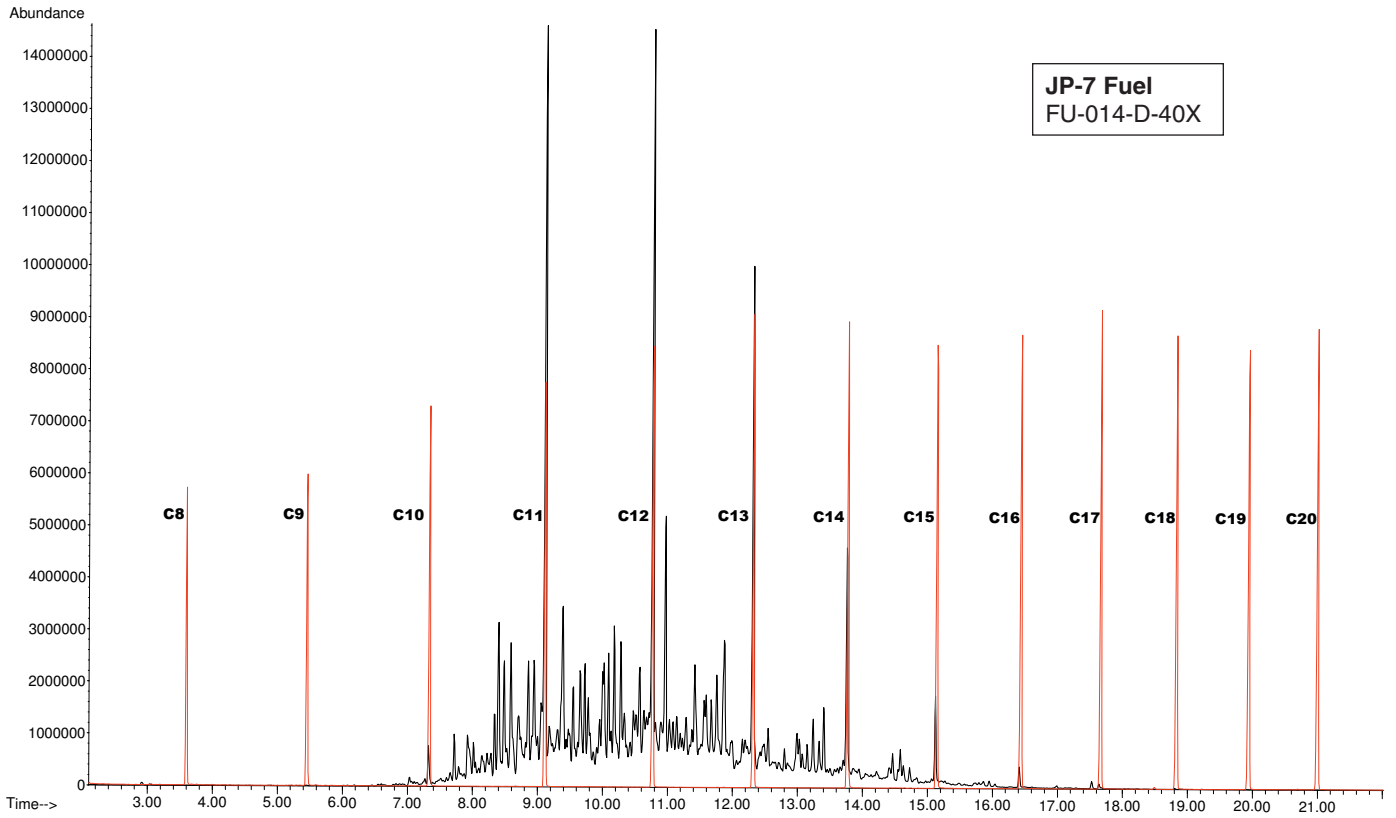
Note: Renewable Aviation Fuel not in set



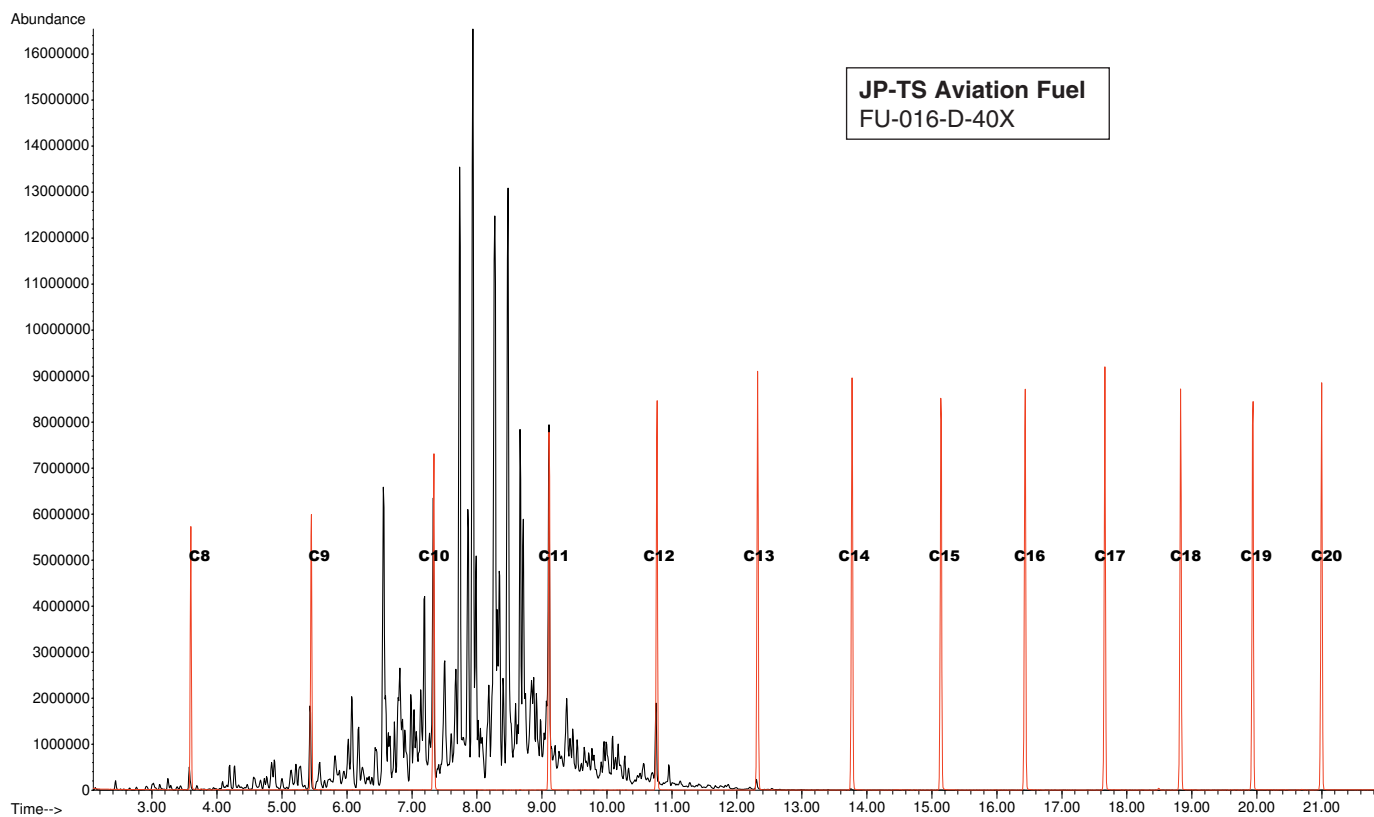
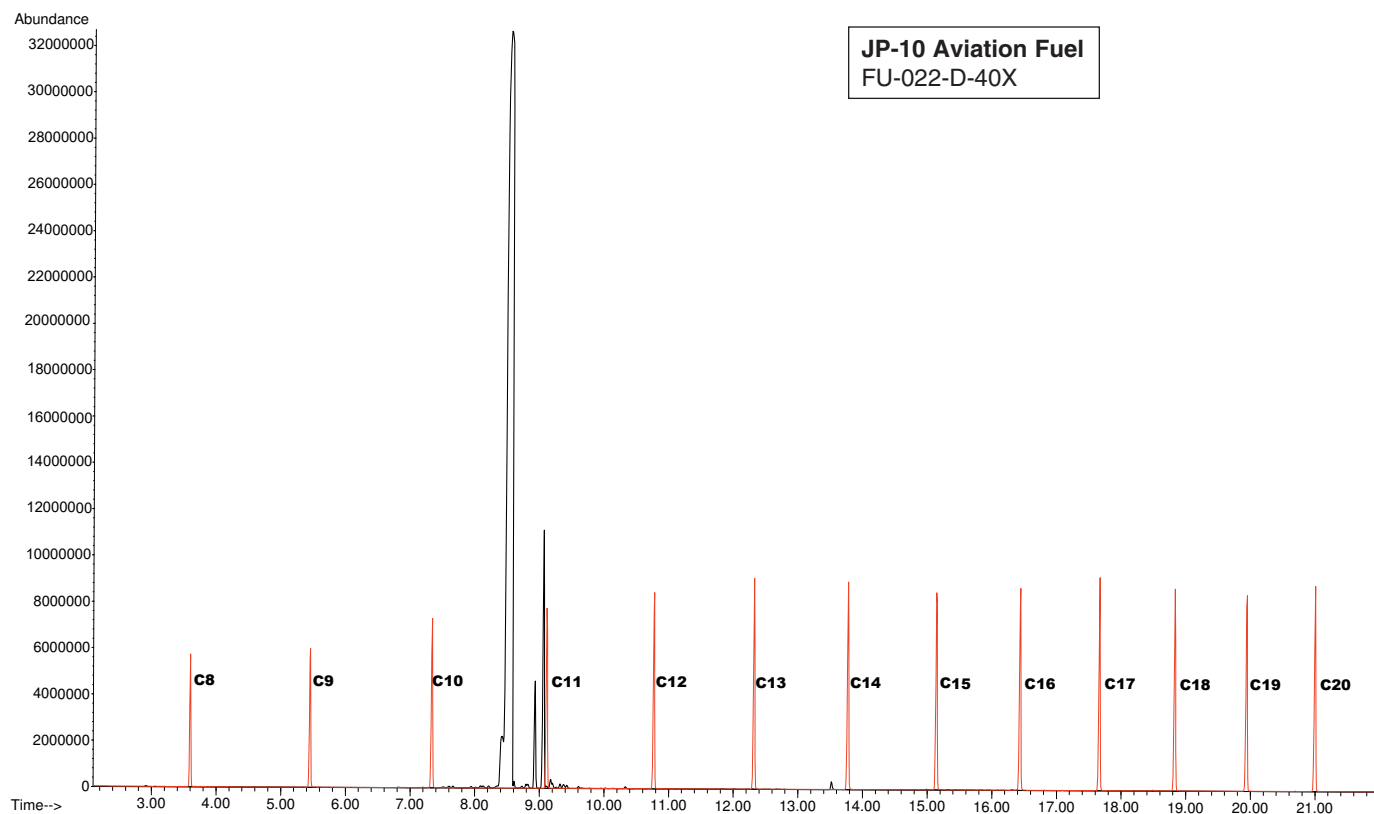
Chromatograms of Aviation Fuels Oils (continued)



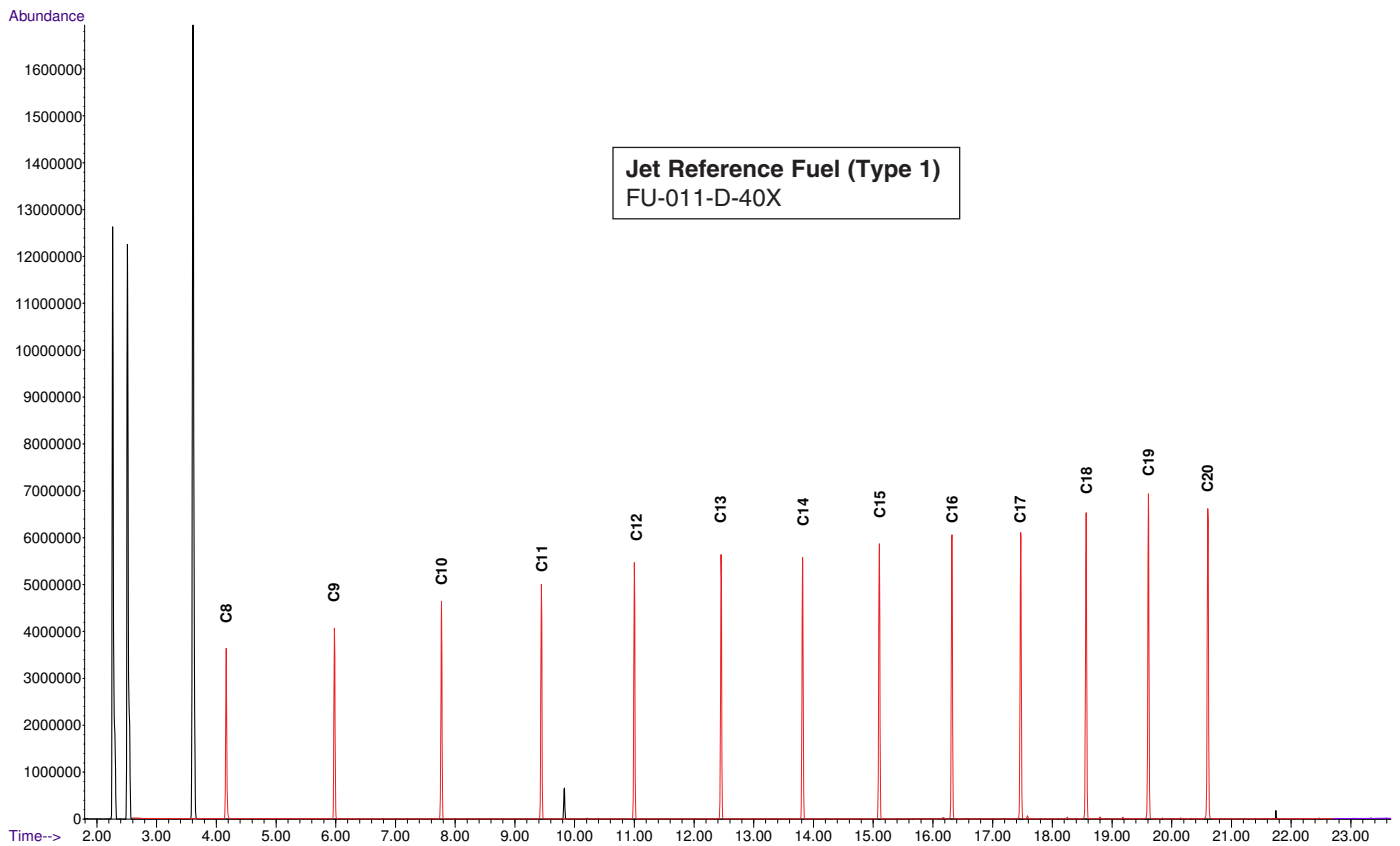
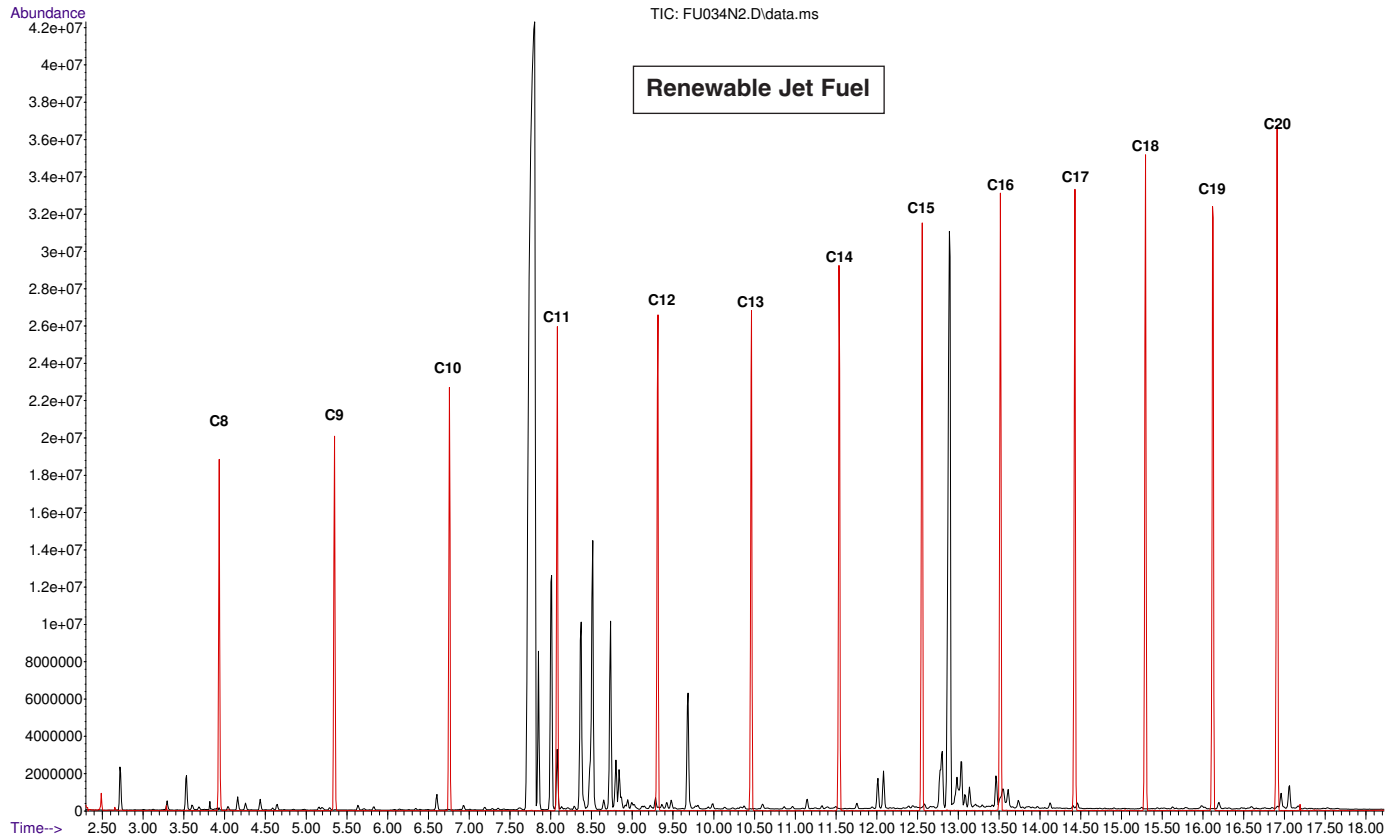
Chromatograms of Aviation Fuels Oils (continued)



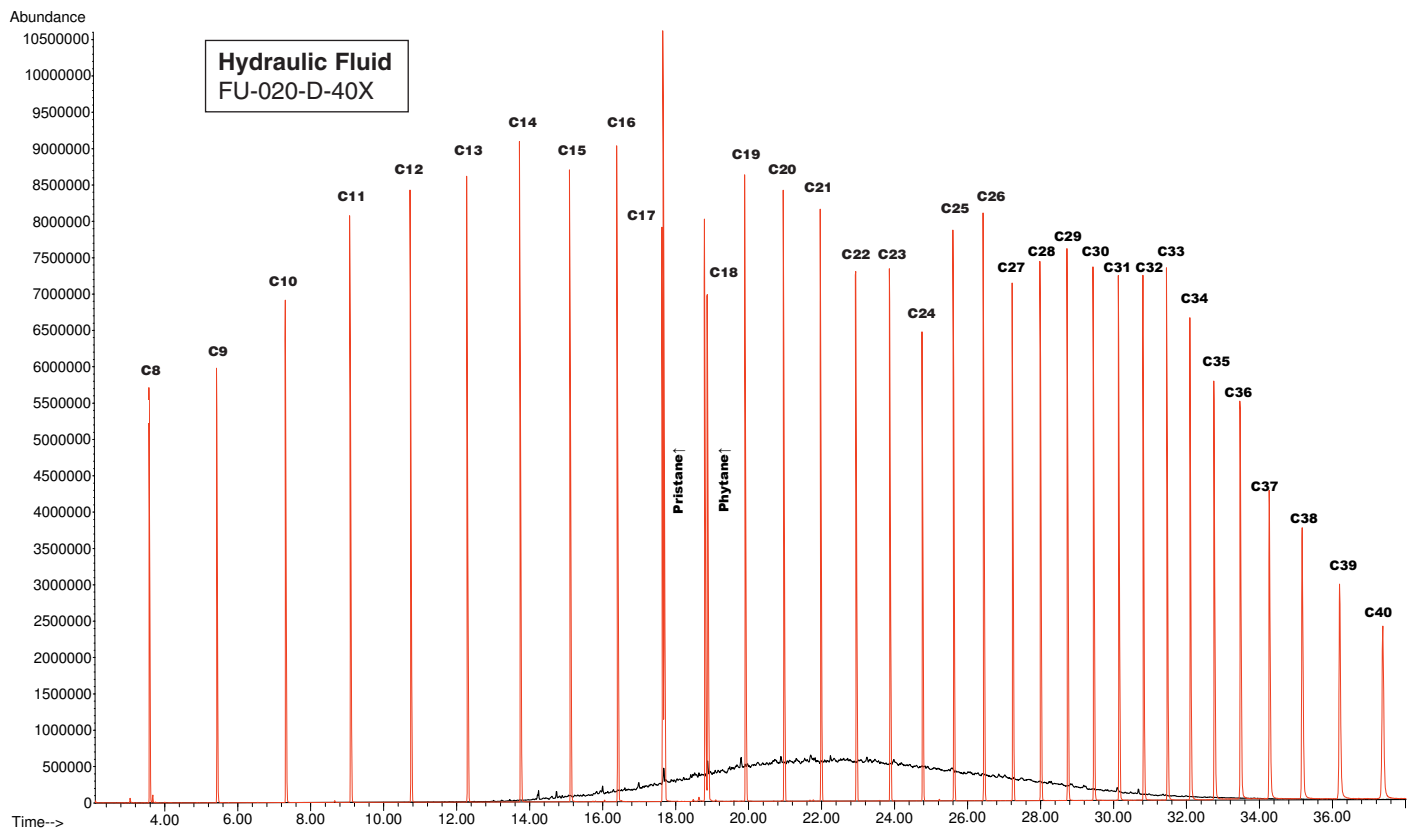
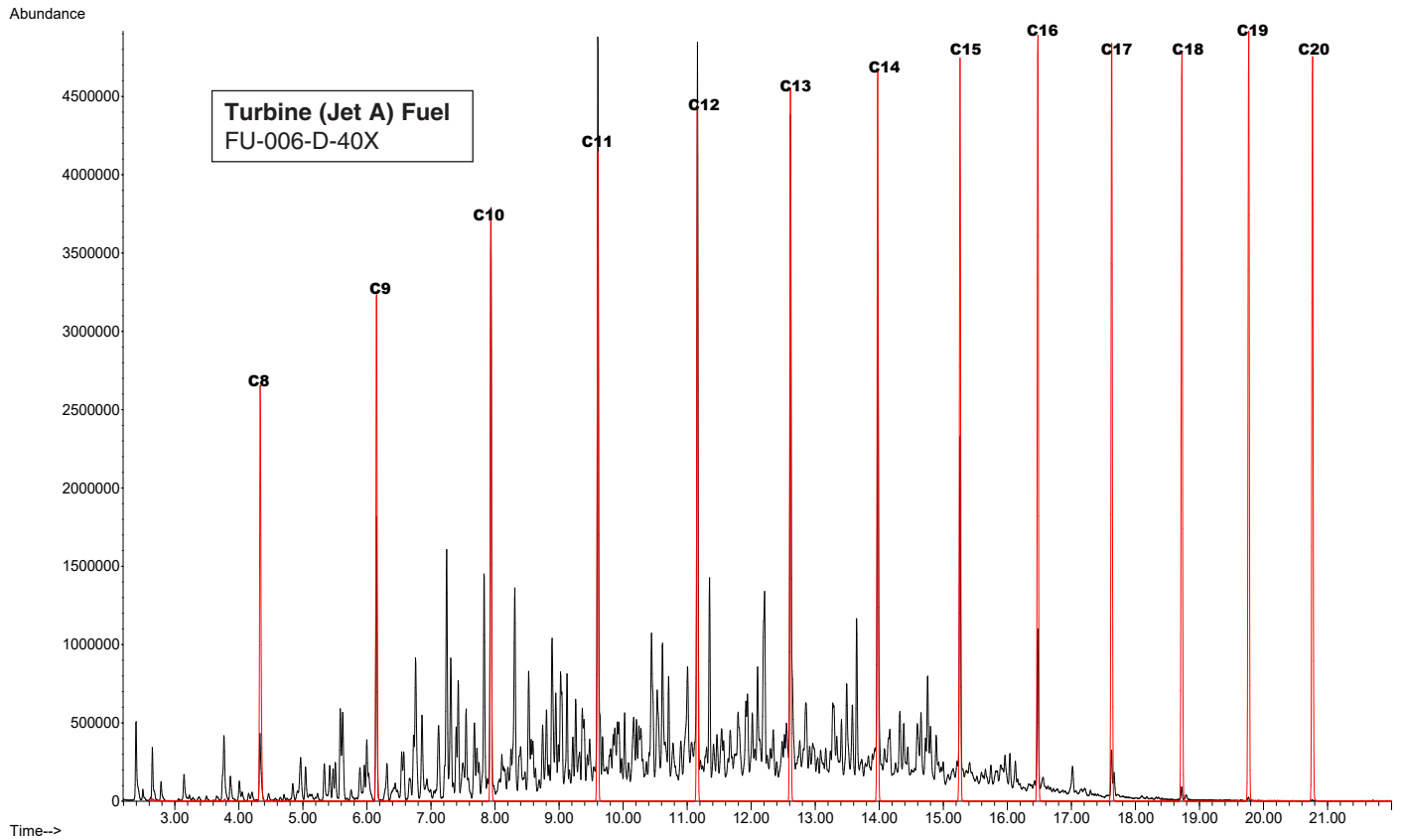
Chromatograms of Aviation Fuels Oils (continued)



Chromatograms of Aviation Fuels Oils (continued)



Chromatograms of Aviation Fuels Oils (continued)



Chromatograms of Household and Industrial Solvents

Household and Industrial Solvents Chromatography

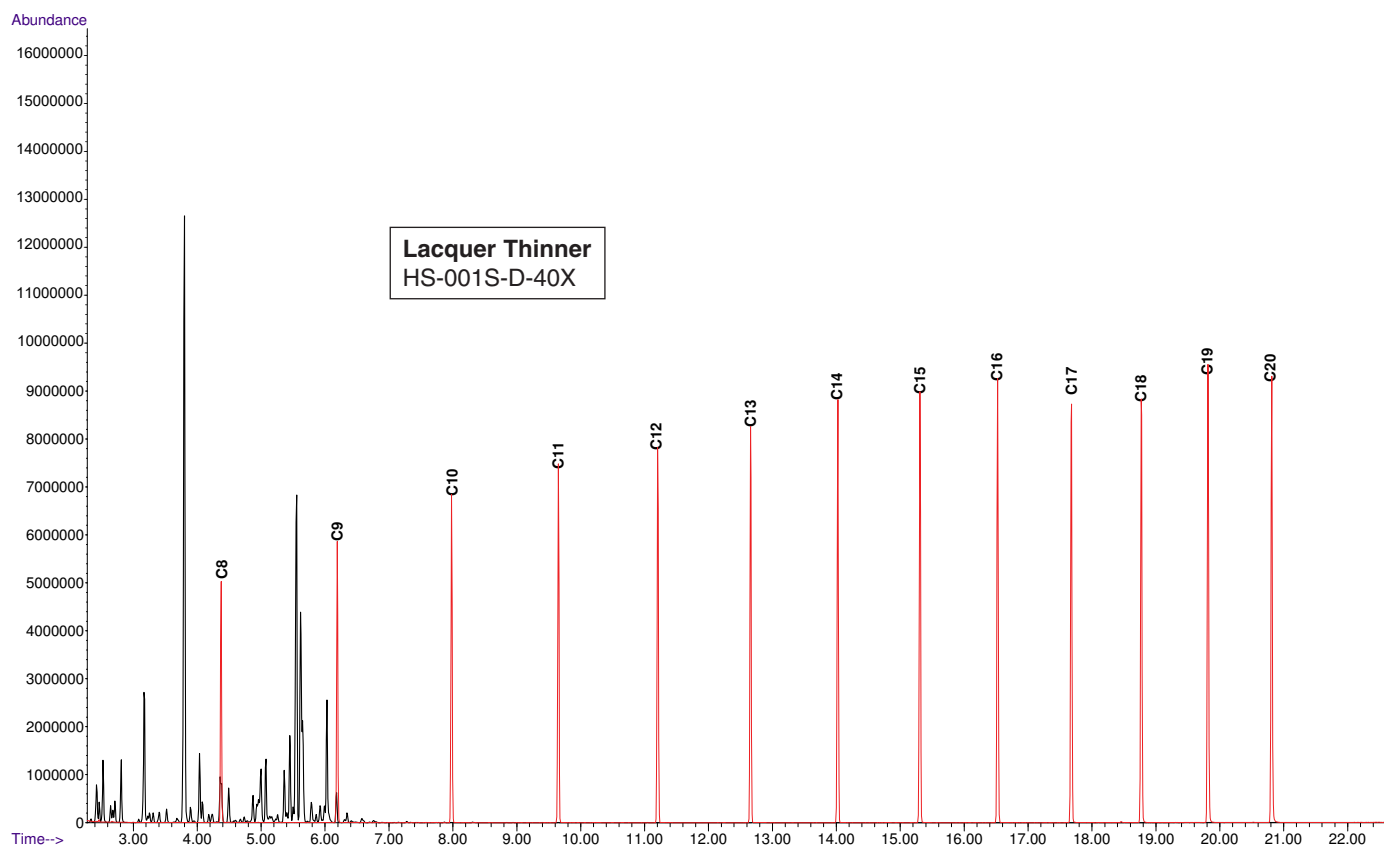
19-21

Lacquer Thinner	19
Mineral Spirits	20
Naphtha	20
Turpentine	21
Stoddard Solvent	21

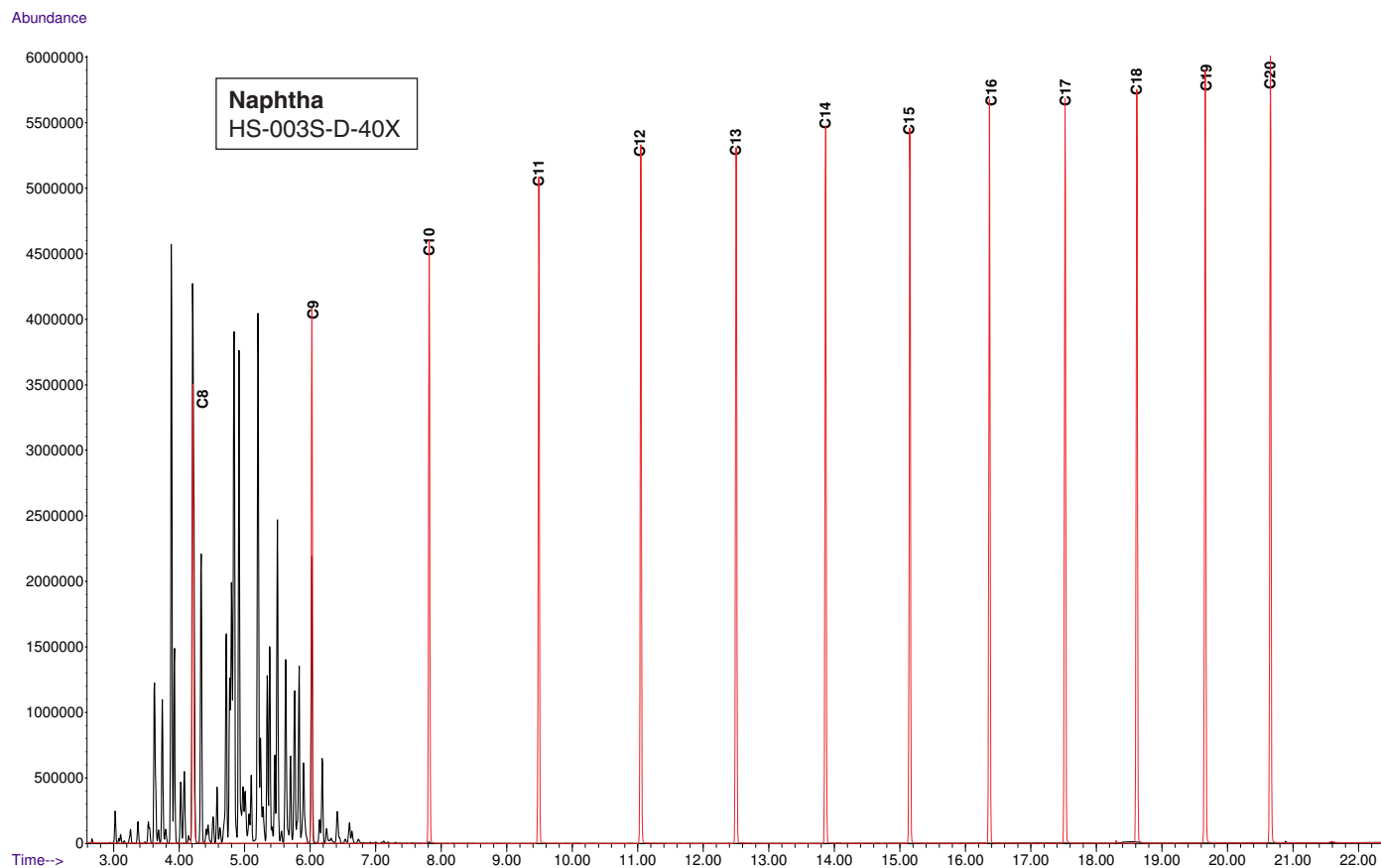
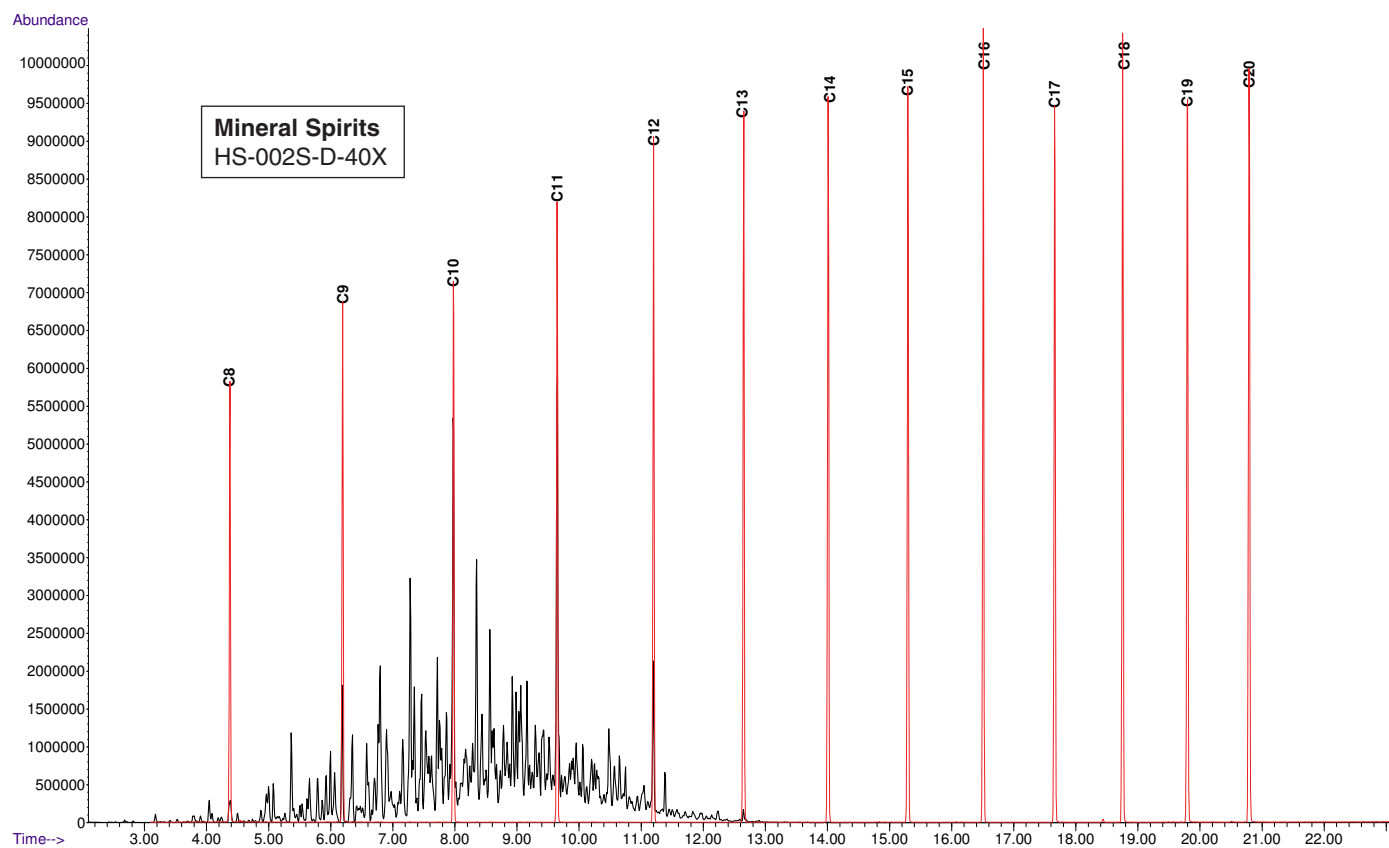
Household and Industrial Solvent Set TPH-004-SET

5 x 1 mL

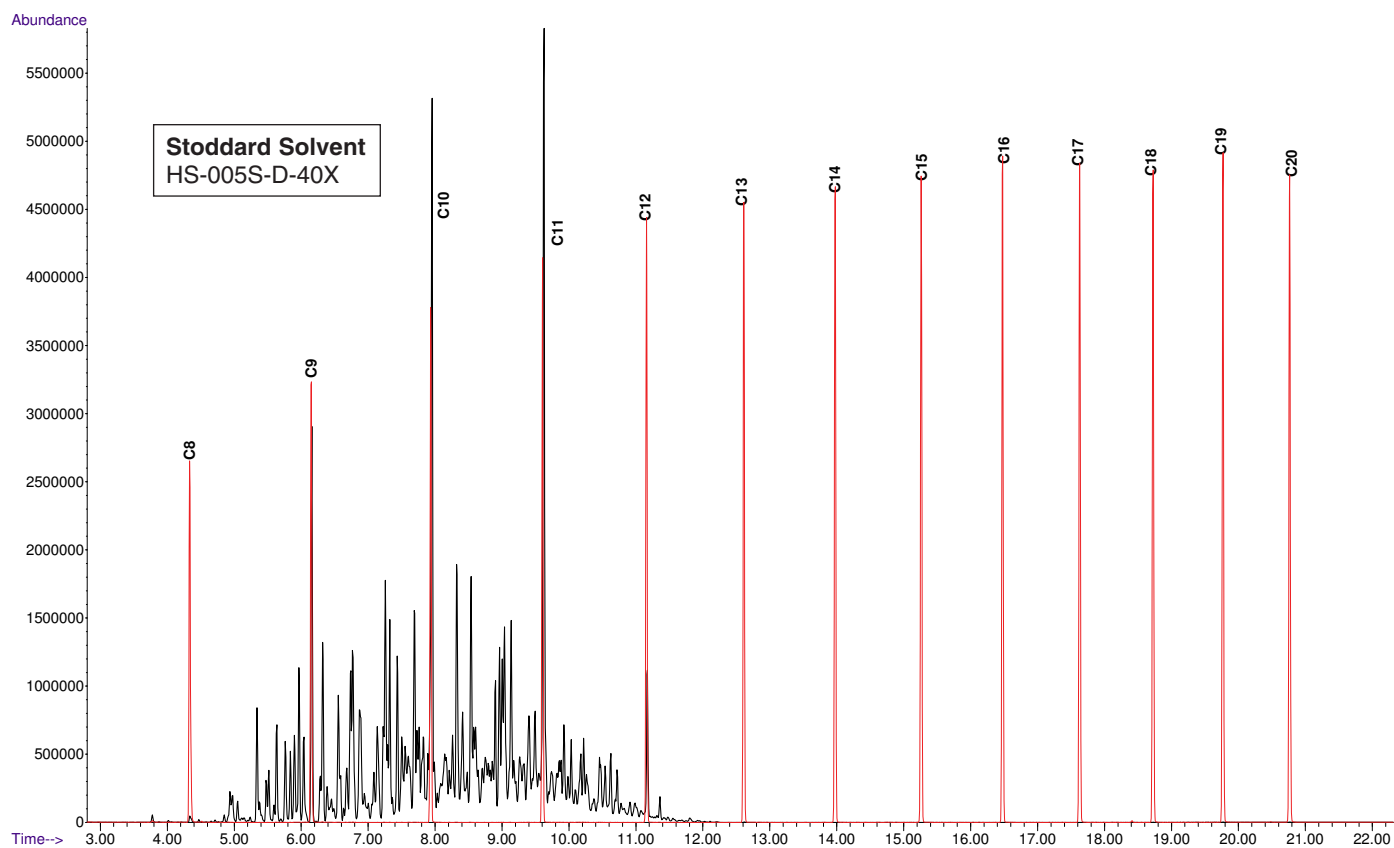
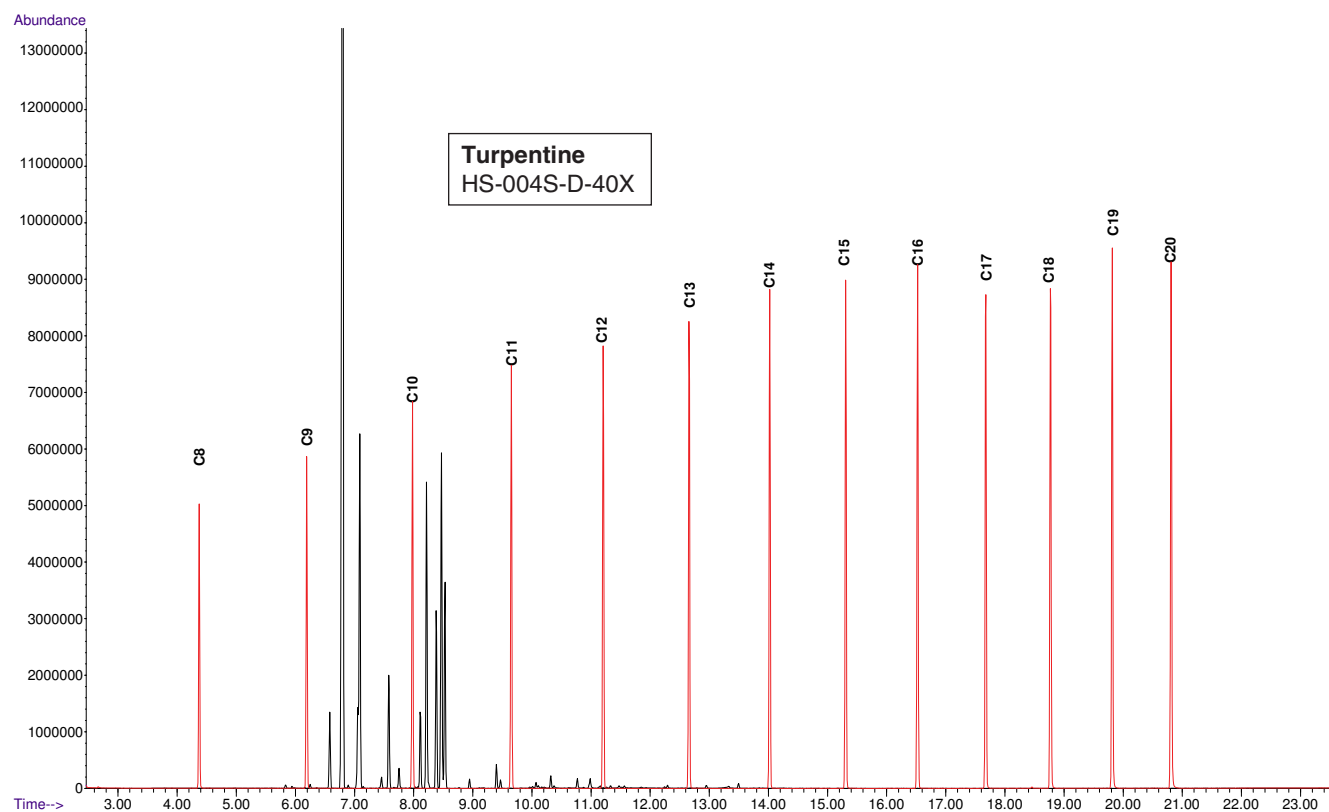
	mg/mL	Solvent	Cat. No.
Lacquer Thinner	20	CH ₂ Cl ₂	HS-001S-D-40X
Mineral Spirits	20	CH ₂ Cl ₂	HS-002S-D-40X
Naphtha	20	CH ₂ Cl ₂	HS-003S-D-40X
Turpentine	20	CH ₂ Cl ₂	HS-004S-D-40X
Stoddard Solvent	20	CH ₂ Cl ₂	HS-005S-D-40X

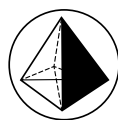


Chromatograms of Household and Industrial Solvents (continued)



Chromatograms of Household and Industrial Solvents (continued)





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