CRC Report No. AVFL-29

ENHANCED SPECIATION OF GASOLINE

Final Report

June 2018

COORDINATING RESEARCH COUNCIL, INC.
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Foreword

This report provides a detailed account of the technical effort undertaken by Joaquin Lubkowitz, Ph.D. and Roberto Meneghini MS.C and the results they produced on behalf of the Coordinating Research Council, Inc. through an agreement with their Advanced/Vehicle/Fuel/Lubricant (AVFL) committee.

The intent of the agreement was for Separation Systems, Inc. to develop an 'enhanced speciation of gasoline method' based on a gas chromatography technique called 'detailed hydrocarbon analysis or DHA and commonly used test method based on it (ASTM D6730-01(2016) to improve the accuracy of the particulate matter (PM) index calculation. The PM Index is a calculation used to determine the contribution of individual hydrocarbons to the formation of particulate matter due to combustion of spark emission fuels.

Dr. Lubkowitz is founder and President of Separation Systems, Inc. (SSI) a small minority owned company located in Gulf Breeze, FL. He's actively participated in ASTM's D02.04 and D02-D subcommittees since 1988 and currently heads the subcommittee D02.04-H (Boiling Point Distribution) a post he's held for the last 12 years. Joaquin received ASTM's prestigious Eagle award for his many contributions to test method development including the pivotal role he played developing DHA test methods including ASTM D6730-01[9].

Roberto Meneghini MS.C holds the position of Principal Software Engineer at Separation Systems. He developed all of the company's software products including Hydrocarbon Expert/MS™ which was used extensively throughout this project.

Preface

The Advanced Vehicle/Fuel/Lubricants Committee (AVFL) of the Coordinating Research Council, Inc. (CRC) publicly issued a request for proposal (RFP) solicitation in June 2016 to private and public companies/organizations deemed with the necessary experience and skills to provide services for the 'enhanced speciation of gasoline'. A number of proposals were evaluated by the Advanced Vehicle Fuel Lubricants Committee (AVFL). The committee decided to choose Separation Systems, Inc. A formal agreement was executed in November 2016.

This report provides a detailed account of the technical efforts undertaken by Separation Systems and the results.

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List of Acronyms and/or Abbreviations

ASTM – American Society for Testing and Materials (a leading international standards organization located in Conshohocken, PA)

AVFL – 29 – Advanced Vehicle/Fuel/Lubricants – of the CRC committee sponsoring this work

CFT – capillary flow technology (sometimes referred to as microfluidics)

CRC – Coordinating Research Council, Inc. (Alpharetta, GA)

DHA – detailed hydrocarbon analysis

D6730-01 (2016) – an ASTM test method entitled "Determination of Individual Components in Spark Ignition Engine Fuels by 100 Meter Capillary (with Pre-Column) High Resolution Gas Chromatography"

EI – electron ionization (type of energy produced in the ion source of a mass spectrometer to fragment components and produce mass spectra)

FID – Flame ionization detector (most commonly used gas chromatography detector; provides linear response to hydrocarbon components)

GC – gas chromatograph, gas chromatography

GC-MS – gas chromatography system in which the effluent of the analytical column flows into a mass spectrometer and components detected

GC-FID/MS – A gas chromatography system in which the effluent from the analytical column is split and directed to FID and MS detectors simultaneously.

HCDX – A retention time/component name 'template' (database) produced by Hydrocarbon Expert™ software. The template is used to identify individual components on the basis of their retention time and retention index. Newly named components are added to the template.

MS – Mass spectrometer, mass spectrometry

MSD – Mass Selective Detector is a single quadrupole mass spectrometer specifically designed for use as a gas chromatography detector. It utilizes electron ionization energy to fragment components separated by the GC column and emanating from it. It can be used in conjunction with a traditional flame ionization detector to identify and quantify individual compounds based on retention time, selected characteristic ions and/or a component's mass (m/z) spectrum. The latter is achieved by using a proprietary software search algorithm to compare the compound's mass spectrum to a comprehensive database/library containing 260,000+ mass spectra to produce probability based matches or through manual examination of the spectrum itself to look for characteristic features (ex. prominent ions and their relative abundance relative to each other).

M/Z – the mass of an ion (Daltons) divided by its charge

PCM – Pressure Control Module - A device used to control gas flow and/or pressure) in a gas chromatograph.

PDMS – polydimethylsiloxane - A non-polar silicone based polymer used in wall coated open tubular (WCOT) gas phase chromatography columns (including the 100 M column(s) used in this project).

PIONA – paraffins, iso-paraffins, olefins, naphthenes and aromatics - An acronym commonly used to describe the GC analysis of hydrocarbons by group type.

PM – Particulate Matter

PMI – Particulate Matter Index

RI – Retention Index; The retention time of an individual hydrocarbon component normalized to the retention times of components eluting before and after it.

SSI – Separation Systems, Inc.

Executive Summary

The goal of the project (AVFL-29) was to develop enhanced speciation of gasoline analysis methodology based on a gas chromatography analysis technique called DHA (detailed hydrocarbon analysis) and a current test method utilizing it (ASTM D6730-01(2016)) to reduce the number of 'unidentified' components typically found (5 wt% or greater) to < 0.5 wt%. A reduction of such magnitude would improve the accuracy of the particulate matter index (PMI) calculation.

In order to achieve this goal, a number of discrete 'research' and 'method development' tasks were undertaken. All of which focused on identifying as many previously unidentified hydrocarbon components as possible through the use of GC-MS. Five (5) gasoline samples were provided by CRC and used to assess progress toward meeting the goal during the course of the project.

Two instrumental systems were used to conduct the study: (1) the 'research system' consisting of a gas chromatograph equipped flame ionization detector (FID) and mass selective detector (MSD) and (2) 'the D6730 system' consisting of a gas chromatograph equipped with a single FID. Both systems were configured in accordance with ASTM D6730-01(2016)

Over 200 individual hydrocarbon components were added to a compound list as it existed at the start of the project including many with boiling points greater than 1-methylnaphthalene which is the last identified compound cited in the ASTM method. The identity of methyl and ethyl substituted naphthalenes were confirmed by preparing individual standards from pure compounds obtained from commercial suppliers and subjecting them to GC-MS analysis and review. Note: a table listing all of the compounds used in this project can be found in Appendix C. The table contains the identity (name), retention time and retention index of 860 compounds. Note, the detailed results including physical characteristics are available in MS Excel format and forwarded to the CRC committee along with the final report.

The addition of more heavy compounds to the compound list produced higher calculated PMI values for all six gasoline samples analyzed in this study. Comparison of PMI calculated before and after addition of these compounds shows increases in PMI ranging from 2 to 29%.

Each sample analysis file contains between 300 and 450 compounds identified from the base list of 860 compounds which required properly 'managing' retention time and retention indices data for ~5,400 compounds identified across the 6 samples analyzed in this project. Due to the large number of component verifications from sample to sample, it was necessary to develop software programs to check the correct identification and consistent location with respect to retention time. This was needed to ensure the identity of a compound previously identified via MS was consistent with the physical and chemical properties of the component eluting immediately before and after it. To the best of our knowledge the use of such an approach is unprecedented.

In addition to the work described above, boiling points and vapor pressure values for all of the individually identified compounds (before the project started as well as the new ones identified as a result of the project) were added[1]). The ability to calculate the particulate matter index for

the five CRC provided gasoline samples or any comparable sample type was added to the Hydrocarbon Expert™ (version 5) software.

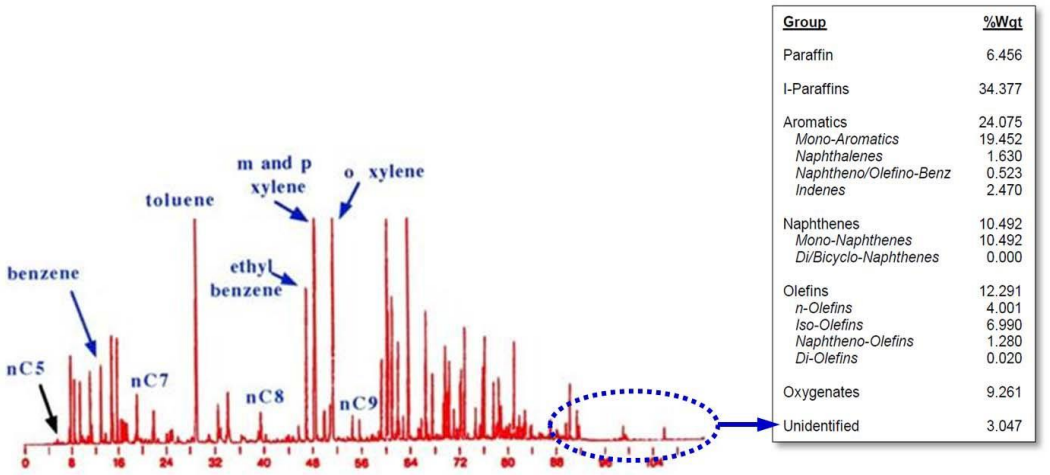
An enhanced retention time/component database was produced which can be used to analyze gasolines and identify 99.5% or greater of the individual components contained in them as well as calculate their respective PMI values. Any of the samples analyzed during this project are suitable for use as a reference material for the enhanced method.

Background [A]

The USEPA, Honda and others have confirmed that the particulate matter Index (PMI) can reasonably predict the relative particulate forming tendency of a gasoline.[2,3,4,5,6] The PMI is a function of the vapor pressure, double bond equivalent (DBE) and concentration of each component in the fuel. Therefore, the accuracy of the PMI is directly related to the accuracy of the analytical method used to separate and quantify the individual components.

Detailed hydrocarbon analysis (DHA) is typically used for this purpose. There are several DHA test methods available of which ASTM D6730-01(2016)[9] is frequently used for gasolines. This gas chromatography based test method is used to identify an individual hydrocarbon compound based on its retention time and retention index and uses the identity to categorize the compound by hydrocarbon group type (ex. paraffins, isoparaffins, aromatics, naphthenes). Unfortunately, many compounds are not identified by this test method, especially those eluting late in the chromatogram or compounds poorly resolved from each other. Even highly skilled labs leave 5% (or greater) of the species unidentified.

Given that many of the components eluting late in the chromatogram can have a substantial contribution to PMI, unidentified or misidentified peaks in this region can result in an inaccurate PMI determination. (See figures below.)



Group	%Wgt
Paraffin	6.456
I-Paraffins	34.377
Aromatics	24.075
Mono-Aromatics	19.452
Naphthalenes	1.630
Naphtheno/Olefino-Benz	0.523
Indenes	2.470
Naphthenes	10.492
Mono-Naphthenes	10.492
Di/Bicyclo-Naphthenes	0.000
Olefins	12.291
n-Olefins	4.001
Iso-Olefins	6.990
Naphtheno-Olefins	1.280
Di-Olefins	0.020
Oxygenates	9.261
Unidentified	3.047

$$PM\ Index = \sum_{i=1}^{n}\left(\frac{DBE_i + 1}{V.P(443K)_i} \times Wt_i\right)$$

- For a constant concentration and vapor pressure, the PM Index factor becomes directly proportional to the DBE term.
- Therefore, if an alkane were to be misidentified as an aromatic, the PM Index factor assigned to that species could be as much as **10x** too high.

	VP (kPa)	DBE*	PMI Factor
n-tetradecane	10.3	0	0.0971
biphenyl	9.87	8	0.912

*DBE = (2C+2-H+N)/2

Note A - The narrative and diagrams on this page courtesy of Coordinating Research Council; Advanced Vehicle Fuels and Lubricants Committee 'Enhanced Speciation of Gasoline' RFP document (Page 3) (June 2016)

Project Objective

The objective of this project was to develop enhanced methodology for the speciation of gasoline based on ASTM D6730-01(2016). Once developed, the methodology would be presented to an appropriate ASTM subcommittee to garner interest and support to develop it into a formal method, conduct an inter-laboratory study ('round robin') to determine precision and bias, obtain approval through balloting process and then be published as an official test method or, more likely, an addendum to ASTM D6730.

Desired attributes of the method:

- It should be capable of being used on a routine basis by a typical chemical analysis laboratory with personnel who possess a fundamental understanding of the theory and practice of high-resolution capillary gas chromatography and prior experience using the DHA technique.
- It should be easy to perform both qualitative and quantitative calibrations. The GC detector used should exhibit a linear response to hydrocarbons to minimize the number of components required in the calibration standard.
- It should produce an accurate quantification of oxygenated components.
- It should be able to separate, identify, and quantify individual hydrocarbon components including isomers to the greatest extent possible. The minimum identification requirements for each component are the compound class it belongs to and its carbon number. At a minimum, 99.5 wt% of the sample must be identified by name or compound class and carbon number.
- It should provide the actual or estimated boiling point for all species.
- It should be capable of quantifying hydrocarbon species with boiling points up to 280°C.

What is detailed hydrocarbon analysis (DHA)?

Detailed hydrocarbon analysis (DHA) utilizes ultra-high resolution capillary gas chromatography to separate and detect individual hydrocarbon components in light hydrocarbon streams. These streams include: virgin naphtha, alkylates, FCC gasoline, gasoline (including oxygenate additives ex. ethanol), reformate with a boiling range up to 225°C. Once separated and detected, individual components are identified by using their retention time to calculate a retention index and comparing it to values found in authoritative sources (ex. Kovats, NIST).

Unlike simulated distillation or 'PIONA' type test methods which only provide summary information such as the boiling point distribution or content characterization by hydrocarbon group type (paraffins, isoparaffins, olefins, naphthenes, aromatics, oxygenates etc.) DHA is the method of choice if individual components must also be identified.

However, DHA has a key shortcoming. It is very difficult to identify a component with a high degree of certainty if it isn't in the reference material used to calibrate the system or its retention index value isn't listed in the peak table/component database the application software (ex. Hydrocarbon Expert) uses to identify the individual components. This is especially problematic when peaks in close proximity to each other are not fully separated (co-eluting species).

Analysts confronted with the need to identify unknown components in gas chromatography increasingly turn to mass spectrometry (MS) detection for help.

MS is used in DHA as a complementary detector to the FID to identify unknown components and co-eluting species. In order to employ MS for DHA analysis, a column identical to the one used for the GC-FID analysis must be installed in the GC-MS system and two separate analysis conducted. Analysts who do this are confronted with the onerous task of transferring information produced by the GC-MS system to the data analysis software utilized by the GC-FID data system. Transferring data is necessary because quantitation using a FID is inherently more reliable and convenient than MS. Data transfer is especially problematic if the GC and GC-MS systems are from different instrument manufacturers. Although the columns used in the GC-FID and GC-MS can be the same (manufacturer, same type, part number etc.), they aren't exactly identical. Subtle differences exist because of the process used to fabricate the column (ex. phase bonding) or due to the wear and tear of repetitive analyses (column ageing). Either or both can produce different retention times from column to column or shifting retention times that must be reconciled before peak identification can be attempted. All of this serves to undermine the ability to utilize the information produced by both systems to identify unknowns or co-eluting peaks. Even if the column effluent from a single column is split between the MS and the FID, the user is usually faced with the challenge of using three separate software systems; one for MS data acquisition and spectral review software, one for GC (FID) data acquisition and DHA software to process detector signals to analyze, assign group type and quantify the final results. Adding to the challenge, GC data handling software is not well designed to process the 400+ peaks typically produced per sample using the DHA technique.

To address DHA's shortcomings, Separation Systems, Inc. improved the technology in two important ways. First, it developed a special software module for use with its Hydrocarbon Expert™ (DHA) software to allow GC-MS and GC-FID signal information to be automatically acquired and simultaneously processed within the same software environment.[8,9,10,11,12] See Figure 1.

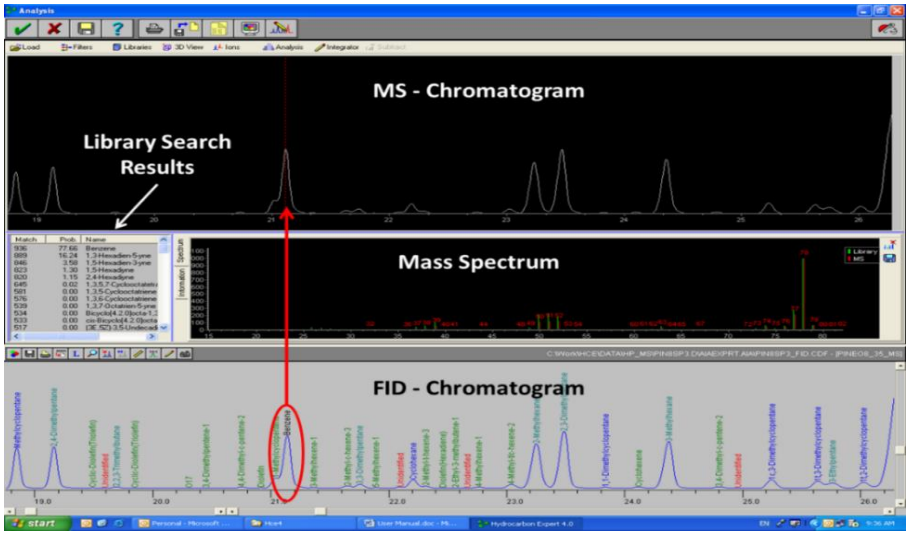


Figure 1 - Hydrocarbon Expert™ with MS software module –workflow integration of GC-FID and MS

The Hydrocarbon Expert™ MS software module made it practical and straightforward for users with a moderate level of GC skill to use both analytical techniques to overcome the inherent limitations of DHA methods.

Second, the company configured, tested and optimized a microfluidic device (Agilent Technologies capillary flow technology (CFT) and SGE's SilFlow™) through which the effluent of the single ultra-high resolution capillary column can be proportionally directed to both the MS and FID simultaneously. See Figure 2.

These tasks resulted in a GC-FID/MS hardware/software system by which a single sample injection will simultaneously produce FID and MS data so unknown components can be identified and easily added to the DHA peak ID/retention timetable.

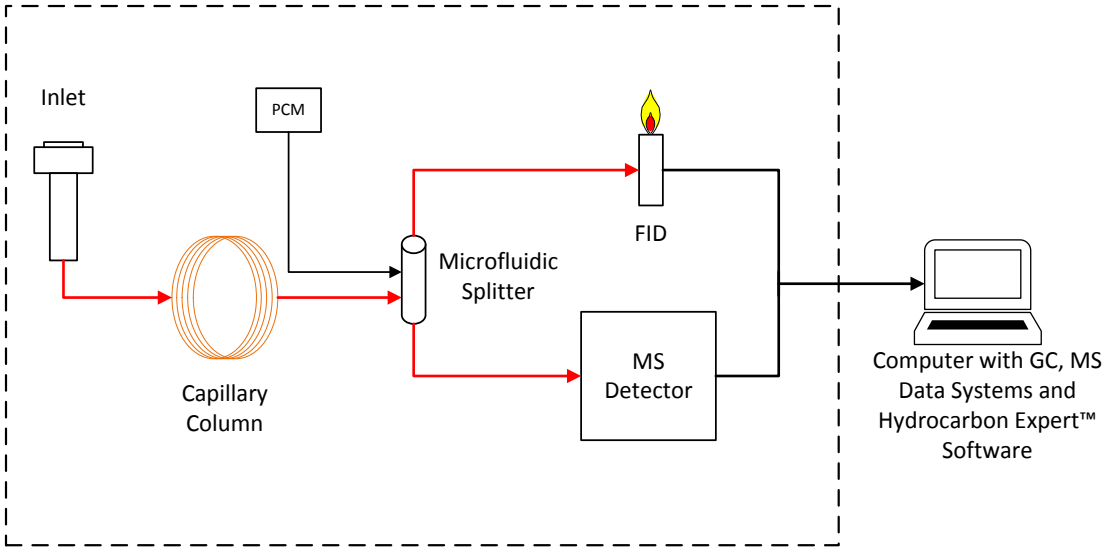


Figure 2 - Flow Schematic of GC-FID/MS System Used for DHA and Unknown Peak Identification

Commercial DHA-FID/MS systems have been successfully used to analyze gasolines as well as other refining streams such as virgin naphtha, alkylates, reformer feed and reformate.

Project Approach

The project consisted of two phases; each with a number of discrete tasks.

Phase One [The 'Research' Phase]

- Analyze gasoline sample(s) provided by CRC in the manner similar to samples sent by the USEPA to SSI (Summer 2016) to use the GC-FID/MS technique to identify unknown compounds. Then use the results to establish a starting point or baseline to assess method development progress during the course of the project.
- Adjust the post-column capillary microfluidic splitter to increase the amount of effluent flowing into the mass spectrometer to increase the signal for components eluting after C10 improving the quality of the spectra produced (ex. increased ion intensities). This was deemed necessary to enhance the ability to identify individual peaks by name using the NIST MS library search algorithm (more definitive search results) and/or via manual review.
- Purchase alkyl substituted naphthalene compounds and prepare individual liquid standards. Analyze the standards by GC-FID/MS and use retention time matching and MS spectra review to confirm identifications previously made. Extend the chromatographic conditions (oven temperature) if need be to identify components with retention times greater than 1-methylnaphthalene. Naphthalene response factors were to be measured and compared to the theoretical response factors.

Phase Two [Developing a Test Method for 'the Enhanced Speciation of Gasoline']

- Using the data/information obtained in Phase 1, produce and refine an 'extended' individual peak table (database) including: retention time, retention indices, group type, carbon number, component name and CAS#. The table will enable anyone with prior experience running the D6730-01(2016) test method and using DHA application software to produce data suitable for use in calculating the PMI via the 'Enhanced Speciation of Gasolines' method. The table will be included in the method.
- Create a special retention time/component database template (HCDX) containing all of the newly identified compounds as well as boiling point and vapor pressure values for each. The HCDX will enable users with Separation Systems' Hydrocarbon Expert™ software to utilize the 'Enhanced Speciation of Gasolines' method to produce more accurate PMI results.
- Produce a reference material for the 'enhanced speciation of gasoline' method.
- Modify SSI's Hydrocarbon Expert™v5 software to produce an estimated boiling point for components identified by group type and carbon number.
- Write an 'Enhanced Speciation of Gasolines' test method utilizing all of the information derived from the tasks above. The method should include required equipment/apparatus, reagents/materials, instrumental setup procedure and operating parameters, system calibration procedure(s), data evaluation criteria and relevant detailed information about the hydrocarbons that can be analyzed using the method.

Equipment and Method Parameters Used for the Project

The GC-MS/FID analysis work was conducted using an Agilent 7890B GC and 5977A MSD; (henceforth referred to as the 'Research System').

Figure 3 - 'Research System' (GC-FID/MSD)

The 'Research System' was comprised of an Agilent 7890B gas chromatograph configured with a split/splitless capillary inlet equipped with a focus liner with fixed immovable glass wool (Separation Systems), single pre-column coupled to a ultra-high resolution capillary column, flame ionization detector, pressure control module (PCM) with CFT (capillary flow technology) based effluent splitter, FID, MS interface and MS detector (MSD). A detailed schematic diagram of this system can be found in Figure 4. A more detailed description of the instrumental components/parts used are in Table 1. Operational parameters are in Table 2.

An additional 'standalone' GC-FID system (henceforth referred to as the 'D6730 System') was used to verify identifications and results. The D6730 system was comprised of an Agilent 6890 GC configured with an inlet/liner and pre-column/analytical column set identical to the one used in the Research System and FID detector. A more detailed description of the instrumental components/parts used can be found in Table 3. The operational parameters used for the D6730 system are in Table 4. Note**:** The operational parameters used with the D6730 system are slightly different from those used in the Research System. **These parameters should be used to replicate the final results obtained in this study.**

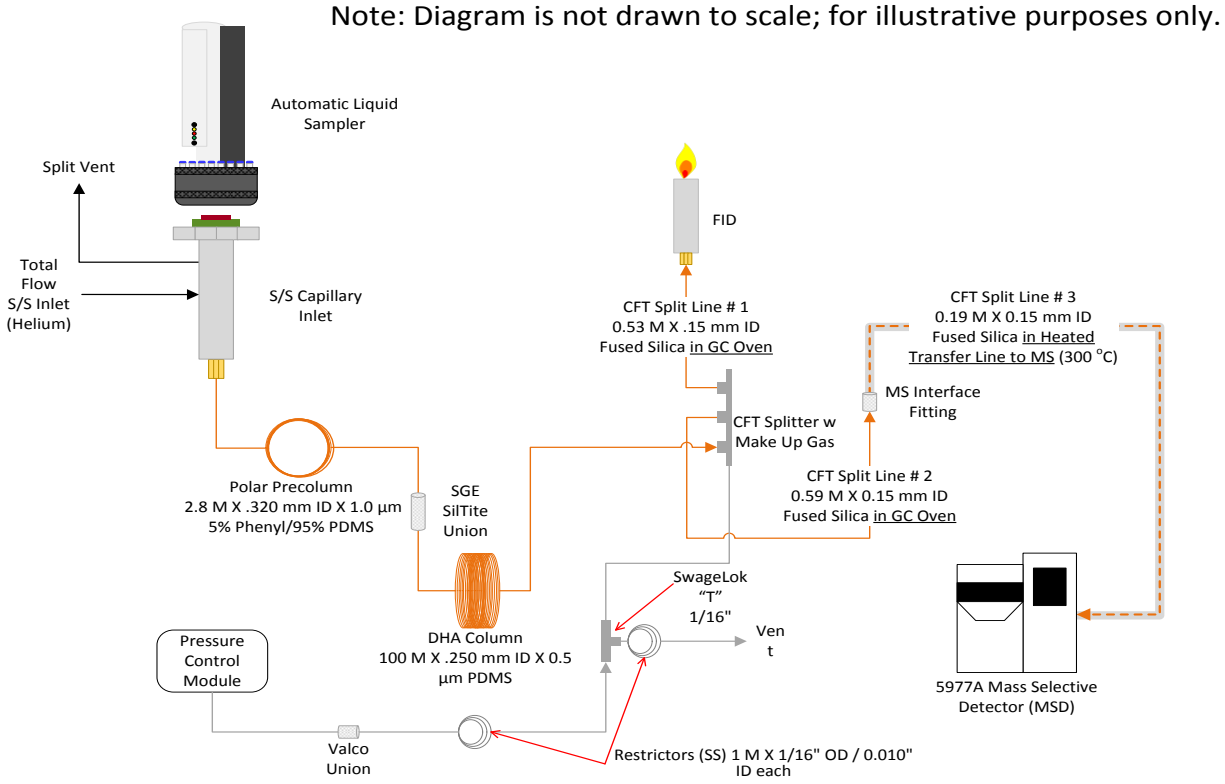


Figure 4 - Schematic of the Research System (GC-FID/MSD)

Table 1 – System Components Used – 'Research System'

Component Description	Supplier	Part Number
7890B gas chromatograph with S/S capillary inlet, (glass liner with non-movable glass wool; Separation Systems, Inc. P/N SS-035-05), flame ionization detector, pressure control module, MS interface	Agilent	G3440B
Pre-column; 2.8 M X 0.25 mm X 1.0 µm X 5% Diphenyl / 95% PDSX	Restek	10196
Analytical column; 100 M X 0.25 mm X 0.5µm-PDMS	Agilent	122-10A6
CFT splitter – 2 way (purged)	Agilent	G3180B
5977A mass selective detector	Agilent	G7076B
7693 automated liquid sampler, injector	Agilent	G4513A
SilTite® Union	SGE	073566
Excel Macro for split calculation	Agilent	G3180B-xls
Deactivated silica tubing; 5M X 0.15 mm ID	Agilent	160-7625-5
SS tubing; 5M X 1/16 inch OD X 0.005-inch ID	Valco	SS-15-005

Table 2 - Operational parameters - 'Research System'

Inlet Temperature = 300 ºC
Inlet Pressure = 40.921 PSI (Constant Pressure Mode)
Transfer line temperature = 300 ºC
PCM flow = 3.6 mL/min
PCM Pressure = 12 psi
'Column 1' = (Pre-column + analytical column) = 102.8 m X 0.25 mm X 0.5µm
'Column 1' flow = 1.78 mL/min at 35 ºC
Split Line #1 (from CFT splitter to FID); 0.59 M X 0.15mm
Split Line #2 (from CFT splitter to MS interface fitting); 0.19 M X 0.15 mm
Split Line #3 (from MS interface fitting to MSD ion source); 0.59 M
Initial MSD vacuum = $1X10^{-5}$ Torr
MSD tuning via 'Autotune' routine
Injection volume 0.5 µL
Split Ratio: 95:1
Initial oven temperature = 5 ºC then hold 10 min
Oven temperature program ramp 1 = 5 ºC/min to 50 ºC then hold 50 min
Oven temperature program 2 = 1.5 ºC/min to 200 ºC then hold 5 min
Oven temperature program ramp 3 = 10 ºC/min to 300 ºC then (final) hold 5 min
FID Temperature = 325 ºC
Air (Zero grade) flow rate = 400 mL/min
H2 (99.9995%) flow rate = 40 mL/min

Table 3 – System Components Used – 'D6730 System'

Component Description	**Supplier**	**Part Number**
6890N gas chromatograph with S/S capillary inlet, (glass liner with non-movable glass wool; Separation Systems; P/N SS-035-05), flame ionization detector, pressure control module, MS interface	Agilent	G3440B
Pre-column; 2.8 M X 0.25 mm X 1.0 µm X 5% Diphenyl / 95%PDSX	Restek	10196
Analytical column; 100 M X 0.2 5mm X 0.5µm-PDMS	Agilent	122-10A6
7693 automated liquid sampler, injector	Agilent	G4513A
SilTite® Union	SGE	073566
SS tubing; 5M X 1/16 inch OD X 0.005-inch ID	Valco	SS-15-005

Table 4 - Operational parameters for 'D6730 System'

Inlet temperature = 300 ºC
Inlet pressure = 45.921 psi Constant Pressure
Retention time methane at 35 ºC is 7.00 min ±0.05 min
Injection volume = 0.5 µL
Split Ratio = 125:1
Initial oven temperature = 5 ºC then hold 10 min
Oven temperature program ramp 1 = 5 ºC/min to 50 ºC then hold 50 min
Oven temperature program ramp 2 = 1.5 ºC/min to 200 ºC then hold 5 min

Table 4 - Operational parameters for 'D6730 System' (Continued)

Oven temperature program ramp 3 = 10 ºC/min to 300 ºC then hold 5 min
FID = 325 ºC
Air (Zero grade) flow rate = 400 mL/min
H2 (99.9995%) flow rate = 40 mL/min

Chemicals, Reagents and Standards

The following chemicals were purchased to verify the identities of alkyl substituted naphthalenes: (Sources = Sigma Aldrich/ St. Louis MO, Alpha Easar/Tewksbury, MA, Fisher Scientific/San Francisco, CA and Glentham Sciences/Wiltshire, United Kingdom):

1-Methylnaphthalene (95% pure)

2,6-Dimethylnaphthalene (99% pure)

2,7-Dimethylnaphthalene (99% pure)

1,3-Dimethylnaphthalene (96% pure)

1,7-Dimethylnaphthalene (99% pure)

1,6-Dimethylnaphthalene (99% pure)

1,4-Dimethylnaphthalene (95% pure)

2,3-Dimethylnaphthalene (97% pure)

1,5-Dimethylnaphthalene (98% pure)

1,2-Dimethylnaphthalene (95% pure)

1,8-Dimethylnaphthalene (95% pure)

1-Ethylnaphthalene (99% pure)

2-Ethylnapthalene (99% pure)

2,6-Diethylnaphthalene (99% pure)

1,4,6,7-Tetramethylnaphthalene (95% pure)

2,3,5-Trimethylnaphthalene (95% pure)

The compounds were individually dissolved in methanol (Fisher Scientific; Methanol Optima® LC/GC 99.98%) to produce concentrations ranging from 0.15 - 0.18% by weight and then used to determine the response factors for analysis.

Note: Due to their toxicity, use extreme caution handling naphthalene compounds.

The paraffins n-tridecane, n-tetradecane, n-pentadecane, n-hexadecane and n-heptadecane (Sigma Aldrich, St. Louis, MO) were used to confirm/validate retention times and retention index values. In order to bracket the retention indices, two dilutions were prepared for each paraffin. First, each paraffin was dissolved in an equal volume of isooctane solvent (Sigma Aldrich, St. Louis, MO). Then 10 µL of the mixture prepared in the first step was added to 2.0 mL of isooctane.

Five gasoline samples representative of commercially available gasolines were obtained from the CRC AVFL-29 committee and labeled CRC#1 through CRC#5. Two of them contain oxygenates. (ethanol in CRC#3 and methyl-*t*-butyl-ether in CRC#4). Additionally, a reference material was prepared by Separation Systems (SD-053-040617ES). It was derived from a gasoline in which alkylate and a mixture of n-paraffins was added. The reference material was sent to Bill Cannella (Chevron) to distribute to CRC members during the course of the project.

Software

Mass Hunter [Agilent Technologies; Version = B07.05.2749 - August 23, 2016] was used to operate the Research System and acquire MS spectra. OpenLab GC Chemstation software [Agilent Technologies; Version = C01.05] was used to acquire the signal produced by the D6730 system. Signal files produced by the OpenLab GC Chemstation software were processed using Hydrocarbon Expert™ [Separation Systems, Inc.; Version = 5.20] which was also used to integrate individual peak areas. The Hydrocarbon Expert™ MS module was used to select and evaluate the MS spectra produced by the Research System by importing the ions from the Mass Hunter software.

All the published response factors listed in ASTM D6730 were used. Some of the response factors for naphthalene compounds were separately determined. (see Naphthalene section).

Results and Discussion

Results and discussion are separated into the following sections:

1. Naphthalene Investigation
2. GC Signal Integration
3. Using a Mass Selective Detector to Identify Sample Components
4. Identifying Components That Yield 'Inconclusive' Results from the NIST Library Search
5. Verifying the Integrity of Component Identifications Final Analysis (Summary by Group Type)
6. Reports for the CRC gasoline samples (CRC#1-5).

Naphthalene Investigation

The results for the analysis of the gasoline samples conducted during the project and as described in the monthly reports were extensively scrutinized. We found that the elution order of naphthalenes to be more complex than previously thought. This is largely attributable to incomplete separation (co-elution) of four di-substituted methylnaphthalenes.

Response factors (in parentheses) were experimentally measured in duplicate for 1-methylnaphthalene (0.8944), 1-ethylnaphthalene (0.8996), 1,3-dimethylnaphthalene (0.8956) and 2,6-diethylnaphthalene (0.8967). Note, the values are lower (6.7% vs. 7.1 %) than the values contained in ASTM D6730 (Table 3). However, all calculations in this report use response factors listed in ASTM D6730.

Table 5 - Retention Indices of Alkyl Substituted Naphthalenes

Naphthalene Component Name	RT, Min	Carbon #	Research Sys RI	D6730 Sys RI	Δ
1-Methylnaphthalene	150.074	13	1304.268	1304.542	-0.274
1-Ethylnaphthalene	158.684	13	1390.250	1390.339	-0.089
2-Ethylnaphthalene	158.923	13	1392.570	1392.824	-0.254
2,6-Dimethylnaphthalene	159.812	14	1401.332	1401.411	-0.079
2,7-Dimethylnaphthalene	159.988	14	1403.268	1403.201	-0.067
1,3-Dimethylnaphthalene	161.293	14	1417.557	1417.559	-0.002
1,7-Dimethylnaphthalene	161.293	14	1417.557	1417.692	-0.135
1,6-Dimethylnaphthalene	161.652	14	1421.468	1421.537	-0.069
1,4-Dimethylnaphthalene	163.264	14	1438.921	1438.886	0.035
2,3-Dimethylnaphthalene	163.264	14	1438.921	1439.160	-0.239
1,5-Dimethylnaphthalene	163.509	14	1441.558	1441.832	-0.274
1,2-Dimethylnaphthalene	164.708	14	1454.409	1454.710	-0.301
1,8-Dimethylnaphthalene	166.549	14	1473.960	1474.353	-0.393
2,3,5-Trimethylnaphthalene	175.197	15	1572.339	1570.748	1.590
2,6-Diethylnaphthalene	177.898	16	1604.361	1606.181	-1.821
1,4,6,7-Tetramethylnaphthalene	183.895	16	1694.533	1694.847	-0.314

We studied the retention indices produced by both the 'Research System' and 'D6730 system'. The retention indices obtained varied between the two systems. We attribute to subtle differences in column flow between the Research System (in which the column outlet is at MS vacuum pressure) and the D6730 GC in which the detector outlet is at atmospheric pressure. The retention indices (Kovats-n-alkanes indices) obtained by the Research System and D6730 System are shown in Table 5.

Note the good agreement of the retention indices produced by both systems. However, the presence of co-eluting compounds (1,3-dimethylnaphthalene and 1,7-dimethylnaphthalene) forced us to reevaluate earlier data. Co-elution is evident from the retention indices values for both compounds; which are the same.

The retention indices for the co-eluting pairs are the same for the Research System but differ slightly for the D6730 system. Also, 1,4-dimethylnaphthalene and 2,3-dimethylnaphthalene co-elute and cannot be resolved further using the 10 ºC/min ramp necessary to elute all of the compounds from the column. No effort was made to change the ramp at this oven temperature to see if further resolution would be possible. We also observed that the relative separation of the isomers is not as much in the Research System compared to the D6730 system.

It is important to note that dimethylnaphthalene compounds are found in almost all crude oils.[12] The most prominent being 1,8-dimethylnaphthalene. Methylnaphthalene content is a geochemical indicator of crude oil maturity. However, this is the only isomer not found in any of the samples. We suspect the absence is probably due to removal during the refining process.

We used pure compounds to elucidate the elution order. We found it relatively easy to single out the individual naphthalenes by selectively monitoring ions (m/z) 115,141,142. However, it is not possible to distinguish isomers if concentrations are < 0.05 wt%.

The characteristic ions (m/z) are present in all di-alkyl-naphthalenes and vary only in small relative intensities. The MS spectral identification software (NIST) relies on the difference in the ion ratios for the masses shown above. This ratio is cannot be reliably assigned to the correct isomer and it is because of this that neat standards were used for identification. It is apparent that some of the identifications reported in literature[7,8] weren't arrived at using pure compounds based on what we observed.

Figure 5 shows the elution order obtained from the D6730 system for the alkyl substituted naphthalenes. The chromatogram was obtained from numerous injections of (12) solutions made from the pure alkyl substituted naphthalenes and used to obtain the correct elution order. The chromatograms also depict the correct co-elution for the naphthalene pairs: (1) 1,3-dimethylnaphthalene and 1,7-dimethylnaphthalene and (2) 1,4-dimethylnaphthalene and 2,3-dimethylnaphthalene.

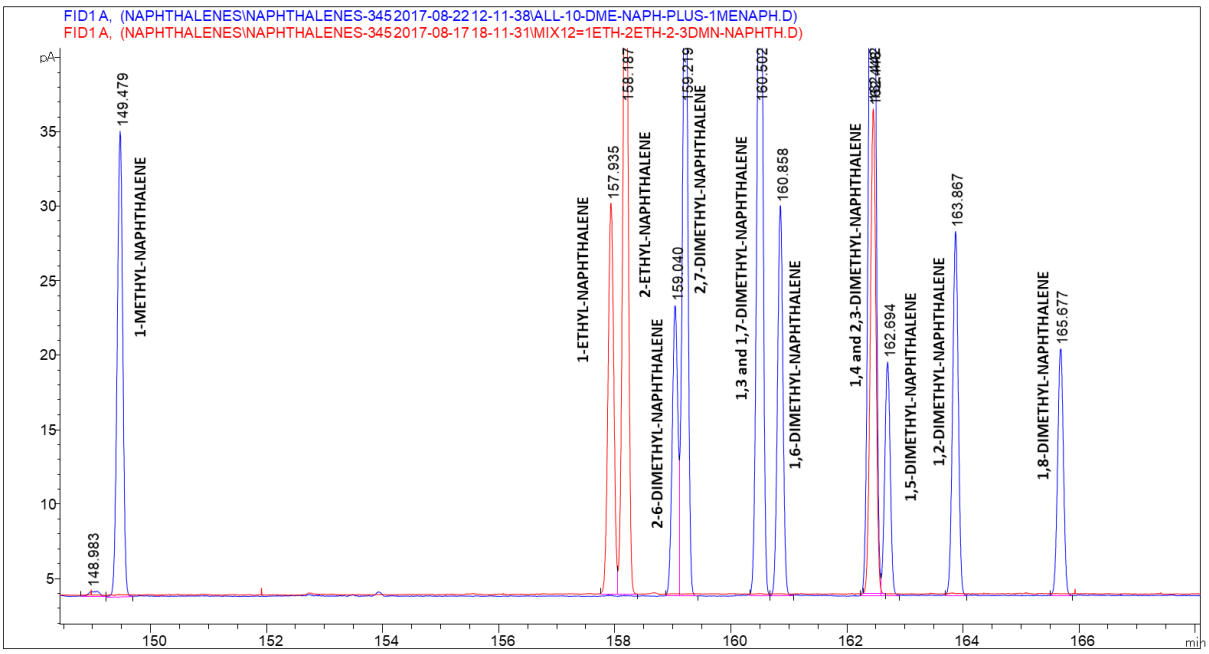


Figure 5 - Chromatogram of the mono and di-methyl naphthalene isomers

Figure 6 shows an overlay of CRC#5 and the alkyl substituted naphthalene standards. The blue trace is the chromatogram of the CRC#5 gasoline sample. The traces in red, green, and purple are the chromatograms of the standards used to confirm the isomer identification. Review of the MS data for this sample confirmed their identities as methylnaphthalenes.

However it is difficult to ascertain whether the co-elution is comprised of a naphthalene pair or not. We also noted that 1,8-dimethylnaphthalene was the only one of the 10 isomers of dimethylnaphthalene absent in the sample which is likely attributable to removal during the refining process.

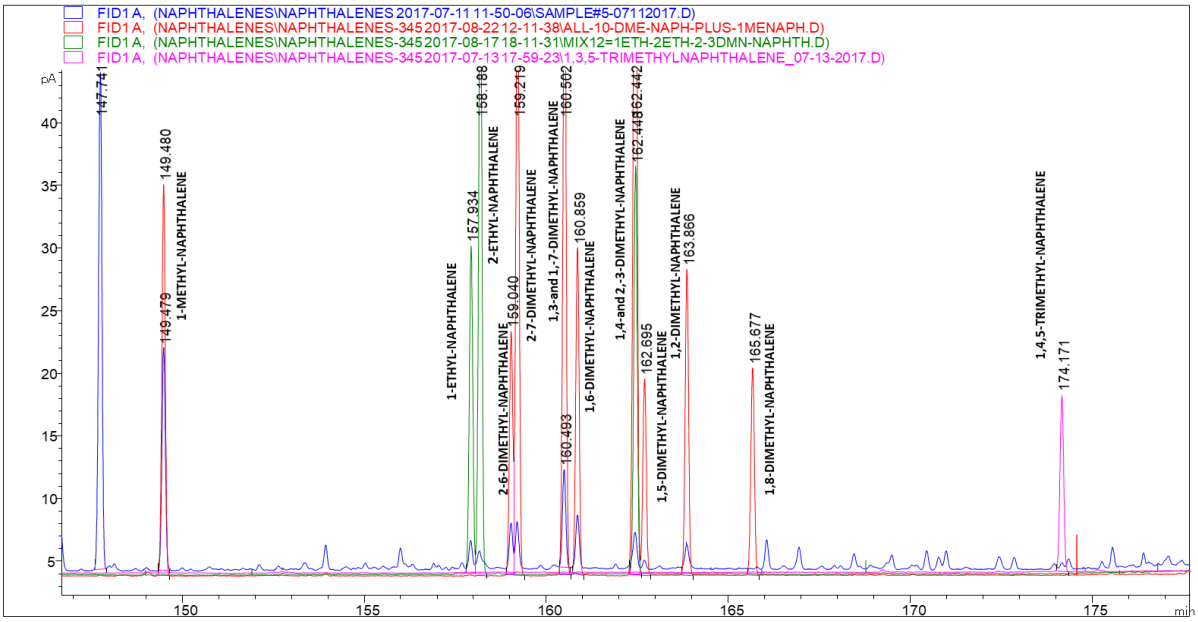


Figure 6 - Chromatogram of CRC#5 with naphthalene standards overlaid

Figure 7 shows the overlay of CRC#4 with the reference chromatogram obtained from pure standards. Note, we cannot confirm that the co-elution obtained with prepared standard solutions also present as co-elutions in the CRC gasoline samples. It is possible that only one of the two isomers is present.

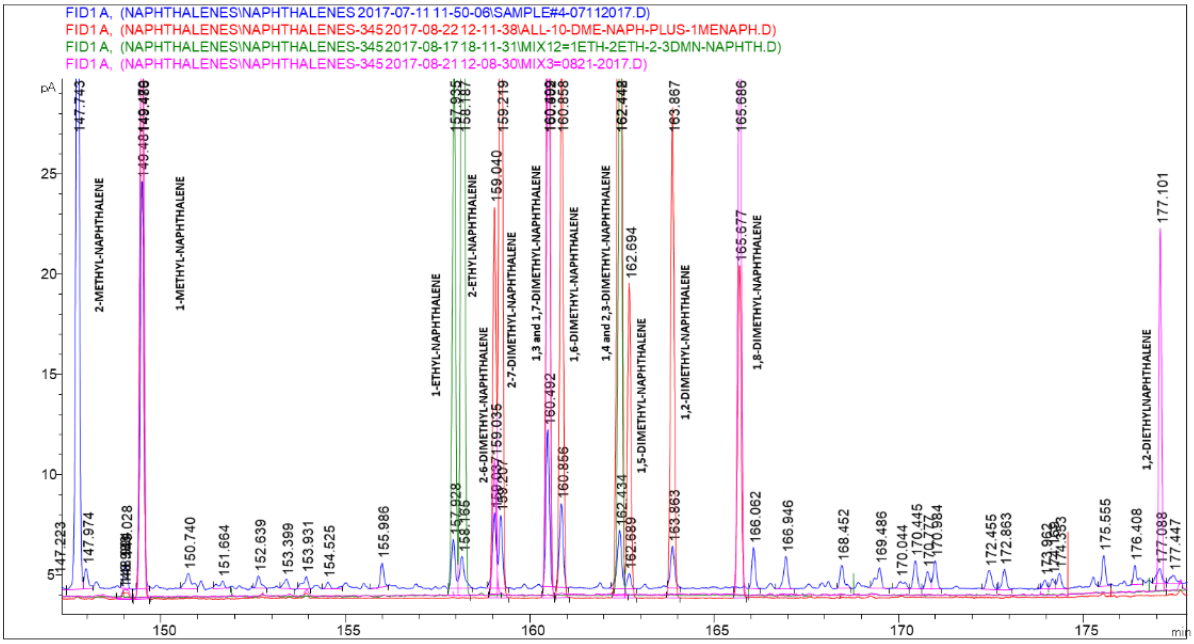


Figure 7 - Chromatogram of CRC#4 with naphthalene standards overlaid

The compounds eluting after naphthalene identified in sample CRC#4 are shown in Table 6. The contribution to the PM index for each compound is also shown in the table as well as the contributions of biphenyl and indanes. Table 6 also shows the contributions of other naphthalene (biphenyl and indanes).

The compounds eluting in this zone in sample CRC#4 have a PM Index of 1.14. Since naphthalene, has a substantial contribution by itself, it is included in this zone. The total PM index for the sample is 2.766. When the other components eluting in this region are added, the contribution is 41.2% of the total (See Table 6 for the complete analysis including the vapor pressures at 443 K.)

Table 6 – Contribution to the PMI of naphthalene, alkyl substituted naphthalenes and other compounds in CRC#4

TIME	CASNO	RI	GROUP	CARBON#	COMPONENT	%WGT	BP (K)	DBE	PMI	VP (at 443 K)
132.43	91-20-3	1171.61	Naphthalenes	10	Naphthalene	0.395	491.15	7	1.111E-01	28.620
132.672	98-19-1	1173.54	Mono-Aromatics	12	1-t-Butyl-3,5-dimethylbenzene	0.022	481.05	4	2.915E-03	37.686
132.973	4175-53-5	1175.94	Indanes	11	1H-Indene, 2,3-dihydro-1,3-dimethyl-	0.024	481.85	5	3.996E-03	36.882
133.172		1177.52	Unidentified	0	Unidentified	0.004	481.85	5		36.882
133.498	6682-71-9	1180.11	Indanes	11	4,7-Dimethyl Indane	0.074	499.75	5	1.959E-02	22.523
133.715	4912-92-9	1181.82	Indanes	11	1,1-Dimethyl Indane	0.028	464.15	5	2.831E-03	58.912
134.153	7364-19-4	1185.28	Mono-Aromatics	12	1t-Butyl-4-ethylbenzene	0.057	484.65	4	8.403E-03	34.190
134.777	99-62-7	1190.19	Mono-Aromatics	12	1,3-Di-n-propylbenzene	0.146	476.15	4	1.713E-02	42.970
134.988	4706-90-5	1191.85	Mono-Aromatics	11	Benzene, 1,3-dimethyl-5-(1-methylethyl)-	0.069	467.05	4	6.364E-03	54.627
136.033	112-40-3	1200	Paraffin	12	n-Dodecane	0.038	488.15	0	1.217E-03	31.079
136.033		1200	Mono-Aromatics	11	C11_Mono-Aromatics(21)	0.035	494.25	5	8.021E-03	26.267
137.173		1210.98	Mono-Aromatics	11	C11_Mono-Aromatics(24)	0.005	465.95	4	4.624E-04	56.217
138	1062949	1218.89	Mono-Aromatics	12	1,3,5-trimethyl-2-propylbenze	0.026	505.25	4	6.784E-03	19.272
138.692	56147-63-8	1225.47	Indanes	11	2-Ethyl-2,3-dihydro-1H-indene	0.018	488.35	5	3.609E-03	30.909
138.958	4830-99-3	1228	Indanes	11	1H-Indene, 1-ethyl-2,3-dihydro-	0.027	495.15	5	6.365E-03	25.618
139.19		1230.19	Unidentified	0	Unidentified	0.017	495.15	5		25.618
139.972		1237.56	Mono-Aromatics	11	C11_Mono-Aromatics(22)	0.007	465.95	4	6.711E-04	56.217
140.72		1244.57	Indanes	11	C11_Indanes(1)	0.065	451.05	5	4.730E-03	82.413
142.25		1258.81	Indanes	11	Diimethyl Indene - 2	0.027	451.05	5	1.969E-03	82.413
142.642	1075-22-5	1262.42	Indanes	11	1H-Indene, 2,3-dihydro-5,6-dimethyl-	0.014	500.75	5	3.821E-03	21.897
143.073	62238-14-6	1266.4	I-Paraffins	13	Decane, 2,3,8-trimethyl-	0.008	495.52	0	3.192E-04	25.356
144.237		1277.06	Indanes	12	C12_Indanes(6)	0.092	451.05	5	6.691E-03	82.413
144.842		1282.57	Indanes	12	C12_Indanes(9)	0.005	451.05	5	3.828E-04	82.413
145.288	90-12-0	1286.62	Naphthalenes	11	2-Methylnaphthalene	0.475	513.15	7	2.411E-01	15.345
145.613		1289.56	Mono-Aromatics	12	C12_Mono-Aromatics(14)	0.012	477.15	4	1.392E-03	41.839
145.843		1291.64	Unidentified	0	Unidentified	0.005	477.15	4		41.839
146.563		1298.12	Indanes	12	C12_Indanes(21)	0.002	451.05	5	1.772E-04	82.413
146.773	629-50-5	1300	Paraffin	13	n-Tridecane	0.011	507.65	0	6.116E-04	17.992
147.022	91-57-6	1302.59	Naphthalenes	11	1-Methylnaphthalene	0.221	513.05	7	1.120E-01	15.390
148.378	22531-20-0	1316.66	Mono-Aromatics	12	Naphthalene, 6-ethyl-1,2,3,4-tetrahydro-	0.004	519.75	5	1.899E-03	12.639
150.243	42775-77-9	1335.8	Mono-Aromatics	13	Naphthalene, 1,2,3,4-tetrahydro-6-propyl-	0.004	537.95	5	2.969E-03	7.265
151.63		1349.88	I-Paraffins	13	C13_I-Paraffins(8)	0.007	495.52	0	2.606E-04	25.356
153.547		1369.12	Unidentified	0	Unidentified	0.026	495.52	0		25.356
155.472	1127-76-0	1388.21	Naphthalenes	12	1-Ethylnaphthalene	0.032	532.25	7	2.617E-02	8.668
155.718	939-27-5	1390.64	Naphthalenes	12	2-Ethylnaphthalene	0.017	530.93	7	1.395E-02	9.026
156.567	581-42-0	1398.97	Naphthalenes	12	Naphthalene,2,6 dimethyl	0.041	535.15	7	3.683E-02	7.926
156.735	582-16-1	1400.72	Naphthalenes	12	Naphthalene,2,7 dimethyl	0.038	536.15	7	3.494E-02	7.684
158.012	575-37-1	1415.36	Naphthalenes	12	Naphthalene,1,7-dimethyl	0.044	535.65	7	3.982E-02	7.804
158.012	575-41-7	1415.36	Naphthalenes	12	Naphthalene, 1,3-dimethyl-	0.044	537.15	7	4.127E-02	7.449
158.368	575-43-9	1419.43	Naphthalenes	12	Naphthalene-1,6-dimethyl	0.045	536.00	7	4.068E-02	7.720
159.933	571-58-4	1437.18	Naphthalenes	12	Naphthalene-1,4-dimethyl	0.018	541.60	7	1.857E-02	6.479
159.933	581-40-8	1437.18	Naphthalenes	12	Naphthalene, 2,3-dimethyl-	0.018	542.05	7	1.876E-02	6.387
160.172	571-61-9	1439.87	Naphthalenes	12	Naphthalene, 1,5-dimethyl-	0.011	538.75	7	1.020E-02	7.086
161.358	573-98-8	1453.19	Naphthalenes	12	Naphthalene, 1,2-dimethyl-	0.022	541.15	7	2.273E-02	6.571
163.598	644-08-6	1478.07	Mono-Aromatics	13	1,1'-Biphenyl, 4-methyl-	0.023	540.95	8	2.651E-02	6.613
164.467	643-58-3	1487.62	Mono-Aromatics	13	1,1'-Biphenyl, 2-methyl-	0.019	528.45	8	1.570E-02	9.734
165.087		1494.41	Unidentified	0	Unidentified	0.003	528.45	8		9.734
165.443		1498.31	Unidentified	0	Unidentified	0.003	528.45	8		9.734
165.957	829-26-5	1503.9	Naphthalenes	13	Naphthalene, 2,3,6-trimethyl-	0.015	536.65	7	1.351E-02	7.565
166.848		1513.57	Unidentified	0	Unidentified	0.006	536.65	7		7.565
167.027		1515.5	Naphthalenes	13	C13_Naphthalenes(5)	0.012	554.25	7	1.661E-02	4.312
167.502		1520.62	Unidentified	0	Unidentified	0.004	554.25	7		4.312
167.673		1522.47	Naphthalenes	13	C13_Naphthalenes(2)	0.003	554.25	7	4.052E-03	4.312
167.908	2131-42-2	1525	Naphthalenes	13	Naphthalene, 1,4,6-trimethyl-	0.017	554.25	7	2.292E-02	4.312
168.25	605-39-0	1528.67	Mono-Aromatics	14	2,2'-Dimethylbiphenyl	0.010	531.00	8	9.053E-03	9.006
168.413	2131-41-1	1530.42	Naphthalenes	13	Naphthalene, 1,4,5-trimethyl-	0.015	563.45	7	2.458E-02	3.175
169.807	2245-38-7	1545.29	Naphthalenes	13	Naphthalene, 1,6,7-trimethyl-	0.013	559.95	7	1.901E-02	3.571
170.175		1549.2	Naphthalenes	13	C13_Naphthalenes(1)	0.009	540.00	7	9.228E-03	6.813
171.218	2027-17-0	1560.23	Naphthalenes	13	Naphthalene, 2-(1-methylethyl)-	0.005	540.00	7	4.670E-03	6.813
171.42		1562.35	Naphthalenes	13	C13_Naphthalenes(4)	0.006	554.25	7	7.944E-03	4.312
171.59	5707-44-8	1564.14	Mono-Aromatics	14	4-Ethylbiphenyl	0.008	564.20	8	1.533E-02	3.096
172.682	612-75-9	1575.59	Mono-Aromatics	14	3,3'-Dimethylbiphenyl	0.004	559.00	8	6.700E-03	3.686
172.997	7383-90-6	1578.88	Mono-Aromatics	14	1,1'-Biphenyl, 3,4'-dimethyl-	0.016	569.00	8	3.238E-02	2.628
174.11	613-33-2	1590.46	Mono-Aromatics	14	4,4'-Dimethylbiphenyl	0.007	568.15	8	1.454E-02	2.706
175.363	21895-16-9	1603.4	Mono-Aromatics	15	Benzene, 1-methyl-3-[(4-methylphenyl)methyl]-	0.000	563.15	8		3.207
176.252		1612.52	Mono-Aromatics	14	C14_Mono-Aromatics(1)	0.009	559.00	8	1.558E-02	3.686
179.518		1645.66	Unidentified	0	Unidentified	0.002	559.00	8		3.686
180.487		1655.37	Unidentified	0	Unidentified	0.004	559.00	8		3.686
182.728		1677.65	Unidentified	0	Unidentified	0.003	559.00	8		3.686
							Naphthalene Total:		1.140E+00	

Table 7 - PM Index Contribution of naphthalene, methyl substituted naphthalenes and other compounds in sample CRC#5

TIME	CASNO	RI	GROUP	CARBON#	COMPONENT	%WGT	BP (K)	DBE	PMI	VP (at 443 K)
132.43	91-20-3	1173.53	Naphthalenes	10	Naphthalene	0.355	494.65	7	1.097E-01	25.977
132.708		1175.75	I-Paraffins	12	C12_I-Paraffins(8)	0.046	470.15	1	1.858E-03	50.364
133.025	4175-53-5	1178.27	Indanes	11	1H-Indene, 2,3-dihydro-1,3-dimethyl-	0.037	481.85	5	6.121E-03	36.882
133.162		1179.36	I-Paraffins	12	C12_I-Paraffins(10)	0.009	470.15	1	3.653E-04	50.364
133.358		1180.92	Mono-Aromatics	12	C12_Mono-Aromatics(19)	0.009	481.05	4	1.175E-03	37.686
133.502	6682-71-9	1182.06	Indanes	11	4,7-Dimethyl Indane	0.043	499.75	5	1.155E-02	22.523
133.72	4912-92-9	1183.78	Indanes	11	1,1-Dimethyl Indane	0.012	464.15	5	1.236E-03	58.912
133.977		1185.81	Mono-Aromatics	12	C12_Mono-Aromatics(20)	0.003	484.65	4	3.844E-04	34.190
134.152		1187.19	Mono-Aromatics	11	C11_Mono-Aromatics(14)	0.038	465.95	4	3.426E-03	56.217
134.775	99-62-7	1192.09	Mono-Aromatics	12	1,3-Di-n-propylbenzene	0.129	476.15	4	1.517E-02	42.970
134.99	4706-90-5	1193.78	Mono-Aromatics	11	Benzene, 1,3-dimethyl-5-(1-methylethyl)-	0.067	467.05	4	6.195E-03	54.627
136.047		1202.49	Mono-Aromatics	11	C11_Mono-Aromatics(23)	0.044	467.05	4	4.050E-03	54.627
137.173	62108-31-0	1213.26	I-Paraffins	13	Heptane, 4-ethyl-2,2,6,6-tetramethyl-	0.008	468.15	0	1.446E-04	53.078
137.998		1221.08	Mono-Aromatics	11	C11_Mono-Aromatics(18)	0.007	465.95	4	6.557E-04	56.217
138.7	56147-63-8	1227.7	Indanes	11	2-Ethyl-2,3-dihydro-1H-indene	0.003	488.35	5	6.766E-04	30.909
138.972	4830-99-3	1230.25	Indanes	11	1H-Indene, 1-ethyl-2,3-dihydro-	0.018	495.15	5	4.122E-03	25.618
140.722		1246.58	Indanes	11	C11_Indanes(3)	0.031	451.05	5	2.282E-03	82.413
142.25	2177-48-2	1260.68	Indanes	11	1-H-Indene,1-3-dimethyl	0.022	502.05	6	7.243E-03	21.107
142.652	1075-22-5	1264.36	Indanes	11	1H-Indene, 2,3-dihydro-5,6-dimethyl-	0.008	500.75	5	2.160E-03	21.897
143.238	62238-14-6	1269.72	I-Paraffins	13	Decane, 2,3,8-trimethyl-	0.004	495.52	0	1.683E-04	25.356
143.54	42775-75-7	1272.46	Indanes	12	Naphthalene, 5-ethyl-1,2,3,4-tetrahydro-	0.008	513.45	5	3.014E-03	15.212
143.993		1276.58	Mono-Aromatics	12	C12_Mono-Aromatics(13)	0.006	477.15	4	7.144E-04	41.839
144.235	700-12-9	1278.76	Mono-Aromatics	11	Pentamethylbenzene	0.084	502.15	4	1.978E-02	21.047
145.29	90-12-0	1288.28	Naphthalenes	11	2-Methylnaphthalene	0.448	513.15	7	2.275E-01	15.345
145.635		1291.37	Mono-Aromatics	12	C12_Mono-Aromatics(14)	0.005	477.15	4	5.595E-04	41.839
145.828	20027-77-4	1293.1	Mono-Aromatics	12	Naphthalene, 1,2,3,4-tetrahydro-5,6-dimethyl-	0.007	527.85	5	3.874E-03	9.913
147.017	91-57-6	1304.37	Naphthalenes	11	1-Methylnaphthalene	0.204	513.05	7	1.032E-01	15.390
149.81		1333.4	I-Paraffins	13	C13_I-Paraffins(3)	0.004	508.55	0	2.035E-04	17.532
151.04		1346.02	Mono-Aromatics	12	C12_Mono-Aromatics(15)	0.009	477.15	4	1.054E-03	41.839
151.632		1352.05	I-Paraffins	13	C13_I-Paraffins(11)	0.026	496.40	0	1.056E-03	24.741
152.163		1357.45	Unidentified	0	Unidentified	0.004	496.40	0		24.741
152.702		1362.9	Unidentified	0	Unidentified	0.011	496.40	0		24.741
153.543		1371.38	Mono-Aromatics	12	C12_Mono-Aromatics(21)	0.023	477.15	8	5.002E-03	41.839
153.82		1374.15	Unidentified	0	Unidentified	0.007	477.15	8		41.839
154		1375.96	Unidentified	0	Unidentified	0.005	477.15	8		41.839
154.588		1381.84	I-Paraffins	13	C13_I-Paraffins(10)	0.005	495.52	0	2.042E-04	25.356
154.702		1382.97	I-Paraffins	13	C13_I-Paraffins(9)	0.002	502.55	0	1.078E-04	20.810
155.46	1127-76-0	1390.51	Naphthalenes	12	1-Ethylnaphthalene	0.029	532.25	7	2.379E-02	8.668
155.712	939-27-5	1393.01	Naphthalenes	12	2-Ethylnaphthalene	0.019	530.93	7	1.489E-02	9.026
155.982		1395.68	Unidentified	0	Unidentified	0.008	530.93	7		9.026
156.568	581-42-0	1401.63	Naphthalenes	12	Naphthalene,2,6 dimethyl	0.039	535.15	7	3.442E-02	7.926
156.737	582-16-1	1403.47	Naphthalenes	12	Naphthalene,2,7 dimethyl	0.040	536.15	7	3.666E-02	7.684
158.012	575-37-1	1417.3	Naphthalenes	12	Naphthalene,1,7-dimethyl	0.046	535.65	7	4.155E-02	7.804
158.012	575-41-7	1417.3	Naphthalenes	12	Naphthalene, 1,3-dimethyl-	0.046	536.15	7	4.205E-02	7.684
158.368	575-43-9	1421.15	Naphthalenes	12	Naphthalene, 1,6-dimethyl-	0.050	537.15	7	4.649E-02	7.449
159.557		1433.92	Indanes	13	C13_Indanes(2)	0.003	451.05	5	2.258E-04	82.413
159.938	571-58-4	1438	Naphthalenes	12	Naphthalene-1,4-dimethyl	0.020	541.60	7	2.123E-02	6.479
159.938	581-40-8	1438	Naphthalenes	12	Naphthalene, 2,3-dimethyl-	0.020	542.05	7	2.145E-02	6.387
160.18	571-61-9	1440.58	Naphthalenes	12	Naphthalene, 1,5-dimethyl-	0.012	538.75	7	1.163E-02	7.086
161.355	573-98-8	1453.06	Naphthalenes	12	Naphthalene, 1,2-dimethyl-	0.024	541.15	7	2.493E-02	6.571
163.602	644-08-6	1476.68	Mono-Aromatics	13	1,1'-Biphenyl, 4-methyl-	0.031	540.95	8	3.505E-02	6.613
164.027	62185-21-1	1481.11	I-Paraffins	12	Octane, 3,4,5,6-tetramethyl-	0.006	472.20	0	1.306E-04	47.716
164.47	643-58-3	1485.72	Mono-Aromatics	13	1,1'-Biphenyl, 2-methyl-	0.025	528.45	8	2.128E-02	9.734
165.088		1492.13	Unidentified	0	Unidentified	0.003	528.45	8		9.734
165.955	829-26-5	1501.07	Naphthalenes	13	Naphthalene, 2,3,6-trimethyl-	0.018	536.65	7	1.644E-02	7.565
166.392		1505.56	Unidentified	0	Unidentified	0.008	536.65	7		7.565
166.853		1510.29	Unidentified	0	Unidentified	0.007	536.65	7		7.565
167.035		1512.15	Naphthalenes	13	C13_Naphthalenes(5)	0.014	540.00	7	1.357E-02	6.813
167.517		1517.06	Unidentified	0	Unidentified	0.004	540.00	7		6.813
167.68		1518.73	Naphthalenes	13	C13_Naphthalenes(2)	0.003	554.25	7	4.321E-03	4.312
167.908	2131-42-2	1521.05	Naphthalenes	13	Naphthalene, 1,4,6-trimethyl-	0.019	554.25	7	2.521E-02	4.312
168.265	605-39-0	1524.68	Mono-Aromatics	14	2,2'-Dimethylbiphenyl	0.013	531.00	8	1.142E-02	9.006
168.413	2131-41-1	1526.18	Naphthalenes	13	Naphthalene, 1,4,5-trimethyl-	0.017	563.45	7	2.756E-02	3.175
169.803	2245-38-7	1540.22	Naphthalenes	13	Naphthalene, 1,6,7-trimethyl-	0.014	559.95	7	2.066E-02	3.571
170.183		1544.04	Naphthalenes	13	C13_Naphthalenes(1)	0.011	540.00	7	1.113E-02	6.813
171.218	2027-17-0	1554.39	Naphthalenes	13	Naphthalene, 2-(1-methylethyl)-	0.005	540.00	7	4.572E-03	6.813
171.417		1556.37	Naphthalenes	13	C13_Naphthalenes(4)	0.005	559.95	7	8.140E-03	3.571
171.6	5707-44-8	1558.19	Mono-Aromatics	14	4-Ethylbiphenyl	0.009	564.20	8	1.654E-02	3.096
172.68	612-75-9	1568.91	Mono-Aromatics	14	3,3'-Dimethylbiphenyl	0.004	562.47	8	6.832E-03	3.282
172.995	7383-90-6	1572.02	Mono-Aromatics	14	1,1'-Biphenyl, 3,4'-dimethyl-	0.019	557.33	8	3.064E-02	3.896
174.108	613-33-2	1582.98	Mono-Aromatics	14	4,4'-Dimethylbiphenyl	0.013	568.00	8	2.460E-02	2.720
174.978		1591.49	Unidentified	0	Unidentified	0.007	568.00	8		2.720
175.388	21895-16-9	1595.49	Mono-Aromatics	15	Benzene, 1-methyl-3-[(4-methylphenyl)methyl]-	0.000	563.15	8		3.207
176.25		1603.86	Mono-Aromatics	14	C14_Mono-Aromatics(1)	0.015	554.00	8	2.311E-02	4.348
177.352		1614.5	Unidentified	0	Unidentified	0.005	554.00	8		4.348
178.01		1620.83	Unidentified	0	Unidentified	0.006	554.00	8		4.348
180.483		1644.39	Unidentified	0	Unidentified	0.003	554.00	8		4.348
							Naphthalene Total:		1.166E+00	

The PM Index contribution for the compounds eluting from naphthalene to the end of the chromatogram is 1.17 in CRC#5 are shown in Table 7. The contribution is not only from the

alkyl substituted naphthalenes but also from other heavy aromatics ex. biphenyls. Since naphthalene is a substantial contributor it is included in this zone. The PMI is 44.0% of the total PMI (2.659). Boiling points, vapor pressures and calculated PMI values[2,4] are listed as well. See Appendix C for further detail about calculating PMI.

The final GC oven temperature ramp enables the analysis to be extended to include heavier components such as C13 naphthalenes and beyond. Note, 1-methylnaphthalene (C11) is the last compound listed in ASTM D6730-01(2016).

GC Signal Integration

It is not practical to use contemporary GC data acquisition software to integrate chromatograms containing many components and 'complexity' without using some level of manual integration. This is certainly the case with DHA.

Despite how well today's ultra-high resolution capillary columns separate individual components they simply cannot resolve all of the components in complex mixtures like gasolines. There are many places in a chromatogram where adjacent peaks only partially separate or, in some cases, not at all. This makes it difficult, if not impossible, for a GC data system to consistently integrate them without manually adjusting integration parameters such as slope sensitivity, peak width, area rejection, tangent skimming/sensitivity and/or creating special timed or manual integration events like manual baseline assignment.

As such, it is necessary for the user to dedicate the time necessary to thoroughly review the chromatogram and manually integrate peaks the GC data acquisition system may do 'incorrectly'.

Although it's impractical to show each and every place in a typical DHA chromatogram where manual integration is appropriate, examples of the most common cases are described below.

It is also important to understand that manual integration adds a subjective element to the analysis which cannot be avoided. And, the fact that reviewers may or may not agree where to specify a manual integration event. For example, where a peak actually begins or ends. However, it is a better alternative than choosing to ignore overlapping peaks when they occur.

Case 1 - Partially Eluting Peak(s)

This is a common phenomenon found throughout DHA chromatograms and can often be resolved by manually 'splitting'' the peak as shown in Figures 8 and 9. The bottom section in these figures is the integrator section of the software display window which shows the peak 'events' automatically assigned by the built in peak integrator or manually using it. Note: any changes in analysis results due to manual integration are not reflected until the integrator section of the software is exited and the file saved. In these figures both peak splitting and manual integration(s) were employed.

It is important to note there's no foolproof means to manually 'split' peaks 'correctly'. The splitting process is very subjective and the ability to consistently apply the technique directly related to the level of experience the user with manual integration. For example, recognizing how important it is to pay close attention to the slope of a co-elution event and the impact a much larger component will have on the peak area vs a much smaller co-eluting peak.

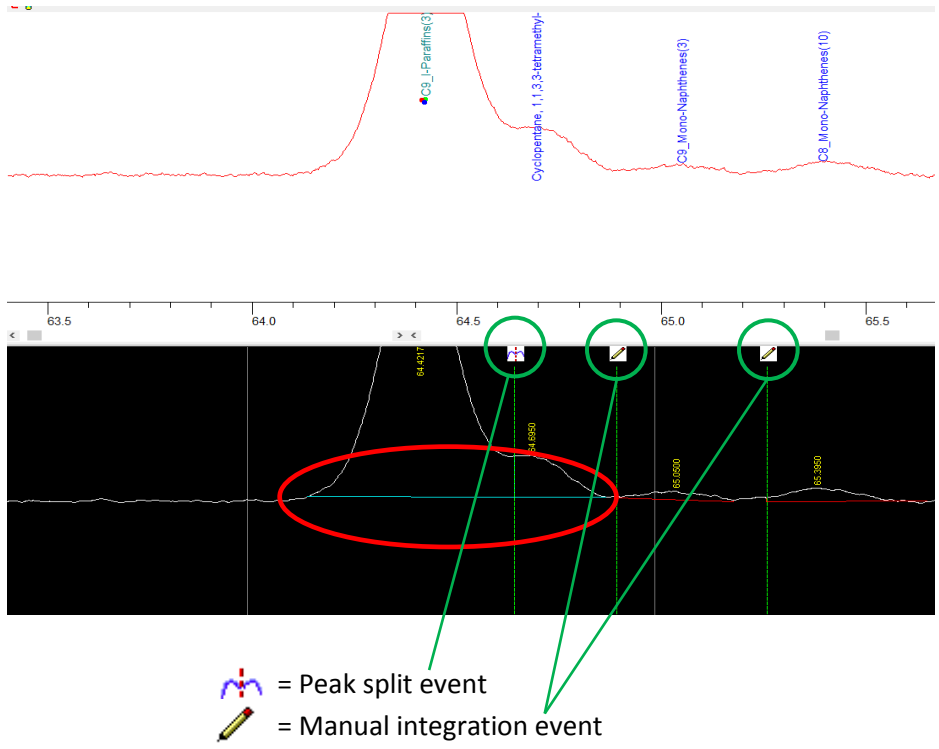


Figure 8 - Using the integrator to 'split' two peaks (red circle) so they can be individually integrated.

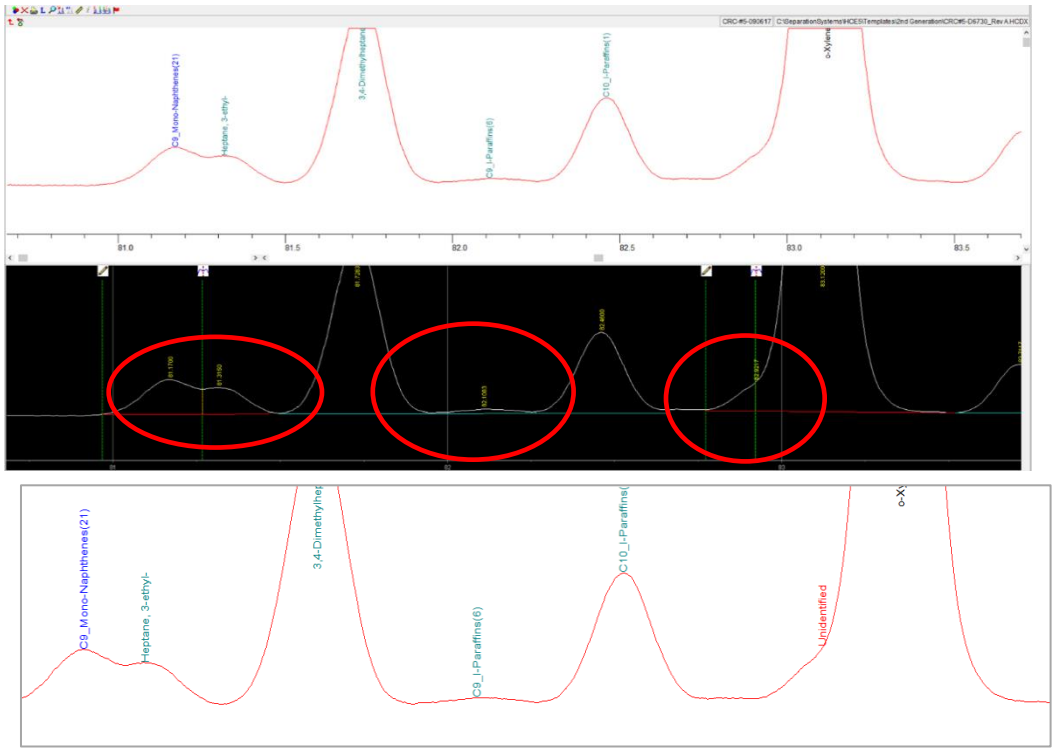


Figure 9 - Another example where poorly resolved peaks had to be 'split' (red circles)

Case 2 - Inability to Integrate Small Peaks

An example is shown in Figure 10. This is most often solved by manually drawing a baseline under each of the peaks. Manually drawn baselines are shown in red under the peaks at retention time 65.050 and 65.395.

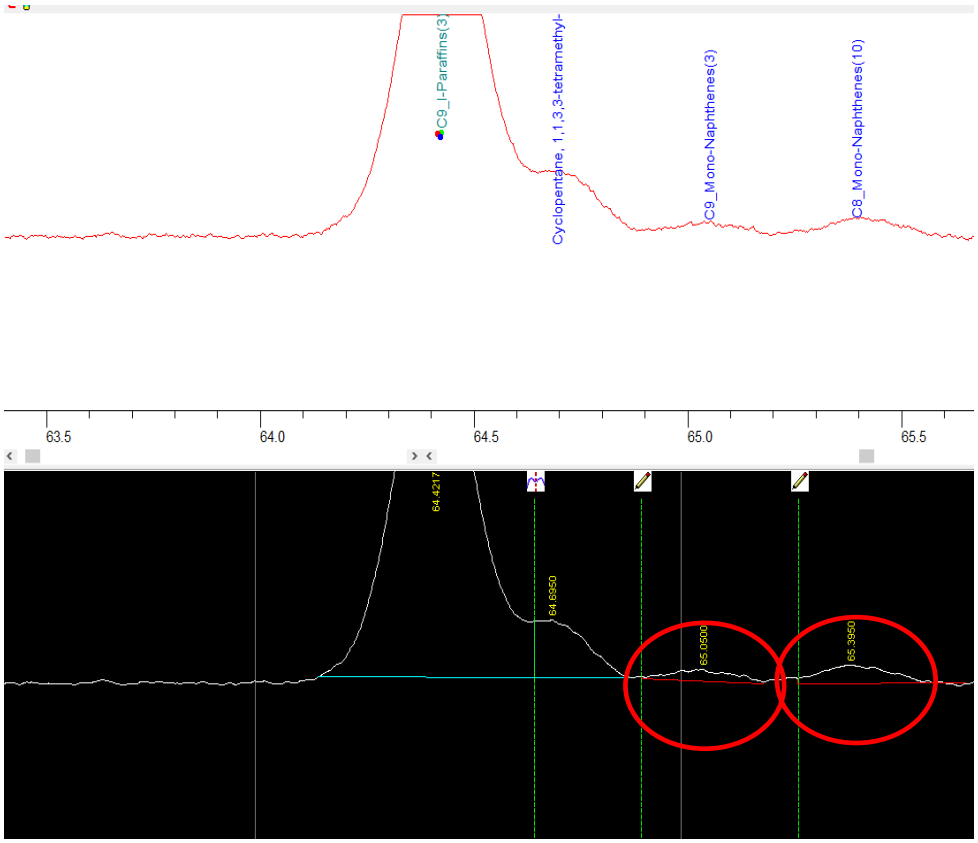


Figure 10 - Manually integrating small peaks

Case 3 - Separation of toluene, 2,3,3-trimethylpentane and 2,3,4-trimethylpentane

This case is especially important because toluene and benzene are regulated compounds (ex EPA).

Refineries use isomerization and alkylation processes to increase the octane number of fuel. Certain precursors produce isomers of isooctane (2,2,4-trimethylpentane). Two of the isomers, 2,3,4-trimethylpentane and 2,3,3-trimethylpentane are likely produced from a single precursor and usually present in similar amounts. This has been documented by Feller[15]. 2,3,3-trimethylpentane is not completely resolved from toluene as shown below (Figure 11). When the amount of 2,3,3-trimethylpentane is small in relation to toluene, the 2,3,3 isomer will not be detected. In cases in which the toluene to 2,3,3 isomer ratio is large, a more accurate toluene measurement can be obtained by subtracting the area of the 2,3,4 isomer from the total area under both peaks.

This is an accepted procedure because the two isomers can coexist in comparable amounts.

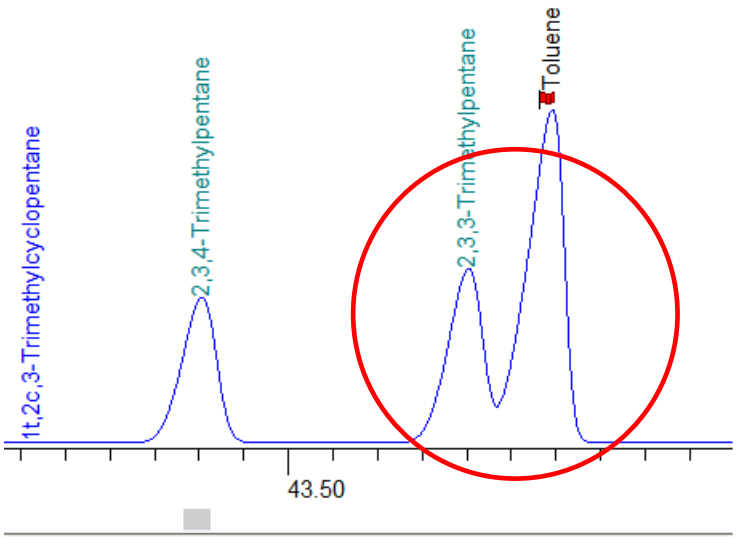


Figure 11 - Separation of 2,3,4 trimethylpentane, 2,3,3 trimethylpentane and toluene

Note: although the official test method for benzene and toluene in gasolines is ASTM D3606, D6730-01(2016) can be used to analyze them when it is not possible to run the specified method. D6730 is used in some other countries to analyze benzene and toluene.

Case 4 - Co-elution of a 'small' peak on the leading or descending edge of a much larger peak

Figure 12 shows an example in which two peaks appear to be one or almost so. This occurs on either side of the large peak and must be manually integrated. Note, this particular correction required two 'splits' to properly represent the poorly resolved peaks. It is possible to activate detection of peak inflexion in the ascending and descending portion of the peak within the software. Doing so may negate the need to manually assign the inflection points in the peak.

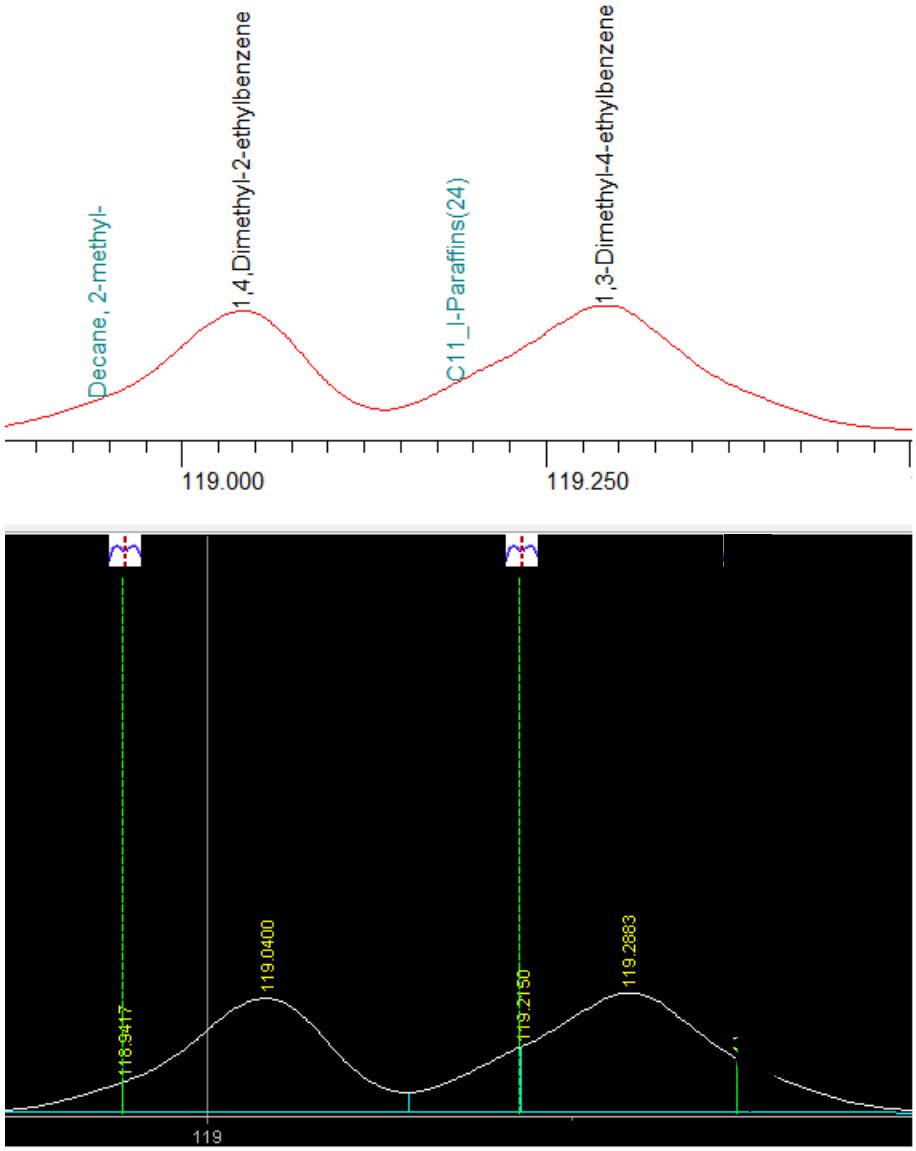


Figure 12 - Peaks that almost completely co-elute

Case 5. - When Co-elution Is Not Obvious

There are times when co-elution occurs but is not at all obvious. In these cases, if the peak is enlarged on screen a very slight shoulder appears on the ascending or descending slope of the peak. Figure 12 shows a good example. Recognizing these cases is especially important for a large peak which can easily 'mask' the presence of other components present in much lower amounts. Figure 13 and Figure 14 show cases in which this phenomenon occurs with two sequential 'large' peaks. Using the software's inflection integration function may facilitate the detection of subtle slope change in the peak.

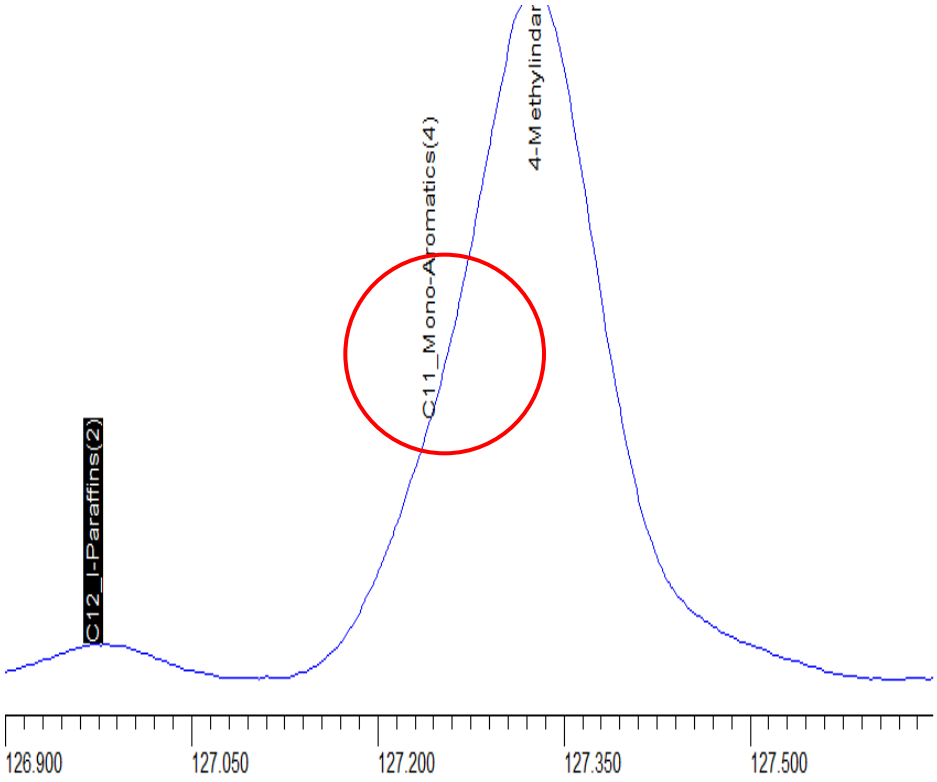


Figure 13 - Correcting a 'side' shoulder

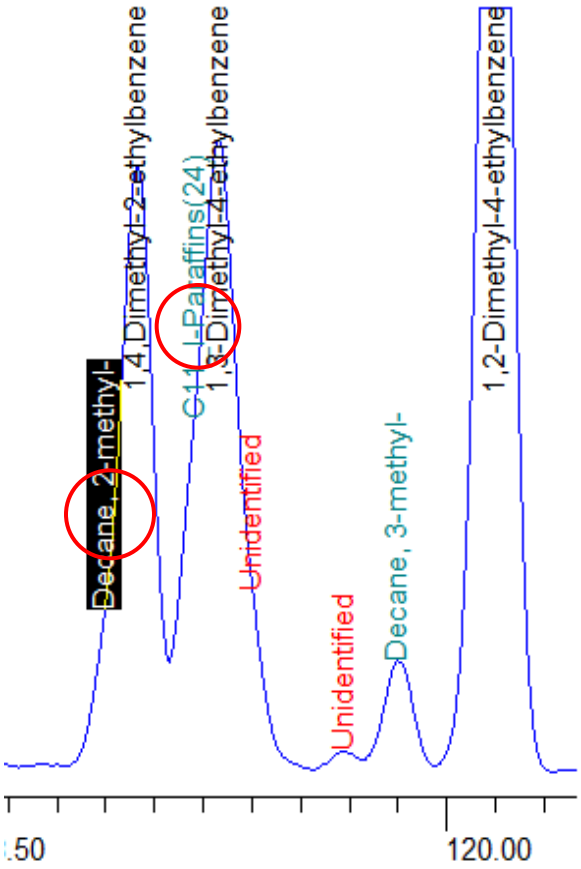


Figure 14 – Properly handling side shoulders

In addition to integrating individual peaks or co-eluting species manually, it can be quite useful to overlay two different chromatograms which makes it somewhat easier to note significant differences between two samples. Figure 15 shows the overlay of sample CRC#1 (blue trace) and sample CRC#5 (pink trace) which clearly shows that 2,4,4-trimethylhexane present in sample CRC#5 is not in sample CRC #1.

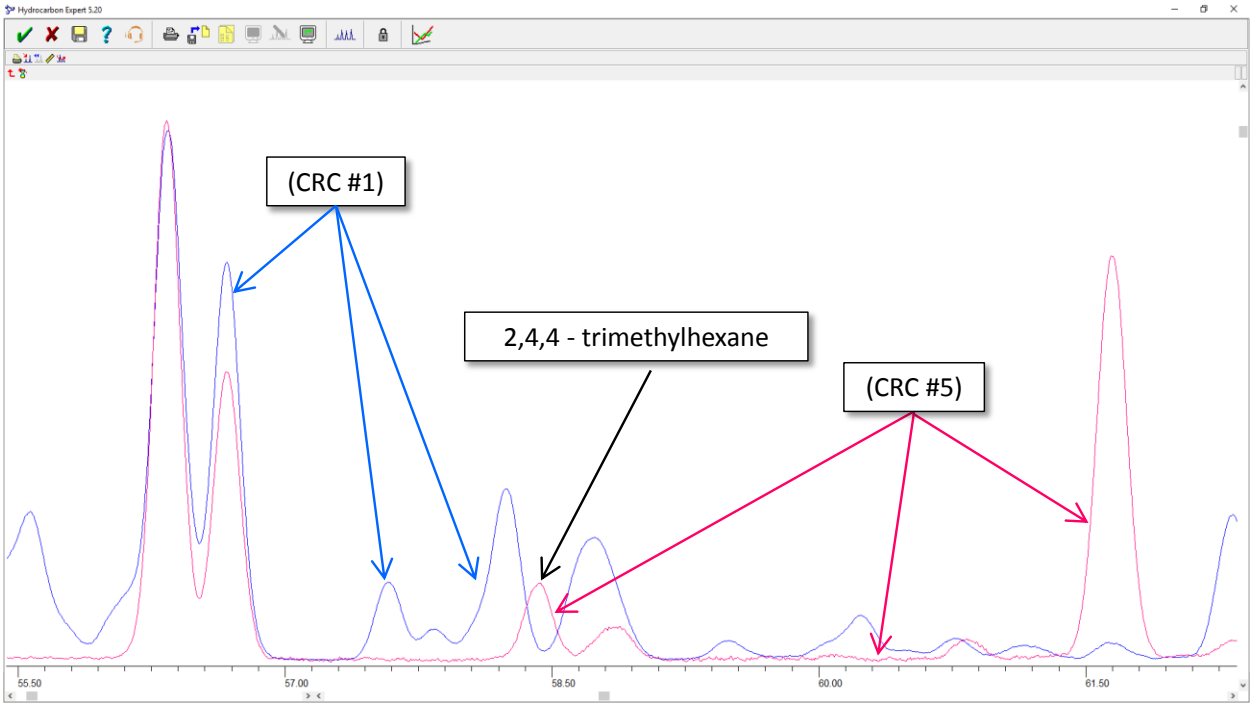


Figure 15 - Overlaying chromatograms to determine the presence or lack of a particular component

Another case when overlaying sample chromatograms makes it easier to distinguish differences is shown in Figure 16.

In this case, overlaying chromatograms helps to discern whether the right side shoulder of the peak for sample CRC#3 (in red) coincides with the peak eluting at the same time in CRC#5 (in blue) identified as 2,4,4-trimethylhexane. Overlaying clearly shows the co-elution and confirms the presence of the 2,4,4-trimethylhexane in both samples.

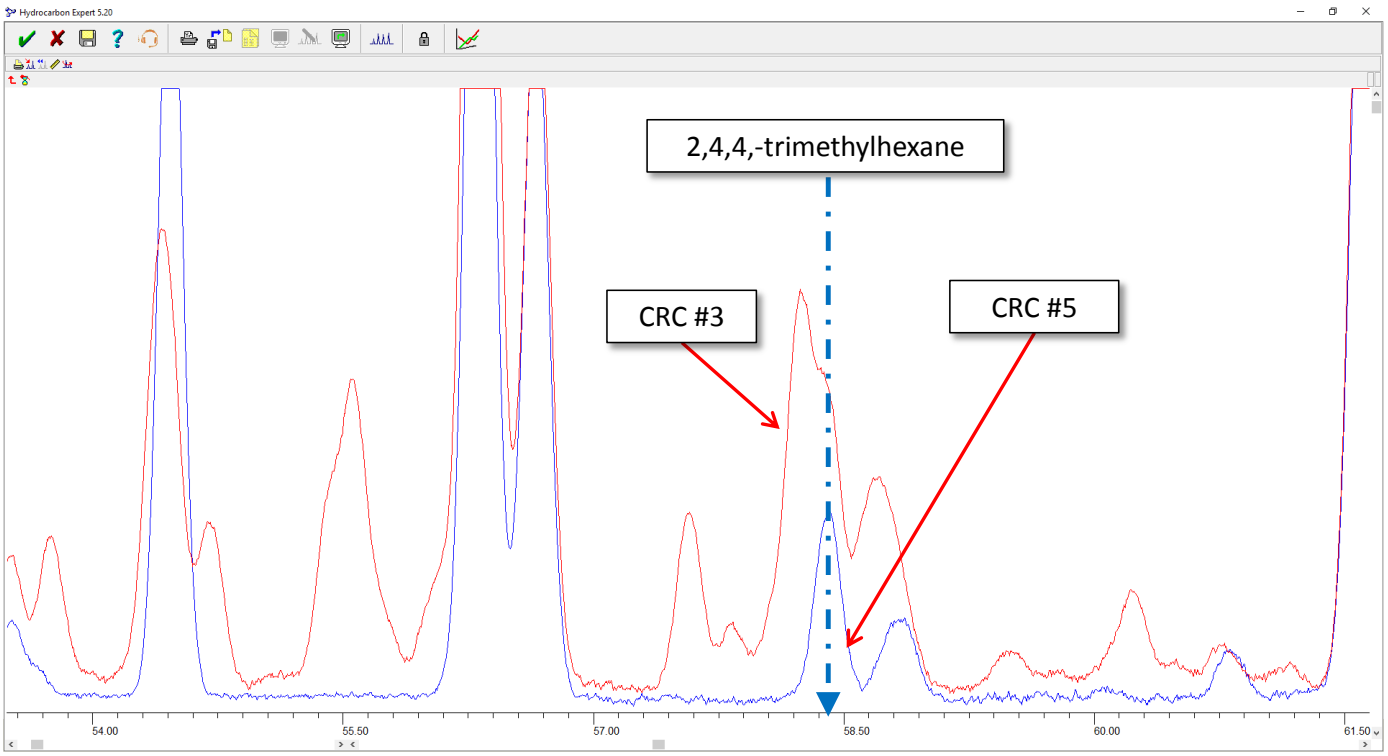


Figure 16 - Overlaying two sample chromatograms; Samples CRC#3 and CRC#5

Using the Mass Selective Detector to Identify Components

Most of the activity for this project centered around the use of the 'Research System' (GC-FID/MS) to identify unknown components in the CRC gasoline samples and reference material. Although it is not our intent to provide a step by step description how each individual identification was made, we believe it is important to describe the process used to do so.

Establishing the identity of an individual hydrocarbon component

1. Run the sample using the GC data system and export the signal file (.CDF)
2. Process the .cdf file using Hydrocarbon Expert/MS™ (HCE/MS) software
   - Chromatogram will be displayed on screen
   - Peaks identified via retention time using component/retention time database are labeled with a compound name; peaks with no corresponding retention time match are labelled 'unidentified'
3. Select an 'unidentified' peak and click on its apex
   - HCE/MS displays the corresponding total ion chromatogram (TIC) (See Figure 17)
   - Mass spectrum corresponding to the apex of the unidentified peak is displayed

4. Conduct a search of the unidentified component's mass spectrum against the NIST/Wiley library
   - A list of possible matches is produced based on match probability % from high to low
   - The sample's mass spectrum and the corresponding library spectrum for the top search result are superimposed so differences in fragmentation pattern and ion intensities can be visually compared.
5. Check the library match probability percentage values to determine if the top 'hit' is significantly greater than the others (see example below) and ~ 40% or higher. Figure 18.
   - If the match probability is significantly higher than the other possibilities and greater than 40%, add the 'identified' component to the component/retention time database
   - If not, a more in-depth review/investigation was undertaken. (See following section)

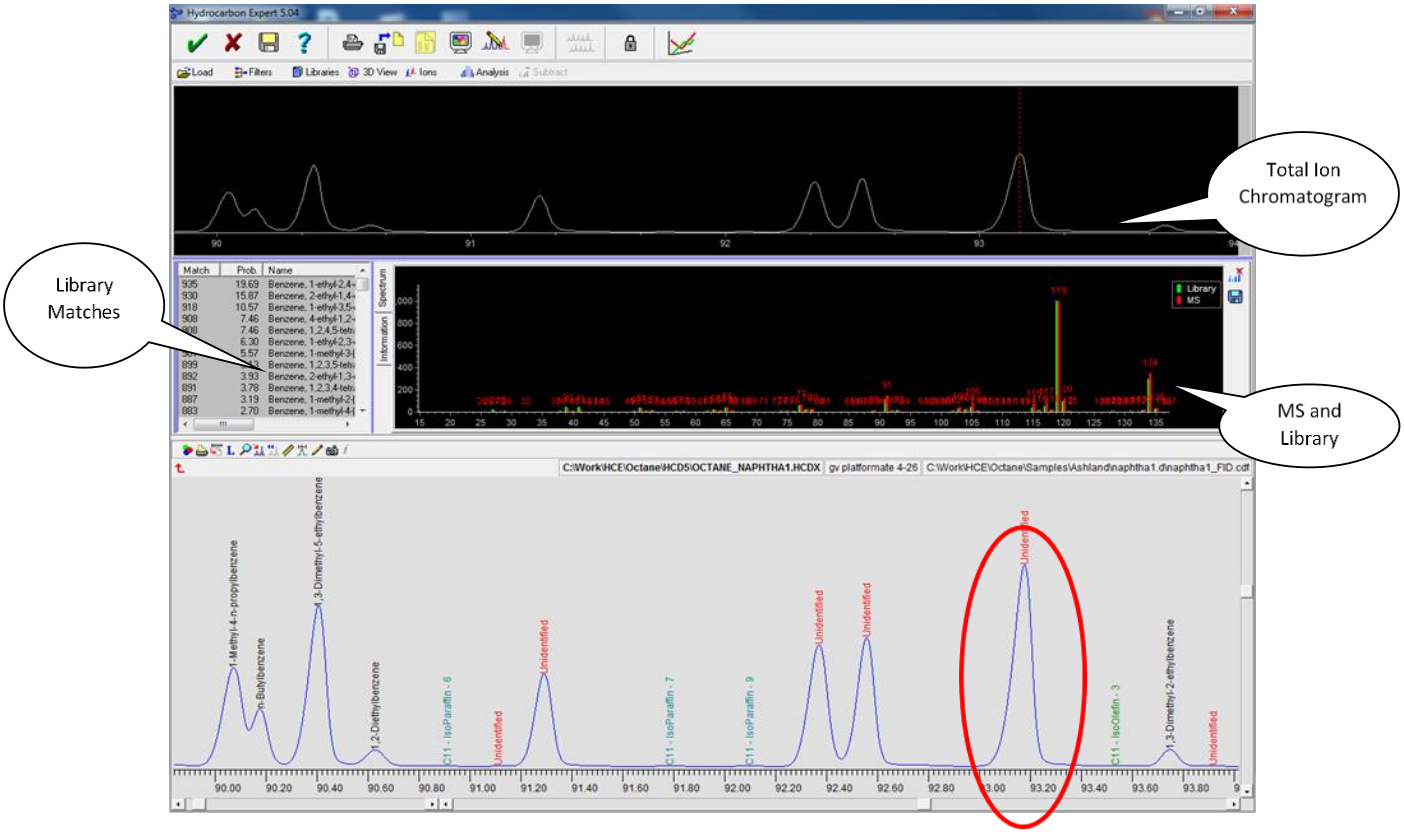


Figure 17 - Hydrocarbon Expert/MS screen showing chromatogram (bottom), total ion chromatogram (top), NIST library search results (left) and MS spectrum of the match with the greatest probability match % overlaid on the MS spectra for the unknown sample

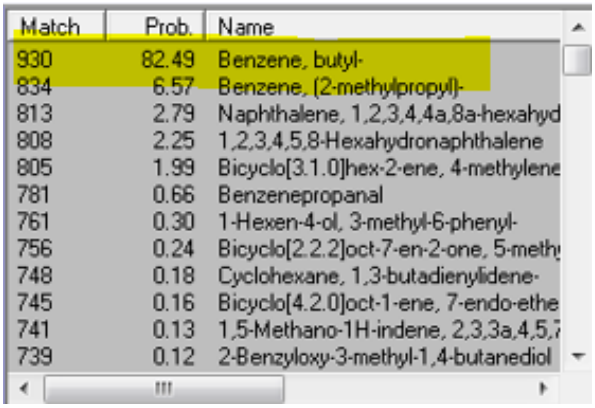


Figure 18 - An example NIST library search results

Identifying Components That Yield 'Inconclusive' Results from the NIST Library Search

A MS library search result with a ≥ 40% match probability criteria was generally accepted and used to identify the unknown component. 40% was selected because library search results for components with concentration ≥ 0.5 wt% almost always produce a match with at least a 40% probability match.

Unfortunately, most of the unidentified components were present in much smaller concentrations producing MS spectra with low ion intensities. Low ion intensities undermine the ability of the NIST library search to yield conclusive results. This was frequently the case in spite of considerable effort to increase the amount of column eluent entering the mass spectrometer (adjusting the effluent splitter or bypassing the FID and directing all of the effluent to the MS). Each time this was encountered, an in-depth investigation was undertaken to identify the component by its actual name or categorize it by group type and carbon number.

An in-depth investigation included: (1) reviewing the MS spectrum for each of the suspected compounds using the CAS number and/or component name (derived from the top yet inconclusive library search result) obtained from the NIST library or other web based sources (ex. NIST WebBook, ChemSpider), (2) selecting the most abundant ions in the MS spectrum, (3) enter the ion set values in the software to produce an extracted ion chromatogram, plot the chromatogram under the total ion chromatogram and (4) closely look at the ion traces and their apexes below the peak(s).

An example can be seen in Figure 19 for three peaks eluting between 61 and 63 minutes. Using the extracted ion chromatogram traces, the middle of the group was identified as a naphthene (blue) and the peaks on either side as isoparaffins (yellow). Since the NIST library search results yielded probabilities of 39%, 37 % and 30 % respectively the individual identities provided by NIST accepted and used. Please note, the ions 57 and 70 are also common to olefins. Since the degree of unsaturation for naphthenes and olefins is the same it may be difficult to assign identity. (See Appendix A for a more detailed summary of the ions used.)

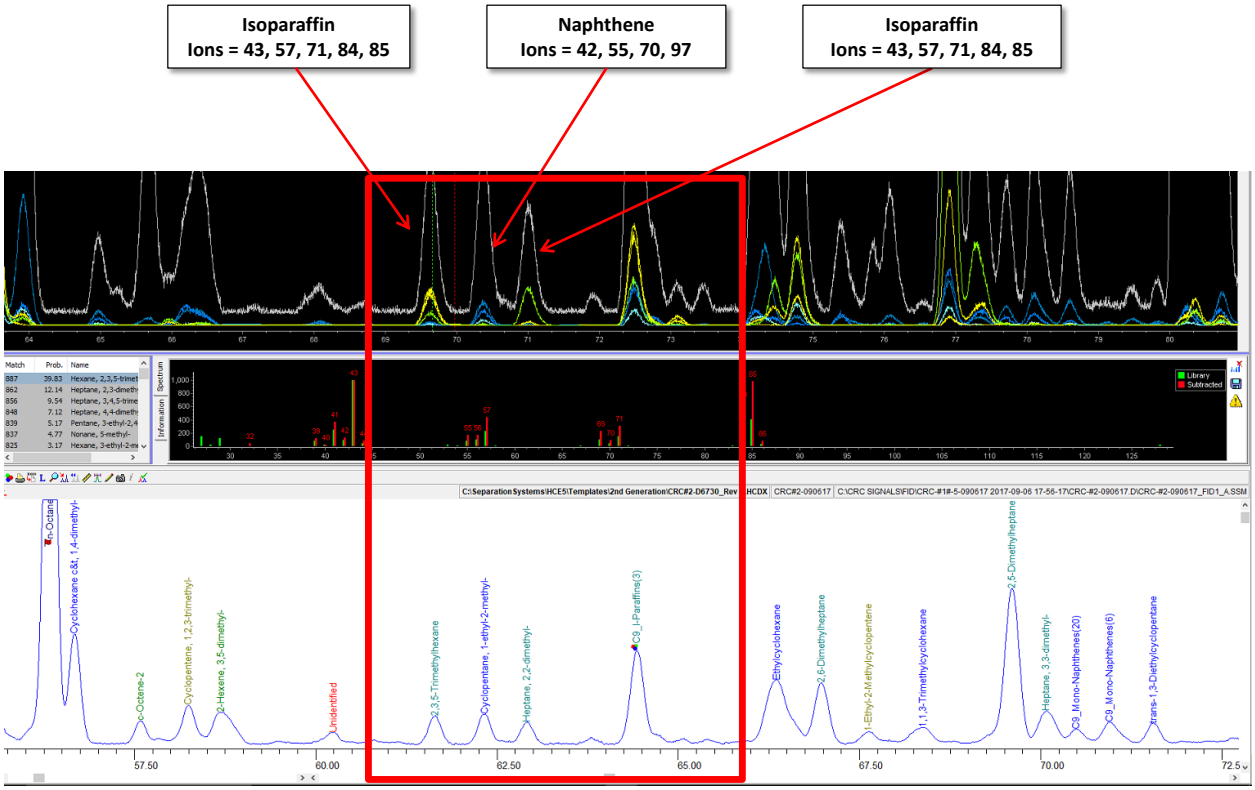


Figure 19 – Using Extracted Ion Current Profiles to Identify Unknown Components

Identifying co-eluting species is important whenever possible. In a co-elution the apex of an extracted ion will not coincide with the apex of one or more other extracted ions. In Figure 19 three different ions series were selected and a corresponding extracted ion current profile plotted under each peak (blue, yellow and green traces). A yellow dotted line is drawn through the apex of each ion series. You'll note the apex of the blue ion trace is different from the yellow ion trace. Also note, the apex of the ion series colored in green is distinct from the other 2 apices. The apex of the blue trace corresponds to an almost imperceptible shoulder on the leading edge of the large peak (isoparaffin). Because it's apex is different than the apex of the yellow ion series trace (indicating a mono-naphthene) there's co-elution with the large isoparaffin peak. The last apex (green colored trace) corresponds to the position of a component (another mono-naphthene) eluting under the descending slope of the large isoparaffin peak. When selecting the individual compound spectrum, it is necessary to subtract neighboring spectra to get an 'interference free' spectrum. Additionally, it is possible to eliminate suspected interference ions to improve the likelihood of correctly identifying an unknown compound. You can use the NIST library to view neighboring spectra and identify ions that may be interfering.

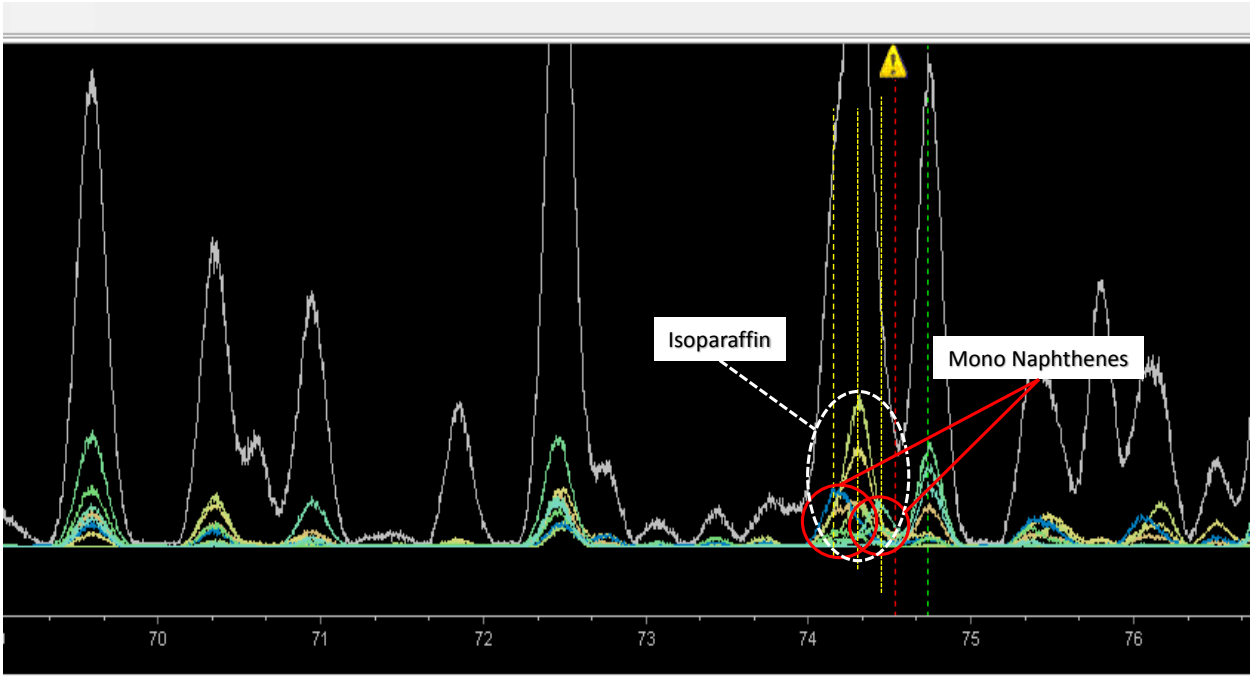


Figure 20 - A case of three co-eluting compounds; 2 mono naphthenes and one isoparaffin

Figure 20 is an example in which components were identified 'generically' due to a low match probability % using the NIST software. The ions 57 (yellow) and 71 (blue) were used for isoparaffin and ions 55 (purple) and 97 (green) were used for the naphthenic component.

The dotted lines drawn through the apexes of two compounds indicate partial separation. The FID chromatogram from the GC-FID system is depicted below the MS extracted ion chromatogram (Figure 21).

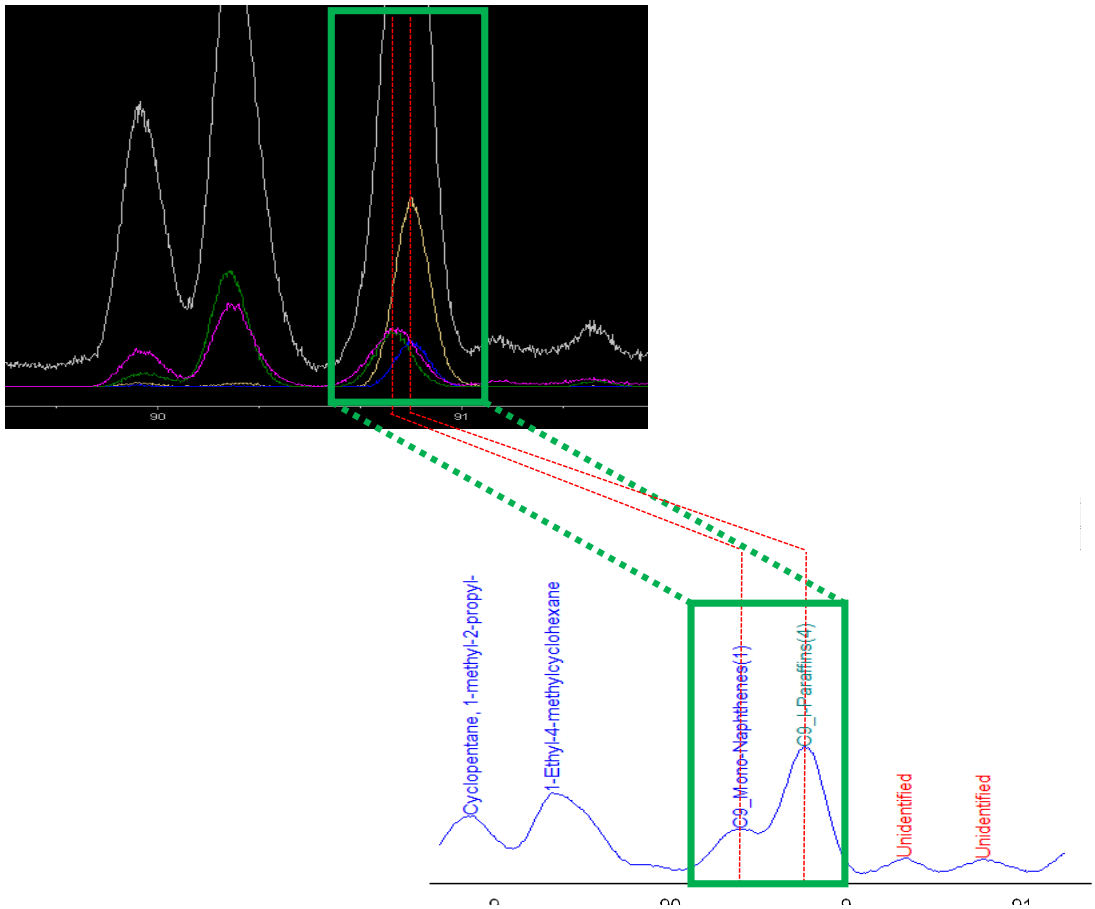


Figure 21– 'Generic' identification of co-eluting species.

GC-MS can be useful to quickly scan a section of the chromatogram where a number of components of the same group type elute. In Figure 22 an extracted ion chromatogram using ions at 91, 105 and 120 is displayed (on the top with black background). These are all alkyl substituted benzenes.

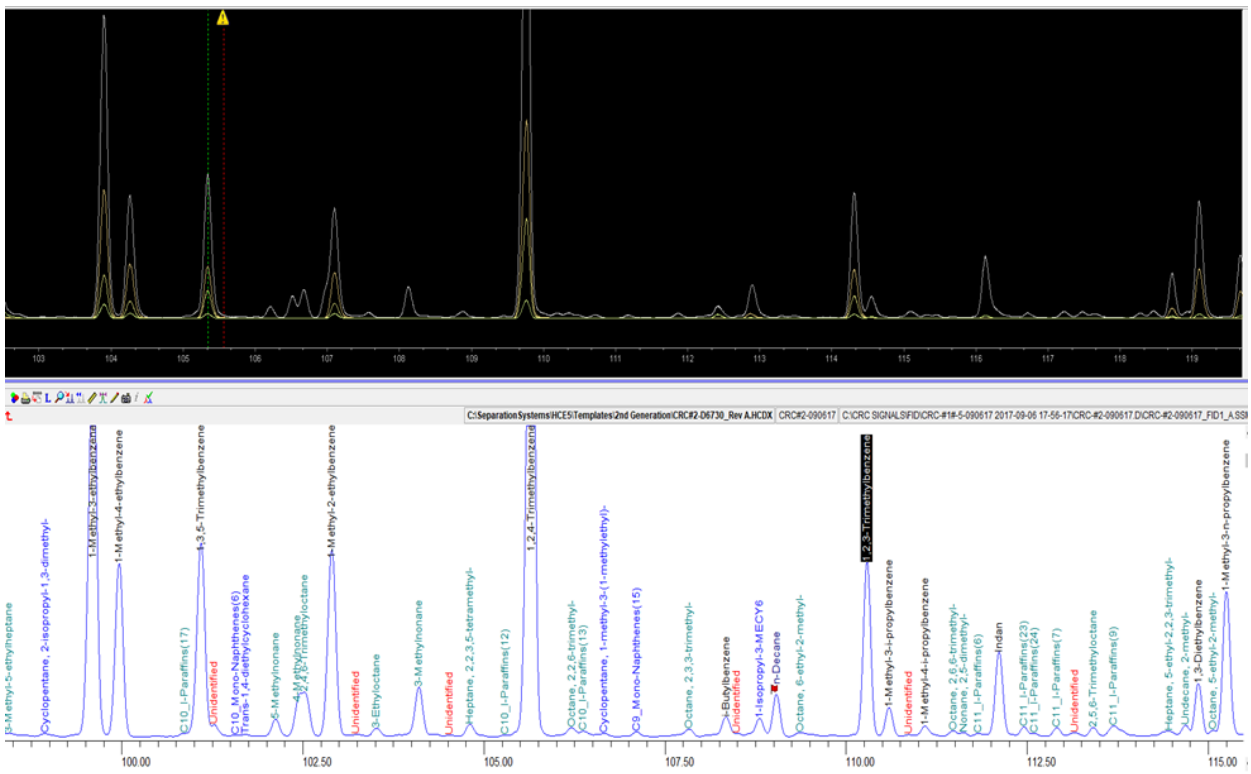


Figure 22 - Extracted ion profile for alkyl substituted benzene

Note, the time axis on the extracted ion chromatogram (top) is different from the time axis for the corresponding D6730 system (GC-FID) chromatogram on the bottom. This retention time difference is the result of choosing the MS ion spectrum from the Research System (GC-FID/MS) but using the chromatogram from the D6730 system. Both the FID and MS signals were obtained under the conditions of ASTM D6730-01(2016). The time discrepancy between the Research System and D6730 System is due to slight differences in the operational parameters between the two needed to ensure the same elution order and separation of critical component pairs.

When the concentration of the compound was low (<0.1 wt.%) and the probably of being able to identify it with a high degree of certainty using MS also low, we had to study the spectra very closely and consider the hydrocarbon types and carbon numbers suggested by NIST. This included inspecting the ions for the unknown component and comparing them with the ions listed in the NIST database. The most intense ions were chosen and plotted under the total ion chromatogram for the compound. Comparing the ions in the compound to the ions reported by NIST enabled us to choose the component's hydrocarbon type by looking for a recognizable MS ion sequence (i.e. +14 series). In a number of cases, we were able to use the presence of a parent ion (M^{+1}) to assign carbon number. In other cases, the carbon number was assigned based on the carbon number equal to the nearest named hydrocarbon compound of the same class. A boiling point was also assigned using the same logic.

Verifying the Integrity of Component Identification

As reported during the project, the CRC gasoline samples were analyzed individually and the identification of unknown components determined separately following the procedures described earlier in this report.

The MS software has no way to know if a name assigned to a newly identified component in the analysis of one of the gasoline samples was added earlier during the analysis of another gasoline sample. That's because each sample analysis has its own retention time/component name identification database template and the templates are not ''connected' in the software.

Therefore, it is quite important to compare the individual component identifications across all of the samples to make sure each component has a unique retention time. It is customary practice to name unknown components without other identification criteria. Doing so can corrupt the database by populating it with the same compound but at different retention times. This must be avoided.

The number of components identified in each of the CRC provided gasolines and reference material is as follows: [Sample# (# components)]: [CRC#1 (409)], [CRC#2 (384)], [CRC#3 (385)], [CRC#4 (368)], [CRC#5 (291)], [Reference Material-SD053 (471)].

When we started to compare the individual sample data files with each other we quickly found many components with the same name/identify had different retention times. Each sample has a database template associated with it from which compound identifications are assigned each containing ~794 components.

We also realized that manually reviewing every single inconsistency would be extremely time consuming potentially adding a month or more to the project timeline. A program was written (HCE 'Merger' – Figure 23) to facilitate our ability to do this.

The program loads multiple Hydrocarbon Expert component database templates and performs a comprehensive cross-check. If a named component (component with a CAS number) was found in multiple samples with a retention time that varied by more than 10 seconds from one another, it was flagged as a potential inconsistency. There were ~200 cases where this occurred.

'HCE Merger' was used to list all components with a retention index value that was either lower or higher than it should be based on its location relative to components before and after. For example, if a component was found to have a retention index of 830 but eluted between n-hexane and n-heptane (which have retention index values of 600 and 700 respectively) it was flagged. As an additional check, a component was flagged if its boiling point was >15 ^{o}C lower or higher than the components eluting before and after it.

Components were also flagged if they had the same retention time (+/- 10 seconds) but a different name or CAS number. These were more than likely cases of co-eluting species. This 'filter' was not applied to components assigned with the same 'generic' name.

Name	CASNO	CRC#1-D6730_Rev A	CRC#2-D6730_Rev A	CRC#3-D6730_Rev A	CRC#4-D6730_Rev A	CRC#5-D6730_Rev A
Naphthalene, 2-ethenyl-	827543		153.915			153.543
Cyclopentane, 1-ethyl-2-methyl-cis	930892		61.638		62.323	
Benzene, (1-ethylpropyl)-	1196583		124.003			123.793
1-Methyl-4-Hexylbenzene	1595013		151.428			151.632
1t,4t-Dimethylcyclohexane	2207047		58.682			58.862
1H-Indene, octahydro-, cis-	4551513		92.265		92.055	
1-Ethyl-2-i-propylbenzene	16021208			123.242	123.538	
1H-Indene, 2,3-dihydro-1,1,4-trimethyl-	16204721		139.380	139.192		
Naphthalene, 6-ethyl-1,2,3,4-tetrahydro-	22531200		151.027		148.378	

Figure 23- HCE 'Merger' Screen Showing Inconsistent Results for CRC#1 - CRC#5

Project Assessment

It is difficult to use the information found in ASTM D6730 -16 (Table A1.1) to determine whether or not the key project goal (to reduce 'unidentified' components to <0.5% by weight) was achieved. This is because there have been no major revisions to the method since its publication in 1995.

Table A1.1 contains: 308 compounds identified by name, 123 compounds with 'generic' names and 171 unidentified components.

A more relevant comparison can be found in Table 8 which shows the analysis results for the 5 CRC samples and the reference standard provided to the CRC at the start of the project ('Before') compared to the final results ('After').

	CRC #1		CRC #2		CRC #3		CRC #4		CRC #5		REF STD	
	Before	After	Before	After	Before	After	Before	After	Before	After	Before	After
GROUP	%WGT	%WGT	%WGT	%WGT	%WGT	%WGT	%WGT	%WGT	%WGT	%WGT	%WGT	%WGT
Paraffin	2.970	3.222	19.268	18.919	6.501	6.219	10.519	10.469	3.912	3.738	13.615	13.612
I-Paraffins	18.383	21.731	37.890	38.628	42.963	42.497	35.745	36.144	53.766	54.729	32.503	32.969
Aromatics	55.564	51.595	28.115	28.565	29.301	28.636	31.963	32.432	30.831	31.323	37.066	37.343
Mono-Aromatics	49.564	46.486	26.221	26.376	27.480	26.219	28.902	29.105	28.053	28.390	34.872	35.129
Naphthalenes	1.153	0.911	0.560	0.939	0.424	0.443	1.232	1.510	1.233	1.463	0.881	0.930
Indanes	4.605	4.027	1.232	1.233	1.308	1.852	1.586	1.817	1.484	1.470	1.205	1.231
Indenes	0.332	0.171	0.102	0.017	0.088	0.121	0.152	0.000	0.060	0.000	0.107	0.052
Naphthenes	9.191	11.623	5.502	5.993	3.783	3.979	7.141	9.075	5.306	5.077	4.834	4.973
Mono-Naphthenes	9.076	11.572	5.485	5.961	3.768	3.972	7.114	9.068	5.289	5.077	4.819	4.957
Di/Bicyclo-Naphthenes	0.115	0.052	0.016	0.033	0.015	0.007	0.027	0.007	0.017	0.000	0.016	0.016
Olefins	9.957	11.394	8.091	7.520	16.050	6.056	6.480	4.596	4.405	4.925	10.867	11.015
n-Olefins	2.252	2.250	2.900	2.724	2.250	2.077	1.430	1.520	0.056	0.010	3.512	3.286
Iso-Olefins	5.572	6.110	4.315	3.895	12.627	2.804	3.602	2.367	0.223	4.813	5.789	5.994
Naphtheno-Olefins	1.589	2.756	0.573	0.863	0.861	1.113	0.803	0.638	3.968	0.102	1.142	1.553
Di-Olefins	0.544	0.278	0.304	0.038	0.312	0.062	0.645	0.071	0.158	0.000	0.425	0.182
Oxygenates	0.000	0.000	0.000	0.000	0.000	12.282	6.410	7.119	0.000	0.000	0.000	0.000
Unidentified	3.845	0.434	1.134	0.374	1.402	0.332	1.743	0.164	1.780	0.208	1.115	0.088
C15+	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
PM Index	3.547	3.685	1.607	2.002	1.513	1.600	2.264	2.908	2.048	2.802	2.268	2.476

Table 8 - Summary of Weight % Values by Group Type for CRC Samples 1-5 and Reference Standard as well as a Comparison of 'Before' (beginning of the project) and 'After' the project (database described in Appendix C).

Table 8 depicts a summary of the 'Before' and 'After' analysis results by hydrocarbon group/sub group type for the five (5) CRC gasolines and the reference standard with breakdown by major group type (PIONA + oxygenates) also graphically represented n Figure 24.

Originally the software did not have sufficient boiling point data to calculate the PM index. However, using a boiling point correlation model developed by Honda and provided to us boiling points were calculated using a polynomial equation (See Appendix C for further detail. The reduction in unidentified components in the samples ranges from a factor of 8 to 3. The difference in the PM index ranges from 4% to 27% which is likely due to the significant reduction

in the number of unidentified components and the resulting change in the composition of the gasolines.

Sample CRC#3 contains MTBE which was missed in the initial analysis and reported incorrectly during one of the monthly project update meetings. This is reflected as a null entry for CRC#4 in Table 8. CRC#4 contains ethanol. The oxygenate response factors were obtained by injecting mixtures of the respective oxygenates with n-heptane at the 2% level resulting in values very close to those listed in D6730-01 (2016).

Identification of additional unknowns resulting in an increase in the calculated PMI value for all the samples.

Figures 24 – 26 breakdown data from Table 8.

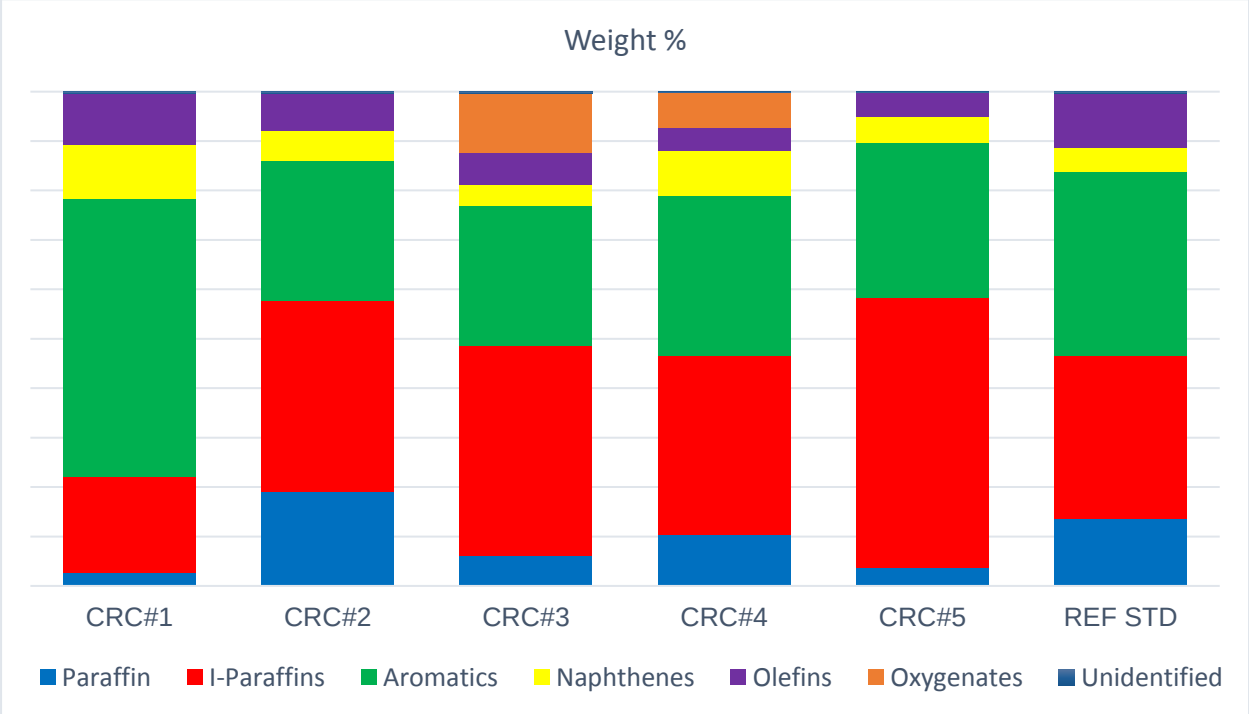


Figure 24 - Breakdown of CRC#1 to CRC#5 and Ref Standard by PIONA + Oxygenates

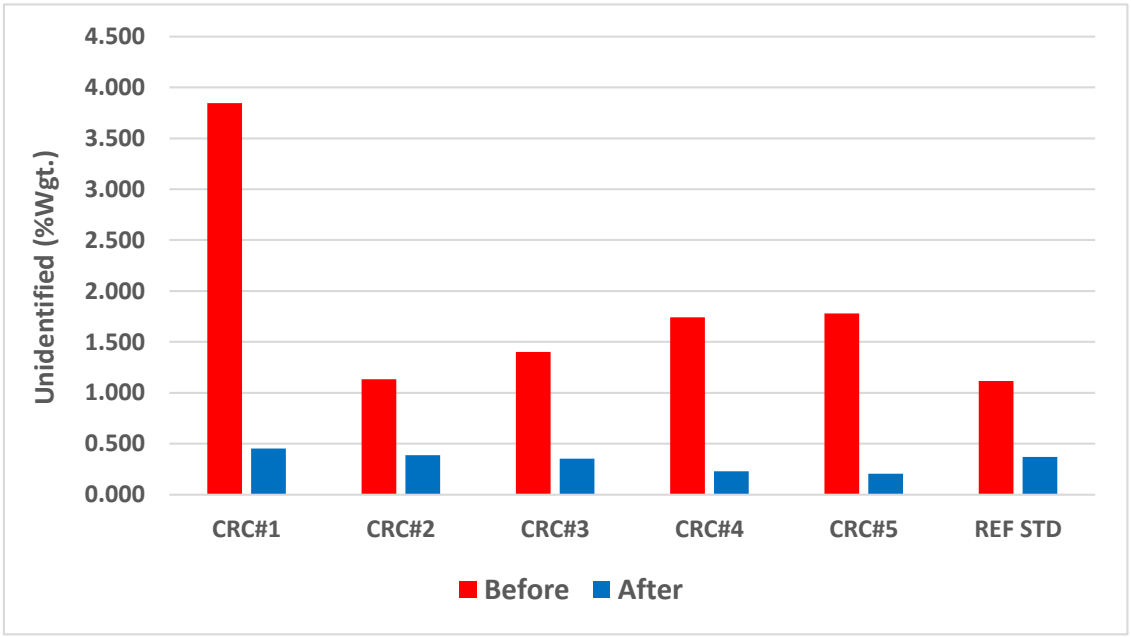


Figure 25 – Reduction in Unidentified Components in CRC#1-5 Gasolines and Reference Standard Before and at the End of the Project.

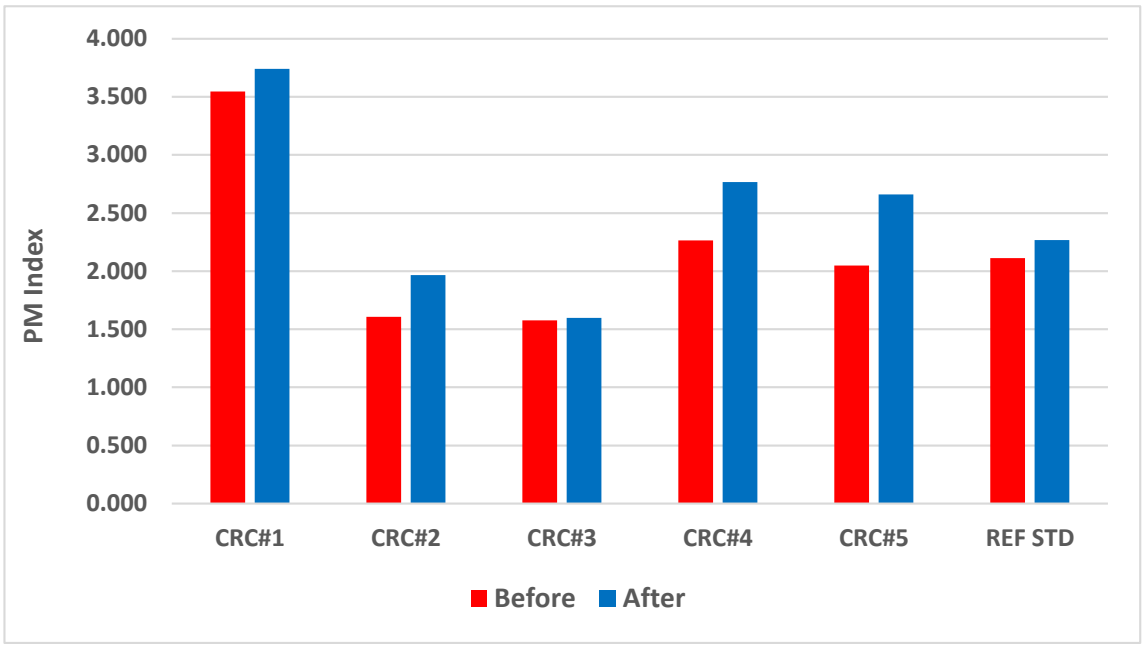


Figure 26 - Change in PM Index for CRC#1-5 Gasolines + Reference Standard Before and at the End of the Project

Final Results for CRC Gasolines Samples Reported by Hydrocarbon Group Type

Note: The final detailed results for CRC#1 through CRC#5 and the reference material are available as individual MS Excel files and were sent with this report.

SUMMARY BY GROUP	CRC #1				
GROUP	**%WGT**	**%VOL**	**%MOL**	**AVG MW**	**AVG SG**
Paraffin	2.787	3.222	2.782	3.115	0.022
I-Paraffins	19.130	21.731	19.159	21.377	0.154
Aromatics	56.338	51.595	53.713	62.956	0.454
Mono-Aromatics	50.125	46.486	48.443	56.013	0.404
Naphthalenes	1.167	0.911	1.000	1.304	0.009
Indanes	4.835	4.027	4.076	5.402	0.039
Indenes	0.212	0.171	0.195	0.237	0.002
Naphthenes	11.077	11.623	11.795	12.378	0.089
Mono-Naphthenes	11.019	11.572	11.748	12.314	0.089
Di/Bicyclo-Naphthenes	0.057	0.052	0.046	0.064	0.000
Olefins	10.226	11.394	12.222	11.427	0.082
n-Olefins	1.912	2.250	2.396	2.137	0.015
Iso-Olefins	5.343	6.110	6.299	5.970	0.043
Naphtheno-Olefins	2.722	2.756	3.232	3.041	0.022
Di-Olefins	0.250	0.278	0.296	0.279	0.002
Oxygenates	0.000	0.000	0.000	0.000	0.000
Unidentified	0.441	0.434	0.329	0.493	0.004
C15+	0.000	0.000	0.000	0.000	0.000

SUMMARY BY GROUP	CRC #2				
GROUP	**%WGT**	**%VOL**	**%MOL**	**AVG MW**	**AVG SG**
Paraffin	18.919	21.696	23.822	17.387	0.135
I-Paraffins	38.628	41.207	38.395	35.500	0.276
Aromatics	28.565	23.290	23.118	26.252	0.204
Mono-Aromatics	26.376	21.707	21.643	24.240	0.189
Naphthalenes	0.939	0.660	0.613	0.863	0.007
Indanes	1.233	0.911	0.851	1.133	0.009
Indenes	0.017	0.012	0.011	0.016	0.000
Naphthenes	5.993	5.624	5.808	5.508	0.043
Mono-Naphthenes	5.961	5.598	5.786	5.478	0.043
Di/Bicyclo-Naphthenes	0.033	0.026	0.022	0.030	0.000
Olefins	7.520	7.855	8.628	6.911	0.054
n-Olefins	2.724	2.985	3.421	2.503	0.019
Iso-Olefins	3.895	4.056	4.278	3.580	0.028
Naphtheno-Olefins	0.863	0.777	0.893	0.794	0.006
Di-Olefins	0.038	0.037	0.036	0.035	0.000
Oxygenates	0.000	0.000	0.000	0.000	0.000
Unidentified	0.374	0.326	0.229	0.344	0.003
C15+	0.000	0.000	0.000	0.000	0.000

SUMMARY BY GROUP	CRC #3				
GROUP	%WGT	%VOL	%MOL	AVG MW	AVG SG
Paraffin	6.219	7.229	8.015	6.081	0.046
I-Paraffins	42.497	45.958	41.808	41.558	0.312
Aromatics	28.636	23.968	24.874	28.003	0.210
Mono-Aromatics	26.219	22.147	23.092	25.640	0.193
Naphthalenes	0.443	0.317	0.323	0.434	0.003
Indanes	1.852	1.405	1.369	1.811	0.014
Indenes	0.121	0.100	0.091	0.118	0.001
Naphthenes	3.979	3.818	3.988	3.891	0.029
Mono-Naphthenes	3.972	3.812	3.983	3.884	0.029
Di/Bicyclo-Naphthenes	0.007	0.006	0.005	0.007	0.000
Olefins	6.056	6.462	7.473	5.922	0.044
n-Olefins	2.077	2.337	2.778	2.031	0.015
Iso-Olefins	2.804	3.035	3.424	2.742	0.021
Naphtheno-Olefins	1.113	1.025	1.198	1.088	0.008
Di-Olefins	0.062	0.065	0.072	0.061	0.000
Oxygenates	12.282	12.267	13.625	12.011	0.090
Unidentified	0.332	0.297	0.216	0.325	0.002
C15+	0.000	0.000	0.000	0.000	0.000

SUMMARY BY GROUP	CRC #4				
GROUP	%WGT	%VOL	%MOL	AVG MW	AVG SG
Paraffin	10.469	11.869	11.150	9.725	0.078
I-Paraffins	36.144	39.892	35.164	33.577	0.270
Aromatics	32.432	27.543	25.865	30.129	0.242
Mono-Aromatics	29.105	25.010	23.602	27.038	0.217
Naphthalenes	1.510	1.125	0.985	1.402	0.011
Indanes	1.817	1.409	1.278	1.688	0.014
Indenes	0.000	0.000	0.000	0.000	0.000
Naphthenes	9.075	8.823	8.140	8.431	0.068
Mono-Naphthenes	9.068	8.817	8.135	8.424	0.068
Di/Bicyclo-Naphthenes	0.007	0.005	0.004	0.006	0.000
Olefins	4.596	4.983	5.224	4.270	0.034
n-Olefins	1.520	1.733	1.896	1.412	0.011
Iso-Olefins	2.367	2.571	2.624	2.199	0.018
Naphtheno-Olefins	0.638	0.607	0.643	0.593	0.005
Di-Olefins	0.071	0.072	0.060	0.066	0.001
Oxygenates	7.119	6.740	14.355	6.613	0.053
Unidentified	0.164	0.150	0.102	0.153	0.001
C15+	0.000	0.000	0.000	0.000	0.000

SUMMARY BY GROUP	CRC #5				
GROUP	%WGT	%VOL	%MOL	AVG MW	AVG SG
Paraffin	3.738	4.463	5.361	3.781	0.027
I-Paraffins	54.729	59.209	56.040	55.358	0.402
Aromatics	31.323	26.213	28.190	31.683	0.230
Mono-Aromatics	28.390	24.036	26.035	28.716	0.209
Naphthalenes	1.463	1.059	1.033	1.480	0.011
Indanes	1.470	1.118	1.122	1.487	0.011
Indenes	0.000	0.000	0.000	0.000	0.000
Naphthenes	5.077	4.903	5.818	5.135	0.037
Mono-Naphthenes	5.077	4.903	5.818	5.135	0.037
Di/Bicyclo-Naphthenes	0.000	0.000	0.000	0.000	0.000
Olefins	4.925	5.026	4.450	4.982	0.036
n-Olefins	0.010	0.010	0.008	0.010	0.000
Iso-Olefins	4.813	4.917	4.356	4.868	0.035
Naphtheno-Olefins	0.102	0.099	0.085	0.103	0.001
Di-Olefins	0.000	0.000	0.000	0.000	0.000
Oxygenates	0.000	0.000	0.000	0.000	0.000
Unidentified	0.208	0.187	0.140	0.211	0.002
C15+	0.000	0.000	0.000	0.000	0.000

SUMMARY BY GROUP	SD-053 REFERENCE STANDARD				
GROUP	%WGT	%VOL	%MOL	AVG MW	AVG SG
Paraffin	13.612	15.444	15.324	13.416	0.101
I-Paraffins	32.969	36.074	32.957	32.494	0.245
Aromatics	37.343	31.738	33.599	36.806	0.278
Mono-Aromatics	35.129	30.071	31.995	34.624	0.261
Naphthalenes	0.930	0.679	0.655	0.917	0.007
Indanes	1.231	0.946	0.907	1.214	0.009
Indenes	0.052	0.041	0.042	0.051	0.000
Naphthenes	4.973	4.845	4.998	4.902	0.037
Mono-Naphthenes	4.957	4.832	4.987	4.886	0.037
Di/Bicyclo-Naphthenes	0.016	0.013	0.011	0.016	0.000
Olefins	11.015	11.820	13.063	10.857	0.082
n-Olefins	3.286	3.718	4.313	3.238	0.024
Iso-Olefins	5.994	6.456	6.856	5.908	0.045
Naphtheno-Olefins	1.553	1.456	1.694	1.530	0.012
Di-Olefins	0.182	0.189	0.200	0.180	0.001
Oxygenates	0.000	0.000	0.000	0.000	0.000
Unidentified	0.088	0.080	0.058	0.087	0.001
C15+	0.000	0.000	0.000	0.000	0.000

Conclusions

- The project results underscore how indispensable GC-MS is for the identification of unknown hydrocarbon components by name or categorizing them by carbon number/group type.

- Although GC-FID or GC-MS can be used for 'enhanced speciation of gasoline' the instrumental operating parameters are slightly different due to the need to retain elution order and meet critical separation criteria.

- Approximately 200 new compounds were individually identified through the course of the project and added to the identification tables which resulted in a reduction in the amount of unidentified components from 1 – 3 % (typically obtained via D6730) to <0.5 %. It is important to note that the characterization '200 new components' was arrived at by comparing the number of identified components in the retention time/component name database contained in Separation Systems Hydrocarbon Expert™ at the end of the project to the number of components contained in it before the project started. Labs using DHA software different from the one used in this project should update their database using the data presented in this project. A complete list of the data base is provided in Appendix C similar the format found in Table 3 in ASTM D6730. The list extends the number of components to 822 compounds.

- Furthermore, many of the compounds eluted after 1-methylnaphthalene and were identified by name and added to the identification tables. This increased PMI values for all 5 samples analyzed in this study. Comparison of the PMI calculated before and after shows increases ranging from 2% for sample CRC#3 to 29% for sample CRC#5.

- In spite of all the effort and time devoted to this project some co-eluting compounds could not be identified with a reasonable degree of certainty. However, the unidentified components comprise a small percentage (<0.5 wt%) of the SD-053 reference material. We believe further investigation is warranted to determine if the unidentified components can be at least categorized by hydrocarbon group and carbon number.

Recommendations

- The results of this project should be presented to ASTM's D02.04 subcommittee (Petroleum Products, Liquid Fuels, and Lubricants -Hydrocarbon Analysis) with the intention of refining and promulgating an 'enhanced DHA of gasolines' methodology by ASTM. We believe the most expeditious way to accomplish this would be to add the method as an addendum to D6730-01(2016).

- Undertake an extensive investigation to determine whether the response factors for naphthalene compounds experimentally measured in this study can be determined with a high degree of precision. And, if so, work with ASTM to determine if the response factor values should replace those currently described in ASTM D6730 (Table 3) (which were used to produce the analysis results in this study). The lower value(s) (6.7 to 7.1%) could significantly affect the accuracy of the PMI calculation.
- Conduct a study to analyze gasoline refinery blend components containing higher amounts (>0.5 wt%) of compounds characterized as 'trace' in this project. The possible outcomes would include the ability to identify some of the compounds by name and not only by Group Type and Carbon Number, improved integration of co-eluting peaks and more accurate determination of vapor pressures and boiling points.

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Appendix

Appendix A

Select MS Ions Used to Identify Components By Hydrocarbon Type

Type of Hydrocarbon	C#	Target Ions (M/E) Most Abundant > > > > > Least Abundant									
Normal Paraffins	4	43	29	27	28	41	39	58	42	15	26
	5	43	42	41	57	39	27	72	55	56	
	6	57	43	41	29	27	56	42	39	86	28
	7	43	41	29	57	27	71	56	42	39	70
	8	43	41	57	29	85	71	27	56	42	39
	9	43	57	41	85	71	29	56	70	42	27
	10	57	43	41	71	85	56	29	55	42	70
	11	57	43	71	41	85	29	56	70	55	42
	12	57	43	71	41	85	55	56	29	70	42
	13	57	43	71	41	85	29	56	55	27	42
	14	57	43	71	85	41	29	55	56	70	42
	15	57	43	71	85	41	29	55	56	70	99
Isoparaffins	4	43	41	42	27	39					
	5	43	42	41	57	27	29	39			
	6	43	57	71	41	29	56	27			
	7	43	57	41	56	42	27	29			
	7	57	43	56	41	85	29	27			
	8	57	56	51	43	29	99	39			
	9	57	43	56	41	29	98	99			
highly branched	9	43	85	41	57	84	27	71	69		
	10	57	43	71	41	70	29				
highly branched	10	43	85	57	41	56	84	39	71	42	69
	11	57	43	85	41	84	56	29	99	71	70
	12	57	43	71	41	85	84	56	55	29	42
	13	43	71	57	70	85	41	55	29	27	56
Olefins	5	42	55	41	70	39	29	27	40		
	6	55	41	42	84	69	56	39	27		
	7	56	41	55	29	42	70	69	57	39	27
	8	43	55	56	70	41	42	69	29	83	39
	9	55	41	56	69	70	39	126	27	42	43
	10	55	69	41	70	43	42	29	57	27	
Iso -Olefins	5	55	70	42	39	41	29	27	53	56	70
	6	55	69	41	56	39	27	84	29	53	
	7	69	41	55	39	98	27	56	83	53	70
	8	56	55	41	69	84	112	70	42	39	43
	9	69	41	56	55	39	126	70	27	67	
	10	55	69	41	70	27	29	140	39	43	83
	11	83	55	69	70	84	41	154	43	56	57
	12	43	69	55	41	56	57	70	29	84	83
Naphtheno-olefins	5	67	68	39	53	41	40	27	42	66	65
	6	67	82	39	41	27	81	54	53	65	51
	7	81	39	27	96	41	53	79	55	67	
	8	67	95	41	110	39	69	66	68	81	55
	9	81	82	67	41	79	95	39	55	124	53
	10	55	67	41	81	82	39	83	57	27	80
Di-Olefins	5	67	68	53	39	40	41	27	51	42	65
	6	67	39	82	41	65	28	53	27	54	81
	7	55	81	39	29	67	54	27	41	53	68
	8	95	41	67	39	55	110	27	53	42	69
	9	69	41	81	67	39	27	80	53	68	29

Type of Hydrocarbon	C#	Target Ions (M/E) Most Abundant > > > > > Least Abundant									
Naphthene	5	41	42	55	70						
	6	41	56	69	84						
	7	41	55	69	83	98					
	8	41	55	69	97	112					
	9	41	55	69	97	126					
	10	41	55	69	97	111	140				
Naphthenes with large side chains	10	41	55	67	82	83	11	140			
	12	27	41	55	69	83	95	109			
Di-Bicyclo-naphthenes	10	67	138	68	82	96	81	41	95	39	55
Mono -Aromatics	6	78	77	51	50	52	39				
	7	91	92	65	39	63	51				
	8	91	106	105	77	65	79				
	9	105	120	119	77	106	91				
	10	119	105	134	91	77	120	106			
	11	133	105	148	91	93	41				
	12	119	134	91	105	39	120	77			
	13	105	106	176	91	92	77	79			
Naphthalene - 1,2,3,4-tetrahydro or tetralin	10	104	132	91	59	39	131				
	12	145	160	132	145	117	119	128			
	13	170	155	153	154	171					
Naphthalenes											
Mono-Alkyl	11	142	141	115	139						
Di-Alkyl	12	156	141	155							
Tri-Alkyl	13	155	170	153	152						
Indanes	9	117	118	115	91	58					
	10	117	132	115	91	39					
	11	131	146	145	115	129	128				
	12	145	160	146	117	91	128				
Indenes	10	130	115	129	128	131					

Note: The information contained in this table is not meant to be used nor should it be used as a sole source for MS spectral interpretation. We encourage interested readers to also utilize 'published' sources. For example: McLafferty, F.W and Turecek, F (1993); 'Interpretation of Mass Spectra 4th Edition; University Science Books, 20 Edgehill Road Mill Valley, CA 94941

Appendix B

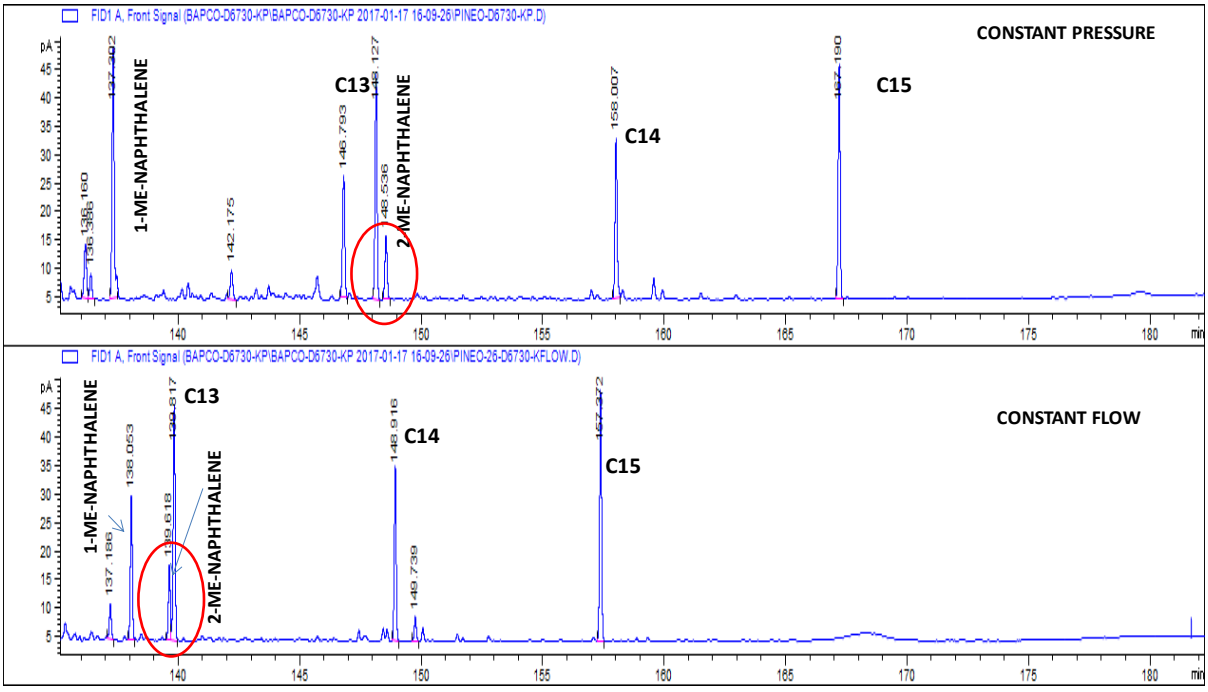
Constant Pressure versus Constant Flow

The following described the use of Constant Pressure or Constant Flow for ASTM D6730-01-16.

When operating the GC using constant (column) pressure, as the temperature of the column is increased flow rate (due to oven temperature programming) through the column decreases. On the other hand, the constant flow is used, as the temperature of the column increases, the flow rate is remains constant. Constant flow is maintained through the use of a digital pneumatic control which changes the column head pressure as needed to ensure a constant flow rate through the column.

Maintaining a constant flow rate is desirable because the optimum flow (usually set at a low column temperature) is maintained throughout the analysis. However, the results below show that critical component separations can be negatively affected. Note in the figure below, the separation of n-C13 and 1-methylnaphthalene was not nearly as good using constant flow as it was using constant pressure.

Because of this phenomenon, all of the analyses conducted in this project were made in the constant pressure mode as stated in the method.



Constant pressure vs constant flow and how each affects the separation of n-C13 and 2-methylnaphthalene

Appendix C

Calculating the Particulate Matter Index (PMI)

$$PMI = \sum_{i=1}^{i=N} \frac{DBEi+1}{VPi_{443K}} \times W_i$$

Where:

- *DBE* is the double bond equivalence of the component.
- VP_{443K} is the Vapor Pressure at 443K in kPa.

  Note: Although the vapor pressure at 443K for an individual component can be calculated from its boiling point using Antoine's Equation (below) values for this study were calculated using a polynomial equation (also below) based on a boiling point / vapor pressure correlation model developed by Honda [2]

- W_i is the % by weight determined from the analysis for the i component
- The product of the two terms in Equation 1 are summed for all components analyzed.

Antoine Equation

$$Log\ P_{10} = A\text{-}B\ /\ (T + C)$$

Where:

- *A, B* and *C* are Antoine Constants[1].
- *T* is the temperature in degrees *C* and *P* is the vapor pressure in mm Hg. The conversion to kPa is 0.1333223 kPa / mm Hg

Polynomial Equation Based on the Honda Correlation Model

= EXP(8.34075219000144E-16*BPK^6 - 2.5368233313227E-12* BPK ^5 + 3.10013311128862E-09* BPK ^4 - 2.02889046987065E-06* BPK ^3 + 0.00074715534189591* BPK ^2 - 0.167354730090773* BPK + 26.0923223622962)

Appendix D

List of all the components in the final database

COMPONENT	RI	TIME	RRF	MW	SG	DBE	VP	PMI Factor
Methane	100.00	6.944	1.1210	16.043	0.4150	0	1683756.034187	5.939103E-07
Ethene	175.17	7.038	0.9800	28.000	0.0013	1	103634.711914	1.929855E-05
Ethane	200.00	7.069	1.0510	30.070	1.0493	0	59130.708114	1.691169E-05
Propene	278.11	7.288	0.9800	42.080	1.4900	1	16956.924549	1.179459E-04
Propane	300.00	7.350	1.0270	44.097	0.4930	0	14398.011154	6.945404E-05
i-Butane	354.37	8.437	1.0150	58.124	0.5509	0	6655.456457	1.502527E-04
Methanol	364.49	8.656	3.2000	32.040	0.7920	0	1154.116353	8.664638E-04
Isobutene	385.80	9.137	0.9800	56.108	0.5890	1	5928.044211	3.373794E-04
Butene-1	387.31	9.172	0.9800	56.108	0.5770	1	5237.389793	3.818696E-04
1,3 BUTADIENE	394.49	9.340	0.9447	54.000	0.6120	2	3918.957873	7.655096E-04
n-Butane	400.00	9.472	1.0150	58.124	0.5730	0	5090.845105	1.964310E-04
Vinyl-Acetylene	407.74	9.817	0.9095	52.032	0.7095	3	4463.527550	8.961522E-04
Cyclobutane	408.69	9.860	0.9799	56.064	0.7038	1	3759.431967	5.319953E-04
t-Butene-2	409.28	9.887	0.9800	56.108	0.5990	1	4925.504236	4.060498E-04
2,2-Dimethylpropane	411.50	9.988	1.0080	72.151	0.5910	0	4250.319227	2.352764E-04
c-Butene-2	422.45	10.507	0.9800	56.108	0.6160	1	4612.073488	4.336444E-04
1,2-Butadiene	438.97	11.340	0.9450	54.092	0.6760	2	3900.880110	7.690572E-04
Ethanol	448.58	11.855	1.6100	46.070	0.7890	0	853.960101	1.171015E-03
3-Methylbutene-1	454.14	12.163	0.9800	70.135	0.6213	1	3158.313500	6.332494E-04
i-Pentane	472.50	13.240	1.0080	72.151	0.6196	0	2523.273101	3.963106E-04
1,4-Pentadiene	474.24	13.346	0.9520	68.119	0.6607	2	2575.048815	1.165026E-03
Butyne-2	475.43	13.420	0.9450	54.092	0.6940	2	2787.173641	1.076359E-03
Pentene-1	488.47	14.253	0.9800	70.135	0.6405	1	2204.597601	9.071950E-04
i-Propanol	489.28	14.307	1.4000	60.110	0.7851	0	578.910151	1.727384E-03
2-Methylbutene-1	495.73	14.740	0.9800	70.135	0.6504	1	2455.918145	8.143594E-04
n-Pentane	500.00	15.033	1.0080	72.151	0.6262	0	2244.560837	4.455215E-04
2-Methyl-1,3-Butadiene	505.21	15.370	0.9520	68.119	0.6790	2	2300.735663	1.303931E-03
t-Pentene-2	509.21	15.633	0.9800	70.135	0.6431	1	2155.673373	9.277843E-04
3,3-Dimethylbutene-1	514.70	16.002	0.9799	84.096	0.6850	1	1962.077649	1.019328E-03
t-Butanol	515.74	16.073	1.3000	74.122	0.7887	0	772.124856	1.295127E-03
c-Pentene-2	517.38	16.185	0.9800	70.135	0.6556	1	2254.668014	8.870486E-04
2-Methylbutene-2	522.34	16.530	0.9800	70.135	0.6600	1	2254.668014	8.870486E-04
1t,3-Pentadiene	525.15	16.728	0.9520	68.119	0.6710	2	1838.882388	1.631426E-03
3-Methylbutadiene-1,2	526.42	16.819	0.9520	68.120	0.6510	2	1872.056201	1.602516E-03
1,3-Cyclopentadiene	535.05	17.447	0.9520	68.064	0.6820	2	1838.882388	1.631426E-03
2,2-Dimethylbutane	537.02	17.593	1.0040	86.178	0.6444	0	1670.557006	5.986027E-04
Cyclopentene	553.86	18.898	0.9520	68.119	0.7740	2	1834.778050	1.635075E-03
n-Propanol	554.73	18.968	1.4000	60.110	0.8053	0	560.870254	1.782944E-03
4-Methylpentene-1-trans	558.26	19.255	0.9800	84.162	0.6650	1	1338.345377	1.494383E-03
3-Methylpentene-1	559.16	19.328	0.9800	84.162	0.6830	1	1403.986966	1.424515E-03
Cyclopentane	563.84	19.717	0.9800	70.135	0.7454	1	1637.355240	1.221482E-03
2,3-Dimethylbutane	566.04	19.902	1.0040	86.178	0.6616	0	1327.954606	7.530378E-04
Methyl-t-butyl ether	567.24	20.003	1.4300	88.150	0.7353	0	1435.609899	6.965681E-04
2,3-Dimethylbutene-1	567.75	20.047	0.9800	84.162	0.6850	1	1422.875713	1.405604E-03
2-Pentene-CIS- ,4-methyl	569.50	20.197	0.9798	84.096	0.6920	1	1379.193101	1.450123E-03
2-Methylpentane	570.73	20.302	1.0040	86.178	0.6550	0	1301.604840	7.682823E-04
4-Methyl-t-pentene-2-E	572.46	20.452	0.9800	84.162	0.6736	1	1097.687455	1.822012E-03
2-Methyl-1,4-pentadiene	579.41	21.064	0.9564	82.146	0.6980	2	1410.255057	2.127275E-03

COMPONENT	RI	TIME	RRF	MW	SG	DBE	VP	PMI Factor
1,5-Hexadiene	579.83	21.102	0.9564	82.146	0.6970	2	1348.817601	2.224170E-03
3-Methylpentane	583.77	21.458	1.0040	86.178	0.6643	0	1214.780368	8.231941E-04
2-Methylpentene-1	588.85	21.927	0.9800	84.162	0.6848	1	1233.866234	1.620921E-03
Hexene-1	589.83	22.018	0.9800	84.162	0.6731	1	1233.866234	1.620921E-03
1c/t,4-Hexadiene	590.72	22.101	0.9564	82.080	0.7000	2	1154.116353	2.599391E-03
2-Butanol	592.14	22.235	1.3000	74.079	0.8063	0	532.404294	1.878272E-03
2-Ethylbutene-1	599.47	22.938	0.9800	84.162	0.6870	1	1233.866234	1.620921E-03
n-Hexane	600.00	22.990	1.0040	86.178	0.6606	0	1062.781439	9.409272E-04
t-Hexene-3	602.51	23.223	0.9800	84.162	0.6940	1	1138.792907	1.756246E-03
c-Hexene-3	603.29	23.297	0.9800	84.162	0.6847	1	1086.976892	1.839966E-03
t-Hexene-2	604.94	23.452	0.9800	84.162	0.6600	1	1081.901620	1.848597E-03
2-Methylpentene-2	607.18	23.663	0.9800	84.162	0.6950	1	1096.465095	1.824043E-03
3-Methylcyclopentene	608.19	23.760	0.9564	82.146	0.8050	2	1156.690112	2.593607E-03
3-Methyl-c-pentene-2	609.82	23.917	0.9800	84.162	0.6980	1	1086.734678	1.840376E-03
4-methylcyclopentene	611.24	24.053	0.9564	82.146	0.8050	2	1136.258729	2.640244E-03
c-Hexene-2	613.67	24.290	0.9800	84.162	0.6920	1	1086.976892	1.839966E-03
iso-Butanol	616.21	24.539	1.3000	74.079	0.8018	0	438.780623	2.279043E-03
1c/t,3-Hexadiene	616.91	24.609	0.9564	82.146	0.7060	2	961.294531	3.120792E-03
4,4-Dimethyl-t-pentene-2	617.73	24.690	0.9800	98.189	0.7120	1	889.021837	2.249664E-03
3,3-Dimethylpentene-1	619.59	24.875	0.9800	98.189	0.7050	1	833.204867	2.400370E-03
2-Pentene, 3-methyl-	619.59	24.875	0.9799	84.000	0.6950	1	1164.445683	1.717555E-03
3-Methyl-t-pentene-2	620.88	25.005	0.9800	84.162	0.6950	1	1164.445683	1.717555E-03
tert-Butyl-Ethyl-Ether	620.97	25.014	1.4300	102.111	0.7360	0	1032.422189	9.685960E-04
2,2-Dimethylpentane	622.75	25.193	1.0000	100.205	0.6950	0	865.493879	1.155410E-03
Methylcyclopentane	624.88	25.410	0.9800	84.162	0.7486	1	991.797150	2.016541E-03
2-Pentene, 4,4-dimethyl-	626.76	25.603	0.9800	98.189	0.7120	1	889.021837	2.249664E-03
2,4-Dimethylpentane	628.92	25.827	1.0000	100.205	0.6910	0	816.591517	1.224602E-03
2-Pentene-c&t-, 4-methyl-	629.74	25.912	0.9800	84.162	0.6920	1	1310.329436	1.526334E-03
2,3,3-Trimethylbutene-1	631.23	26.068	0.9800	98.189	0.7060	1	838.815850	2.384314E-03
4-Methyl-1,3-pentadiene	633.10	26.265	0.9564	82.146	0.7070	2	893.003746	3.359448E-03
2,2,3-Trimethylbutane	633.34	26.290	1.0000	100.205	0.6930	0	794.943716	1.257951E-03
1,3-Pentadiene, 2-methyl-, (E)-	634.64	26.428	0.9564	82.146	0.6940	2	923.431957	3.248750E-03
C6_Naphtheno-Olefins(1)	636.84	26.663	0.9800	82.146	0.7622	2	1156.690112	2.593607E-03
3,4-Dimethylpentene-1	640.22	27.028	0.9800	98.189	0.7010	1	833.204867	2.400370E-03
C6_Naphtheno-Olefins(2)	641.32	27.148	0.9800	82.146	0.7622	2	1156.690112	2.593607E-03
2,4-Dimethylpentene-1	644.76	27.527	0.9800	98.189	0.7040	1	736.607489	2.715150E-03
C6_Naphtheno-Olefins(3)	646.18	27.683	0.9800	82.146	0.7622	2	1156.690112	2.593607E-03
1,3-Pentadiene, 2,3-dimethyl-	646.18	27.683	0.9598	96.180	1.0000	2	705.689647	4.251161E-03
1-Methylcyclopentene	647.24	27.802	0.9570	82.146	0.8210	2	855.871875	3.505198E-03
Benzene	648.88	27.987	0.9100	78.048	0.8756	4	823.934804	6.068441E-03
3-Ethylpentene-1	650.02	28.115	0.9800	98.189	0.7030	1	731.665424	2.733490E-03
3-Methylhexene-1	650.25	28.141	0.9800	98.189	0.7030	1	731.665424	2.733490E-03
5-Methylhexene-1	650.62	28.183	0.9800	98.189	0.7030	1	733.309179	2.727363E-03
3,3-Dimethylpentane	652.40	28.385	1.0000	100.205	0.6950	0	720.259208	1.388389E-03
n-Butanol	652.85	28.437	1.2950	74.120	0.8098	0	351.993925	2.840958E-03
2-Pentene, 2,4-dimethyl-	652.85	28.437	0.9800	98.189	0.7120	1	765.233268	2.613582E-03
C7_Iso-Olefins(1)	653.34	28.493	0.9800	98.189	0.7120	1	765.233268	2.613582E-03
1-Pentene, 2,3-dimethyl-	655.18	28.705	0.9800	98.189	0.7040	1	736.607489	2.715150E-03
Cyclohexane	656.74	28.885	0.9800	84.162	0.7785	1	812.943931	2.460194E-03
cis-2-Methyl-hexene-3	659.08	29.158	0.9800	98.189	0.7110	1	683.986835	2.924033E-03
1,4-Hexadiene, 2-methyl-	661.00	29.385	0.9598	96.096	0.7500	2	703.789919	4.262636E-03
1,4-Pentadiene, 3,3-dimethyl-	662.25	29.533	0.9598	96.096	0.7150	2	861.632413	3.481763E-03
2-Hexene, 4-methyl-, (E)-	664.57	29.810	0.9800	98.189	0.7110	1	683.986835	2.924033E-03
2-Methyl-t-hexene-3(1)	665.96	29.977	0.9800	98.189	0.7110	1	683.986835	2.924033E-03
2-Methylhexane	665.96	29.977	1.0000	100.205	0.6930	0	658.324211	1.519008E-03
3-Methyl-3-hexene	665.97	29.978	0.9798	98.186	0.7000	1	560.616514	3.567501E-03
4-Methylhexene-1	666.30	30.018	0.9800	98.189	0.7030	1	731.665424	2.733490E-03
1,6-Heptadiene	666.63	30.058	0.9598	96.096	0.7160	2	632.170658	4.745554E-03
2,3-Dimethylpentane	667.49	30.162	1.0000	100.205	0.6910	0	662.783952	1.508787E-03
4,4-Dimethyl-c-pentene-2	668.98	30.344	0.9800	98.189	0.7039	1	700.477358	2.855196E-03
4-Methyl-t/c-hexene-2	669.15	30.364	0.9800	98.189	0.7110	1	683.986835	2.924033E-03

COMPONENT	RI	TIME	RRF	MW	SG	DBE	VP	PMI Factor
5-Methyl-t-hexene-2	669.33	30.386	0.9800	98.189	0.6971	1	657.879842	3.040069E-03
1,1-Dimethylcyclopentane	670.25	30.498	0.9800	98.189	0.7720	1	697.963684	2.865479E-03
TAME	672.23	30.743	1.4300	102.111	0.7660	0	717.032217	1.394637E-03
Cyclohexene	673.04	30.843	0.9564	82.146	0.8110	2	728.388676	4.118680E-03
3-Methylhexane	674.64	31.042	1.0000	100.205	0.6930	0	649.491902	1.539665E-03
3,4-Dimethyl-c-pentene-2	678.36	31.510	0.9800	98.189	0.7120	1	699.533700	2.859047E-03
1,5-Heptadiene	678.36	31.510	0.9598	96.096	0.7240	2	652.423156	4.598243E-03
C6-Diolefin-1	679.19	31.616	0.9564	82.080	0.7900	2	913.177651	3.285232E-03
1t,3-Dimethylcyclopentane	681.09	31.858	0.9800	98.189	0.7620	1	635.026109	3.149477E-03
1c,3-Dimethylcyclopentane	683.96	32.228	0.9800	98.189	0.7620	1	648.031068	3.086272E-03
3-Ethylpentane	685.24	32.395	1.0000	100.205	0.6930	0	626.497023	1.596177E-03
1t,2-Dimethylcyclopentane	686.89	32.610	0.9800	98.189	0.7620	1	632.170658	3.163703E-03
2,2,4-Trimethylpentane	688.12	32.772	0.9980	114.232	0.6919	0	550.806557	1.815519E-03
Heptene-1	688.17	32.778	0.9800	98.189	0.6970	1	608.396163	3.287332E-03
Cyclopropane, butyl-	688.57	32.832	0.9800	98.189	0.7920	1	537.252801	3.722642E-03
Cyclopropane, 1,1-diethyl-	689.00	32.888	0.9798	98.000	0.7740	1	691.717811	2.891352E-03
Isopropylcyclobutane	689.31	32.929	0.9800	98.000	0.7970	1	569.821299	3.509872E-03
3-Methyl-c-hexene-3	694.54	33.630	0.9800	98.189	0.7140	1	611.147586	3.272532E-03
t-Heptene-3	697.78	34.070	0.9800	98.189	0.7026	1	580.219931	3.446969E-03
2-Methylhexene-1	698.23	34.133	0.9800	98.189	0.7060	1	646.573420	3.093230E-03
3,5-Dimethylcyclopentene	698.78	34.208	0.9598	96.173	0.7830	2	573.958976	5.226854E-03
2-pentyne,4,4-dimethyl	699.29	34.279	0.9598	96.096	0.7540	2	772.124856	3.885382E-03
n-Heptane	700.00	34.377	1.0000	100.205	0.6795	0	545.840224	1.832038E-03
c-Heptene-3	700.14	34.400	0.9800	98.189	0.7130	1	597.509802	3.347225E-03
Cyclobutane, (1-methylethylidene)-	700.61	34.480	0.9598	96.096	0.7830	2	432.706966	6.933098E-03
3-Methyl-c-hexene-2	701.94	34.708	0.9800	98.189	0.7140	1	559.602661	3.573964E-03
2-Methyl-2-hexene	702.90	34.872	0.9800	98.189	0.7140	1	584.166469	3.423682E-03
3-Methyl-t-hexene-3	704.39	35.130	0.9800	98.189	0.7140	1	609.770373	3.279923E-03
t-Heptene-2	705.84	35.382	0.9800	98.189	0.7057	1	651.395761	3.070330E-03
3-Ethylpentene-2	708.52	35.853	0.9800	98.189	0.7140	1	611.147586	3.272532E-03
(Z)-4-Methyl-2-hexene	708.52	35.853	0.9798	98.189	0.7110	1	683.986835	2.924033E-03
Cyclopentene, 1,5-dimethyl-	708.98	35.935	0.9598	96.096	0.8010	2	503.041794	5.963719E-03
1-Pentene, 2,4,4-trimethyl-	709.06	35.948	0.9798	112.000	0.7150	1	508.786785	3.930920E-03
2-Pentene, 3,4-dimethyl-, (E)-	711.68	36.417	0.9800	98.000	0.7322	1	659.659067	3.031869E-03
2-Ethyl-3-methylbutene-1	711.72	36.425	0.9800	98.189	0.7040	1	736.607489	2.715150E-03
3-Methyl-t-hexene-2	712.08	36.488	0.9800	98.189	0.7188	1	653.157973	3.062046E-03
2-Heptene	712.08	36.488	0.9799	98.000	0.7130	1	544.605402	3.672384E-03
2,3-Dimethylpentene-2	713.19	36.690	0.9800	98.189	0.7150	1	558.337832	3.582061E-03
c-Heptene-2	713.62	36.767	0.9800	98.189	0.7130	1	545.840224	3.664076E-03
3-Ethylcyclopentene	715.52	37.113	0.9598	96.173	0.8040	2	553.306031	5.421954E-03
Cyclobutane, 1-ethyl-3-methylene-	716.21	37.242	0.9598	96.173	0.7830	2	568.791387	5.274341E-03
1c,2-Dimethylcyclopentane	717.06	37.397	0.9800	98.189	0.7620	1	560.870254	3.565887E-03
Methylcyclohexane	717.81	37.537	0.9800	98.189	0.7694	1	515.764078	3.877742E-03
2,2-Dimethylhexane	719.67	37.882	0.9980	114.232	0.7110	0	462.423762	2.162519E-03
1,1,3-Trimethylcyclopentane	720.36	38.012	0.9800	112.216	0.7620	1	470.930018	4.246916E-03
Butane, 2,2,3,3-tetramethyl-	723.73	38.650	0.9980	114.232	0.7100	0	450.967832	2.217453E-03
2-Pentene, 3,4,4-trimethyl-	725.04	38.900	0.9800	112.000	0.7350	1	431.028693	4.640062E-03
1,3-Dimethyl-1-cyclohexene	725.68	39.023	0.9623	110.173	0.8000	2	285.003996	1.052617E-02
Ethylcyclopentane	728.49	39.568	0.9800	98.189	0.7770	1	486.178428	4.113716E-03
2,5-Dimethylhexane	729.14	39.697	0.9980	114.232	0.7070	0	427.886469	2.337069E-03
2,2,3-Trimethylpentane	730.25	39.913	0.9980	114.232	0.7090	0	420.126463	2.380236E-03
2,2,3,4-Tetramethylpentane	730.77	40.017	0.9960	128.259	0.7200	0	240.751666	4.153658E-03
2,4-Dimethylhexane	730.99	40.060	0.9980	114.232	0.7070	0	424.960541	2.353160E-03
Cyclohexene, 3-methyl-	731.73	40.207	0.9598	96.000	0.8030	2	477.407992	6.283933E-03
1,4-Heptadiene	732.65	40.390	0.9800	96.170	0.7000	2	615.574926	4.873493E-03
3-Heptyne, 5-methyl-	733.43	40.545	0.9623	110.200	1.0000	2	317.927683	9.436108E-03
Cyclohexene, 4-methyl-	734.53	40.767	0.9598	96.189	0.8030	2	477.407992	6.283933E-03
1,4-Cyclohexadiene, 1-methyl-	736.12	41.088	0.9396	94.080	0.8480	3	404.080633	9.899014E-03
Cyclopentane, 1,2,4-trimethyl-, (1α,2ß,4α)-	736.49	41.163	0.9800	112.000	0.7540	1	362.705281	5.514119E-03
4-Methyl-2-heptene	737.23	41.314	0.9799	112.128	0.7250	1	372.010404	5.376194E-03

COMPONENT	RI	TIME	RRF	MW	SG	DBE	VP	PMI Factor
3-Heptene, 2-methyl-	737.31	41.329	0.9799	112.128	0.7250	1	372.010404	5.376194E-03
1c,2t,4-Trimethylcyclopentane	737.32	41.332	0.9800	112.216	0.7540	1	359.376877	5.565188E-03
3,3-Dimethylhexane	737.58	41.385	0.9980	114.232	0.7110	0	408.738183	2.446554E-03
Cyclopentane, 1,3-bis(methylene)-	739.87	41.855	0.9396	94.000	0.7514	3	473.295422	8.451381E-03
3-Hexene, 3,4-dimethyl-, (Z)-	741.80	42.257	0.9800	112.000	0.7290	1	317.927683	6.290739E-03
2-Hexene, 2,4-dimethyl-	742.51	42.405	0.9800	112.128	0.7260	1	413.446983	4.837380E-03
1t,2c,3-Trimethylcyclopentane	743.60	42.633	0.9800	112.216	0.7540	1	362.705281	5.514119E-03
1-Heptene, 3-methyl-	745.19	42.970	0.9798	112.000	0.7190	1	396.733790	5.041164E-03
2,3,4-Trimethylpentane	746.15	43.173	0.9980	114.232	0.7060	0	386.839760	2.585050E-03
Cyclopentene, 4,4-dimethyl-	747.29	43.417	0.9598	96.096	0.7980	2	694.833925	4.317578E-03
2,3-Dimethyl-1-hexene	747.29	43.417	0.9800	112.128	0.7190	1	399.473786	5.006586E-03
5-Methyl-c-hexene-2	747.29	43.417	0.9800	98.189	0.7110	1	683.986835	2.924033E-03
1-Ethylcyclopentene	748.75	43.732	0.9598	96.096	0.8170	2	450.967832	6.652359E-03
2,3,3-Trimethylpentane	750.25	44.055	0.9980	114.232	0.7090	0	375.450118	2.663470E-03
Toluene	751.65	44.362	0.9200	92.143	0.8623	4	413.446983	1.209345E-02
4-Ethyl-2-hexene	752.37	44.521	0.9800	112.128	0.7250	1	369.450341	5.413447E-03
1,1,2-Trimethylcyclopentane	752.71	44.594	0.9800	112.216	0.7620	1	407.802590	4.904334E-03
2-Pentene, 3-ethyl-2-methyl-	752.71	44.594	0.9799	112.128	0.7190	1	399.473786	5.006586E-03
5,5-Dimethyl-1,3-hexadiene	753.04	44.667	0.9623	110.000	0.7370	2	367.752966	8.157650E-03
3-Ethyl-3-Hexene	754.34	44.955	0.9799	112.128	0.7280	1	365.220820	5.476139E-03
4-methyl-2-heptene(1)	755.17	45.138	0.9799	112.200	0.7250	1	372.010404	5.376194E-03
2,3-Dimethylhexane	757.09	45.568	0.9980	114.232	0.7070	0	373.726490	2.675754E-03
2-Methyl-3-ethylpentane	758.27	45.835	0.9980	114.232	0.7121	0	373.726490	2.675754E-03
2-Hexene, 2,5-dimethyl-	759.32	46.073	0.9799	112.128	0.7260	1	379.792392	5.266035E-03
Cyclohexene, 1-methyl-	761.37	46.543	0.9598	96.096	0.8100	2	419.165977	7.157069E-03
3-Methyl-3-ethylpentane	761.37	46.543	0.9975	114.232	0.7110	0	348.759135	2.867308E-03
2,3-Dimethyl-2-hexene	763.01	46.920	0.9799	112.128	0.7290	1	317.927683	6.290739E-03
2-Methylheptane	763.22	46.970	0.9980	114.232	0.7090	0	351.182563	2.847522E-03
4-Methylheptane	764.75	47.327	0.9980	114.232	0.7090	0	356.899673	2.801908E-03
Hexane, 2,3,3-trimethyl-	765.95	47.607	0.9980	128.000	0.7220	0	219.053933	4.565086E-03
3,4-Dimethylhexane	766.50	47.737	0.9980	114.232	0.7070	0	360.206242	2.776187E-03
1c,2c,4-Trimethylcyclopentane	769.05	48.342	0.9800	112.216	0.7620	1	371.753639	5.379907E-03
C7_Naphtheno-Olefins(1)	769.11	48.355	0.9598	96.096	0.8100	2	419.165977	7.157069E-03
3,4-Dimethyl-t-2-hexene	769.18	48.372	0.9800	112.220	0.7260	1	379.792392	5.266035E-03
1c,2t,3-Trimethylcyclopentane	769.52	48.453	0.9800	112.216	0.7550	1	362.371124	5.519204E-03
3-Hexyne, 2-methyl-	769.67	48.488	0.9598	96.096	0.7520	2	562.140617	5.336743E-03
3-Methylheptane	771.03	48.817	0.9980	114.232	0.7090	0	341.583904	2.927538E-03
1t,3-Dimethylcyclohexane	771.76	48.993	0.9800	112.216	0.7660	1	290.369902	6.887766E-03
3-Ethylhexane	772.22	49.103	0.9980	114.232	0.7090	0	352.807070	2.834410E-03
i-Propylcyclopentane	772.69	49.217	0.9800	112.216	0.7960	1	295.143384	6.776367E-03
1t,2-Dimethylcyclohexane	773.55	49.427	0.9800	112.216	0.7660	1	290.369902	6.887766E-03
1,3-dimethyl-c-cyclohexane	774.72	49.713	0.9800	112.216	0.7660	1	332.234946	6.019836E-03
1,3-Octadiene	775.35	49.869	0.9623	110.200	0.7380	2	279.079533	1.074962E-02
Heptane, 4-methylene-	776.59	50.175	0.9800	112.000	0.7196	1	460.845326	4.339851E-03
2,2,4-Trimethylhexane	778.20	50.574	0.9960	128.259	0.7220	0	293.088579	3.411938E-03
C8_Mono-Naphthenes(1)	778.23	50.583	0.9800	112.216	0.7625	1	337.658526	5.923144E-03
t-Octene-2	779.40	50.875	0.9800	112.216	0.7270	1	326.137895	6.132375E-03
1,1-Dimethylcyclohexane	780.49	51.150	0.9800	112.216	0.7700	1	348.759135	5.734617E-03
1-Heptene, 2-methyl-	782.19	51.582	0.9800	112.128	0.7210	1	351.182563	5.695044E-03
2,2,5-Trimethylhexane	782.42	51.638	0.9960	128.259	0.7220	0	302.795011	3.302564E-03
1,1-Methylethylcyclopentane	783.64	51.950	0.9800	112.216	0.7750	1	342.374166	5.841562E-03
3c-Ethylmethylcyclopentane	784.29	52.118	0.9800	112.216	0.7670	1	333.776036	5.992042E-03
3t-Ethylmethylcyclopentane	786.56	52.707	0.9800	112.216	0.7670	1	333.776036	5.992042E-03
5-Methyl-3-heptene	786.80	52.769	0.9800	112.220	0.7650	1	391.217670	5.112244E-03
1c,4-Dimethylcyclohexane	787.96	53.072	0.9800	112.216	0.7660	1	290.369902	6.887766E-03
C9_I-Paraffins(1)	789.60	53.502	0.9960	128.259	0.7389	0	245.905105	4.066609E-03
C8_Mono-Naphthenes(2)	790.38	53.710	0.9800	112.216	0.7660	1	290.369902	6.887766E-03
3-Heptene, 4-methyl-	790.49	53.738	0.9800	112.220	0.7280	1	333.004644	6.005922E-03
1,4-Hexadiene, 2,3-dimethyl-	792.82	54.359	0.9623	110.200	0.7370	2	381.542669	7.862817E-03
C8_Naphtheno-Olefins(1)	792.89	54.380	0.9623	110.112	0.8020	2	258.943888	1.158552E-02

COMPONENT	RI	TIME	RRF	MW	SG	DBE	VP	PMI Factor
C8_Naphtheno-Olefins(2)	792.98	54.404	0.9623	110.112	0.8020	2	258.943888	1.158552E-02
Cyclohexane, 1,2-dimethyl-	793.19	54.460	0.9800	112.000	0.7660	1	290.369902	6.887766E-03
1,3-Dimethylcyclohexane,c&t	793.54	54.560	0.9800	112.000	0.7660	1	290.369902	6.887766E-03
cis-1-Butyl-2-methylcyclopropane	793.62	54.580	0.9800	112.000	0.7828	1	406.309896	4.922351E-03
C8_Mono-Naphthenes(3)	794.04	54.697	0.9800	112.000	0.7828	1	406.309896	4.922351E-03
t-Octene-4	794.12	54.718	0.9800	112.216	0.7150	1	315.722805	6.334671E-03
Octene-1	795.59	55.112	0.9800	112.220	0.7149	1	323.879009	6.175145E-03
Cyclohexene, 3-ethyl-	796.11	55.253	0.9623	110.112	0.8020	2	258.943888	1.158552E-02
3,5,5-Trimethylhexene-1	796.46	55.346	0.9800	126.240	0.7310	1	282.356363	7.083247E-03
3-Heptene, 3-methyl-	796.66	55.400	0.9800	112.000	0.7280	1	333.004644	6.005922E-03
3-Octene, (Z)-	797.20	55.548	0.9800	112.220	0.7270	1	326.137895	6.132375E-03
c-Octene-4	798.04	55.780	0.9800	112.216	0.7270	1	326.137895	6.132375E-03
trans-3,5-DimethylCyclohexene	798.86	56.005	0.9623	110.200	0.7880	2	314.260952	9.546207E-03
2-Heptene, 3-methyl-	798.88	56.011	0.9800	112.220	0.7280	1	333.004644	6.005922E-03
n-Octane	800.00	56.322	0.9980	114.232	0.6986	0	296.520825	3.372444E-03
Cyclohexane c&t, 1,4-dimethyl-	801.30	56.658	0.9800	112.216	0.7740	1	324.630316	6.160854E-03
2-Hexene, 2,5,5-trimethyl-	804.09	57.391	0.9800	126.144	0.7400	1	239.620367	8.346536E-03
Cyclopentane, 1,1,3,4-tetramet	804.75	57.565	0.9800	126.243	0.7550	1	265.083894	7.544781E-03
2,3,4-Trimethylhexane	804.76	57.567	0.9960	128.259	0.7190	0	215.962632	4.630431E-03
c-Octene-2	804.76	57.568	0.9800	112.216	0.7270	1	293.772004	6.808001E-03
C8_Iso-Olefins(1)	805.73	57.823	0.9800	112.216	0.7704	1	352.807070	5.668821E-03
2,4-Octadiene	805.77	57.835	0.9623	110.000	0.7450	2	258.943888	1.158552E-02
Cyclopentene, 1,2,3-trimethyl-	807.26	58.233	0.9623	110.173	0.7980	2	329.935976	9.092673E-03
Hexane, 2,4,4-trimethyl-	807.92	58.410	0.9960	128.255	0.7000	0	276.483999	3.616846E-03
C9_Iso-Olefins(1)	808.72	58.623	0.9800	126.144	0.7400	1	239.620367	8.346536E-03
2-Hexene, 3,5-dimethyl-	808.83	58.655	0.9800	112.216	0.7704	1	392.296994	5.098178E-03
2-Ethylhexene-1	809.03	58.708	0.9800	112.220	0.7210	1	351.182563	5.695044E-03
1-Ethyl-5-methylcyclopentene	809.11	58.728	0.9623	110.173	0.7514	2	271.933042	1.103213E-02
Cyclopentane, (1-methylbutyl)-	809.45	58.823	0.9800	140.000	0.8060	1	93.003083	2.150466E-02
1t,4t-Dimethylcyclohexane	809.60	58.862	0.9800	112.216	0.7660	1	337.658526	5.923144E-03
C8_Iso-Olefins(2)	811.87	59.480	0.9800	112.216	0.7704	1	352.807070	5.668821E-03
t-Octene-3	814.62	60.235	0.9800	112.216	0.7270	1	326.137895	6.132375E-03
1,3-Cyclopentadiene, 1,2-dimet	815.69	60.532	0.9396	94.080	0.8460	3	455.101795	8.789242E-03
Cyclohexene, 1-ethyl-	816.52	60.763	0.9623	110.112	0.8140	2	234.038617	1.281840E-02
C8_Mono-Naphthenes(4)	816.67	60.807	0.9800	112.216	0.7690	1	323.879009	6.175145E-03
Cyclopentene, 1-(1-methylethyl)-	817.82	61.128	0.9623	110.000	0.8340	2	289.693973	1.035576E-02
2,3,5-Trimethylhexane	819.62	61.635	0.9960	128.259	0.7190	0	255.324598	3.916583E-03
Cyclopentane, 1-ethyl-2-methyl-cis	820.58	61.908	0.9800	112.216	0.7670	1	302.795011	6.605129E-03
3,3-Dimethylheptene-1	821.10	62.056	0.9800	126.240	0.7000	1	249.985062	8.000478E-03
Cyclopentane, 1-ethyl-2-methyl-	822.01	62.317	0.9800	112.216	0.7670	1	302.795011	6.605129E-03
C8_Iso-Olefins(3)	822.95	62.587	0.9800	112.216	0.7800	1	178.042793	1.123325E-02
3-Octyne, 6-methyl-	824.04	62.902	0.9642	124.000	0.7322	2	183.675057	1.633319E-02
Heptane, 2,2-dimethyl-	824.07	62.908	0.9960	128.259	0.7210	0	252.641521	3.958178E-03
Cyclohexene, 3,5-dimethyl-	824.10	62.917	0.9623	110.197	0.7000	2	308.262578	9.731963E-03
C9_I-Paraffins(2)	824.13	62.927	0.9960	128.259	0.7190	0	255.324598	3.916583E-03
1c,2-Dimethylcyclohexane	826.53	63.624	0.9800	112.216	0.7660	1	290.369902	6.887766E-03
2,4-Dimethylheptane	827.16	63.808	0.9960	128.259	0.7210	0	242.458058	4.124425E-03
1,4-Dimethyl-1-cyclohexene	827.18	63.815	0.9623	110.112	0.8000	2	285.003996	1.052617E-02
C9_I-Paraffins(3)	829.23	64.427	0.9960	128.259	0.7105	0	247.645907	4.038024E-03
C8_Naphtheno-Olefins(3)	829.23	64.427	0.9623	110.200	0.7322	2	349.565172	8.582091E-03
C9_Mono-Naphthenes(1)	830.03	64.662	0.9800	126.144	0.7962	1	265.705400	7.527133E-03
Cyclopentane, 1,1,3,3-tetramethyl-	830.16	64.702	0.9800	126.239	0.8000	1	348.759135	5.734617E-03
C9_Mono-Naphthenes(2)	831.35	65.056	0.9800	126.144	0.7962	1	265.705400	7.527133E-03
1,4-Pentadiene, 2,3,4-trimethyl-	832.45	65.384	0.9623	110.112	0.7200	2	503.384727	5.959656E-03
C9_Mono-Naphthenes(3)	832.47	65.389	0.9800	126.144	0.7962	1	265.705400	7.527133E-03
C9_Mono-Naphthenes(4)	832.53	65.407	0.9800	126.243	0.7697	1	196.940742	1.015534E-02
Ethylcyclohexane	835.69	66.360	0.9800	112.216	0.7880	1	267.578188	7.474451E-03
n-Propylcyclopentane	835.71	66.367	0.9800	112.216	0.7850	1	257.732111	7.759995E-03
2,2,3-Trimethylhexane	836.77	66.691	0.9960	128.259	0.7220	0	241.887998	4.134145E-03
2,6-Dimethylheptane	837.69	66.973	0.9960	128.259	0.7210	0	233.487230	4.282889E-03

COMPONENT	RI	TIME	RRF	MW	SG	DBE	VP	PMI Factor
1-Ethyl-2-Methylcyclopentene	839.80	67.625	0.9955	128.160	0.7240	0	234.038617	4.272799E-03
Methyl ethyl cyclopentene	841.59	68.183	0.9800	110.197	0.8000	2	272.569709	1.100636E-02
C8_Naphtheno-Olefins(4)	841.85	68.265	0.9800	110.000	0.7322	2	349.565172	8.582091E-03
1,1,3-Trimethylcyclohexane	842.01	68.315	0.9800	126.243	0.7650	1	215.962632	9.260861E-03
1c,3c,5-Trimethylcyclohexane	842.27	68.398	0.9800	126.243	0.7697	1	196.940742	1.015534E-02
C9_Mono-Naphthenes(5)	843.36	68.740	0.9800	126.243	0.7722	1	234.591229	8.525468E-03
3,5-Dimethyl-3-heptene	845.02	69.268	0.9800	126.240	0.6826	1	230.367617	8.681776E-03
C9_Mono-Naphthenes(6)	845.35	69.373	0.9800	126.243	0.7697	1	196.940742	1.015534E-02
2,5-Dimethylheptane	846.08	69.607	0.9960	128.160	0.7210	0	230.204519	4.343963E-03
Heptane, 3,3-dimethyl-	847.56	70.080	0.9960	128.000	0.7240	0	223.240450	4.479475E-03
1,1,4-Trimethylcyclohexane	848.79	70.485	0.9800	126.243	0.7650	1	234.591229	8.525468E-03
C9_Mono-Naphthenes(7)	848.88	70.516	0.9800	126.243	0.7722	1	234.591229	8.525468E-03
Cyclopentene, 1-propyl-	849.74	70.788	0.9623	110.112	0.8210	2	247.064353	1.214259E-02
C9_Mono-Naphthenes(8)	850.26	70.956	0.9800	126.243	0.7722	1	234.591229	8.525468E-03
C9_Mono-Naphthenes(9)	850.31	70.974	0.9800	126.243	0.7722	1	234.591229	8.525468E-03
C9_Mono-Naphthenes(10)	850.37	70.992	0.9800	126.243	0.7722	1	234.591229	8.525468E-03
2-Methyloctene-1	851.78	71.458	0.9800	126.240	0.7330	1	195.910784	1.020873E-02
trans-1,3-Diethylcyclopentane	852.14	71.577	0.9800	126.144	0.8802	1	187.671672	1.065691E-02
C9_Iso-Olefins(2)	853.34	71.977	0.9800	126.240	0.7330	1	195.910784	1.020873E-02
3-Heptene, 2,6-dimethyl-	855.47	72.673	0.9800	126.240	0.7360	1	234.591229	8.525468E-03
4-Nonene	855.47	72.673	0.9800	126.144	0.7390	1	181.924516	1.099357E-02
C9_Mono-Naphthenes(11)	856.51	73.022	0.9799	126.243	0.8802	1	187.671672	1.065691E-02
3-Ethyl-3-methylheptane	856.57	73.043	0.9930	142.176	0.7340	0	116.047539	8.617158E-03
2,3-Dimethylheptene-2	856.58	73.047	0.9800	126.240	0.7410	1	184.556236	1.083681E-02
Ethylbenzene	858.16	73.578	0.9270	106.168	0.8626	4	228.040243	2.192595E-02
1c,2t,4t-Trimethylcyclohexane	859.62	74.073	0.9800	126.243	0.7580	1	194.051070	1.030657E-02
C9_Mono-Naphthenes(12)	861.64	74.767	0.9800	126.243	0.7722	1	234.591229	8.525468E-03
3-Heptene, 4-ethyl-	861.71	74.788	0.9800	126.144	0.7400	1	185.885438	1.075932E-02
Hexane, 3-ethyl-2-methyl-	862.90	75.198	0.9930	128.000	0.7210	0	216.474983	4.619471E-03
Cyclohexane, 1,3,5-trimethyl-, (1α,3α,5ß)-	863.59	75.437	0.9800	126.000	0.7590	1	210.901443	9.483102E-03
C10_I-Paraffins(1)	865.30	76.032	0.9940	142.286	0.7276	0	127.417326	7.848226E-03
m-Xylene	866.81	76.562	0.9270	106.168	0.8698	4	218.535842	2.287954E-02
p-Xylene	867.69	76.873	0.9270	106.168	0.8610	4	210.351571	2.376973E-02
3,5-Dimethylheptane	869.60	77.552	0.9960	128.160	0.7210	0	229.119975	4.364526E-03
1-Heptene, 5-methyl-	870.33	77.812	0.9800	112.000	0.7190	1	396.733790	5.041164E-03
C9_I-Paraffins(4)	870.38	77.830	0.9960	128.160	0.7210	0	229.119975	4.364526E-03
1-Methyl-2-propyl-cyclopentan	870.45	77.855	0.9800	126.243	0.8022	1	156.711467	1.276231E-02
C9_Mono-Naphthenes(13)	871.60	78.268	0.9800	126.243	0.7722	1	234.591229	8.525468E-03
C9_Mono-Naphthenes(14)	871.67	78.292	0.9800	126.243	0.8022	1	156.711467	1.276231E-02
Hexane, 2-methyl-4-methylene-	871.90	78.375	0.9800	112.128	0.7322	1	465.490113	4.296547E-03
4-Ethylheptane	872.42	78.562	0.9960	128.259	0.7220	0	202.552368	4.936995E-03
C9_Mono-Naphthenes(15)	872.73	78.673	0.9800	126.243	0.8022	1	156.711467	1.276231E-02
3,3-Diethylpentane	872.80	78.698	0.9960	128.000	0.7240	0	175.077462	5.711757E-03
C9_Mono-Naphthenes(16)	872.80	78.700	0.9800	126.243	0.8022	1	156.711467	1.276231E-02
C9_Mono-Naphthenes(17)	872.87	78.725	0.9800	126.243	0.8022	1	156.711467	1.276231E-02
Cyclopentane, 1-methyl-3-(2-methyl-2-propenyl)-	872.89	78.733	0.9658	138.000	0.8000	2	109.631888	2.736430E-02
Nonene-1	873.41	78.920	0.9800	126.241	0.7433	1	176.342609	1.134156E-02
2-Heptene, 2,6-dimethyl-	874.01	79.137	0.9800	126.144	0.6826	1	230.367617	8.681776E-03
trans-2-Methyl-3-octene	874.06	79.155	0.9800	126.000	0.7370	1	206.932986	9.664965E-03
4-Methyloctane	875.03	79.512	0.9960	128.259	0.7220	0	200.633516	4.984212E-03
2,3-Dimethylheptane	875.12	79.544	0.9960	128.259	0.7210	0	205.951893	4.855503E-03
2-Methyloctane	875.90	79.828	0.9960	128.259	0.7220	0	192.667170	5.190298E-03
C9_Naphtheno-Olefins(1)	876.68	80.117	0.9800	124.000	0.7322	2	349.565172	8.582091E-03
C9_Naphtheno-Olefins(2)	876.79	80.155	0.9800	124.000	0.7322	2	349.565172	8.582091E-03
C9_Naphtheno-Olefins(3)	876.90	80.198	0.9800	124.000	0.7322	2	349.565172	8.582091E-03
3-Hexene, 2,3-dimethyl-	877.46	80.405	0.9800	112.128	0.7260	1	379.792392	5.266035E-03
i-Butylcyclopentane	877.51	80.423	0.9800	126.243	0.7900	1	163.278100	1.224904E-02
3-Hexene, 3-ethyl-2,5-dimethyl-	878.47	80.777	0.9800	140.000	0.6826	1	134.432452	1.487736E-02
C9_Mono-Naphthenes(18)	879.40	81.125	0.9800	126.243	0.7900	1	163.278100	1.224904E-02
C9_Mono-Naphthenes(19)	879.53	81.170	0.9800	126.243	0.7722	1	234.591229	8.525468E-03

COMPONENT	RI	TIME	RRF	MW	SG	DBE	VP	PMI Factor
Heptane, 3-ethyl-	879.97	81.337	0.9960	128.259	0.7220	0	194.051070	5.153283E-03
3,4-Dimethylheptane	881.02	81.728	0.9960	128.259	0.7210	0	205.462987	4.867057E-03
3-Methyloctane	881.05	81.742	0.9960	128.259	0.7220	0	191.749720	5.215131E-03
3-Heptyne, 5-ethyl-5-methyl-	881.96	82.085	0.9658	138.144	0.7810	2	144.311680	2.078834E-02
Pentane, 2,3,3,4-tetramethyl-	882.96	82.460	0.9940	128.000	0.7200	0	202.071046	4.948755E-03
2,6-Dimethylheptene-1	882.98	82.470	0.9800	126.240	0.7320	1	222.186820	9.001434E-03
1c,2t,4c-Trimethylcyclohexane	883.64	82.720	0.9800	126.243	0.7590	1	210.901443	9.483102E-03
o-Xylene	884.79	83.158	0.9270	106.168	0.8802	4	194.051070	2.576641E-02
Octane, 3,4-dimethyl-	886.23	83.712	0.9940	142.000	0.7320	0	118.944360	8.407292E-03
C9_Iso-Olefins(3)	886.26	83.722	0.9800	126.241	0.6826	1	184.998310	1.081091E-02
2,2,4-trimethylheptane	886.87	83.958	0.9940	142.286	0.7330	0	167.260104	5.978712E-03
2,4-Dimethylheptene-1	887.90	84.354	0.9800	126.240	0.7320	1	222.186820	9.001434E-03
Cyclohexane, 1-ethyl-2-methyl-	887.94	84.372	0.9800	126.243	0.7690	1	160.931641	1.242764E-02
Cyclopentane, 1-methyl-2-propyl-	888.56	84.612	0.9799	126.144	0.7750	1	168.472307	1.187139E-02
C9_Mono-Naphthenes(20)	889.24	84.877	0.9798	126.000	0.7690	1	160.931641	1.242764E-02
1-Ethyl-4-methylcyclohexane	889.33	84.912	0.9798	126.000	0.7690	1	160.931641	1.242764E-02
C9_Mono-Naphthenes(21)	890.03	85.183	0.9798	126.000	0.7690	1	160.931641	1.242764E-02
1,1,2-Trimethylcyclohexane	890.70	85.447	0.9800	126.243	0.7650	1	184.115152	1.086277E-02
cis-1-Ethyl-3-methyl-cyclohexane	890.79	85.482	0.9800	126.243	0.7690	1	160.931641	1.242764E-02
Octane, 3,3-dimethyl-	891.32	85.690	0.9940	142.286	0.7340	0	125.555755	7.964589E-03
1α,2ß,3α,4ß-Tetramethylcyclopentane	892.15	86.017	0.9800	126.243	0.7480	1	234.591229	8.525468E-03
t-Nonene-3	892.84	86.292	0.9800	126.241	0.7390	1	181.924516	1.099357E-02
trans-1,2-Diethyl cyclopentane	893.23	86.448	0.9800	126.243	0.7722	1	195.071853	1.025263E-02
Cyclohexane, 1-ethyl-2-methyl-, cis-	893.52	86.560	0.9798	126.000	0.7690	1	141.875240	1.409689E-02
Cyclohexane, 1-isopropyl-1-methyl-	894.01	86.755	0.9800	140.000	0.8000	1	118.068330	1.693934E-02
Cyclohexane, 1-methyl-4-(1-methylethyl)-, trans-	894.01	86.758	0.9800	140.000	0.8039	1	104.998953	1.904781E-02
trans-4-Nonene	896.17	87.622	0.9800	126.241	0.6826	1	227.340988	8.797358E-03
c-Nonene-2	896.87	87.940	0.9800	126.243	0.7390	1	162.100900	1.233799E-02
C10_Iso-Olefins(1)	896.90	87.953	0.9800	140.270	0.7013	1	176.342609	1.134156E-02
t-Butylbenzene	897.20	88.051	0.9330	134.112	0.8665	4	106.153009	4.710182E-02
C10_Iso-Olefins(2)	897.37	88.107	0.9800	140.270	0.7013	1	176.342609	1.134156E-02
cis-4-Nonene	897.39	88.117	0.9800	126.241	0.7390	1	181.924516	1.099357E-02
3,7-Dimethyloctene-1	897.50	88.159	0.9800	140.270	0.7400	1	141.186195	1.416569E-02
cis-3-Nonene	897.89	88.317	0.9800	126.241	0.6826	1	227.340988	8.797358E-03
2-Methyl-2-octene	898.48	88.557	0.9800	126.000	0.7400	1	176.342609	1.134156E-02
1-ethyl-4-CIS-methylcyclohexane	898.48	88.558	0.9800	126.243	0.7700	1	160.776336	1.243964E-02
C9_Mono-Naphthenes(22)	899.01	88.772	0.9800	126.243	0.7700	1	160.776336	1.243964E-02
Heptane, 3,3,5-trimethyl-	899.01	88.775	0.9940	142.286	0.7330	0	142.567420	7.014225E-03
n-Nonane	900.00	89.178	0.9960	128.259	0.7176	0	157.470994	6.350376E-03
Heptane, 2,5,5-trimethyl-	902.18	89.571	0.9940	142.286	0.7330	0	164.067336	6.095058E-03
1,1-Methylethylcyclohexane	902.72	89.667	0.9800	126.243	0.7770	1	155.578593	1.285524E-02
C9_Iso-Olefins(4)	904.31	89.955	0.9800	126.000	0.7400	1	176.342609	1.134156E-02
t-Nonene-2	904.37	89.965	0.9800	126.243	0.7390	1	189.473990	1.055554E-02
i-Butylcyclohexane	905.65	90.198	0.9800	140.270	0.7900	1	97.289397	2.055722E-02
2-Nonene, 3-methyl-, (E)-	906.01	90.263	0.9800	140.000	0.7800	1	131.571435	1.520087E-02
Cyclohexane, 1-ethyl-4-methyl-, trans-	906.46	90.345	0.9800	126.243	0.7690	1	160.931641	1.242764E-02
Decene-1	908.24	90.668	0.9799	140.270	0.7408	1	103.032974	1.941126E-02
i-Propylbenzene	913.22	91.582	0.9330	120.195	0.8618	4	154.827599	3.229398E-02
C10_n-Olefins(1)	914.35	91.790	0.9799	140.270	0.7408	1	103.032974	1.941126E-02
Cyclohexene,3-propyl-	915.60	92.020	0.9642	124.000	0.8070	2	144.662913	2.073787E-02
C9_Mono-Naphthenes(23)	915.74	92.047	0.9800	126.243	0.7690	1	160.931641	1.242764E-02
1H-Indene, octahydro-, cis-	915.75	92.048	0.9642	124.000	0.8820	2	125.555755	2.389377E-02
C10_I-Paraffins(2)	915.75	92.048	0.9940	142.286	0.7330	0	164.067336	6.095058E-03
C9_Naphtheno-Olefins(4)	915.76	92.050	0.9642	124.000	0.8180	2	131.217824	2.286275E-02
1H-Indene, octahydro-, trans-	915.76	92.050	0.9642	124.000	0.8820	2	125.555755	2.389377E-02
C10_I-Paraffins(3)	916.53	92.202	0.9940	142.176	0.7245	0	138.799041	7.204661E-03
C9_Mono-Naphthenes(24)	916.74	92.243	0.9800	126.243	0.7690	1	160.931641	1.242764E-02
C10_I-Paraffins(4)	916.93	92.280	0.9940	142.176	0.7245	0	138.799041	7.204661E-03
Propylcyclohexane	918.59	92.575	0.9800	126.243	0.7840	1	145.367773	1.375821E-02
3-Hexene, 2,2-dimethyl-, (E)-	918.59	92.576	0.9800	112.000	0.7800	1	417.060290	4.795470E-03

COMPONENT	RI	TIME	RRF	MW	SG	DBE	VP	PMI Factor
Heptane, 2,3,5-trimethyl-	921.18	93.058	0.9940	142.286	0.7300	0	135.454044	7.382578E-03
C10_I-Paraffins(5)	923.12	93.423	0.9940	142.286	0.7245	0	177.744157	5.626064E-03
C10_I-Paraffins(6)	923.23	93.443	0.9943	142.200	0.7245	0	177.744157	5.626064E-03
2,2-Dimethyloctane	923.32	93.460	0.9940	142.286	0.7340	0	141.530327	7.065623E-03
Heptane, 2,4,6-trimethyl-	923.92	93.573	0.9940	142.286	0.7300	0	168.067329	5.949996E-03
Cyclohexene,1-propyl-	925.15	93.805	0.9642	124.000	0.8180	2	131.217824	2.286275E-02
1,6-Octadiene, 2,5-dimethyl-, (E)-	926.08	93.980	0.9658	138.000	0.7013	2	144.206465	2.080351E-02
C10_I-Paraffins(7)	928.85	94.326	0.9940	142.286	0.7276	0	127.417326	7.848226E-03
1-Ethyl-3-methylcyclohexane (c,t)	928.93	94.337	0.9800	126.239	0.8000	1	161.866415	1.235587E-02
C9_Mono-Naphthenes(25)	930.30	94.507	0.9800	126.243	0.8000	1	184.115152	1.086277E-02
C10_I-Paraffins(8)	930.30	94.782	0.9940	142.286	0.7300	0	138.799041	7.204661E-03
C9_Mono-Naphthenes(26)	931.43	94.782	0.9800	126.243	0.8000	1	184.115152	1.086277E-02
C9_Mono-Naphthenes(27)	932.08	95.108	0.9799	126.243	0.8062	1	155.578593	1.285524E-02
t-2,2,5,5-Tetramethylhexene-3	932.12	95.130	0.9800	140.270	0.7480	1	168.878198	1.184285E-02
C10_I-Paraffins(9)	932.19	95.143	0.9940	142.286	0.7276	0	127.417326	7.848226E-03
C10_I-Paraffins(10)	933.99	95.488	0.9940	142.286	0.7276	0	127.417326	7.848226E-03
C10_I-Paraffins(11)	934.14	95.517	0.9940	142.286	0.7276	0	127.417326	7.848226E-03
2,3,6-trimethylheptane	936.61	95.992	0.9940	142.286	0.7300	0	138.799041	7.204661E-03
1,2,3,5-t-Tetramethylcyclohex	937.28	96.121	0.9800	140.270	0.8000	1	127.417326	1.569645E-02
2,4-Dimethyloctane	937.58	96.179	0.9940	142.286	0.7000	0	140.500273	7.117424E-03
2,7-dimethyloctane	937.80	96.223	0.9940	142.286	0.7320	0	133.483275	7.491575E-03
C10_Mono-Naphthenes(1)	940.10	96.668	0.9800	140.270	0.7960	1	97.289397	2.055722E-02
Cyclooctane, 1,2-dimethyl-	941.19	96.881	0.9800	140.160	0.7722	1	81.232318	2.462074E-02
2,5-Dimethyloctane	941.76	96.992	0.9940	142.286	0.7320	0	133.483275	7.491575E-03
2,6-Dimethyloctane	941.77	96.993	0.9940	142.176	0.7320	0	129.621632	7.714762E-03
Hexane, 3,3,4-trimethyl-	943.11	97.255	0.9940	128.000	0.7220	0	210.401504	4.752818E-03
C10_Mono-Naphthenes(2)	943.72	97.375	0.9800	140.270	0.7960	1	97.289397	2.055722E-02
C10_I-Paraffins(12)	943.74	97.378	0.9940	142.286	0.7276	0	127.417326	7.848226E-03
C10_Mono-Naphthenes(3)	943.81	97.393	0.9800	140.160	0.7722	1	81.232318	2.462074E-02
C9_Mono-Naphthenes(28)	944.57	97.542	0.9800	126.243	0.8000	1	184.115152	1.086277E-02
3-Octene, 4-ethyl-	944.64	97.555	0.9798	140.000	0.7500	1	105.103384	1.902888E-02
n-Propylbenzene	946.88	97.997	0.9330	120.195	0.8660	4	127.105290	3.933747E-02
3-Methyl-5-ethylheptane	949.21	98.457	0.9940	142.286	0.7320	0	130.577163	7.658307E-03
3,6-Dimethyloctane	949.56	98.525	0.9940	142.286	0.7320	0	126.173447	7.925598E-03
4-Octene, 2,3,6-trimethyl-	950.16	98.645	0.9800	154.292	1.0000	1	86.463676	2.313110E-02
Cyclohexane, 1-ethyl-2,3-dimethyl-	950.34	98.680	0.9800	140.266	0.8000	1	113.048613	1.769150E-02
Cyclopentane, 2-isopropyl-1,3-dimethyl-	951.63	98.937	0.9799	140.000	0.7302	1	126.949540	1.575429E-02
1-Octene, 3-methyl-	952.67	99.144	0.9799	126.000	0.7000	1	220.615145	9.065561E-03
1-Methyl-3-ethylbenzene	954.92	99.593	0.9330	120.195	0.8670	4	124.634494	4.011731E-02
3-Nonene, 3-methyl-, (E)-	956.15	99.839	0.9799	140.270	0.7400	1	131.571435	1.520087E-02
1-Methyl-4-ethylbenzene	956.71	99.953	0.9330	120.195	0.8600	4	122.509295	4.081323E-02
Cyclohexane, 1,1,3,5-tetramethyl-, trans-	959.02	100.417	0.9800	140.266	0.8000	1	140.705723	1.421406E-02
1,5-Heptadiene, 2,6-dimethyl-	959.33	100.480	0.9642	124.000	0.7500	2	202.071046	1.484626E-02
C10_I-Paraffins(13)	961.13	100.845	0.9940	142.000	0.7320	0	118.944360	8.407292E-03
C10_I-Paraffins(14)	961.24	100.867	0.9940	142.000	0.7320	0	118.944360	8.407292E-03
1-Octene, 4-methyl-	961.53	100.927	0.9799	126.000	0.7310	1	220.615145	9.065561E-03
1,3,5-Trimethylbenzene	962.30	101.083	0.9330	120.195	0.8637	4	109.089873	4.583377E-02
C10_I-Paraffins(15)	963.23	101.272	0.9940	142.286	0.7320	0	115.761494	8.638451E-03
C10_Mono-Naphthenes(4)	964.59	101.548	0.9799	140.000	0.8000	1	90.926180	2.199587E-02
C10_Mono-Naphthenes(5)	964.69	101.570	0.9799	140.000	0.8000	1	90.926180	2.199587E-02
Trans-1,4-diethylcyclohexane	965.32	101.698	0.9799	140.000	0.8000	1	90.926180	2.199587E-02
2,3,3-Trimethyl-1-hexene	966.11	101.860	0.9799	126.144	0.7310	1	282.356363	7.083247E-03
4-Decene	966.29	101.897	0.9799	140.270	0.7408	1	131.185722	1.524556E-02
2,3-Dimethyloctane(1)	966.68	101.977	0.9940	142.286	0.7320	0	115.761494	8.638451E-03
2,3-Dimethyl-2-octene	966.97	102.037	0.9800	140.270	0.7500	1	109.089873	1.833351E-02
5-Methylnonane	967.33	102.110	0.9940	142.286	0.7326	0	113.496617	8.810835E-03
4-Methylnonane	969.35	102.525	0.9940	142.176	1.4150	0	110.997888	9.009180E-03
2,4,6-Trimethyloctane	969.35	102.527	0.9940	156.313	0.7390	0	95.123866	1.051261E-02
2-Methylnonane	970.60	102.785	0.9940	142.286	0.7264	0	110.997888	9.009180E-03
1-Methyl-2-ethylbenzene	971.10	102.888	0.9330	120.195	0.8807	4	116.621601	4.287370E-02

COMPONENT	RI	TIME	RRF	MW	SG	DBE	VP	PMI Factor
Cyclopentane, 1-methyl-3-(2-methylpropyl)-	972.78	103.235	0.9800	140.266	0.7000	1	166.296223	1.202673E-02
3-Ethyloctane	974.07	103.503	0.9940	142.286	0.7330	0	109.631888	9.121434E-03
3-Octyne, 2,2-dimethyl-	974.98	103.693	0.9658	138.144	0.7810	2	144.311680	2.078834E-02
3-Methylnonane	976.89	104.092	0.9940	142.286	0.7334	0	106.153009	9.420364E-03
4-Octene, 2,6-dimethyl-, [S-(Z)]-	977.84	104.292	0.9800	140.000	0.7013	1	134.038929	1.492104E-02
C10_Mono-Naphthenes(6)	978.90	104.513	0.9800	140.270	0.8000	1	98.021337	2.040372E-02
Heptane, 2,2,3,5-tetramethyl-	980.26	104.800	0.9940	156.286	0.7334	0	91.338091	1.094833E-02
C10_Mono-Naphthenes(7)	980.81	104.917	0.9800	140.270	0.8000	1	98.021337	2.040372E-02
3-Ethyl-2-methylheptene-2	982.50	105.273	0.9800	140.270	0.7500	1	100.247909	1.995054E-02
C10_I-Paraffins(16)	982.50	105.273	0.9940	142.286	0.7334	0	106.153009	9.420364E-03
Benzene, 2-propenyl-	983.05	105.389	0.9173	118.080	0.9060	5	106.946604	5.610276E-02
C11_I-Paraffins(1)	983.21	105.423	0.9930	156.313	0.7440	0	70.562958	1.417174E-02
1,2,4-Trimethylbenzene	984.32	105.660	0.9330	120.195	0.8758	4	105.626986	4.733639E-02
1-Octene, 2,6-dimethyl-	986.87	106.203	0.9800	140.000	0.7013	1	159.500413	1.253915E-02
C10_I-Paraffins(17)	987.47	106.332	0.9940	142.286	0.7334	0	106.153009	9.420364E-03
Octane, 2,2,6-trimethyl-	987.60	106.358	0.9940	156.000	0.7420	0	94.886029	1.053896E-02
C11_I-Paraffins(2)	987.87	106.417	0.9940	156.000	0.7420	0	94.886029	1.053896E-02
C10_I-Paraffins(18)	988.51	106.555	0.9940	142.286	0.7334	0	106.153009	9.420364E-03
Cyclopentane, 1-methyl-3-(1-methylethyl)-	989.01	106.662	0.9800	126.243	0.8000	1	197.128553	1.014566E-02
C9_Mono-Naphthenes(29)	989.89	106.853	0.9800	126.243	0.8000	1	197.128553	1.014566E-02
C9_Mono-Naphthenes(30)	991.06	107.108	0.9800	126.243	0.8000	1	184.115152	1.086277E-02
Cyclopentane, 1,1,3,4-tetramethyl-, trans-	992.70	107.457	0.9800	126.000	0.7550	1	265.083894	7.544781E-03
trans-4-Decene	993.52	107.633	0.9799	140.270	0.7400	1	105.626986	1.893456E-02
2-Octene, 3,7-dimethyl-, (Z)-	993.72	107.677	0.9800	140.000	0.7013	1	132.994775	1.503818E-02
Octane, 2,3,3-trimethyl-	994.44	107.833	0.9940	156.000	0.7300	0	90.334233	1.107000E-02
2,2,3-trimethyloctane	995.41	108.043	0.9930	156.313	0.7000	0	78.938004	1.266817E-02
C9_Mono-Naphthenes(31)	995.79	108.127	0.9800	126.000	0.7550	1	265.083894	7.544781E-03
3-Heptene, 4-propyl-	996.05	108.182	0.9799	140.000	0.7500	1	127.105290	1.573499E-02
2,4,4-Trimethyl-1-hexene	996.22	108.220	0.9799	126.000	0.7330	1	251.753089	7.944292E-03
trans-3-Decene	996.29	108.234	0.9799	140.270	0.7490	1	103.032974	1.941126E-02
i-Butylbenzene	996.77	108.338	0.9380	134.222	0.8620	4	87.780660	5.696016E-02
C11_I-Paraffins(3)	997.47	108.493	0.9930	156.192	0.7440	0	70.562958	1.417174E-02
1-Isopropyl-3-MECY6	998.86	108.795	0.9898	140.000	0.8000	1	101.783605	1.964953E-02
sec-Butylbenzene	998.90	108.803	0.9380	134.222	0.8580	4	92.537787	5.403198E-02
n-Decane	1000.00	109.045	0.9940	142.286	0.7300	0	88.892305	1.124957E-02
C11_I-Paraffins(4)	1002.29	109.362	0.9930	156.313	0.7000	0	78.938004	1.266817E-02
Octane, 6-ethyl-2-methyl-	1003.39	109.513	0.9930	156.000	0.7440	0	84.202864	1.187608E-02
C10_I-Paraffins(19)	1005.22	109.768	0.9940	142.286	0.7334	0	106.153009	9.420364E-03
C11_I-Paraffins(5)	1005.52	109.810	0.9930	156.313	0.7440	0	70.562958	1.417174E-02
C10_Mono-Naphthenes(8)	1005.54	109.812	0.9800	140.270	0.8010	1	79.541201	2.514420E-02
4-Octene, 2,2,3,7-tetramethyl-, [S-(E)]-	1006.66	109.968	0.9799	168.000	0.7408	1	45.484561	4.397096E-02
1,2,3-Trimethylbenzene	1008.99	110.293	0.9330	120.195	0.8944	4	88.668939	5.638953E-02
1-Methyl-3-i-propylbenzene	1011.16	110.597	0.9380	134.222	0.8610	4	88.446092	5.653161E-02
C10_Mono-Aromatics(1)	1013.10	110.868	0.9380	134.222	0.8610	4	88.446092	5.653161E-02
C11_I-Paraffins(6)	1013.21	110.883	0.9930	156.313	0.7440	0	70.562958	1.417174E-02
1-Methyl-4-i-propylbenzene	1014.68	111.090	0.9380	134.222	0.8573	4	86.463676	5.782775E-02
Nonane, 2,5-dimethyl-	1017.43	111.477	0.9930	156.313	0.7410	0	79.339663	1.260404E-02
Octane, 2,6,6-trimethyl-	1017.46	111.482	0.9930	156.000	0.7440	0	90.334233	1.107000E-02
C11_I-Paraffins(7)	1018.50	111.628	0.9930	156.313	0.7440	0	70.562958	1.417174E-02
C11_I-Paraffins(8)	1019.83	111.823	0.9930	156.313	0.7440	0	70.562958	1.417174E-02
C11_I-Paraffins(9)	1019.99	111.845	0.9930	156.313	0.7440	0	70.562958	1.417174E-02
Cyclohexane, butylidene-	1020.74	111.948	0.9658	138.144	0.8140	2	67.189458	4.464986E-02
Indan	1021.95	112.117	0.9180	118.080	0.9970	5	85.380185	7.027392E-02
sec-Butylcyclohexane	1023.94	112.408	0.9800	140.270	0.8010	1	79.541201	2.514420E-02
C11_I-Paraffins(10)	1024.30	112.460	0.9930	156.313	0.7410	0	79.339663	1.260404E-02
C10_Mono-Naphthenes(9)	1025.22	112.589	0.9800	140.270	0.8010	1	79.541201	2.514420E-02
C11_I-Paraffins(11)	1025.36	112.608	0.9930	156.313	0.7410	0	79.339663	1.260404E-02
C11_I-Paraffins(12)	1027.51	112.908	0.9930	156.313	0.7440	0	70.562958	1.417174E-02
1-Methyl-2-i-propylbenzene	1029.12	113.138	0.9380	134.222	0.8766	4	81.789567	6.113249E-02
Indene	1029.13	113.140	0.9016	116.064	0.9968	6	75.023484	9.330412E-02

COMPONENT	RI	TIME	RRF	MW	SG	DBE	VP	PMI Factor
2,5,6-Trimethyloctane	1031.09	113.422	0.9930	156.313	0.7440	0	85.143509	1.174488E-02
C11_I-Paraffins(13)	1033.00	113.702	0.9930	156.313	0.7440	0	70.562958	1.417174E-02
C11_I-Paraffins(14)	1033.14	113.720	0.9930	156.313	0.7440	0	70.562958	1.417174E-02
n-ButylCyclohexane	1033.75	113.803	0.9800	140.160	0.7920	1	77.350089	2.585647E-02
Cyclopentane, (2-methylbutyl)-	1034.77	113.950	0.9800	140.000	0.8140	1	100.774149	1.984636E-02
Heptane, 5-ethyl-2,2,3-trimethyl-	1038.24	114.452	0.9930	170.208	0.7440	0	50.762975	1.969940E-02
Undecane, 2-methyl-	1039.90	114.693	0.9930	170.000	0.7500	0	36.683089	2.726052E-02
1,3-Diethylbenzene	1041.14	114.873	0.9380	134.222	0.8602	4	74.832548	6.681585E-02
Octane, 5-ethyl-2-methyl-	1042.53	115.075	0.9930	156.000	0.7410	0	81.789567	1.222650E-02
1-Methyl-3-n-propylbenzene	1043.80	115.260	0.9380	134.222	0.8650	4	71.106810	7.031675E-02
Nonane, 3,7-dimethyl-	1046.26	115.619	0.9930	156.313	0.7410	0	71.837965	1.392022E-02
1-Methyl-4-n-propylbenzene	1047.67	115.827	0.9380	134.222	0.8650	4	70.202525	7.122251E-02
n-Butylbenzene	1048.72	115.980	0.9380	134.222	0.8601	4	71.837965	6.960108E-02
1,4-Diethylbenzene	1048.76	115.987	0.9380	134.222	0.8620	4	92.537787	5.403198E-02
1,3-Dimethyl-5-ethylbenzene	1050.82	116.288	0.9380	134.222	0.8670	4	69.486752	7.195616E-02
1,2-Diethylbenzene	1053.19	116.638	0.9380	134.222	0.8799	4	71.471525	6.995793E-02
C10_Mono-Aromatics(2)	1054.39	116.815	0.9380	134.222	0.8799	4	71.471525	6.995793E-02
Cyclohexane, 1-methyl-4-(1-methylethenyl)-, cis-	1054.43	116.822	0.9660	138.250	0.8000	2	104.192874	2.879276E-02
C10_Mono-Aromatics(3)	1055.49	116.978	0.9380	134.222	0.8799	4	71.471525	6.995793E-02
C11_I-Paraffins(15)	1057.00	117.202	0.9930	156.313	0.7440	0	70.562958	1.417174E-02
t-Decahydronaphthalene	1057.09	117.215	0.9658	138.144	0.8965	2	59.095693	5.076512E-02
C11_I-Paraffins(16)	1057.19	117.230	0.9930	156.313	0.7440	0	70.562958	1.417174E-02
C11_I-Paraffins(17)	1058.07	117.360	0.9930	156.313	0.7440	0	70.562958	1.417174E-02
1-Methyl-2-n-propylbenzene	1059.33	117.548	0.9380	134.222	0.8650	4	66.177858	7.555397E-02
C11_I-Paraffins(18)	1060.61	117.743	0.9930	156.313	0.7440	0	70.562958	1.417174E-02
C10_I-Paraffins(20)	1060.84	117.778	0.9940	142.176	0.7320	0	129.621632	7.714762E-03
Decane, 5-methyl-	1062.17	117.972	0.9930	156.000	0.7420	0	66.862142	1.495615E-02
C9_Mono-Aromatics(1)	1063.91	118.232	0.9330	120.195	0.8944	4	86.245965	5.797373E-02
Octane, 2,3,7-trimethyl-	1063.95	118.237	0.9930	156.313	0.7390	0	79.541201	1.257210E-02
C11_Iso-Olefins(1)	1063.97	118.240	0.9930	154.300	0.7400	1	58.000682	3.448235E-02
Decane, 4-methyl-	1065.35	118.447	0.9932	156.000	0.7420	0	64.661762	1.546509E-02
Nonane, 2,3-dimethyl-	1065.79	118.513	0.9932	156.000	0.7410	0	65.500037	1.526717E-02
2-Octene, 2,3,7-trimethyl-	1066.51	118.621	0.9799	154.000	0.7400	1	75.387502	2.652960E-02
C11_I-Paraffins(19)	1067.31	118.742	0.9930	156.313	0.7440	0	70.562958	1.417174E-02
Decane, 2-methyl-	1068.70	118.950	0.9932	156.000	0.7440	0	83.271842	1.200886E-02
1,4,Dimethyl-2-ethylbenzene	1069.32	119.043	0.9380	134.222	0.8670	4	65.500037	7.633584E-02
C11_I-Paraffins(20)	1070.46	119.215	0.9932	156.000	0.7410	0	65.500037	1.526717E-02
1,3-Dimethyl-4-ethylbenzene	1070.92	119.285	0.9380	134.222	0.8670	4	63.833387	7.832892E-02
Benzene, (2-methyl-1-propenyl)-	1070.98	119.293	0.9235	132.000	0.9010	5	63.833387	9.399470E-02
C10_Mono-Aromatics(4)	1071.69	119.402	0.9380	134.222	0.8772	4	65.500037	7.633584E-02
C10_Mono-Aromatics(5)	1073.48	119.673	0.9380	134.222	0.8772	4	65.500037	7.633584E-02
Decane, 3-methyl-	1074.64	119.848	0.9932	156.000	0.7420	0	61.885029	1.615900E-02
1,2-Dimethyl-4-ethylbenzene	1076.64	120.152	0.9380	134.222	0.8670	4	61.247854	8.163551E-02
Indan, 1-methyl-	1079.46	120.582	0.9180	132.096	0.9540	5	55.344343	1.084122E-01
Decane, 2,3,4-trimethyl-	1082.23	121.005	0.9930	184.000	0.7440	0	25.355613	3.943900E-02
1-Methyl-4-t-butylbenzene	1082.31	121.017	0.9420	148.240	0.8612	4	56.217084	8.894093E-02
C11_I-Paraffins(21)	1083.87	121.257	0.9930	156.313	0.7440	0	70.562958	1.417174E-02
C11_I-Paraffins(22)	1084.24	121.313	0.9930	156.313	0.7440	0	70.562958	1.417174E-02
Cyclopropane, 1,2-dimethyl-1-pentyl-	1086.26	121.623	0.9800	140.160	0.8140	1	137.250891	1.457185E-02
Cyclopentane, 1,2-dimethyl-3-(1-methylethyl)-	1086.77	121.702	0.9798	140.000	1.0000	1	126.949540	1.575429E-02
1-Undecene, 7-methyl-	1087.99	121.889	0.9799	168.192	0.7570	1	40.736120	4.909648E-02
α,ß,ß-Trimethylstyrene	1088.98	122.043	0.9287	146.112	0.8770	5	57.850083	1.037164E-01
C11_I-Paraffins(23)	1089.05	122.053	0.9932	156.000	0.7410	0	65.500037	1.526717E-02
1-Octene, 6-methyl-	1089.73	122.158	0.9799	126.144	0.7000	1	220.615145	9.065561E-03
Undecane, 4-methyl-	1090.46	122.272	0.9930	170.000	0.7500	0	36.387163	2.748222E-02
C9_Iso-Olefins(5)	1090.72	122.312	0.9799	126.144	0.7000	1	220.615145	9.065561E-03
C10_Indanes(1)	1090.89	122.338	0.9180	136.234	0.9600	3	88.959417	4.496432E-02
Decane, 2,3,6-trimethyl-	1091.16	122.379	0.9930	184.000	0.7440	0	70.562958	1.417174E-02
1-Ethyl-3-i-propylbenzene	1093.07	122.677	0.9420	148.240	0.9000	4	42.741779	1.169816E-01
1,2-Dimethyl-3-ethylbenzene	1094.95	122.968	0.9380	134.222	0.8670	4	57.400444	8.710734E-02

COMPONENT	RI	TIME	RRF	MW	SG	DBE	VP	PMI Factor
1-Ethyl-2-i-propylbenzene	1097.17	123.315	0.9420	148.240	0.9000	4	42.741779	1.169816E-01
C12_I-Paraffins(1)	1097.88	123.425	0.9916	170.340	0.7440	0	70.562958	1.417174E-02
(1,2-dimethylpropyl)benzene	1098.56	123.532	0.9420	148.240	0.8570	4	66.519189	7.516628E-02
C12_I-Paraffins(2)	1098.60	123.538	0.9930	170.000	0.7500	0	36.387163	2.748222E-02
n-Undecane	1100.00	123.757	0.9930	156.313	0.7402	0	51.840398	1.928998E-02
C11_Mono-Aromatics(1)	1100.31	123.793	0.9420	148.240	0.8570	4	66.519189	7.516628E-02
Benzene, (1-ethylpropyl)-	1102.10	124.002	0.9416	148.128	0.8590	4	64.495298	7.752503E-02
C12_I-Paraffins(3)	1102.27	124.022	0.9916	170.340	0.7440	0	70.562958	1.417174E-02
4,7-Methano-1H-indene, octahydro-	1103.04	124.111	0.9180	136.234	0.9600	3	88.959417	4.496432E-02
Benzene, 2,4-dimethyl-1-(1-methylpropyl)-	1105.37	124.385	0.9416	162.144	0.8600	4	26.931510	1.856561E-01
1,2,3,5-Tetramethylbenzene	1107.03	124.580	0.9380	134.222	0.8910	4	47.527241	1.052028E-01
1-Ethyl-4-i-propylbenzene	1107.03	124.580	0.9420	148.240	0.8600	4	50.364276	9.927672E-02
1,2,4,5-Tetramethylbenzene	1111.04	125.052	0.9380	134.112	0.8875	4	51.704580	9.670323E-02
Benzene, 1-methyl-4-(2-methylpropyl)-	1112.58	125.234	0.9420	148.240	0.8620	4	51.704580	9.670323E-02
trans-4a-Methyl-decahydronaphthalene	1113.25	125.313	0.9800	152.277	1.0000	2	49.445144	6.067330E-02
C11_Mono-Aromatics(2)	1114.26	125.433	0.9420	148.240	0.8590	4	59.991594	8.334501E-02
1-t-Butyl-2-methylbenzene	1115.73	125.607	0.9420	148.240	0.8590	4	59.991594	8.334501E-02
Decane, 2,5-dimethyl-	1116.74	125.726	0.9930	170.208	0.7490	0	47.905265	2.087453E-02
1H-Indene,2,3-dihydro-2,2-dime	1118.59	125.945	0.9287	146.112	0.9310	5	45.195996	1.327551E-01
C11_I-Paraffins(24)	1120.02	126.115	0.9930	156.192	0.7410	0	70.562958	1.417174E-02
C11_Mono-Aromatics(3)	1120.06	126.120	0.9420	148.240	0.8900	4	54.484083	9.176992E-02
C11_I-Paraffins(25)	1121.17	126.253	0.9930	156.192	0.7410	0	70.562958	1.417174E-02
Nonane, 4,5-dimethyl-	1122.83	126.451	0.9930	156.192	0.7410	0	70.562958	1.417174E-02
C11_Mono-Aromatics(4)	1124.66	126.669	0.9420	148.240	0.8900	4	54.484083	9.176992E-02
Decane, 5,6-dimethyl-	1125.89	126.815	0.9930	170.000	0.7490	0	41.727900	2.396478E-02
C12_I-Paraffins(4)	1126.10	126.840	0.9930	170.300	0.7440	0	70.562958	1.417174E-02
1H-Indene, 2,3-dihydro-1,2-dim	1126.15	126.847	0.9287	146.286	0.9220	5	39.872729	1.504788E-01
2-Undecene, (E)-	1127.00	126.948	0.9799	154.176	0.7408	1	74.092179	2.699340E-02
C12_I-Paraffins(5)	1127.18	126.970	0.9930	170.300	0.7440	0	70.562958	1.417174E-02
Benzene, 1-ethyl-4-(2-methylpropyl)-	1129.35	127.230	0.9420	162.000	0.8900	4	19.310174	2.589309E-01
5-Methylindan	1130.13	127.323	0.9235	132.200	0.9800	5	42.401336	1.415050E-01
4-Methylindan	1130.14	127.325	0.9235	132.200	0.9800	5	39.553306	1.516940E-01
C11_Mono-Naphthenes(1)	1133.33	127.708	0.9930	156.000	0.7440	0	70.562958	1.417174E-02
C12_Mono-Aromatics(1)	1133.36	127.712	0.9450	162.272	0.8900	4	41.839454	1.195044E-01
C12_I-Paraffins(6)	1133.41	127.718	0.9916	170.340	0.7440	0	70.562958	1.417174E-02
Benzene, 1,3-diethyl-5-methyl-	1135.00	127.910	0.9420	148.240	0.8650	4	43.199603	1.157418E-01
C11_Mono-Aromatics(5)	1136.33	128.085	0.9420	148.240	0.8650	4	43.199603	1.157418E-01
C11_Mono-Aromatics(6)	1136.62	128.117	0.9420	148.240	0.8650	4	43.199603	1.157418E-01
Octane, 2,3,6,7-tetramethyl-	1136.76	128.133	0.9930	170.000	0.7440	0	47.715909	2.095737E-02
Benzene, 1-(1,1-dimethylethyl)-3-methyl-	1137.92	128.262	0.9420	148.240	0.8590	4	62.366913	8.017072E-02
C10_Indenes(1)	1138.01	128.273	0.9095	130.000	0.8900	6	56.496081	1.239024E-01
1H-Indene, 1-methyl-	1139.32	128.432	0.9095	130.000	0.8900	6	56.496081	1.239024E-01
C11_Mono-Aromatics(7)	1139.36	128.437	0.9420	148.240	0.8590	4	62.366913	8.017072E-02
C10_Mono-Aromatics(6)	1139.68	128.475	0.9380	134.222	0.8670	4	60.303414	8.291405E-02
2-Methylindan	1141.16	128.655	0.9235	132.200	0.9540	5	53.776614	1.115727E-01
1H-Indene, 3-methyl-	1144.09	129.010	0.9095	130.186	1.0020	6	40.086990	1.746202E-01
1,3-Dimethyl-2-ethylbenzene	1145.30	129.158	0.9380	134.222	0.8670	4	60.303414	8.291405E-02
5-Ethyldecane	1148.60	129.560	0.9930	170.340	1.0000	0	46.078972	2.170187E-02
C11_Mono-Naphthenes(2)	1148.66	129.568	0.9930	156.313	0.7440	0	70.562958	1.417174E-02
Benzene, 1,4-dimethyl-2-(1-methylethyl)-	1150.07	129.740	0.9380	148.000	0.8610	4	51.433925	9.721210E-02
Benzene, (1-methylbutyl)-	1151.59	129.927	0.9420	148.000	0.8900	4	41.649975	1.200481E-01
n-Pentylbenzene	1151.61	129.928	0.9420	148.240	0.8630	4	40.302305	1.240624E-01
Naphthalene, 1,2,3,4-tetrahydro	1152.25	130.007	0.9180	132.096	0.9702	5	35.320707	1.698720E-01
Benzene, 4-ethenyl-1,2-dimethyl-	1152.94	130.092	0.9235	132.096	0.8930	5	47.778951	1.255783E-01
C10_Mono-Aromatics(7)	1153.67	130.182	0.9376	134.222	0.8900	4	60.459883	8.269946E-02
1,4-diethyl-2-methylbenzene	1154.80	130.320	0.9420	148.240	0.8650	4	38.921484	1.284638E-01
Benzene, 1-ethyl-3-(1-methylethyl)-	1155.82	130.445	0.9420	148.240	0.8600	4	56.658187	8.824850E-02
C10_I-Paraffins(21)	1158.04	130.727	0.9940	142.286	0.7530	0	29.990406	3.334400E-02
Heptane, 3-ethyl-2-methyl-	1158.82	130.818	0.9940	142.176	0.7320	0	122.810816	8.142605E-03
Benzene, (1,1-dimethylpropyl)-	1159.36	130.882	0.9420	148.240	0.8580	4	60.459883	8.269946E-02

COMPONENT	RI	TIME	RRF	MW	SG	DBE	VP	PMI Factor
2,4-diethyl-1-methylbenzene	1161.25	131.115	0.9420	148.240	0.8650	4	39.765993	1.257356E-01
Decane, 4-ethyl-	1163.16	131.352	0.9932	170.335	1.0000	0	46.078972	2.170187E-02
C11_Mono-Aromatics(8)	1165.32	131.632	0.9420	148.128	0.8900	4	35.608684	1.404152E-01
C12_I-Paraffins(7)	1165.98	131.709	0.9932	170.335	1.0000	0	46.078972	2.170187E-02
Undecane, 2,7-dimethyl-	1167.15	131.847	0.9907	184.224	0.7530	0	25.046529	3.992569E-02
1-Methyl-2-n-butylbenzene	1168.03	131.957	0.9420	162.144	0.8701	4	41.839454	1.195044E-01
1-methyl-4-(1-methylpropyl)be	1168.05	131.958	0.9420	148.240	0.8600	4	51.840398	9.644988E-02
1,4-Di-i-propylbenzene	1171.13	132.342	0.9450	162.272	0.8568	4	35.320707	1.415600E-01
Naphthalene	1171.84	132.432	0.8960	128.174	1.0370	7	25.977026	3.079644E-01
C12_I-Paraffins(8)	1173.70	132.663	0.9916	170.340	0.7400	0	50.364276	1.985534E-02
1-t-Butyl-3,5-dimethylbenzene	1173.72	132.667	0.9450	162.272	0.8600	4	37.685497	1.326770E-01
C12_I-Paraffins(9)	1174.06	132.708	0.9916	170.340	0.7400	0	50.364276	1.985534E-02
1H-Indene, 2,3-dihydro-1,6-dimethyl-	1176.21	132.978	0.9287	146.200	0.9440	5	32.378827	1.853063E-01
1H-Indene, 2,3-dihydro-1,3-dimethyl-	1176.21	132.978	0.9287	146.000	0.9220	5	36.881595	1.626828E-01
C12_I-Paraffins(10)	1177.67	133.162	0.9916	170.340	0.7400	0	50.364276	1.985534E-02
C12_Mono-Aromatics(2)	1179.24	133.358	0.9450	162.272	0.8600	4	37.685497	1.326770E-01
4,7-Dimethyl Indane	1180.38	133.502	0.9287	146.200	0.9670	5	22.523061	2.663936E-01
1,1-Dimethyl Indane	1182.10	133.718	0.9287	146.112	0.9310	5	58.911879	1.018470E-01
C12_Mono-Aromatics(3)	1184.14	133.977	0.9450	162.272	0.8580	4	34.189989	1.462416E-01
1t-Butyl-4-ethylbenzene	1185.59	134.160	0.9450	162.272	0.8580	4	34.189989	1.462416E-01
C12_Indanes(1)	1186.38	134.260	0.9329	160.260	0.9640	5	82.412878	7.280416E-02
1,3-Di-n-propylbenzene	1190.40	134.770	0.9450	162.272	0.8559	4	42.970132	1.163599E-01
Benzene, 1-ethyl-2,4,5-trimethyl-	1192.16	134.993	0.9420	148.240	0.8660	4	32.823195	1.523313E-01
Benzene, 1,3-dimethyl-5-(1-methylethyl)-	1192.16	134.993	0.9420	148.000	0.8610	4	54.626600	9.153050E-02
4-Octene, 2,3,6,7-tetramethyl-	1194.00	135.228	0.9799	168.000	0.7400	1	42.730391	4.680510E-02
C12_Iso-Olefins(1)	1196.05	135.490	0.9930	168.200	0.7400	1	58.000682	3.448235E-02
C11_Mono-Aromatics(9)	1196.11	135.497	0.9420	148.000	0.8610	4	54.626600	9.153050E-02
n-Dodecane	1200.00	135.995	0.9920	170.340	0.7495	0	31.078524	3.217656E-02
C11_Mono-Aromatics(10)	1200.02	135.997	0.9240	146.112	0.9350	5	26.267371	2.284203E-01
C11_Mono-Aromatics(11)	1200.37	136.033	0.9240	146.112	0.9350	5	26.267371	2.284203E-01
Benzene, (3,3-dimethylbutyl)-	1202.42	136.247	0.9420	162.144	0.8500	4	24.052125	2.078818E-01
C12_Mono-Aromatics(4)	1204.04	136.415	0.9416	162.000	0.9000	4	37.888965	1.319645E-01
1H-Indene, 2,3-dihydro-1,1,3-trimethyl-	1207.46	136.772	0.9329	160.000	0.9050	5	29.826130	2.011659E-01
Benzene, (1,3-dimethylbutyl)-	1207.51	136.777	0.9416	162.000	0.9000	4	37.888965	1.319645E-01
Naphthalene, 1,2,3,4-tetrahydro-2-methyl-	1207.55	136.782	0.9240	146.112	0.9350	5	26.267371	2.284203E-01
Benzene, 2,4-dimethyl-1-(1-methylethyl)-	1210.22	137.060	0.9416	148.000	0.8610	4	47.276749	1.057602E-01
n-propyl indane	1211.09	137.152	0.9329	160.200	0.9000	5	18.251881	3.287332E-01
Naphthalene, 1,2,3,4-tetrahydro-1-methyl-	1211.15	137.158	0.9420	146.229	0.8000	5	26.738091	2.243990E-01
Heptane, 4-ethyl-2,2,6,6-tetramethyl-	1211.30	137.173	0.9930	184.361	0.8000	0	53.077603	1.884034E-02
C11_Mono-Aromatics(12)	1213.29	137.382	0.9420	148.240	0.8500	4	56.217084	8.894093E-02
C11_Mono-Aromatics(13)	1213.49	137.404	0.9420	148.240	0.8500	4	56.217084	8.894093E-02
Decane, 2,5,9-trimethyl-	1216.58	137.730	0.9930	184.361	0.8000	0	34.563159	2.893254E-02
C11_Mono-Aromatics(14)	1217.08	137.783	0.9420	148.240	0.8500	4	56.217084	8.894093E-02
1,3,5-Triethylbenzene	1217.64	137.842	0.9450	162.272	0.8897	4	31.939967	1.565437E-01
1,3,5-trimethyl-2-propylbenze	1219.20	138.003	0.9450	162.272	0.8650	4	19.271633	2.594487E-01
Octane, 2,3,6-trimethyl-	1222.03	138.302	0.9932	156.192	0.7390	0	77.546951	1.289541E-02
C12_Indanes(2)	1223.40	138.447	0.9180	160.200	0.9640	5	82.412878	7.280416E-02
2,6-Dimethyldecane	1224.19	138.531	0.9932	170.000	0.7490	0	45.677876	2.189244E-02
Decane, 3,7-dimethyl-	1224.23	138.535	0.9932	170.000	0.7490	0	42.970132	2.327198E-02
2-Ethyl-2,3-dihydro-1H-indene	1225.71	138.692	0.9287	146.112	0.9360	5	30.908806	1.941194E-01
1H-Indene, 1-ethyl-2,3-dihydro-	1228.24	138.960	0.9287	146.112	0.9360	5	25.618215	2.342084E-01
C12_Mono-Aromatics(5)	1230.41	139.190	0.9450	162.272	0.8900	4	41.839454	1.195044E-01
1H-Indene, 2,3-dihydro-1,1,4-trimethyl-	1230.43	139.192	0.9329	160.000	0.9640	5	13.476920	4.452056E-01
1-Methyl-4-n-pentylbenzene	1232.04	139.363	0.9450	162.272	0.9000	4	22.459737	2.226206E-01
C12_Mono-Aromatics(6)	1232.21	139.382	0.9450	162.272	0.8900	4	41.839454	1.195044E-01
C12_Indanes(3)	1232.90	139.455	0.9180	160.200	0.9640	5	82.412878	7.280416E-02
C12_Indanes(4)	1233.18	139.485	0.9180	160.200	0.9640	5	82.412878	7.280416E-02
1-H-Indene-1-Ethyl	1233.28	139.495	0.9180	144.217	1.0000	6	18.568470	3.769831E-01
Benzene, 1,4-dimethyl-2-(2-methylpropyl)-	1237.79	139.977	0.9450	162.000	0.8620	4	25.263933	1.979106E-01
C12_Mono-Aromatics(7)	1239.12	140.118	0.9450	162.272	0.8900	4	41.839454	1.195044E-01

COMPONENT	RI	TIME	RRF	MW	SG	DBE	VP	PMI Factor
C12_Mono-Aromatics(8)	1239.74	140.185	0.9450	162.272	0.8900	4	41.839454	1.195044E-01
1H-Indene, 2,3-dihydro-1,1,5-trimethyl-	1240.90	140.309	0.9329	160.000	0.9640	5	24.914127	2.408272E-01
Benzene, (1-ethyl-1-methylpropyl)-	1243.55	140.593	0.9450	162.000	0.8570	4	40.736120	1.227412E-01
C11_Indanes(1)	1244.73	140.725	0.9180	146.112	0.9640	5	82.412878	7.280416E-02
Benzene, 3-ethyl-1,2,4,5-tetramethyl-	1248.40	141.115	0.9450	162.000	0.8900	4	12.338964	4.052204E-01
Benzene, (1,1-dimethylbutyl)-	1248.73	141.151	0.9450	162.270	0.8570	4	40.194515	1.243951E-01
Benzene, (1,1,2-trimethylpropyl)-	1248.81	141.160	0.9450	162.144	0.9640	4	24.350000	2.053388E-01
Benzene, (2-ethylbutyl)-	1250.51	141.343	0.9450	162.000	0.8600	4	28.541219	1.751852E-01
C12_Mono-Aromatics(9)	1252.98	141.610	0.9450	162.271	0.8580	4	37.584139	1.330348E-01
Dodecane, 6-methyl-	1255.03	141.832	0.9930	184.224	1.2210	0	23.691096	4.220995E-02
Benzene, (1-methylpentyl)-	1255.12	141.842	0.9450	162.271	0.8580	4	37.584139	1.330348E-01
2,3-Dimethyldecane	1257.40	142.088	0.9930	170.208	0.7490	0	37.584139	2.660697E-02
n-Hexylbenzene	1257.51	142.101	0.9450	162.272	0.8610	4	22.906437	2.182793E-01
Decane, 2,4-dimethyl-	1258.36	142.193	0.9930	170.208	0.7490	0	46.042376	2.171912E-02
1-H-Indene,1-3-dimethyl	1258.93	142.255	0.9180	144.200	0.9620	6	21.107014	3.316433E-01
1H-Indene, 2,3-dihydro-4,6-dimethyl-	1262.27	142.618	0.9287	146.000	0.9670	5	23.492666	2.553989E-01
1H-Indene, 2,3-dihydro-5,6-dimethyl-	1262.58	142.652	0.9287	146.112	0.9670	5	21.897080	2.740091E-01
Decane, 2,3,8-trimethyl-	1266.51	143.080	0.9932	184.000	0.7400	0	25.355613	3.943900E-02
Benzene, 1-(1-methylethenyl)-4-(1-methylethyl)-	1269.37	143.393	0.9329	160.000	0.8640	5	26.856968	2.234057E-01
Naphthalene, 5-ethyl-1,2,3,4-tetrahydro-	1270.71	143.540	0.9329	160.128	0.9470	5	15.211829	3.944299E-01
C13_I-Paraffins(1)	1270.88	143.558	0.9910	184.370	0.7560	0	17.532188	5.703795E-02
C12_Mono-Aromatics(10)	1270.95	143.567	0.9329	160.000	0.8640	5	26.856968	2.234057E-01
C12_Mono-Aromatics(11)	1273.19	143.813	0.9450	162.272	0.8900	4	41.839454	1.195044E-01
Benzene, 1-(1-methylethenyl)-2-(1-methylethyl)-	1274.70	143.978	0.9329	160.000	0.9640	5	21.293019	2.817825E-01
C12_Mono-Aromatics(12)	1275.91	144.112	0.9450	162.272	0.8900	4	41.839454	1.195044E-01
C12_Mono-Aromatics(13)	1276.32	144.157	0.9450	162.272	0.8900	4	41.839454	1.195044E-01
Indane,4,5,7-trimethyl	1276.68	144.196	0.9329	160.200	0.9570	5	11.768179	5.098495E-01
1,2,4-Triethylbenzene	1277.03	144.234	0.9450	162.272	0.8630	4	28.541219	1.751852E-01
C12_Indanes(5)	1277.05	144.237	0.9329	160.260	0.9640	5	82.412878	7.280416E-02
Pentamethylbenzene	1277.16	144.248	0.9420	148.240	0.8670	4	21.047330	2.375598E-01
C12_Indanes(6)	1282.53	144.848	0.9180	160.000	0.9640	5	82.412878	7.280416E-02
2-Methylnaphthalene	1286.58	145.290	0.9030	142.080	1.0200	7	15.345431	5.213278E-01
C12_Mono-Aromatics(14)	1289.24	145.573	0.9450	162.272	0.8900	4	41.839454	1.195044E-01
C12_Mono-Aromatics(15)	1289.49	145.600	0.9450	162.272	0.8900	4	41.839454	1.195044E-01
C12_Mono-Aromatics(16)	1289.76	145.632	0.9450	162.272	0.8900	4	41.839454	1.195044E-01
Naphthalene, 1,2,3,4-tetrahydro-5,6-dimethyl-	1291.75	145.865	0.9329	160.000	0.9490	5	9.913369	6.052433E-01
1H-Indene, 2,3-dihydro-1,4,7-trimethyl-	1298.14	146.578	0.9329	160.255	0.9360	5	17.034038	3.522359E-01
n-Tridecane	1300.00	146.787	0.9910	184.370	0.7564	0	17.991818	5.558082E-02
1-Methylnaphthalene	1302.45	147.020	0.9030	142.080	1.0058	7	15.390202	5.198113E-01
Naphthalene, 1,2,3,4-tetrahydro-1,8-dimethyl-	1304.04	147.172	0.9329	160.000	0.9280	5	14.602225	4.108963E-01
C13_I-Paraffins(2)	1305.94	147.353	0.9910	184.370	0.7560	0	17.532188	5.703795E-02
Naphthalene, 1,2,3,4-tetrahydro-2,6-dimethyl-	1306.83	147.439	0.9240	160.128	0.9695	5	11.959284	5.017023E-01
C12_Indanes(7)	1307.33	147.487	0.9180	160.128	0.9640	5	82.412878	7.280416E-02
Naphthalene, 1,2,3,4-tetrahydro-1,1-dimethyl-	1316.56	148.373	0.9240	160.128	0.9170	5	25.977026	2.309733E-01
Naphthalene, 6-ethyl-1,2,3,4-tetrahydro-	1316.61	148.378	0.9240	160.128	0.9470	5	12.639302	4.747098E-01
1H-Indene, 2,3-dihydro-4-propyl-	1319.73	148.678	0.9329	160.000	0.9640	5	11.817456	5.077235E-01
1H-Indene, 1-ethyl-2,3-dihydro-1-methyl-	1320.33	148.736	0.9330	160.255	1.0000	5	29.990406	2.000640E-01
1H-Indene, 2,3-dihydro-1,5,7-trimethyl-	1323.95	149.087	0.9329	160.000	0.9360	5	16.693034	3.594314E-01
Naphthalene, 1-ethyl-1,2,3,4-tetrahydro-	1325.86	149.272	0.9237	160.000	0.9210	5	15.480099	3.875944E-01
Undecane, 5-ethyl-	1328.13	149.492	0.9910	184.000	1.0000	0	24.740886	4.041892E-02
C13_I-Paraffins(3)	1331.37	149.807	0.9910	184.370	0.7560	0	17.532188	5.703795E-02
Naphthalene, 1,2,3,4-tetrahydro-6-propyl-	1335.97	150.255	0.9365	174.000	0.9390	5	7.265096	8.258666E-01
C12_Indanes(8)	1343.71	151.012	0.9180	160.200	0.9640	5	82.412878	7.280416E-02
C12_Mono-Aromatics(17)	1344.00	151.040	0.9450	162.272	0.8900	4	41.839454	1.195044E-01
1-Methyl-4-Hexylbenzene	1347.92	151.425	0.9450	176.200	0.8610	4	13.019241	3.840470E-01
C13_I-Paraffins(4)	1350.01	151.633	0.9910	184.000	0.7560	0	25.355613	3.943900E-02
Naphthalene, 2-ethyl-1,2,3,4-tetrahydro-	1353.27	151.952	0.9240	160.128	0.9210	5	17.735132	3.383115E-01
C13_Mono-Naphthenes(1)	1356.18	152.238	0.9799	182.351	0.8000	1	40.736120	4.909648E-02
Benzene, 1,2,4-trimethyl-5-(1-methylethyl)-	1356.19	152.240	0.9450	162.000	0.8610	4	27.840882	1.795920E-01
Benzene, (2,4-dimethylpentyl)-	1361.07	152.723	0.9450	176.000	0.8570	4	18.890051	2.646896E-01

COMPONENT	RI	TIME	RRF	MW	SG	DBE	VP	PMI Factor
Octane, 3-ethyl-2,7-dimethyl-	1361.20	152.735	0.9910	170.000	0.7560	0	47.164424	2.120242E-02
2,4,6-Trimethyl-1-nonene	1364.00	153.014	0.9799	168.000	0.7400	1	51.043788	3.918204E-02
Undecane, 3-ethyl-	1365.93	153.205	0.9910	184.000	0.7570	0	20.810125	4.805353E-02
Acenaphthene	1367.00	153.312	0.9030	154.080	1.0242	8	19.772548	4.551765E-01
1,1'-Biphenyl	1369.37	153.548	0.9040	154.210	1.0410	8	9.823537	9.161670E-01
Naphthalene, 2-ethenyl-	1373.11	153.922	0.8977	154.080	1.0000	8	6.168536	1.459017E+00
Undecane, 2,8-dimethyl-	1373.19	153.930	0.9907	184.361	0.8000	0	25.046529	3.992569E-02
C13_I-Paraffins(5)	1379.77	154.597	0.9910	184.000	0.7560	0	25.355613	3.943900E-02
C13_I-Paraffins(6)	1380.90	154.712	0.9910	184.000	0.7570	0	20.810125	4.805353E-02
1-Ethylnaphthalene	1388.53	155.470	0.9095	156.096	0.9990	7	8.667610	9.229765E-01
Decane, 2,3,5-trimethyl-	1388.79	155.496	0.9910	184.000	0.7560	0	25.355613	3.943900E-02
2-Ethylnaphthalene	1390.96	155.715	0.9095	156.096	0.9922	7	9.025530	8.863746E-01
n-Tetradecane	1400.00	156.632	0.9900	198.390	0.7628	0	10.756043	9.297099E-02
Naphthalene,2,6 dimethyl	1400.00	156.632	0.9095	156.224	1.0000	7	7.926041	1.009331E+00
Naphthalene,2,7 dimethyl	1401.56	156.770	0.9095	156.224	1.0000	7	7.683983	1.041127E+00
1H-Indene, 2,3-dihydro-1,1,6-trimethyl-	1412.65	157.761	0.9180	160.255	0.8000	5	5031.110610	1.192580E-03
Naphthalene,1,7-dimethyl	1415.49	158.015	0.9095	156.224	1.0000	7	7.804161	1.025094E+00
Naphthalene, 1,3-dimethyl-	1415.49	158.015	0.9095	156.000	1.0000	7	7.683983	1.041127E+00
Naphthalene, 1,6-dimethyl-	1419.44	158.370	0.9095	156.000	1.0030	7	7.448643	1.074021E+00
C13_Indanes(1)	1432.58	159.555	0.9180	174.200	0.9640	5	82.412878	7.280416E-02
Naphthalene-1,4-dimethyl	1436.77	159.935	0.9095	156.227	1.0000	7	6.478552	1.234844E+00
Naphthalene, 2,3-dimethyl-	1436.77	159.935	0.9095	156.224	1.0000	7	6.387125	1.252520E+00
Naphthalene, 1,5-dimethyl-	1439.54	160.187	0.9095	156.000	1.0000	7	7.085656	1.129042E+00
Naphthalene, 1,2-dimethyl-	1452.34	161.355	0.9095	156.000	1.0130	7	6.571163	1.217441E+00
1,1'-Biphenyl, 2-methyl-	1470.76	163.051	0.9040	168.096	1.0110	8	9.734443	9.245521E-01
1,1'-Biphenyl, 3-methyl-	1476.81	163.612	0.9040	168.000	0.9830	8	5.660429	1.589986E+00
Naphthalene, 1,8-dimethyl-	1479.11	163.826	0.9095	156.000	1.0000	7	6.052183	1.321837E+00
Octane, 3,4,5,6-tetramethyl-	1481.45	164.043	0.9910	170.000	0.7560	0	47.715909	2.095737E-02
1,1'-Biphenyl, 4-methyl-	1485.95	164.463	0.9040	168.096	0.9830	8	6.612707	1.361016E+00
Naphthalene, 1-propyl-	1491.06	164.941	0.9240	170.000	0.9840	7	5.207276	1.536312E+00
n-Pentadecane	1500.00	165.780	0.9900	212.420	0.7690	0	6.052183	1.652296E-01
Naphthalene, 2,3,6-trimethyl-	1501.61	165.955	0.9240	170.112	0.9870	7	7.565484	1.057434E+00
C13_Naphthalenes(1)	1511.32	167.017	0.9240	170.250	0.9750	7	6.813309	1.174173E+00
C13_Naphthalenes(2)	1511.49	167.035	0.9240	170.250	0.9750	7	6.813309	1.174173E+00
Azulene, 4,6,8-trimethyl-	1514.74	167.392	0.9240	170.112	0.9870	7	3.829606	2.088988E+00
C13_Naphthalenes(3)	1517.30	167.673	0.9240	170.300	0.9870	7	4.312458	1.855091E+00
Naphthalene, 1,4,6-trimethyl-	1519.48	167.913	0.9240	170.300	0.9870	7	4.312458	1.855091E+00
2,2'-Dimethylbiphenyl	1522.68	168.267	0.9040	182.260	0.9890	8	9.006218	9.993096E-01
Naphthalene, 1,4,5-trimethyl-	1524.08	168.422	0.9149	170.250	0.9870	7	3.175131	2.519581E+00
C13_Naphthalenes(4)	1536.50	169.800	0.9240	170.112	0.9870	7	3.571092	2.240211E+00
C13_Naphthalenes(5)	1539.86	170.190	0.9149	170.255	0.9750	7	6.813309	1.174173E+00
Naphthalene, 2-(1-methylethyl)-	1549.32	171.235	0.9240	170.250	0.9750	7	6.813309	1.174173E+00
Naphthalene, 1,6,7-trimethyl-	1551.09	171.435	0.9240	170.112	0.9870	7	3.571092	2.240211E+00
4-Ethylbiphenyl	1552.57	171.602	0.9040	182.261	0.9700	8	3.095639	2.907315E+00
3,3'-Dimethylbiphenyl	1564.61	172.963	0.9040	182.260	0.9990	8	3.281784	2.742411E+00
1,1'-Biphenyl, 3,4'-dimethyl-	1568.34	173.387	0.9040	182.261	0.9990	8	3.896181	2.309954E+00
1,1'-Biphenyl, 2,4'-dimethyl-	1569.89	173.564	0.9040	182.261	0.9000	8	4.347952	2.069940E+00
4,4'-Dimethylbiphenyl	1581.28	174.867	0.9040	182.261	0.9900	8	2.719881	3.308968E+00
Naphthalene, 2,6-diethyl	1582.37	174.992	0.9240	184.280	0.9740	7	2.743270	2.916228E+00
Benzene, 1-methyl-3-[(4-methylphenyl)methyl]-	1586.56	175.473	0.9142	196.293	0.8000	8	3.207442	2.805974E+00
C14_Mono-Aromatics(1)	1593.29	176.257	0.9040	182.261	0.9000	8	4.347952	2.069940E+00
Hexadecane	1600.00	177.034	0.9887	226.448	0.7734	0	3.607028	2.772366E-01
1,4,6,7-tetramethylnaphthalene	1629.44	180.483	0.9195	184.282	1.0000	7	2.056715	3.889699E+00