Overview

This workbook is an automated and annotated tool for processing individual samples using the sufficiency method. Use of this workbook requires ChemStation Percent Reports for the TIC and EIPs.

To begin, save this workbook as the indvidual Sample ID/Name being processed and make sure to retain an unused template of this workbook for additional and/or future samples.

Notes:
-This workbook will only allow the processing of one sample; this is not a batch tool.

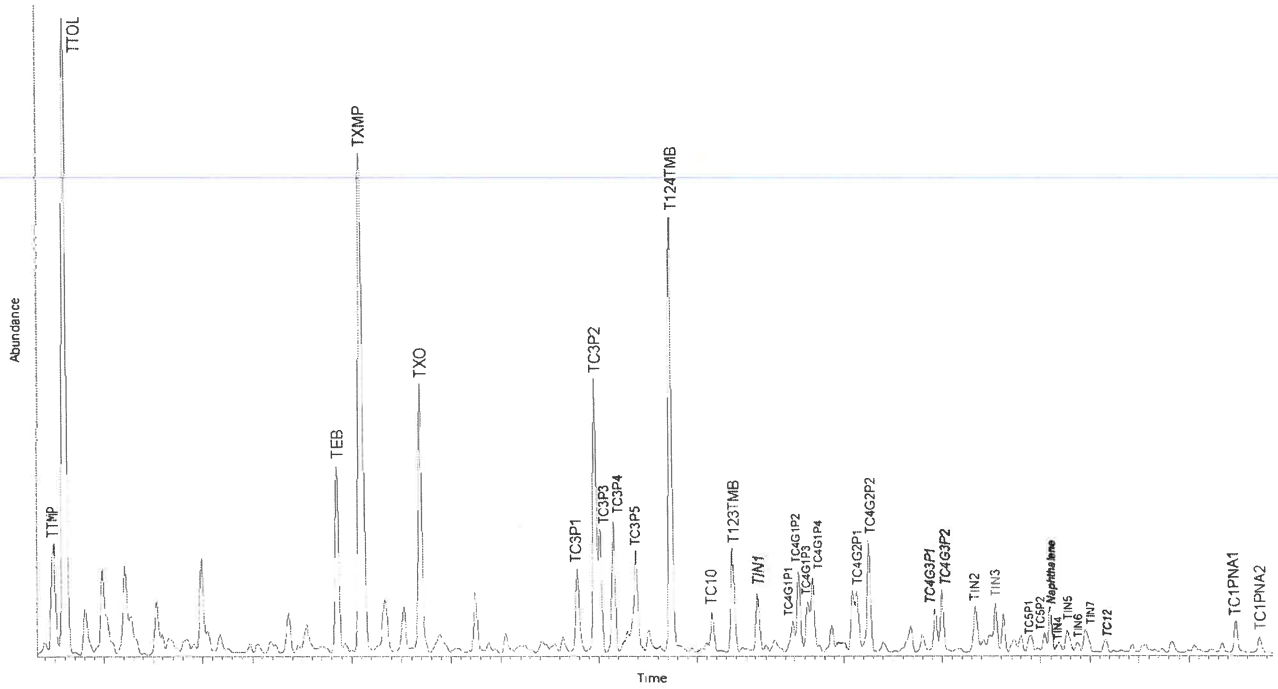
-The Peak Maps worksheet has a labeled TIC and labeled EIPs showing all of the peaks of interest.

-The Retention Time worksheet is for collecting retention times (RTs) in one place. RTs documented in the Retention Time worksheet can be copied and pasted to the appropriate TIC or EIP worksheet.

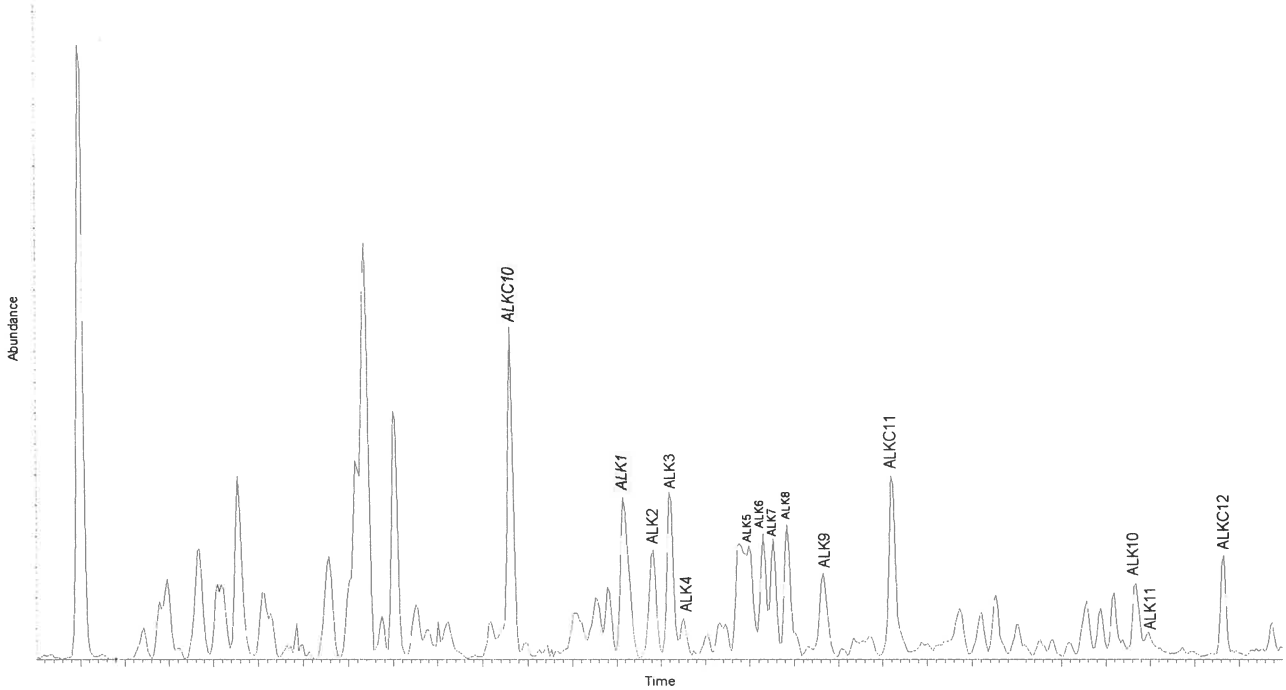
-The formula will search up to 1100 rows of data therefore you cannot integrate more than 1100 peaks.

Representative data of a 50% evaporated gasoline sample is shown. The designated peak code, where T=TIC, ALK=Alkane, AR=Aromatic, IN=Indane, and PNA=Polynuclear Aromatic, is followed by letters or numbers representing either the known composition of the peak, or in cases where the number of isomers preclude a known composition, letters or numbers to denote the peak. Grayed labels indicate peaks that are not included in the final statistical analyses due to lack of statistical significance or lack of elution-based paired peak.

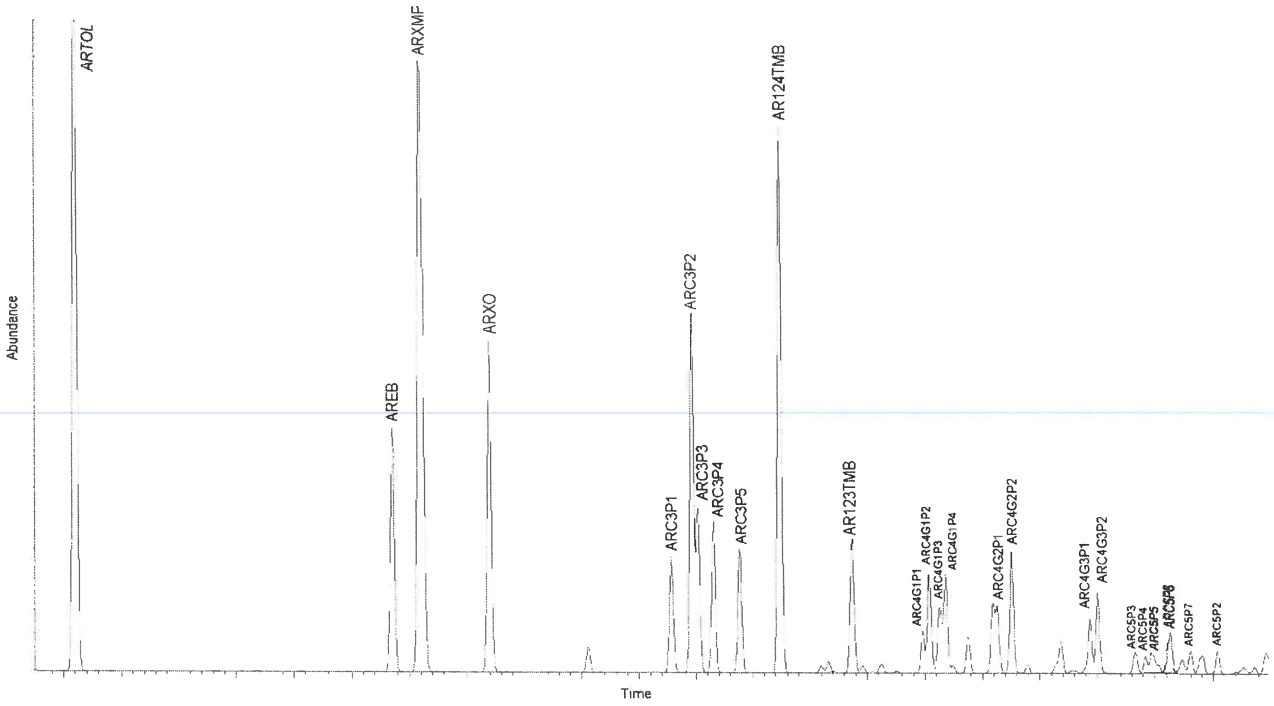
TIC



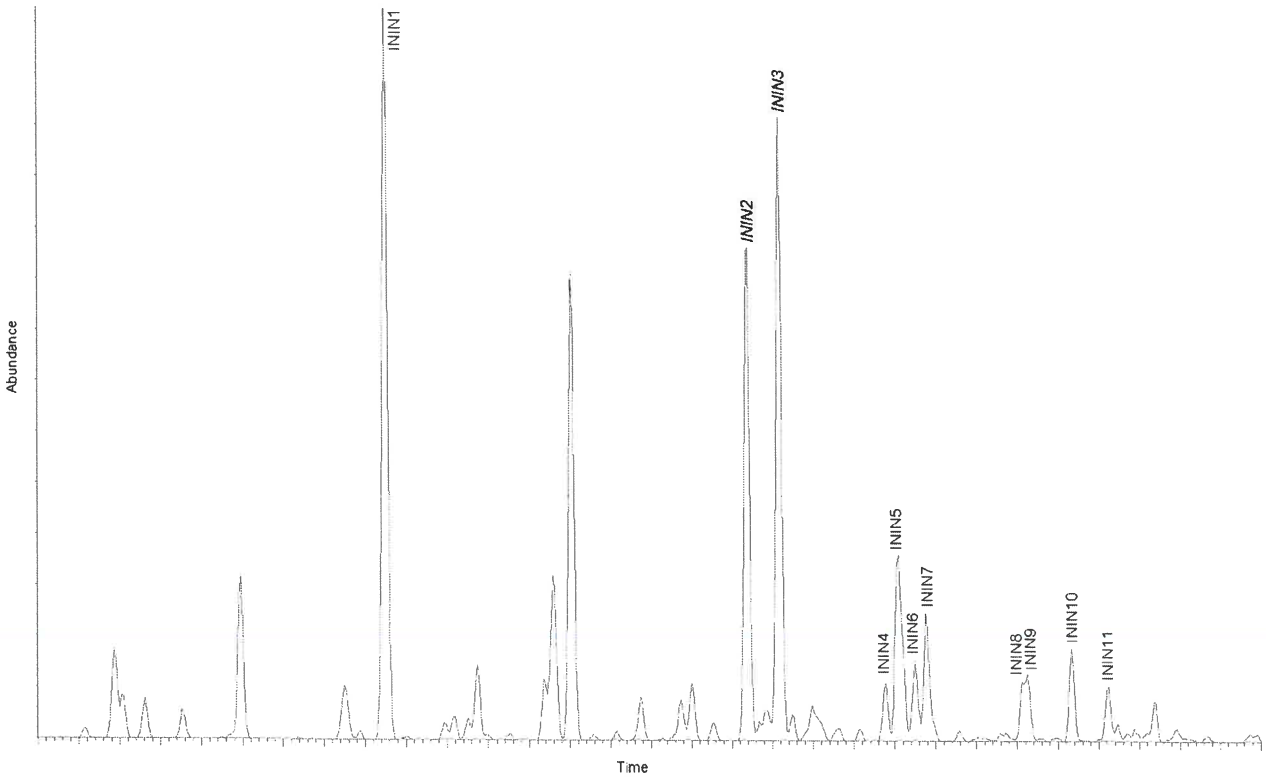
Alkane



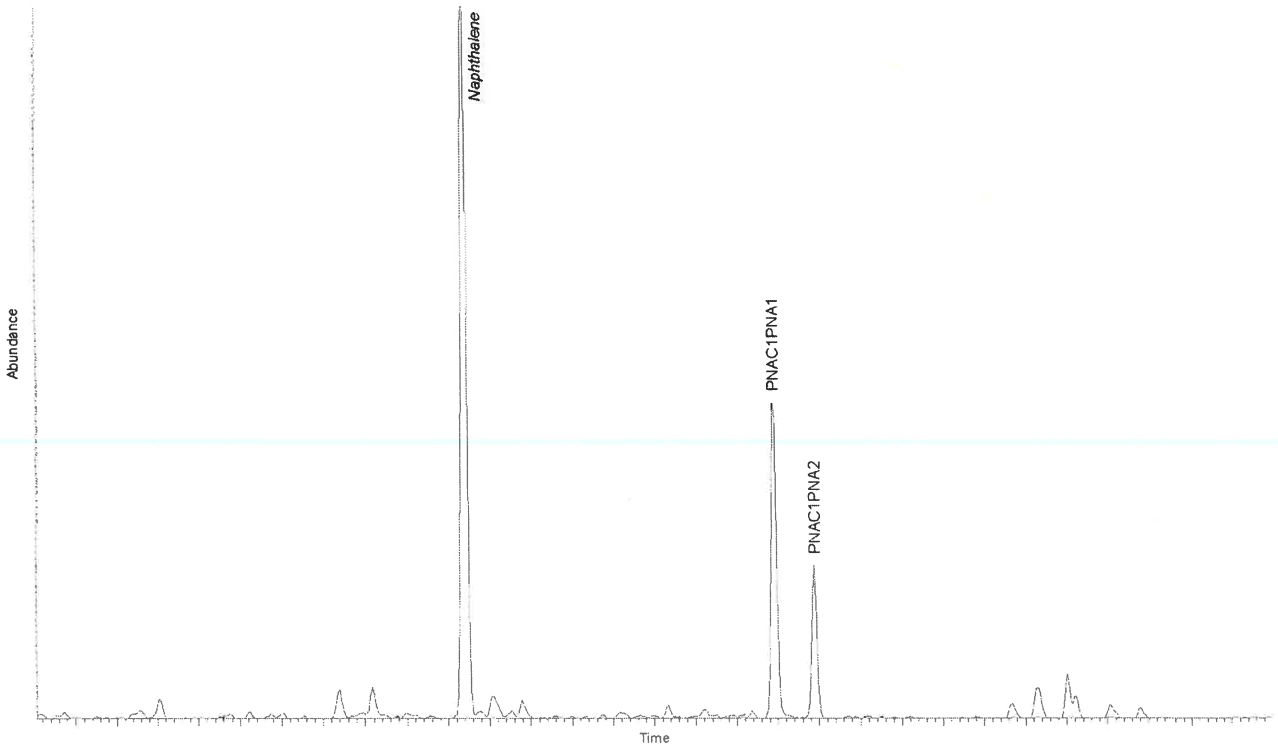
Aromatic



Indane



Polynuclear Aromatic



Retention Time Worksheet

This worksheet is not linked to any subsequent worksheets and is meant to serve as an area to collect all of the RTs in one place.

RTs documented in this Retention Time worksheet may be copied and pasted to the appropriate TIC or EIP worksheet.

Retention time cells are grayed for peaks that are not included in the calculation of points. Entries for these peaks are optional.

TIC (T)	
TMP	
Toluene (TOL)	
Ethylbenzene (EB)	
Xylenes (XMP)	
Xylene (XO)	
C3P1	
C3P2	
C3P3	
C3P4	
C3P5	
124TMB	
C10	
123TMB	
Indane (IN1)	
C4G1P1	
C4G1P2	
C4G1P3	
C4G1P4	
C4G2P1	
C4G2P2	
C4G3P1	
C4G3P2	
IN2	
IN3	
C5P1	
C5P2	
Naphthalene	
IN4	
IN5	
IN6	
IN7	
C12	
C1PNA1	
C1PNA2	

Alkanes (ALK)	
C10	
ALK1	
ALK2	
ALK3	
ALK4	
ALK5	
ALK6	
ALK7	
ALK8	
ALK9	
C11	
ALK10	
ALK11	
C12	

Aromatic (AR)	
Toluene (TOL)	
Ethylbenzene (EB)	
Xylenes (XMP)	
Xylene (XO)	
C3P1	
C3P2	
C3P3	
C3P4	
C3P5	
124TMB	
123TMB	
C4G1P1	
C4G1P2	
C4G1P3	
C4G1P4	
C4G2P1	
C4G2P2	
C4G3P1	
C4G3P2	
C5P3	
C5P4	
C5P5	
C5P6	
C5P7	
C5P2	

Indane (IN)	
IN1	
IN2	
IN3	
IN4	
IN5	
IN6	
IN7	
IN8	
IN9	
IN10	
IN11	

PNA (PNA)	
Naphthalene	
C1PNA1	
C1PNA2	

Total Ion Chromatogram (TIC)

Peak #	R.T. Min	First Scan	Max Scan	Last Scan	PK TY		Peak Height	Corr. Area
---	---	---	---	---	---	---	---	---

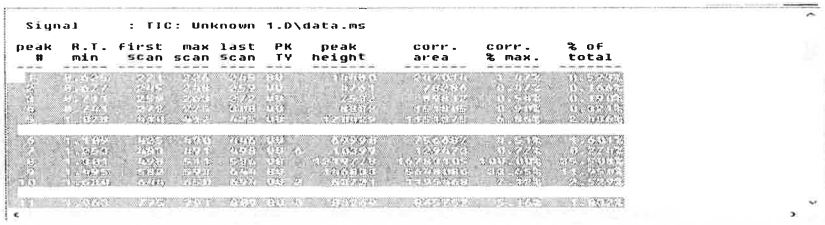
Corr. % Max % of Total
--- ---

TIC (T)		
Peak Name	RT	Abundance
TMP		#N/A
Toluene (TOL)		#N/A
Ethylbenzene (EB)		#N/A
Xylenes (XMP)		#N/A
Xylene (XO)		#N/A
C3P1		#N/A
C3P2		#N/A
C3P3		#N/A
C3P4		#N/A
C3P5		#N/A
124TMB		#N/A
C10		#N/A
123TMB		#N/A
Indane (IN1)		#N/A
C4G1P1		#N/A
C4G1P2		#N/A
C4G1P3		#N/A
C4G1P4		#N/A
C4G2P1		#N/A
C4G2P2		#N/A
C4G3P1		#N/A
C4G3P2		#N/A
IN2		#N/A
IN3		#N/A
C5P1		#N/A
C5P2		#N/A
Naphthalene		#N/A
IN4		#N/A
IN5		#N/A
IN6		#N/A
IN7		#N/A
C12		#N/A
C1PNA1		#N/A
C1PNA2		#N/A

Instructions:

Type the RTs to the third decimal place in the cells for the corresponding peak of interest (Example: Toluene 3.034) OR if you collected the RTs in the "Retention Time" worksheet, copy and paste the RTs to the correct cells in this worksheet.

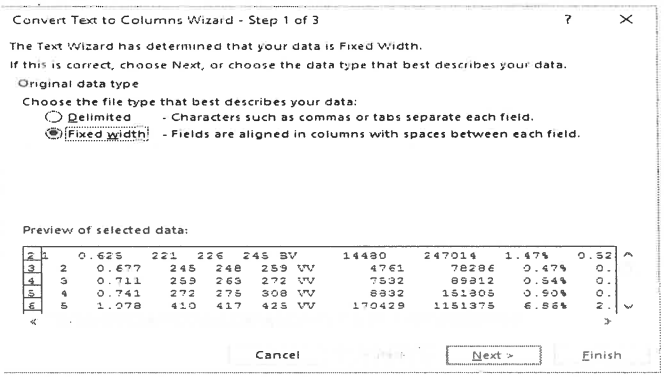
Pull the Percent Report in Chemstation. Select the area from the first peak to the last peak, omitting the headers (shown below):



Copy (Ctrl+C) the selected area. In the corresponding Excel worksheet, paste (Ctrl+V) the Percent Report in the A3 cell. Make sure that the A column is selected from A3 to A#, where # is the last row of the pasted Percent Report (shown below):

Peak #	R.T. Min	First Scan	Max Scan	Last Scan	PK TY	Peak Height	Corr. Area	Corr. % Max	% of Total
1	1.249	485	492	509	BV	182416	3329637	3.89%	1.207%
2	1.908	509	517	537	VV	2 259585	5294694	8.85%	2.743%
3	1.371	537	543	573	PV	2 2747497	40167094	67.11%	20.807%
4	1.466	573	583	683	VB	3 2196585	24574567	41.06%	12.730%
5	2.141	831	841	852	BV	4 157632	3109033	5.19%	1.611%
6	2.214	852	858	867	VV	402170	6143196	10.26%	3.182%
7	2.315	874	880	899	VB	3 95829	2168808	3.62%	1.123%
8	2.466	899	913	925	BB	730355	12529071	20.93%	6.490%
9	2.703	952	966	986	BB	3 507586	10668732	17.83%	5.527%
10	2.842	986	997	999	BV	3 133470	1745175	2.92%	0.904%
11	2.864	999	1002	1012	VV	159685	2669073	4.46%	1.383%
12	3.106	1045	1056	1066	BV	3489706	59850016	100.00%	31.003%
13	4.286	1313	1318	1326	BB	66040	923490	1.54%	0.478%
14	4.745	1413	1421	1431	BB	1846288	20874043	34.88%	10.813%

With the A column selected, choose the Data tab in Excel (between Formulas and Review) and click "Text to Columns", this opens following dialog box:



Click "Next" until "Finish" is the only option, then click "Finish". This will sort the data into the individual columns of data.

Abundance will autopopulate next to the RT for a given peak.

Leave #N/A errors in the Abundance column for any uncalled peaks. Replace #N/A errors with the manually calculated peak height for peaks that wouldn't integrate.

Repeat the above process for each of the EIPs, then proceed to the Sufficiency Tab to see final results.

Notes:

-Enter the Retention Time to the third decimal place (Examples: C3P3: 5.191)
-Leave RT cells blank when peaks are not called
-DO NOT delete or move columns or rows
-Double check that Column G aligned properly; correct any errant numbers
-Edits to the RTs or Percent Report can be made at anytime
-Entering or pasting copied RTs and pasting Percent Reports can be done in any order
-Hidden worksheets between the TIC/EIP worksheets and the Sufficiency worksheet include the Data, Ratio, Log, STD, and Points worksheets.
-If you accidentally clear a formula cell so that it is blank, a #NUM error will appear in the Sufficiency Sheet. To correct this there are three options:

Option #1: Undo (Ctrl+Z)
Option #2: Select the cell above the blank cell and drag the right corner down; this should populate an #N/A error, but will copy the incorrect formula, including the value in the above cell, if one is present
Option #3: Type #N/A into the blank cell (this will not correct the deleted formula, which is ok if no value is needed in that cell)

-If a formula is accidentally deleted, selecting the above cell and dragging down will copy the exact formula from the above cell. If a formula that is needed is accidentally deleted, Undo (Ctrl+Z) is the best option to replace the original formula. Otherwise, the formula will need to be corrected.
-Save one copy of this workbook per sample and always retain one original copy as a back up template
-Cells are grayed for peaks that are not included in the points calculations. These are optional.

Alkane EIP

Peak #	R.T. Min	First Scan	Max Scan	Last Scan	PK TY		Peak Height	Corr. Area

Corr. % Max % of Total
--- ---

Alkane (ALK)		
Peak Name	RT	Abundance
C10		#N/A
ALK1		#N/A
ALK2		#N/A
ALK3		#N/A
ALK4		#N/A
ALK5		#N/A
ALK6		#N/A
ALK7		#N/A
ALK8		#N/A
ALK9		#N/A
C11		#N/A
ALK10		#N/A
ALK11		#N/A
C12		#N/A

Aromatic EIP

Peak #	R.T. Min	First Scan	Max Scan	Last Scan	PK TY		Peak Height	Corr. Area
---	---	---	---	---	---	---	---	---

Corr. % Max % of Total
--- ---

Aromatic (AR)		
Peak Name	RT	Abundance
Toluene (TOL)		#N/A
Ethylbenzene (EB)		#N/A
Xylenes (XMP)		#N/A
Xylene (XO)		#N/A
C3P1		#N/A
C3P2		#N/A
C3P3		#N/A
C3P4		#N/A
C3P5		#N/A
124TMB		#N/A
123TMB		#N/A
C4G1P1		#N/A
C4G1P2		#N/A
C4G1P3		#N/A
C4G1P4		#N/A
C4G2P1		#N/A
C4G2P2		#N/A
C4G3P1		#N/A
C4G3P2		#N/A
C5P3		#N/A
C5P4		#N/A
C5P5		#N/A
C5P6		#N/A
C5P7		#N/A
C5P2		#N/A

Indane EIP

Peak #	R.T. Min	First Scan	Max Scan	Last Scan	PK TY		Peak Height	Corr. Area
---	---	---	---	---	---	---	---	---

Corr. % Max % of Total
--- ---

Indane (IN)		
Peak Name	RT	Abundance
IN1		#N/A
IN2		#N/A
IN3		#N/A
IN4		#N/A
IN5		#N/A
IN6		#N/A
IN7		#N/A
IN8		#N/A
IN9		#N/A
IN10		#N/A
IN11		#N/A

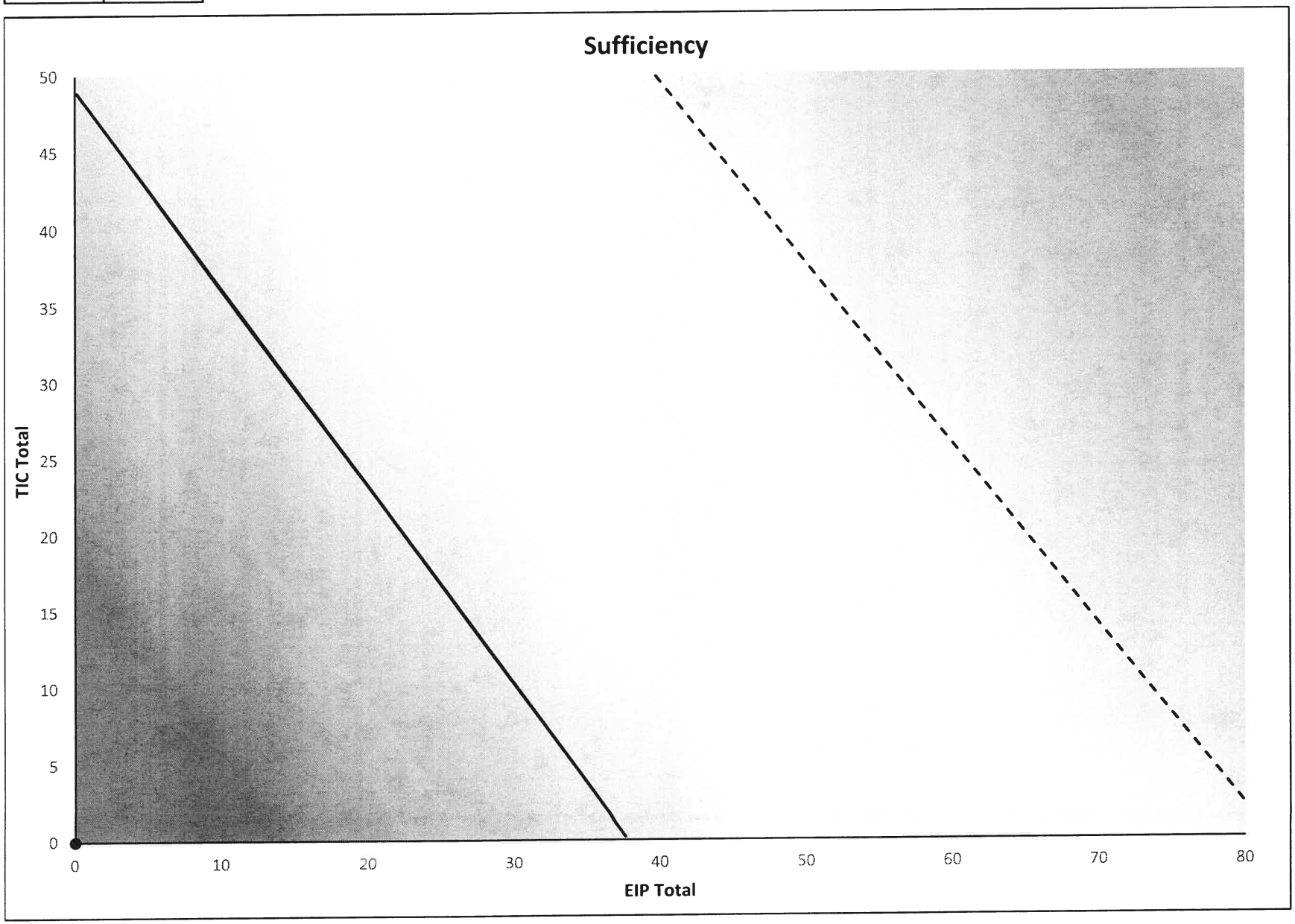
PNA EIP

Peak #	R.T. Min	First Scan	Max Scan	Last Scan	PK TY		Peak Height	Corr. Area
---	---	---	---	---	---	---	---	---

Corr. % Max % of Total
--- ---

PNA (PNA)		
Peak Name	RT	Abundance
Naphthalene		#N/A
C1PNA1		#N/A
C1PNA2		#N/A

EIP Total	TIC Total
0	0



TIC		
Peak Ratio	Ratio Value	Points
TTMP:TTOL		0
TEB:TXMP		0
TXMP:TXO		0
TC3P1:TC3P2		0
TC3P2:TC3P3		0
TC3P3:TC3P4		0
TC3P4:TC3P5		0
TC3P5:T124TMB		0
TC3P2:T124TMB		0
T124TMB:T123TMB		0
TC10:T123TMB		0
T123TMB:TIN1		0
TC4G1P1:TC4G1P2		0
TC4G1P2:TC4G1P3		0
TC4G1P3:TC4G1P4		0
TC4G2P1:TC4G2P2		0
TIN2:TIN3		0
TC5P1:TC5P2		0
TIN4:TIN5		0
TIN5:TIN6		0
TIN6:TIN7		0
TC1PNA1:TC1PNA2		0

Aromatic		
Peak Ratio	Ratio Value	Points
AREB:ARXMP		0
ARXMP:ARXO		0
ARC3P1:ARC3P2		0
ARC3P2:ARC3P3		0
ARC3P4:ARC3P5		0
ARC3P5:AR124TMB		0
ARC3P2:AR124TMB		0
AR124TMB:AR123TMB		0
ARC4G1P1:ARC4G1P2		0
ARC4G1P2:ARC4G1P3		0
ARC4G1P3:ARC4G1P4		0
ARC4G2P1:ARC4G2P2		0
ARC4G3P1:ARC4G3P2		0
ARC5P3:ARC5P4		0
ARC5P7:ARC5P2		0

Alkanes		
Peak Ratio	Ratio Value	Points
ALK2:ALK3		O
ALK3:ALK4		O
ALK4:ALK5		O
ALK5:ALK7		O
ALK6:ALK8		O
ALK7:ALK9		O
ALKC11:ALKC12		O
ALK10:ALK11		O

Indane		
Peak Ratio	Ratio Value	Points
ININ4:ININ5		0
ININ5:ININ6		0
ININ6:ININ7		0
ININ8:ININ9		0
ININ9:ININ10		0
ININ10:ININ11		0

PNA		
Peak Ratio	Ratio Value	Points
PNAC1PNA1:PNAC1PNA2		0

Other		
Peak Ratio	Ratio Value	Points
AR123TMB: ININ1		0

This Spreadsheet is an autopopulated summary of all the data. It is linked to the relevant worksheets. Do not move, delete, or clear any cells.

A key for the highlighted point cells is defined in the "Points Color Key" table.

Points Color Key	
Green	Highest Points
Yellow	Medium Points
Orange	Lowest Points
Red	Scored Zero
No Color-Zero	Uncalled Peak Zero