

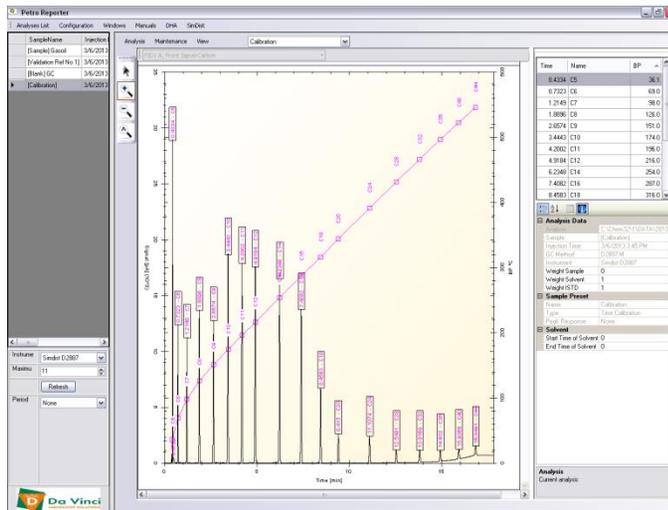


**Da Vinci**  
LABORATORY SOLUTIONS

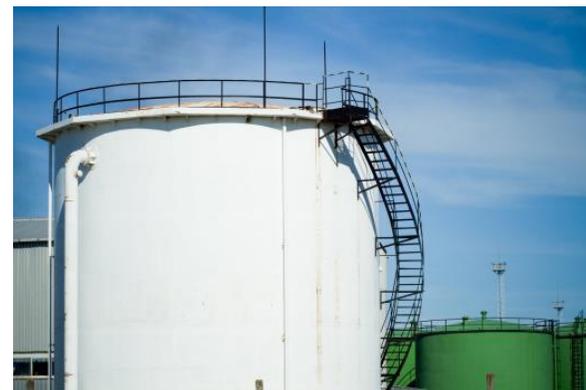
  
**Ingeniería Analítica**  
Chromatography & Spectrometry

  
**Agilent Technologies**  
Channel Partner

# An introduction to DVLS PetroReporter© software



## PetroReporter



PetroReporter automates the data processing of various sample types:

- SimDist, DHA and Gas applications, all within the same program
- Includes Standard (ASTM, IP, GPA etc.) databases and formulas
- Includes predefined methods (presets)
- Allows analysis-based customization
- Compatible with multiple data platforms (CDS)
- Available as stand-alone or network (C/S) application

# CDS - PetroReporter Compatibility

- Agilent ChemStation
- Agilent EZChrom Elite
- Agilent OpenLab ChemStation
- Agilent OpenLab EZchrom

## Simdist / DHA applications

Da Vinci participates in both ASTM and CEN, to follow international regulations and develop new methods where necessary.

SimDist		DHA
ASTM D2887	IP 406	ASTM D5134
ASTM D3710	IP 480	ASTM D6729
ASTM D5442	IP 507	ASTM D6730
ASTM D6352	IP 545	ASTM D6733
ASTM D7096	EN 15199-1/2/3	
ASTM D7169	DIN 51.435	
ASTM D7213	IP 601	
ASTM D7500		

## Simdist / DHA Report Options

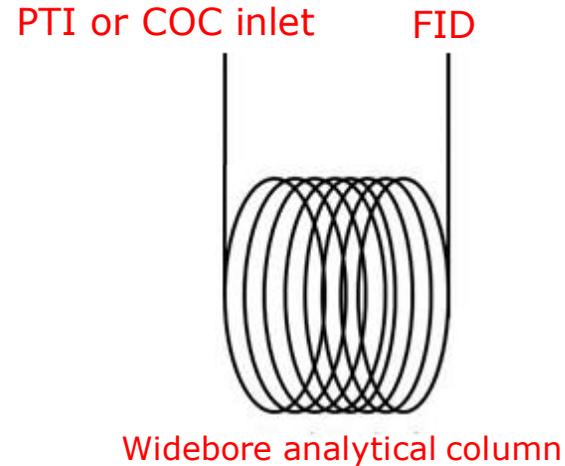
SimDist	DHA
Boiling point distribution (°C/°F)	PNA, NPIPNA, PIONAX: mass%, vol%, mole%
Cutpoints	Individual hydrocarbons
Validation report for known samples	True boiling point (°C/°F)
Volume correlation for customizable (ASTM D86, D86/STP 577, D1160)	Reid vapor pressure
Flashpoint correlation (D93, D56, D3984)	Specific gravity
Motor oil volatility (D6417)	Heating values
Noack evaporation loss (DIN 51.581)	Octane number
Wax content (D5442)	Bromine number
Crude oil DHA merge	Export to *.CSV, *.PDF or *.XLS
Export to *.CSV, *.PDF or *.XLS	

# SimDist Application

- Determines
  - Boiling point range (IBP – FBP)
  - BP distribution yield (mass%)
- Purpose
  - Used for optimizing distillation process parameters
  - Used for quality control of refinery streams
  - Measures cross-contaminations
- Market Area
  - Refinery laboratories
  - Independent laboratories
  - Chemical plants (consumes naphtha for plastics)

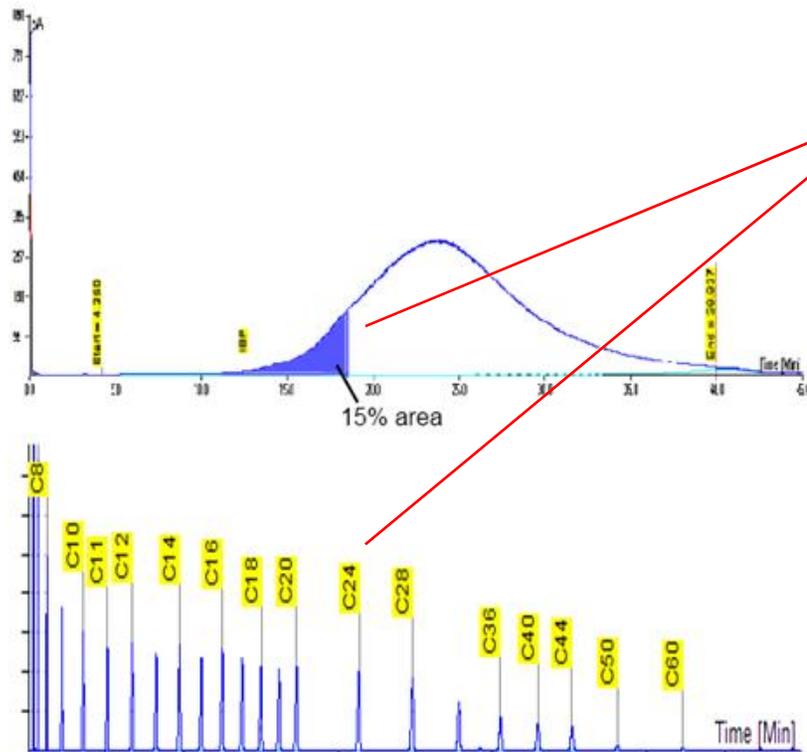
# Hardware

- No sample split
- Standard column and detector
- Autosampler injection
- Non-polar column
- Inlet and oven temperature ramping
- Relatively high temperatures (350-430 °C)



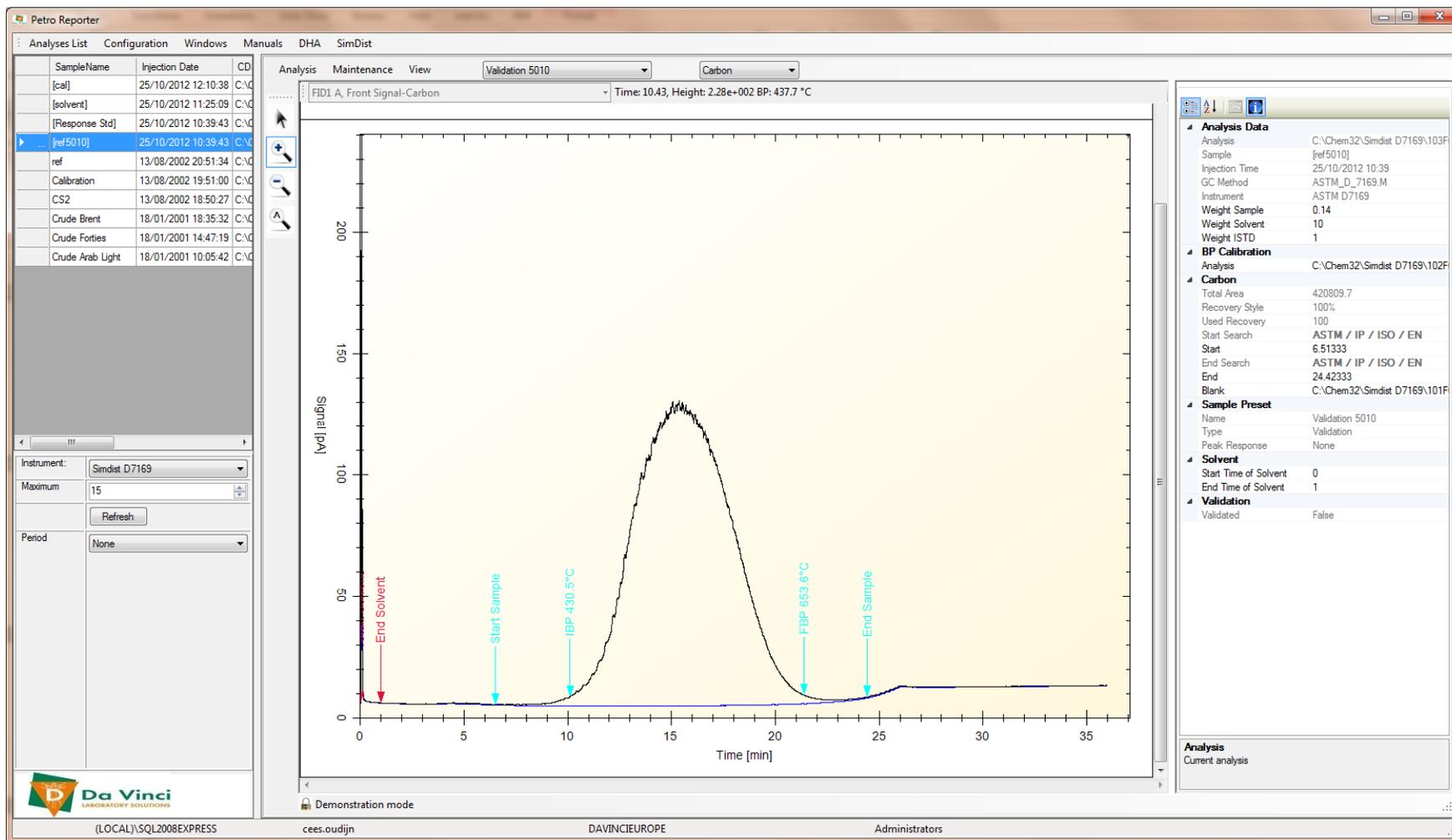
## Background

- Sample area is calculated after blank subtraction
- Sample area is divided into segments (e.g. 15%)
- Segment boiling point is calculated using n-paraffin elution times
- IBP and FBP is defined as 0.5% and 99.5% of total area



15% of the sample eluted at the boiling point of C24 (391 °C)

# PetroReporter - Main SimDist Menu



Sample list

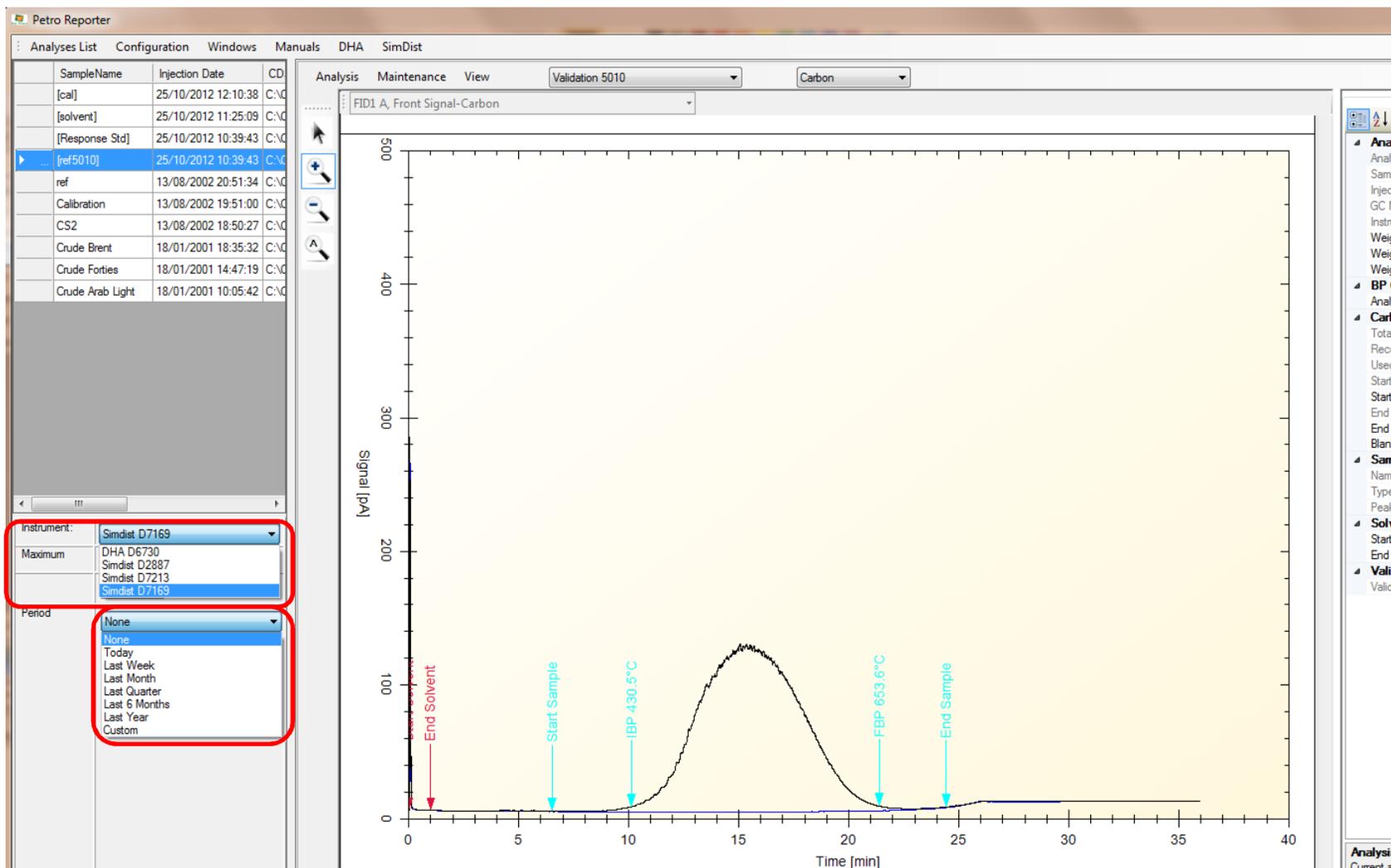


Chromatogram

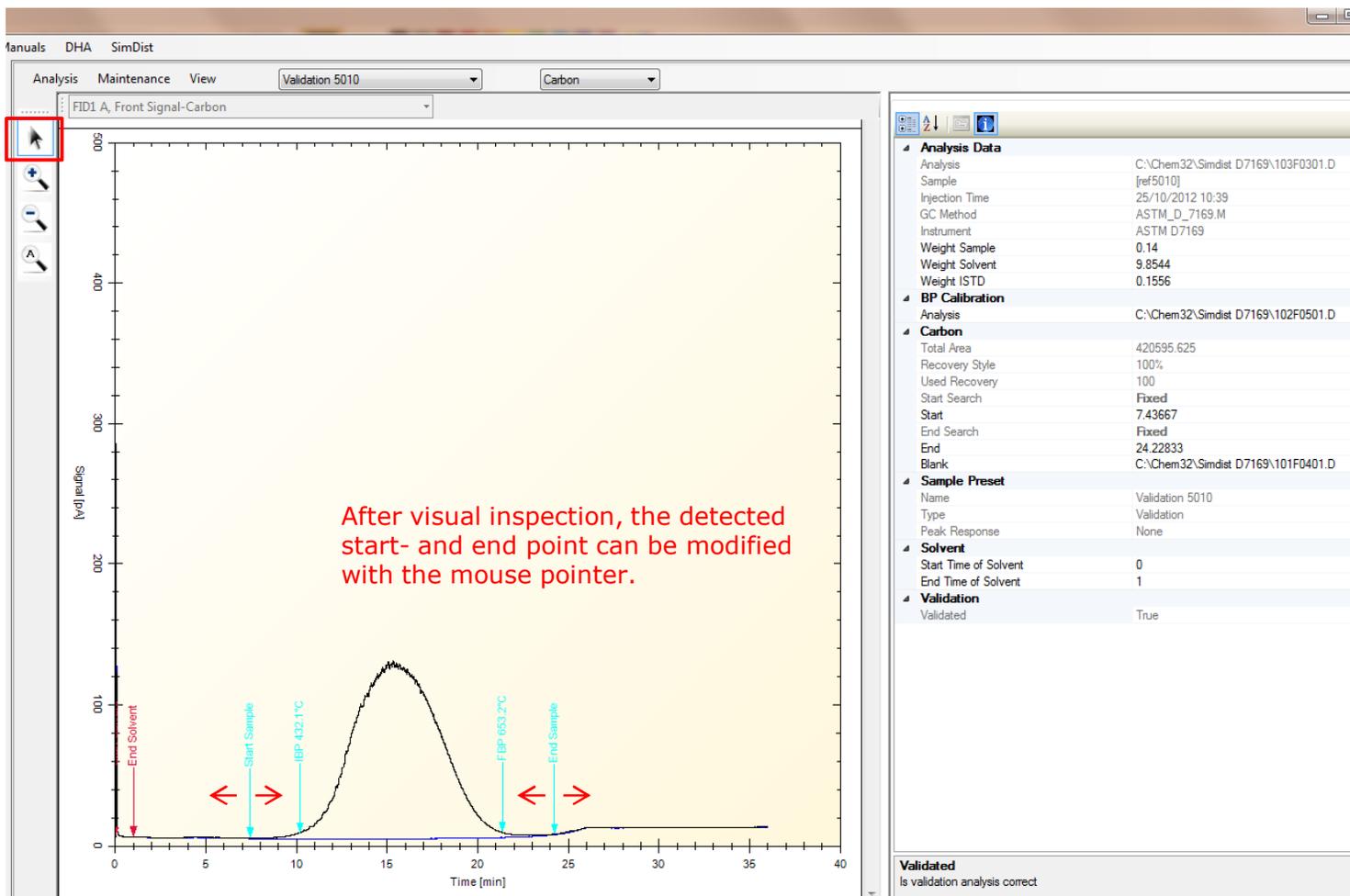
Sample details



# Instrument Selection Menu & Data Filter



# SimDist Sample Details

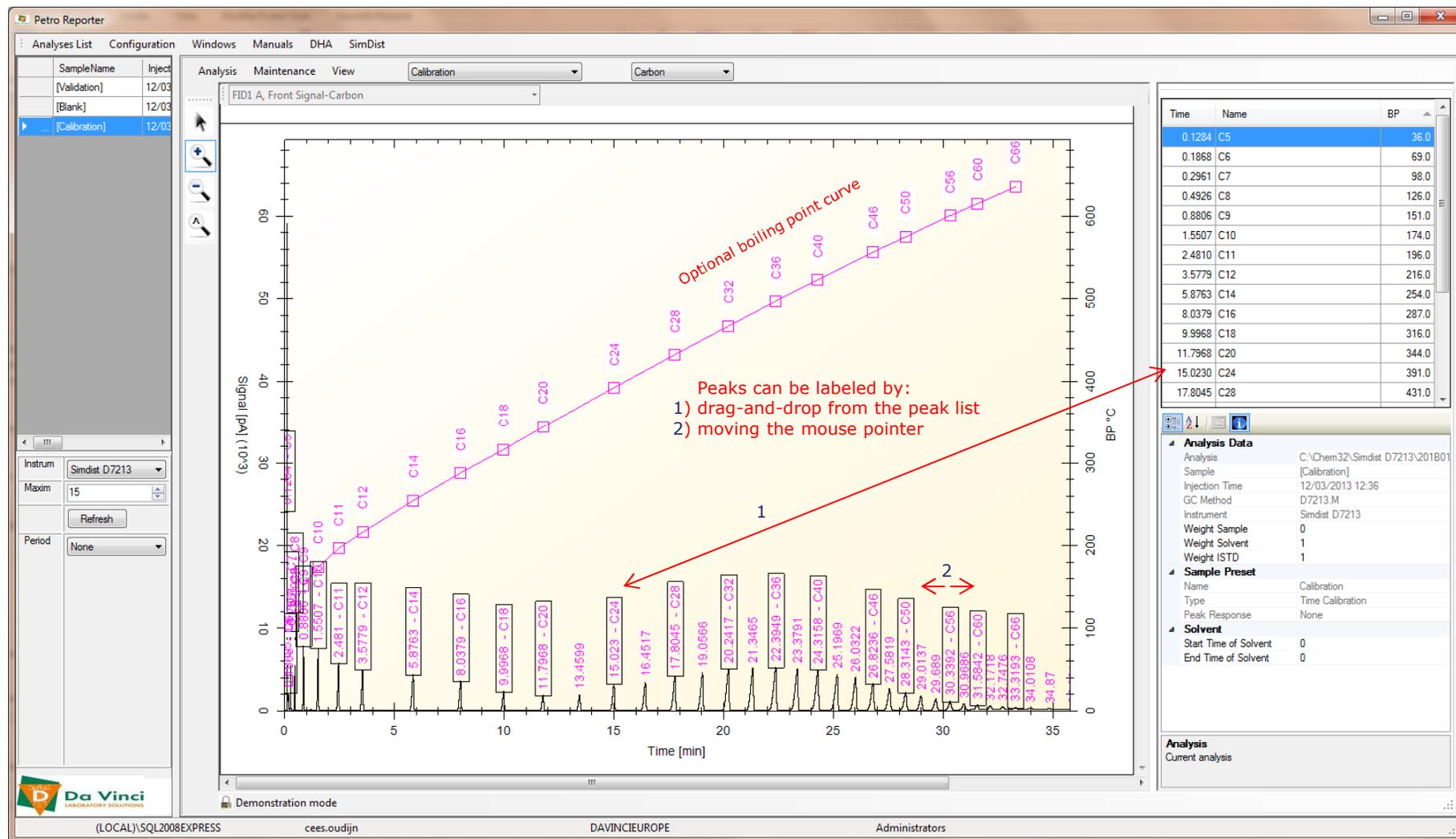


← Sample depending information

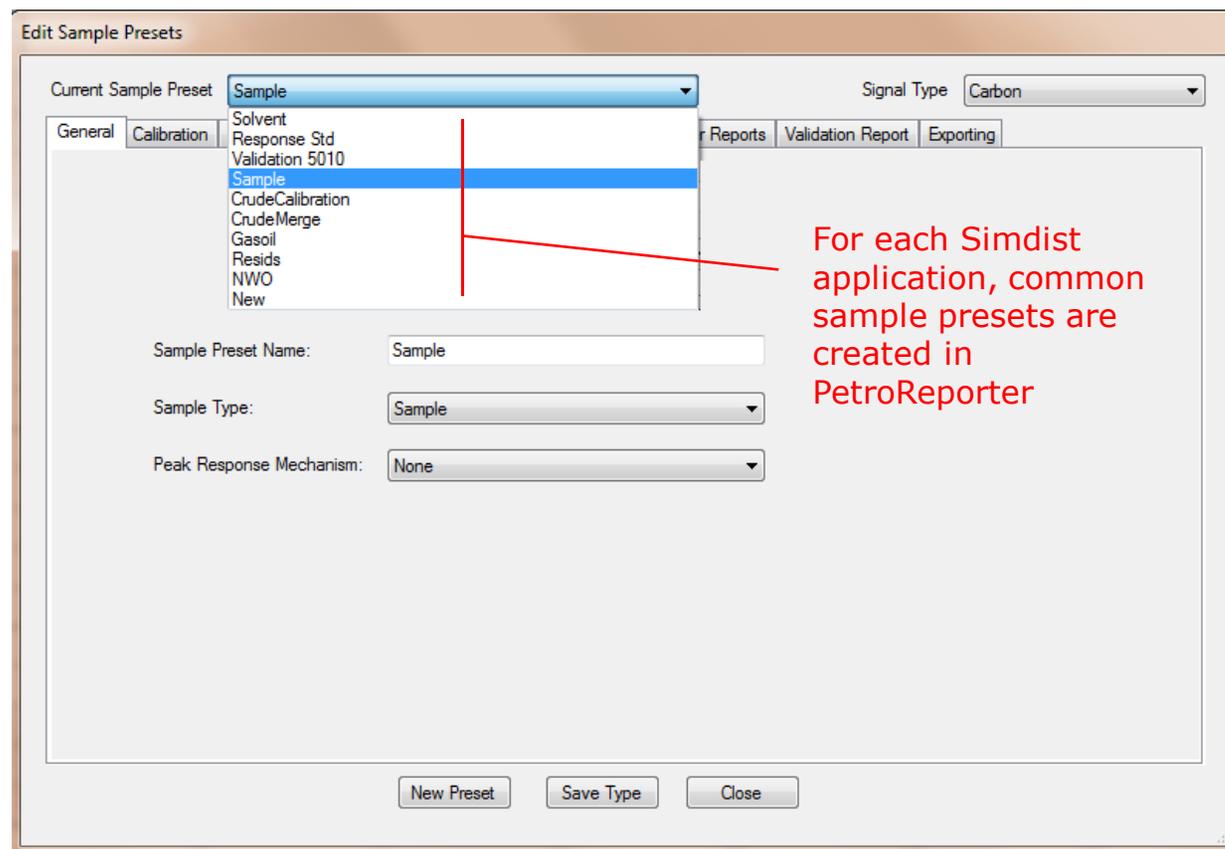
← Startpoint and endpoint times can be modified after processing

←

# SimDist Calibration



# Simdist Sample Preset Editor (1)



## Simdist Sample Preset Editor (2)

Edit Sample Presets

Current Sample Preset:  Signal Type:

General | Calibration | **Signal Processing** | General Reports | Distillation Reports | Other Reports | Validation Report | Exporting

<b>Baseline Correction</b> <input checked="" type="checkbox"/> Subtract Blank	<b>Start Elution Search</b> Location: <input type="text" value="6.500"/> <input type="text" value="Minutes"/> Search: <input type="text" value="ASTM / IP / ISO / EN"/>	<b>Recovery Calculation</b> Style: <input type="text" value="ASTM D5307"/> Recovery [%]: <input type="text" value="100.0000"/> Merge Temperature [°C]: <input type="text" value="0.0"/>
<b>Solvent Correction</b> Start Solvent Time [min]: <input type="text" value="0.000"/> End Solvent Time [min]: <input type="text" value="1.000"/> Quench Factor: <input type="text" value="2.85"/>	<b>End Elution Search</b> Location: <input type="text" value="24.500"/> <input type="text" value="Minutes"/> Search: <input type="text" value="ASTM / IP / ISO / EN"/>	<b>ISTD Information</b> ISTD 1 BP [°C]: <input type="text" value="254.0"/> ISTD 2 BP [°C]: <input type="text" value="302.0"/> ISTD Conc [mass%]: <input type="text" value="100.000"/>

Blank handling

Start/End settings

Recovery calculation

## SimDist Sample Preset Editor (3)

Current Sample Preset: Sample | Signal Type: Carbon

General | Calibration | Signal Processing | General Reports | **Distillation Reports** | Other Reports | Validation Report | Exporting

**TBP Distillation Percent**

- Show Report
- Page Break Before
- Percent Interval: 1.0

**Alkane Profile**

- Show Report
- Page Break Before
- First Carbon: 17
- Last Carbon: 44
- Peak Width: 0.2

**TBP Distillation Temperature**

- Show Report
- Page Break Before
- Boiling Point Interval: 10.0

**Volume Correlation**

- Show Report
- Page Break Before
- Use Model: ASTM D86 Jetfuel and Diesels (D2887-6a)

New Preset | Save Type | Close

TBP & cutpoint reports

Correlations & Alkane content

## SimDist Sample Preset Editor (4)

Current Sample Preset: Sample      Signal Type: Carbon

General   Calibration   Signal Processing   General Reports   Distillation Reports   **Other Reports**   Validation Report   Exporting

**Chromatogram**

Show Report       Page Break Before

Merge with Special Plot

**X-Axis**      **Y-Axis**

Automatic       Automatic

Minimum: 0.0      Minimum: 0.0

Maximum: 0.0      Maximum: 500.0

Step [min]: 0.0

**Special Reporting Options**

Page Break Before

Flash Point: ASTM D56 Flashpoint

Motor Oil Volatility (ASTM D6417)

Noack Evaporation Loss (DIN 51.581)

New Preset   Save Type   Close

Chromatogram output

Special calculations

## SimDist Sample Preset Editor (5)

Current Sample Preset: Sample      Signal Type: Carbon

General | Calibration | Signal Processing | General Reports | Distillation Reports | Other Reports | **Validation Report** | Exporting

Validation

Show Report

Page Break Before

	Recovery	Target [°C]	Deviation [°C]
▶	0.5	430.0	5.0
	5.0	478.0	3.0
	10.0	492.0	3.0
	20.0	510.0	3.0
	30.0	524.0	4.0
	40.0	537.0	4.0
	50.0	548.0	4.0
	60.0	560.0	4.0
	70.0	572.0	4.0
	80.0	585.0	4.0
	90.0	602.0	4.0

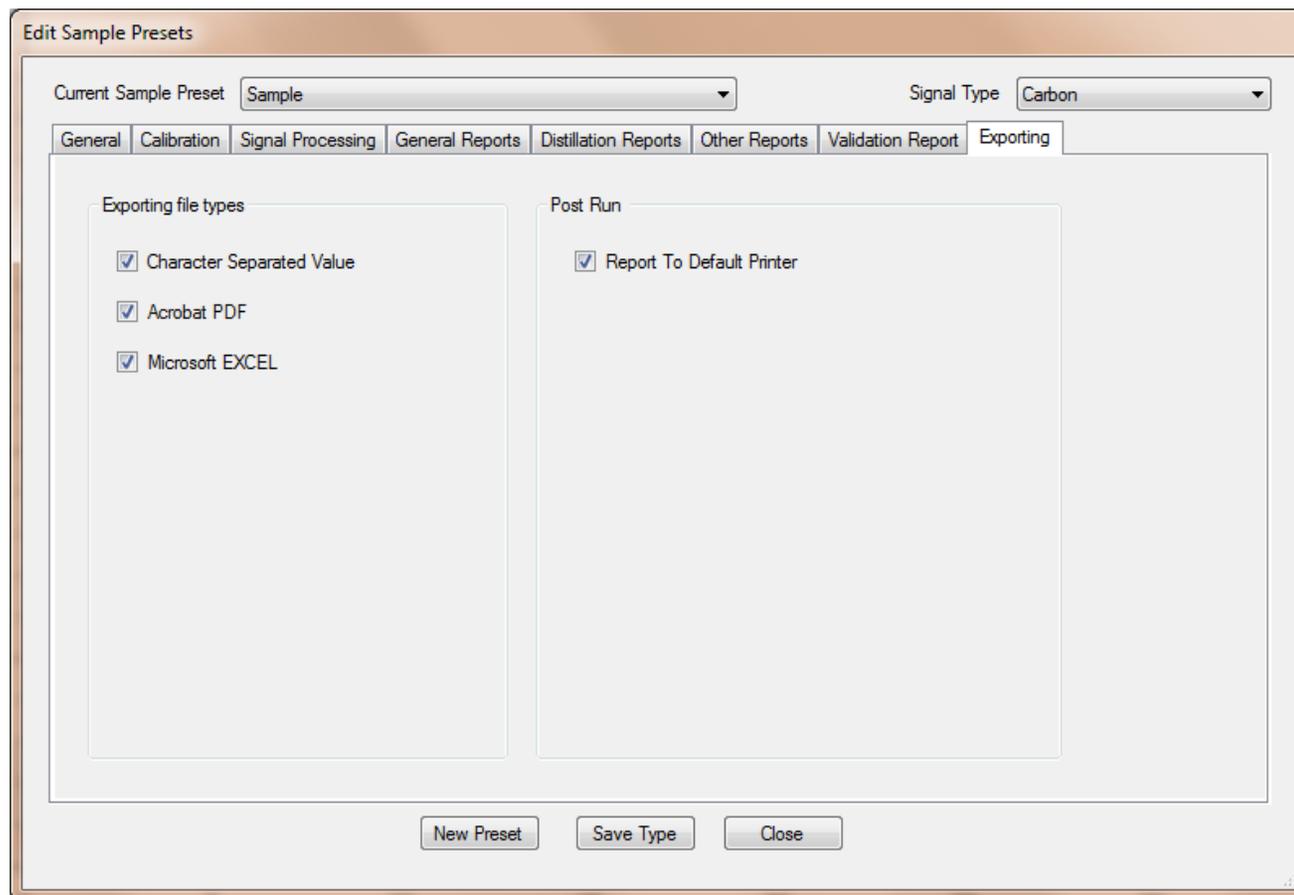
Add

Remove

New Preset    Save Type    Close

Validation settings for known or site specific samples

## SimDist Sample Preset Editor (6)



Export to LIMS properties

# Customizable Correlation

Select: ASTM D86 Jetfuel and Diesels (D2887-6a) [New] [Delete]

Correlation Model  
Target Application: ASTM D86  
Name: ASTM D86 Jetfuel and Diesels (D2887-6a)

Calculation Base  
 °C  °F

	Report Value	Result	User	Factor [0]	Mass% [0]	Factor [1]	Mass% [1]	Factor [2]
▶	0.5	0	1.00	25.35100	0.0	0.32216	0.5	0.71187
	5	0	1.00	18.82200	0.0	0.06602	0.5	0.15803
	10	0	1.00	15.17300	0.0	0.20149	5.0	0.30606
	20	0	1.00	13.14100	0.0	0.22677	10.0	0.29042
	30	0	1.00	5.77660	0.0	0.37218	20.0	0.30313
	50	0	1.00	6.37530	0.0	0.07763	30.0	0.68984

[Add] [Delete]

[Correlate] [Save] [Close]

# Reporting

The screenshot displays the Petro Reporter interface. On the left, a table lists sample names and injection numbers. The main area shows a chromatogram with a single prominent peak. A context menu is open over the peak, listing several actions. A red box highlights the 'Show Report' option, with a red arrow pointing to it and a text label. The chromatogram includes several key markers: 'End Solvent' at approximately 5 minutes, 'Start Sample' at approximately 8 minutes, 'IBP 432.1 °C' at approximately 10 minutes, 'FBP 663.2 °C' at approximately 22 minutes, and 'End Sample' at approximately 25 minutes. The y-axis is labeled 'Signal [pA]' and the x-axis is 'Time [min]'. The status bar at the bottom indicates 'Demonstration mode' and provides system information.

SampleName	Inj
[cal]	25
[solvent]	25
[Response Std]	25
[ref5010]	25
ref	13
Calibration	13
CS2	13
Crude Brent	18
Crude Forties	18
Crude Arab Light	18

Analysis: Validation 5010, Carbon

Time: 0.97, Height: 2.41e+002 BP: 205.4 °C

Signal [pA]

Time [min]

End Solvent

Start Sample

IBP 432.1 °C

FBP 663.2 °C

End Sample

Refresh Integration Peaks

Export Report F5

Show Report F6

Reset Properties

Update Link in Method Set

Close Analysis F4

On-screen report or export to LIMS

Demonstration mode

(LOCAL)\SQL2008EXPRESS cees.oudijn DAVINCIEUROPE Administrators

# Onscreen Reporting

The screenshot displays a series of overlapping report windows from the Da Vinci Laboratory Solutions software. The windows are titled 'ASTM D2887' and '[Sample] Gasoil'. The reports include:

- Sample Details:** Sample Preset: Sample, Method: D2887.M, Analyst.
- Description:** Channel: Carbon, BP Calibration, Blank, Validation, Start Elution Time, End Elution Time, Total Area, Used Recovery.
- Distribution Report:**

Rec Mass%	TBP °C
IBP	119.3
5.0	184.9
10.0	209.8
15.0	226.2
20.0	237.0
25.0	248.3
- Cut Point Distribution:**

BP °C	Recov Mass%
119.3	0.5
140.0	1.1
160.0	2.2
180.0	4.3
- ASTM D86 Jetfuel and:**

Rec Vol%	BP °C
IBP	186.5
5.0	219.4
10.0	231.0
- Special Calculations:**
  - Property: ASTM D93 Flashpoint, Motor Oil Volatility
- Chromatogram:** FID1 A, Front Signal-Carbon. The plot shows detector response versus time (min) with various peaks labeled with retention times and properties.

Footer text in the reports includes: 'Created by Da Vinci Laboratory Solutions - 1.0.0' and 'Created by Da Vinci Laboratory Solutions - 1'.

# Validation Report



**ASTMD2887**

[Validation Ref No 1]  
 06/03/2013 16:40:47

---

C:\Chem32\Simdist D2887\205B0801.D

Sample Preset	Validation Ref No 1	Bottle	
Method	D2887.M	Sample Weight	-
Analyst		SolventWeight	1.0000
		ISTD Weight	1.0000

Description

**Channel: Carbon**

BP Calibration C:\Chem32\Simdist D2887\204B0601.D  
 Blank C:\Chem32\Simdist D2887\NV-B0701.D  
 Validation C:\Chem32\Simdist D2887\205B0801.D 06/03/2013 16:40:47 validated  
 Start Elution Time 0.825  
 End Elution Time 16.064  
 Total Area 7.1609e+007  
 Used Recovery 100.0

---

**Validation Report**

Recov Mass%	Target °C	Max Δ °C	Found °C	Δ °C
IBP	115.0	7.6	115.1	0.1
5.0	151.0	3.8	150.9	-0.1
10.0	176.0	4.1	176.0	0.0
20.0	224.0	4.9	226.1	2.1
30.0	259.0	4.7	261.6	2.6
40.0	289.0	4.3	290.9	1.9
50.0	312.0	4.3	313.6	1.6
60.0	332.0	4.3	332.3	0.3
70.0	354.0	4.3	355.4	1.4
80.0	378.0	4.3	379.7	1.7
90.0	407.0	4.3	409.0	2.0
95.0	428.0	5.0	431.2	3.2
FBP	475.0	11.8	480.3	5.3

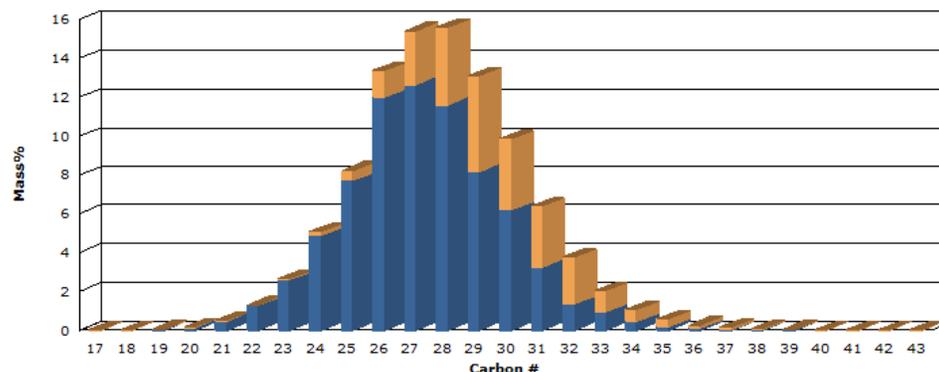
---

Created by Da Vinci Laboratory Solutions - 100      Page 1 of 2      02/04/2013 09:41:31

Validation info always present on sample reports.

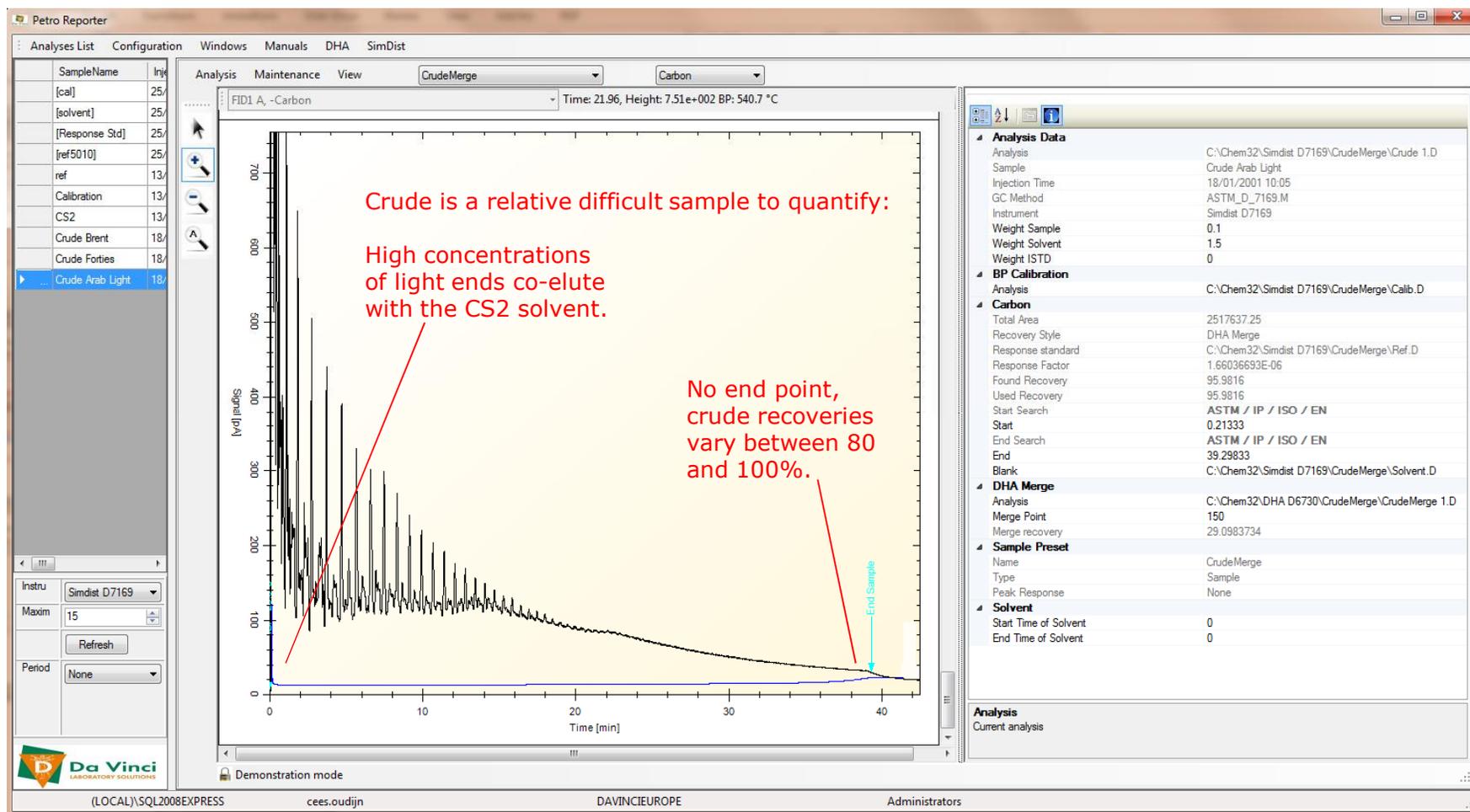
# Wax Content Report (ASTM D5442)

## Alkane Profile Report

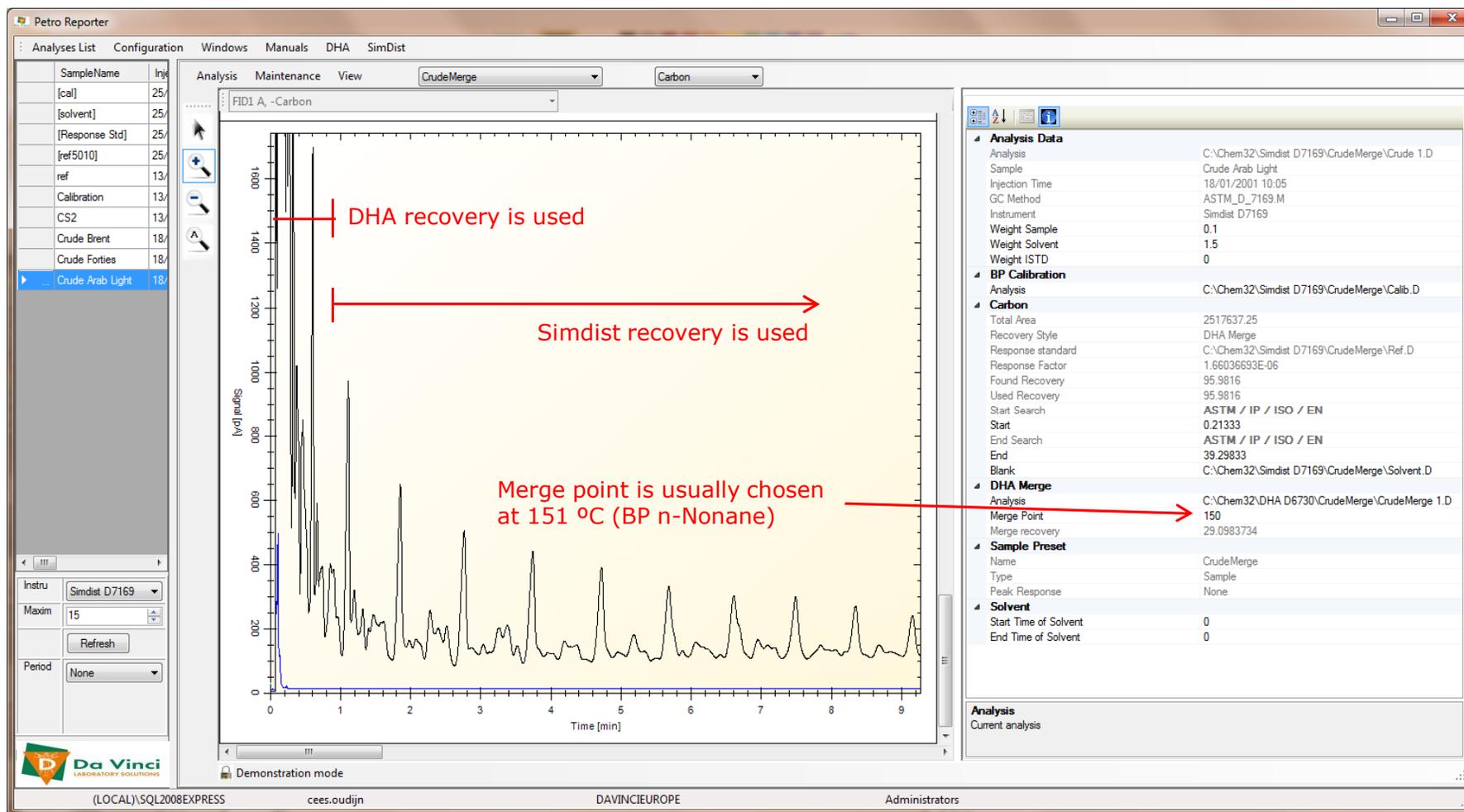


Carbon	Normals	Unknowns	Total
17	0.006	0.015	0.021
18	0.008	0.036	0.044
19	0.029	0.044	0.072
20	0.131	0.043	0.174
21	0.476	0.048	0.524
22	1.257	0.054	1.311
23	2.576	0.087	2.663
24	4.881	0.182	5.063
25	7.712	0.510	8.222
26	11.989	1.384	13.373
27	12.642	2.769	15.412
28	11.598	3.967	15.565
29	8.145	4.958	13.103
30	6.190	3.669	9.860
31	3.258	3.123	6.381
32	1.340	2.440	3.779
33	0.921	1.097	2.019
34	0.453	0.626	1.079
35	0.184	0.393	0.576
36	0.093	0.183	0.276
37	0.049	0.131	0.180
38	0.024	0.091	0.115
39	0.015	0.044	0.059
40	0.010	0.044	0.054
41	0.007	0.020	0.027
42	0.006	0.026	0.032
43	0.004	0.010	0.014
	<b>74.010</b>	<b>25,99</b>	<b>100,00</b>

# SimDist Crude Calculations (1)



## SimDist Crude Calculations (2)



# Crude SimDist - DHA merge report



ASTMD7169

Crude Brent  
18/01/2001 18:35:32

C:\Chem32\Simdist D7169\CrudeMerge\Crude 3.D

Sample Preset	CrudeMerge	Bottle	
Method	ASTM_D_7169.M	Sample Weight	0.1000
Analyst	Za	SolventWeight	1.3000
		ISTD Weight	-

Description Crude Brent

**Channel: Carbon**  
 BP Calibration C:\Chem32\Simdist D7169\CrudeMerge\Calib.D  
 Blank C:\Chem32\Simdist D7169\CrudeMerge\Solvent.D  
 Response C:\Chem32\Simdist D7169\CrudeMerge\Ref.D  
 DHA C:\Chem32\DHA D6730\CrudeMerge\CrudeMerge 3.D  
 Start Elution Time 0.213  
 End Elution Time 39.298  
 Total Area 2.5183e+006  
 Response Factor 1.6604e-006  
 Found Recovery 92.8  
 DHA Recovery at 150 34.3  
 SimDist Recovery 58.5  
 Total Recovery 92.8  
 Used Recovery 92.8

Combined  
Simdist / DHA  
recovery

## Distribution Report

Rec Mass%	TBP °C						
1.0	-36.5	24.0	100.3	47.0	241.5	70.0	420.1
2.0	-9.2	25.0	103.3	48.0	249.3	71.0	428.7
3.0	-4.8	26.0	106.4	49.0	255.9	72.0	437.2
4.0	0.1	27.0	109.1	50.0	263.2	73.0	446.1
5.0	17.4	28.0	115.8	51.0	269.4	74.0	455.6
6.0	29.0	29.0	124.2	52.0	277.5	75.0	465.9
7.0	32.1	30.0	124.7	53.0	285.5	76.0	476.4
8.0	35.2	31.0	125.2	54.0	292.6	77.0	486.9
9.0	52.4	32.0	126.6	55.0	300.2	78.0	498.3
10.0	61.1	33.0	137.0	56.0	305.2	79.0	511.1
11.0	64.4	34.0	147.3	57.0	313.6	80.0	525.7
12.0	66.8	35.0	156.0	58.0	319.1	81.0	541.4
13.0	69.2	36.0	161.7	59.0	327.9	82.0	553.6
14.0	71.7	37.0	169.8	60.0	335.2	83.0	566.1
15.0	80.3	38.0	175.0	61.0	343.1	84.0	579.4
16.0	80.7	39.0	179.2	62.0	352.4	85.0	593.5
17.0	90.3	40.0	186.1	63.0	360.2	86.0	608.7
18.0	92.0	41.0	191.5	64.0	368.2	87.0	624.7
19.0	94.6	42.0	202.1	65.0	377.7	88.0	641.8
20.0	97.6	43.0	214.2	66.0	386.4	89.0	660.2
21.0	98.6	44.0	220.0	67.0	395.0	90.0	681.2
22.0	98.8	45.0	226.8	68.0	403.5	91.0	704.3
23.0	99.0	46.0	232.6	69.0	411.8		

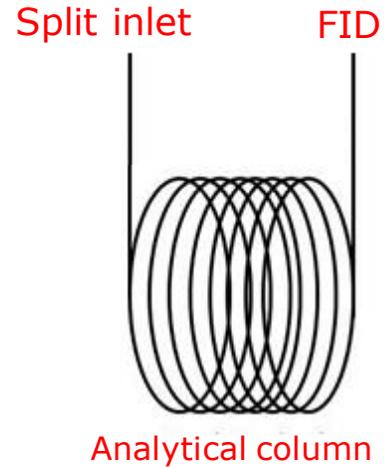
DHA true  
boiling point  
results

# DHA Application

- Determines
  - Component identification up to tridecane
  - Component concentration (mass%, vol%, mol%)
- Purpose
  - Used for quality control of refinery streams, mostly related to the gasoline blending pool
  - Used for quality control of finished gasoline
- Market Area
  - Refinery laboratories
  - Independent laboratories
  - Chemical plants (consumes naphtha for plastics)
  - Solvent plants (feedstock evaluation)

# Hardware

- Relatively simple setup
- Standard GC parts (except crude method)
- Autosampler injection
- Electronic pressure control
- Mostly non-polar columns
- Sometimes an additional polar pre-column is used



## Background

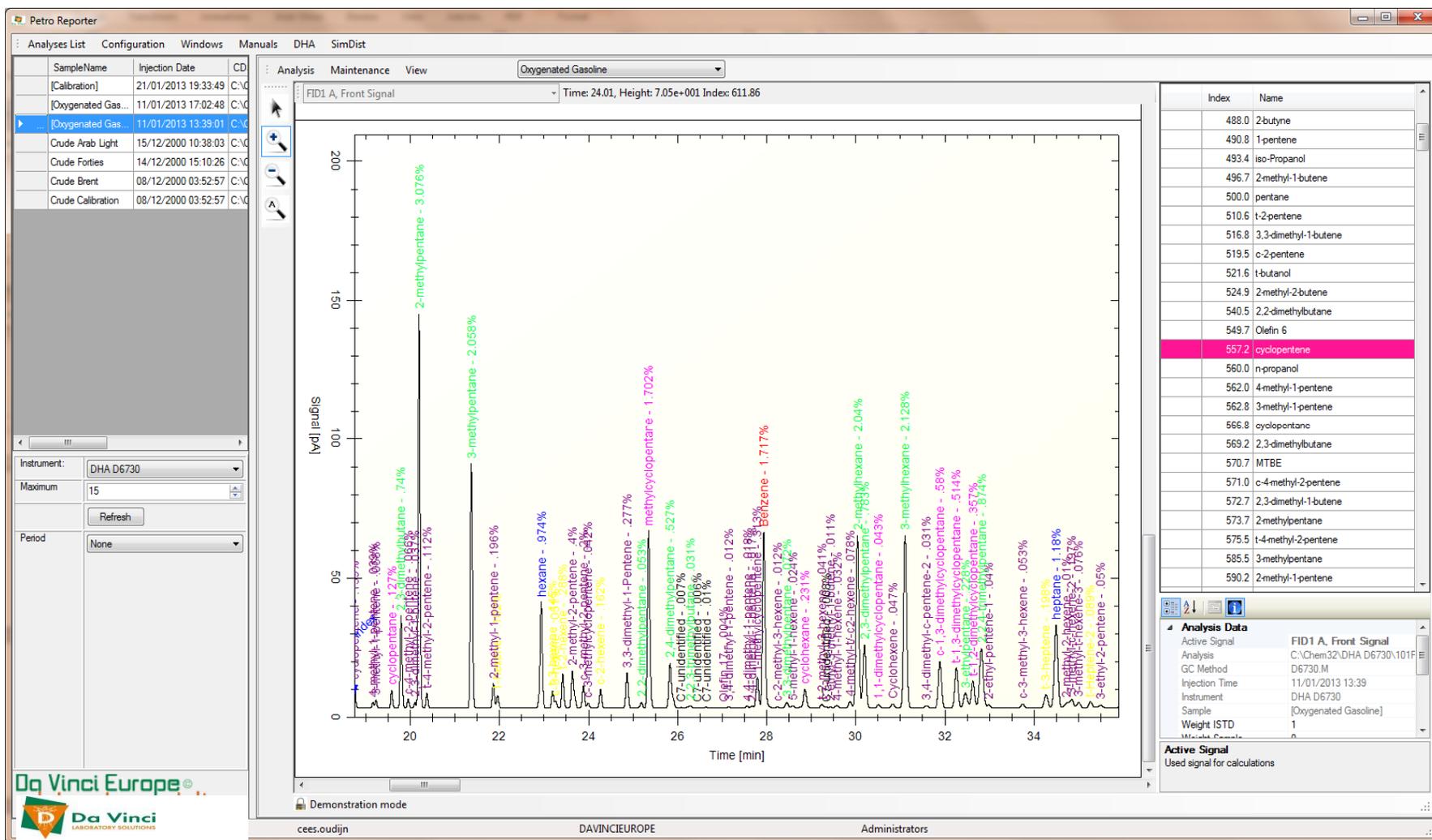
- Peak identification using Kovats Retention Indices (RI)

$$RI = 100 * \left[ C_1 + (C_2 - C_1) * \frac{(\text{Log}(t - t_0) - \text{Log}(t_1 - t_0))}{(\text{Log}(t_2 - t_0) - \text{Log}(t_1 - t_0))} \right]$$

- RI unknown peak (*I*) calculated from:
  - Retention time unknown peak
  - Retention time n-paraffin eluting before and after unknown peak
- RI unaffected in case of (small) retention time shifts
- Calculated RI is matched against a database in the software

Index	CompName	Group	RRF	MolWt	BP °C	Density	RON	MON	Vapor Pres	Gross Heating	Nett Heating
411.4	t-2-butene	normal Olefin	0.8742	56.1	1.0	0.6112	153.0	130.0	49.9	20700.29	19389
414.3	2,2-dimethylpropane	iso Paraffin	0.8995	72.1	9.5	0.5974	83.5	80.2	36.7	20898.41	19369
425.8	c-2-butene	normal Olefin	0.8742	56.1	3.7	0.6286	153.0	130.0	45.8	20726.29	19415
436.6	1,2-butadiene	di Olefin	0.8431	54.1	10.9	0.6576	185.0	135.0	36.8	20586.82	19567
445.4	ethanol	Oxygenate	1.8620	46.1	78.3	0.7967	126.0	102.0	2.3	12727.62	11530
456.2	cyclobutane	cyclo Paraffin	0.8742	56.1	12.6	0.6999	100.0	100.0	34.1	20987.29	19676
457.7	3-methyl-1-butene	iso Olefin	0.8739	70.1	20.0	0.6322	129.0	125.0	26.4	20469.75	19158
474.7	iso Pentane	iso Paraffin	0.8995	72.1	27.8	0.6247	92.3	90.3	20.4	20833.41	19304
481.9	1,4-Pentadiene	di Olefin	0.8490	68.1	26.0	0.6663	180.0	160.0	21.9	20113.22	19033

# PetroReporter Main DHA Menu

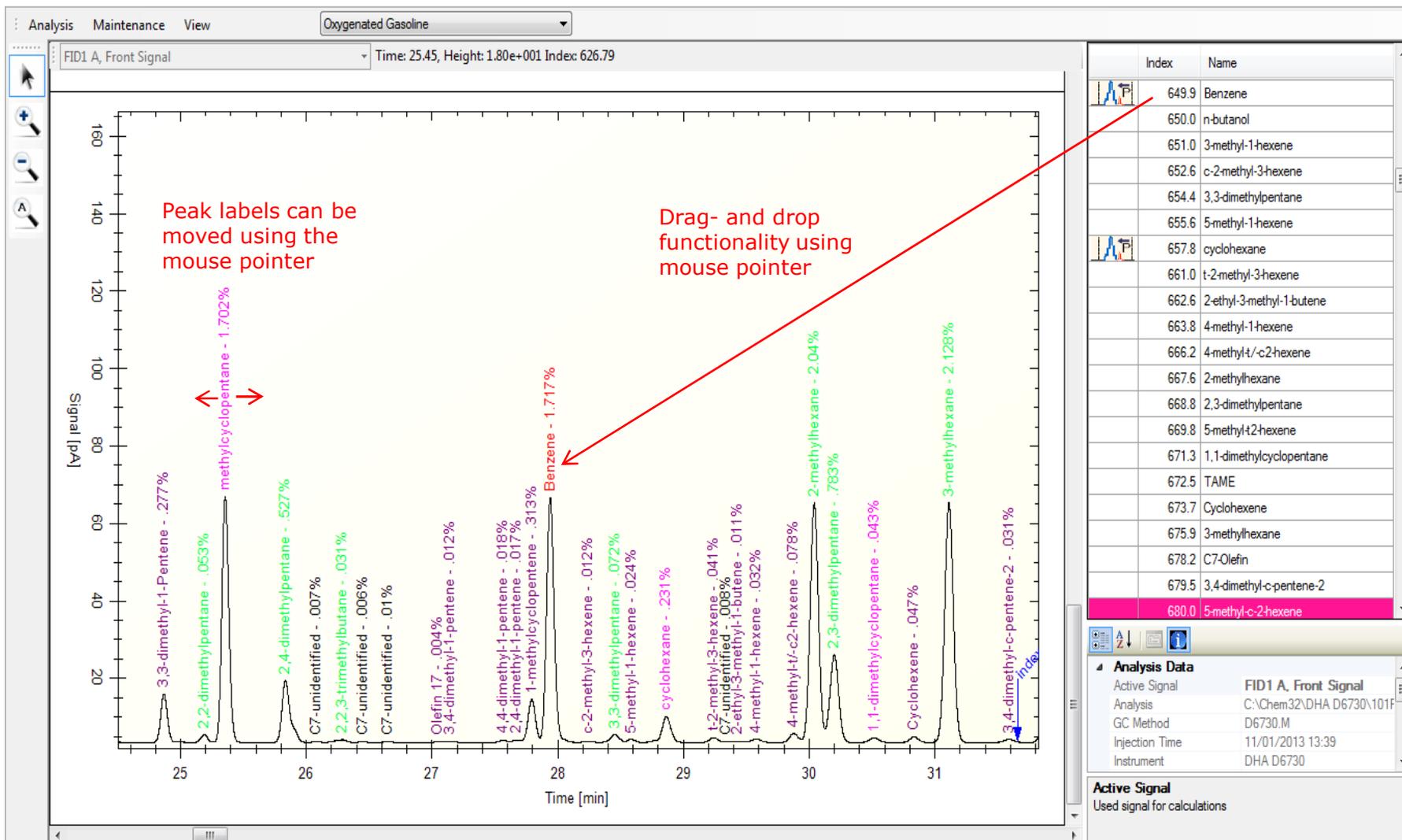


Sample list

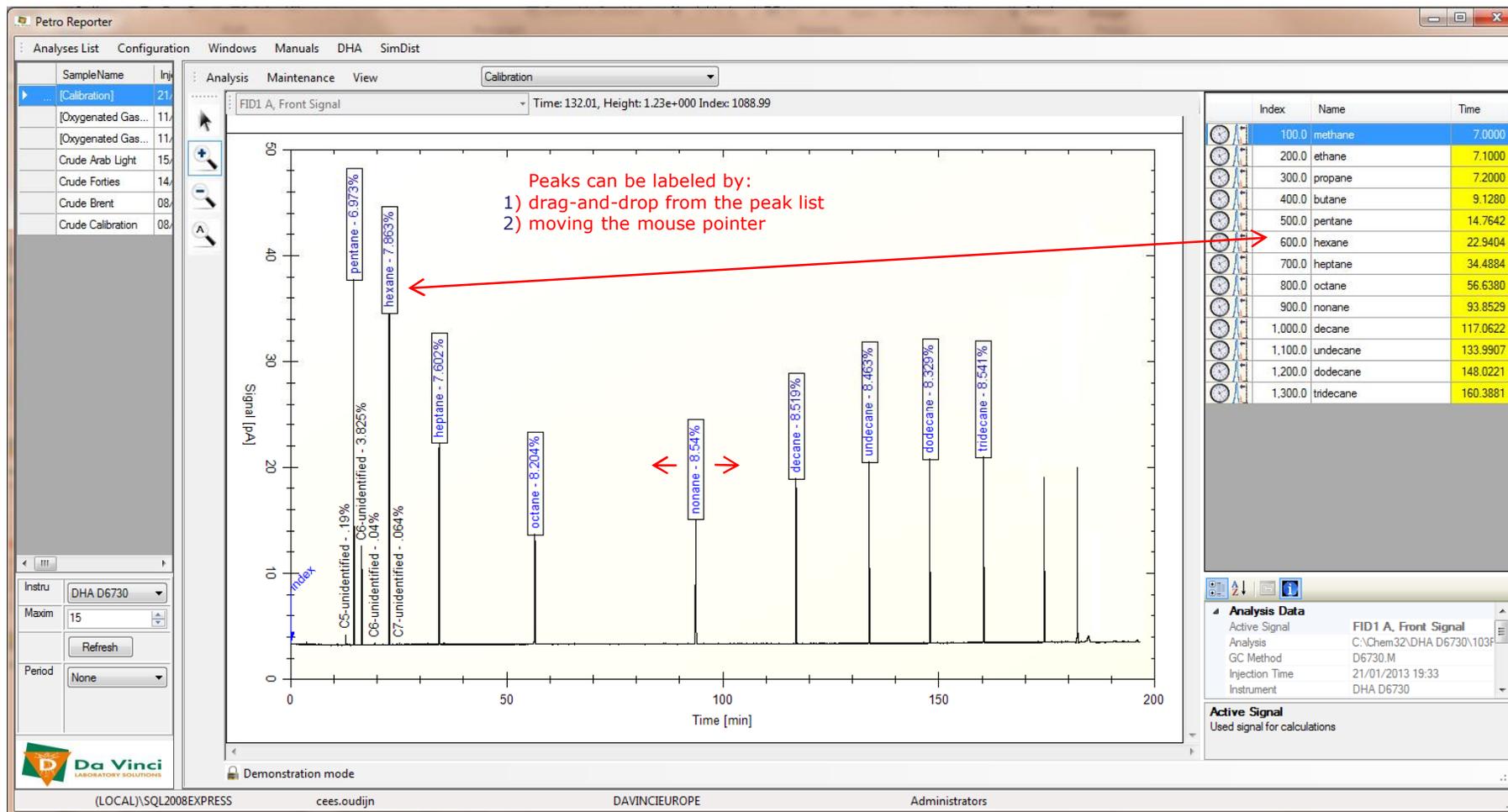
Chromatogram

Sample details

# DHA Sample Details



# DHA Calibration



# DHA Sample Preset Editor (1)

Edit Sample Presets

Current Sample Preset: Oxygenated Gasoline

General | Group Filter | Primary Components | Index Windows | Peak / Group Report | Other Reports | Exports

Group Name	Select
normal Paraffin	<input checked="" type="checkbox"/>
iso Paraffin	<input checked="" type="checkbox"/>
cyclo Paraffin	<input checked="" type="checkbox"/>
normal Olefin	<input type="checkbox"/>
iso Olefin	<input type="checkbox"/>
cyclo Olefin	<input type="checkbox"/>
Aromatics	<input checked="" type="checkbox"/>
Oxygenate	<input checked="" type="checkbox"/>
di Olefin	<input type="checkbox"/>

By selecting only sample-applicable components, the peak RI matching process becomes more robust.

New Preset | Save Type | Close

## DHA Sample Preset Editor (2)

Edit Sample Presets

Current Sample Preset: Oxygenated Gasoline

General Group Filter Primary Components Index Windows Peak / Group Report Other Reports Exports

Preset Components:

Index	Name
100.0	methane
200.0	ethane
300.0	propane
366.1	isoButane
378.8	methanol
400.0	butane
415.1	2,2-dimethylpropane
455.3	ethanol
477.5	isoPentane
483.0	ethylcyclopropane
493.4	iso-Propanol
500.0	pentane
521.6	t-butanol
540.5	2,2-dimethylbutane
560.0	n-propanol
566.8	cyclopentane

Primary Preset Components:

Index	Usage	Name
649.9	Main Component	Benzene
657.8	Main Component	cyclohexane
751.8	Main Component	toluene
854.7	Main Component	ethylbenzene
864.2	Main Component	m-xylene
883.5	Main Component	o-xylene

Primary components will first be matched with unknown peaks, which reduces the chance of misidentification for major peaks.

New Preset Save Type Close

## DHA Sample Preset Editor (3)

Current Sample Preset: Oxygenated Gasoline

General | Group Filter | Primary Components | **Index Windows** | Peak / Group Report | Other Reports | Exports

Index	Window
0.0	15.0
400.0	5.0
550.0	4.0
750.0	3.0
800.0	1.5
1,500.0	0.5

Add Delete

New Preset Save Type Close

Flexibility on the RI matching windows allows for more accurate identification (to areas of the chromatogram with more peaks present).

## DHA Sample Preset Editor (4)

Edit Sample Presets

Current Sample Preset: Oxygenated Gasoline

General | Group Filter | Primary Components | Index Windows | **Peak / Group Report** | Other Reports | Exports

**Group Report**

Report Style: PIONAX

Maximum Carbon Group: 13

Show Mass% Report

Show Volume% Report

Show Mol% Report

---

Group (PIONA) report settings

**Peak Report**

Show Peak Report  Page Break Before

Selected Report Columns:

Report Column	Selected
Name	<input checked="" type="checkbox"/>
#	<input checked="" type="checkbox"/>
Index	<input checked="" type="checkbox"/>
Time	<input checked="" type="checkbox"/>
Area	<input checked="" type="checkbox"/>
Mass%	<input checked="" type="checkbox"/>
Vol%	<input checked="" type="checkbox"/>
Mol%	<input checked="" type="checkbox"/>

↑

↓

---

Individual hydrocarbon report settings

New Preset Save Type Close



## DHA Sample Preset Editor (6)

Edit Sample Presets

Current Sample Preset: Oxygenated Gasoline

General | Group Filter | Primary Components | Index Windows | Peak / Group Report | Other Reports | Exports

Exporting file types

- Character Separated Value
- Acrobat PDF
- Microsoft EXCEL

Post Run

- Report To Default Printer

Export to LIMS properties

New Preset | Save Type | Close

# Component Database Editor

The screenshot shows the Petro Reporter software interface. The main window displays a chromatogram with a signal intensity of 600 pA over a time range of 0 to 200 minutes. A 'Component Database Editor' window is overlaid on the chromatogram, showing a table of components. The table has the following columns: Delete, Index, CompName, Group, RRF, MolWt, BP °C, Density, RON, and MON. The 'ASTM D 6730' standard is highlighted in the title bar of the editor window. A red text box at the bottom of the editor window states: 'Per application, properties of components can be modified in the database.'

Delete	Index	CompName	Group	RRF	MolWt	BP °C	Density	RON	MON
<input type="checkbox"/>	100.0	methane	normal Paraffin	1.0000	16.0	-161.5	0.3000	101.0	100
<input type="checkbox"/>	178.1	ethene	normal Olefin	0.8727	28.0	-103.7	0.3500	180.0	160
<input type="checkbox"/>	200.0	ethane	normal Paraffin	0.9372	30.1	-89.0	0.3562	101.6	100
<input type="checkbox"/>	284.0	propene	normal Olefin	0.8727	42.0	-47.7	0.5210	180.0	160
<input type="checkbox"/>	300.0	C3-unidentified	Unknown	0.8743	42.1	-42.0	0.5070	88.0	79
<input type="checkbox"/>	300.0	propane	normal Paraffin	0.9162	44.1	-42.0	0.5070	88.0	79
<input type="checkbox"/>	313.1	propadiene	di Olefin	0.8332	40.1	-34.5	0.5997	220.0	200
<input type="checkbox"/>	366.1	isoButane	iso Paraffin	0.9057	58.1	-11.7	0.5629	100.1	97
<input type="checkbox"/>	378.8	methanol	Oxygenate	2.6720	32.0	65.0	0.7965	128.0	101
<input type="checkbox"/>	386.9	1-butyne	normal Olefin	0.8431	54.1	8.1	0.6959	180.0	130
<input type="checkbox"/>	390.7	1-butene	normal Olefin	0.8742	56.1	-6.3	0.6005	144.0	126
<input type="checkbox"/>	391.5	isobutene	iso Olefin	0.8742	56.1	-6.9	0.6013	170.0	139
<input type="checkbox"/>	394.9	1,3-butadiene	di Olefin	0.8431	54.1	-4.4	0.6273	190.0	140
<input type="checkbox"/>	400.0	butane	normal Paraffin	0.9057	58.1	-0.5	0.5840	66.0	60
<input type="checkbox"/>	400.0	C4-unidentified	Unknown	0.8429	54.1	-0.5	0.5840	150.0	130
<input type="checkbox"/>	409.0	VinylAcetylene	iso Olefin	0.8119	52.1	5.1	0.6500	150.0	130
<input type="checkbox"/>	412.1	1,2-butene	normal Olefin	0.8742	56.1	1.0	0.6112	153.0	130

Per application, properties of components can be modified in the database.



# Onscreen reporting



[Oxygenated Gasoline]  
1/11/2013 5:02:48PM

C:\Chem32\1\DATA\20130104\_GCB\_D6730-7\102F0201.D

Sample Preset Oxygenated Gasoline  
Method D6730.M  
Analyst  
Description  
Calibration C:\Chem32\1\

Bottle  
Sample Weight  
ISTD Weight 1.0000



[Oxygenated Gasoline]  
1/11/2013 5:02:48PM

C:\Chem32\1\DATA\20130104\_GCB\_D6730-7\102F0201.D

## Group Report in Mass%

	n-Par	i-Par
C2	0.00	0.00
C3	0.01	0.00
C4	1.39	0.11
C5	0.87	9.76
C6	0.90	5.43
C7	1.11	5.51
C8	0.84	5.13
C9	0.29	2.43
C10	0.11	0.67
C11	0.04	0.20
C12	0.03	0.19
C13	0.03	0.01
Total	5.61	29.43

## Detailed Peak Report

#	Index	Time	Area
1	300.0	7.208	1.003E+000
2	364.8	8.225	1.453E+001
3	390.0	8.874	1.056E+001
4	400.0	9.185	1.882E+002
5	411.6	9.571	8.880E-001
6	414.5	9.675	3.221E+000
7	426.8	10.154	1.706E+000
8	454.5	11.494	6.317E-001
9	460.5	11.839	8.266E+000
10	477.1	12.918	1.330E+003
11	490.8	13.970	3.214E+001
12	496.7	14.471	6.037E+001
13	500.1	14.767	1.188E+002
14	506.1	15.118	2.181E+000
15	510.6	15.396	9.014E+001
16	516.8	15.786	2.623E+000
17	519.6	15.965	4.984E+001
18	521.5	16.086	5.931E+000
19	524.9	16.320	1.253E+002
20	528.0	16.530	2.220E+000
21	538.0	17.248	7.888E-001
22	540.6	17.435	7.967E+000
23	557.2	18.757	2.129E+001
24	561.9	19.167	5.189E+000
25	562.7	19.237	7.667E+000
26	566.7	19.591	1.601E+001
27	569.0	19.800	9.319E+001
28	570.8	19.962	8.709E+000
29	572.4	20.112	4.996E+000
30	573.4	20.204	3.852E+002
31	575.3	20.380	1.484E+001
32	585.4	21.376	2.590E+002
33	590.2	21.873	2.534E+001
34	591.1	21.967	1.323E+001
35	600.1	22.947	1.242E+002
36	603.0	23.203	1.881E+001
37	603.7	23.270	6.534E+000
38	605.5	23.431	3.741E+001
39	607.9	23.647	5.189E+001
40	610.6	23.895	2.605E+001
41	611.7	23.999	5.651E+000
42	614.7	24.280	2.116E+001
43	620.7	24.859	1.262E+003
44	624.1	25.192	7.049E+000
45	625.8	25.367	2.227E+002
46	630.5	25.844	6.866E+001

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[Oxygenated Gasoline]  
1/11/2013 5:02:48PM

C:\Chem32\1\DATA\20130104\_GCB\_D6730-7\102F0201.D

## Boiling Point Distribution Report

Perc	TBP (mass) [°C]	TBP (vol) [°C]	Perc
	-8.7	-9.6	34.0
	-4.9	-6.7	35.0
	20.3	-0.7	36.0
	21.1	20.6	37.0
	21.9	21.2	38.0
	22.7	21.9	39.0
	23.5	22.6	40.0
	24.3	23.2	41.0
	25.1	23.9	42.0
	25.9	24.6	43.0
	26.7	25.2	44.0
	27.5	25.9	45.0
	30.8	26.6	46.0
	36.1	27.2	47.0
	36.6	28.8	48.0
	43.9	34.8	49.0
	58.0	36.2	50.0
	59.1	36.7	51.0
	59.7	44.0	52.0
	60.5	57.9	53.0
	62.6	59.0	54.0
	63.3	59.5	55.0
	68.2	60.0	56.0
	68.7	62.2	57.0
	70.4	62.8	58.0
	70.5	65.8	59.0
	70.5	68.3	60.0
	70.6	68.7	61.0
	70.6	70.4	62.0
	70.7	70.5	63.0
	70.7	70.5	64.0
	70.8	70.6	65.0
	70.8	70.6	66.0
	70.9	70.7	67.0



[Oxygenated Gasoline]  
1/11/2013 5:02:48PM

C:\Chem32\1\DATA\20130104\_GCB\_D6730-7\102F0201.D

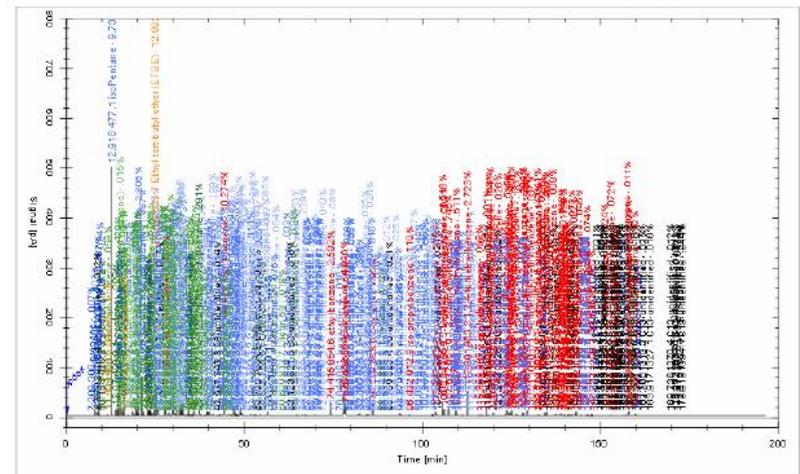
## Calculations

Specific Gravity 0.7521  
Reid Vapor Pressure 5.4  
Motor Octane Number 89.4  
Research Octane Number 98.2  
Gross Heating Value 44,656.4  
Nett Heating Value 41,886.5  
Bromine Number 17.8



[Oxygenated Gasoline]  
1/11/2013 5:02:48PM

C:\Chem32\1\DATA\20130104\_GCB\_D6730-7\102F0201.D



# Easy Setup and Configuration

The screenshot shows the Petro Reporter software interface. The 'Configuration' menu is open, and 'Setup Instruments' is selected. The 'Instrument Editor' dialog box is displayed, showing a table of instruments and a form for instrument details.

Instrument Name	Plugin	Data System	Auto Print	Data Path
DHA D6730	ASTM D 6730	Chemstation	<input type="checkbox"/>	C:\Chem32\DHA D6730
Simdist D2887	ASTM D2887	Chemstation	<input type="checkbox"/>	C:\Chem32\Simdist D2887
Simdist D7213	ASTM D7213	Chemstation	<input type="checkbox"/>	C:\Chem32\Simdist D7213
Simdist D7169	ASTM D7169	Chemstation	<input type="checkbox"/>	C:\Chem32\Simdist D7169

Instrument Editor Form:

Instrument Name: Simdist D7169  
Main Application: ASTM D7169  
Data System: EZChrom  
CDS Data Path: C:\Chem32\Simdist D7169

Licenses:

Serial Number: 670556AD

Name	Licenses	Used
DHA	10	1
SimDist	10	3

In this screen all instruments are created and configured.

Part of the configuration is the application and CDS selection.

It also shows the number of licenses available.

# Optional Other Configuration Features

The screenshot shows the Petro Reporter configuration interface with several key areas highlighted by red boxes and arrows:

- Select Users:** A section for selecting users from the company domain. It includes a 'Use Domain' checkbox, a domain name field (DAVINCEUROPE), and a search button. A tooltip indicates 'The domain name'. Below this is a table of 'Computer Users' with columns for Name and Email.
- Petro Reporter Users:** A table showing selected users with columns for UserName, User Group, and Domain. The user 'cees oudijn' is selected, with 'Administrators' as the group and 'DAVINCEUROPE' as the domain.
- Available Users:** A table of available users with columns for UserName and Domain. 'cees oudijn' is selected from the 'DAVINCEUROPE' domain.
- Instrument Users:** A table of instrument users with columns for User Name and Domain. 'cees oudijn' is selected from the 'DAVINCEUROPE' domain.
- Select User Group:** A dropdown menu set to 'Analysts'.
- Module Access:** A table defining shortcuts and accessibility for various modules.
- Peak Appearance:** A table defining the appearance of peaks in the chromatogram.

**Configuration Tables:**

**Computer Users:**

Name	Email
Jemey van den Berg	jemey.v.d.berg@davincieurope.com
Jobs	jobs@davincieurope.com
Kim Engeldal	kim.engeldal@davincieurope.com

**Petro Reporter Users:**

UserName	User Group	Domain
cees oudijn	Administrators	DAVINCEUROPE

**Available Users:**

UserName	Domain
cees oudijn	DAVINCEUROPE

**Instrument Users:**

User Name	Domain
cees oudijn	DAVINCEUROPE

**Select User Group:** Analysts

**Module Access:**

ModuleName	Description	Accessible	Function Key
DHA	Closes the analysis	<input checked="" type="checkbox"/>	F4
DHA	Adds the analysis as link in the method set	<input checked="" type="checkbox"/>	None
DHA	Sample presets editor	<input checked="" type="checkbox"/>	F2
DHA	Component editor	<input checked="" type="checkbox"/>	None
DHA	Instrument Method Link editor	<input checked="" type="checkbox"/>	None

**Peak Appearance:**

Name	Short	Color
normal Paraffin	nP	Blue
iso Paraffin	iP	Green
cyclo Paraffin	cP	Magenta
normal Olefin	nO	Yellow
iso Olefin	iO	Purple
cyclo Olefin	cO	Red
Aromatics	Ar	Red

Select PetroReporter users from the company domain.

Select users per instrument.

Define shortcuts & accessibility per user.

Choose the appearance of the peaks in the chromatogram.

# Active Signal Storage

Instrument Name: DHA D6730

Method Mapping Calibration Sets

Calibration Mapping Table:

GC Method	Signal Name	Enable	Calibration Set
DHACFE.M	FID1 A,	<input checked="" type="checkbox"/>	New Set 5
D6730.M	FID1 A, Front Signal	<input checked="" type="checkbox"/>	New Set 3

Add Delete

Close

For each GC method, the information in the Method Links editor is automatically updated after the analysis is imported in PetroReporter.

# Manuals Available Inside PetroReporter

The screenshot displays the Petro Reporter software interface. The 'Manuals' menu is open, showing options for 'User Manual PetroReporter', 'User Manual DHA', and 'User Manual SimDist'. The 'Contents' window is open, displaying a table of contents for the 'User Manual Petro Reporter' document. The table lists various sections and their corresponding page numbers. The interface also shows a chromatogram plot on the left and a 'Properties' window on the right.

Section	Page
CONTENTS	2
INTRODUCTION	4
SUPPORTED WINDOWS VERSIONS	4
HARDWARE LICENSE	4
INSTALLED SOFTWARE PACKAGES	4
SOFTWARE COMPONENTS	5
License Service	5
Auto-Processing Service	5
USER AUTHENTICATION MODELS	6
Using a Windows Domain server for user authentication	6
Using a Local Windows Account	7
Using SQL authentication	7
PETRO REPORTER MAIN	9
EDITOR LAYOUT	9
MENUS	9
WINDOWS SIZING	10
CHANGING THE COMPANY LOGO	10
GENERAL OPERATION	12
PERFORM ANALYSIS ON DATA SYSTEM	12
IMPORT DATA INTO PETROREPORTER INSTRUMENT	12
CONNECT ANALYSIS TO APPLICATION AND SAMPLE PRESET	12
CONNECT ANALYSIS WITH CALIBRATION ANALYSES	12
PERFORM BASIC CALCULATIONS	13
PERFORM REPORTING AND EXPORTING	13
SAMPLE PRESETS	14
DEFINITION	14
ANALYSIS TYPES	14
HOW TO USE THE PRESET	14
PRESET LEVELS ON APPLICATION - ANALYSIS	14
CONFIGURATION MENU	16
SQL SERVER CONNECTION	16
AUTO-PROCESS SERVICE	16
LICENSE SERVICE	18
USER CONFIGURATION	20
Adding or modifying Users	20
GROUP ACCESS EDITOR	21
INSTRUMENTS USERS EDITOR	23
GROUP TYPE EDITOR	23
THE ANALYSIS LIST MENU	27
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DELETING ANALYSES FROM THE SYSTEM	29
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