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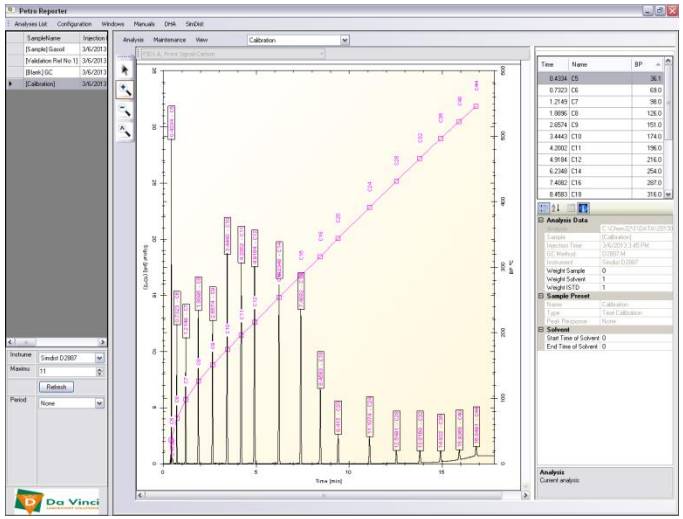
An introduction to DVLS PetroReporter© software



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

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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

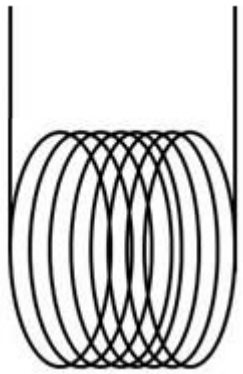
- Determines
  - Boiling point range (IBP – FBP)
  - BP distribution yield (mass%)

- 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

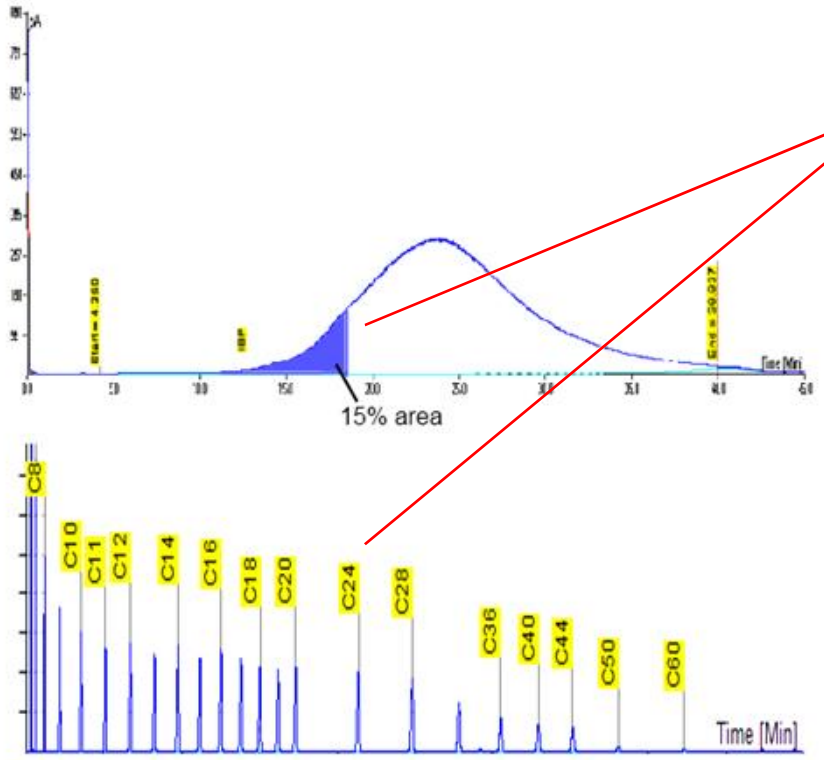
- No sample split
- Standard column and detector
- Autosampler injection
- Non-polar column
- Inlet and oven temperature ramping
- Relatively high temperatures (350-430 ºC)



Widebore analytical column

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 ºC)

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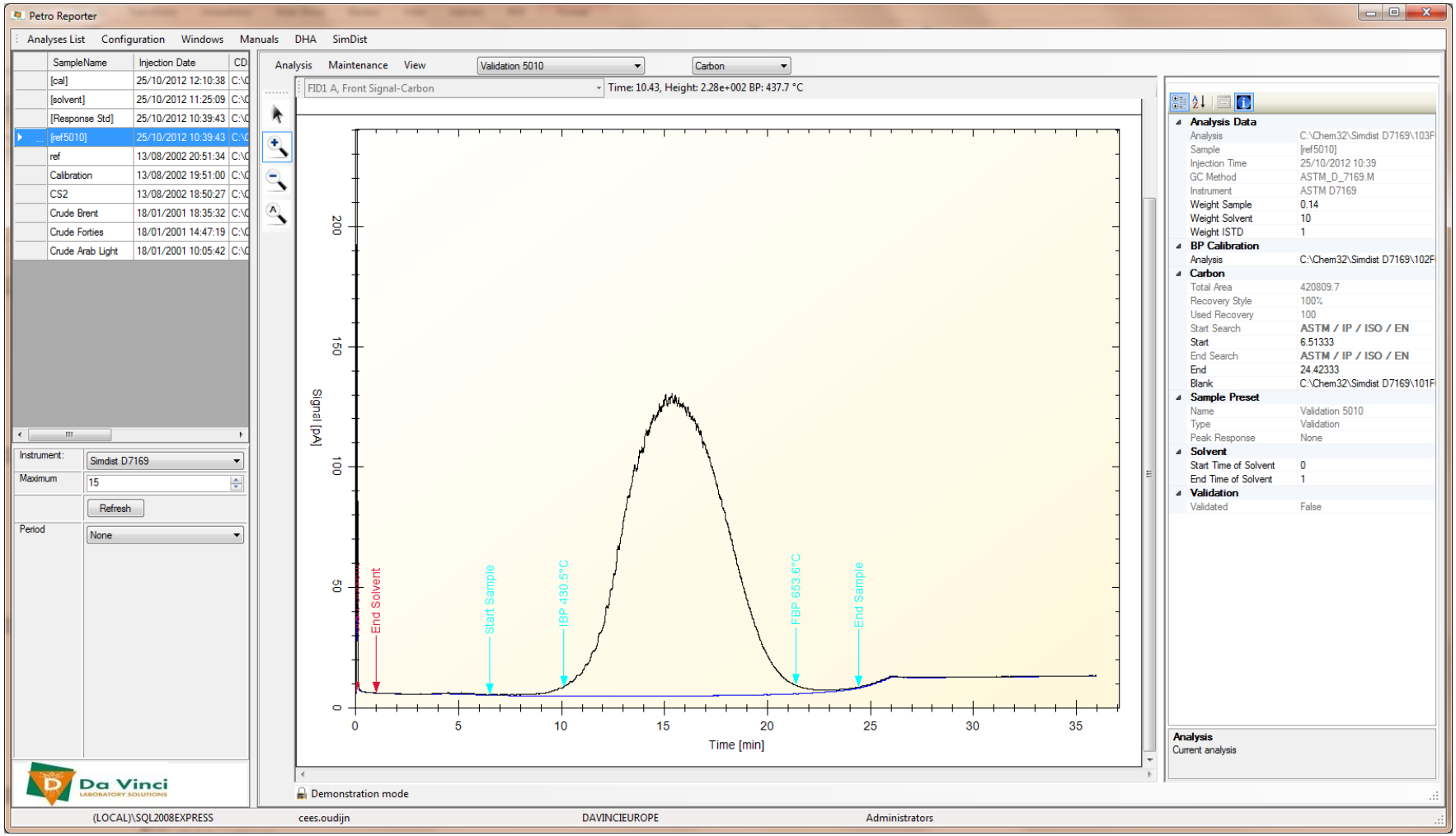
PetroReporter - Main SimDist Menu



Sample list

Chromatogram

Sample details

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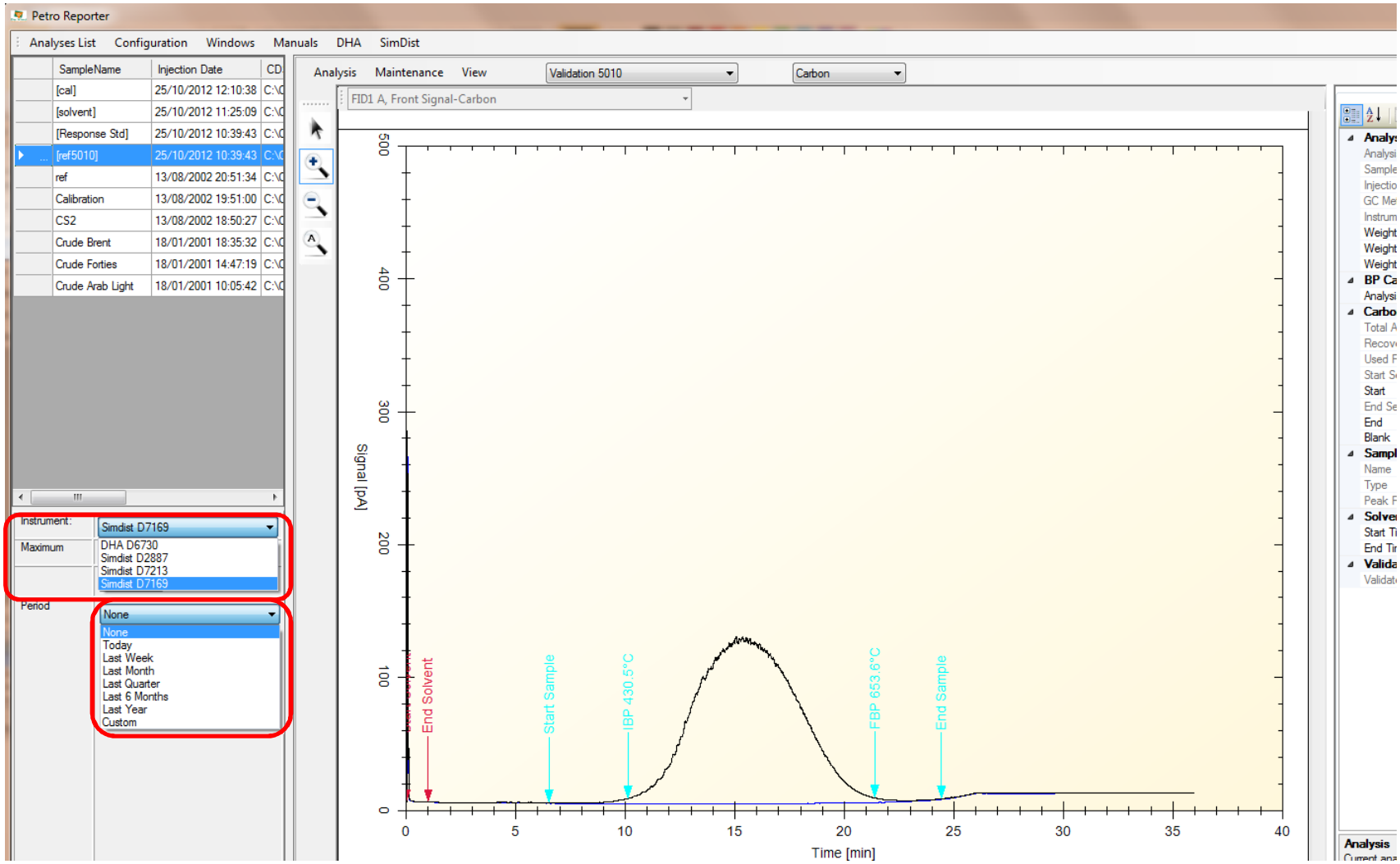
Instrument Selection Menu & Data Filter



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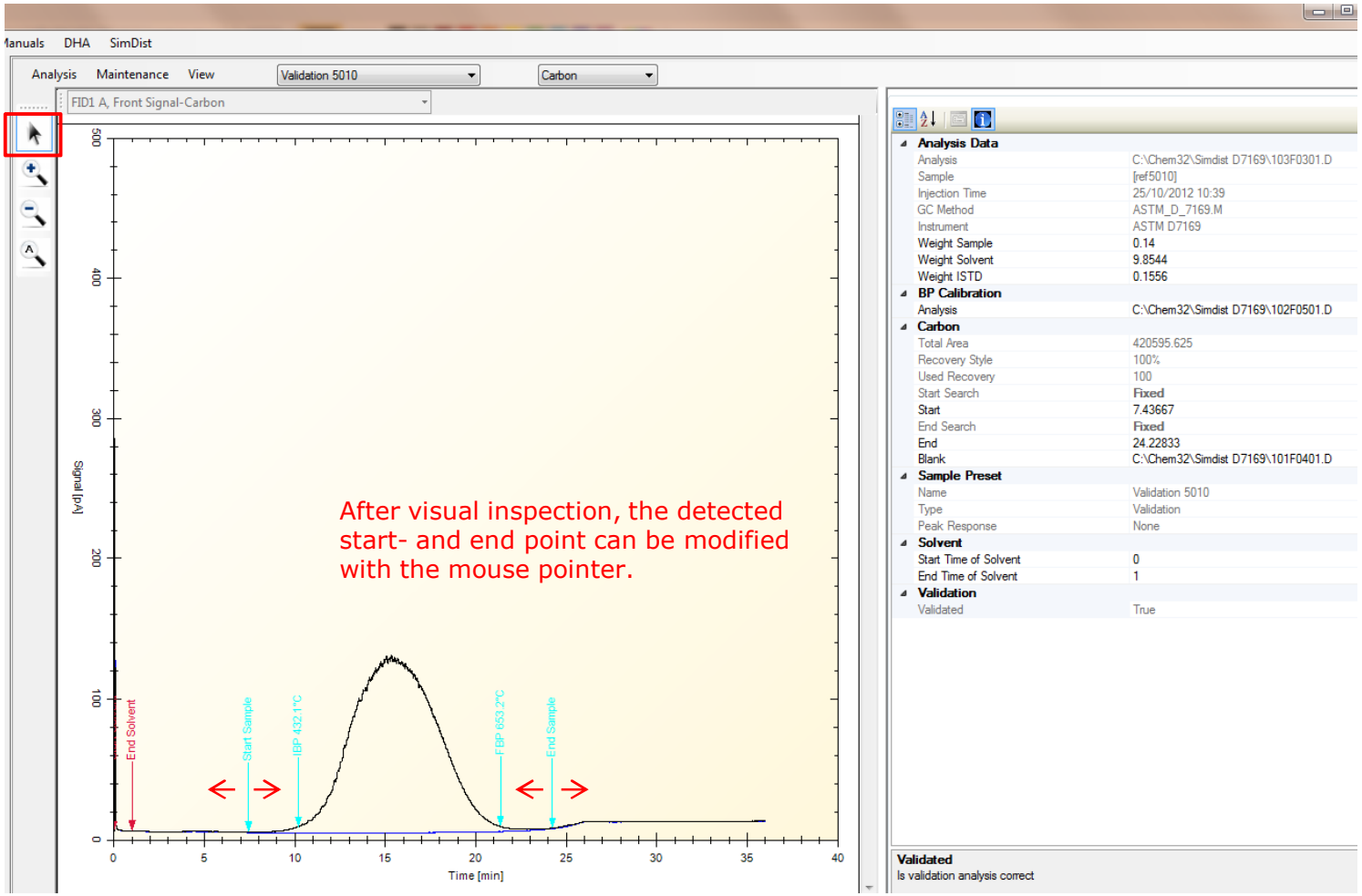
SimDist Sample Details



Sample depending information

Startpoint and endpoint times can be modified after processing

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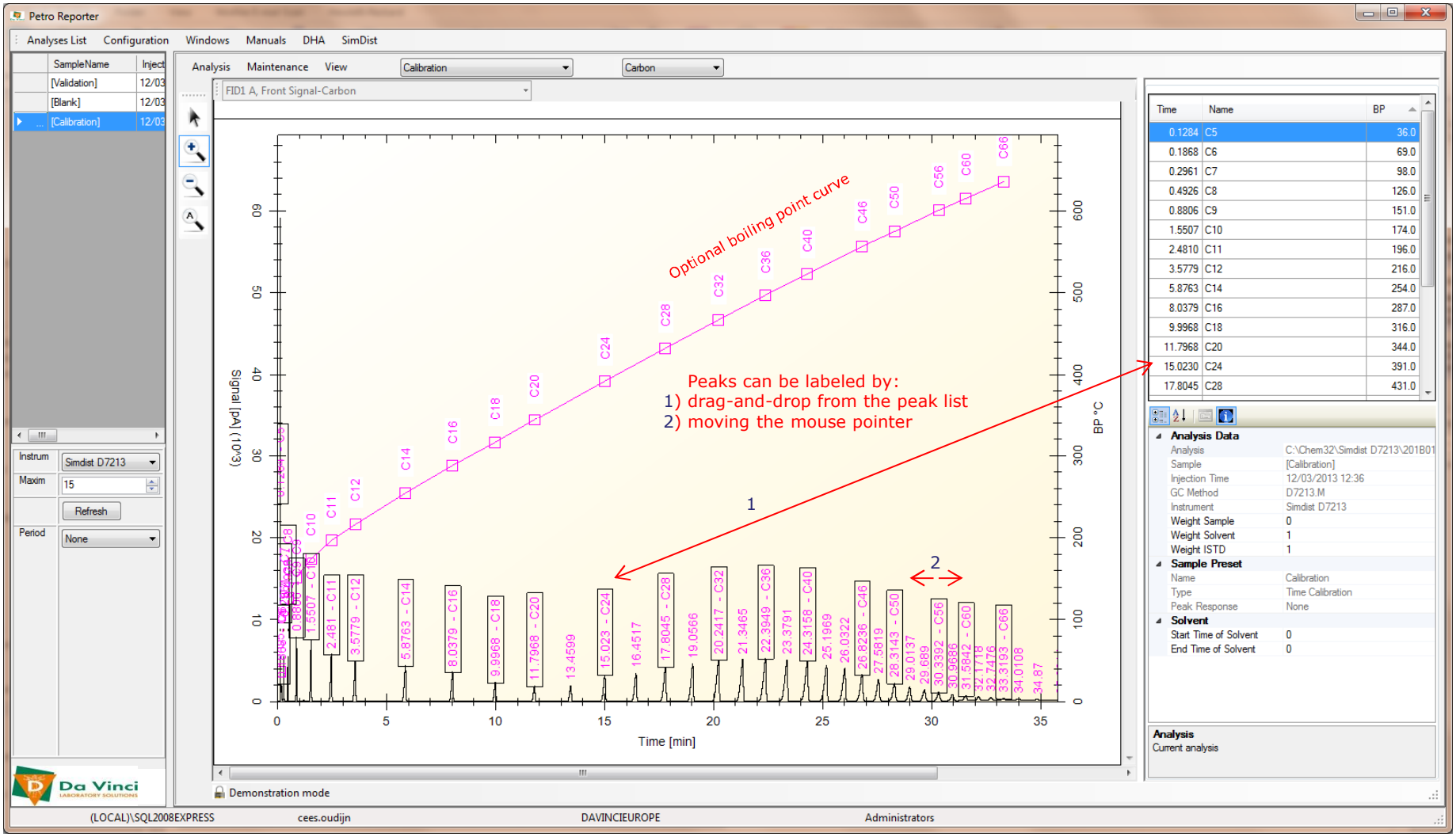
SimDist Calibration



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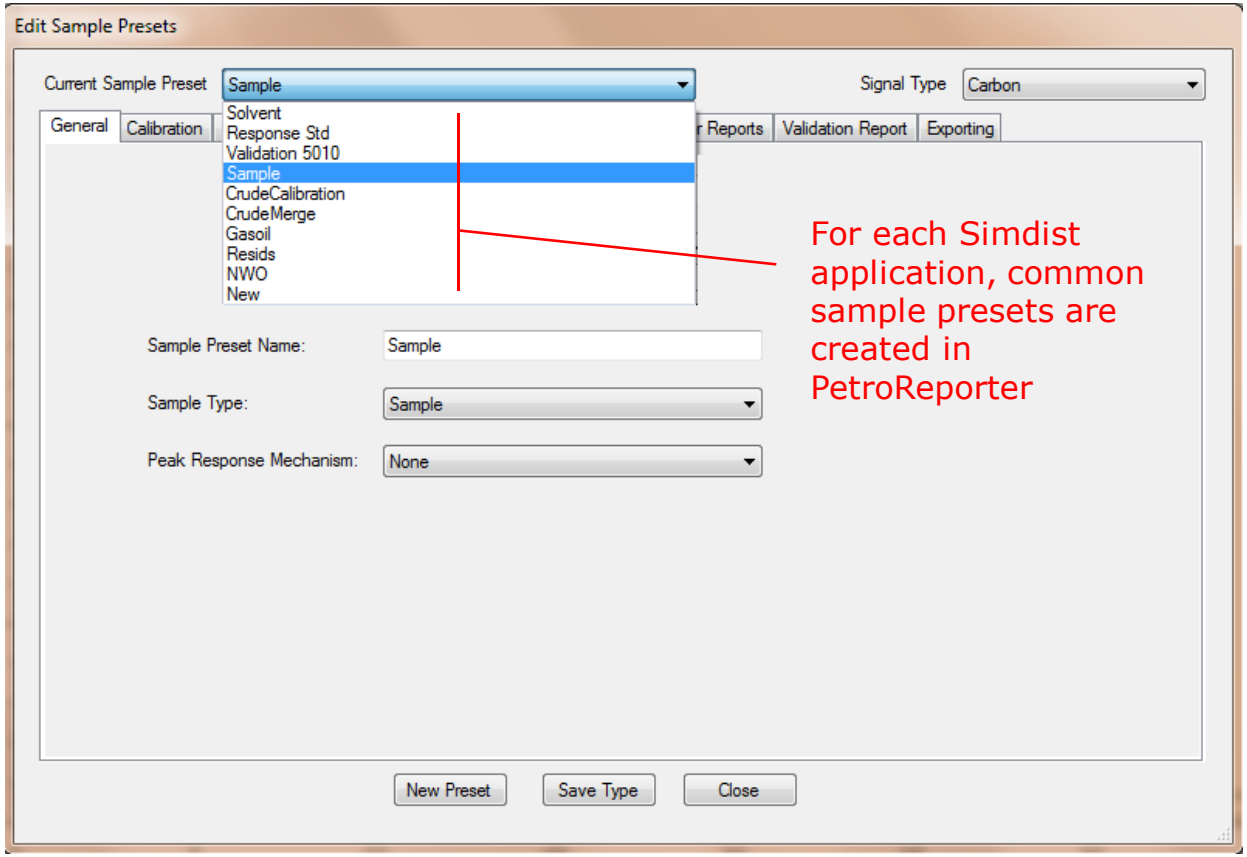
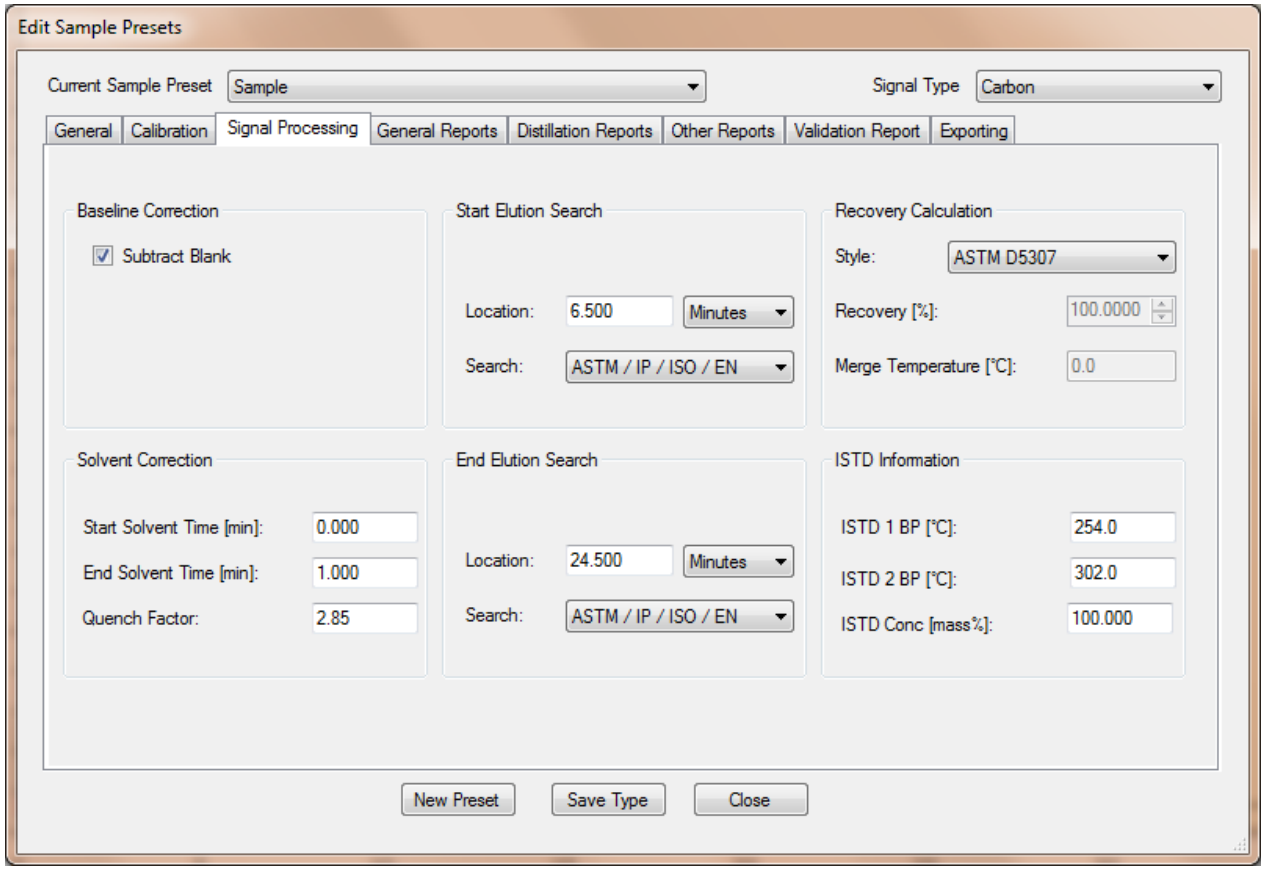
Simdist Sample Preset Editor (1)



Simdist Sample Preset Editor (2)

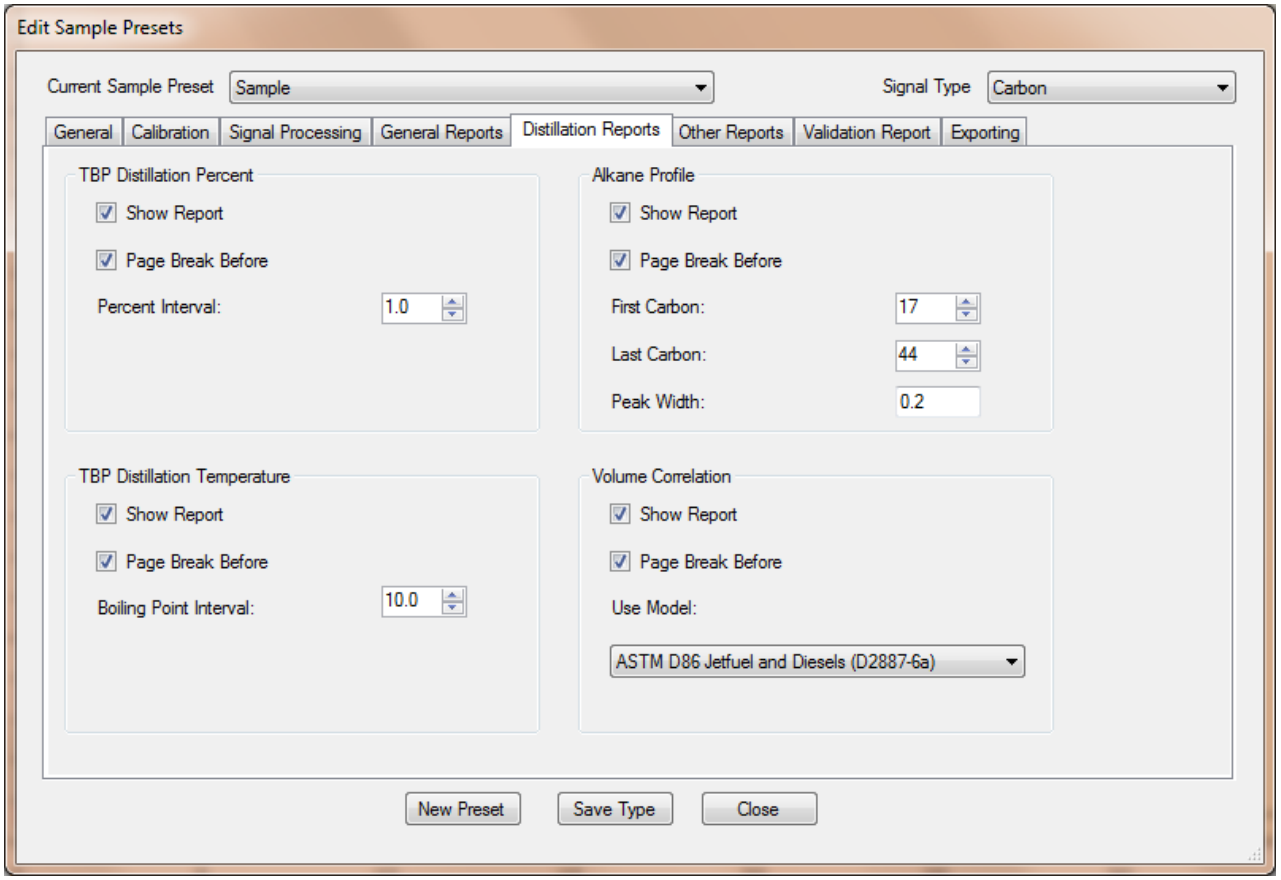


Blank handling

Start/End settings

Recovery calculation

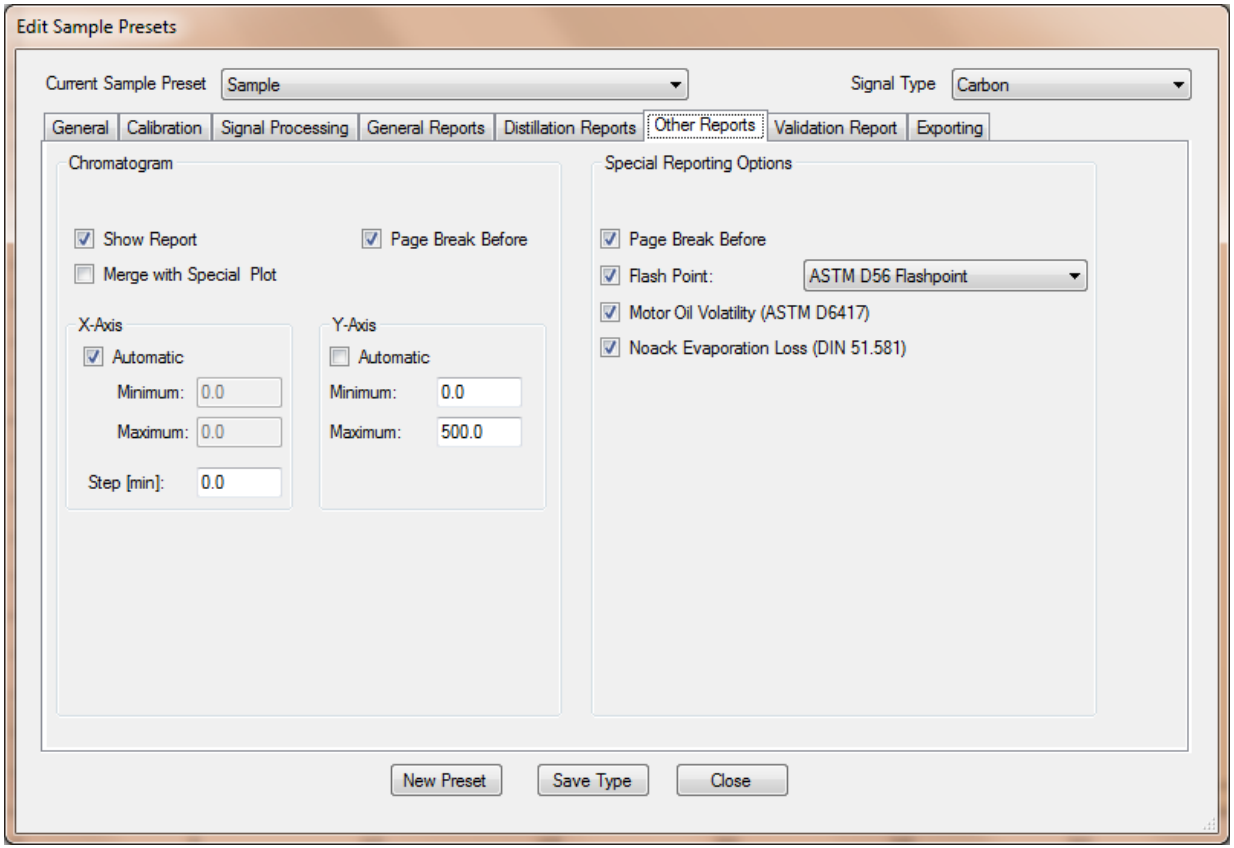
SimDist Sample Preset Editor (3)



TBP & cutpoint reports

Correlations & Alkane content

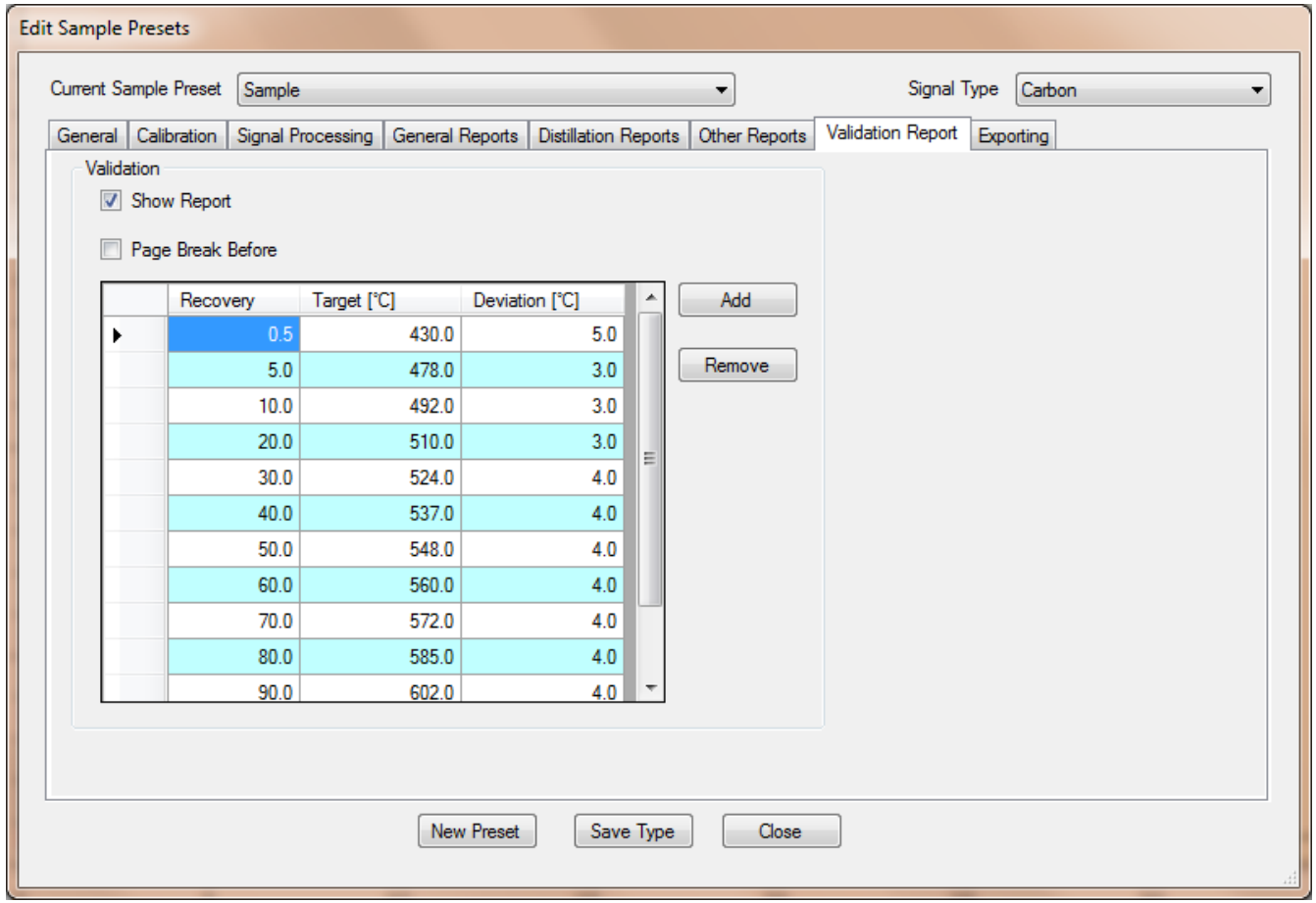
SimDist Sample Preset Editor (4)



Chromatogram output

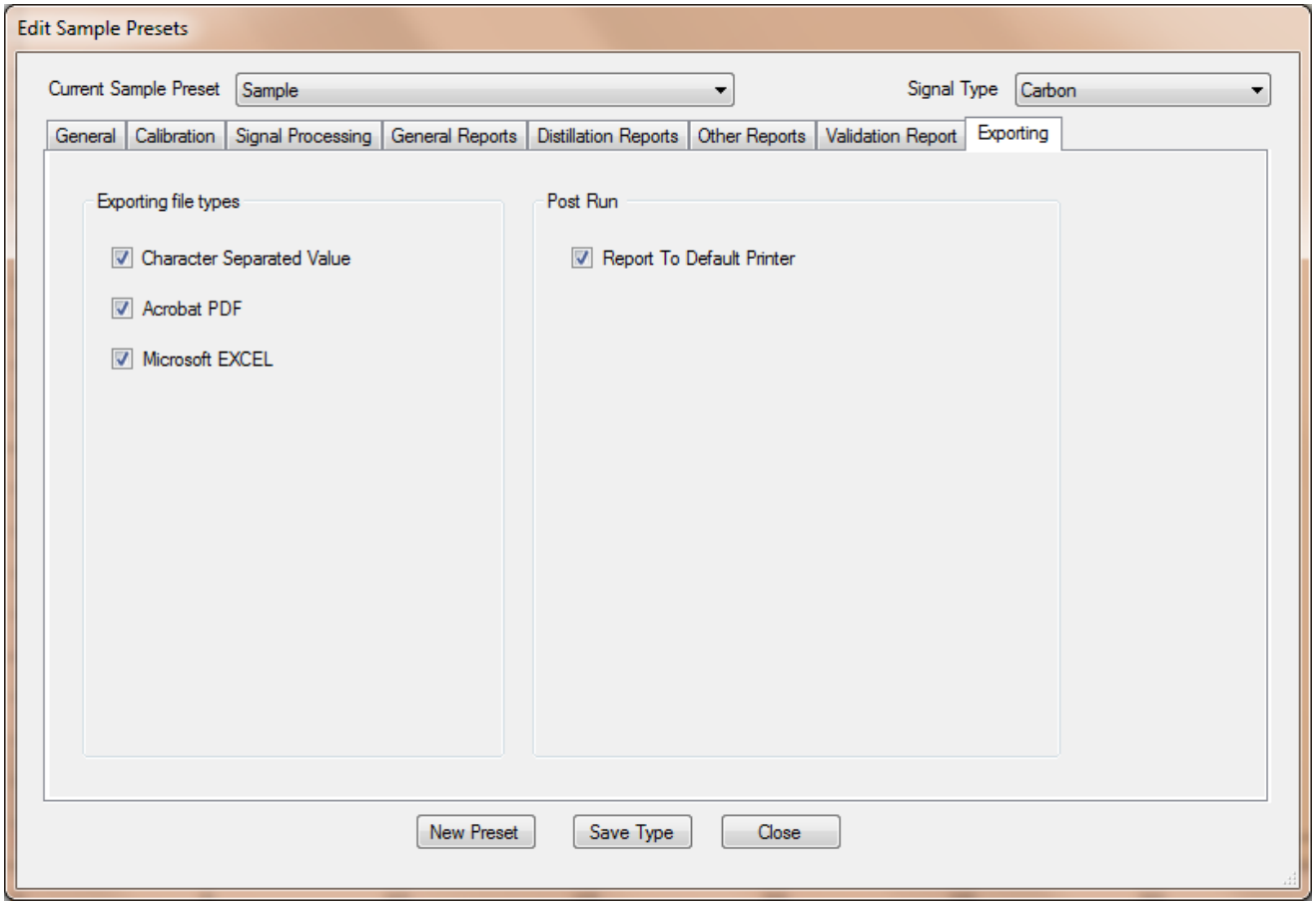
Special calculations

SimDist Sample Preset Editor (5)



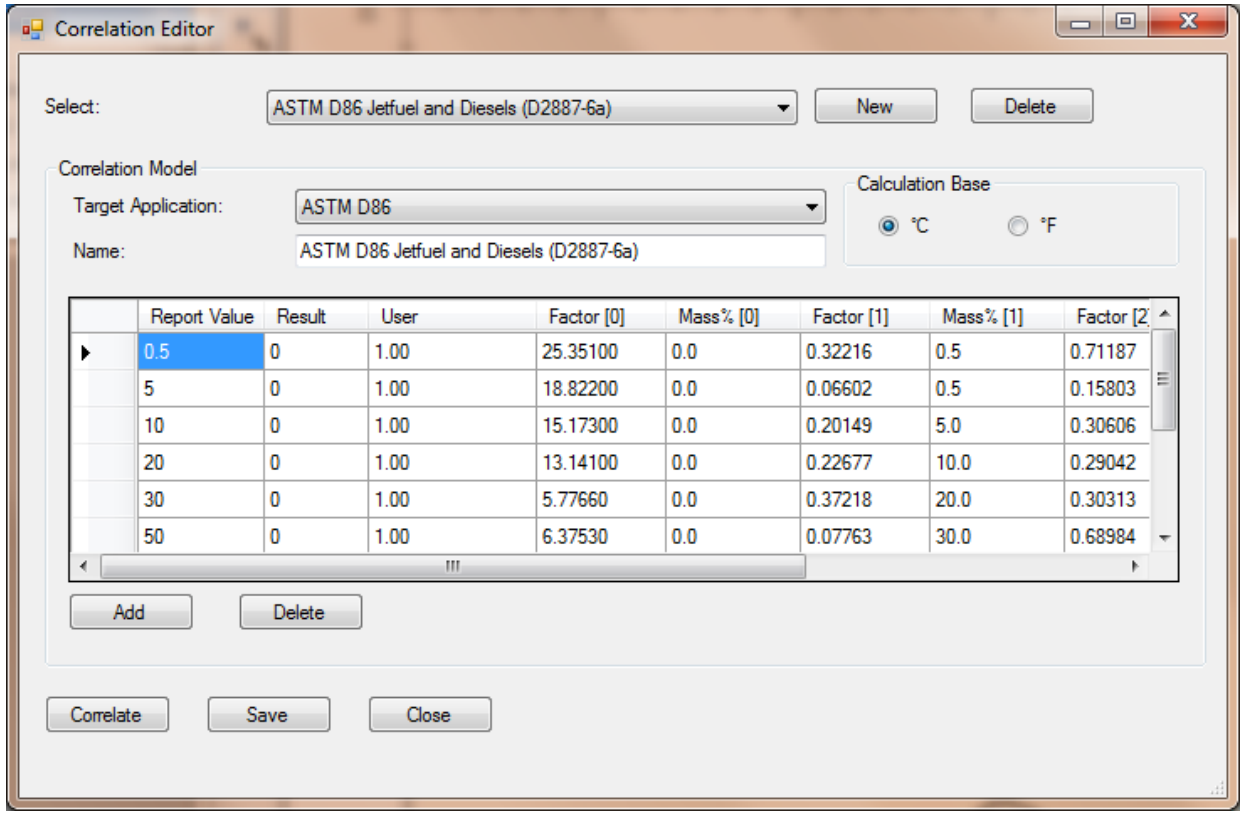
Validation settings for known or site specific samples

SimDist Sample Preset Editor (6)

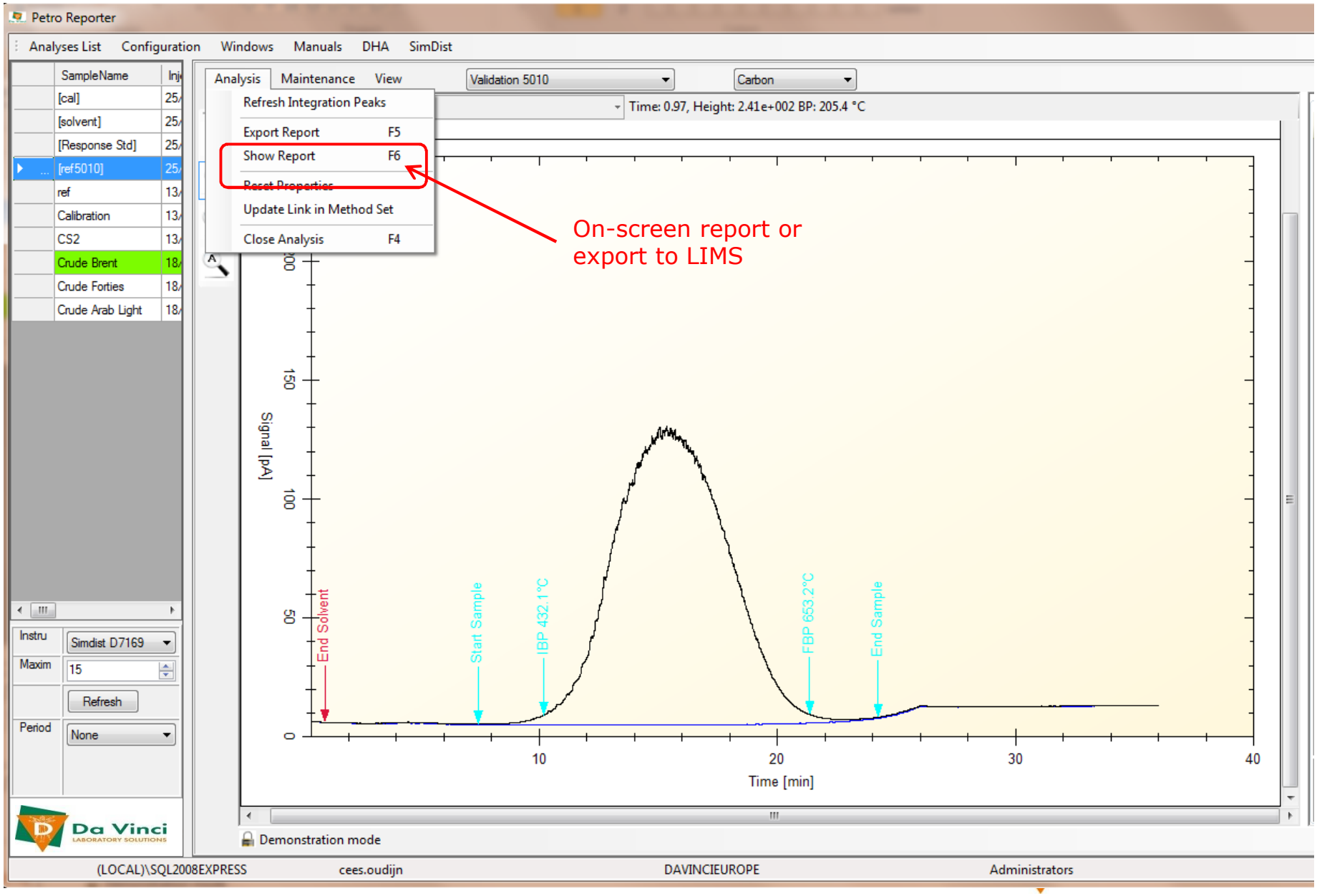


Export to LIMS properties

Customizable Correlation



Reporting


Petro Reporter
Analyses List
Configuration
Windows
Manuals
DHA
SimDist
SampleName
[cal]
[solvent]
[Response Std]
[ref5010]
ref
Calibration
CS2
Crude Brent
Crude Forties
Crude Arab Light
Analysis
Maintenance
View
Validation 5010
Carbon
Refresh Integration Peaks
Export Report F5
Show Report F6
Reset Properties
Update Link in Method Set
Close Analysis F4
Time: 0.97, Height: 2.41e+002 BP: 205.4 °C
On-screen report or
export to LIMS
Signal [pA]
Time [min]
End Solvent
Start Sample
IBP 432.1°C
FBP 653.2°C
End Sample
Instru
Simdist D7169
Maxim
15
Refresh
Period
None
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Demonstration mode
(LOCAL)\SQL2008EXPRESS
cees.oudijn
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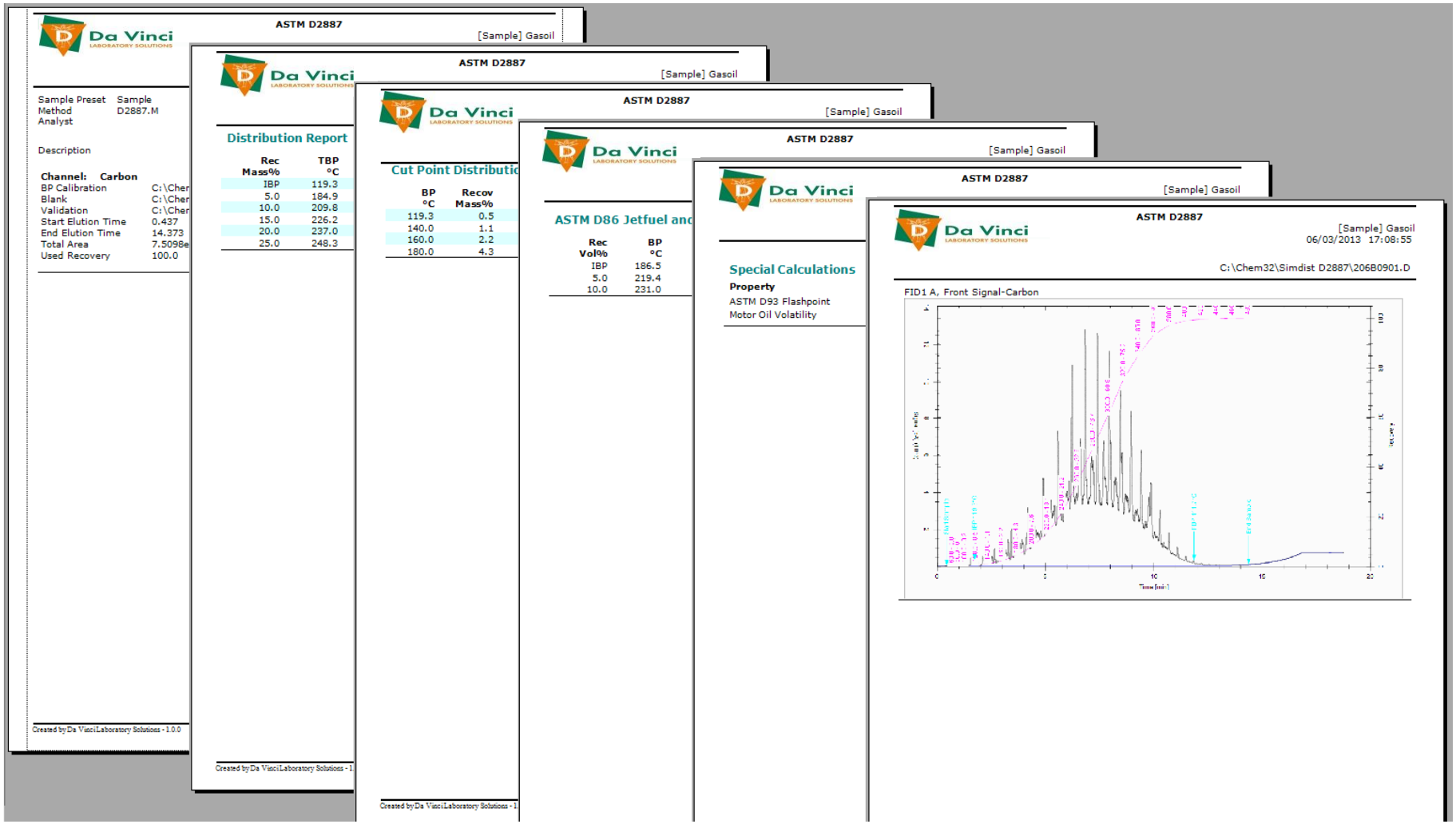
Administrators

Onscreen Reporting



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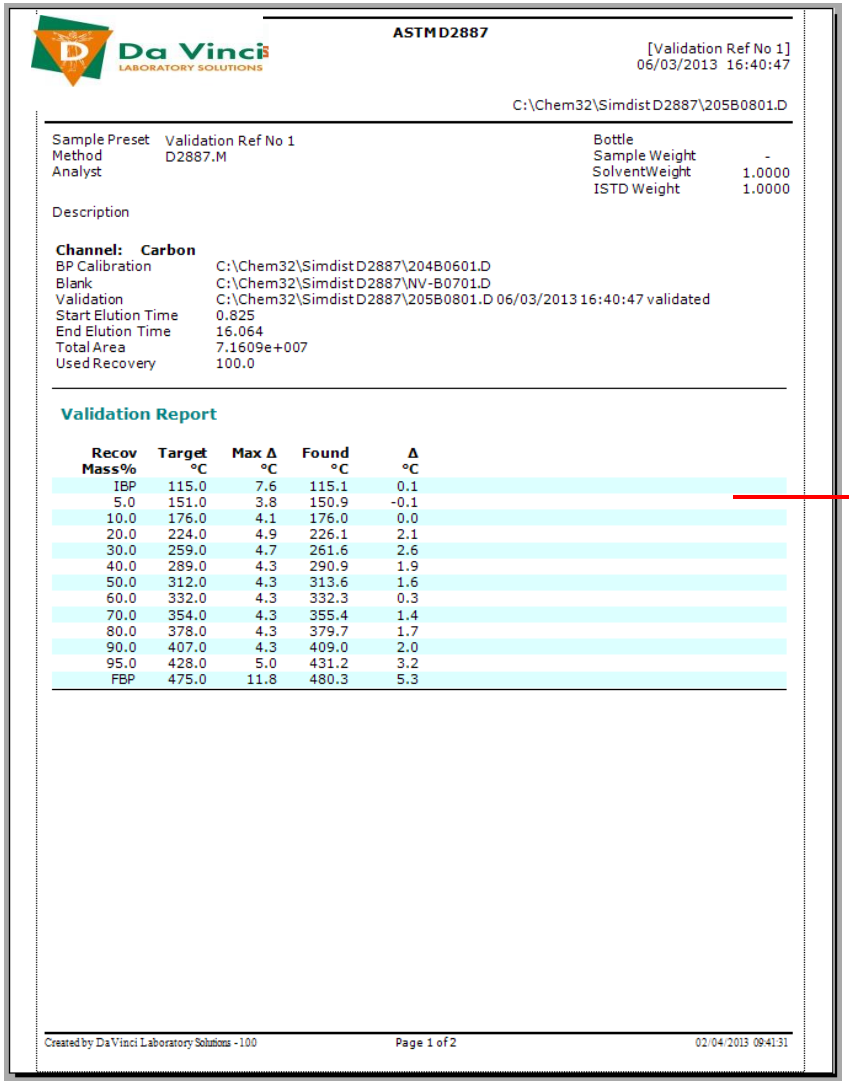
Validation Report



ASTM D2887

[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

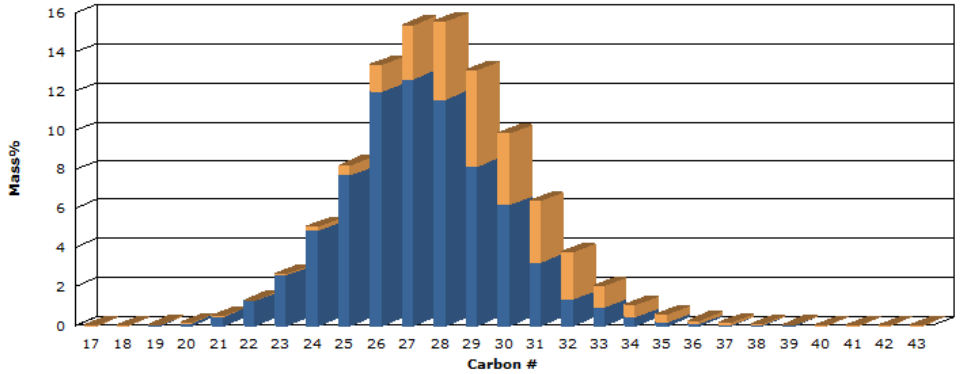
Recov Mass%	Target °C	Max Δ °C	Found °C	Δ °C
IBP	115.0	7.6	115.1	0.1
5.0	151.0	3.8	150.9	-0.1
10.0	176.0	4.1	176.0	0.0
20.0	224.0	4.9	226.1	2.1
30.0	259.0	4.7	261.6	2.6
40.0	289.0	4.3	290.9	1.9
50.0	312.0	4.3	313.6	1.6
60.0	332.0	4.3	332.3	0.3
70.0	354.0	4.3	355.4	1.4
80.0	378.0	4.3	379.7	1.7
90.0	407.0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

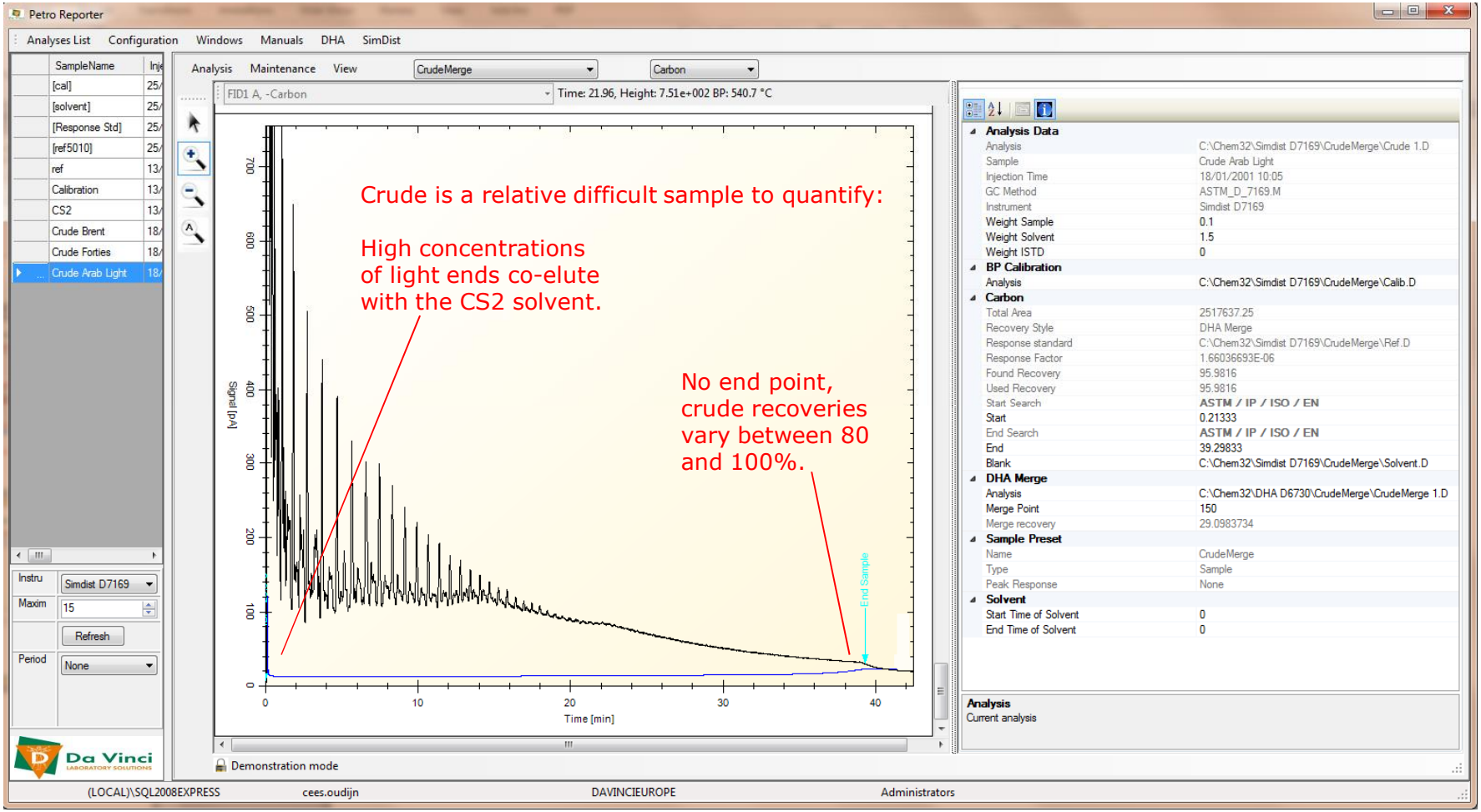
Wax Content Report (ASTM D5442)

Alkane Profile Report

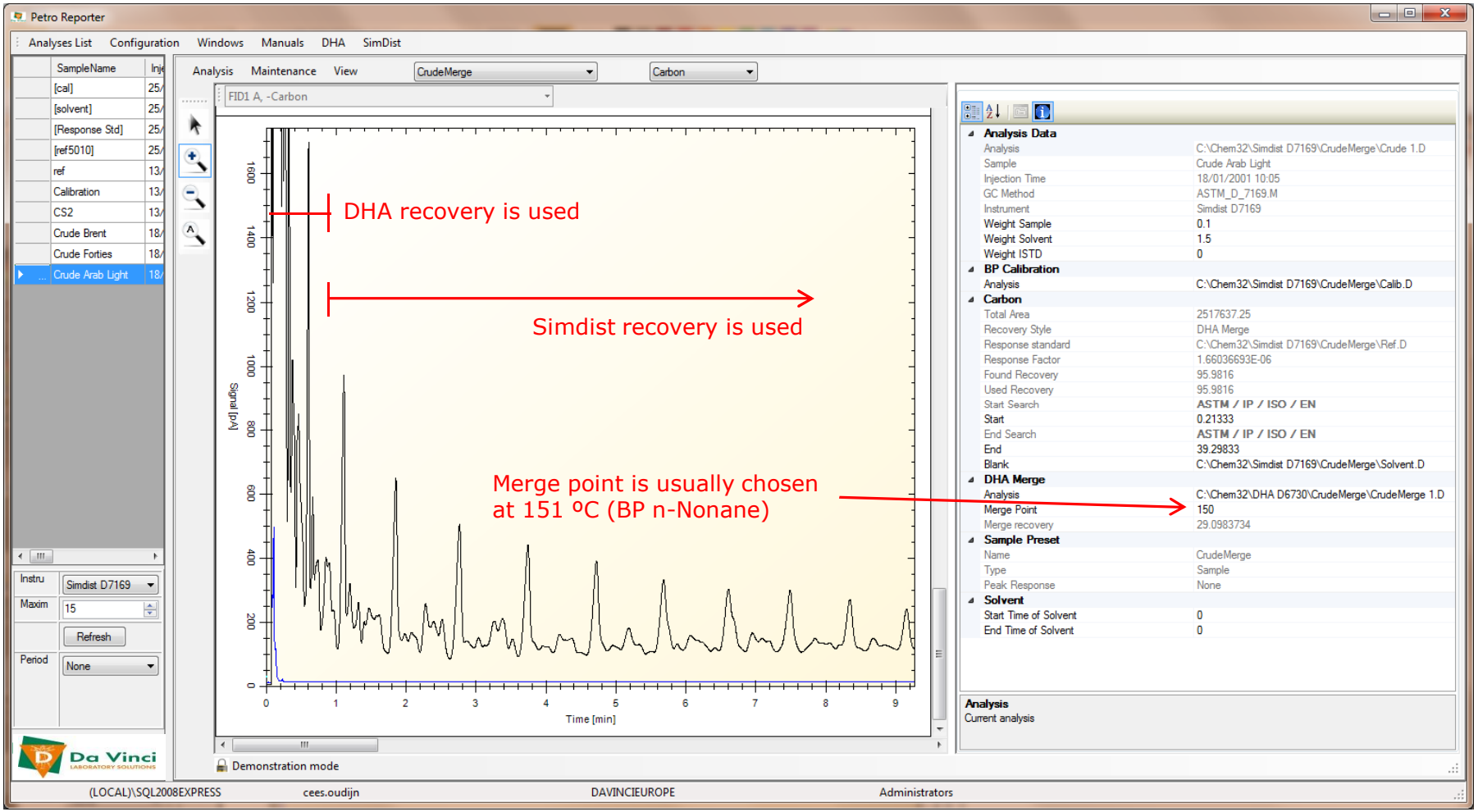


Carbon	Normals	Unknowns	Total
17	0.006	0.015	0.021
18	0.008	0.036	0.044
19	0.029	0.044	0.072
20	0.131	0.043	0.174
21	0.476	0.048	0.524
22	1.257	0.054	1.311
23	2.576	0.087	2.663
24	4.881	0.182	5.063
25	7.712	0.510	8.222
26	11.989	1.384	13.373
27	12.642	2.769	15.412
28	11.598	3.967	15.565
29	8.145	4.958	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
	74.010	**25,99**	**100,00**

SimDist Crude Calculations (1)



SimDist Crude Calculations (2)



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Crude SimDist - DHA merge report

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ASTM D7169

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

DHA true boiling point results

Rec Mass%	TBP °C	Rec Mass%	TBP °C	Rec Mass%	TBP °C	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 Application

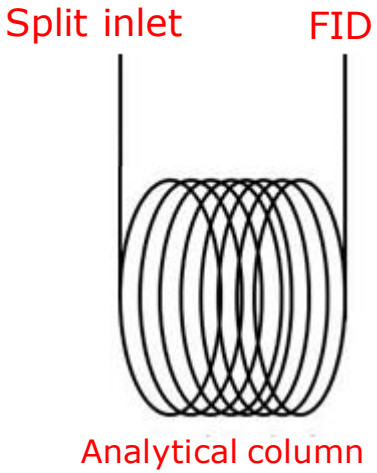
- Determines
  - Component identification up to tridecane
  - Component concentration (mass%, vol%, mol%)

- 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)

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

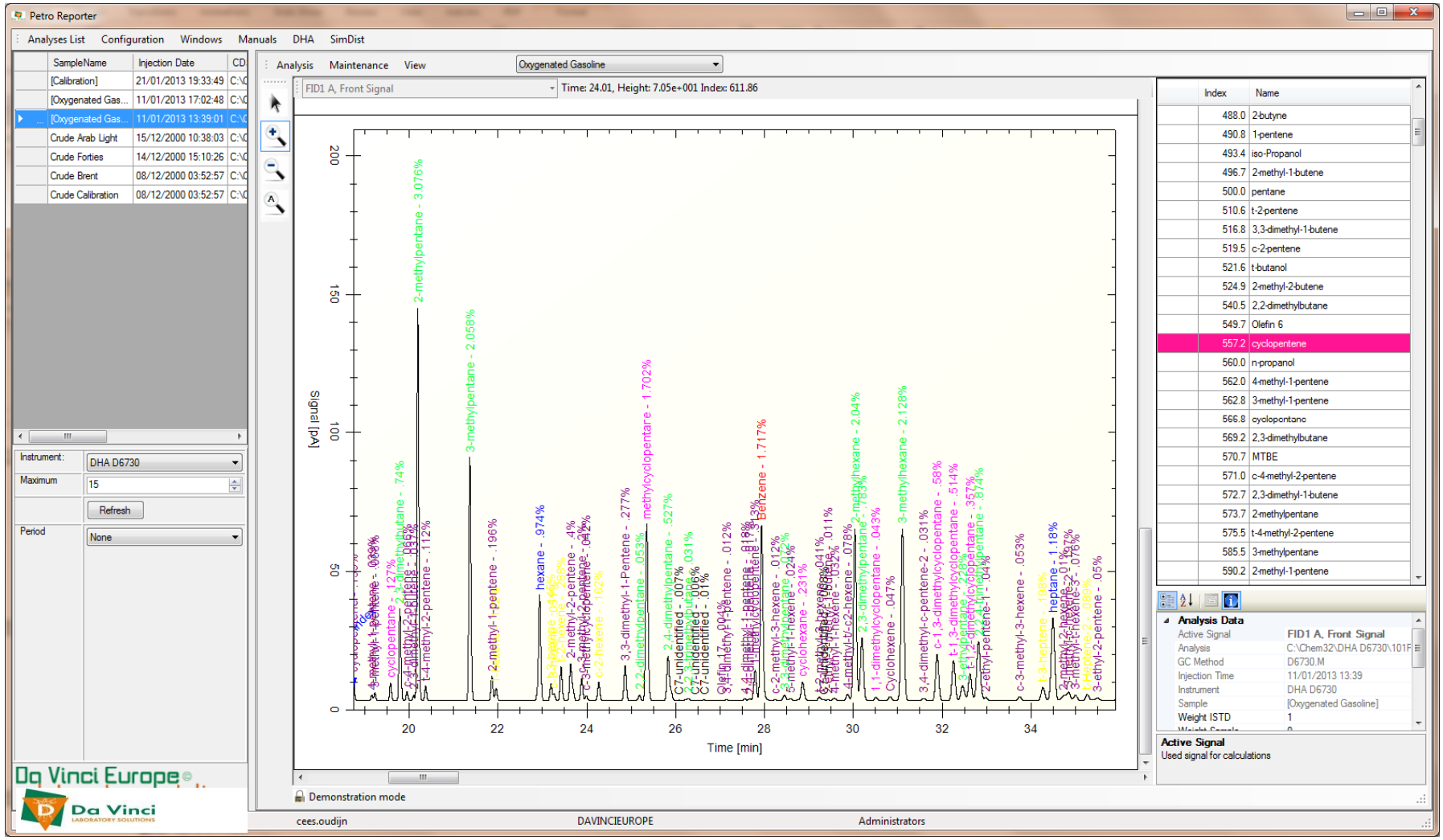
- RI unknown peak (*I*) calculated from:
  - Retention time unknown peak
  - Retention time n-paraffin eluting before and after unknown peak

- <u>RI unaffected in case of (small) retention time shifts</u>

- 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	isoPentane	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

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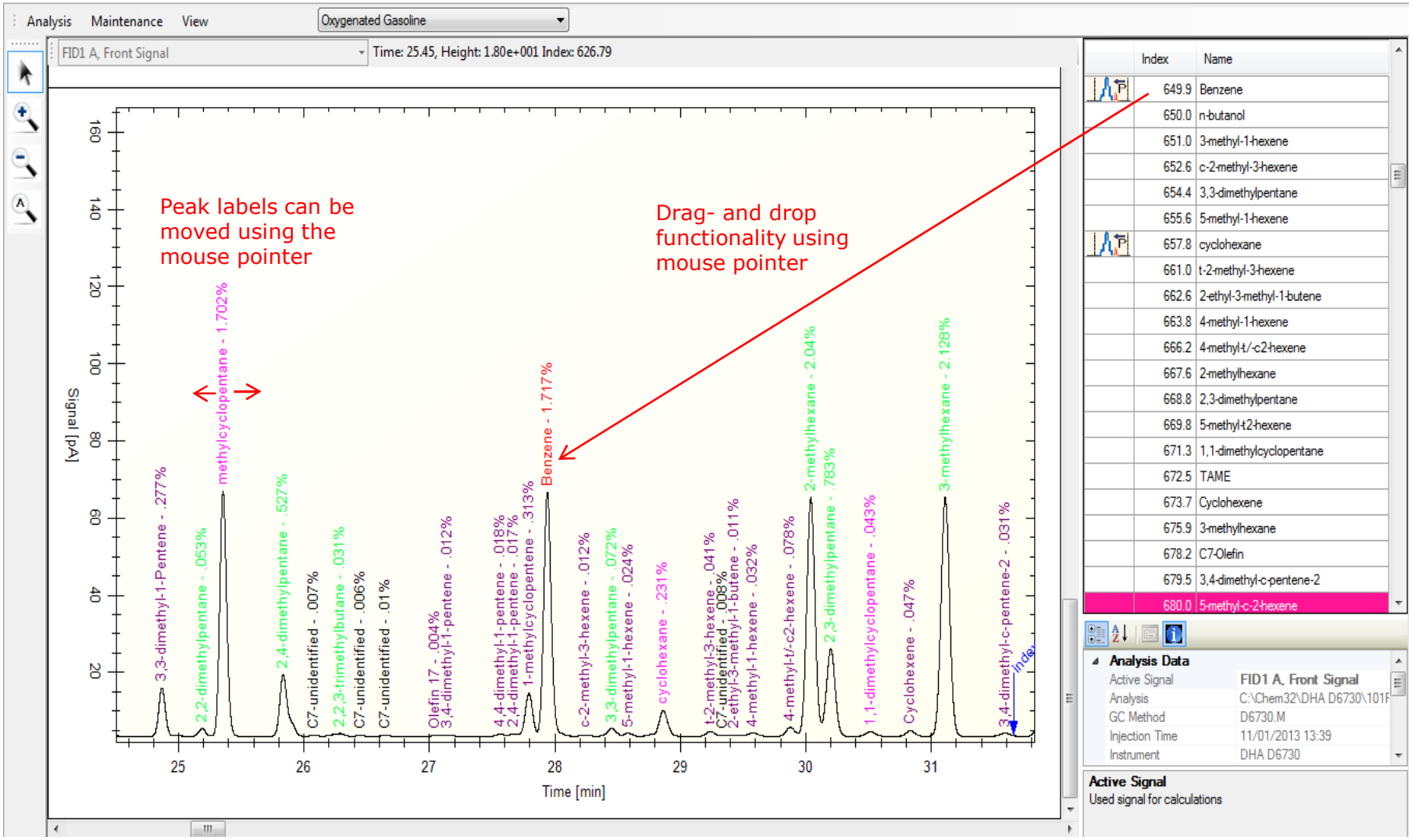
DHA Sample Details



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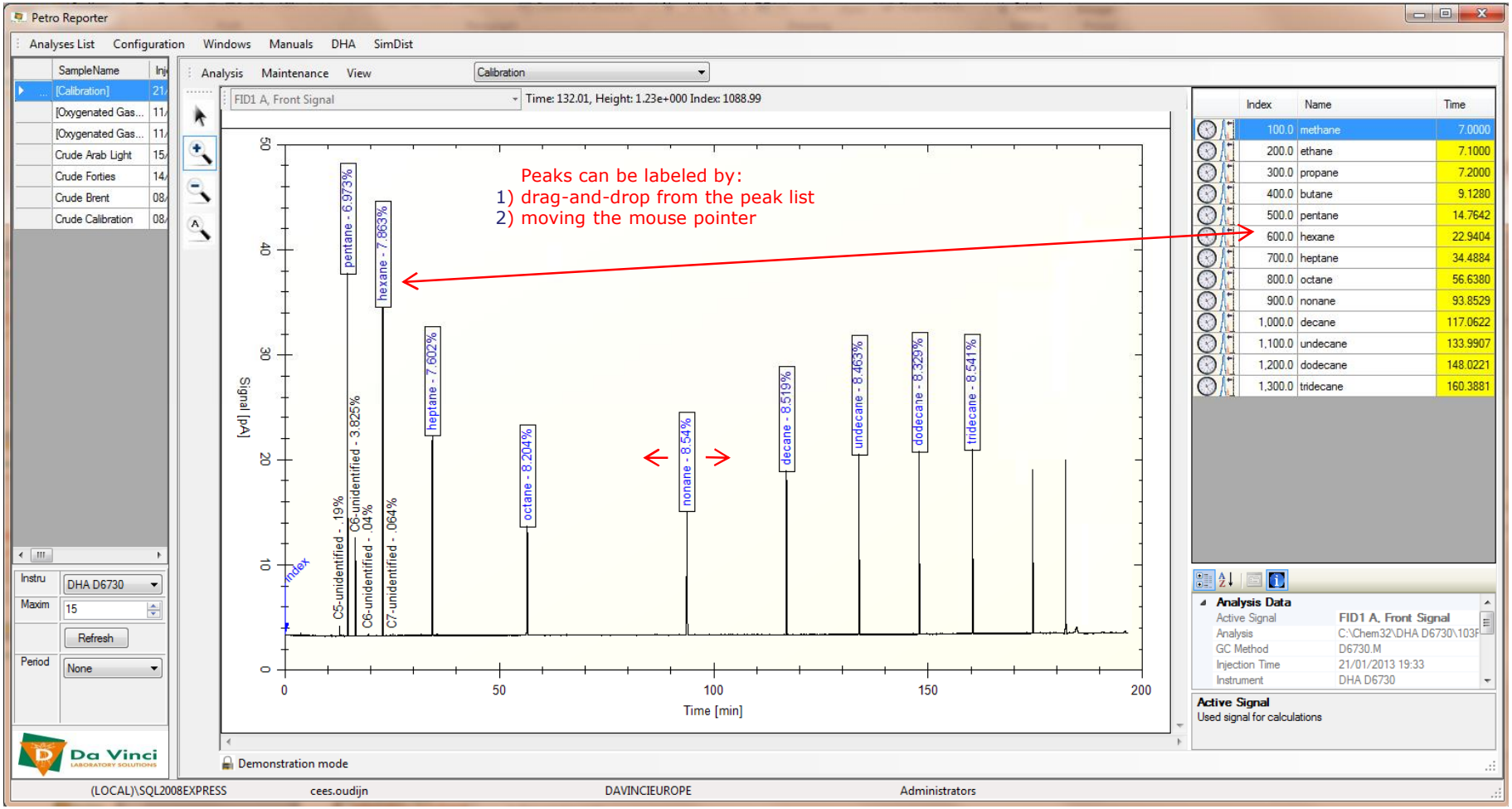
DHA Calibration



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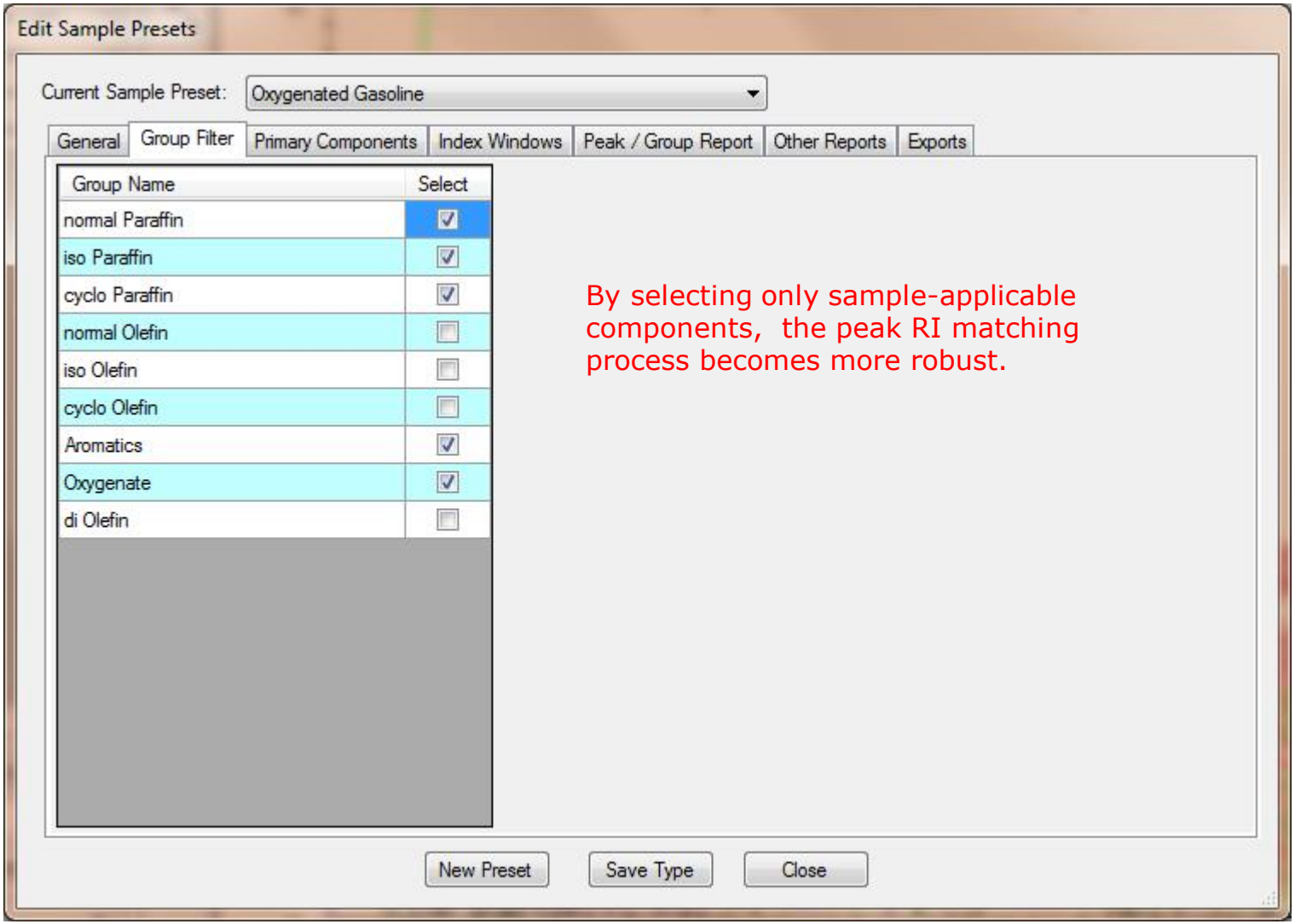
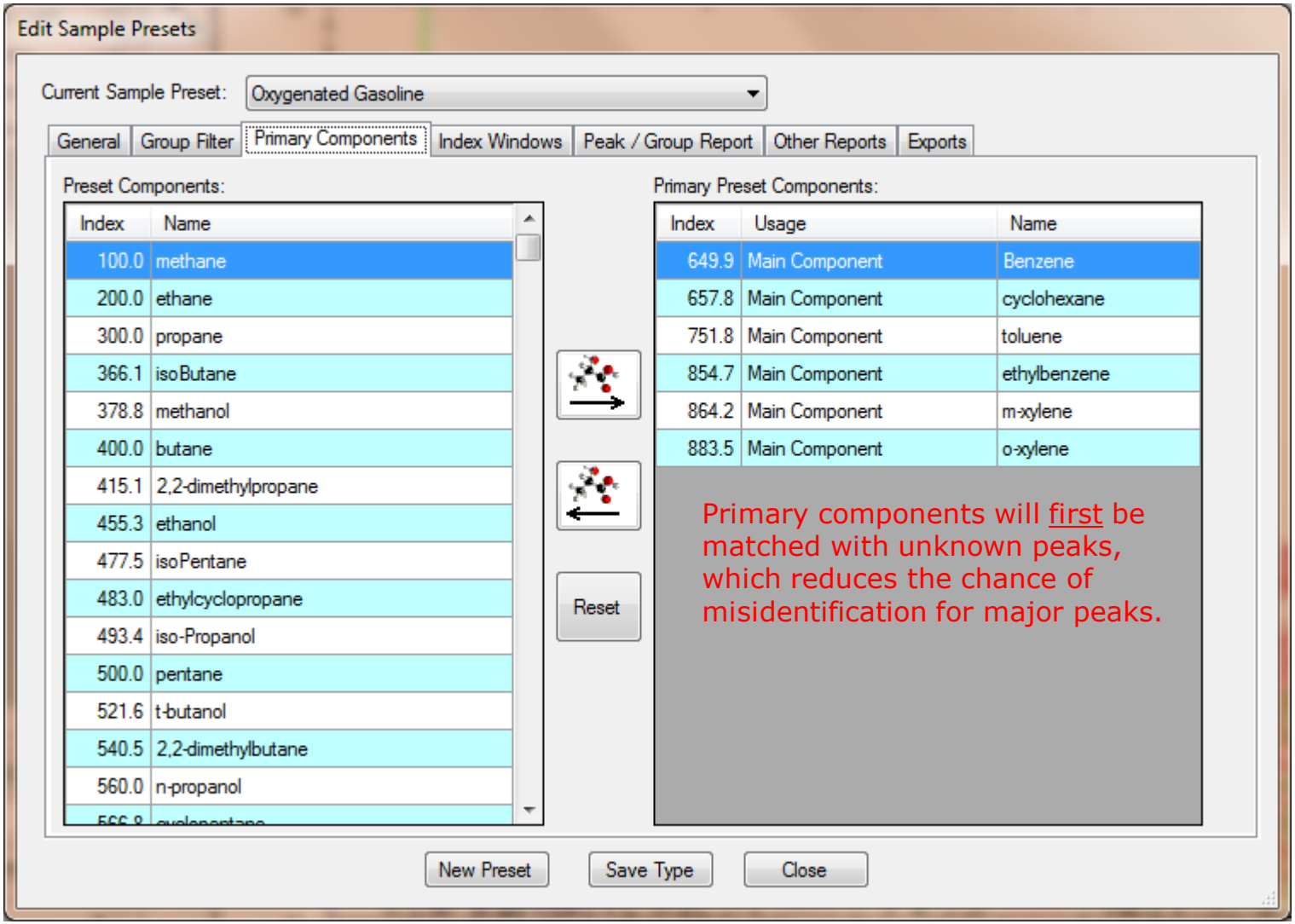
DHA Sample Preset Editor (1)



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

DHA Sample Preset Editor (2)



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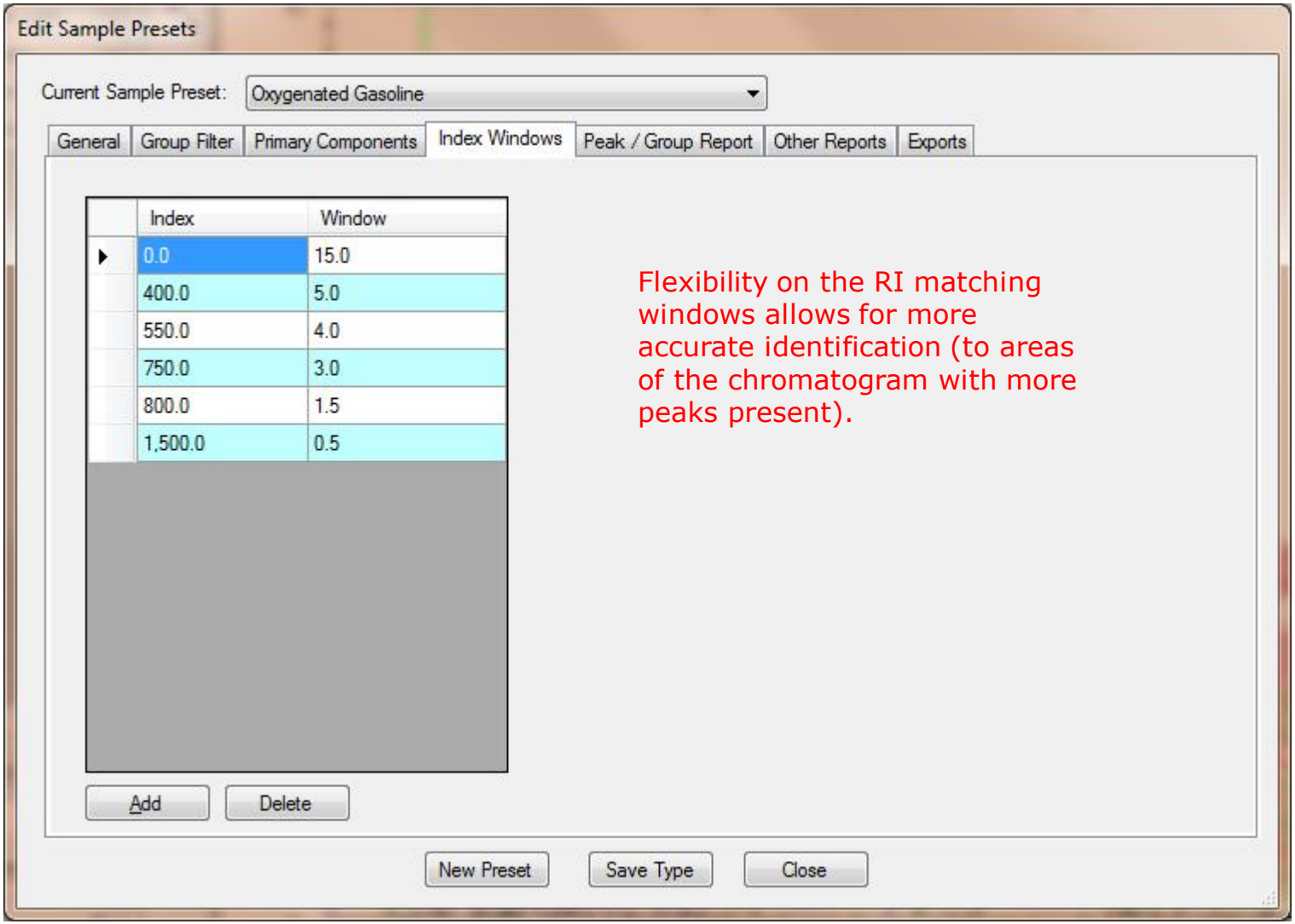
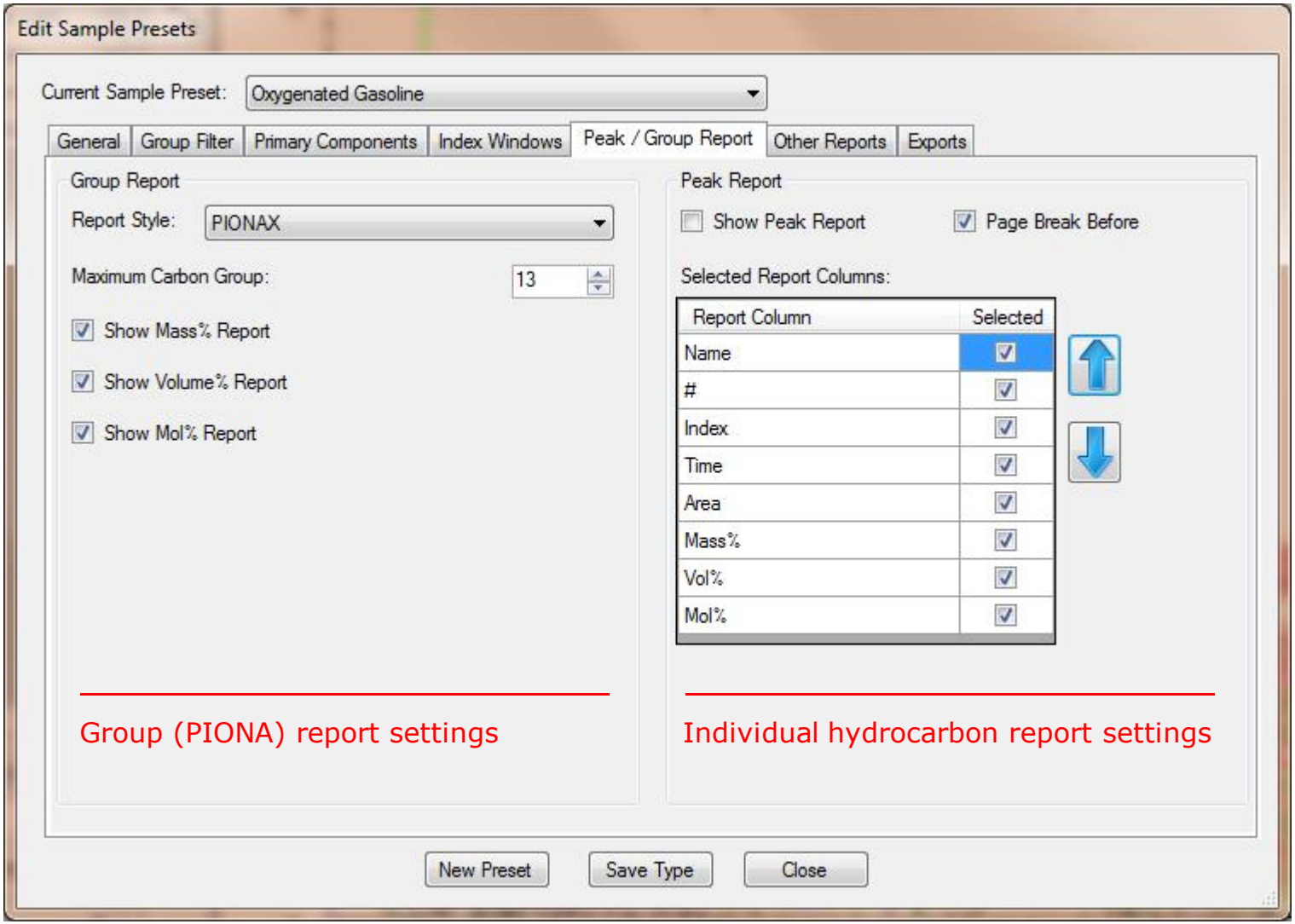
DHA Sample Preset Editor (3)



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

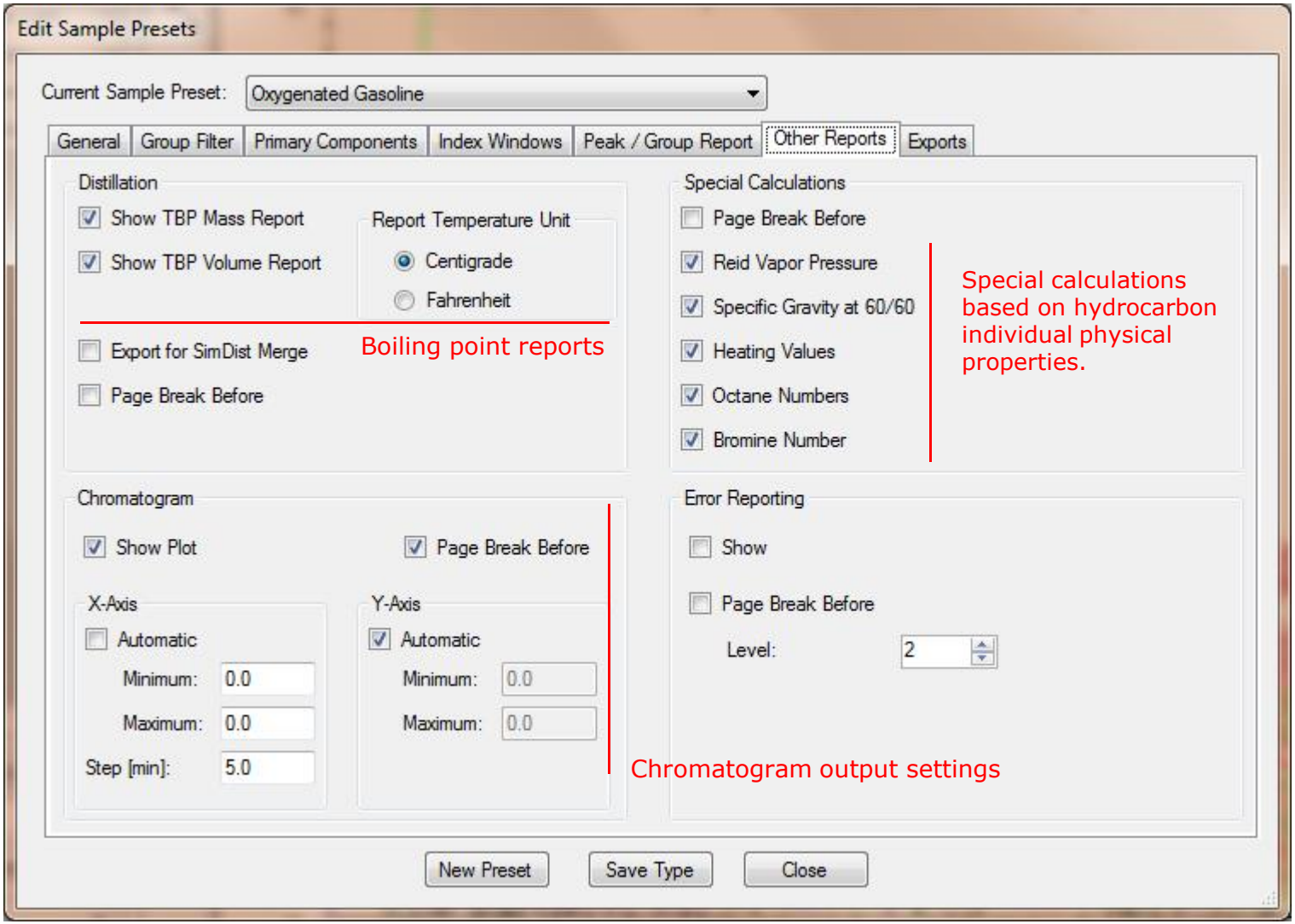
DHA Sample Preset Editor (4)



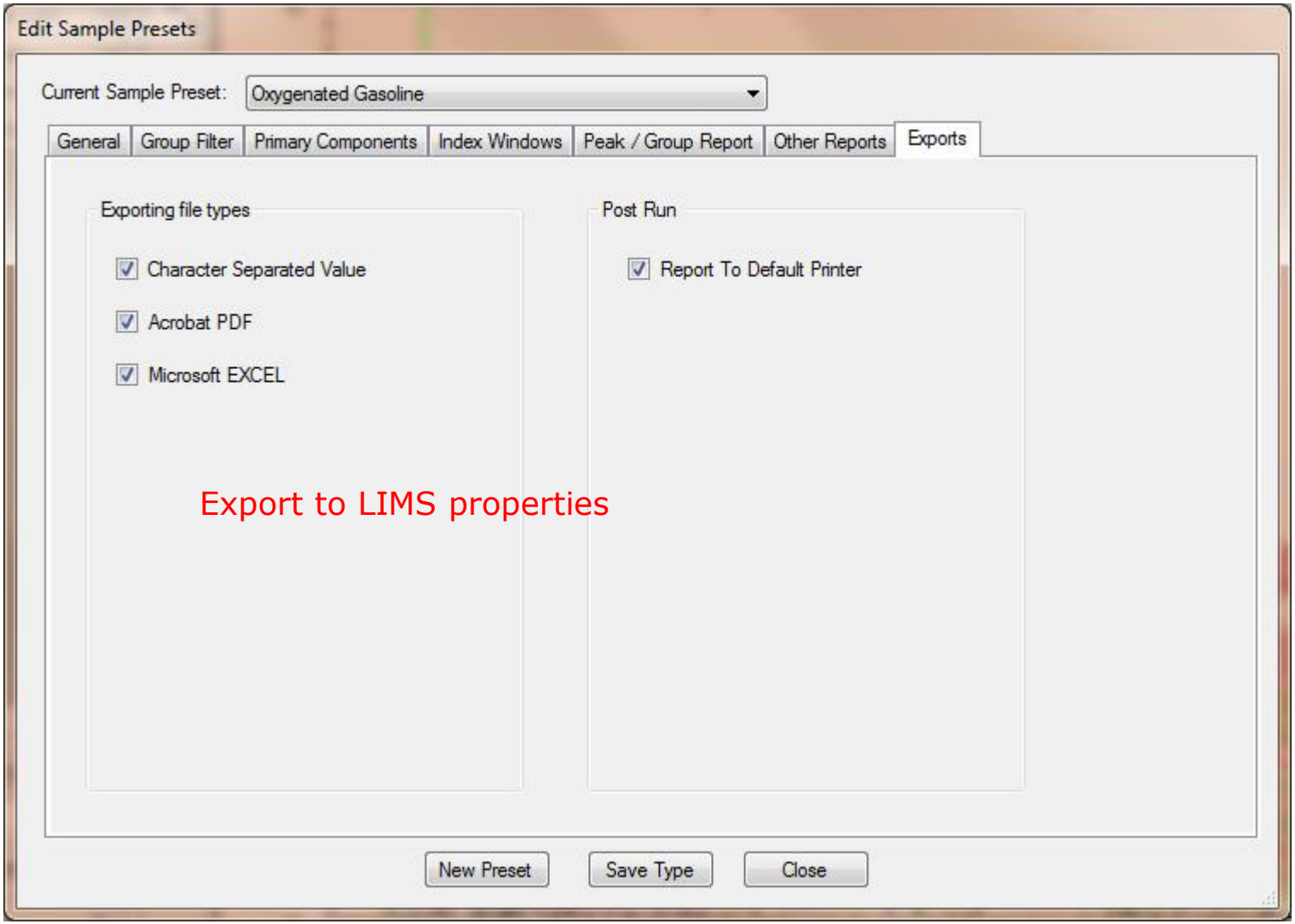
Group (PIONA) report settings

Individual hydrocarbon report settings

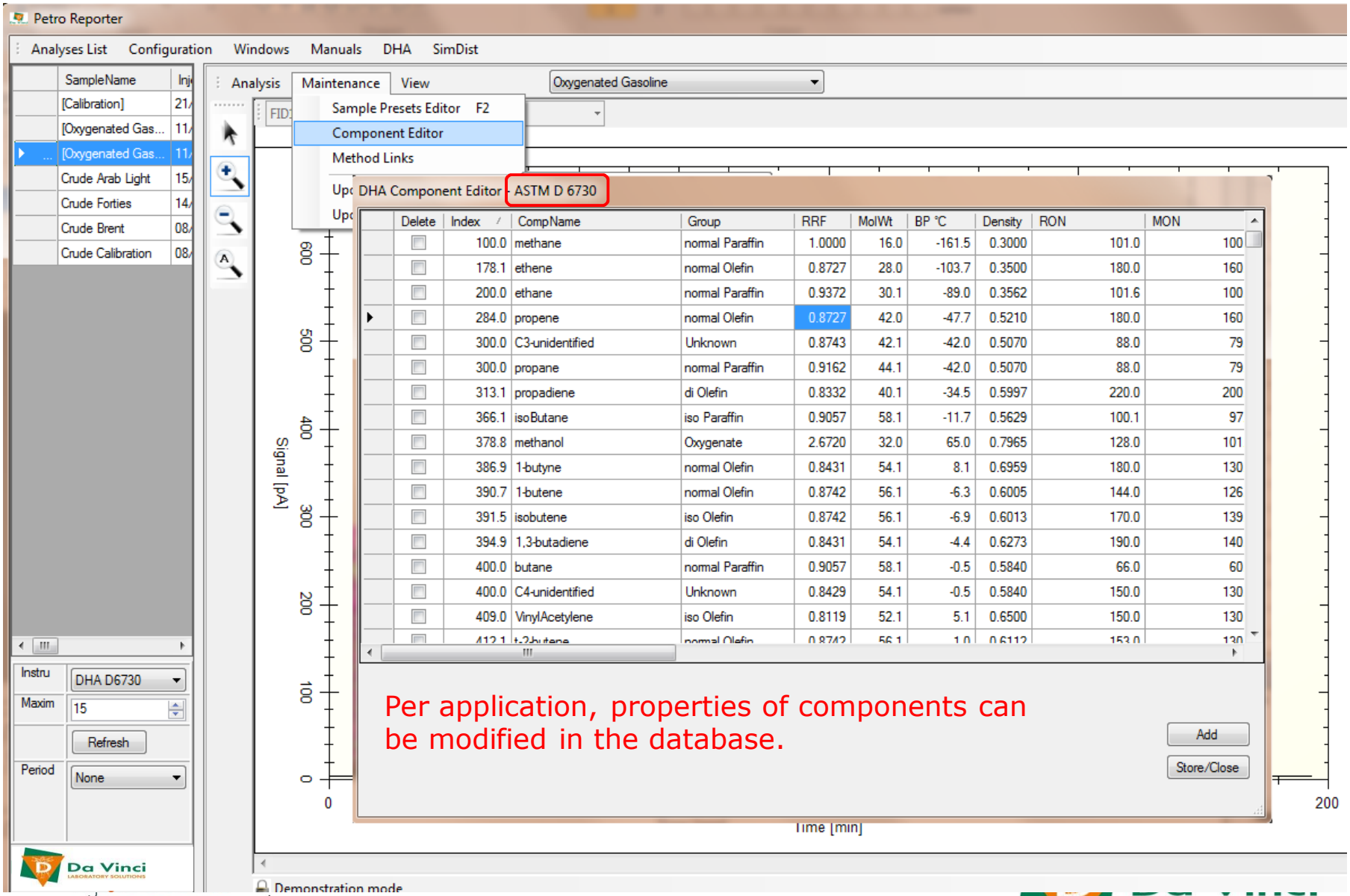
DHA Sample Preset Editor (5)



DHA Sample Preset Editor (6)



Component Database Editor



Onscreen reporting

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

C:\Chem32\1\DATA\20130104_GCB_D6730-7\102F0201.D

Sample Preset	Oxygenated Gasoline	Bottle	
Method	D6730.M	Sample Weight	-
Analyst		ISTD Weight	1.0000
Description			
Calibration	C:\Chem32\1\		

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

Group Report in Volume%

	n-Par	i-Par
C2	0.00	0.00
C3	0.01	0.00
C4	1.79	0.14
C5	1.04	11.75
C6	1.03	6.16
C7	1.22	6.01
C8	0.90	5.45
C9	0.30	2.53
C10	0.11	0.69
C11	0.04	0.20
C12	0.03	0.19
C13	0.03	0.01
Total	6.48	33.14

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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	1.691E+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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Boiling Point Distribution Report

Perc	TBP (mass) [°C]	TBP (vol) [°C]	Perc
IBP	-8.7	-9.6	34.0
1.0	-4.9	-6.7	35.0
2.0	20.3	-0.7	36.0
3.0	21.1	20.6	37.0
4.0	21.9	21.2	38.0
5.0	22.7	21.9	39.0
6.0	23.5	22.6	40.0
7.0	24.3	23.2	41.0
8.0	25.1	23.9	42.0
9.0	25.9	24.6	43.0
10.0	26.7	25.2	44.0
11.0	27.5	25.9	45.0
12.0	30.8	26.6	46.0
13.0	36.1	27.2	47.0
14.0	36.6	28.8	48.0
15.0	43.9	34.8	49.0
16.0	58.0	36.2	50.0
17.0	59.1	36.7	51.0
18.0	59.7	44.0	52.0
19.0	60.5	57.9	53.0
20.0	62.6	59.0	54.0
21.0	63.3	59.5	55.0
22.0	68.2	60.0	56.0
23.0	68.7	62.2	57.0
24.0	70.4	62.8	58.0
25.0	70.5	65.8	59.0
26.0	70.5	68.3	60.0
27.0	70.6	68.7	61.0
28.0	70.6	70.4	62.0
29.0	70.7	70.5	63.0
30.0	70.7	70.5	64.0
31.0	70.8	70.6	65.0
32.0	70.8	70.6	66.0
33.0	70.9	70.7	67.0

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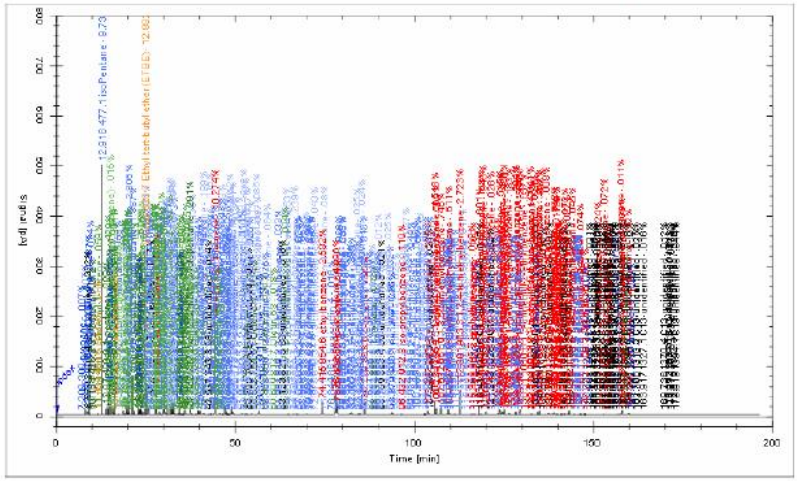
Calculations

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



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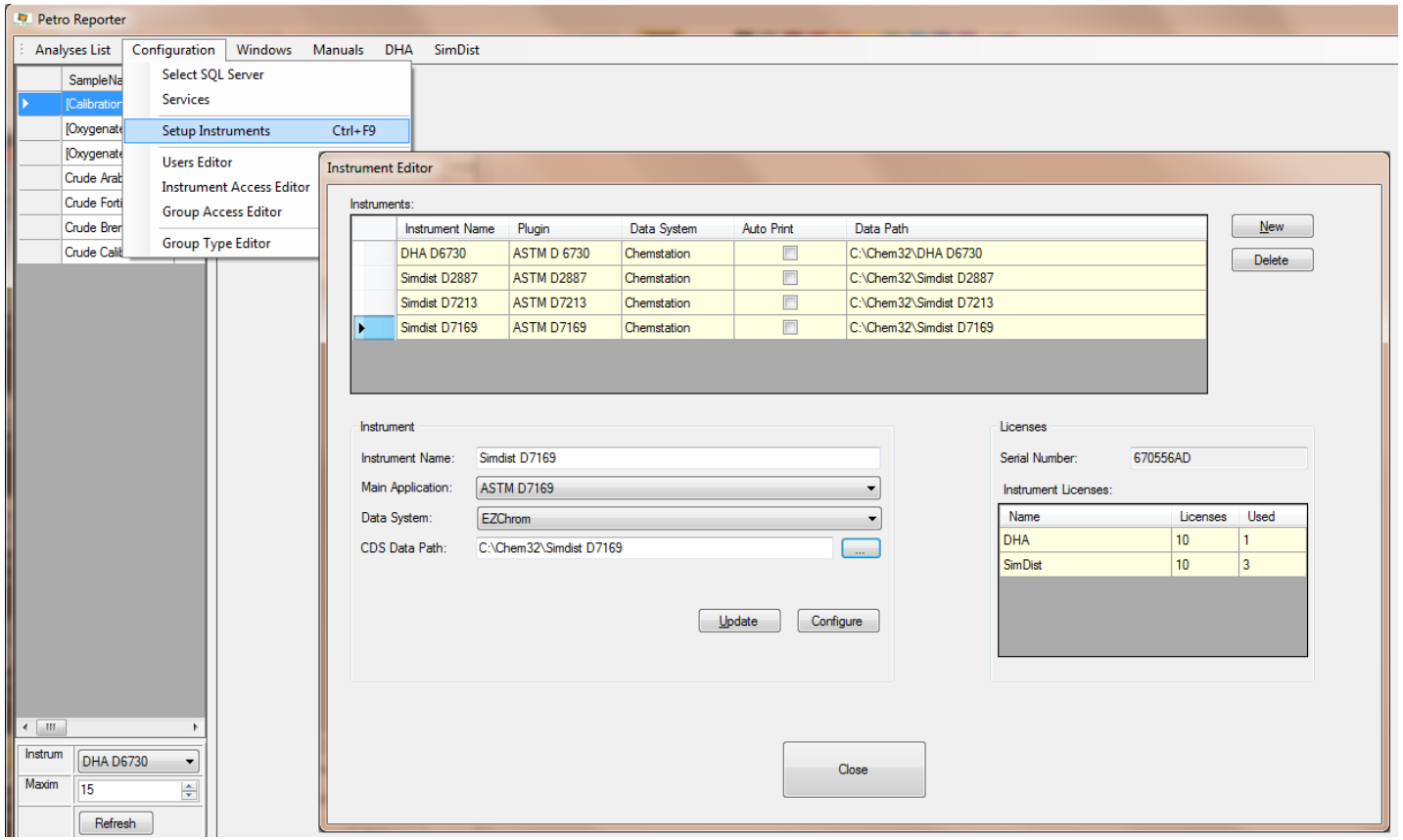
Easy Setup and Configuration

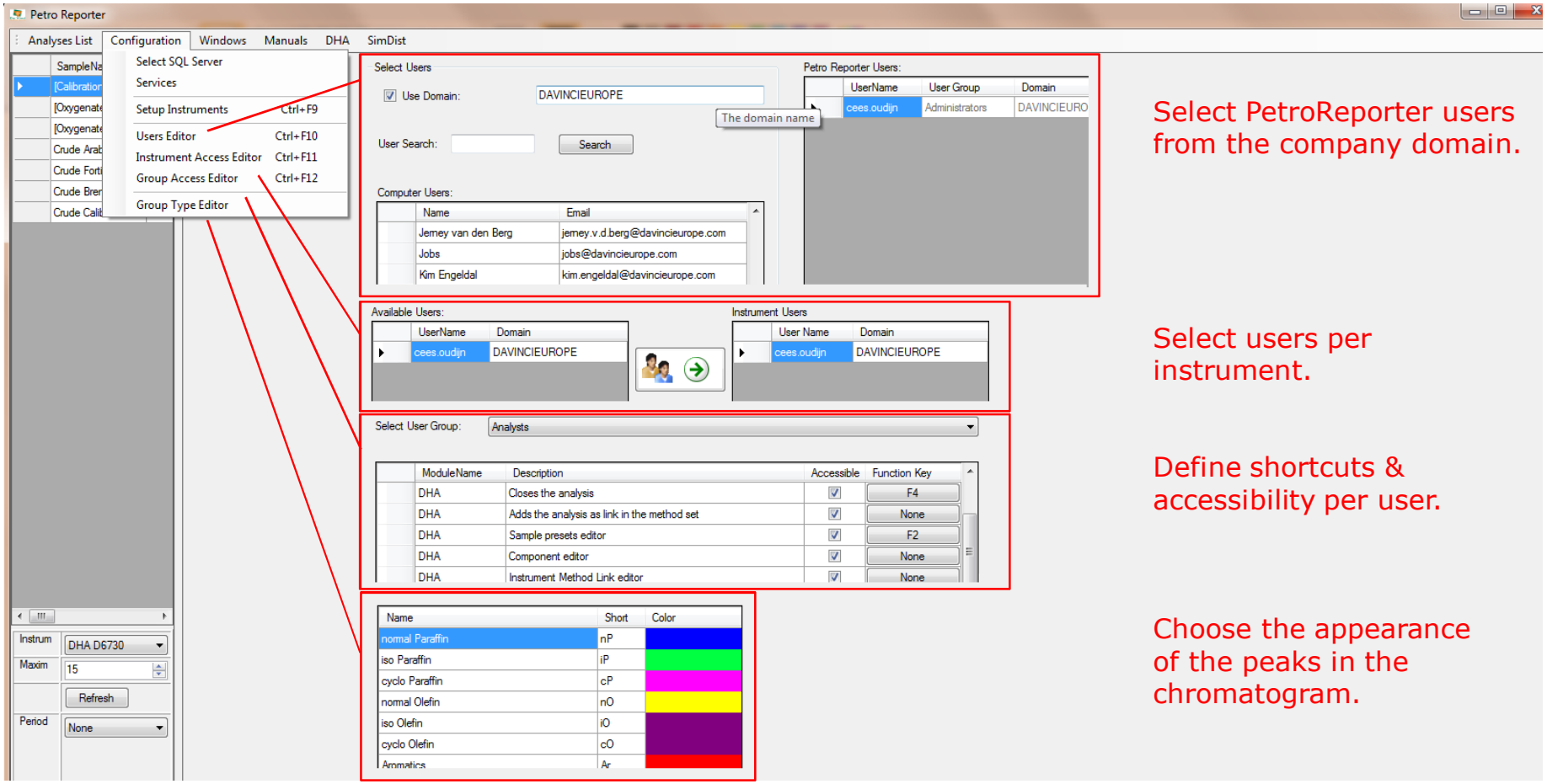


In this screen all instruments are created and configured.

Part of the configuration is the application and CDS selection.

It also shows the number of licenses available.

Optional Other Configuration Features



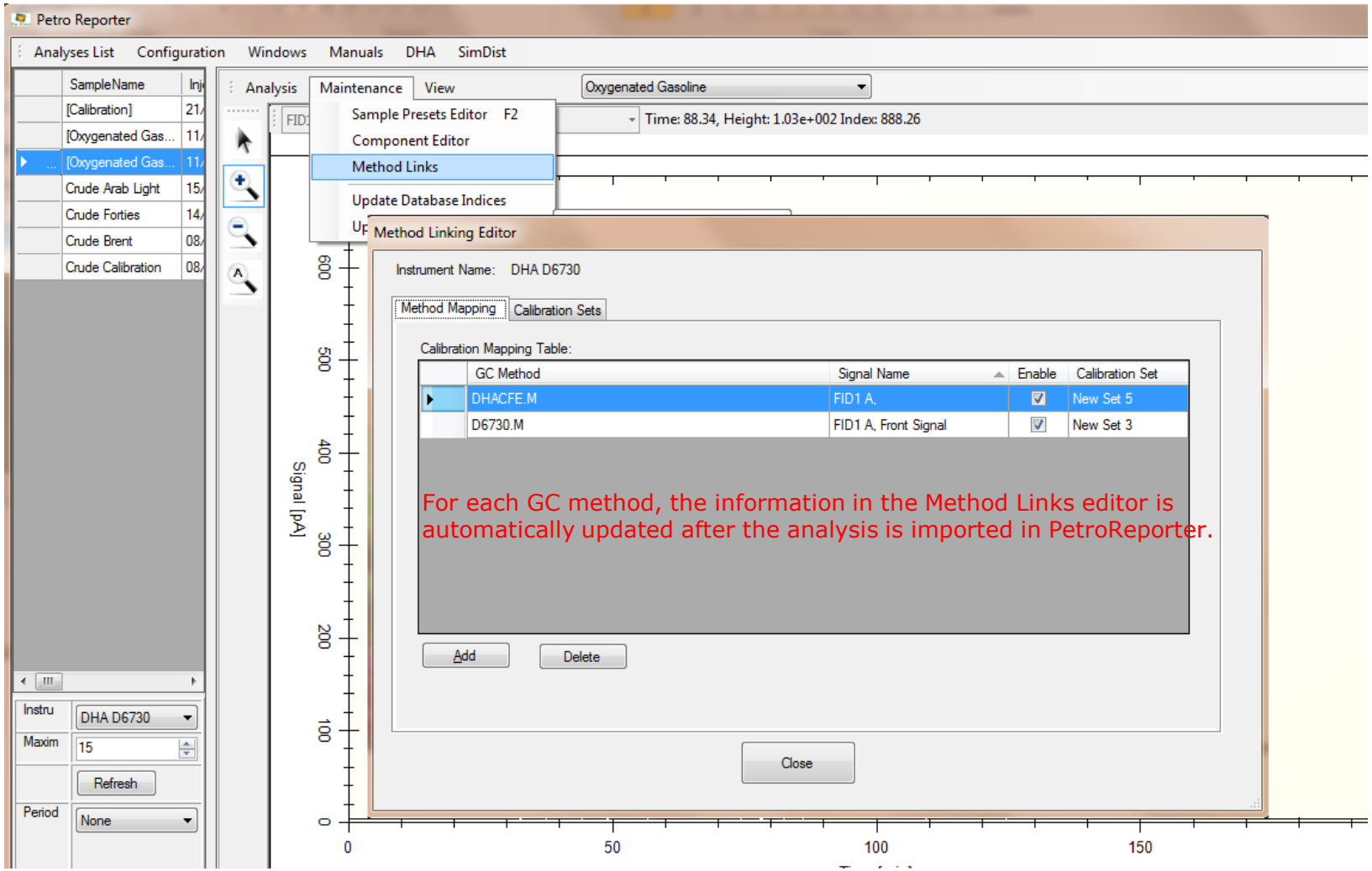
Select PetroReporter users from the company domain.

Select users per instrument.

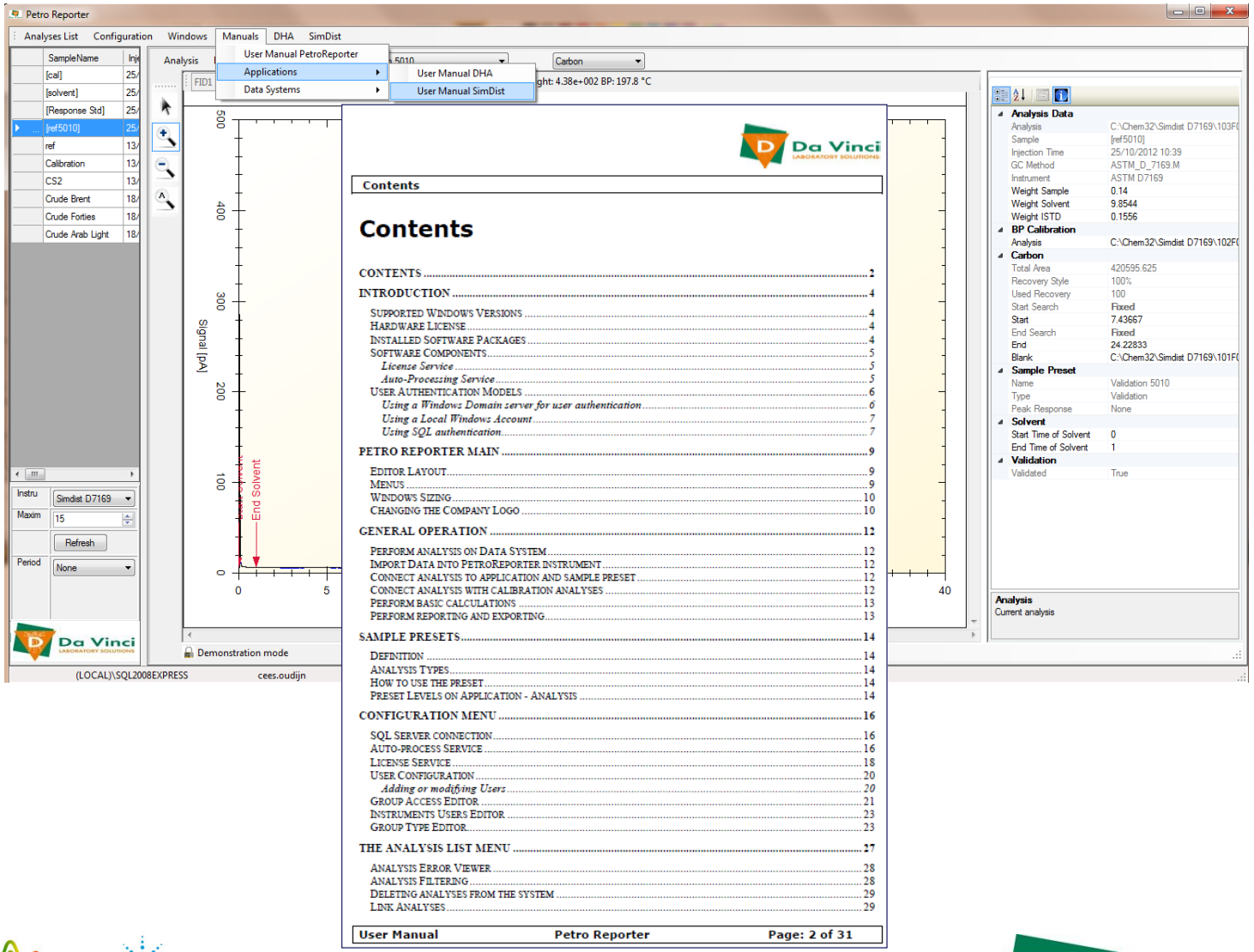
Define shortcuts & accessibility per user.

Choose the appearance of the peaks in the chromatogram.

Active Signal Storage



Manuals Available Inside PetroReporter



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