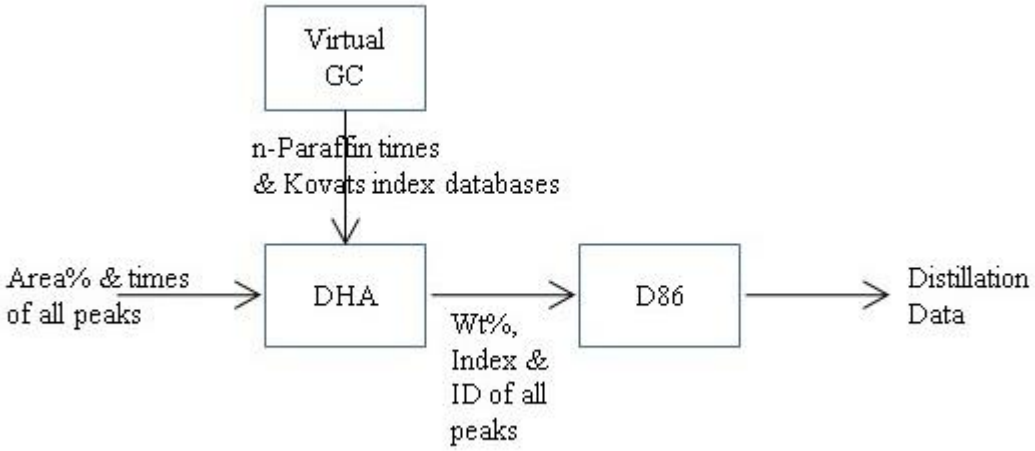
Quick Reference Guide

DHAtoD86 1.1.6

www.StillPeaks.com

StillPeaks DHAtoD86 software consists of 3 apps that read peak integrator data from Chromatographic Data Systems (CDS) and calculate a D86 report of your sample:



Virtual GC is a computer model of a Dimethylsilicone coated capillary gas chromatographic column. Kovats index databases and n-Paraffin retention times are calculated from GC configuration input and an isothermal Kovats index database. The GC configuration should match the actual GC configuration. Column aging is accounted for with film thickness. Copy the Virtual GC window to your lab journal.

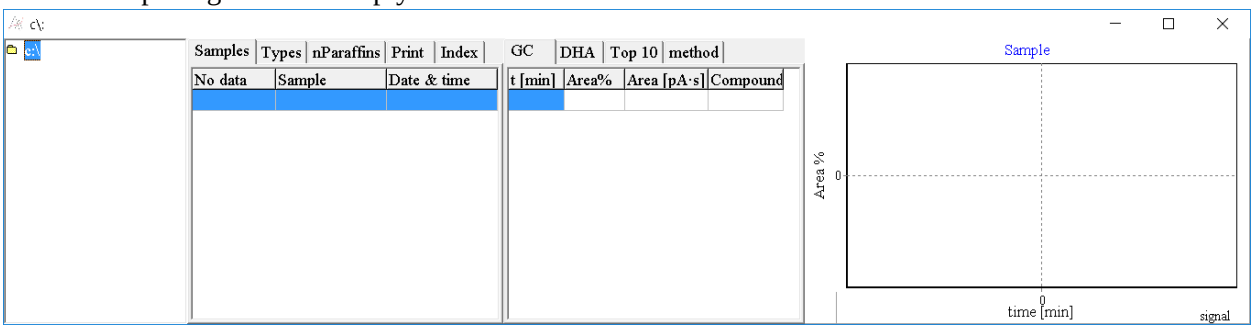
DHA Detailed Hydrocarbon Analysis software reads the GC integration file. Peaks are identified by shortlist, pattern and Kovats index database. From DHA, Virtual GC and D86 can be started.

D86 The Fugacity-Film model uses the DHA output of the sample to calculate the distillation curve of the sample. The D86 report is shown on screen and written to the sample folder. To keep the same numbers, you can enter D86 distillation data and offsets are calculated. D86 set points and off sets are managed per sample type.

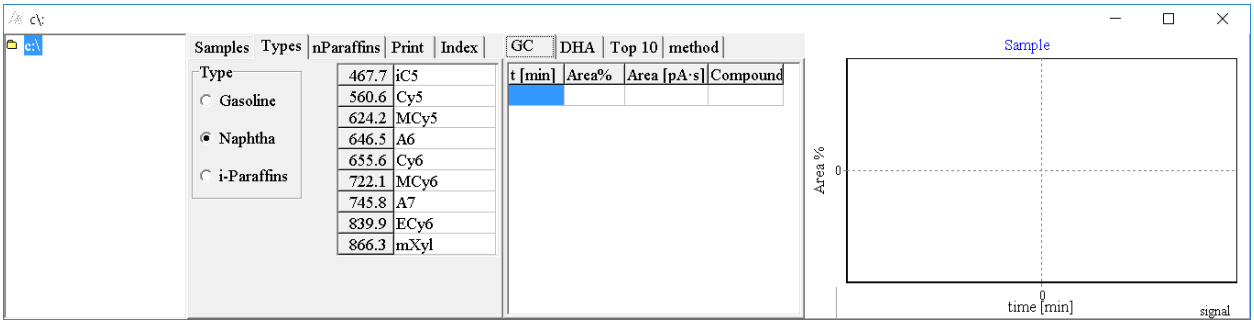
Content

1.DHA Detailed Hydrocarbon Analysis

The DHA opening screen is empty:

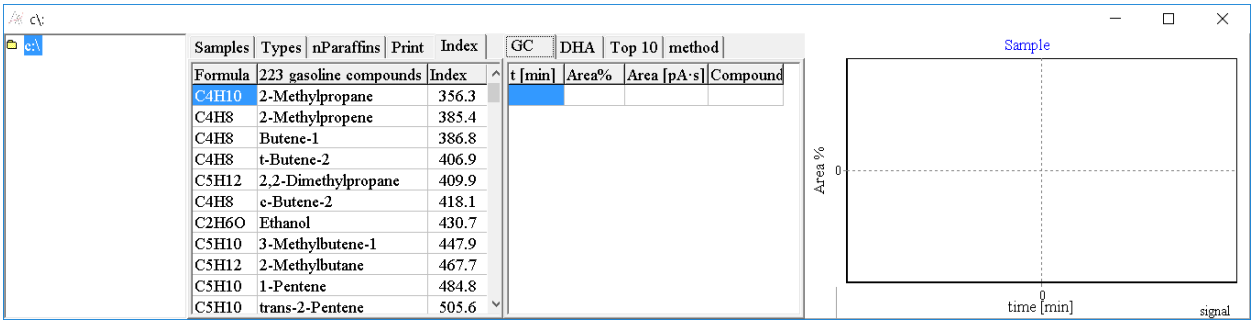


The Types tabsheet allows you to select your sample type. The typical shortlist of big peaks is displayed:



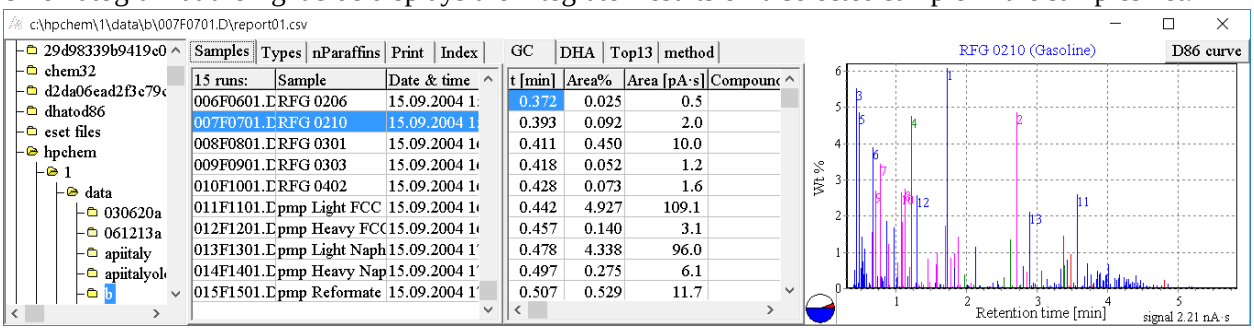
Use *i*-Paraffins for Alkylates and Isomerates.

Sample type selection also changes the Kovats index database for peak identification:



The Kovats index database does not contain the *n*-Paraffins (indices follow from carbon number I=100c).

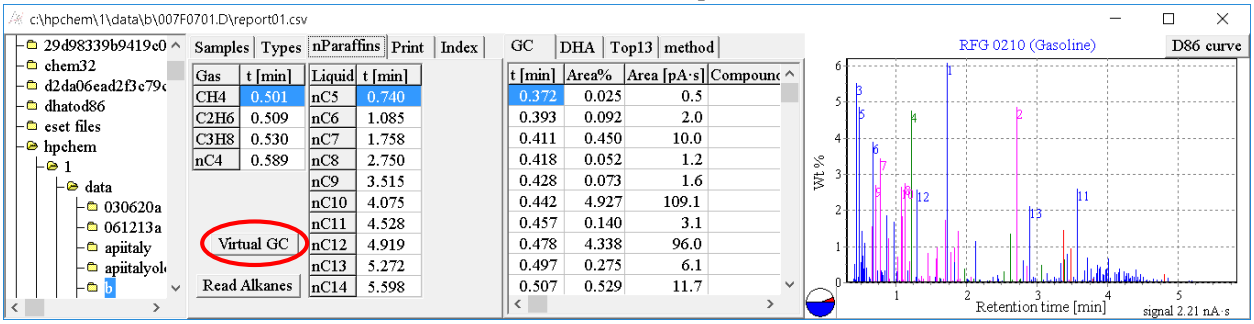
Use directory tree at the left side to select your ChemStation or OpenLab analysis sequence. The chromatogram at the right side displays the integrator results of a selected sample in the samples list:



The white slice of the small circle at the left bottom of the chromatogram indicates almost 50% of the sample peaks are not identified.

2.Virtual GC: *n*-Paraffin Times & Kovats Index

Click the nParaffins tab sheet of the left hand side tab lineup:



n-Paraffin retention times are displayed, along with a Virtual GC button and a Read Alkanes button.

The right side tab sheet lineup shows the measured GC peak times and peak Area of sample RFG 0210 located in the path displayed in the window title. The peak identity result is shown in the 4th column.

The measured first peak time in the GC table is before CH4 time, hence the n-paraffin times needs to be adjusted. Please lookup the GC method used to acquire the GC data. The Virtual GC button enables you to adjust the methane time at 35°C to the 0.35 minute setpoint:

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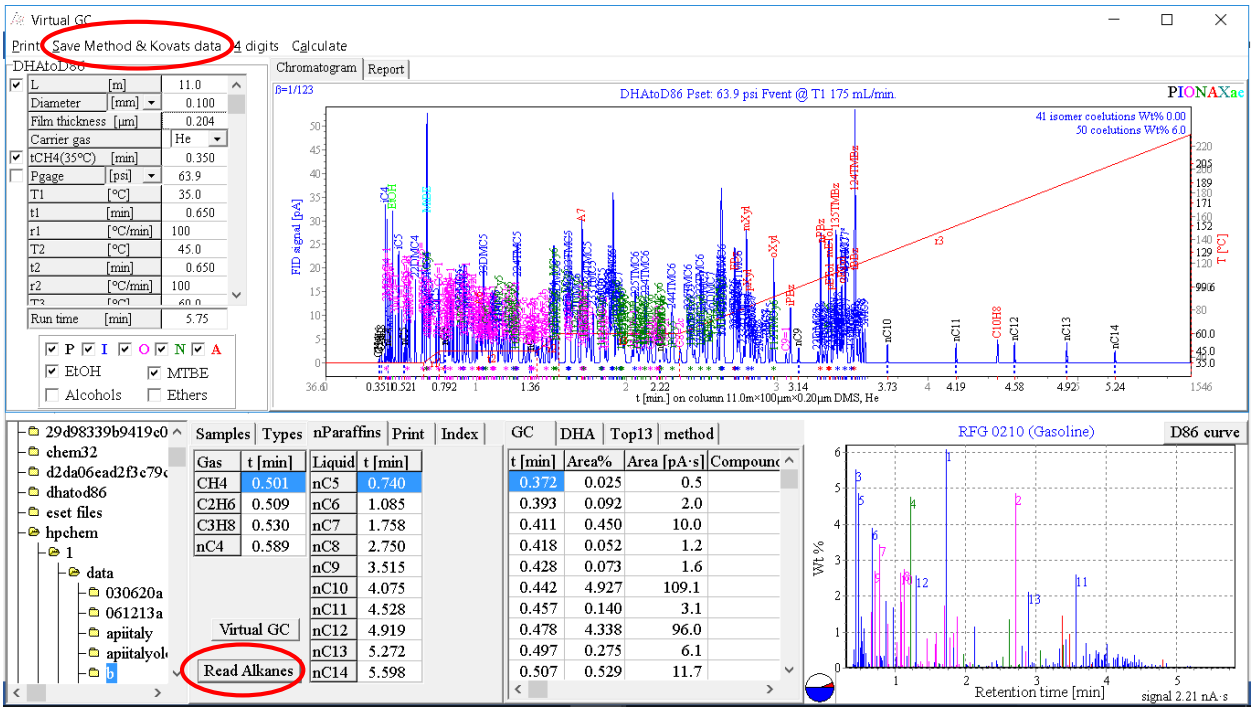
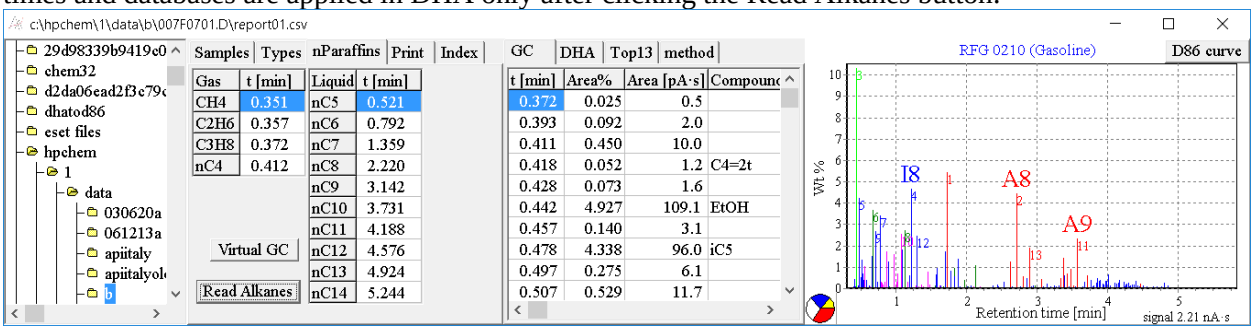
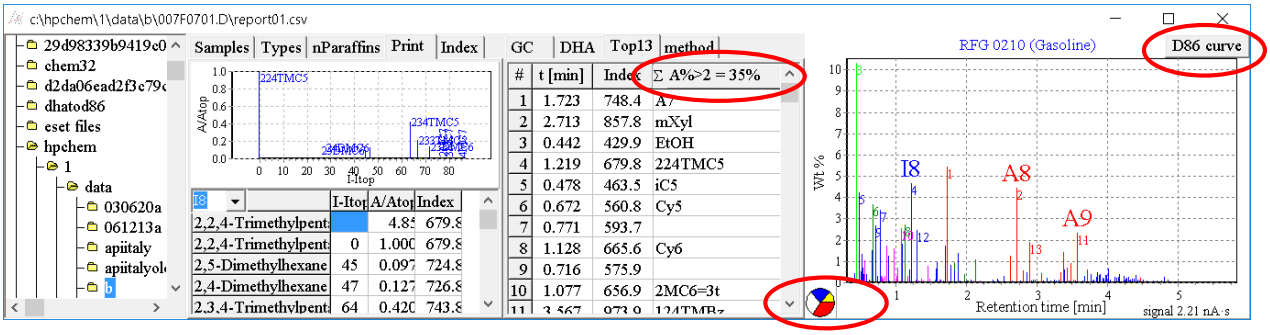


Select the Save Method & Kovats index data menu option of Virtual GC. Times and databases are filed. Select the Print option of the Virtual GC menu to keep track of the n-Paraffin calculations. The n-Paraffin times and databases are applied in DHA only after clicking the Read Alkanes button:



3.DHA Peak Identification

The Peak ID pie chart has a red part for the big peaks, a yellow part for the pattern recognition, a blue part for the small peaks with Kovats index and a white part for the unidentified peaks. In this sample 13 peaks have Area% > 2, corresponding 35% red part of the pie chart:

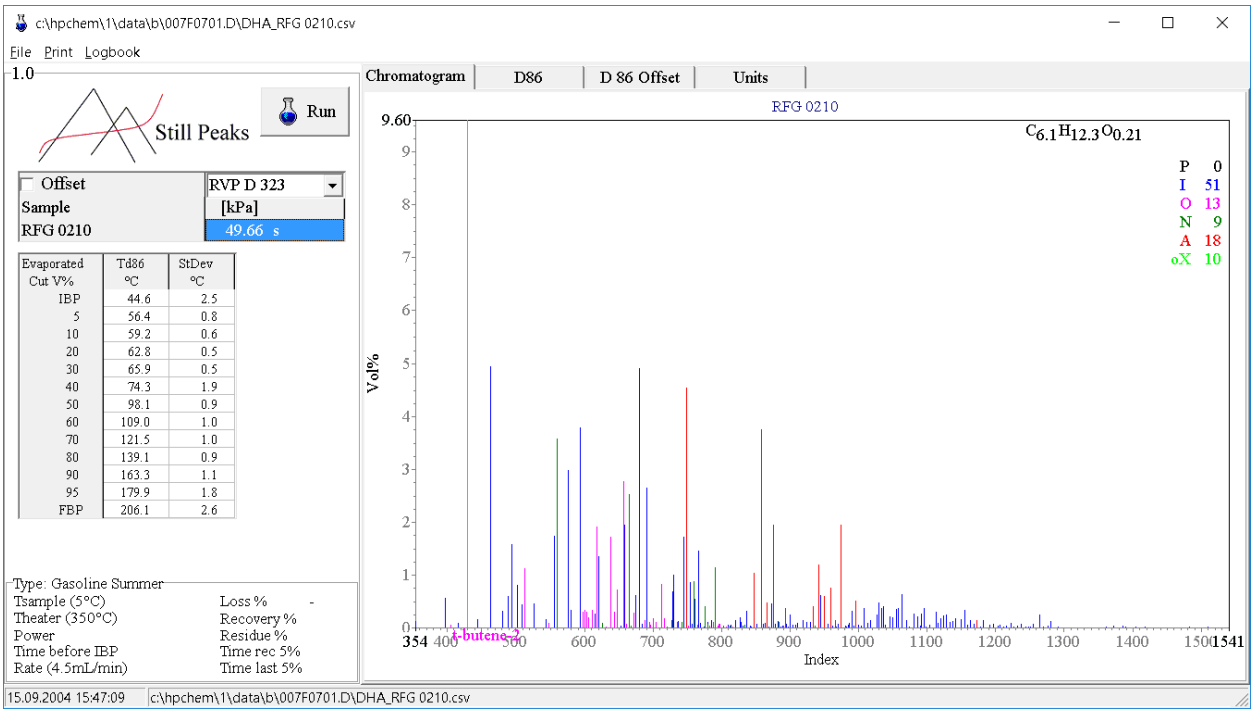


The left hand tab sheet Print is selected, where the hard coded I8 pattern is selected. This pattern is recognized in this sample and marked with I8. The yellow part of the ID pie indicates that about 20% of the peaks in this sample are identified by peak recognition of the Iso-octanes (I8), Xylenes and Ethylbenzene (A8, A9).

☞NOTE The D86 curve button appears only if less than 50% of the peaks is unknown.

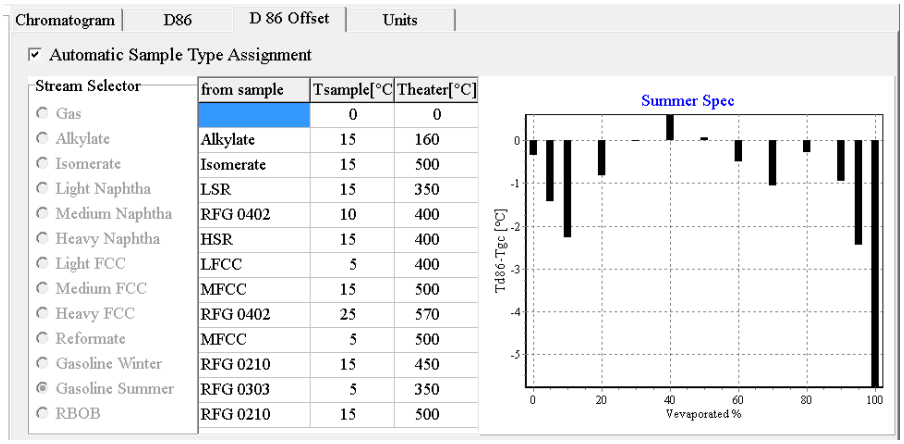
4.D86 Sample Type Setpoints

Clicking the D86 button opens the D86 page, showing the sample and available D86 data:



Evaporated Cut V%	Td86 °C	StDev °C
IBP	44.6	2.5
5	56.4	0.8
10	59.2	0.6
20	62.8	0.5
30	65.9	0.5
40	74.3	1.9
50	98.1	0.9
60	109.0	1.0
70	121.5	1.0
80	139.1	0.9
90	163.3	1.1
95	179.9	1.8
FBP	206.1	2.6

The sample has been recognized as Summer Spec gasoline and the ASTM D86 cross check data are displayed at the left side. The setpoints and offsets for this summer gasoline are found in the D 86 Offset tabsheet:



Stream Selector	from sample	Tsample[°C]	Theater[°C]
Gas		0	0
Alkylate	Alkylate	15	160
Isomerate	Isomerate	15	500
Light Naphtha	LSR	15	350
Medium Naphtha	RFG 0402	10	400
Heavy Naphtha	HSR	15	400
Light FCC	LFCC	5	400
Medium FCC	MFCC	15	500
Heavy FCC	RFG 0402	25	570
Reformate	MFCC	5	500
Gasoline Winter	RFG 0210	15	450
Gasoline Summer	RFG 0303	5	350
RBOB	RFG 0210	15	500

ASTA can be switched off by unchecking the Automatic Sample Type Assignment checkbox:

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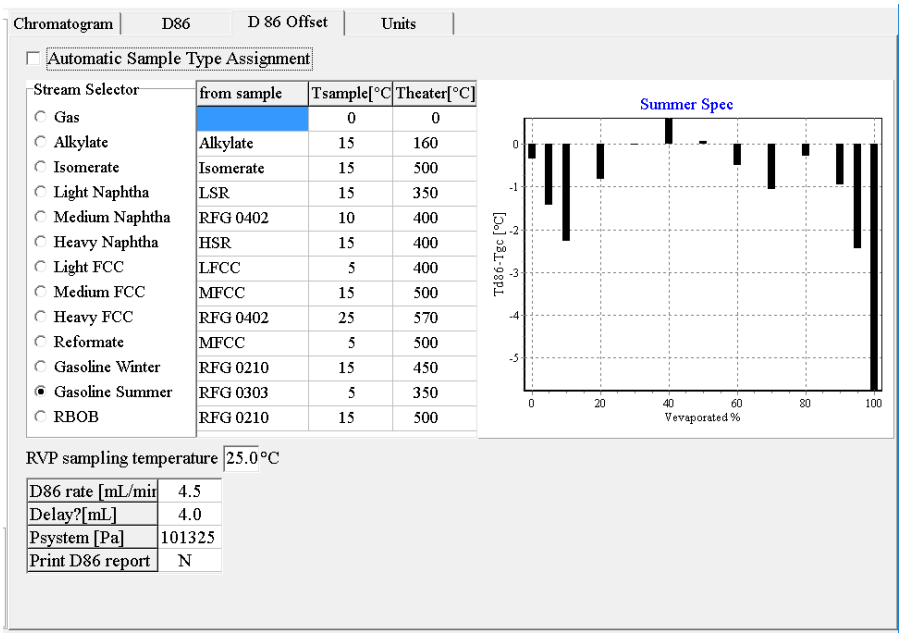


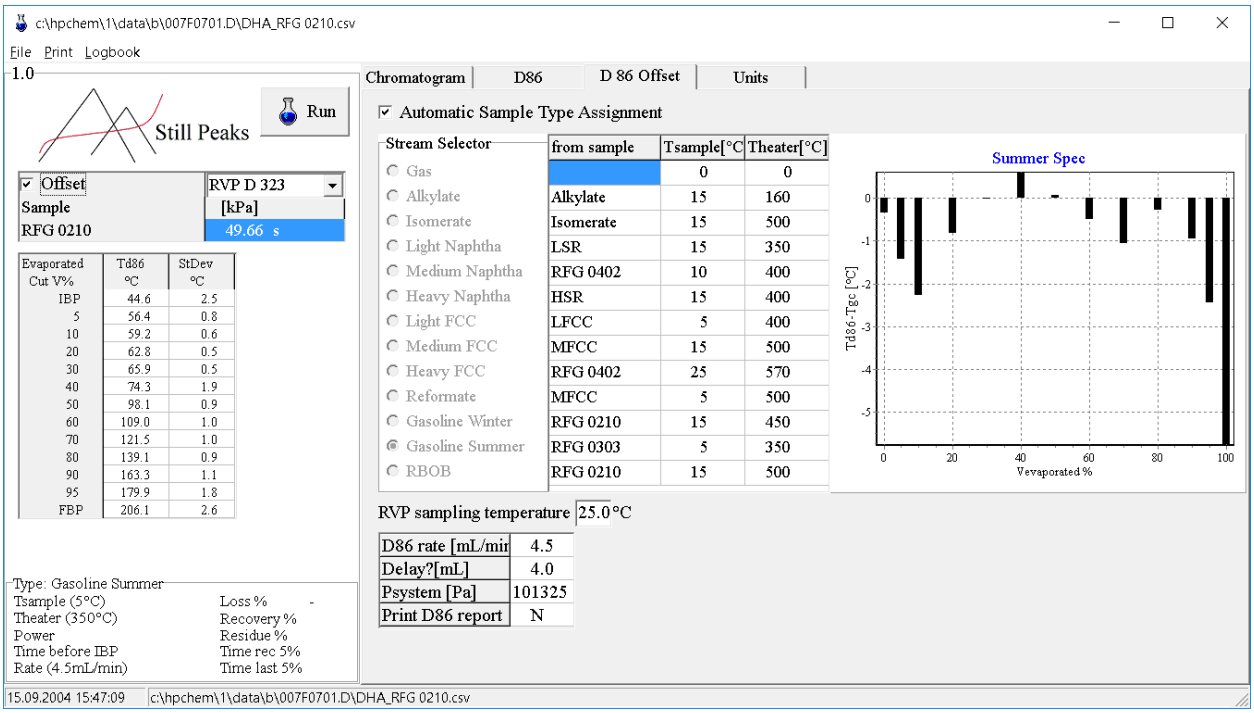
The ASTA check will stay checked or unchecked.

Now waith ASTA unchecked, all sampletype specific setpoints can be selected allowing you to run a gasoline with reformate setpoints.

The setpoint selection and the value of the setpoints is retained in the D86 software.

Tsample is the Sample Temperature, Theater is the heater temperature before IBP.

The offset shown at the right side can be applied to the final D86 report by checking the Offset checkbox:



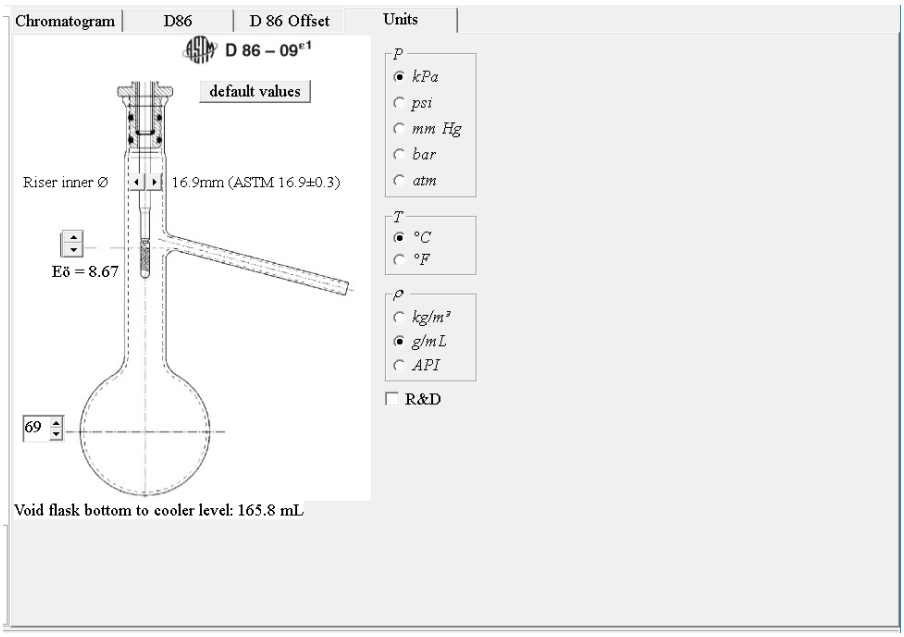
With this check, the offsets are applied to the final D86 caculation. Offset is found by entering ASTM D 86 data and can be applied to tune DHAtoD86 even closer to your D 86 numbers.

5.D86 Property Units and Thermometer Shift

The units of the properties P, T and density can be selected in the Units tabsheet.

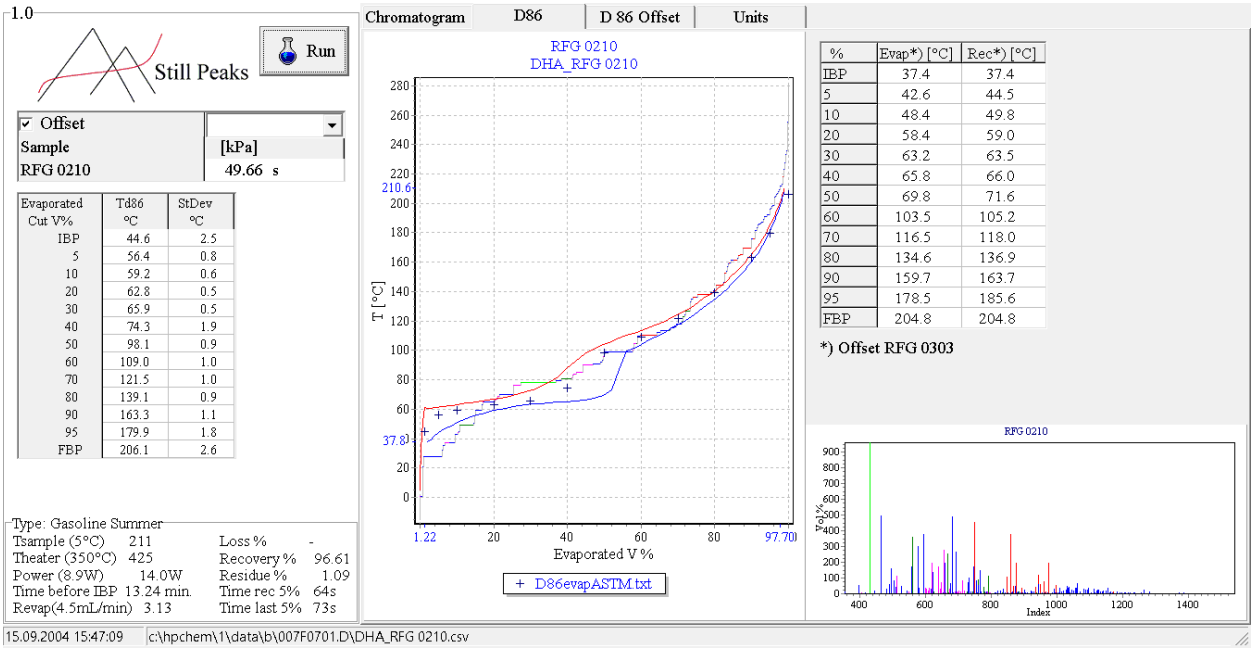
Eö is a dimensionless number, related to droplet size. The bigger the droplet at the virtual thermometer tip, the lower the temperature.

The Eö number shifts the calculated D86 curve down. Any changes are saved and applied ever after. Droplet size can be restored to default values by hitting the default values button.

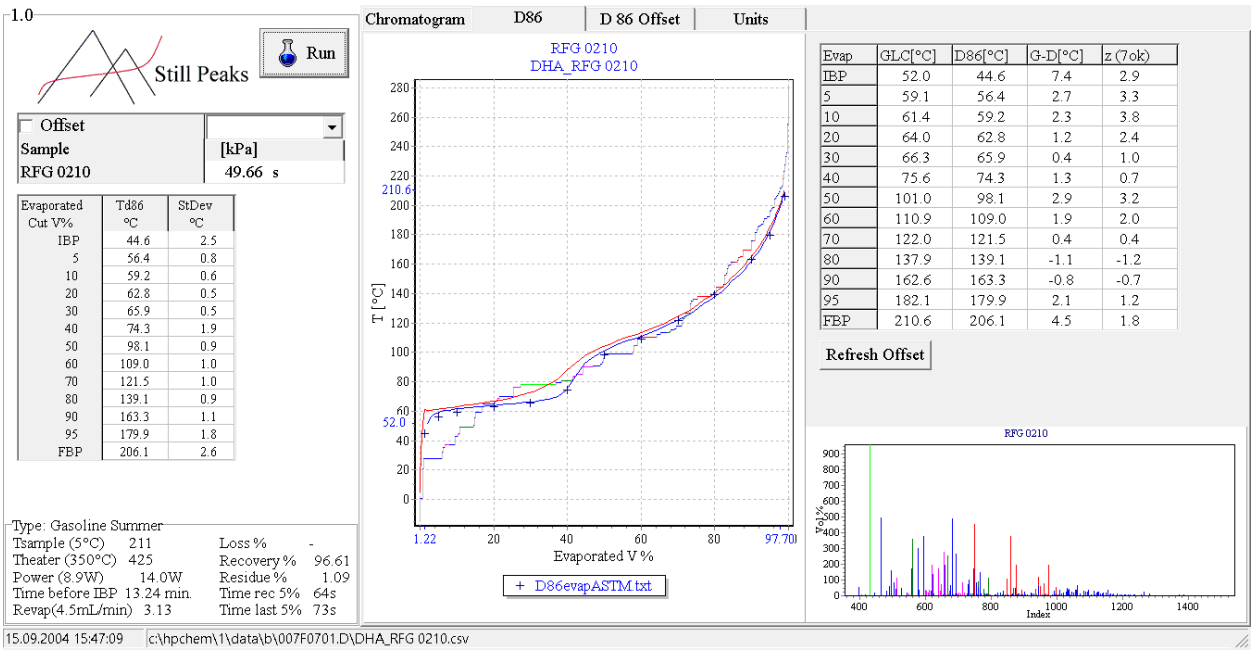


6.D86 Calculation and Setpoint Adjustents

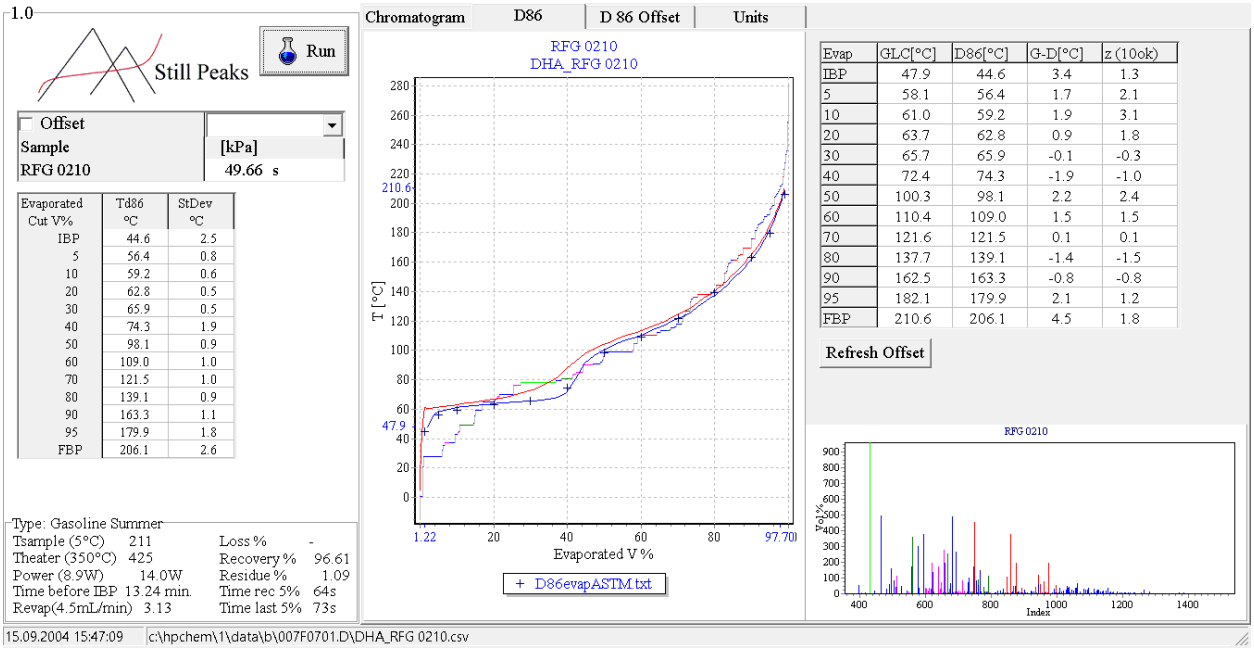
The Eö number from chapter 5 is much too high, shifting the calculated D86 curve down:



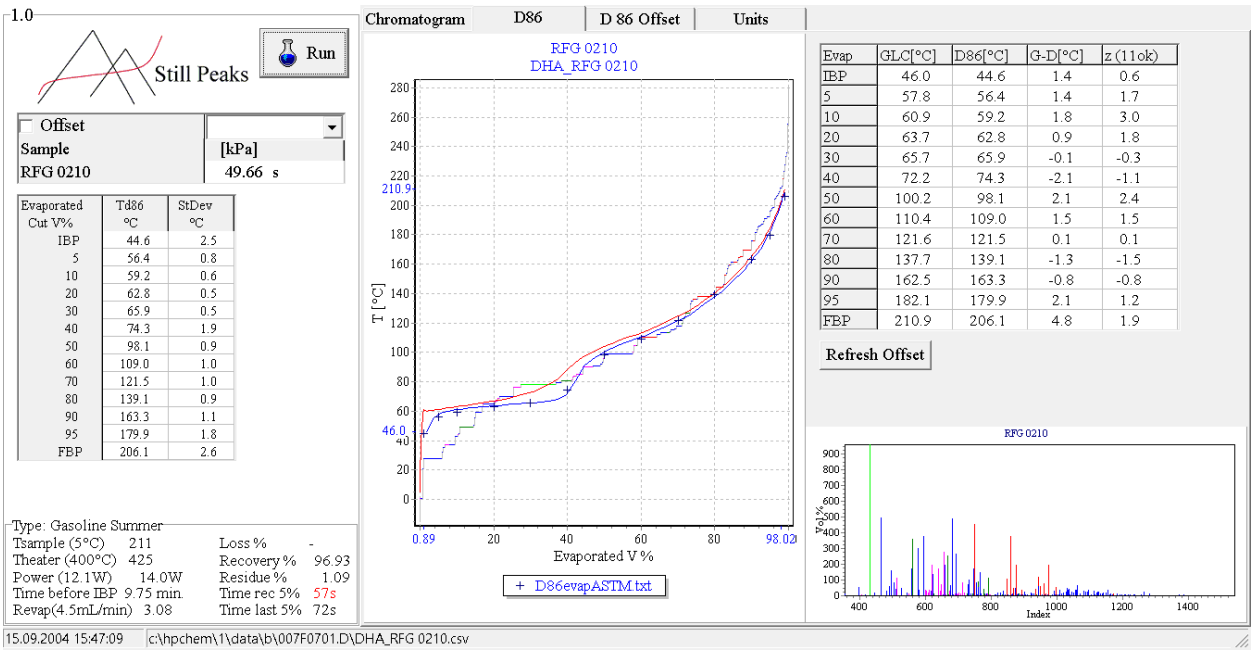
So we hit the default values button (chapter 5, Eö = 1) and re-run the D86:



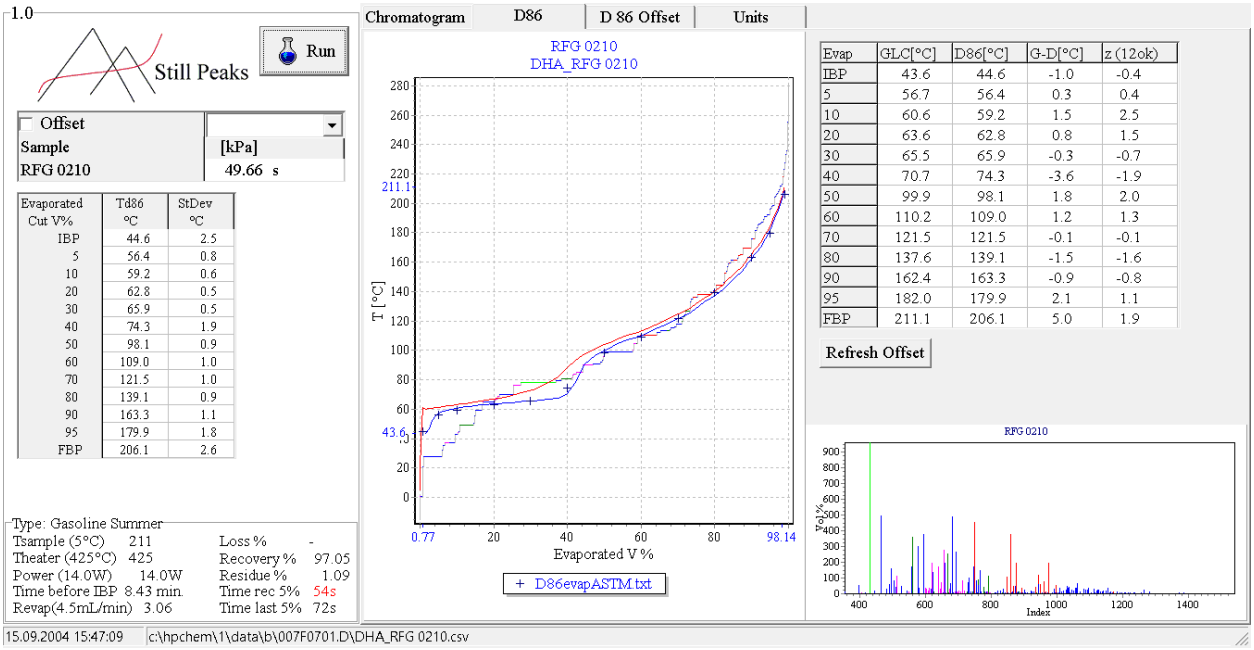
Maybe Eö = 1.666 is better:



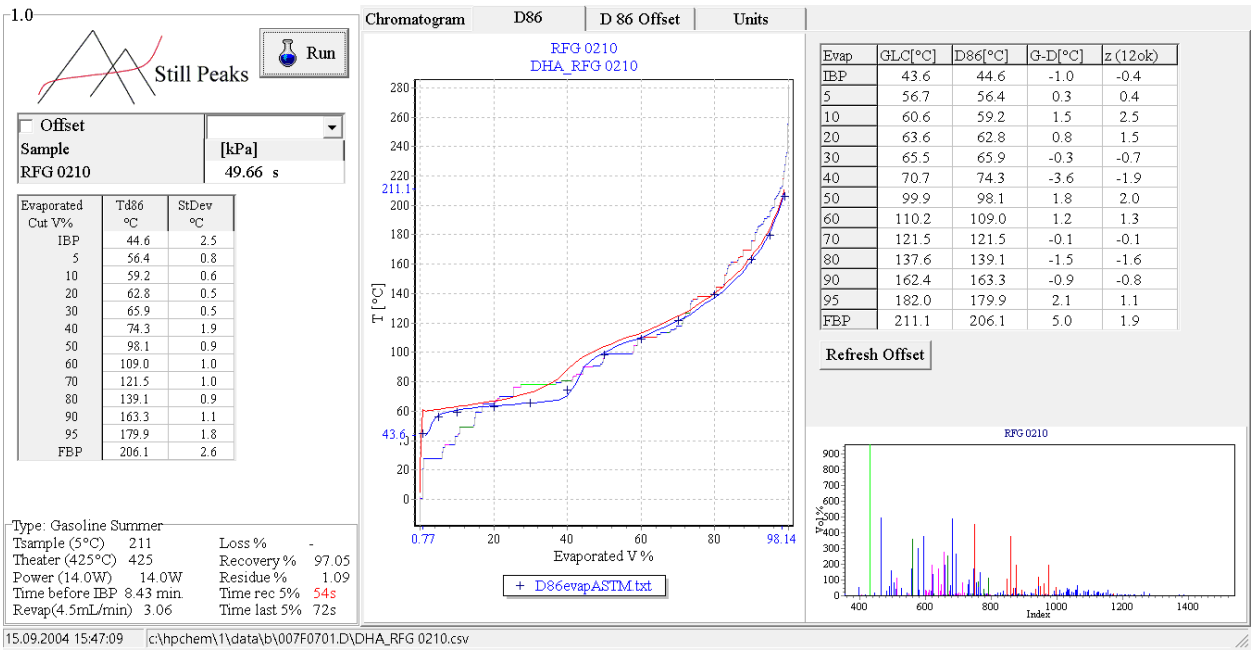
Now we have 10 temperatures within the -2<z<2 range. The IBP is overestimated, so we take an initial heater temperature of 400°C:



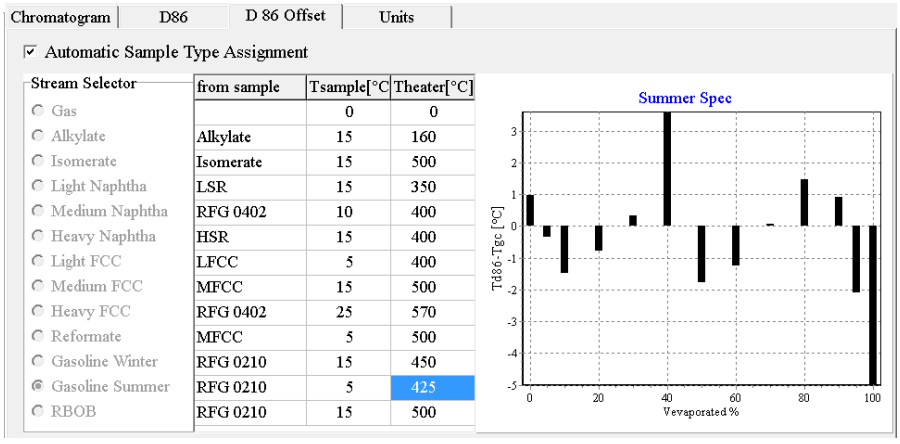
The repair of the 10% may be found by adding another 25°C to Theater:



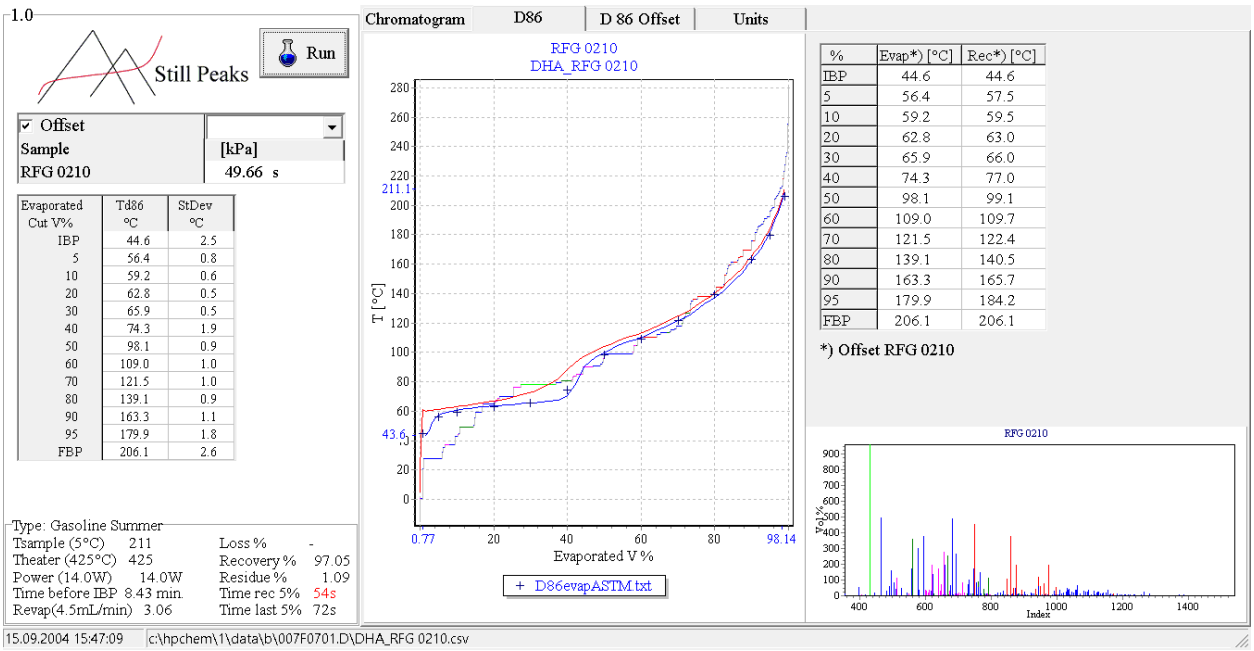
Next we change the Delay setpoint and the Eo number in a last effort to get closer to the ASTM D 86 data:



To repair the last differnces, offset is refreshed by clicking the Refresh Offset, and we the result is:



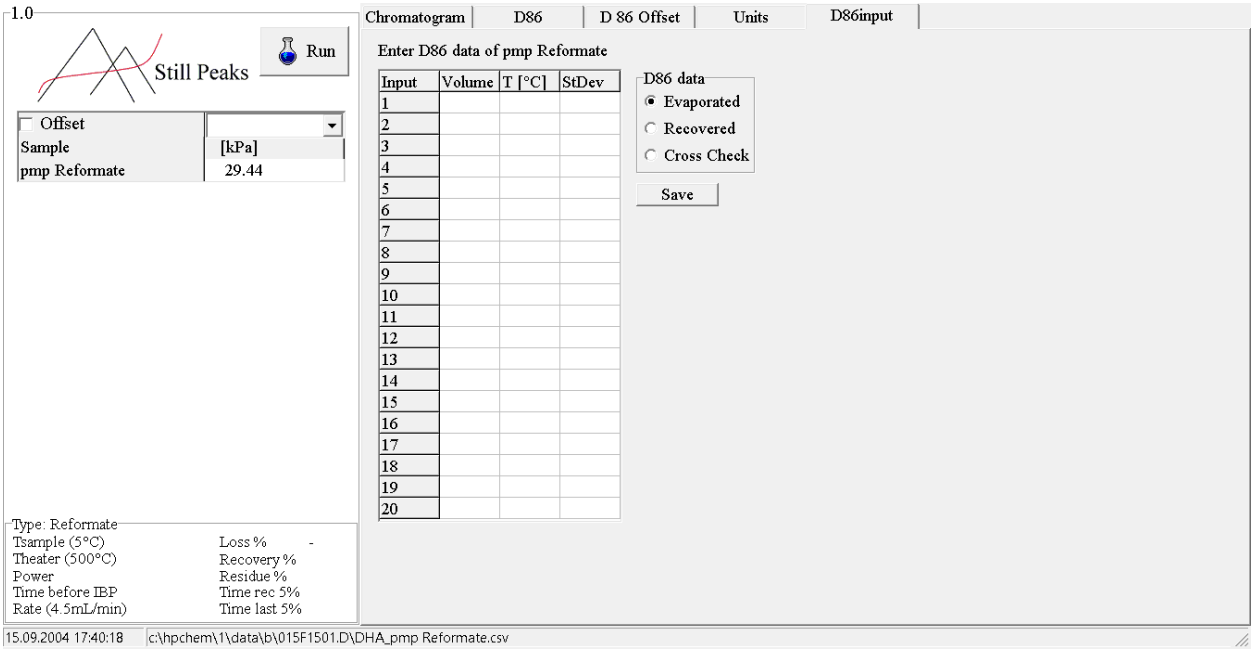
The offset values are the negative values of the G-D data column in above D86 report. When we recalculate using these offsets we get:



As expected, exactly the correct values, because the RFG 0210 offsets are used.

7.D86 Physical Data Input

Physical D86 data can be entered to determine the setponts and the offsets of a sample type:



The entry of data should be evaporated data beginning with IBP a number of volumes and temperatures ending with FBP. Hit save to store this data with the samplename for later reference. Every following calculation with the same sample name will be compared to these distillatin data. Sample names and data can be removed from the file D86evaporateDHAtoD86.txt. Only evaporated data and crosscheck data can be entered, the recovered data entry is not yet implemented.