

Customize Your Data to Fit Your Workflow

Agilent OpenLAB CDS Intelligent Reporter

Agilent OpenLAB Intelligence Reporter Client [LR User (BUILT-IN\lruser), Account: xtr1]

File Edit View Report Layout Projects Result Query Options Help

<New Filter>

Filter Definition Results Editor Preview

untitled.rdl *

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Report Items

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Sequence Summary Report

Creation Date: 2/12/2009 8:10:56 AM

Body

Sequence Name: LIR-2008-1 2008-10-15 11:51:46
Description: Third Sequence for Agilent OL Reporting
Acq. Date: 2/08/2007 1:26:00 PM
Acquired by: R. Honsberg

Summary Results per Compound

Name: des-hyd cis tramadol (C)

Name	Inj	RT	Area	Height	Amount	Unit	Vial
Standard L1	1	2.517	0.6835	0.5073	0.816	P1-F-04	P1-F-04
Standard L2	1	2.518	0.1001	0.0801	0.103	P1-F-05	P1-F-05
LOD	1	2.518	0.4565	0.3307	0.537	P1-F-06	P1-F-06
Standard L1	1	2.518	0.6723	0.5028	0.808	P1-F-04	P1-F-04
Standard L2	1	2.517	0.0778	0.0598	0.082	P1-F-05	P1-F-05
Sample 1	1	2.516	0.1765	0.1171	0.203	P1-E-01	P1-E-01
Sample 1	2	2.519	0.1674	0.1157	0.192	P1-E-01	P1-E-01

Footer

Auto Query

OpenLAB CDS Intelligent Reporter

What is it about?

Enable extended reporting and knowledge generation via

- search-based report content selection
- condense information by visualizing key results (e.g. in trend charts)
- decision-based result presentation (flag outliers, automatically sort results by pass/fail criteria, etc.)
- custom calculation (e.g. summary calculations, statistics and complex reports like Dissolution Tests)

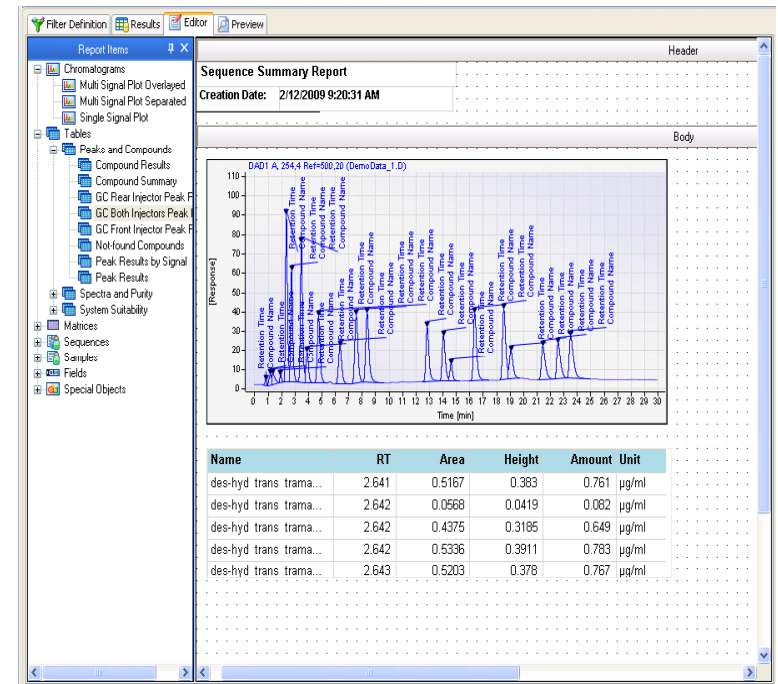
OpenLAB CDS Intelligent Reporter is an included stand alone reporting engine starting with OLCDS A.01.xx

OpenLAB CDS Intelligent Reporter Features

- Search-based reporting
- Simple and advanced calculations
- Trend charts
- Direct Integration into OLCDS A.01.xx (and above)
- Reporting of chromatograms for one or multiple injections
- Easy to use Report Template Editor integrated into the Client
- Reporting of Calibration Curves
- Reporting of Spectra
- OpenLAB CDS Intelligent Reporter reporting without connection to a database

New Report Template Editor

- New editor embedded directly into the OpenLAB CDS A.01.xx Client
- Focus on ease of use
- Preview of report with data selected in the client
- Lots of preconfigured “Snippets” like tables, signal plots etc make template creation fast and easy
- Supports custom calculations



Template Editor Details

Report item tree with "Snippets"

Sequence Summary Report
Creation Date: 2/12/2009 9:20:31 AM

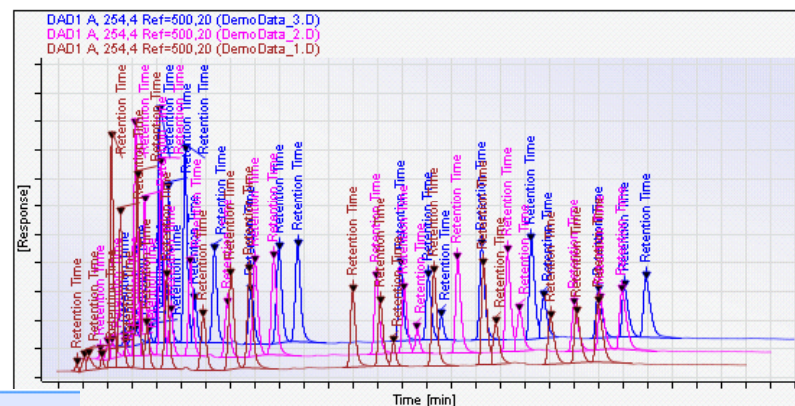
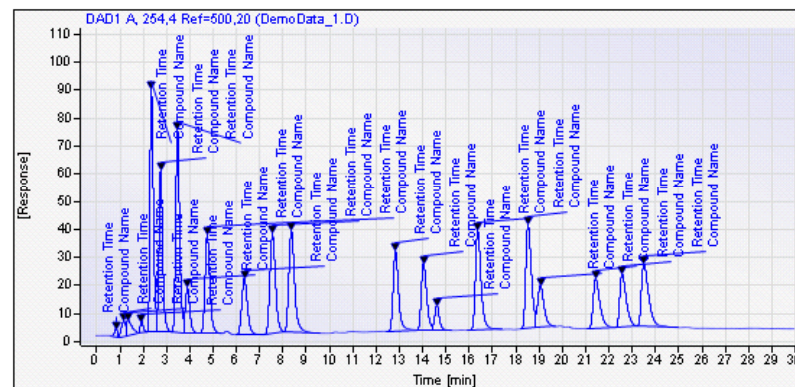
Chromatogram Data: DAD1 A, 254.4 Ref=500.20 (DemoData_1.D)

Name	RT	Area	Height	Amount Unit
des-hyd trans trama...	2.641	0.5167	0.383	0.761 µg/ml
des-hyd trans trama...	2.642	0.0568	0.0419	0.082 µg/ml
des-hyd trans trama...	2.642	0.4375	0.3185	0.649 µg/ml
des-hyd trans trama...	2.642	0.5336	0.3911	0.783 µg/ml
des-hyd trans trama...	2.643	0.5203	0.378	0.767 µg/ml

WYSIWYG editing pane

Chromatogram Reporting

- Reporting of one or multiple signals from one or multiples injections
- Overlaid, separated or stacked layout
- Extensive signal scaling, grouping and labeling options
 - Custom peak label formulas
- Filtering of signals for sample names, signal name etc.



Single and Multi-Signal Plots

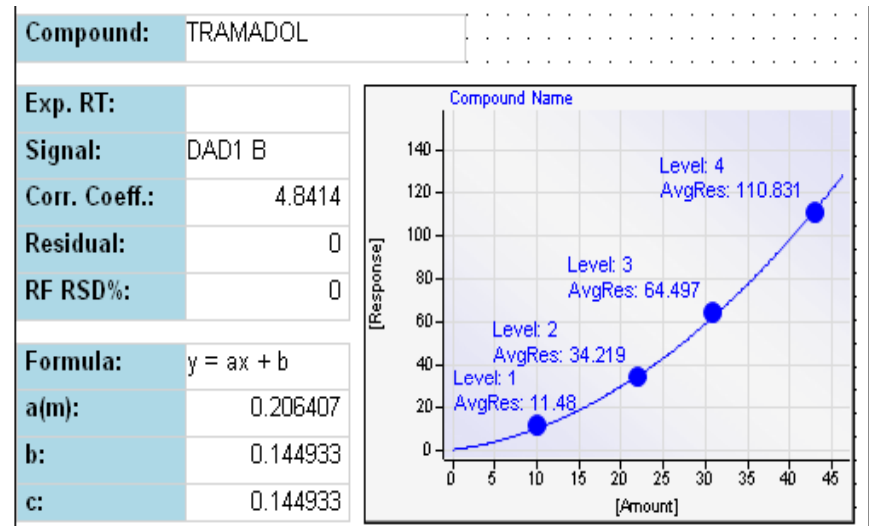
Peak Labels

Label 1:	Retention Time	▼	<input type="button" value="fx..."/>
Label 2:	Compound Name	▼	<input type="button" value="fx..."/>
Label 3:	No Label	▼	<input type="button" value="fx..."/>

Peak Labeling options

Other Features

- Reporting of Calibration Curves
 - Plot of single curves per compound
 - Overlay of curves from multiple compounds
 - Various annotation options for the curve
- Reporting of Spectra
 - Plots one or multiple spectra of a single peak or compound
 - Allows to select which peak spectra to show
- OLIR Client without direct database connection



Wide Range of reporting capabilities

OpenLAB CDS Intelligent Reporter offers a wide range of reporting capabilities covering

- Single injection reports with chromatograms, spectra and calibration curves
- Sequence summary reports with statistics, calculations and trend chart reports
- Flagging of outliers or out of spec values

Impurity Profiling with complex calculations

Impurity Profiling

Creation Date: 11/22/2007 4:11:39 PM



Applied rules for calibration test
 2.1 The precision of area must be < 5 % rsd above the 0.03 % level for all Impurities.
 2.2 Precision of area must be < 20 % rsd below the 0.03 % level for all Impurities.
 2.3 The precision of area must be < 1 % rsd for the main compound.
 2.4 The precision for retention times should be < 0.5% rsd.

Calculations:

% Level = Amount(measured Impurity)/Calibration Amount(Main Compound)*100

Control Sample Test

Failed tests are marked red

	Amount	Resolution	S/N	% Level LOD
des-hyd c/c tramadol (C)	5.089	7.391	23.561	S/N Missing
des-hyd trans tramadol (B)	4.692	3.791	17.606	10.585
o-desm tramadol (D)	5.326	4.363	18.644	S/N Missing
TRAMADOL	5.634	5.890	12.160	S/N Missing
trans-tramadol (A)	5.055	6.822	17.575	9.933

List of NOT found compounds is empty

Applied rules for control sample test

3.1 Resolution for all peaks must be > 2.
 3.2 Limit of detection must be < 0.01 % level for all Impurities.

Calculations:

% Level LOD = (Amount(Impurity)*2SignalToNoise (Impurity))/Amount(MainCompound)*100

Sample Test

Failed tests are marked red

	Sample 1	Sample 2	Sample 3	Sample 4	Sample 5	Sample 6
TRAMADOL	1012.339	1009.025	1018.611	1017.147	1009.324	1018.067
Impurity des-hyd c/c tramadol (C) % level	0.02004	0.06943	0.03075	0.04538	0.05640	0.02395
Impurity des-hyd trans tramadol (B) % level	0.01997	0.06327	0.02872	0.04323	0.05149	0.02266
Impurity o-desm tramadol (D) % level	0.01424	0.06639	0.02515	0.04221	0.05236	0.01748
Impurity trans-tramadol (A) % level	0.01896	0.06834	0.02968	0.04382	0.05248	0.02359
Total Impurity %	0.073	0.267	0.114	0.175	0.213	0.088

Applied rules for above sample tests

4.5 Determination of the amount of the main compound in ug/mL.
 4.6 Determination of the Impurity level in %.
 4.7 Percentage of allowed total Impurity amount must be < 0.5 %.

Impurity-Profiling-LimitsParams

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Impurity Profiling

Creation Date: 11/22/2007 4:11:39 PM



Main compound		Sample 1	Sample 2	Sample 3	Sample 4	Sample 5	Sample 6
TRAMADOL	RSD (Area)	0.094	0.287	0.159	0.203	0.180	0.149
	RSD (RT)	1.461	1.445	1.355	1.149	1.110	1.038
Impurities							
	RSD (Area)	5.689	2.690	3.440	3.464	1.494	5.499
des-hyd c/c tramadol (C)	RSD (RT)	0.776	0.765	0.747	0.664	0.627	0.605
	RSD (Area)	10.076	1.993	5.585	2.185	3.353	5.906
des-hyd trans tramadol (B)	RSD (RT)	0.723	0.715	0.682	0.623	0.583	0.565
	RSD (Area)	2.716	2.975	4.183	5.651	2.087	4.367
o-desm tramadol (D)	RSD (RT)	1.942	1.934	1.868	1.601	1.524	1.471
	RSD (Area)	0.094	0.287	0.159	0.203	0.180	0.149
TRAMADOL	RSD (RT)	1.461	1.445	1.355	1.149	1.110	1.038
	RSD (Area)	7.269	6.668	5.663	1.269	2.306	4.417
trans-tramadol (A)	RSD (RT)	1.295	1.303	1.222	1.032	1.006	0.930
	RSD (Area) Min	0.094	0.287	0.159	0.203	0.180	0.149
	RSD (Area) Max	10.076	6.668	5.663	5.651	3.353	5.906
	RSD (RT) Min	0.723	0.715	0.682	0.623	0.583	0.565
	RSD (RT) Max	1.942	1.934	1.868	1.601	1.524	1.471
	Count	5.000	5.000	5.000	5.000	5.000	5.000

List of NOT found compounds is empty

Applied rules for above sample tests

4.1 Area precision of the main compound must be < 1 % rsd.
 4.2 Retention time precision must be < 0.5 % rsd.
 4.3a Precision for areas of impurities from 0.05 up to the 0.4 % level must be < 10 % rsd
 4.3b precision below 0.05 % down to the 0.02% level area precision should be < 20 % rsd
 4.4 Retention time precision for impurities must be < 0.5 % rsd

Impurity-Profiling-LimitsParams

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Flagging of out of spec values

- Flag outliers by pass/fail criteria using conditional formatting
- Automatically sort results, etc.

System Suitability Test Failed tests are marked red

	Amount	RSD(RT)	RSD(Area)	HW-Resolution	PW	k'	S/N
des-hyd cis tramadol (C)	0.804	0.019	1.456	15.247	-0.041	21.547	10.076
des-hyd trans tramadol (B)	0.748	0.025	1.846	3.854	-0.135	22.639	7.584
o-desm tramadol (D)	0.816	0.059	2.648		0.281	7.088	7.813
TRAMADOL	1004.590	0.057	0.099		42.381	5.150	2094.055
trans- tramadol (A)	0.812	0.065	2.346	6.892	0.100	11.992	7.931

List of NOT found compounds is empty

Applied rules for system suitability test
 1.1 Precision of areas must be < 2 % rsd
 1.2 Precision of retention times must be < 0.5 % rsd
 1.3 Resolution must be > 2 for all peaks
 1.4 Maximum peak width must be < 0.08 min at half height.
 1.5 k' must be 5 < k' < 25
 1.6 Signal-to-noise ratio must be > 50 for all peaks

Calibration Test Failed tests are marked red

Compound and Calibration lvl	Amount	% Level	RSD(RT)	RSD(Area)
des-hyd cis tramadol (C)	1	0.821	0.082	0.285
	2	0.104	0.103	25.604
des-hyd trans tramadol (B)	1	0.765	0.076	1.992
	2	0.079	0.078	17.515
o-desm tramadol (D)	1	0.815	0.081	1.359
	2	0.093	0.092	14.671
TRAMADOL	1	1000.474	100.000	0.300
	2	100.654	100.000	0.082
trans- tramadol (A)	1	0.831	0.083	4.311
	2	0.089	0.089	13.703

All calibrated compounds found

Method Development Report

- Summary table with overview of found peaks and the sum of peak resolution
- Summary bubble plot shows a graphical representation of the results
 - Size of the bubble shows the sum of all peak resolution values.
 - The bigger the bubble the better the peak separation in the chromatogram

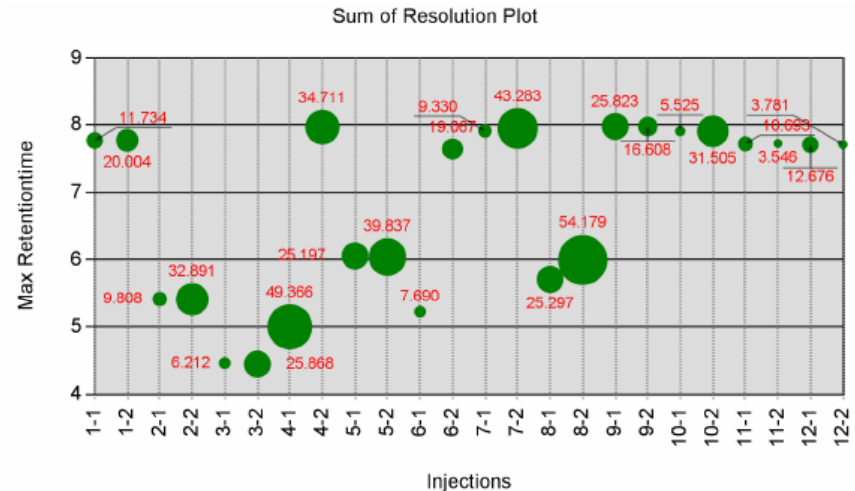
Method Development Results Summary

Sequence : METOPROLOL100N2008-07-30

Signal: DAD1 B, Sig=230,10 Ref=360,100

Min. Area%: 0.5

# Column / Solvent	# of peaks	Sum Resolution	Max RT
1-1 Chromatographic column: Zorbax SB C18, 2.1x50mm, 1.8µm Solvents: 95% A1: H2O (water+0.2%tfa), 5% B1: ACN (*0,16% TFA)	13	3.488	7.769
1-2 Chromatographic column: Zorbax SB C18, 2.1x50mm, 1.8µm Solvents: 95% A1: H2O (water+0.2%tfa), 5% B1: ACN (*0,16% TFA)	9	5.090	7.771
2-1 Chromatographic column: Zorbax Eclipse Plus, 2.1x50mm, 1.8µm Solvents: 95% A1: H2O (water+0.2%tfa), 5% B1: ACN (*0,16% TFA)	11	6.275	2.866



Normalized RGA Report for Gas Analysis

- Reports Gas Analyzer results
- Groups compounds into categories
- Automatically does an Air correction of the results based on a set limit
- Calculates summary results

Compound list

Oxygen limit exceeded, Air Corrected values used (.01 Mole)

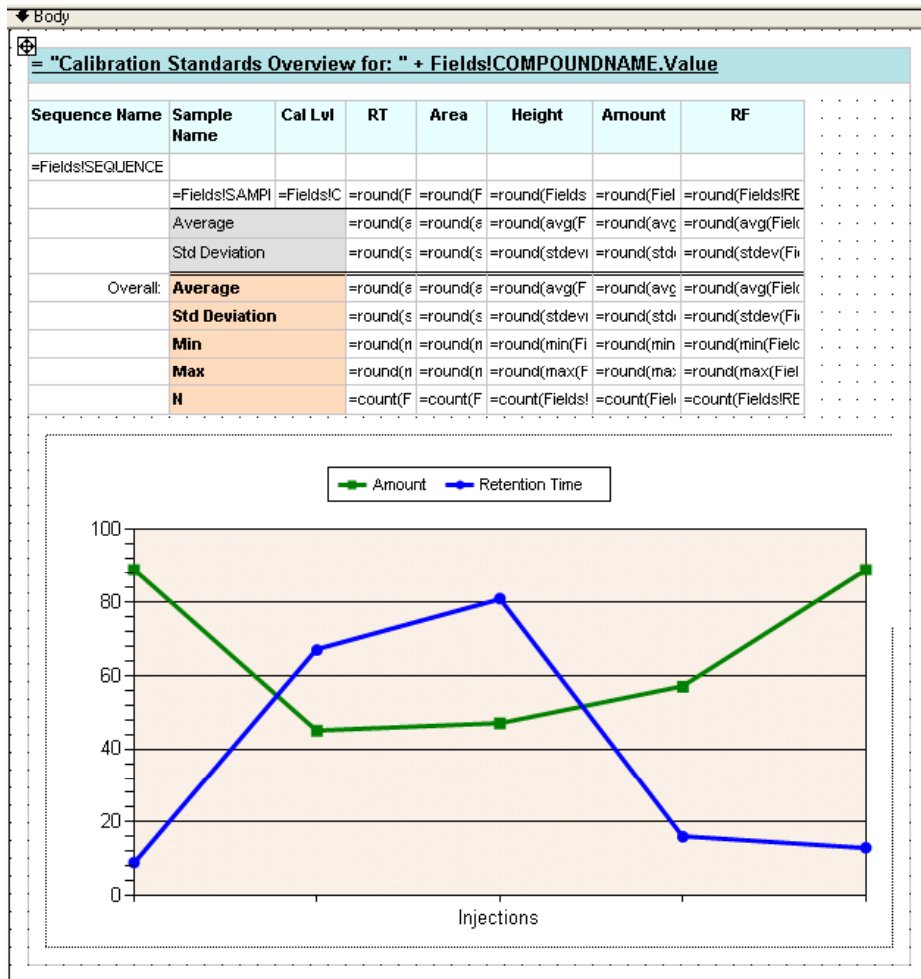
Inert Gases	Ret. time	Area	Mole%	N-Mole%	N-Wt%	N-Vol%
Carbon dioxide	0.436	220274	4.03	4.09	5.44	4.8
Hydrogen	0.731	1801817	22.2	22.55	1.37	0.06
Oxygen	0.903	23021	0.01	0	0	0
Nitrogen	1.056	48546	2.03	2.03	1.72	0.96
Carbon monoxide	1.608	20605	1.99	2.02	1.71	0.96
Total Inert Gases		2114263	30.26	30.68	10.24	6.78

Saturated Hydrocarbons	Ret. time	Area	Mole%	N-Mole%	N-Wt%	N-Vol%
n-Propane	0.403	216547	8.03	8.16	10.87	9.61
Iso-butane	0.509	1427703	7.98	8.1	13.74	15.46
Ethane	0.511	151415	1.98	2.01	1.83	1.1
n-Butane	0.554	66389	2.01	2.04	3.59	4.18
iso-Pentane	0.905	71625	1.99	2.02	4.41	6.38
n-Pentane	0.960	150927	3.99	4.05	9.2	13.32
Methane	1.386	445047	18.98	19.28	9.35	3.01
Total Saturated Hydrocarbons		2529653	44.96	45.66	52.98	53.05

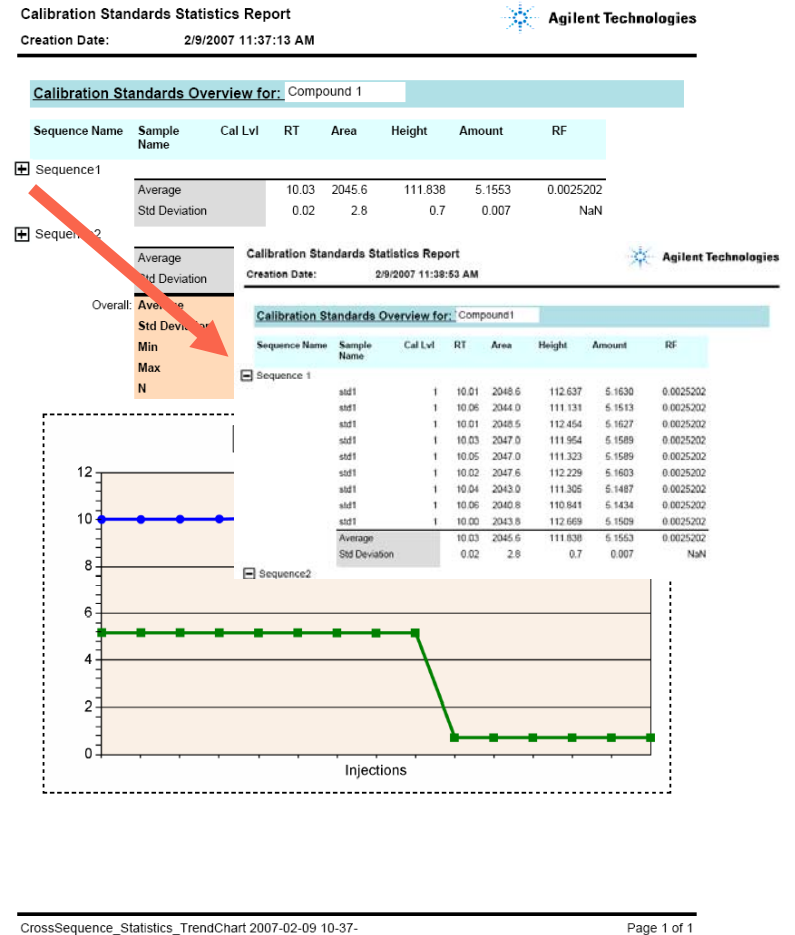
Unsaturated Hydrocarbons	Ret. time	Area	Mole%	N-Mole%	N-Wt%	N-Vol%
Total		5428898	98.51	100	100	100

Real density of gas 0.5808 kg/m3
Molar weight of mixture 33.0885 g/mol
Superior molar calorific value 6065.4 kJ/mol

Sequence Statistics with Trend Chart



Report template



Reports with interactive elements when viewed in the reporting client!

What does OpenLAB CDS Intelligent Reporter deliver?

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