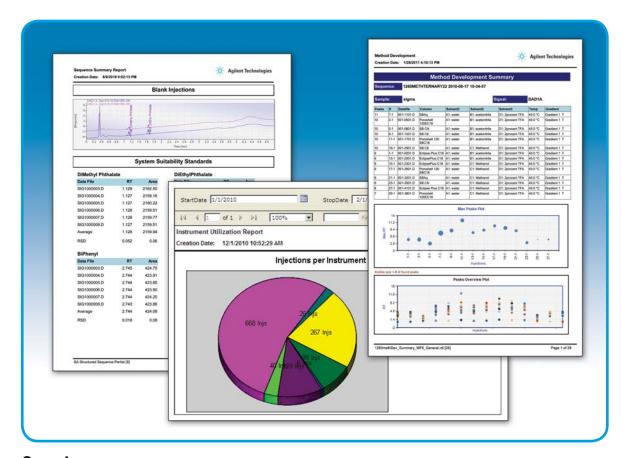


Agilent OpenLAB Intelligent Reporter

Report Compendium



Overview

A key challenge laboratories are facing is to turn raw analytical data into meaningful and actionable information. Meaningful report generation is a daily activity that occupies analysts in all fields, including: Pharmaceutical, Hydrocarbon processing, Bioanalytical, Biofuels, Academic, Environmental, and Contract organizations to name a few. User's workflows require reporting tools that handle calculations of varying complexity, they may require aggregation of content from varied sources, and reports may need to be exchanged with internal or external collaborators, or used as official records for submission to regulatory agencies.



A reporting engine that does not address these requirements, therefore, can severely impact results, regardless of the capability of the data system that produces the raw data. Agilent's OpenLAB Intelligent Reporter addresses the challenges as it allows users in the laboratory to easily create reporting templates for complex reports. In addition, OpenLAB Intelligent Reporter relies on common resources that can be used both by a scalable data system (OpenLAB CDS) as well as an Enterprise Content Management system (OpenLAB ECM).

This document is designed to provide an overview of the many different reports possible with Agilent OpenLAB Intelligent Reporter. For improved usability and expandability, the document consists of a Report Summary table—one for standard workstation, sequence based reports; the other for enterprise level, query-driven reports with links to more detailed views of each report. A brief description of each report, illustrative pages and many more detailed links are displayed in each section. At the end of each report section are links back to the main Report Summary table.

Report Summary Table

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Title (Link)	Features	Users Benefitting	Applicable Industry
<u>Dual Display</u>	Dual channel displays different data perspectives	All	All
LC Diagnosis Report		Routine	All
Minor Component Analysis	Combined benefit of sensitive instrument with intelligent reporting	All	All
Performance Report	Column performance viewed from various λ using DAD	R&D, all	All
Simple Purity	Known/unknown peaks ratioed	All	All
Raw Material Purity	Known/unknown peaks ratioed	Mfg, production	Pharma; foods; Contract
Suitability & Stability	Extensive compound analysis	Regulated users	Pharma; Energy; Contract
Manual Integration Summary	Standards, QC, Samples, manual integration, statistics	Lab Manager	All
Seq Summary/Limits	Statistics, special calc	High throughput	All
Seq Summary/Long	Statistic, more detail	Routine	All
Structured Sequences	Defined sections; Sys Suit; Column Performance	Regulated users	Pharma; Environmental; Contract
BTU (Calorific Value) Calculation	Gross BTU/ft ³ value, average Molecular Weight, and Specific Gravity	Lab; field	Energy; HPI
Method Development Summary	Method and separation optimization; column, solvent usage; graphic displays	R&D Lab Management	All
Impurity Profiling	System Suitability; Conditional formatting	R&D, QC	All

Enterprise level – central database, query-based (OpenLAB ECM Intelligent Reporter)²

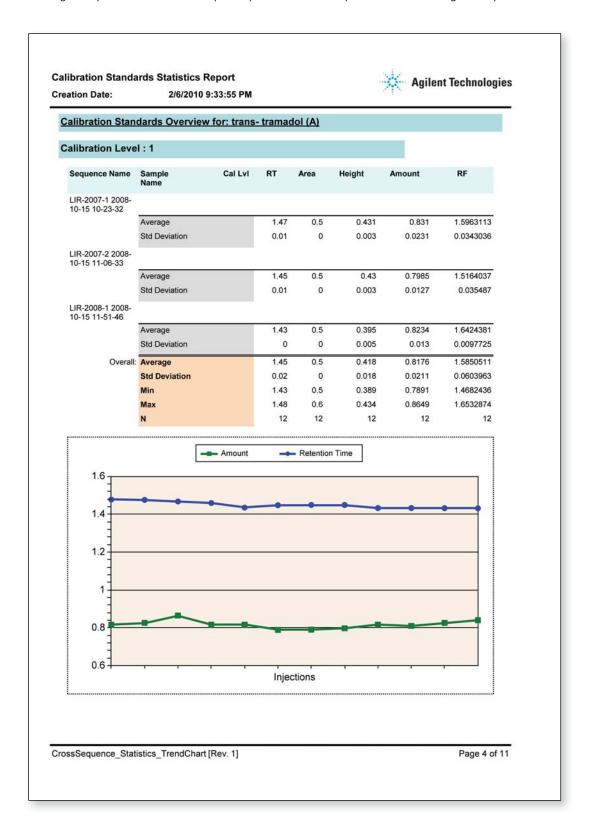
the state of the s			
Title (Link)	Features	Users Benefitting	Applicable Industry
Column Usage Check	Usage summaries, graphics, statistics	Lab Managers	All
Instrument Utilization	Administrative usage summary	IT dept	All
Dissolution Summary	Aggregate sample IDs; Stats	Regulated users	Pharma; Contract
Calibration Standards Report	Cross-sequence; Trend Charting; Statistics	Lab users	Pharma; Bio; Energy; Academic

¹ All features shown are available in OpenLAB CDS; sequence based reports are portable to database, query-based OpenLAB ECM Intelligent Reporter.

² Requires central database and query-based OpenLAB ECM Intelligent Reporter. The templates are often adaptable to OpenLAB CDS Intelligent Reporter. Check with your local specialist to ensure portability.

Calibration Standards Report

The report shown below was created using a template that was modified in Microsoft® Business Intelligence Studio. This illustrates how OpenLAB ECM Intelligent Reporter can aggregate results and information from different sequences stored in OpenLAB ECM. For single sequences, the same capability is available in OpenLAB CDS Intelligent Reporter.



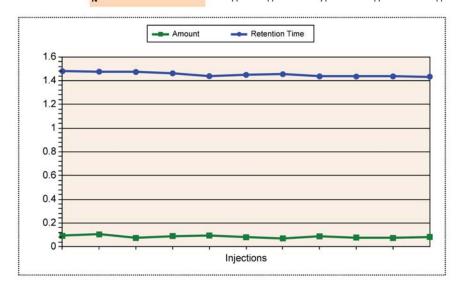


Calibration Standards Statistics Report Creation Date: 2/6/2010 9:33:55 PM



Calibration Level : 2

Sequence Name	Sample Name	Cal Lvi	RT	Area	Height	Amount	RF
LIR-2007-1 2008- 10-15 10-23-32							
	Average		1.47	0.1	0.046	0.0894	1.4759325
	Std Deviation		0.01	0	0.003	0.0126	0.0262966
LIR-2007-2 2008- 10-15 11-06-33							
	Average		1.45	0.1	0.041	0.0812	1.3962796
	Std Deviation		0.01	0	0.002	0.0122	0.067252
LIR-2008-1 2008- 10-15 11-51-46							
	Average		1.43	0	0.04	0.0797	1.6222997
	Std Deviation		0	0	0.003	0.006	0.0399246
Overall:	Average		1.45	0.1	0.042	0.0836	1.5074334
	Std Deviation		0.02	0	0.004	0.0104	0.1047444
	Min		1.43	0	0.037	0.0699	1.3294235
	Max		1.48	0.1	0.05	0.1037	1.6567221
	N		11	11	11	11	11



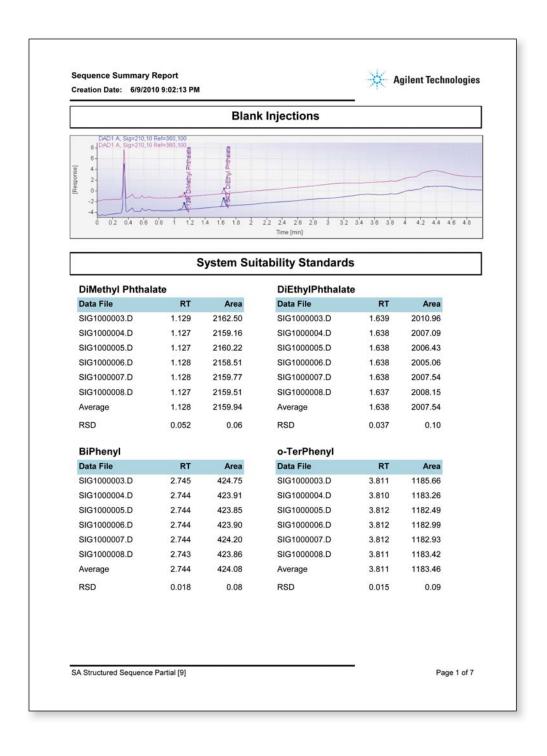
CrossSequence_Statistics_TrendChart [Rev. 1]

Page 5 of 11



Structured Sequences

This example is ideal for more complex analyses or in regulated laboratories. The user can create structured data sets which must be reported in a series of structured report sections. In this case we show the analysis of phthalates and partition the report template into a graphic region showing a blank run in 2 channel overlaid mode, followed by a tabular section with summary and statistics for only System Suitability standards, then another tabular section with performance parameters for target phthalates. The OpenLAB Intelligent Reporter makes it easy to create specific subsets of injections within the sequence, calculate and format appropriate report sections, and assemble the sections into a complete report for the sequence.





Sequence Summary Report Creation Date: 6/9/2010 05:18:19 PM



Resolution Standard

DataFileName

SIG1000008.D

Name	RT	Area	Plates	Resolution	Tailing
DiMethyl Phthalate	1.127	2159.5122	5249	3.86	1.07
DiEthyl Phthalate	1.637	2008.1476	8924	3.94	1.05
BiPhenyl	2.743	423.8644	18814	14.81	1.03
o-TerPhenyl	3.811	1183.4171	38410	13.53	1.02

SA Structured Sequence Partial [8]

Page 1 of 6



Dissolution Summary

Routine dissolution testing of pharmaceutical products can be tedious from the post-analysis, data handling perspective. The OpenLAB Intelligent Reporter enables the analyst to quickly organize results by vessel and sampling time point, perform statistics, and generate graphic views that clearly show compound dissolution over time. In addition, volume compensation is possible when aliquots reach the threshold specified by pharmacopeia norms. The extract below shows the summary and graphic displays possible. The specific example utilizes an aggregation capability available in OpenLAB ECM Intelligent Reporter. An added benefit could be that of Interactive Fields enabling the reviewer to choose data display options prior to printing the report (e.g. the aliquot time or vessel numbers could be interactive). An adaptation of this template enables usability in a smaller deployment. These capabilities prove valuable in determining the bioavailability of drugs in the QA/QC setting.



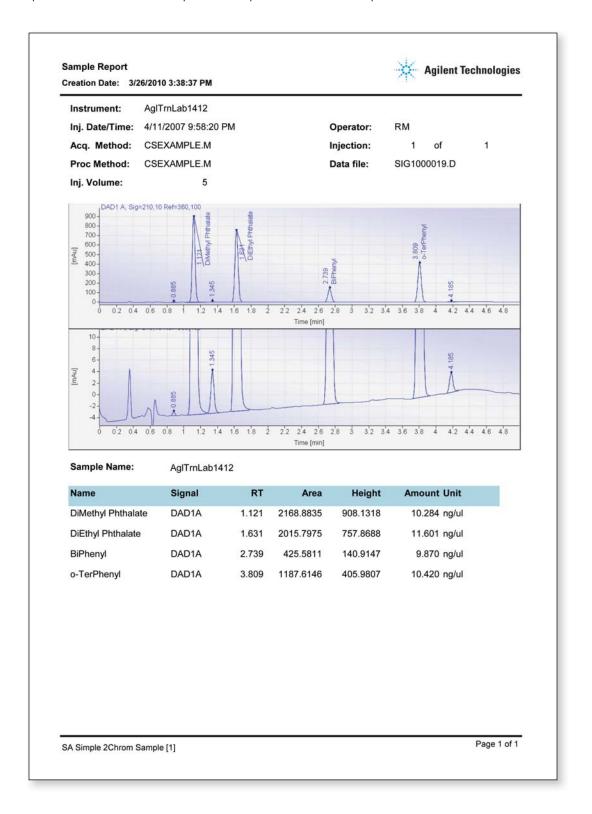
The final output combines tabular and graphic results in a multi-page report.





Dual Chromatogram

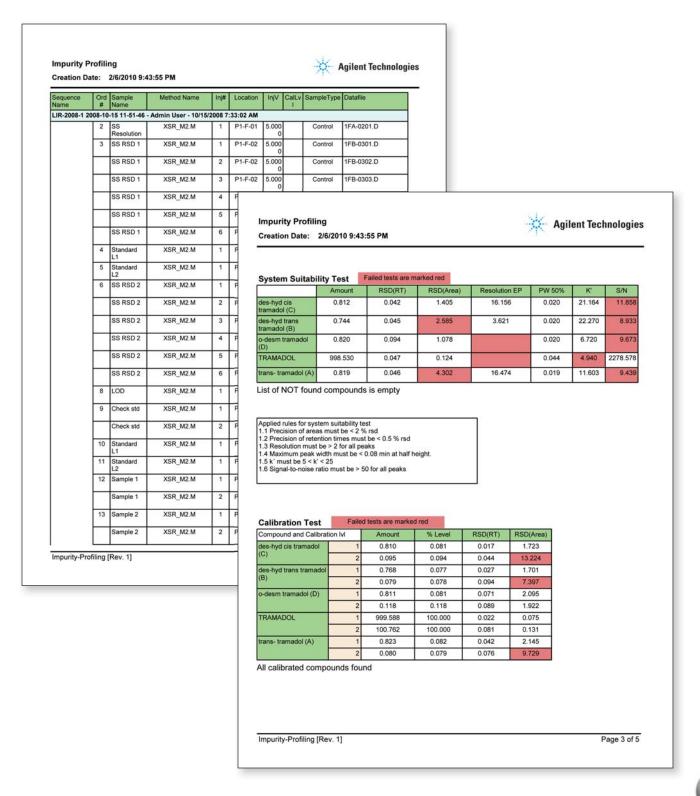
The ability to easily display different perspectives of the same data file enables the analyst to gain a better understanding and improve actionable knowledge about the sample. In this example two graphic regions are displayed. The overall chromatogram is on top. A more focused region on the bottom. In this way peak distortion, or the appearance of an unexpected component, such as the small peak at 1.345 minutes, may indicate a problem with the sample.





Impurity Profiling

This report takes full advantage of the OpenLAB Intelligent Reporter capability to provide fully automated, self-documenting reports with conditional formatting that highlights anomalous or out-of-specification results requiring attention or further action.





Impurity Profiling

Creation Date: 2/6/2010 9:43:55 PM



Agilent Technologies

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 EP	S/N	% Level LOD
des-hyd cis tramadol (C)	5.022	7.551	17.685	10.334
des-hyd trans tramadol (B)	4.595	3.663	13.135	12.729
o-desm tramadol (D)	5.144	4.085	14.604	12.818
TRAMADOL	5.496	5.683	9.742	20.529
trans- tramadol (A)	5.198	7.400	13.547	13.962

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 impurit

Calculations: %Level LOD=(Amount(impurity)*2/SignalToNoise(impurity)*2

Sample Test	Failed tests are marked			
	Sample 1	Sample 2		
TRAMADOL	1015.185	1009.053		
Impurity des-hyd cis tram	0.01944	0.07045		
Impurity des-hyd trans tr	0.01969	0.06352		
Impurity o-desm tramado	0.01592	0.06597		
Impurity trans- tramadol (0.02079	0.06856		
Total Impurity %	0.076	0.268		

Applied rules for above sample tests
4.5 Determination of the amount of the main compound in
4.6 Determination of the impurity level in %.
4.7 Percentage of allowed total impurity amount must be

Main compound	Sample 1	Sample
Main compound	Cumpic 1	Cumpi

Impurity-Profiling [Rev. 1]

Impurity Profiling

Creation Date: 2/6/2010 9:43:55 PM



Agilent Technologies

Main compor	und	Sample 1	Sample 2	Sample 3	Sample 4	Sample 5	Sample 6
TRAMADOL	RSD(Area)	0.032	0.140	0.084	0.111	0.049	0.222
	RSD(RT)	0.033	0.028	0.054	0.171	0.053	0.024
Impurities		Sample 1	Sample 2	Sample 3	Sample 4	Sample 5	Sample 6
des-hyd cis	RSD(Area)	3.758	3.569	4.500	1.377	2.451	2.116
tramadol (C)	RSD(RT)	0.086	0.032	0.039	0.080	0.006	0.008
des-hyd trans	RSD(Area)	13,676	1.685	3.020	2.442	3.822	6.687
tramadol (B)	RSD(RT)	0.095	0.039	0.035	0.078	0.007	0.015
o-desm	RSD(Area)	1.860	1.587	4.453	0.372	0.942	3.784
tramadol (D)	RSD(RT)	0.011	0.192	0.017	0.101	0.032	0.151
TRAMADOL	RSD(Area)	0.032	0.140	0.084	0.111	0.049	0.222
	RSD(RT)	0.033	0.028	0.054	0.171	0.053	0.024
trans- tramadol	RSD(Area)	12.542	0.836	2.155	1.365	1.203	1.929
(A)	RSD(RT)	0.007	0.047	0.091	0.146	0.056	0.059
R	SD(Area) Min	0.032	0.140	0.084	0.111	0.049	0.222
RSD(Area) Max RSD(RT) Min RSD(RT) Max Count		13.676	3.569	4.500	2.442	3.822	6.687
		0.007	0.028	0.017	0.078	0.006	0.008
		0.095	0.192	0.091	0.171	0.056	0.151
		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. 4.2 Retention time precision must be < 0.5 % rsd. 4.3 a Precision for areas of impurities from 0.05 up to the 0.4 % level must be < 10 % rsd 4.3 b 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

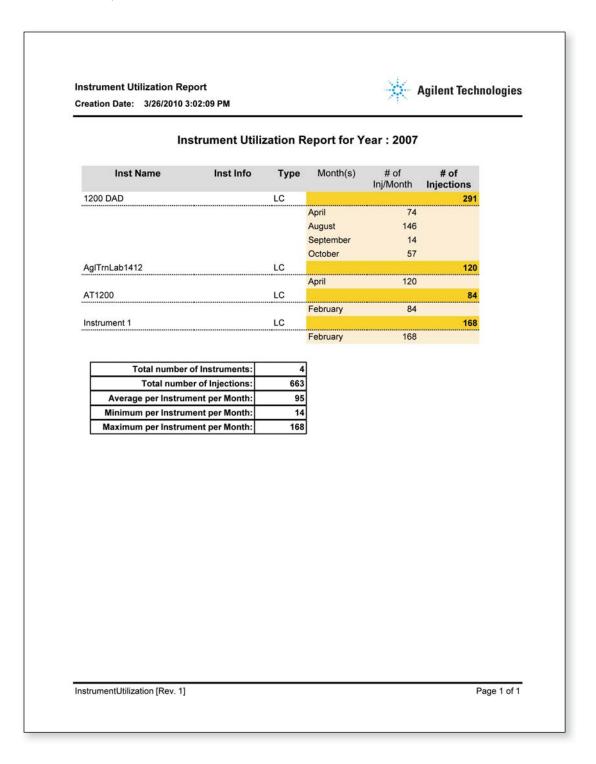
Impurity-Profiling [Rev. 1]

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Instrument Utilization

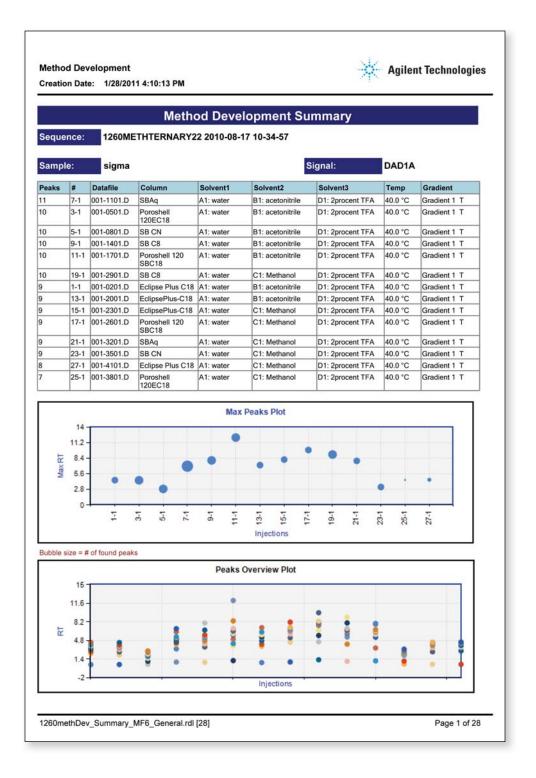
While many report templates are designed for the analyst, utilization reports provide an overview of the usage of each instrument to the lab manager and can be used to balance resources, justify additional equipment or manpower, and determine service intervals. An added benefit is that of Interactive Fields that enable the reviewer to choose data display options prior to printing the report (e.g. the report year could be interactive). The example below provides the Lab Manager a rapid overview of the status of instruments in the enterprise.



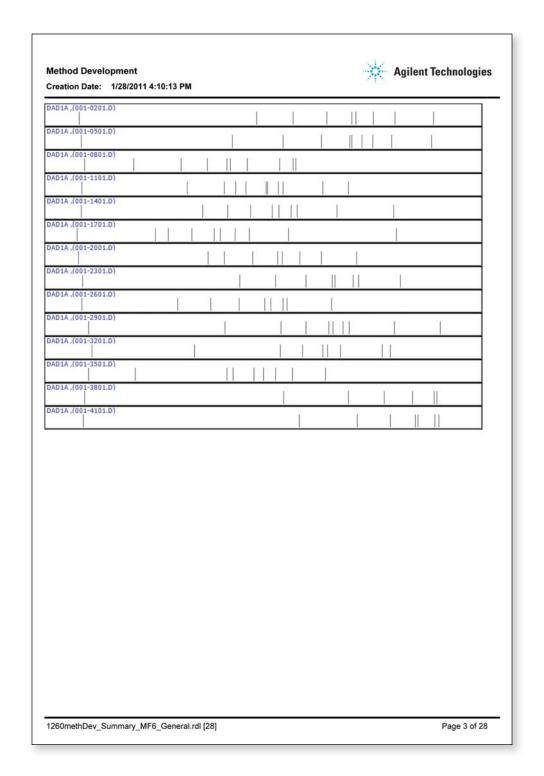


Method Development Summary

This Method Development Report provides an extensive summary of the data to enable the analyst to easily determine the optimum conditions for a separation. For example, the data in the table below are sorted by the number of peaks so that those injections with the maximum number of peaks appear at the top of the table. The bubble plot below the table gives the user a indication of which injections have the maximum number of peaks (size of the bubble) with a short duration of the run (y-axis). The lower plot gives the user an indication of the spread of the peaks for each injection.









Agilent Technologies **Method Development** Creation Date: 1/28/2011 4:10:13 PM Individual Results sorted for max number of peaks (best first) Data file Column Solvent1 Solvent2 Solvent3 Temp Gradient 001-1101.D SBAq A1: water B1: acetonitrile D1: 2procent TFA 40.0 °C Gradient 1 T DAD1 A, Sig=254,10 Ref=360,100 120 -100 3.271 MAU 60-0.867 40-20-2.5 7.5 8.5 N/A Column Solvent1 Solvent2 Solvent3 Gradient Data file Temp 001-0501.D Poroshell 120EC18 A1: water B1: acetonitrile D1: 2procent TFA 40.0 °C Gradient 1 T DAD1 A, Sig=254,10 Ref=360,100 120-100-80-2.157 4.439 60-3.181 0.42 40-20-2.2 2.4 2.6 2.8 1.2 1.4 1.6 3.2 3.4 3.6 3.8 4.2 4.4 4.6 Data file Column Solvent1 Solvent2 Solvent3 Temp Gradient 001-0801.D SB CN A1: water B1: acetonitrile D1: 2procent TFA Gradient 1 T 100 90-80-70-60-1.024 50-40-12.82 30-10.06 20-10-1.2 1.4 1.6 1.8 2 2.2 2.4 2.6 2.8 3 3.2 3.4 3.6 3.8 4 4.2 4.4 4.6 4.8 N/A

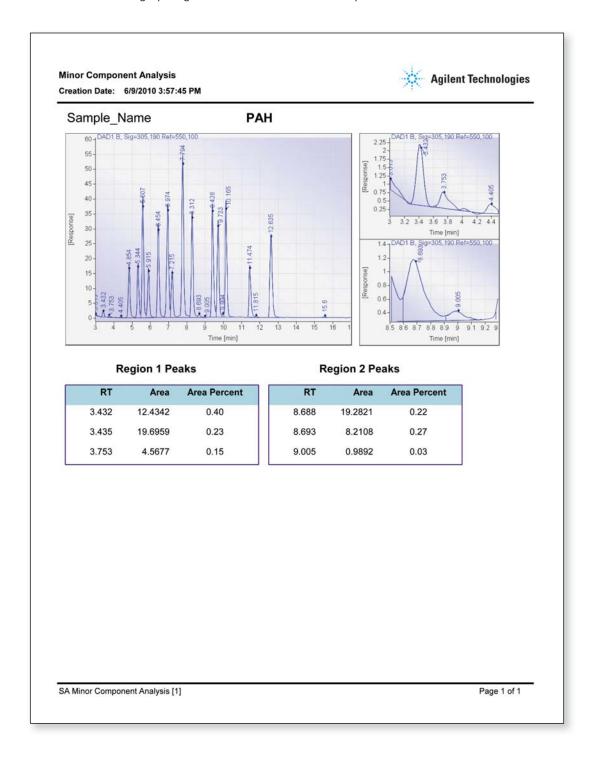
1260methDev_Summary_MF6_General.rdl [28]

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Minor Component Analysis

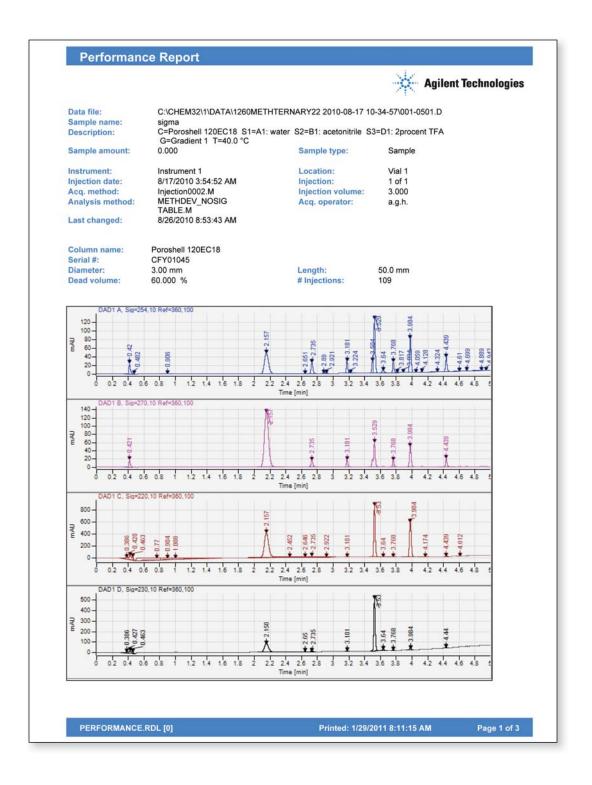
Below is an example of the benefit of excellent sensitivity of Agilent instrumentation combined with the power of the OpenLAB Intelligent Reporter. The DAD enables detection of trace levels of components while the report displays a chromatographic overview in combination with two highly magnified areas to determine the presence of contaminants.



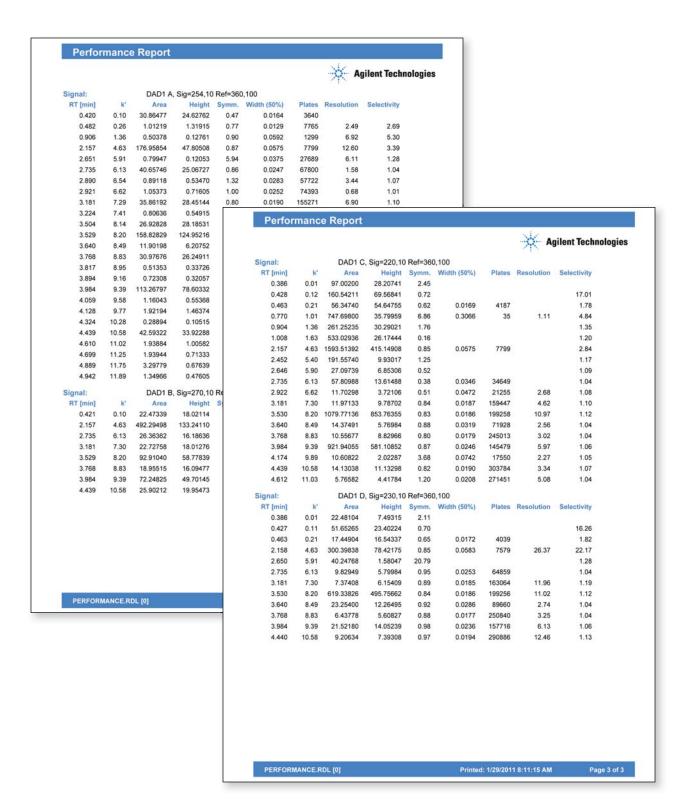


Performance Report

Method and column performance are quickly reviewed using a report template that provides separate chromatograms for different wavelength and column performance results including peak symmetry, theoretical plates, resolution and selectivity.



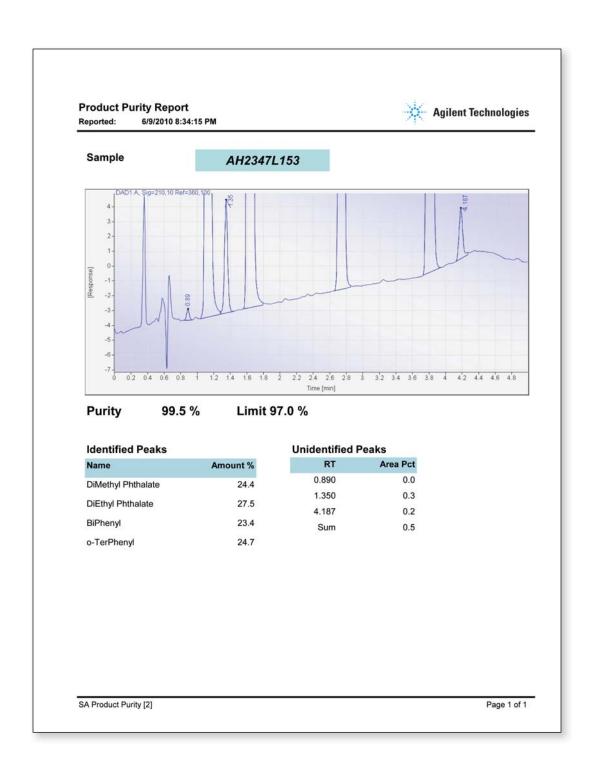






Simple Purity Report

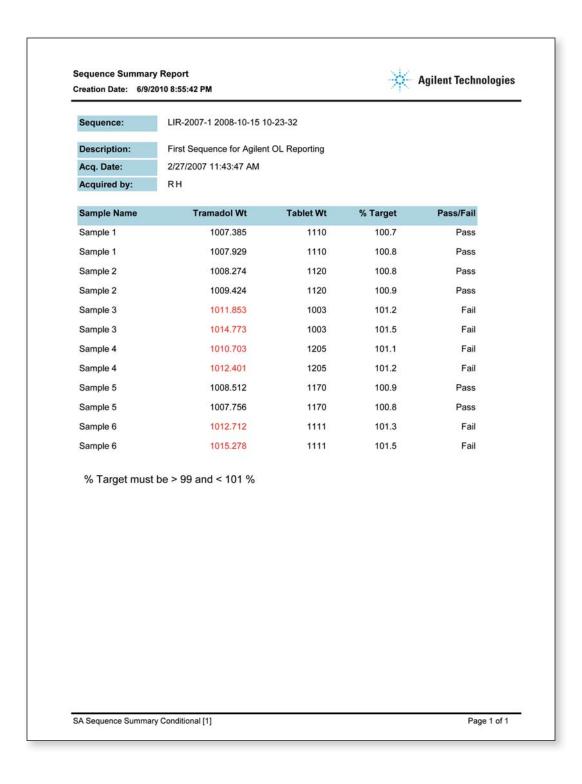
In this example, a simple purity determination is performed by taking into account known and unknown peaks and reporting the ratio as a percentage. This type of report can speed certification of incoming raw material in the pharmaceutical and food industry. The report is minimized to show only a magnified region of the chromatogram and a ratio of the area % of unknown to known components. For quick confirmation, the result and acceptance limit are shown.





Sequence Summary with Limits

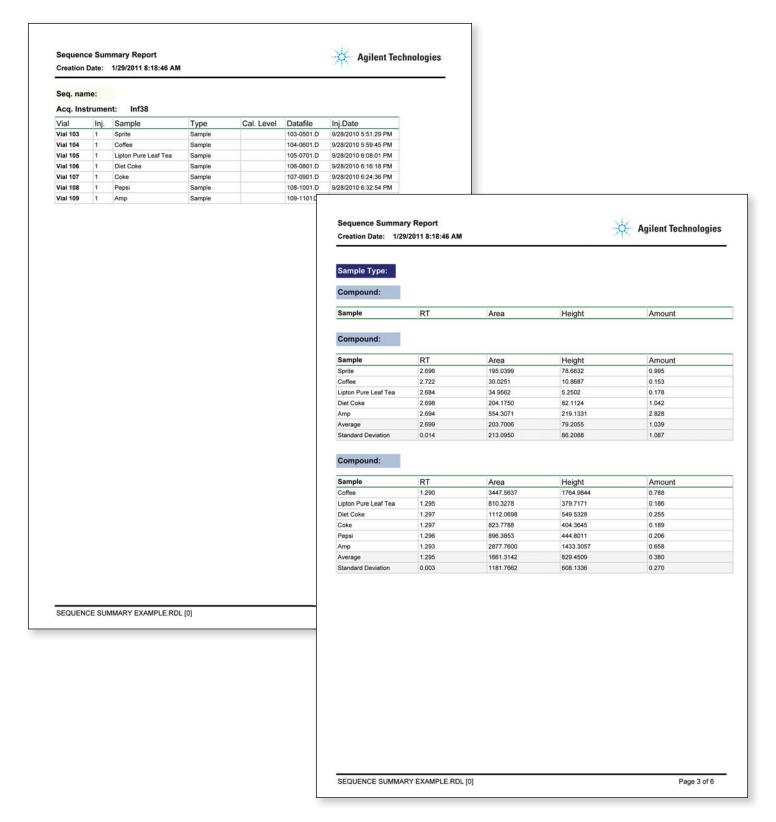
The OpenLAB Intelligent Reporter is the ideal tool to summarize lengthy sequences, perform secondary calculations on target compounds, and display results conditionally on pre-set acceptance limits.





Sequence Summary – Long Form

These different templates are used to determine comparative levels of components in various beverages. Varying levels of detail facilitates a comparison between different types of soft drinks.





Sequence Summary Report Creation Date: 1/29/2011 8:28:09 AM



Sequence: CAFF_SODA 2010-09-28 A1

Description:

Acq. Date: 9/28/2010 5:18:11 PM by: SB

#	Sample	Vial	Injs	Cal Lvi	Datafile	
1	Caffeine Standard 250ug/ml .5ul	Vial 101	1	- 1	101-0101.D	
2	Caffeine Standard 250ug/ml 1ul	Vial 101	1	1	101-0201.D	
3	Caffeine Standard 250ug/ml 3ul	Vial 101	1	1	101-0301.D	
4	Caffeine Standard 250ug/ml 5ul	Vial 102	1	- 1	102-	-
5	Sprite	Vial 103	1		103-	
6	Coffee	Vial 104	1		104-	
7	Lipton Pure Leaf Tea	Vial 105	- 1		105-	
8	Diet Coke	Vial 106	1		106-	
9	Coke	Vial 107	1		107-	
10	Pepsi	Vial 108	1		108-	
11	Amp	Vial 109	1		109-	
12	Caffeine Standard 250ug/ml .5ul	Vial 101	1	1	101-	
13	Caffeine Standard 250ug/ml 1ul	Vial 101	1	- 1	101-	
14	Caffeine Standard 250ug/ml 3ul	Vial 101	1	1	101-	
15	Caffeine Standard 250ug/ml 5ul	Vial 102	1	1	102-	

Sequence Summary Report
Creation Date: 1/29/2011 8:23:23 AM

Agilent Technologies

Sequence Name CAFF_SODA 2010-09-28 A1

Seq Acquired By Steve Brown

Seq Acquired Date 9/28/2010 10:18:11 PM

Sample Name	Compound	RT	Area	Height	Amount	Unit
Caffeine Standard 250ug/ml .5ul	Caffeine	1.294	537.303	268.135	0.12	ug/ml
Caffeine Standard 250ug/ml 1ul	Caffeine	1.293	1076.098	538.029	0.21	ug/ml
Caffeine Standard 250ug/ml 3ul	Caffeine	1.293	3236.960	1620.167	0.65	ug/ml
Caffeine Standard 250ug/ml 5ul	Caffeine	1.295	5432.336	2713.158	1.33	ug/ml
Sprite	Benzoate	2.696	195.040	78.663	1.00	ug/ml
Coffee	Caffeine	1.290	3447.564	1764.984	0.79	ug/ml
Coffee	Benzoate	2.722	30.025	10.869	0.15	ug/ml
Lipton Pure Leaf Tea	Caffeine	1.295	810.328	379.717	0.19	ug/ml
Lipton Pure Leaf Tea	Benzoate	2.684	34.956	5.250	0.18	ug/ml
Diet Coke	Caffeine	1.297	1112.070	549.533	0.25	ug/ml
Diet Coke	Benzoate	2.698	204.175	82.112	1.04	ug/ml
Coke	Caffeine	1.297	823.779	404.364	0.19	ug/ml
Pepsi	Caffeine	1.296	896.385	444.801	0.21	ug/ml
Amp	Caffeine	1.293	2877.760	1433.306	0.66	ug/ml
Amp	Benzoate	2.694	554.307	219.133	2.83	ug/ml
Caffeine Standard 250ug/ml .5ul	Caffeine	1.296	526.626	261.166	0.12	ug/ml
Caffeine Standard 250ug/ml 1ul	Caffeine	1.295	1067.522	533.253	0.24	ug/ml
Caffeine Standard 250ug/ml 3ul	Caffeine	1.294	3253.161	1625.220	0.74	ug/ml
Caffeine Standard 250ug/ml 5ul	Caffeine	1.293	5449.240	2712.749	1.25	ug/ml

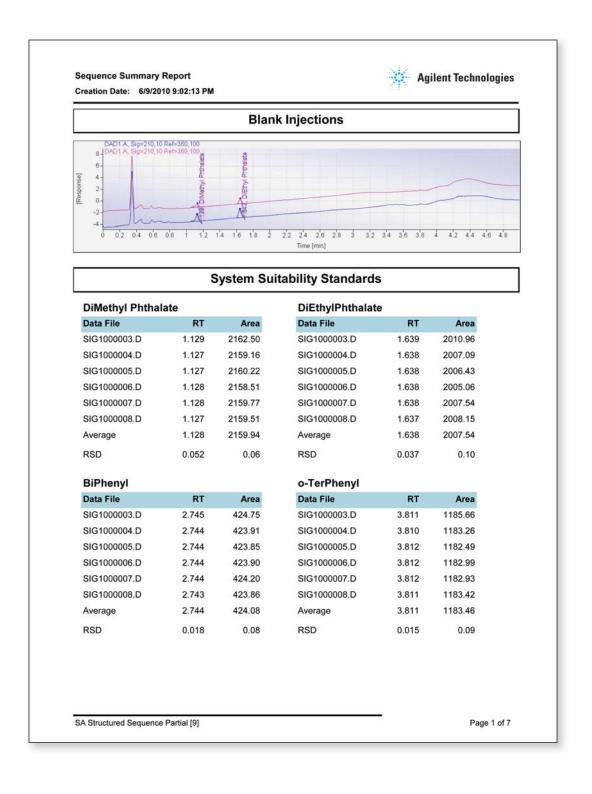
EXAMPLE SEQ SUMMARY 3.RDL [0]

0-SEQ-SUMMARY.RDL [1] Page 1 of 4



Detailed System Suitability and Stability

Extensive system suitability reporting shows the data in a tabular fashion. Graphics are used to show area stability and peak symmetry with inflection points.

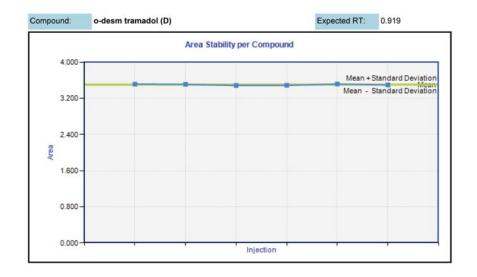




System Suitability and Area Stability per Compound



Compound	Compound: o-desm tramadol (D)						
Sample	Vial	lnj#	RT	Area	Tailing Factor	k'	
SS RSD 2	P1-F-03	1	0.921	3.513	1.11	7.104	
SS RSD 2	P1-F-03	2	0.922	3.507	1.11	7.113	
SS RSD 2	P1-F-03	3	0.92	3.483	1.11	7.093	į.
SS RSD 2	P1-F-03	4	0.919	3.485	1.11	7.091	
SS RSD 2	P1-F-03	5	0.92	3.515	1.11	7.096	
SS RSD 2	P1-F-03	6	0.92	3.494	1.11	7.094	
		Average	0.920	3.500	1.11	7.099	
		Standard D	0.001	0.014	0.00	0.008	

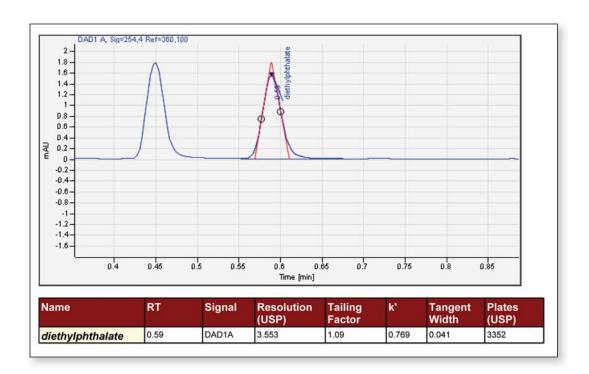


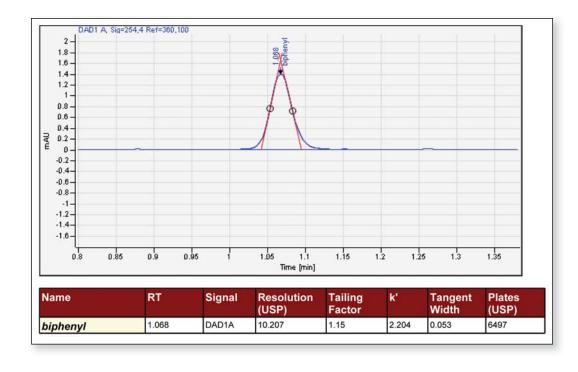
SystemSuit&AreaStabilityPerCompound.rdl [3]

Printed: 2/18/2011 3:13:58 PM

Page 1 of 4



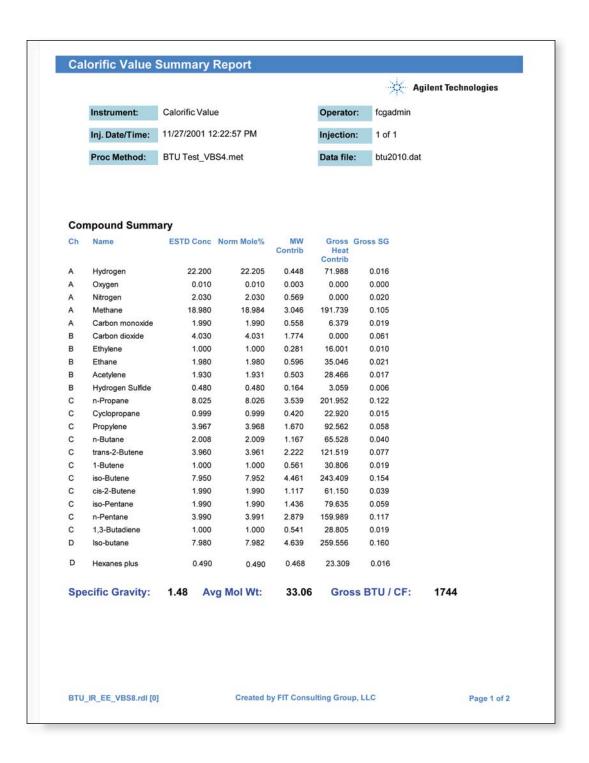






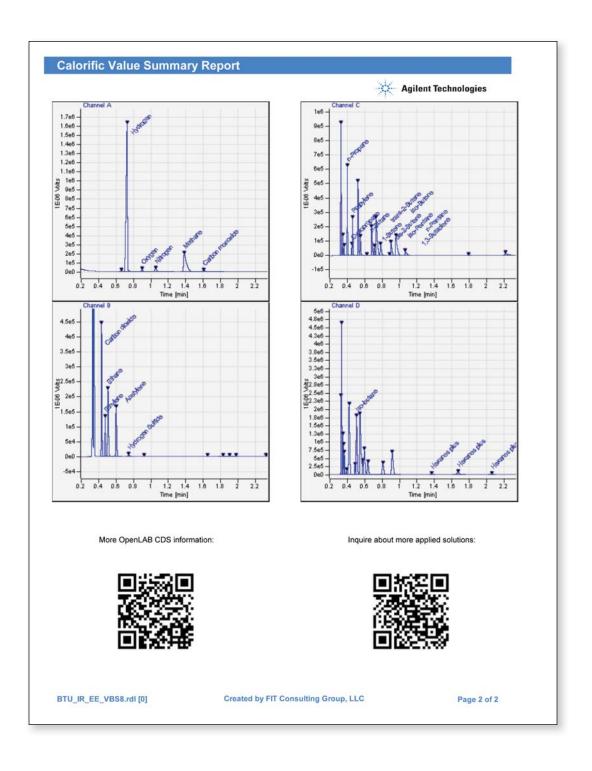
Concise Calorific Analysis

RGA, NGA and BTU analyses require complex calculations designed to yield a final, actionable piece of information that determines the quality of a fuel or gas sample. In this example, the OpenLAB Intelligent Reporter provides a concise result consisting of gross BTU/ft³ value along, average molecular weight, and specific gravity. The report computes 3 physical constants for each of 22 components, and a hexanes-plus group from OpenLAB CDS EZChrom Edition.





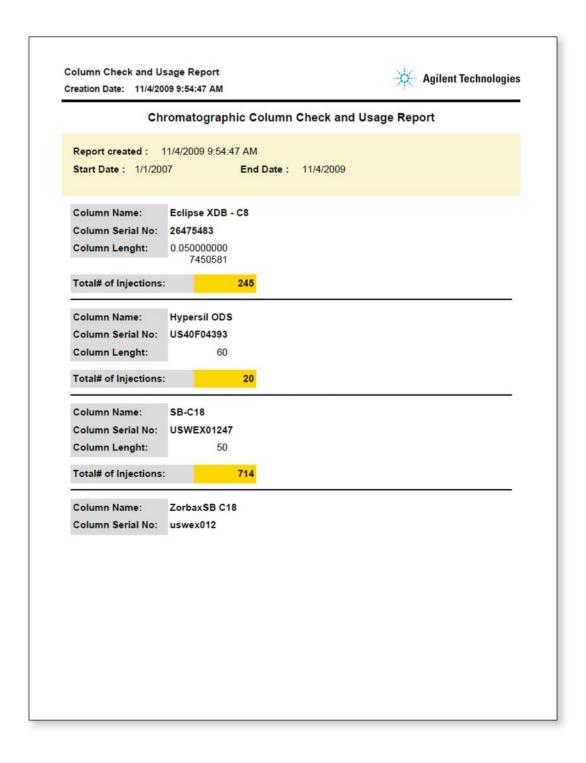
Intelligent reporting also allows the insertion of additional graphics such as logos or bar codes. The example shown includes QR codes that enable a smart phone to quickly access additional details.



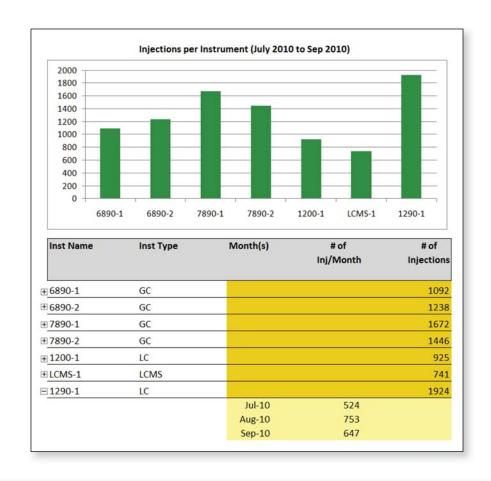


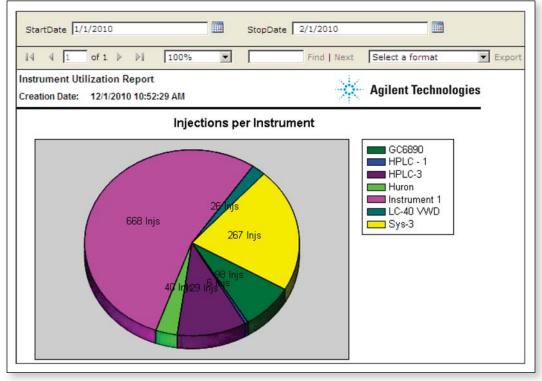
Column Usage Check

Lab managers will benefit significantly from periodic checks of column usage in the laboratory. By combining statistics, summaries, and graphic displays this Column Usage Check report allows the lab manager to easily get an overview of the distribution of resources, determine service intervals, and to make more efficient use of lab resources.

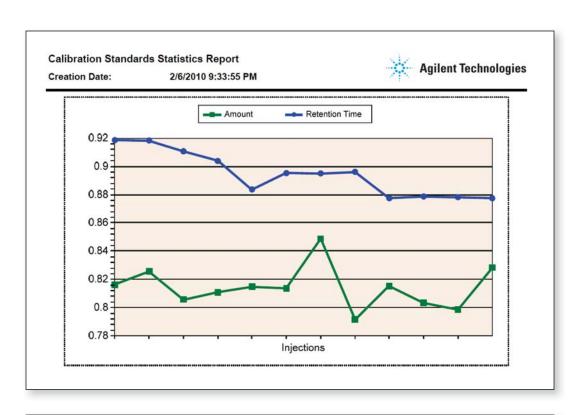










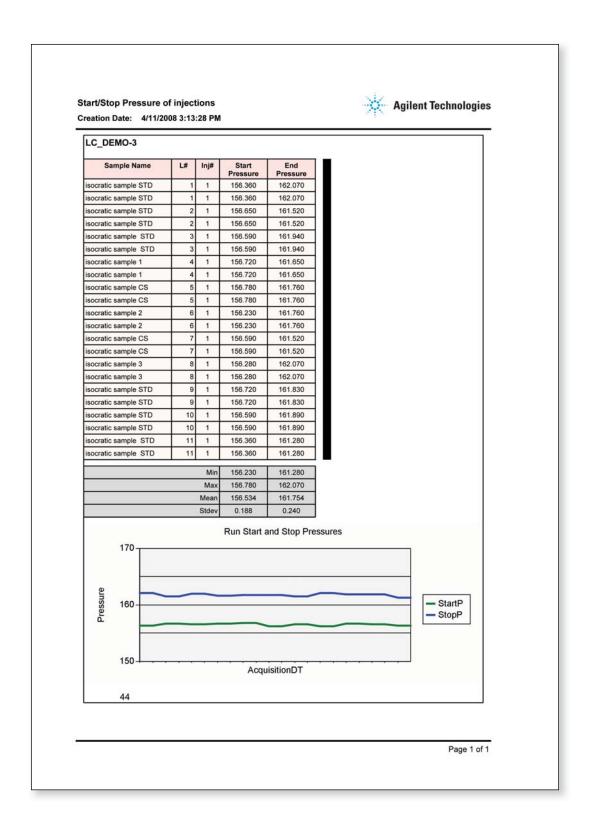


Column Name: Column Serial No:		Eclipse XDB - C8					
		26475483					
Instrument	Acq	Method		Plates USP	Plates EP		
A1100_6							
\Mast		_Data\ICM er\dissoluti eophyl_caff	Overall Average:	5732	5998		
	inet		Overall Average:	5778	6033		
Column Nan	ne:	Hypersil ODS					
Column Serial No:		US40F04393					
Instrument	Acq	Method		Plates USP	Plates EP		
AglTmLab1412							
	CSEX	(AMPLE.M	Overall Average:	0	0		
Column Nan	ne:	SB-C18			-		
Column Seri	al No:	USWEX01247					
Instrument	Acq I	Method		Plates USP	Plates EP		
Instrument 1			<u> </u>				
	XSR_M1.M		Overall Average:	53038	55700		
AT1200							
	XSR	M2.M	Overall Average:	45894	48465		



LC Diagnosis Report

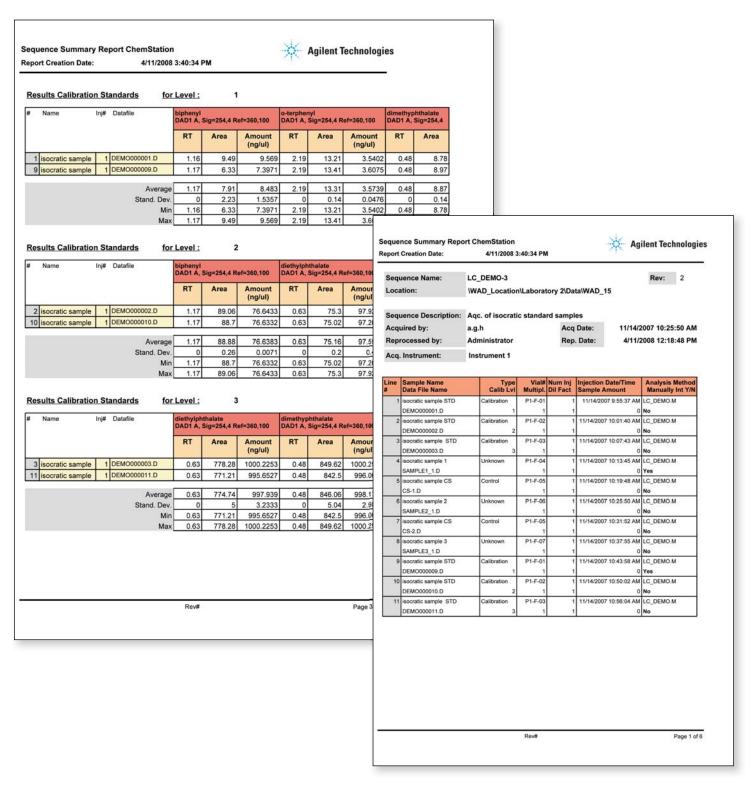
The 'health' of a chromatograph is reviewed in this report focusing on minimum and maximum pressure and on the variations in pressure over the course of numerous runs.





Manual Integration Summary

All the unknowns, calibration standards, and QC standard are analyzed by setting manual integration parameters. The report summarizes results by type of run.





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