

Improving Return on Investment with Smart, Integrated InfinityLab Solutions

Incremental Economic Value of the Agilent 1260 Infinity II Prime LC and the InfinityLab LC/MSD iQ

Introduction

Agilent InfinityLab LC series products provide superior efficiency for liquid chromatography analyses. In 2017, a new member of the InfinityLab LC series—the Agilent 1260 Infinity II Prime LC—was introduced. The 1260 Infinity II Prime LC provides high-end InfinityLab LC technology for routine analysis. This new instrument is the most capable and convenient LC in the 1260 Infinity II LC family.

In contrast to other LC instruments designed for routine analyses, typically with a 400 or 600 bar pressure range, the 1260 Infinity II Prime LC allows operation in an extended pressure range up to 800 bar. The system combines the advantages of flexible quaternary solvent mixing with mixing performance that resembles a binary, high-pressure mixing pump. The system comes with features that automate daily tasks, such as BlendAssist, to create consistent mobile phase mixing and an automatic purge function that can be started remotely. Furthermore, easy column exchange and superior sample logistics help reduce errors and prevent system downtime. The 1260 Infinity II Prime LC even provides Intelligent System Emulation Technology (ISET), which enables seamless method transfer to and from other LC systems. ISET helps reduce the tremendous effort required to revalidate methods transferred to a different generation or type of HPLC or UHPLC.

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Economic Advantages of 1260 Infinity II Prime LC

This white paper illustrates how the new capabilities of the 1260 Infinity II Prime LC can sum up to over 80,000 USD of incremental economic value per year compared to a conventional LC system. This economic value includes the following aspects: 1) reduced cost of operation; 2) reduced downtime; 3) more samples per day; and 4) the utilization of one system for many methods. This white paper can serve as a resource for lab managers while calculating the financial benefit of replacing their current instrumentation with the 1260 Infinity II Prime LC.



Figure 1. The 1260 Infinity II LC has received the 2018 Scientists' Choice Award for Best New Separations Product.

As workflows, number of samples, and instrument utilization differ significantly from lab to lab, it is difficult to calculate an economic value that is applicable to all labs. Therefore, this paper uses a representative sample throughput and instrument utilization as an example with the assumptions shown in Table 1. Conservative assumptions were used, so that the results would apply to many labs. Therefore, for laboratories with greater sample throughput than shown in Table 1, the incremental economic value of a 1260 Infinity II Prime LC may be significantly higher than calculated here.

Table 1. Assumptions of laboratory sample throughput and instrument use per system.

Please enter your own values in the highlighted fields. Use the button below to reset the table to default.

Parameter		Value
Cycle time for typical sample analysis in minutes		
Sample runs per day		
Revenue per sample		
Profit margin		
Solvent use	in liters per day	
	in liters per year	
Yearly column use		
Percentage of time allocated for method development		
Numbers of purges	per day	
	per year	
Yearly number of troubleshooting incidents that can be solved with Lab Advisor		
Solvent cost per liter		

Reduced cost of operation

Consumables and spare parts contribute significantly to the total cost for the operation of an analytical laboratory. For LC analysis, this includes the cost of solvents, columns, fittings, and so on. This section describes how two design features of the 1260 Infinity II Prime LC reduce these operating costs.

BlendAssist

BlendAssist is a software feature that is available for the Agilent 1260 Infinity II Flexible Pump. It delivers automatic blending of buffer or additive concentrations without manual interaction. BlendAssist therefore simplifies LC workflows and accelerates method development. Instead of manually preparing many different solvent bottles with different concentrations of buffers or additives, only four solutions (pure solvent and concentrated stock solution) need to be prepared. After entering the stock concentration and the desired concentration into the BlendAssist software, the instrument delivers the required mobile phase composition required for each specific analysis. In this way, solvent purchase and disposal costs can be significantly reduced compared to the manual premixing approach (see Table 2).

Table 2. Economic value of reducing consumable cost with BlendAssist and InfinityLab fittings.

Please enter your own values in the highlighted fields. Use the button below to reset the table to default.

	Parameter	Value
BlendAssist	Solvents saved by BlendAssist compared to standard blending for method development per year	
	Total solvent cost per year	
	Solvent cost saving using 1260 Infinity II Prime LC with BlendAssist per year	
InfinityLab fittings	Average percentage of column destruction during column exchange	
	Cost per column	
	Column cost saving with InfinityLab fittings per year	
	Saved cost of fittings from other vendors	
Total	Consumable cost saving per year	

Expressing this value economically varies depending on the number of method development tasks. Typical method development tasks include evaluating six concentrations of buffer/additive. In a premixing approach, up to 12 solvent bottles (two for each concentration) would need to be prepared by laboratory staff; alternatively, with BlendAssist, only four solvent solutions need to be prepared. Assuming only 50% of the premixed bottle contents are consumed during the experiment, BlendAssist offers a 33% reduction in solvent consumption. Taking the assumption shown in Table 1, 130 L solvent per instrument and 50% of instrument utilization is for method development, resulting in a saving of 1,122 USD per system per year. In addition, pipette tips, filter membranes, and even bottle washing contribute to further savings, which are not considered here.

InfinityLab fittings

An incorrectly installed column can lead to peak tailing, peak broadening, split peaks, and carryover. Sometimes, faulty connections can also cause damage to the column. InfinityLab Quick Connect and Quick Turn fittings (Figure 2) simplify installation, ensuring a dead-volume-free column connection up to 1300 bar. These fittings reduce the failure rate during column exchange and decrease associated costs caused by destroyed columns.



Figure 2. Agilent InfinityLab Quick Connect fitting.

As shown in Table 1, an average of 12 columns are assumed to be connected to each LC system per year. It is assumed that the LC system is run 70% of the time by experienced analysts and 30% of the time by unexperienced operators, and that InfinityLab fittings reduce the failure rate of unexperienced operators from 15 to 0%. InfinityLab fittings result in a decrease of 4.5% in the failure rate for each LC system, saving 0.54 columns per system per year. A conventional column costs 500 USD. Therefore, InfinityLab fittings provide a saving of 270 USD in column cost per system per year.

In addition, InfinityLab fittings can be used for columns from many vendors, so there is no need to purchase extra fittings from other vendors. Assuming that columns from two other vendors are used on each system, InfinityLab fittings help to save 700 USD per year.

The economic value of decreased downtime

Every time an LC system goes into error mode or must be stopped due to malfunction for maintenance purposes, it results in potential economic loss. In this section, three features of the 1260 Infinity II Prime LC that reduce system downtime are highlighted. These aspects enable laboratories to analyze more samples in less time and provide internal or external customers with answers more quickly.

Automatic solvent purge

The 1260 Infinity II Flexible Pump has an integrated multipurpose valve. With this valve, a simple click in the user interface of the software begins an automatic purge without requiring direct interaction with the instrument in the lab. By doing this, at least 1 min can be saved during each purge. Assuming one purge per working system per day as shown in Table 1, up to 260 min can be saved every year using the automatic purge feature.

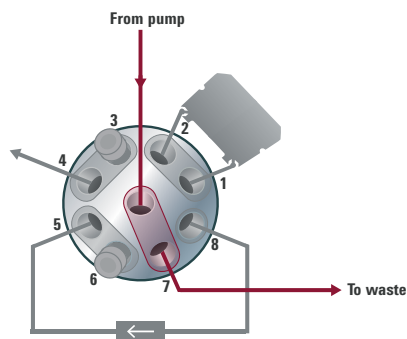


Figure 3. Valve position in purge mode.

InfinityLab fittings

As already mentioned, InfinityLab Quick Connect and Quick Turn fittings ensure that every user achieves a perfect column connection every time a column is exchanged, regardless of experience. No tool or special training is required. Column connections are therefore done quickly and significant time saving can be expected. As previously mentioned, it is assumed that an LC is operated 70% of the time by experienced operators and 30% by inexperienced users.

If InfinityLab fittings reduce the time to install a column for experienced operators by 0.5 min and for inexperienced operators by 1.5 min, 0.8 min is saved on average for each connection of a column. Therefore, if 150 column connections are performed on each system per year, 120 min are saved annually.

Lab Advisor

Lab managers increasingly recognize the importance of preventive maintenance of LC systems to avoid unplanned instrument downtime. When instruments are unexpectedly in an error state, troubleshooting can be time-consuming. Agilent Lab Advisor is software designed for performing calibration, diagnosis, and maintenance of Agilent LC instruments. Lab Advisor provides a series of tests and tools to assist an operator or Field Service Engineer while troubleshooting. This software expedites instrument repair and reduces downtime during troubleshooting. In Table 1, it is assumed that troubleshooting is required 0–1 times per year and that troubleshooting is completed with Lab Advisor within 2–3 hours. This is compared to a manual approach without Lab Advisor, where troubleshooting may take up to 1–2 days (16 working hours) of downtime (including contacting engineers, making an appointment, the engineers' visit, etc.). Lab Advisor therefore reduces downtime by 840 min (14 hours) for each LC instrument annually.

To summarize, the three features provided with the 1260 Infinity II Prime LC listed in Table 3 reduce downtime by 1,220 min per year. Assuming a typical sample analysis cycle time of 25 min, 49 more samples could be analyzed per year, if downtime could be avoided. As shown in Table 1, a service lab charges on average 40 USD per sample. This avoided downtime therefore represents 1,952 USD of incremental revenue annually. Recognizing that there are normally large fixed human resource and infrastructure costs, the assumption shown in Table 1 is that the revenue is associated with a 20% profit margin. Thus, 390 USD of incremental profit is gained per year.

Table 3. Economic value of incremental profit with automatic purge, InfinityLab fittings, and Lab Advisor.

Please enter your own values in the highlighted fields. Use the button below to reset the table to default.

	Parameter	Value
Automatic purge	Reduced time for each purge in minutes	
	Numbers of purges	per day
		per year
	Saved time with automatic purge per year in minutes	
InfinityLab fittings	Reduced time for each column connection procedure in minutes	
	Number of connecting incidents per year	
	Total saved time with InfinityLab fittings per year in minutes	
Lab Advisor	Number of troubleshooting incidents that can be solved with Lab Advisor per year	
	Saved time with Lab Advisor per year in minutes	
Total	Saved time per year in minutes	
	Cycle time for typical sample analysis in minutes	
	Number of incremental samples that could be run	
	Assumed revenue per sample	
	Incremental revenue per year	
	Incremental profit per year	

The value of higher sample throughput per day

Lab managers understand that high-throughput analysis can contribute significantly to the economic success of a laboratory and an analysis cycle time consists of sample injection, gradient run time, column wash, and equilibration. The following two sections will describe how the 800-bar capability and the automated column regeneration with dual-needle injection can provide higher sample throughput.

Up to 800 bar for columns with smaller particles

1260 Infinity II Prime LC offers ultimate performance for flow rates up to 5 mL/min within a pressure range of up to 800 bar. Smaller particle columns can be applied with the 1260 Infinity II Prime LC for faster analysis compared to conventional 400 or 600 bar LC systems. Assuming, as shown in Table 1, that a sample analysis cycle takes 25 min under 600 bar pressure, the 1260 Infinity II Flexible Pump saves around 7 min per sample run.

Automated column regeneration and dual-needle injection

With automated column regeneration (ACR), a setup of two pumps and two columns is used to optimize run times through reduction of idle times. This is achieved through overlapping the time needed for regeneration of a first column with the gradient separation of the next sample on a second, similar column. By doing this, the total analysis time can be reduced, since the time needed for column wash and re-equilibration can be minimized. With the dual-needle option of InfinityLab Multisamplers, a further time optimization can be achieved. The Smart Overlap high-throughput mode provides simultaneous analysis on the first flowpath and overlapped sample draw using the second flowpath preparing the next run.

As shown in an [Agilent application note](#), a 60% time saving can be achieved using alternating column regeneration with dual-needle injection for a fast run. For common methods (15 min analysis, 10 min column wash, and re-equilibration), 40% of analysis cycle time can be saved by combining ACR with dual-needle injection. It is assumed that ACR with dual-needle injection is not applied for method development, which is thought to represent 50% of use annually (Table 1). The cost of the extra pump and column will also be considered while calculating the economic value.

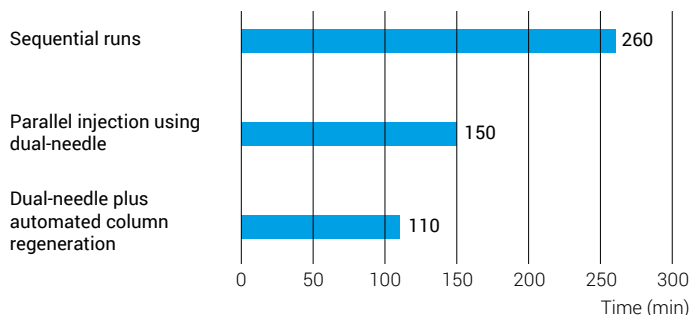


Figure 4. Time savings for ultrahigh throughput over 100 injections using alternating column regeneration.

As shown in Table 1, it is assumed that the cycle time for sample analysis is 25 min and that labs run 20 samples per day on one LC instrument. If using smaller particle columns saves 7 min per run, a cycle time of 18 min can be achieved. This shorter cycle time results in an increase of seven to eight incremental samples per day. For 50% of the time annually (130 days), we do not take ACR and dual-needle into account. For the other 130 working days, ACR and dual-needle brings a 40% further reduction of analysis cycle time. That equates to 26 incremental samples per day. All together, it is possible to run 4,290 samples more per year. Taking the assumption of sample revenue and profit margin shown in Table 1 and cutting the cost of the extra pump and column for ACR, this represents 150,600 USD incremental revenue and 30,120 USD of incremental profit per year (see Table 4).

Table 4. Economic value of more samples per day with 800 bar, ACR, and dual-needle injection.

	Parameter	Value
800 bar	Analysis time reduction in minutes	
ACR and dual-needle	Injector overlap time saving per analysis	
	Cost for extra pump needed	
	Cost for extra column needed per year	
Total	Incremental samples per year that could be run with 800 bar and ACR with dual-needle injection per year	
	Incremental revenue per year	
	Incremental profit per year	

The value of applying one system for many methods

Intelligent System Emulation Technology (ISET)

ISET provides the 1260 Infinity II Prime LC with the unique capability to emulate other LC systems. It creates the possibility to seamlessly transfer methods from one LC to another LC instrument without risk. There are different ways to apply ISET: the first is to run existing methods developed on a different LC system directly on the 1260 Infinity II Prime LC without modification. The alternative is to develop methods on the 1260 Infinity II Prime LC for other target systems without the necessity to re-adjust the method on the target system. Therefore, a single 1260 Infinity II Prime LC with ISET functionality can replace several other LC instruments. Moreover, working on only one system simplifies the overall lab workflow, saving space, and reducing the cost of instruments, training, repair parts, maintenance, etc. For this calculation, it is assumed that the ISET feature of the 1260 Infinity II Prime LC could help to avoid the purchase of one extra LC of different origin per year. The average LC price is estimated to be 50,000 USD, training for new instrumentation is 450 USD, and maintenance and other costs is 2,000 USD. Therefore, the 1260 Infinity II Prime LC with ISET could help to reduce total spending by up to 52,450 USD per year (see Table 5).

Table 5. Economic value of applying one system for different methods with ISET.

Please enter your own values in the highlighted fields. Use the button below to reset the table to default.

Features	Parameter	Value
ISET	Fewer number of LC systems purchased per year	
	Saved spending per system	
	Saved training costs per system	
	Yearly saved maintenance cost per system	
	Cost saving per year	

Incremental economic value with the 1260 Infinity II Prime LC

The calculations performed in the previous sections of this white paper highlight how the InfinityLab LC technology of the 1260 Infinity II Prime LC could contribute to achieve more than 80,000 USD incremental economic value per year compared to a conventional LC system (see Table 6).

In addition, there are many other features designed into the 1260 Infinity II Prime LC that should be considered, because they can provide further economic benefit. For example, InfinityLab Quick Change valves significantly reduce the need for column exchanges, resulting in time saved and in a reduction of column-related failure rates. The InfinityLab Companion is another option that can help to save time through direct control by a local interface, which can be operated remotely or via mobile. However, these savings are not considered in this paper, because of the high variability from lab to lab.

On top of the directly calculated economic values, important features of the 1260 Infinity II Prime LC can contribute to extra benefits: binary-like mixing performance for higher precision and accuracy of results; smaller delay volume compared to other quaternary systems; lowest carryover from sample to sample; and the superior sensitivity and extended linear range in DAD detection.

In summary, the 1260 Infinity II Prime LC streamlines LC workflows in analytical labs and simplifies the daily life of operators, resulting in reduced failure rates and ultimately leading to more consistent and reliable results.

Table 6. Estimated economic value of using an Agilent 1260 Infinity II Prime LC.

Features	Parameter	Value
BlendAssist InfinityLab fittings	Operating cost savings	
Automatic purge InfinityLab fittings Lab Advisor	Reduced downtime savings	
Automated column regeneration Dual-needle injection	Higher sample throughput	
ISET	Reduced cost for extra instruments	
	Total incremental economic value per year	

Efficiency Increase and Financial Benefits of moving to Mass Detection with the InfinityLab LC/MSD iQ

The compact and intuitive InfinityLab LC/MSD iQ is the perfect partner for labs performing small molecule analysis in pharmaceutical drug discovery, development, and QA/QC labs as well as academia, food, and chemical/materials labs that need mass spectral information for making data-driven decisions. Unlike other complicated and costly LC/MS and LC/MS/MS systems that require extensive MS knowledge, the InfinityLab LC/MSD iQ is specifically designed for chemists, chromatographers, and new users looking for more throughput and improved financials in their lab operation.



Figure 5. Agilent InfinityLab LC/MSD iQ with the 1260 Infinity II Prime LC in the InfinityLab Flex Bench MS.

The addition of mass detection to UV-based methods can greatly improve the efficiency of chromatography and the financial results of the lab operation. With added mass information, even coeluting species can be easily distinguished by their mass, permitting shorter chromatographic separations and allowing for an overall increase in sample throughput. As a result, more analyses can be performed per day, per instrument, increasing the lab's throughput while reducing costs, which improves overall financial performance.

When used in conjunction with Agilent MassHunter WalkUp software, chemists and scientists can quickly submit their samples in four easy steps. All the user must do is log in, choose an analysis method, enter the sample information, and place the sample in the automated liquid sampler. The system automatically generates and emails a report that assists the user in determining the presence or absence of both desired and undesired sample components.

The InfinityLab LC/MSD iQ also provides more certainty in analytical results. For example, compounds that respond poorly to UV detectors can be detected by mass spectrometry. In addition, mass detection can detect trace compounds, sometimes at levels 100 times better than UV only-based workflows. Finally, where multiple analytes are analyzed, such as in reaction monitoring or chemical synthesis verification, using mass detection instead of UV detection provides you with molecular weight, structural information, and selectivity, replacing the use of chemical standards and retention time to identify peaks. MS provides direct mass information to determine which peaks are the compounds of interest, further saving time and maximizing sample throughput.

The addition of the Agilent InfinityLab Flex Bench MS further optimizes your whole lab set-up. You can now keep your InfinityLab LC/MSD Series systems in one stack with easy access to all areas. This saves over 2 hours of maintenance time without the need to remove modules for routine maintenance.

Table 7. InfinityLab LC/MSD iQ Cost-Saving.

Please enter your own values in the highlighted fields. Use the button below to reset the table to default.

Parameter	LC/UV Approach	LC/MSD iQ
Run time for a typical sample in minutes		
Average number of samples per day		
Time taken to run sample set in minutes *		
Sample revenue per sample		
Total revenue per day		
Working days per year		
Additional yearly revenue potential		

* LC/UV run time includes 3mins re-equilibration time per run

Economic value of InfinityLab Poroshell 120 columns

Superficially porous particle (SPP) LC columns can generate high efficiency at lower pressure, relative to their totally porous particle (TPP) column counterparts. The higher efficiency can be used to speed up analyses or improve results—giving better resolution and sensitivity.



Figure 6. InfinityLab Poroshell 120 columns.

Changing from a totally porous column to a superficially porous column, such as [InfinityLab Poroshell 120](#), is another option for achieving incremental economic value. For example, let's refer back to the assumptions made in Table 1 of this paper. This lab currently does 20 samples runs per day. If this lab is currently using 5 µm TPP columns to do these runs, by migrating to 2.7 µm InfinityLab Poroshell columns, they could save ~37.5% of run time and solvents used. These numbers are averaged from different comparison experiments that were performed.

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Printed in the USA, February 24, 2020
5994-1796EN
DE.2958796296

