



# Benchtop NMR Spectroscopy Market Analysis

Ease of Use and Low Cost Boosts Growth

A Frost & Sullivan White Paper

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## INTRODUCTION

Miniaturization is a paradigm in the scientific instrumentation world today. The convenient nature of compact instruments is gaining importance in the chemical laboratories, testing environments as well as process environments. These are attributed to the increased accessibility, affordability and often ease of use that generally increases efficiency. Although one of the later analytical techniques to be miniaturized, this is also the case in Nuclear Magnetic Resonance (NMR) Spectroscopy, with the emergence of a new class of NMR technology: the compact, benchtop NMR spectrometer.

The nuclear spin and resultant magnetic properties of atomic nuclides was first discovered in the 1920s and was exploited throughout the 1950s and beyond in the development of the now well-known technique referred to as NMR. NMR Spectroscopy is invaluable in identifying unknown chemical compounds because it is an extremely information rich technique providing evidence of the individual building blocks within a molecule, the intramolecular connectivity of these components, as well as the relative amount of each component. NMR Spectroscopy, not well known outside of chemistry, is the same technique of MRI, but instead of considering a human 'sample' to afford a diagnostic image, NMR Spectroscopy analyzes a chemical sample to generate a spectrum detailing sample composition. Subsequently, NMR has been widely adopted technique in academic and governmental research to elucidate and/or confirm molecular structure and to determine sample purity. Although less common in industry, NMR Spectroscopy is an important component in many fields.

NMR Spectroscopy currently represents the largest market segment in the well-established molecular spectroscopy vertical, with the majority of users coming from academic research or pharmaceuticals. Prior to 2010, NMR spectrometers were predominately represented by high-field, superconducting instruments. These extremely powerful, very large magnets that are expensive, both in capital costs as well as operating expenditures, require dedicated personnel to maintain the magnet with frequent cryogen fills. Resultantly, this technique has remained limited to centralized analytical facilities where experts collect and interpret data.

The benchtop NMR spectrometer adds a new layer of NMR workflow that can begin to address the cost, accessibility and requisite knowledge limitations of high-field NMR spectrometers. With its price point, low maintenance requirements, and small footprint benchtop NMR spectrometers are poised to expand the NMR market into numerous fields. First adopters were primarily in academic teaching, but the development of software and hardware features has lead to wider adoption of these instruments in chemical research, QA/QC, and process chemistry.

One of the key potential opportunities for growth in this market is the influence of Internet of Things (IoT) and its implications. Ubiquity, return on investment (ROI) and security are factors to be considered and that can drive the demand for IoT. Integrated with IoT, the importance of analytical instruments increases as the Ethernet allows for higher manufacturing gains with better performance than legacy technologies.

This position paper focuses on the rapidly growing benchtop NMR market. Benchtop NMR spectrometers were first commercialized in 2012 and have advanced quickly since that time. The goal is to elucidate the benefits of benchtop NMR spectrometers and its various application areas driving growth. The white paper aims to be a key resource for organizations interested in NMR spectroscopy and how the market lies ahead for benchtop NMR spectrometers.

# 1

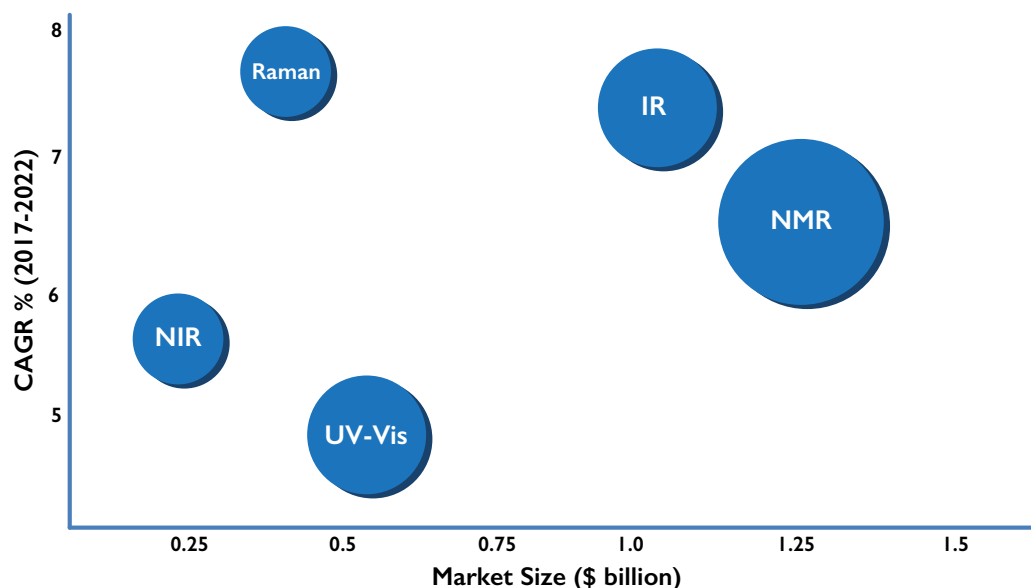
## IMPORTANCE OF NMR SPECTROSCOPY – GAINING MOMENTUM IN COMPACT NMR SPECTROMETERS

NMR spectroscopy is renowned for determining chemical structure and molecular configuration. NMR technology can be classified into 3 categories:

- Relaxometers - low-field, low-resolution
- Benchtop NMR spectrometers – low-field, high-resolution (sometimes referred to as medium resolution)
- Superconducting NMR spectrometers – high-field, high-resolution

Low-resolution NMR spectroscopy, measures bulk sample properties (e.g., viscosity of petroleum or solid fat content of chocolate) and does not provide specific chemical structure information. High-resolution NMR spectroscopy, on the other hand, can also be used to determine bulk property measurements like the low-resolution relaxometers, but additionally they can be used to learn information about the individual chemical components of, or speciate a sample. In other words, the high-resolution NMR enables intramolecular structural connectivity data of a chemical compound to be determined. The difference between low-field and high-field NMR spectrometers is governed by the physics behind the NMR experiment. As the field increases (i.e., the strength of the magnetic field), more atomic nuclei are observed in each experiment, ultimately resulting in better sensitivity. Additionally, higher-field results in better resolution of the chemical shifts. Thus, while both low-field (benchtop) and high-field (super-conducting) high-resolution NMR spectrometers provide structural data; the higher-field magnets can be used for more complex chemical compounds that are found in lower concentrations (e.g., identifying natural products extracted from sea sponges). Regardless, there are a vast number of applications that do not require higher-fields and are more than sufficiently addressed by low-field instruments.

Molecular Spectroscopy Market: Market Sizing, Global 2016










The three key factors propelling the demand for benchtop instruments are accessibility, portability, and ease-of-use. Although a new class of instrument, imparting knowledge and increasing confidence among end users in using benchtop instruments is expected to exponentially increase the use of these instruments both in new applications where NMR spectroscopy has not been previously used, but also as a pre-screening tool to reduce outsourcing costs or free up time on busy high-field NMR spectrometers.

## 2

### BUSINESS BENEFITS – ADVANTAGES OF NMR SPECTROSCOPY OVER OTHER ANALYTICAL METHODS

While NMR Spectroscopy remains the most commonly reported technique in organic and inorganic synthetic research, its adoption in industry has lagged behind. This is primarily due to the economic realities of super-conducting technology. The driving force behind increasing the use of NMR spectroscopy, either to replace, compliment or simplify other existing analytical techniques is three-fold, it: 1) elucidates connectivity within a molecule; 2) is quantitative without calibration; and 3) has output that is not masked by turbid or inhomogeneous solutions. Additionally, sample preparation is simple, and the experiment is non-destructive, allowing the user to recover samples after analysis. The primary limitation is that it is considered a less sensitive technique when compared to UV-Vis or MS, see table 1.

Table 1: Comparison of Selected Molecular Spectroscopy Techniques

 Technique	 Principle	 Sample Prep	 Sensitivity	 Advantages	 Disadvantages	 Primary Application(s)
Infrared Spectroscopy (IR)	Observes vibrational excitation of a molecule upon absorption of quantized light 190- 780 nm	Easy, different preps (e.g., pellet, Nujol mull result in different spectra and masking agents)	Mid-to-low sensitivity	<ul style="list-style-type: none"> <li>Well-established chemometric methods and libraries of compounds</li> <li>Accessibility of instrumentation</li> </ul>	<ul style="list-style-type: none"> <li>Evidence of functional groups but not connectivity or number</li> <li>Extensive calibration required for quantification</li> <li>Depending on sampling method, sample may or may not be recovered</li> </ul>	Identifying presence or absence of specific functional groups
Mass Spectrometry (MS)	Determination of mass/charge ratio for ionized molecular fragments	Difficult, m/z intensity often operator-dependent	Sensitive	<ul style="list-style-type: none"> <li>Isotopic patterns help facilitate structural elucidation</li> </ul>	<ul style="list-style-type: none"> <li>Only see molecules and fragments that can be ionized</li> <li>Extensive calibration required for quantification</li> <li>Analyte cannot be recovered, sample destructive</li> </ul>	Chemical analysis and confirmation
Nuclear Magnetic Resonance (NMR)	Absorption of radio frequency radiation due to changes in spin states of atomic nuclides	Easy, repeatable	Low sensitivity	<ul style="list-style-type: none"> <li>Full structural characterization</li> <li>Quantitative without calibration</li> <li>Sample can be recovered, non-destructive</li> </ul>	<ul style="list-style-type: none"> <li>Sensitivity</li> <li>Access to traditional NMR equipment</li> </ul>	Full structure elucidation and molecular configuration determination
Ultra-violet Spectroscopy (UV-Vis)	Absorption of light particles at quantized wavelengths indicative of electronic transition of a chromophore	Slow, often operator-dependent	Extremely sensitive	<ul style="list-style-type: none"> <li>Electronic information (e.g., band gap, conjugation)</li> <li>Sample can be recovered, non-destructive</li> </ul>	<ul style="list-style-type: none"> <li>Evidence of chromophore but not molecular structure</li> <li>Quantitative via Beer's Law</li> </ul>	Electronic materials characterization and detector for HPLC

NMR Spectroscopy is a non-targeted technique that can be used to examine an analyte, looking most commonly at  $^1\text{H}$  or  $^{13}\text{C}$ , but also at  $^7\text{Li}$ ,  $^{11}\text{B}$ ,  $^{19}\text{F}$ , and  $^{31}\text{P}$  nuclides, as well as many others.  $^1\text{H}$  NMR Spectroscopy observes hydrogen atoms, commonly referred to as 'protons' and is the most commonly observed nucleus to retrieve the structural information of the molecules giving the ubiquitous nature of hydrogen atoms.

Being a non-destructive testing mechanism, NMR spectroscopy allows recovery of an analyte after analysis, as opposed to a destructive method like MS. In order to overcome the barriers to adoption of NMR Spectroscopy in industry, there needs to be better accessibility, simplification of operation and maintenance and better education about the relative advantages of NMR Spectroscopy. In market surveys, apparent clients suggested they would want to take stock of the benchtop NMR for at least a year before shifting to NMR technology. Vendors selling the benchtop NMR spectrometers have a herculean task of tutoring the users, and developing application case-studies and proof-of-concepts such that the technology may reap its full benefit as a supplementary tool for high-field NMR and a disruptive innovation for quantitative techniques like high-performance liquid chromatography (HPLC). Nevertheless, this trend is witnessing a gradual change thereby raising the prediction of the growth rate to high double digits each year.

One of the prominent reasons for the acceptance of benchtop NMR is its accelerated result delivery besides being cryogen-free. This omits the need for a cooling apparatus and weekly cryogen fills. In real-time industrial lab applications where the results are required rapidly without commodity detriment, NMR can provide data in as little as 15 seconds.

Internet of Things (IoT) is a popular trend influencing the growth of the analytical instrumentation market. Driving the future of this market is the lab virtualization using automated sample changes. The cloud spectrum sharing assisted by the IoT helps implement the differential mathematical analysis adeptly.

### 3

## NMR SPECTROSCOPY MARKET – DRIVING FACTORS AND KEY VENDORS










NMR spectroscopy forms the largest segment in the molecular spectroscopy market, including UV-Vis, IR, Near-IR, and Raman spectroscopy. The key end users of these instruments are: (i) synthetic chemists (including academic research, pharmaceuticals, biotechnology, petrochemicals, cosmetic and personal care, materials chemists and polymers); and (ii) quality assurance personnel (including environmental testing, food and beverage testing).

NMR spectroscopy is an effective tool in pharmaceutical industry for drug discovery and efficacy. Drug regulations in the pharmaceutical industry will become more stringent in the developed and developing countries. This will drive the demand for molecular analysis spectrometers. Similarly, the need for these instruments in the academics especially in undergraduate courses are gaining momentum that will enable students to get hands-on experience and thereby use these instruments effectively in their work life. However, these large instruments are highly expensive and require skilled personnel. In such a scenario, benchtop NMR spectrometers have emerged as the best-in-class solution especially for low field and less sensitive applications. They are compact in nature and also low cost that is ideal for academics.

In addition, benchtop NMR is a supplementary tool to expand NMR into new applications in pharmaceuticals, academics, polymer research, reaction monitoring, and food among others. It is widely available to applications where it's not feasible to have a high-field NMR due to its expensive costs incurred.

Academics and pharmaceuticals compose >60% of the existing NMR market. The demand is filled by the two existing super-conducting NMR magnet vendors: Bruker and JEOL; but there are many remaining Varian/Agilent/Oxford Instruments systems that remain in the field. In the almost nascent benchtop arena, however, the vendors are Nanalysis Corp., Magritek Ltd., Thermo Fisher Scientific, Inc., and Oxford Instruments Plc.

Benchtop NMR Spectroscopy Market: Company Portfolio Analysis, Global 2016

 Company	 Product Name	 Key End Users	 Uniqueness	 Price Range
	<ul style="list-style-type: none"> <li>• NMRReady-60e</li> <li>• NMRReady-60PRO</li> </ul>	<ul style="list-style-type: none"> <li>• Academic teaching</li> <li>• Pharmaceuticals</li> <li>• Chemical Producers</li> </ul>	<ul style="list-style-type: none"> <li>• Lightweight</li> <li>• All-in-one</li> <li>• Brand Image, especially in USA</li> <li>• High-connectivity</li> <li>• Vision of application development</li> </ul>	US \$45,000 to US \$70,000
	<ul style="list-style-type: none"> <li>• Spinsolve 43</li> <li>• Spinsolve 60</li> <li>• Spinsolve 80</li> <li>• Spinsolve ULTRA</li> </ul>	<ul style="list-style-type: none"> <li>• Academic teaching</li> <li>• Academic research</li> <li>• Pharmaceuticals</li> </ul>	<ul style="list-style-type: none"> <li>• Brand image, especially in Europe</li> <li>• Different models for various applications</li> </ul>	US \$45,000 to US \$125,000
	<ul style="list-style-type: none"> <li>• Pulsar</li> </ul>	<ul style="list-style-type: none"> <li>• Academic teaching</li> <li>• Pharmaceuticals</li> <li>• Food Science</li> </ul>	<ul style="list-style-type: none"> <li>• Good portfolio of NMR analyzers as well</li> </ul>	US \$70,000 to US \$80,000
	<ul style="list-style-type: none"> <li>• picoSpin™ 45 Series II</li> <li>• picoSpin™ 80 Series II</li> </ul>	<ul style="list-style-type: none"> <li>• Academics</li> </ul>	<ul style="list-style-type: none"> <li>• Global recognition in analytical instrumentation market</li> </ul>	US \$25,000 to US \$50,000

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**'BENCHTOP' IS THE KEY**

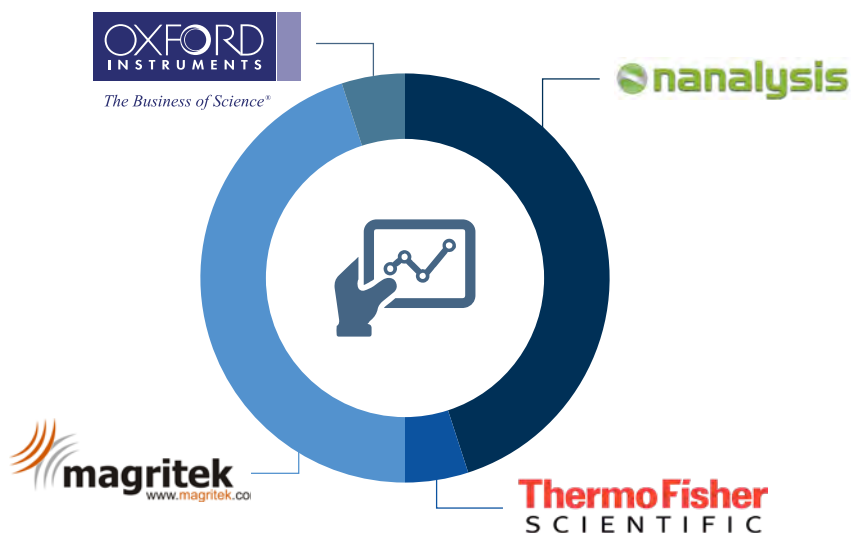
Accessibility, compactness, connectivity, low maintenance requirements and cost are the key determinants in the value proposition benchtop NMR. They have found immense use first in academic teaching, but increasingly in the chemical industry including pharmaceuticals, chemical, food & beverage, environmental and biotechnology among others.

In the past, NMR spectrometers were rarely used especially due to cost-constraints in quality control analysis. However, with the benchtop option made available, it has become easy to analyze data with effective results at a low cost.

Although lower-resolution, accessibility and affordability are the key reasons why benchtop NMR spectroscopy are desirable for some applications relative to high-field NMR spectroscopy. Both the capital cost as well as the operating expenditures involved with using a benchtop NMR is far less than that of its high-field counterpart and several start-ups and applications that require comparatively less sensitive data are well benefited with the benchtop version.

Nanalysis is the market leader in this segment contributing a little over 45 percent in 2016. Nanalysis' key focus area is North America with majority of its client based in this region. It is closely followed by Magritek that has more revenues generated from the European region comparatively. Thermo and Oxford Instruments stand in distant third and fourth positions respectively.

### Benchtop NMR Spectroscopy Market: Company Market Share, Global 2016



## 5

### END-USER APPROACH – FINDING THE RIGHT SOLUTION

As mentioned previously, academic teaching currently represents the most important source of revenue for benchtop NMR. As NMR spectrometers are the most commonly used analytical technique in synthetic chemistry, and given the amount of information that can be extracted from a single spectrum, this technique is an important component to organic, inorganic, physical, analytical, pharmaceutical and biochemistry teaching curricula. The value proposition where students prepare their own samples and then immediately collect their own data is immediately apparent to chemical instructors.

The second segment where benchtop NMR spectrometers gained traction was in synthetic start-ups and SMEs. These companies have either an overbooked high-field NMR spectrometer facility or no accessible high-field NMR instrument. They are faced with either purchasing a high-field spectrometer or outsourcing their analysis needs. The ROI of the benchtop NMR instrument is then realized in both money and time, considerably reducing courier and outsourcing costs.

Benchtop NMR spectrometers are also being explored for a number of applications where it can be turned into an analyzer for quantitative applications, for example determination of ratios of cannabinoids in cannabis oil is faster and more repeatable using benchtop NMR spectroscopy relative to the more conventional HPLC.

Benchtop NMR spectrometers are also being explored for use in the process industry in addition to or instead of other techniques like IR or Raman spectroscopy. This is expected to witness significant growth with automation. Manufacturing is slowly returning back to the US where more analytical instruments will find focus. Nanalysis is working with BASF in Ludwigshafen in this regard in a project to develop a process-NMR-system.

Automation and remote control of process instruments is critical to avoid delays and also minimize direct intervention of humans in hazardous conditions. 'React NMR' is a product under development between BASF and Nanalysis to convert the existing commercial NMRReady-60e benchtop NMR spectrometer, into a process hardened online NMR tool. This requires hardware modifications, temperature control and a centralized software interface that can be controlled through proprietary process automation. This tool can be used to increase safety, product yield and facilitate reaction self-optimization.



With Internet of Things (IoT) becoming a key trend in the analytical instrumentation market, it will allow users with more instant data, safety to technicians and quick data transfer and analysis. Today companies are well established in remote diagnostics, remote training and similar activities for their customers. It is established through remote accessibility through Ethernet port via Wi-Fi. Mobile data connectivity for the analysis of NMR spectroscopy is an upcoming trend that will provide instant access to data analysis and reports. With the support of IoT, customers can exchange and analyze data remotely from a centralized location. With the compact benchtop NMR spectrometers becoming more sophisticated with features and functionalities, they are expected to become more prominent in laboratories with the advent of IoT when remote diagnosis comes into play in the analytical sector.

The United States is forecasted to hold 35 % of the global pharmaceutical market and will continue to remain the largest pharmaceutical market in the world. High throughput and low-level detection are key decisive factors that influence the purchase decision of molecular analysis spectrometers. Manufacturing of pharmaceutical drugs will increase in the United States which will increase demand for quality control analysis with analytical instrumentation.

## 6

### EXAMPLES OF SUCCESS STORIES

Started in 2009, Nanalysis is one of the successful companies in the NMR spectroscopy market today. They have two main benchtop NMR spectrometers: the NMRReady-60e and the NMRReady-60PRO. Nanalysis' NMRReady-60 family of NMR spectrometers is ideal for applications including teaching, academic research, oil & gas, pharmaceuticals, chemical, biotech and food science to name a few.

Less sensitive, low cost, compact, faster analysis time and ease of use are the key advantages of Nanalysis NMR benchtop spectrometers. Nanalysis also partners with accessory manufacturers that help them provide a holistic approach and a one-shop-stop solution provider that makes it easy for customers to get the entire product package at a single place.

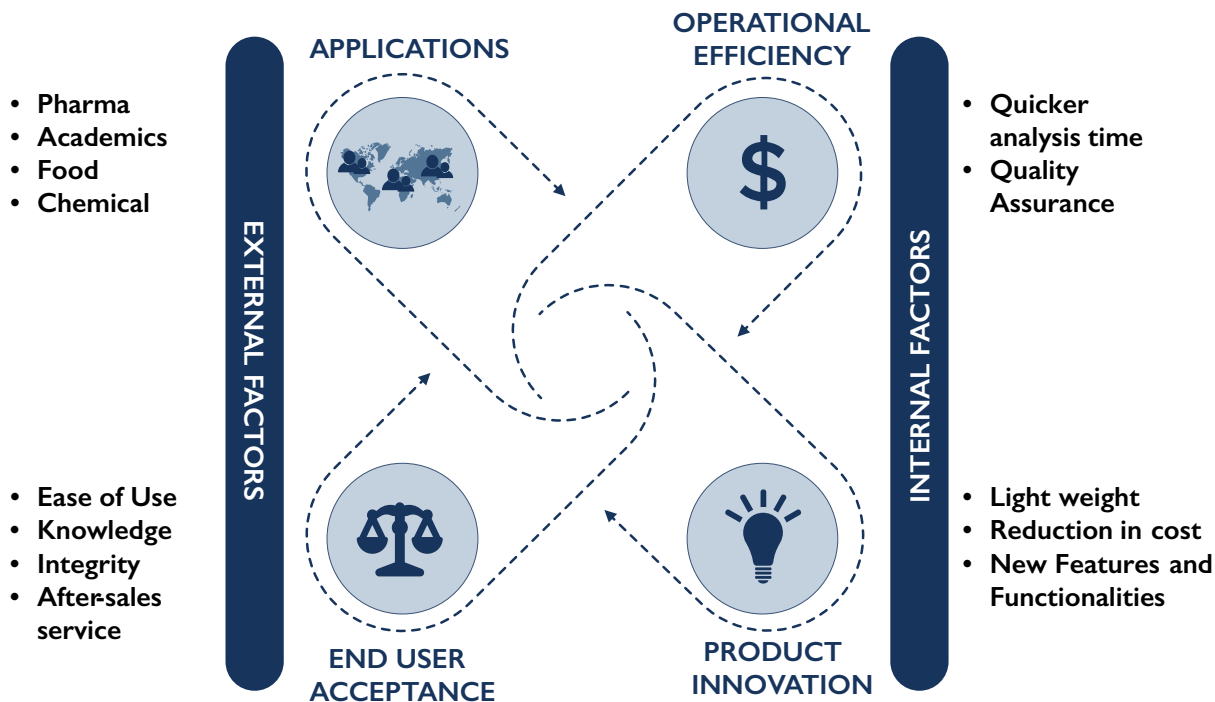
Nanalysis' aim is to convert their spectrometer into an analyzer, where technicians can get answers without expertise in the technique. This requires the development of NMR specific databases, the generation of chemometric methods and increased programmability of interface to make it easier to use. In this regard, Nanalysis developed the NMRReady-CONNECT that is an open application programmatic interface that allows users to integrate it to their centralized system and programs specific experiments. This way, the clients are able to acquire and process data manually or automatically from a centralized location. It can also be combined with other analysis software including MATLAB or Microsoft Visual Studio for example. On the other hand, Nanalysis' NMRReady-flow kit helps users to convert the NMRReady products into an online detector to analyze in real-time. This tool kit can also be paired with other analytical techniques thereby making it even more effective for a centralized laboratory system.

Dr. Hamish Christie of the University of Arizona was an early adopter of benchtop NMR and has incorporated the technique into the organic chemistry undergraduate teaching labs for the last 3 years with great success. The program now has 6 instruments serving 8 labs. He has seen that students can now understand NMR better, due to more frequent use of the method, enabled by the ready accessibility and ease of use of the benchtop spectrometers. "Based on my understanding of other benchtop NMR instruments, my impression is that Nanalysis' benchtop products stand out against other company products mainly due to the instrument being an all-in-one (no additional computer), compact unit." – Dr. Christie, The University of Arizona.

Dover Chemical Corporation, on the other hand, is newer to benchtop NMR and have been using a  $^1\text{H}/^{31}\text{P}$  NMRReady-60PRO QA/QC to look for decomposition products in their phosphorus containing compounds. "Nanalysis has very good customer service and a clear design of the instrument. The instrument is all in one self-contained unit, which makes it very attractive to

use and maintain. It's hard to get such companies to work with you before a purchase to understand the instrument in your facility. We worked with them for at least 6 months; they were very patient with us, answered all our questions, ran our samples for free and that's to me makes them stand apart." – Jacob Lance, Dover Chemical Corporation

Benchtop NMR Spectroscopy Market: Factors for Growth, Global 2016

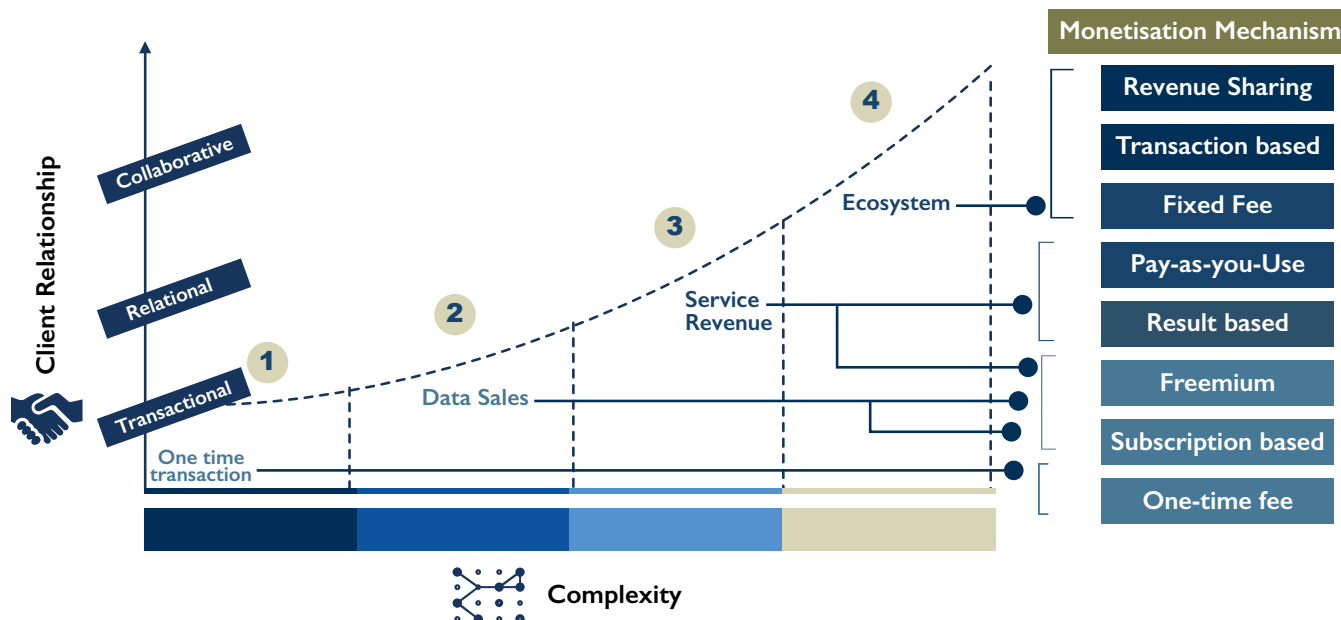


## 7

### INTERNET OF THINGS - THE CROSS-POLLINATION OF IDEAS, TECHNOLOGIES, AND PROCESSES

Centralization, remote monitoring, enhanced flexibility and ease of maintenance are some of the key advantages of IoT. The future lies in cloud computing by integrating decentralized systems into a single platform. IoT helps in analyzing huge amount of data quickly and effectively. Software inclusion makes the products a part of the community rather than an individual user. With lab virtualization, samples can be test virtually from anywhere and automated sample changes can be performed effectively without the need for a physical presence. Cloud is slowly becoming a model accepted by several industrial end-users. Real-time data analysis is another advantage where the results can be sent across the internet instantly and avoid delays in decision making. Lowered CAPEX and OPEX, greater agility, and reduced time to market are some of the crucial benefits that cloud offers.

Internet of Industrial Things: Mind-Set Shift, Global, 2014-2022



## LAST WORD

Miniaturized instruments with lower footprint will be in demand, driven by the portability and field analysis option. Today, one of the key criteria while selecting NMR spectrometers is not just the size of the magnet but also the dimensions of the system. The compact size of the instruments boosts higher sales as lesser space is required to use them. Vendors who develop benchtop NMR with more ease of use, that provide faster results with increase in accuracy are expected to gain market share.

Thus, NMR spectroscopy, a technique that has been around for over 6 decades but largely allocated into the labs of experts, is finding new applications through compact benchtop form factors. The use of benchtop NMR spectrometers in academics has achieved great success and there is increasing opportunity in the fields of industrial including pharma, chemical, food & beverage, environmental and biotechnology among others. The growth in this market is expected to cross double digits with focus on accuracy and ease of use.


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