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FEATURE

Chemometrics & Fast Analytics: A New Scenario in Business Intelligence

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A new analytical scenario

We are in the world of information. Data intelligence is the great asset of our time and it will be no different in our area of expertise. Analytical chemistry, driven by chemometrics, will follow the same path and provide unprecedented and essential information for the sustainability of companies.

In recent years, trends in analytical chemistry have emerged with important advances in speed, cost, intelligence and simplicity. In fact, it is a great "virtuous circle", where fast analysis generates increased analytical capacity and lower operating costs, large amounts and a high quality of data produce extraordinary databases, chemical data science opens up possibilities for augmented intelligence, and finally, in the real world, if the solution is not simple and robust, it will probably not go any further.

OpenScience works in partnership with the main players in the market. The idea is to bring the successful experience of applied research in tobacco business to leverage open innovation programs in many segments of industry, food, agribusiness and other bioeconomic issues. It is important to say that these initiatives have the support of an exceptional group of professionals who contribute to this reality, with many national and international references in analytical chemistry, chemometrics and businesses. They are researchers, professors, senior managers, R&D directors, entrepreneurs, innovation managers, government leaders, and technology providers, as well as chemical data scientists.

The next leap in chemical intelligence

The best way to move on to the new scenario is to take a step back and review some paradigms in applied analytical chemistry. Historically, we have learned to think in a univariate way: "one thing at a time". In business, it is no different; complex problems are often divided and addressed as their parts. Based on this concept, the questions demand traditional analytical methods which are selective, slow and laborious. For the same reason, they are disconnected from their original complexity, and often underestimated, after major simplifications. Consequently, what we have achieved is only a poor approximation of reality.

On the other hand, through a more holistic assessment, we realize that food, beverages and ingredients have complex chemical signatures that can provide information, with a cause/effect, of each stage of the business. The chemical composition related to food can reveal its sensory attributes, nutritional value, and special products, among others. Therefore, a deeper analysis of molecular markers can guide plant breeding, management practices and the influence of environmental factors. In addition, chemical, physical and microbiological processes leave "chemical marks" that can be measured using advanced analytical techniques and chemical intelligence.

In this way, the new approaches provide comprehensive and bidirectional analysis (i.e., top-down and bottom-up), eliminate slow and costly sample preparation steps, and can provide a large amount of chemical data. Therefore, we can transform chemical data into business information through chemical data science. Figure 1 presents the summarized scheme of the analytical approaches to business intelligence.

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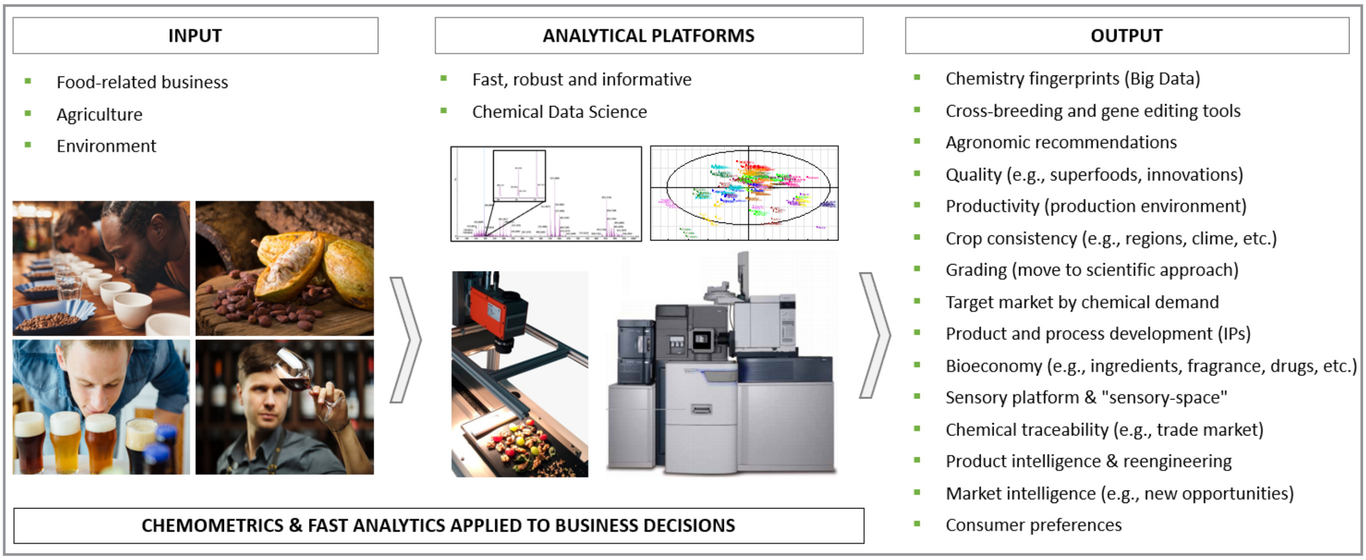

Figure 1. Analytical approaches to business intelligence.

Affording this scenario, it is important to pay attention to the level of complexity involved in choosing the technique and extracting the chemical information associated with the business objectives. It is not a simple data science work. Many current attempts are simply frustrated by the lack of technical knowledge and, mainly, by the absence of a culture of innovation and market, which makes it possible to understand the problems and their solutions in a realistic and scientifically robust way.

Open innovation in analytical chemistry

In this new scenario, our goal is to build a modern analytical chemistry, to leverage the agribusiness bioeconomy and create new action standards for food-related business. For this, we believe that analytical chemists will be the new protagonists in business intelligence. Therefore, we must be prepared to influence our business environments, through articulation between important stakeholders, connecting scientific knowledge to social demands, in a transparent and efficient manner.

In open science and innovation, it is important to be guided in an aggregating environment between the science and technology institutions, startups and big companies that seek products and services in an assertive and sustainable way. However, the success of these initiatives depends on correct managerial decisions and both public and private policies of investing in science, technology and innovation.

In the next sections, we will present some areas of opportunity that range from farming to the consumer. Furthermore, it is not just abstract, but issues that we have been privileged to innovate in the past two decades in real business scenarios.

New analytical tools in agriculture and food

The genetic potential of a crop depends on a complexity of factors which define the characteristics of the production: the phenotype. In pre-breeding work, analytical tools play an important role in the discovery of new marker compounds and in rapid screening for genetic crossbreeding. The time window for crossing is generally short and marker profiles are often complex. Thus, high-throughput tools are usually necessary. In this sense, new approaches to high resolution mass spectrometry in real-time have been emerging, which guarantee high analytical capacity with unprecedented information. An example where fast screening tools were used to patent new hybrid tobacco plants with innovative taste profile has been previously reported [1].

The concept can be used for various applications where it is necessary to find compositions or properties relevant to-quality, productivity or resistance of food and ingredients to pests and diseases, and lots of applications. These approaches are also important for monitoring new gene editing programs. In both cases, the idea is to recognize the latent variables which pinpoint the root cause for genetic improvement and, at the same time, avoid undesirable new compounds via the expression of new metabolic pathways, ensuring quality and environmental safety necessary for the expected objective.

From a scientific point of view, we can define agricultural strategies and practices based on experimental design and cause/effect relationships in management. Environmental factors, soil fertility, and other characteristics can define new production standards, treatments and processes used in the food generation. This scenario aims to use new-to-the-world chemical simulation tools based on target production, carbon sustainability and return on agricultural investments.

After defining the target metabolic profiles for production, we can apply the concept to the crop quality index. The objective is to quantify the quality of production for each farmer or group of producers. This can be used to verify the farmer's assertiveness to apply the technological package, or assess regional production trends. In the same way, it is possible to categorize raw materials and even determine the value of the product quality using objective methods of analysis. An example is the modernization of product classification guidelines, often based on sensory and subjective characteristics. In addition, we can use multivariate management tools and assess the factors that truly impact the value of commodities and return on investment for rural producers, strengthening national production. These previous concepts are some examples of the tobacco industry and patented analytical platforms [2].

Product and process intelligence

After business and scientific definitions, we can implement new tools for product inspection, traceability and certifications in real-time or at high throughput. In this case, the development of an analytical approach to estimate a wide range of quality parameters can increase the capacity of material inspection to much higher levels than currently reported. For example, the present spectroscopic imaging techniques can simultaneously monitor dozens of parameters and provide an accurate dashboard of products and processes performance. The new approaches open up opportunities for extensive sample monitoring due to low analysis costs and high analytical capacity. This is a clear opportunity for many segments. In this way, the new analytical tools are important to leverage the digital transformation and innovation in both agriculture and industry environments. The following publications from British American Tobacco describe online systems using hyperspectral imaging [3,4]. Let's see the point of view of real-time analytical technologies in the highlighted box.

Real-time analytical technologies

Hyperspectral imaging technologies are critical to accelerate business decisions on quality control and automation for Industry 4.0. According to Luiz Felipe Merenholz de Aquino, who provides this type of technology in Brazil: "chemical imaging is a mandatory tech for leading companies. In the Agro sector, we help producers of feed, food, fruits to check quality parameters in real time such as sugars, fat, moisture and many others, allowing automated machines to select and separate products according to their quality. In the pharmaceutical industry, the efficiency of the mixture of active ingredients is checked in real-time, ensuring products to meet QC standards."

However, spectroscopy may not always be satisfactory. In industry, an extremely important area is related to product and competitor intelligence. The use of advanced instrumental techniques of chemical fingerprints, combined with predictive models and databases, can determine the composition of complex formulations. In other words, the composition of products, quality of ingredients, or even the processes used can be evaluated through the chemical composition of the products. In this case, the most promising technologies (High Resolution Mass Spectrometry – HRMS) are being improved to provide incredibly fast and powerful molecular data. On the other hand, some of these approaches are described in the industry for crop quality and the monitoring of toxic compounds [5,6].

In addition to product quality or formulations, we can create objective sensory assessment tools. The subjective sensory panels, through specialists, are generally expensive, have low analytical capacity and can often expose the worker to unnecessary work risks. In some cases, they can be biased or have high subjectivity and imprecision. Thus, employing chemical fingerprint methods can dramatically increase the ability to evaluate products on a routine basis, allowing the appropriate use of specialized human resources to practice more qualified activities, for example, products with sensory innovation [7]. In addition, a deep dive in molecular knowledge was used to understand the chemical contributions and sensory characterizations. In the next paper, you can see an example of this platform [8].

Once fast and objective methods have been implemented, accurate sensory information can be used to determine the "sensory space" of a product: sensory 4.0. Through chemical signatures, products and processes can be objectively understood and protected based on chemical characteristics that define the novelty of the process or product in intellectual property [9].

Thus, it is possible to project quality through product categories, differences in origin and competitive positioning. A new area of opportunity purposes to the possibility of using the databases generated by the above technologies, to design (*in silico*) new products with desired characteristics. These approaches can drastically reduce the cycle of developing new products and bringing competitive advantages to companies. The same concept can be used to recommend best practices, processes and product formulations. An augmented intelligence point of view is shown in the highlighted box.

Augmented intelligence point of view

According to Guilherme Post Sabin, founder of OpenScience: "Artificial intelligence has been gaining ground in all areas of activities. However, our proposal goes further. We want to value human experience, empirical knowledge, the learning accumulated over the years, in the art of producing food. The proposal is to bring augmented intelligence to business, that is, to enhance the human capacity to make plans, analysis and make decisions, driven by artificial intelligence of chemical data. As protagonists on this path, we believe that our approaches based on chemical intelligence can interact to people and transform the way we produce food and do business!"

Finally, the new analytical platforms can be used for product intelligence, market mapping and consumer preferences. Once consumer preferences and market opportunities are defined, it is possible to describe the action standards in product development or reengineering. In addition, raw material management, harvest volumes and service to markets can be more accurately predicted when simulated by a chemical database suitable for the definition of commodity logistics, national brands, premium products, and trade market relationship, among others.

Analytical trends and main motivations of stakeholders

What is the future of applied analytical chemistry? This is an issue that we will address shortly. For now, let's think about the different angles from which we can look at analytical chemistry, from the point of view of the professional environment in which we are inserted in the different areas; this is the first clue to try to answer the question.

Therefore, if you are an academic researcher, a reference in the field of analytical chemistry and chemometrics, you will probably be concerned with showing the best performance in terms of speed, precision and analytical cost to obtain information with less effort and cost than is currently possible (i.e., analytical democratization). It is likely that you are focused on the technique and method used to obtain the best information, and on the analytical advantages until the moment at which you provide the result. Let's see the academic point of view in the highlighted box.

Academic point of view

According to Professor Leandro Wang Hantao, University of Campinas, recent advances in separation science have imposed new requirements for method development, which has ultimately altered the essence of contemporary analytical chemistry. Advances in column technology and multidimensional instrumentation, including high-resolution mass spectrometers, have led to the achievement of unprecedented peak capacities and fast analyses. Today, fast analyses can be routinely performed with the development of modern and powerful analytical instruments. This reality challenges the fundamental pillars of method development. In the near future, if not now, sampling and sample preparation and data processing will be the limiting steps in modern analytical methods. Today, these two steps are already considered the most time-consuming stages and responsible for most of the errors in an analytical measurement.

Please let us consider the following scenario. Considering that an analyst can obtain a chemical fingerprint in under 10 seconds, it is still feasible to consider traditional liquid-liquid and solid-liquid extractions. Researchers will need to revise the requirements for sampling and sample preparation to improve sample throughput, while preserving the accuracy and precision of the method. Today, sampling and sample preparation comprise an amazing scope of techniques and methods used for the isolation of analytes in complex matrices. Numerous formats and configurations are available, ranging from immobilized sorbent-extractions, 3D-printed sampling devices, acoustic-assisted sampling, laser assisted desorption/ionization, just to name a few. It is imperative that sample preparation bypasses the use of solvents and other consumables to support a sustainable work environment. Also, automation is key to improve productivity and feature attractive operational expenditure.

Analytical chemistry has evolved too much to be restrained for QA/QC purposes only. This field of research is the embodiment of applied chemistry and it will gain much attention in improving business intelligence in smart-industries. How are researchers going to tackle the hundreds of files generated weekly, if not daily, in their laboratory? How can we extract the most meaningful information from chemical measurements and establish statistically valid models and interpretations of such “big data”? We are incapable of quickly determining multivariate behaviors in data using univariate methods. Multivariate data analysis using chemometrics will be unavoidable in modern analytical chemistry. There are endless opportunities for chemometric processing to improve the analytical workflow in laboratories, even in the seemingly distant applications of water research, like effect-directed analysis.

Similarly, a technology company will want to produce equipment or software that is simple and robust to use and will also believe that a higher throughput and lower operating cost approach will increase the analytical capacity to measure more and better. This certainly benefits the customer. But what kind of business intelligence does the customer need? Will this company need to update its technology base? These are non-trivial questions and are worth thinking about! So, let’s see the cutting-edge technological point of view in the highlighted box.

Cutting-edge technologies point of view

According to Jane Finzi, Market Development Lead at Waters Corporation, to unlock the potential of science today, more than an instrument of excellent technical precision is necessary; we need to drive greater collaboration to help to uncover the needs of the next generation of scientific advances. With the collaboration of customers, the development of complete solutions according to the real needs of the market is faster and more efficient. Creation of new products, development of prototypes and continuous improvement of existing solutions are built with the help of customers who are in different institutions around the globe, such as Universities, Research Centers, Hospitals and Industry, with the goal of delivering benefit to the customer and society. In addition to the most diverse collaborations, Waters created Immerse, a new innovation and research laboratory, which includes the Waters Innovation Response team, whose team works closely with several researchers to provide the technology and experience necessary to make new ones advances in science a reality. In this way, new-to-the-world analytical platforms based on high resolution mass spectrometry are giving us unprecedented multidimensional information, as well as real-time possibilities for business intelligence.

However, if you are a consumer goods company or government institution linked to a country's bioeconomy, you will think about Market Intelligence. This is very clear for the food, energy and agribusiness industry. However, intelligence will also be part of the analytical service labs and in the pharmaceutical industry through PAT and QbD. Finally, this subject has already been discussed by the major laboratories of clinical analyses and personalized medicine. Let's hear the views of a senior scientist who works in a Fast Moving Consumer Goods (FMCG) industry.

FMCG's senior scientist point of view

Nadir Hermes, Senior Scientist at British American Tobacco, describes this new scenario: "The century-old tobacco industry has been transformed in the last years. Consumers increasingly have a choice between a single agricultural product (cigarette) and new categories of tobacco and nicotine products. A trigger of this transformation was the access to evolving new technologies coupled with the continuing historical commitment of tobacco product manufacturers to provide adult consumers with a wide range of potentially reduced risk products as compared to continued cigarette smoking. The new product portfolio includes vapor, tobacco free nicotine pouches and tobacco heating products that have shown a reduction in emissions of 90-95%* of certain harmful compounds found in cigarette smoke [10,11], and which have demanded, from an analytical perspective, more sensitive and robust methods, and shorter turnarounds. A new set of methods for the new categories had to be implemented, at the speed required by the pace of the innovation and scheduled product launches. The dynamic of the new market, fast technology changes and speed of change in response to consumer demand required an Analytics Strategy/Program able to identify sound innovative capabilities to quickly support all stages of product development, manufacturing and quality control. The advances in the traditional Analytical Chemistry approaches can cope with the given challenges, but not necessarily at the right pace to win in this new market. All advantages of chemometrics and fast analytics approaches to support business intelligence is clearly the way to follow."

Note:

*Comparison of smoke from a scientific standard reference cigarette (approximately 9 mg tar) and emissions from glo™ and Vype ePen™ products, in terms of the average of the 9 harmful components the World Health Organisation recommends to reduce in cigarette smoke.

Now, it is worth reflecting on the following: what kind of information can chemical intelligence bring us? For this, we need to understand the chemistry and type of information that each technique can provide to assist in this new scenario. From a technological point of view, we must increasingly migrate to top-down analytical platforms. This will have an impact on today's laboratories, which are usually bottom-up.

Furthermore, to complete the professional scenario, we cannot forget the current model of open innovation where startups, small companies and analytical intelligence consultants sit, who can operate with agility and low cost. Also, it is true that both scientists and impresarios want to act in this segment, but there is a big gap of understanding between them. It is necessary to convince investors that current investments are insufficient, and that chemical intelligence is the most scalable model that we can produce in this area. Any serious scientist who knows business will say: science takes time and is worth investing in!

Moreover, we must remember that success depends on the established metrics. Interestingly, accelerators of open innovation are increasingly parameterized "inside the box". Therefore, we need to understand the problem and propose the goals and metrics that will lead us to the solutions we need in the near future; otherwise, we will lose the race! Let's see analytical intelligence according Ministry of Agriculture, Livestock and Food Supply in the highlighted box.

Analytical intelligence - new paradigm for value chains

According to Cleber Oliveira Soares, Director of Innovation at the Ministry of Agriculture, Livestock and Supply: "For this decade, drivers powered by innovation will be levers to raise the bar for food security and humanity development on the globe. This new logic will expand the prominent position of analytical science in relation to technological, economic, social and environmental aspects. Countless value chains will have to transform.

In agriculture, food and the bioeconomy the drivers associated with sustainability supported by the analysis of the product's life cycle – from field to table – with efficient use of inputs will make a difference in the production equation. The bioeconomy and the use of advanced biology technologies will improve genetic, zootechnical and health aspects. For the same purpose, the use of biological engineering tools using RNA, DNA, proteins and subunits of molecules for vaccines and other bio-applications. Bio-based inputs will make up this contemporary arsenal enhanced by the use of probiotics, biofilms, sanitizers, enzymes, proteins to prevent pathogens and parasites, and may even be used to mitigate greenhouse gases.

Transformations that do not require digital. Increasingly, digital and analytics will make all the difference in the contemporary economic sectors. The increase in global demand for food brings another innovative perspective - advances and opportunities in food tech. Innovations in processes such as conservation, maturation, traceability, intelligent packaging and other applications will also be common in production chains and their products. A new paradigm is born supported by analytical intelligence!"

In conclusion, let's return to the initial question: what is the future of applied analytical chemistry? In this direction, there are no surprises, although someone may disagree. As in all other areas of our society: "follow the funding!" The industry will be more successful and sustainable when it knows how to use chemical intelligence! Technology companies which see this opportunity will focus on world-class comprehensive platforms. Universities will continue to discover the foundations for the greater effectiveness of new scientific and technological solutions. Finally, the business style startups will continue to evolve towards self-knowledge and maturity, discovering the confusing paths between opportunities and purpose!

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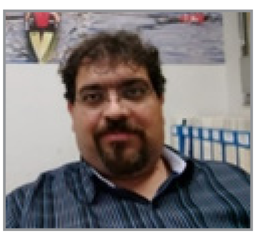
Key Players and Stakeholders

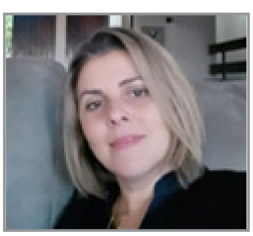
Cleber Oliveira Soares, PhD

Executive with 20 years of experience in Science, Technology & Innovation, Strategic Management, Agriculture & Business, developed in Brazilian agribusiness, with significant experience at Embrapa and IICA - Inter-American Institute for Agricultural Cooperation, currently at the Brazilian Ministry of Agriculture, Livestock and Food Supply.



Guilherme Post Sabin, PhD

Founder of OpenScience and senior scientist with 19 years' experience in analytical science for business and academic settings. In 2017, he won the "Sir Charles Ellis Award", in recognition of the best scientist in global R&D at the British American Tobacco. In 2018, he decided to work widely through chemical data science for big companies. Also, he is visiting professor at Unicamp and co-advisor for chemometrics and fast analytics applied to business intelligence.

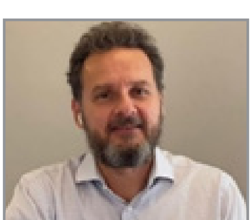


Jane Kelly Finzi, MSc

Market Development lead at Waters, she is responsible for business development in Brazil. Demonstrated history of working in the research industry. Strong sales professional skilled in Good Laboratory Practice (GLP), Liquid Chromatography-Mass Spectrometry (LC-MS), Protein and small molecule Chemistry, Validation, and GC-MS. LC-MS Hardware knowledge and field service experience.

Leandro Wang Hantao, PhD

Professor of Chemistry at the Institute of Chemistry, State University of Campinas (IQ-UNICAMP). His studies aim to sample preparation for analysis of organic compounds, chromatographic techniques, mass spectrometry and data processing. Among the awards, the 2018 Power List "TOP 40 UNDER 40" (Analytical Scientist) and 2019 The "John Phillips Award" stand out.



Luiz Felipe Merenholz de Aquino

Entrepreneur who dedicated his life to advanced analytical technologies since his youth and has always loved to participate in high end projects and research. He has founded ASTRO34 in 2003 with the purpose of selling scientific instruments like hyperspectral cameras. Today he is dedicating his time to develop solutions to serve Agro, Pharma, and Food among others.

Nadir Hermes, PhD

Senior Scientist – PRRP* Analytical at British American Tobacco (UK). Nadir is about to complete 30 years of experience in Analytical Chemistry. He started his career working for the University of Santa Cruz do Sul (RS, Brazil), where he was technical responsible for the Analytical Centre and Professor of Analytical Chemistry in the last years. After 17 years, he joined Souza Cruz Company (BAT Brazil). In 13 years at BAT, one of the remarkable achievements was the transformation of the labs he managed or have technically supported. The views expressed in this article do not necessary represent the views of BAT.

*PRRP – Potentially Reduced Risk Product.