COAST Student Innovation Award 2017

COAST Student Innovation Award (CSIA)
During the COAST Education Event, nominated students will present their internship results. The talent student who has performed the best internship, has been the most innovative and gives the best presentation will win the award. Representatives of COAST participants that are regularly involved in our education programs will form the jury.

Event details Education Event:
When: Thursday 13 April 2017, 13:00 - 18:00 hrs
Where: Hogeschool Utrecht, Heidelberglaan 7 Utrecht

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Understanding Aqueous SEC-MS Elution and Ionization Behavior of Biomacromolecules

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Analysis of proteins in native-like conditions free of organic solvents is becoming more and more necessary not only at the quality control stage, but also throughout the discovery and design stages of therapeutic proteins (Heck, 2008). Size-exclusion chromatography (SEC) is a very powerful tool to characterize proteins, as well as their aggregation and fragmentation (Hong, 2012). To ensure identification of separated species, the hyphenation with mass spectrometry (MS) would be advantageous (García, 2005). Interestingly, little has been written on the direct coupling of SEC with MS under aqueous conditions for protein characterization.

The aim of this study is to gain a better understanding of the effect of mobile phase additives on the ionization and separation of water-soluble biopolymers in SEC-MS. In order to ensure SEC-MS coupling under native conditions a variety of volatile salts at varying pH and concentrations were tested (Arakawa T. E., 2010 ). The extent of the non-ideal SEC behavior - due to electrostatic and hydrophobic interactions - is correlated to the retention behavior and analyte peak shape. The protein charge state distribution in direct infusion MS experiments give an insight whether true native MS conditions are approached. All information is brought together in SEC-MS analysis of intact proteins, showing the influence of separation conditions on data quality. Future steps are focusing on the optimization of trapped ion mobility in order to gain more insight on the aggregation and the conformational changes of the proteins both in the gas.

References


4 Improved anthropogenic gadolinium quantification with ICP-MS

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The Netherlands consists of a compact delta area in which the Meuse, Rhine and Scheldt flows into the polder areas. In order to map the different water contributions in a certain polder area, the waters have to be characterized. The characterization is performed by the determination of the gadolinium concentration that serves as a geochemical tracer [1]. Currently, the water originated from rivers shows a positive gadolinium anomaly due to the discharge of gadolinium-containing substances for MRI purposes [2]. Deltares is specialized in making a detailed water balance for complex hydrological systems by the determination of this gadolinium anomaly in certain pools performed by ICP-MS. This is performed by the quantification of the rare-earth elements (REEs) in water and determining the relative enrichment of gadolinium as anthropogenic gadolinium (Gd-DTPA) concentration. However, waters with high REEs concentration show little or no gadolinium anomaly making it impossible to determine the anthropogenic gadolinium concentration. This effect is associated with the content colloidal/nanoparticulate matter [3].

During this study, a sample preparation method is developed in order to reduce the high REE concentration so that the anthropogenic gadolinium concentration can be determined for waters with high colloidal/nanoparticulate content. Several sample preparation methods such as (ultra)filtration, chemical oxidation and ion exchange chromatography were performed and discussed.

References


Development of a Sample Preparation Technique for Silver Nanoparticles

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The consumer market is increasingly using metal nanoparticles in products. For example, silver nanoparticles have antibacterial properties and as such is used in washing detergents and air conditioners. Thus, nanoparticles are possibly ending up in the environment via diffuse emissions [1]. Therefore, analytical techniques are important that can analyze particle concentration, particle size, and size distribution. By operating inductive coupled plasma – mass spectrometry (ICP-MS) in non-conventional settings, this technique is able to determine the before mentioned parameters. The so-called single particle ICP-MS (spICP-MS) can be performed without modifying the instrumentation [2]. However, ions interfere with the analysis by increasing the total background, increasing the difficulty of detecting smaller particles. The ions that are present could have different sources, present by nature or because of dissolving nanoparticles. Therefore, an ion exchange column was tested to assess the functionality of removing ions. The restriction of the column is that the nanoparticles must remain intact. Hence, the possibility of an (on-line) IEC coupled with spICP-MS method for lowering the ionic background was assessed.

References


Evaluation of Translocation Properties of a Gut-on-a-Chip Intestinal Barrier Model

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Microfluidic devices have the potential to adopt more accurate physiological conditions of the human intestine through the use of continuous flow and by producing mechanical stress to the cells [1]. The dynamic microenvironment in the chip has been previously described to highly influence cellular behaviour [2]. Due to this reason, this study was set to evaluate the translocation properties of a microfluidic gut-on-chip device recently developed at RIKILT-Wageningen University, in comparison with the conventional static Transwells. The dynamic \textit{in vitro} model consisted of a microchip with a porous membrane assembled and connected to a syringe pump system. This allowed for constant flows to be streamed through the apical and basolateral side of the membrane, thereby feeding the cells with fresh medium and producing mechanical shear stress. Antipyrine, a highly permeable model drug, was used to investigate the translocation across Caco-2 intestinal cells, together with a low permeability marker, Lucifer Yellow, commonly used to assess the monolayer integrity.

The results showed comparable permeability coefficients in the two \textit{in vitro} models. The translocation of Antipyrine revealed a similar linear transport trend in Transwell inserts and gut-on-chip. Well-formed tight junctions, characteristic of differentiated Caco-2 cells, were suggested by permeation of Lucifer Yellow, revealing insignificant amounts translocated across the Caco-2 monolayer upon a 24hr exposure time. The Papp values determined for Lucifer Yellow correlated well in the two \textit{in vitro} models. These findings support the potential use of the gut-on-chip device, showing great promise for kinetic bioavailability studies in the future. Furthermore, the use of gut-on-chip showed advantages in obtaining more automised conditions and a minimal consumption of reagents, as compared to the traditional Transwells model.

References


ANALYZING AMMONIA IN BREATH SAMPLES WITH LASER SPECTROSCOPY
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As long as there has been the transportation of goods, transportation of illegal goods has been a problem. One group of illegal products that are still transported nowadays is drugs. The transport of drugs can be done in packages on or in the body [1]. Especially this internal smuggling is hard to intercept because it can only be detected via an interrogation and a complete body scan. The body scanner is a luxury that not every airport has. Airports that do have a body scanner select people to go through it, based on their behaviour.

The people that transport drugs inside their body, also called couriers, swallow packages filled with drugs [2]. These packages, or pallets, must stay inside the stomach for as long as possible. If they are excreted before the courier reaches the delivery point the packages are lost. This requires the couriers to fast from the time they ingest the pallets, until the time of arrival. The fasting causes the ratios of the molecules in a breath to shift.

The customs office wants to use this shift, and perhaps molecules that are specific for the packaging materials of the pallets, to detect drug traffickers with a breath test. A breath test would be easy to perform, it is faster and less invasive than the body scans and interrogations. It is hypothesised that the biggest concentration shift can be found in the trace gases in a breath.

During fasting, several of these gases, like acetone and ammonia are excreted at a higher concentration than in a normal person [3]. The focus in this study lay with ammonia, because acetone had been researched before. Ammonia are transported via the bloodstream towards the liver to be excreted via urine. During transportation, it also passes the lungs where a part of the ammonia diffuses into the lung. That part will, in turn, be exhaled. The name of ammonia, and other organic compounds that can be found in breath is Volatile Organic Compounds (VOCs).

In this study, a detection system was modified and tested to detect ammonia in breath from test subjects. The testing was done with people that fasted up to 15 hours. The same people were also asked for a breath sample without any fasting.

References
ANALYSIS OF NANOPARTICLES BY COMPREHENSIVE TWO-DIMENSIONAL LIQUID CHROMATOGRAPHY

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Within the Making Analytically Incompatible Approaches Compatible (MANIAC) project, completely different and incompatible separation systems are combined into a single, highly efficient and extensively optimized instrument. Amongst the investigated applications is the analysis of complex polymeric nanoparticles encountered in coating formulations. A large number of sample dimensions are found in these complex samples such as the particle-size distribution, the chemical (surface) composition(s), charge and molecular weight.

An effective technique for the analysis of complex mixtures is comprehensive two-dimensional liquid chromatography (LC\texttimes LC). In LC\texttimes LC, a modulator is used to couple the two separation dimensions with different time scales (spanning about two orders of magnitude). The potential of modulators can be further enhanced by allowing fast, controlled chemical reactions to take place. To resolve the incompatibility, various chemical and physical processes are integrated with (multi-dimensional) separation systems allowing complex mixtures to be analyzed.

In our study, we use hydrodynamic chromatography (HDC) to separate the nanoparticles based on size. Next, the modulator is used to dissolve the nanoparticle dispersions, yielding a homogeneous molecular solution. These molecules are then separated in the second dimension based on their chemical composition, by LC (e.g. SEC, RPLC) or by LC\texttimes LC (e.g. RPLC\texttimes SEC), in combination with MS detection when appropriate. However, a successful application of the above-mentioned techniques faces a number of challenges, including solvent and sample incompatibility between the two dimensions. In this study, these challenges are all addressed.
Desorption Atmospheric Pressure Chemical Ionisation (DAPCI) is a technique without the need to perform sample clean-up and chromatography before analysis [1]. This research explores the use of DAPCI. The technique DAPCI is investigated to see whether it can be used as a replacement and/or extension to current analyses. Current analyses are based on a primary extraction of the sample with, for instance, Liquid-Liquid Extraction followed by a concentration step [2]. This is mostly done with Solid-Phase Extraction. The final analysis is carried out with Liquid Chromatography-Mass Spectrometry. Therefore, pesticides, growth promoters, antibiotics and other compounds will be analysed. Some matrices such as apples, pears and meat are tested as well to check if the technique DAPCI is suitable and perform well for this research. The final goal of this research is to use DAPCI to analyse samples in the field. The results of DAPCI tested are interesting for laboratories engaged in this type of analysis. It is expected that the investigated technique will give a higher recovery and maximizes the number of compounds introduced into the Mass Spectrometer (MS) [3]. Upon completion of the testing, it will be clear if DAPCI can replace or extend current analysis. The performance of this technique will be clarified as well. DAPCI may be quicker, simpler, easier and can contribute to a more environmentally friendly analysis since there is no need of harmful solvents. In this research, the Ambient Ionisation MS technique DAPCI is investigated for different compounds and matrix combinations. A portable solution to ionise samples for MS will be demonstrated and discussed.

References


Development of a combined XRF/NIR system for the feed industry
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PANalytical got an assignment of SoilCares research to develop a combined XRF/NIR instrument for the feed industry. This instrument will provide the feed industry more knowledge on what is in the feed and what it needs to modify the feed. With the XRF was looked at the repeatability of the sample preparation, to determine the influence of the sample preparation. Therefore, the following question raised: How much different is using liquid cups as sample preparation in comparison to the pressed pellets sample preparation? To answer this question the repeatability was measured for both the instrument and the analyst. NIR is a very sensitive method with a lot of parameters that have an influence on the spectra [1]. For getting a better understanding of these parameters the following question was set up: what are the optimum settings (distance, angle, and sample movement) for the probe to the sample? To answer that question the spread, reflectance and noise area were investigated. The NIR measurements were done by a step by step process. The parameters that were tested: angle (horizontal (30, 45, 90), Vertical (20, 45)), distance (0 mm, 2 mm, 6 mm and 8 mm), Sample movement (fixed, rotate, load/unload and spinner). Each parameter was 10 times measured for better indication on the spread, noise area and the reflectance.

The data of the XRF showed variation in the repeatability for each element and sample. There was no trend in the results. That concludes to: The heterogeneity of the samples plays a major part in the repeatability of the sample preparation for XRF. The NIR data were compared with each other. The angle vertical 20 was overall the best. This angle had the lowest reflection, spread and noise area. The optimum distance lay between the 2 and 6 mm. The spread and average standard deviation for these distances was small. The reflectance was also low. The fixed position was used to test which angle and distance was better, this to eliminate other factors. The spinner had a wider spread than the fixed, but it measures the whole perimeter of the sample cup and thus provides more knowledge on the sample. It only needs further investigation.

Reference

Implementation of Near Infra-Red spectroscopy to increase the efficiency of the Quality Control department

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Sonneborn Refined Products is a world leader in the manufacture of high-purity specialty hydrocarbons. Sonneborn’s QC and Development work follows the methods of ASTM and the European Pharmacopeia requiring a large number of analyses. The use of NIR has shown to be a time saving technique in other companies.

This is the reason Sonneborn is interested to evaluate whether NIR techniques can improve the efficiency of the QC department of the laboratory. This has not been tried before with these types of hydrocarbons.

NIR is a secondary or indirect analytical method, i.e. to obtain the desired information; their spectra have to be compared to primary or reference methods. Therefore, chemo metrics are applied to the spectra to determine the desired parameters. One of the most important advantages of NIR analysis is the simplicity of sample preparation, easy use and rapid time analysis.\textsuperscript{[1]}

A method was developed for the calibration of three products, base oils, white oils and petrolatum. Measurements were carried out on two types of equipment from two companies were the reference database was uploaded. After PLS procession of the responses and further results processing, it was concluded that NIR could substitute not only chemical but also physical properties analyses.\textsuperscript{[2]}

Although at first the development of a NIR method takes time, samples and well educated staff. Long term it could substitute 17 of the 23 methods tested. Some of these old methods are labor-intensive, require time and are expensive while NIR methods are not. Coming to the conclusion that the implementation of a Near Infra-Red spectroscopy would increase not only the efficiency but in some cases also decrease standard deviations of the Quality Control Department.

References

\textsuperscript{[1]} Yves Roggo, Pascal Chalus, Lene Maurer, Nadine Jent, A review of infrared spectroscopy and chemometrics in pharmaceutical technologies. Journal of Pharmaceutical and Biomedical Analysis, 44(3), 683-700. DOI: 10.1016/j.jpba.2007.03.023

Study into the use of co-polyamides for low temperature selective laser sintering (3D printing)

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A new additive manufacturing (AM) system is under development where selective laser sintering (SLS) will be used to create layers. Currently SLS of polymers is done at 173°C which makes it difficult to integrate other systems in the building chamber, e.g. electronics. Therefore, polymers are under investigation that can be sintered at low temperatures resulting in end products with well enough mechanical properties.

During this project four different commercial available co-polyamides are under investigation. The goal of this project is to link the chemical structure of the different co-polyamides to the sintering behavior and end-product mechanical properties. In this way, ideally, polymers of the same class could be selected more easily in the future. Sintering behavior, which includes powder deposition, will be rated on a scale of 0-5 where 0 corresponds to “sintering impossible” and 5 corresponds to “similar behavior as the currently used PA2200”. Mechanical properties of interest are elasticity, tensile strength, and dimensional accuracy and will be compared to the currently used PA2200.

The hypothesis is that there is a correlation between the chemical structure of the co-polyamides and selected mechanical properties. The sintering behavior will be mostly dependent on the particle shape and size distribution, and thermal behavior of the co-polyamides.

The chemical structure will be determined with IR and \textsuperscript{13}C-NMR and thermal behavior with DSC and if necessary rheology experiments. The powders will be optimized by measuring their particle size distribution and create well flowing powders. This is done by measuring the angle of repose and combining different sieve fractions or by using additives. The SLS operating parameters will be optimized empirically for each powder to obtain a mapping of the earlier described mechanical properties at different operating parameters.

References

