



**Pierre Giusti** is a PhD in analytical chemistry, head of the TRTG separation and molecular identification service at TotalEnergies and Director of Research at the CNRS, he is co-founder and director of the iC2MC joint laboratory. He is interested in the molecular characterization of complex matrices in the field of energy and its decarbonation. He is a specialist in analytical sciences for TotalEnergies.

**Brice Bouyssiere** is a professor of analytical chemistry at the institute of analytical sciences and physical chemistry for environment and materials (University of Pau and Adour Countries / CNRS), his research focuses on the characterization of complex matrices and development of hyphenated techniques between separation device and detection techniques. He is also Vice President Science with and for the society and open science at UPPA and co-founder and co-director of the iC2MC joint laboratory.





**Carlos Afonso** is a professor of analytical chemistry at the COBRA laboratory (Université de Rouen/ CNRS/INSA), his research focuses on developments in ultra-high resolution molecular mass spectrometry and ion mobility spectrometry. He is particularly interested in ionization and activation methods, especially for highly complex organic mixtures characterization. He is deputy director of the CNRS Infranalytics research infrastructure, in charge of the FTICR division, and is co-founder and co-director of the iC2MC joint laboratory.

**Ryan Rodgers** is a PhD in analytical chemistry and researcher at the National High Magnetic Field Laboratory (Florida State University), he is one of the world specialists in very high resolution mass spectrometry (FTICR MS). His research focuses on the characterization of complex matrices by FTICR MS. He is co-founder and co-director of the iC2MC joint laboratory and holds the international chair of High Resolution Mass Spectrometry at UPPA.





**Julien Maillard** is a PhD in analytical chemistry, he is a research engineer in the high-resolution mass spectrometry laboratory of TotalEnergies in Gonfreville. He is interested in the molecular characterization of complex matrices in the field of new energies.

**Mélanie Mignot** Mélanie Mignot obtained her PhD in analytical chemistry in December, 2016 and spent one year as temporary assistant professor at IUT Rouen in 2017. In 2017-2018, she received a MSCA Postdoctoral Fellowship in KU Leuven and in 2019, she became assistant professor and since 2023, associate professor at COBRA laboratory, INSA Rouen. Her current research areas include the instrumental and/or methodological developments, especially by chromatography hyphenated with high resolution mass spectrometry, for environmental or energy applications.





Attracted to science since childhood, after my high school diploma, I pursued a degree in geology before continuing my studies with a Master's in Communication and Scientific Culture at Grenoble. After graduating, my first job took me to Pau, where I began contributing to the journal Ebullition(s) as a SAPS mediator at the CCSTI Laqc Odyssée - Science Odyssée. Today, deeply committed to the project, I continue to work on the journal alongside my role as a scientific mediator in the Var.

## SUPER SPECTROMETER ARRIVES IN IC2MC LABS

Santa Claus is a little early this year. After weeks of loud noises, drilling, and pouring of a thick concrete slab for support, he's finally delivered the present...

In Rouen, Normandy, the COBRA laboratory has just installed a FT-ICR mass spectrometer equipped with an 18-tesla (T) magnet (the 2nd highest field in the world), i.e. around 1,800 times stronger than the magnetic field created by a fridge magnet. In parallel, at the Université de Pau et des Pays de l'Adour, in southern Aquitaine, as well as at the Gonfreville l'Orcher site of TotalEnergies research laboratories, received its little brothers, two 12 T's, which have just been installed as well. These three instruments complete iC2MC's fleet of FT-ICR MS instruments, along with the 21 T already in place at Florida State University's National High Magnetic Field Laboratory (NHMFL). But what's the point of these longawaited high magnetic field machines in these 4 laboratories?

These devices are very high-resolution, high-precision, mass spectrometers. They can analyze and identify the individual components present in a complex sample. Unlike other mass spectrometers, these particular models contain extremely powerful superconducting magnets. They have large metal coils made of an alloy of niobium and titanium, several hundred kilometers in length, each weighing several tons. When an electric current flows through a coil, it produces a magnetic field, but would also emit heat - the Joule effect. However, when the coil is cooled to -269°C using liquid helium, it becomes superconducting, i.e. its electrical resistance becomes zero, and it no longer emits heat. This makes it possible to use an electric current of over 200 A to create a magnet with a very high magnetic field. Under these cold conditions, the huge coil is a superconducting magnet that produces a very stable and powerful magnetic field for science. But the technology doesn't stop there!

Known by its full name, Fourier Transform Ion Cyclotron Resonance Mass Spectrometer (or FT-ICR MS), this instrument performs mass spectrometry by combining the use of



the superconducting magnet with a mathematical operation called the Fourier transform.

Invented by Marshall and Comisarow at the University of British Columbia in 1974. this instrument is used to study molecules, i.e. combinations of atoms. A molecule is made up of several atoms linked together by chemical bonds. Each molecule has a mass, corresponding to the sum of the masses of its constituent atoms. The aim of this super spectrometer is to measure the mass of molecules with the utmost precision, in order to elucidate their molecular composition. In addition, this instrument has a very high resolution, i.e. it is capable of separating molecules whose masses are very close (less than a single electron), which is essential for the analysis of very complex samples made up of tens of thousands of different molecules.

## STATE-OF-THE-ART TECHNOLOGY

Thanks to its high dynamic range, this instrument can detect molecules present in a mixture, even in very small quantities. Furthermore, the high measurement accuracy of this instrument makes it very easy to determine the molecular formula of each molecule that makes up our sample, i.e. determining which types of atoms they contain, and how many of each type! Whereas an imprecise instrument would only provide molecular masses with a single digit after the decimal point, a FT-ICR spectrometer gives a value with 7 digits after the decimal point! This drastically reduces the possible atomic combinations for a given mass. This distinction is also made possible by the fact that the error, i.e. the difference between the theoretical mass and the experimentally measured mass, is less than 1 ppm (parts per million). This means that the measured error rate is less than 1 for every million units measured, making this super spectrometer one of the most accurate measuring instruments available!

At the same time, the very high field strength of the magnet gives the device a resolution of well over a million. Such high resolution enables very fine signals to be obtained, enabling molecules with very similar masses to be differentiated. With complex mixtures such as soils or combustion fumes containing



## THE FTICR MS IS A MULTITASKING ENGINE!



tens of thousands of molecules, the need for resolution is paramount.

This instrument enables us both to separate each molecule in a highly complex mixture and to assign a molecular formula to each signal, thus deciphering the molecular composition of a sample. It's a bit like wearing glasses for a short-sighted person... The contours are much sharper, more precise, and we're able to distinguish the details of an object and not just its overall shape.

## HOW DOES IT WORK IN PRACTICE?

To begin with, you need to dilute the sample in a solvent. This is a bit like diluting grenadine in water, so that it's not too sweet. Next, the sample is introduced into the ionization source using a syringe. Naturally, a molecule is electrically neutral; it has no charge. But we can add charges to it, for example, by associating it with other charged species in the sample, so that our molecule becomes an ion. This step is important because the electric and magnetic fields used by the instrument would not be able to act on molecules without an electric charge, and the analysis would not work. Once the molecules have been ionized, the great journey begins, all the way to the heart of the spectrometer. Once in the center of the magnet, the ions will spin and travel tens of kilometers! But for the measurements to go smoothly, they must not encounter any obstacles, which is only possible in a very high vacuum corresponding to 13 orders of magnitude less than atmospheric pressure! To achieve this, the instrument is equipped with very powerful vacuum pumps called turbomolecular pumps.

To determine the mass of ions, we measure their rotational frequency, which depends on their mass. By applying a mathematical operation known as the Fourier transform, it is possible to determine the frequency of each ion, enabling us to calculate their mass using a very simple calculation. Of course, for this to work at its best, expert users must be able to optimize the acquisition parameters to ensure optimum ion transmission, and the instrument must be very well calibrated to obtain highly accurate measurements. To achieve this, reference molecules with known masses are used.

The instrument generates a huge amount of data. To manage this data more easily, the international laboratory iC2MC (International Complex Matrices Molecular Characterization) has developed software capable of determining molecular formulas and representing the data obtained in the form of molecular maps, to facilitate comparison between samples.

These new spectrometers will enable us to push back the boundaries of molecular characterization and explore in greater detail highly complex samples in the healthcare, energy and environment sectors, and many others!

























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KanKr, whose real name is Simon Baert, is an author. He is the scriptwriter of the duo Plop & KanKr, formed with the cartoonist Julie Besombes, alias Plop. Together, they regularly publish in regional, national, and international press (Le Monde, Siné Mensuel, Le Temps, Sud Ouest dimanche, Le Sans-culotte 85, L'Anjou Laïque, La Galipote, La Gazette du Béarn des gaves...) and on television (Une semaine dans le monde on France 24). They are members of the Cartooning for Peace and Cartoon Movement networks. He also scripts scientific popular comics for the University of Pau and the Pays de l'Adour within the framework of the Science with, and for Society label.

Sébastien Tessier signs his comic books under the pseudonym **DAMOUR**, his mother's maiden name. Born in La Roche-sur-Yon in 1972, a passionate amateur of drawing, he came to study plastic arts in 1990 in Bordeaux where he still resides. He decided to live from his passion for comics and met Delcourt Editions at the Angoulême fair in 1994. This was the beginning of a long collaboration with the scriptwriter Jean-Pierre Pécau on the series Nash and Le Testament du Docteur M. He has produced 28 albums to date, with various scriptwriters and illustrators, including the series Pinkerton, La Cagoule, un Fascisme à la française at Glénat, as well as two historical albums, Kennedy with Sylvain Runberg as scriptwriter and L'Etincelle de Saint-Sardos, of which he is the author, at Sud-Ouest editions. He is passionate about history and has been working on historical projects for several years.

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**Plop**, whose real name is Julie Besombes, is a press cartoonist, illustrator and graphic designer. Together with KanKr, she forms the duo Plop & KanKr, who publish in the regional, national and international press (*Le Monde, Siné Mensuel, Le Temps, Sud Ouest dimanche, Le Sans-culotte 85, L'Anjou, Laïque, La Galipote...*) and for television (Une semaine dans le monde on France 24). She also produces press cartoons and popular science cartoons for the University of Pau and the Pays de l'Adour as part of the Science with and for Society label Science avec et pour la société.

**Cai Jiao Ping** is a teacher of Chinese and French. As an interpreter and translator, she teaches at the University of Pau and the Adour Region (UPPA), the Confucius Institute of Pau Pyrénées, and the University of Free Time of Aquitaine. She trains future language teachers in the French as a Foreign Language (FLE) program and conducts workshops and numerous seminars. Additionally, as a self-employed professional, she shares Chinese culture through courses for all ages and audiences.

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**Thomas Ferreira** is editor and graphic designer at Presses universitaires de Pau et des pays de l'Adour (PUPPA). In particular, he helped to create the comic strip magazine *Ebullition(s)*, for which he is artistic director. He is also an illustrator and graphic designer under the name Atelier Decafé.

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