Written on 16 January 2026

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News

Innovation and Industry

Analysis and characterization | Chemical analysis | Mathematics and IT | Software design

Chemists examine numerous mixtures of substances using increasingly sophisticated analytical tools that enable them to produce an identity card for the samples (gas, liquid, solid) analyzed. Unfortunately, to store test results, instruments utilize proprietary formats that are difficult to read and use outside of the software provided with these instruments. To simplify access to data, initiatives such as that of the Allotrope Foundation are emerging. An IFPEN

team is participating in this initiative and developing open source utilities for chromatography data. Explanations.

Analytical chemistry: a broad diversity of approaches

The analysis of gas, liquid or solid mixtures enables **their constituent elements to be identified, characterized, and quantified**, even when these mixtures contain hundreds of different substances in varying proportions. Chemists use specific equipment depending on the nature of the samples, be they fluids or solid materials such as catalysts or polymers.
IFPEN has **state-of-the-art analytical equipment**, covering various types of spectroscopy (IR, UV-Vis, Raman), chromatography, mass spectrometry and NMR, as well as electron microscopy. These instruments provide complex data, analyzed by sophisticated algorithms to produce a precise identity card for the samples, with research still ongoing to optimize their use.

Numerous proprietary formats

There are several challenges associated with analysis data, including **the diversity of proprietary formats**, their constant evolution, and their lack of interoperability. "*This makes it difficult to compare and aggregate data from different devices, and difficult to share this data between applications or experts*", explains Maxime Visconte, from the Information and Digital Systems Department. "*Developing converters for these formats is also very time-consuming. An ideal solution would be **a standardized exchange format for each area of analysis**.*"
Gas chromatography is a good candidate for data format standardization due to its widespread use and the diversity of proprietary formats associated with different devices. Used in a variety of fields (perfumery, wine-making, biology, etc.), **this technique makes it possible to separate, identify and quantify the volatile molecules present in a sample**. "*At IFPEN, more than fifteen different formats have been identified for gas chromatographs*", notes Maxime Visconte.

Towards a data standard for gas chromatography

A project team, *LabVision*, has been set up within IFPEN's IT department to simplify data reading and visualization, starting with gas chromatography.
The approach chosen was to adopt **the standardized exchange model proposed by the Allotrope Foundation** for this type of data. This model (*ADM - Allotrope Data Model*) is available in two formats: one containing text only (*ASM - Allotrope Simple Model*) and one combining text and binary data (*ADF - Allotrope Data Format*).
The *LabVision* project team, with technical support from Tech' Advantage, has developed ASM format converters for **the most common formats used by gas chromatography analyzers**[1], and data models to facilitate the use of ASM format files. These data models are available as Open Source in three programming languages: Java, Typescript and Python. Developers can then use these converters as they see fit in their own applications (machine learning, visualization, etc.).
These converters have also enabled the *LabVision* project team to contribute to a database containing numerous analysis results, made available to IFPEN chemists.

Allotrope Foundation and IFPEN: a shared vision

Founded in 2012, the Allotrope Foundation is an international consortium of companies that use analytical equipment (pharmaceutical, biopharmaceutical industries, etc.), instrument suppliers and software publishers established **to simplify the exchange of laboratory data**. The goal is to develop new approaches to improve data access, interoperability and integrity through standardization, an innovation driver. IFPEN shares this vision and contributes to defining and disseminating the Allotrope Foundation's standards, notably by participating in the chromatography working group.

Optimized sharing of scientific results

The *LabVision* project team initiative is part of a broader drive by IFPEN to promote open science, notably through an **Open Access platform**[2] where researchers are encouraged to submit their scientific publications. Open Source libraries developed at IFPEN are also available on GitHub, as well as the Arcane computing platform, developed in close collaboration with the CEA.
The tools provided by the LabVision project team will facilitate **the availability of laboratory data to a broad community of researchers**. These developments mark the first step in an ongoing process to incorporate more analysis techniques and formats. "*The hope is that new partners will sign up to this initiative and join the existing teams in order to accelerate the implementation of these standards*", concludes Maxime Visconte.

[1] The Java version of the GC to ASM format converter is available on GitHub at this address: GC2ASM : GC to Allotrope Simple Model converter. This converter processes data from Agilent's Chemstation and OpenLab software.

[2] HAL IFPE Portal

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16 January 2026

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