



# Metabolite identification to enhance and accelerate small molecule biomarker discovery

Accurate metabolite identification is needed to **maximize the impact of discovery metabolomics and lipidomics**, to effectively map the role of key biomarkers identified in a study and support translation to clinical use.

Sapient has focused extensively on building capabilities to **enhance the speed, quality, and extent of metabolite identification** so that more statistically significant metabolites and lipids can be effectively interrogated and advanced to validation studies.

The goal of nontargeted metabolomic or lipidomic studies is to discover the most biologically important signals in a patient population, whether they are known molecules or yet to be chemically identified.

With Sapient's rapid liquid chromatography-mass spectrometry (rLC-MS) systems, we can now measure >15,000 chromatographic features in a single sample, greatly expanding biomarker discovery potential but also increasing the likelihood of finding important but unidentified molecules.

Metabolite identification is central towards understanding the biological role of molecules of interest and to effectively map their involvement in disease processes. Accuracy in this process is critical to ensure that misidentifications or false hits do not lead researchers astray, and also that the biomarker can be reproducibly measured in validation studies.

**Sapient's metabolite identification capabilities have been developed to maximize definitive identifications for a study and elucidate more unknown molecules to advance novel discoveries.**

## Expanding identification to enhance your discovery insights

### Comprehensive Metabolite Standards Library of >10,000 reference standards

- Enriched for key human and preclinical metabolic pathways, biochemical processes, and disease drivers
- Ranging from endogenous human metabolites to molecules originating from plants, food, FDA approved drugs, and environmental toxicants
- All standards have been extensively analyzed using Sapient's rLC-MS instrumentation

### >1,000 Tier 1 metabolite identifications

Leveraging three chemical parameters – including retention time (RT), MS1 mass-to-charge ratio (m/z), and MS2 chemical fingerprint – and computational mapping between metabolites assayed in biological samples and Sapient's Metabolite Standards Library

### Database of >6 million MS2 spectra

Representing over 600,000 compounds that is used for putative structural identification of unidentified metabolites and lipids

# Accelerating **insights**, improving **translatability**.

The scale and accuracy with which we can perform metabolite identification brings critical scientific value to discovery screenings, in two key ways:

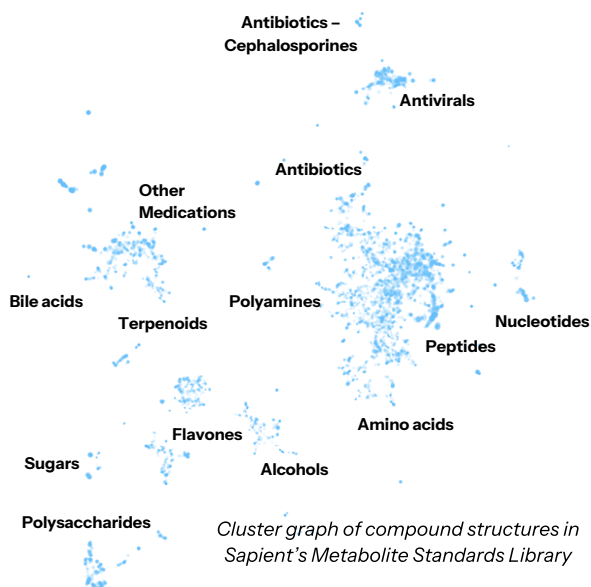
## Tier 1 identifications at the **highest confidence levels**.

By generating multi-parameter rLC-MS data on greater than 10,000 chemical reference standards, we are able to assign MSI Tier 1 identification to over 1,000 metabolites and lipids that are routinely measured in plasma and tissue biosamples. This approach provides **the highest possible confidence in the biomarker's identity** so it can be quickly made actionable to advance the given drug development program.

All identified compounds undergo **rigorous quality control** including visual inspection of peak shape and retention time consistency across all samples, as well as confirmation that no identified compound represents an isotope, adduct, or in-source fragment of another signal.

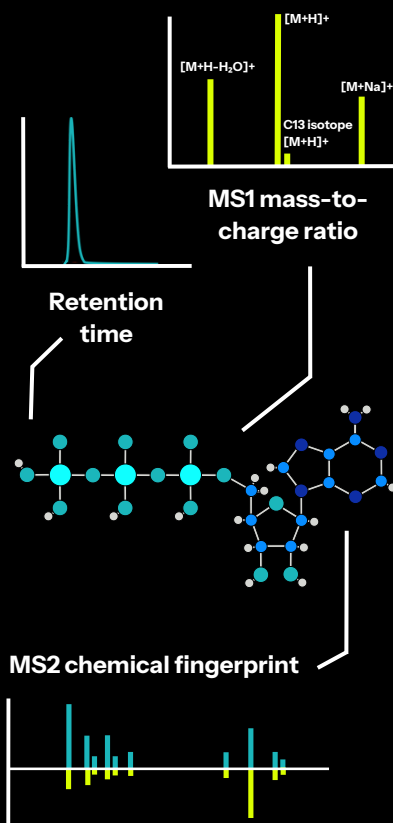
## Extensive data to **amplify discovery potential** among unannotated molecules.

For those molecules that remain unannotated, Sapient can continue to provide putative structural and pathway information. Leveraging Sapient's database of more than 6 million MS2 spectra across more than 600,000 compounds, we can provide **putative structural insights for hundreds to thousands of additional metabolites**, enabling advancement of novel discoveries.



## What makes an identification Tier 1?

The molecule is matched to a reference standard under the same analytical conditions via multiple chemical parameters including:



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To identify and advance robust small molecule biomarkers with confidence, make Sapient your discovery partner.