

SIRIUS

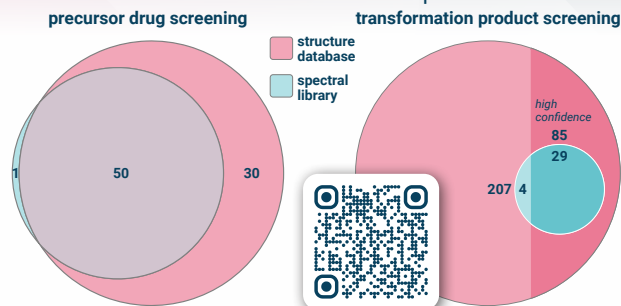
Applications

Transformation Products

Non-targeted screening for transformation products with SIRIUS

Integrated precursor and transformation / degradation product screening:

- BioTransformer 3.0 integration for transformation product candidate generation.
- *De novo* molecular formula assignment for unknowns.
- Transformation product database search.
- Compound class prediction for novel contaminants.
- Multiple validation levels for structural annotations.



Application Note:

Detecting pharmaceuticals and their transformation products with SIRIUS

Early Drug Discovery

Barcode-free screening for early drug discovery using SIRIUS

Affinity selection screening for early drug discovery:

- Screening massive chemical libraries in a single experiment.
- Target protein exposed to a compound pool.
- Binding ligands are identified based on DNA- or RNA-barcodes.
- **Drawback:** Synthetic complexity and biased binding results.

New decoding solution: Self-Encoded Libraries (SELs):

- No external decoding tags or genetic labels.
- Ligands are directly identified based on their characteristic MS/MS spectrum.
- Structure elucidation of selected ligands with SIRIUS.
- Faster and more cost-effective.
- Suitable for previously intractable targets.

SEL Case Studies:
Going barcode-free:
screening massive small
molecule libraries for
early drug discovery



CAIX: known oncology target with established binders
Screening a ~500,000-member library for CAIX ligands.

Identification and validation of several nanomolar binders (e.g. 4-sulfamoylbenzoic acid).

SELs are suitable for high-throughput applications.

FEN1: DNA-processing enzyme considered
inaccessible to traditional barcode-based screening.
Targeting FEN1 with a focused 4,000-member library.
Identification of two compounds that inhibit its activity.

SELs have the potential to unlock challenging drug targets that were previously intractable.

PFAS, E&Ls, Contaminants

Detecting PFAS, extractables & leachables, and unknown contaminants with SIRIUS

Advanced PFAS detection:

- Automated PFAS flagging during pre-processing.
- Molecular clusters visualized using Kendrick Mass Defect plots.

Extractables & Leachables detection:

- Targeted contaminant screening for known, prevalent contaminants.
- Comprehensive non-targeted analysis for unexpected or unknown contaminants.



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SIRIUS Discoveries



Independent research groups using the SIRIUS software framework to enhance their small molecule data analysis.

Mapping the ISS metabolome uncovering its vast chemical “dark matter”



Understanding the invisible ecosystems of space habitats has become critical for astronaut health. The International Space Station (ISS) is a closed microbial and chemical environment unlike anything on Earth. This study mapped the ISS microbiome and metabolome in unprecedented detail using SIRIUS.

Decoding the influence of gut microbiota on drug efficacy



In pharmacology, one of the most significant challenges is the variability in how patients respond to the same drug. Emerging research points to a hidden player: the human gut microbiota. Using SIRIUS, researchers investigated how gut microbiota alter the chemical structure of GPCR drugs.

Investigating the efficacy of abatement systems at fluoropolymer plants



Fluoropolymer production plants have invested in abatement systems to curtail the emission of PFAS. In a screening approach using SIRIUS, researchers detected a homologous series of previously overlooked polymerization byproducts and reveal a more complex emission profile than previously understood.

Mapping the chemical space of biomes



“Biotics” have gained attention for their potential to enhance skin health. SIRIUS identifies changes in the skin metabolome that are more pronounced than changes in the microbial composition, suggesting that even subtle shifts in microbial abundance can lead to significant effects on the skin.

Screening extractables and leachables in liquor products



Understanding the potential presence of unexpected E&Ls in our food and drinks is paramount. Alcoholic beverages are of particular concern due to their increased affinity and extended storage periods. SIRIUS predicts chemical structures to identify unexpected contaminants and ensure safety of our food.

Investigating biotransformation of antibiotics in wastewater



Conventional treatment methods are often unable to adequately remove antibiotics from wastewater, which perpetuates resistance. SIRIUS identifies degradation products from fungal biotransformation as a promising alternative wastewater treatment method.

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