The cutting-edge software for automated identification of small molecules



SIRIUS is your all-in-one software solution for comprehensive small molecule annotation.

## WHY CHOOSE SIRIUS?

Best in class: Our methods are best-in-class and published in leading scientific journals.

**Beyond spectral libraries:** SIRIUS helps you reveal novel small molecules instead of limiting your analysis to common compounds with reference standards in spectral libraries.

Al-based: SIRIUS is based on profound algorithms and machine learning models developed through decades of research.

### YOUR ADVANTAGES

Fully automate your analysis: Accelerate your workflow with our software, delivering faster, more precise insights while eliminating hours of tedious manual work.

Unlock your instrument's full potential: Our software enhances annotation quality, maximizing the insights gained from your measurements.

Gain confidence: Our automated confidence score evaluates annotation accuracy, ensuring reliable and trustworthy results.

## **APPLICATION AREAS & CASE STUDIES**

contaminants, leachables & extractables, PFAS, impurities, ... 

Screening for plastic-related contaminants in liquor products

CASE STUDY

As we are becoming increasingly conscious of what we consume, understanding the potential presence of unexpected extractables and leachables in our food and drinks is paramount. SIRIUS predicts chemical structures of unknowns to identify unexpected contaminants and ensure food safety.

DENTIFY

new bioactive substances, drug leads, biomarkers, ...

### Revealing novel bioactive molecules hidden in the coral reef

**CASE STUDY** 

Marine microorganisms offer a rich source of bioactive molecules with unique structures and remarkable biological activity. To narrow down the search to the most promising microorganisms, SIRIUS is annotating natural products to estimate the chemical potential of microbial extracts.

degredation products, toxins, drugs, pesticides, ...

### Identifying unstable metabolites in long-term storage samples

**CASE STUDY** 

Neonatal dried blood spots are important for newborn screening and a powerful source for investigating metabolic etiologies of various diseases. SIRIUS helps tracking the stability of metabolites to carefully monitor the effect of storage time on metabolite levels.



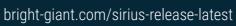
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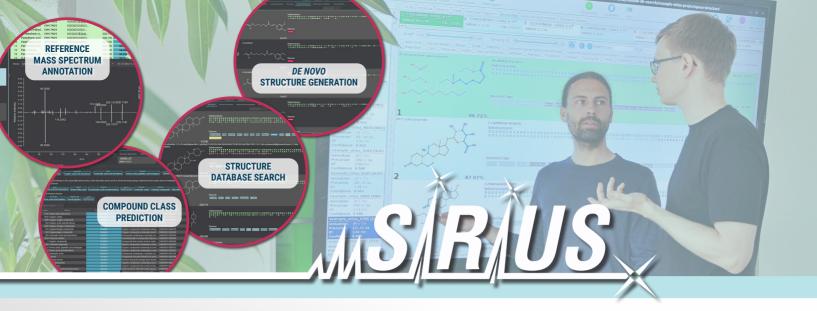
info@bright-giant.com



bright-giant.com







### **ALL-IN-ONE SOLUTION**

SIRIUS is the all-in-one solution for comprehensive small molecule annotation **from suspects to novel molecules**.

# Molecules with reference standards in spectral libraries

Annotation based on spectral libraries (including your in-house libraries) is seamlessly integrated into the full annotation workflow.

# Molecules only catalogued in structure databases

Beyond spectral libraries: Tap into the vast potential of structure databases and expand your analysis beyond known reference standards.

# Molecules that are previously undiscovered or not yet elucidated

Beyond structure databases: Push the boundaries of discovery with advanced tools for analyzing and elucidating novel molecules.

### **OUR SERVICES**

### **Software and interfaces**

SIRIUS is a free, open-source software suite for analyzing LC-MS/MS data of small molecules that supports all operating systems and offers multiple interfaces (GUI, CLI, API) catering to beginners, experts, and programmers alike.

### Licences

Bright Giant GmbH is the only license provider for SIRIUS web services for advanced structure elucidation features and related SaaS solutions for non-academic users.

#### **Custom services**

We provide custom hosting of our software solutions, custom tailored workflows and reporting, custom structure database generation and custom training of machine learning models to include clients' own reference data. Get your personalized structure elucidation workflow.

### TRUSTED BY USERS WORLDWIDE



SIRIUS is widely recognized and trusted within the scientific community, processing millions of queries each year.



**CONTACT US:** 



info@bright-giant.com



bright-giant.com



