

# メタボロームリポジトリの 設計と機能

|      |          |
|------|----------|
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# 関連サイト MetaboLights

2012年よりスタート、あらゆる生物種の総合リポジトリ

Chris Steinbeck と Reza Salekらがスタート

代謝物のリストなど、データは充実

投稿者はISA-TOOLSによりメタデータを作成（けっこう大変）


>90% が論文成果

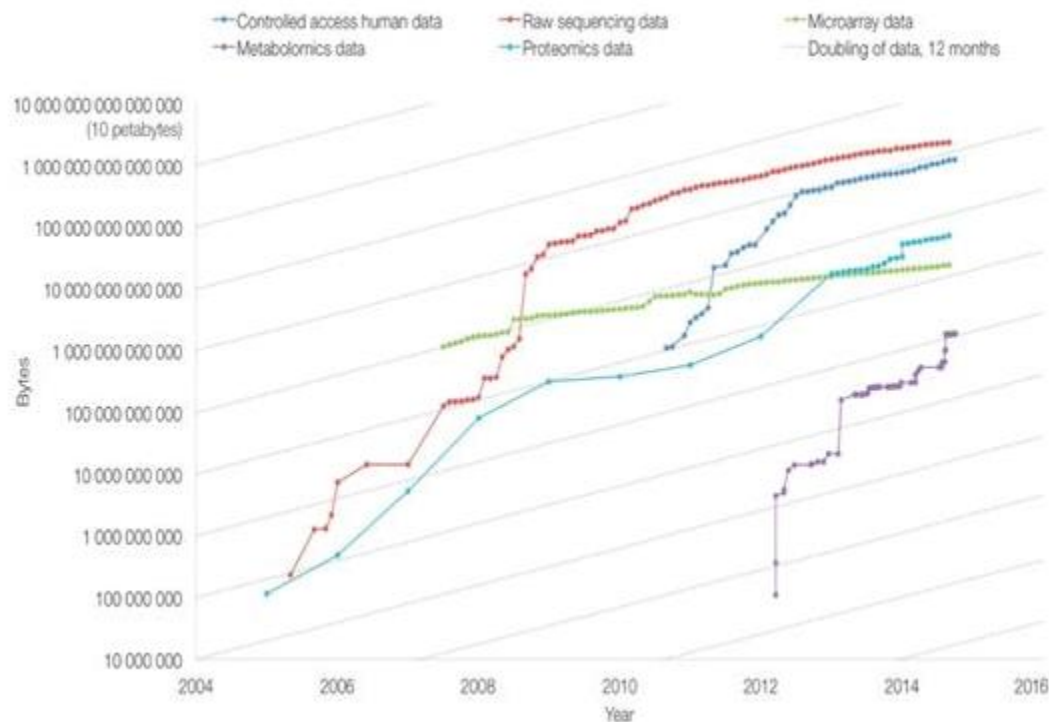


## MetaboLights

MetaboLights is a database for Metabolomics experiments and derived information. The database is cross-species.

## Download

 **Pre-packaged ISAcreator download.** To make it easy for new users, please download and just unzip the pre-packaged ISAcreator with plugin and configurations.



# 関連サイト Metabolomics Workbench

NIH Common Fund による  
主にヒト・データ  
< 20% が論文化  
(NIHポリシーによる公開)

メタデータはエクセルで  
アップロード可  
サイト上でデータ解析が  
可能(クラウドコンピュー  
ティング)

しかし、メタデータが不足  
再解析も難しい



The screenshot shows the homepage of the Metabolomics Workbench. At the top left is a circular logo with the text 'Metabolomics Workbench' and a molecular structure. To the right, the title 'METABOLOMICS WORKBENCH' is displayed in large white letters against a background of a dry, cracked landscape. Below the title is a navigation menu with links: Home, NIH Data Repository, Databases, Protocols, Standards, Tools, Training / Events, and a partially visible 'F'. A welcome message reads: 'Welcome to the UCSD Metabolomics Workbench, a resource sponsored by the Common Fund of the National Institutes of Health'. Below this is a section titled 'NIH Metabolomics Data Repository' with three buttons: 'Upload and Manage Studies', 'Browse and Search Studies', and 'Analyze Studies'. At the bottom is a 'Metabolomics News' section with a dated announcement: '02-11-2018 - Research Associate for Metabolomics Research - The Sumner Lab at the University of North Carolina at Chapel Hill Nutrition Research Institute is seeking an individual who is highly skilled and experienced in mass spectrometry methods to serve as a Research Associate for metabolomics research. The Research Associate will be responsible for the development and optimization of mass spectrometry methods for metabolomics research.'

結局、リサイクルが難しい

1. 生データの取得法、フォーマットが多様
2. データの統合が困難  
(マイクロアレイに酷似)

MetabolomeXchange 

An international data aggregation and notification service for metabolomics.

## 目標

- 論文投稿時に登録するリポジトリ
- 統合解析のできるデータサーバ
  - 生データに解析結果や測定法がぶら下がる構造 (Metabolonoteの分類法)
  - 解析結果(例えばスペクトル、化合物リスト)の検索
  - データ登録者へのリワード

# 2020年までのマイルストーン

いずれも国際標準が前提

**遺伝研：** 恒久的なデータ・リポジトリの開設（遺伝研アドレス）

初期データ： 理研CSRSおよびかずさDNA研のデータ  
（MassBase, DropMet, Komics）

投稿データ： 共同研究先を優先

プロジェクトデータ： AMED微生物叢領域との連携

**かずさ：** 保有するメタボロームデータの再解析

PowerGet等、ソフトウェアのアップデート 遺伝研でリリース

**理研：** 保有するメタボロームデータの再解析 理研でリリース

**奈良先：** 生体活性オントロジー構築、メタ代謝マップ構築

# MetaboBank 全体構想

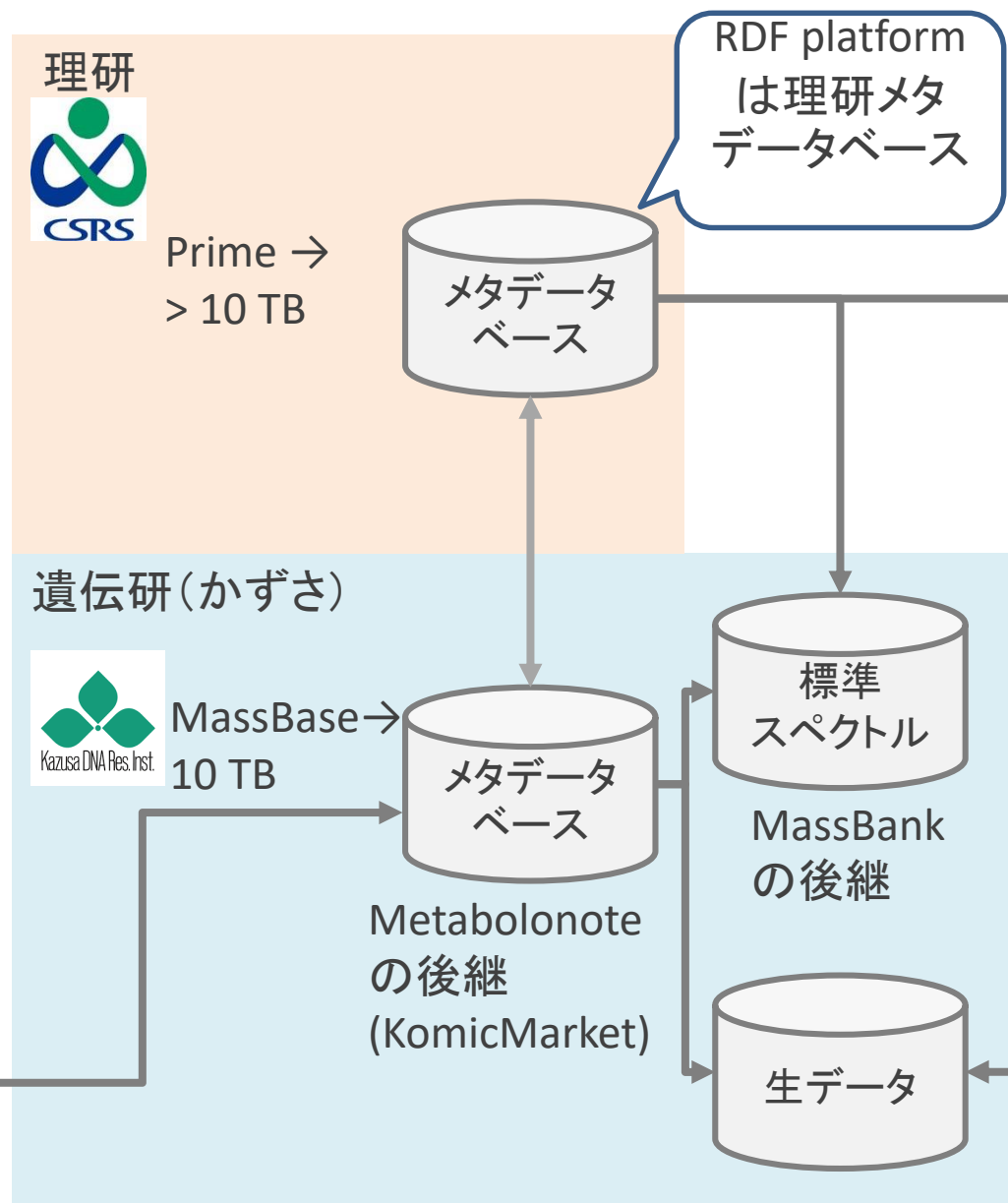
欧州のMetaboLights, 米国のMetabolomics Workbenchに並ぶ、生データのリポジトリ。  
DDBJサービスとして開設。  
平成31~2年度には、一般からの投稿を受付。

標準スペクトルのサーバは、MassBank wikiという名前でも継続

データはOmics DI (omicsdi.org)およびmetabolomeXchangeに登録。

今年度は植物のメタデータ作成と、フォーマット決定。  
来年度以降、医薬学のメタボロミクスへ拡張

  
ユーザー



# メタデータ登録処理



ユーザ



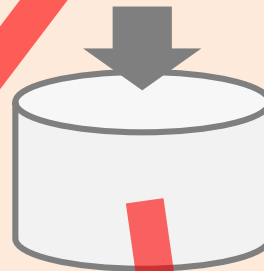
メタデータ  
登録用Excel



登録



内部処理用  
Excel



RDF  
データベース

検索・データ入手



MetaboBankシステム

| 1                            | 2          | 3      | 4   | 5   | 6   | 7   | 8   | 9   | 10  | 11  | 12  | 13  | 14  | 15  | 16  | 17  | 18  | 19  | 20  | 21  | 22  | 23  | 24  | 25  |
|------------------------------|------------|--------|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Biological Sample            | 生物サンプル     | proton | plant organ                                   | plant tissue part                             | transcription factor                          | transcription factor                          | transcription factor                          | transcription factor                          | transcription factor                          | transcription factor                          | transcription factor                          | transcription factor                          | transcription factor                          | transcription factor                          | transcription factor                          | transcription factor                          | transcription factor                          | transcription factor                          | transcription factor                          | transcription factor                          | transcription factor                          | transcription factor                          | transcription factor                          | transcription factor                          |
| 生物サンプル                       | 生物サンプルID   | 種別     | 植物器官  | 植物組織  | 転写因子  | 転写因子  | 転写因子  | 転写因子  | 転写因子  | 転写因子  | 転写因子  | 転写因子  | 転写因子  | 転写因子  | 転写因子  | 転写因子  | 転写因子  | 転写因子  | 転写因子  | 転写因子  | 転写因子  | 転写因子  | 転写因子  | 転写因子  |
| BiologicalSample             | identifier | file   | accession                                     | accession                                     | accession                                     | accession                                     | accession                                     | accession                                     | accession                                     | accession                                     | accession                                     | accession                                     | accession                                     | accession                                     | accession                                     | accession                                     | accession                                     | accession                                     | accession                                     | accession                                     | accession                                     | accession                                     | accession                                     | accession                                     |
| en_bioscience:SE46_QC_L_18_1 | "1_18_1"   | Col-0  | https://url.iobio.library.org/iobio/FO_000806 | https://url.iobio.library.org/iobio/FO_000806 | https://url.iobio.library.org/iobio/FO_000806 | https://url.iobio.library.org/iobio/FO_000806 | https://url.iobio.library.org/iobio/FO_000806 | https://url.iobio.library.org/iobio/FO_000806 | https://url.iobio.library.org/iobio/FO_000806 | https://url.iobio.library.org/iobio/FO_000806 | https://url.iobio.library.org/iobio/FO_000806 | https://url.iobio.library.org/iobio/FO_000806 | https://url.iobio.library.org/iobio/FO_000806 | https://url.iobio.library.org/iobio/FO_000806 | https://url.iobio.library.org/iobio/FO_000806 | https://url.iobio.library.org/iobio/FO_000806 | https://url.iobio.library.org/iobio/FO_000806 | https://url.iobio.library.org/iobio/FO_000806 | https://url.iobio.library.org/iobio/FO_000806 | https://url.iobio.library.org/iobio/FO_000806 | https://url.iobio.library.org/iobio/FO_000806 | https://url.iobio.library.org/iobio/FO_000806 | https://url.iobio.library.org/iobio/FO_000806 | https://url.iobio.library.org/iobio/FO_000806 |

**RIKEN Plant Metabolomics MetaDatabase**

Search

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| Experiment ID                                     | title            | comment   | description                                       | measurement type     | technology type                     |
|---|------------------|---|---|----------------------|-------------------------------------|
| GC-TOF/MS analysis                                | "RPMM0001 GC-MS" | GC-TOF/MS analysis                                | Non-targeted analysis of metabolites by GC-TOF/MS | metabolite profiling | chromatography<br>mass spectrometry |
| Non-targeted analysis of metabolites by GC-TOF/MS | "RPMM0002"       | Non-targeted analysis of metabolites by GC-TOF/MS | Non-targeted analysis of metabolites by GC-TOF/MS | metabolite profiling | chromatography<br>mass spectrometry |
| Non-targeted analysis of metabolites by GC-TOF/MS | "RPMM0003_GC"    | Non-targeted analysis of metabolites by GC-TOF/MS | Non-targeted analysis of metabolites by GC-TOF/MS | metabolite profiling | chromatography<br>mass spectrometry |
| GC-TOF-MS analysis                                | "RPMM0004"       | GC-TOF-MS analysis                                | GC-TOF-MS analysis                                | metabolite profiling | chromatography<br>mass spectrometry |

# メタデータ項目検討

MetaboBankMetadataTest.xlsx - Excel

|    | B                         | C                   | J          | K  | L                         | M           | N                | O          | P      | Q  | R       | S       | T        | U                      |
|----|---------------------------|---------------------|------------|--|---------------------------|-------------|------------------|------------|--------|--|---------|---------|----------|------------------------|
| 1  | Biological Sample         | biological sample   | genotype   | plant organ                                | plant tissmutant transgre | levartreatm | growth condition |            |        |  | day len | dark L  | humidity | development stage      |
| 2  | 生物サンプル                    | 生物サンプルID            | 遺伝型        | 植物器官                                       | 植物組織 変異体 形質転              | 関連遺伝        | 処理               | 生育条件       |        |  | 日長      | 暗時間     | 湿度       | 生育段階                   |
| 3  |                           | dcterms: identifier | genotype   | plantOrgan                                 | plantTissmutant transgre  | levartreatm | growthCondition  |            |        |  | dayLen  | darkLer | humidity | developmentStage       |
| 4  | BiologicalSample          | xsd:string          | xsd:string | owl:Class                                  | owl:Class                 | xsd:string  | xsd:string       | xsd:string | Treatm | xsd:string   | xsd:du  | xsd:du  | Humidit  | xsd:string             |
| 20 | pm_biosamp:SE46_GC_L_18_1 | "L_18_1"            | Col-0      | http://purl.obo.library.org/obo/PO_0009006 |                           |             |                  |            |        | "The sterilized seeds were stratified at 5 degrees C for 2 d, and were successively sown on Murashige and Skoog (MS) medium containing 1% sucrose. Plants saw on the plate were grown in controlled growth chambers for 18 days. Aerial parts were harvested 6 h after the onset of the bright phase." | PT16H   | PT8H    |          | "18 days after sowing" |
| 21 | pm_biosamp:SE46_GC_L_19_1 | "L_19_1"            | Col-0      | http://purl.obo.library.org/obo/PO_0009006 |                           |             |                  |            |        | "The sterilized seeds were stratified at 5 degrees C for 2 d, and were successively sown on Murashige and Skoog (MS) medium containing 1% sucrose. Plants saw on the plate were grown in controlled growth chambers for 18 days. Aerial parts were harvested 6 h after the onset of the bright phase." | PT16H   | PT8H    |          | "18 days after sowing" |
| 22 | pm_biosamp:SE46_GC_L_20_1 | "L_20_1"            | Col-0      | http://purl.obo.library.org/obo/PO_0009006 |                           |             |                  |            |        | "The sterilized seeds were stratified at 5 degrees C for 2 d, and were successively sown on Murashige and Skoog (MS) medium containing 1% sucrose. Plants saw on the plate were grown in controlled growth chambers for 18 days. Aerial parts were harvested 6 h after the onset of the bright phase." | PT16H   | PT8H    |          | "18 days after sowing" |
| 23 | pm_biosamp:SE46_GC_L_21_1 | "L_21_1"            | tt4        | http://purl.obo.library.org/obo/PO_0009006 |                           |             |                  |            |        | "The sterilized seeds were stratified at 5 degrees C for 2 d, and were successively sown on Murashige and Skoog (MS) medium containing 1% sucrose. Plants saw on the plate were grown in controlled growth chambers for 18 days. Aerial parts were harvested 6 h after the onset of the bright phase." | PT16H   | PT8H    |          | "18 days after sowing" |
| 24 | pm_biosamp:SE46_GC_L_22_1 | "L_22_1"            | tt4        | http://purl.obo.library.org/obo/PO_0009006 |                           |             |                  |            |        | "The sterilized seeds were stratified at 5 degrees C for 2 d, and were successively sown on Murashige and Skoog (MS) medium containing 1% sucrose. Plants saw on the plate were grown in controlled growth chambers for 18 days. Aerial parts were harvested 6 h after the onset of the bright phase." | PT16H   | PT8H    |          | "18 days after sowing" |
| 25 | pm_biosamp:SE46_GC_L_23_1 | "L_23_1"            | tt4        | http://purl.obo.library.org/obo/PO_0009006 |                           |             |                  |            |        | "The sterilized seeds were stratified at 5 degrees C for 2 d, and were successively sown on Murashige and Skoog (MS) medium containing 1% sucrose. Plants saw on the plate were grown in controlled growth chambers for 18 days. Aerial parts were harvested 6 h after the onset of the bright phase." | PT16H   | PT8H    |          | "18 days after sowing" |

準備完了



# RIKEN Plant Metabolite Database



Database

## RIKEN Plant Metabolomics MetaDatabase

RIKEN Plant Metabolomics MetaDatabase



Search

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Fix Heading  Show URI

| Experiment  | experiment ID  | title   | comment | description   | measurement type   | technology type  |
|---|--|---|---------|---|--|--|
| <ul style="list-style-type: none"><li>GC-TOF/MS analysis</li></ul>                                | <ul style="list-style-type: none"><li>"RPMM0001 GC-MS"</li></ul> | <ul style="list-style-type: none"><li>GC-TOF/MS analysis</li></ul>                                |         | <ul style="list-style-type: none"><li>Non-targeted analysis of metabolites by GC-TOF-MS</li></ul> | <ul style="list-style-type: none"><li>metabolite profiling</li></ul> | <ul style="list-style-type: none"><li>chromatography</li><li>mass spectrometry</li></ul> |
| <ul style="list-style-type: none"><li>Non-targeted analysis of metabolites by GC-TOF-MS</li></ul> | <ul style="list-style-type: none"><li>"RPMM0002"</li></ul>       | <ul style="list-style-type: none"><li>Non-targeted analysis of metabolites by GC-TOF-MS</li></ul> |         | <ul style="list-style-type: none"><li>Non-targeted analysis of metabolites by GC-TOF-MS</li></ul> | <ul style="list-style-type: none"><li>metabolite profiling</li></ul> | <ul style="list-style-type: none"><li>chromatography</li><li>mass spectrometry</li></ul> |
| <ul style="list-style-type: none"><li>Non-targeted analysis of metabolites by GC-TOF-MS</li></ul> | <ul style="list-style-type: none"><li>"RPMM0003_GC"</li></ul>    | <ul style="list-style-type: none"><li>Non-targeted analysis of metabolites by GC-TOF-MS</li></ul> |         | <ul style="list-style-type: none"><li>Non-targeted analysis of metabolites by GC-TOF-MS</li></ul> | <ul style="list-style-type: none"><li>metabolite profiling</li></ul> | <ul style="list-style-type: none"><li>chromatography</li><li>mass spectrometry</li></ul> |
| <ul style="list-style-type: none"><li>GC-TOF-MS analysis</li></ul>                                | <ul style="list-style-type: none"><li>"RPMM0004"</li></ul>       | <ul style="list-style-type: none"><li>GC-TOF-MS analysis</li></ul>                                |         | <ul style="list-style-type: none"><li>GC-TOF-MS analysis</li></ul>                                | <ul style="list-style-type: none"><li>metabolite profiling</li></ul> | <ul style="list-style-type: none"><li>chromatography</li><li>mass spectrometry</li></ul> |



RIKEN MetaDatabase

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