資料科學統計合作社

生物資訊與數據分析

Metabolomics Data Analysis Ⅰ

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2025.6.10

Outline

01 代謝體學簡介

02 實驗分析平台

03 代謝體資料庫

04 資料分析平台

01

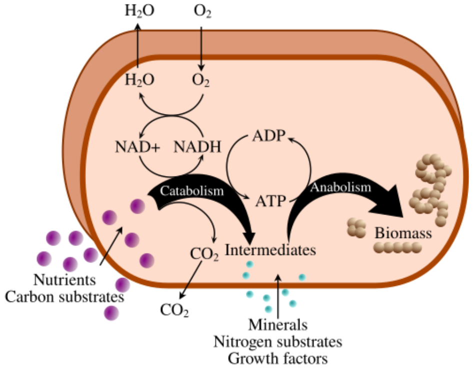
代謝體學
(Metabolomics)

代謝 (Metabolism)

- **代謝**是指**生物體內所有化學反應的總稱**，這些反應可分為兩大類：
  - **分解代謝（Catabolism）**：將大分子（如碳水化合物、脂肪、蛋白質）**分解成小分子**，**並釋放能量（如 ATP）**。
  - **合成代謝（Anabolism）**：將小分子**合成成大分子**（如細胞組成物質），此過程**需要消耗能量**。

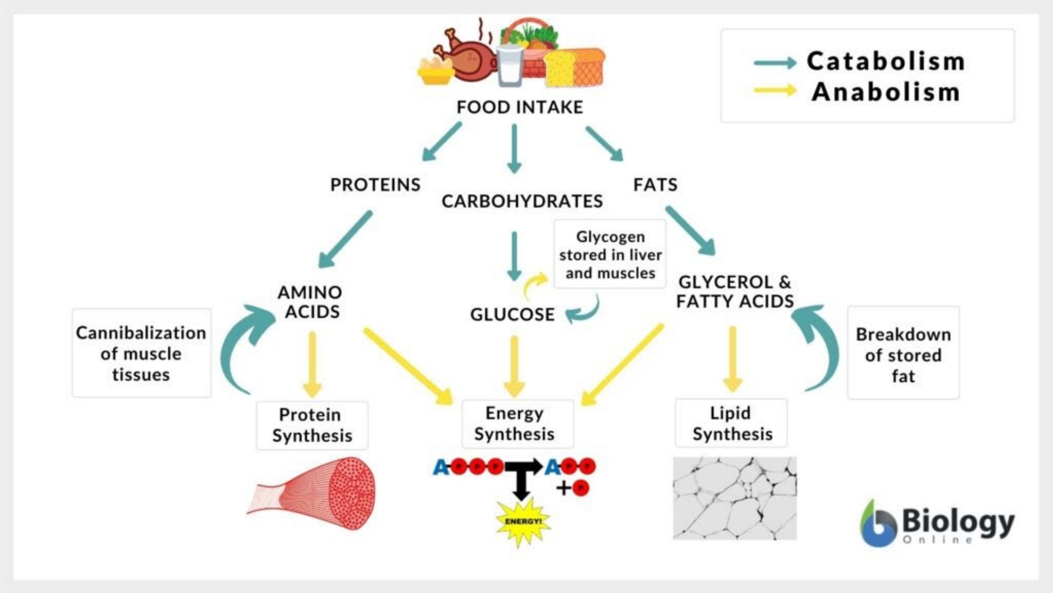
這些反應使得生物能夠維持生命、成長、修復與繁殖。

Simplified view of cellular metabolism



H_2O
O_2
H_2O
O_2
NAD+
NADH
ADP
Catabolism
ATP
Anabolism
Biomass
CO_2
Intermediates
Nutrients
Carbon substrates
CO_2
Minerals
Nitrogen substrates
Growth factors

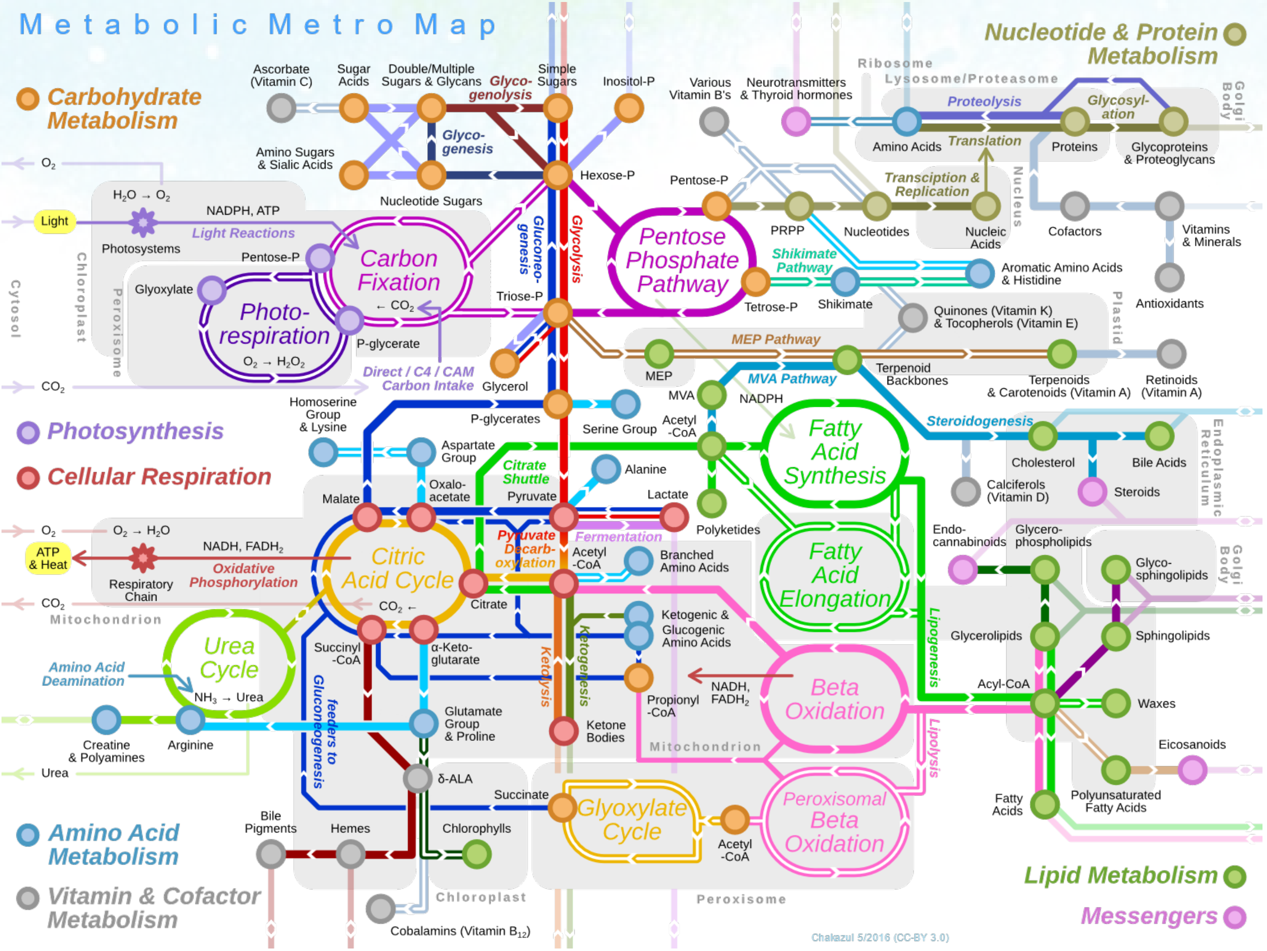
https://en.m.wikipedia.org/wiki/Metabolism



Catabolism
Anabolism
FOOD INTAKE
PROTEINS
CARBOHYDRATES
FATS
Glycogen stored in liver and muscles
AMINO ACIDS
GLUCOSE
GLYCEROL & FATTY ACIDS
Cannibalization of muscle tissues
Breakdown of stored fat
Protein Synthesis
Energy Synthesis
Lipid Synthesis
ENERGY!
Biology Online

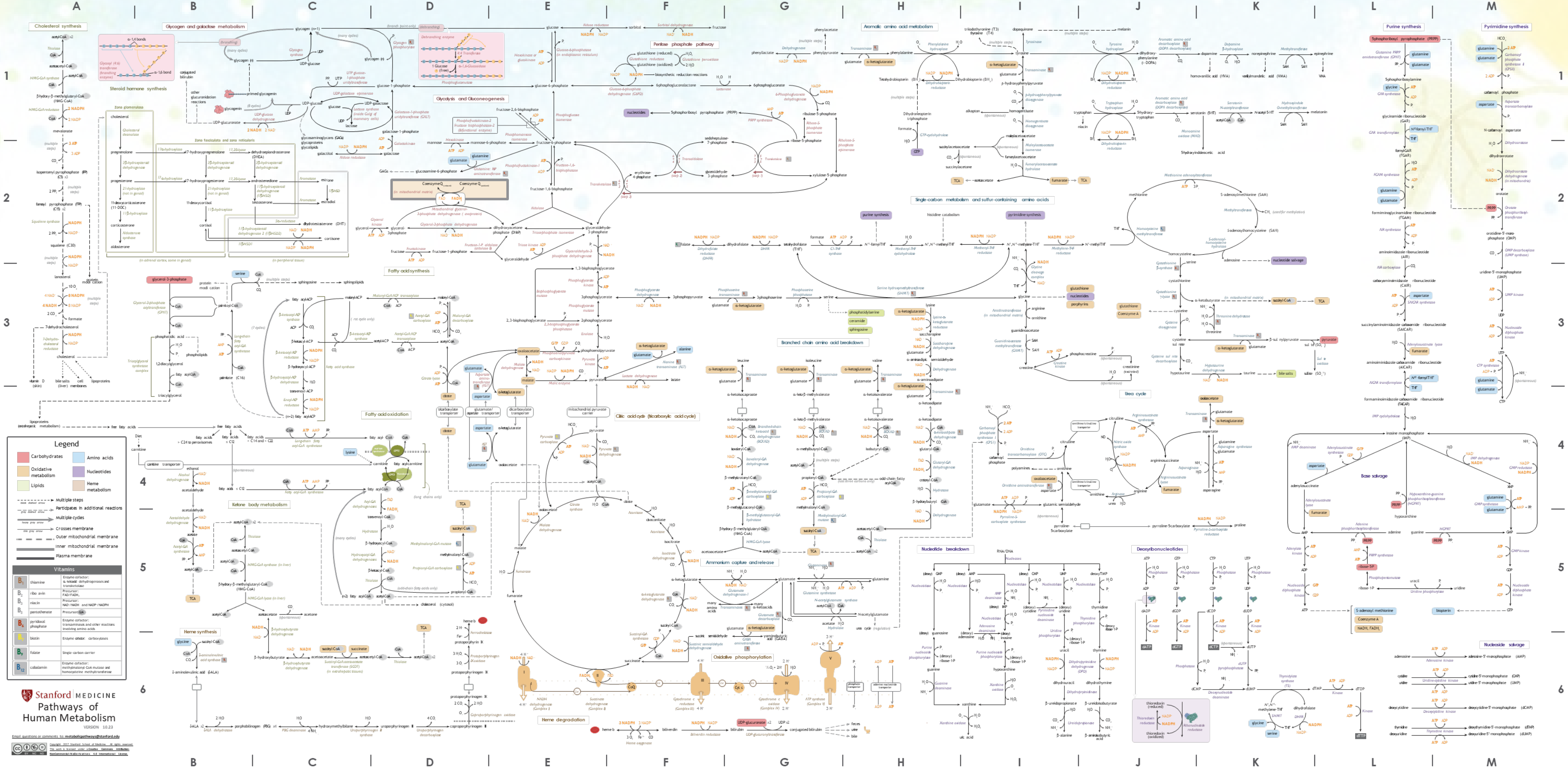
https://www.biologyonline.com/dictionary/metabolism

Cellular metabolic pathways


Metabolic Metro Map
Carbohydrate Metabolism
Photosynthesis
Cellular Respiration
Amino Acid Metabolism
Vitamin & Cofactor Metabolism
Nucleotide & Protein Metabolism
Lipid Metabolism
Messengers
Ascorbate (Vitamin C)
Sugar Acids
Double/Multiple Sugars & Glycans
Glyco-genolysis
Simple Sugars
Inositol-P
Amino Sugars & Sialic Acids
Glyco-genesis
Hexose-P
Nucleotide Sugars
O_2
$H_2O \rightarrow O_2$
Light
NADPH, ATP
Light Reactions
Photosystems
Pentose-P
Carbon Fixation
$\leftarrow CO_2$
Glyoxylate
Photo-respiration
$O_2 \rightarrow H_2O_2$
P-glycerate
Direct / C4 / CAM Carbon Intake
CO_2
Cytosol
Chloroplast
Peroxisome
Gluconeo-genesis
Glycolysis
Triose-P
Glycerol
Pentose Phosphate Pathway
Pentose-P
Tetrose-P
PRPP
Nucleotides
Shikimate Pathway
Shikimate
Aromatic Amino Acids & Histidine
Various Vitamin B's
Neurotransmitters & Thyroid hormones
Ribosome
Lysosome/Proteasome
Proteolysis
Glycosyl-ation
Amino Acids
Translation
Proteins
Glycoproteins & Proteoglycans
Golgi Body
Transcription & Replication
Nucleus
Nucleic Acids
Cofactors
Vitamins & Minerals
Antioxidants
Quinones (Vitamin K) & Tocopherols (Vitamin E)
Plastid
MEP Pathway
MEP
Terpenoid Backbones
Terpenoids & Carotenoids (Vitamin A)
Retinoids (Vitamin A)
MVA
MVA Pathway
NADPH
Acetyl -CoA
Fatty Acid Synthesis
Steroidogenesis
Cholesterol
Bile Acids
Calciferols (Vitamin D)
Steroids
Endoplasmic Reticulum
Homoserine Group & Lysine
P-glycerates
Serine Group
Aspartate Group
Citrate Shuttle
Oxalo-acetate
Pyruvate
Alanine
Lactate
Malate
Polyketides
Pyruvate Decarb-oxylation
Fermentation
Acetyl -CoA
Branched Amino Acids
Fatty Acid Elongation
O_2
$O_2 \rightarrow H_2O$
NADH, $FADH_2$
ATP & Heat
Oxidative Phosphorylation
Respiratory Chain
CO_2
Mitochondrion
Citric Acid Cycle
$CO_2 \leftarrow$
Citrate
Endo-cannabinoids
Glycero-phospholipids
Glyco-sphingolipids
Golgi Body
Urea Cycle
Amino Acid Deamination
$NH_3 \rightarrow$ Urea
Succinyl -CoA
α-Keto-glutarate
Ketolysis
Ketogenesis
Ketogenic & Glucogenic Amino Acids
Glycerolipids
Sphingolipids
Lipogenesis
Acyl-CoA
Waxes
Creatine & Polyamines
Arginine
Urea
Gluconeogenesis
feeders to
Glutamate Group & Proline
Propionyl -CoA
NADH, $FADH_2$
Beta Oxidation
Ketone Bodies
Mitochondrion
Lipolysis
Eicosanoids
δ-ALA
Succinate
Glyoxylate Cycle
Acetyl -CoA
Peroxisomal Beta Oxidation
Fatty Acids
Polyunsaturated Fatty Acids
Bile Pigments
Hemes
Chlorophylls
Chloroplast
Peroxisome
Cobalamins (Vitamin B_{12})
Chakazul 5/2016 (CC-BY 3.0)

https://en.m.wikipedia.org/wiki/Metabolic_pathway

Metabolic Pathways Map


A B C D E F G H I J K L M
Cholesterol synthesis
Glycogen and galactose metabolism
Steroid hormone synthesis
Glycolysis and Gluconeogenesis
Pentose phosphate pathway
Aromatic amino acid metabolism
Purine synthesis
Pyrimidine synthesis
Fatty acid synthesis
Single-carbon metabolism and sulfur-containing amino acids
Branched chain amino acid breakdown
Fatty acid oxidation
Citric acid cycle (tricarboxylic acid cycle)
Urea cycle
Ketone body metabolism
Ammonium capture and release
Heme synthesis
Oxidative phosphorylation
Heme degradation
Nucleotide breakdown
Deoxyribonucleotides
Base salvage
Nucleoside salvage
Legend
Carbohydrates
Amino acids
Oxidative metabolism
Nucleotides
Lipids
Heme metabolism
Multiple steps
Participates in additional reactions
Multiple cycles
Crosses membrane
Outer mitochondrial membrane
Inner mitochondrial membrane
Plasma membrane
Vitamins
B_1 thiamine
B_2 riboflavin
B_3 niacin
B_5 pantothenate
B_6 pyridoxal phosphate
B_7 biotin
B_9 folate
B_{12} cobalamin
Stanford MEDICINE
Pathways of Human Metabolism
VERSION 10.23

https://mededucation.stanford.edu/pathways-download/

常見細胞代謝路徑（Cellular Metabolic Pathways）

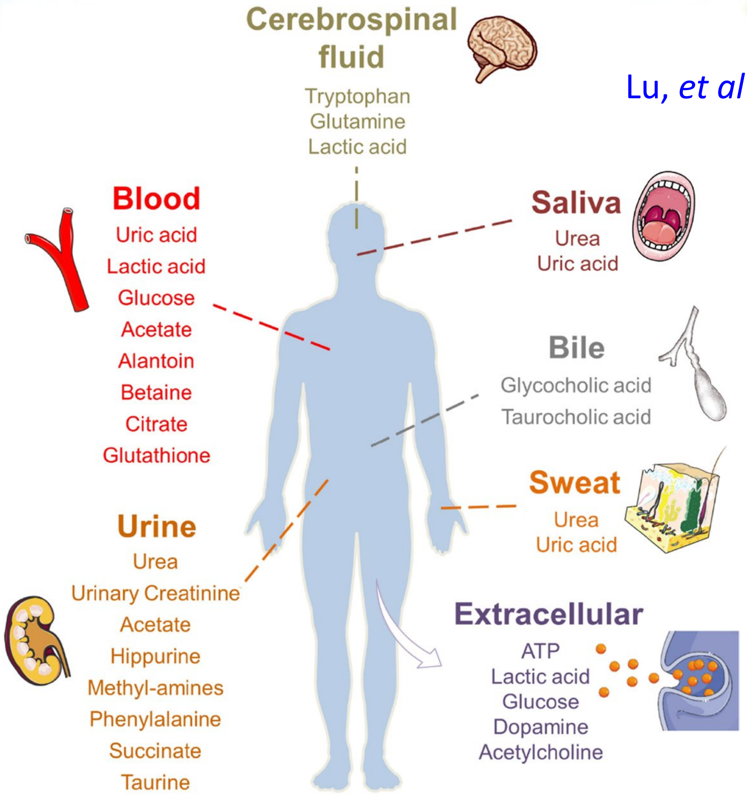
代謝途徑	主要功能	發生位置
糖解作用 Glycolysis	分解葡萄糖產生能量（ATP）	細胞質 (cytosol)
三羧酸循環 TCA cycle	完整氧化有機物產生 NADH/$FADH_2$	粒線體 (mitochondria)
電子傳遞鏈 ETC	利用 NADH/$FADH_2$ 產生 ATP	粒線體內膜
脂肪酸合成與氧化	合成或分解脂質作為能量來源	細胞質/粒線體
蛋白質代謝	胺基酸分解或合成	多處（細胞質等）

- ➔ **Metabolite (代謝物)**
- ➔ **Metabolome (代謝體)**
- ➔ **Metabolomics (代謝體學)**

Metabolite

- **Metabolites** are small molecules involved in metabolism processes [Wishart, 2007].

代謝物是指在生物體內進行代謝反應時所產生或使用的小分子化合物。這些小分子參與細胞內的各種生化反應，對生命活動至關重要。


Cerebrospinal fluid
Tryptophan
Glutamine
Lactic acid
Blood
Uric acid
Lactic acid
Glucose
Acetate
Alantoin
Betaine
Citrate
Glutathione
Saliva
Urea
Uric acid
Bile
Glycocholic acid
Taurocholic acid
Sweat
Urea
Uric acid
Urine
Urea
Urinary Creatinine
Acetate
Hippurine
Methyl-amines
Phenylalanine
Succinate
Taurine
Extracellular
ATP
Lactic acid
Glucose
Dopamine
Acetylcholine

Lu, *et al.*, 2022

https://www.sciencedirect.com/science/article/pii/S2590006422000035

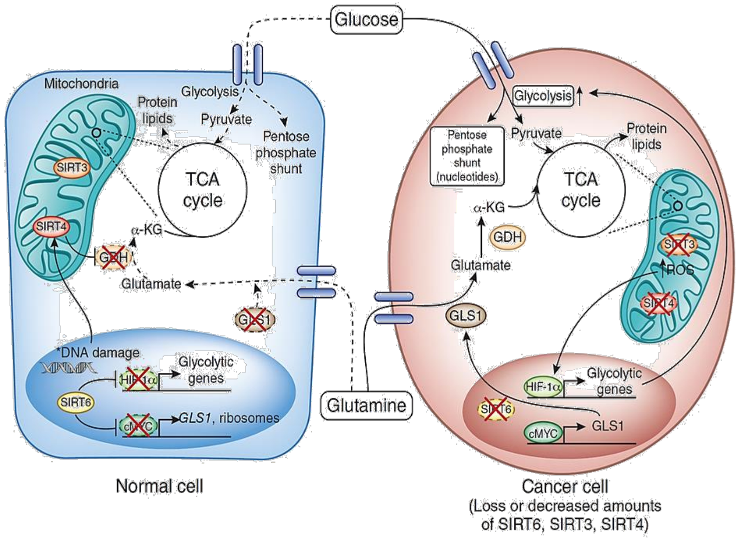
分類（Types of Metabolites）

分類	說明	英文註解
主要代謝物	與細胞生長、能量轉換直接相關的代謝物	Primary metabolites
次級代謝物	非必要但有特定功能，如防禦或訊號分子（例：抗生素、黑色素）	Secondary metabolites
內生代謝物	由體內自然產生的代謝物	Endogenous metabolites
外源代謝物	來自飲食、藥物、毒物等外部來源的代謝物	Exogenous metabolites

Metabolome

- **Metabolome**, typically defined as a collection of **all metabolites** produced by cells, offers a window to investigate cellular biochemistry and how the mechanistic biochemistry relates to **cellular phenotype**

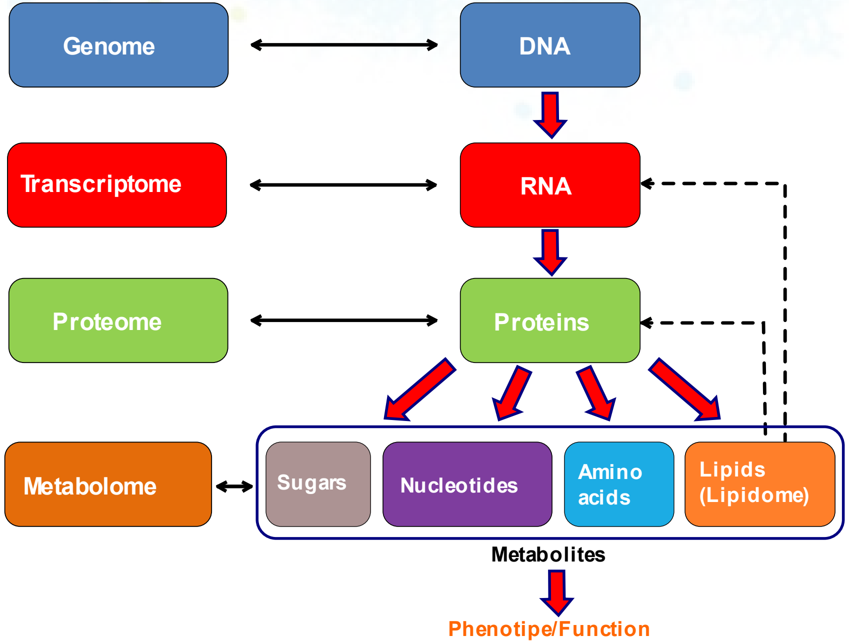
[Oliver et al., 1998; Patti et al., 2012].


Glucose
Mitochondria
Protein lipids
Glycolysis
Pyruvate
Pentose phosphate shunt
SIRT3
TCA cycle
SIRT4
α-KG
GDH
Glutamate
GLS1
DNA damage
HIF-1α
Glycolytic genes
SIRT6
cMYC
GLS1, ribosomes
Glutamine
Glycolysis
Pentose phosphate shunt (nucleotides)
Pyruvate
Protein lipids
TCA cycle
α-KG
GDH
Glutamate
SIRT3
ROS
SIRT4
GLS1
HIF-1α
Glycolytic genes
SIRT6
cMYC
GLS1
Normal cell
Cancer cell
(Loss or decreased amounts of SIRT6, SIRT3, SIRT4)

Nature Medicine, 2014

代謝體（Metabolome）是指某一個生物體、細胞、組織或體液中，在特定時間與條件下所包含的所有代謝物的總和。它反映了生物系統在分子層次的動態生理狀態。

Metabolome


Genome
DNA
Transcriptome
RNA
Proteome
Proteins
Metabolome
Sugars
Nucleotides
Amino acids
Lipids (Lipidome)
Metabolites
Phenotipe/Function

https://en.m.wikipedia.org/wiki/Metabolome

特性	說明
變化迅速	受飲食、壓力、藥物、疾病狀態等快速影響
反映生理現象	是最接近「表現型」的分子層級資料
資料複雜且異質	含極廣範圍的化學性質與濃度（nM 到 mM）
需要高靈敏度分析技術	如質譜（MS）與核磁共振（NMR）

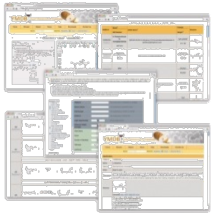
🧠 為什麼要研究 Metabolome？

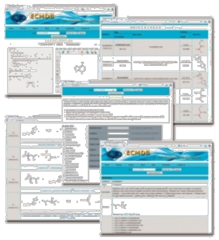
- 🔍 疾病早期偵測 (biomarker discovery)
- 💊 藥物作用與代謝機制研究 (pharmacometabolomics)
- 🧫 個人化醫療與營養建議 (precision medicine & nutrition)
- 🌱 植物與微生物代謝工程 (metabolic engineering)

Metabolome

- Because metabolome is also largely determined by genome, different species have different metabolomes.

- Metabolome databases of some species have been constructed
  - Yeast Metabolome Database (YMDB)
  - E. coli Metabolome Database (ECMDB)
  - Human Metabolome Database (HMDB)
  - MassBank Database
  - METLIN (METabolite LINk) Metabolomics Database

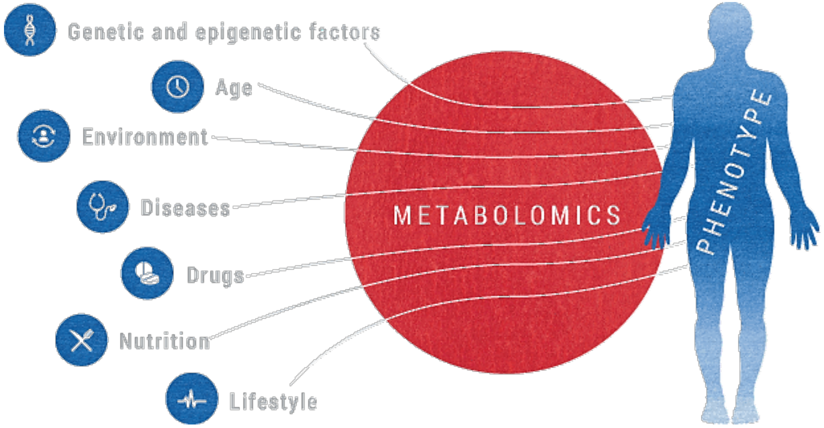




Metabolomics

- Metabolomics was developed in the early 2000s as one of the OMICS tools.
- Metabolomics is the comprehensive and quantitative analysis of all metabolites in a biological system, providing a snapshot of the physiological or pathological state under specific conditions.

Metabolomics 代謝體學發展於兩千年初。它所涵蓋的範圍很廣，因為代謝體除了與phenotype相關之外，另外也跟**基因**，**生理因素**以及許多**外在環境**因素有關。
例如， 年紀、環境暴露、服用藥物等等。
因此，研究這些不同面向與代謝體之間的研究，即稱為**代謝體學**。


Genetic and epigenetic factors
Age
Environment
Diseases
Drugs
Nutrition
Lifestyle
METABOLOMICS
PHENOTYPE

http://www.metanomics-health.com/en/why-metabolomics.html

02

實驗分析平台
(Analytical Platforms)

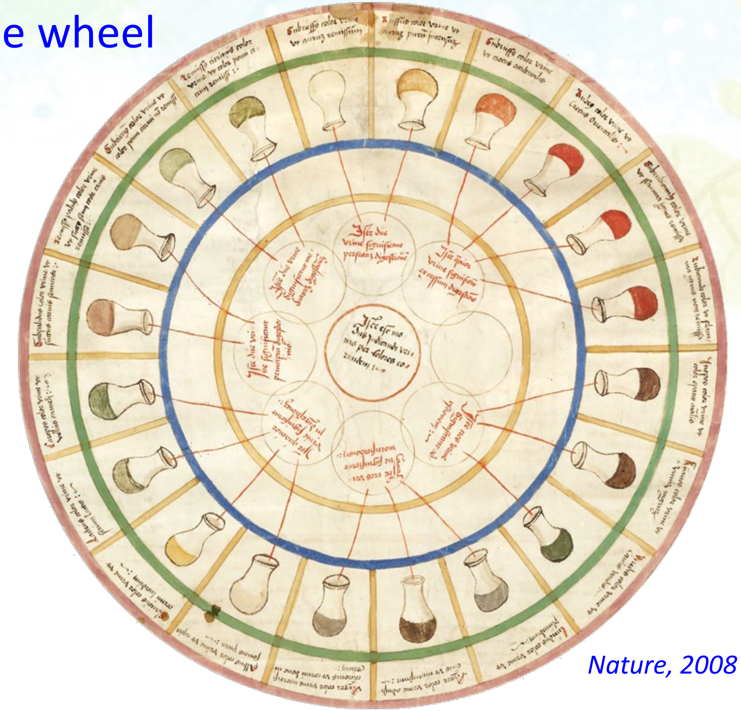
Metabolomics

🏺 古人如何研究「代謝物」？

- **觀察體液（Humorism）與尿液顏色**
  - 在**古希臘醫學**中，醫師會觀察病人的尿液、汗液與糞便，來推斷體內「體液平衡」是否失衡。這些實際上就是**內源代謝物**的早期應用。
  - 尿液中氣味變化、顏色變深或混濁，常被用作疾病診斷指標。
  - 例如：尿中有甜味 → 現在我們知道這是糖尿病的徵象（尿中有葡萄糖）。
  - 🕮 現代對這種方法稱為 **Uroscopy**，可追溯至公元前400年，希波克拉底時代。

- **中醫辨證論治：望聞問切**
  - 會透過觀察舌苔、氣味、脈象，來判斷內臟氣血與代謝是否順暢。
  - 這些方法反映了對內在代謝狀態的整體感知。
  - 例如：「肝鬱氣滯」可對應現代人壓力造成的內分泌與代謝失調。
  - 🕮 在《黃帝內經》中，就有「五臟化五味、五色、五氣」的描述，可視為早期代謝與健康關係的理解。

Urine wheel



Nature, 2008

區域	顏色範例（例）	對應診斷
1	淡黃色	健康、飲水多
5	深黃色	脫水、發熱
8	混濁白色	泌尿道感染、膿尿
12	紅色或血色	尿血、腎臟疾病
16	黑色或深紫色	嚴重肝病、代謝異常
20	綠色或藍色	藥物影響或細菌感染

This urine wheel was published in 1506 by **Ullrich Pinder**, in his book ***Epiphanie Medicorum***. It describes the possible colours, smells and tastes of urine, and uses them to diagnose disease.

Metabolomics

現階段常見代謝物偵測技術

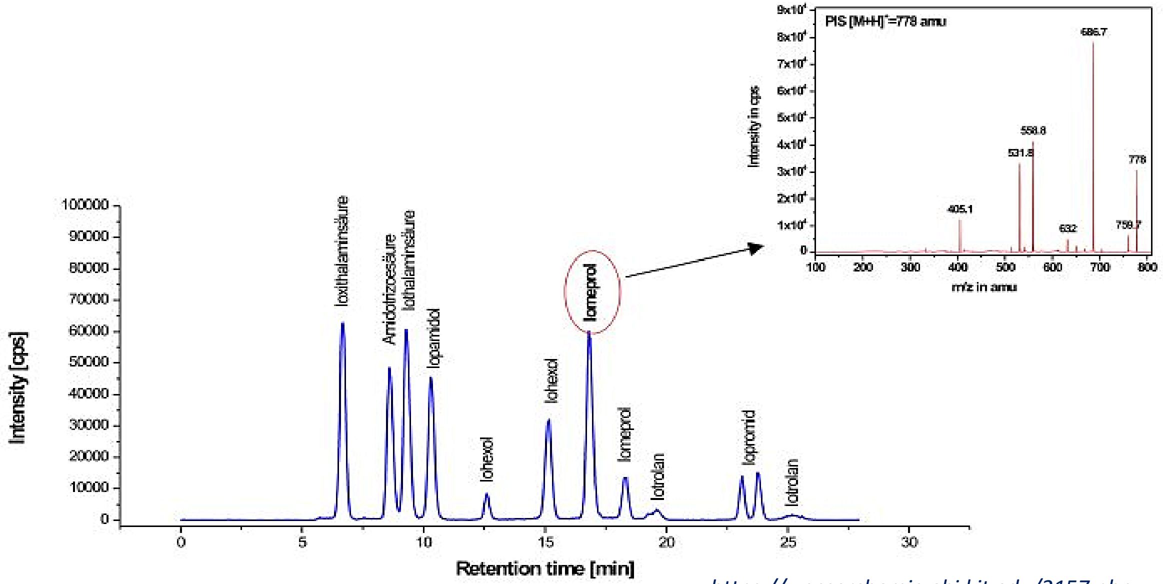
補充說明

- **LC-MS** 最常用於代謝體學研究，能夠廣泛偵測多種極性與非極性小分子。
- **NMR** 精確度高，適合做定量與結構分析，但靈敏度較低，可搭配 LC-MS 多平台統合。
- **Direct MS**（如 DESI-MS、DART-MS）正快速崛起於食品、毒物、現場鑑定領域。
- **FTIR/Raman** 與 **酵素法/ELISA** 多用於品質管控或臨床快篩，但無法進行大範圍代謝物探索。

技術名稱	使用頻率	原理簡介	應用領域	優點	缺點
LC-MS（液相層析質譜）	✔ 常常用	以液相層析分離代謝物，接質譜分析其質荷比（m/z）	臨床診斷、代謝體學、藥物代謝	靈敏度高、覆蓋範圍廣、定性定量皆可	設備昂貴、需複雜樣本前處理與校正
GC-MS（氣相層析質譜）	✔ 常用	揮發性代謝物進行氣相層析與質譜分析	食品、毒物、揮發性代謝物分析	高解析度、數據穩定、資料庫豐富	需衍生化處理、不適極性代謝物
CE-MS（毛細管電泳-質譜）	△ 次要	帶電分子以電泳方式分離後，進入質譜	小分子離子、極性代謝物	分離力高、樣本用量低	重現性低，技術操作困難
NMR（核磁共振）	✔ 常用	檢測核磁共振訊號，非破壞性分析分子結構與濃度	結構分析、定量代謝體學	無需標準品、非破壞性、可回收樣本	靈敏度較低、儀器成本高
FTIR / Raman（紅外與拉曼光譜）	△ 補充用法	利用分子振動產生的光譜「指紋」特徵	食品品質、細胞狀態篩檢	無需標記、快速、不需高耗材	分辨率與特異性低、結構類似物難區分
Direct MS（直接進樣質譜）	✔ 新興應用	樣本不經層析，直接進入質譜（如DART-MS）	快速毒物篩檢、現場分析	快速、不需分離、可現場應用	背景雜訊高、定量困難、結構辨識有限
色層法（**TLC, HPLC**）	△ 傳統技術	靠薄層或高效液相分離代謝物	基礎化學實驗、藥品品質分析	操作簡便、視覺化結果明確	靈敏度與通量較低、不適高通量代謝體學
ELISA / 酵素比色法	△ 特定用途	利用抗體或酵素專一性檢測特定代謝物	單一代謝物量測（如葡萄糖、乳酸）	簡單快速、特異性高、適合臨床快速測定	只能分析單一目標，無法做廣泛篩查

Analytical Platforms

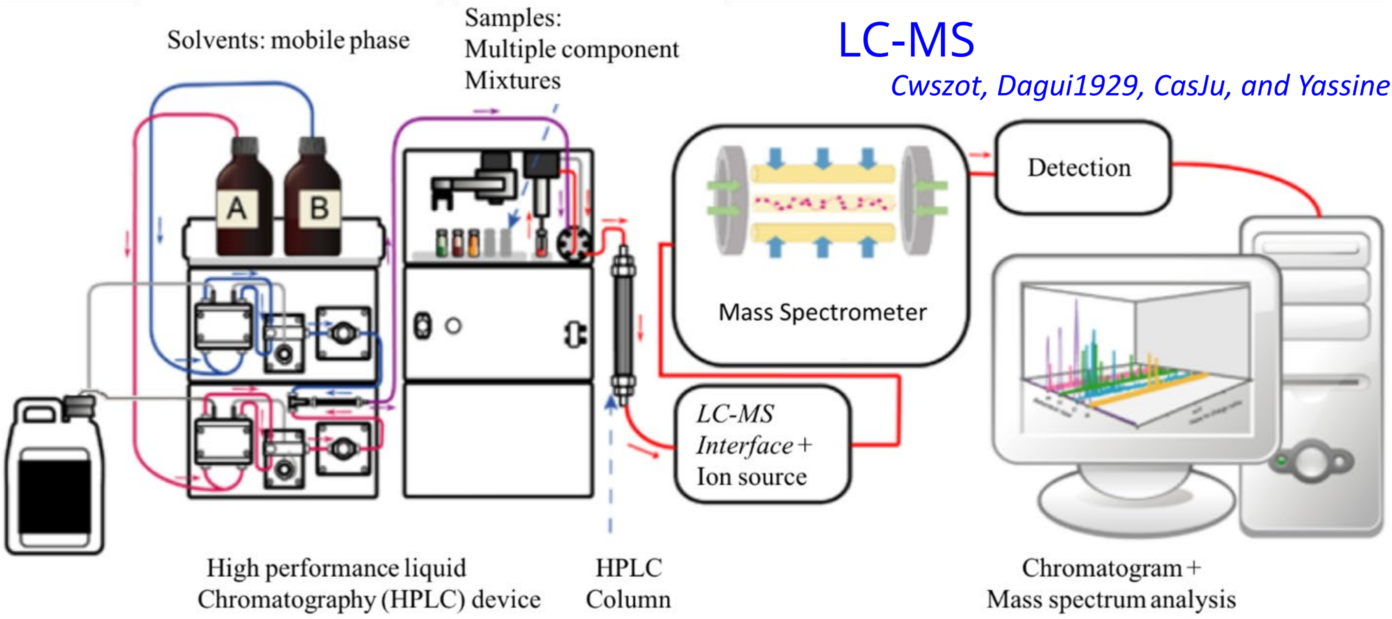
- 在代謝體學（metabolomics）中，研究者需要分析體內數百至數千種**代謝物**（metabolites）的種類與濃度。由於這些代謝物性質各異，包括極性、揮發性、分子量大小等，因此需要**高靈敏且可分離複雜混合物**的技術。



https://wasserchemie.ebi.kit.edu/2157.php

Analytical Platforms Liquid/Gas Chromatography-Mass Spectrometry

- **LC-MS** and **GC-MS** are the most popular experiment platforms for metabolomics studies.
  - High sensitivity and selectivity in rapidly separating and quantifying target or non-target compounds, including metabolites and lipids, in biological fluids [Hird et al., 2014].


Solvents: mobile phase
Samples:
Multiple component
Mixtures
A
B
Mass Spectrometer
Detection
LC-MS
Interface +
Ion source
High performance liquid
Chromatography (HPLC) device
HPLC
Column
Chromatogram +
Mass spectrum analysis

LC-MS

Cwszot, Dagui1929, CasJu, and YassineMrabet

https://en.wikipedia.org/wiki/Liquid_chromatography-mass_spectrometry

Analytical Platforms

- **LC-MS（液相層析-質譜聯用，Liquid Chromatography-Mass Spectrometry）**是一種將液相層析（LC）與質譜儀（MS）結合的分析技術，用於分離並檢測樣本中的代謝物。

基本流程

Step 1：樣本處理

生物樣本（如血漿、尿液、細胞萃取）經過離心、蛋白沉澱、過濾或萃取後，得到代謝物溶液。

Step 2：液相層析（LC）分離代謝物

代謝物經過**色譜柱（column）**，依據其**極性**、**疏水性**或**大小**被分離，不同分子在不同時間（**保留時間**）流出。（例如：水溶性的胺基酸 vs 脂溶性的脂肪酸）

💬 **關鍵詞：Retention time（保留時間）**

Step 3：質譜偵測（MS）

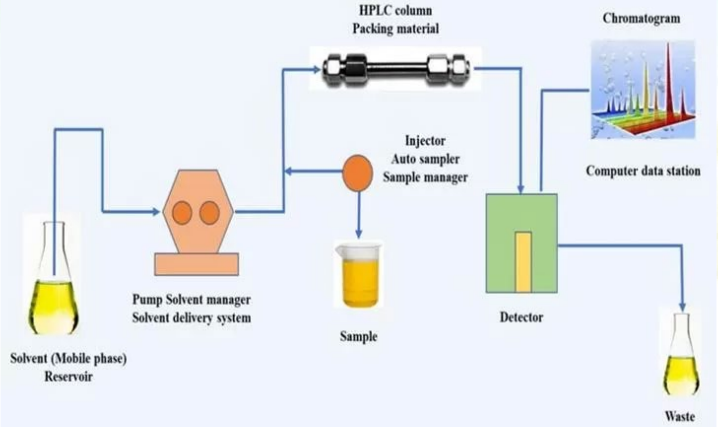
流出的代謝物經**電灑游離（ESI）**變成帶電離子，進入質譜儀中。

質譜儀測量每個離子的 **質荷比（mass-to-charge ratio, m/z）**，得到：

- **MS1：分子離子的 m/z 值與強度（定性 + 定量）**
- **MS2（MS/MS）：碎裂離子的圖譜，用於結構鑑定**

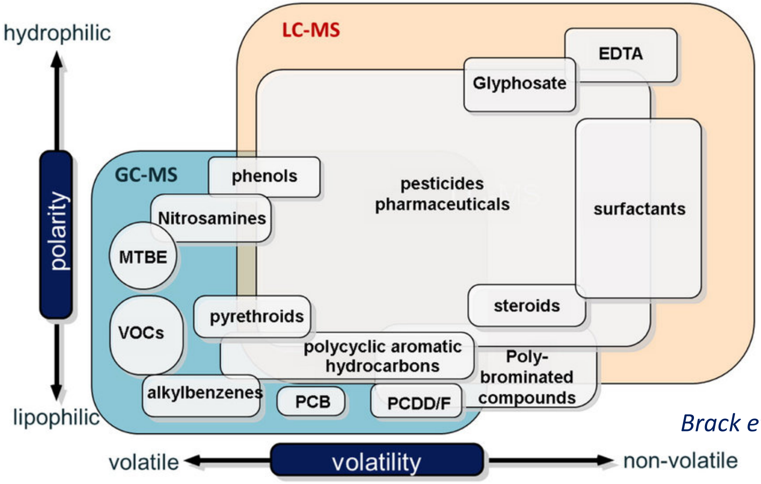
💬 **MS1：定量、MS2：定性結構鑑定**

Schematic Representation of High-Performance Liquid Chromatography


HPLC column
Packing material
Chromatogram
Injector
Auto sampler
Sample manager
Computer data station
Pump Solvent manager
Solvent delivery system
Sample
Detector
Solvent (Mobile phase)
Reservoir
Waste

https://www.metwarebio.com/mastering-chromatography-principles-types-applications/

GC-MS 和 LC-MS 技術在疏水性和揮發性兩個維度上的應用


hydrophilic
lipophilic
polarity
volatile
volatility
non-volatile
LC-MS
GC-MS
EDTA
Glyphosate
phenols
pesticides
pharmaceuticals
surfactants
Nitrosamines
MTBE
VOCs
pyrethroids
steroids
polycyclic aromatic hydrocarbons
Poly-brominated compounds
alkylbenzenes
PCB
PCDD/F

Brack et al., 2016

Analytical Platforms

LC-MS/MS
（Liquid Chromatography–Tandem Mass Spectrometry）

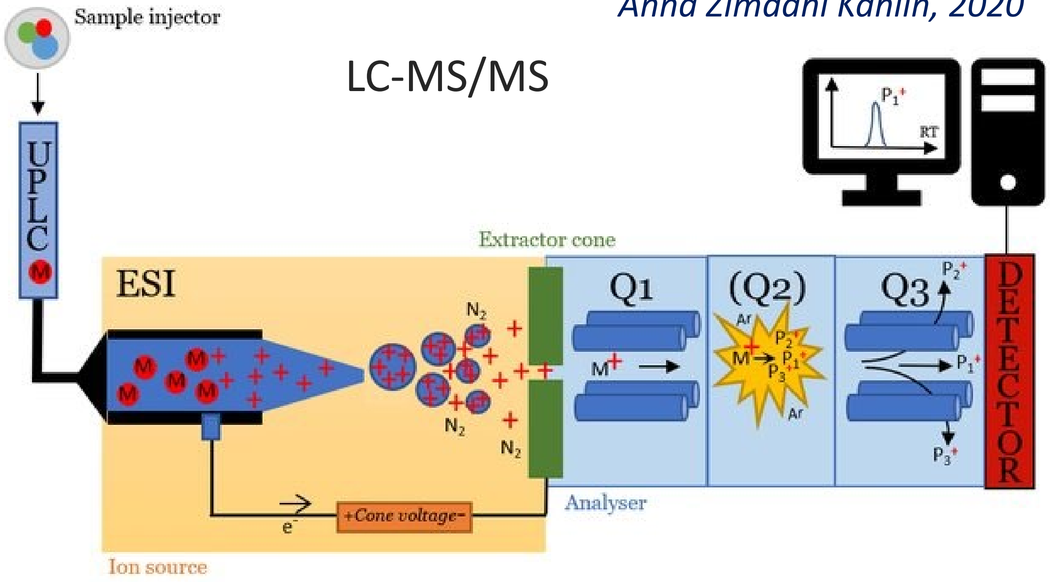
MS/MS（串聯質譜）

➤ 利用兩級質譜儀（MS1 → MS2）來分析每個代謝物的結構與訊號強度。

MS/MS 怎麼運作？

- **MS1**：先選出一個特定的離子（母離子 precursor ion）。
- **碰撞室（Collision Cell）**：讓母離子與氣體碰撞，斷裂成片段（碎片離子 fragment ions）。
- **MS2**：分析這些碎片，來判斷其化學結構與身分。

Anna Zimdahl Kahlin, 2020


Sample injector
LC-MS/MS
UPLC
M
ESI
Extractor cone
N_2
M^+
Q1
(Q2)
Ar
P_2^+
P_1^+
P_3^+
Q3
RT
DETECTOR
e⁻
+Cone voltage−
Analyser
Ion source

https://www.researchgate.net/publication/339747713_Pharmacogenetic_studies_of_thiopurine_methyltransferase_genotype-phenotype_concordance_and_effect_of_methotrexate_on_thiopurine_metabolism/figures?lo=1

Analytical Platforms

LC-MS 實驗資料

1.原始資料（Raw Data）

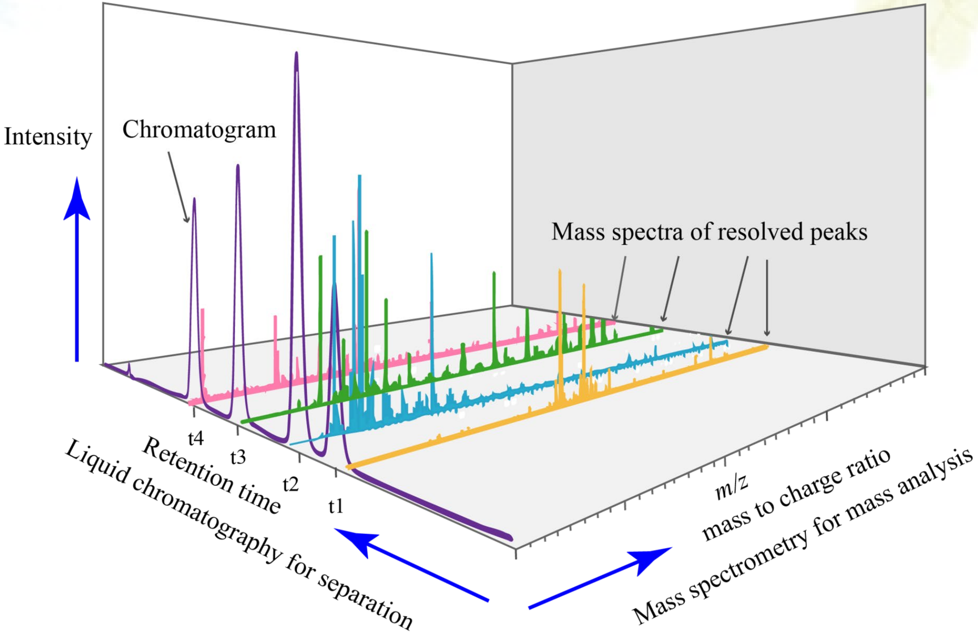
- 包含 MS1 與 MS2 的完整質譜掃描訊號
- 通常為儀器廠牌專屬格式（如 .raw, .d, .wiff）
- 需透過軟體轉檔與解析

2.特徵變數（Features）

- 每個 Feature 通常對應一個代謝物訊號
- 主要變數：
  - m/z：質量電荷比 (mass-to-charge ratio)
  - Retention Time (RT)：色譜保留時間
  - Intensity / Area：離子訊號強度或面積
  - Feature ID：特徵代碼（如 F001）

LC–MS spectrum of each resolved peak

Daniel Norena-Caro, 2017


Intensity
Chromatogram
Mass spectra of resolved peaks
t4
t3
t2
t1
Retention time
Liquid chromatography for separation
m/z
mass to charge ratio
Mass spectrometry for mass analysis

https://en.wikipedia.org/wiki/Liquid_chromatography%E2%80%93mass_spectrometry

Analytical Platforms

Total Intensity（總強度）是什麼？

- 指的是在一個樣本的 LC-MS 分析中，所有偵測到的離子訊號強度的**總和**，通常用來表示整體代謝物含量的總量。

🧬可用來評估樣本的整體代謝活性（metabolic activity）或代謝量豐富度

- 常見於品質管控（Quality Control, QC）
- 偵測是否有批次效應（Batch Effect）或注射量的不一致
- 做為樣本均一化的依據（如 Total Ion Normalization）

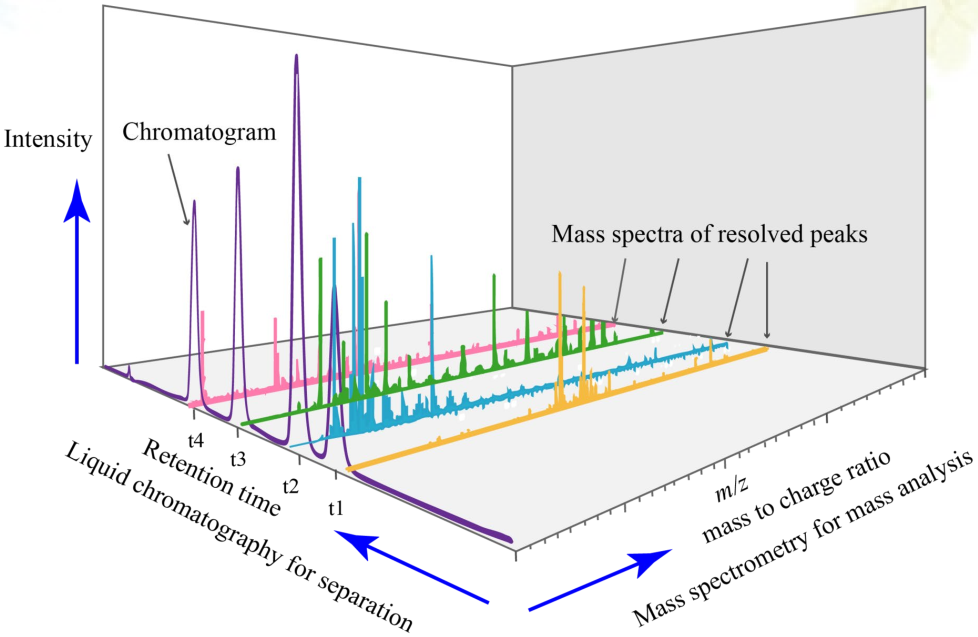
Total Ion Chromatogram（總離子色譜圖）是什麼？

- **TIC** 是 LC-MS 或 GC-MS 實驗中最基本也最常見的一種色譜圖（Chromatogram）。
- 它呈現在整個實驗掃描過程中，每個保留時間點（Retention Time, RT）所偵測到的**全部離子訊號強度的總和**。

🧬可檢查峰形是否正常、有無污染、基線是否穩定

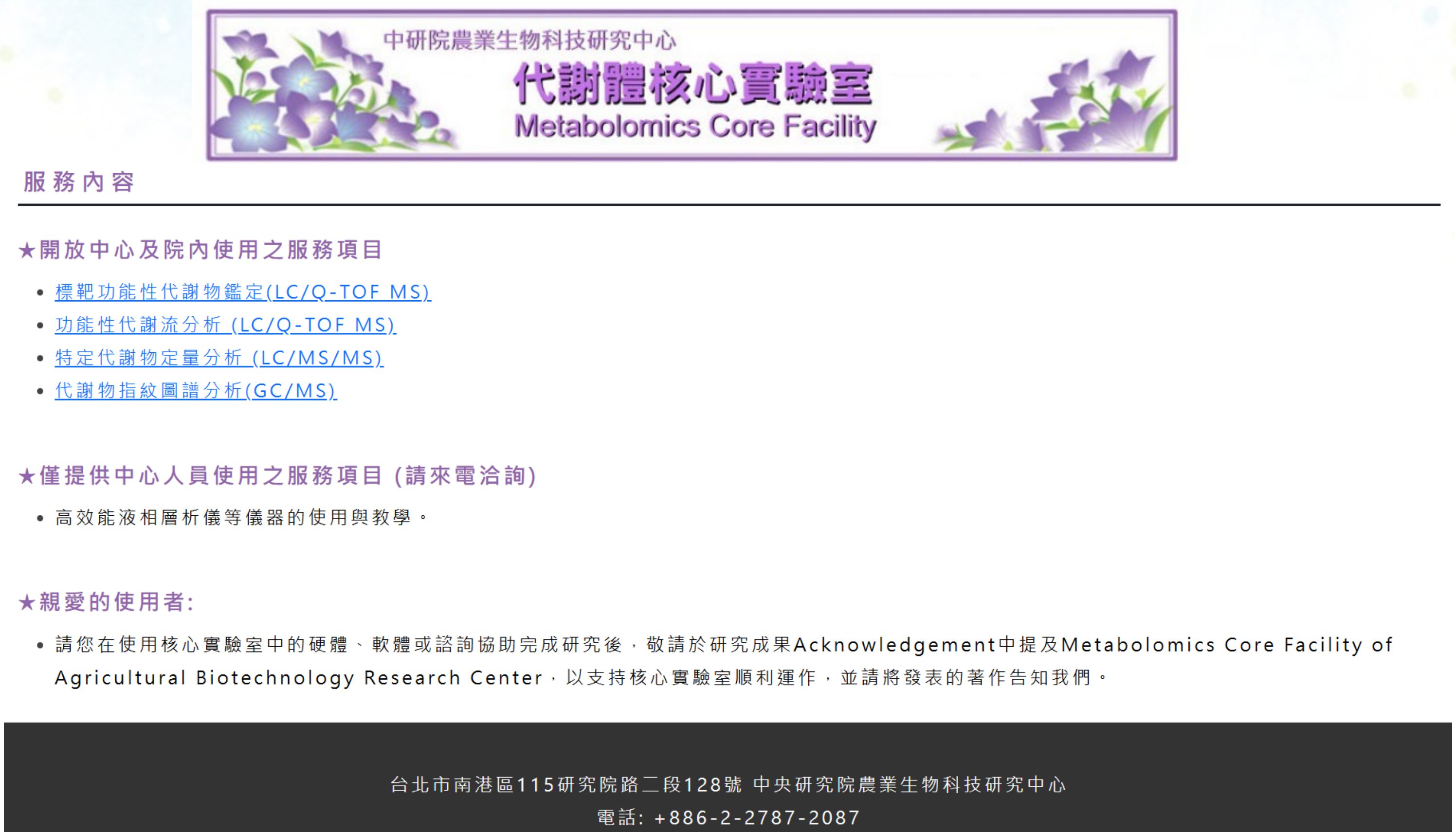
LC–MS spectrum of each resolved peak

Daniel Norena-Caro, 2017


Intensity
Chromatogram
Mass spectra of resolved peaks
t4
t3
t2
t1
Retention time
Liquid chromatography for separation
m/z
mass to charge ratio
Mass spectrometry for mass analysis

https://en.wikipedia.org/wiki/Liquid_chromatography%E2%80%93mass_spectrometry

Analytical Platforms



中研院農業生物科技研究中心

代謝體核心實驗室

Metabolomics Core Facility

服務內容

★開放中心及院內使用之服務項目

- 標靶功能性代謝物鑑定(LC/Q-TOF MS)
- 功能性代謝流分析 (LC/Q-TOF MS)
- 特定代謝物定量分析 (LC/MS/MS)
- 代謝物指紋圖譜分析(GC/MS)

★僅提供中心人員使用之服務項目 (請來電洽詢)

- 高效能液相層析儀等儀器的使用與教學 。

★親愛的使用者:

- 請您在使用核心實驗室中的硬體、軟體或諮詢協助完成研究後，敬請於研究成果Acknowledgement中提及Metabolomics Core Facility of Agricultural Biotechnology Research Center，以支持核心實驗室順利運作，並請將發表的著作告知我們。

台北市南港區115研究院路二段128號 中央研究院農業生物科技研究中心
電話: +886-2-2787-2087

https://abrc.sinica.edu.tw/metabolomics/

資料類型與變數

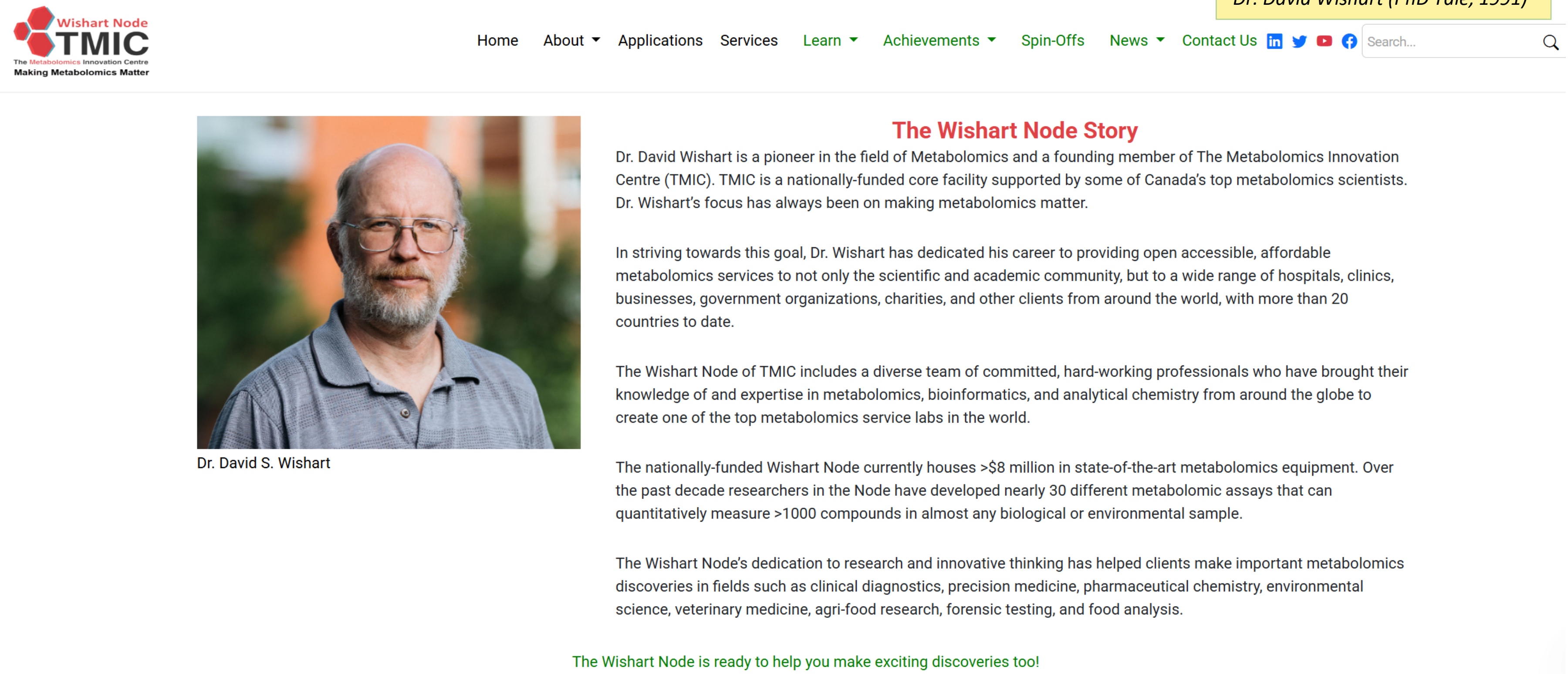
資料類型	**描述**	**主要變數（Variables）**	**說明**
Raw Data（原始檔案）	原始質譜數據，需經解析軟體轉換與擷取	N/A（需處理後擷取）	包含 MS1、MS2 訊號與掃描資訊
MS1 資料（全離子掃描）	母離子質荷比與強度	m/z, Retention Time (RT), Intensity, Area	用於定量分析與描繪 chromatogram
MS2 資料（碎裂譜）	選定母離子的碎片圖譜	Precursor m/z, Fragment m/z, Fragment Intensity	用於代謝物鑑定與比對資料庫
Chromatogram（色譜圖）	離子訊號 vs. 保留時間	RT, Intensity（或 Total Intensity）	包含 TIC / XIC，常用於觀察峰型
Feature Table（峰表 / 變數表）	經過 peak picking + alignment 處理後的資料矩陣	Feature ID, m/z, RT, Intensity in Sample A/B/..., Area, Signal-to-noise ratio	是進入統計與機器學習的主要資料
Metabolite Identification（代謝物鑑定）	比對資料庫後之化學資訊與鑑定層級	Putative Metabolite ID, HMDB/KEGG ID, Confidence Level, Adduct, Formula, Mass error	幫助賦予生物意義與路徑分析基礎
Statistical Summary（統計衍生變數）	統計分析所產生的變數	Log2 Intensity, Fold Change, p-value, FDR, VIP, AUC	差異分析與生物標記探索的依據

03

代謝體資料庫
(Database)

The Metabolomics Innovation Centre

Dr. David Wishart (PhD Yale, 1991)



Dr. David S. Wishart

The Wishart Node Story

Dr. David Wishart is a pioneer in the field of Metabolomics and a founding member of The Metabolomics Innovation Centre (TMIC). TMIC is a nationally-funded core facility supported by some of Canada's top metabolomics scientists. Dr. Wishart's focus has always been on making metabolomics matter.

In striving towards this goal, Dr. Wishart has dedicated his career to providing open accessible, affordable metabolomics services to not only the scientific and academic community, but to a wide range of hospitals, clinics, businesses, government organizations, charities, and other clients from around the world, with more than 20 countries to date.

The Wishart Node of TMIC includes a diverse team of committed, hard-working professionals who have brought their knowledge of and expertise in metabolomics, bioinformatics, and analytical chemistry from around the globe to create one of the top metabolomics service labs in the world.

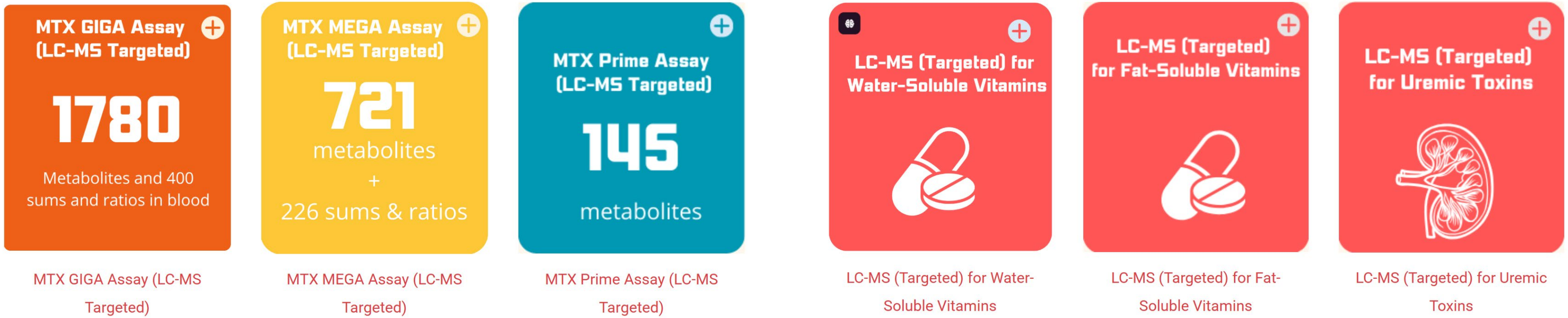
The nationally-funded Wishart Node currently houses >$8 million in state-of-the-art metabolomics equipment. Over the past decade researchers in the Node have developed nearly 30 different metabolomic assays that can quantitatively measure >1000 compounds in almost any biological or environmental sample.

The Wishart Node's dedication to research and innovative thinking has helped clients make important metabolomics discoveries in fields such as clinical diagnostics, precision medicine, pharmaceutical chemistry, environmental science, veterinary medicine, agri-food research, forensic testing, and food analysis.

The Wishart Node is ready to help you make exciting discoveries too!

https://www.tmicwishartnode.ca/about-us/

The Metabolomics Innovation Centre



MTX GIGA Assay (LC-MS Targeted)
1780
Metabolites and 400 sums and ratios in blood

MTX MEGA Assay (LC-MS Targeted)
721
metabolites
+
226 sums & ratios

MTX Prime Assay (LC-MS Targeted)
145
metabolites

LC-MS (Targeted) for Water-Soluble Vitamins

LC-MS (Targeted) for Fat-Soluble Vitamins

LC-MS (Targeted) for Uremic Toxins

MTX GIGA Assay (LC-MS Targeted)

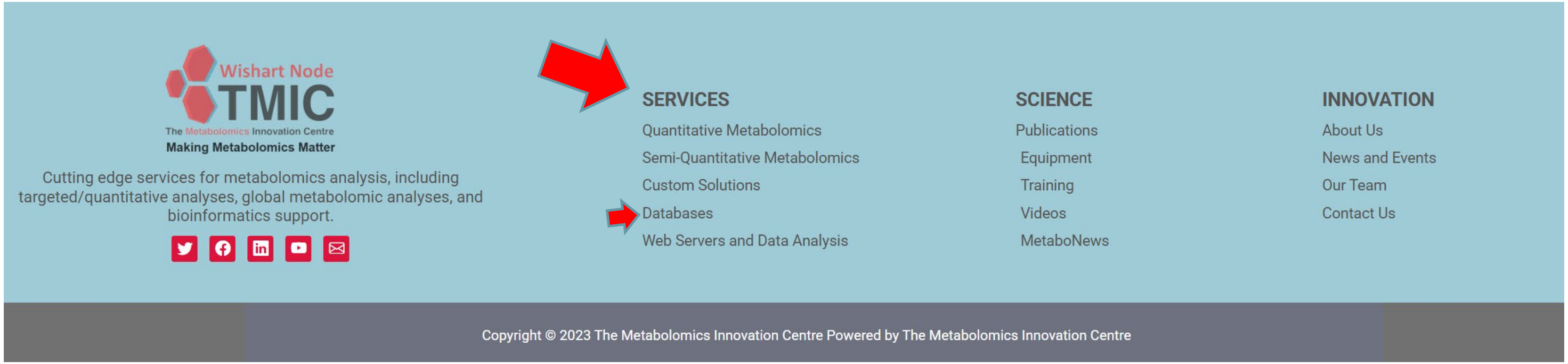
MTX MEGA Assay (LC-MS Targeted)

MTX Prime Assay (LC-MS Targeted)

LC-MS (Targeted) for Water-Soluble Vitamins

LC-MS (Targeted) for Fat-Soluble Vitamins

LC-MS (Targeted) for Uremic Toxins



Wishart Node TMIC
The Metabolomics Innovation Centre
Making Metabolomics Matter

Cutting edge services for metabolomics analysis, including targeted/quantitative analyses, global metabolomic analyses, and bioinformatics support.

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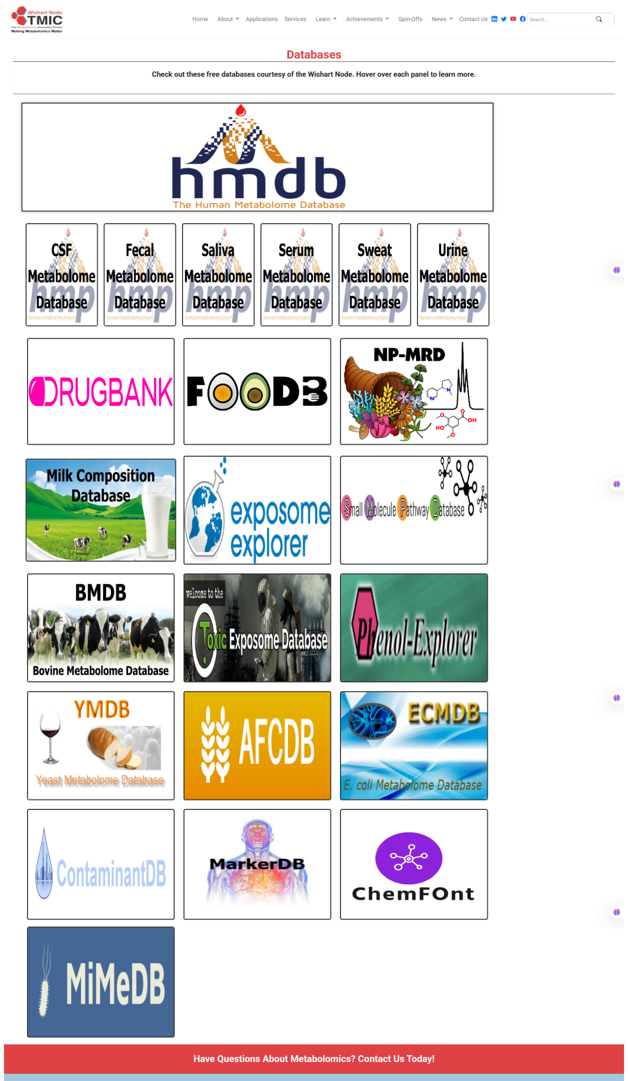
https://www.tmicwishartnode.ca/services/

TMIC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Check out these free databases courtesy of the Wishart Node. Hover over each panel to learn more.

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Saliva Metabolome Database
Serum Metabolome Database
Sweat Metabolome Database
Urine Metabolome Database
DRUGBANK
FOODB
NP-MRD
Milk Composition Database
exposome explorer
Small Molecule Pathway Database
BMDB
Bovine Metabolome Database
welcome to the Toxic Exposome Database
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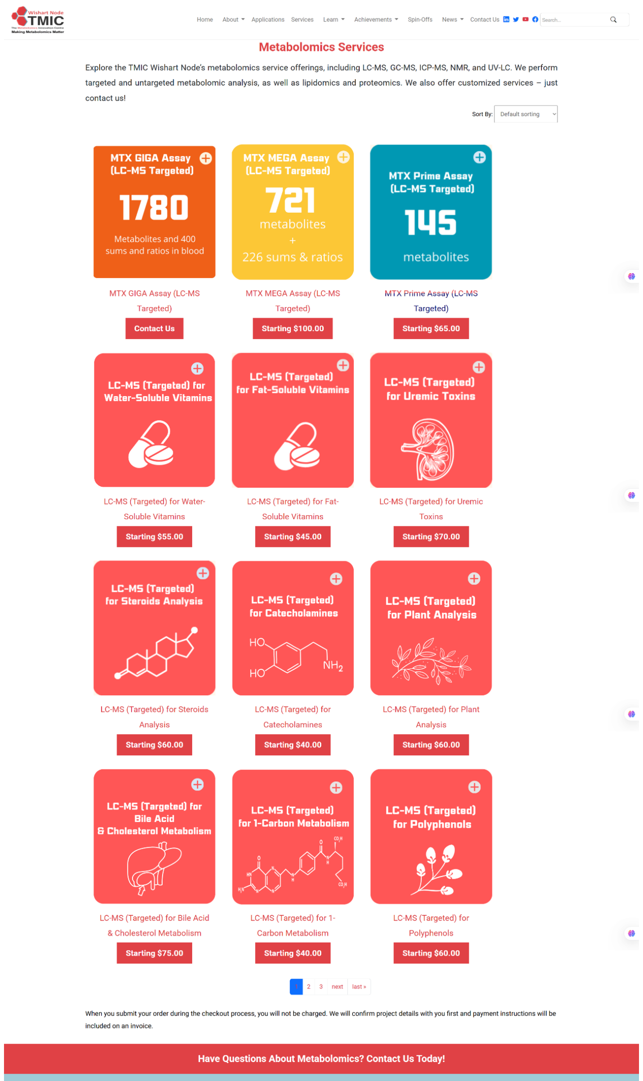
MarkerDB
ChemFOnt
MiMeDB

Have Questions About Metabolomics? Contact Us Today!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1780
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metabolites
+
226 sums & ratios
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145
metabolites
LC-MS (Targeted) for Water-Soluble Vitamins
LC-MS (Targeted) for Fat-Soluble Vitamins
LC-MS (Targeted) for Uremic Toxins
LC-MS (Targeted) for Steroids Analysis
LC-MS (Targeted) for Catecholamines
HO
HO
NH2
LC-MS (Targeted) for Plant Analysis
LC-MS (Targeted) for Bile Acid & Cholesterol Metabolism
LC-MS (Targeted) for 1-Carbon Metabolism
LC-MS (Targeted) for Polyphenols

MTX GIGA Assay (LC-MS Targeted)
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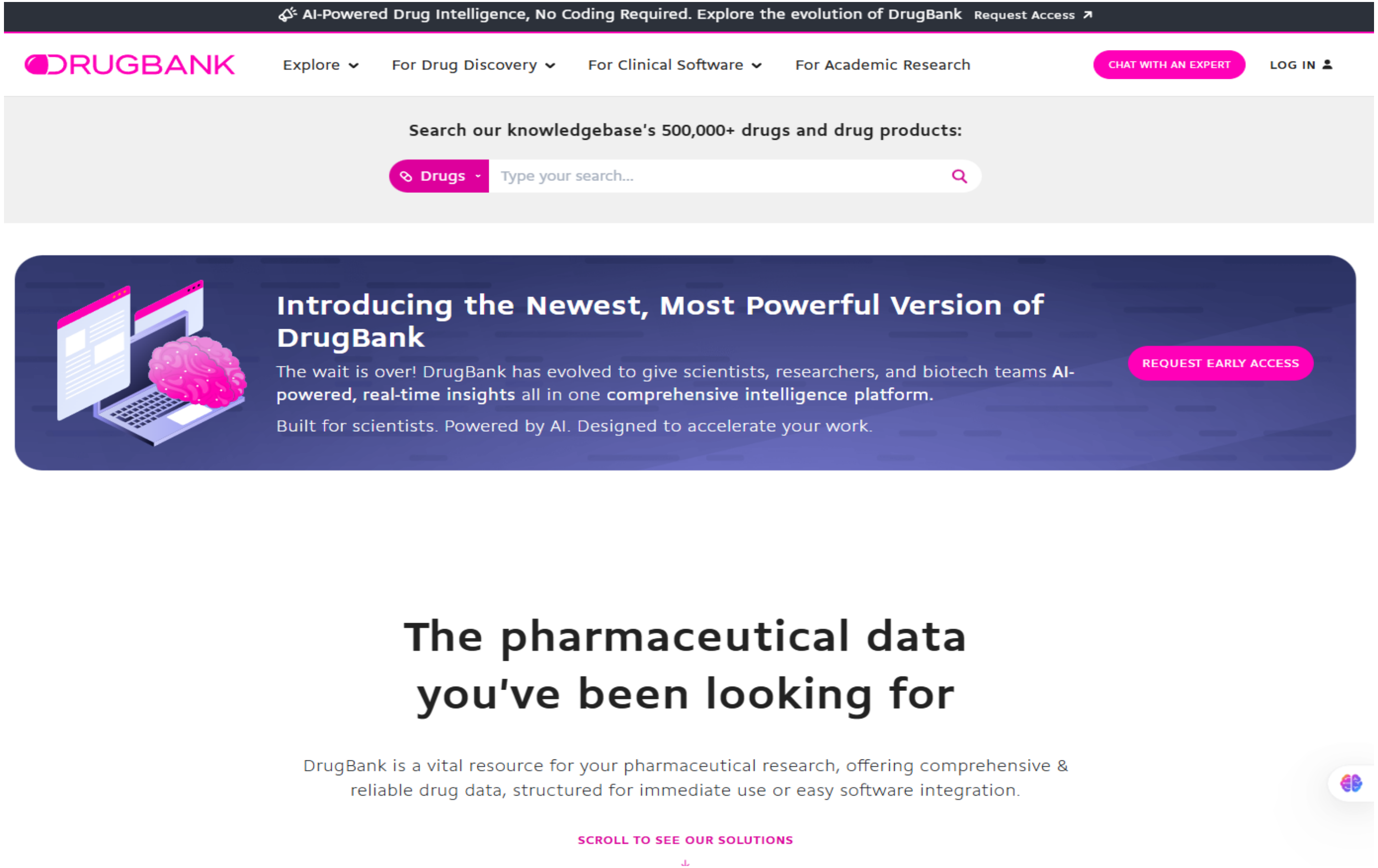
DRUGBANK

DrugBank 是一個重要的藥物研究資源，提供全面且可靠的藥物數據。包含結構化的藥物資訊及其作用靶點，有助於加速藥物研究和改善醫療保健服務。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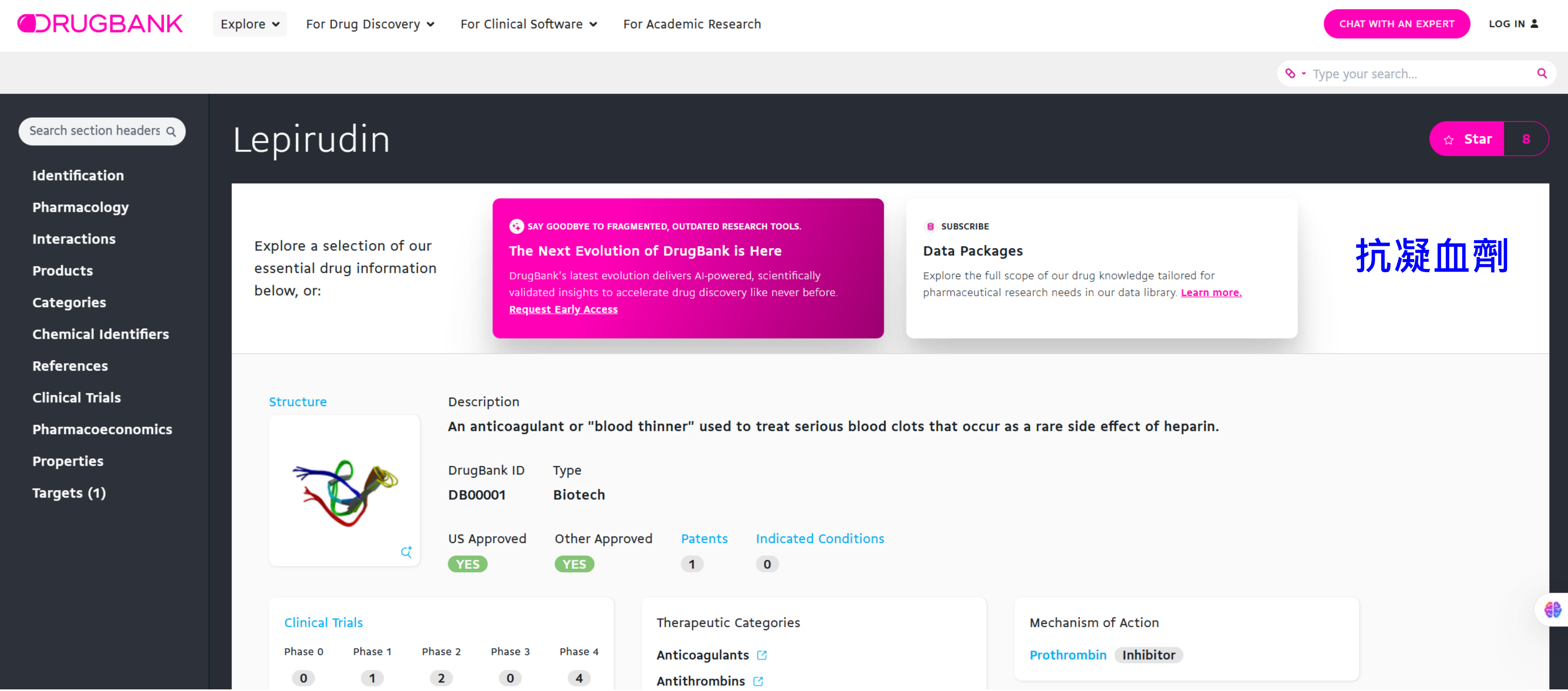
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Lepirudin

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抗凝血劑

Structure

Description

An anticoagulant or "blood thinner" used to treat serious blood clots that occur as a rare side effect of heparin.

DrugBank ID	Type
DB00001	Biotech

US Approved	Other Approved	Patents	Indicated Conditions
YES	YES	1	0

Clinical Trials

Phase 0	Phase 1	Phase 2	Phase 3	Phase 4
0	1	2	0	4

Therapeutic Categories

Anticoagulants

Antithrombins

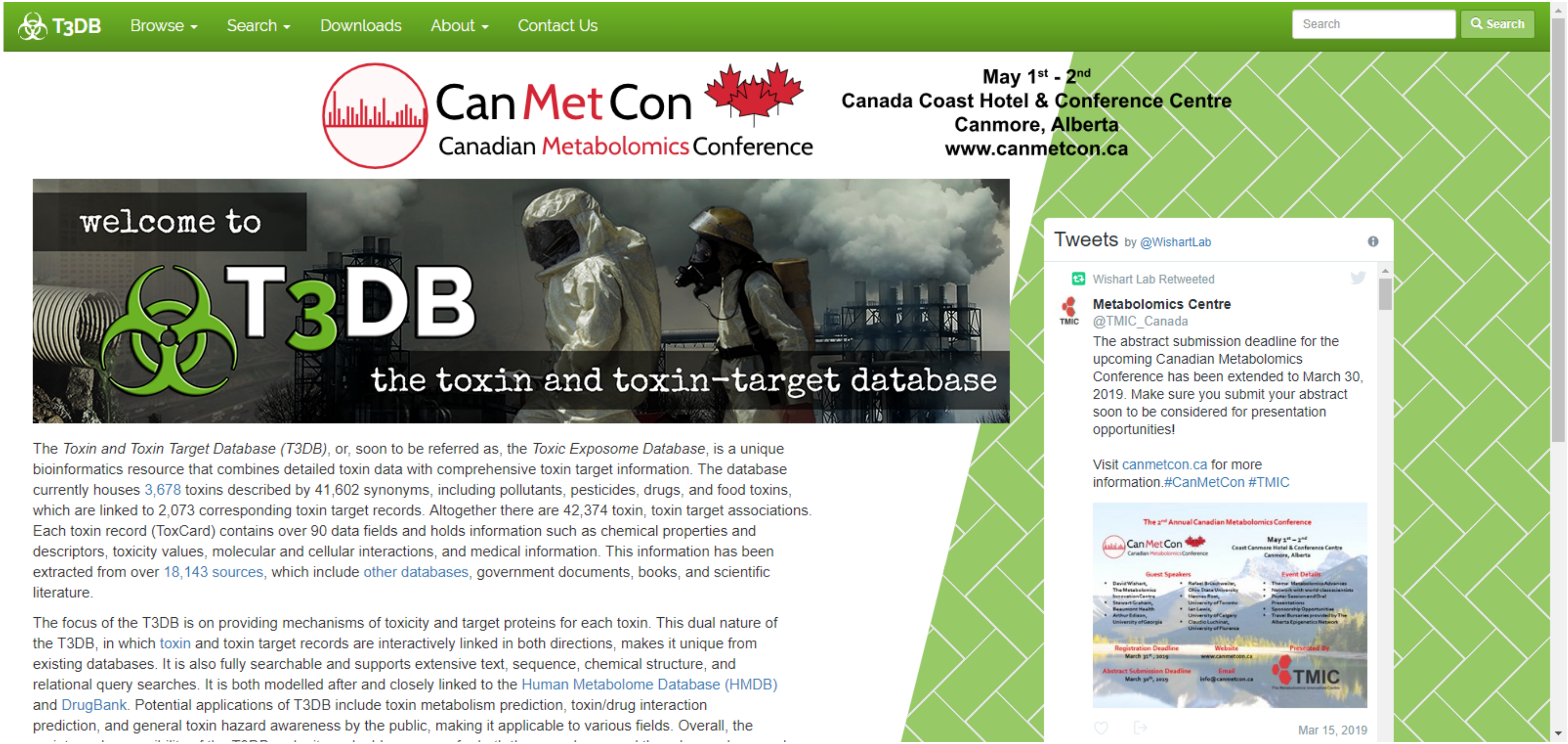
Mechanism of Action

Prothrombin **Inhibitor**

https://go.drugbank.com/drugs/DB00001

T3DB

T3DB 是一個關於毒素的資料庫，專注於毒理學機制及常見毒物的目標蛋白質。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welcome to
T3DB
the toxin and toxin-target database

The *Toxin and Toxin Target Database (T3DB)*, or, soon to be referred as, the *Toxic Exposome Database*, is a unique bioinformatics resource that combines detailed toxin data with comprehensive toxin target information. The database currently houses 3,678 toxins described by 41,602 synonyms, including pollutants, pesticides, drugs, and food toxins, which are linked to 2,073 corresponding toxin target records. Altogether there are 42,374 toxin, toxin target associations. Each toxin record (ToxCard) contains over 90 data fields and holds information such as chemical properties and descriptors, toxicity values, molecular and cellular interactions, and medical information. This information has been extracted from over 18,143 sources, which include other databases, government documents, books, and scientific literature.

The focus of the T3DB is on providing mechanisms of toxicity and target proteins for each toxin. This dual nature of the T3DB, in which toxin and toxin target records are interactively linked in both directions, makes it unique from existing databases. It is also fully searchable and supports extensive text, sequence, chemical structure, and relational query searches. It is both modelled after and closely linked to the Human Metabolome Database (HMDB) and DrugBank. Potential applications of T3DB include toxin metabolism prediction, toxin/drug interaction prediction, and general toxin hazard awareness by the public, making it applicable to various fields. Overall, the

Tweets by @WishartLab

Wishart Lab Retweeted

Metabolomics Centre @TMIC_Canada

The abstract submission deadline for the upcoming Canadian Metabolomics Conference has been extended to March 30, 2019. Make sure you submit your abstract soon to be considered for presentation opportunities!

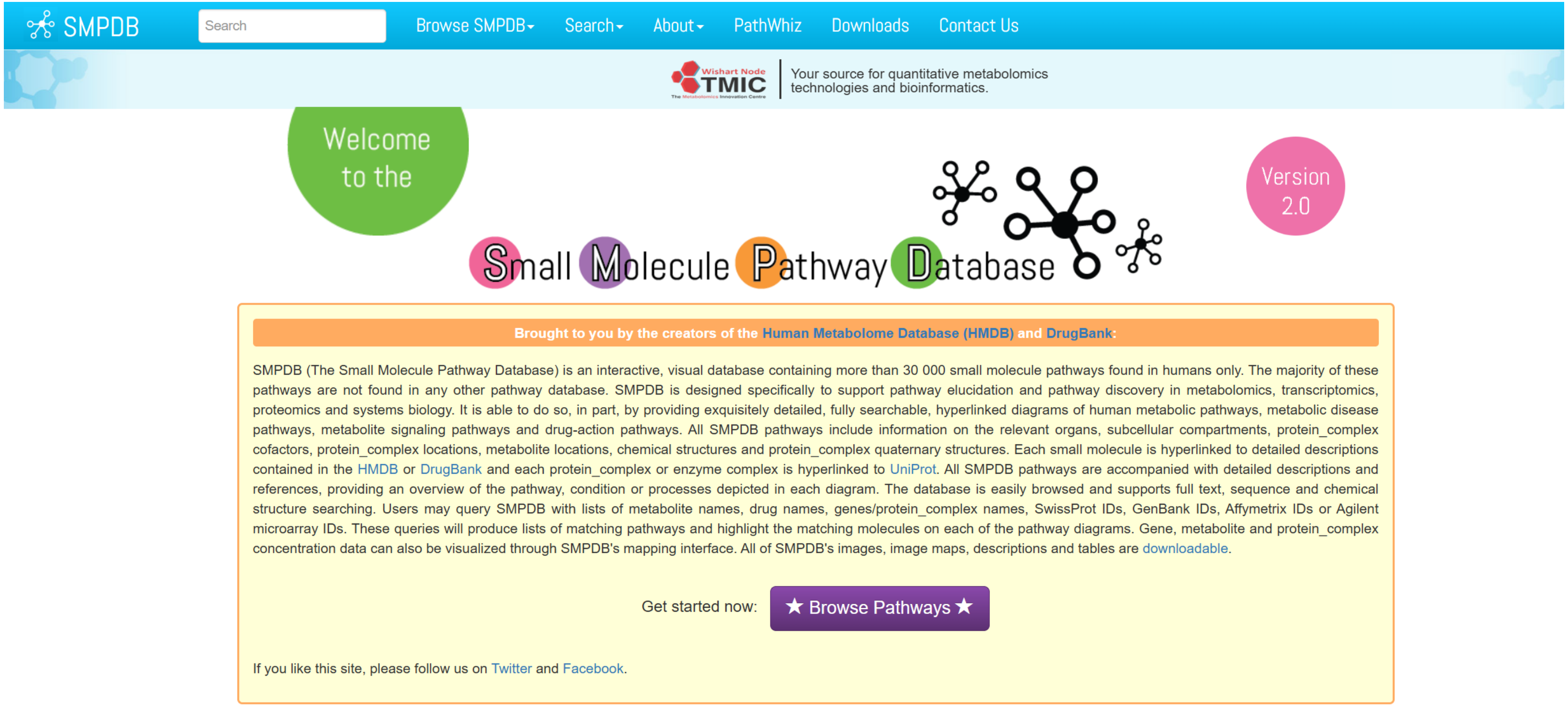
Visit canmetcon.ca for more information.#CanMetCon #TMIC

Mar 15, 2019

SMPDB

SMPDB (Small Molecule Pathway Database) 是一個互動式、視覺化的資料庫，收錄了超過 30,000 個存在於人類體內的**小分子代謝途徑**。這個資料庫是全面、高品質且可免費存取的線上資源，有助於研究者探索人類的代謝過程，提供重要的生物化學資訊。

SMPDB 的設計著重於**視覺化**，使得研究人員更容易理解複雜的代謝途徑。這資料庫涵蓋了廣泛的小分子，並幫助揭示這些分子在生物系統中的作用。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Small Molecule Pathway Database

Brought to you by the creators of the Human Metabolome Database (HMDB) and DrugBank:

SMPDB (The Small Molecule Pathway Database) is an interactive, visual database containing more than 30 000 small molecule pathways found in humans only. The majority of these pathways are not found in any other pathway database. SMPDB is designed specifically to support pathway elucidation and pathway discovery in metabolomics, transcriptomics, proteomics and systems biology. It is able to do so, in part, by providing exquisitely detailed, fully searchable, hyperlinked diagrams of human metabolic pathways, metabolic disease pathways, metabolite signaling pathways and drug-action pathways. All SMPDB pathways include information on the relevant organs, subcellular compartments, protein_complex cofactors, protein_complex locations, metabolite locations, chemical structures and protein_complex quaternary structures. Each small molecule is hyperlinked to detailed descriptions contained in the HMDB or DrugBank and each protein_complex or enzyme complex is hyperlinked to UniProt. All SMPDB pathways are accompanied with detailed descriptions and references, providing an overview of the pathway, condition or processes depicted in each diagram. The database is easily browsed and supports full text, sequence and chemical structure searching. Users may query SMPDB with lists of metabolite names, drug names, genes/protein_complex names, SwissProt IDs, GenBank IDs, Affymetrix IDs or Agilent microarray IDs. These queries will produce lists of matching pathways and highlight the matching molecules on each of the pathway diagrams. Gene, metabolite and protein_complex concentration data can also be visualized through SMPDB's mapping interface. All of SMPDB's images, image maps, descriptions and tables are downloadable.

Get started now: ★ Browse Pathways ★

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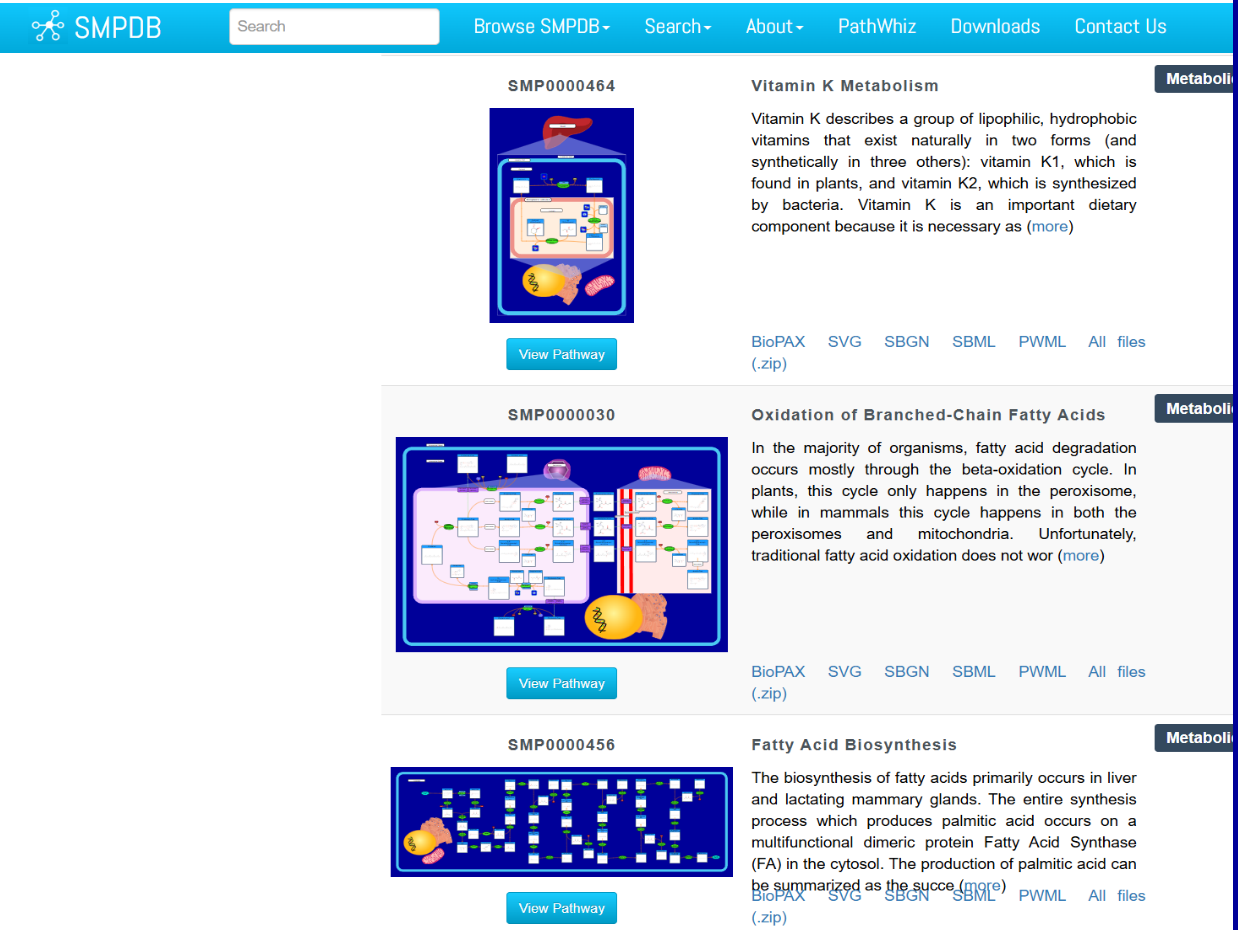
SMPDB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SMP0000464

Vitamin K Metabolism

Vitamin K describes a group of lipophilic, hydrophobic vitamins that exist naturally in two forms (and synthetically in three others): vitamin K1, which is found in plants, and vitamin K2, which is synthesized by bacteria. Vitamin K is an important dietary component because it is necessary as (more)

BioPAX SVG SBGN SBML PWML All files (.zip)

SMP0000030

Oxidation of Branched-Chain Fatty Acids

In the majority of organisms, fatty acid degradation occurs mostly through the beta-oxidation cycle. In plants, this cycle only happens in the peroxisome, while in mammals this cycle happens in both the peroxisomes and mitochondria. Unfortunately, traditional fatty acid oxidation does not wor (more)

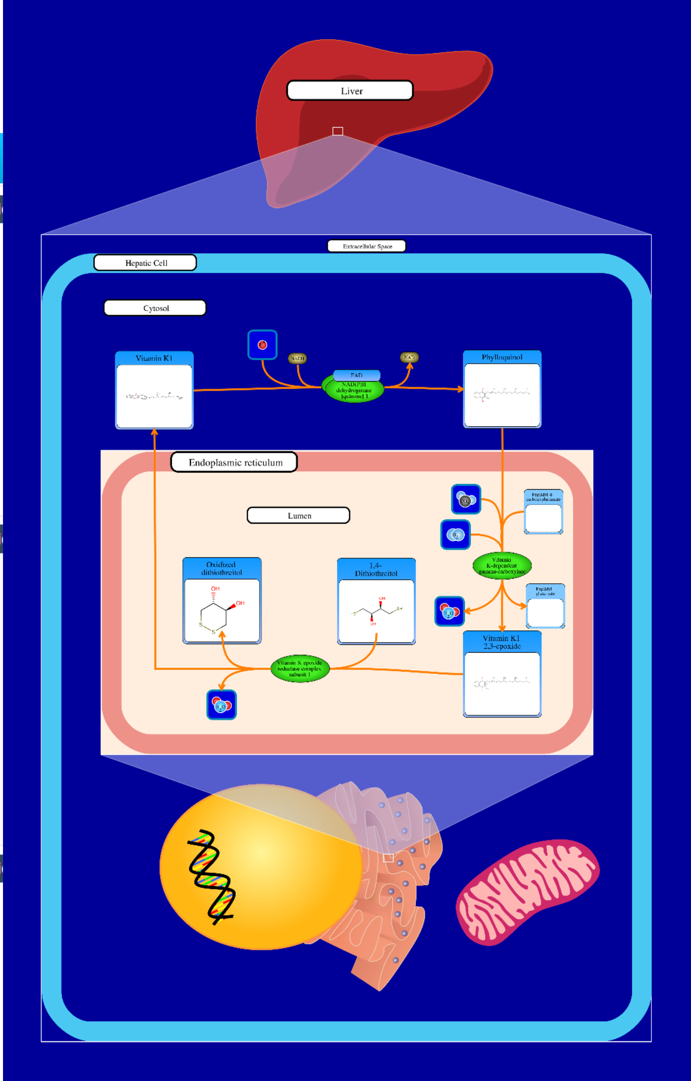
BioPAX SVG SBGN SBML PWML All files (.zip)

SMP0000456

Fatty Acid Biosynthesis

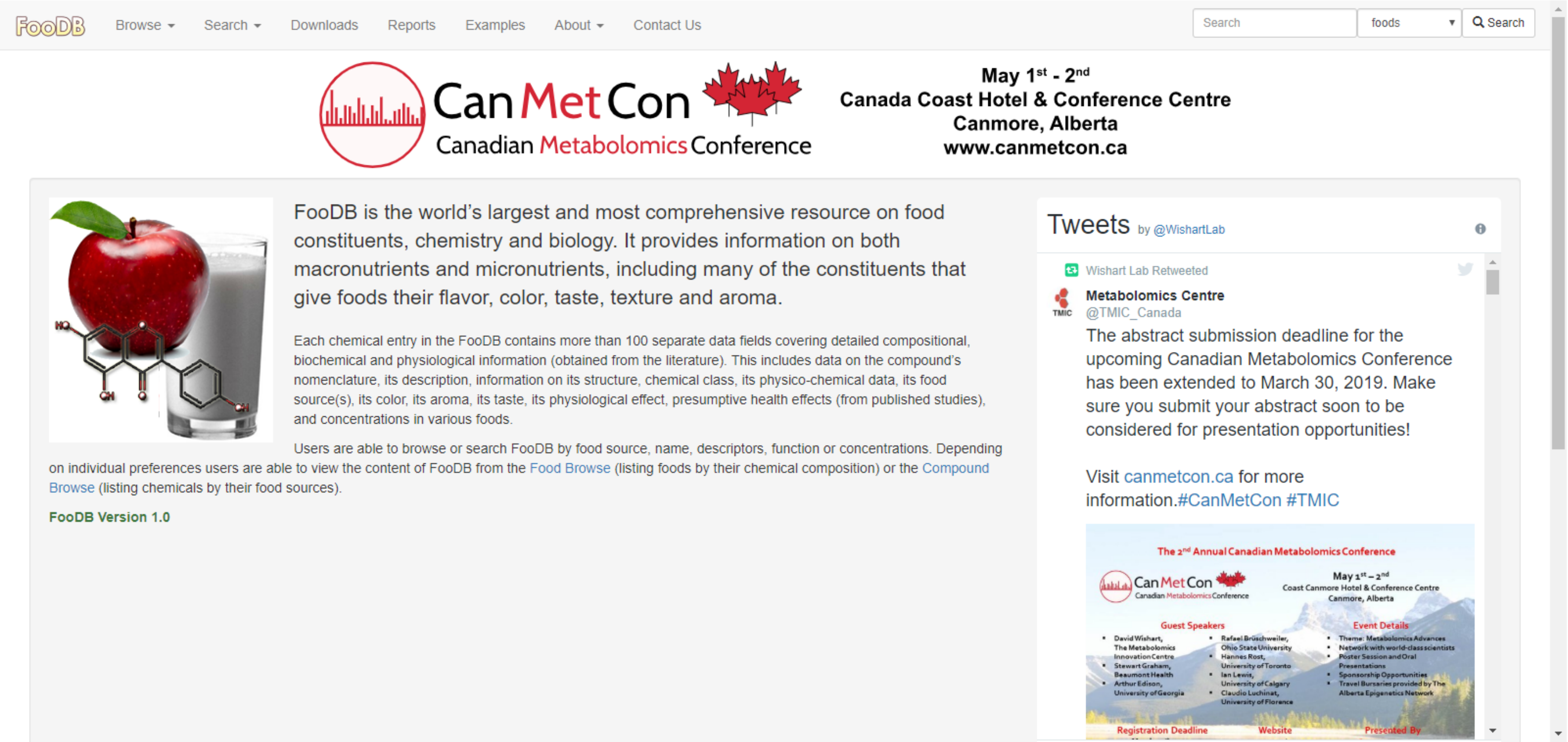
The biosynthesis of fatty acids primarily occurs in liver and lactating mammary glands. The entire synthesis process which produces palmitic acid occurs on a multifunctional dimeric protein Fatty Acid Synthase (FA) in the cytosol. The production of palmitic acid can be summarized as the succe (more)

BioPAX SVG SBGN SBML PWML All files (.zip)


Liver
Extracellular Space
Hepatic Cell
Cytosol
Vitamin K1
NADH
NAD
FAD
NAD(P)H dehydrogenase [quinone] 1
Phylloquinol
Endoplasmic reticulum
Lumen
Oxidized dithiothreitol
1,4-Dithiothreitol
Vitamin K-dependent gamma-carboxylase
Vitamin K epoxide reductase complex subunit 1
Vitamin K1 2,3-epoxide

FooDB

FooDB（食品數據庫）涵蓋了常見食物的化學成分資訊，包括大量關於營養素和微量營養素的詳細資料。包含食品成分、化學和生物學資源，提供有關食物組成及特性的詳盡資訊。
該資料庫涵蓋了食物中的各種化學物質，為研究人員和對食物成分感興趣的人士提供了重要的參考。



Can Met Con
Canadian Metabolomics Conference
May 1^{st} - 2^{nd}
Canada Coast Hotel & Conference Centre
Canmore, Alberta
www.canmetcon.ca

FooDB is the world's largest and most comprehensive resource on food constituents, chemistry and biology. It provides information on both macronutrients and micronutrients, including many of the constituents that give foods their flavor, color, taste, texture and aroma.

Each chemical entry in the FooDB contains more than 100 separate data fields covering detailed compositional, biochemical and physiological information (obtained from the literature). This includes data on the compound's nomenclature, its description, information on its structure, chemical class, its physico-chemical data, its food source(s), its color, its aroma, its taste, its physiological effect, presumptive health effects (from published studies), and concentrations in various foods.

Users are able to browse or search FooDB by food source, name, descriptors, function or concentrations. Depending on individual preferences users are able to view the content of FooDB from the Food Browse (listing foods by their chemical composition) or the Compound Browse (listing chemicals by their food sources).

FooDB Version 1.0

Tweets by @WishartLab

Wishart Lab Retweeted

Metabolomics Centre
@TMIC_Canada

The abstract submission deadline for the upcoming Canadian Metabolomics Conference has been extended to March 30, 2019. Make sure you submit your abstract soon to be considered for presentation opportunities!

Visit canmetcon.ca for more information.#CanMetCon #TMIC

The 2^{nd} Annual Canadian Metabolomics Conference

Can Met Con
Canadian Metabolomics Conference

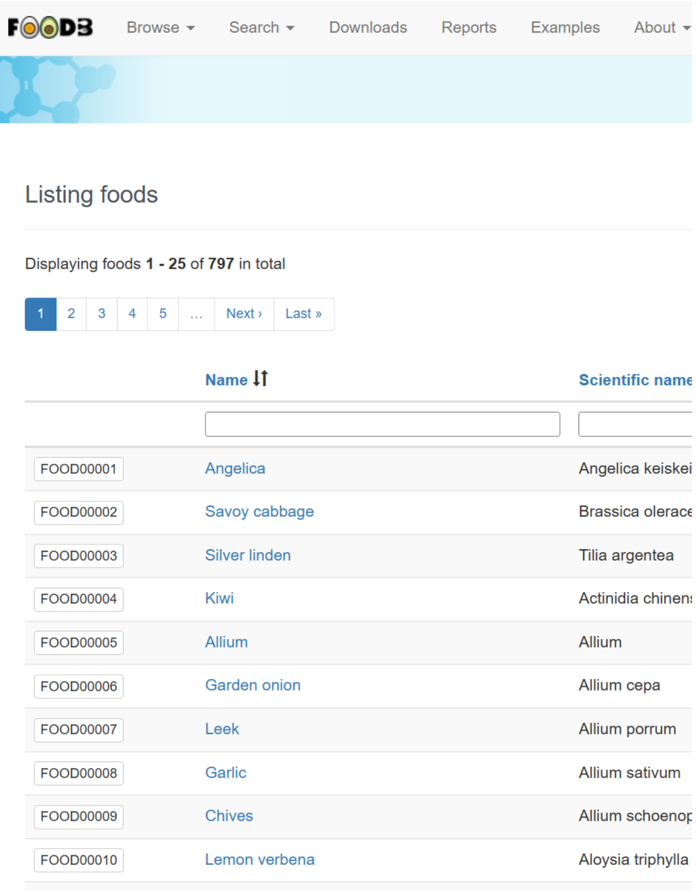
May 1^{st} – 2^{nd}
Coast Canmore Hotel & Conference Centre
Canmore, Alberta

Guest Speakers
- David Wishart, The Metabolomics Innovation Centre
- Stewart Graham, Beaumont Health
- Arthur Edison, University of Georgia
- Rafael Brüschweiler, Ohio State University
- Hannes Rost, University of Toronto
- Ian Lewis, University of Calgary
- Claudio Luchinat, University of Florence

Event Details
- Theme: Metabolomics Advances
- Network with world-class scientists
- Poster Session and Oral Presentations
- Sponsorship Opportunities
- Travel Bursaries provided by The Alberta Epigenetics Network

Registration Deadline
Website
Presented By

FooDB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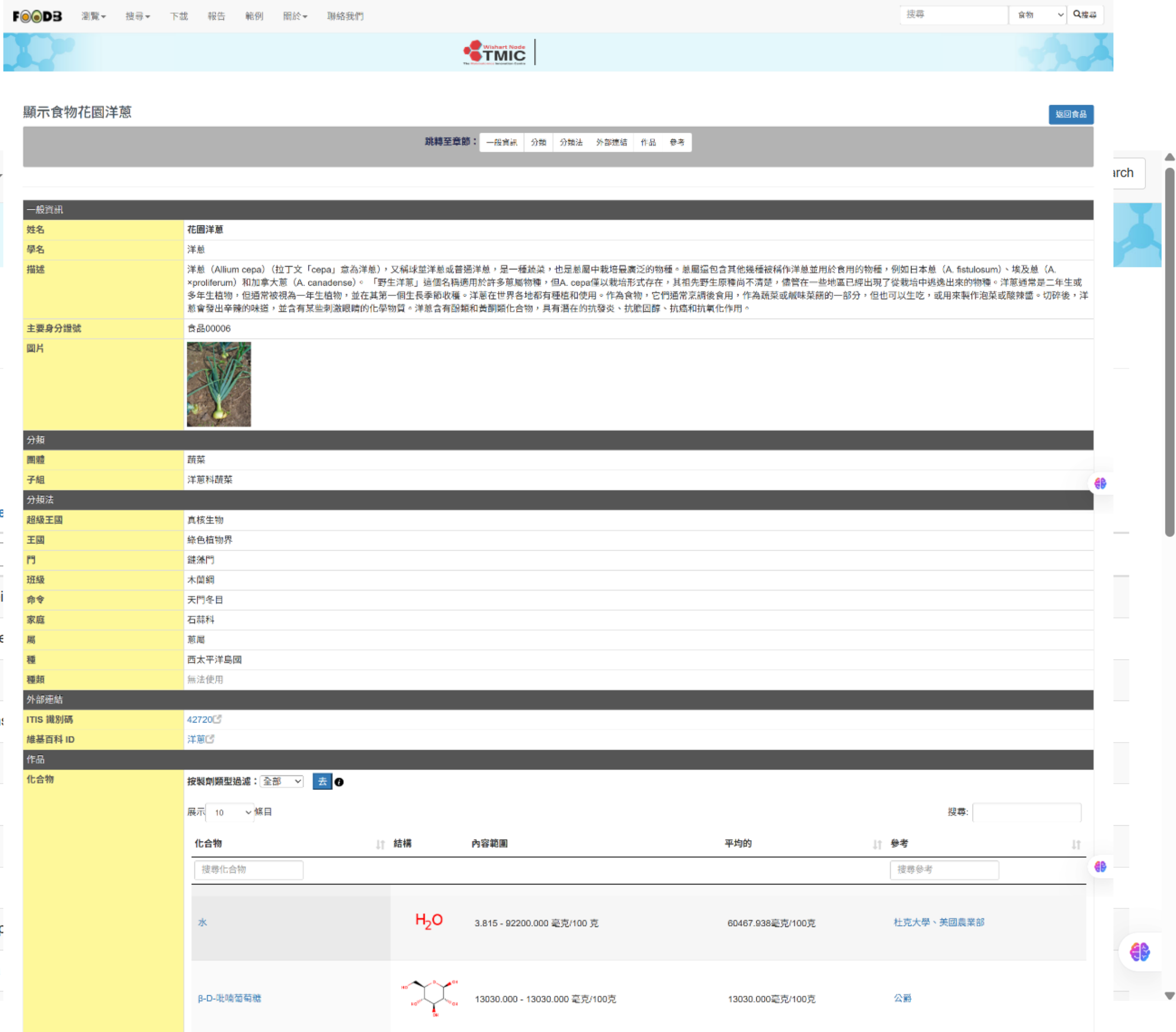
About

Listing foods

Displaying foods **1 - 25** of **797** in total

1
2
3
4
5
…
Next ›
Last »

	Name	**Scientific name**
FOOD00001	Angelica	Angelica keiskei
FOOD00002	Savoy cabbage	Brassica olerace
FOOD00003	Silver linden	Tilia argentea
FOOD00004	Kiwi	Actinidia chinens
FOOD00005	Allium	Allium
FOOD00006	Garden onion	Allium cepa
FOOD00007	Leek	Allium porrum
FOOD00008	Garlic	Allium sativum
FOOD00009	Chives	Allium schoenop
FOOD00010	Lemon verbena	Aloysia triphylla


FOODB
瀏覽
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下載
報告
範例
關於
聯絡我們
搜尋
食物
搜尋
Wishart Node
TMIC
返回食品
跳轉至章節：
一般資訊
分類
分類法
外部連結
作品
參考

顯示食物花園洋蔥

一般資訊	
姓名	**花園洋蔥**
學名	洋蔥
描述	洋蔥（Allium cepa）（拉丁文「cepa」意為洋蔥），又稱球莖洋蔥或普通洋蔥，是一種蔬菜，也是蔥屬中栽培最廣泛的物種。蔥屬還包含其他幾種被稱作洋蔥並用於食用的物種，例如日本蔥（A. fistulosum）、埃及蔥（A. ×proliferum）和加拿大蔥（A. canadense）。「野生洋蔥」這個名稱適用於許多蔥屬物種，但A. cepa僅以栽培形式存在，其祖先野生原種尚不清楚，儘管在一些地區已經出現了從栽培中逃逸出來的物種。洋蔥通常是二年生或多年生植物，但通常被視為一年生植物，並在其第一個生長季節收穫。洋蔥在世界各地都有種植和使用。作為食物，它們通常烹調後食用，作為蔬菜或鹹味菜餚的一部分，但也可以生吃，或用來製作泡菜或酸辣醬。切碎後，洋蔥會發出辛辣的味道，並含有某些刺激眼睛的化學物質。洋蔥含有酚類和黃酮類化合物，具有潛在的抗發炎、抗膽固醇、抗癌和抗氧化作用。
主要身分證號	食品00006
圖片	
分類	
團體	蔬菜
子組	洋蔥科蔬菜
分類法	
超級王國	真核生物
王國	綠色植物界
門	鏈黴門
班級	木蘭綱
命令	天門冬目
家庭	石蒜科
屬	蔥屬
種	西太平洋島國
種類	無法使用
外部連結	
ITIS 識別碼	42720
維基百科 ID	洋蔥
作品	
化合物	按製劑類型過濾：全部 去

展示 10 條目 搜尋:

化合物	結構	內容範圍	平均的	參考
水	H_2O	3.815 - 92200.000 毫克/100 克	60467.938毫克/100克	杜克大學、美國農業部
β-D-吡喃葡萄糖		13030.000 - 13030.000 毫克/100克	13030.000毫克/100克	公爵

Yeast, Bovine & E. Coli

YMDB
Yeast Metabolome Database
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Browse
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About
Help
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Yeast Metabolome Database

The **Y**east **M**etabolome **D**ata**b**ase (**YMDB**) is a manually curated database of small molecule metabolites found in or produced by Saccharomyces cerevisiae(also known as Baker's yeast and Brewer's yeast). This database covers metabolites described in textbooks, scientific journals, metabolic reconstructions and other electronic databases. YMDB contains metabolites arising from normal S. cerevisiae metabolism under defined laboratory conditions as well as metabolites generated by S. cerevisiae when used in baking and in the production of wines, beers and spirits. YMDB currently contains 2010 small molecules with 857 associated enzymes and 138 associated transporters.

References:

1. Jewison T, Neveu V, Lee J, Knox C, Liu P, Mandal R, Murthy RK, Sinelnikov I, Guo AC, Wilson M, Djoumbou Y and Wishart DS. "YMDB: The Yeast Metabolome Database". Nucleic Acids Res. 2012 Jan;40(Database issue):D815-20
2. Wiki: http://en.wikipedia.org/wiki/YMDB

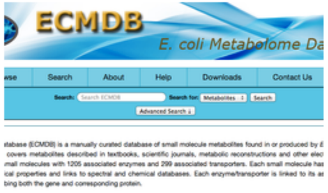
Metabolomics Toolbox
BMDB Browse
Downloads
Bovine Metabolome Database
hmp
Browsing metabolites

Bovine Metabolome Database (BMDB)

The **B**ovine **M**etabolome **D**ata**b**ase (**BMDB**) The Bovine Metabolome Database (BMDB) is a freely available electronic database containing detailed information about small molecule metabolites found in beef and dairy cattle. The information includes literature and experimentally derived information on bovine meat, bovine serum, bovine milk, bovine urine and bovine ruminal fluid.

References:

1. http://en.wikipedia.org/wiki/Bovine_Metabolome_Database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Metabolites
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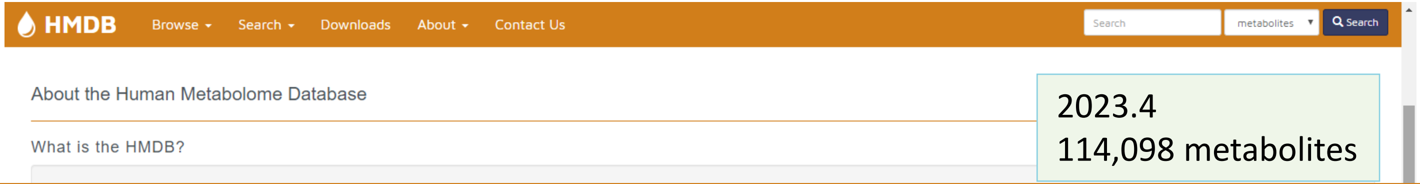
E. coli Metabolome Database (ECMDB)

E. **c**oli **M**etabolome **D**ata**b**ase (**ECMDB**) is a freely available eletronic database containing detailed information about the >3,700 metabolites found in E. coli (strain K12, MG1655). The information includes literature and experimentally derived information on the chemical data, spectral data and the molecular/biochemistry data.

References :

1. Sajed, T., Marcu, A., Ramirez, M., Pon, A., Guo, A., Knox, C., Wilson, M., Grant, J., Djoumbou, Y. and Wishart, D. ECMDB 2.0: A richer resource for understanding the biochemistry of *E. coli*. *Nucleic Acids Res*. 2016 Jan 4;44(D1):D495-501.
2. ECMDB: The E. coli Metabolome Database. Guo AC, Jewison T, Wilson M, Liu Y, Knox C, Djoumbou Y, Lo P, Mandal R, Krishnamurthy R, Wishart DS. Nucleic Acids Res. 2012 Oct 29.
3. Wiki: https://en.wikipedia.org/wiki/E._Coli_Metabolome_Database

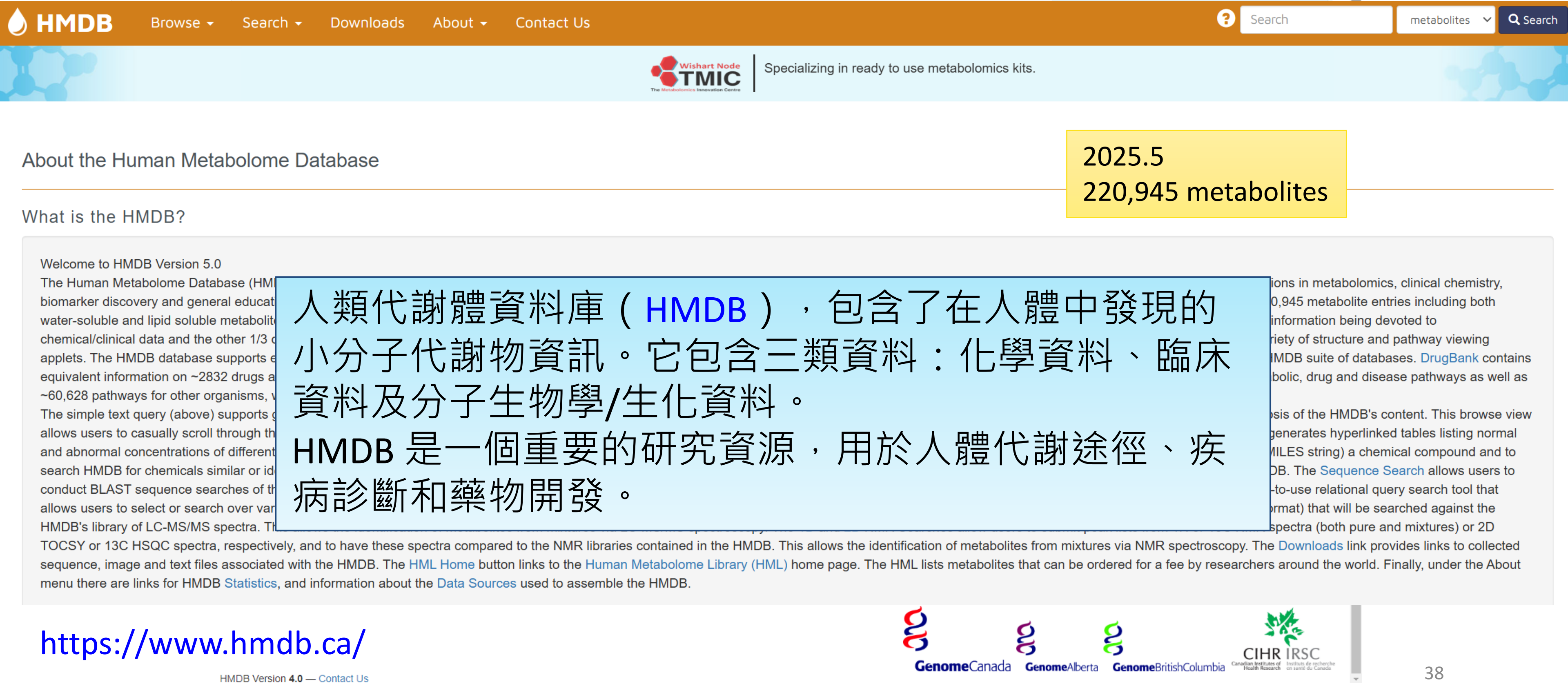
HMDB



About the Human Metabolome Database

What is the HMDB?

2023.4
114,098 metabolites



Specializing in ready to use metabolomics kits.

About the Human Metabolome Database

What is the HMDB?

2025.5
220,945 metabolites

Welcome to HMDB Version 5.0
The Human Metabolome Database (HM … ions in metabolomics, clinical chemistry,
biomarker discovery and general educat … 0,945 metabolite entries including both
water-soluble and lipid soluble metabolit … information being devoted to
chemical/clinical data and the other 1/3 c … riety of structure and pathway viewing
applets. The HMDB database supports e … MDB suite of databases. DrugBank contains
equivalent information on ~2832 drugs a … bolic, drug and disease pathways as well as
~60,628 pathways for other organisms, v
The simple text query (above) supports g … sis of the HMDB's content. This browse view
allows users to casually scroll through th … generates hyperlinked tables listing normal
and abnormal concentrations of different … MILES string) a chemical compound and to
search HMDB for chemicals similar or id … DB. The Sequence Search allows users to
conduct BLAST sequence searches of th … -to-use relational query search tool that
allows users to select or search over var … rmat) that will be searched against the
HMDB's library of LC-MS/MS spectra. Th … spectra (both pure and mixtures) or 2D
TOCSY or 13C HSQC spectra, respectively, and to have these spectra compared to the NMR libraries contained in the HMDB. This allows the identification of metabolites from mixtures via NMR spectroscopy. The Downloads link provides links to collected sequence, image and text files associated with the HMDB. The HML Home button links to the Human Metabolome Library (HML) home page. The HML lists metabolites that can be ordered for a fee by researchers around the world. Finally, under the About menu there are links for HMDB Statistics, and information about the Data Sources used to assemble the HMDB.

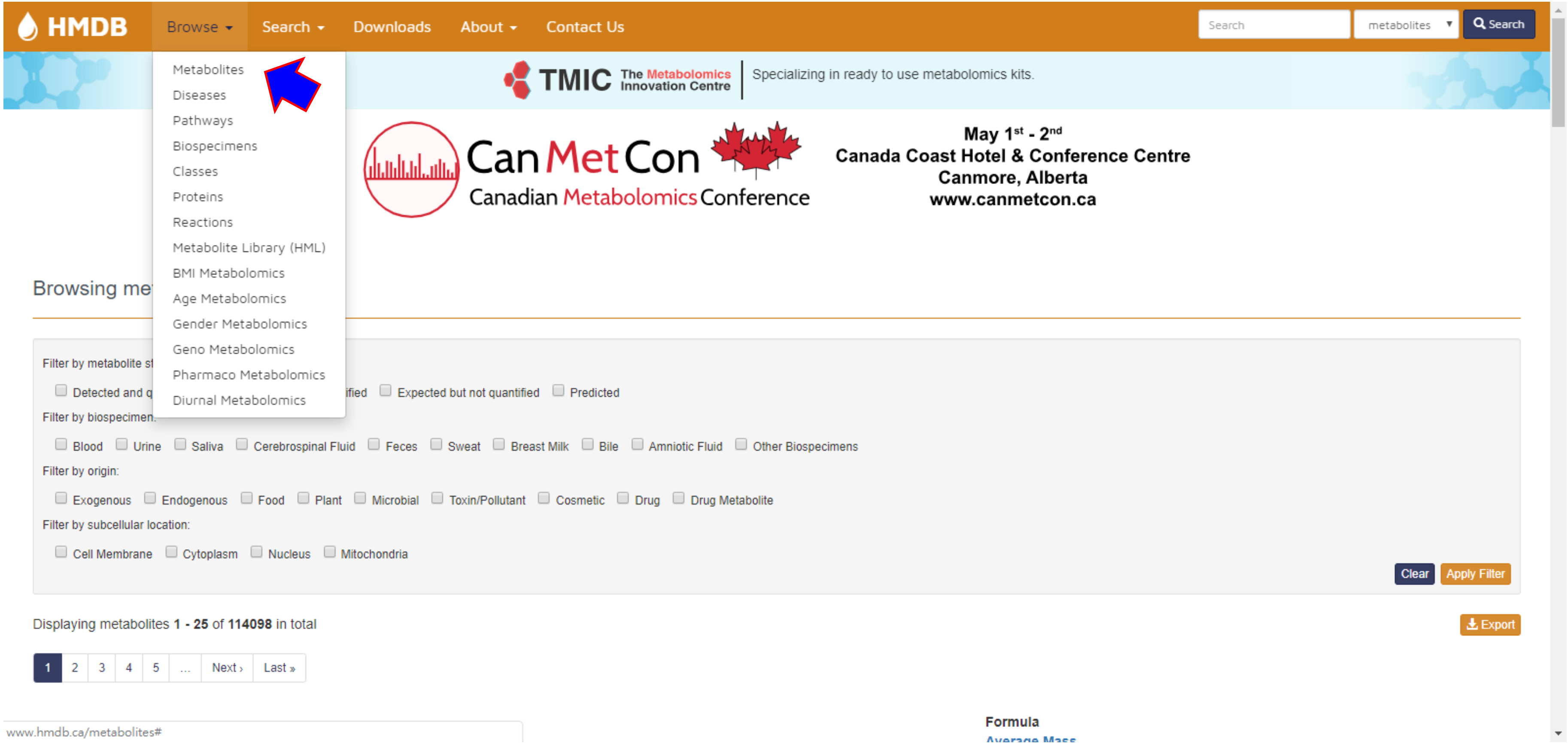
人類代謝體資料庫（HMDB），包含了在人體中發現的小分子代謝物資訊。它包含三類資料：化學資料、臨床資料及分子生物學/生化資料。

HMDB 是一個重要的研究資源，用於人體代謝途徑、疾病診斷和藥物開發。

https://www.hmdb.ca/

HMDB Version **4.0** — Contact Us

HMDB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metabolites
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Diseases
Pathways
Biospecimens
Classes
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Reactions
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2
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☐ Detected and q ified ☐ Expected but not quantified ☐ Predicted

Filter by biospecimen:

☐ Blood ☐ Urine ☐ Saliva ☐ Cerebrospinal Fluid ☐ Feces ☐ Sweat ☐ Breast Milk ☐ Bile ☐ Amniotic Fluid ☐ Other Biospecimens

Filter by origin:

☐ Exogenous ☐ Endogenous ☐ Food ☐ Plant ☐ Microbial ☐ Toxin/Pollutant ☐ Cosmetic ☐ Drug ☐ Drug Metabolite

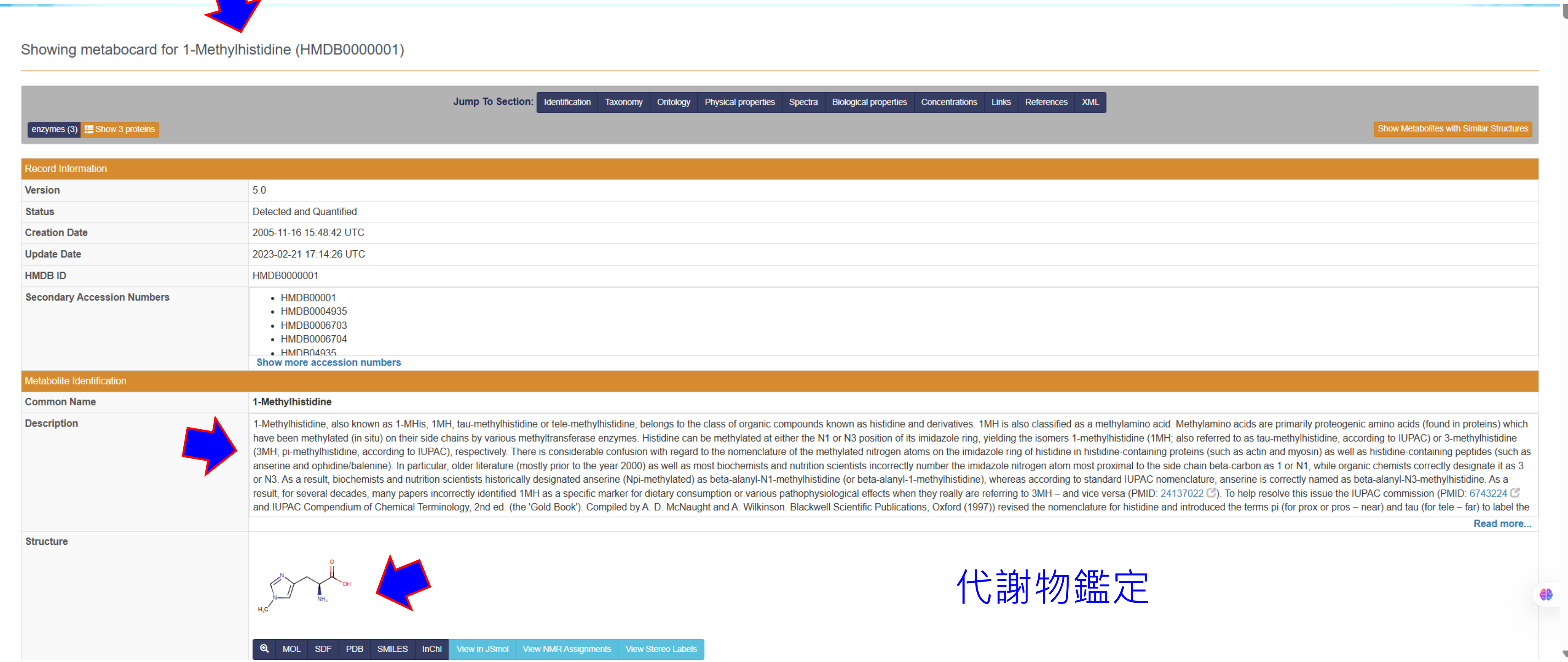
Filter by subcellular location:

☐ Cell Membrane ☐ Cytoplasm ☐ Nucleus ☐ Mitochondria

Displaying metabolites **1 - 25** of **114098** in total

HMDB

甲基氨基酸主要指蛋白質中的蛋白原性氨基酸，其側鏈已被各種甲基轉移酶原位甲基化。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Identification
Taxonomy
Ontology
Physical properties
Spectra
Biological properties
Concentrations
Links
References
XML
enzymes (3)
Show 3 proteins
Show Metabolites with Similar Structures
MOL
SDF
PDB
SMILES
InChI
View in JSmol
View NMR Assignments
View Stereo Labels
O
OH
N
N
NH₂
H₃C

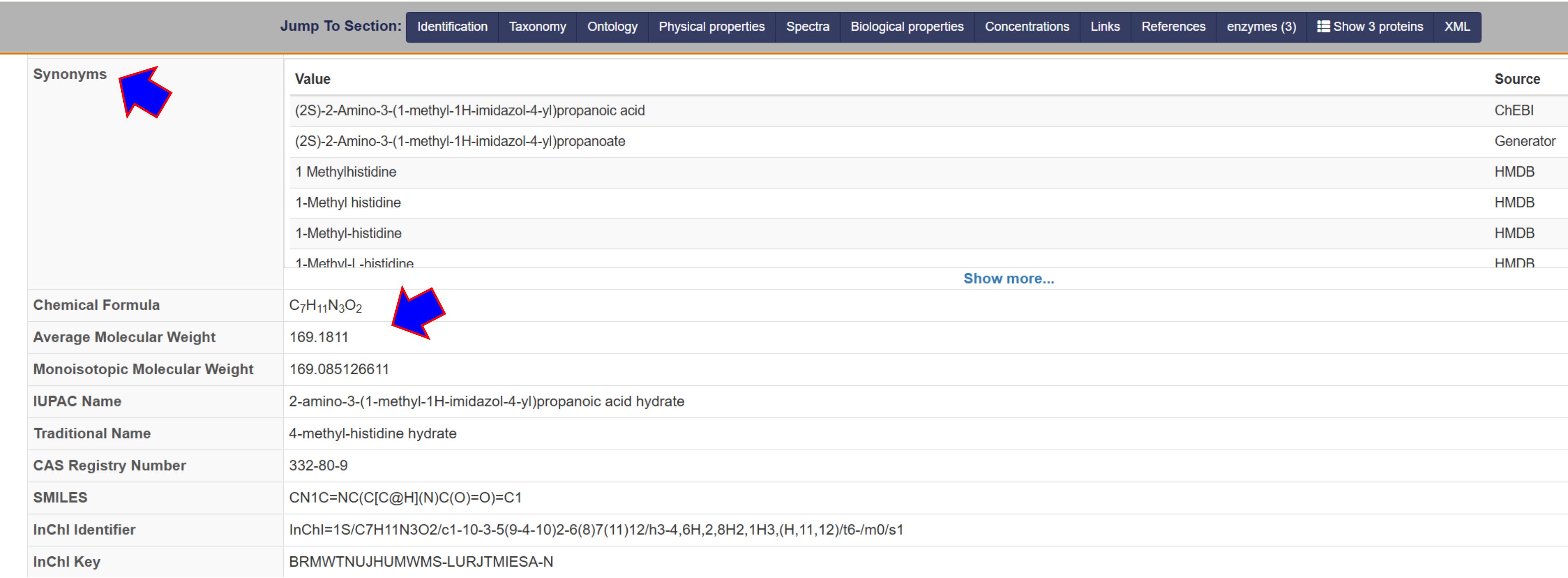
Showing metabocard for 1-Methylhistidine (HMDB0000001)

Record Information	
Version	5.0
Status	Detected and Quantified
Creation Date	2005-11-16 15:48:42 UTC
Update Date	2023-02-21 17:14:26 UTC
HMDB ID	HMDB0000001
Secondary Accession Numbers	• HMDB00001 • HMDB0004935 • HMDB0006703 • HMDB0006704 • HMDB04935 Show more accession numbers

Metabolite Identification	
Common Name	**1-Methylhistidine**
Description	1-Methylhistidine, also known as 1-MHis, 1MH, tau-methylhistidine or tele-methylhistidine, belongs to the class of organic compounds known as histidine and derivatives. 1MH is also classified as a methylamino acid. Methylamino acids are primarily proteogenic amino acids (found in proteins) which have been methylated (in situ) on their side chains by various methyltransferase enzymes. Histidine can be methylated at either the N1 or N3 position of its imidazole ring, yielding the isomers 1-methylhistidine (1MH; also referred to as tau-methylhistidine, according to IUPAC) or 3-methylhistidine (3MH; pi-methylhistidine, according to IUPAC), respectively. There is considerable confusion with regard to the nomenclature of the methylated nitrogen atoms on the imidazole ring of histidine in histidine-containing proteins (such as actin and myosin) as well as histidine-containing peptides (such as anserine and ophidine/balenine). In particular, older literature (mostly prior to the year 2000) as well as most biochemists and nutrition scientists incorrectly number the imidazole nitrogen atom most proximal to the side chain beta-carbon as 1 or N1, while organic chemists correctly designate it as 3 or N3. As a result, biochemists and nutrition scientists historically designated anserine (Npi-methylated) as beta-alanyl-N1-methylhistidine (or beta-alanyl-1-methylhistidine), whereas according to standard IUPAC nomenclature, anserine is correctly named as beta-alanyl-N3-methylhistidine. As a result, for several decades, many papers incorrectly identified 1MH as a specific marker for dietary consumption or various pathophysiological effects when they really are referring to 3MH – and vice versa (PMID: 24137022). To help resolve this issue the IUPAC commission (PMID: 6743224 and IUPAC Compendium of Chemical Terminology, 2nd ed. (the 'Gold Book'). Compiled by A. D. McNaught and A. Wilkinson. Blackwell Scientific Publications, Oxford (1997)) revised the nomenclature for histidine and introduced the terms pi (for prox or pros – near) and tau (for tele – far) to label the Read more...
Structure	

代謝物鑑定

HMDB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Identification
Taxonomy
Ontology
Physical properties
Spectra
Biological properties
Concentrations
Links
References
enzymes (3)
Show 3 proteins
XML
Show more...

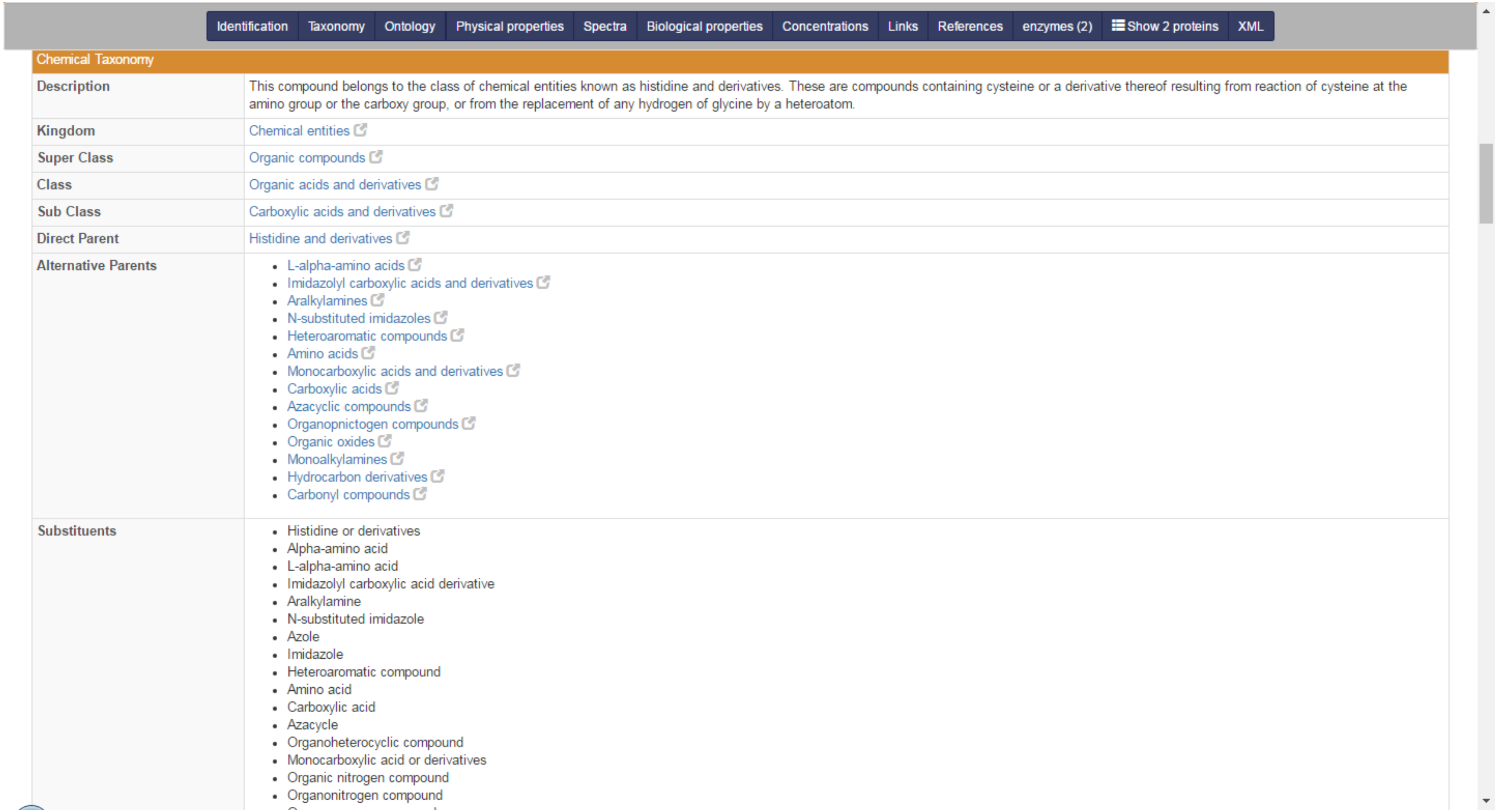
Synonyms

Value	Source
(2S)-2-Amino-3-(1-methyl-1H-imidazol-4-yl)propanoic acid	ChEBI
(2S)-2-Amino-3-(1-methyl-1H-imidazol-4-yl)propanoate	Generator
1 Methylhistidine	HMDB
1-Methyl histidine	HMDB
1-Methyl-histidine	HMDB
1-Methyl-L-histidine	HMDB

Chemical Formula	$C_7H_{11}N_3O_2$
Average Molecular Weight	169.1811
Monoisotopic Molecular Weight	169.085126611
IUPAC Name	2-amino-3-(1-methyl-1H-imidazol-4-yl)propanoic acid hydrate
Traditional Name	4-methyl-histidine hydrate
CAS Registry Number	332-80-9
SMILES	CN1C=NC(C[C@H](N)C(O)=O)=C1
InChI Identifier	InChI=1S/C7H11N3O2/c1-10-3-5(9-4-10)2-6(8)7(11)12/h3-4,6H,2,8H2,1H3,(H,11,12)/t6-/m0/s1
InChI Key	BRMWTNUJHUMWMS-LURJTMIESA-N

HMDB

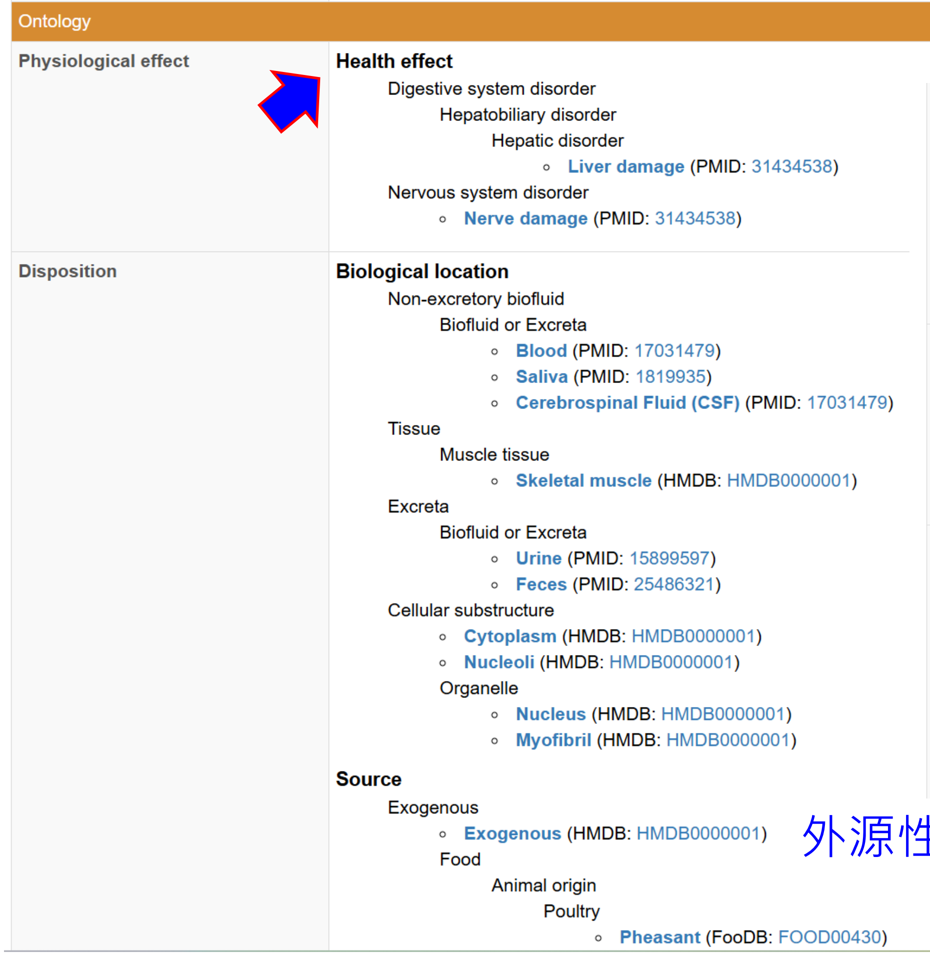
化學分類學


Identification
Taxonomy
Ontology
Physical properties
Spectra
Biological properties
Concentrations
Links
References
enzymes (2)
Show 2 proteins
XML

Chemical Taxonomy

Description	This compound belongs to the class of chemical entities known as histidine and derivatives. These are compounds containing cysteine or a derivative thereof resulting from reaction of cysteine at the amino group or the carboxy group, or from the replacement of any hydrogen of glycine by a heteroatom.
Kingdom	Chemical entities
Super Class	Organic compounds
Class	Organic acids and derivatives
Sub Class	Carboxylic acids and derivatives
Direct Parent	Histidine and derivatives
Alternative Parents	L-alpha-amino acids Imidazolyl carboxylic acids and derivatives Aralkylamines N-substituted imidazoles Heteroaromatic compounds Amino acids Monocarboxylic acids and derivatives Carboxylic acids Azacyclic compounds Organopnictogen compounds Organic oxides Monoalkylamines Hydrocarbon derivatives Carbonyl compounds
Substituents	Histidine or derivatives Alpha-amino acid L-alpha-amino acid Imidazolyl carboxylic acid derivative Aralkylamine N-substituted imidazole Azole Imidazole Heteroaromatic compound Amino acid Carboxylic acid Azacycle Organoheterocyclic compound Monocarboxylic acid or derivatives Organic nitrogen compound Organonitrogen compound

HMDB



Ontology

Physiological effect

Health effect

- Digestive system disorder
  - Hepatobiliary disorder
    - Hepatic disorder
      - **Liver damage** (PMID: 31434538)
- Nervous system disorder
  - **Nerve damage** (PMID: 31434538)

Disposition

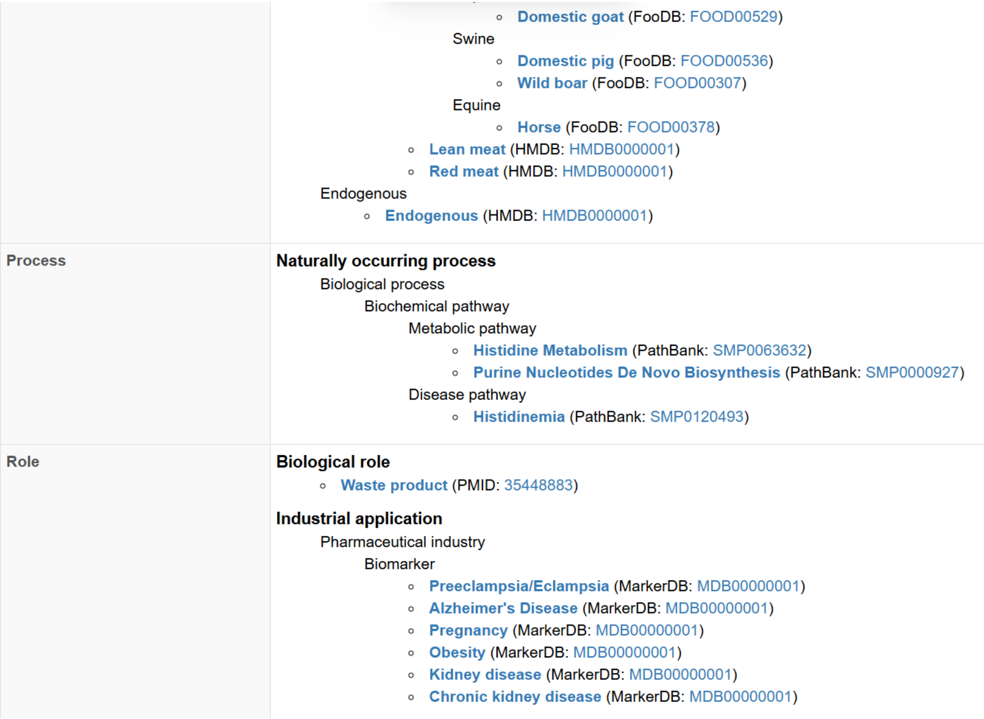
Biological location

- Non-excretory biofluid
  - Biofluid or Excreta
    - **Blood** (PMID: 17031479)
    - **Saliva** (PMID: 1819935)
    - **Cerebrospinal Fluid (CSF)** (PMID: 17031479)
- Tissue
  - Muscle tissue
    - **Skeletal muscle** (HMDB: HMDB0000001)
- Excreta
  - Biofluid or Excreta
    - **Urine** (PMID: 15899597)
    - **Feces** (PMID: 25486321)
- Cellular substructure
  - **Cytoplasm** (HMDB: HMDB0000001)
  - **Nucleoli** (HMDB: HMDB0000001)
  - Organelle
    - **Nucleus** (HMDB: HMDB0000001)
    - **Myofibril** (HMDB: HMDB0000001)

Source

- Exogenous
  - **Exogenous** (HMDB: HMDB0000001)
  - Food
    - Animal origin
      - Poultry
        - **Pheasant** (FooDB: FOOD00430)

外源性



- **Domestic goat** (FooDB: FOOD00529)
- Swine
  - **Domestic pig** (FooDB: FOOD00536)
  - **Wild boar** (FooDB: FOOD00307)
- Equine
  - **Horse** (FooDB: FOOD00378)
- **Lean meat** (HMDB: HMDB0000001)
- **Red meat** (HMDB: HMDB0000001)
- Endogenous
  - **Endogenous** (HMDB: HMDB0000001)

Process

Naturally occurring process

- Biological process
  - Biochemical pathway
    - Metabolic pathway
      - **Histidine Metabolism** (PathBank: SMP0063632)
      - **Purine Nucleotides De Novo Biosynthesis** (PathBank: SMP0000927)
    - Disease pathway
      - **Histidinemia** (PathBank: SMP0120493)

Role

Biological role

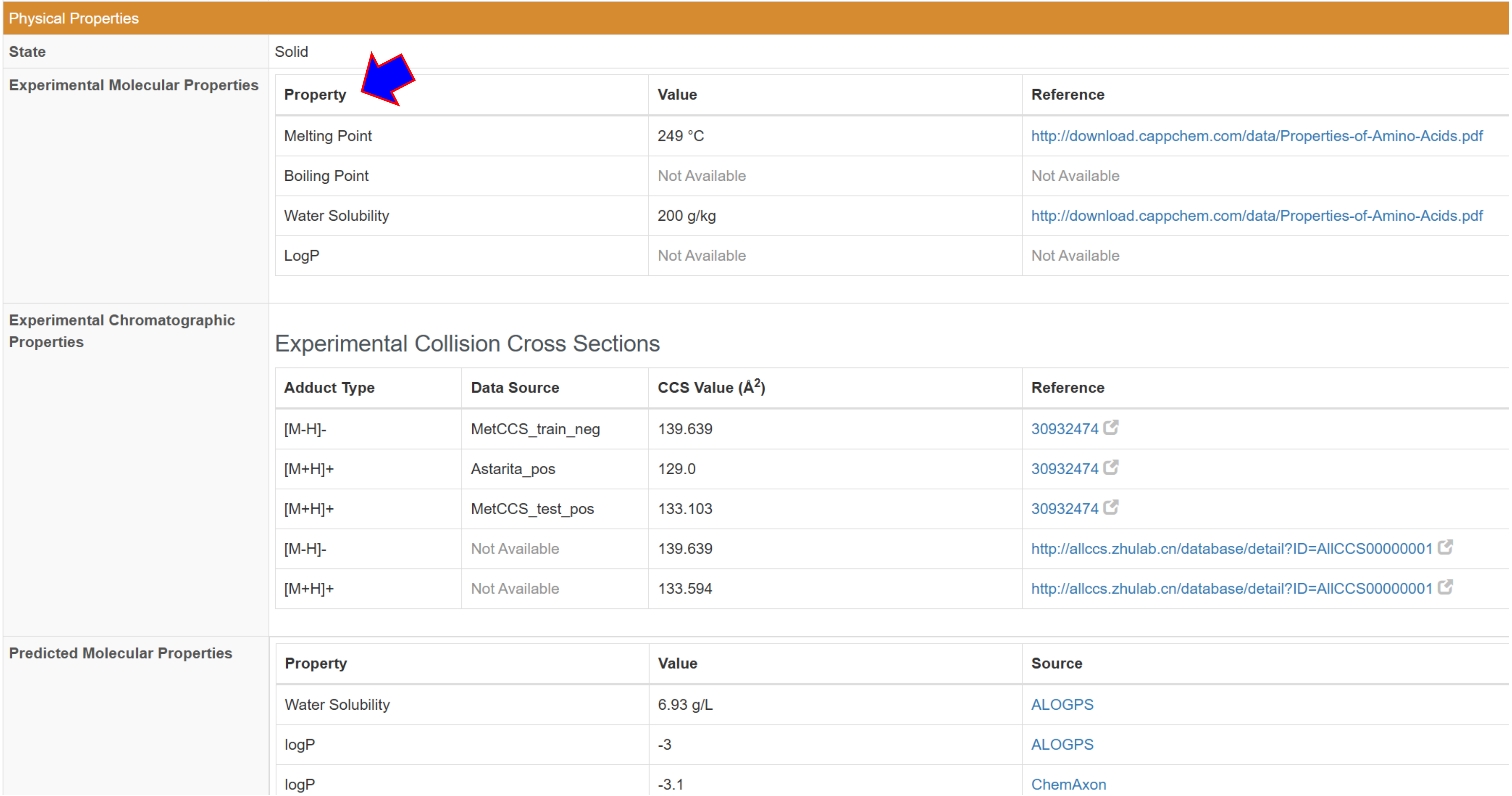
- **Waste product** (PMID: 35448883)

Industrial application

- Pharmaceutical industry
  - Biomarker
    - **Preeclampsia/Eclampsia** (MarkerDB: MDB00000001)
    - **Alzheimer's Disease** (MarkerDB: MDB00000001)
    - **Pregnancy** (MarkerDB: MDB00000001)
    - **Obesity** (MarkerDB: MDB00000001)
    - **Kidney disease** (MarkerDB: MDB00000001)
    - **Chronic kidney disease** (MarkerDB: MDB00000001)

HMDB

物理性質



Physical Properties

State: Solid

Experimental Molecular Properties

Property	Value	Reference
Melting Point	249 °C	http://download.cappchem.com/data/Properties-of-Amino-Acids.pdf
Boiling Point	Not Available	Not Available
Water Solubility	200 g/kg	http://download.cappchem.com/data/Properties-of-Amino-Acids.pdf
LogP	Not Available	Not Available

Experimental Chromatographic Properties

Experimental Collision Cross Sections

Adduct Type	Data Source	CCS Value (Å^2)	Reference
[M-H]-	MetCCS_train_neg	139.639	30932474
[M+H]+	Astarita_pos	129.0	30932474
[M+H]+	MetCCS_test_pos	133.103	30932474
[M-H]-	Not Available	139.639	http://allccs.zhulab.cn/database/detail?ID=AllCCS00000001
[M+H]+	Not Available	133.594	http://allccs.zhulab.cn/database/detail?ID=AllCCS00000001

Predicted Molecular Properties

Property	Value	Source
Water Solubility	6.93 g/L	ALOGPS
logP	-3	ALOGPS
logP	-3.1	ChemAxon

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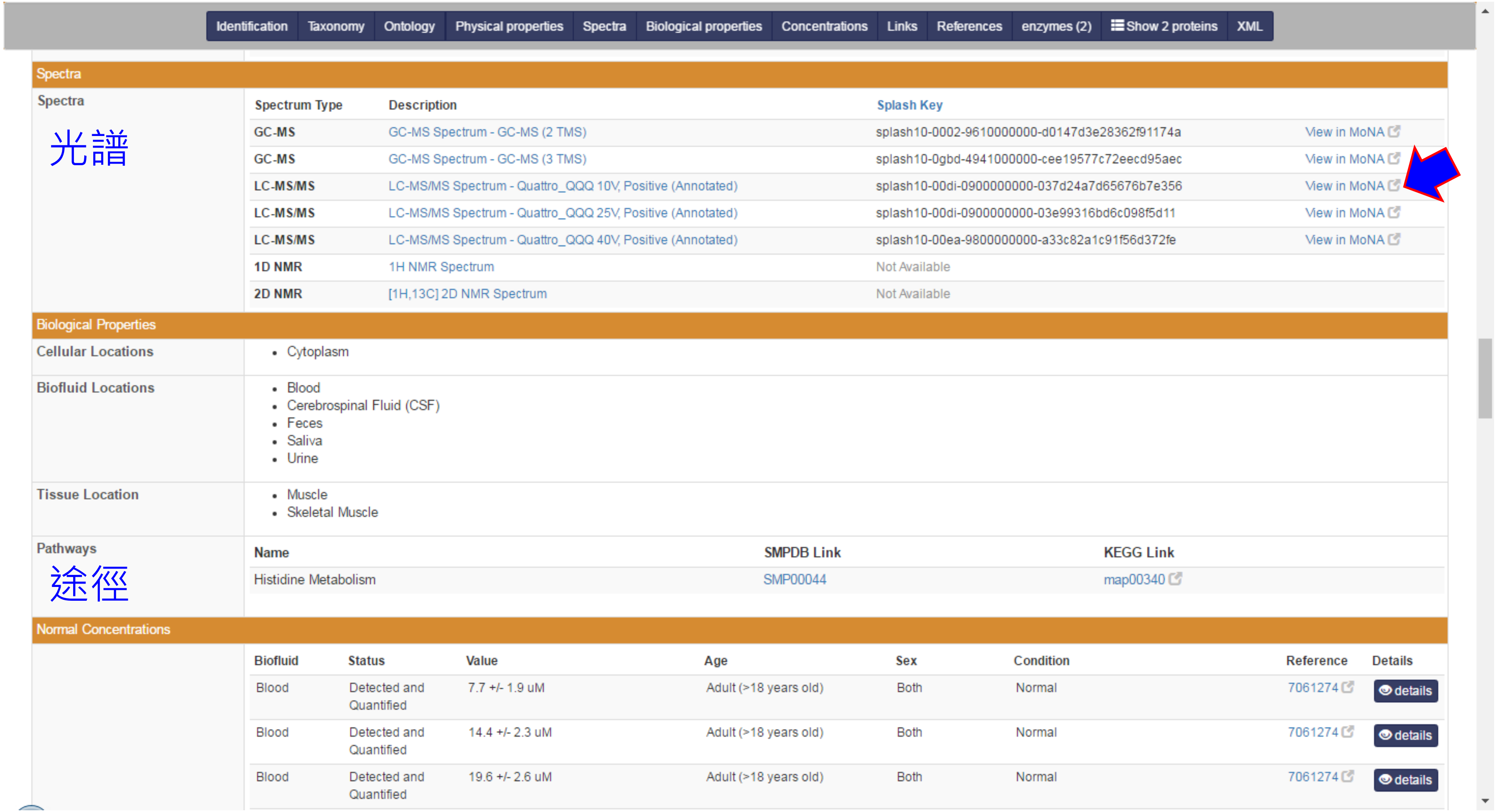

Identification
Taxonomy
Ontology
Physical properties
Spectra
Biological properties
Concentrations
Links
References
enzymes (2)
Show 2 proteins
XML

Spectra

Spectra

光譜

Spectrum Type	Description	Splash Key	
GC-MS	GC-MS Spectrum - GC-MS (2 TMS)	splash10-0002-9610000000-d0147d3e28362f91174a	View in MoNA
GC-MS	GC-MS Spectrum - GC-MS (3 TMS)	splash10-0gbd-4941000000-cee19577c72eecd95aec	View in MoNA
LC-MS/MS	LC-MS/MS Spectrum - Quattro_QQQ 10V, Positive (Annotated)	splash10-00di-0900000000-037d24a7d65676b7e356	View in MoNA
LC-MS/MS	LC-MS/MS Spectrum - Quattro_QQQ 25V, Positive (Annotated)	splash10-00di-0900000000-03e99316bd6c098f5d11	View in MoNA
LC-MS/MS	LC-MS/MS Spectrum - Quattro_QQQ 40V, Positive (Annotated)	splash10-00ea-9800000000-a33c82a1c91f56d372fe	View in MoNA
1D NMR	1H NMR Spectrum	Not Available	
2D NMR	[1H,13C] 2D NMR Spectrum	Not Available	

Biological Properties

Cellular Locations

- Cytoplasm

Biofluid Locations

- Blood
- Cerebrospinal Fluid (CSF)
- Feces
- Saliva
- Urine

Tissue Location

- Muscle
- Skeletal Muscle

Pathways

途徑

Name	SMPDB Link	KEGG Link
Histidine Metabolism	SMP00044	map00340

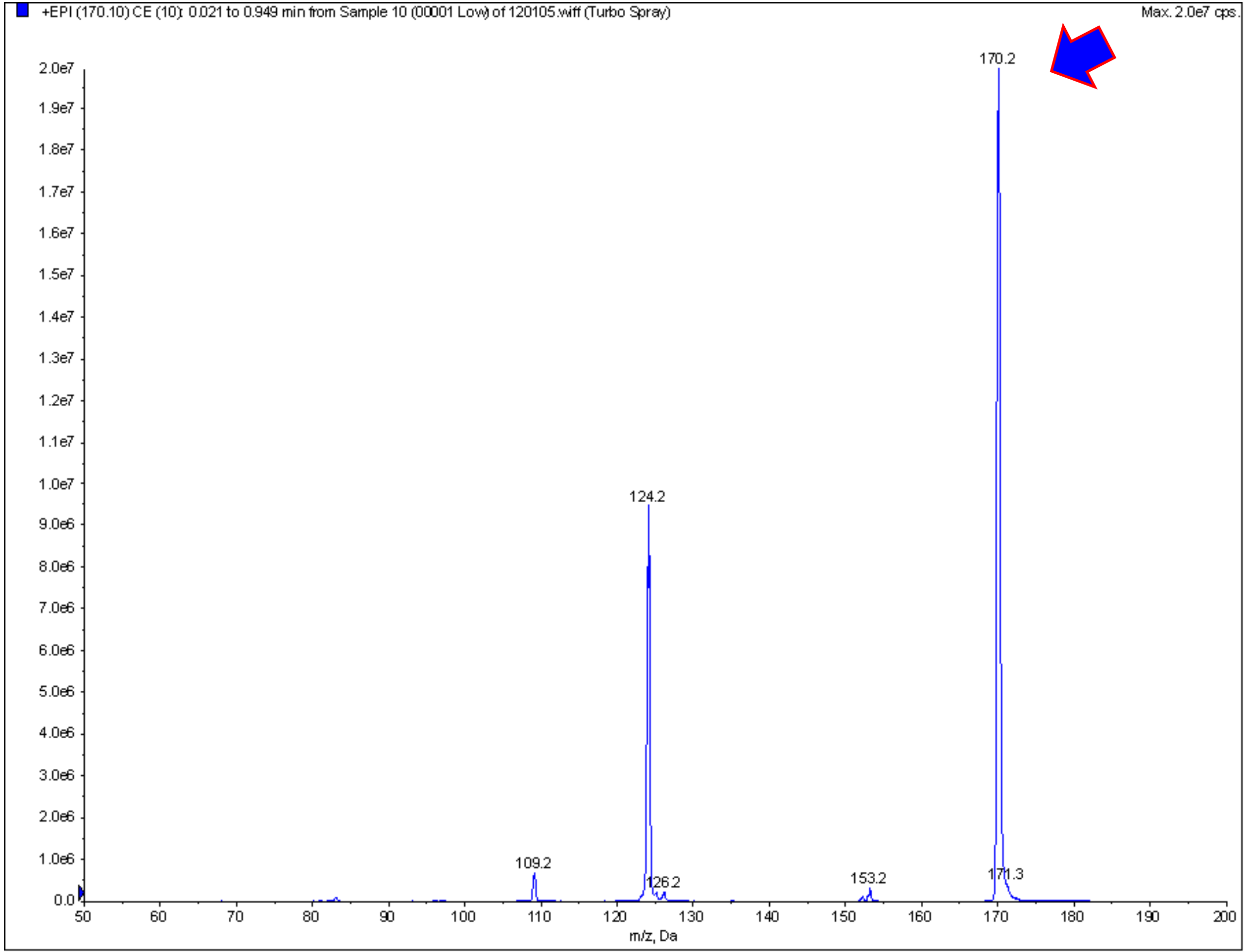
Normal Concentrations

Biofluid	Status	Value	Age	Sex	Condition	Reference	Details
Blood	Detected and Quantified	7.7 +/- 1.9 uM	Adult (>18 years old)	Both	Normal	7061274	details
Blood	Detected and Quantified	14.4 +/- 2.3 uM	Adult (>18 years old)	Both	Normal	7061274	details
Blood	Detected and Quantified	19.6 +/- 2.6 uM	Adult (>18 years old)	Both	Normal	7061274	details

HMDB

LC-MS/MS Spectrum

質譜光譜



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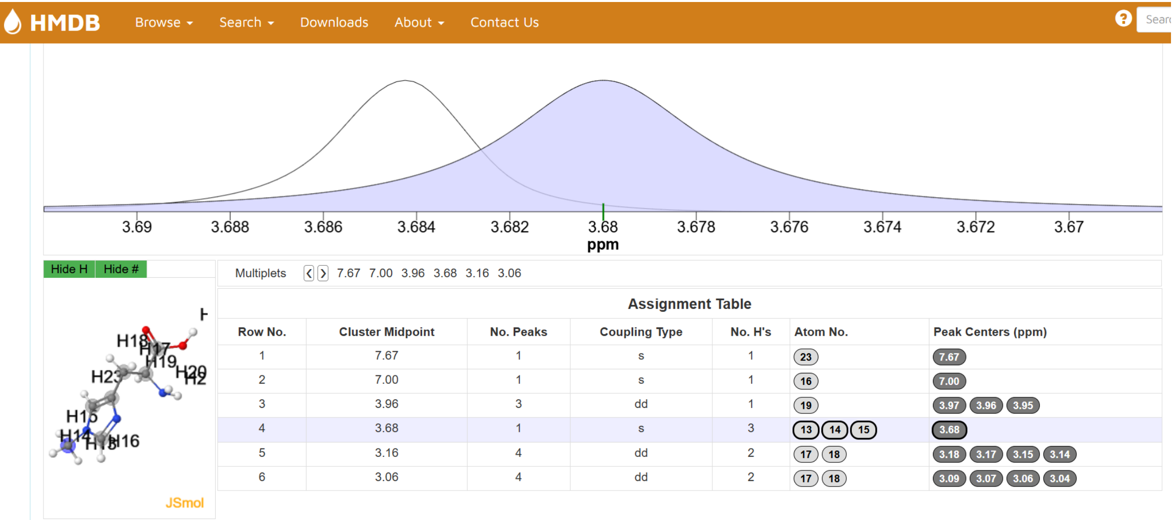
1H NMR Spectrum (1D, 500 MHz, H2O, experimental)

NMR光譜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3.69
3.688
3.686
3.684
3.682
3.68
3.678
3.676
3.674
3.672
3.67
ppm
Hide H
Hide #
JSmol

Multiplets 7.67 7.00 3.96 3.68 3.16 3.06

Assignment Table

Row No.	Cluster Midpoint	No. Peaks	Coupling Type	No. H's	Atom No.	Peak Centers (ppm)
1	7.67	1	s	1	23	7.67
2	7.00	1	s	1	16	7.00
3	3.96	3	dd	1	19	3.97 3.96 3.95
4	3.68	1	s	3	13 14 15	3.68
5	3.16	4	dd	2	17 18	3.18 3.17 3.15 3.14
6	3.06	4	dd	2	17 18	3.09 3.07 3.06 3.04

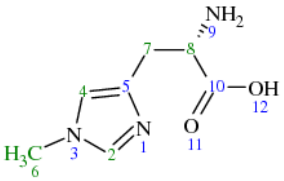
1-Methylhistidine

HMDB00001

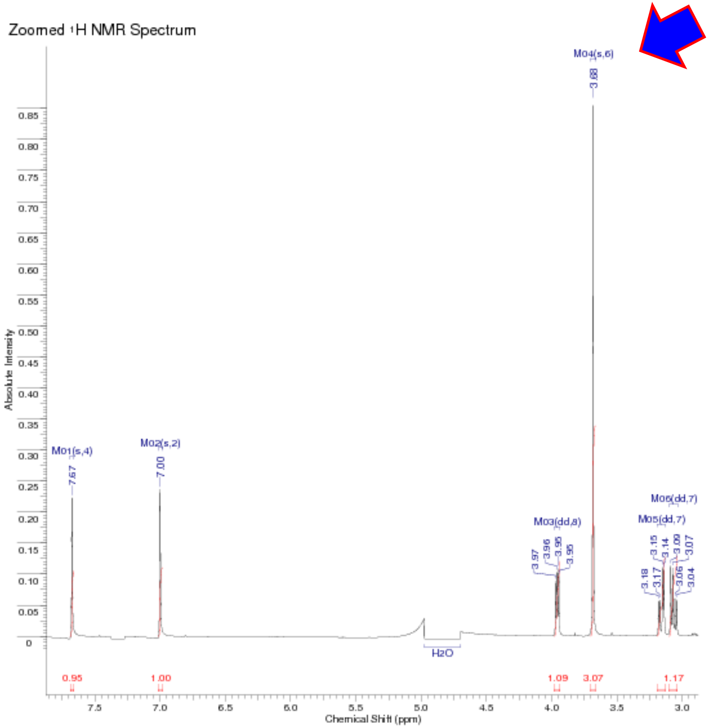
1H NMR Spectrum: 500MHz in H2O

Sample: ~50mM in H2O and pH 7.10

Referenced to DSS


NH2
9
7
8
4
5
10
OH
12
N
N
1
O
11
H3C
6
3
2

Zoomed 1H NMR Spectrum



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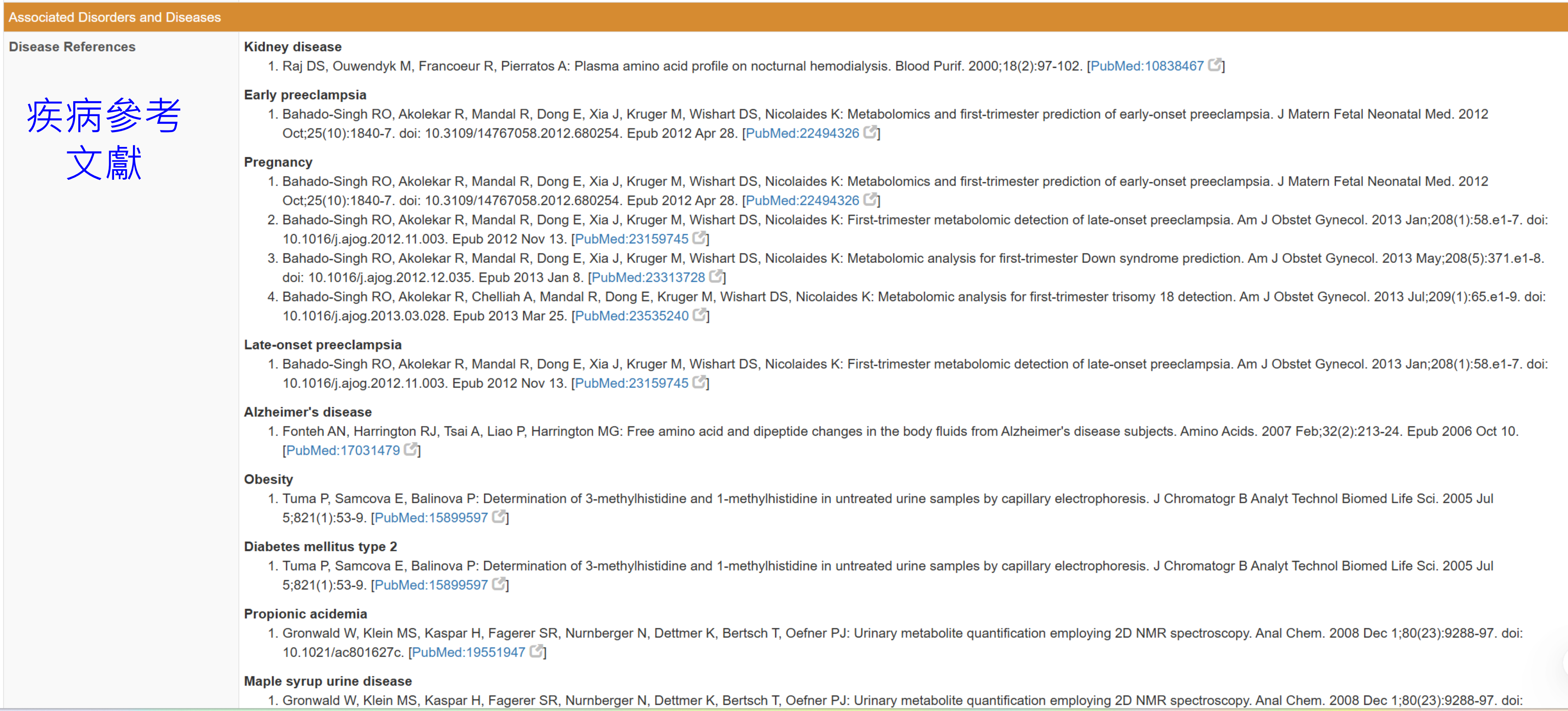

Associated Disorders and Diseases

Disease References

疾病參考文獻

Kidney disease

1. Raj DS, Ouwendyk M, Francoeur R, Pierratos A: Plasma amino acid profile on nocturnal hemodialysis. Blood Purif. 2000;18(2):97-102. [PubMed:10838467]

Early preeclampsia

1. Bahado-Singh RO, Akolekar R, Mandal R, Dong E, Xia J, Kruger M, Wishart DS, Nicolaides K: Metabolomics and first-trimester prediction of early-onset preeclampsia. J Matern Fetal Neonatal Med. 2012 Oct;25(10):1840-7. doi: 10.3109/14767058.2012.680254. Epub 2012 Apr 28. [PubMed:22494326]

Pregnancy

1. Bahado-Singh RO, Akolekar R, Mandal R, Dong E, Xia J, Kruger M, Wishart DS, Nicolaides K: Metabolomics and first-trimester prediction of early-onset preeclampsia. J Matern Fetal Neonatal Med. 2012 Oct;25(10):1840-7. doi: 10.3109/14767058.2012.680254. Epub 2012 Apr 28. [PubMed:22494326]
2. Bahado-Singh RO, Akolekar R, Mandal R, Dong E, Xia J, Kruger M, Wishart DS, Nicolaides K: First-trimester metabolomic detection of late-onset preeclampsia. Am J Obstet Gynecol. 2013 Jan;208(1):58.e1-7. doi: 10.1016/j.ajog.2012.11.003. Epub 2012 Nov 13. [PubMed:23159745]
3. Bahado-Singh RO, Akolekar R, Mandal R, Dong E, Xia J, Kruger M, Wishart DS, Nicolaides K: Metabolomic analysis for first-trimester Down syndrome prediction. Am J Obstet Gynecol. 2013 May;208(5):371.e1-8. doi: 10.1016/j.ajog.2012.12.035. Epub 2013 Jan 8. [PubMed:23313728]
4. Bahado-Singh RO, Akolekar R, Chelliah A, Mandal R, Dong E, Kruger M, Wishart DS, Nicolaides K: Metabolomic analysis for first-trimester trisomy 18 detection. Am J Obstet Gynecol. 2013 Jul;209(1):65.e1-9. doi: 10.1016/j.ajog.2013.03.028. Epub 2013 Mar 25. [PubMed:23535240]

Late-onset preeclampsia

1. Bahado-Singh RO, Akolekar R, Mandal R, Dong E, Xia J, Kruger M, Wishart DS, Nicolaides K: First-trimester metabolomic detection of late-onset preeclampsia. Am J Obstet Gynecol. 2013 Jan;208(1):58.e1-7. doi: 10.1016/j.ajog.2012.11.003. Epub 2012 Nov 13. [PubMed:23159745]

Alzheimer's disease

1. Fonteh AN, Harrington RJ, Tsai A, Liao P, Harrington MG: Free amino acid and dipeptide changes in the body fluids from Alzheimer's disease subjects. Amino Acids. 2007 Feb;32(2):213-24. Epub 2006 Oct 10. [PubMed:17031479]

Obesity

1. Tuma P, Samcova E, Balinova P: Determination of 3-methylhistidine and 1-methylhistidine in untreated urine samples by capillary electrophoresis. J Chromatogr B Analyt Technol Biomed Life Sci. 2005 Jul 5;821(1):53-9. [PubMed:15899597]

Diabetes mellitus type 2

1. Tuma P, Samcova E, Balinova P: Determination of 3-methylhistidine and 1-methylhistidine in untreated urine samples by capillary electrophoresis. J Chromatogr B Analyt Technol Biomed Life Sci. 2005 Jul 5;821(1):53-9. [PubMed:15899597]

Propionic acidemia

1. Gronwald W, Klein MS, Kaspar H, Fagerer SR, Nurnberger N, Dettmer K, Bertsch T, Oefner PJ: Urinary metabolite quantification employing 2D NMR spectroscopy. Anal Chem. 2008 Dec 1;80(23):9288-97. doi: 10.1021/ac801627c. [PubMed:19551947]

Maple syrup urine disease

1. Gronwald W, Klein MS, Kaspar H, Fagerer SR, Nurnberger N, Dettmer K, Bertsch T, Oefner PJ: Urinary metabolite quantification employing 2D NMR spectroscopy. Anal Chem. 2008 Dec 1;80(23):9288-97. doi:

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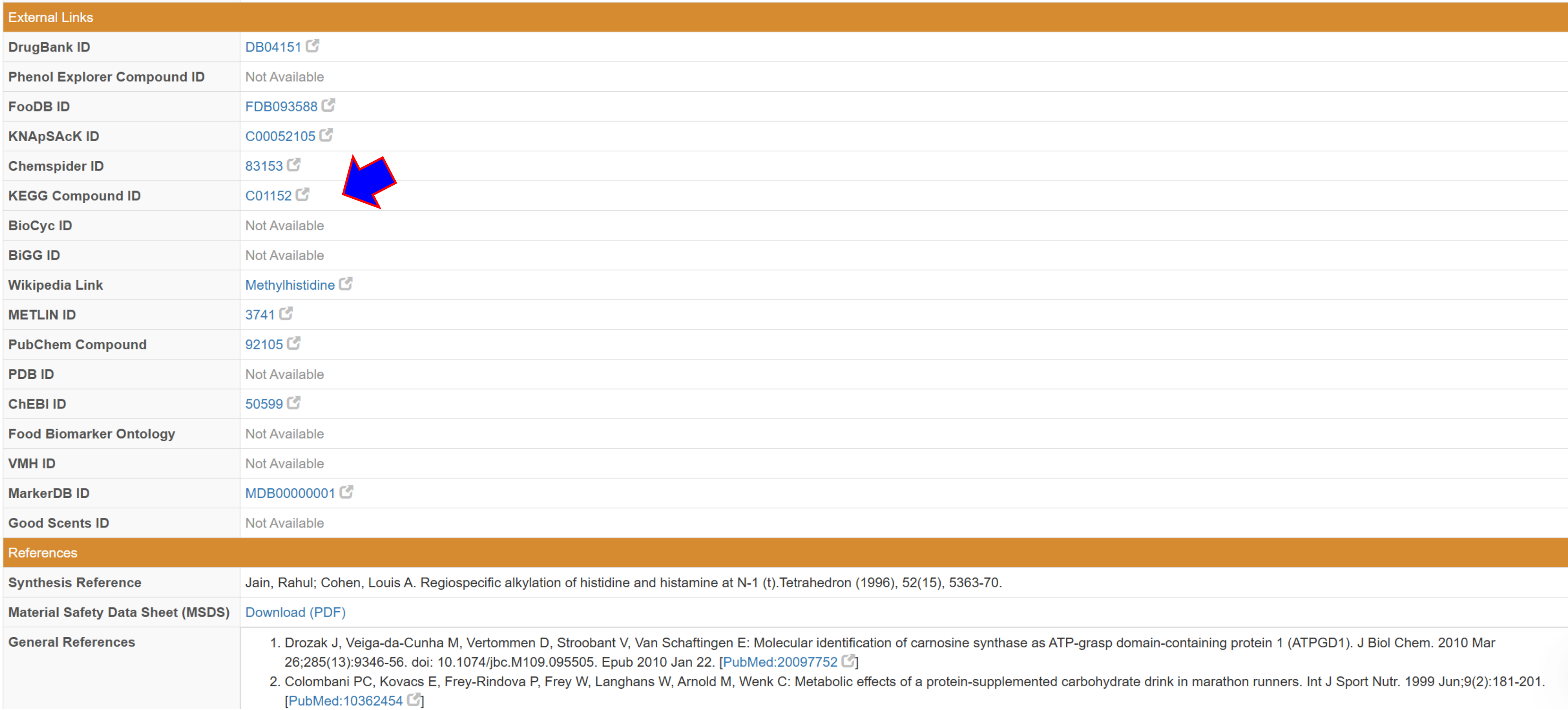

External Links	
DrugBank ID	DB04151
Phenol Explorer Compound ID	Not Available
FooDB ID	FDB093588
KNApSAcK ID	C00052105
Chemspider ID	83153
KEGG Compound ID	C01152
BioCyc ID	Not Available
BiGG ID	Not Available
Wikipedia Link	Methylhistidine
METLIN ID	3741
PubChem Compound	92105
PDB ID	Not Available
ChEBI ID	50599
Food Biomarker Ontology	Not Available
VMH ID	Not Available
MarkerDB ID	MDB00000001
Good Scents ID	Not Available
References	
Synthesis Reference	Jain, Rahul; Cohen, Louis A. Regiospecific alkylation of histidine and histamine at N-1 (t).Tetrahedron (1996), 52(15), 5363-70.
Material Safety Data Sheet (MSDS)	Download (PDF)
General References	1. Drozak J, Veiga-da-Cunha M, Vertommen D, Stroobant V, Van Schaftingen E: Molecular identification of carnosine synthase as ATP-grasp domain-containing protein 1 (ATPGD1). J Biol Chem. 2010 Mar 26;285(13):9346-56. doi: 10.1074/jbc.M109.095505. Epub 2010 Jan 22. [PubMed:20097752] 2. Colombani PC, Kovacs E, Frey-Rindova P, Frey W, Langhans W, Arnold M, Wenk C: Metabolic effects of a protein-supplemented carbohydrate drink in marathon runners. Int J Sport Nutr. 1999 Jun;9(2):181-201. [PubMed:10362454]

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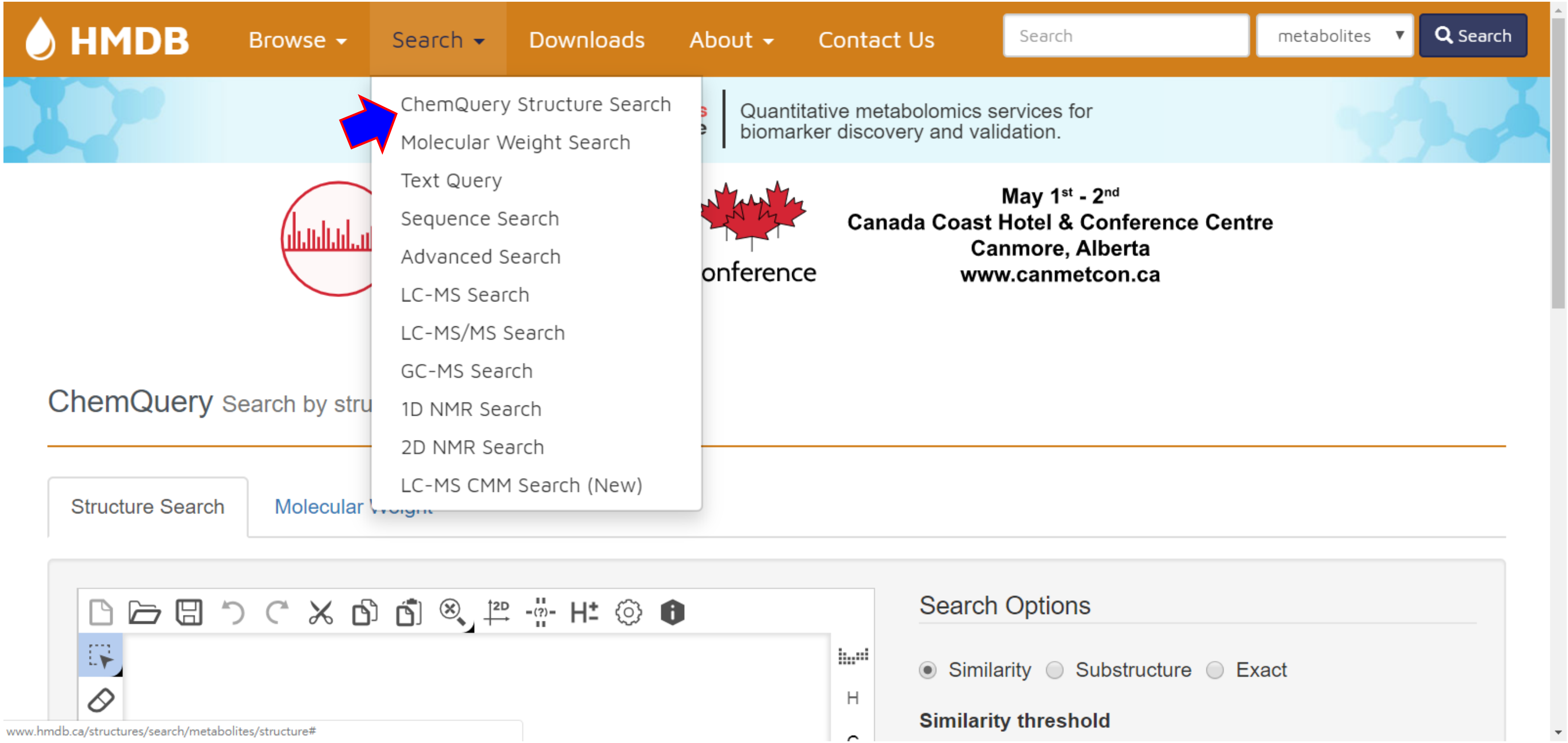

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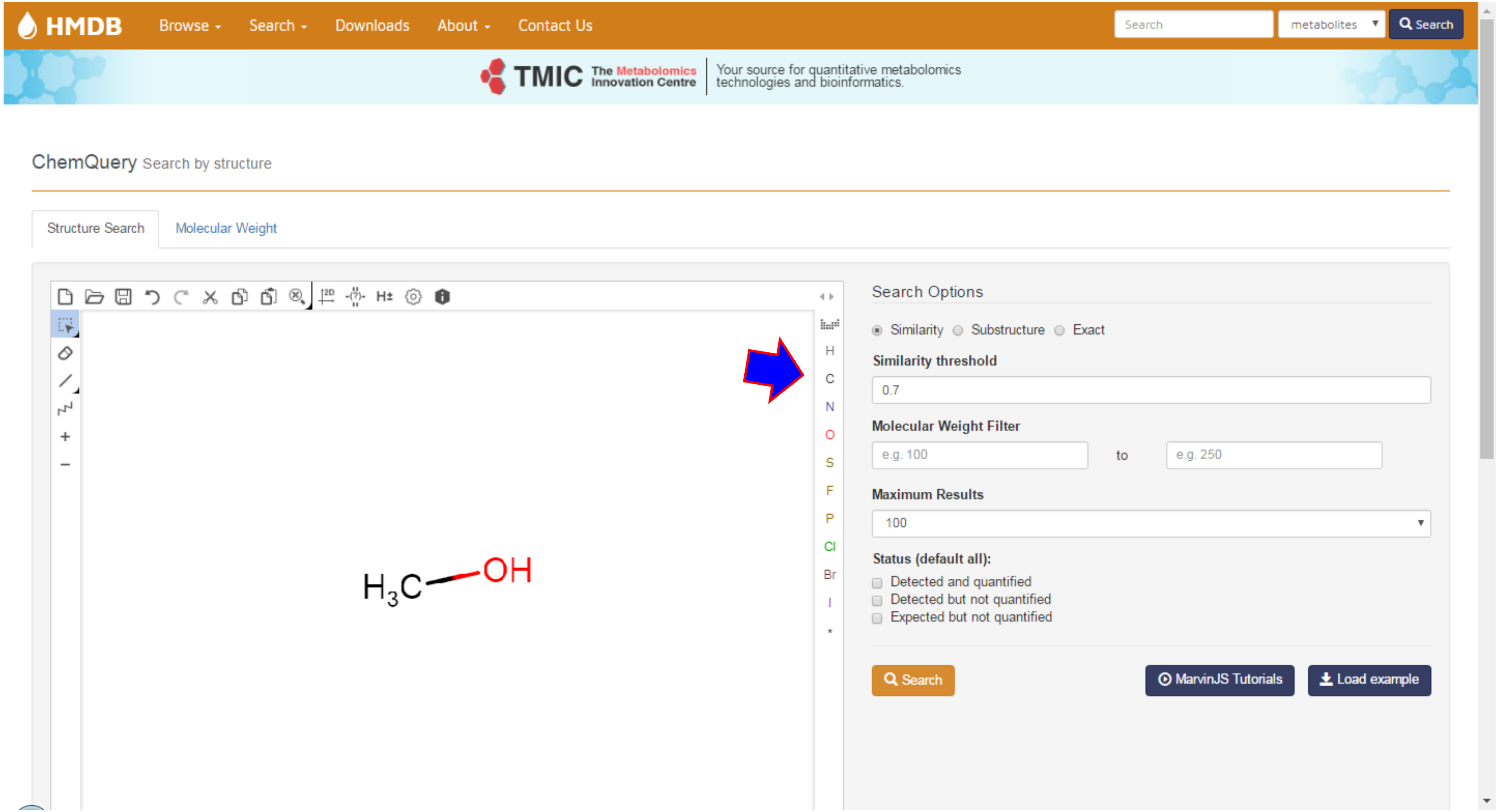
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$H_3C—OH$

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0.7

Molecular Weight Filter

e.g. 100 to e.g. 250

Maximum Results

100

Status (default all):

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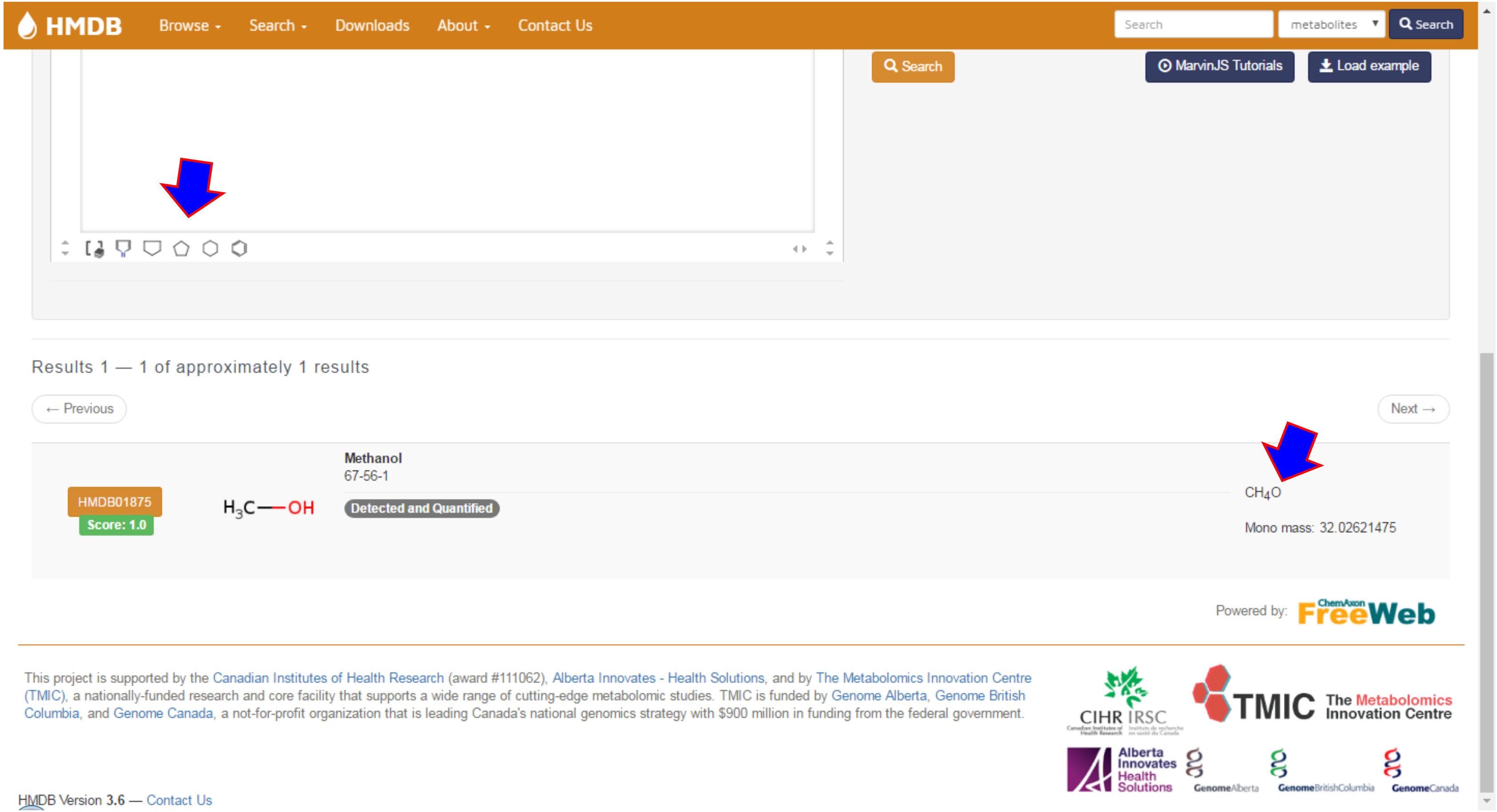
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Results 1 — 1 of approximately 1 results

Methanol
67-56-1

$H_3C—OH$

CH_4O

Mono mass: 32.02621475

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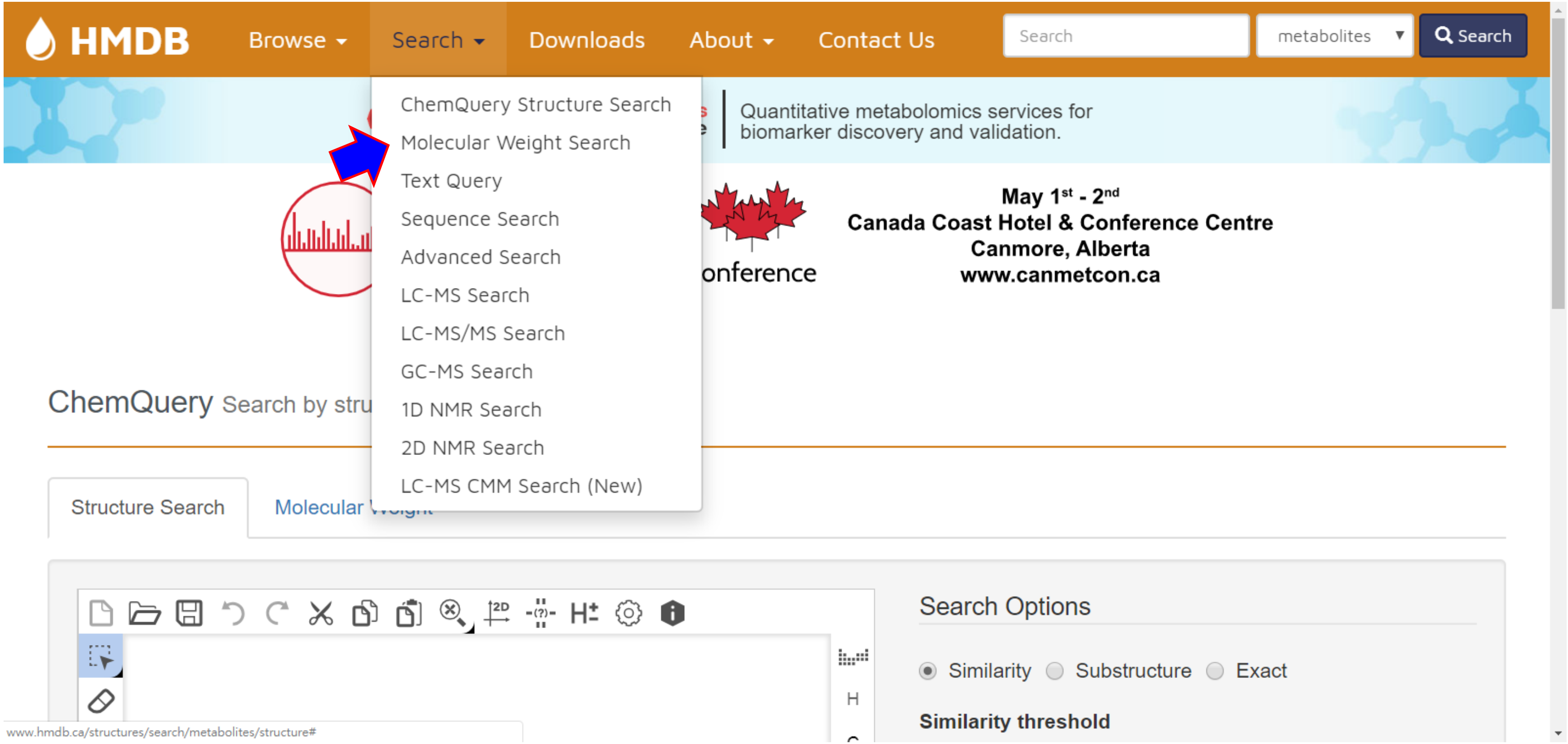

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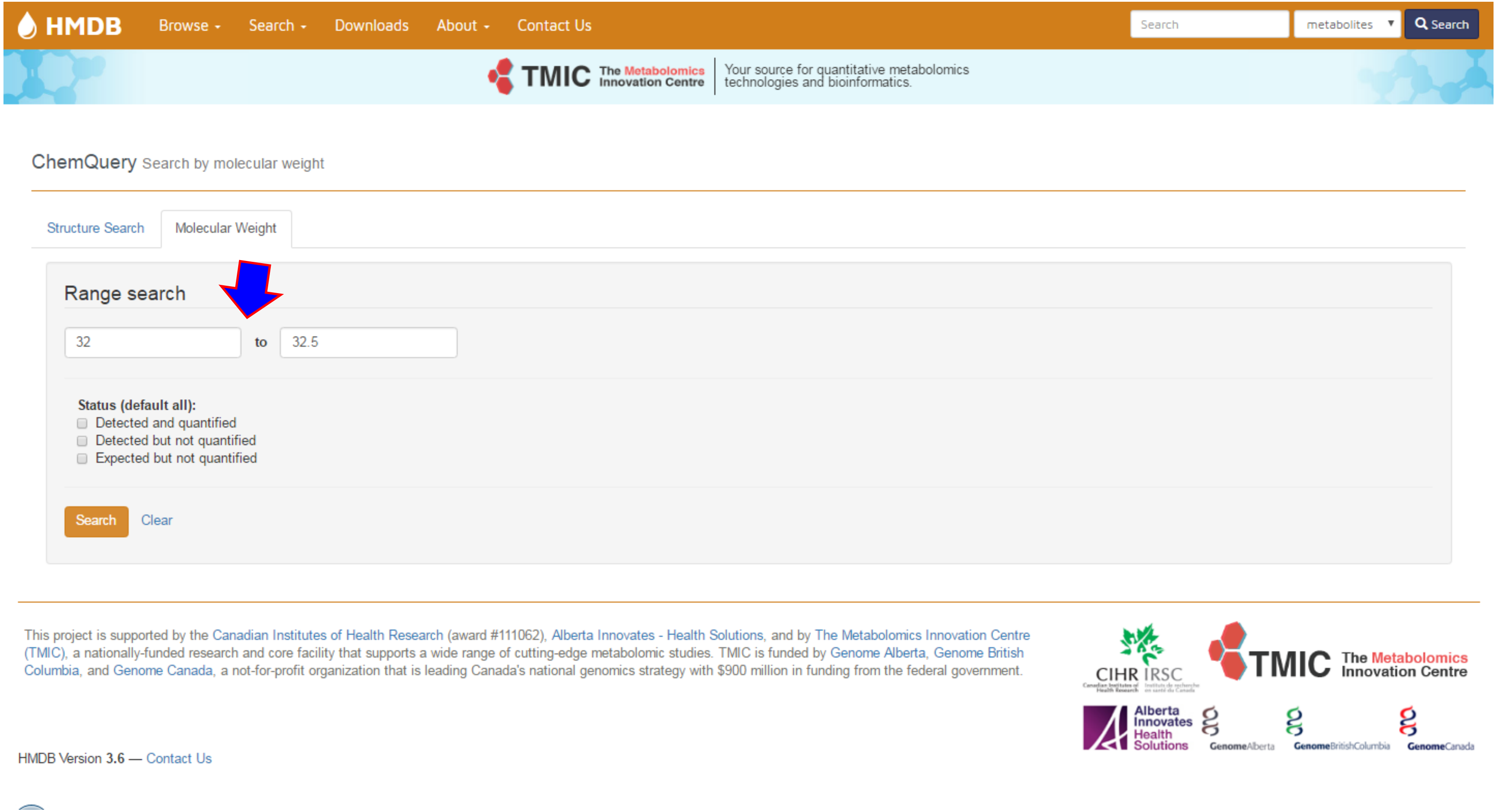
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Status (default all):
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☐ Expected but not quantified

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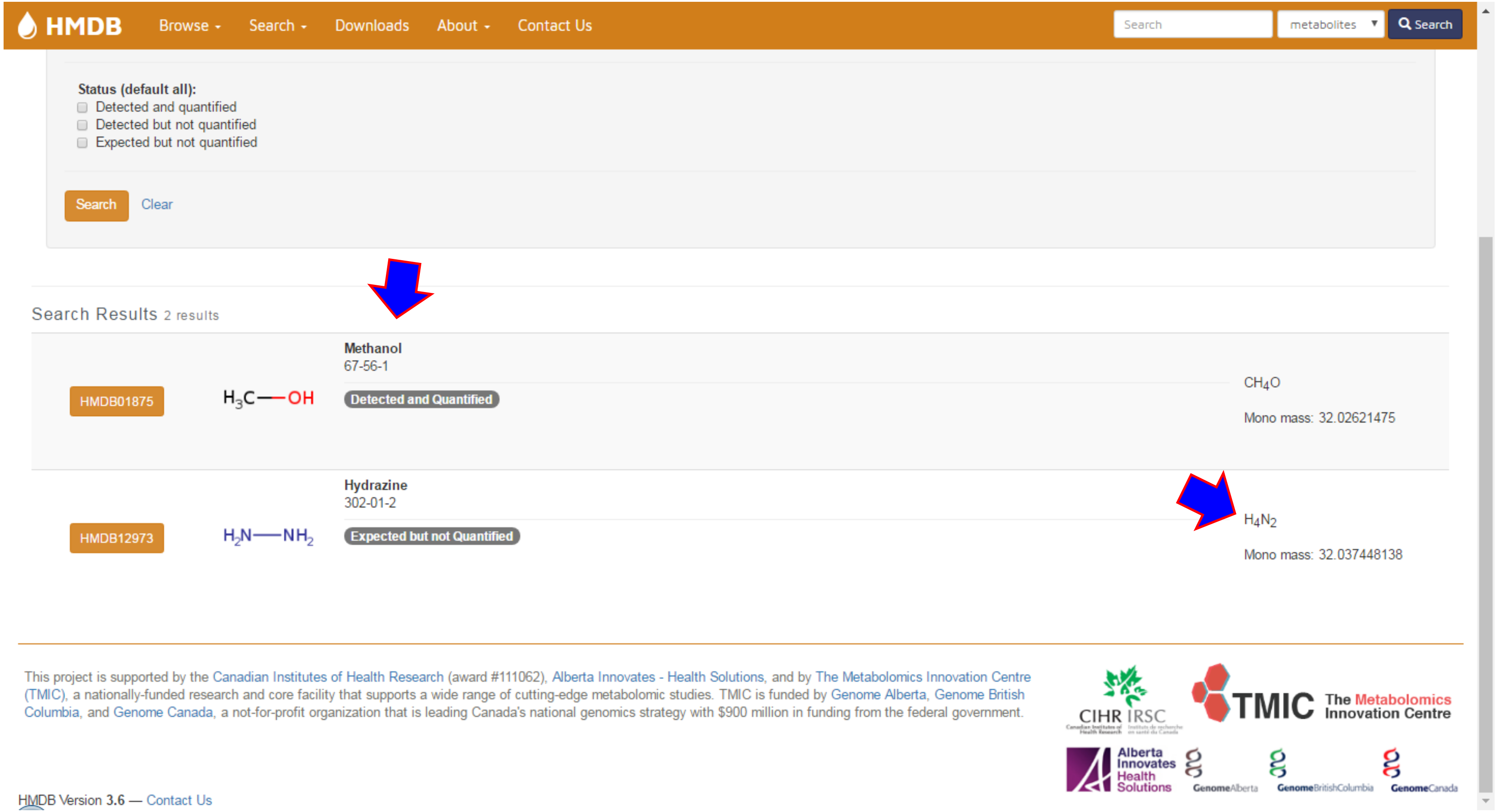

Status (default all):
☐ Detected and quantified
☐ Detected but not quantified
☐ Expected but not quantified

Search Results 2 results

HMDB01875	$H_3C—OH$	**Methanol** 67-56-1 Detected and Quantified	CH_4O Mono mass: 32.02621475
HMDB12973	$H_2N—NH_2$	**Hydrazine** 302-01-2 Expected but not Quantified	H_4N_2 Mono mass: 32.037448138

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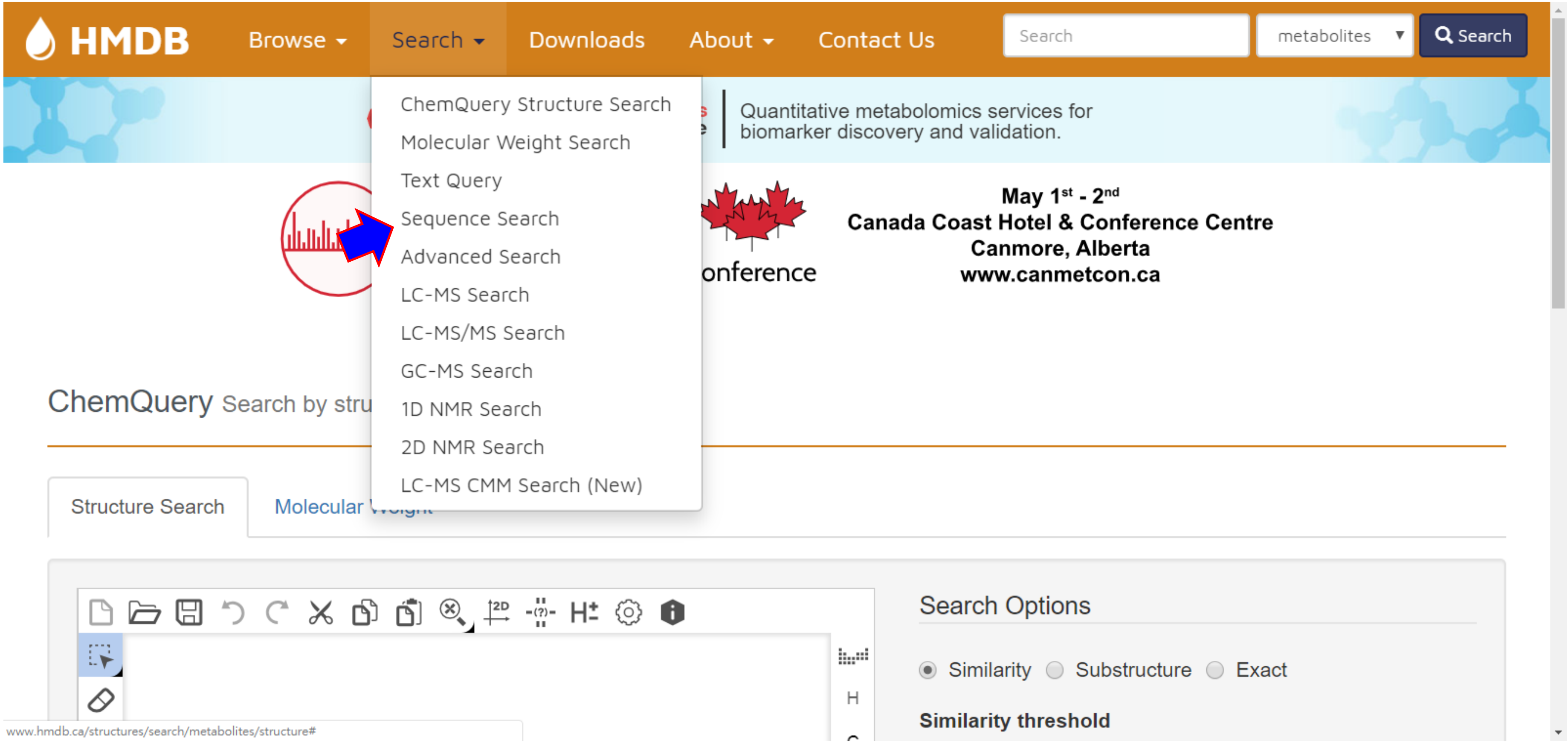
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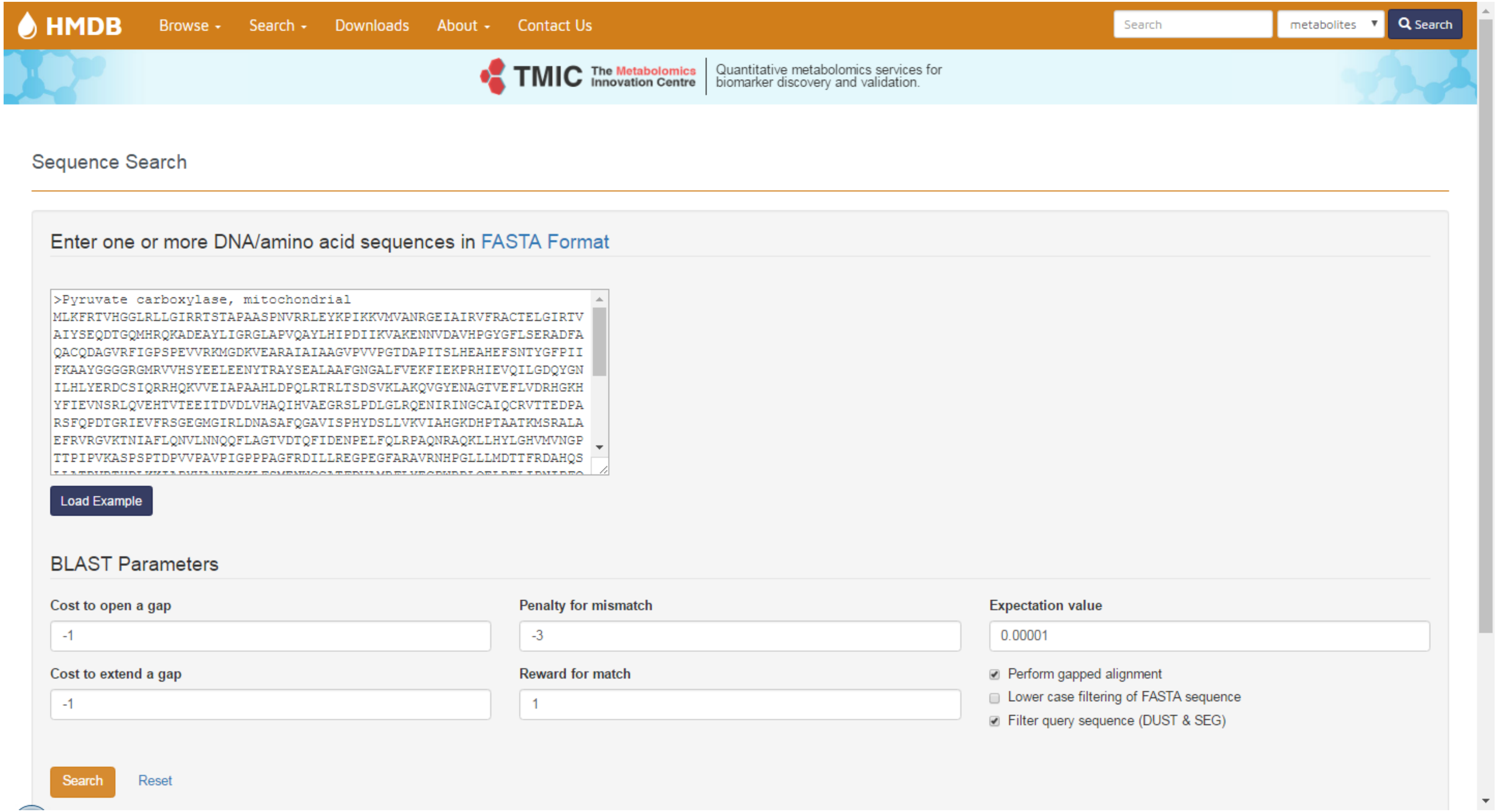
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Sequence Search

Enter one or more DNA/amino acid sequences in FASTA Format

```
>Pyruvate carboxylase, mitochondrial
MLKFRTVHGGLRLLGIRRTSTAPAASPNVRRLEYKPIKKVMVANRGEIAIRVFRACTELGIRTV
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QACQDAGVRFIGPSPEVVRKMGDKVEARAIAIAAGVPVVPGTDAPITSLHEAHEFSNTYGFPII
FKAAYGGGGRGMRVVHSYEELEENYTRAYSEALAAFGNGALFVEKFIEKPRHIEVQILGDQYGN
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YFIEVNSRLQVEHTVTEEITDVDLVHAQIHVAEGRSLPDLGLRQENIRINGCAIQCRVTTEDPA
RSFQPDTGRIEVFRSGEGMGIRLDNASAFQGAVISPHYDSLLVKVIAHGKDHPTAATKMSRALA
EFRVRGVKTNIAFLQNVLNNQQFLAGTVDTQFIDENPELFQLRPAQNRAQKLLHYLGHVMVNGP
TTPIPVKASPSPTDPVVPAVPIGPPPAGFRDILLREGPEGFARAVRNHPGLLLMDTTFRDAHQS
```

Load Example

BLAST Parameters

Cost to open a gap: -1

Penalty for mismatch: -3

Expectation value: 0.00001

Cost to extend a gap: -1

Reward for match: 1

☑ Perform gapped alignment
☐ Lower case filtering of FASTA sequence
☑ Filter query sequence (DUST & SEG)

Search
Reset

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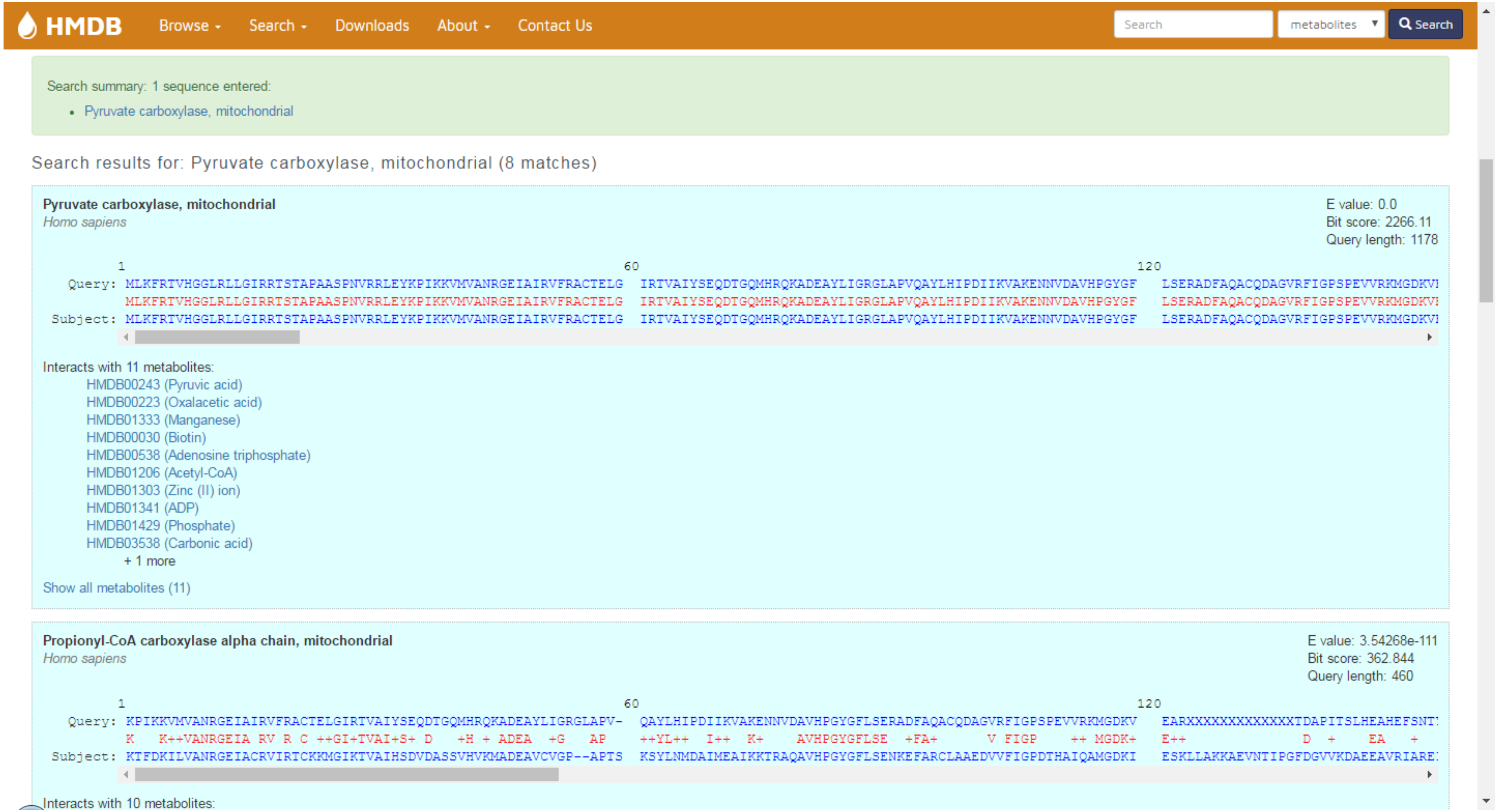

Search summary: 1 sequence entered:

- Pyruvate carboxylase, mitochondrial

Search results for: Pyruvate carboxylase, mitochondrial (8 matches)

Pyruvate carboxylase, mitochondrial
Homo sapiens

E value: 0.0
Bit score: 2266.11
Query length: 1178

```
           1                                                           60                                                          120
   Query:  MLKFRTVHGGLRLLGIRRTSTAPAASPNVRRLEYKPIKKVMVANRGEIAIRVFRACTELG  IRTVAIYSEQDTGQMHRQKADEAYLIGRGLAPVQAYLHIPDIIKVAKENNVDAVHPGYGF  LSERADFAQACQDAGVRFIGPSPEVVRKMGDKV
           MLKFRTVHGGLRLLGIRRTSTAPAASPNVRRLEYKPIKKVMVANRGEIAIRVFRACTELG  IRTVAIYSEQDTGQMHRQKADEAYLIGRGLAPVQAYLHIPDIIKVAKENNVDAVHPGYGF  LSERADFAQACQDAGVRFIGPSPEVVRKMGDKV
 Subject:  MLKFRTVHGGLRLLGIRRTSTAPAASPNVRRLEYKPIKKVMVANRGEIAIRVFRACTELG  IRTVAIYSEQDTGQMHRQKADEAYLIGRGLAPVQAYLHIPDIIKVAKENNVDAVHPGYGF  LSERADFAQACQDAGVRFIGPSPEVVRKMGDKV
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Interacts with 11 metabolites:
HMDB00243 (Pyruvic acid)
HMDB00223 (Oxalacetic acid)
HMDB01333 (Manganese)
HMDB00030 (Biotin)
HMDB00538 (Adenosine triphosphate)
HMDB01206 (Acetyl-CoA)
HMDB01303 (Zinc (II) ion)
HMDB01341 (ADP)
HMDB01429 (Phosphate)
HMDB03538 (Carbonic acid)
+ 1 more

Show all metabolites (11)

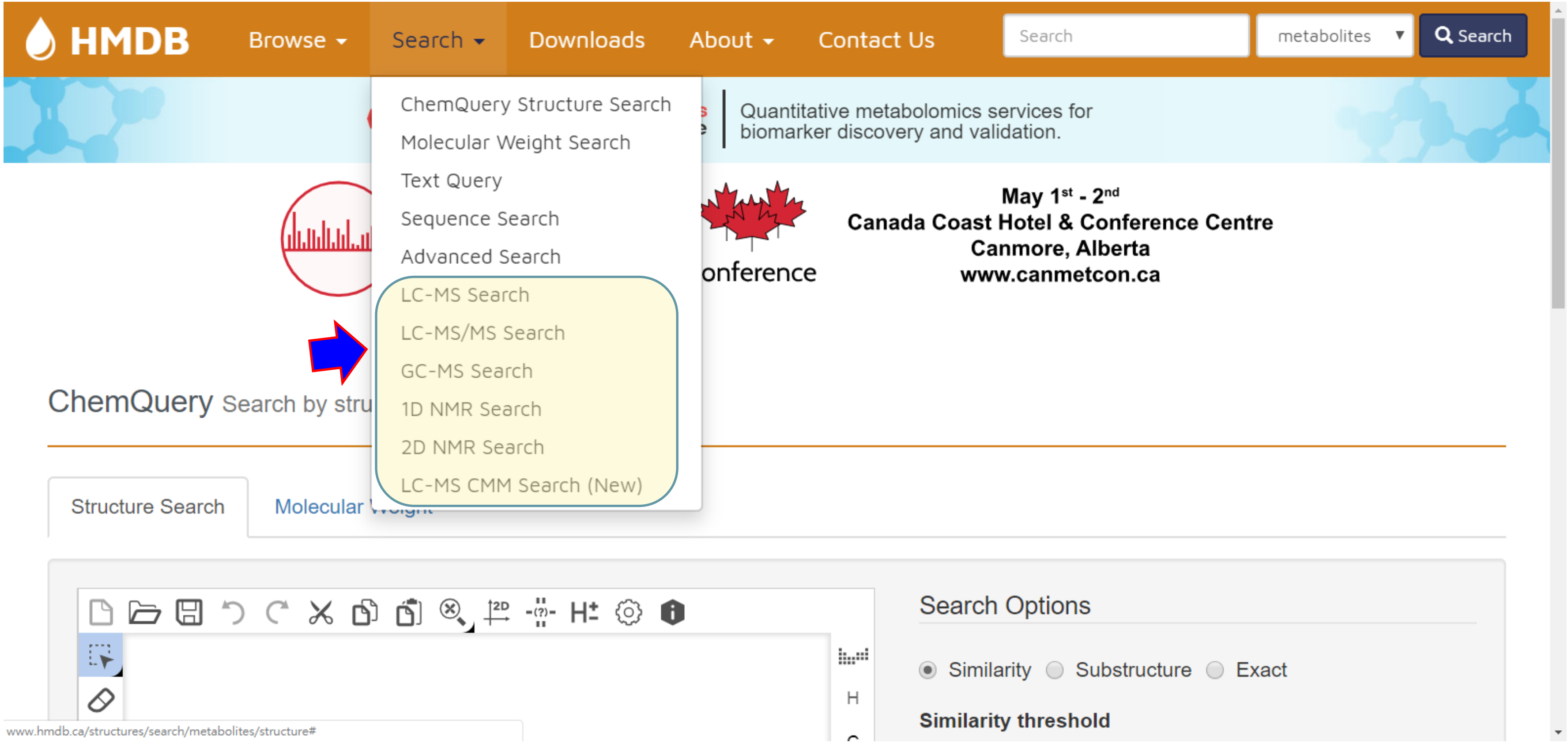
Propionyl-CoA carboxylase alpha chain, mitochondrial
Homo sapiens

E value: 3.54268e-111
Bit score: 362.844
Query length: 460

```
           1                                                           60                                                          120
   Query:  KPIKKVMVANRGEIAIRVFRACTELGIRTVAIYSEQDTGQMHRQKADEAYLIGRGLAPV-  QAYLHIPDIIKVAKENNVDAVHPGYGFLSERADFAQACQDAGVRFIGPSPEVVRKMGDKV  EARXXXXXXXXXXXXXTDAPITSLHEAHEFSNT
           K   K++VANRGEIA RV R C ++GI+TVAI+S+ D   +H + ADEA  +G   AP    ++YL++  I++  K+    AVHPGYGFLSE  +FA+      V FIGP    ++ MGDK+  E++              D  +    EA   +
 Subject:  KTFDKILVANRGEIACRVIRTCKKMGIKTVAIHSDVDASSVHVKMADEAVCVGP--APTS  KSYLNMDAIMEAIKKTRAQAVHPGYGFLSENKEFARCLAAEDVVFIGPDTHAIQAMGDKI  ESKLLAKKAEVNTIPGFDGVVKDAEEAVRIARE
```

Interacts with 10 metabolites:

HMDB


HMDB
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ChemQuery Structure Search
Molecular Weight Search
Text Query
Sequence Search
Advanced Search
LC-MS Search
LC-MS/MS Search
GC-MS Search
1D NMR Search
2D NMR Search
LC-MS CMM Search (New)
Structure Search
Molecular Weight
Search Options
Similarity
Substructure
Exact
Similarity threshold
H

Quantitative metabolomics services for biomarker discovery and validation.

onference

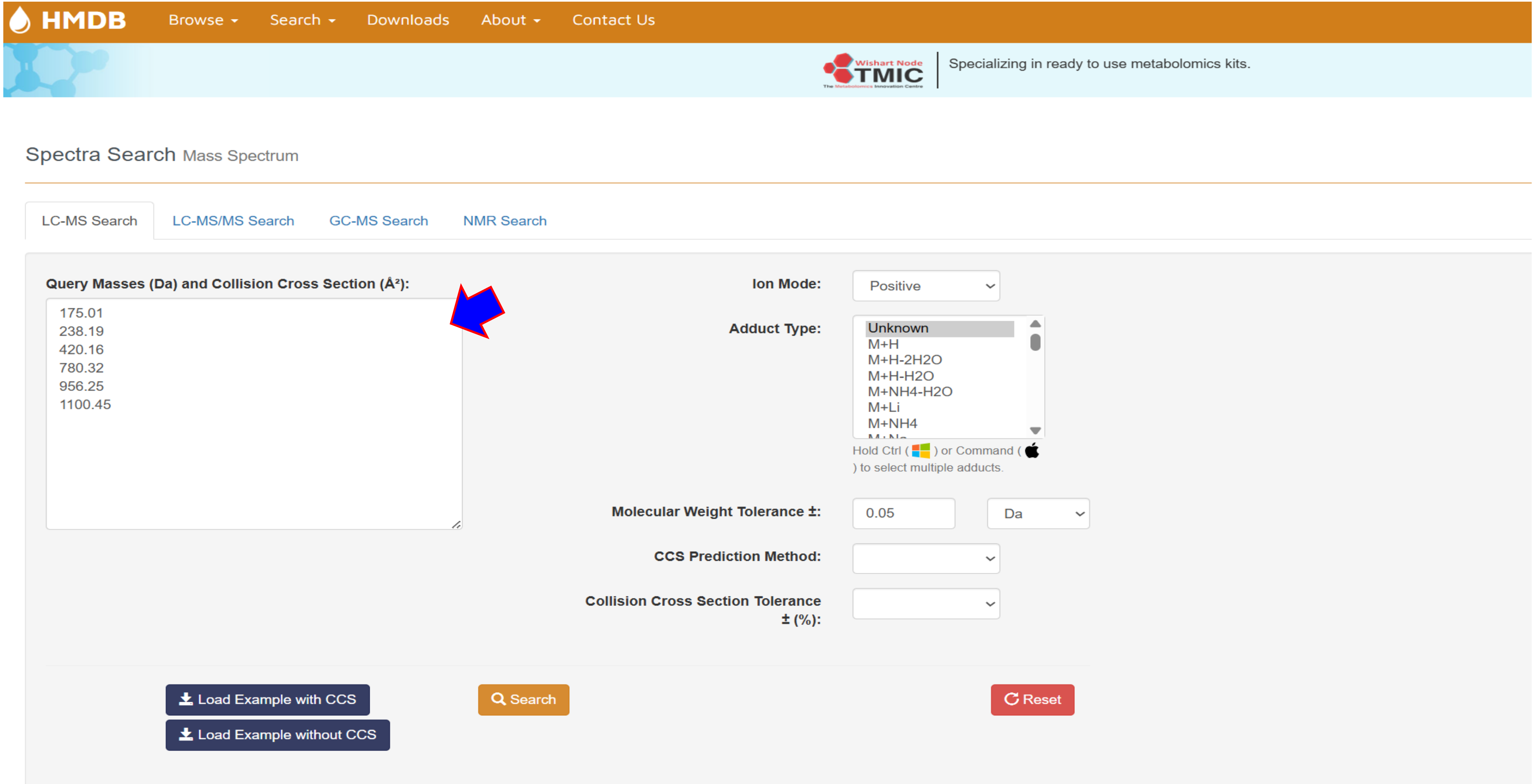
May 1st - 2nd
Canada Coast Hotel & Conference Centre
Canmore, Alberta
www.canmetcon.ca

ChemQuery Search by stru

○ Similarity ○ Substructure ○ Exact

www.hmdb.ca/structures/search/metabolites/structure#

HMDB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The Metabolomics Innovation Centre

Specializing in ready to use metabolomics kits.

Spectra Search Mass Spectrum

LC-MS Search | LC-MS/MS Search | GC-MS Search | NMR Search

Query Masses (Da) and Collision Cross Section (Å²):

175.01
238.19
420.16
780.32
956.25
1100.45

Ion Mode: Positive

Adduct Type: Unknown, M+H, M+H-2H2O, M+H-H2O, M+NH4-H2O, M+Li, M+NH4

Hold Ctrl ( ) or Command ( ) to select multiple adducts.

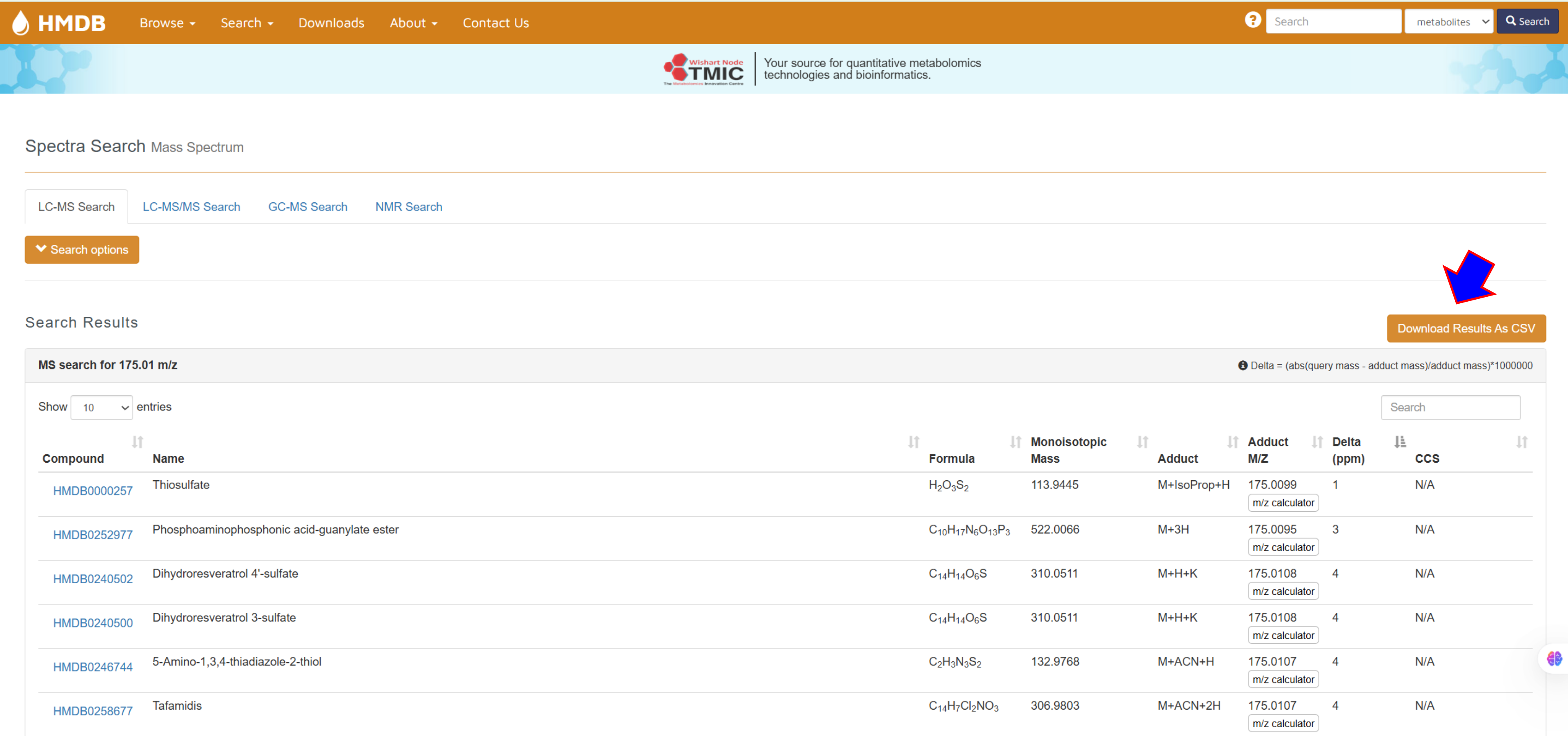
Molecular Weight Tolerance ±: 0.05 Da

CCS Prediction Method:

Collision Cross Section Tolerance ± (%):

Load Example with CCS
Load Example without CCS
Search
Reset

HMDB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Your source for quantitative metabolomics technologies and bioinformatics.

Spectra Search Mass Spectrum

LC-MS Search
LC-MS/MS Search
GC-MS Search
NMR Search
Search options

Search Results

Download Results As CSV

MS search for 175.01 m/z

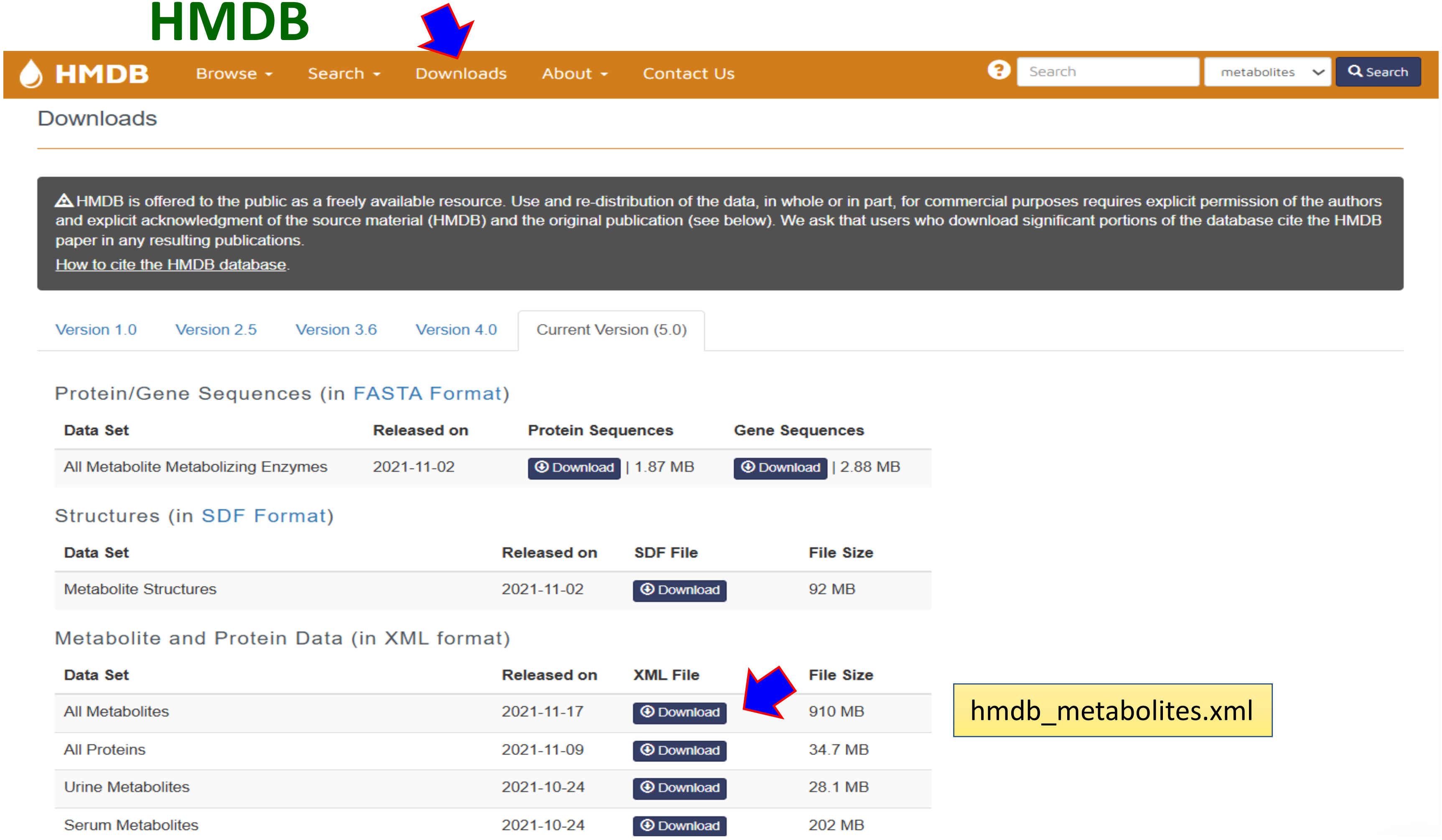
Delta = (abs(query mass - adduct mass)/adduct mass)*1000000

Show 10 entries

Search

Compound	Name	Formula	Monoisotopic Mass	Adduct	Adduct M/Z	Delta (ppm)	CCS
HMDB0000257	Thiosulfate	$H_2O_3S_2$	113.9445	M+IsoProp+H	175.0099 m/z calculator	1	N/A
HMDB0252977	Phosphoaminophosphonic acid-guanylate ester	$C_{10}H_{17}N_6O_{13}P_3$	522.0066	M+3H	175.0095 m/z calculator	3	N/A
HMDB0240502	Dihydroresveratrol 4'-sulfate	$C_{14}H_{14}O_6S$	310.0511	M+H+K	175.0108 m/z calculator	4	N/A
HMDB0240500	Dihydroresveratrol 3-sulfate	$C_{14}H_{14}O_6S$	310.0511	M+H+K	175.0108 m/z calculator	4	N/A
HMDB0246744	5-Amino-1,3,4-thiadiazole-2-thiol	$C_2H_3N_3S_2$	132.9768	M+ACN+H	175.0107 m/z calculator	4	N/A
HMDB0258677	Tafamidis	$C_{14}H_7Cl_2NO_3$	306.9803	M+ACN+2H	175.0107 m/z calculator	4	N/A

HMDB



Downloads

⚠ HMDB is offered to the public as a freely available resource. Use and re-distribution of the data, in whole or in part, for commercial purposes requires explicit permission of the authors and explicit acknowledgment of the source material (HMDB) and the original publication (see below). We ask that users who download significant portions of the database cite the HMDB paper in any resulting publications.

How to cite the HMDB database.

Version 1.0 | Version 2.5 | Version 3.6 | Version 4.0 | Current Version (5.0)

Protein/Gene Sequences (in FASTA Format)

Data Set	Released on	Protein Sequences	Gene Sequences
All Metabolite Metabolizing Enzymes	2021-11-02	Download | 1.87 MB	Download | 2.88 MB

Structures (in SDF Format)

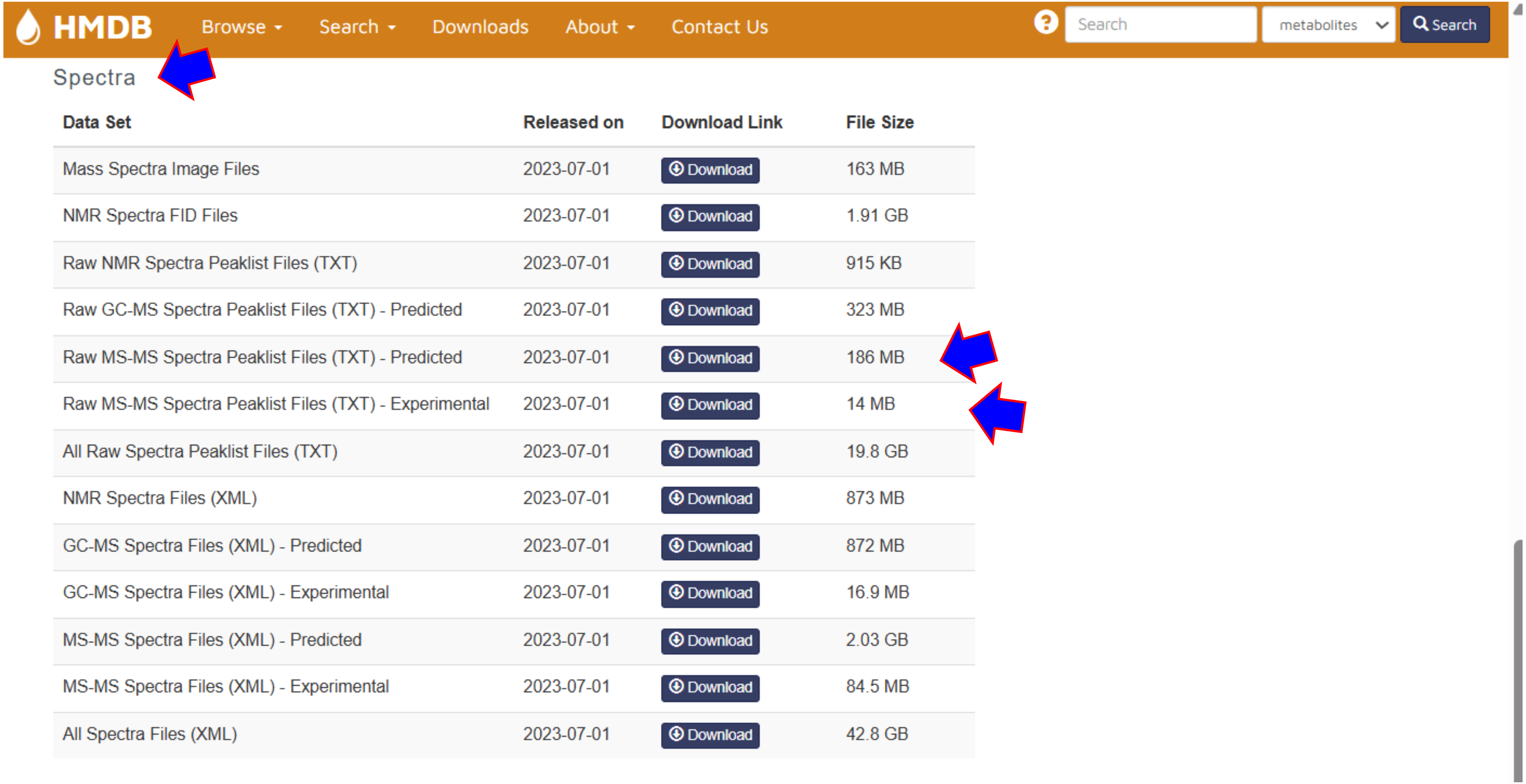
Data Set	Released on	SDF File	File Size
Metabolite Structures	2021-11-02	Download	92 MB

Metabolite and Protein Data (in XML format)

Data Set	Released on	XML File	File Size
All Metabolites	2021-11-17	Download	910 MB
All Proteins	2021-11-09	Download	34.7 MB
Urine Metabolites	2021-10-24	Download	28.1 MB
Serum Metabolites	2021-10-24	Download	202 MB

hmdb_metabolites.xml

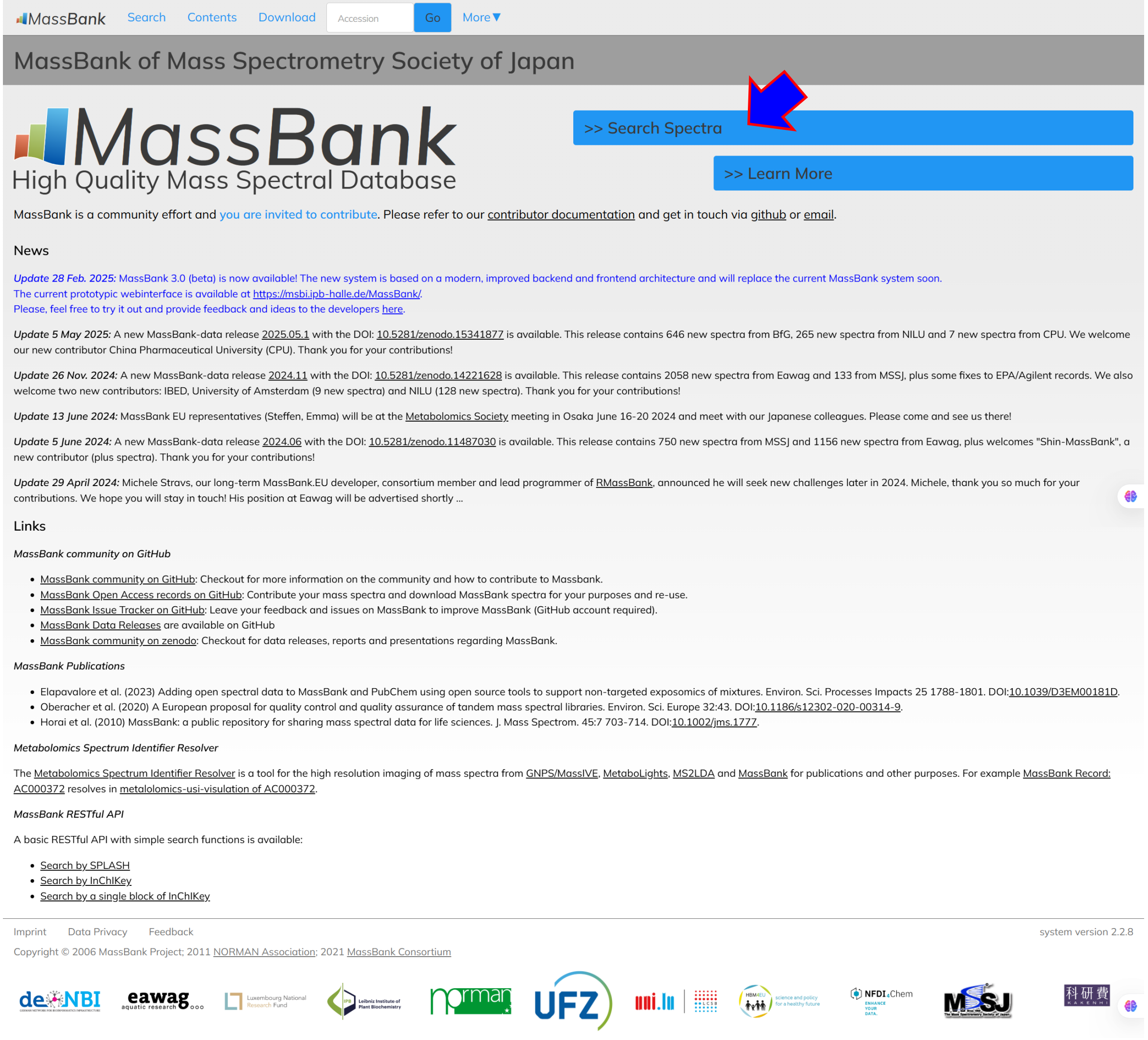
HMDB



Spectra

Data Set	Released on	Download Link	File Size
Mass Spectra Image Files	2023-07-01	Download	163 MB
NMR Spectra FID Files	2023-07-01	Download	1.91 GB
Raw NMR Spectra Peaklist Files (TXT)	2023-07-01	Download	915 KB
Raw GC-MS Spectra Peaklist Files (TXT) - Predicted	2023-07-01	Download	323 MB
Raw MS-MS Spectra Peaklist Files (TXT) - Predicted	2023-07-01	Download	186 MB
Raw MS-MS Spectra Peaklist Files (TXT) - Experimental	2023-07-01	Download	14 MB
All Raw Spectra Peaklist Files (TXT)	2023-07-01	Download	19.8 GB
NMR Spectra Files (XML)	2023-07-01	Download	873 MB
GC-MS Spectra Files (XML) - Predicted	2023-07-01	Download	872 MB
GC-MS Spectra Files (XML) - Experimental	2023-07-01	Download	16.9 MB
MS-MS Spectra Files (XML) - Predicted	2023-07-01	Download	2.03 GB
MS-MS Spectra Files (XML) - Experimental	2023-07-01	Download	84.5 MB
All Spectra Files (XML)	2023-07-01	Download	42.8 GB

MassBank



MassBank of Mass Spectrometry Society of Japan

MassBank
High Quality Mass Spectral Database

MassBank is a community effort and you are invited to contribute. Please refer to our contributor documentation and get in touch via github or email.

News

Update 28 Feb. 2025: MassBank 3.0 (beta) is now available! The new system is based on a modern, improved backend and frontend architecture and will replace the current MassBank system soon.
The current prototypic webinterface is available at https://msbi.ipb-halle.de/MassBank/.
Please, feel free to try it out and provide feedback and ideas to the developers here.

Update 5 May 2025: A new MassBank-data release 2025.05.1 with the DOI: 10.5281/zenodo.15341877 is available. This release contains 646 new spectra from BfG, 265 new spectra from NILU and 7 new spectra from CPU. We welcome our new contributor China Pharmaceutical University (CPU). Thank you for your contributions!

Update 26 Nov. 2024: A new MassBank-data release 2024.11 with the DOI: 10.5281/zenodo.14221628 is available. This release contains 2058 new spectra from Eawag and 133 from MSSJ, plus some fixes to EPA/Agilent records. We also welcome two new contributors: IBED, University of Amsterdam (9 new spectra) and NILU (128 new spectra). Thank you for your contributions!

Update 13 June 2024: MassBank EU representatives (Steffen, Emma) will be at the Metabolomics Society meeting in Osaka June 16-20 2024 and meet with our Japanese colleagues. Please come and see us there!

Update 5 June 2024: A new MassBank-data release 2024.06 with the DOI: 10.5281/zenodo.11487030 is available. This release contains 750 new spectra from MSSJ and 1156 new spectra from Eawag, plus welcomes "Shin-MassBank", a new contributor (plus spectra). Thank you for your contributions!

Update 29 April 2024: Michele Stravs, our long-term MassBank.EU developer, consortium member and lead programmer of RMassBank, announced he will seek new challenges later in 2024. Michele, thank you so much for your contributions. We hope you will stay in touch! His position at Eawag will be advertised shortly ...

Links

MassBank community on GitHub

- MassBank community on GitHub: Checkout for more information on the community and how to contribute to Massbank.
- MassBank Open Access records on GitHub: Contribute your mass spectra and download MassBank spectra for your purposes and re-use.
- MassBank Issue Tracker on GitHub: Leave your feedback and issues on MassBank to improve MassBank (GitHub account required).
- MassBank Data Releases are available on GitHub
- MassBank community on zenodo: Checkout for data releases, reports and presentations regarding MassBank.

MassBank Publications

- Elapavalore et al. (2023) Adding open spectral data to MassBank and PubChem using open source tools to support non-targeted exposomics of mixtures. Environ. Sci. Processes Impacts 25 1788-1801. DOI:10.1039/D3EM00181D.
- Oberacher et al. (2020) A European proposal for quality control and quality assurance of tandem mass spectral libraries. Environ. Sci. Europe 32:43. DOI:10.1186/s12302-020-00314-9.
- Horai et al. (2010) MassBank: a public repository for sharing mass spectral data for life sciences. J. Mass Spectrom. 45:7 703-714. DOI:10.1002/jms.1777.

Metabolomics Spectrum Identifier Resolver

The Metabolomics Spectrum Identifier Resolver is a tool for the high resolution imaging of mass spectra from GNPS/MassIVE, MetaboLights, MS2LDA and MassBank for publications and other purposes. For example MassBank Record: AC000372 resolves in metalolomics-usi-visulation of AC000372.

MassBank RESTful API

A basic RESTful API with simple search functions is available:

- Search by SPLASH
- Search by InChIKey
- Search by a single block of InChIKey

Imprint Data Privacy Feedback system version 2.2.8

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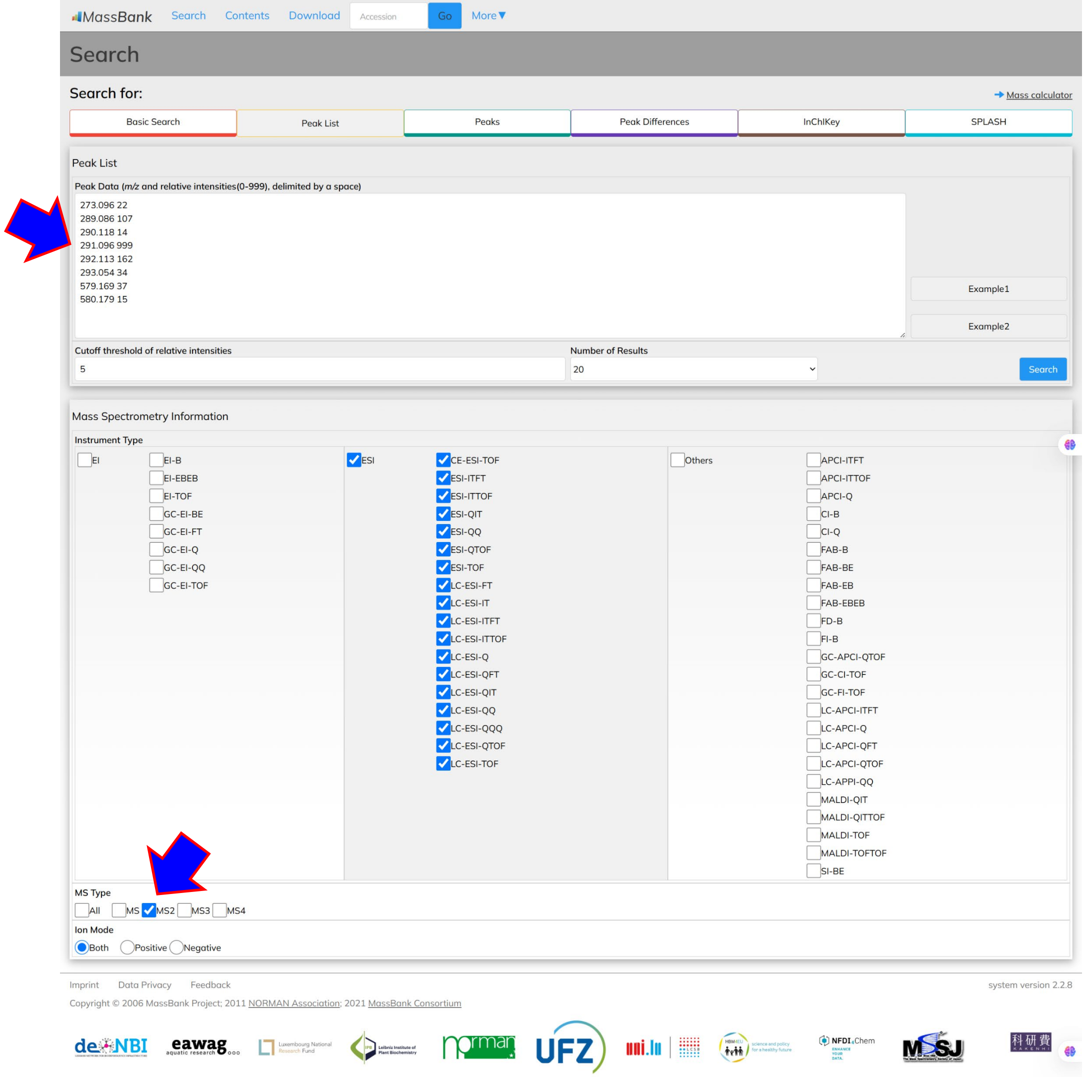
MassBank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Contents
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Accession
Go
More ▾
Search
Mass calculator
Basic Search
Peak List
Peaks
Peak Differences
InChIKey
SPLASH
Example1
Example2
Search
Imprint
Data Privacy
Feedback
system version 2.2.8

Search for:

Peak List

Peak Data (*m/z* and relative intensities(0-999), delimited by a space)

```
273.096 22
289.086 107
290.118 14
291.096 999
292.113 162
293.054 34
579.169 37
580.179 15
```

Cutoff threshold of relative intensities: 5

Number of Results: 20

Mass Spectrometry Information

Instrument Type

☐ EI
- ☐ EI-B
- ☐ EI-EBEB
- ☐ EI-TOF
- ☐ GC-EI-BE
- ☐ GC-EI-FT
- ☐ GC-EI-Q
- ☐ GC-EI-QQ
- ☐ GC-EI-TOF

☑ ESI
- ☑ CE-ESI-TOF
- ☑ ESI-ITFT
- ☑ ESI-ITTOF
- ☑ ESI-QIT
- ☑ ESI-QQ
- ☑ ESI-QTOF
- ☑ ESI-TOF
- ☑ LC-ESI-FT
- ☑ LC-ESI-IT
- ☑ LC-ESI-ITFT
- ☑ LC-ESI-ITTOF
- ☑ LC-ESI-Q
- ☑ LC-ESI-QFT
- ☑ LC-ESI-QIT
- ☑ LC-ESI-QQ
- ☑ LC-ESI-QQQ
- ☑ LC-ESI-QTOF
- ☑ LC-ESI-TOF

☐ Others
- ☐ APCI-ITFT
- ☐ APCI-ITTOF
- ☐ APCI-Q
- ☐ CI-B
- ☐ CI-Q
- ☐ FAB-B
- ☐ FAB-BE
- ☐ FAB-EB
- ☐ FAB-EBEB
- ☐ FD-B
- ☐ FI-B
- ☐ GC-APCI-QTOF
- ☐ GC-CI-TOF
- ☐ GC-FI-TOF
- ☐ LC-APCI-ITFT
- ☐ LC-APCI-Q
- ☐ LC-APCI-QFT
- ☐ LC-APCI-QTOF
- ☐ LC-APPI-QQ
- ☐ MALDI-QIT
- ☐ MALDI-QITTOF
- ☐ MALDI-TOF
- ☐ MALDI-TOFTOF
- ☐ SI-BE

MS Type

☐ All ☐ MS ☑ MS2 ☐ MS3 ☐ MS4

Ion Mode

● Both ○ Positive ○ Negative

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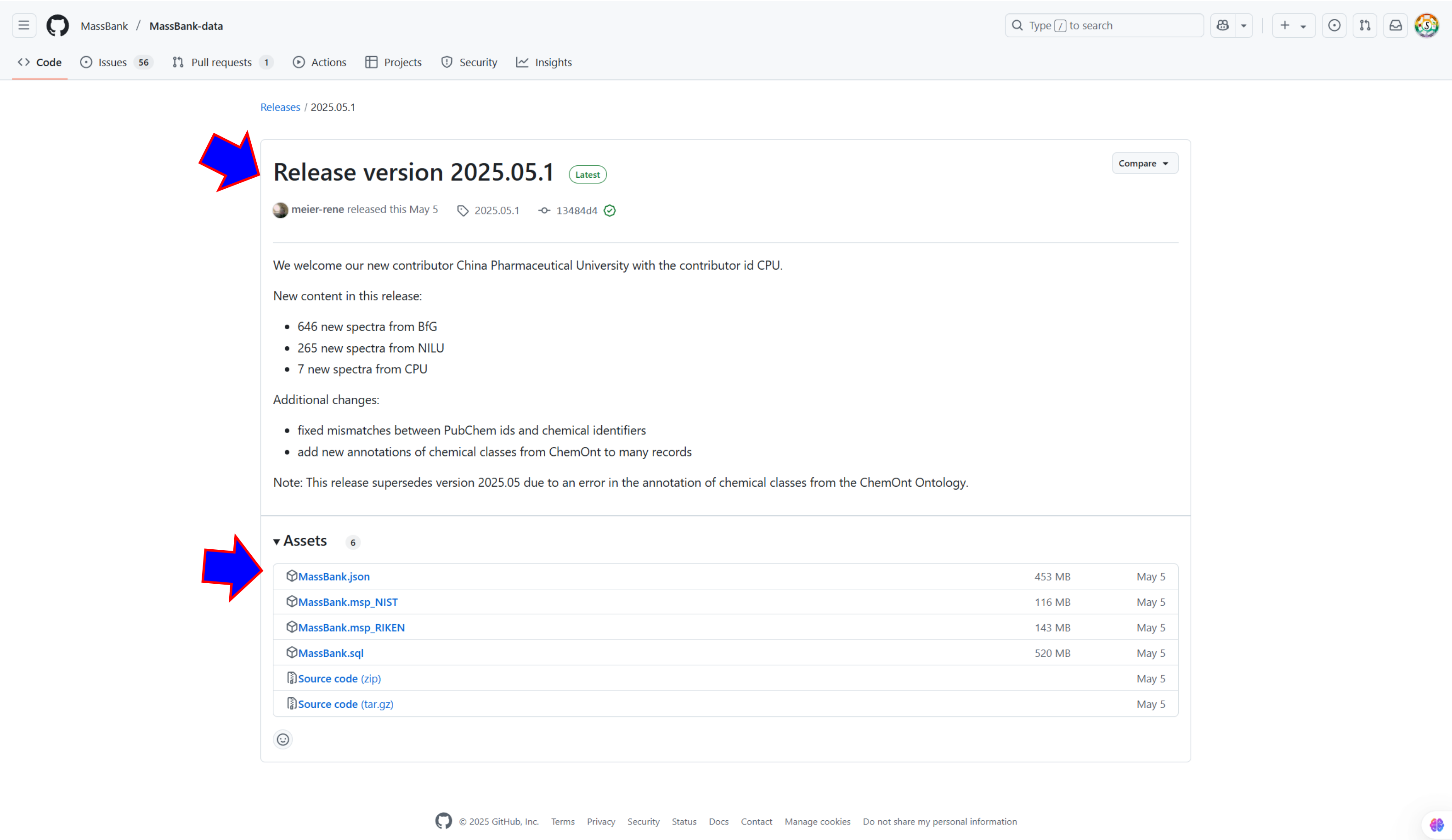
MassBank


MassBank / MassBank-data
Type / to search
Code
Issues 56
Pull requests 1
Actions
Projects
Security
Insights
Compare
Latest

Releases / 2025.05.1

Release version 2025.05.1

meier-rene released this May 5 2025.05.1 13484d4

We welcome our new contributor China Pharmaceutical University with the contributor id CPU.

New content in this release:

- 646 new spectra from BfG
- 265 new spectra from NILU
- 7 new spectra from CPU

Additional changes:

- fixed mismatches between PubChem ids and chemical identifiers
- add new annotations of chemical classes from ChemOnt to many records

Note: This release supersedes version 2025.05 due to an error in the annotation of chemical classes from the ChemOnt Ontology.

Assets 6

MassBank.json	453 MB	May 5
MassBank.msp_NIST	116 MB	May 5
MassBank.msp_RIKEN	143 MB	May 5
MassBank.sql	520 MB	May 5
Source code (zip)		May 5
Source code (tar.gz)		May 5

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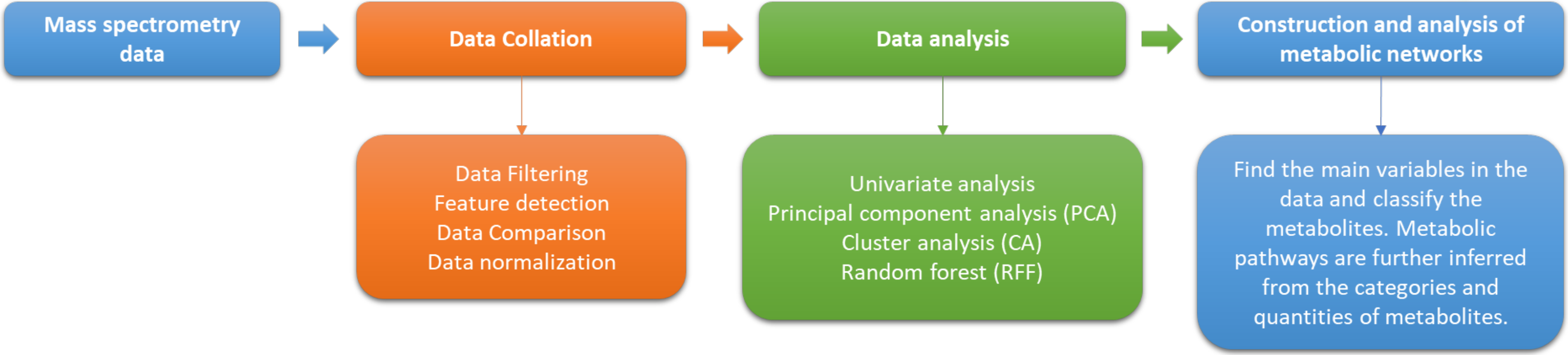
04

資料分析平台

(Analysis)

Metabolomics Workflow



Mass spectrometry data

Data Collation

Data Filtering
Feature detection
Data Comparison
Data normalization

Data analysis

Univariate analysis
Principal component analysis (PCA)
Cluster analysis (CA)
Random forest (RFF)

Construction and analysis of metabolic networks

Find the main variables in the data and classify the metabolites. Metabolic pathways are further inferred from the categories and quantities of metabolites.

https://metabolomics.creative-proteomics.com/metabolomics-data-analysis.htm

商用 / 收費軟體（Commercial / Licensed）

軟體名稱	類型	核心功能	適用說明
Compound Discoverer (Thermo)	商業全流程分析平台	Data processing, compound ID, pathway analysis	配合 Thermo LC-MS 系統，用於藥物代謝與生醫代謝研究
Progenesis QI (Waters)	多樣品定量與統計分析	Peak alignment, annotation, statistics	搭配 Waters 儀器，直覺式操作，支持多樣品比較
MarkerLynx (Waters)	資料處理與統計	Feature extraction, PLS-DA, trend analysis	老牌但穩定，適合熟悉 Waters 生態者
SIMCA (Sartorius)	多變量統計分析	PCA, PLS, OPLS, clustering	適合統計建模、品質控制與臨床研究者
Metabolon (平台服務)	商業服務	代謝物定量鑑定與報告	提供端到端代謝分析服務，包含標準化報告與 pathway insight
MassHunter (Agilent)	資料前處理與定量	整合 GC-MS/LC-MS 資料處理與鑑定	搭配 Agilent 儀器使用，穩定性高
Bruker TopSpin	儀器廠商整合軟體	• 原始 NMR 數據處理 • 結構分析 • 與 AMIX 模組結合進行代謝分析	為 Bruker NMR 儀器原廠軟體，整合性高，支援全套流程。
BATMAN (R Package)	半開源貝葉斯方法分析套件	• NMR 光譜解卷積 • 代謝物定量（基於 Bayesian 模型）	適用於程式熟練者，適合科研應用與方法學開發，部分版本有商業擴展授權。

與儀器深度整合、操作簡便、自動化程度高，能快速產出高品質且可重現的分析結果。

免費 / 開源軟體（Open-source / Freeware）

軟體名稱	類型	核心功能	適用說明
XCMS (R package)	資料前處理	Peak detection, alignment, RT correction	開源 R 套件，適合有程式基礎者，搭配 CAMERA 可進行同位素與離子標註
MS-DIAL	全流程分析	Peak picking, alignment, MS/MS 鑑定	圖形化友善介面，支援多平台與 MS2 分析
MZmine 2 / 3	全流程分析	Peak picking, filtering, network 連結	適用 LC-MS/MS 資料，整合 GNPS，跨平台支援
MetaboAnalyst	統計分析 & pathway	多變量分析、代謝途徑、機器學習	Web-based，簡單操作，適合生醫研究者
GNPS (Global Natural Products Social)	MS/MS 資料挖掘	Feature-based molecular networking (FBMN)	適合天然物與二級代謝物分析，可視化碎片網絡
SMART 2.0（中研院）	全流程統計平台	QC、多樣化統計分析、整合分析	GUI介面、適合大學與醫院單位使用
NMRProcFlow	NMR 專用	對齊、baseline 校正、bucketting	專為 NMR data 設計，圖形操作介面
Workflow4Metabolomics	工作流程平台	多步驟整合（XCMS, CAMERA, PLS等）	基於 Galaxy 平台，適合教學與 reproducibility

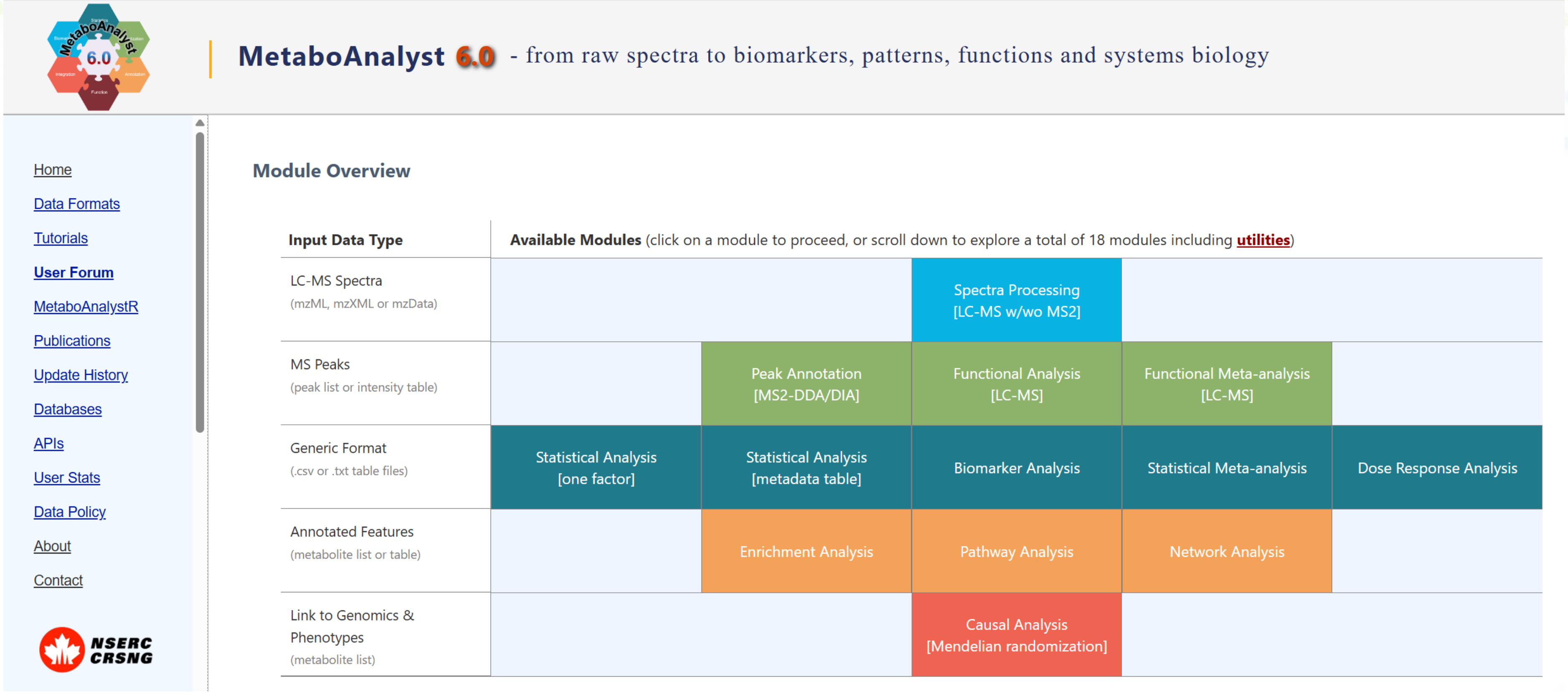
優點: 開放原始碼、無成本，並具高度彈性與可自訂性，適合研究創新與方法開發。

商用 vs 開源代謝物鑑定精確度比較表

分析平台	MS1 精準質量比對	MS/MS 鑑定準確性	Retention Time 比對	同位素 & adduct 標註	Fragment 結構推論	資料庫整合能力	MSI 等級支援	發表接受度	使用門檻與自動化	成本
商用軟體（Compound Discoverer, MassHunter）	☑ 儀器整合良好，ppm 精度高	☑ 商業資料庫支援，fragment 解譯佳	☑ 支援標準品 retention index	☑ 高準確性，自動化整合	☑ FISh Scoring, SIRIUS 模型內建	☑ 內建 HMDB, KEGG, mzCloud 等	☑ 易達 MSI Level 1/2	☑ 臨床/期刊接受度高	☑ 介面友善，自動流程多	$ 昂貴，需授權
開源軟體（MS-DIAL, MZmine, XCMS）	☑ 高解析資料支援，參數敏感	⚠ 依賴公開資料庫，準確性略低	⚠ 多需手動比對或補充資料	⚠ 有功能但較難整合多形式	⚠ 支援 SIRIUS，需進階操作	⚠ 多數需使用者串接外部庫	⚠ 多為 Level 2/3，少 Level 1	☑ 被接受，但需說明流程	⚠ 需熟悉設定與流程	💡 免費，社群活躍

「開源工具雖鑑定精度略低，但擁有高度彈性、透明性與學術友善性，是創新與教育研究的重要利器。」

MetaboAnalyst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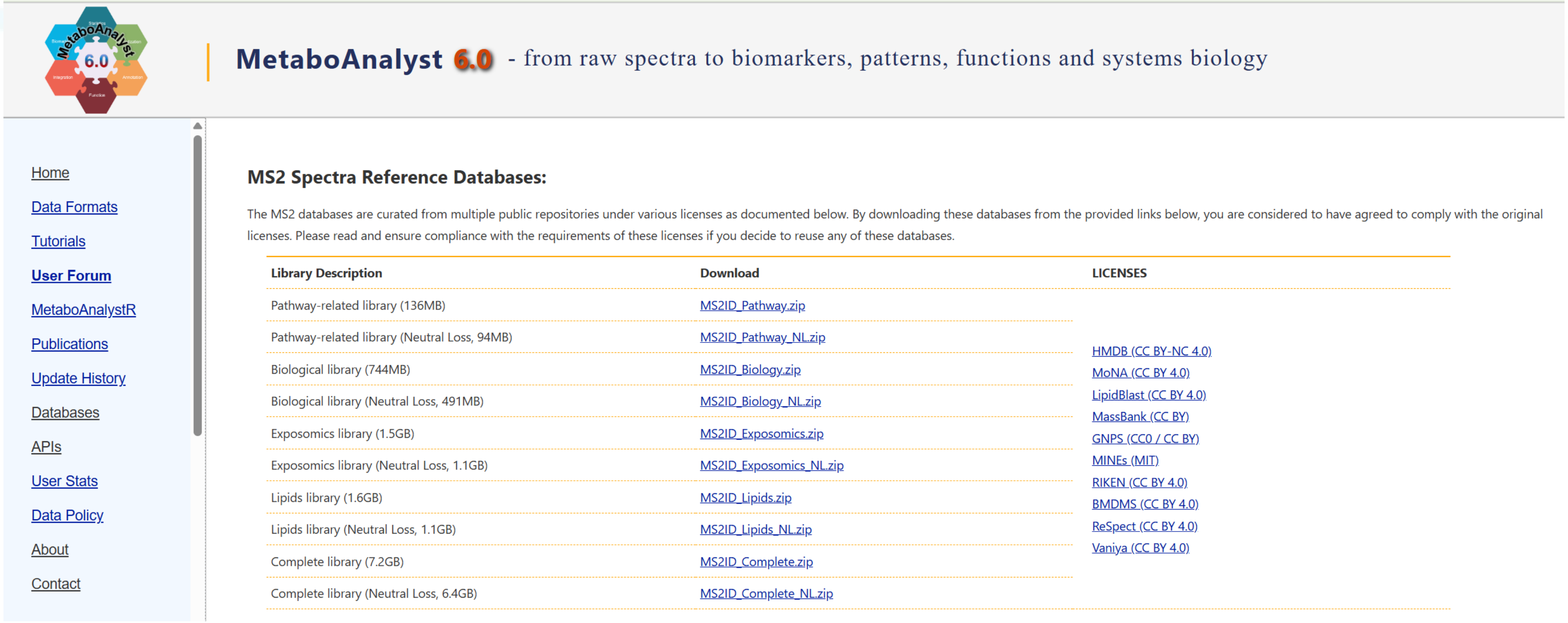
MetaboAnalyst 6.0 - from raw spectra to biomarkers, patterns, functions and systems biology

Module Overview

Input Data Type	**Available Modules** (click on a module to proceed, or scroll down to explore a total of 18 modules including **utilities**)				
LC-MS Spectra (mzML, mzXML or mzData)			Spectra Processing [LC-MS w/wo MS2]		
MS Peaks (peak list or intensity table)		Peak Annotation [MS2-DDA/DIA]	Functional Analysis [LC-MS]	Functional Meta-analysis [LC-MS]	
Generic Format (.csv or .txt table files)	Statistical Analysis [one factor]	Statistical Analysis [metadata table]	Biomarker Analysis	Statistical Meta-analysis	Dose Response Analysis
Annotated Features (metabolite list or table)		Enrichment Analysis	Pathway Analysis	Network Analysis	
Link to Genomics & Phenotypes (metabolite list)			Causal Analysis [Mendelian randomization]		

https://www.metaboanalyst.ca/home.xhtml

MetaboAnalyst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MetaboAnalyst 6.0 - from raw spectra to biomarkers, patterns, functions and systems biology

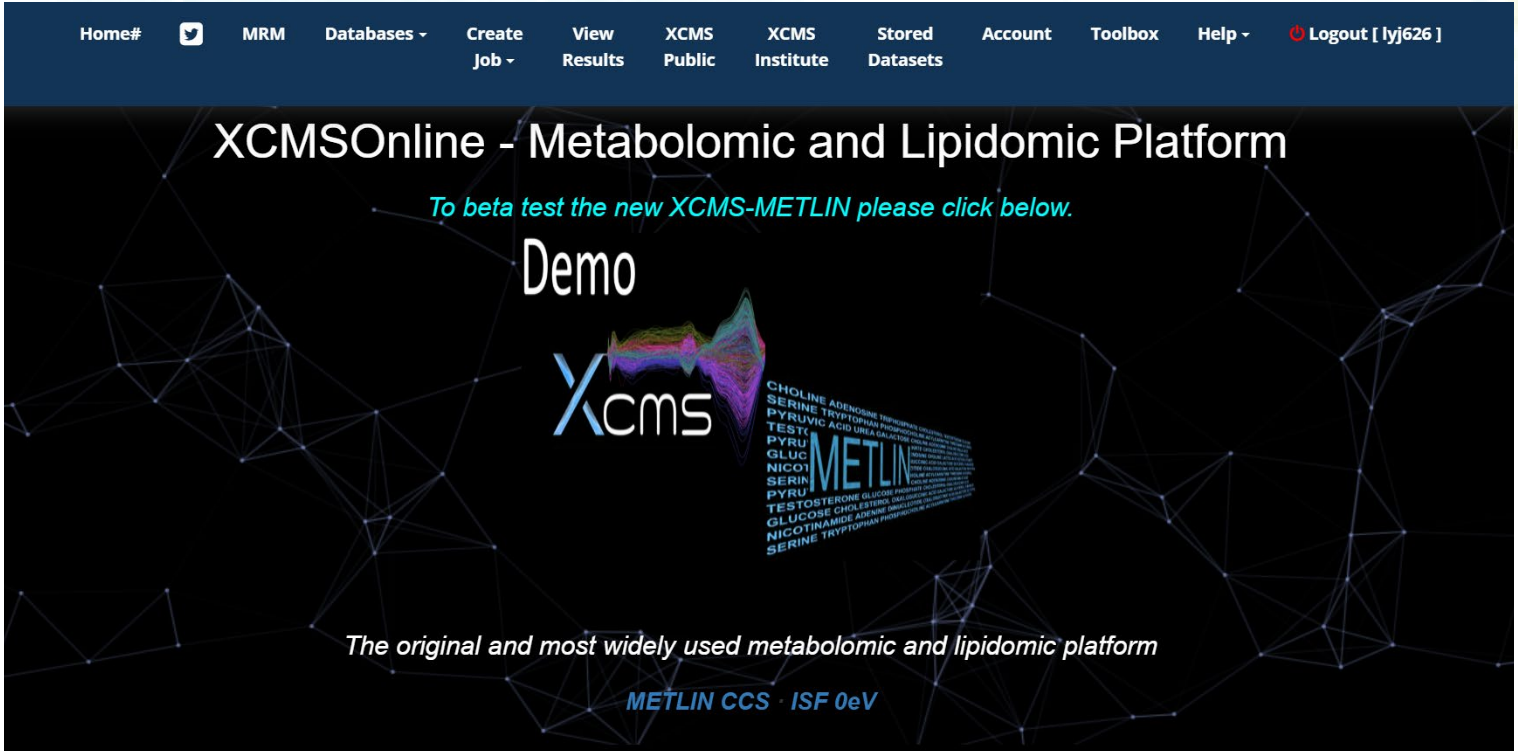
MS2 Spectra Reference Databases:

The MS2 databases are curated from multiple public repositories under various licenses as documented below. By downloading these databases from the provided links below, you are considered to have agreed to comply with the original licenses. Please read and ensure compliance with the requirements of these licenses if you decide to reuse any of these databases.

Library Description	Download	LICENSES
Pathway-related library (136MB)	MS2ID_Pathway.zip	HMDB (CC BY-NC 4.0) MoNA (CC BY 4.0) LipidBlast (CC BY 4.0) MassBank (CC BY) GNPS (CC0 / CC BY) MINEs (MIT) RIKEN (CC BY 4.0) BMDMS (CC BY 4.0) ReSpect (CC BY 4.0) Vaniya (CC BY 4.0)
Pathway-related library (Neutral Loss, 94MB)	MS2ID_Pathway_NL.zip	
Biological library (744MB)	MS2ID_Biology.zip	
Biological library (Neutral Loss, 491MB)	MS2ID_Biology_NL.zip	
Exposomics library (1.5GB)	MS2ID_Exposomics.zip	
Exposomics library (Neutral Loss, 1.1GB)	MS2ID_Exposomics_NL.zip	
Lipids library (1.6GB)	MS2ID_Lipids.zip	
Lipids library (Neutral Loss, 1.1GB)	MS2ID_Lipids_NL.zip	
Complete library (7.2GB)	MS2ID_Complete.zip	
Complete library (Neutral Loss, 6.4GB)	MS2ID_Complete_NL.zip	

https://www.metaboanalyst.ca/docs/Databases.xhtml

XCMS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XCMSOnline - Metabolomic and Lipidomic Platform

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Xcms
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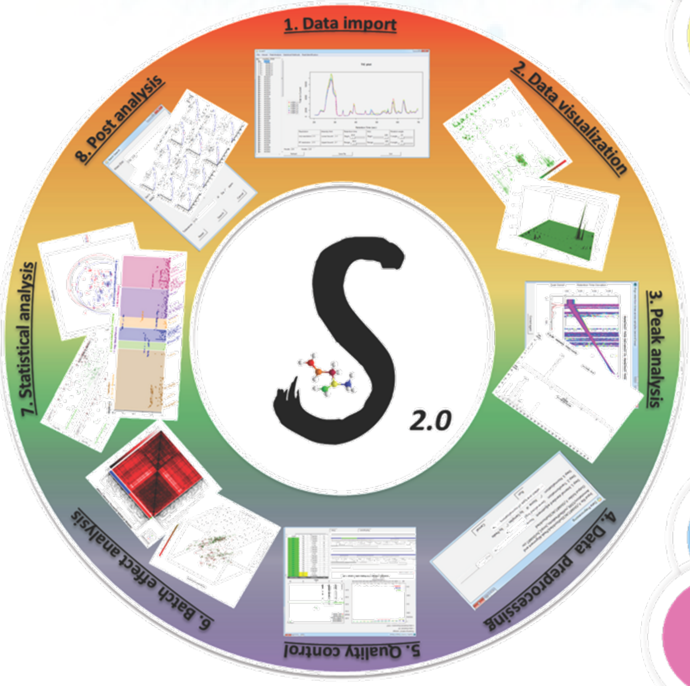
METLIN CCS · ISF 0eV

https://xcmsonline.scripps.edu/landing_page.php?pgcontent=mainPage

SMART

Intelligent Metabolomics Analytical System


1. Data import
2. Data visualization
3. Peak analysis
4. Data preprocessing
5. Quality control
6. Batch effect analysis
7. Statistical analysis
8. Post analysis
2.0

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https://staff.stat.sinica.edu.tw/hsinchou/metabolomics/SMART.htm

THANK YOU!

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