

# XCMS Online & METLIN: Resources for web-based metabolomic data processing

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<http://xcmsonline.scripps.edu> | <http://metlin.scripps.edu>

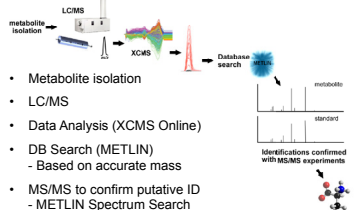
## Introduction

The profiling of small molecules, known as metabolomics, provides a tool to study cellular metabolism and has particular power for investigating biochemical applications related to the clinical laboratory. Technological advances in mass spectrometry and bioinformatic processing over the past decade have enabled rapid growth of the field and facilitated identification, quantification, and classification of thousands of metabolites. Metabolomic data can be used for diagnostic screening, drug discovery and development, clinical toxicology, nutrition studies and quantitative phenotyping of plants or microbes. The identification of metabolites, however, is a bottleneck in metabolomic experiments, largely due to the limited size, functionality, and usability of metabolite databases. To facilitate this effort, we have developed a new web-based platform for untargeted metabolomic data, called XCMS Online. Furthermore, a new scoring system has been integrated into the METLIN MS/MS database that allows for ranking of user MS/MS spectra against the METLIN database for automated quality control of metabolite identification

## Preliminary Data

**METLIN<sup>1</sup>**, a freely accessible web-based metabolite data repository. Currently METLIN contains  
 Total Metabolites: **45,282**  
 Total Metabolites with **High Resolution** MS/MS: **7,568**  
 Total MS/MS spectra: **38,464**

## Data Processing Workflow



## Acknowledgement

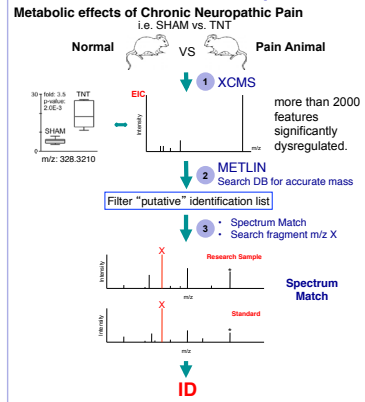
Financial support from the National Institutes of Health, the Department of Energy, and the California Institute for Regenerative Medicine

## References

- Smith, Colin et al. (2005) METLIN A Metabolite Mass Spectral Database. *Theor. Drug Monit.* **27**: 747-751.
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- Miyasaka, Roman et al. (2009) X-Rank: A Robust Algorithm for Small Molecule Identification Using Tandem Mass Spectrometry. *Anal. Chem.* **81**: 7604-7610.
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## Results

### An Overview: Chronic Neuropathic Pain



### 1 XCMS / XCMSOnline

Upload Data  
 Select Parameters  
 View/Download Results

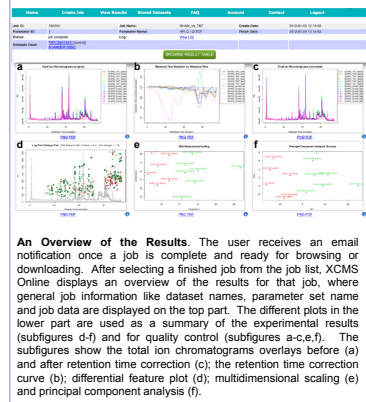
Data is compressed and encrypted on the client side and uploaded through a secure SSL connection.

Predefined parameter sets for different instrument setups are available and can be customized.

An email notification is sent once the job is complete. Results can be browsed online, shared with other users or downloaded for import into other programs (e.g. Excel).

**Overview.** XCMS<sup>2</sup> is a software program that performs nonlinear retention time alignment, feature detection, and feature matching for LC/MS data. Without using internal standards, the method dynamically identifies hundreds of endogenous metabolites for use as standards, calculating a nonlinear retention time correction profile for each sample. The processing of metabolomic data using XCMS Online is organized in three simple steps: data upload, parameter selection and result interpretation.

### View Results



### Result Table

DOWNLOAD RESULT TABLE

**Result Table.** The list of differentially regulated metabolites can be directly viewed in the web browser as described in the figure above. Users can filter the features by fold change, *p*-value, *m/z*, etc., then click each row to verify the EIC (displayed on the upper right), Box-and-Whisker Plot (displayed on the center right), and putatively identified metabolites (displayed on the bottom right) from METLIN database for further investigation.

### 2 METLIN – SIMPLE / BATCH SEARCH

Masses: 328.3211, 328.3212, 328.3213, 328.3214, 328.3215, 328.3216, 328.3217, 328.3218, 328.3219, 328.3220, 328.3221, 328.3222, 328.3223, 328.3224, 328.3225, 328.3226, 328.3227, 328.3228, 328.3229, 328.3230, 328.3231, 328.3232, 328.3233, 328.3234, 328.3235, 328.3236, 328.3237, 328.3238, 328.3239, 328.3240, 328.3241, 328.3242, 328.3243, 328.3244, 328.3245, 328.3246, 328.3247, 328.3248, 328.3249, 328.3250, 328.3251, 328.3252, 328.3253, 328.3254, 328.3255, 328.3256, 328.3257, 328.3258, 328.3259, 328.3260, 328.3261, 328.3262, 328.3263, 328.3264, 328.3265, 328.3266, 328.3267, 328.3268, 328.3269, 328.3270, 328.3271, 328.3272, 328.3273, 328.3274, 328.3275, 328.3276, 328.3277, 328.3278, 328.3279, 328.3280, 328.3281, 328.3282, 328.3283, 328.3284, 328.3285, 328.3286, 328.3287, 328.3288, 328.3289, 328.3290, 328.3291, 328.3292, 328.3293, 328.3294, 328.3295, 328.3296, 328.3297, 328.3298, 328.3299, 328.3300, 328.3301, 328.3302, 328.3303, 328.3304, 328.3305, 328.3306, 328.3307, 328.3308, 328.3309, 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