

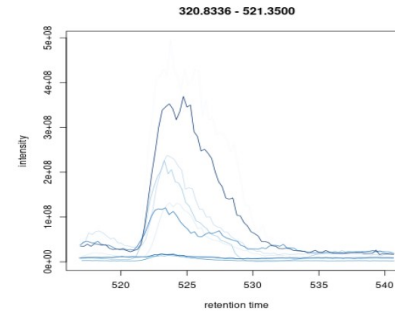
Indian Metabolome Data Archive (IMDA)

Data Submission Tutorial

ABOUT US


Indian Metabolome Data Archive (IMDA) is an effort by Indian Biological Data Center (IBDC), Regional Centre for Biotechnology, Faridabad to catalogue Metabolome data and their associated experimental metadata with various parameters including (experimental conditions, sample details and instrument characteristics) of mass spectrometer and NMR techniques. IMDA accepts raw data as well as processed data of MS and NMR. The raw data can be uploaded in the form of binary files and processed data in the form of quantitated metabolite concentrations, MS peak height/area values, LC retention time, NMR binned areas etc. A unique and persistent IBDC accession will be assigned on data submission to IMDA.

GET STARTED




Submit new study

Browse study

 Browse Data

View Details

 Data Submission Overview

View Details

Data Submission Process

Fill the Registration form (New User)



Register

Username*

Required. 150 characters or fewer. Letters, digits and @/./+/-/_ only.

Email*

First name*

Last name*

Organization*

Designation*

Password*

Your password must contain at least 8 characters.
Your password can't be a commonly used password.
Your password can't be entirely numeric.

Password confirmation*

Enter the same password as before, for verification.

Country*

Orcid*

Already have an account? [Log In](#)

(* = Mandatory to be filled)

Data Submission Process



The screenshot displays the website interface for the Indian Metabolome Data Archive (IMDA). At the top right, there are links for [Login](#) and [User Registration](#). The main navigation bar includes [HOME](#), [SUBMIT](#), [BROWSE](#), [HELP](#), [IBDC](#), and [CONTACT US](#). The IMDA logo (Indian Metabolome Data Archive) is on the left, and the BDC logo (Indian Biological Data Centre) is on the right. The central focus is the "Log In" form, which includes fields for "Username*" and "Password*", a "LogIn" button, and links for "Forgot Password? [Reset Now](#)", "Don't have an account? [Register Now](#)", and "Resend activation link to admin? [Resend Link](#)". The footer contains the copyright notice "© Copyright 2023 IMDA Team" and social media icons for Facebook, Twitter, Instagram, and LinkedIn.

Data Submission Process



Indian Metabolome Data Archive Toggle Menu shivani Logout

CORE

- Home
- Dashboard
- Project
- Study
- Author
- Sample
- Experiment
- Accessions
- Edit File Data

TOOLS

- Submit New Data
- Register Project**
- Register Study
- Register Sample
- Register Experiment
- FTP Files Upload
- Map Uploaded Files
- Submitted Data

My Data Step 1: Project Step 2: Study Step 3: Sample Step 4: Experiment/Files

Project

Fields marked as * are required

Title*	Project Contributors*
Research Area*	Funding Source*

Biological Sciences

Project Description*

Submit

[Return to home](#)

(* = Mandatory to be filled)

Data Submission Process



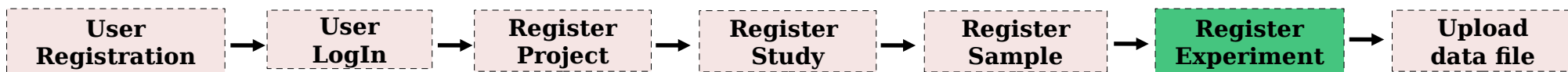
The screenshot shows the 'Sample' registration form in the Indian Metabolome Data Archive. The interface includes a navigation menu on the left with sections for CORE (Home, Dashboard, Project, Study, Author, Sample, Experiment, Accessions) and TOOLS (Submit New Data, Register Project, Register Study, Register Sample, Register Experiment, FTP Files Upload, Map Uploaded Files, Submitted Data). The main content area features a progress bar with four steps: My Data, Step 1: Project, Step 2: Study, Step 3: Sample (current), and Step 4: Experiment/Files. A 'Download Sample file Template' link is visible. The form fields include: 'Select Study*' (dropdown), 'Source*' (text), 'Organism Name*' (text), and 'Taxonomy ID*' (text). An 'Additional Information' text area is present. A 'Sample File Template' section contains a 'Browse...' button and the text 'No file selected.' A 'Submit' button and a 'Return to home' link are at the bottom.

Upload the filled Sample file template

Do not leave any cell blank in the Sample file template
Alternately use "NA" for any missing or blank value.

(* = Mandatory to be filled)

Data Submission Process



Indian Metabolome Data Archive Toggle Menu shivani Logout

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TOOLS

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My Data Step 1: Project Step 2: Study Step 3: Sample Step 4: Experiment/Files

[Download MS file Template](#)
[Download NMR file Template](#)

Experiment

Fields marked as * are required

Select Technique*

Study

Metabolite / Compound File MS/NMR File Template

No file selected. --- No file selected. ---

[Return to home](#)

Select technique used to generate data either by Mass Spectrometer(MS) or Nuclear Magnetic Resonance (NMR)

Upload the file containing the list of metabolites with ChEBI identifier and their associated parameters identified in the study

Upload the filled MS/NMR file template

(* = Mandatory to be filled)

Experiment File Template for MS and NMR

	A	B	C	D	E	F	G	H	I	J	K	L	M	N
1	Sample id	Sample Name	Reference Standard	Chromatography Inst	Column Model	Column Type	Mass Spectrometer Type	MS Instrument Name	MS Instrument Type	MS Ionization Method	Ion Mode/Scan	Data Transformation(Software)	MS Data File Name	Md5checksum
2	810													
3	811													
4														
5														
6														

CORE

- Home
- Dashboard
- Project
- Study
- Author
- Sample
- Experiment
- Accessions

TOOLS

- Edit File Data
- Submit New Data

OTHER

- Browse Lists

My Data My Project My Study Authors My Sample Experiment Accession List Submit New Data

Sample

Samples Uploaded: 2

List of Available Sample

Search Text

Search

Search from Project Summary



Sr.No	Sample ID	Study ID	Sample Name	Sample Type	Experimental Condition	Time of treatment	Variant/Variety	Gender	Age	Replicates	Storage Conditions	Upload Date	Edit
1	810	IMS_100010	KO-1	breast cancer cells	Treated with miRNA Precursor	24 hrs	NA	NA	NA	NA	-20C	May 17, 2024	Edit
2	811	IMS_100010	WT-1	breast cancer cells	Untreated	NA	NA	NA	NA	NA	-20C	May 17, 2024	Edit

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
1	Sample id	Sample Name	Reference Standard	NMR Instrument Name	NMR Type	NMR Experiment Type	NMR Spectrometer Frequency	NMR Probe	NMR Probe Temperature	NMR Solvent	NMR Tube Size	Data Transformation	NMR Data File Name	Md5checksum	
2	810														
3	811														
4															
5															
6															

Fill the sample id for each sample from the "My Sample" section of the dashboard

Do not leave any cell blank in excel file templates. Alternately use "NA" for any missing or blank value.




Instructions to calculate md5Checksum value:

Toggle Menu  Mayuri  Logout

My Data Step 1: Project Step 2: Study Step 3: Sample Step 4: Experiment/Files

Calculate MD5Checksum for Your Files Here

Select your operating system to download the script for compressing your data and verifying its integrity. This tool automatically zips any uncompressed folders and calculates the MD5 checksum for both files and folders in your directory, ensuring that your data remains secure and unaltered before deposition or transfer.

-  [Download Script for Windows](#)
-  [Download Script for macOS](#)
-  [Download Script for Linux](#)

Instructions to calculate md5Checksum value for data files (in linux, windows and mac system) is given on the pages named as Zip and md5checksum

Data Submission Process



The screenshot displays the 'Indian Metabolome Data Archive' web interface. At the top, a navigation bar includes 'Toggle Menu', a user profile 'shivani', and a 'Logout' button. A progress indicator shows the current step as 'Step 4: Experiment/Files'. The main content area is titled 'FTP Details' and contains the following text:

Dear shivani

Your FTP Details are as below:

HOSTNAME: 14.139.42.253
USERNAME: IBDCM_100006
Password: LyVqL3gfRu

Please click the link to Map the uploaded file : [Map Uploaded Files](#)

Two red arrows point from explanatory text boxes to the interface. The first arrow points to the FTP details box, and the second points to the 'Map Uploaded Files' link.

After filling all the details of data file, user will get FTP details to upload data file and the link to map the uploaded file

Map Uploaded File: Match mdchecksum value of the uploaded file

FTP Files Upload

IBDCM_100003@14.139.42.253 - FileZilla

File Edit View Transfer Server Bookmarks Help

Host: 14.139.42.253 Username: IBDCM_1000 Password: Port: Quickconnect

Status: Starting upload of /home/ibdc/download/ibdc/Control1.mzML
Status: File transfer successful, transferred 4.7 KB in 1 second
Status: Retrieving directory listing of "/IMDA/IBDCM_100003/IMDA/IMP_100005/IMS_100005"...
Status: Directory listing of "/IMDA/IBDCM_100003/IMDA/IMP_100005/IMS_100005" successful
Status: Disconnected from server
Status: Connection closed by server

Local site: / Remote site: /IMDA/IBDCM_100003/IMDA/IMP_100005/IMS_100005

bin
boot
cdrom
dev
etc
home
ibdc

Filename	Filesize	Filetype	Last modified
tmp		Directory	11/03/23 15:40...
run		Directory	11/03/23 06:48...
dev		Directory	10/10/23 03:46...
sys		Directory	09/15/23 16:20...
proc		Directory	09/15/23 16:20...
snap		Directory	02/22/23 15:36...
etc		Directory	02/10/23 10:08...
bin		Directory	02/10/23 10:07...
opt		Directory	02/10/23 10:07...
lib		Directory	01/05/23 14:54...
sbin		Directory	01/05/23 13:18...
lib64		Directory	01/05/23 13:18...
media		Directory	12/16/22 11:17...
root		Directory	10/12/22 10:10...
boot		Directory	07/01/22 06:58...
home		Directory	07/01/22 06:54...
cdrom		Directory	07/01/22 06:54...
lost+found		Directory	07/01/22 06:52...
var		Directory	04/19/22 15:37...
usr		Directory	04/19/22 15:32...
srv		Directory	04/19/22 15:32...

24 directories

IMDA
IBDCM_100003
IMDA
IMP_100005
IMS_100005

Filename	Filesize	Filetype	Last modified	Permission	Owner/Grou
..					
Control1.mzML	4.7 KB	mzML-file	11/03/23 20:...	-rw-----	1004 1004
Sample1.mzML	14.3 MB	mzML-file	11/03/23 20:...	-rw-----	1004 1004

2 files. Total size: 14.3 MB









Server/Local file	Directio	Remote file	Size	Priority	Status
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Queued files Failed transfers Successful transfers (4)

Transfer all the data files in the study folder of IMDA

Final Submission

CORE

-  Home
-  Dashboard
-  Project
-  Study
-  Author
-  Sample
-  Experiment
-  Accessions

 [Edit File Data](#) 

TOOLS

 [Submit New Data](#) 

OTHER

 [Browse Lists](#) 

 [Update List](#)

Please click the link to Finalized the submission

Study ID: IMS_100001

[Validate All Files for This Study](#)

Sr No.	FTP Run ID	File Name	Status
1	IMR_100001	Sample1.mzml	Unmapped
2	IMR_101067	cbbc	Unmapped

Study ID: IMS_100021

[Validate All Files for This Study](#)

Sr No.	FTP Run ID	File Name	Status
1	IMR_101133	S001.mzML	Unmapped
2	IMR_101134	S002.mzML	Unmapped
3	IMR_101135	S003.mzML	Unmapped
4	IMR_101136	S004.mzML	Unmapped
5	IMR_101137	S005.mzML	Unmapped

After uploading the data file using FTP, please click the link to validate the data file and finalized the submission

User Dashboard

CORE

 Home

 Dashboard

 Project

 Study

 Sample

 Experiment

TOOLS

 Submit New Data 

 Edit File Data 

OTHER

 Browse Lists 

 Create Lists 

[Go back](#)

My Data My Project My Study My Sample Experiment **Submit New Data**

project Project Uploaded: 1	Study Studies Uploaded: 1	Sample Samples Uploaded: 2	Experiment Techniques Uploaded: 2	Files Files Uploaded: 2
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Sr.No	Project ID	Study ID	Study Title	Study Type	Date of Submission
1	IMP_100002	IMS_100002	Metabolomic analysis of particulate matter in the NPSG during a 2017 cruise on the R/V Kilo Moana as part of the MESOSCOPE program	Mass Spectrometry (MS)	Oct 23, 2023

Click Study ID to get the submitted study details

Study Details

Study

Study uploaded by : shivani

Study ID : IMS_100002

Title : Metabolomic analysis of particulate matter in the NPSG during a 2017 cruise on the R/V Kilo Moana as part of the MESOSCOPE program

Summary : Targeted and untargeted analysis of metabolomics samples from the North Pacific Subtropical Gyre taken during the 2017 June/July SCOPE cruise on the R/V Kilo Moana (KM1709) across a mesoscale eddy dipole, with high-resolution depth profile sampling across the DCM in the center of each eddy. Particulate matter was collected on 0.2um filters and extracted using a modified Bligh & Dyer before analysis on a QE Orbitrap. Results show significant changes in the absolute quantity and relative composition of particles in the gyre between anticyclonic and cyclonic eddies.

Keywords : Targeted, untargeted analysis, MESOSCOPE program

Publication : NA

Release Date : Oct. 25, 2023

Study Type : Mass Spectrometry (MS)

Data Type : Targeted

IBSC Approval : 435345

Author List

Project

Edit Study

Navigation: My Data | **My Project** | My Study | Authors | My Sample | Experiment | Accession List | Submit New Data

Project
Project Uploaded: 1

List of Available Project

Search Text

[Search](#)

Search from Title and Project Description

Sr.No	Project ID	Title	Funding_Source	Project Description	Project Contributors	Research Area	Upload Date	Edit
1	IMP_100012	Study the role of miRNAs in breast cancer	DBT, India	study the role of mirna	Dr. Shivani Sharma	Biological Sciences	May 17, 2024	Edit

TOOLS
[Submit New Data](#)

Navigation: My Data | My Project | My Study | Authors | **My Sample** | Experiment | Accession List | Submit New Data

Sample
Samples Uploaded: 2

List of Available Sample

Search Text

[Search](#)



Search from Protocol Summary

Sr.No	Sample ID	Study ID	Sample Name	Sample Type	Experimental Condition	Time of treatment	Variant/Variety	Gender	Age	Replicates	Storage Conditions	Upload Date	Edit
1	810	IMS_100010	KO-1	breast cancer cells	Treated with miRNA Precursor	24 hrs	NA	NA	NA	NA	-20C	May 17, 2024	Edit
2	811	IMS_100010	WT-1	breast cancer cells	Untreated	NA	NA	NA	NA	NA	-20C	May 17, 2024	Edit


OTHER
[Browse Lists](#)

The project, study, sample and experiment can be edited directly from user dashboard and the edit link would be active during the submission process only

Edit Run information and metabolite/compound file

Indian Metabolome Data Archive Toggle Menu  shivani  Logout

CORE

- Home
- Dashboard
- Project
- Study
- Author
- Sample
- Experiment
- Accessions
- Edit File Data 
- Edit Run**
- Edit/Update Metabolite/Compound File

Edit upload Run


Fields marked as * are required

Select Run*

Ftp filename

Mdchecksum

[Return to home](#)

Indian Metabolome Data Archive Toggle Menu  shivani  Logout

CORE

- Home
- Dashboard
- Project
- Study
- Author
- Sample
- Experiment
- Accessions
- Edit File Data 
- Edit Run
- Edit/Update Metabolite/Compound File**

Edit Metabolite/Compound

Fields marked as * are required

Study

Compounds document

[Return to home](#)

Run refers to the data file

Browse and Update List

The screenshot shows the 'Indian Metabolome Data Archive' interface. On the left is a blue sidebar menu with sections: CORE (Home, Dashboard, Project, Study, Sample, Experiment), TOOLS (Submit New Data, Edit File Data), and OTHER (Browse Lists, Update List). The 'Update List' option is highlighted. The main content area is titled 'Please Request the Master Value to Update' and contains two input fields: 'Type*' with the value 'NMRInstrument' and 'Name*'. A green 'Submit' button is located below the fields. A red arrow points from the 'Update List' menu item to the form, and another red arrow points from the 'Submit' button to a text box.

New terms (related to organism, source and Instrument) which are not listed in the database can be updated by submitting the request of new term

Add the name and type of new term (related to organism, source and Instrument) and click submit

List will be updated only after the verification by database administration