

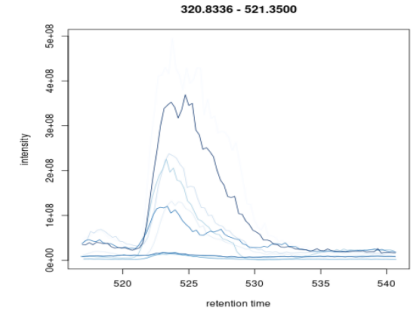
Indian Metabolome Data Archive (IMDA)

Data Submission Tutorial

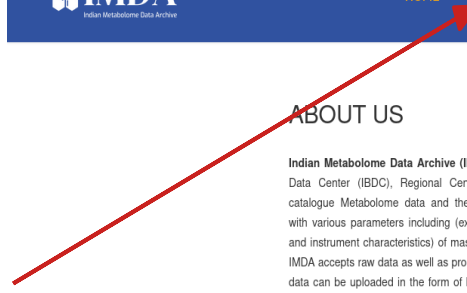
ABOUT US

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

Data Submission Overview

View Details

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). The header includes navigation links for [HOME](#), [SUBMIT](#), [BROWSE](#), [HELP](#), [IBDC](#), and [CONTACT US](#). The IMDA logo is on the left, and the Indian Biological Data Centre (IBDC) logo is on the right. In the top right corner, there are links for [Login](#) and [User Registration](#).

The main content area features a 'Log In' form with the following fields and options:

- Username***: A text input field.
- Password***: A password input field.
- Login**: A button to submit the login information.
- [Forgot Password? Reset Now](#): A link for password recovery.
- [Don't have an account? Register Now](#): A link for new user registration.
- [Resend activation link to admin? Resend Link](#): A link for account activation.

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

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

Project

Fields marked as * are required

Title*	Project Contributors*
<input type="text"/>	<input type="text"/>
Research Area*	Funding Source*
<input type="text" value="Biological Sciences"/>	<input type="text"/>
Project Description*	
<input type="text"/>	

[Return to home](#)

(* = Mandatory to be filled)

Data Submission Process



Indian Metabolome Data Archive Toggle Menu shivani Logout

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OTHER

- Browse Lists
- Update List

• Successfully Uploaded the Project Data.The Unique Project id is : 'IMP_100012'

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

Study

Fields marked as * are required

Select Project*

Title*

Study Type*

Data Type*

Keywords*

Summary (Max. 500 words only)*

Publication

Release Date*

IEC/IBSC Approval Number

IBSC Approval document

Author List

First Name*

Last Name*

Email*

Organization Name*

Designation*

Others

Add Author Remove Author

Submit

[Return to home](#)

Data Submission Process



The screenshot shows the 'Sample' registration form on the Indian Metabolome Data Archive website. The page features a blue header with the site name and user information, and a left sidebar with navigation options. A progress bar at the top indicates the current step is 'Step 3: Sample'. The form includes fields for 'Select Study*', 'Source*', 'Organism Name*', and 'Taxonomy ID*', along with an 'Additional Information' text area and a 'Sample File Template' upload section. A red arrow points to the 'Submit' button.

Upload the filled Sample file template

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

(* = Mandatory to be filled)

Data Submission Process



The screenshot shows the 'Indian Metabolome Data Archive' website interface. A progress bar at the top indicates the current step: 'Step 4: Experiment/Files'. The main content area is titled 'Experiment' and contains a form with the following fields:

- Select Technique***: A dropdown menu with a red arrow pointing to it from a text box below.
- Study**: A text input field with a red arrow pointing to it from a text box below.
- Metabolite / Compound File**: A file upload field with a 'Browse...' button and 'No file selected.' text. A red arrow points to it from a text box below.
- MS/NMR File Template**: A file upload field with a 'Browse...' button and 'No file selected.' text. A red arrow points to it from a text box below.
- Submit**: A blue button.
- Return to home**: A blue link.

On the left sidebar, the 'Register Experiment' option is highlighted in green. Below the sidebar, there are three text boxes with red arrows pointing to the form fields:

- Select technique used to generate data either by Mass Spectrometer(MS) or Nuclear Magnetic Resonance (NMR)** (points to 'Select Technique*')
- Upload the file containing the list of metabolites with ChEBI identifier and their associated parameters and identified in the study** (points to 'Metabolite / Compound File')
- Upload the filled MS/NMR file template** (points to '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 Standar	Chromatography Inst	Column Model	Column Type	Mass Spectrometer Type	MS Instrument Name	MS Instrument Type	MS Ionization Method	Ion Model/Scan	Data Transformation(Software)	MS Data File Nam	Md5checksum
2	810													
3	811													
4														
5														
6														

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

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 Transformatio	NMR Data File Na	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.

Data Submission Process



The screenshot displays the 'Indian Metabolome Data Archive' interface. A progress bar at the top indicates the current step: 'Step 1: Project'. The main content area is titled 'FTP Details' and contains the following information:

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 the text boxes below to the 'Map Uploaded Files' link and the FTP details box.

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

Local site tree:
- /
- bin
- boot
- cdrom
- dev
- etc
- home
- ibdc

Remote site tree:
- /
- ? /
- ? /IMDA
- ? /IMDA/IBDCM_100003
- ? /IMDA/IBDCM_100003/IMDA
- ? /IMDA/IBDCM_100003/IMDA/IMP_100005
- ? /IMDA/IBDCM_100003/IMDA/IMP_100005/IMS_100005

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

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

Queued files Failed transfers Successful transfers (4)

Transfer all the data files in the study folder of IMDA

Final Submission

Indian Metabolome Data Archive Toggle Menu shivani Logout

CORE

- Home
- Dashboard
- Project
- Study
- Sample
- Experiment

TOOLS

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

OTHER

- Browse Lists
- Create Lists

Please click the link to Finalized the submission

Sr No.	FTP Run ID	File Name	Status
1	JMR_100005	Sam_1.mzML	Unmapped
2	JMR_100006	CTL_1.mzML	Unmapped

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

Indian Metabolome Data Archive Toggle Menu shivani Logout

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OTHER

- Browse Lists
- Create Lists

Final Submission

File name	MD5 Checksum	
Sam_1.mzML	c4743c3cfc978f6f239059c3628f20e4	<input type="button" value="Submit"/>

Click on Submit button for the final submission

User Dashboard

- CORE
 - Home
 - Dashboard
 - Project
 - Study
 - Sample
 - Experiment
- TOOLS
 - Submit New Data
 - Edit File Data
- OTHER
 - Browse Lists
 - Create Lists

- 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

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

[Go back](#)

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: CORE | Home | Dashboard | Project | Study | Author | Sample | Experiment | Accessions | Edit File Data | TOOLS | Submit New Data

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

Navigation: CORE | Home | Dashboard | Project | Study | Author | Sample | Experiment | Accessions | Edit File Data | TOOLS | 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 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

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' website. On the left is a blue sidebar menu with categories: 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