



Standard Operating Procedure (SOP)
for
Metabolomics data submission
to
Indian Metabolome Data Archive (IMDA)
Version_0.1
2023



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Introduction to Indian Metabolome Data Archive

Indian Metabolome Data Archive (IMDA) is an effort by Indian Biological Data Center (IBDC), Regional Centre for Biotechnology, Faridabad to catalogue metabolomics 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 (preferable Mzml format). 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. The portal can be accessed at <https://ibdc.dbtindia.gov.in/imda/>.

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

Browse Data
View Details

Data Submission Overview
View Details

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Figure 1. Snapshot of home page of IMDA.

Getting started on the submission

User Registration

To create a new account, user has to fill all the asterisk marked mandatory fields (including Username, Email, Organisation, Password and Orcid etc.) mentioned on user registration page. After successful registration, user will get the account activation link from the IBDC support team on the registered e-mail address. On clicking the link user can confirm the activation of account on the IMDA portal.

Register

Username*

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

Email*

First name*

Last name*

Organization*

Select Organization

Designation*

Others

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*

India

Orcid*

Sign Up

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

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Figure 2. Snapshot of user registration page of IMDA.

User Login

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User can enter their specified username and password (mentioned on the registration page) for directly login to the IMDA portal. Additional links such as forgot password, to create a new account and their activation are provided on the same page.

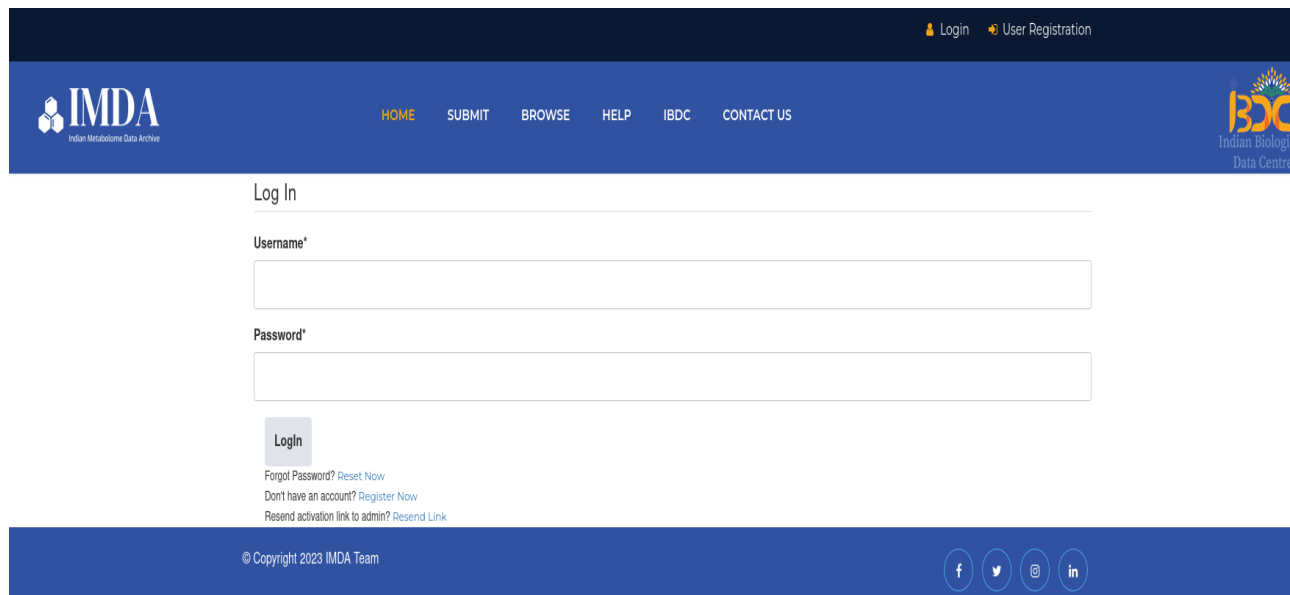
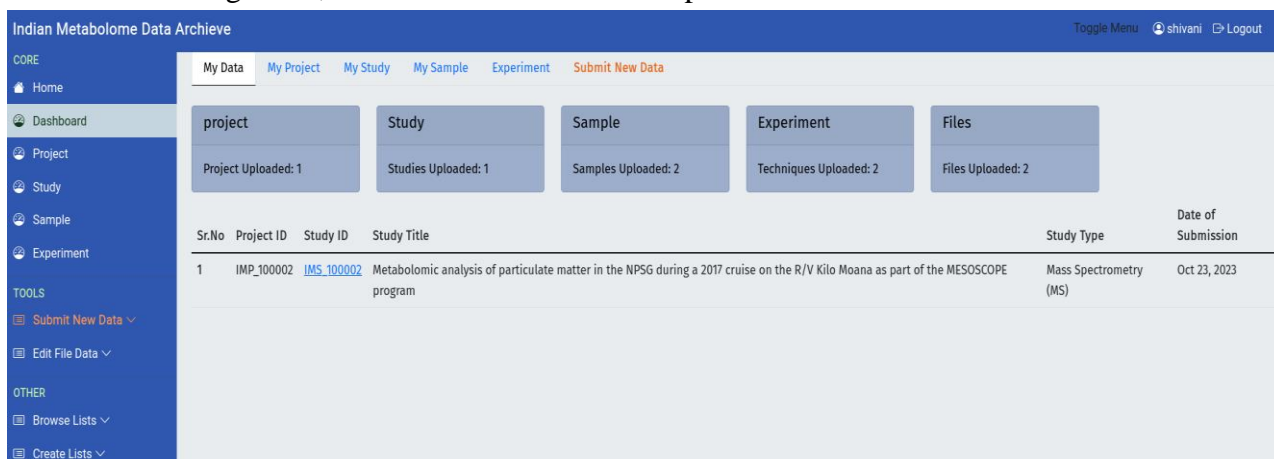


Figure 3. Snapshot of LogIn page of IMDA.

User Dashboard

on successful login, users are directed to the dashboard of the portal where user can access the details of their submitted data and its associated project, study, sample and experiment. On the side panel of the dashboard the link for data submission “submit new data” as well as in the browse list section detailed list of organism, source and instruments are provided.



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

Figure 4. Snapshot of dashboard page of IMDA.

Stepwise submission process: For every new data submission, IMDA requires registration of the study and its associated metadata. The fields marked with asterisk are mandatory to be filled.

Step 1. Project Registration

To start with new submission select **submit new data** link given in the side panel as well as on the top panel of the dashboard page, the information of the project are required to be filled by the user. The fields marked with asterisk are mandatory to filled.

Toggle Menu shivani Logout

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*

Project Description*

Submit

[Return to home](#)

Figure 5. Snapshot of project registration page of IMDA.

Step 2. Study Registration

To register a new study, user has to fill the details of the study i.e. title, summary, type of the study and data including Release date (the date when the study may be made available to the public) of the study.

Once the study is successfully registered, a unique study accession id will be assigned to user.

Toggle Menu shivani Logout

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*

Add Author Remove Author

Submit

[Return to home](#)

Figure 5. Snapshot of study registration page of IMDA.

Step 3. Sample Registration

For sample registration, excel file template named as sample file template is provided where user can fill the information regarding sample preparation including sample type, experimental condition, replicates, storage condition and their protocol summary. The link to download the template is provided on the top left corner of the sample registration page. Sample accession id will be given on the submission of sample details. Users are requested to submit two separate entries for the sample information in case of the study having more than one organism or source.

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

[Download Sample file Template](#)

Sample

Fields marked as * are required

Select Study*

Source*

Organism Name*

Taxonomy ID*

Additional Information

Sample File Template

No file selected. ---

[Return to home](#)

Figure 6. Snapshot of sample registration page of IMDA.

Step 4. Experiment Registration

For experiment registration, first user needs to specify the technique (Mass Spectrometry or Nuclear Magnetic Resonance Spectrometry) used to generate the data files. Once user select the technique, metadata fields related to specified technique needs to be filled (in the excel file templates) with their sample Ids provided in the section named as “My Sample” on the user dashboard and upload on the same page. Two separate excel file templates download links for mass spectrometry and NMR are provided on the top left corner of the page. User will get an experiment id after the submission of all metadata fields related to specified technique.

Download MS file Template
Download NMR file Template

Experiment

Fields marked as * are required

Select Technique*

Study

Metabolite / Compound File

MS/NMR File Template

Browse... No file selected. ---

Browse... No file selected. ---

Submit

[Return to home](#)

Figure 7. Snapshot of experiment registration page of IMDA.

Step 5. Upload Data

Before uploading the data file, please review the following information:

- Each sample should have a corresponding raw/processed data file.
- An open source format submission (mzML/nmrML) is encouraged, as long as the raw data and open format contain the same level of information. Otherwise all file formats of MS and NMR are acceptable.
- Calculate the md5 checksum of the data file.

The final step of submission is to upload the data file to the FTP server through FTP client. Before uploading the data file, metabolite file consisting of metabolite information identified in the study should be uploaded and the file name should be mentioned in the column named as metabolite file name. All the relevant information of the metabolite file and data file (metabolite file name, MS/NMR file name, md5checksum value) needs to be filled in the same page for further proceedings.

When you request to upload the data file, you will get the FTP credentials on the FTP files Upload pages and on the user's registered e-mail. (As dummy FTP credential is given below)

```
HOSTNAME: 14.139.42.253  
USERNAME: IBDCM_100006  
Password: LyVqL3gfRu
```

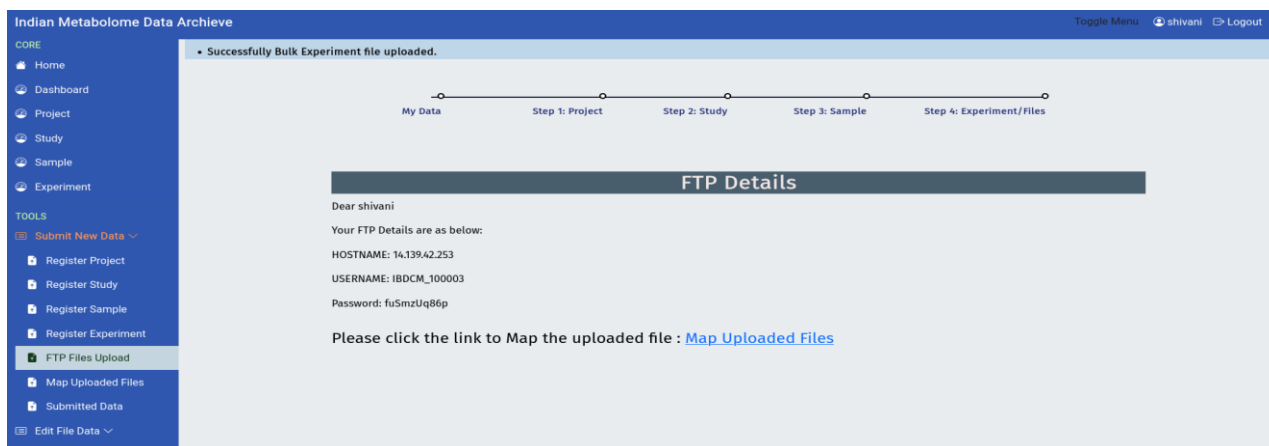


Figure 8. FTP credential details (As dummy)

To transfer the file on FTP, user has to click the project folder first (already displayed on the FTP page) and then select/click the study folder where all the data files can be dragged and dropped simultaneously. After successful transfer of the data file, user needs to map the uploaded file for the final submission.

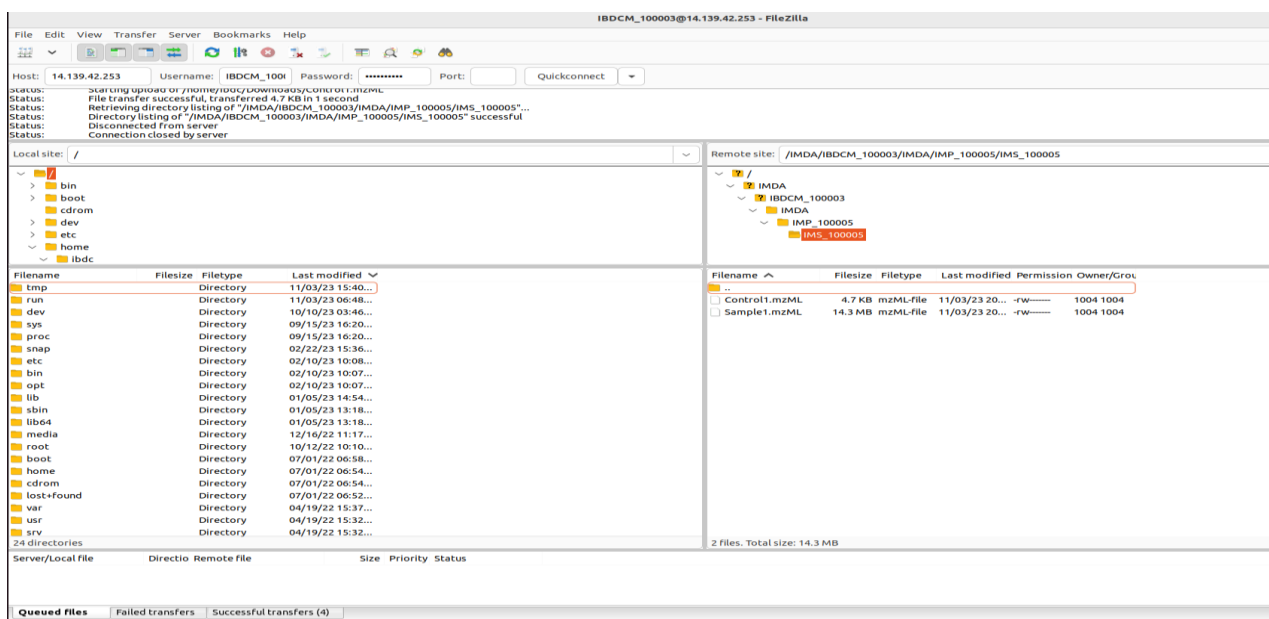


Figure 9. Snapshot of FTP data files upload page

Browse and Update list (Source, Organism, MS/NMR Instrument)

This section deals with the submission of new terms related to source, organism and MS/NMR Instrument which might not be listed in the database.

Before submission, users are advised to search the term in the section 'Browse list'. If the term is not existed in the list. the user can user submit the name and type of the new term in the given columns

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on the suggested term page, then the automated request will be send to database administration. Once the administrator verify the submitted term then only the list will be updated with new term.

Indian Metabolome Data Archive

Toggle Menu shivani Logout

CORE

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

TOOLS

- Submit New Data
- Edit File Data

OTHER

- Browse Lists
- Update List

Please Request the Master Value to Update

Type*
NMRInstrument

Name*

Submit

Figure 10. Browse and Update List of organism, source and instrument.

5. Edit Study

User can edit project, study, sample and experiment information directly from their dashboard. The process of editing will be providing during the submission process. Once the submission of the data files has been done the edit option will be automatically inactive.

The options to edit file data/Run and metabolite/compound file is provided in the side panel of the dashboard named as Edit file 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_100014	Study the role of miRNAs in breast cancer	DBT, India	study the role of miRNA in breast cancer	Dr. Shivani Sharma	Biological Sciences	May 13, 2024	Edit

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My Data My Project **My Study** Authors My Sample Experiment Accession List [Submit New Data](#)

Study

Studies Uploaded: 1

List of Available Study

Search Text

[Search](#)

Search from Title and Summary

Sr.No	Study ID	Title	Summary	Keywords	Publication	Release Date	Upload Date	Edit
1	IMS_100016	Study the role of miRNAs in breast cancer	Study the role of miRNAs in breast cancer	mirna, cancer	NA	May 18, 2024	May 13, 2024	Edit

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	923	IMS_100016	WT-1	breast cancer cells	Untreated	NA	NA	NA	NA	NA	-20C	May 13, 2024	Edit
2	922	IMS_100016	KO-1	breast cancer cells	Treated with miRNA Precursor	24 hrs	NA	NA	NA	NA	-20C	May 13, 2024	Edit

My Data My Project My Study Authors My Sample **Experiment** Accession List [Submit New Data](#)

Select Technique*

MS (Mass Spectrometry)

Mass Spectrometry

Sr.No	Study	Sample	Mass Spectrometry Id	Mass Spectrometer Type	MSInstrument Name	Instrument Type	Ionization Method	Binary Data Format MS	Upload Date	Edit/Update
1	IMS_100016	IMSM_100923 (923)	IME_100579	GCMS (Gas Chromatography -Mass Spectrometry)	Agilent 5975C	TOF	Electrospray Ionization - ESI	NA	May 13, 2024	Edit
2	IMS_100016	IMSM_100922 (922)	IME_100578	GCMS (Gas Chromatography -Mass Spectrometry)	Agilent 5975C	TOF	Electrospray Ionization - ESI	NA	May 13, 2024	Edit

Figure 11. Edit options in the user's dashboard.

The figure displays two screenshots of the Indian Metabolome Data Archive (IMDA) user dashboard. Both screenshots show a navigation menu on the left with categories: CORE (Home, Dashboard, Project, Study, Author, Sample, Experiment, Accessions, Edit File Data, Edit Run, Edit/Update Metabolite/Compound File), TOOLS (Submit New Data), and OTHER (Browse Lists, Update List). The top screenshot is titled 'Edit upload Run' and contains the following form fields: 'Select Run*' (with a dropdown arrow), 'Ftp filename', and 'Mdchecksum'. A 'Submit' button and a 'Return to home' link are located below the fields. The bottom screenshot is titled 'Edit Metabolite/Compound' and contains the following form fields: 'Study' (with a dropdown arrow) and 'Compounds document' (with a 'Browse...' button and the text 'No file selected. ---'). A 'Submit' button and a 'Return to home' link are located below the fields.

Figure 12. Edit file data options in the user's dashboard.

User Manual and Submission overview tutorial (PDF)

To guide users through the process of data submission, the detailed standard operating procedures and data submission tutorial (PDF) are available in the top bar (Help section) and bottom bar (data submission overview tab) of the IMDA home page.

Impotent Note:

- Do not edit or change the format of the Excel template files for sample, MS and NMR.
- The asterisk marked fields are mandatory to be filled.
- Do not leave any cell blank in excel file templates. Alternately use NA instead of missing or blank values in your data.
- MD5Checksum value should be in the lower case.

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- Name of the file to be uploaded on FTP server should be same as mentioned in the excel file templates.
- Name of the data files should be different from one another.
- Do not leave any blank space in all the files name. Alternately use ‘_’ instead of blank space.
- In case of more than one organism or source in study, users are requested to register and fill the separate excel file template.

□