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

IMDA: Table of Content

Introduction to Indian Metabolome Data Archive

Indian Metabolome Data Archieve (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 (preferrable 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/.

 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.

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.
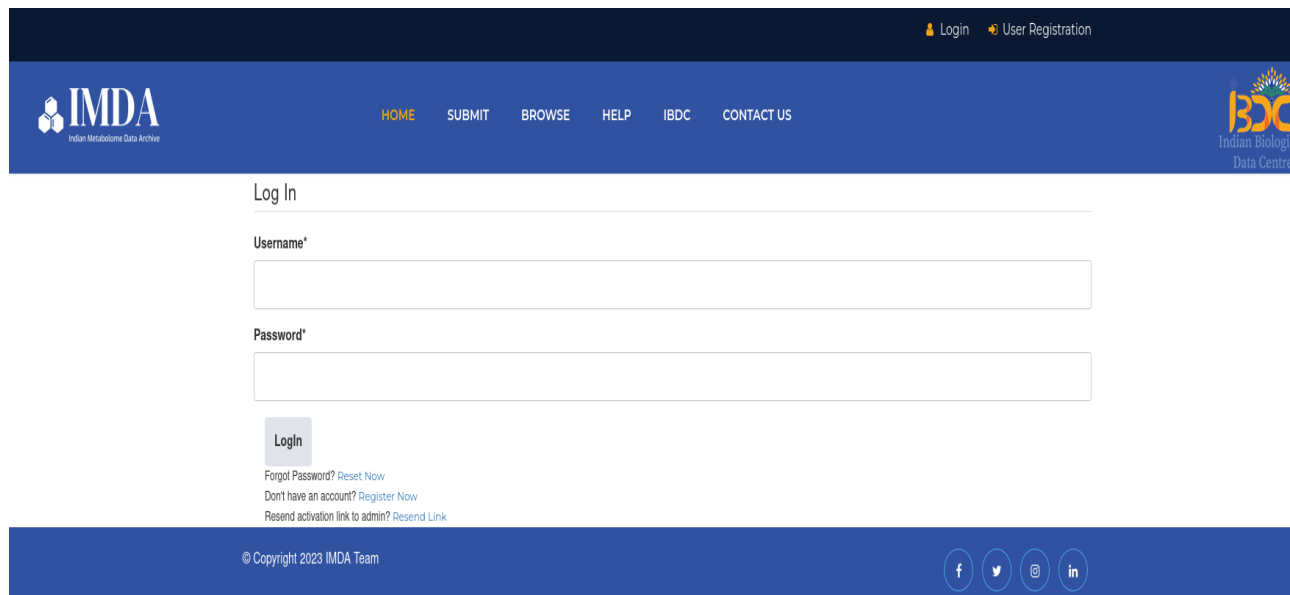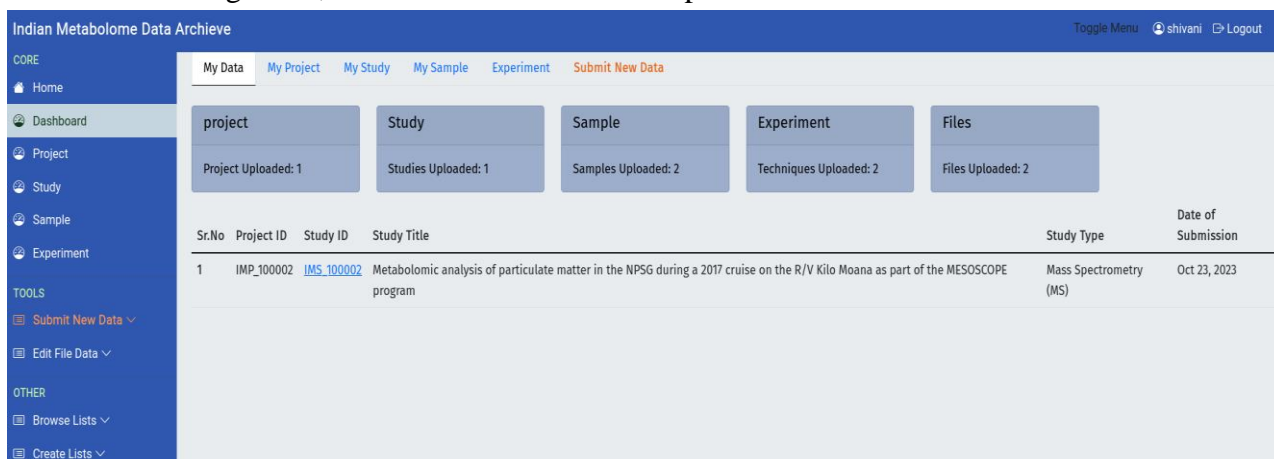
Figure 3. Snapshot of LogIn page of IMDA.

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.

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.

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 sucessfully registered, a unique study accession id will be asssigned to user.

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 preperation 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 seperate entries for the sample information in case of the study having more than one organism or source.

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 seperate 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.

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 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
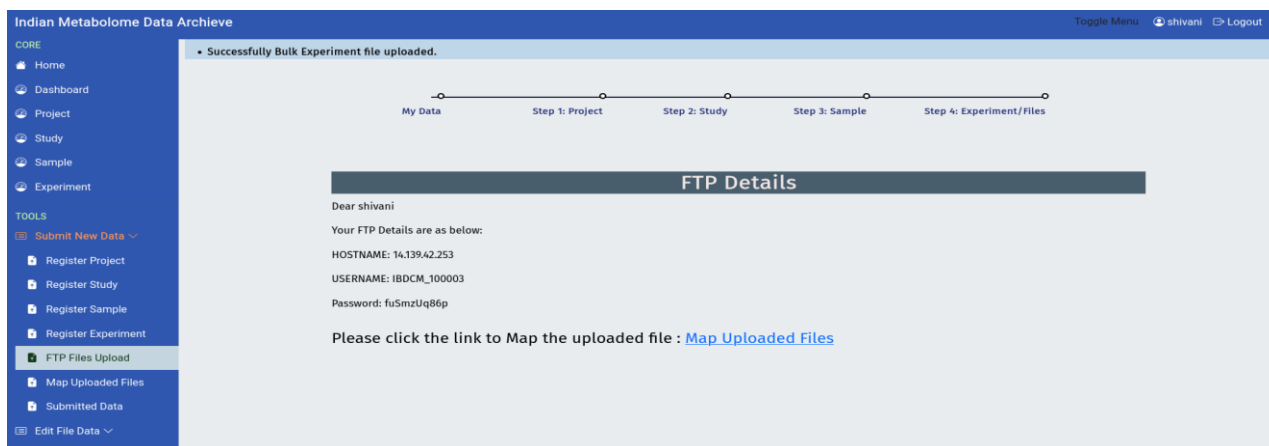USERNAME: IBDCM_100006
Password: LyVqL3gfRu

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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.
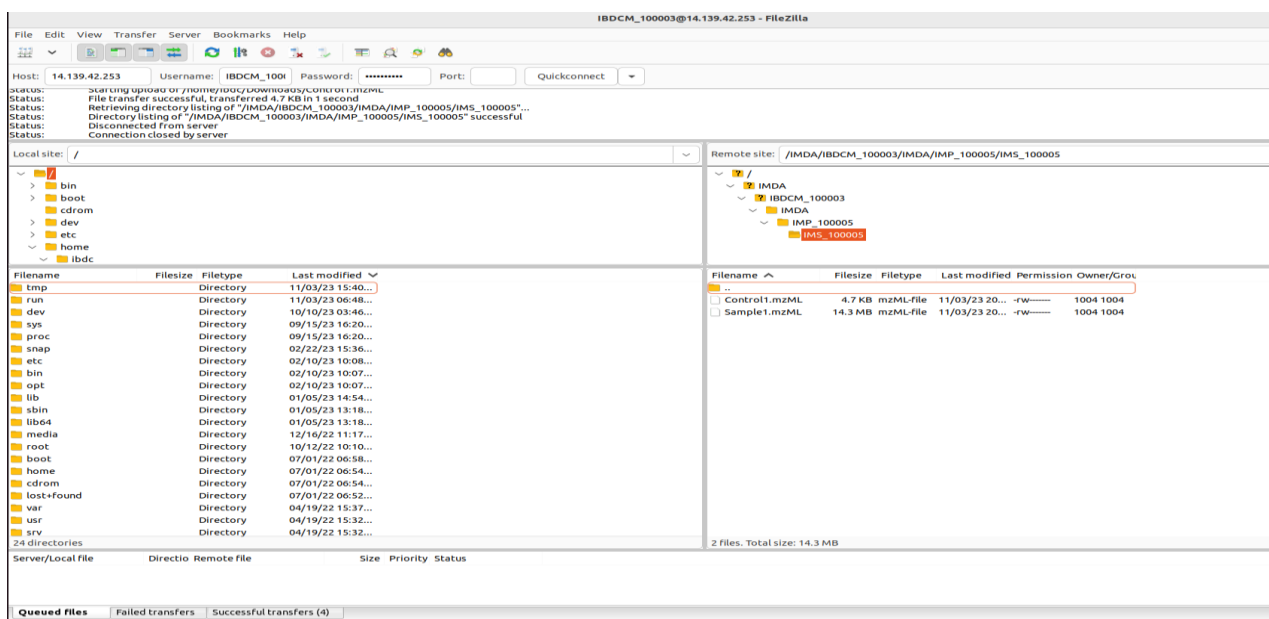

Figure 9. Snapshot of FTP data files upload page

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 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

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.

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

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.

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.

Impotant 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.

- 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 seperate excel file template.