

A brief report of 7thworkshop on CCPM

CCPM-7 “Launch of CCPM v4.4”

April 10, 2017

This workshop “CCPM-7 held on 10th April 2017” consists of one day workshop at two different places IIIT Hyderabad and JNU Delhi both online and offline, was organized as Launch of CCPMv4.4 of the LIMS platform to its potential workshop participants including experimentalist.

Announcement and Invitations with program outline were sent well in advance to most of the PI's and Experimentalist (**Appendix 1 a – c**). Reminder mails were also sent. Announcements and workshop details were also displayed on the CCPM portal

Each potential participant was contacted and given an option to choose a mode (online / offline) as well as place (IIIT Hyderabad/ JNU Delhi) of their convenience for workshop participation through the workshop portal.

A total of 40 participants, including three faculty members and several research group members of PIs, registered at both venues (JNU and IIIT-H) combined. Three registrants attended online, whereas all others attended the workshop physically. All the researchers attended both the morning as well as the afternoon sessions. Among morning session attendees there were several students who were exposed to the area of Metabolomics and to the CCPM portal.

Program Details – Workshop Schedule

Inaugural Session

10:00 AM – 10:15 AM	Welcome addresses By: Prof. Indira Ghosh, Dr. Meenakshi Munshi
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Morning Session

10:15 AM – 10:20 AM	Introduction to CCPM version 4.4 By: Prof. Abhijit Mitra
10:20 AM – 10:40 AM	Technical innovations and enhancements By: Prof. Vikram Pudi and IT team
10:40 AM – 11:30 AM	Walk through of new functionalities Bio team CCPM (Coordinated by Dr. Kapil Sharma)
11:30 AM – 11:45 AM	Tea Break
11:45 AM – 1:15 PM	Interaction and feedback from experts and experimentalists. By: CCPM PIs (Prof. Indira Ghosh, Prof. Abhijit Mitra, Prof. Nita Parekh and Prof. Vikram Pudi)

1:15 PM – 2:00 PM

Lunch Break

Afternoon Session

2:00 PM – 2:45 PM

Tutorial Presentation
By: Dr. Kapil Sharma

2:45 PM – 4:30 PM

Physical/Online workshop
(Participants to upload their data and use portal functionalities for analysis)
Team CCPM (Coordinated by Dr. Kapil Sharma at IIIT-Hyderabad & Isha Saini at JNU)

Morning Session

The morning session was conducted using Live Google hangout session (For online participants) and contents are available at <https://www.youtube.com/watch?v=2p--A8Uo54o&t=2350s> (39:11min)

Inauguration and introduction: The coordinating PI of the project CCPM, Prof. Indira Ghosh (Professor, School Computational and Integrative Sciences, JNU) thanked DBT for funding the project, and, highlighting how the project has become a good example of Computer Science and Domain Science groups working together, welcomed Dr. Meenakshi Munshi (Director at DBT Govt. of India) to inaugurate the workshop CCPM-7 and E-launch the CCPM version 4.4. After a ceremonious e-launch of the latest version of CCPM, version v4.4, Dr. Munshi spoke at length outlining the laudatory progress of the project since its genesis. Objective of this project include development of a metabolomics relational database and statistical tool for analyzing plant metabolomics data and studying metabolomics pathways and their network properties. The latest release, CCPMv4.4, is nearly fully developed and is equipped new functionalities like NMR Module, Multi-Group, KEGG Module, Metabolite Correlation Edge list, Filtration and Bulk Upload to accept metabolomics data from experimentalists. In continuation with Dr. Meenakshi Munshi, Prof. Indira Ghosh also added that the portal is ready for phase 2 which will involve industry to test the viability of developing it into a professional platform, ready to serve both academic as well as corporate research. The next logical steps should involve securing IPR and ensuring self sustainability through industrial collaborations and to produce a business model as suggested by DBT-Task force committee. She also thanked all the active working members at IIITH and JNU for making “Launch of CCPM v4.4” successful.

Prof Abhijit Mitra gave an introduction to CCPM version 4.4, sharing in brief the highlights of “Launch of CCPM v4.4”. Prof. Vikram Pudi listed different technological innovations, which have been incorporated while planning and developing the software, and explained the related issues in a simplified fashion. This was followed up by the IT team who shared the technical aspects of the software and its working efficiency, data security and development platform. On behalf of the bio-team, Dr. Kapil Sharma explained the new added functionalities to CCPM v4.4 and their research importance and aspects to metabolomics.

Interactions with and feedback from experimentalists and experts

After the brief overview of the why and what of the project "Computational Core for Plant Metabolomics", Prof. Mitra initiated the interaction session. The context was set by indicating that the CCPMv4.4 portal is ready after complete optimization of existing functionalities and incorporation of newly added functionalities. Decisions taken during CCPM-6 were reinforced during the interaction session. Additional decisions were also taken:

- 1. New Functionalities have been implemented. These include Bulk Upload, NMR Module, KEGG Module Integration, Metabolite Correlation Edge list, Filtration Module and Multi-Group functionalities, etc. They need to be optimized.**
- 2. The software now needs testing with bulk upload from the experimentalists**
- 3. Constant dialogue should take place between the CCPM team members and portal users.**
- 4. Data Security Concepts, which were proposed, have been added to the portal. They need to be properly reviewed during the workshop.**

As experimentalists there were Prof. R.P Sharma (UoH) at IIIT-H. and Dr. Ashwini Pareek from JNU. Prof. Indira Ghosh coordinated the interactions from JNU. From IIIT-H the discussions were coordinated by Prof. Abhijit Mitra along with Dr. Nita Parekh and Dr. Vikram Pudi. Dr. Kapil Sharma gave his inputs on behalf of the bio-team.

Participants from online and physical are allowed to ask their questions and queries regarding the CCPM v4.4 portal in online live session. Prof. R.P Sharma shared his feedback regarding the new added functionalities of the portal sharing real time scenario data analysis and the importance of the KEGG pathway module for their research.

Few important questions are recorded during online live session are in appendix-2a:

Afternoon Session

Tutorial and Hands on session

(Also conducted over Hangouts by share screen function for online participants)

- The tutorial was presented by Dr. Kapil Sharma. The printout of the tutorial was given to the physical participants as hand out. The soft copy of the tutorial is available in the portal. The new functionalities and their importance were explained in detail during the presentation.
 - The following Demos related to new added functional features of CCPM v4.4 were presented:
 - (a) Unpublished Projects
 - (b) Other online participants were asked to carry their own data for uploading them into portal and doing several kind of analysis followed with pathway analysis.
 - Handouts for DEMO were distributed to all the participants.
- (Appendix-2b_WorkshopHandout)**

The hands on session was for participants to explore and test all updated and newly added functionalities on the workshop portals at JNU and IIIT-H respectively. Participants were provided with pre-authenticated secured login accounts which were to be kept activated for 15 days for submitting their unpublished data and doing statistical, pathway and metabolite identification analysis in CCPM portal. Extensive and detailed discussions went on during the hands-on session and covered topics such as related to bulk data upload, multi-group analysis, NMR Module and NMR format conversion tool, KEGG Module Integration, Metabolite Correlation Edgelist and security features of CCPM tool along with Filtration Module.

Follow up action plan to contribute further to the project's objectives

The suggestion and feedback from the participants are noted will be incorporated into the CCPM portal.

Conclusions:

The one day workshops at both the places were successful. Valuable suggestions received will enable us to improve the prototype development. Pre-release of CCPM v4.4 was praised and appreciated by faculties and researchers in metabolomics community.

Appendix 1a

Workshop Announcement



Computational Core for Plant Metabolomics



Sponsored by DBT Govt. of India

Announcing CCPM-7 Workshop

Launch of CCPM version 4.4

On 10th April 2017

*Conducted jointly by JNU Delhi and IIIT-H
Physical & ONLINE*

We are pleased to announce the seventh one day workshop (CCPM 7), based on CCPM v4.4 <metabolomics.iiit.ac.in>, entitled as '**Launch of CCPM version 4.4**' to be organized concurrently (both online as well as physical hands on) at JNU Delhi & IIIT Hyderabad on **Monday 10th April 2017**. All the presentations and activities will also be streamed through Google Hangout/YouTube for online participants.

There will be no registration fees, and local hospitality will be taken care of. However, participants are requested to fill in the online registration form, available at the workshop portal, <to be announced*>, for arrangements and logistics. The portal will have all requisite information about the workshop. All participants are welcome to the workshop venues (Hyderabad/Delhi) according to their convenience, for those who cannot make it physically, we have arranged for interactive online session using Hangouts (link to be announced). Please bring your laptop in case you plan to physically attend the hands on session.

Depending on your convenience for hands on and online participation, you may register for either of the two modes. Especially participants from Hyderabad or Delhi are strongly encouraged to participate physically at their respective workshop venues. In case you are registering for the online mode, please provide your Hangouts/Gmail account and test it beforehand; so that you and your team members can participate in the workshop virtually.

Please mark your calendars and save the date to attend the CCPM7 Workshop '**Launch of CCPM version 4.4**' on **10th April 2017**. A detailed program schedule will follow soon.

The portal <to be announced*> has all the necessary information about the workshop. We look forward for your active participation in the workshop.

With Best Regards
Sincerely,

Dr. Indira Ghosh
School of Computational & Integrative Sciences
Jawaharlal Nehru University
New Delhi 110067
Phone: +91-9971287771; 011-2673 8707
Email: indira0654@gmail.com

Dr. Abhijit Mitra,
Center for Computational Natural Sciences and
Bioinformatics, IIIT Hyderabad
Gachibowli, Hyderabad - 500032
Phone: +91-40-6653 1156(O)/ 1201(R)
Email: abi_chem@iiit.ac.in

Appendix 1b

Workshop Invitation



Computational Core for Plant Metabolomics



Sponsored by DBT Govt. of India

Invitation for CCPM-7 Workshop

Launch of CCPM version 4.4

On 10th April, 2017

*Conducted jointly by IIIT-H and JNU Delhi
(Physical and Online)*

As you are aware, “**Computational Core for Plant Metabolomics (CCPM)**” is a collaborative project being implemented jointly by IIIT-H and JNU Delhi. Funded by the Department of Biotechnology (DBT), Government of India, the goal of the project is to create a national computational facility to support collaborative initiatives in Plant Metabolomics. The implementation involves development of a LIMS platform integrated with databases and tools required for storage, retrieval and analysis of metabolomics data as per the International Metabolomics Standards Initiative (MSI) guidelines.

Regarding this, by now you must have received the announcement of the **7th Workshop (CCPM-7)** – “**Launch of CCPM version 4.4**” **scheduled on 10th April, 2017** concurrently at IIIT-H and JNU Delhi. Based on suggestions received during the previous workshop CCPM-6 on version 3.4 from DBT experts and users who were requested to test the version with live data, an updated version CCPM v4.4 was initiated in January 2017. With nearly all modules incorporated in this version along with suggestions, we have planned workshop CCPM-7 as “Launch of CCPM version 4.4” to showcase new functionalities.

This will be a one day workshop. The morning session will have presentations followed by interaction with experimentalists and experts. In the afternoon session we will have online and hands on sessions at IIIT-H and JNU Delhi.

We invite you to participate in this workshop, along with your colleagues and project personnel. You may also participate online by going to this link (<http://metabolomics.iiit.ac.in/workshop>) where the morning session will be broadcasted. The participants coming to attend the hands on session are requested to come with laptops. They are also requested to come with the raw data to test the functionality of the CCPM portal. For afternoon hands-on session, online participants are requested to connect on Hangouts (ccpm7workshop@gmail.com) or YouTube (<https://www.youtube.com/watch?v=vSpkid5K-lc>). Kindly refer to the following link for registration (<http://metabolomics.iiit.ac.in/workshopregistration>). The workshop schedule is enclosed in the next page.

For further details on the workshop or for any assistance in registration or usage, please contact:

JNU Delhi: Ms. Isha Saini
Email: sainiisha22@gmail.com
Phone: +91 8569909875

IIIT Hyderabad: Dr. Kapil Sharma
Email: kapil05vats@gmail.com
Phone: +91 9912104813

Your presence in this workshop and your feedback is very important for the success of the project. We look forward to seeing you.

With Best Regards
Sincerely,

Dr. Indira Ghosh
School of Computational & Integrative Sciences
Jawaharlal Nehru University
New Delhi 110067
Phone: +91-9971287771; 011-2673 8707
Email: indira0654@gmail.com

Dr. Abhijit Mitra,
Center for Computational Natural Sciences and
Bioinformatics, IIIT Hyderabad
Gachibowli, Hyderabad - 500032
Phone: +91-9866406028, 040-6653 1201 (R)
Email: abi_chem@iiit.ac.in

Appendix 1c

Program Details



Computational Core for Plant Metabolomics



Sponsored by DBT Govt. of India

Workshop Schedule

Inaugural Session

- 10:00 AM – 10:15 AM Welcome addresses
- Prof. Indira Ghosh
 - Dr. Meenakshi Munshi

Morning Session

- 10:15 AM – 10:20 AM Introduction to CCPM version 4.4
- Prof. Abhijit Mitra
- 10:20 AM – 10:40 AM Technical innovations and enhancements
- Prof. Vikram Pudi and IT team
- 10:40 AM – 11:30 AM Walk through of new functionalities
- Bio team CCPM (Coordinated by Dr. Kapil Sharma)
- 11:30 AM – 11:45 AM Tea Break
- 11:45 AM – 1:15 PM Interaction and feedback from experts and experimentalists.
Hosted by CCPM PIs (Prof. Indira Ghosh, Prof. Abhijit Mitra, Prof. Nita Parekh and Prof. Vikram Pudi)
- 1:15 PM – 2:00 PM Lunch Break

Afternoon Session

- 2:00 PM – 2:45 PM Tutorial Presentation
- Dr. Kapil Sharma
- 2:45 PM – 4:30 PM Physical/Online workshop
(Participants to upload their data and use portal functionalities for analysis)
Team CCPM (Coordinated by Dr. Kapil Sharma at IIIT-Hyderabad & Isha Saini at JNU)

Appendix-2a

Questions and Comments during “Interaction with Experimentalists”:

1. During Bulk raw data upload, how many files and how fast can be uploaded? If there is discontinuation of internet connection during upload, will it resume from that point of upload?

Answer: As such there is no-limit but upload limits might get imposed based on institute internet connections and firewall. It was tested up to 60GB of data upload per instance/upload. Yes, it will resume from that point of upload.

2. Can we integrate PLANTCYC database in CCPM tool locally?

Answer: Integrating PLANTCYC by downloading the database is not maintainable. It is possible to link to the PLANTCYC API. In PLANTCYC, the links aren't stable. For PLANT Reactome it is possible.

3. How many digits are to be considered while displaying the values in Filtration Table UI (eg: Fold change, RT, P-value, etc).

Answer: Currently, it displays upto 12 digits after decimal.

4. What are the file formats supported by CCPM for Pre-processing Module?

Answer: .netCDF, .mzML, .mzXML, .mzDATA are the supported file formats. File conversion module is also available in CCPM Portal under Tools > Format Conversion which does the same.

5. How many digits difference is considered while finding the difference in two close data samples (for GC, LC, NMR)?

Answer: By default python considers upto 15 digits after decimal to prevent duplicity in the datasets.

6. Some participants asked about Proteomic data analysis in CCPM v4.4 portal and their KEGG pathway analysis. PI's from IIITH end shared their views saying in Metabolomics tool Proteomics data analysis is not allowed or not feasible. But, KEGG pathway analysis can be done along-with cytoscape analysis. But, generally these things are preferred for metabolomics data not for proteomics data, as this is Plant metabolomics tool.

Workshop Handout

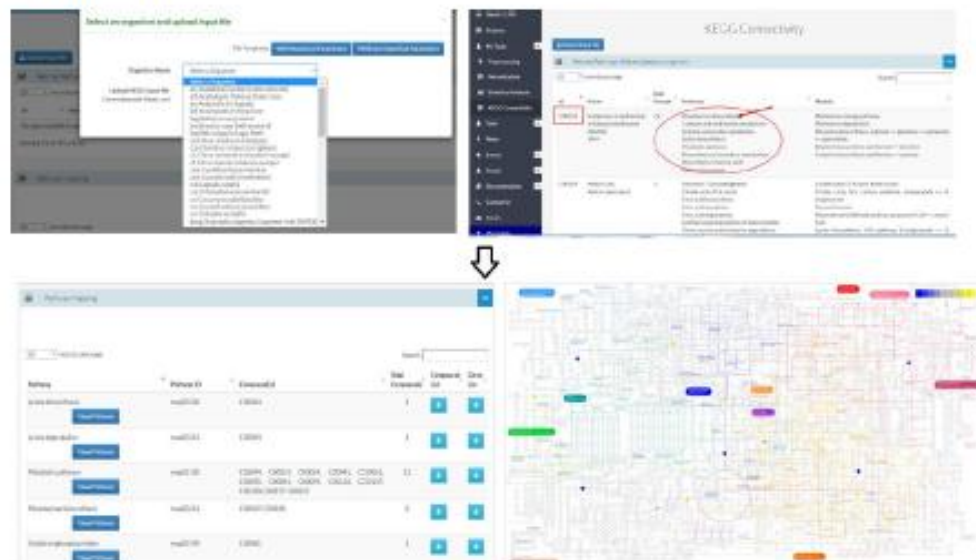
“Workshop Manual”

```

graph LR
    M1["MODULE I:  
Data Upload  
Meta Data, Instrument data ,  
Bulk Upload"] --> PMI["Peak to Metabolite  
Identification"]
    M2["MODULE II:  
Data Pre-Processing"] --> PMI
    PMI --> M3["MODULE III:  
Data Pre-treatment and  
Statistical Analysis"]
    PMI --> M4["MODULE IV:  
Data Integration  
Pathway Connectivity"]
  
```

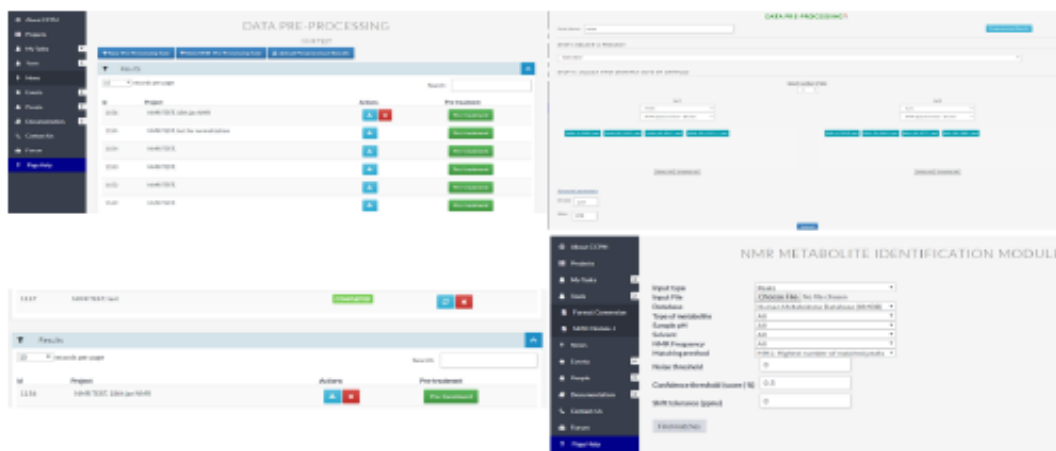
1. KEGG Module Integration:

The KEGG module can be used for mapping and visualizing a given set of metabolites on to KEGG pathways. The user can upload a list of metabolites along with fold-change/p values (optional) to retrieve the associated KEGG pathways and modules. In case no information is available for the given species, mapping can be done on the KEGG Reference Pathway. The fold-change/p values can be used for rendering the visualization of pathway maps



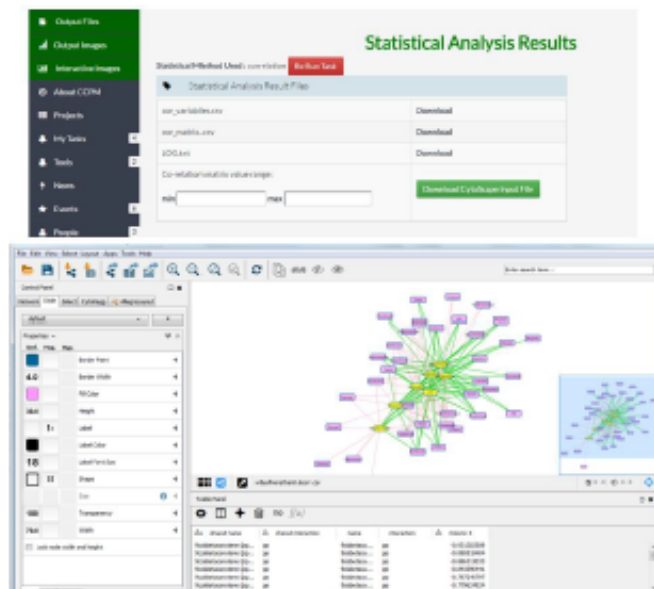
2. NMR Module:

NMR Metabolite identification tool uses the open source metabohunter scripts for semi-automatic assignment of 1D NMR spectra of metabolites. The metabolite identification interface search two major publicly available NMR database (HMDB: Human Metabolome Database and MMCD: Madison Metabolomics Consortium Database) in background and display the result output from the selected database based on user input parameters. This tool for metabolite identification is based on spectra or peak lists with different search methods and with possibility for peak drift in a user defined spectral range.



3. Metabolite Correlation Edgelist:

This feature can be used to export metabolite correlation matrix as an edge list with user-defined cut-offs for correlation values. The edge list can be used as an input to network visualization softwares, such as Cytoscape.



4. Multigroup:

Multigroup comparison allows user for the identification of differentially expressed metabolite features across multiple classes of data. multigroup analysis aims to identify differences between groups and reveal the diversity of metabolic patterns across different groups.

Add Preprocessing Task

Study Name:

☒ Single Project
☐ Cross Project

STEP-I: SELECT A PROJECT

Project 04: Metabolome profiling using LC-MS in *Arabidopsis* overaccumulating and lacking flavonoids

STEP-II: SELECT TWO DISTINCT SETS OF SAMPLES
(SAMPLES IN BOTH SETS MUST BE OF SAME TYPE, E.G., POS-POS OR NEG-NEG)

Select Number Of Sets: 4

Set1

dCol0

UPLC/UHD Q-TOF

RN_25 RN_26 RN_27

Set2

dpop1Dtt4

UPLC/UHD Q-TOF

RN_34 RN_35 RN_36

5. Bulk Upload:

Meta data for multiple groups and its samples in a project can be uploaded as a single .csv file by the user. The corresponding file can be uploaded by clicking the button **Choose File** followed by clicking **Upload Bulk Data**. User can also upload Multiple Raw files with a group simultaneously using this Bulk Upload option.

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GROUPS & SAMPLES

Create New Group

Search Samples

+ 1

+ 2

+ 3

GROUP DETAILS

1 (A)

email@null.kapil.tham@gmail.com

MS2 leaf phytochemicals

No. of samples (maximum): 3

phenotype samples

edit group

add new sample

delete

Upload Bulk Data

Upload Raw Data

Supported raw data formats are CDF,mzData,mzXML

Select Instrument

HPLC/Q-TOF

Select Raw bulk data

Upload Raw Data

Supported raw data formats are CDF,mzData,mzXML

Select Instrument

HPLC/Q-TOF

Select Raw bulk data

A_1.cdf

A_2.cdf

A_3.cdf