

A training session report on  
**Characterization Techniques and Advance in  
Research (MRS/Metabolomics)**

Under STUTI program funded by DST



In association with  
**Indian Institute of Technology, Gandhinagar**  
(Project Management Unit)



Co-ordinated by  
**Dr. Anjani Kumar Tiwari**  
**Prof. Gajanan Pandey**  
Department of Chemistry  
Babasaheb Bhimrao Ambedkar University  
(A Central University), Lucknow India

**22<sup>nd</sup> to 28<sup>th</sup> September 2022**

## Acknowledgement

Department of Chemistry, BBAU Lucknow conveys gratitude for the encouragement and support received during the execution of this training program. First and foremost, we want to express our sincere appreciation to the Department of Science and Technology (DST) for entrusting us with this project. We would like to thank to **Prof. Sanjay Singh** (Honorable Vice-chancellor), Babasaheb Bhimrao Ambedkar University (A Central University), Lucknow for encouraging to host DST-STUTI program. The DST-STUTI training program was coordinated by **Dr. Anjani Kumar Tiwari** with the support of Head, Department of Chemistry, Babasaheb Bhimrao Ambedkar University (A Central University), Lucknow. The workshop was conducted on the “Characterization Techniques and Advance in Research (MRS/Metabolomics)” on the instrument funded by the FIST program (Sanction No.: SR/FST/CS-I/2019/112). Organizing team acknowledge the contributions of the experts, teaching staff, non-teaching staff and research scholars of the department for execution of the successful program to achieve the objectives of the DST-STUTI. We are thankful to **Prof. Raja Roy** (Ex Director, Centre of Biomedical Research, Lucknow) for accepting our invitation as chairperson of inaugural ceremony. We would also like to thank to all the members of organizing team. Our sincere thanks to finance section of our university. We also acknowledge IIT, Gandhinagar for their constant support and guidance.

### Coordinators

Dr. Anjani Kumar Tiwari

Prof. Gajanan Pandey

## ***Summary***

The goal of this training session is to popularize BET Surface Area and NMR facilities among students, faculty, scientists and industry professionals through a week-long training workshop. The “*Characterization Techniques and Advance in Research (MRS/Metabolomics)*” workshop was conducted in the department of Chemistry at BBAU, Lucknow from 22<sup>nd</sup> to 28<sup>th</sup> September 2022 and comprised of lectures and hands on training sessions. This initiative is funded by Department of Science & Technology under the program ***STUTI*** (*Synergistic Training Program Utilizing the Scientific and Technological Infrastructure*). All the guidance and support were provided by IIT Gandhinagar. The participants were introduced to the basic concepts and various functions of BET Surface Area Analyzer and Nuclear magnetic resonance (NMR) through demonstration and hands-on session on data analysis and interpretation of results useful for sample investigation. The focus of this workshop was to have “*a balance between theory and practical training on the equipment. Emphasis is on hands-on use of equipment for demonstration/characterization by each participant and analysis of participant’s samples*”.

## Introduction

Department of Chemistry Babasaheb Bhimrao Ambedkar University conducted 7-day long workshop on DST-FIST funded instrument ‘Characterization Techniques and Advance in Research (MRS/Metabolomics)’ workshop in its campus. About 35 participants from around 24 Institutes, faculty members, postdoctoral researchers, and doctoral students have participated in this training workshop were invited (**Annex-1**). The following workshop's activities took place from 22<sup>nd</sup> to 28<sup>th</sup> September 2022 (**Annex-2 & 3**). This report provides a quick overview of inauguration, the lecture and technical sessions.

- Lecture Session

The inauguration ceremony was started with invocation followed by lightning of *Kulgeet* by dignitaries. **Prof. Raja Roy** (Ex. CBMR Director, Lucknow) explained the basics of NMR and its applications in different fields of research. **Dr. Bikash Baishya** (CBMR, Lucknow) gave a talk on the essential principles and physics behind the operation of Nuclear Magnetic Resonance (NMR). **Dr. H M Gauniyal** (Scientist, CDRI Lucknow) has discussed about different aspects of NMR operation with demonstration. **Dr. Nihar Ranjan** (NIPER, Lucknow) has explained about the JEOL NMR setup and its various aspects. **Prof R.P. Tripathi** (Ex Senior Scientist, CDRI, Lucknow) discussed about 2D/3D NMR applications. **Dr. Sanjeev Kumar Shukla** (Sr. Scientist, CDRI, Lucknow) has explained about the MRS/Metabolomics with different examples. **Senior Specialist Engineer** (JEOL, Asia) explained about the processing software with its demonstration. **Dr. Chandra Shekhar Pati Tripathi and Prof. Vinod Kumar Tiwari** (Professors BHU Varanasi) explained about the basics and principles of BET surface analyzer and its applications.

- Technical Session

On the **first day**, after inauguration of the workshop, the participants were exposed to various labs of the institutes and interaction with about their research problems. Dr. Anjani (Asistant Professor, BBAU) gave an overview on the STUTI and its activities funded by DST. Dr. Anjani also gave brief about DST and its initiatives on S&T infrastructure. **Second day**, the participants were taken to the laboratory and demonstrated the working principle of NMR and understanding about its software. On the **Third** day, the participants were showed how to obtain data from the software and precautions that needs to be taken to avoid errors. In the **fourth** day's session, participants were instructed on how to operate BET surface analyzer and obtain the data known and data from an unknown sample. On **fifth** and **Sixth** day, the samples bought by the participants were characterized so as to provide hands-on training on the samples preparation and operation of the instruments. On the **Seventh day**, a concluding session held with all the participants including certification and a session on Questions and Answers on technical and software difficulties.

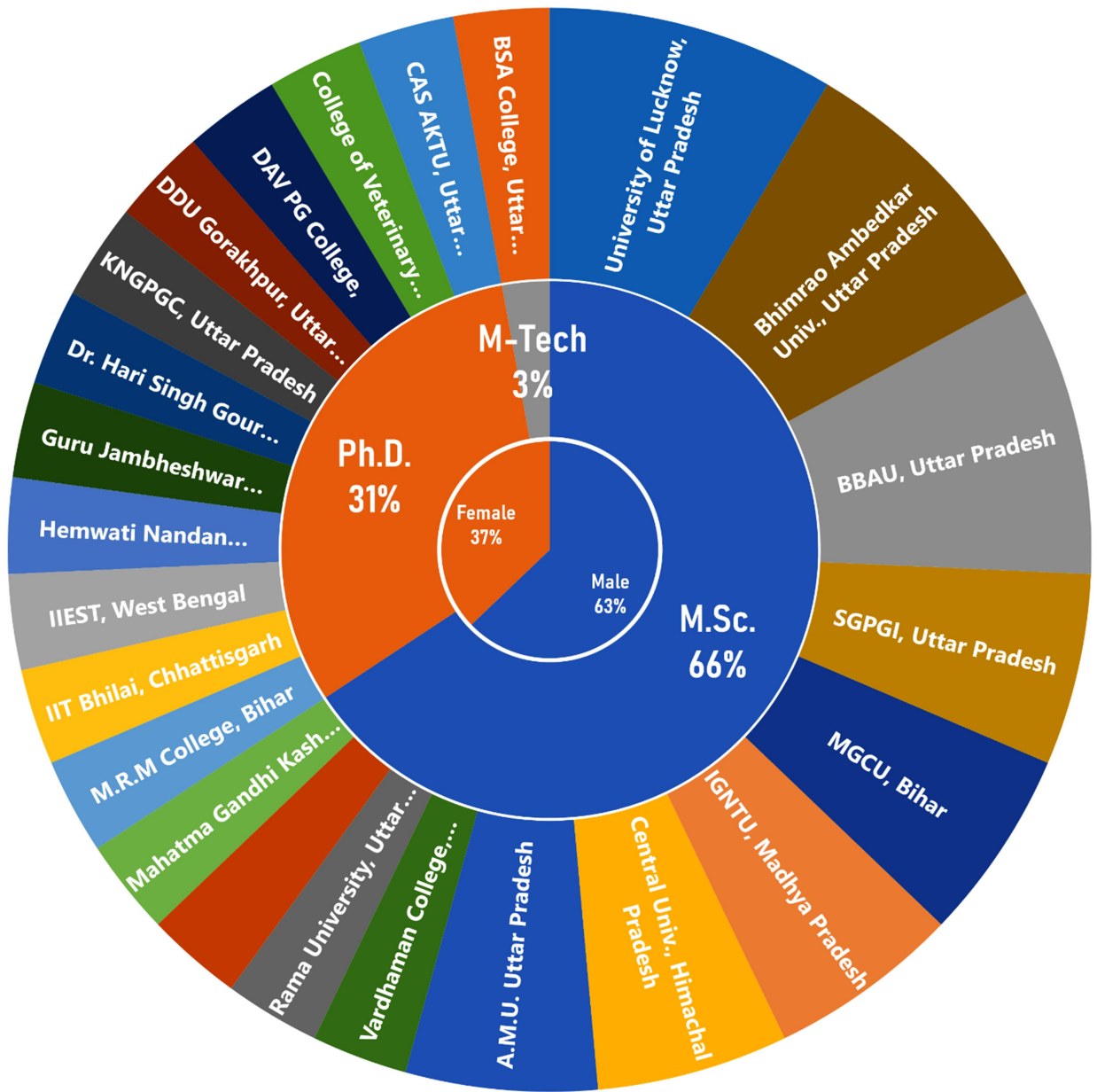
- Types of samples tested

During the technical session, all of the participants expressed an interest in learning from the workshop and more than 10 samples were characterized and tested. It includes: Medicinal Compunds using BET analyzer (such as, small and Nano-scale material compound).

## *Outcome of the workshop*

The STUTI workshop attracted participants from 24 different institutes (**Figure 1**). About 33 participants enrolled and attended the training sessions. The goal of this training event was to bring together participants from many disciplines and raise awareness of the institute's advanced facilities. Throughout the sessions, participants asked major questions regarding theoretical and practical aspects NMR and Bet Surface Analyzer instrumentation techniques. Finally, the feedback from the participants was considered in the evaluation of workshop (**Annex-4**). The majority of the participants was pleased with the training session and suggested that more workshops be held in the future. Few participants also suggested for organizing such a workshop/training session on more troubleshooting techniques of data collection and on other instruments.





**Figure 1:** Participants registered for the workshop from 24 different institutes.

# Annex 1: Brochure for the program.

## ABOUT BBAU:

Babasaheb Bhimrao Ambedkar University was established by an Act passed by the parliament (No. 58 of 1994). The University came in to existence on 10.01.1996 vide GOI, Ministry of HRD, Education Department Notification No. 5-16/GOI/des/U-1 dated 05.01.1996. The basic philosophy and policies of the University are spelt out and enshrined in the University Act and Statutes. The University offers graduate and post-graduate students the knowledge and skills needed to succeed as persons and professionals, and the values and sensitivity necessary to serve the society.

## Objective:

This is a 7-day program aimed to provide hands-on training to the participants on DST funded instruments to promote the expansion of R&D Infrastructure at academic institutions by ensuring transparent access to S&T facilities. STUTI program is also intended to build human resources and its knowledge capacity through open access of S&T Infrastructure across the country. The main focus is to be on Scientists/Professors/ PhDs and Post Doc Fellows actively involved in research across various institutions in the country.

## Scope of the Workshop:

STUTI training includes both theoretical and practical sessions for in-depth knowledge of the instrument and its applications.

Faculty/experts will demonstrate their knowledge of the subject and give appropriate study material to participants, along with an introduction to the instrument's basic fundamentals.

Participants will use the lab facilities and also be allowed to bring their research samples for examination/characterization from the existing S&T facilities.



**HANDS ON TRAINING ON**  
**CHARACTERIZATION TECHNIQUES AND ADVANCE APPLICATION IN RESEARCH (MRS/ METABOLOMIC)**  
*(7-days Training program)*  
 Hosted By  
**Babasaheb Bhimrao Ambedkar University Lucknow**  
 Department of Chemistry  
**Sep 22<sup>nd</sup> to 28<sup>th</sup>, 2022**  
*under STUTI Program*  
*(Synergistic Training program Utilizing the Scientific and Technological Infrastructure)*  
 Department of Science and Technology,  
 Government of India, New Delhi  
 In collaboration with:  
 Indian Institute of Technology Gandhinagar




**Chief Patron,**  
**Prof. Sanjay Singh,**  
 Vice-Chancellor, BBAU

**Chairperson**  
**Prof. Gajanan Pandey**  
 Head, Department of Chemistry,  
 BBAU

**Coordinator**  
**Dr. Anjani Kumar Tiwari**  
 Department of Chemistry, BBAU

**List of Speakers**



**Tentative schedule of workshop**

<p><b>Session I</b>                      + Welcome note                      + Introduction with Participants and Host Center</p> <p><b>Session III</b>                      + Structure elucidation using NMR spectroscopy</p> <p><b>Session V</b>                      + NMR Based Metabolomics</p> <p><b>Session VII</b>                      + Analysis of different structures : small and large</p> <p><b>Session IX</b>                      + NMR &amp; drug discovery</p> <p><b>Session XI</b>                      + Principal of HCT Surface analysis</p> <p><b>Session XII</b>                      + Characterization of different materials/polymers</p>	<p><b>Session II</b>                      + Basics of NMR and NMR Instrumentation</p> <p><b>Session IV</b>                      + 2D NMR &amp; Applications for Small Molecules</p> <p><b>Session VI</b>                      + Hands-on experience and demonstration</p> <p><b>Session VIII</b>                      + Solving small molecule structures using NMR: A tutorial for young researchers</p> <p><b>Session X</b>                      + MRI and in-vivo MRS</p> <p><b>Session XIII</b>                      + Hands-on experience on HCT</p> <p><b>Session XIV</b>                      + Processing and Presentation of NMR/HCT Data in different Applications</p>
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Registration Link: <https://forms.gle/tw2AB1KxZdDbJdeXA>

Venue: **Conference Hall, Old Administrative Building, BBAU Lucknow-226025, U.P**  
 Organizing Secretaries: **Dr. Jyoti Pandey, Dr Shailesh Kumar, Dr Preeti Gupta & Dr Jawahar Lal**

For further queries, feel free to contact us on: Email: [stuti@bbaulko@gmail.com](mailto:stuti@bbaulko@gmail.com) Website: [www.bbau.ac.in](http://www.bbau.ac.in)

## Outcome of the Workshop:

By the end of the workshop, the participants will be able to:

1. Practice good laboratory methods for sample preparation and its preservation.
2. Design of experiments for a thorough understanding of step by step manner.
3. Understanding the basic operations of the instruments and know-how to operate, troubleshoot along with maintenance of the instrument.
4. Critical evaluation of the experimental approaches and data analysis.

## Registration Procedure:

- Interested candidates have to fill the online form (link given below) on or before **(08/09/2022)**.
- Candidates will be selected according to eligibility and available seats. The confirmation of selection will be communicated to the selected candidates by **(10/09/2022)** through email ([stuti@bbaulko@gmail.com](mailto:stuti@bbaulko@gmail.com))

## General Information:

- There is no registration fee
- Mode of the training program will be offline.
- Number of participants is limited to 50 and selection will be based on a screening process of their resume.
- Registration Kit, Course material and Certificate of participation will be provided to the participants.
- Local Hospitality: (Accommodation & Meal) will be provided. The train fare (AC 3-Tier) by shortest route will be reimbursed to the selected outstation participants.



**Annex 2: List of participants registered and their attendance during the workshop.**

Sr. No.	Candidate Name	Gender	Educational Qualification	University/Institute
1	Rambabu kusuma	Male	M.Sc. (Chemistry)	Aligarh Muslim University, Uttar Pradesh
2	Yashvant Kashyap	Male	M.Sc. (Chemistry)	
3	Anupama Anjali	Female	M.Sc. (Organic Chemistry)	BSA College Of Engineering & Technology, Mathura, Uttar Pradesh
4	Sakshi	Female	M.Sc. (Chemistry)	Babasaheb Bhimrao Ambedkar University Lucknow, Uttar Pradesh
5	Shiv Kumar Jayant	Male	Ph.D. (Biochemistry)	
6	Subrata Ghosh	Male	Ph.D. (Chemistry)	
7	Madan Singh	Male	Ph.D. (Chemistry)	Central University of Himachal Pradesh, Shahpur Campus, Himachal Pradesh
8	Mahendra Vyas	Male	Ph.D. (Chemistry)	
9	Ravi Prakash	Male	Ph.D. (Chemistry)	Centre for Advanced Studies, AKTU, Uttar Pradesh
10	Shashikant Shingdilwar	Male	M.Sc. (Organic Chemistry)	College of Veterinary Science and Animal Husbandry, Ayodhya, Uttar Pradesh
11	Munish Sharma	Male	M.Sc. (Botany)	D. A. V. P. G. College Gorakhpur, Uttar Pradesh
12	Praveen kumar	Male	M.Sc. (Chemistry)	Deen Dayal Upadhyay Gorakhpur University, Gorakhpur, Uttar Pradesh
13	Munna Prasad Gupt	Male	Ph.D. (Organic Chemistry)	Kashi Naresh Government PG College, Gyanpur, Bhadohi, Uttar Pradesh
14	Poonam Shukla	Female	Ph.D. (Chemistry)	Dr. Bhimrao Ambedkar University, Agra, Uttar Pradesh
15	Rakesh Kumar Gupta	Male	M.Sc. (Veterinary Pathology)	
16	Babita Chaudhary	Female	Ph.D. (Organic Chemistry)	
17	Nidhi Awasthi	Female	Ph.D. (Physics)	Dr. Hari Singh Gour University, Sagar, Madhya Pradesh
18	Swati	Female	M.Sc. (Chemistry)	Guru Jambheshwar University of Science & Technology, Hisar, Haryana
19	Nitya arora	Female	M.Sc. (Biotechnology)	Hemwati Nandan Bahuguna Govt. P.G. College, Prayagraj, Uttar Pradesh
20	Sanjeev Kumar Patel	Male	M. Pharm (Chemistry)	Indira Gandhi National Tribal University, Madhya Pradesh
21	Meenakshi	Female	M.Sc. (Microbiology)	
22	Divya Varshney	Female	M.Sc. (Microbiology)	Indian Institute of Engineering Science and Technology, Howrah, West Bengal
23	Alok Kumar	Male	M.Sc. (Material Science & Tech)	Indian Institute of Technology Bhilai, Chhattisgarh
24	Sanjeev Porwal	Male	Ph.D. (Chemistry)	M.R.M College/Lalit Narayan Mithila University, Bihar
25	Sudeshana	Female	M.Sc. (Organic Chemistry)	Mahatma Gandhi Kashi Vidyapith University, Varanasi, Uttar Pradesh
26	Vipul Vaibhav Mishra	Male	M-Tech (Nanotechnology)	Mahatma Gandhi Central University, Motihari, Bihar
27	Vaibhav Pandey	Male	M.Sc. (Chemistry)	
28	Huda khanam	Female	M.Sc. (Chemistry)	NIT Warangal, Telangana State
29	Mohd Faheem	Male	M.Sc. (Chemistry)	Rama University, Mandhana, Kanpur, Uttar Pradesh
30	Akanksha Mishra	Female	M.Sc. (Chemistry)	SGPGI, Lucknow, Uttar Pradesh
31	Neelam Gautam	Female	M.Sc. (Chemistry)	
32	Hariom Kumar	Male	M.Sc. (Chemistry)	
33	Alok Kumar Singh	Male	Ph.D. (Chemistry)	University of Lucknow, Uttar Pradesh
34	Vijay Kumar	Male	M.Sc. (Chemistry)	
35	Pradeep Kumar Pandey	Male	M.Sc. (Chemistry)	Vardhaman College, Bijnor, Uttar Pradesh

### Annex 3: Scheduled activities during the workshop.

Day 1	Day 2	Day 3	Day 4
8.30 am: Registration 9.00 am: Inaugural session 10.00 am: Introduction 10.30 am: Expert Lecture (S-1) 11.30 am: Expert Lecture-(S-2) 12.30pm: Lunch 2.00 pm: Hands on training 4.00 pm: Tea break 4.30 pm : Campus visit	9.00 am: Expert Lecture (S-3) 10.00am: Tea break 10.30am: Expert Lecture-(S-4) 12.30pm: Lunch 2.00 pm : Hands on training 4.00 pm : Tea break	9.00 am: Expert Lecture (S-5) 10.00 am: Tea break 10.30am: Expert Lecture-(S-6) 12.30pm: Lunch 2.00 pm: Hands on training 4.00 pm: Tea break	9.00am: Expert Lecture (S-7) 10.00 am: Tea break 10.30 am: Expert Lecture-(S-8) 12.30pm: Lunch 2.00 pm: Hands on training 4.00 pm: Tea break
Day-5	Day 6	Day 7	
9.00am: Expert Lecture (S-9) 10.00am: Tea break 10.30am: Expert Lecture-(S-10) 12.30pm: Lunch 2.00 pm; Hands on training 4.00 pm : Tea break	9.00am: Expert Lecture (S-11) 10.00am: Tea break 10.30am: Expert Lecture-(S-12) 12.30pm: Lunch 2.00 pm: Hands on training 4.00 pm: Tea break	9.00am: Interactive session 11.00am: Tea break 11.30 am: closing remarks	

#### Annex 4: Feedback summary

Sr. No.	Content	% Rating
1.	Overall grading of the programme with reference to relevance of course module/content etc	98 % rated above 8 points
2.	Overall grading of the facilities provided by the institute i.e. Hostel, mess, class rooms, transport/infrastructure etc.	99 % rated above 8 points
3.	Overall grading of the faculty members conducting the training	99 % rated above 8 points
4.	How do you rate the overall training methodology	97 % rated above 8 points
5.	How far the field visit is relevant and related to your research study	98 % rated above 8 points
6.	Usefulness of this training in your current role	99 % rated above 8 points
7.	Usefulness of this training in future work/job you may handle	98 % rated above 8 points
8.	How far have you benefitted from interaction with the fellow participants of the training	97 % rated above 8 points
9.	How far the course material supplied relevant and related to the training curriculum	99 % rated above 8 points
10.	Overall grading of the process of training	99 % rated above 8 points
11.	Your recommendation to your peers/colleagues for the training programme	96 % rated above 8 points