

**National Level Hands-on Training Program**

**On**

**“Mass Spectrometry”**

**Organized by**

**Division of Biological Sciences, Indian Institute of Sciences (IISc),  
Bangalore**

**And**

**JSS Academy of higher education and research (JSS AHER), Mysuru**

**Sponsored by**

**The Department of Science and Technology, Synergistic Training program  
Utilizing the Scientific and Technological Infrastructure (DST-STUTI)  
scheme**

## Program Schedule

	<b>MASS SPEC WORKSHOP SCHEDULE 2nd - 8th January 2023</b>
<b>2nd Jan 2023 Monday</b>	
09.00 - 9.30 am	Registration
09.30 - 10.30 am	Lecture 1: Lecture by - Prof. P. Balaram
10.30 - 11.15 am	Lecture 2: Introduction to mass spectrometry (Instrumentation and Types) - Mr. Venkatesh (Bruker)
	Tea Break
11.30 - 12.15 pm	Lecture 3: Introduction to MALDI Mr. Venkatesh (Bruker)
12.15 - 12.45 pm	Workshop Inauguration
	Lunch break
2.00 - 5.00 pm	Lab/ Demo/Hands-on session
<b>3rd Jan 2023 Tuesday</b>	
09.30 - 10.15 am	Lecture 4 : Concept and instrumentation of GC/Q-TOF and applications -Chandrashekar (Agilent)
10.15 - 11.00 am	Lecture 5 : Metabolite workflow solution by GC/MS - Chandrasekar (Agilent)
11.00 - 11.30 am	Talk by SCIEX
	Tea break
11.45 - 1.00 pm	Lab/ Demo/Hands-on session
	Lunch break
2.00 - 5.00 pm	Lab/ Demo/Hands-on session
<b>4th Jan 2023 Wednesday</b>	
09.30 - 10.15 am	Lecture 6 : Mass Spectrometry in Metabolomics - Dr. Vinay Bulusu
10.15 - 11.00 am	Lecture 7 : Using omics to investigate a novel glycode program in early breast cancer migration - Dr. Ramray Bhat
11.00 - 11.30 pm	Talk by Bruker
	Tea break
11.45 - 1.00 pm	Lab/ Demo/Hands-on session
	Lunch break
2.00 - 5.00 pm	Lab/ Demo/Hands-on session
<b>5th Jan 2023 Thursday</b>	
09.30 - 10.15 am	Lecture 8: Delineating Protein PTMs using High Resolution Orbitrap Mass spectrometry. Dr. Saravanan Kumar (Thermo scientific)
10.15 - 11.00 am	Lecture 9: Single Cell Proteomics workflow to interrogate the granularity of biological systems. - Dr. Sarvanan Kumar (Thermo scientific)
11.00 - 11.30	Talk by Thermofisher scientific

	Tea break
11.45 - 1.00 pm	Lab/ Demo/Hands-on session
	Lunch break
2.00 - 5.00 pm	Lab/ Demo/Hands-on session
<b>6th Jan 2023 Friday</b>	
9.00 - 6.00 pm	SITE VISIT - SCIEX MASS SPECTROMETRY FACILITY
<b>7th Jan 2023 Saturday</b>	
09.30 - 10.15 am	Lecture 10 – Do’s and Don’ts in proteomics and Mass spectrometry Dr.Sushma IISc
10.15 - 11.00 am	Lecture 11 - An overview on de-novo and data based guided sequencing of peptides and proteins by mass spectrometry – Dr.Sanjeev Kumar - NCBS
	Tea break
11.30 - 12.15 pm	Lecture 12 - Mass spectrometry based site-specific N-glyco profiling of proteins Dr.Gnanesh Kumar from CFTRI
12.15 - 1.00 pm	Lecture 13 - Analysis lectures - Talk by valerian Chem - Gagandeep
	Lunch break
2.00 - 2.45 pm	Lecture 14 - Analysis lectures - Talk by valerian Chem - Gagandeep
	Tea break/ CLOSE
<b>8th Jan 2023 Sunday</b>	
9.30 - 12.00	Lab/ Demo/Hands-on session
12.00-12.30 pm	Valedictory
	Lunch

## List of Participants

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## Report

### Day 1 (02.01.2023)

The DST STUTI Training programme on “Mass Spectrometry” mainly focused to train the participants on basics of Mass Spectrometry, profiling small molecule and protein by MALDI and LCQTOF, Profiling of volatile compounds by GCMS and acquisition and data analysis by effective lectures and hands on sessions. The brochure for the training programme was widely circulated through the JSS AHER website as well as on social media platforms, WhatsApp groups, etc. For the training programme, more than 150 applications were received out of which 30 participants were selected. The participants were Faculty Members, Teaching Assistants, Research Scholars, Post-doctoral Fellows and Post Graduate students from chemistry and Life Sciences backgrounds. All except the in-house participants were accommodated in the Hoysala Guest House at IISc Campus.



### **Inauguration of the DST STUTI training program**

The Registrar, Dr. Manjunatha B, presided over the programme insisting on the utilization of the instrumentation facilities at IISc, the importance of knowledge enhancement and how such events are helpful in bringing all the resources and the knowledge under one roof. Finally, Dr Dhanya B E, Project co-ordinator proposed the Vote of Thanks.

The schedule of the programme included four - five sessions per day with resource lectures in the first & second session followed by hands on training for the third & fourth sessions. The participants we offered working tea and lunch at the respective venues of the sessions.



The day one started with a lecture by Prof. Padmanabhan Balam National Centre for Biological Sciences, Bangalore. He gave a talk about “Mass spectrometry in the analysis of peptides and proteins”. He provided all the basic knowledge about the Mass Spectrometry and gave his insights about basic principles of polypeptide fragmentation in the gas phase, a prerequisite for peptide sequencing followed by interaction of participants

The second lecture was delivered by Mr. Venkatesh Sankarasetty, Bruker India Scientific Pvt. Ltd on the “Basics of Mass Spectrometry and its applications”, which gave the participants a detailed view of Mass Spectrometry instrumentation, workflow, varieties starting from Single Quadrupole to FTMS. He also spoke about MALDI (Matrix Assisted Laser Desorption/Ionization) which is a soft ionization technique in biological mass spectrometry. It is generally combined with TOF-MS (Time-of-flight mass spectrometry) technology to determine the molecular mass or better mass-to-charge ratio ( $m/z$ ) of analytes and its applications.



**Mr. Venkatesh Sankarasetty, Bruker India Scientific Pvt. Ltd delivering his talk**

The participants were divided into 4 groups as there was 4 main demo instruments i.e. Orbitrap fusion, GCMS, MALDI TOF and LC-ESI QTOF. All the participants are trained about each equipment's instrumentation and working methodologies. This demonstration carried out from 2<sup>nd</sup> January to 5<sup>th</sup> January, in four days all the four groups were demonstrated each instrument per day, which is carried over in a rotational manner.

Orbitrap fusion, GCMS, MALDI TOF and LC-ESI QTOF instruments were explained and demonstrated by Dr. Saravanan Kumar and his team members from Thermo Fisher Scientific India, Chandrasekar kandaswamy from Agilent Technologies, Mr. Venkatesh Sankarasetty from Bruker India Scientific Pvt. Ltd respectively for the four consecutive days. The participants were given an in-depth knowledge of the instrumentation, key features, and the applications of each instrument and all the sessions were open to interaction, so the participants utilized it thoroughly to get all their doubts cleared.





**Orbitrap fusion, By Dr Sarvanan Kumar (Thermo scientific)**

### **Day 2 (03-01-2023)**

The day two started with the resource lecture on “GC/QTOF and its applications” by Chandrasekar kandaswamy, Product Manager- GC GCMS, Agilent Technologies. He explained how GC/QTOF is used as an analytical tool to identify the unknown volatile compounds and its applications. Also spoke on “Metabolite workflow solution by GC/MS” as how Gas chromatography–Mass spectrometry (GC–MS) based metabolite profiling of biological or plant samples is one of the key technologies for metabolite profiling. After that another lecture was delivered by Jayant of SCIEX. Then it was followed by Demonstration session.



**Concept and instrumentation of GCMS and applications – Chandrashekar (Agilent)**

### **Day 3 (04-01-2023)**

Day 3 started with the lecture session by Prof. Paturu Kondaiah, he spoke about the cancer, characteristics of cancerous cells and how mass spectrometry is used for the study of metabolomics. Followed by a talk by Dr. Vinay Bulusu, Assistant Professor, Indian Institute of Science Education and Research, Berhampur. He spoke about the basics of a metabolomics pipeline and gave some examples from his own research experience. This was followed by a talk by Sricharan Nethala, Bruker India Scientific Pvt. Ltd on “Bruker’s next gen mass spectrometry solutions - Enhancing workflow capabilities for Translational Mass Spectrometry.



**Talk by Prof. Paturu Kondaiah**

#### **Day 4 (05-01-2023)**

The day 4 started with theoretical session on “Delineating Protein PTMs using High Resolution Orbitrap Mass spectrometry” by Dr. Saravanan Kumar from Thermo Fisher Scientific India, which gave the participants an insight of recent advancements in fragmentation principles such as EThCD, PTCR, UVPD coupled to ultra-high-resolution mass spectrometry which has been shown to yield complementary and less complex fragmentation information.

He also spoke on “Single cell proteomics workflow to interrogate the granularity of biological systems” as how the recent developments in Liquid chromatography, High-Resolution Mass spectrometry (LC-HRMS) and automated sample preparation tools helping the researchers to

assess & get 1000 proteins qualitatively and quantitatively from single cell. Then it was followed by demonstration sessions.



**Explanation of MALDI-TOF Instrumentation and Its working mechanism**

### **Day 5 (06-01-2023)**

On day 5, all the participants were made to visit the Mass Spec facility at SCIEX for which a bus has been arranged from Division of Biological Sciences, IISc to SCIEX. We have reached SCIEX around 10:00 AM. There they have arranged the theoretical sessions on many topics which were very intense and helpful for many of the participants in their research. In the beginning a talk was delivered on “Introduction to the mass spectrometry and its general applications” followed by “Mass spectrometry platforms from SCIEX and applications” In the middle the participants were made to visit lab and get the demonstration of their advanced instruments. Again, the theoretical session “LC-MS applications in BioPharma “followed by “Introduction to Capillary Electrophoresis and its applications” and they have also covered

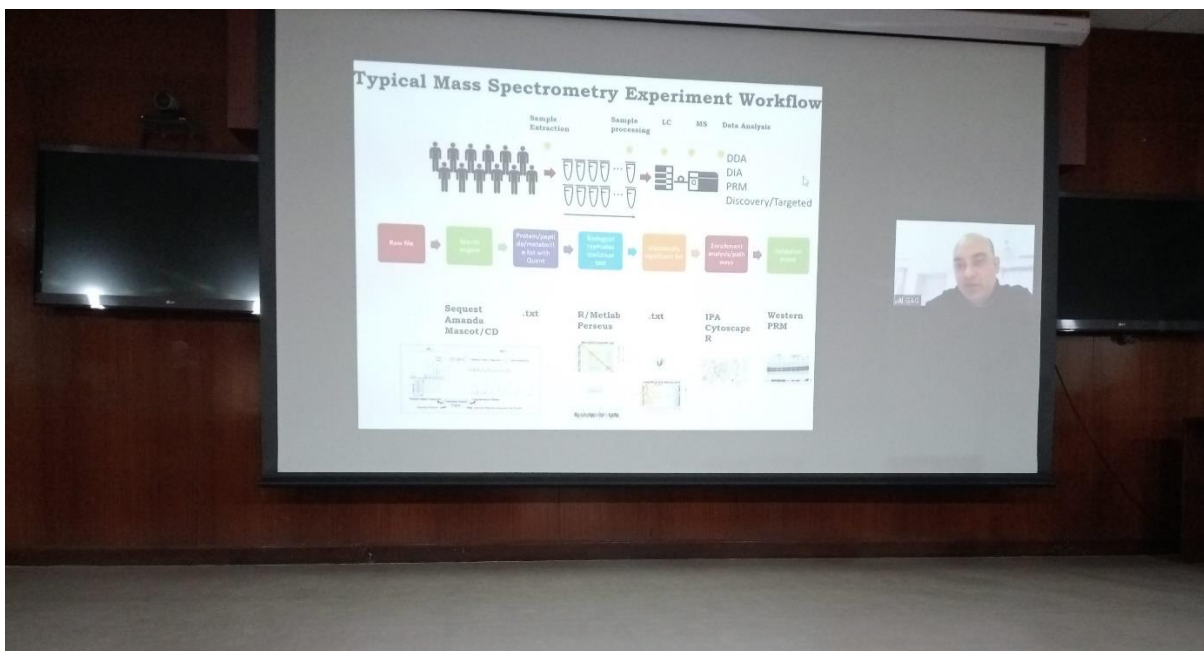
many other aspects. The participants got many of their doubts cleared. Overall, it was a very knowledgeable & a fruitful day.



**SITE VISIT Mass Spec facility at SCIEX SPECTROMETRY FACILITY**

### **Day 6 (07-01-2023)**

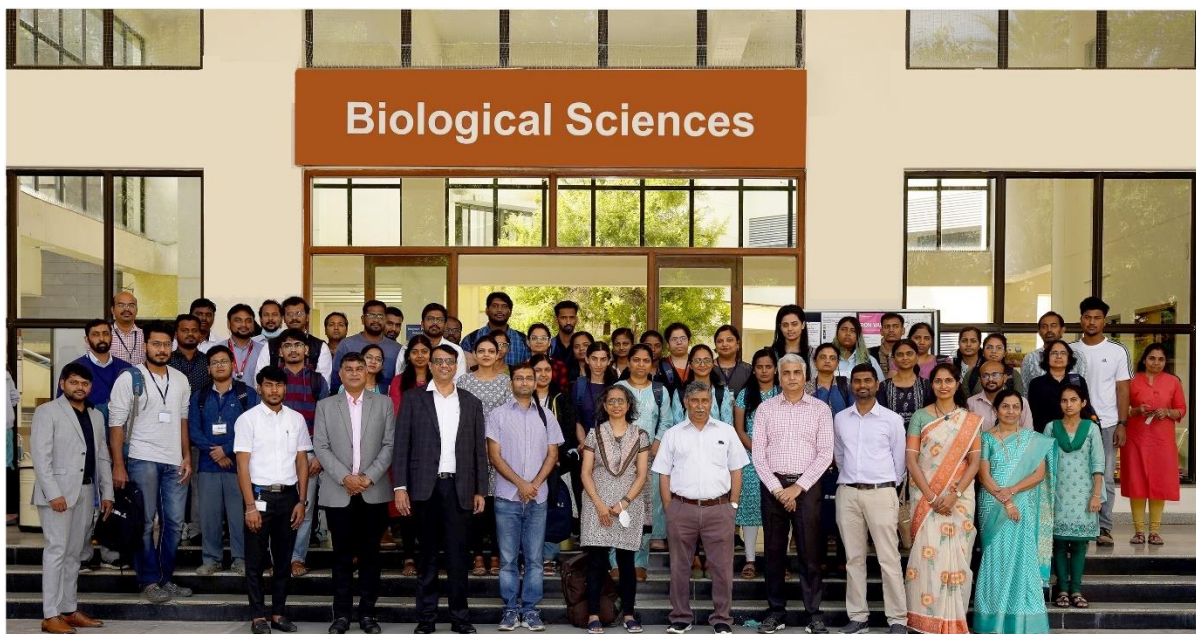
The day started with lecture session by Dr Ramray Bhat on “Using omics to investigate a novel glycode program in early breast cancer migration”, which was an intensive session, after which the session was open for discussion by which the participants were benefitted. The next session was on “Choosing the Right Bio separation Method In Proteomics” delivered by Dr Sushma Krishnan, which gave the participants a detailed view about principles, and methods for biomolecule separation, particularly protein purification and also about different types of chromatographic matrices, especially monolithic supports. After which a talk on “Data analysis tools for proteomics experiments by “Dr.Gagan Deep Jhingan (Valerian Chem Pvt Ltd) was held through Online Mode.



### Day 7 (08-02-2023)

On day seven participants were informed to gather at the mass spec facility, IISc so that the participants got all their basic doubts cleared by Mrs Sunitha Prakash and Mr Muralidaran who are the technical staffs of Mass Spec facility, IISc.





## *Workshop on Mass Spectrometry*

2nd - 8th January 2023

Biological Sciences Auditorium, Indian Institute of Science, Bengaluru