

FACT SHEET/ TERMS AND CONDITIONS
High Resolution Mass Spectrometry (HRMS) Services
(Revised: 12th October, 2024)

FEATURES

- HRMS will be performed on an Agilent QTOF (model number: 6540 UHD or 6550 UHD). UHPLC, nanoLC models are available as front end with ESI, API, APPI & ASAP as source of Ionization. GC-MS will be performed on Agilent 7890 A & 5977 B equipped with Headspace and Liquid Sampler.
- High Resolution Mass Analysis for
 - Synthetic organic samples (MS and tandem MS)
 - Peptide and intact protein analysis
 - Peptide mass fingerprinting using tandem MS
 - Natural Product extracts (Only MS)
- GC MS and LC MS with established protocols and methods can also be undertaken on a case to case basis. Contact CAMS for further details.
- Do It Yourself (DIY) Data Processing & Analysis using the following Software: Spectrum Mill, BioConfirm, Mass Profiler Professional
- CAMS & Venture Center will be willing to work with researchers on new method development and other analytical requirements using MS. These exercises need to be discussed separately with the Venture Center management.
- Venture Center only supports researchers with scientific data. Venture Center is not an accredited testing lab. Venture Center does not provide certificates. This data cannot be used for any certifications/ approvals. Venture Center does not offer to certify or confirm data in front of any agency or any court of law.

ELIGIBILITY

- The MS service is open to all technology developers, entrepreneurs, academic institutes, researchers and industries. However, priority shall be given to:
 - Proof-of-concept studies aiming to create to start-ups
 - Requests from incubatee companies (resident and AIP)
- Venture Center retains the right to refuse applications without providing a reason.

TERMS & PRICING

GENERAL CONDITIONS:

- This service sheet only offers standardized experimental protocols on Mass Spectrometry available with Venture Center. The terms and conditions are specifically for these standardized studies. All publications, posters and presentations by researchers using MS data from Venture Center are expected to acknowledge use of Venture Center facilities as follows in the acknowledgement section: "Mass Spectrometry analysis were performed by at the DBT-BIRAC supported Center for Applications of Mass Spectrometry (CAMS) at Venture Center BioIncubator at CSIR-NCL, Pune, India"
Any analysis involving intellectual inputs relating to design of experiments or new method development etc are treated different from the above mentioned standardized studies. Such collaborative efforts involving Venture Center staff have to be approved by the Venture Center management on a case-to-case basis. The terms of engagement shall be different in these cases.

- Typically, in these cases, Venture Center requires that all publications, posters and presentations by researchers using Mass Spectrometry data generated with intellectual contributions from Venture Center staff be acknowledged through co-authorship.
- Experiments can fail for various reasons. Venture Center shall not be liable for the loss of samples and time in this case.

HOW TO APPLY?

- Request a discussion meeting with the Manager of the Center for Applications of Mass Spectrometry (CAMS). Understand what can and cannot be done at CAMS.
- Fill and submit application form. Venture Center raises an invoice against this application form. Payments are expected in full in advance prior to start of MS analysis.

PAYMENT TERMS

- All services are offered against advance payment in full. Service tax and other taxes applicable at the prevailing rate shall be in addition to the above.
- Payment via a) Demand Draft, b) Cheque payable in Pune or at par or c) bank transfer are possible. All payments have to be made in the name of “**Entrepreneurship Development Center**”
- Booking once made shall not be transferrable or payment made thereof shall be non- refundable. On the occasional case where Venture Center is unable to carry out the experiment due to equipment failure or contamination or absence of staff, Venture Center shall inform the applicant immediately and refund the payments made to it.

USAGE TERMS

- Service users shall not (intentionally or otherwise) do or say anything to suggest that
- Venture Center or CSIR-NCL has any connection to the samples being studied.
- Venture Center shall maintain records of MS data for each applicant. These will be made available to the applicant prior to billing. User agrees that in case of any dispute, Venture Center’s assessment of the number of samples / number of hours and fees applicable will be considered final and the same shall be used for billing purposes.
- Venture Center reserves the right to deny use of its services at its sole discretion, without providing any reason whatsoever. In case of scheduling conflicts, Venture Center will be the sole and final authority on the schedule and availability of the MS analysis

SAMPLE HANDLING

- It is the sole responsibility of the customer to clearly label the sample at the time of submission; once the sample is received no changes in the labeling will be allowed or done by analyst.
- Sample label should in minimum contain Name, Quantity, storage conditions and any handling precaution if applicable
- Samples, if left any after analysis will be stored at specified conditions up till ONE MONTH after the dispatch of the results. After the storage period is over the sample will be handed over to the concerned department for destruction.
- All sample preparation is to be done by the client. Samples are to be provided in LC-MS grade solvents and in ready to inject form only preferably filtered through a 0.22u filter.

DATA POLICY

- Processed data files will be provided in pdf and/or excel format to the applicant only.
- If the client requires the raw data of the analysis they may specify it at the time of sample submission and the same can be provided to the applicant at a Fee of Rs. 500/-
- Raw data & processed data files will be stored at our end till SIX MONTHS from the time of analysis. The files would be then permanently deleted.
- If the client requires the Calibration record of the Instrument they may specify it at the time of sample submission and the same can be provided to the applicant at a Fee of Rs. 5000/-

DISCOUNTS

- Venture Centre's standard discounts shall apply. See latest discounts at: <http://www.venturecenter.co.in/discounts.php>
- Only one discount may be availed at a time.
- Photocopies of Valid ID card and letter of support on company's /Institute's letter head should be submitted for availing discount facility

It is hereby declared that the undersigned has read and understood the terms and conditions and the Pricing as mentioned in Annexure (I, II, III) of Venture Center's HRMS services and accepts the same.

For and on Behalf of
(Name of the Company)

(Name of the authorized signatory)

ANNEXURE-I PRICE LIST FOR HRMS SERVICES

Qualitative LC-MS services

Small Molecules Analysis (Molecules having mass less than 3200 Da)

Service code	Service	Available resource	Price	Deliverables	Requirement from client
SM01	Mass determination only using direct injection (No LC)	ESI/APCI/ASAP Ionization source	Rs. 500/- per sample per polarity	MS spectra/report in pdf or excel	Sample solubility Polarity of molecules Expected molecular weight and formula
SM02	MS/MS of two masses using direct injection (No LC)	ESI/APCI/ASAP Ionization source CID fragmentation	Rs. 1500/- per sample per polarity	MS spectra /report in pdf or excel	Sample solubility List of m/z or mass for ms/ms

Service code	Service	Available resource	Price		Deliverables	Requirement from client
SM03	Mass determination and separation using UPLC-MS	ESI/APCI Ionization source Column: see the annexure	Run time	Price per sample	Analysis report in pdf or excel MS spectra in excel or pdf of all LC peaks	Sample solubility Polarity of molecules Expected molecular weight and formula Client can provide their own method suitable for column.
			0-15 min	1500		
			15.1-30 min	2500		
			30.1-60 min	3500		
		<ul style="list-style-type: none"> Price is for single polarity (positive or negative ion mode) Extra charges beyond 60 min: Rs. 1000/30min Replicate: similar charges 				
SM04	Mass determination, Fragmentation (MS/MS) and separation using UPLC-MS	ESI/APCI Ionization source Column: see the annexure Method: Auto MS/MS of all major ions	Run time	Price per sample	Analysis report in pdf or excel MS spectra in excel or pdf of all LC peaks MS/MS spectra in excel or pdf of all LC peaks	Sample solubility Polarity of molecules Client can provide their own method suitable for column.
			0-15 min	2500		
			15.1-30 min	3500		
			30.1-60 min	4500		
		<ul style="list-style-type: none"> Price is for single polarity (positive or negative ion mode) Extra charges beyond 60 min: Rs. 1000/30min Replicate: similar charges 				

Service code	Service	Available resource	Price		Deliverables	Requirement from client
SM05	Mass determination and separation using UPLC-UV-MS	DAD, ESI/APCI Ionization source Column: see the annexure	Run time	Price per sample	Analysis report in pdf or excel UV & MS spectra in excel or pdf of all observed peaks	Sample solubility Polarity of molecules Expected molecular weight and formula Client can provide their own method suitable for column.
			0-15 min	2500		
			15.1-30 min	3500		
			30.1-60 min	4500		
		<ul style="list-style-type: none"> Price is for single polarity (positive or negative ion mode) Extra charges beyond 60 min: Rs. 1000/30min Replicate: similar charges 				
SM06	Mass determination, Fragmentation (MS/MS) and separation using UPLC-UV-MS	DAD, ESI/APCI Ionization source Column: see the annexure Method: Auto MS/MS of all major ions	Run time	Price per sample	Analysis report in pdf or excel UV & MS spectra in excel or pdf of all Observed peaks MS/MS spectra in excel or pdf of all Observed peaks	Sample solubility Polarity of molecules Client can provide their own method suitable for column.
			0-15 min	3500		
			15.1-30 min	4500		
			30.1-60 min	5500		
		<ul style="list-style-type: none"> Price is for single polarity (positive or negative ion mode) Extra charges beyond 60 min: Rs. 1000/30min Replicate: similar charges 				

Service code	Service	Available resource	Price	Deliverables	Requirement from client
MA01	Metabolite screening with exact mass (only MS)	ESI/APCI Ionization source with UPLC Column: see the annexure Matching with METLIN database /Lipidmap/Database provided by client	Rs. 2500/- per sample per polarity <ul style="list-style-type: none"> Extra charges beyond 30 min: Rs. 500/30min Replicate: similar charges 	Exact mass and isotopic pattern based Compound screening report in excel	Ready to inject sample extracted in solvent compatible with MS For powdered samples, solubility is required λ_{\max}
MA02	Untargeted Metabolomics (only MS)	ESI/APCI/ASAP Ionization source with UPLC Column: see the annexure Matching with METLIN database /Lipidmap/Database provided by client	Rs. 10000/- per sample <ul style="list-style-type: none"> Includes duplicate run of 30 min for positive and negative ion mode Extra charges beyond 30 min: Rs. 500/30min 	Exact mass and isotopic pattern based Metabolite identification Fold change analysis	Ready to inject sample extracted in solvent compatible with MS For powdered samples, solubility is required λ_{\max}

Service code	Service	Available resource	Price	Deliverables	Requirement from client
MA03	Metabolite screening with exact mass by UPLC-UV-MS	DAD, ESI/APCI Ionization source with UPLC Column: see the annexure Matching with METLIN database /Lipidmap/Database provided by client	Rs. 3500/- per sample per polarity <ul style="list-style-type: none"> Extra charges beyond 30 min: Rs. 1000/30min Replicate: similar charges 	UV Profile, Exact mass and isotopic pattern based Compound screening report in excel	Ready to inject sample extracted in solvent compatible with MS For powdered samples, solubility is required λ_{max}
MA04	Untargeted Metabolomics UPLC-UV-MS	DAD, ESI/APCI/ASAP Ionization source with UPLC Column: see the annexure Matching with METLIN database /Lipidmap/Database provided by client	Rs. 14000/- per sample <ul style="list-style-type: none"> Includes duplicate run of 30 min for positive and negative ion mode Extra charges beyond 30 min: Rs. 1000/30min 	UV Profile, Exact mass and isotopic pattern based Metabolite identification Fold change analysis	Ready to inject sample extracted in solvent compatible with MS For powdered samples, solubility is required λ_{max}

Proteomics: (Biomolecules (protein/peptide) having mass more than 3200 Da)

Service code	Service	Available resource	Price		Deliverables	Requirement from client
			Standard Run time	Price per sample		
PA01	Peptide mass fingerprinting, Identification with Spectrum Mill software	ESI/Nano ESI Ionization source with UPLC/ Nano flow LC Column: see the annexure	0-15 min	2000	Matching report in HTML format with protein sequence given by client or relevant protein database	Proteolytic digest sample in buffer/solvent compatible with MS (see annexure) Or lyophilized sample
			15.1-30 min	3000		
			30.1-60 min	4000		
			Extra charges beyond 60 min: Rs. 1000/30min			
PA02	Peptide Sequencing using data dependent LC-MS/MS	ESI/Nano ESI Ionization source with UPLC/ Nano flow LC Column: see the annexure	0-15 min	2000	Matching report in HTML or excel using spectrum mill software with protein sequence given by client or relevant protein database	Proteolytic digest sample in buffer/solvent compatible with MS (see annexure) Or lyophilized sample
			15.1-30 min	3000		
			30.1-60 min	4000		
			60.1-120 min	6500		
			120.1-180 min	8000		
			Extra charges beyond 60 min: Rs. 1000/30min			
PA03	Intact protein mass determination	ESI/Nano ESI Ionization source with UPLC/ Nano flow LC Column: see the annexure	0-30 min	4000	Deconvoluted mass spectra in pdf or excel	Purified protein sample in buffer/solvent compatible with MS (see annexure) Or lyophilized sample
			30.1-60 min	6000		
			Extra charges beyond 60 min: Rs. 1000/30min			
			Standard Run time			
			Direct injection	2500		

Service code	Service	Available resource	Price		Deliverables	Requirement from client
PA04	Peptide mass fingerprinting, Identification with Spectrum Mill software	DAD, ESI/Nano ESI Ionization source with UPLC/ Nano flow LC Column: see the annexure	Standard Run time	Price per sample	Matching report in HTML format with protein sequence given by client or relevant protein database	Proteolytic digest sample in buffer/solvent compatible with MS Or lyophilized sample λ_{max}
			0-15 min	3000		
			15.1-30 min	4000		
			30.1-60 min	5000		
			Extra charges beyond 60 min: Rs. 2000/30min			
PA05	Peptide Sequencing using data dependent LC-MS/MS	DAD, ESI/Nano ESI Ionization source with UPLC/ Nano flow LC Column: see the annexure	Standard Run time	Price per sample	Matching report in HTML or excel using spectrum mill software with protein sequence given by client or relevant protein database	Proteolytic digest sample in buffer/solvent compatible with MS Or lyophilized sample λ_{max}
			0-15 min	3000		
			15.1-30 min	4000		
			30.1-60 min	5000		
			60.1-120 min	7500		
PA06	Intact protein mass determination	DAD, ESI/Nano ESI Ionization source with UPLC/ Nano flow LC Column: see the annexure	120.1-180 min	9000	Deconvoluted mass spectra in pdf or excel	Purified protein sample in buffer/solvent compatible with MS Or lyophilized sample λ_{max}
			Standard Run time	Price per sample		
			Direct injection	3500		
			0-30 min	5000		
			30.1-60 min	7000		
			Extra charges beyond 60 min: Rs. 2000/30min			

Small Molecules quantitative analysis (Molecules having mass less than 3200 Da)

Service code	Service	Available resource	Price	Deliverables	Requirement from client
SMQ01	Method development UPLC-MS	ESI/APCI Ionization source	Rs. 3000/- per hour	Valid method for quantitative analysis	Standards or reference material Sample solubility Polarity of molecules Expected molecular weight and formula
SMQ02	Quantitative UPLC-MS for small molecules using UPLC	ESI/APCI Ionization source	Rs. 4000/- per hour	Quantitative report based on EIC of molecules in pdf or excel	Standards or reference material Sample solubility Polarity of molecules Expected molecular weight and formula
SMQ03	Method optimization by UPLC- UV-MS	DAD, ESI/APCI Ionization source	Rs. 4000/- per hour	Valid method for quantitative analysis	Standards or reference material Sample solubility Polarity of molecules Expected molecular weight and formula & λ_{max}
SMQ04	Quantitative UPLC-UV-MS for small molecules	DAD, ESI/APCI Ionization source	Rs. 5000/- per hour	Quantitative report based on EIC and UV of molecules in pdf or excel	Standards or reference material Sample solubility Polarity of molecules Expected molecular weight and formula & λ_{max}

Large molecules quantitative analysis (protein/peptide) having mass more than 3200 Da

Service code	Service	Available resource	Price	Deliverables	Requirement from client
LMQ01	Method development UPLC-MS	ESI/Nano flow Ionization source	Rs. 4000/- per hour	Valid method for quantitative analysis	Standards or reference material Sample solubility Polarity of molecules Expected molecular wt. and formula
LMQ02	Quantitative UPLC-MS for large molecule	ESI source	Rs. 5000/- per hour	Quantitative report based on EIC of molecules in pdf or excel	Standards or reference material Sample solubility Polarity of molecules Expected molecular wt. and formula
LMQ03	Method optimization UPLC-UV-MS	DAD, ESI/Nano flow Ionization source	Rs. 5000/- per hour	Valid method for quantitative analysis	Standards or reference material Sample solubility Polarity of molecules Expected molecular wt. and formula λ_{\max}
LMQ04	Quantitative UPLC-UV-MS for large molecules	DAD, ESI source	Rs. 6000/- per hour	Quantitative report based on EIC & UV of molecules in pdf or excel	Standards or reference material Sample solubility Polarity of molecules Expected molecular wt. and formula λ_{\max}

ANNEXURE-II: PRICE LIST FOR GC-MS SERVICES

Service code	Service	Available resource	Price		Deliverables	Requirement from client
			Run time	Price per sample		
GC-01	GC-MS analysis	EI source NIST 2017 Library	0-15 min	1000	GC Chromatogram NIST Library search for 10 peaks	Sample solubility Expected molecular weight and formula
			15.1-30 min	1500		
			Extra every 15 min	500		
GC-02	GC-MS analysis of plant extract	EI source NIST 2017 Library	Run time	Price per sample	GC Chromatogram NIST Library search	Sample prepared in GC compatible solvent
			60 min	4000		
GC-03	Headspace GC-MS analysis	EI source NIST 2017 Library	Run time	Price per sample	GC Chromatogram NIST Library search for 10 peaks	Expected molecular weight
			0-15 min	1500		
			15.1-30 min	2000		
			Extra every 15 min	500		

Service code	Service	Available resource	Price	Deliverables	Requirement from client
GC-04	Method development	EI source NIST 2017 Library	Rs. 3000/- per hour	Valid method for quantitative analysis	Standards or reference material
GC-05	Quantitative GC-MS	EI source NIST 2017 Library	Rs. 4000/- per hour	Quantitative analysis report	Standards or reference material
GC-06	Identification and Quantification of Short Chain Fatty Acids (SCFA)	EI source NIST 2017 Library	Rs. 18000/- for five samples with single point quantification	Identification and quantification of acetate, butyrate, propionate; Chromatogram and MS spectra; Additional Identification of target peaks with NIST reference database; Consultation on sample preparation	Ready to inject samples

ANNEXURE-III: PRICE LIST FOR DATA ANALYSIS & INTERPRETATION

Service code	Service	Available Software	Price	Deliverables	Requirement from client
DA-01	Do It Yourself (DIY) - Data Processing & Analysis	Spectrum Mill; BioConfirm; Mass Profiler Professional (MPP)	Rs. 1,000/- per hour	Brief Technical Training by the CAMS team to give an overview of the software; Separate folder will be made for the client , where the raw data and processed data will be stored; Data will be stored for a period of six months, after which the files will be deleted permanently.	Data files in the required & compatible format; formatted pen drive/external hard disk
DA-02	Advisory Services for Data Analysis & Interpretation	Spectrum Mill; BioConfirm; Mass Profiler Professional (MPP)	TBD	TBD	TBD

IMPORTANT

- Prior appointment is mandatory to avail the above DIY services. Appointments will be allocated on the availability of the Data Analysis Computer Systems .

ANNEXURE-IV: AVAILABLE COLUMNS FOR LC-MS

MAKE	BRAND	STATIONARY PHASE	DIMENSION
AGILENT	ZORBAX	SB-C18	150mm X 0.5mm, 5u
AGILENT	ZORBAX RRHD	HILIC PLUS	100mm X 2.1 mm, 1.8u
AGILENT	ZORBAX ECLIPSE	XDB-C18	150mm X 3.0mm , 3.5u
AGILENT	ZORBAX RRHD	HILIC 300	100 mm x 2.1mm, 1.8u
AGILENT	ZORBAX RRHT	SB-Aq	100 mm X 3.0mm, 1.8 u
AGILENT	ADVANCE BIO	RP-mAb C4	75mm X 2.1mm, 3.5u
AGILENT	ZORBAX RRHT	SB-C18	100 mm X 2.1mm, 1.8u
AGILENT	ZORBAX	EXTENDED C18	50mm X 2.1mm, 1.8u
AGILENT	POROSHELL 120	EC-C18	50mm X 3.0mm, 2.7u
PHENOMENEX	LUNA	C18 (2)	250mm X 4.6mm, 5u
AGILENT	ZORBAX HILIC GUARD COLOUMN	HILIC PLUS	5mm X 2.1mm, 1.8u
AGILENT	ZORBAX ECLIPSE PLUS GUARD COLOUMN	ECLIPSE PLUS C18	5mm X 2.1mm, 1.8u
BENSON	BP-100 H ⁺ CARBOHYDRATE COLOUMN	POLYMERIC	150 mm X 7.8mm, 5u
	ZORBAX 300 (AGILENT BIOLC)	SB-C18	150 mm X 0.1mm, 3.5u
AGILENT	ZORBAX ECLIPSE PLUS	C8	150mm X 2.1mm, 1.8u
AGILENT	ZORBAX RX-SIL	SILICA	250mm X 4.6mm, 5u
AGILENT	POROSHELL 120	HILIC-Z	100 mm X 3.0mm, 2.7 u
AGILENT	ZORBAX 300 (AGILENT BIOLC)	SB-C18	150 mm X 0.075mm, 3.5 u
AGILENT	POROSHELL HPH	C18	100 mm X 4.6mm, 2.7u
AGILENT	ZORBAX ECLIPSE PLUS RRHD`	C18	150 mm X 2.1mm, 1.8u
AGILENT	ZORBAX RRHT	EXTENDED C18	50mm X 2.1mm, 1.8u
AGILENT	ZORBAX 300 (AGILENT BIOLC)	SB-C18	50mm X 0.075 mm , 3.5u

ANNEXURE V: Solvents compatibles LC-MS

S.No.	Buffers	Solvent
1.	Ammonium acetate	Acetonitrile
2.	Ammonium Formate	Methanol
3.	Ammonium biocarbonate	Isopropanol
4.		Ethyl Acetate
5.		Dichloromethane
6.		Chloroform
7.		Formic acid
8.		Hexane
9.		Toluene
10.		Cyclohexane
11.		Water (Deionized)

ANNEXURE VI: Solvents compatibles LC-MS

Solvent	Formula	MW (Da)	Boiling Point (°C)	UV Cutoff (nm)
Acetonitrile	CH ₃ CN	41.05	81.6	190
Chloroform	CHCl ₃	119.38	61.7	245
Dichloromethane	CH ₂ Cl ₂	84.93	40.0	235
Ethanol	CH ₃ CH ₂ OH	46.08	78.5	210
Ethyl acetate	CH ₃ CO ₂ CH ₂ CH ₃	88.12	77.1	260
Diethyl ether	(CH ₃ CH ₂) ₂ O	74.12	34.5	220
Heptane	CH ₃ (CH ₂) ₅ CH ₃	100.21	98.4	200
Hexane	CH ₃ (CH ₂) ₄ CH ₃	86.18	69	200
Isopropanol	CH ₃ CH(OH)CH ₃	60.11	82.4	210
Methanol	CH ₃ OH	32.04	65	205
<i>n</i> -Propanol	CH ₃ CH ₂ CH ₂ OH	60.11	97.4	210
Tetrahydrofuran	C ₄ H ₈ O	72.12	66	215
Toluene	C ₆ H ₅ (CH ₃)	92.15	110.6	285
Water	H ₂ O	18.02	100	none

ANNEXURE VII: LC-MS compatible volatile buffers

1 to 10 mM buffer concentration is usually recommended for LC/MS

Volatile Buffer	Structure	p <i>K_a</i>	Buffer Range
Trifluoroacetic acid	CF ₃ CO ₂ H	0.5	3.8–5.8
Formic acid	HCO ₂ H	3.8	—
Ammonium formate	HCO ₂ NH ₄	3.8	2.8–4.8
Acetic acid	CH ₃ CO ₂ H	4.8	—
Ammonium acetate	CH ₃ CO ₂ NH ₄	4.8	3.8–5.8
4-Methylmorpholine	OC ₄ H ₈ N(CH ₃)	8.4	7.4–9.4
Ammonium bicarbonate	NH ₄ CO ₃ H	6.3/9.2/10.3	6.8–11.3
Ammonium acetate	CH ₃ CO ₂ NH ₄	9.2	8.2–10.2
Ammonium formate	HCO ₂ NH ₄	9.2	8.2–10.2
1-Methylpiperidine	C ₅ H ₁₀ N(CH ₃)	10.1	10.0–12.0
Triethylammonium acetate	CH ₃ CO ₂ NH(CH ₃) ₃	11.0	10.0–12.0
Pyrrolidine	C ₄ H ₈ NH	11.3	10.3–12.3