

Price List: Mass Spectrometry Services

(From 1st April 2019 to 31 March 2020)

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. 1000/- 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
SM03	Mass determination and separation using UPLC	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.
			15 min	1500		
			30 min	2500		
			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. 500/30min • Replicate: similar charges 			

Service code	Service	Available resource	Price	Deliverables	Requirement from client								
SM04	Mass determination, Fragmentation (MS/MS) and separation using UPLC	ESI/APCI Ionization source Column: see the annexure Method: Auto MS/MS of all major ions	<table border="1"> <thead> <tr> <th>Run time</th> <th>Price per sample</th> </tr> </thead> <tbody> <tr> <td>15 min</td> <td>2500</td> </tr> <tr> <td>30 min</td> <td>3500</td> </tr> <tr> <td>60 min</td> <td>4500</td> </tr> </tbody> </table> <ul style="list-style-type: none"> • Price is for single polarity (positive or negative ion mode) • Extra charges beyond 60 min: Rs. 500/30min • Replicate: similar charges 	Run time	Price per sample	15 min	2500	30 min	3500	60 min	4500	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.
Run time	Price per sample												
15 min	2500												
30 min	3500												
60 min	4500												

Metabolites analysis (Molecules having mass less than 3200 Da)

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
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

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	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
			30 min	3000		
			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	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
			30 min	3000		
			60 min	4000		
			120 min	6500		
			180 min	8000		
PA03	Intact protein mass determination	ESI/Nano ESI Ionization source with UPLC/ Nano flow LC Column: see the annexure	Standard Run time	Price per sample	Deconvoluted mass spectra in pdf or excel	Purified protein sample in buffer/solvent compatible with MS (see annexure) Or lyophilized sample
			Direct injection	2500		
			30 min	4000		
			60 min	6000		
Extra charges beyond 60 min: Rs. 1000/30min						

Quantitative LC-MS services

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

Service code	Service	Available resource	Price	Deliverables	Requirement from client
SMQ01	Method development	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 LC-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

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	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 weight and formula
LMQ02	Quantitative LC-MS for large molecules using UPLC	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 weight and formula
LMQ03	Quantitative LC-MS for large molecules using Nano Flow LC	NanoESI source	Rs. 6000/- 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

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	Run time	Price per sample	GC Chromatogram NIST Library search for 10 peaks	Sample solubility Expected molecular weight and formula
			15 min	1000		
			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
			15 min	1500		
			30 min	2000		
			Extra every 15 min	500		
GC-03	Method development	EI source NIST 2017 Library	Rs. 3000/- per hour		Valid method for quantitative analysis	Standards or reference material
GC-04	Quantitative GC-MS	EI source NIST 2017 Library	Rs. 4000/- per hour		Quantitative analysis report	Standards or reference material

Annexures

Available column for LC-MS and GC-MS

LC Columns	
S.No.	Column description
1.	Agilent Zorbax C18 2.1x50mm 1.8 um
2.	
3.	
4.	
5.	
6.	

Available solvent and buffers for LC-MS at CAMS

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)

Solvents And Volatile Buffers compatibles LC-MS

1 to 10 mM buffer concentration is usually recommended for 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

LC-MS compatible volatile buffers

Volatile Buffer	Structure	pK_a	Buffer Range
Trifluoroacetic acid	CF_3CO_2H	0.5	3.8–5.8
Formic acid	HCO_2H	3.8	—
Ammonium formate	HCO_2NH_4	3.8	2.8–4.8
Acetic acid	CH_3CO_2H	4.8	—
Ammonium acetate	$CH_3CO_2NH_4$	4.8	3.8–5.8
4-Methylmorpholine	$OC_4H_8N(CH_3)$	8.4	7.4–9.4
Ammonium bicarbonate	NH_4CO_3H	6.3/9.2/10.3	6.8–11.3
Ammonium acetate	$CH_3CO_2NH_4$	9.2	8.2–10.2
Ammonium formate	HCO_2NH_4	9.2	8.2–10.2
1-Methylpiperidine	$C_5H_{10}N(CH_3)$	10.1	10.0–12.0
Triethylammonium acetate	$CH_3CO_2NH(CH_3)_3$	11.0	10.0–12.0
Pyrrolidine	C_4H_8NH	11.3	10.3–12.3

Format for list of molecules (provide in Excel)

Molecule	Formula	CAS ID (optional)
Caffeine	C ₈ H ₁₀ N ₄ O ₂	58-08-2