MassTech

Breakfast Seminar

@ Room 213C

SPME analysis on a portable mass spectrometer.

Enrico Davoli

June 3rd 2024

IMN ISTITUTO DI RICERCHE FARMACOLOGICHE MARIO NEGRI · IRCCS

Mass Spectrometry Research Center for Health & Environment

MS4HE

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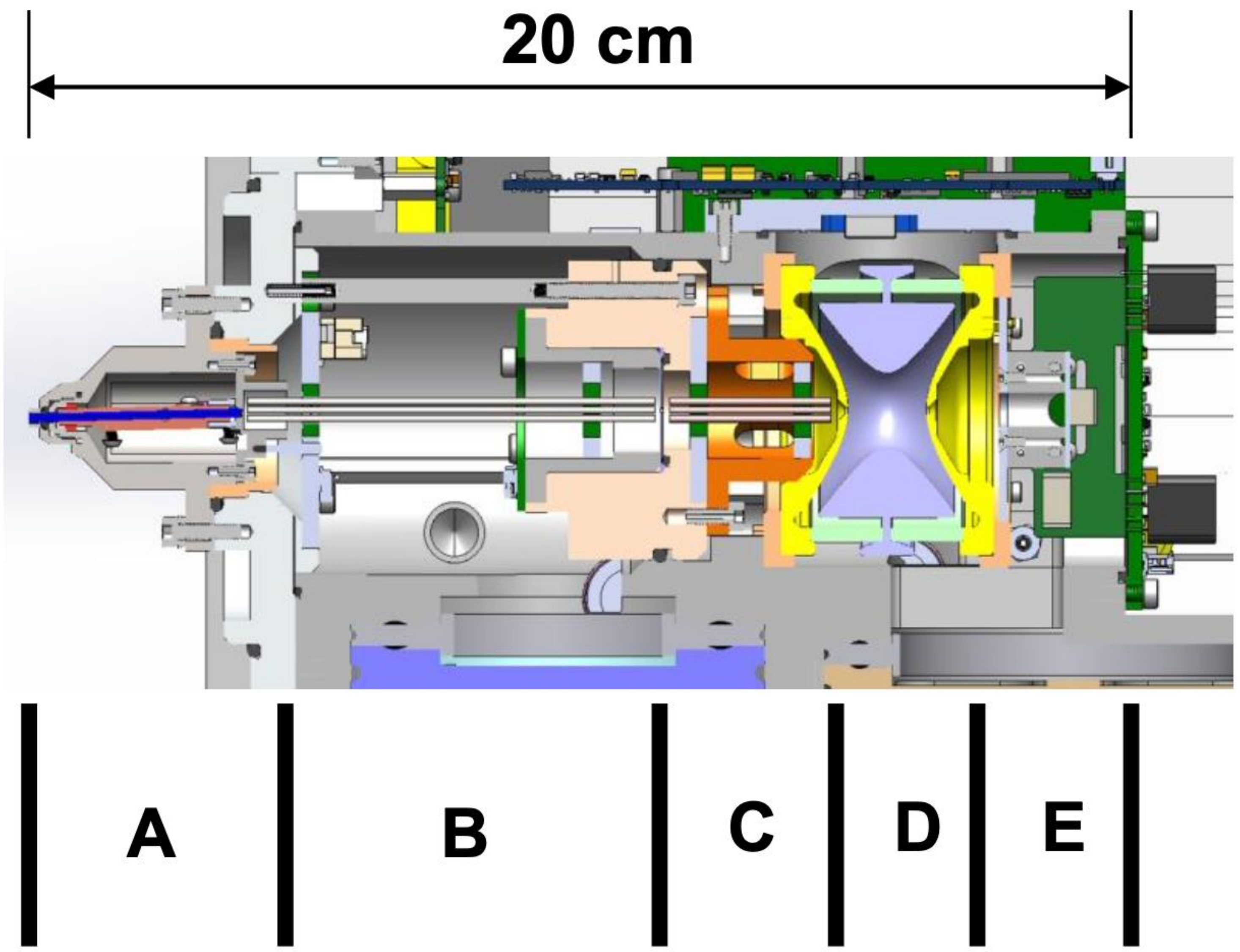
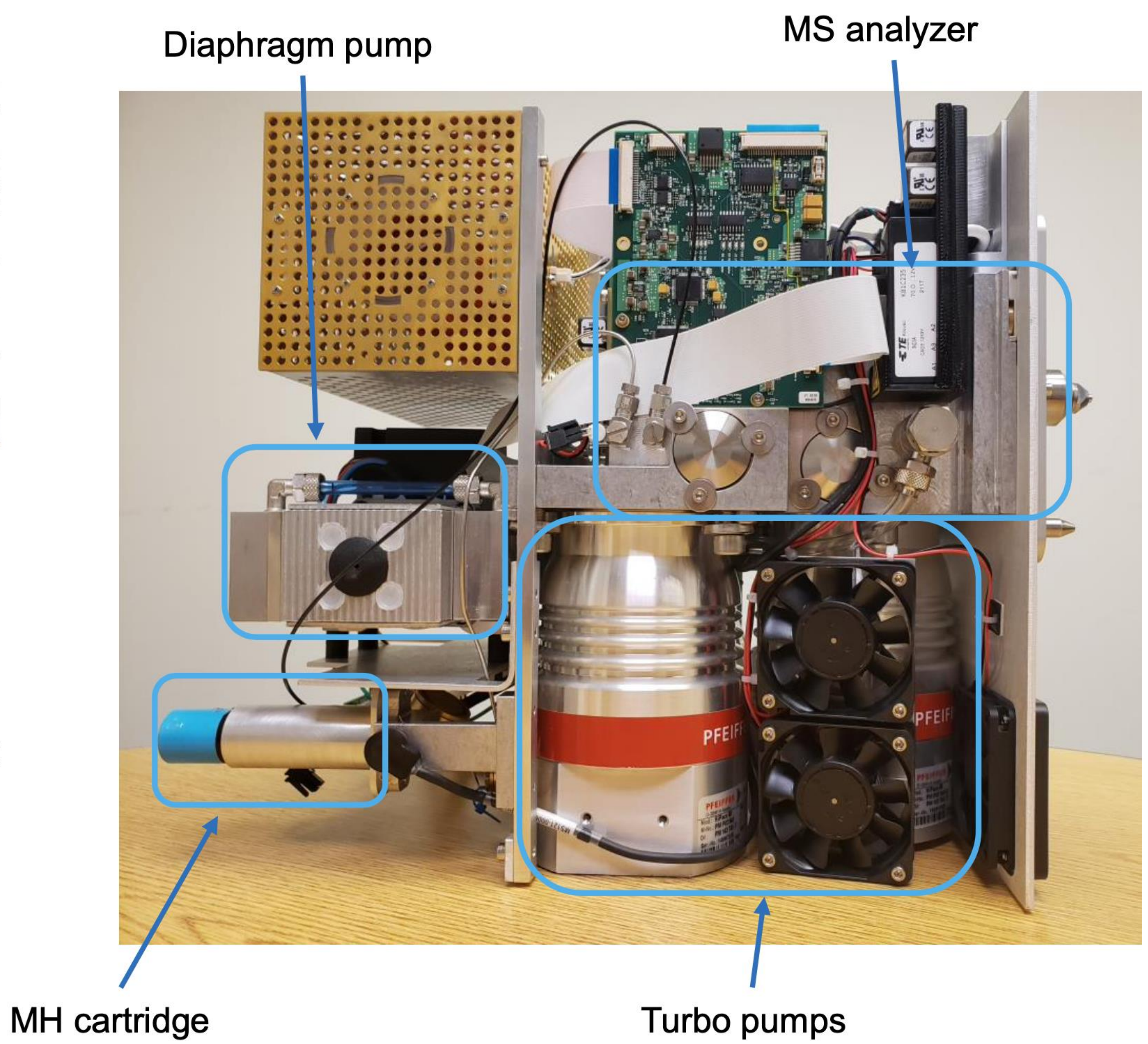
Environmental Health Sciences Department


DHL
FLYER

INSIDE THE MassTech MTE-30 Explorer



A. **Cone, heating elements and inlet capillary**
B. **Inlet hexapole ion guide and conductance limit**
C. **MS analyzer hexapole ion guide**
D. **Ion trap mass analyzer**
E. **Ion detector**



MTE-30 SPECIFICATIONS

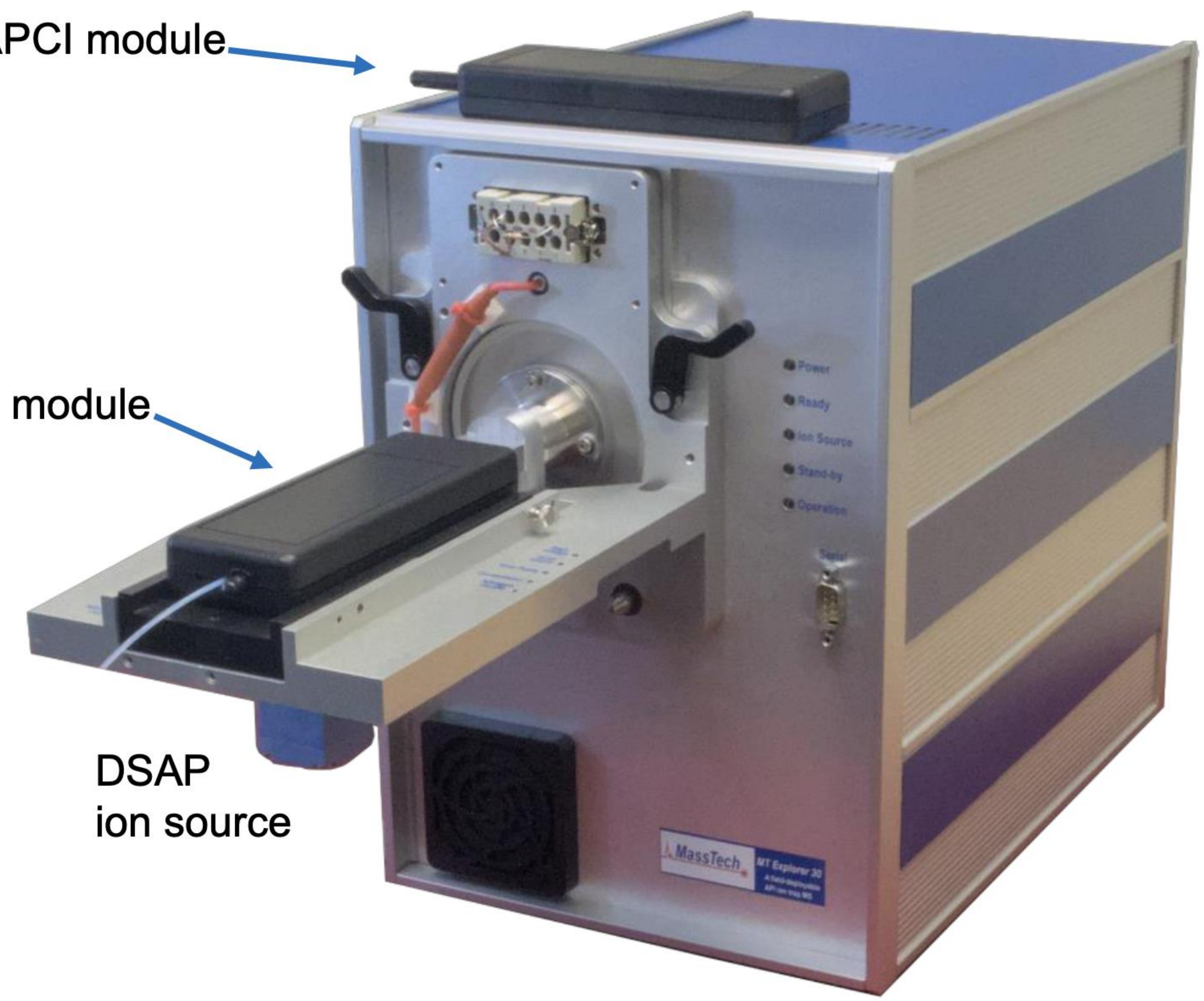
- Atmospheric pressure interface (API)
- MS and MS/MS modes of operation
- Mass range: 35-2,000 Da
- Mass accuracy 0.3 Da
- Weight 37 lb
- Dimensions 8”x12”x13”
- Power AC or battery (250W max)

MassTech MTE-30 Explorer

APCI module

sESI module

DSAP
ion source

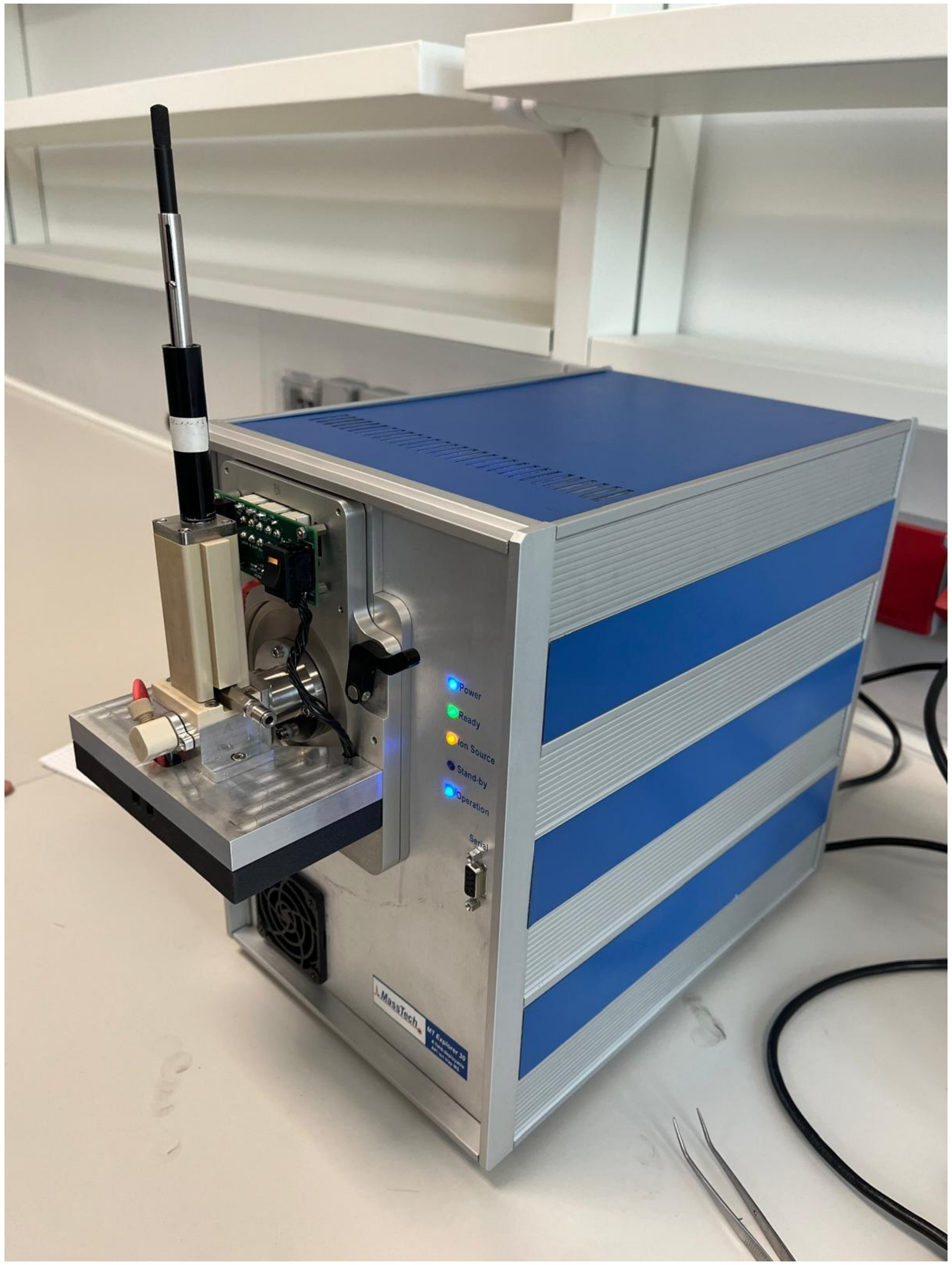


MTE30

0.8 cu.ft.
37 lb

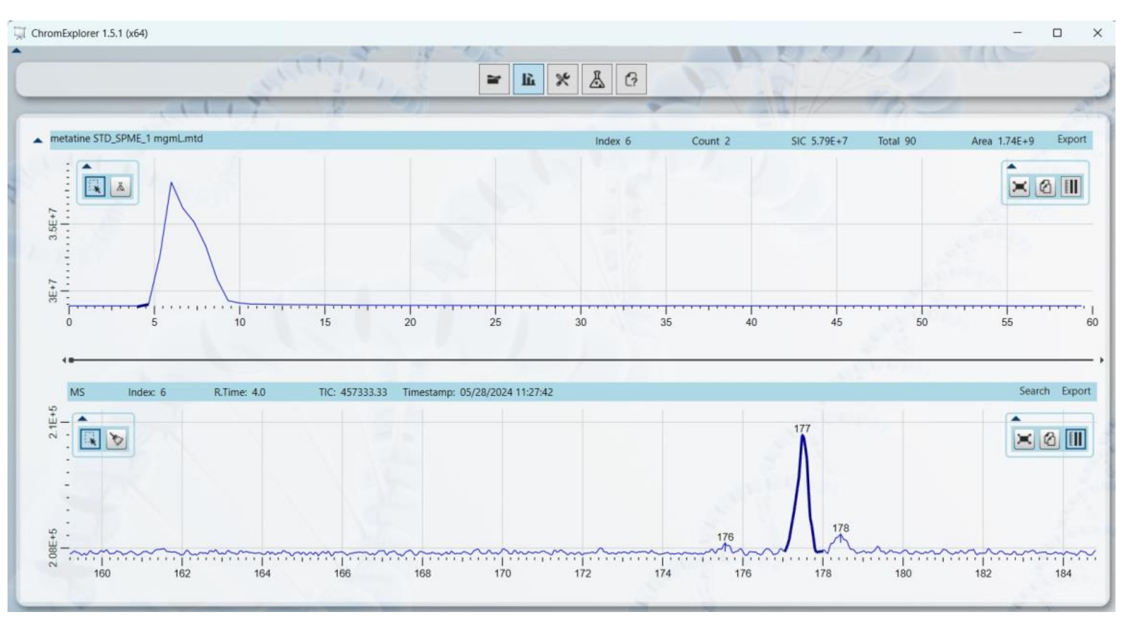
MassTech

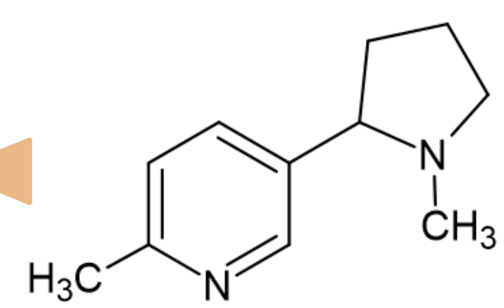
MTE-30 with APCI source modified to accept SPME



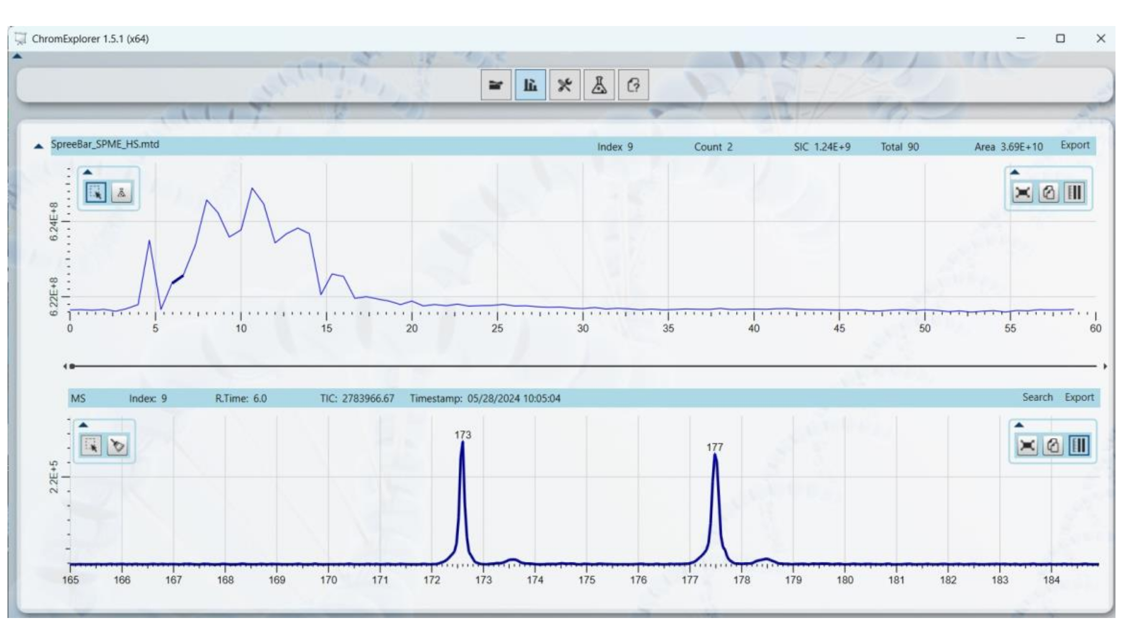
HS-SPME - FULL SCAN

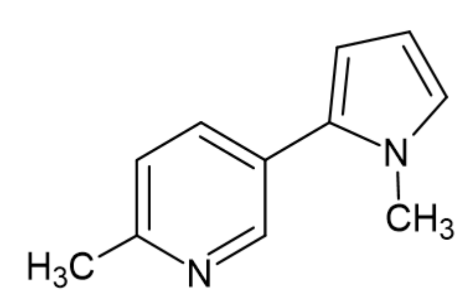
‘ Absence ‘ of nicotine in E-Liquids – PMTA exempt product





Pure STD 6-methyl nicotine (metatine m/z $M+H^+$ 177)



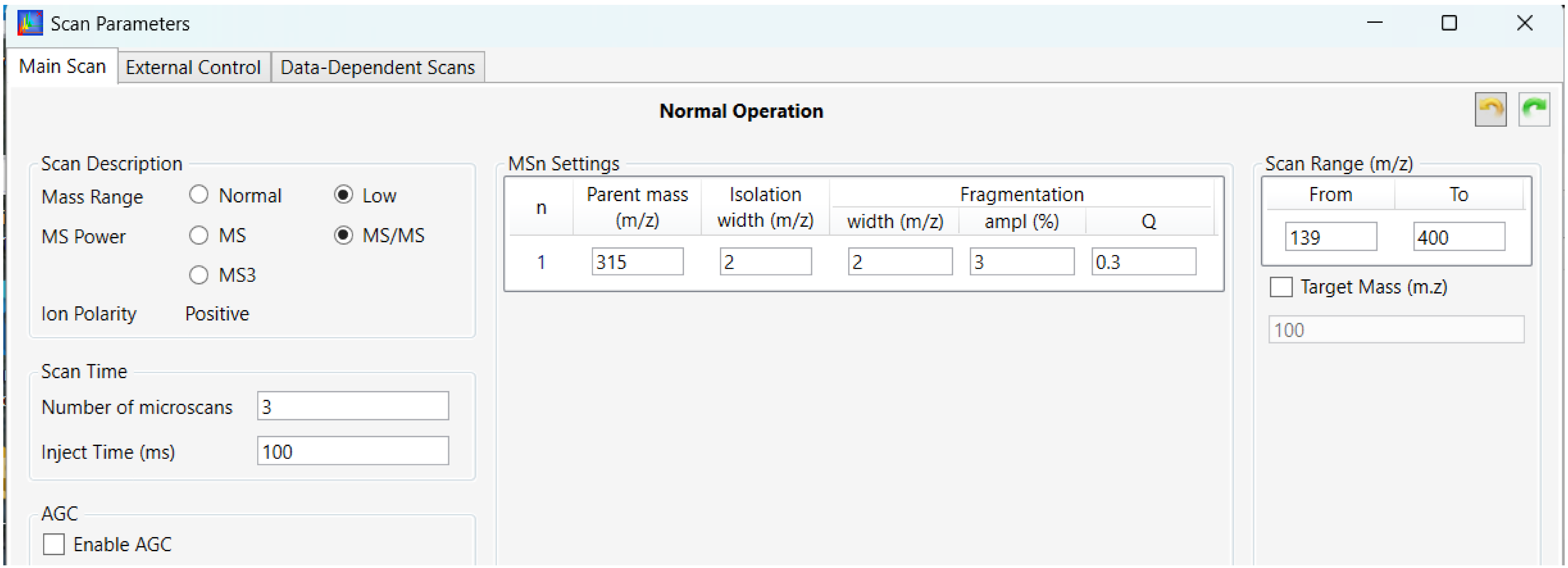


metatine + dehydrogenation product (metatyrine m/z $M+H^+$ 173)

- **In 2022, the FDA required a premarket tobacco product application (PMTA) for all tobacco products containing nicotine or nicotine synthetic forms commercialized in the United States.**
- **Tobacco industry has begun developing new compounds as alternative to nicotine or synthetic nicotine derivates, to override the existing tobacco product regulation.**
- **In 2023, the e-cigarette market in the USA saw the introduction of a new product named SpreeBar, declared as PMTA exempt due to the absence of Nicotine.**
- **In SpreeBar products, Nicotine was replaced by metatine (6-methyl nicotine)**

HS-SPME of 6-methyl nicotine and of e-liquid. Results verified by HR GC/MS.

SPME - MS/MS parameters for cannabidiol (CBD)



CBD MS/MS - 100 ng/mL in water

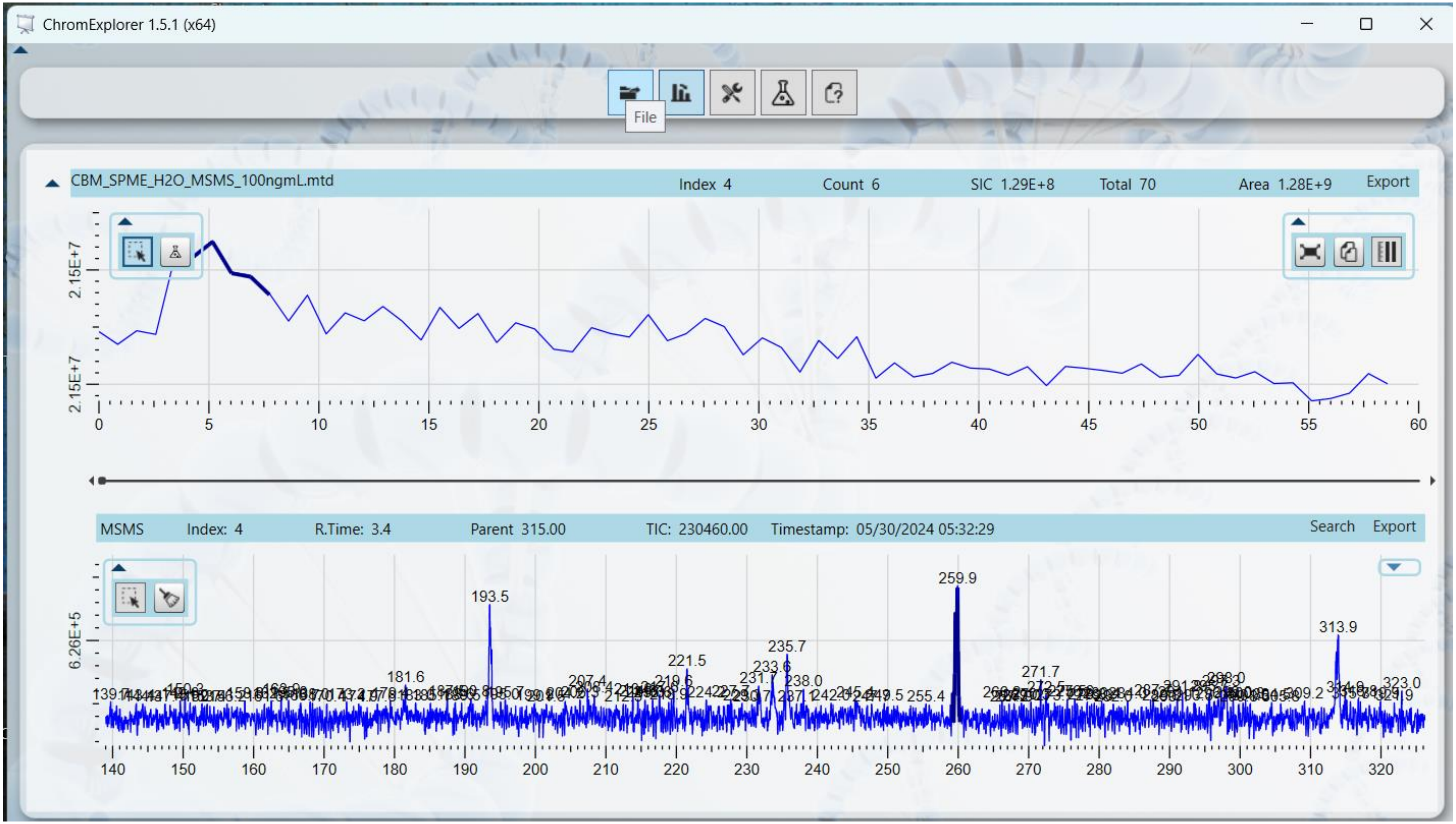


Table 2

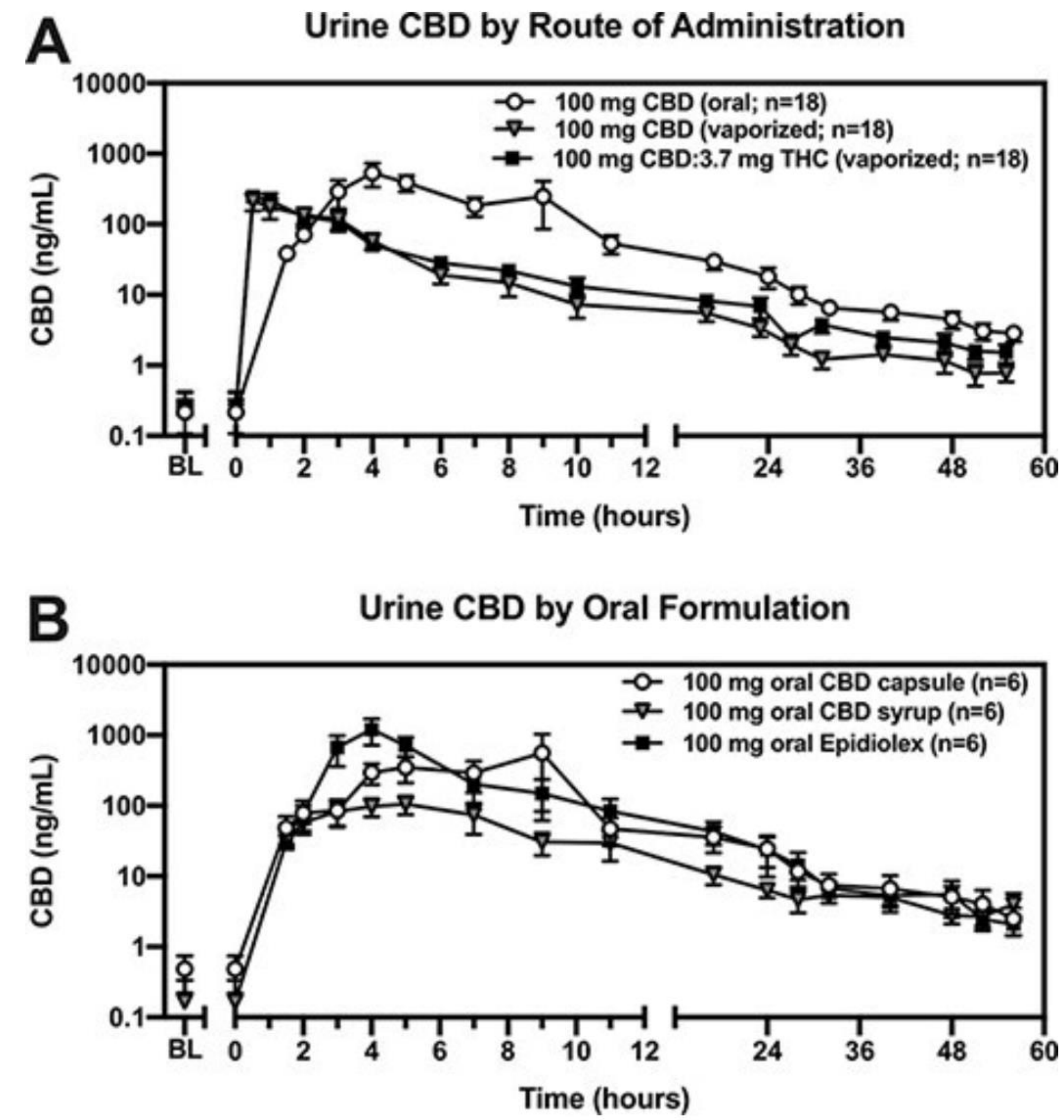
Comparison of limits of detection and quantification of several methods.

Analyte	Sample Amount (mL)	LOD (ng/mL)	LLOQ (ng/mL)	Method of Detection	Reference
CBD		1.00			
THC		1.00			
CBN	1.00	1.00	ns	LC-MS/MS	[38]
11-OH-THC		1.00			
THC-COOH		5.00			
CBD		3.00	10.00		
THC		3.00	8.00		
CBN	0.09	4.00 *	9.00	LC-MS/MS	[39]
11-OH-THC		3.00	9.00		
THC-COOH		2.00 *	6.00 *		
CBD		3.00	9.00		
THC		2.00	8.00		
CBN	1.00	4.00 *	12.00	LC-MS/MS	[40]
11-OH-THC		2.00 *	6.00		
THC-COOH		2.00 *	6.00 *		
CBD		5.00	16.00		
THC		3.00	9.00		
CBN	2.00	5.00	18.00	GC-MS	[41]
11-OH-THC		2.60 *	8.70		
THC-COOH		4.50 *	15.00		
CBD		2.00			
THC		1.00			
CBN	0.20	2.00 *	**	LC-MS/MS	[42]
11-OH-THC		2.00			
THC-COOH		1.00 *			

Open in a separate window

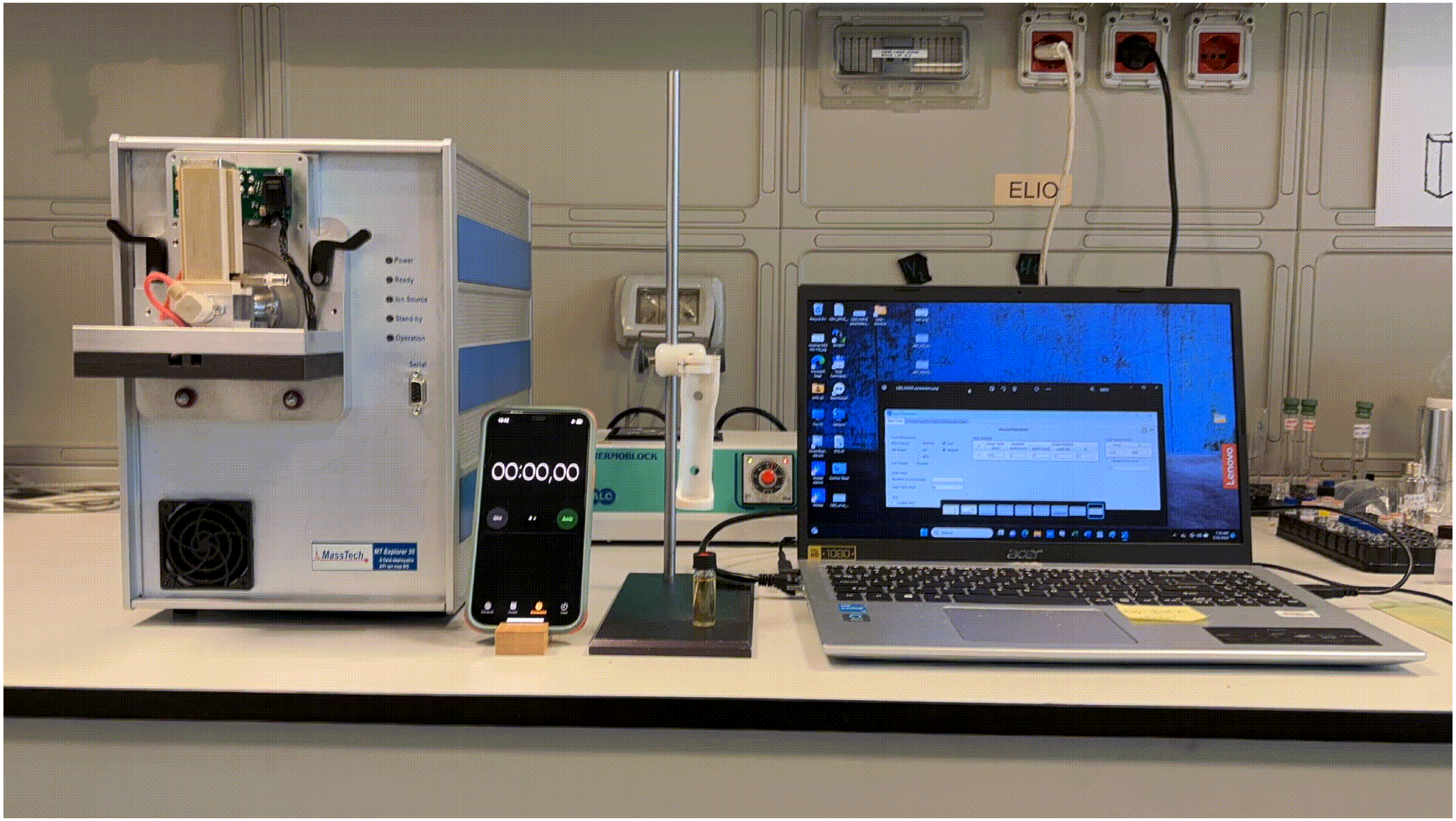
* lower limits than the present work; ** LOD values are the same as LLOQ; ns: not specified.

Rosendo LM et al. The Determination of Cannabinoids in Urine Samples Using Microextraction by Packed Sorbent and Gas Chromatography-Mass Spectrometry. Molecules. 2022 Aug 27;27(17):5503.

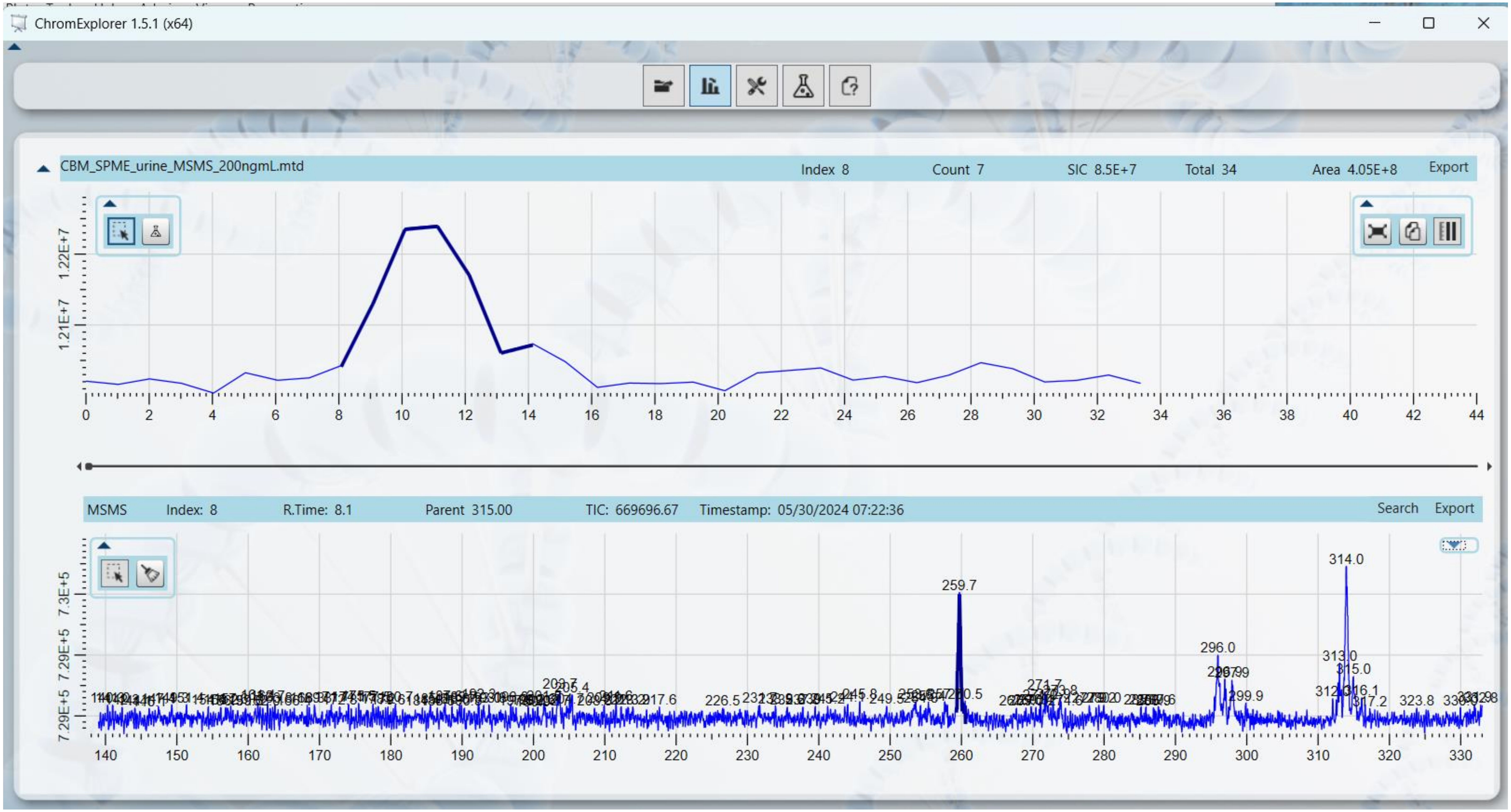


Sholler DJ et al. Urinary Pharmacokinetic Profile of Cannabidiol (CBD), Δ9-Tetrahydrocannabinol (THC) and Their Metabolites following Oral and Vaporized CBD and Vaporized CBD-Dominant Cannabis Administration. J Anal Toxicol. 2022 May 20;46(5):494-503.

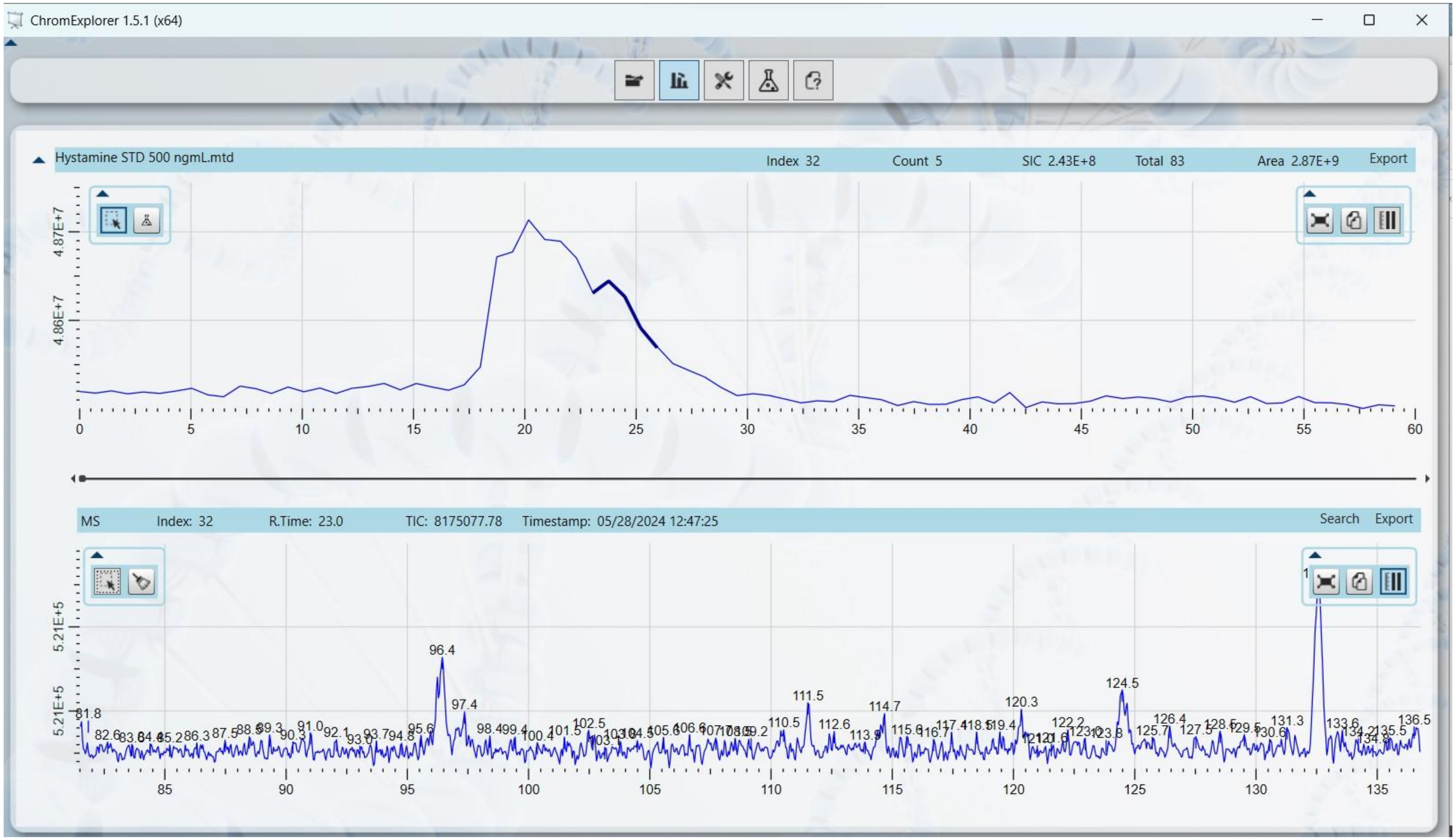
CBD MS/MS - 200 ng/mL in urine



CBD MS/MS - 200 ng/mL in urine



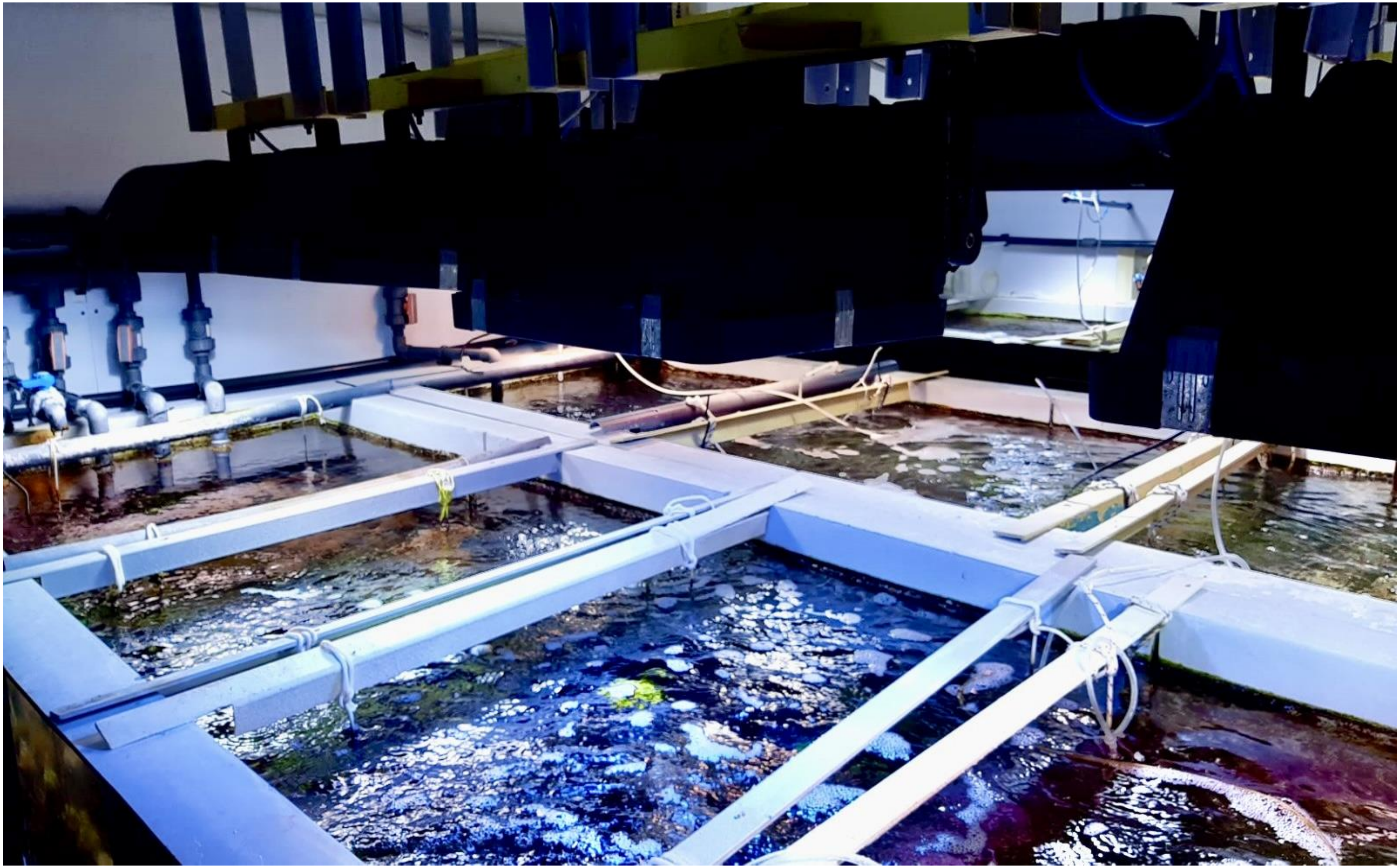
Fish and histamine intolerance



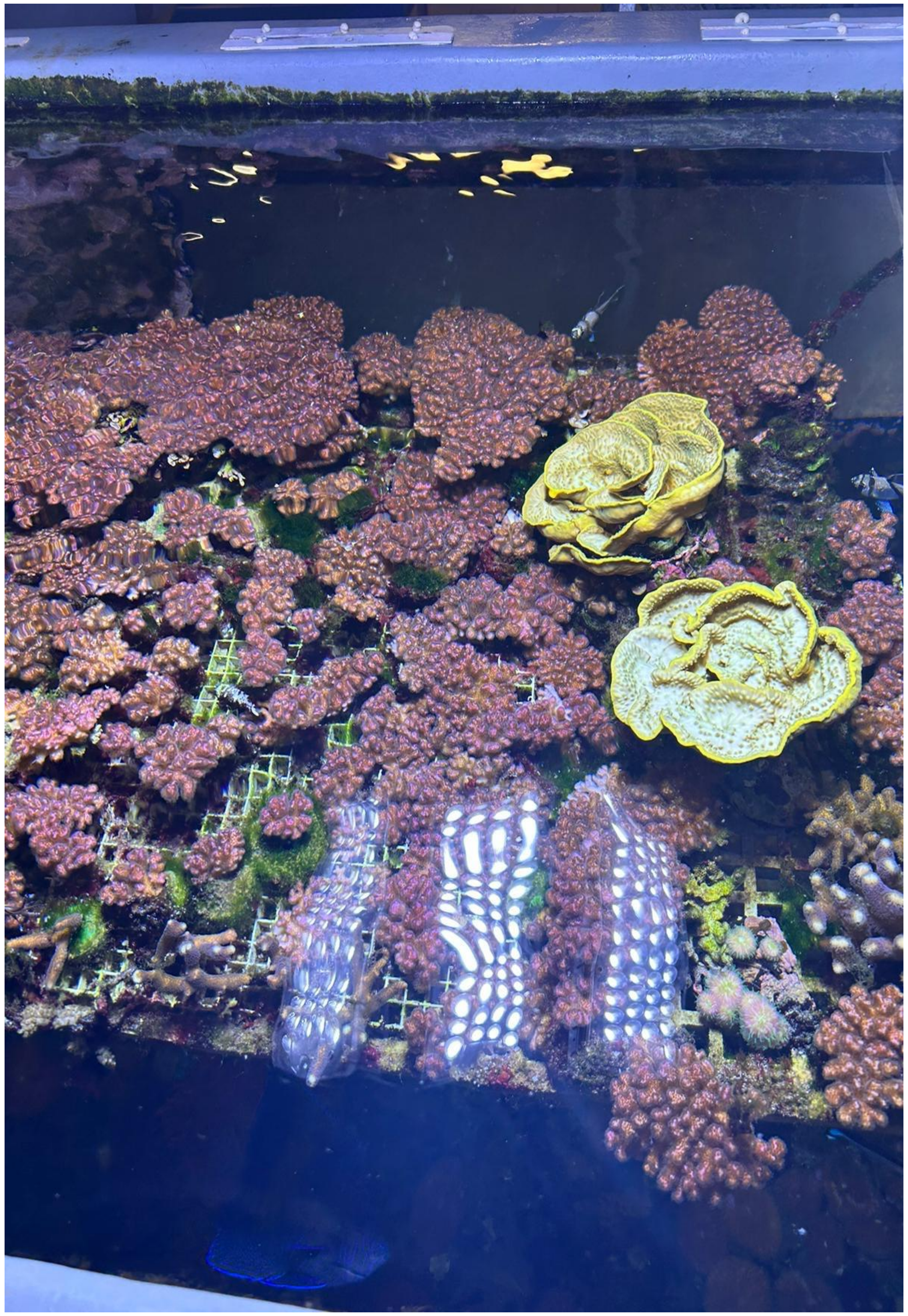
Hystamine 5 ppb in water. Head space sampling.
Limits in EU are 200 ppm in fish

Beyond the laboratory. MTE-30 at the aquarium.

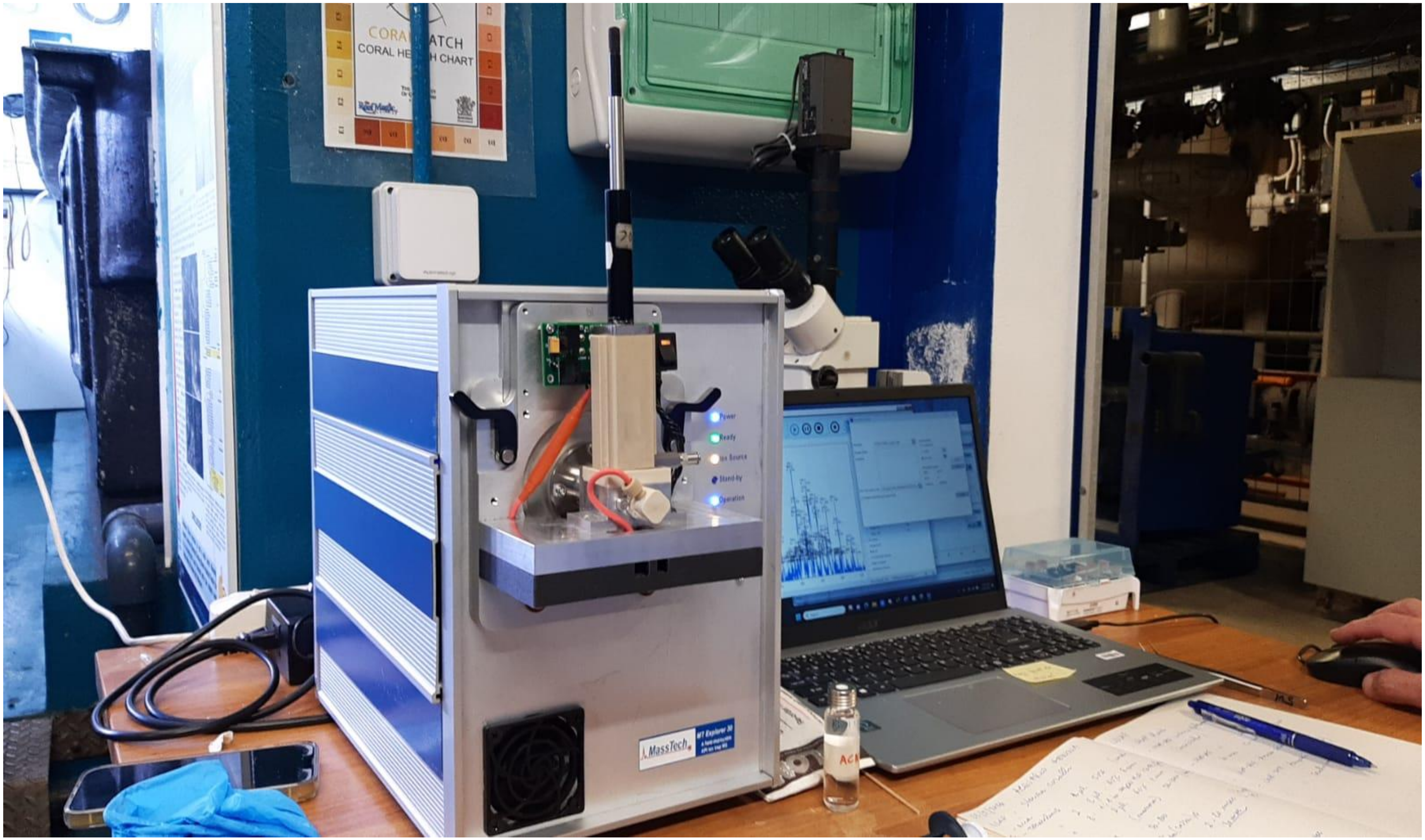
CORALS TANKS



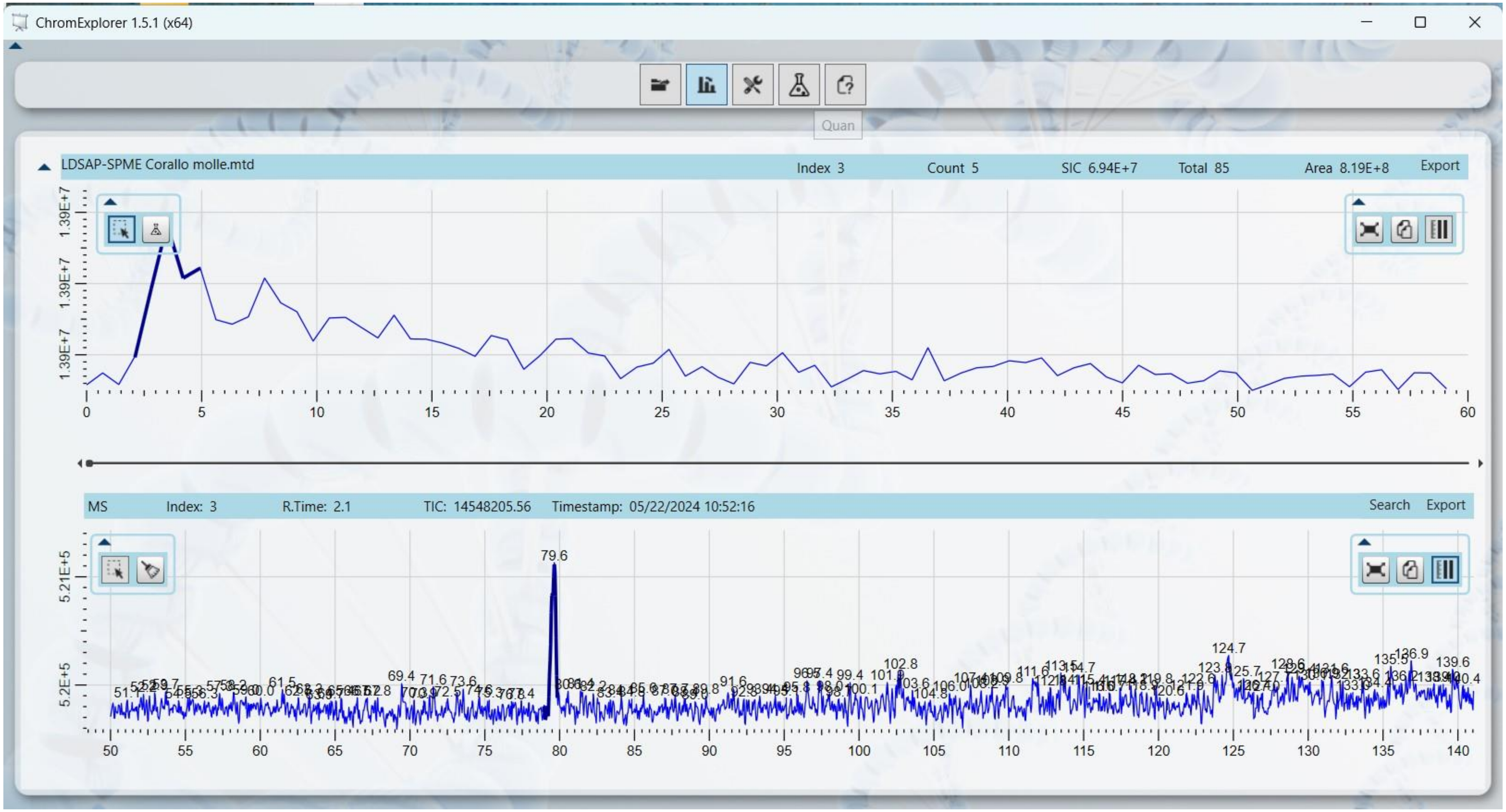
BABY CORALS GROWING



ON-SITE ANALYSIS



DMSO PRESENCE IN THE CORALS ROOM HEADSPACE



ECOPHYSIOLOGY AND ECOLOGICAL ASPECTS OF DMS - DMSO

SCIENTIFIC REPORTS

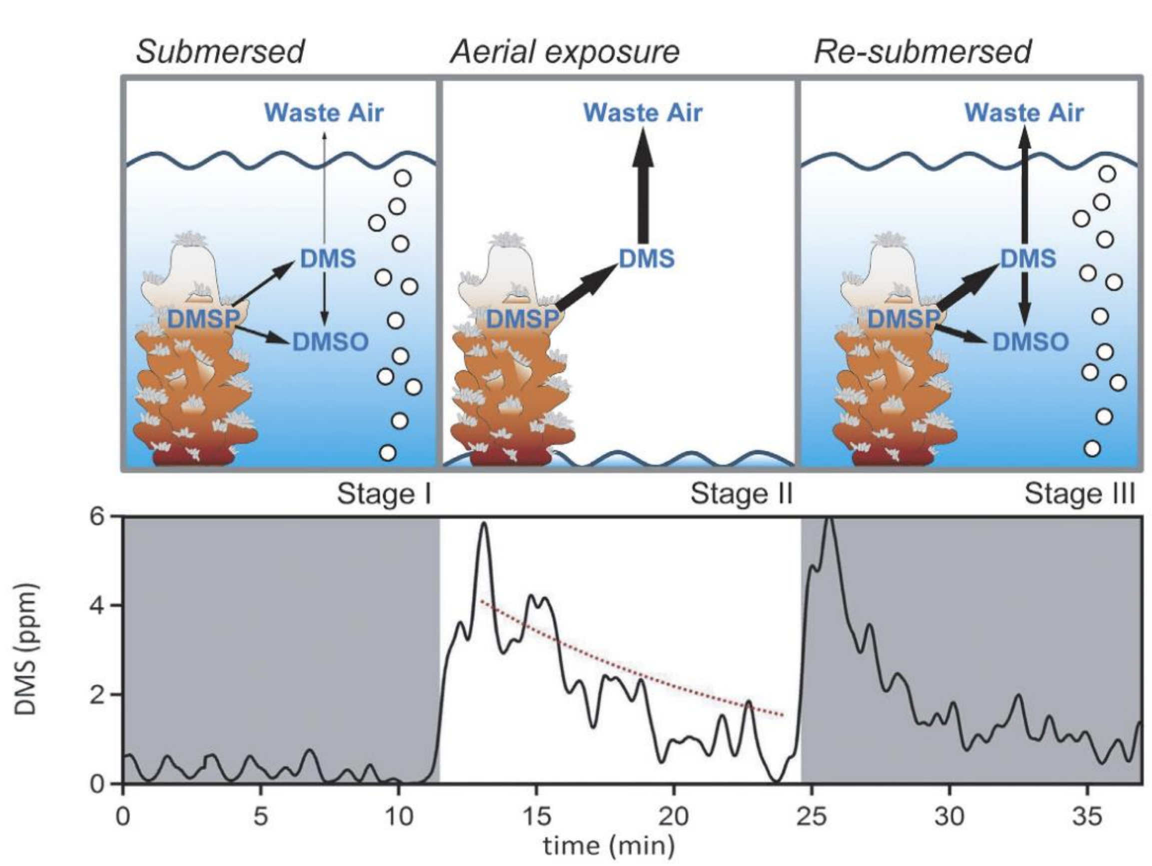
OPEN

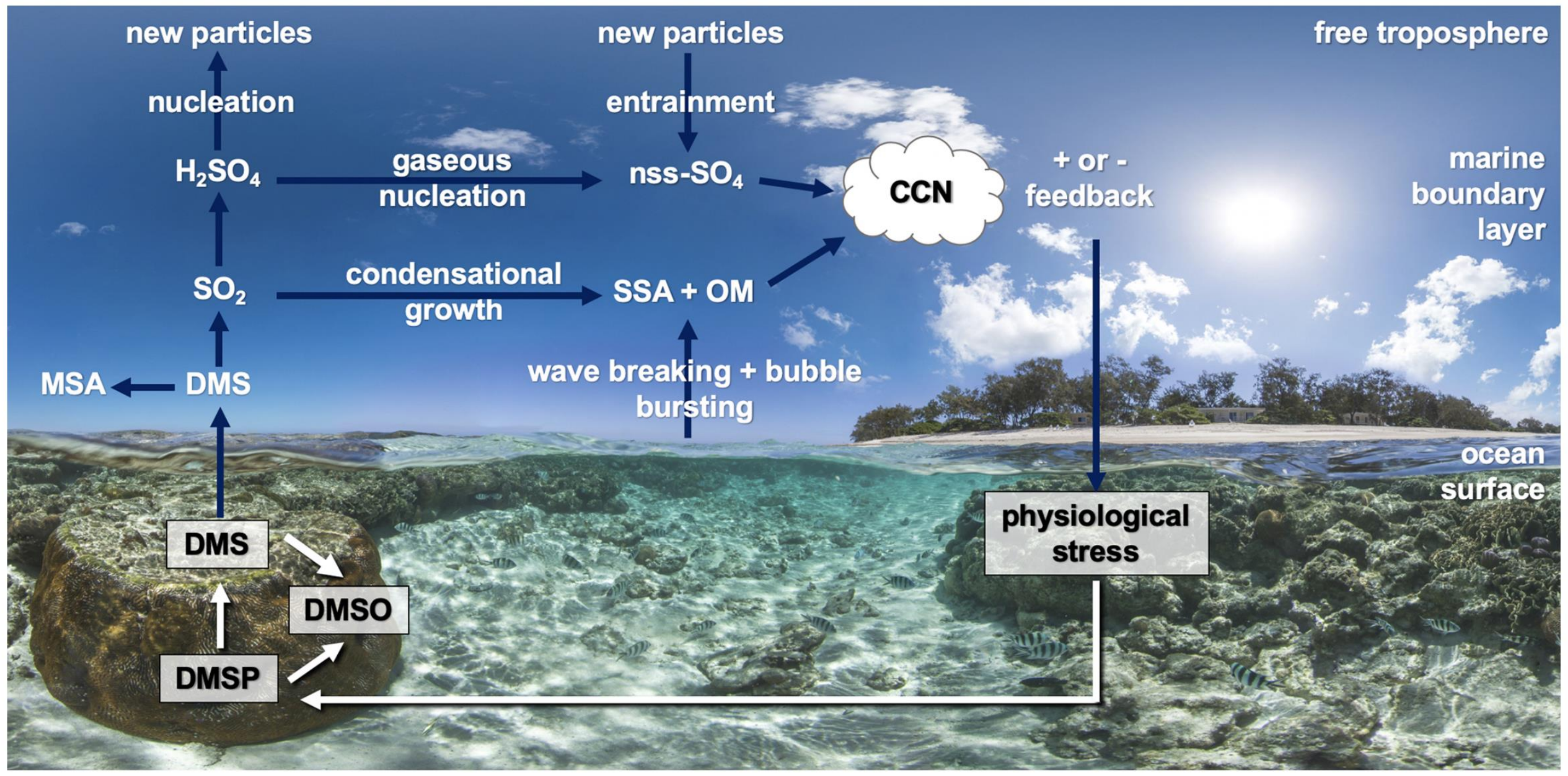
Air exposure of coral is a significant source of dimethylsulfide (DMS) to the atmosphere

Received: 01 April 2016
Accepted: 10 October 2016
Published: 31 October 2016

Frances E. Hopkins[1], Thomas G. Bell[1], Mingxi Yang[1], David J. Suggett[2,3] & Michael Steinke[2]

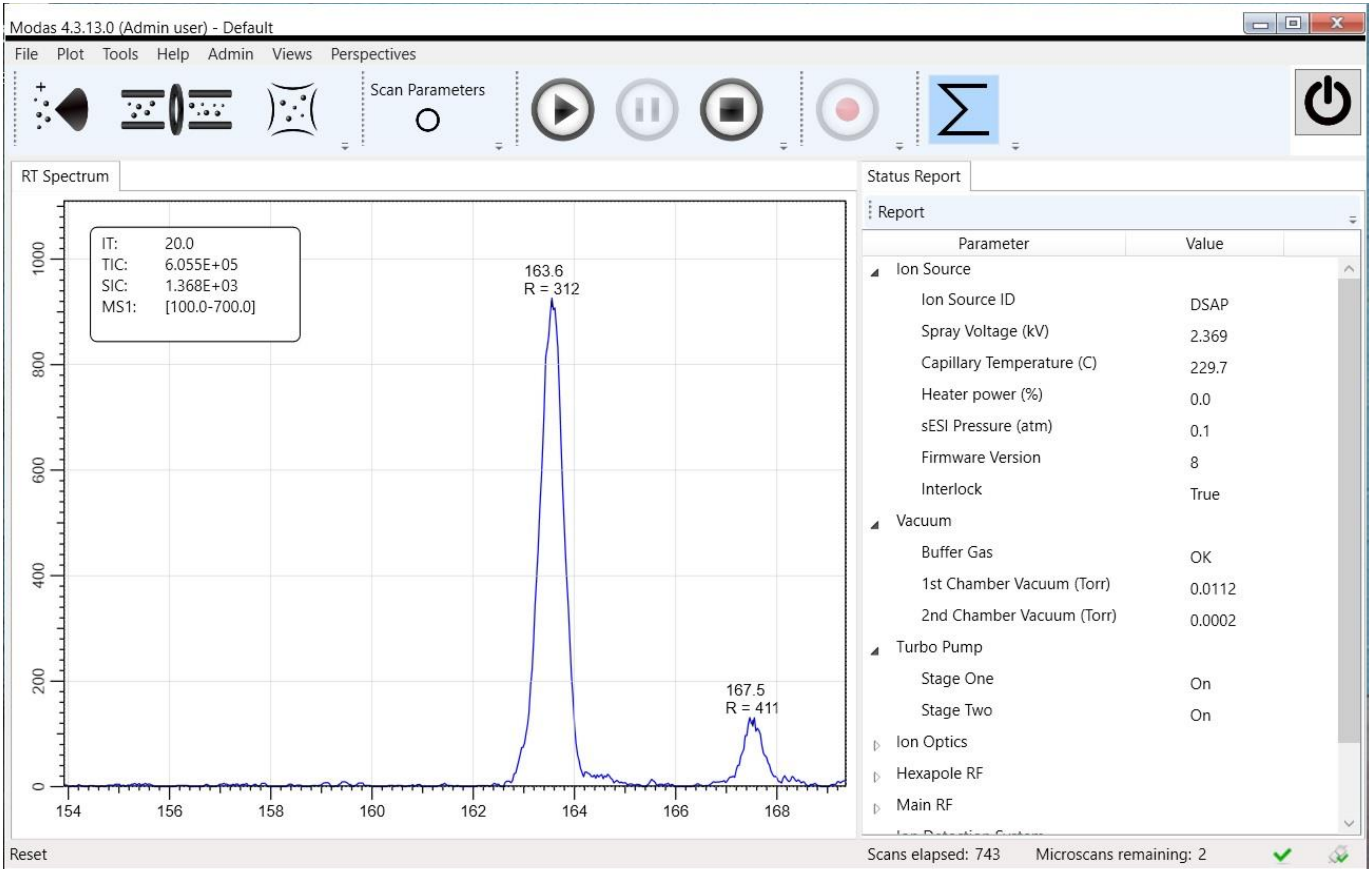
Corals are prolific producers of dimethylsulfoniopropionate (DMSP). High atmospheric concentrations of the DMSP breakdown product dimethylsulfide (DMS) have been linked to coral reefs during low tides. DMS is a potentially key sulfur source to the tropical atmosphere, but DMS emission from corals during tidal exposure is not well quantified. Here we show that gas phase DMS concentrations (DMS_{gas}) increased by an order of magnitude when three Indo-Pacific corals were exposed to air in laboratory experiments. Upon re-submersion, an additional rapid rise in DMS_{gas} was observed, reflecting increased production by the coral and/or dissolution of DMS-rich mucus formed by the coral during air exposure. Depletion in DMS following re-submersion was likely due to biologically-driven conversion of DMS to dimethylsulfoxide (DMSO). Fast Repetition Rate fluorometry showed downregulated photosynthesis during air exposure but rapid recovery upon re-submersion, suggesting that DMS enhances coral tolerance to oxidative stress during a process that can induce photoinhibition. We estimate that DMS emission from exposed coral reefs may be comparable in magnitude to emissions from other marine DMS hotspots. Coral DMS emission likely comprises a regular and significant source of sulfur to the tropical marine atmosphere, which is currently unrecognised in global DMS emission estimates and Earth System Models.



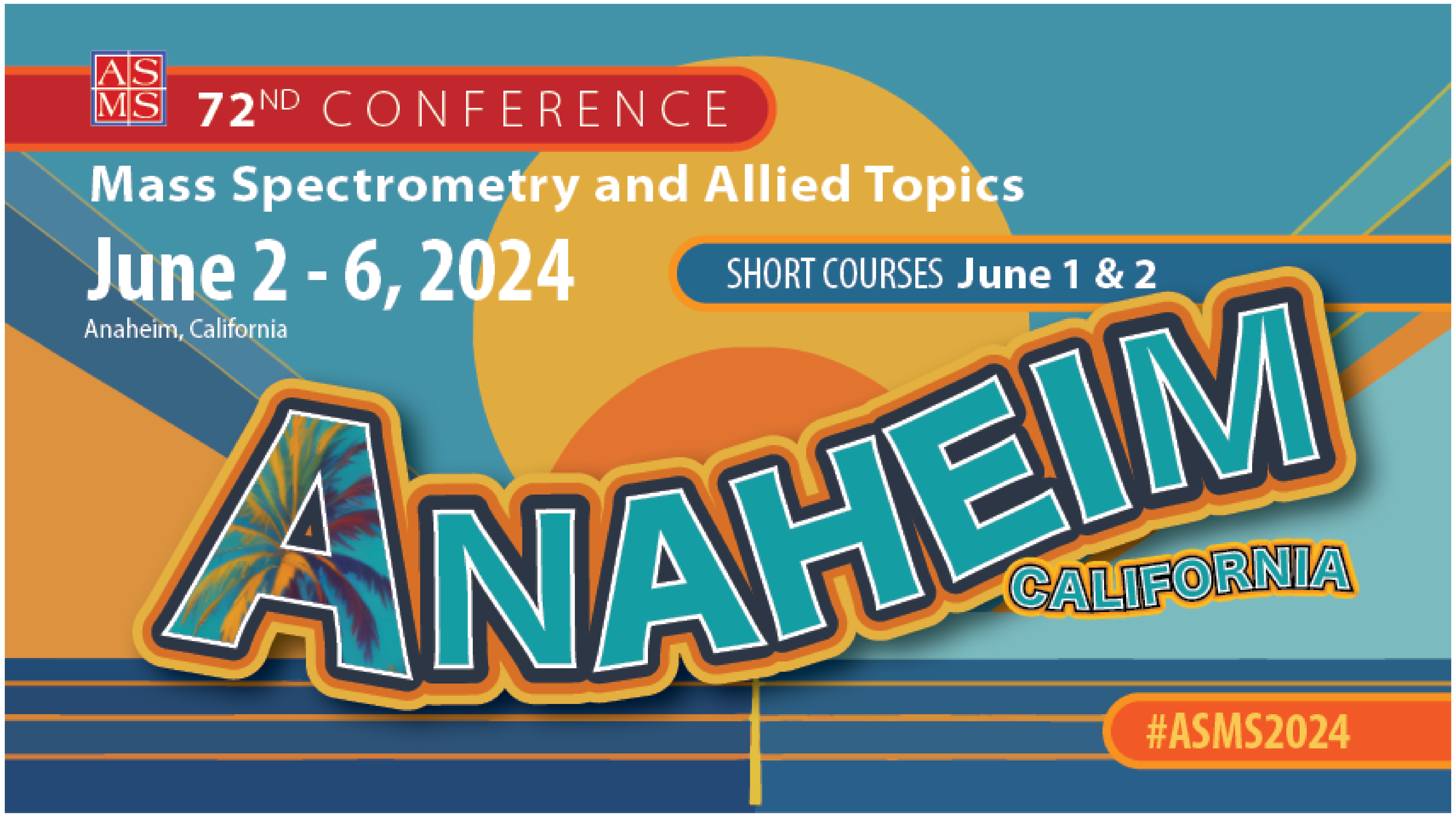


Jackson et al. Biogeosciences, 17, 2181–2204, 2020

QUANTITATIVE ANALYSIS - STD Nicotine 30 ng / Nicotine D_4 10 ng



More questions? Want more applications?



Visit me at POSTER WP436

Portable Instrumentation for SPME Analysis: Beyond the Laboratory

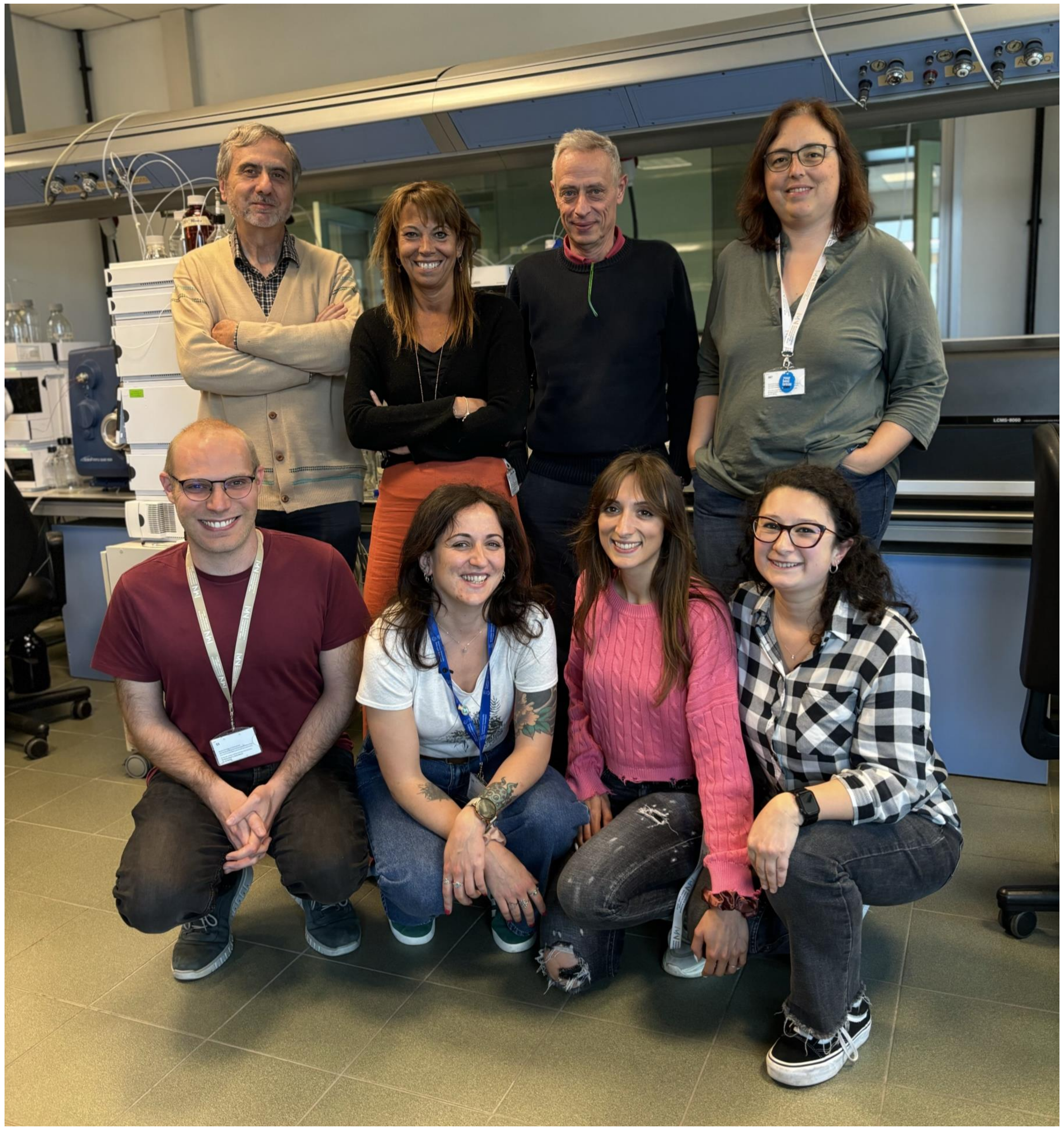
THANKS

Prof. Claudio Medana

Prof. Francesco Saliu

Victor Laiko, Ph.D.
Vladimir Doroshenko, Ph.D.

THANKS



ASMS Mass Spectrometry & Allied Topics

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Anaheim CA

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Breakfast Seminar

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6/3 MONDAY
7:00-08:15 AM PST

ENRICO DAVOLI
Istituto Mario Negri, Milan, Italy
SPME analysis on a portable MS/MS instrument

CALEIGH O'CONNOR
MassTech Inc., MD, USA
Expanding Analytical Frontiers: Showcasing the Portability and Versatility of Miniature Ion Trap Mass Spectrometry

NIVEDITA BHATTACHARYA
Barefeet Analytics Private Limited, India
Applications of AP/MALDI with triple quadrupole mass analyzers

RUSS KIBBE
North Carolina State University, USA
Software for efficient AP/MALDI MSI data analysis

PETER VERHAERT
ProteoFormiX, Belgium
AP/MALDI: Connecting a variety of mass spectrometers globally with MSI

6/4 TUESDAY
7:00-08:15 AM PST

GILLES FRACHE
Luxembourg Institute of Science and Technology
AP/MALDI coupled with Orbitraps: Principle, applications and current developments

ERIN SEELEY
University of Texas, Austin, USA
Sequential Imaging with AP/MALDI for Enhanced Tissue Characterization

ALICE PASSONI
Istituto Mario Negri, Milan, Italy
Imaging Investigations Using AP/MALDI: Drugs and Metabolites Distribution

TIMO HUANG
University of Wisconsin-Madison, USA
In situ deciphering protein glycosylation signatures in human ovarian cancer via combined MALDI MS imaging and tandem MS

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