MT Explorer 30: A Portable Tandem Mass Spectrometer - Development and Applications

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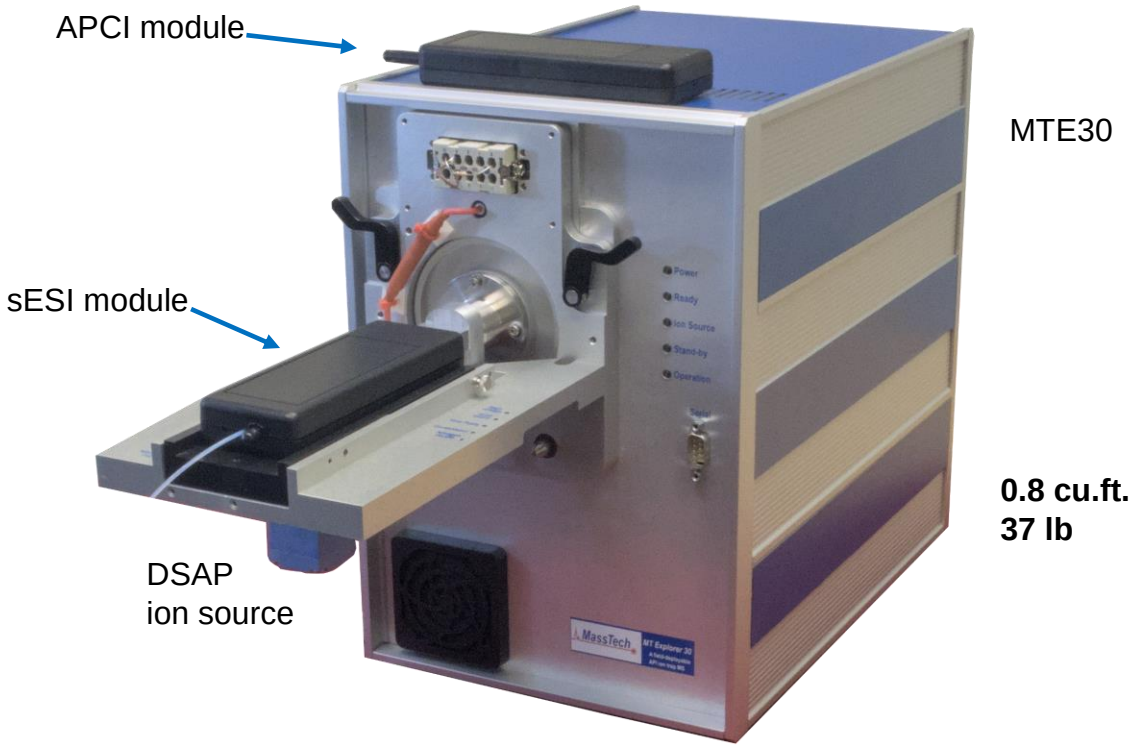
MT Explorer 30 (MTE30) with DSAP ion source



- **Field-deployable instrument (0.8 cu.ft, 37 lb.) for**
  - ✓ **small molecule analysis**
  - ✓ **biomolecule analysis**
- **Sensitivity comparable with that of commercial desktops**
- **Interfacing with all atmospheric pressure (AP) ionization techniques**
- **Providing software tools for custom application software development**

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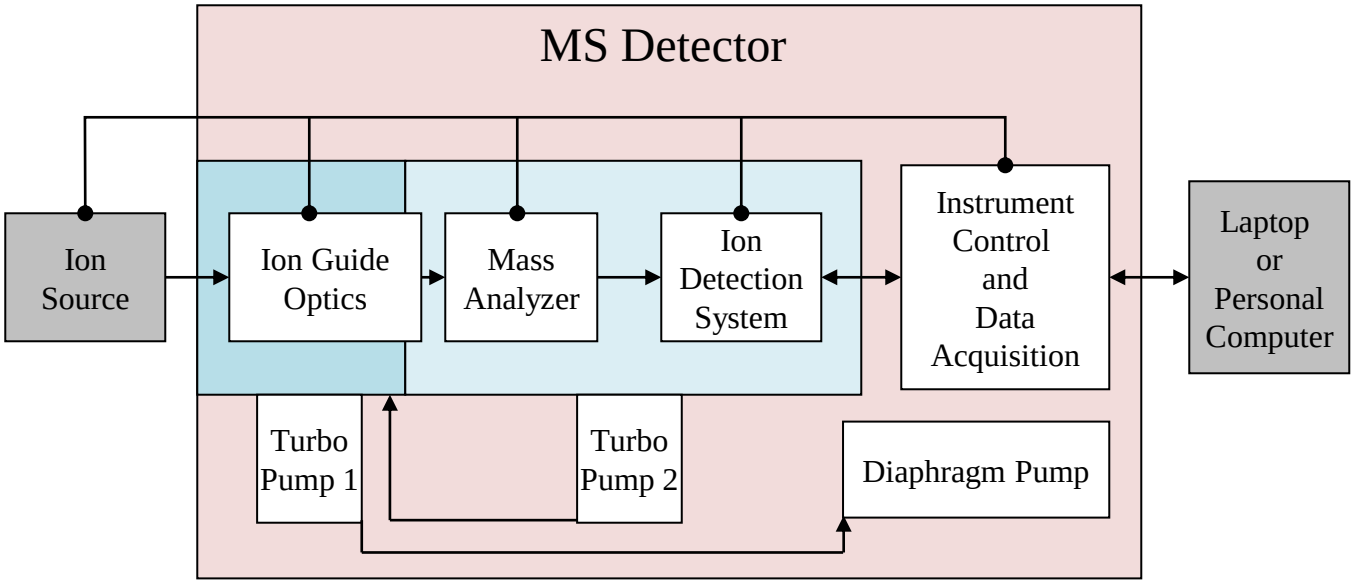
MTE30 Block Diagram



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Two-chamber Vacuum System

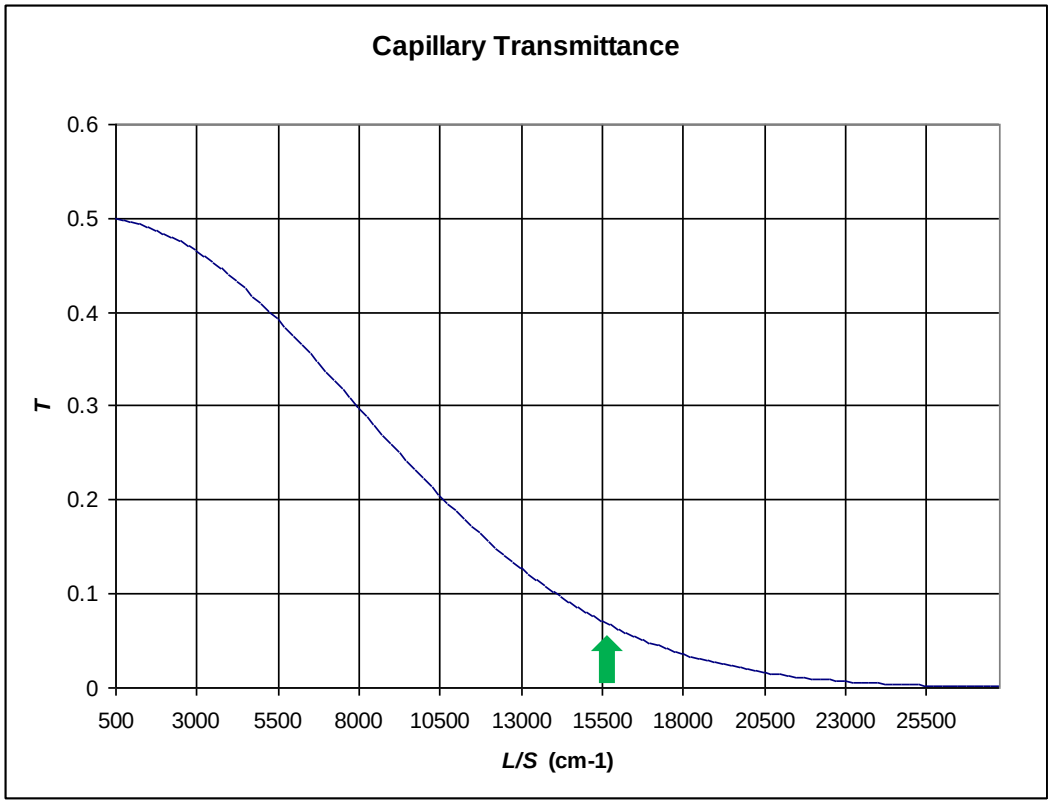
Ion transmission through a capillary[1]:

$$T \approx 0.5 \exp\left[-\frac{18.16\,DLP}{Q}\right]$$

Gas flow load:

$$Q = \left(\frac{S^2}{8\pi\mu L}\right) P_{av}\,\Delta P$$

[1]Lin, Sunner, J. Am. Soc. Mass Spectrom. 1994, vol. 5, pp. 873-885



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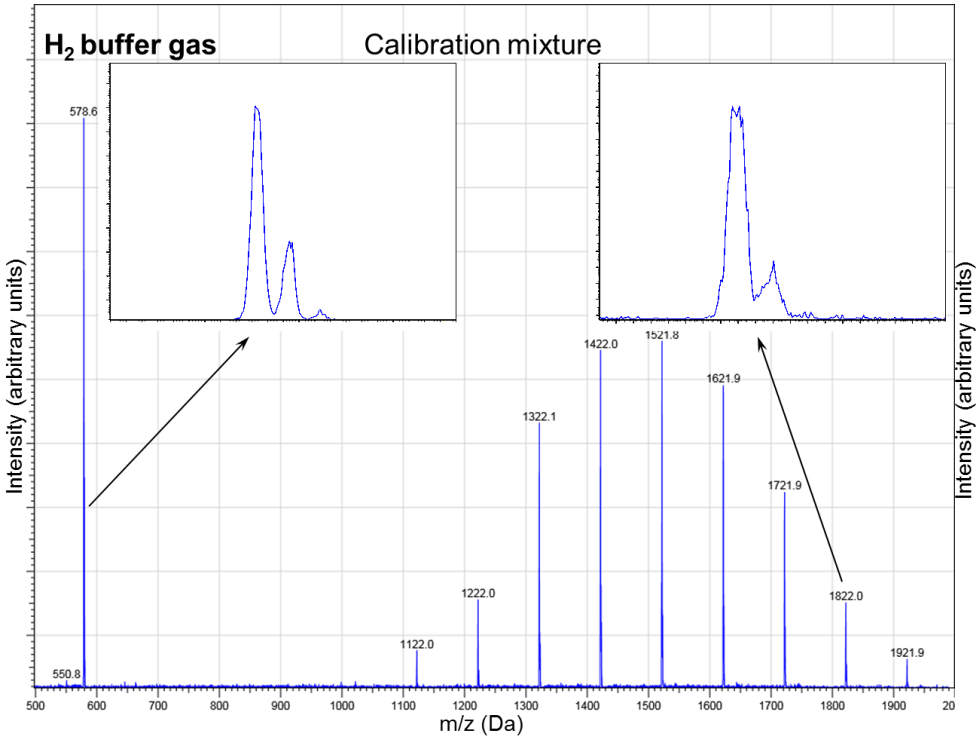
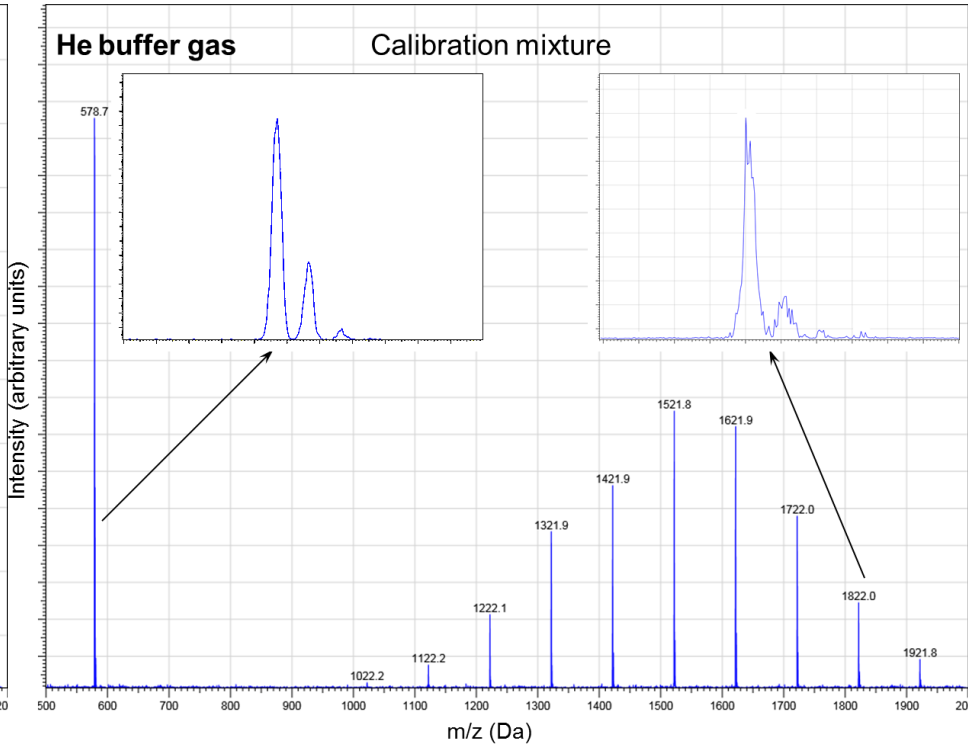
Hydrogen as a Buffer Gas: MS





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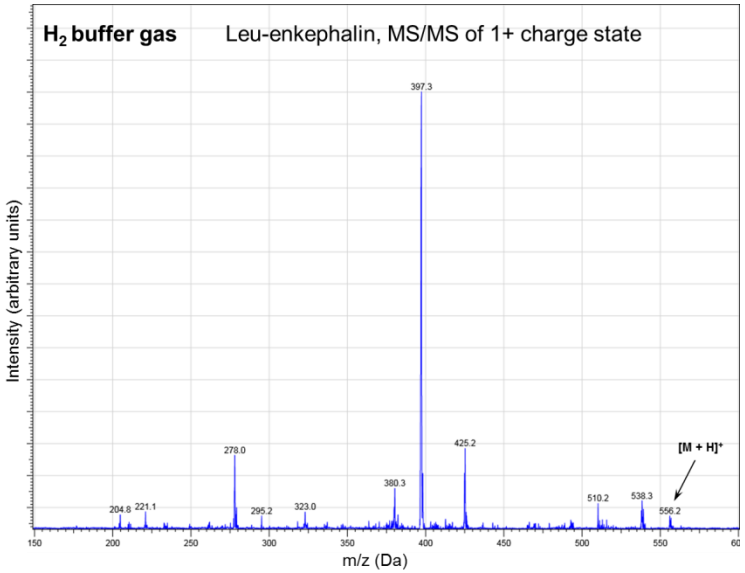
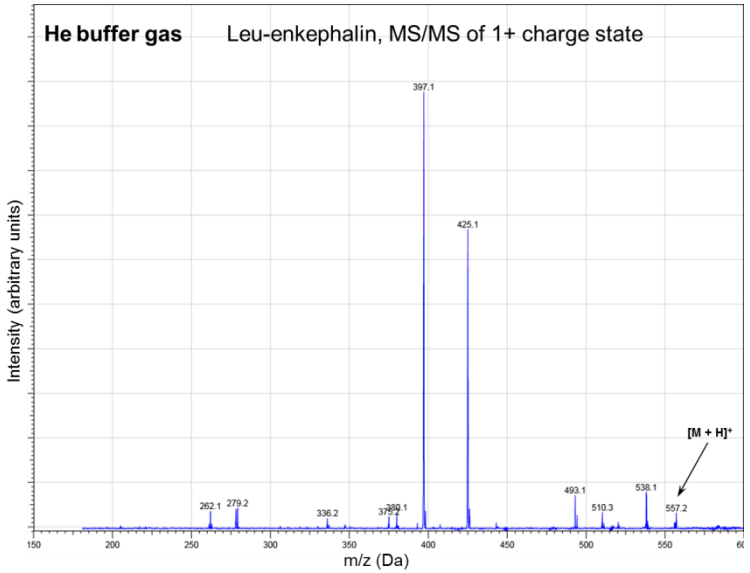
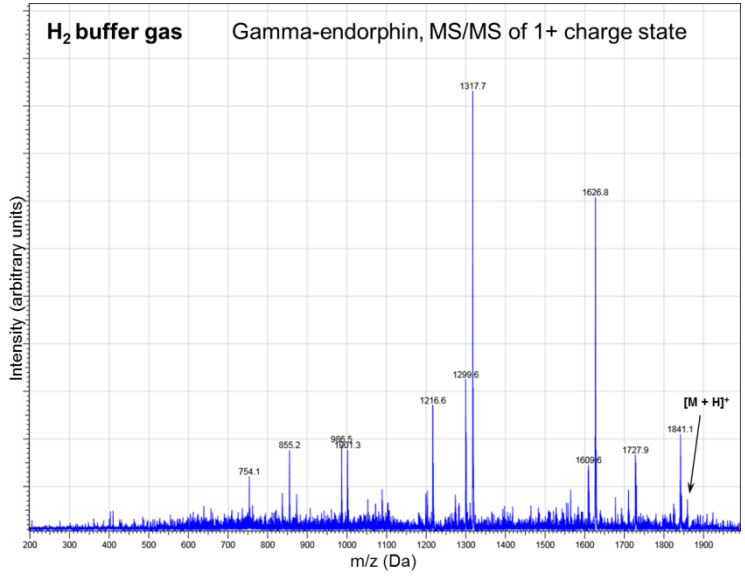
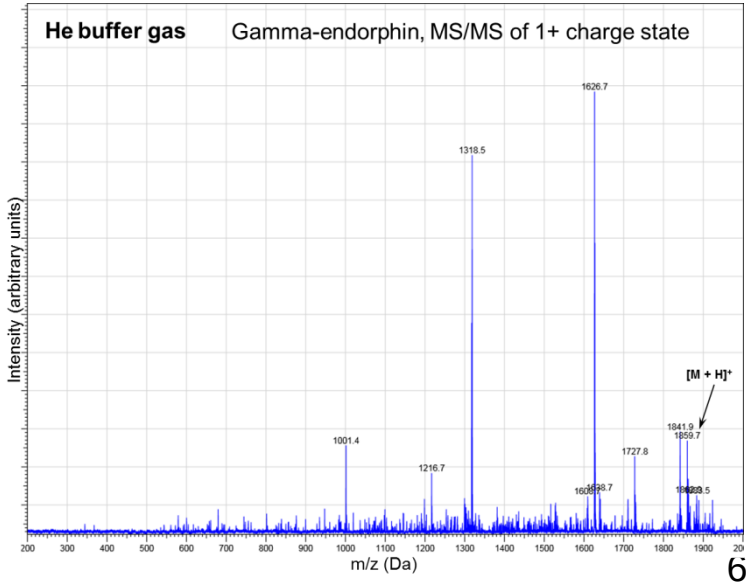
Hydrogen as a Buffer Gas: MS/MS









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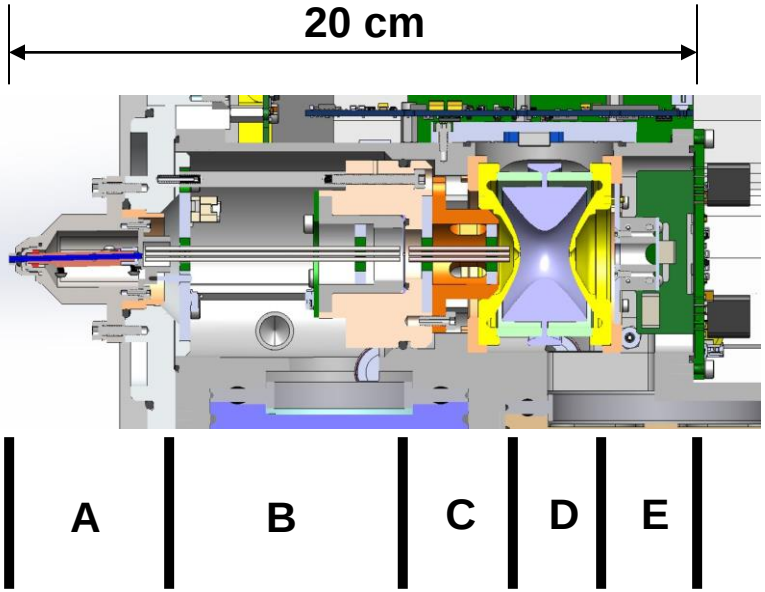
MTE30 Design Features



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

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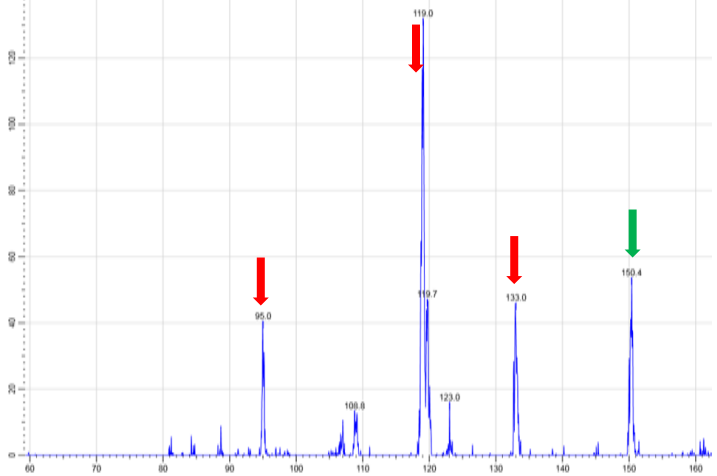
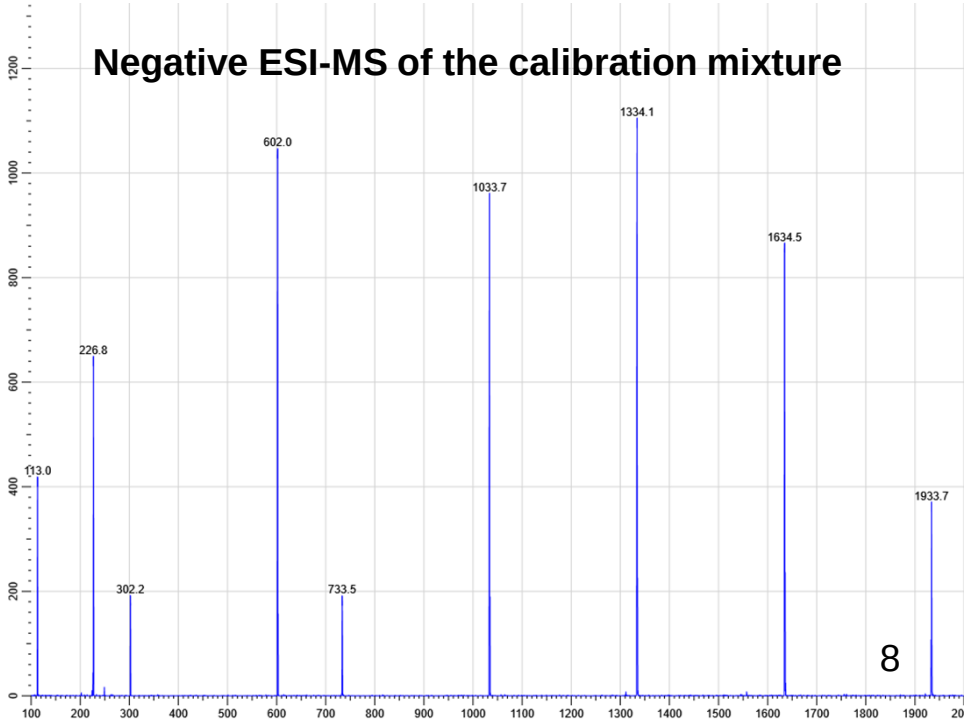
MTE30: Specifications

- Atmospheric pressure interface (API)
- MS and MS/MS modes of operation
- Mass range: 35-2,000 Da
- Mass accuracy 0.3 Da
- Mass resolution 0.5 Da
- Weight 37 lb
- Dimensions 8”x12”x13”
- Power AC or battery (250W max)

APCI-MS/MS of Methamphetamine, 2ng



Negative ESI-MS of the calibration mixture



MTE30 Configurations

ESI
nanoESI

SICRIT™

AP-MALDI

sESI

DART

APCI

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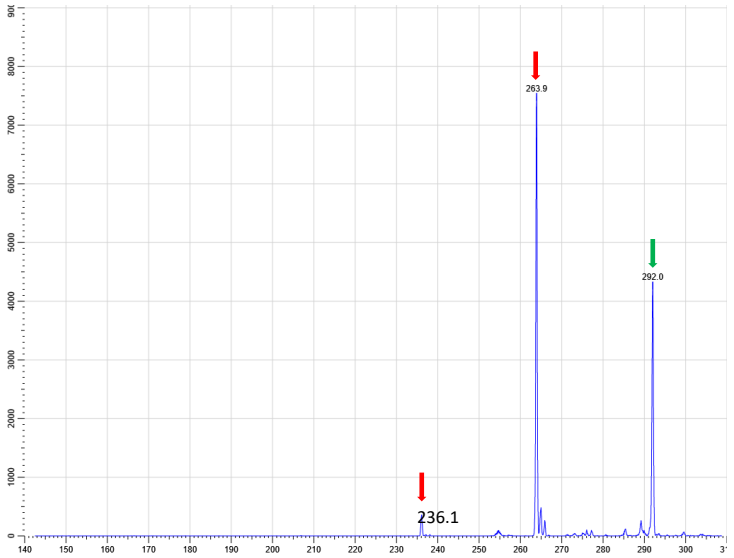
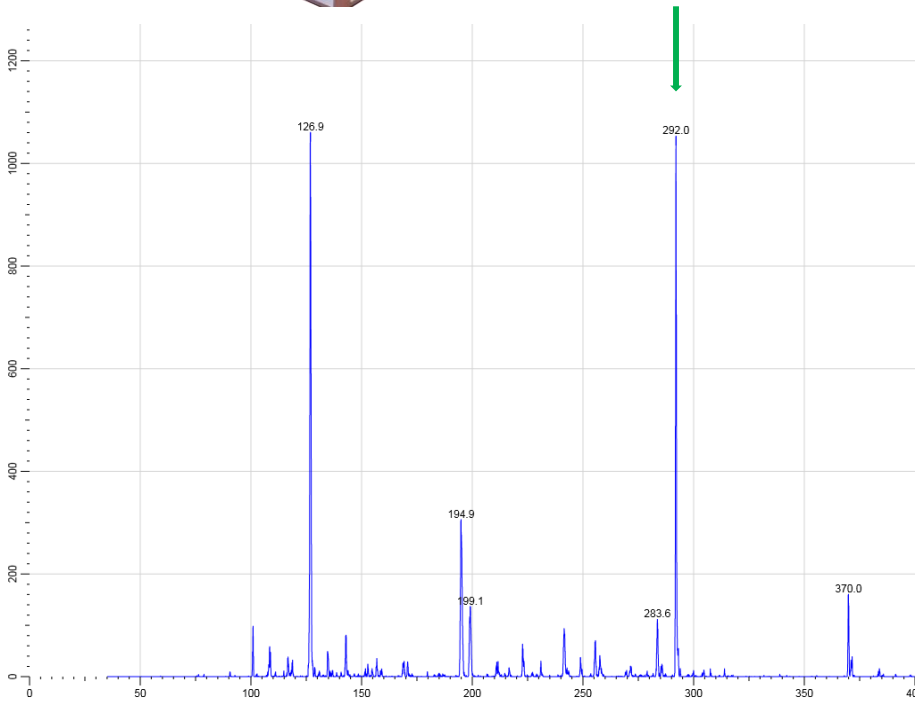
MTE30 Interfaced with DS-APCI Ion Source



Parathion, 2ng
+ ve ion mode MS/MS



Parathion, 2ng
+ ve ion mode MS

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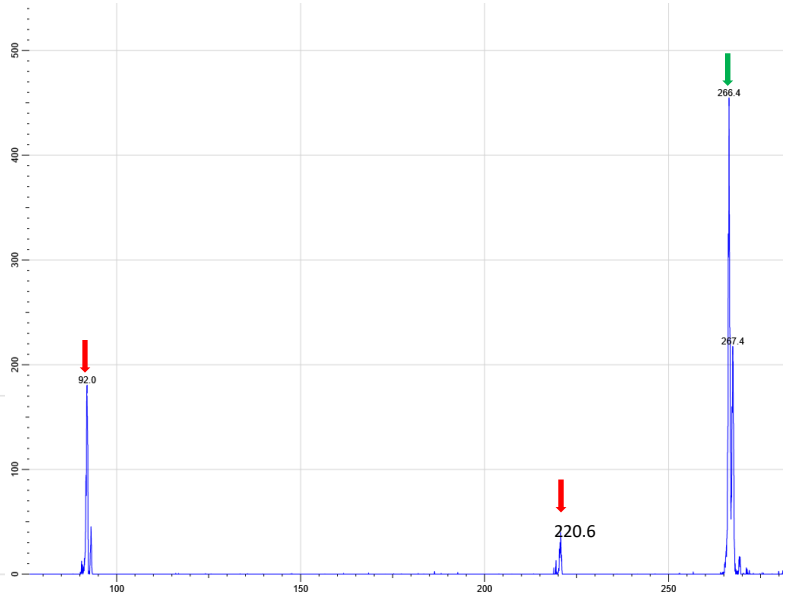
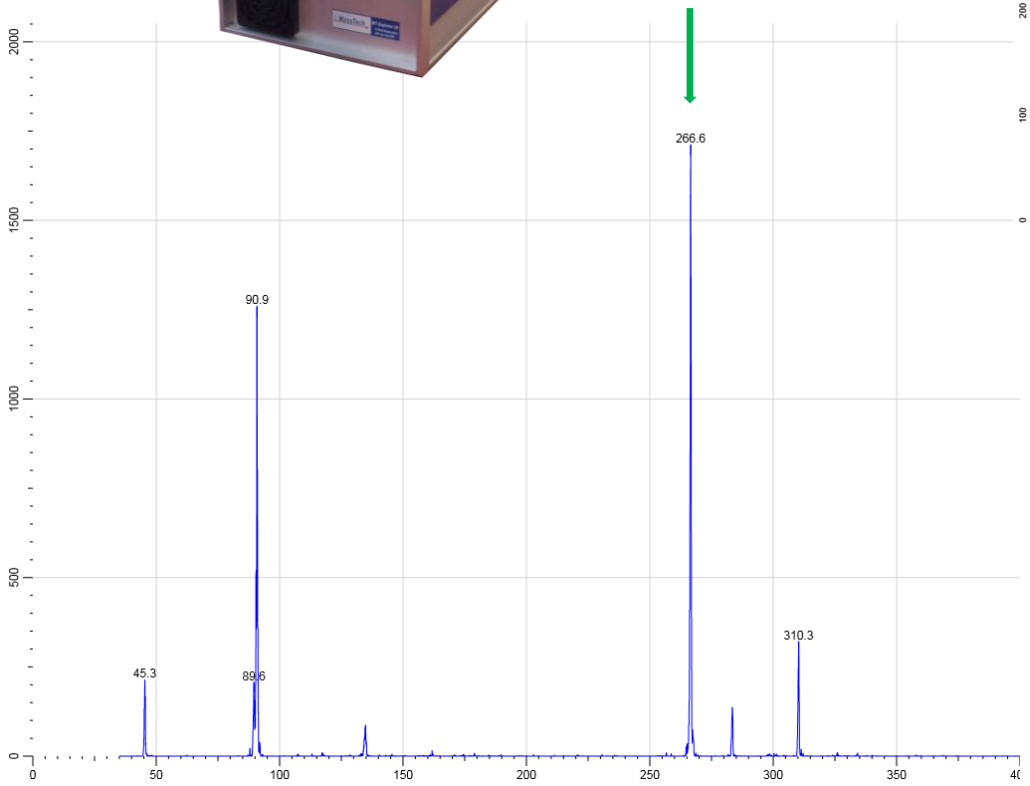
MTE30 Interfaced with DS-sESI Ion Source



RDX 2 ng
- ve ion mode MS/MS



RDX 2 ng
- ve ion mode MS

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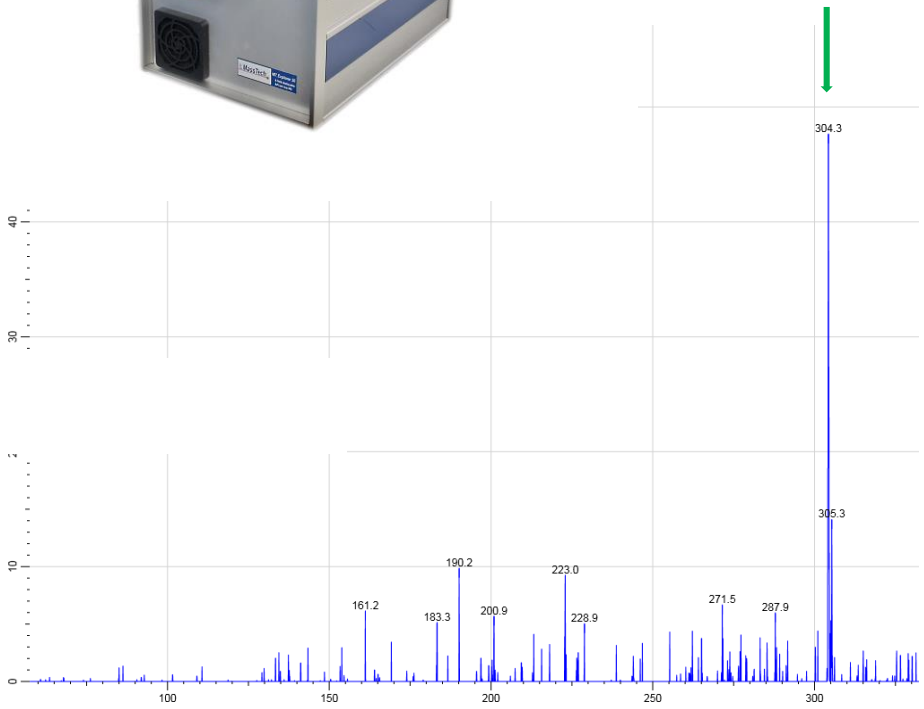
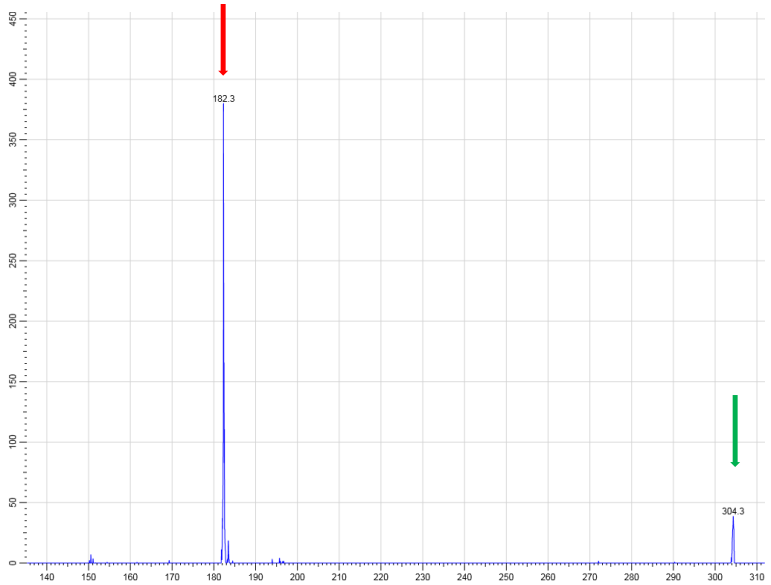
MTE30 Interfaced with Plasmion SICRIT™ Ion Source



Cocaine 500 pg
+ ve ion mode MS



Cocaine 500 pg
+ ve ion mode MS/MS

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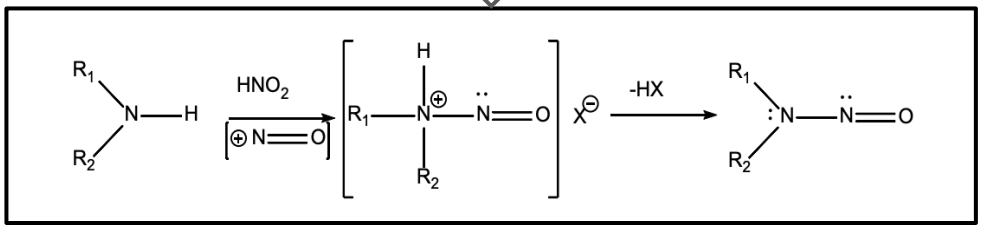
Pharmaceutical Impurities
Nitrosamines

- Class of genotoxic compounds
- Potent (Probable) Carcinogens (International Agency for Research on Cancer (IARC))
- Found in drinking water, beer, fried food, cigarettes, meat, and evidently, certain pharmaceutical agents

- 2020 FDA recall of Ranitidine due to unacceptable levels of Nitrosamines
- Increasingly discovered at many different stages of pharmaceutical development
- Any process that uses nitrites in the presence of secondary, tertiary, or quaternary amines risks the formation of Nitrosamines (FDA)

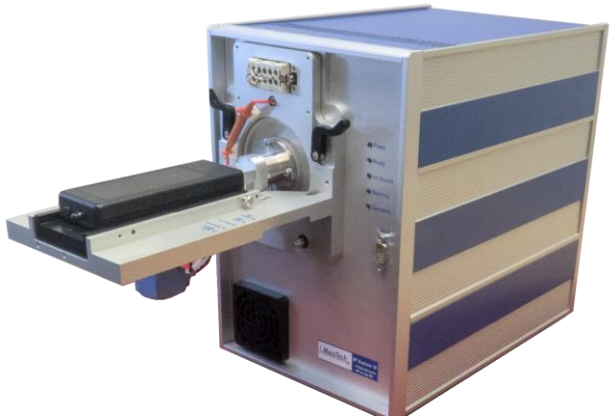


Via US Food and Drug Administration

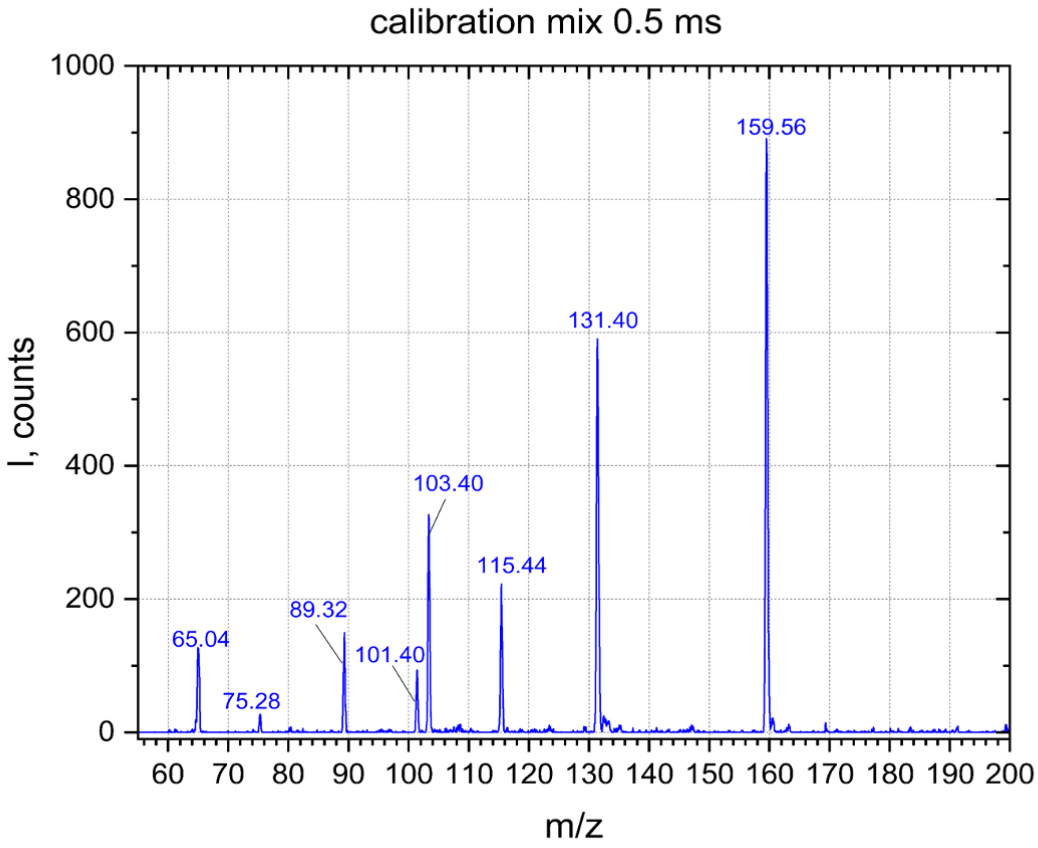
Businessweek
Business

A New Contaminant Found in Popular Drugs Could Cost Big Pharma Millions

Nitrosamines, linked to cancer, have surfaced in Zantac, Januvia, and generic valsartan.



0.5 ppm MS – N-Nitrosamine impurity standards (7) from Restek



Rudimentary LOD Table

Nitrosamine	FDA AI (ng/day)	Observed Mass (m/z)	Limit of Detection FS (ppm/ppb)	Limit of Detection SIM (ppm)
NDMA	96	75.3	-	0.1 ppm
NMEA	-	89.1	0.4 ppm	50 ppb
NPYR	-	101.1	0.1 ppb	-
NDEA	26.5	103.4	0.1 ppm	0.1 ppm
NPIP	-	115.2	0.1 ppb	-
NDPA	26.5	131.1	5 ppb	0.1 ppb
NDBA	-	159.1	0.1 ppb	-

MS/MS, 1ppm

Nitrosamine	Nominal Mass (amu)	Exact Mass $[M+H]^+$	Observed $[M+H]^+$ (*m/z*)	MS Mode (FS/SIM[1])	MS/MS Expected Product Ion (*m/z*)	MS/MS Observed Product Ion[2] (*m/z*)	CE (%)
NDMA	74.08	75.08	75.3	SIM	43, 58	58	16
NMEA	88.11	89.11	89.1	SIM	61	60.7	16
NPYR	100.12	101.12	101.1	FS	55.1	55.1,75.2	16
NDEA	102.14	103.14	103.4	FS	75.1	75.2	16
NPIP	114.15	115.15	115.2	FS	69.1	69.1	16
NDPA	130.19	131.19	131.1	FS	-	89.1	16
NDBA	158.24	159.24	159.1	FS	103.1	103.2	25

Thank you