Broadband, Fully Automated Identification of Drugs Using a Field Deployable DART-ITMS

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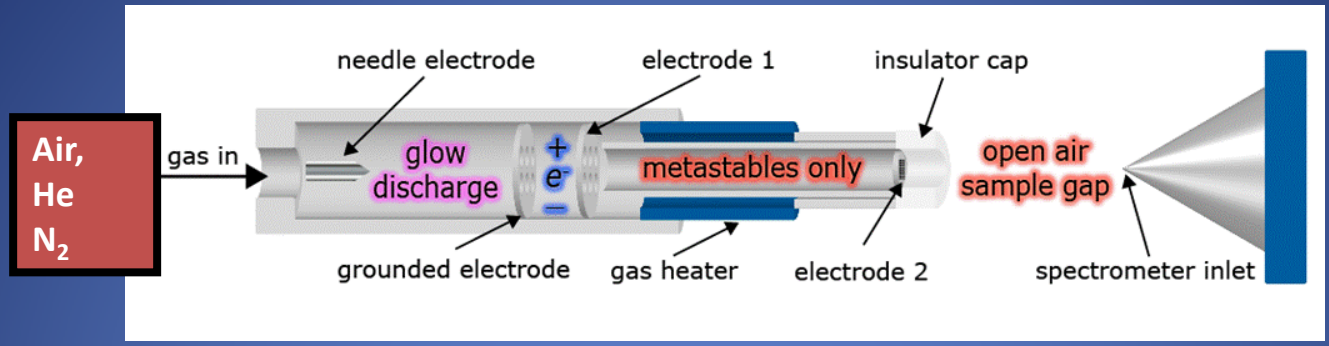
apmaldi.com

Harsh Environment Mass Spectrometry Workshop, Baltimore, MD, USA

September 15th, 2015

DART: Direct Analysis in Real Time



DART Schematic (Image Courtesy of- Ionsense)

- No Sample preparation
- Liquid or solid sample introduction
- Air, Nitrogen or Helium gas input

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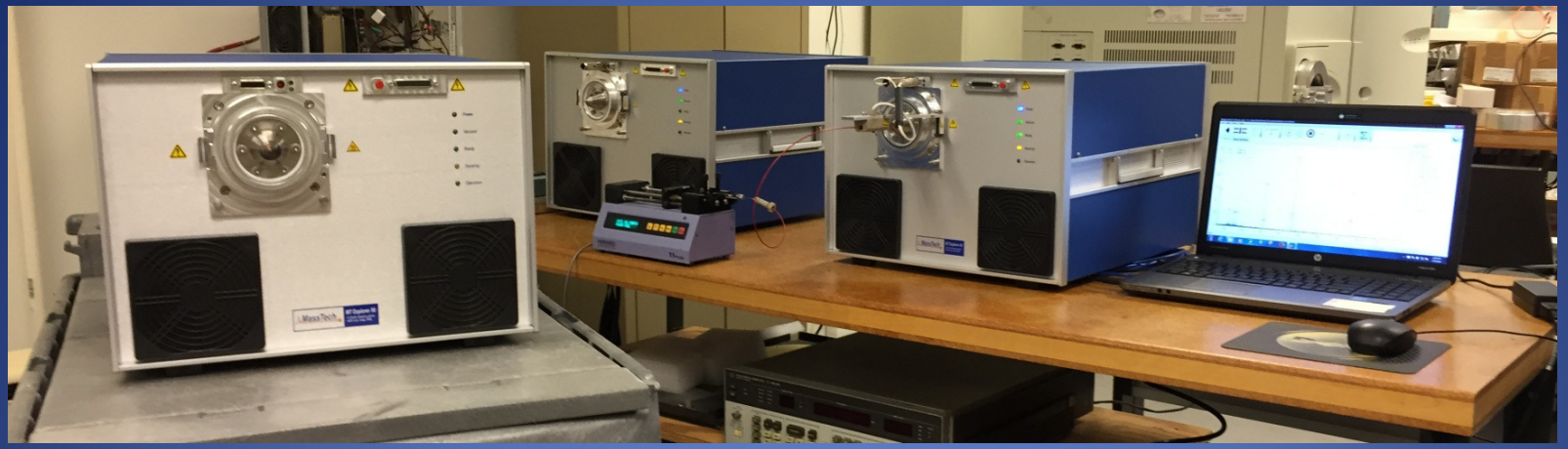
MTE 50: Specifications



- Atmospheric pressure interface (API)
- MS , MS/MS and MS^3 modes of operation
- Mass range: 30-2,500 Da
- Mass accuracy 0.3 Da
- Weight 75 lb
- Dimensions 12”x17”x20”
- Power 100-300W

DS-APCI

DART

AP-MALDI

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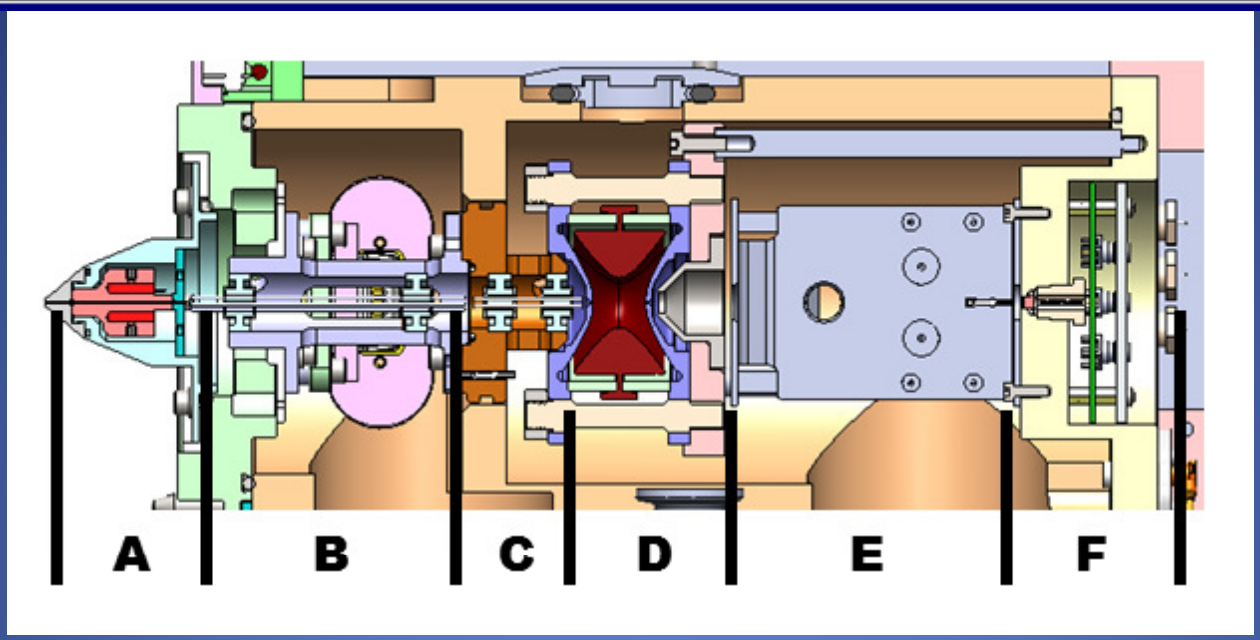
MTE 50 : Mass Spectrometer Built for Mobility



A. Cone, heating elements and inlet capillary
B. Ion optics: inlet hexapole ion guide and conductance limit orifice
C. Ion Optics: MS analyzer hexapole ion guide
D. Ion trap mass analyzer
E. Conversion dynode and electron multiplier
F. Pre-amplifier

- Two vacuum chamber design (U.S. Patent 8,471,199)
- Bounded hydrogen (metal hydride) cartridge as a source for buffer gas (U.S. Patent 8,476,586)

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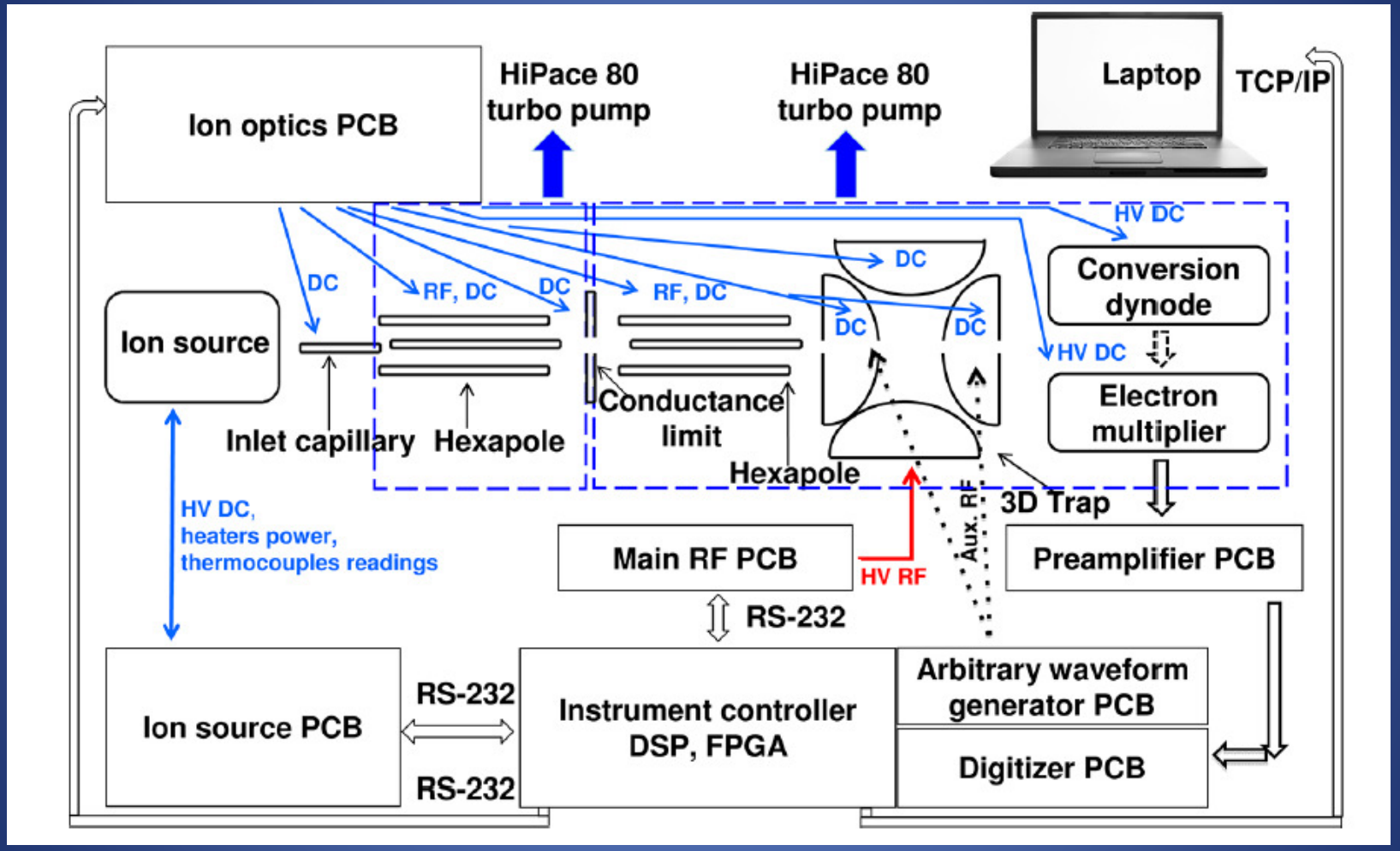
Misharin et al. *Anal. Chem.*, **2012**, *84* (22), pp 10105–10112

MTE 50 : Mass Spectrometer Built for Mobility



- **Two vacuum chamber design (U.S. Patent 8,471,199)**
- **Bounded hydrogen (metal hydride) cartridge as a source for buffer gas (U.S. Patent 8,476,586)**

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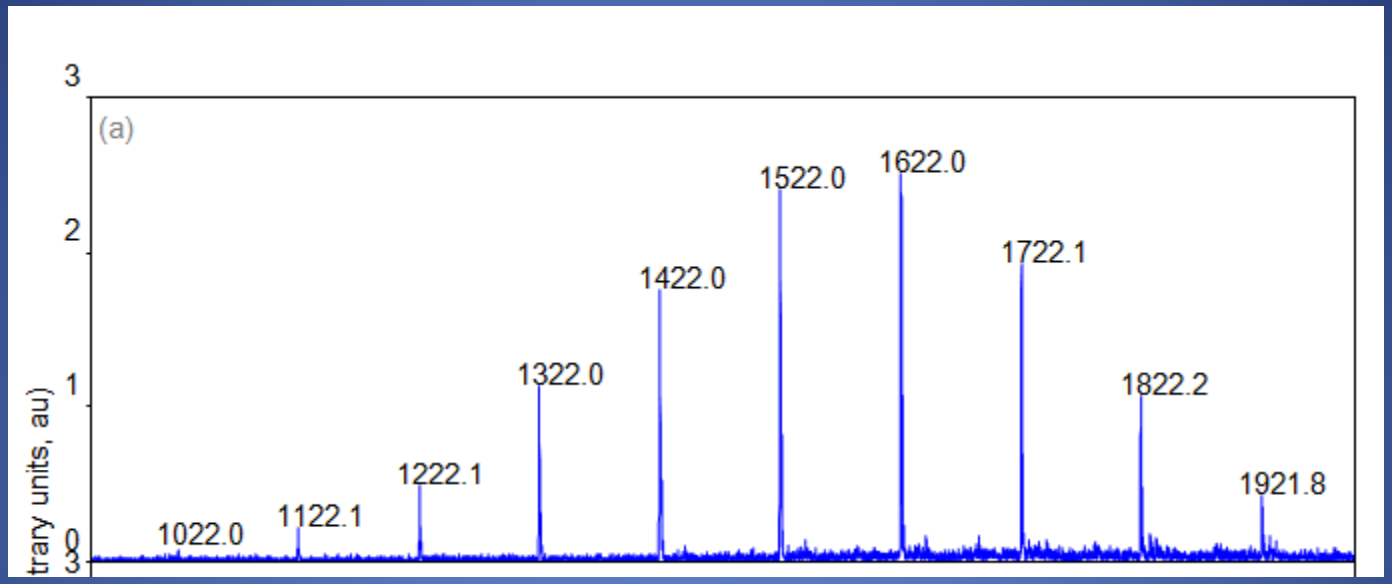
Misharin et al. *Anal. Chem.*, **2012**, *84* (22), pp 10105–10112

MTE50: Broadband MS/MS



ESI-MS of the calibration mixture (Ultramark)

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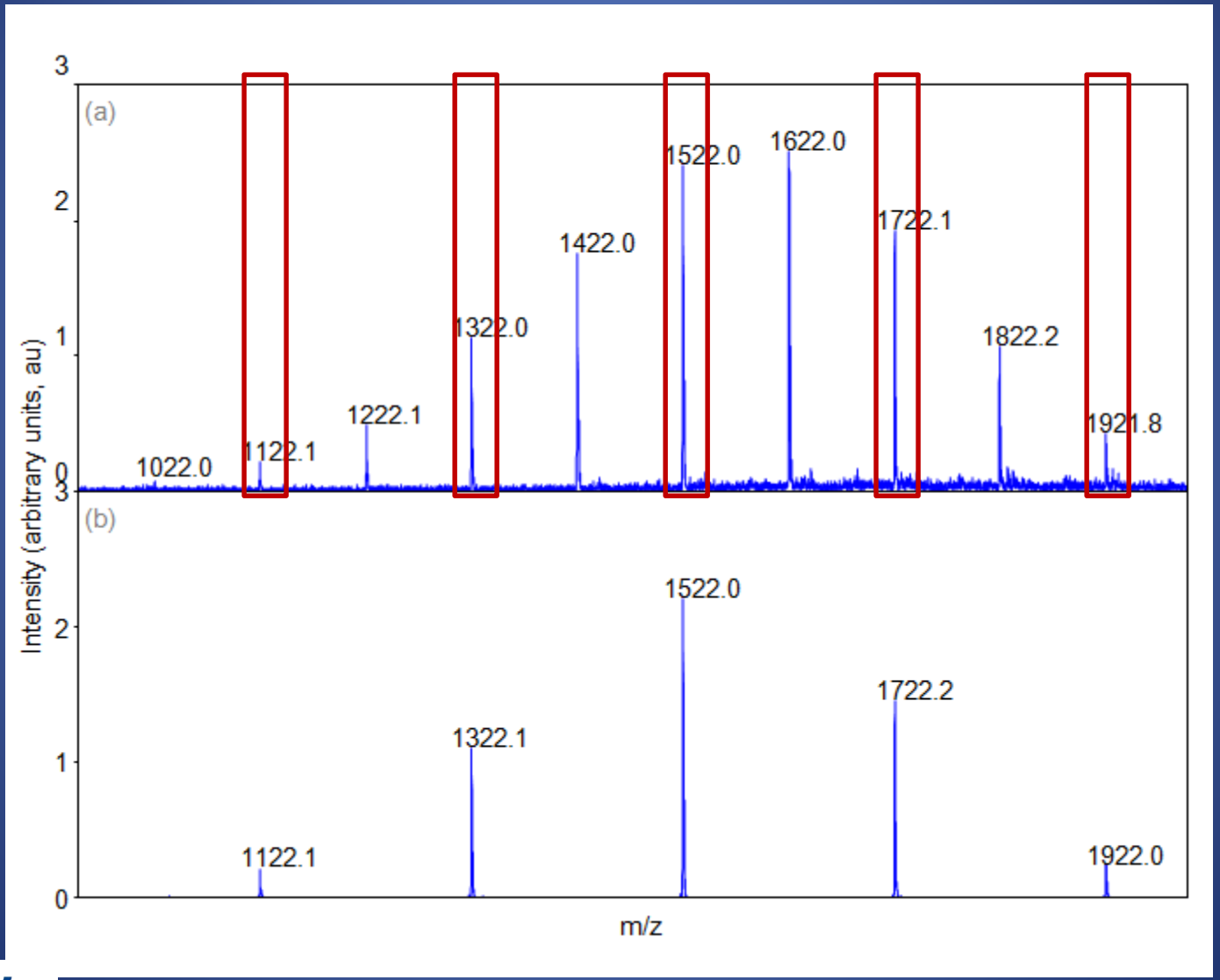
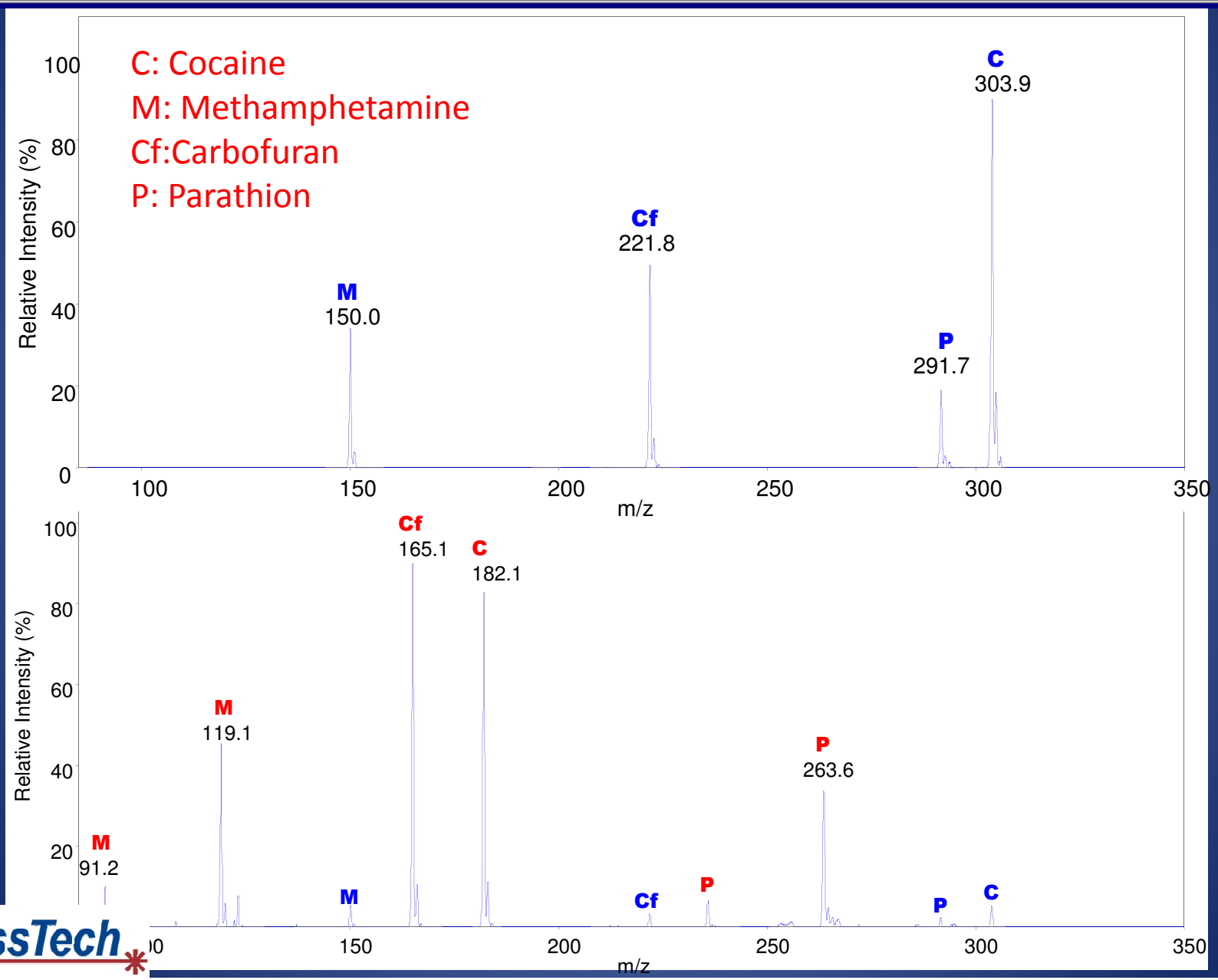
MTE50: Broadband MS/MS

ESI-MS of the calibration mixture



MTE50: Broadband MS/MS



DART-MTE 50

No pumps under the table, nothing hiding in the back

(except a small nitrogen cylinder)

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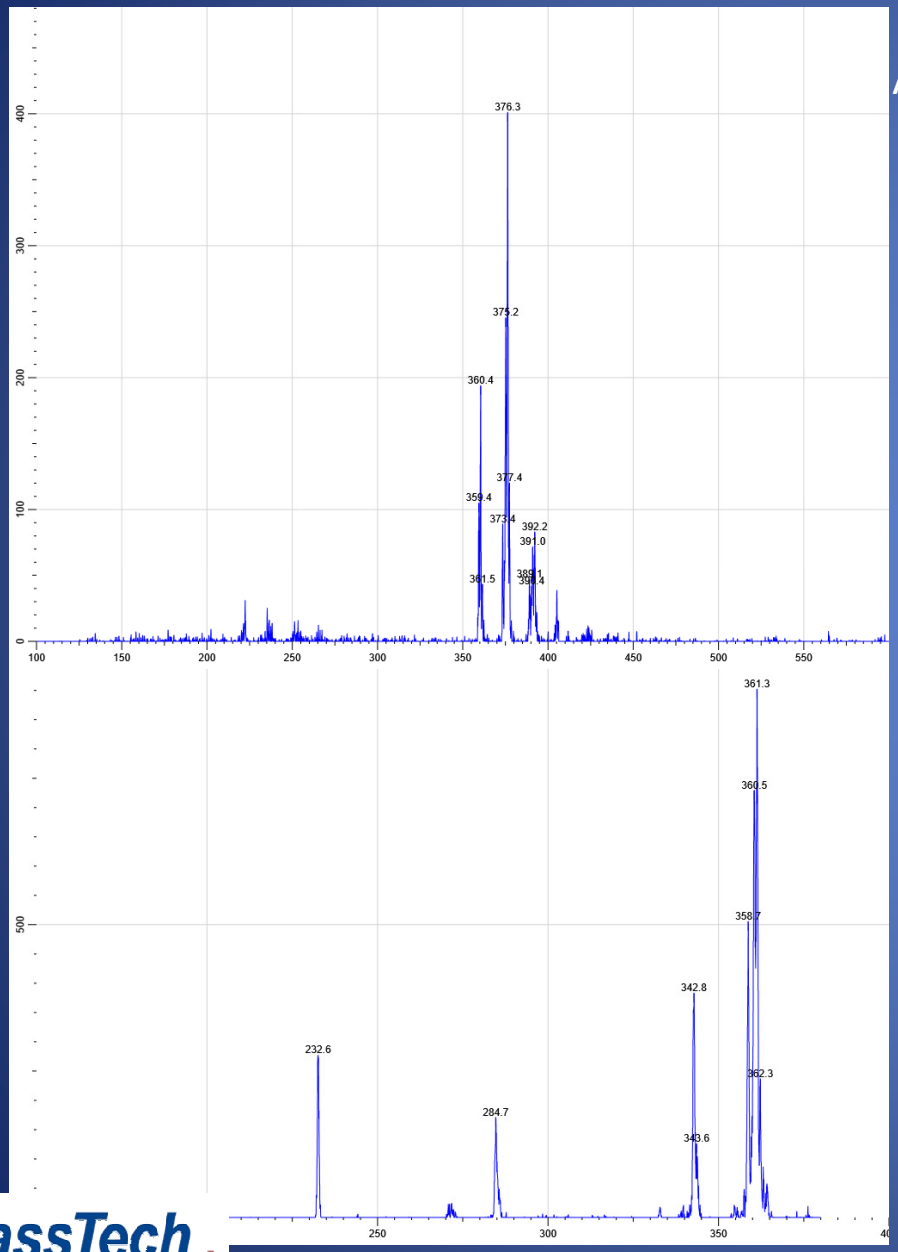
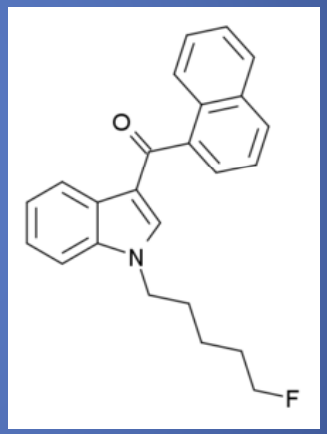
MTE50 Interfaced with DART Ion Source

Examples of User Library Spectra



AM2201

IUPAC name:
1-[(5-Fluoropentyl)-1H-indol-3-yl]-(naphthalen-1-yl)methanone



AM2201
(MSMS)

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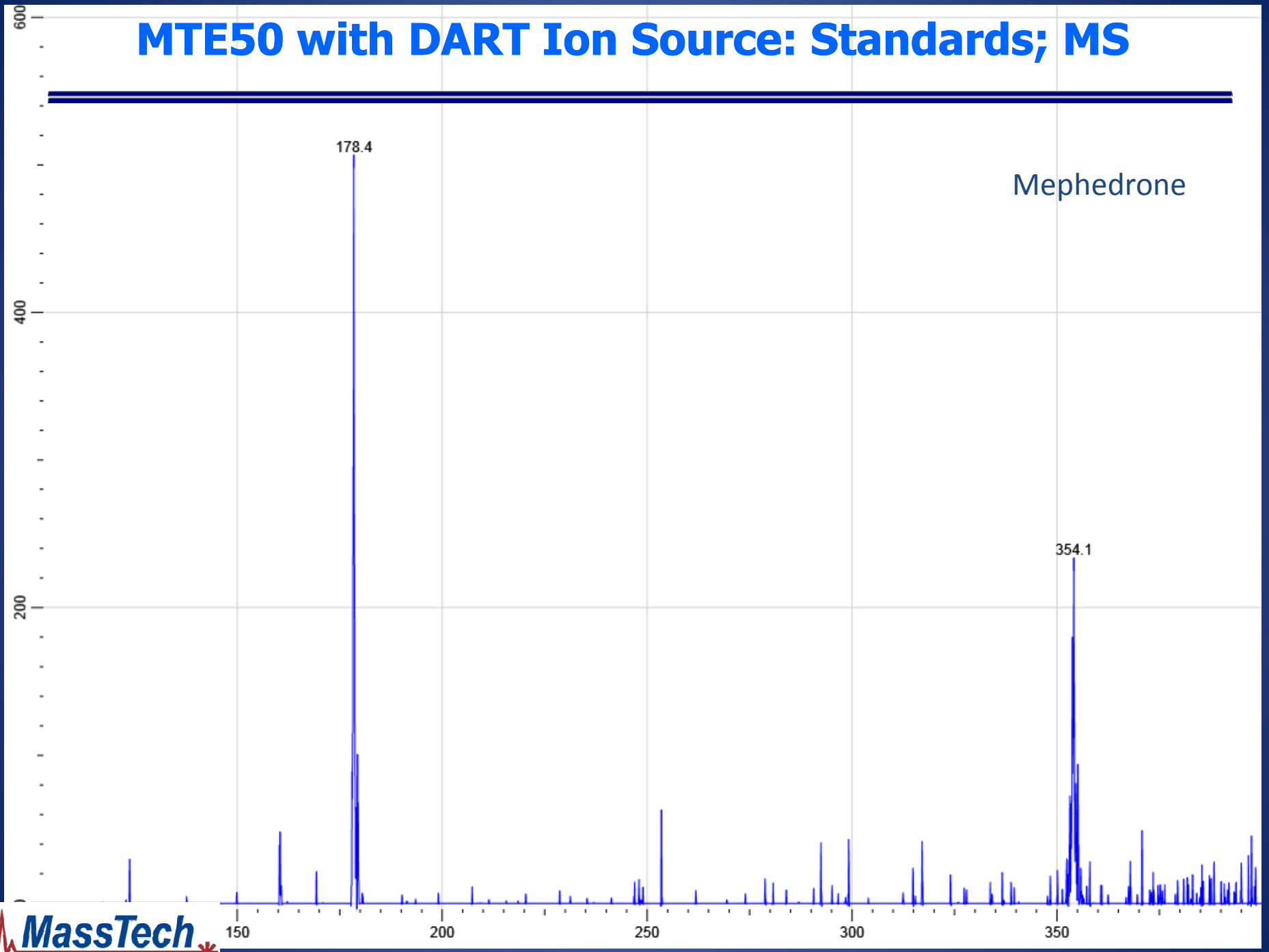
MTE50 with DART Ion Source: Standards; MS



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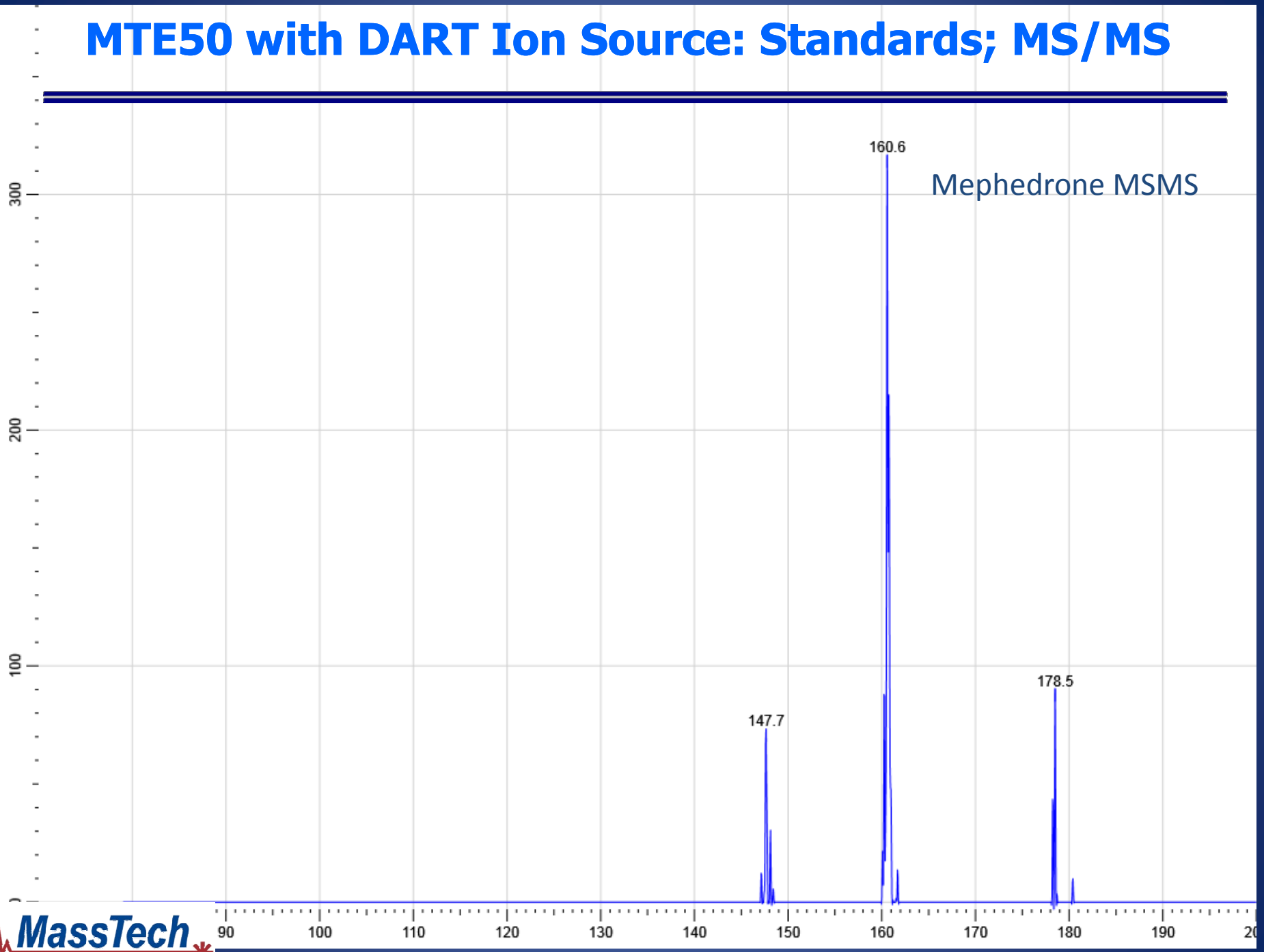
MTE50 with DART Ion Source: Standards; MS/MS



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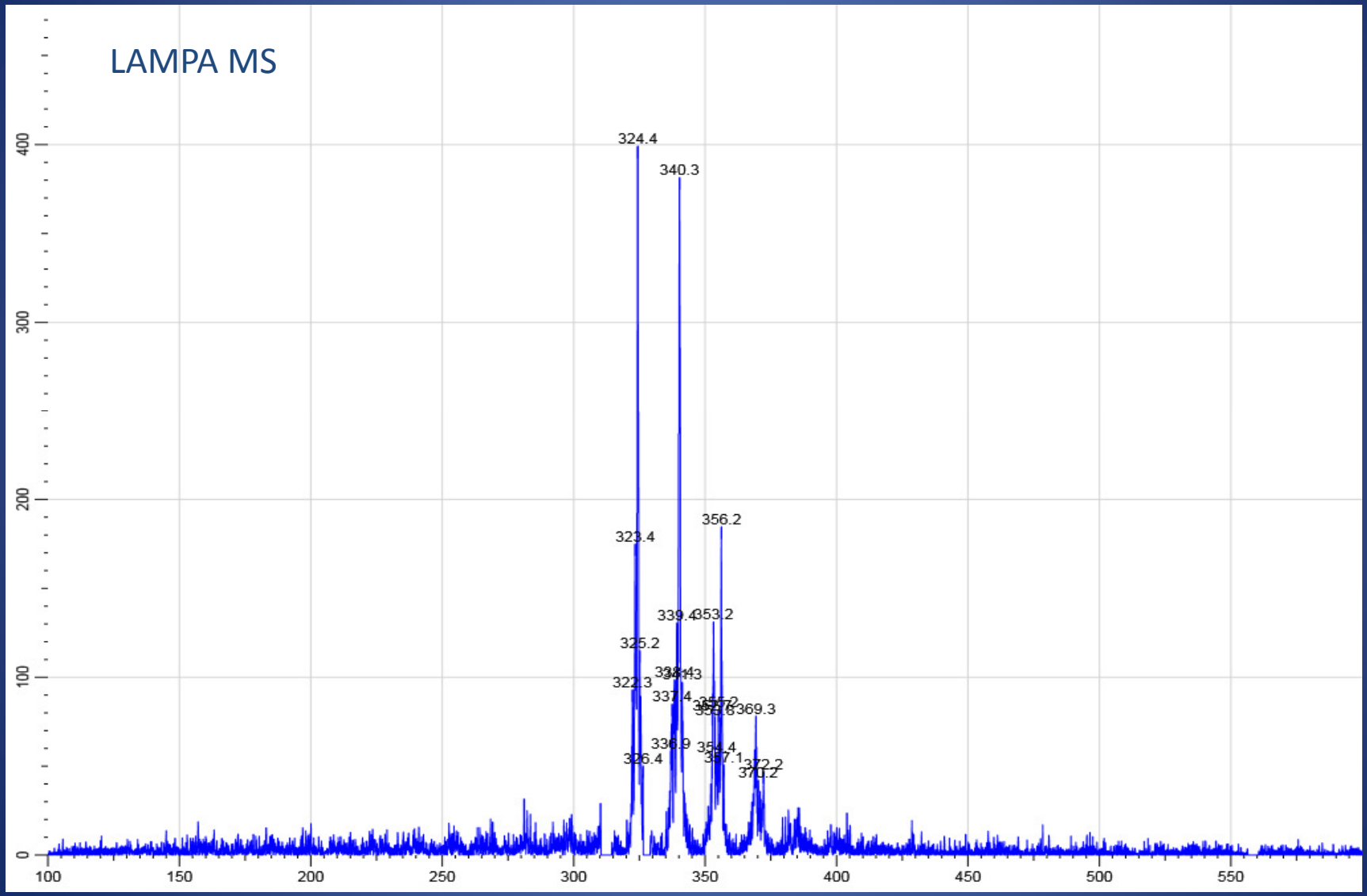
MTE50 with DART Ion Source: Standards; MS/MS



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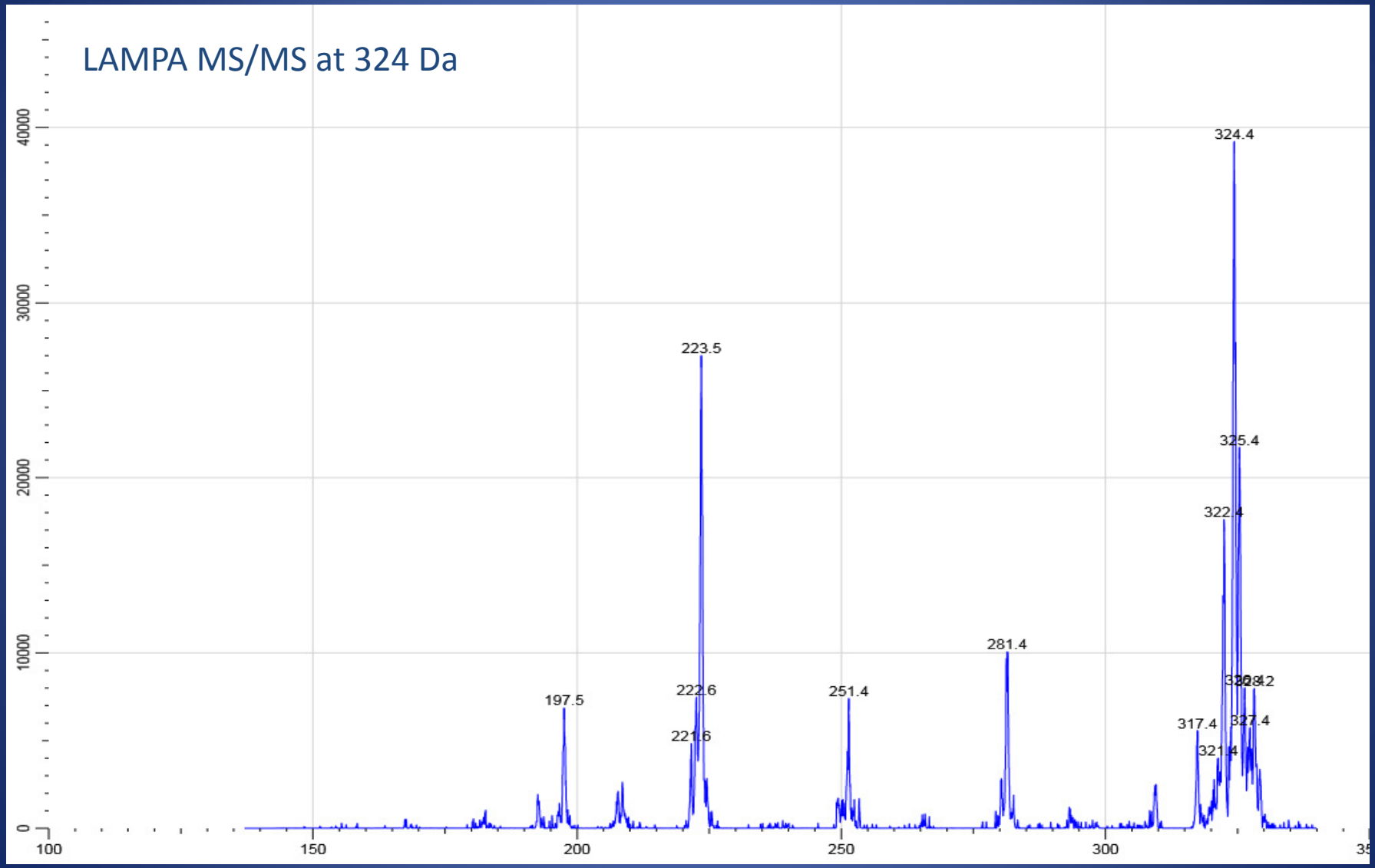
MTE50 with DART Ion Source: Standards; MS/MS

LAMPA MS/MS at 324 Da



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DART –ITMS : Observed Ions

Compounds Tested	MW	MS Ions observed	MSMS parent	MSMS fragments	Mass Loss	Optimum Frg
Cocaine	303	304	304	182	122	7
LAMPA	323	324,340,356,372,388	324	281,251,223,197	42,72,104,127	5
Methcathinone	163	165, 326	164	147	17	3
Mephedrone	177	178,354	178	160	18	3
Methylone	207	208,414	208	190,160	18,48	3
MDMA	193	194,414,449?	194	163	31	3
MDEA	207	208	208	163	45	3
MDA	179	180,163	180	163	17	3
Oxycodone	315	316	316	298	18	7
Methamphetamine	149	150.7, 303.9	150.7	135,119	15,31	5
Amphetamine	135	136,270	136	119	17	3
Caffeine	195	196, 390	196	139,110	57,86	5
Scopolamine	303	304	304	138	166	7
Diazepam	284	285,304	285.6	257,222, 193,182,154	28, 63, 93, 102,130	10
Heroin	369	370	370	328,310, 268	52, 60, 102	7.5
Morphine	285.3	286, 302,319	286	229,201,183	57,85,103	7
Acetaminophen	151	152,302	152	110, 75	42	3
LSD	323	324,340,356,372,388	324	281,251,223,197	42,72,104,127	5
Sudafed-pseudoephedrine	165	166, 358,403, 447	166.5	148,5	124.5	5
Acetaminophen-powder	151	152,302	152	152,110	42	3
5APDB	177	178,354	178	161	17	5
6APDB	177	178,354	178	161	17	5
5APB	175	176,350	176	159	17	5
Methadrone	193	194	194	176	18	5
251NBOMe	424	425.8, 427.7	425	291	134	6
THC	313	314	314	297, 259	18, 55	5
Alprazolam	308	309	309	281, 274	28, 35	6
AM2201	359	360	360	360, 342, 284,232	18, 76, 128	5
JWH 210	369	370, 388	370	370, 353, 312, 214, 183	17, 58, 156, 187	6
N,N Dimethyl Cathinone	177	178, 195	178	133, 105	45,73	5

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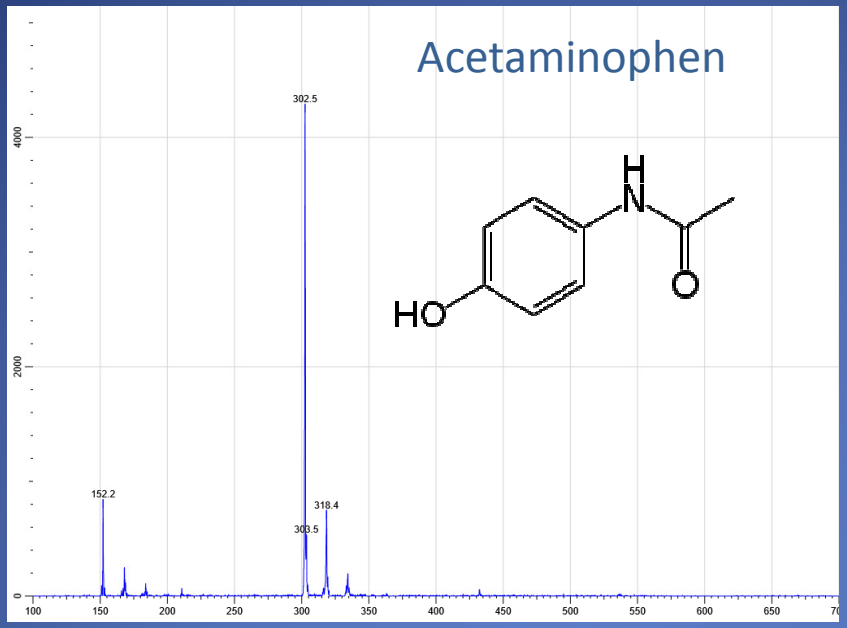
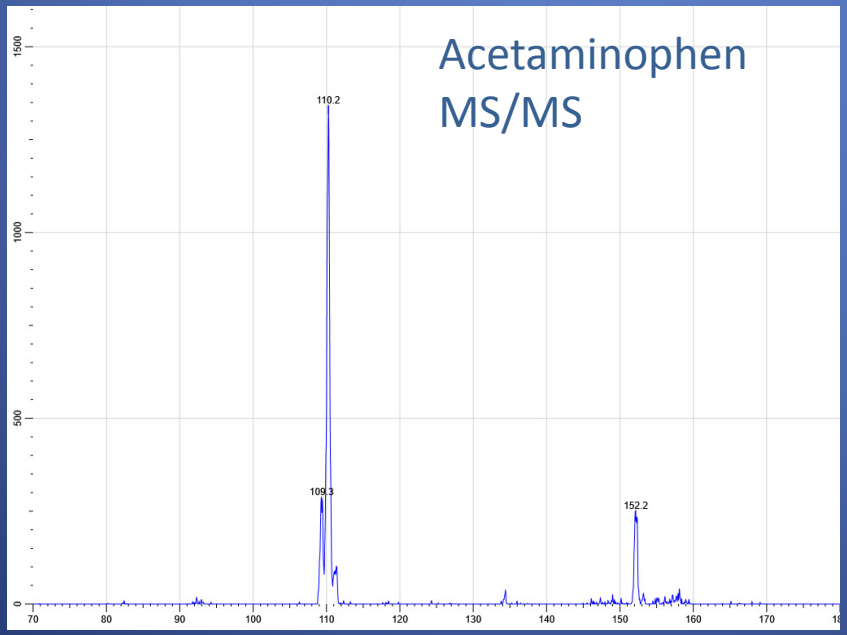
Tablet sampling





Tablets sampled directly by rubbing them onto the Open Spot card

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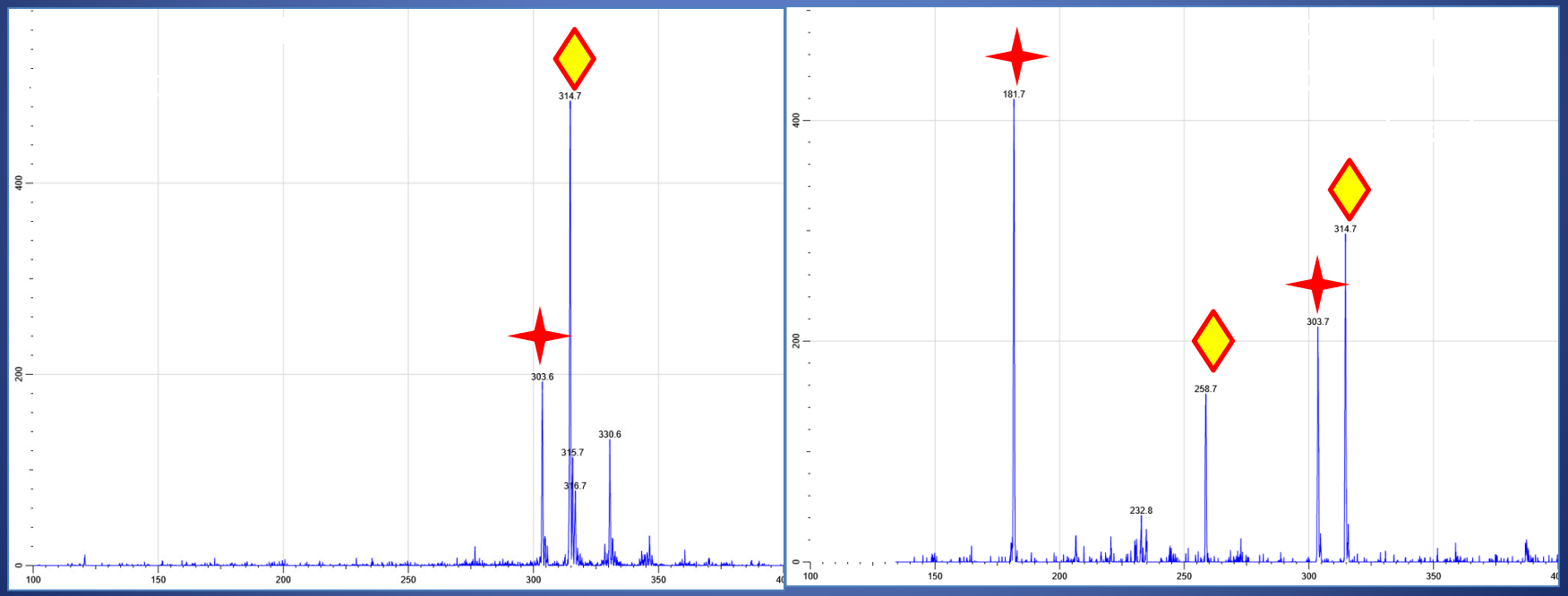
DART-ITMS: Broadband MS/MS

The unique feature of the system is its ability to do broadband MS/MS analysis. (isolating multiple parent ions simultaneously and then fragmenting them). This increases the number of targets being monitored as well as throughput. Below is the MS and MS/MS spectrum of a mixture of cocaine and THC.



Cocaine and its fragments

THC and its fragments

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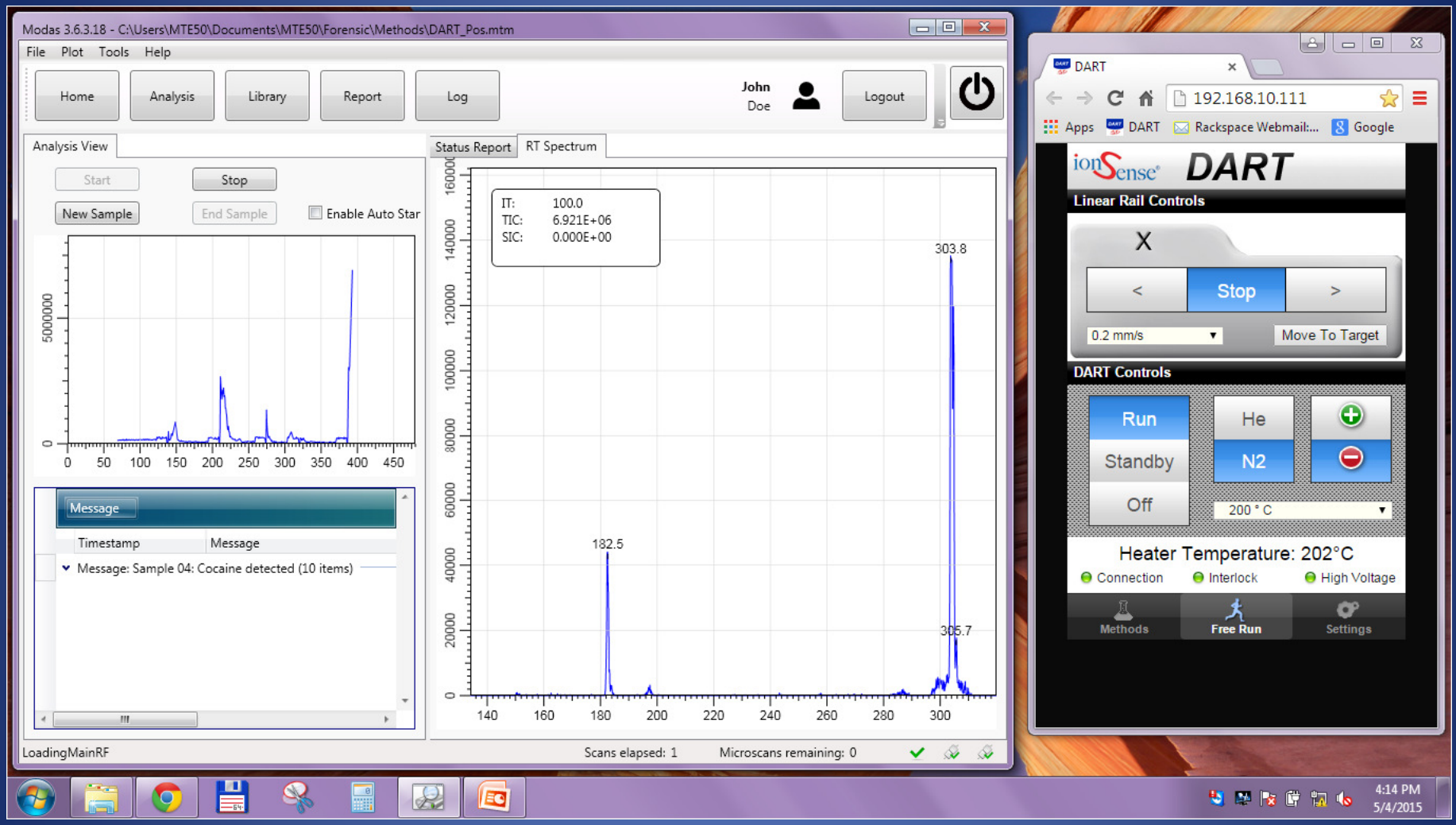
DART-ITMS: Software Operation



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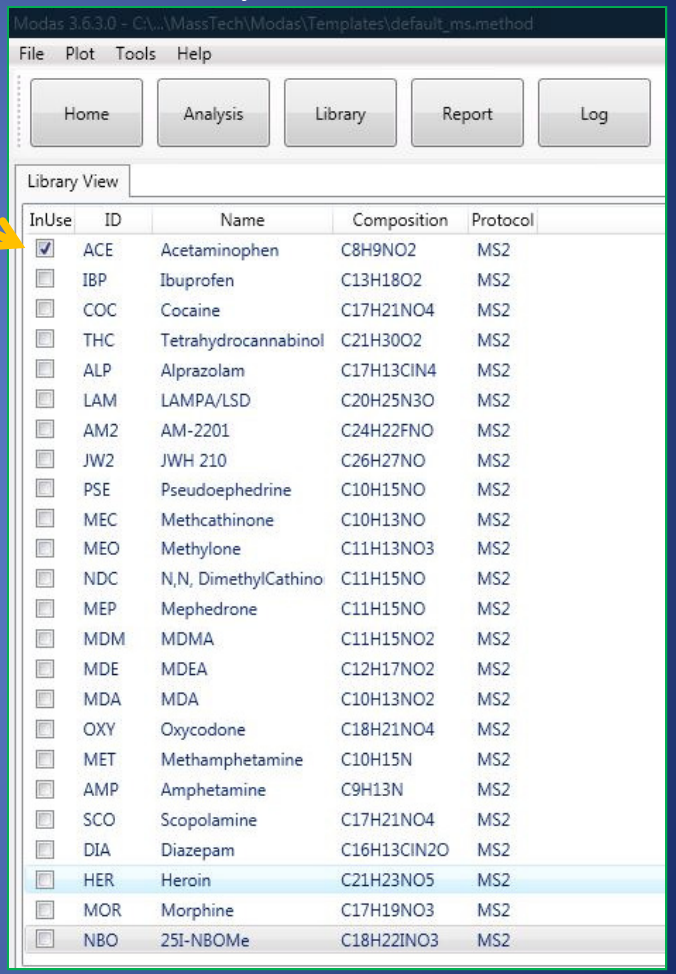
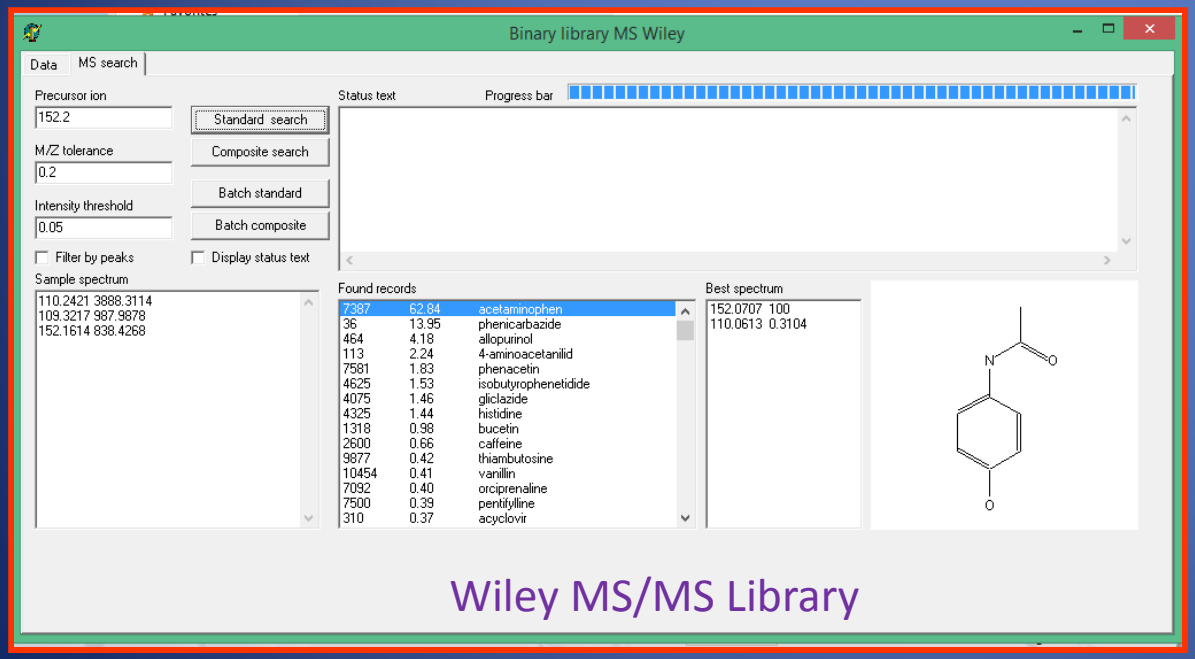
DART-ITMS: Library Options

Target specific monitoring can be done by checking appropriate boxes.

User Generated Library





Wiley MS/MS Library

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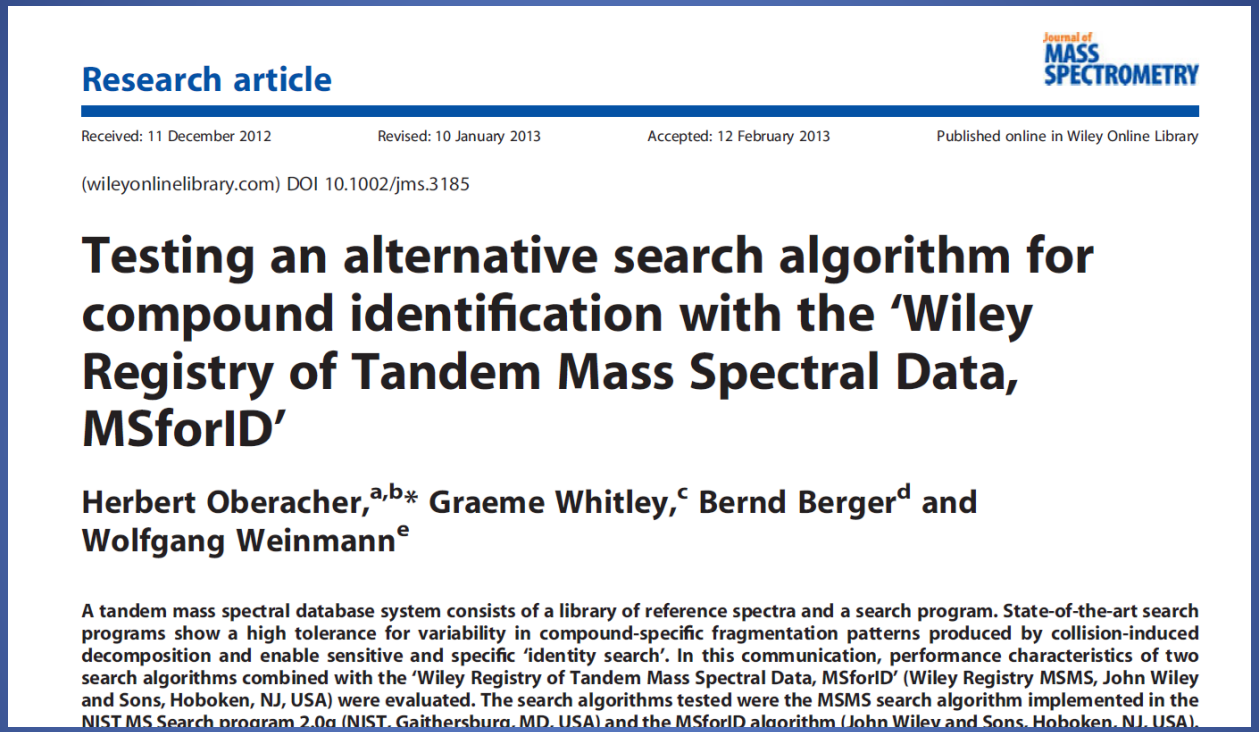
DART-ITMS: Library Options



Research article

Journal of MASS SPECTROMETRY

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Testing an alternative search algorithm for compound identification with the 'Wiley Registry of Tandem Mass Spectral Data, MSforID'

Herbert Oberacher,[a,b]* Graeme Whitley,[c] Bernd Berger[d] and Wolfgang Weinmann[e]

A tandem mass spectral database system consists of a library of reference spectra and a search program. State-of-the-art search programs show a high tolerance for variability in compound-specific fragmentation patterns produced by collision-induced decomposition and enable sensitive and specific 'identity search'. In this communication, performance characteristics of two search algorithms combined with the 'Wiley Registry of Tandem Mass Spectral Data, MSforID' (Wiley Registry MSMS, John Wiley and Sons, Hoboken, NJ, USA) were evaluated. The search algorithms tested were the MSMS search algorithm implemented in the NIST MS Search program 2.0g (NIST, Gaithersburg, MD, USA) and the MSforID algorithm (John Wiley and Sons, Hoboken, NJ, USA).

J. Mass Spectrom 2013, 48, 487-496

J. Mass Spectrom 2013, 48, 497-504

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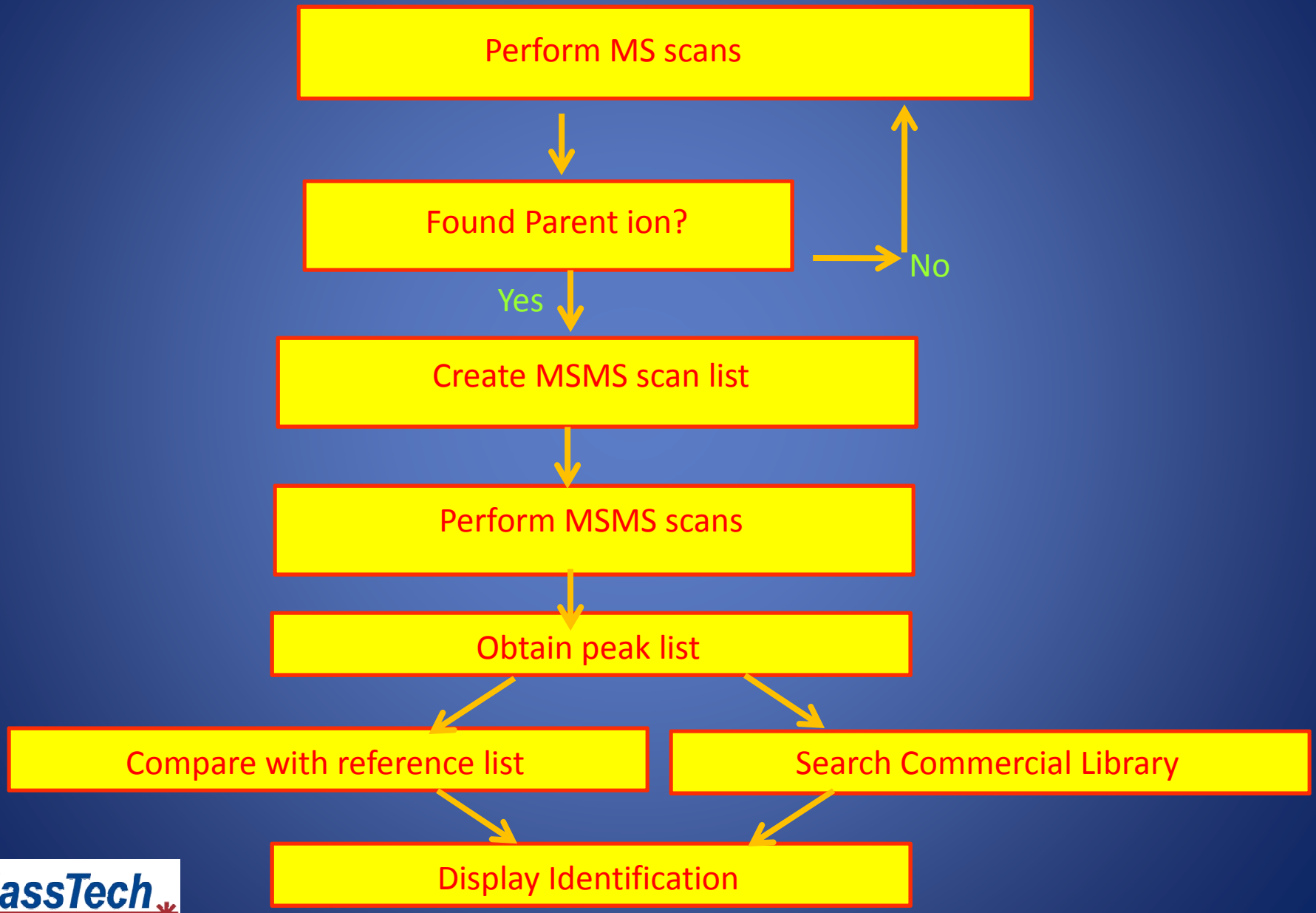
Library Search Procedure



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DART-ITMS: Library Identification

- No parent ion- no MS-MS interrogation.

  -User can select – to accommodate unknowns

- Signal processing is automatically done to remove to reduce influence of electronic noise.
- User library simply looks for match; no intensity information is used. (using intensity values can be helpful)
- Wiley library output is sorted by *ramp* values

(relative average match probability). Top on the list is picked if the ramp value is >40. (needs further work)

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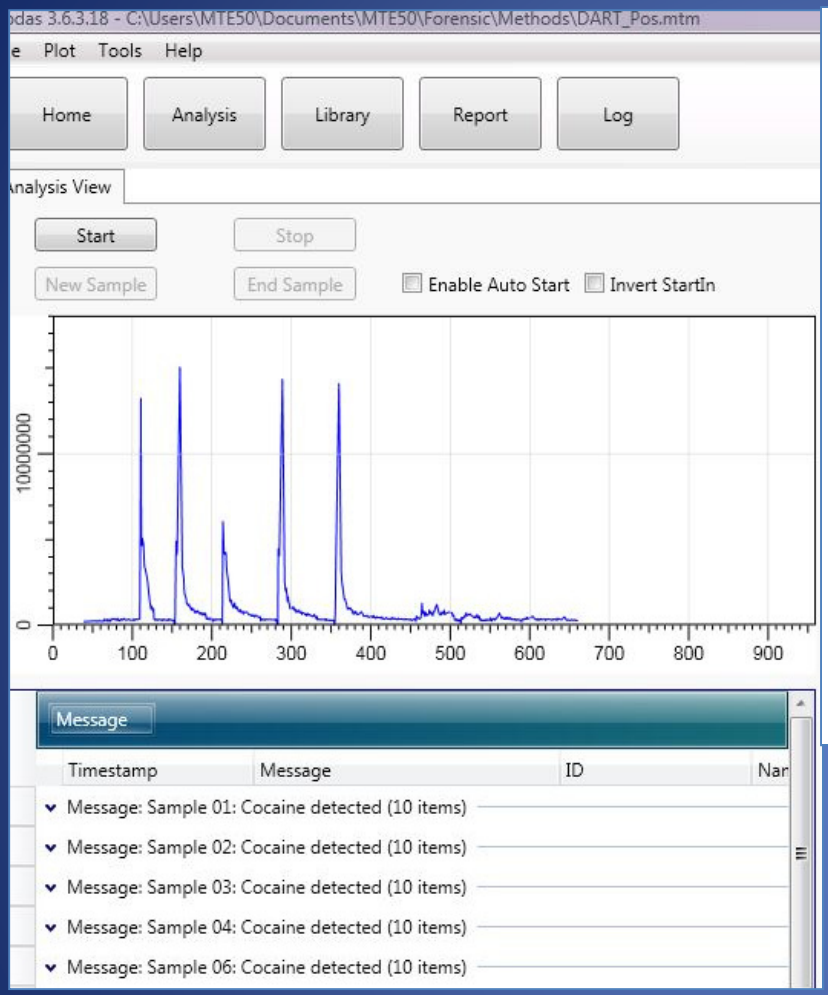
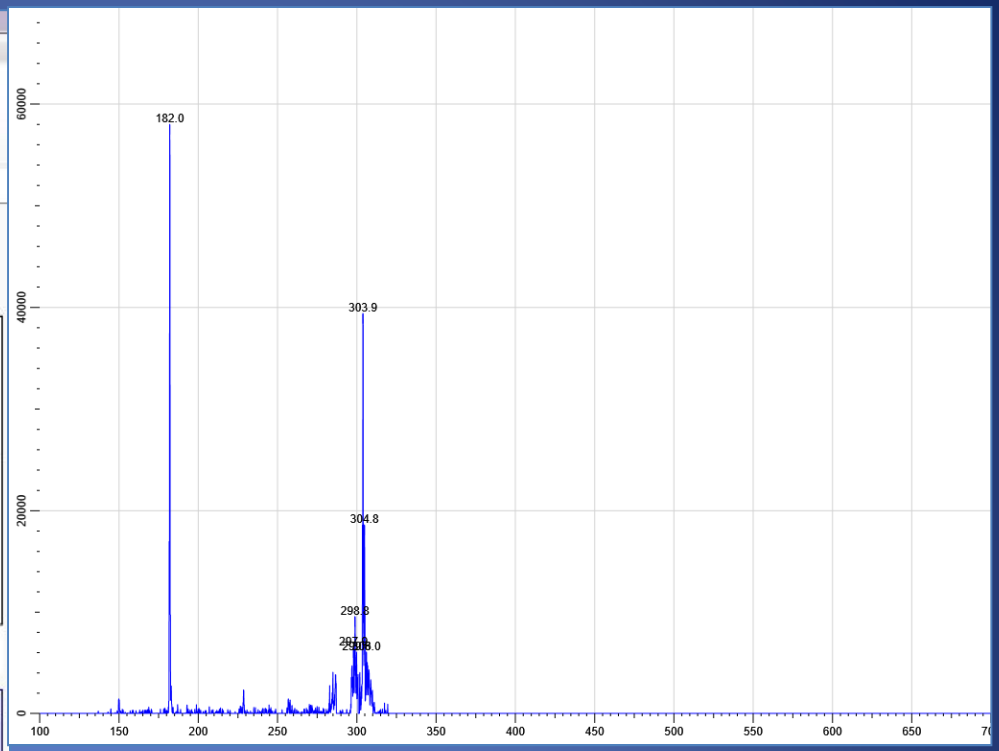
DART-ITMS: Software Operation





Replicates of same sample automatically detected by the software; liquid sample spotted on the Open Spot card.

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Conclusions

- DART and Ion trap MS can be used for a mobile system
- On board libraries are available for target identification (including Wiley MS/MS library)
- Multiple targets can be interrogated simultaneously by Broadband MS/MS

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thank you -gracias - danke -谢谢- спасибо -teşekkürler

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