

## Analysis of explosives, drugs, pesticides and chemical warfare simulants using Direct Sampling Atmospheric Pressure (DSAP) source with APCI and sESI modules coupled to MT Explorer 30 (MTE30) Mass Spectrometer

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### Overview

A portable mass spectrometer, MT Explorer 30 (MTE30), recently developed by MassTech Inc, was interfaced with a direct sampling atmospheric pressure (DSAP) ionization source using atmospheric pressure chemical ionization (APCI) as well as secondary electrospray ionization (sESI) cartridges. Sensitive MS and MS/MS detection of explosive materials, drugs, pesticides, and chemical warfare simulants was performed using the DS-APCI and DS-sESI ionization sources.

### Keywords:

MT Explorer 30  
MTE30  
DSAP source  
DS-APCI  
DS-sESI  
Explosives  
Drugs  
Pesticides  
CWA simulants

## **Introduction:**

MTE30, the MassTech Inc's recent product, is a portable, field-deployable mass spectrometer. MTE30 utilizes the ion trap as the mass analyzer. This makes possible working at higher gas pressures with lower power consumption and reduction in weight<sup>1</sup>. Most importantly, MTE30 offers tandem mass spectrometry capabilities<sup>1</sup>.

MTE30 also allows interfacing different ambient ionization sources. In our previous studies, we have successfully interfaced MT Explorer product series with Direct Analysis in Real Time (DART)<sup>1</sup>, APCI<sup>2</sup> and micro-electro-mechanical system (MEMS) gas chromatography<sup>3</sup> sources. Our field-deployable mass spectrometer, MT Explorer series found major applications in niche areas such as on-site forensics, drug regulatory bodies, public safety research<sup>1-3</sup>.

In this application note, in addition to APCI, we demonstrate interfacing of sESI source with MTE30 for the analysis of explosive materials, drugs, pesticides, and chemical warfare agent simulants.

## **Experimental:**

### **Chemicals**

Explosives: trinitrotoluene (TNT) and royal demolition eXplosive (RDX). Drugs: cocaine and methamphetamine. Pesticides: parathion. A chemical warfare agent (CWA) simulant: methyl salicylate. HPLC grade water, acetonitrile and formic acid. All chemicals were purchased from Aldrich-Sigma (USA).

### **Preparation of Solutions**

TNT and RDX were prepared by diluting stock solutions with acetonitrile. An acetonitrile/water (1:1, v/v) solution with 0.1% of formic acid was prepared as sESI spraying solution.

### **Sample Preparation**

Sample solution was deposited on a disposable glass slide and allowed to dry. Then the “loaded” slide was inserted into the source for MS data acquisition. The source cartridge heater was kept on for 30 seconds at 30 W. In DS-APCI analysis, laboratory air corona discharge between tungsten needle placed coaxially with MS inlet at a 3-mm distance was used. In DS-sESI analysis, laboratory air electrospray from stainless steel needle (OD 127  $\mu\text{m}$ , ID 50  $\mu\text{m}$ ) was mounted coaxially with the MS inlet at a 3-mm distance. The sESI flow rate was kept at 0.5-0.7  $\mu\text{L}/\text{min}$ .

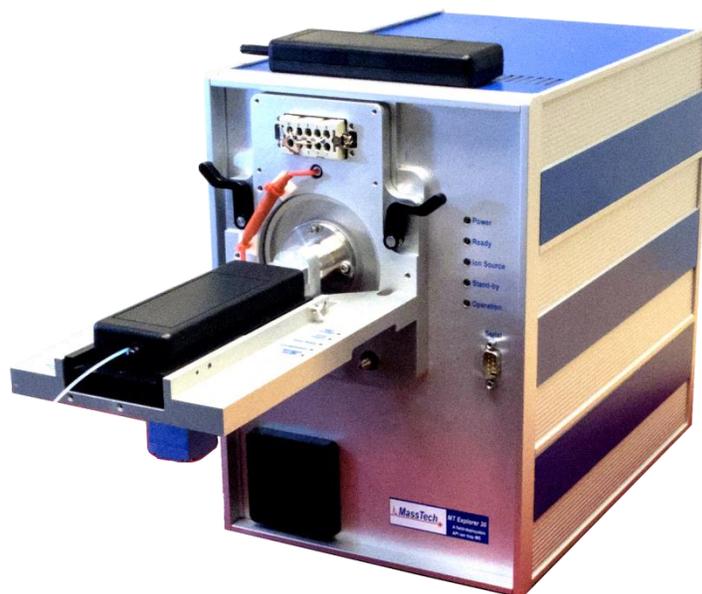


Figure 1: DSAP sESI cartridge hyphenated with MTE30 system. The APCI cartridge is featured on the instrument top.

## Mass Spectrometry

All mass spectrometry experiments were carried out on a MTE30 (MassTech Inc., Columbia, MD, USA) coupled to the DSAP source equipped with APCI and sESI cartridges. A representative picture of DSAP with sESI cartridge hyphenated with MTE30 is shown in Figure 1 with the APCI cartridge featured on the instrument top. In the MS analyses of samples, 3 micro-scans were combined in a single MTE30 scan, total scan duration being less than 1 second.

## Software and Data processing

The data were acquired in MS and MS/MS modes using the MODAS software version 4.0.7.0. The qualitative data analysis was performed using ChromExplorer 1.5.1 software.

## Results and Discussion:

### Detection of Explosives

TNT was detected using DSAP with APCI cartridge. The negative molecular ion  $[M-H]^-$  of TNT was observed at  $m/z$  226.3 at 2 ng, see Figure 2(a). The fragment ions of TNT were detected at  $m/z$  198.4 and  $m/z$  136.8 at the loaded amount of 200 pg, see Figure 2(b). RDX was detected using DSAP with sESI cartridge. The negative molecular adduct ion of RDX was observed at  $m/z$  266.6, see Figure 3(a). The MS/MS ion of RDX was detected at  $m/z$  220.7, see Figure 3(b). Both MS and MS/MS were observed at loaded amount of 2 ng.

### Detection of Drugs

Cocaine and methamphetamine were detected using DSAP with APCI cartridge. The molecular ion  $[M+H]^+$  of cocaine was observed at  $m/z$  304.5, see Figure 4(a). The fragment ion of cocaine was observed at  $m/z$  182.0 (Figure 4(b)). Both MS and MS/MS were observed at a loaded amount of 200 pg. The molecular ion  $[M+H]^+$  of methamphetamine was observed at  $m/z$  149.9, see Figure 5(a). The fragment ions of methamphetamine were detected at  $m/z$  133.0, 119.0, and 95.0, see Figure 5(b). Both MS and MS/MS were observed at 2 ng.

### Detection of Pesticides

Parathion was detected using DSAP with APCI cartridge. The molecular ion  $[M+H]^+$  of parathion was observed at  $m/z$  292.0, see Figure 6(a). The MS/MS fragment ions of parathion were detected at  $m/z$  263.9 and 236.0, see Figure 6(b).

### Detection of Chemical Warfare Agent Simulant

Methyl salicylate was detected using DSAP with APCI cartridge. The molecular ion  $[M+H]^+$  of methyl salicylate was observed at  $m/z$  152.8, see Figure 7(a). The MS/MS fragment ions of methyl salicylate was detected at  $m/z$  121.1, see Figure 7(b). Both MS and MS/MS of methyl salicylate were observed at a concentration of 2 ng.

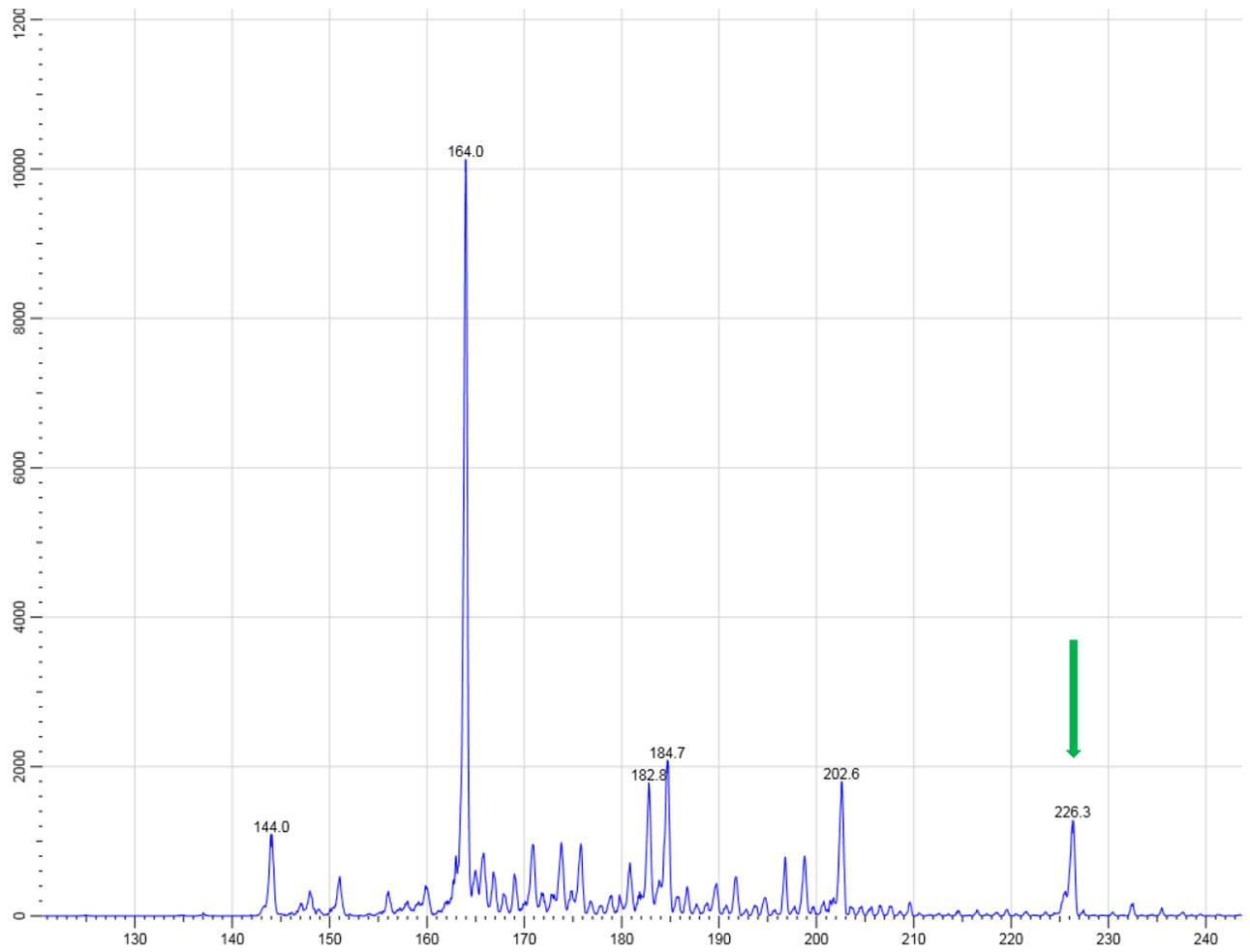


Figure 2 (a): Mass spectrum of TNT explosive by DSAP with APCI cartridge in a negative ion mode at 2 ng sample load. The green arrow indicates molecular ion.

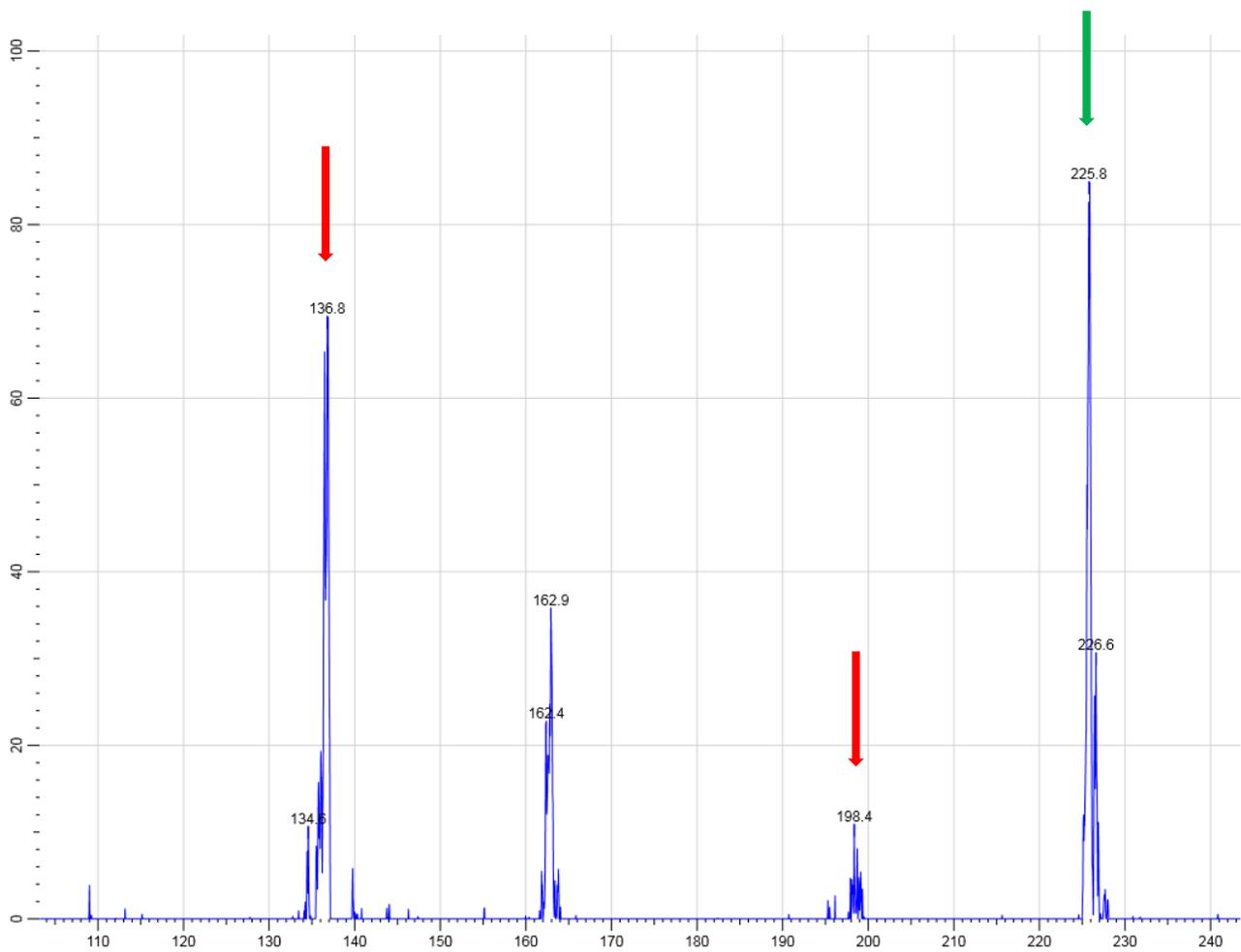


Figure 2 (b): Tandem mass spectrum of TNT explosive by DSAP with APCI cartridge in a negative ion mode at 200 pg sample load. The green arrow indicates parent ion and red arrow indicates fragment ions.

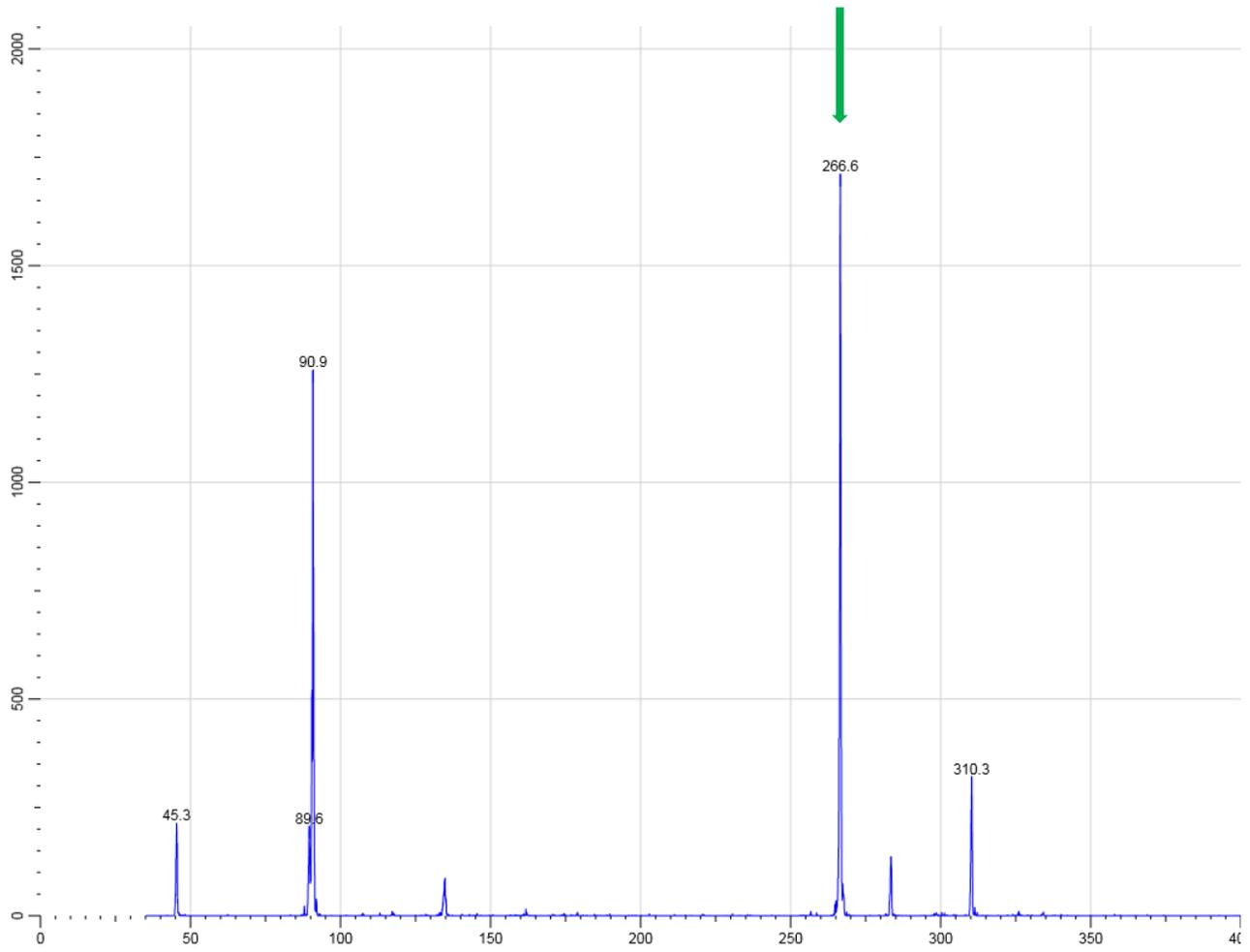


Figure 3 (a): Mass spectrum of RDX explosive by DSAP with sESI cartridge in a negative ion mode at 2 ng sample load. The green arrow indicates molecular adduct ion.

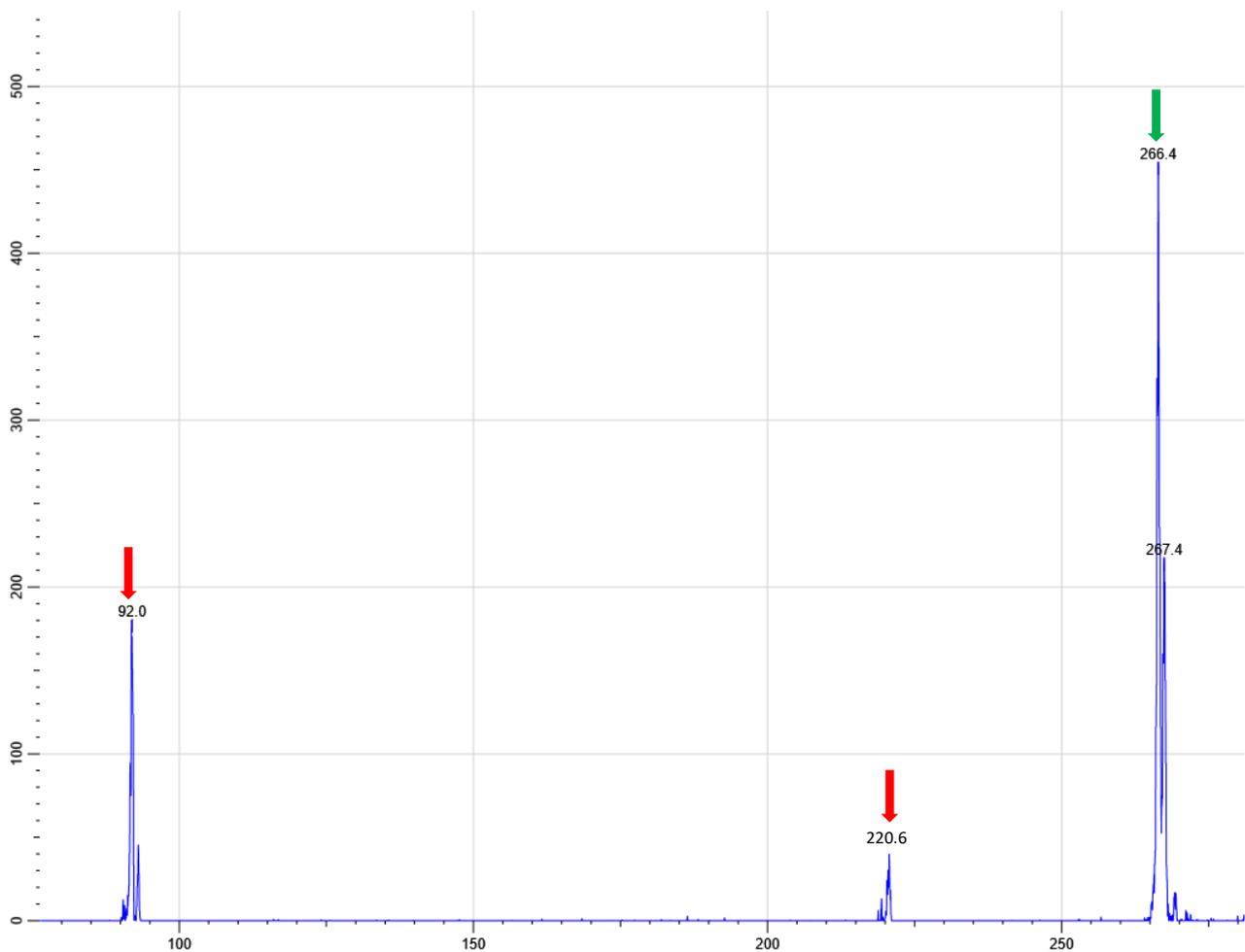


Figure 3 (b): Tandem mass spectrum of RDX explosive by DSAP with sESI cartridge in a negative ion mode at 2 ng sample load. The green arrow indicates the parent ion and red arrow indicates molecular ions.

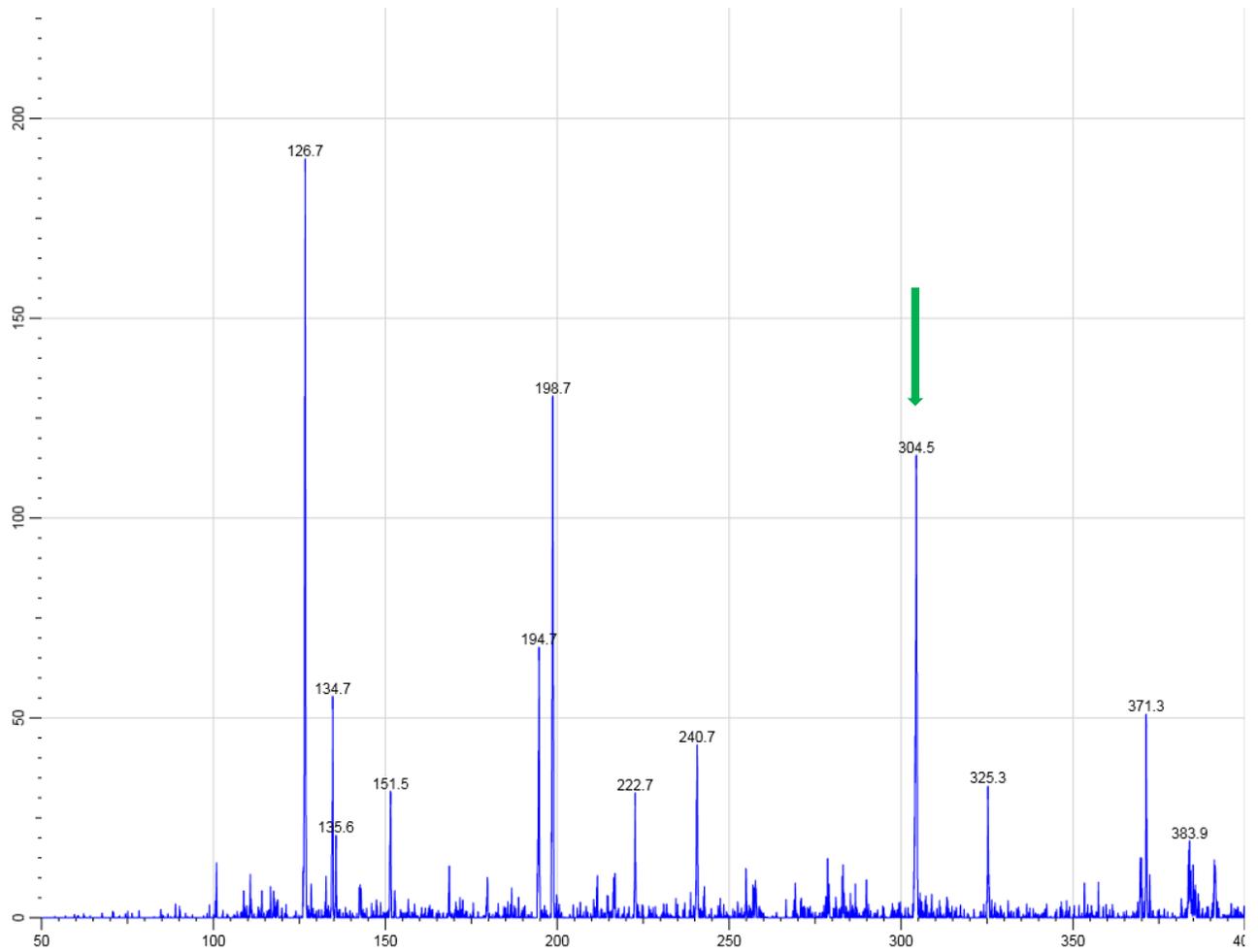


Figure 4 (a): Mass spectrum of Cocaine drug by DSAP with APCI cartridge in a positive ion mode at 200 pg sample load. The green arrow indicates molecular ion.

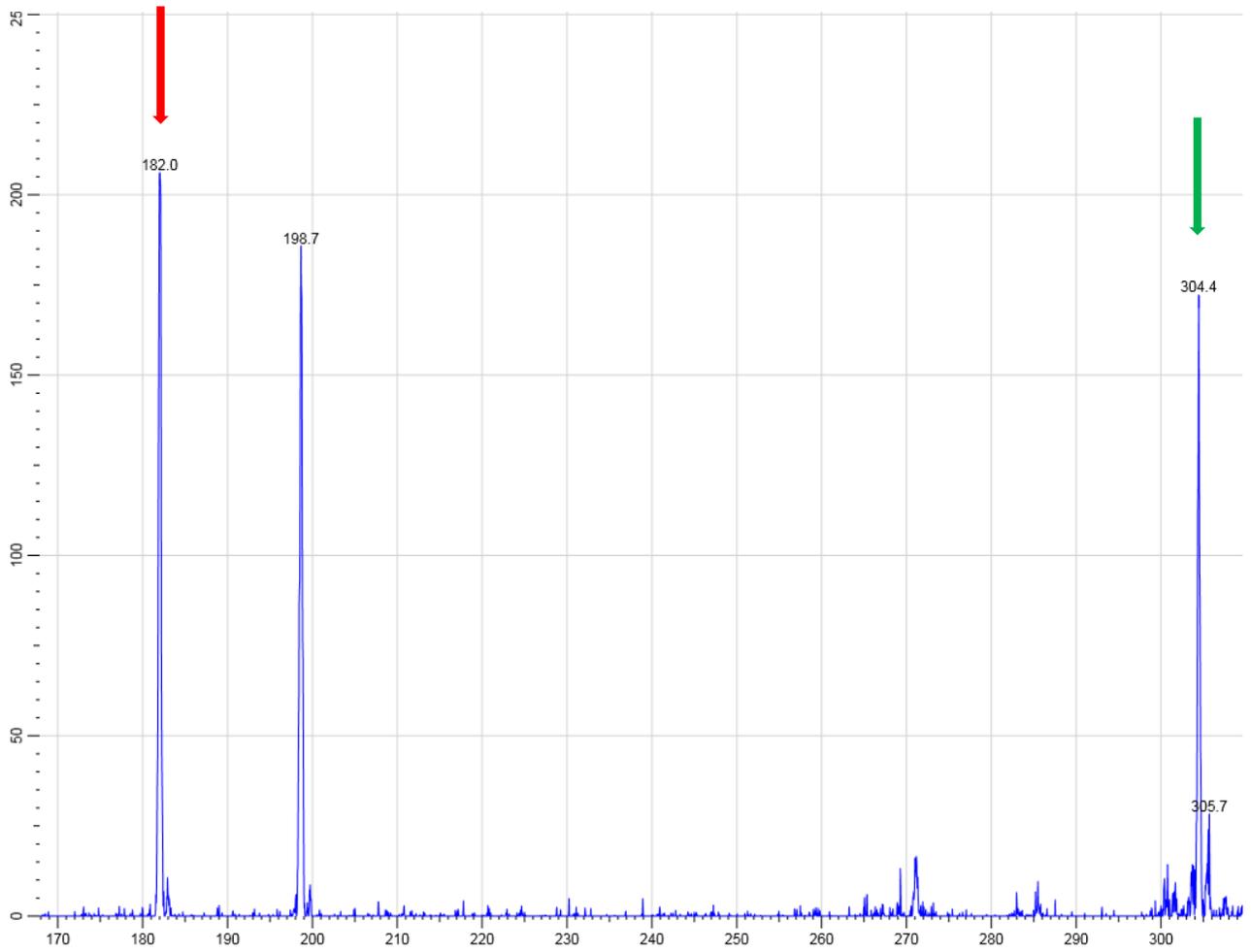


Figure 4 (b): Tandem mass spectrum of Cocaine drug by DSAP with APCI cartridge in a positive ion mode at 200 pg sample load. The green arrow indicates molecular ion and red arrow indicates fragment ion.

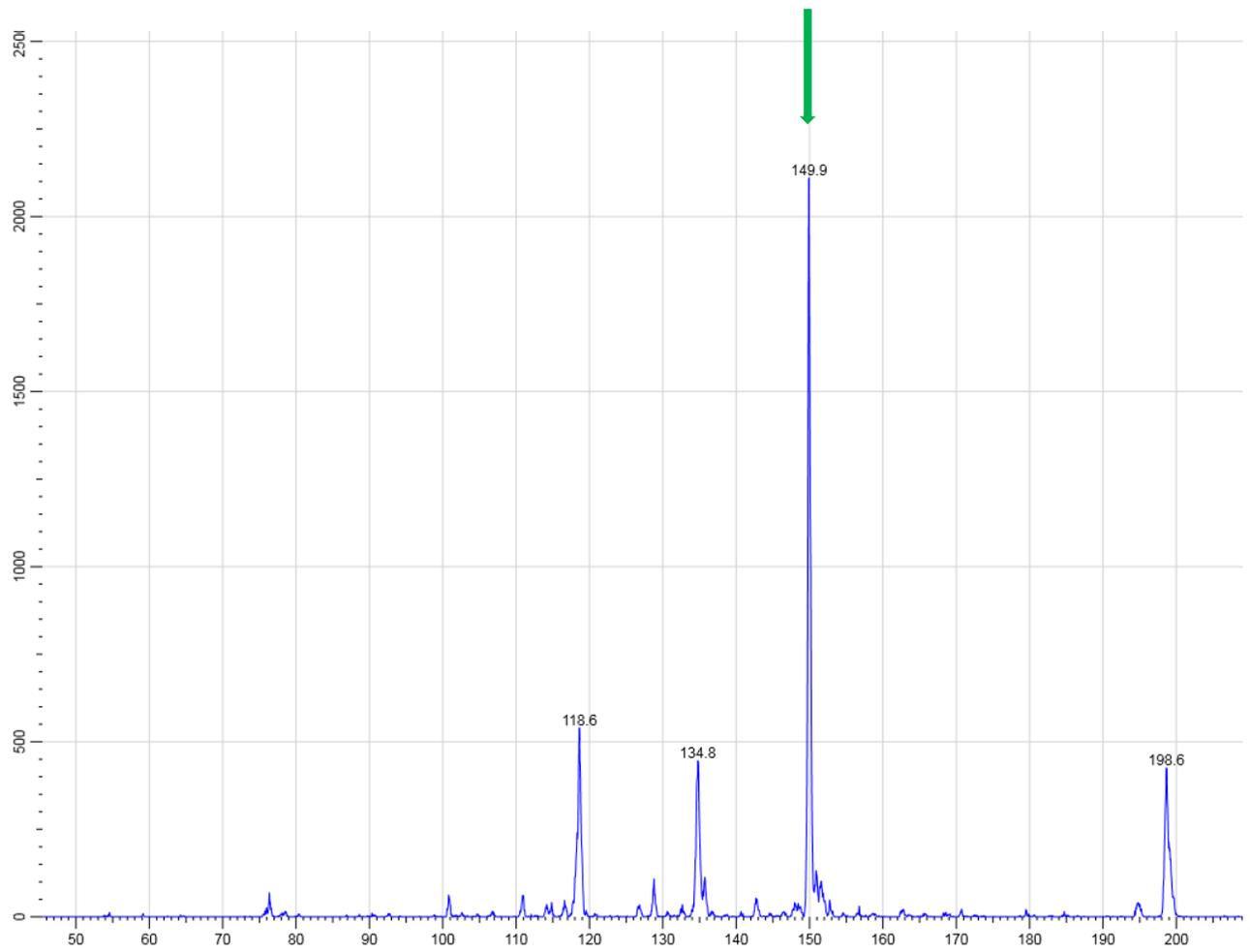


Figure 5 (a): Mass spectrum of Methamphetamine drug by DSAP with APCI cartridge in a positive ion mode at 2 ng sample load. The green arrow indicates molecular ion.

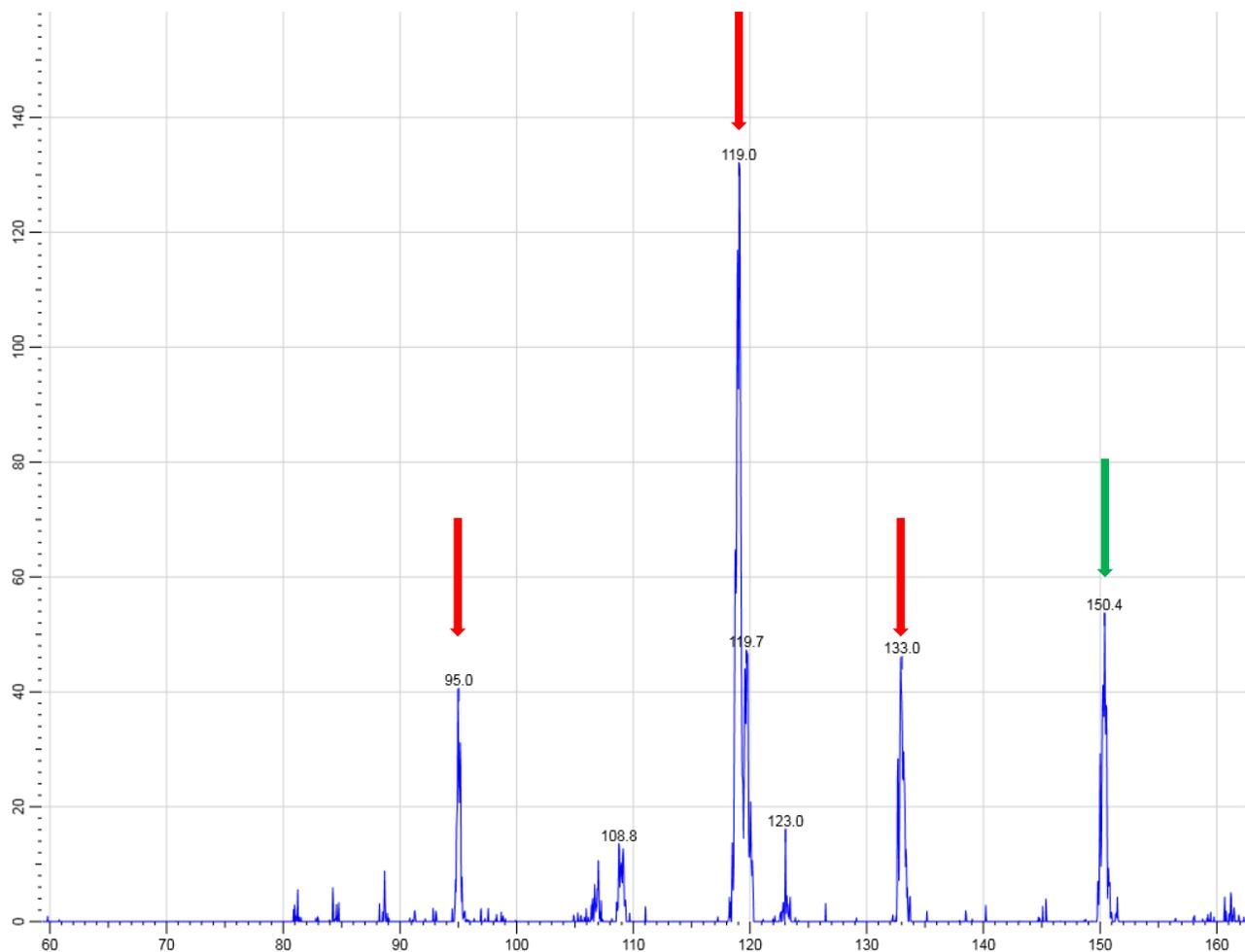


Figure 5 (b): Tandem mass spectrum of Methamphetamine drug by DSAP with APCI cartridge in a positive ion mode at 2 ng sample load. The green arrow indicates molecular ion and red arrow indicates fragment ions.

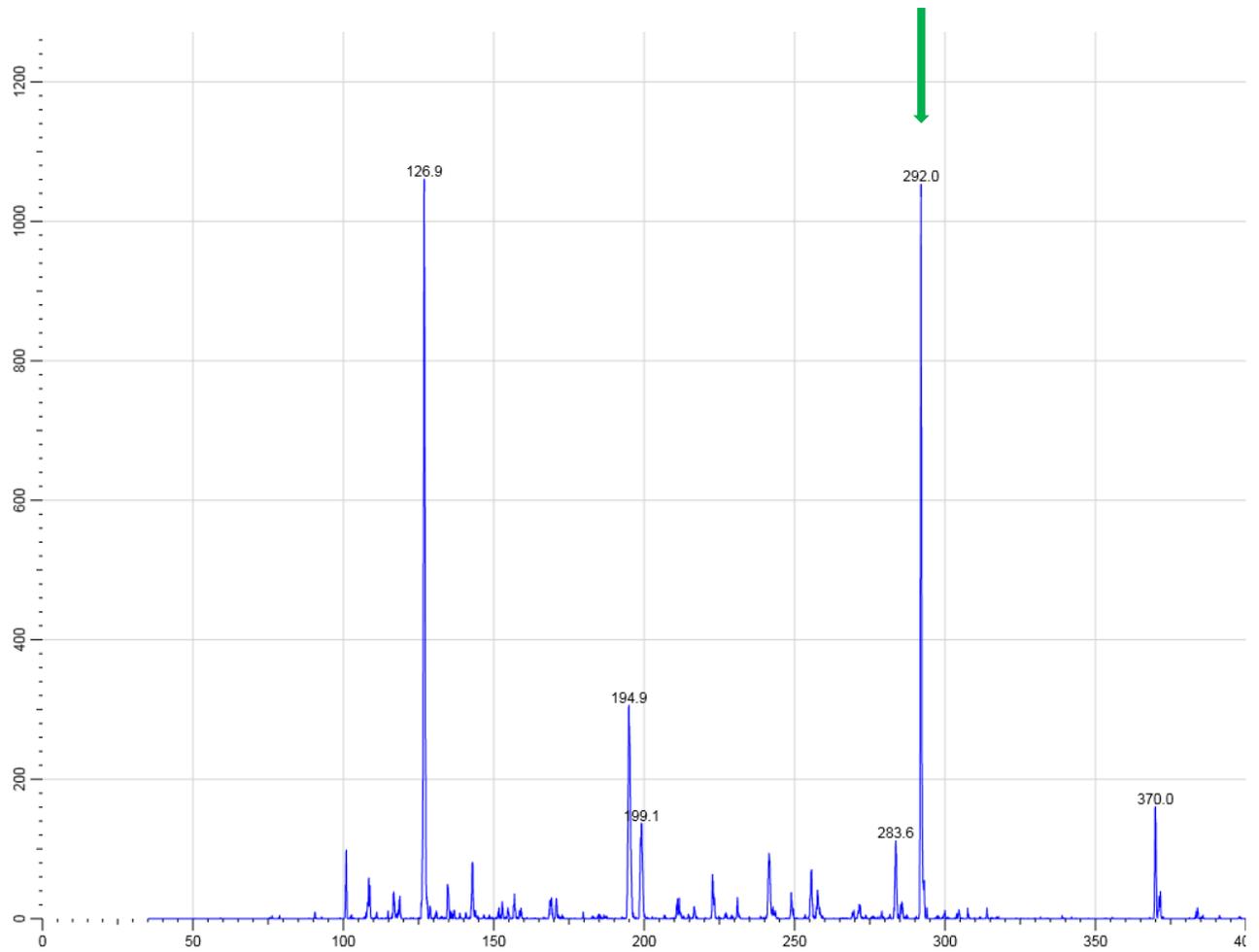


Figure 6 (a): Mass spectrum of Parathion pesticide by DSAP with APCI cartridge in a positive ion mode at 2 ng sample load. The green arrow indicates molecular ion.

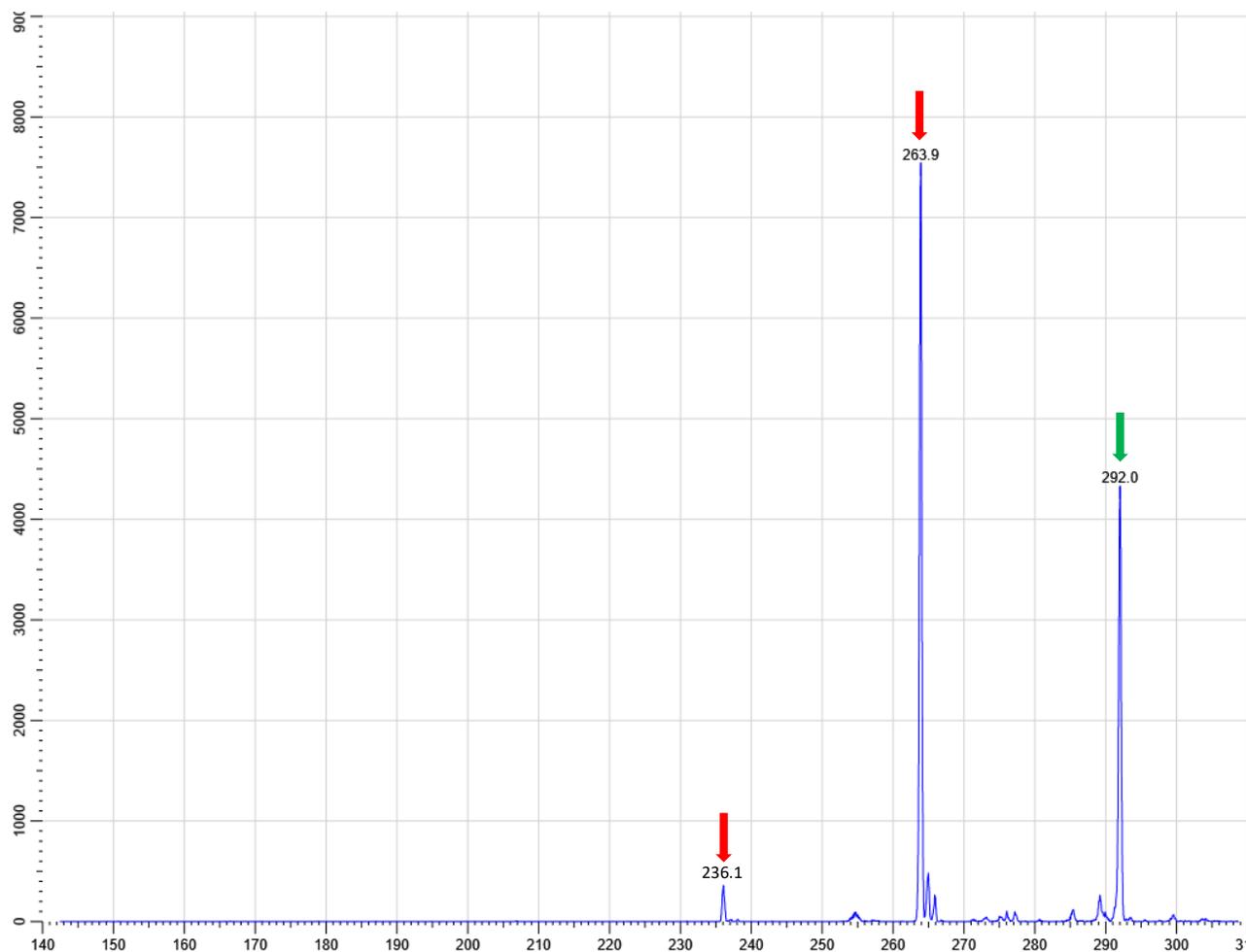


Figure 6 (b): Tandem mass spectrum of Parathion drug by DSAP with APCI cartridge in a positive ion mode at 2 ng sample load. The green arrow indicates molecular ion and red arrow indicates fragment ions.

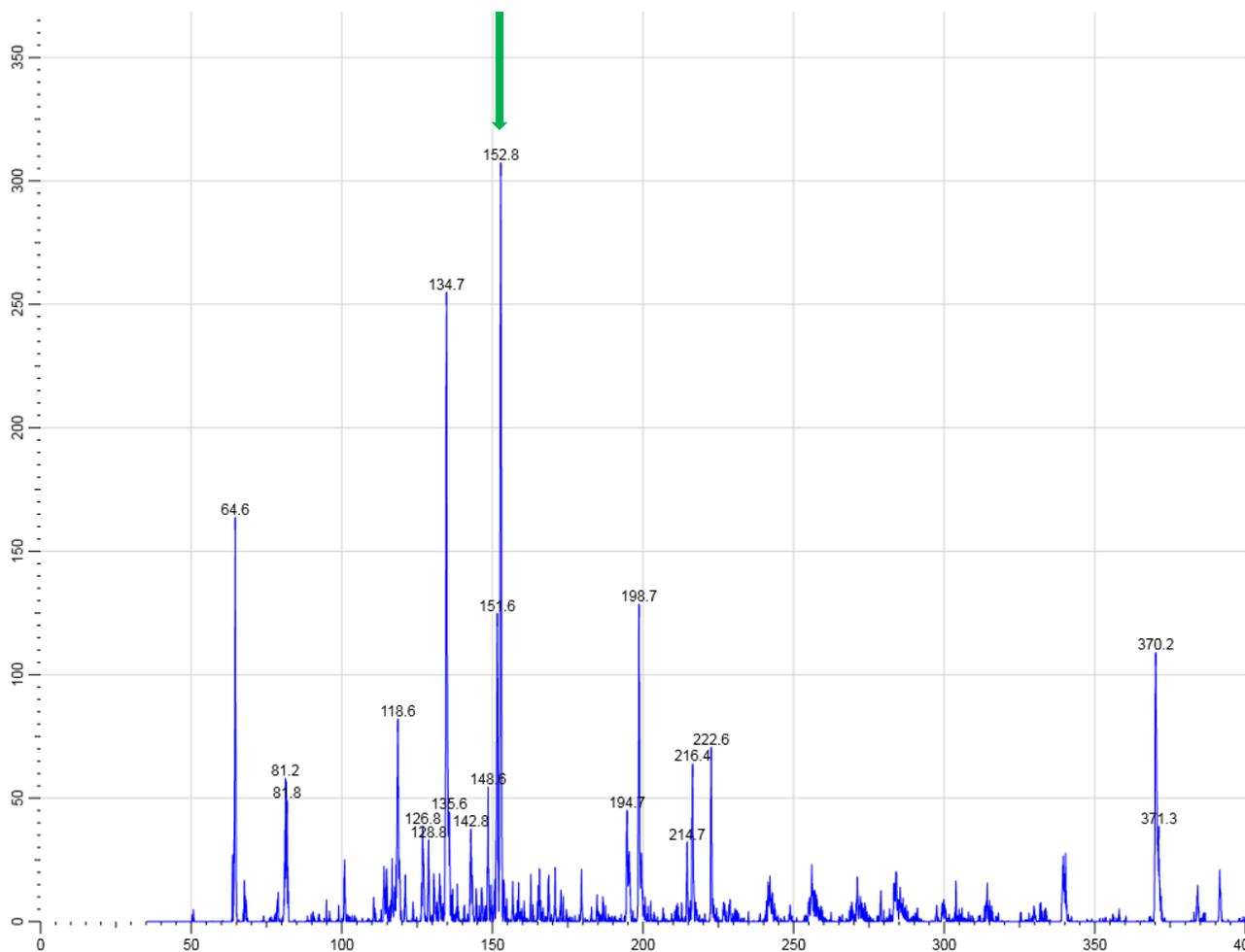


Figure 7 (a): Mass spectrum of methyl salicylate, a CWA simulant by DSAP with APCI cartridge in a positive ion mode at 2 ng sample load. The green arrow indicates molecular ion.

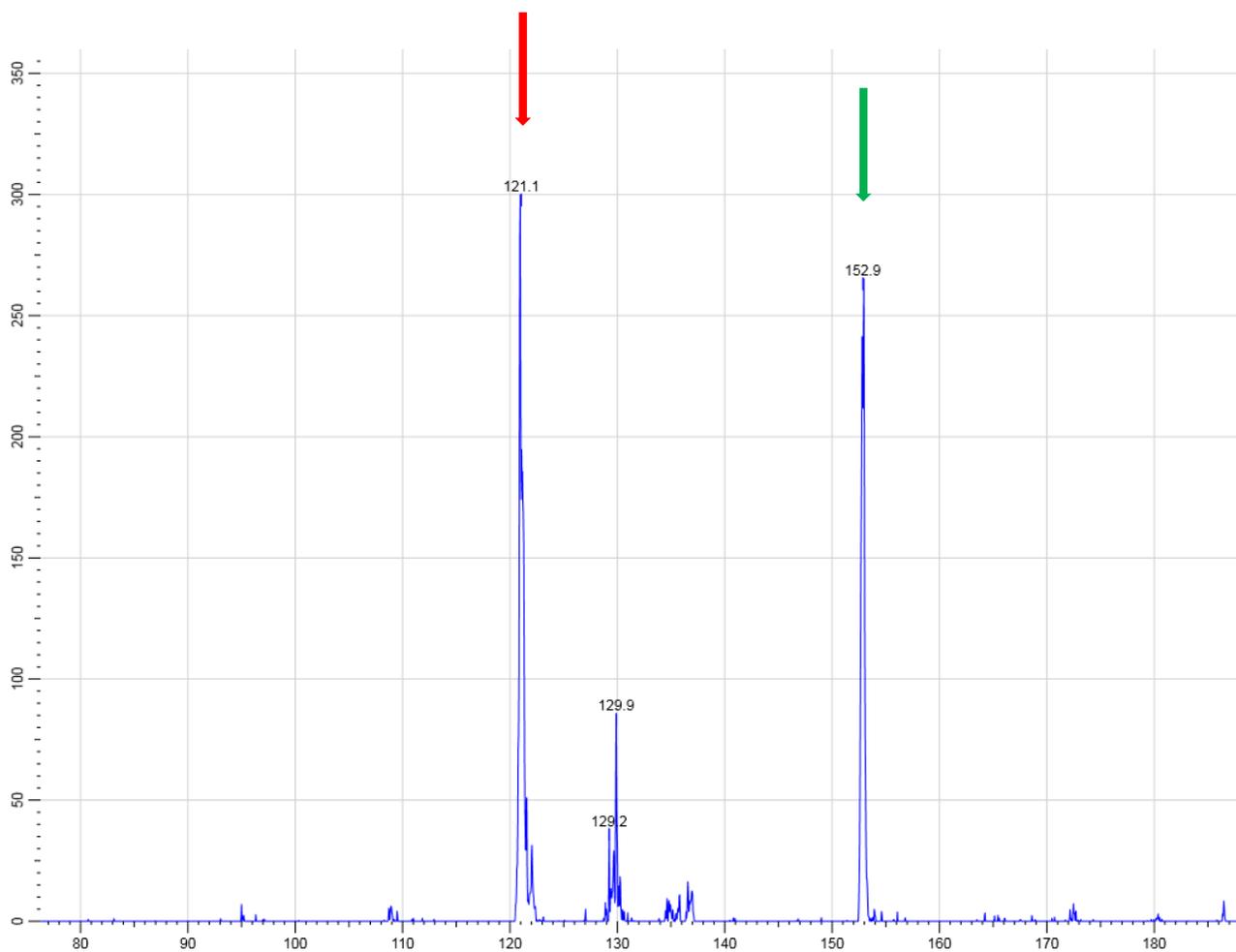


Figure 7 (b): Tandem mass spectrum of methyl salicylate, a CWA simulant by DSAP with APCI cartridge in a positive ion mode at 2 ng sample load. The green arrow indicates molecular ion and red arrow indicates fragment ions.

### Summary:

With the above results, we have demonstrated the analytical capabilities of MTE30 utilizing DSAP source equipped and APCI/sESI ionization modules. The MS/MS analyses performed in MTE30 provide identification and quantitation of explosives, drugs, pesticides, as well as CWA simulants. Direct sampling (DSAP) has been demonstrated to be a simple, yet powerful technique for both MS and MS/MS analyses performed in MTE30.

### References:

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