Forensic Technology Testing & Evaluation Report Form

Report Date: 12/14/2007

Project Information

Title: The Constellation Technology CT-1128 Portable GC-MS Evaluation
Evaluation Type: Instrumentation
Stakeholder(s): Constellation Technology, NFSTC Mobile Laboratory Project
Start Date: 10/17/2007 End Date: 10/24/2007

Manufacturer Information

Manufacturer: Constellation Technology
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Evaluation Overview

The National Forensic Science Technology Center (NFSTC) conducted an assessment on the CT-1128 portable gas chromatograph-mass spectrometer (GC-MS) manufactured by Constellation Technology. Due to a short timeframe of instrument availability and a malfunctioning split valve, the study was limited in scope.

The purpose of this performance evaluation was to determine the suitability of this chemical detection system for use in the analysis and identification of forensically relevant chemical compounds. The samples used during this assessment were selected to be a small representative subset from each of the following forensic classification groups: drugs of abuse, ignitable liquids, and explosives.

The following observations were noted during the evaluation process:

- The instrument is engineered to be utilized in a non-traditional laboratory environment, making it capable of operating under field conditions that most ordinary laboratory bench top GC-MS instrumentation would be unable to handle.
- The CT-1128 utilizes a Varian 1177 injector as well as an Agilent 5973N Mass Selective Detector.
- This system comes equipped with an internal hydrogen gas cylinder that can provide several days supply of carrier gas.
- Operation of the CT-1128 requires the utilization of two separate software platforms:
    - Chemstation/E (MS)
    - Constellation Technology GC Software (GC).

- The instrument performed adequately for the analysis and identification of drugs of abuse, ignitable liquids, and explosives. More information regarding the strengths, opportunities for improvement, and instrument limitations can be obtained within the Findings section of this document.

Evaluation Team

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NFSTC Laboratory Manager

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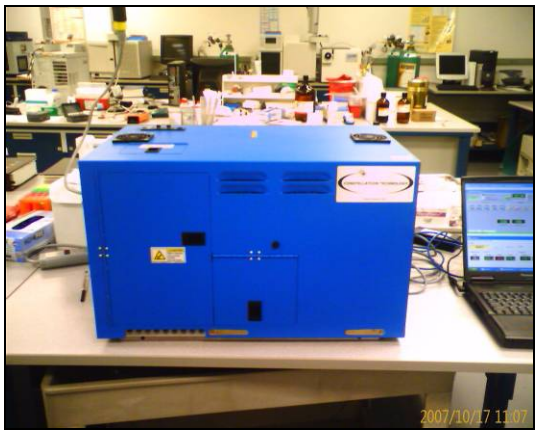
Product Specifications

Photo(s) of product:



Product Name: **CT-1128 Portable GC-MS Chemical Detection System**
Model No.: **CT-1128**
Serial/Lot No.: **Not provided by manufacturer**

Brief Description

The CT-1128 Chemical Detection System is a bench top GC-MS manufactured with enhanced engineering specifications that, when coupled with an optional anti-vibration vehicle mounting system, allows for its safe portability and usage in field environments.

By combining a gas chromatograph (GC) equipped with a Varian 1177 split/splitless injector, to an Agilent 5973N mass spectrometer detector (MSD), this self contained all-in-one GC-MS instrument can separate and identify individual compounds from complex sample mixtures originating from gas, liquid, or solid matrices.

The GC portion of the CT-1128, utilizing differences in the affinity of each mixture component for the fused silica of the capillary column, is responsible for the separation of each of the individual sample constituents. As each component exits the column into the MS detector, the compound is ionized and fragmented. The CT-1128 mass spectrometer is an Agilent 5973N MSD that is equipped with a quadrapole capable of scanning ion fragments within the mass range of 1.8 to 800 m/z. Final compound spectra, composed of ion fragments, can be searched against a spectral database(s) for definitive chemical compound identification.

Product Uses Per Manufacturer
Environmental assessments, arms control and non-proliferation activities, as well as detecting and identifying hazardous substances released during an accident or terrorist attack.

Dimensions: 26 in. x 16.5 in. x 15.5 in.
Weight: 75 pounds
Storage Conditions: Not applicable
Operational Conditions: 10-35°C @ 5-95 % humidity
Power Requirements: 99-127 volts
Cost: Information not provided by manufacturer

Evaluation

Objective(s):

- To assess the CT-1128 GC-MS for forensic applications in the analysis and identification of:
  - Drugs of abuse
  - Ignitable liquids
  - Explosives
- To provide user feedback to the manufacturer
- To assess instrument for mobile laboratory applications

Instrument setup performed by:

☑ Manufacturer ☐ Manufacturer & NFSTC Lab Staff ☐ NFSTC Lab Staff Only

Instrument setup comment(s):

The instrument was transported from Constellation Technologies to the NFSTC laboratory facility by vehicle.

The following components were provided with the CT-1128:

- Laptop computer equipped with Windows XP, HP Chemstation/E and Constellation Technology GC software
- Hardware and software user manuals
- A second hydrogen gas cylinder

The instrument was placed on a laboratory bench and connected to power. The laptop computer was connected by an Ethernet cable to establish PC-to-instrument communication. Once control of the

instrument was established, the pumpdown command was executed. The CT-1128 took approximately 25-30 minutes to reach operational readiness.

Level of operator knowledge as set by manufacturer:

☐ Non-Scientist ☑ Technician ☐ Scientist

Standards, controls and samples used in evaluation:

Drugs of Abuse	
Alprazolam	Hydromorphone
Methamphetamine	Phentermine
Drug Mix (Methamphetamine, Benzocaine, Cocaine, Diazepam, Testosterone Proprionate)	

Ignitable Liquids	
NFSTC Fire Debris Test Mix (C_6-C_{28} n-alkanes, toluene, p-xylene, o-ethyltoluene, m-ethyltoluene, 1,2,4-trimethylbenzene and C_6-C_{20} even alkanes in $MeCl_2$)	
Ronsonol Lighter Fluid	Sunnyside Kerosene
Texaco Diesel	Lamplight Lamp Oil

Explosives
Explosives Mix A (2-Amino-4,6-dinitrotoluene, 1,3-Dinitrobenzene, 2,4-Dinitrotoluene, HMX, Nitrobenzene, RDX, 1,3,5-Trinitrobenzene, 2,4,6-Trinitrotoluene)
Explosives Mix B (4-Amino-2,6-dinitrotoluene, 2,6-Dinitrotoluene, 2-Nitrotoluene, 3-Nitrotoluene, 4-Nitrotoluene, Tetryl)
2,6-Dinitrotoluene 500ng/mL

Equipment and Consumables:

- Fisherbrand 10x75mm Borosilicate Glass disposable culture tubes
- Fisher Scientific Optima Acetonitrile
- Fisher Scientific Certified ACS Methanol
- National Scientific Company 2.0mL 12x32mm Amber Vials with PTFE/Silicone Septa
- Eppendorff epTIPS 10uL - 1000uL PCR clean disposable pipette tips
- Eppendorff Research Pro 100/1000 uL
- Fisher Scientific ACS Grade Methylene Chloride
- 0.5 M NaOH
- Analytical Balance
- Hamilton 1uL syringe
- 30m 95% dimethyl polysiloxane/5% diphenyl polysiloxane GC column
  (Column was installed by manufacturer; no other information was provided)

Synopsis of Experiment(s):

Experiments were designed to assess the ability of the CT-1128 to separate and produce quality ion spectra for the identification of forensically relevant compounds. The samples used during this brief assessment were selected to be a small representative subset from each of the following forensic classification groups: drugs of abuse, ignitable liquids, and explosives.

This abbreviated evaluation was divided into three separate parts based on the different classifications of the substances being analyzed. Appropriate solutions were made up at known concentrations and each sample was manually injected at a volume of 1 uL using a Hamilton 1 uL syringe. Listed below are all of the names of the methods used during the evaluation process. The NFSTC Fire Debris parameters for both the GC and MS methods have been given in detail.

GC Method(s)	MS Method(s)
NFSTCDRUG Injector temperature: 280°C Transfer line temperature: 280°C Column: 130.0 °C (Hold 1.0 min.) to 325.0 °C @ 35.0°C /min (Hold 5.0 min) Total Run Time: 11.0 minutes	**NFSTCDrugMS.M** Solvent Delay: 1.50 minutes Scan range: 50 – 450 m/z Total Run Time: 11.0 minutes
NFSTCEXPLOSIVE Injector temperature: 150°C Transfer line temperature: 280°C Column: 40.0 °C (Hold 0.5 min.) to 150 °C@ 60.0°C /min (Hold 3.5 min) 150 °C to 250.0 °C @ 60.0°C /min (Hold 4.0 min) Total Run Time: 14.0 minutes	**NFSTCEXPLOSIVESMS.M** Solvent Delay: 1.50 minutes Scan range: 50 – 450 m/z Total Run Time: 14.0 minutes
NFSTCFIRE: Injector temperature: 250°C Transfer line temperature: 280°C Column: 35.0 °C (Hold 4.0 min.) to 325.0 °C @ 25.0°C /min (Hold 5.0 min) Total Run Time: 24.4 minutes	**NFSTCFIREDEBRISMS.M:** Solvent Delay: 1.50 minutes Scan range: 50 – 450 m/z Total Run Time: 24.4 minutes

Part I: Drugs of Abuse

- 1 mg/mL solutions of each of the different drug standards were made up using, an analytical balance, 10.0 mg of analyte, A.C.S. grade methanol, and a 10.0 mL volumetric flask.

Part II: Explosives

- Explosive samples were prepared by pipetting 15 uL of neat explosive reference standard into 15 uL of acetonitrile, resulting in a concentration of 500 ug/mL.

Part III: Ignitable liquids

- Ignitable liquids samples were prepared by pipetting 20 uL of neat reference standard into 1.5 mL of pentane.

The TIC and spectra illustrated in figures 1-3 below are representative sampling of the data obtained during the CT-1128 assessment.

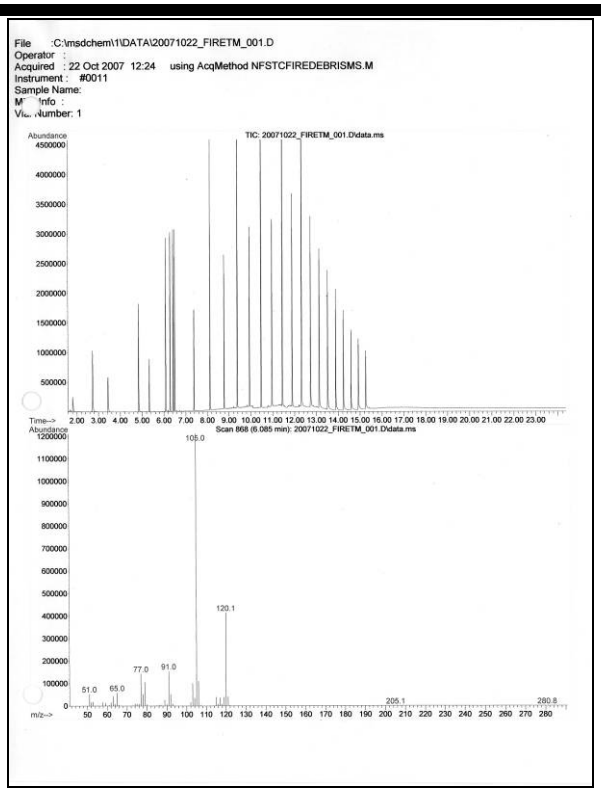


Figure 1: Hydrocarbon Test Mixture (Fire Debris)

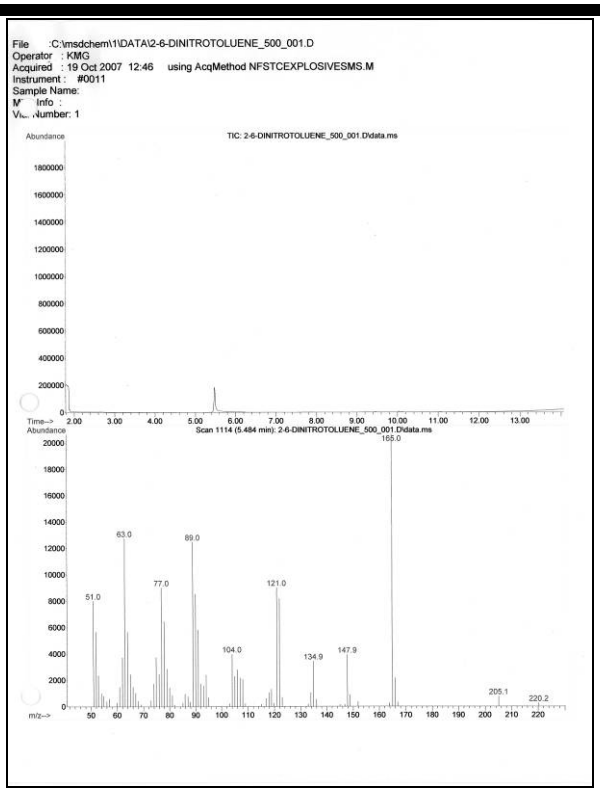


Figure 2: 2,6-dinitrotoluene (Explosive)

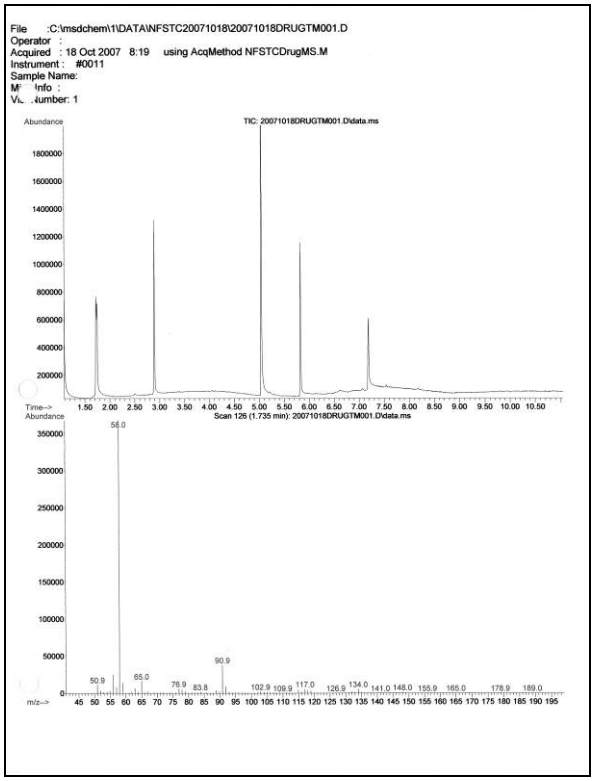


Figure 3: Drug Test Mixture

Findings

Strengths:

- The instrument is engineered to be utilized in a non-traditional laboratory environment, making it capable of operating under field conditions that most ordinary laboratory bench top GC-MS instrumentation would be unable to handle.
- This system comes equipped with an internal hydrogen gas cylinder that can provide several days supply of carrier gas. This feature not only allows for the storage of the carrier gas supply directly within the instrument, but totally eliminates the need to have a burdensome external gas cylinder and/or other gas generating equipment. Another feature of the gas system is that the small gas cylinder is attached to the CT-1128 with a quick connection system, which allows for rapid (< 1 minute) tank change-out, when needed.
- The CT-1128 utilizes a Varian 1177 injector as well as an Agilent 5973N Mass Selective Detector. Not only are these components known for their excellent performance capabilities, but when replacement parts are needed they can be purchased from vendors other than the manufacturer.
- The operational mass scan range of the CT-1128 is from 1.6 to 800 amu.
- Unit power-up to sample injection time was noted to be approximately 25-30 minutes. Typical GC-MS systems require lengthier pump down times to remove residual air and water before sample injection can occur.
- For routine maintenance or repair, the entire protective housing around the instrument can be completely removed, creating easily accessible service areas.
- The instrument is capable of performing real-time snapshot analysis of unknown spectra, allowing for the identification of the unknown compound through direct spectral library comparison. The MSD ChemStation incorporates the NIST/EPA/NIH and/or user-defined compound libraries to create a searchable spectral database consisting of numerous compounds.
- The column oven is capable of reaching temperatures up to 325 °C. These temperatures are necessary for late eluting compounds like anabolic steroids, some benzodiazepines, and heavy petroleum distillates.
- The CT-1128 has an integrated heater/mixer component located in the exterior housing of the instrument that allows for the extraction of volatile compounds from either liquid or solid matrices.
- The integrated Agilent MS possesses a dual filament assembly instead of a single filament assembly.
- The instrument uses a small internalized rough pump and two turbomolecular pumps that are housed within the instrument, eliminating the need for a heavy external vacuum pump and lengthy pumpdown times.
- The CT-1128 GC-MS is quite compact and possesses a manageable footprint requiring a relatively small workspace.

Opportunities For Improvement:

- Operation of the CT-1128 requires the utilization of two separate software platforms: Chemstation/E and Constellation Technology GC Software. Integration of the two separate software platforms would render the system more functional and user friendly. The development of two separate methods (one for the GC and one for the MS) is cumbersome and could be potentially disastrous if the user is not aware of the necessary method selections for each component.

- The performance of a split sample injection on this system requires an awkward and time consuming manual process with the usage of the adjustable purge flow regulator and a flow meter. A programmable flow control system within the GC method software would be a more suitable means of performing this function.
- Approximately 21.5 minutes was required to cool the column from an end of run temperature of 325 °C to an initial start temperature of 40 °C. A much faster cooling technique (use of a larger oven exhaust fan, internal column oven cooling fan, or by other means) is needed to shorten column cooling lag time between sample runs.
- Manual injection of samples was required on the CT-1128. After injecting the sample, the run is not initiated and data collection does not begin until the operator activates the start button within the GC software. An electronic start button in close proximity to the injection port would better facilitate the process of injecting the sample and activating the data collection software simultaneously.
- A small removable or integrated autosampler would be beneficial to laboratory efficiency for multiple sample analyses.

Limitations:

- The CT-1128 cannot be operated by non-scientists or non-technical personnel. A much more simplistic user interface would be needed to allow non-scientists to operate this unit; however, the manufacturer has clearly stated that this instrument does require technician level expertise.
- Although the manufacturer characterizes the ease of mobility of this system, safe relocation of the 75 pound instrument still requires a two member team.
- During the evaluation, it was noted that the GC-MS software platform did not possess the capabilities of easily restricting access to users of different levels of expertise. Once proven GC/MS methods or spectral libraries have been developed and established, a lower level user should not be able to modify them easily.
- The CT-1128 GC software allows a scientist to develop methods with only up to two temperature programmable ramp steps. Most GC systems have the capability of performing multiple ramp steps within a method and are not restricted to only two.

Training Requirements:

- The depth and length of training will depend on the desired level of the end user.
- An operator who possessed a technician level of expertise can quickly be trained to a level that would allow them to competently perform simple sample preparation, sample introduction, data collection, and basic data interpretation. However, some instrument maintenance, troubleshooting, method development, and advanced data interpretation would require more extensive scientific knowledge.

Health and Safety Issues:

- The CT-1128, like any other GC-MS, does have potential safety and health risks associated with its usage. The operator (no matter what their skill level may be), should be provided the appropriate training to prevent any unnecessary injuries due to chemical, extreme heat, or high voltage exposures.
- Given the brief one week assessment period of this GC/MS, the user manual was not reviewed for safety warnings or cautions that a user would be made aware of while operating this equipment. Most instrument manufacturers, who consider safety a top priority, provide user manuals that

address all necessary warnings and cautions with easily identifiable safety symbols.