

QuickProbe Technology for Direct, Real-Time MS Analysis

QuickProbe Comprehensive e-Book



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QuickProbe Technology for direct, real-time MS analysis of powders, solids, and liquids

Maximizing productivity is a critical goal for Forensic labs that face large sets of samples and growing caseloads day after day. QuickProbe is a cost-effective alternative for rapid screening without the need for sample preparation that results in reviewable MS data in under a minute. It is positioned primarily to forensic customers who need to rapidly identify samples such as seized drugs comprising unknown powders, liquids and solids and want a lower cost fast analysis solution that is easy to learn and operate.

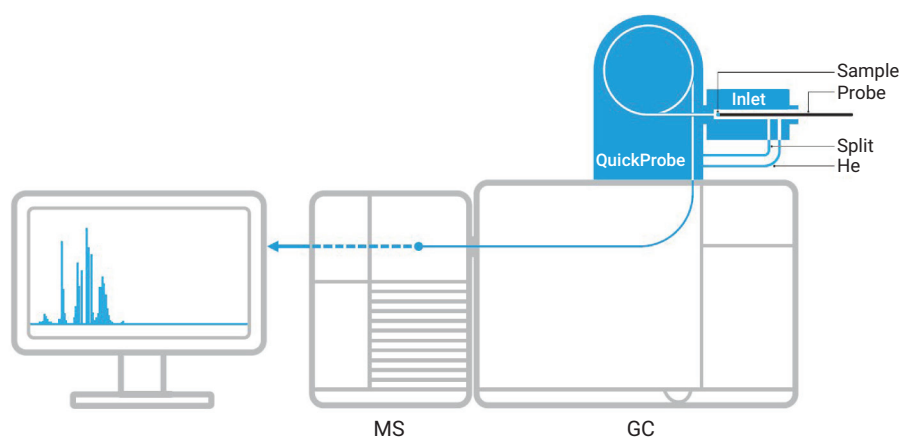


QuickProbe sits on the front detector position on the GC. The technology comprises of a QuickProbe inlet that open to ambient air and provides rapid heating and vaporization of the sample inserted. The inlet is mounted next to the QuickProbe GC that comprises of a short 1.3 m column that is able to ramp up to 350 degrees in a matter of seconds and provides separation of the mixture that is introduced.

This is followed by Mass spectrometry detection and compound identification using EI libraries like NIST and Wiley to identify names and structures even at the isomer level. The accessory enhances the value of our GC/MSD solutions for our customers.

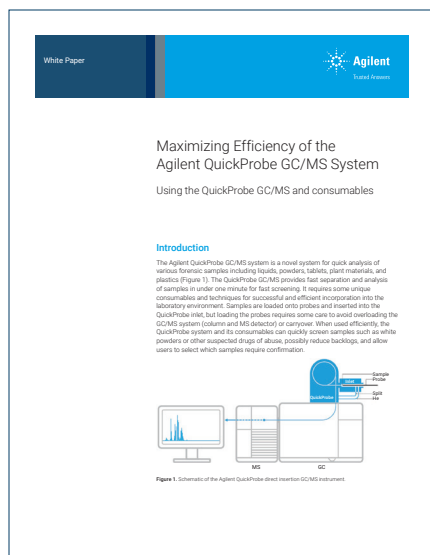
QuickProbe is a direct insertion solution for MS and can be added to existing and new GC/MSDs for the direct real-time analysis of powders, solids, and liquids.

G3971A	QuickProbe (Software Driver: MH GC/MS Acquisition 10.0)
G3971-60200	Probe holder
G5190-5118	Insertion Probe Round Tip (for Tablets and Liquids)
G5190-5113	Insertion Probe Pocket Tip (for Powders)
G5190-5104	Specialty Liner with Frit
G3903-61006	DB-1HT 0.25mm x 0.1um x 2m
G3903-61007	DB-1msUI 0.18mm x 0.18 um x 1m



Schematic of the Agilent QuickProbe direct insertion GC/MS instrument.

White Paper



Maximizing Efficiency of the Agilent QuickProbe GC/MS System

The Agilent QuickProbe GC/MS system is a novel system for quick analysis of various forensic samples including liquids, powders, tablets, plant materials, and plastics (Figure 1). The QuickProbe GC/MS provides fast separation and analysis of samples in under one minute for fast screening. It requires some unique consumables and techniques for successful and efficient incorporation into the laboratory environment. This comprehensive white paper outlines how users can efficiently use the QuickProbe system and its consumables to quickly screen samples, mitigate carryover, possibly reduce backlogs, and allow users to select which samples require confirmation.

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Brochure



Fast Analysis Workflow with No Sample Preparation for Forensic Applications Using QuickProbe GC/MS

This brochure describes QuickProbe technology that enables you to identify compounds with little or no sample preparation. Learn how you can enjoy the speed and simplicity of direct sample analysis on a GC/MS platform that has been a workhorse in your laboratory for decades.

Download

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Video



Innovation Minute – QuickProbe Technology

Is your forensic lab struggling with a growing caseload of samples that require fast, accurate analysis? Now you can enjoy the speed and simplicity of direct sample analysis on the GC/MSD platform that has been a workhorse in your laboratory for decades.

In this innovation minute, we will discuss QuickProbe, a real-time MS analysis technique that enables you to rapidly identify compounds with little or no sample preparation

Watch now

www.agilent.com/en/video/quickprobe-gc-ms-technology

Fast Analysis Workflow with No Sample Preparation for Forensic Applications Using QuickProbe GC/MS

Author

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Abstract

This Application Note describes a straightforward, quick workflow for drug analysis using the Agilent QuickProbe GC/MS system without sample preparation. Sub-minute analysis was possible for complicated samples of seized drugs, including edible cannabis, black tar heroin, and magic mushroom.

Introduction

The need for fast analysis for the identification of compounds in a variety of samples has been increasing over time, especially for seized drugs.^{1,2} Positive identification of drugs and other chemicals in bulk samples is critical during screening in crime laboratories. Conventional drug analysis often requires sample preparation that includes dissolution, dilution, and several reagent-based assays to classify the type of drugs, followed by gas chromatography/mass spectrometry (GC/MS) analysis or other techniques for confirmation.^{3,4} The QuickProbe GC/MS demonstrates a simple and fast analysis workflow that does not require sample preparation.

Experimental

Samples

A variety of drug samples were analyzed including prescription drugs in tablet form (Oxycodone and Vicodin) and seized drugs from criminal cases such as black tar heroin, magic mushrooms, and a cannabis edible (cookie) (Figure 1).

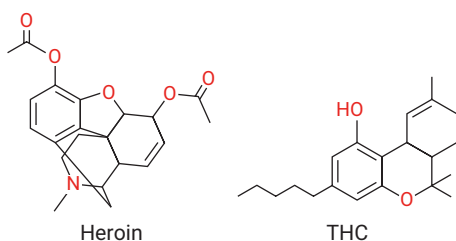


Figure 1. Chemical structures of two drug compounds tested in this study.

Instrument

QuickProbe is installed on the detector slot on top of the GC of a GC/MS system (Figure 2). It consists of a heated inlet open to the atmosphere, with a constant helium flow that prevents air intrusion. The system uses a short capillary column (Agilent J&W DB-1ht, ~1.5 m × 0.25 mm, 0.10 μm) that is rapidly heated (up to 16 °C/s or 960 °C/min), allowing for basic chromatographic separation in under one minute. Individual samples (liquid, solid, and powder) were touched with a

glass probe (Figure 3) and introduced into the QuickProbe inlet for three to six seconds for vaporization prior to data acquisition with the GC/MS. Little to no sample preparation was required. Compound identification was achieved through searches performed through standard GC/MS data analysis packages (Agilent MassHunter Qualitative Analysis, Quantitative Analysis, and Unknowns Analysis software) and against the NIST or Wiley libraries.

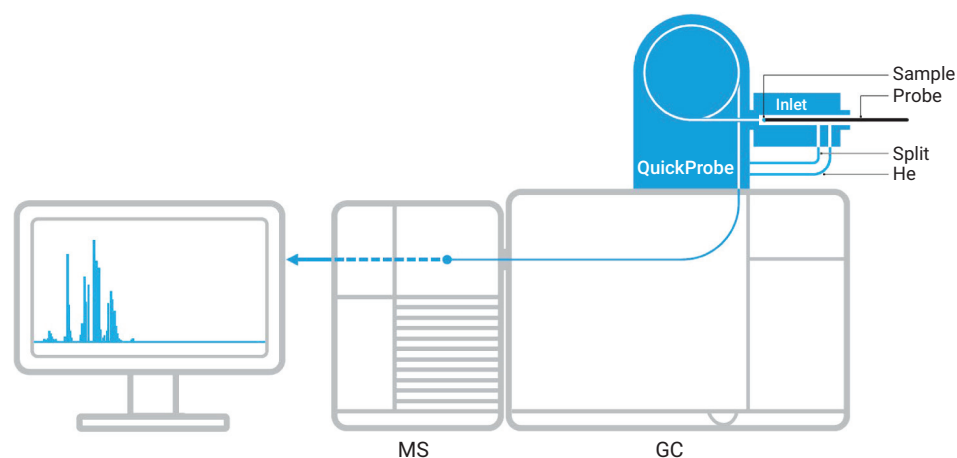


Figure 2. Schematic for the Agilent QuickProbe GC/MS system configuration.

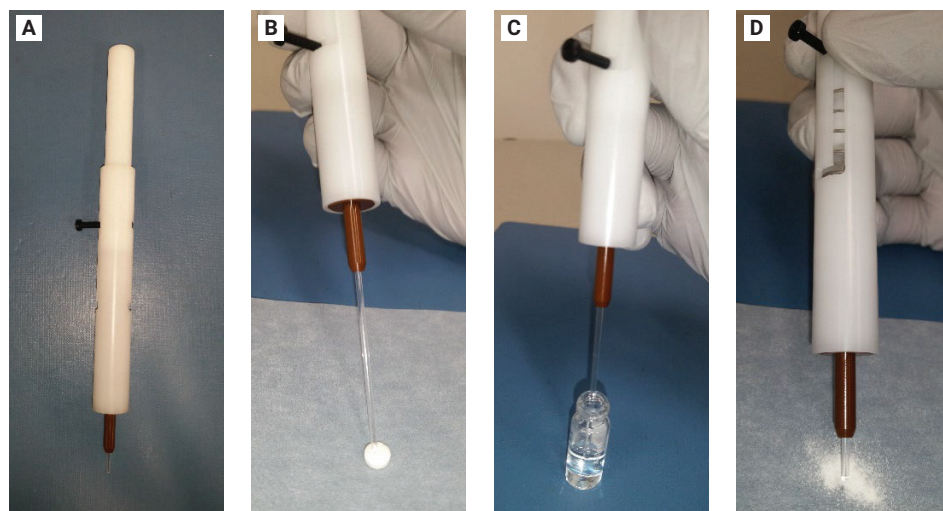


Figure 3. Sample preparation consists of touching the sample with a glass probe in a probe holder (A) as shown for B) solid (tablet), C) liquid, or D) powder (pulverized tablet).

Results and discussion

The analysis of a pulverized Vicodin tablet (5:300 mg of hydrocodone:acetaminophen) with no sample preparation in under one minute resulted in chromatographic separation of the two main components, namely acetaminophen and hydrocodone, thereby demonstrating the capabilities of QuickProbe GC/MS (Figure 4). Additionally, the two active ingredients were identified with a NIST library match of >90 even when the hydrocodone accounted to <2% by weight of acetaminophen.

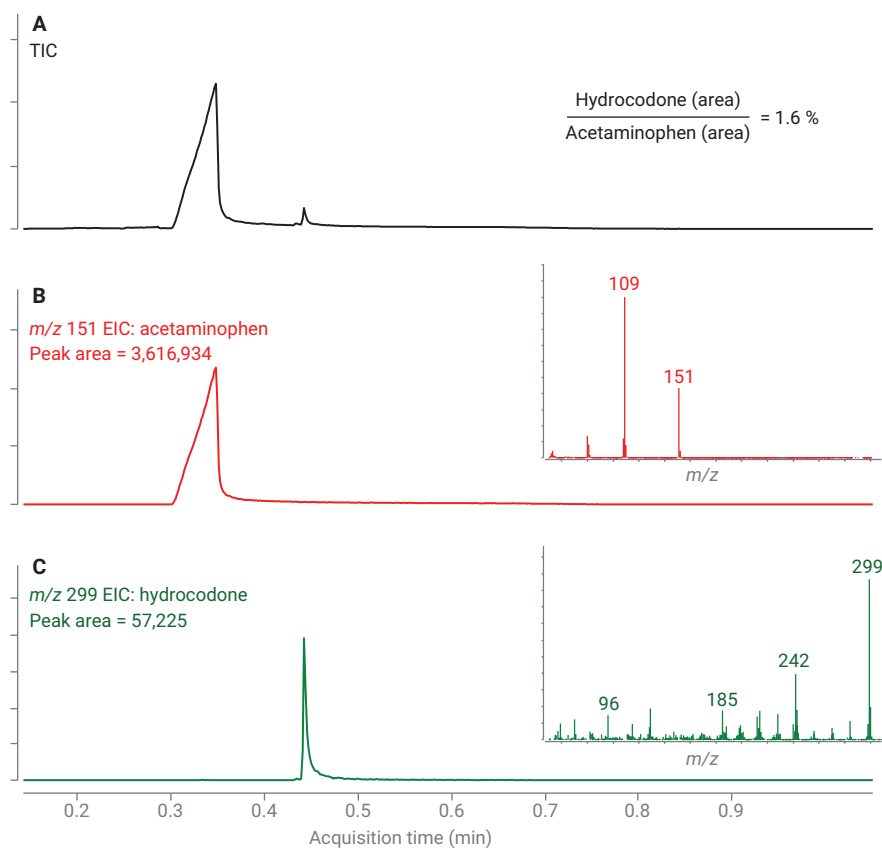


Figure 4. Pulverized Vicodin tablet (5:300 mg of hydrocodone:acetaminophen) analysis in ~one minute. A) Total ion chromatogram (TIC). Extracted ion chromatograms (EIC) for acetaminophen *m/z* 151 (B) and hydrocodone *m/z* 299 (C). NIST library match >90 for both components.

The combination of fast analysis with minimal sample preparation, basic chromatographic separation, and library searches allows for the development of simple, forensically sound workflows (Figure 5). Fast screening workflow analysis in under five minutes includes the following steps:

1. System blank
2. Probe blank
3. Sample
4. System blank

Figure 5 shows the analysis of an Oxycodone tablet using the workflow. Blank runs show background peaks such as phthalates and organic acids. The sample extracted spectrum was identified as Oxycodone with a NIST library match of 93. The final system blank shows the system is back to normal background levels, and is ready for the next screening analysis.

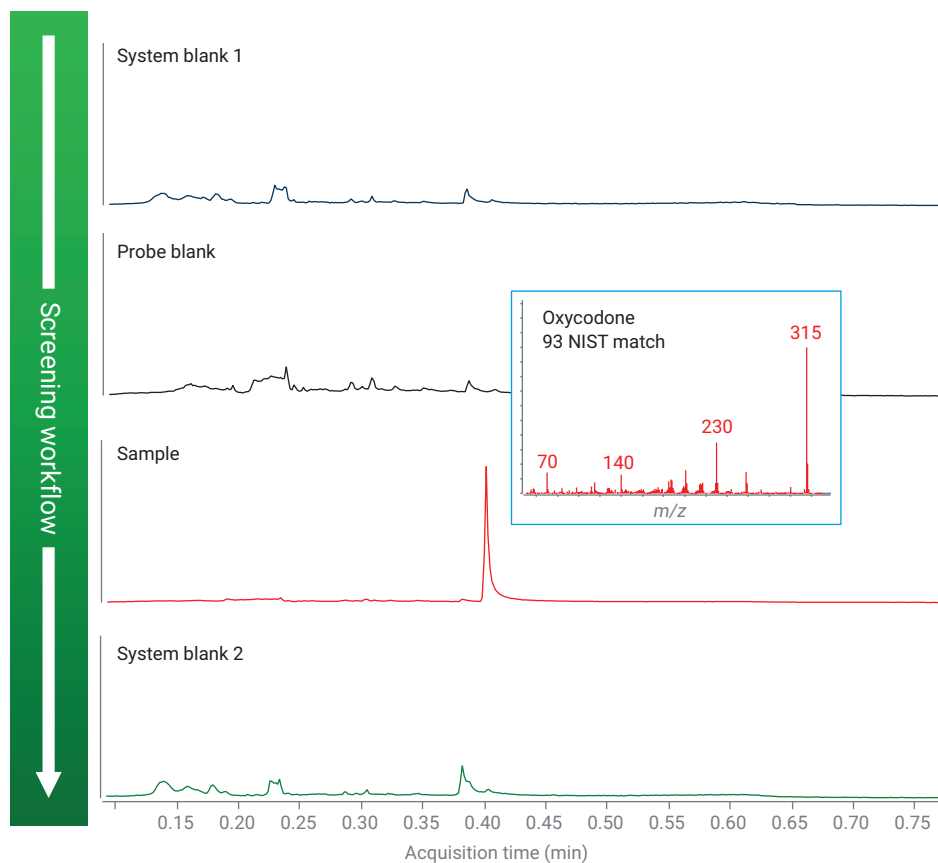


Figure 5. Screening workflow analysis of an Oxycodone tablet in <five minutes.

The fast workflow was applied to seized drug samples from forensic cases. Figure 6 shows the analysis of a cannabis edible (cookie), black tar heroin and “magic” mushroom using MassHunter Unknowns Analysis software. Note that major and minor components were identified with high NIST library match scores. For example, the analysis of the cannabis edible showed THC/dronabinol, cannabichromene, and cholesterol in the sample. Heroin, acetylcodeine, 6-monoacetylmorphine, papaverine, and noscapine were identified in the black tar heroin sample. In the “magic” mushroom analysis, psilocin was identified, even though it was not a major peak. Table 1 shows the summary of results of a variety of seized drug samples and tablets.

Table 1. Summary of the screening analysis results of forensic case samples and prescription drugs.

Sample	Compound	NIST Library Match	Formula
Back Tar Heroin	Acetylcodeine	97	C ₂₀ H ₂₃ NO ₄
	6-Monoacetylmorphine (6-MAM)	98	C ₁₉ H ₂₁ NO ₄
	Diacetylmorphine (Heroin)	98	C ₂₁ H ₂₃ NO ₅
	Papaverine	93	C ₂₀ H ₂₁ NO ₄
	Noscapine	98	C ₂₂ H ₂₃ NO ₇
Cannabis Edible	Dronabinol	99	C ₂₁ H ₃₀ O ₂
	Cannabichromene	89	C ₂₁ H ₃₀ O ₂
“Magic” Mushroom	Psilocin	90	C ₁₂ H ₁₆ N ₂ O
Cocaine Powder	Cocaine	98	C ₁₇ H ₂₁ NO ₄
	Tetramisole	97	C ₁₁ H ₁₂ N ₂ S
Red Tablet	Sildenafil (Viagra)	92	C ₂₂ H ₃₀ N ₆ O ₄ S
Tablet (Alprazolam)	Alprazolam	99	C ₁₇ H ₁₃ ClN ₄
Tablet (Oxycodone)	Oxycodone	97	C ₁₈ H ₂₁ NO ₄
Tablet (Vicodin)	Acetaminophen	99	C ₈ H ₉ NO ₂
	Hydrocodone	96	C ₁₈ H ₂₁ NO ₃

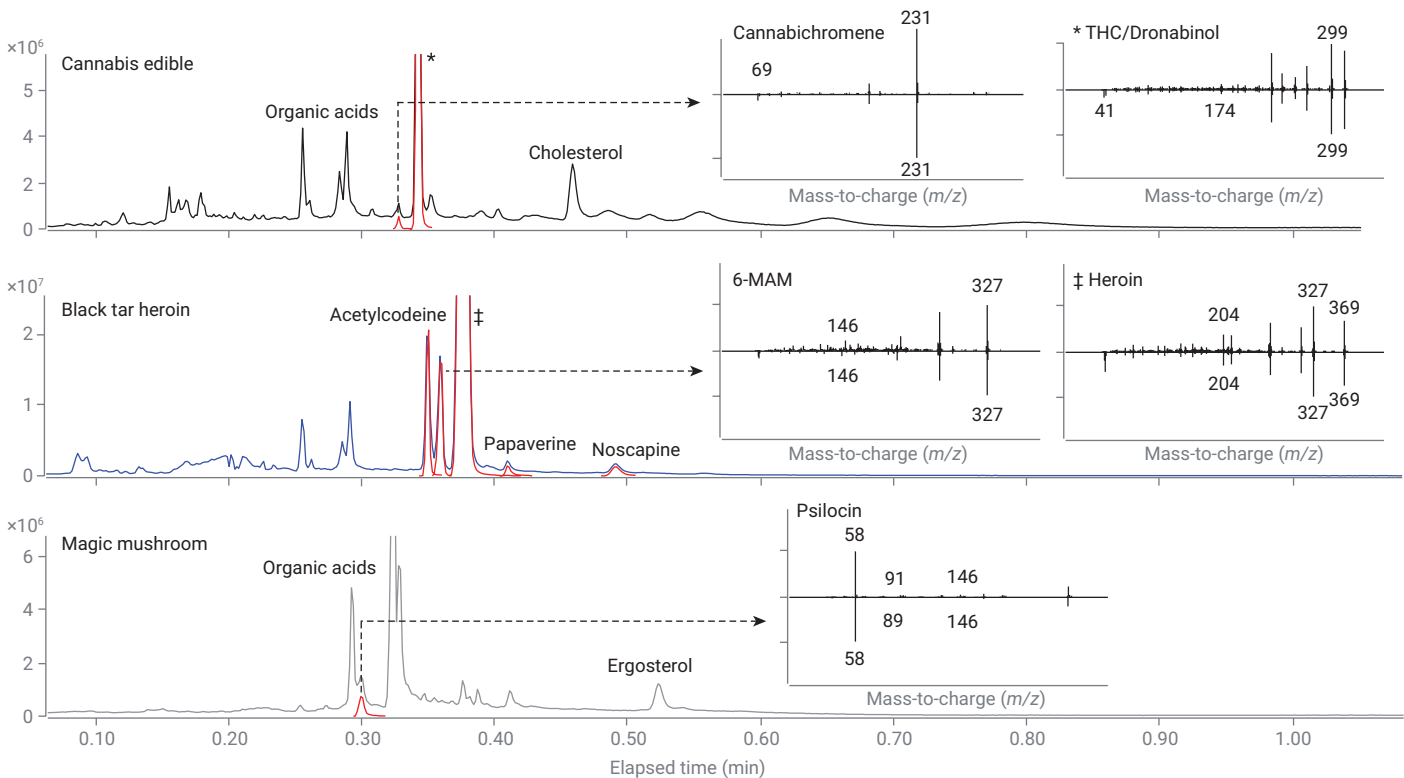


Figure 6. Sub-minute fast screening analysis (without sample preparation) of various forensic case samples including a cannabis edible, black tar heroin, and “magic” mushroom. Comparison spectra (head-to-tail) are shown for the main target compounds in each sample.

The positive identification of the main components can guide the analyst to specific sample preparation procedures or confirmation methods as in the tablets analysis examples. Furthermore, extensive time savings could be achieved in the sub-minute screening analysis of seized drugs for complicated samples (such as cannabis edible, black tar heroin, and “magic” mushroom).

Conclusion

Fast sample analysis with little to no sample preparation was demonstrated in the screening of tablets and seized drugs in bulk samples of different physical states (solid, gel, or powder). The analyses were performed rapidly with the positive identification of drug components by NIST library match and known origin. A fast and forensically sound analysis workflow was shown for screening that involved: 1) system blank; 2) probe blank; 3) sample; and 4) system blank.

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3. Scientific Working Group for the Analysis of Seized Drugs (SWGDRUG) Recommendations, United States Department of Justice Drug Enforcement Administration, 7th ed., **2016** (<http://www.swgdrug.org/Documents/SWGDRUG%20Recommendations%20Version%207-1.pdf>)
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60-Second Screening of Foods Using the Agilent QuickProbe GC/MS System

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Abstract

The Agilent QuickProbe, a direct insertion sampling device for GC/MS, was evaluated for the screening of nonextracted food samples. Foods analysis benefits from fast screening because it quickly identifies samples that are suspect and require further investigation.

Introduction

Typical GC/MS screening of foods and botanicals requires sample preparation such as QuEChERS or other liquid extraction methods. Using the QuickProbe system enables a simple and fast screening analysis that requires no sample preparation. The QuickProbe unit contains a short GC column, and is mounted on the top of the oven of either an Agilent 5975 or 5977 GC/MSD instrument. Sampling is accomplished by touching the sample with a glass probe and inserting the probe into an open atmosphere heated inlet. Ultra fast heating of the column in the presence of helium flow accomplishes the separation of sample components. Data acquisition and analysis is performed using Agilent MassHunter Workstation Acquisition and Unknowns Analysis software, and spectra are identified by searching against user or commercial libraries. Many food sample types have been studied including various oils, spice mixes, beverages, plant material, and flavorings. Samples may consist of either unprepped samples before extraction, as described here, or extracts resulting from the existing laboratory workflow.

Experimental

An Agilent 5977B single quadrupole mass spectrometer was coupled to an Agilent 7890B GC instrument equipped with a separate QuickProbe control unit (Figure 1). The QuickProbe system (G3971A) had an open inlet containing a specialty liner with frit (5190-5104), as shown in Figure 2, a 1.5 m × 0.25 mm, 0.1 μm DB-1HT column, and a 0.7 m × 0.18 mm, 0.18 μm DB1-MS column used as a restrictor into the mass spectrometer.

Helium was used as the carrier gas. The GC/MS system was autotuned. Round tip, glass sample probes (5190-5118) were obtained in touchless packaging (Figure 3), and were held using the QuickProbe holder (G3971-60200) shown in Figure 4, that works as the sample insertion device. Pocket tip probes (5190-5113) contain an indentation or “pocket” at the tip, and are useful for powders. Table 1 lists instrument conditions. Some variations in column temperature hold time and ramp rate were also used.



Figure 1. Agilent QuickProbe (G3971A) device mounted on an Agilent 5977 GC/MS system.



Figure 2. Specialty liner with frit (5190-5104).



Figure 3. Sample probes in touchless packaging (round tip, 5190-5118; pocket tip, 5190-5113).

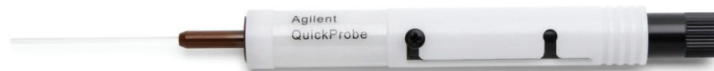


Figure 4. Probe holder shown in loading position with inserted probe on left side (G3971-60200).

Sampling was performed by first inserting a glass probe into the probe holder then, while in loading position (Figure 4), scraping the probe along the solid food or plant material. In a liquid sample, the tip of the probe was dipped into the liquid. Powdered or granular samples were loaded by rubbing the glass probe with sample or tapping the pocket tip probe into the sample. Sample introduction was performed by first retracting the glass probe into the holder. The start button on the QuickProbe unit and the plunger on the probe holder were simultaneously depressed to start the run and position the probe into the hottest part of the inlet. Insertion time was generally five seconds, but this could be varied as required. MassHunter Workstation Acquisition and Unknown Analysis software were used for data acquisition and processing. A minimum match factor of 60 was used for NIST library matches.

Results and discussion

Various food components were easily differentiated using the QuickProbe GC/MS system. The chromatograms resulted from analysis of nonextracted food samples. They demonstrate the power of chromatographic separation coupled with mass spectral

deconvolution to screen highly complex samples and identify targets (Figures 5 to 9). NIST library match scores for each component are in parentheses. As a demonstration, several types of oils such as fish, sesame seed, and vegetable were differentiated using the GC/MS QuickProbe system.

Table 1. Instrument conditions.

QuickProbe and GC Conditions	
Inlet Temperature	250 °C (isothermal only)
Injection Mode	Split (the split is fixed at ~1:10)
Column Temperature	35 °C, hold for 6 seconds 4 °C/sec to 325 °C, hold for 0 seconds (or extended hold)
Run Time	Generally 40 to 60 seconds
Transfer Line Temperature	280 °C
MS Conditions	
Ion Source Temperature	280 °C
Quadrupole Temperature	150 °C
Ionization	El mode
EMV Mode	Gain factor
Gain Factor	10 (should be lowest value required to detect peaks of interest; minimum is 0.05)
Solvent Delay	0 minutes
Scan Type	Scan (38 to 550 μ , 6,250 μ /sec)
Scans Per Second	9.7

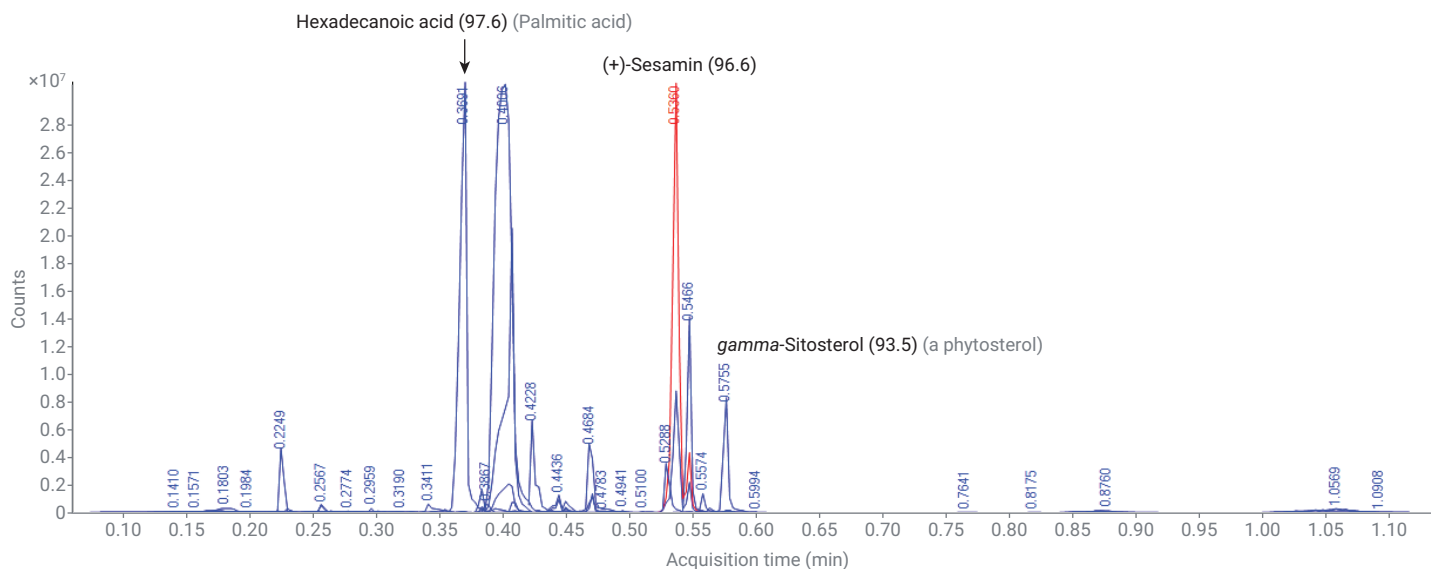


Figure 5. Sesame seed oil. The characteristic component sesamin is identified with a high library match score of 96.6.

This was due to the presence of characteristic components such as sesamin, in sesame seed oil (Figure 5), and cholesterol in fish oil (Figure 6). The profile for vegetable oil shown in Figure 7 shows a peak for 2,4-decadienal, which is formed upon oxidation and contributes to the characteristic aroma of fried foods.

Plant material was able to be screened for components by manually crushing a leaf around the glass probe. The characteristic compound umbellunone was found in California Bay Laurel leaf (Figure 8); this compound differentiates this species from the true bay leaf, or *Laurus nobilis*.¹ Native Americans

used the California Bay Laurel leaves for various medicinal purposes due to their curative properties. This species is sometimes known as the "headache tree" because umbellunone can cause headaches in some sensitive individuals. Methyl eugenol was also determined to be a major constituent of the sample.

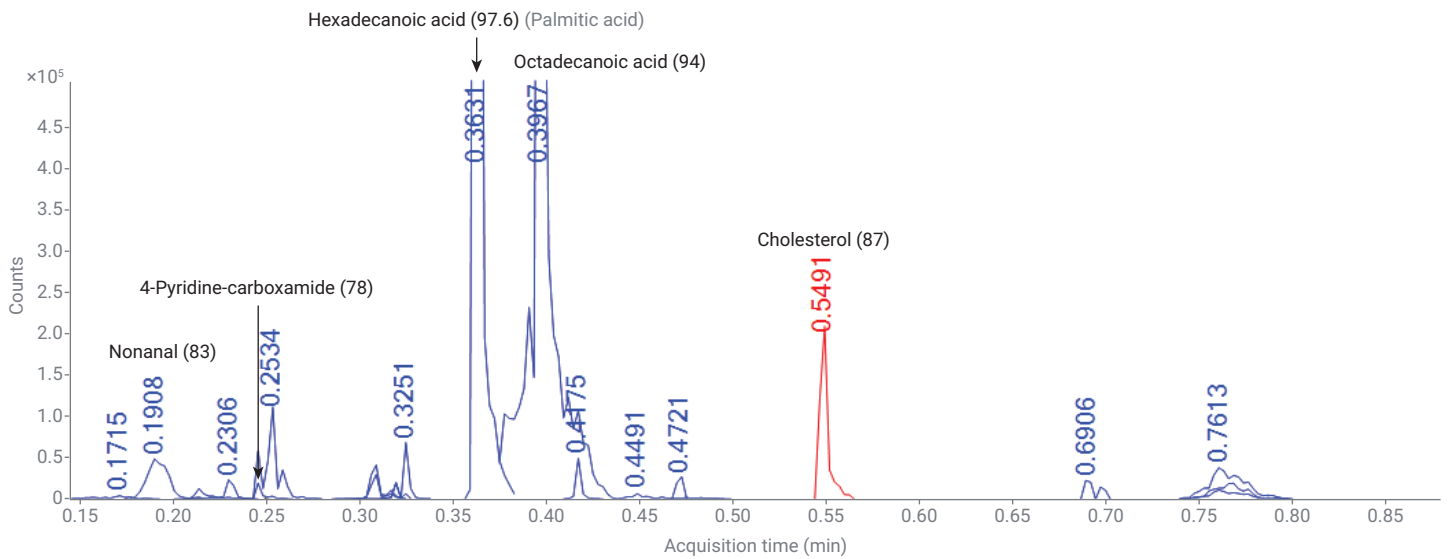


Figure 6. Commercial fish oil showing a peak for cholesterol.

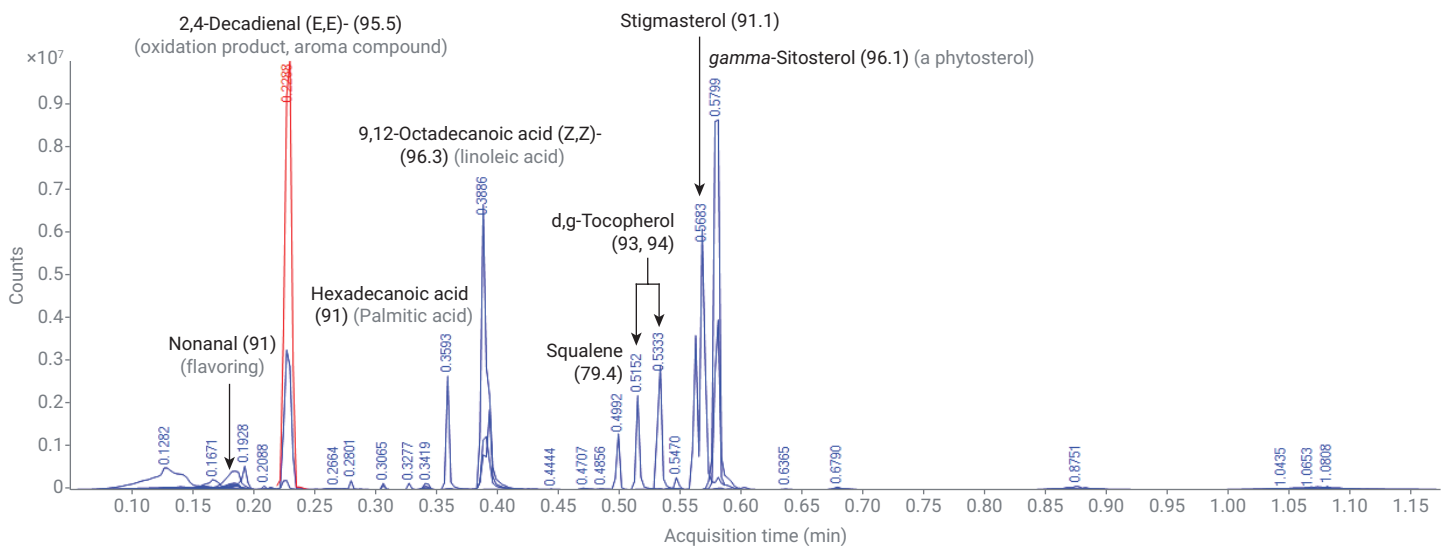


Figure 7. Vegetable oil profile (cottonseed).

Figure 9 shows a chromatogram for a peppery spice rub mix. The compound piperine, from black pepper, was determined in this sample along with *n*-isobutyl-2,4-decadienamide, which is found in herbs and spices. Vitamin E was also detected, and had a library match score of 81.

The QuickProbe GC/MS system successfully characterized several food samples in under one minute without the need for sample preparation. Diverse sample types such as liquids (oils), granular or whole food, and plant material were sampled using a

round tip or pocket tip glass probe. Other means of sampling solid plant material (i.e., cannabis), using a thermal desorption technique, have been used with success, and are described elsewhere (Agilent publication 5994-1357EN).

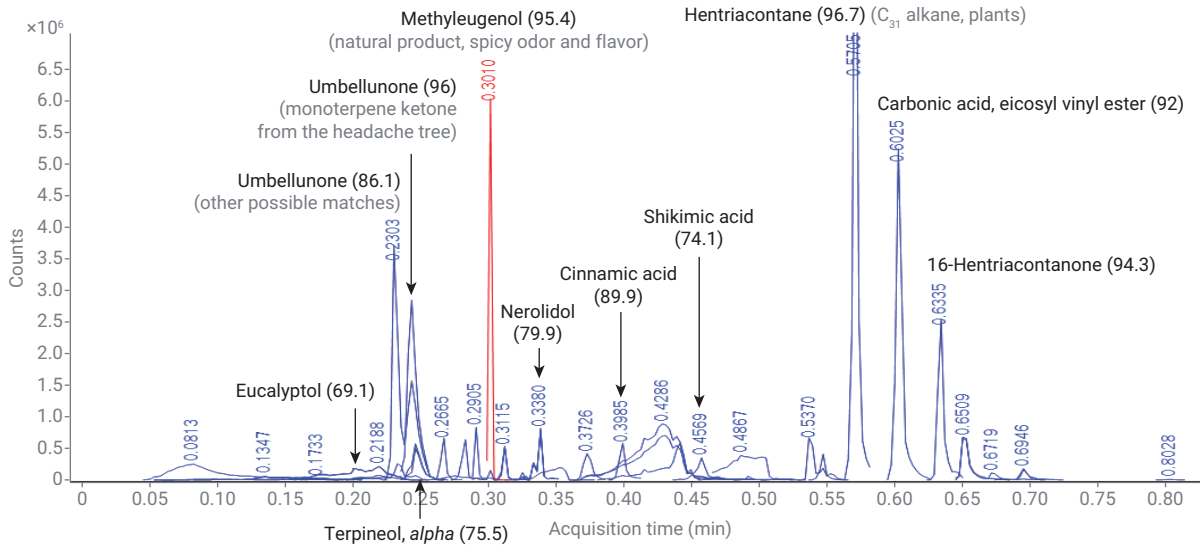


Figure 8. Leaf from the California Bay Laurel (headache tree).

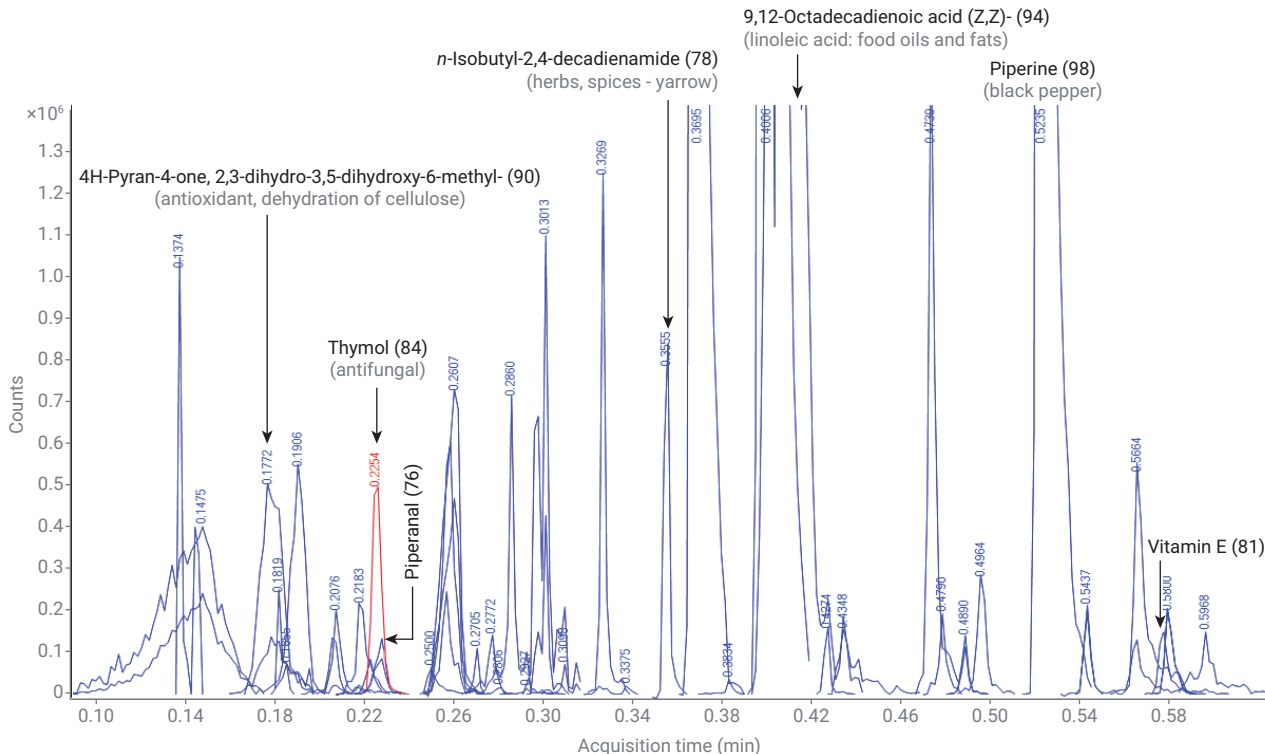


Figure 9. Spice rub mix with black pepper.

Conclusion

The power of the Agilent QuickProbe GC/MS system lies in its ability to quickly chromatograph complex foods and plants, without prior extraction, using a short GC column coupled to a mass spectrometer. Characteristic sample components were identified using Agilent Unknowns Analysis software with spectral match against the NIST library. Thus, a 60-second food screen is made possible using the QuickProbe GC/MS system.

Reference

1. Wang, M. *et al.* Application of GC/Q-TOFQ Combined with Advanced Data Mining and Chemometric Tools in the Characterization and Quality Control of Bay Leaves. *Planta Med* **2018** Sep, *84(14)*, 1045–1054. doi: 10.1055/a-0585-5987. Epub 2018 Mar 14.

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Increasing Throughput for Forensic Screening of Raw Case Samples Using the Agilent QuickProbe GC/MS System

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Abstract

Forensic analysis prescreening using the Agilent QuickProbe GC/MS system allows a simple and fast analysis workflow that does not require sample preparation. The technique of ultrafast chromatographic separation resulting in library-searchable mass spectra permits the development of a forensically sound screening process. Because the QuickProbe GC/MS eliminates the need for preparation steps and reagent-based assays prior to confirmation testing, laboratory productivity can be significantly increased. The Alabama Department of Forensic Science (ADFS) requires reviewable data at all phases of the forensic analysis to increase defensibility in court, and spectra resulting from QuickProbe GC/MS screening satisfy this requirement.

Introduction

Criminal justice laboratories traditionally have used a sample analysis workflow that includes visual examination, weight measurement, and a number of presumptive tests prior to any subsequent confirmation through extraction and GC/MS analysis. In response to the NAS report and in preparation for accreditation under ISO 17025, the ADFS rewrote operating procedures to require reviewable data at all phases of the forensic analysis. Evaluation of the QuickProbe GC/MS (Figure 1) provided a means of prescreening seized samples with resulting mass spectra without any extraction required, which could lead to maximized throughput.

Experimental

The QuickProbe unit is installed on the detector slot on top of the GC instrument of a GC/MS system (Figure 2). It consists of a heated inlet open to the atmosphere, with a constant helium flow that prevents air intrusion. The system uses a short capillary column (Agilent J&W DB-1ht, 1.5 m × 0.25 mm, 0.10 μm) that is rapidly heated (up to 16 °C/s or 960 °C/min), allowing chromatographic separation in under one minute. Individual samples (liquid, solid, and powder) were touched with a glass probe (Figure 3) and introduced into the QuickProbe inlet for three to six seconds for vaporization prior to data acquisition with the GC/MS. Little to no sample preparation was required. A glass probe was first inserted into the probe holder, then, while in loading position (Figure 3), was dipped into a liquid sample, or scraped along a solid sample or plant material. Powdered or granular samples were sampled using pocket-tip probes, which have a small indentation in the tip for a cupped design. Sample introduction was performed by first retracting the



Figure 1. Agilent QuickProbe unit (G3971A) mounted on an Agilent 5977 GC/MS system.

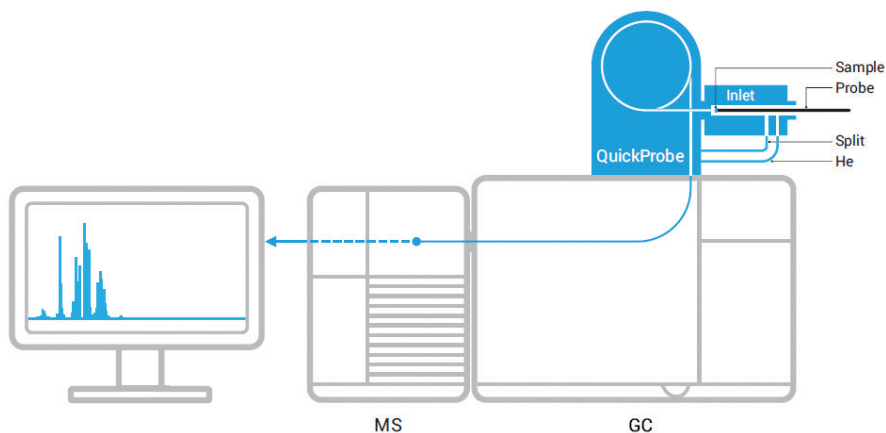


Figure 2. Schematic of QuickProbe direct insertion GC/MS instrument.



Figure 3. Sample probes in touchless packaging (A) and probe holder (B).

glass probe into the holder. The start button on the QuickProbe unit and the plunger on the probe holder were simultaneously depressed to start the run and to position the probe into the hottest part of the inlet. Insertion time was generally five seconds, but this time could be varied as required. Compound identification was achieved through searches performed through standard GC/MS data analysis packages: Agilent ChemStation, MassHunter Qualitative Analysis, Quantitative Analysis, and Unknowns Analysis software. A minimum match factor of 80 was used for the American Academy of Forensic Sciences (AAFS) and Cayman Chemical (Cayman) drug library matches.

Results and discussion

Case samples used in this study are those which had been previously analyzed, adjudicated, and turned into research samples. Sampling handling is critical to forensically sound analysis and probe-loading technique varies with sample type and the desired screen. The suggested workflow is: 1) run system blank, 2) run probe blank, 3) run sample, and 4) run blank. After system blanks are completed, the user may perform probe holder blanks to ensure absence of contamination of the holder tip, which may be rinsed with water or solvent for cleaning. Sample types including bulk materials and seized drugs are diverse in nature and a given screen may require a logistical approach. For example, sampling both the interior and exterior of a tablet may provide information regarding tablet components, previous handling, and storage environment. In certain cases, scraping the exterior surface with a scalpel can expose the interior ingredients.

Plant materials, such as cannabis and hemp, may be sampled by simply scraping or rubbing the material with the tip of the probe. In the case of cannabis, THC is normally the most intense peak in the chromatogram. THC and cannabidiol can be distinguished, however further sample evaluation would be required to determine whether plant material is industrial hemp or marijuana (the latter being defined as $\geq 0.3\%$ THC by dry weight). The QuickProbe GC/MS can separate and lead to identification of the major component, THC, however it is not yet clear if it would be useful for a more accurate, quantitative purpose.

Due to the static nature of certain powdered samples such as cocaine, the probe holder was rinsed with water in between samples to prevent contamination. Alternatively, powders could be dissolved in 1 mL of methanol. Selected results for seized samples are shown in Figures 4 and 5.



Figure 4A. Seized sample of powdered cocaine, which was sampled using a pocket tip probe. The probe was then placed against a piece of clean weigh paper, pocket tip facing down, and rinsed twice with methanol. Once the probe dried, it was inserted into the probe holder, which was previously cleaned with water and dried with a laboratory wipe.

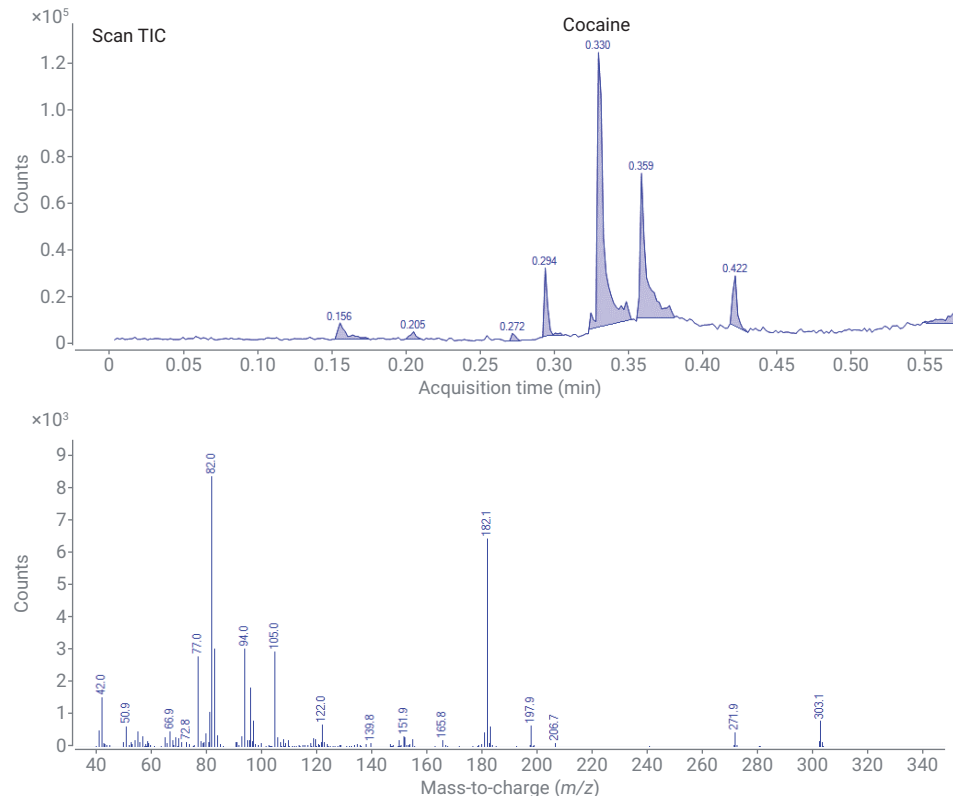


Figure 4B. Chromatographic and spectral results for the same sample of powdered cocaine. The cocaine peak elutes at 0.330 minutes. and the AAFS library match score is 99.

Resulting spectra of raw or dissolved samples provided excellent library match scores against AAFS and Cayman drug libraries. Therefore, any extraction steps could be eliminated in the screening process. Sample throughput was significantly increased since typical analysis time for a sample is one minute, while the total analysis time is three to four minutes, including analysis of appropriate blanks (system, probe, and any solvent if used).

Implementation of the QuickProbe GC/MS in a drug chemistry lab will result in quantifiable benefits such as the generation of reviewable spectra for case screening and the possibility of screening samples for which there had been no prior screening technique available, such as synthetic cannabinoids.

Table 1 provides results for case samples, including library match scores that were evaluated in this study. Results highlighted in yellow indicate that identified compounds did not match the known identification of the case samples (which had previously been adjudicated and turned into test samples for this study). Some missed identifications are readily explained. For example, clonazepam elutes late and is challenging by GC/MS. GHB must be derivatized to perform GC/MS analysis, and methamphetamine in lighter fluid is overwhelmed by the propane peak. Nicotinamide is a cutting agent for pseudoephedrine (some of the latter may be observed in a sample). However, QuickProbe correctly identified 83% of the samples studied.

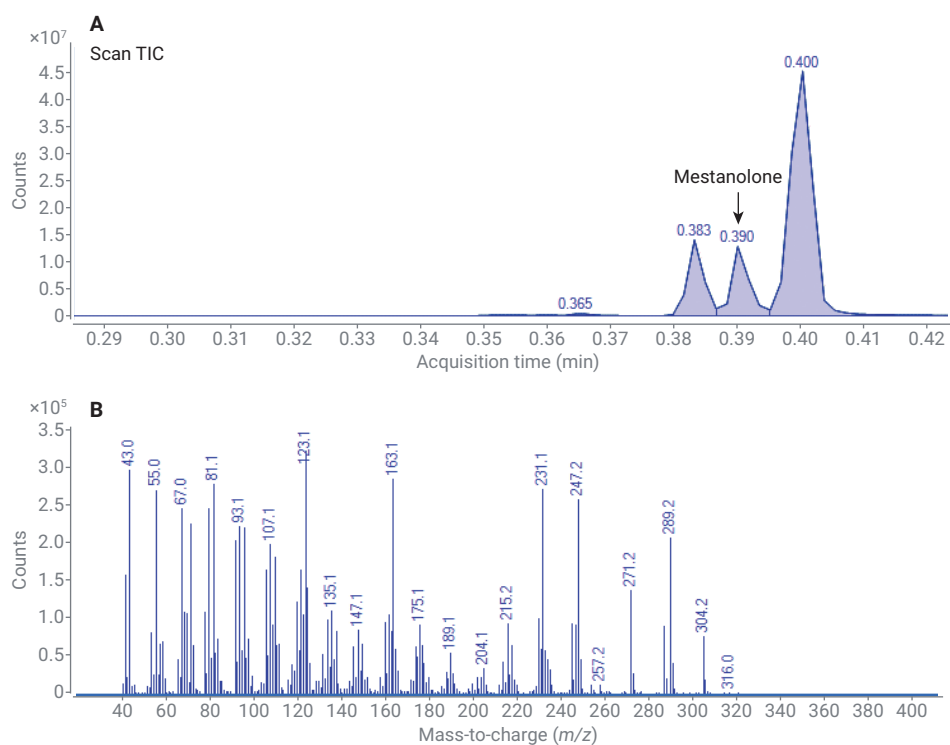


Figure 5. Chromatographic (zoomed in) and spectral results for a sample containing mestanolone. The mestanolone peak elutes at 0.390 minutes, and the AAFS library match score is 91.

Table 1. Case sample (previously adjudicated) results, including library match scores.

Sample	Major Identified Compound(s)	Identification
13HQ00031-1	Amobarbital (91), secobarbital (91)	Amobarbital Sodium
13HQ00048-1	Chlordiazepoxide (87)	Chlordiazepoxide
13HQ00114-1	Hexanedioic acid (93)	Plant material
13HQ00128-1	Stearic acid (89)	Clonazepam
13HQ00170-1	Lorazepam (99)	Lorazepam
13HQ00180-1	Oxazepam (72)	Oxazepam
13HQ00289-1	JWH250 (80)	JWH 250
13HQ00411-1	Morphine (98)	Morphine
13HQ00434-1	Phenobarbital (96)	Phenobarbital
13HQ00505-1	Pentobarbital (72)	Pentobarbital
13HQ00522-1	PCP (phencyclidine) (92), cyclohexene (95)	Phencyclidine
13HQ00525-1	Ketamine (97)	Meth, ketamine
13HQ00552-1	Dimethyl sulfone (90), nicotinamide (96), methamphetamine (64)	Meth, nicotinamide
13HQ00581-1	Temazepam (99)	Temazepam
13HQ00584-1	PCP (phencyclidine) (96)	Phencyclidine
13HQ00591-1	Pentobarbital (91)	Pentobarbital
13HQ00611-1	Benzoic acid (90), cocaine (99), anhydroecgonine methyl ester(98), benzoylcegonine (96)	Cocaine
13HQ00615-1	Cocaine (99)	Cocaine HCl
13HQ00622-1	Dimethyl sulfone (76), nicotinamide (96), methamphetamine (93)	Methamphetamine, nicotinamide
13HQ00866-2	Hexanedioic acid (47)	GHB/H ₂ O/CHCl ₃
13HQ00869-1	Pseudoephedrine (83)	Pseudoephedrine

Sample	Major Identified Compound(s)	Identification
13HQ00881-1	Guaiaphenesin (98)	Guaphenesin
13HQ00893-1	Mestanolone (91)	Mestanolone
13HQ00912-1	Hexanedioic acid (86)	Sodium bicarbonate
13HQ00933-1	Testosterone propionate (99), testosterone enanthate (72)	Steroid
13HQ00938-1	Diisooctyl adipate (72), hexanedioic acid (80)	Hydromorphone
13HQ00949-1	Dodecanoic acid (86)	Trenbolone
13HQ00970-1	Nandrolone decanoate (99)	Nandrolone decanoate
13HQ00972-1	Bezyl benzoate (98), testosterone cypionate (99)	Testosterone
13HQ00975-1	Nicotinamide (98)	Pseudoephedrine
13HQ01188-1	Codeine(97)	Codeine sulfate
13HQ01192-1	Hydromorphone (99)	Dilaudid
13HQ01193-1	Ketamine (97)	Ketamine
13HQ01195-1	heroin(99)	Heroin
13HQ01198-1	Benzophenone (91), nordiazepam (99)	Clorazepate
13HQ01217-1	AM2201 (99)	AM2201
13HQ01231-1	AM2201 (99)	AM2201
13HQ01238-1	Hexanedioic acid (86)	Negative
14HQ00003-1	1,4-Butanediol (83)	1,4-Butanediol
15HQ00097-1	Heroin (99)	Heroin and lactose
16HQ00095-1	Propane (78)	Meth in lighter fluid
16HQ00197-1	Caffeine (97)	Suspected kratom
16HQ00197-8	Hexanedioic acid (62)	Suspected kratom
18HQ00193-1	1-Di-Cyclobutanol (72)	Plant material
18HQ00195-1	Cannabidiol (90)	Relax gummies
18HQ00203-1	Hexanedioic acid (91)	Brownie
18HQ00204-1	Theobromine (95), glycerine (83)	Kush cakes
18HQ00216-1	Cannabidiol (93)	Pharxma
18HQ00218-1	Propylene glycol (86)	CBD Drip Gold
19HQ00057-1	Acetaminophen (87)	Hydrocodone/APAP syrup
HW250	Cannabidiol (98)	Cannabidiol
HW750	Cannabidiol (97)	Cannabidiol

As a result of evaluating the QuickProbe screening method, a complete workflow may be recommended for drug analysis case work. The diagram in Figure 6 shows that cases would be triaged by a screen team prior to analysis, instead of each case screened separately by the analyst as in traditional case analyses. QuickProbe GC/MS can be the screening technique used for any sample containing powders, liquids, or unknown plant materials. Following triage, a different analyst would perform the drug screening. This new workflow would limit the tasks necessary for each analyst, allowing the screen team to sort cases into batches for the analyst prior to the run. This, in turn, would add redundancy to the analysis and reduce employee workload.

The transition from a single analyst to a team of analysts per case would improve productivity. Cases could be sorted effectively into batches following the first sampling without extraction, allowing the confirmation analyst to test an entire batch of cases in sequence. QuickProbe screening generates reviewable data that can be recorded and stored with the batch for further reference. Since a minimum of two scientists would be involved in each case, there is increased confidence in analyte determination as an additional scientist would now confirm the evidence description.

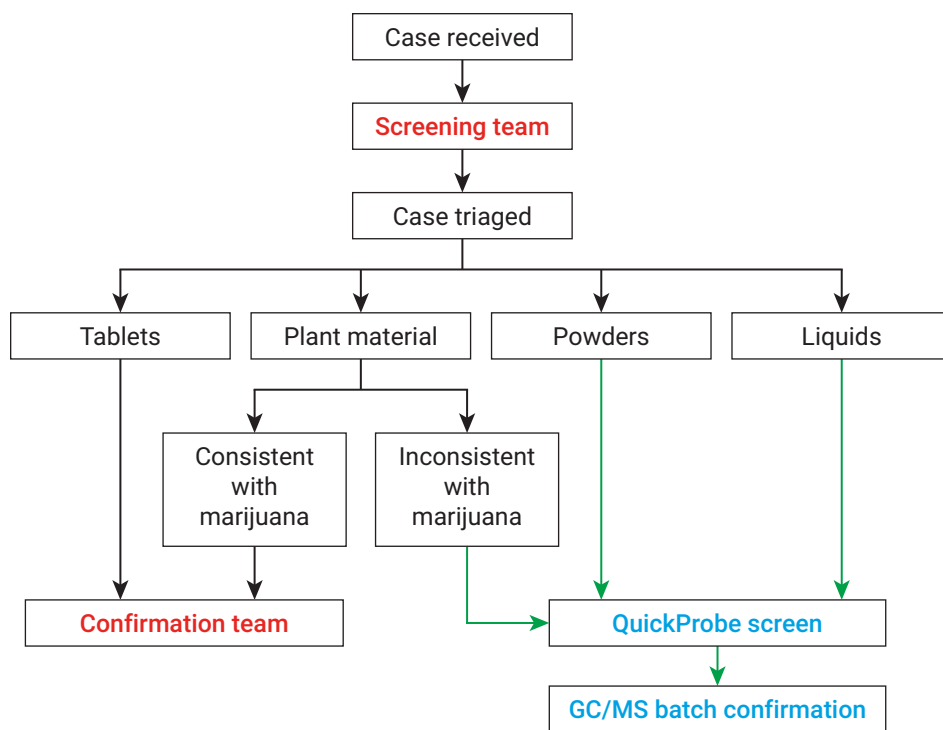


Figure 6. Recommended laboratory workflow.

Conclusion

It has been demonstrated that the QuickProbe GC/MS system screening method provides advantages over traditional screening techniques in forensic drug chemistry labs. The method provides a single screening test for a wide range of analytes, as well as reviewable data that can be recorded and stored with the case records. It also provides the ability to screen for emerging analytes that do not have a traditional screening technique, such as synthetic cannabinoids.

Using the QuickProbe GC/MS system as the screening choice increases confidence in the results since library-searchable mass spectra are generated with every run. The workflow developed as a result of this method improves productivity and confidence in analytical results.

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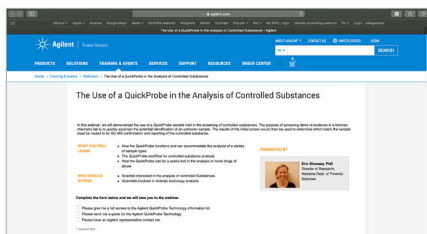
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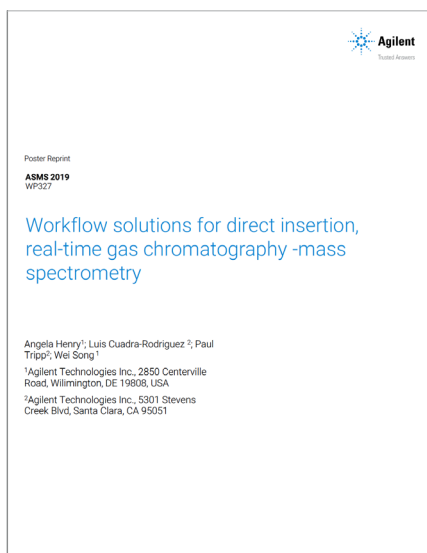
The Use of a QuickProbe in the Analysis of Controlled Substance

Watch Erin Shonsey from the Alabama Dept of Forensic Sciences demonstrate the use of a QuickProbe in the screening of controlled substances. The purpose of screening items of evidence in a forensic chemistry lab is to quickly ascertain the potential identification of an unknown sample. The results of the initial screen would then be used to determine which batch the sample must be routed to for GC-MS confirmation and reporting of the controlled substance.

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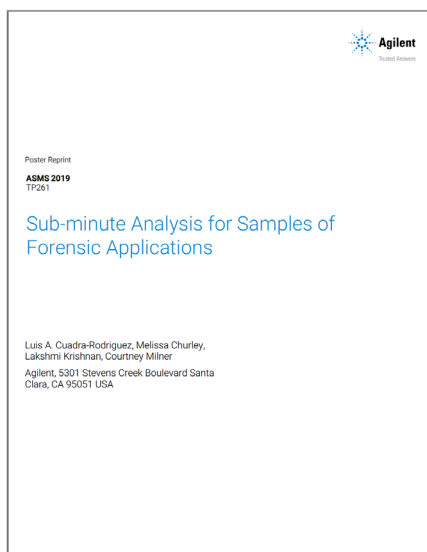
Workflow solutions for direct insertion, real-time gas chromatography-mass spectrometry

The need for fast screening of samples is desired across many fields of study, from crime laboratories analysis of seized drugs, to verifying RoHS compliance of plastic commodities. Conventional screening with gas chromatography-mass spectrometry (GC/MS) requires sample preparation of dissolution, dilution and/or headspace sampling and long GC analysis times. Typical application of direct insertion real-time MS provides quick analysis of various sample types but does not have chromatographic separation of the analytes, causing increased time of human review. Direct insertion GC/MS is an easy-to-use screening techniques, and offers fast analysis with GC separation and mass spectral confirmation in under a minute.

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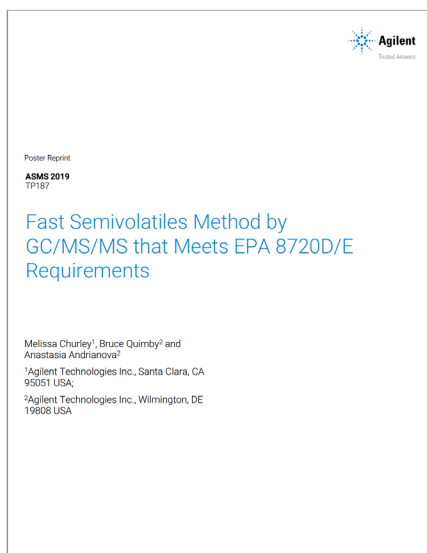


Sub-minute Analysis for Samples of Forensic Applications

The last two decades have seen a steady increase in the need for fast and accurate identification of compounds in a variety of samples and mixtures, especially in forensic laboratories. Positive identification of chemical components in bulk samples is critical during the screening process. Conventional analysis often requires sample preparation that includes dissolution, dilution and physical characterization followed by GC/MS analysis for confirmation. A simple and fast screening analysis that requires little to no sample preparation is demonstrated with a unique direct insertion GC/MS system. Compound identification of prescription drugs and standards is achieved through the routinely used NIST library search when using single quadrupole (SQ) mass spectrometer.

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