Memorandum

MIAMI-DADE COUNTY

Date:	May 6, 2014
To:	Honorable Chairwoman Rebeca Sosa and Members, Board of County Commissioners
From:	Carlos A. Gimenez Mayor
Subject:	Retroactive Application to Apply For, Receive, and Expend Funds From the National Institute of Justice Paul Coverdell Forensic Science Improvement Grants Program

Agenda Item No. 3(B)(9)

Recommendation

It is recommended that the Board of County Commissioners approve the attached Resolution retroactively authorizing the County Mayor's or the County Mayor's designee action to apply for, receive, and expend funds in the amount of up to $175,000 from the National Institute of Justice (NIJ) Paul Coverdell Forensic Science Improvement Grants Program to support Medical Examiner Department and authorizing the County Mayor or the County Mayor's designee to exercise and execute necessary applications, agreements and Memoranda of Understanding (and modifications thereto) to accomplish the purposes of the grant. The grant period will be effective October 1 through September 30 of the grant award year and does not require any matching local or in-kind funds.

Scope

The grant will provide countywide services.

Fiscal Impact/Funding Source

This grant will provide up to $175,000 in federal funds to implement the proposed project. The grant does not require any matching local or in-kind funds. The funding source is the Department of Justice, National Institute of Justice.

Track Record/Monitor

The Accountant 3 of the Medical Examiner Department, Yeseny Serra, will monitor the grant.

Background

The Paul Coverdell Forensic Science Improvement Grants Program awards grants to states and units of local government to help improve the quality and timeliness of forensic science and medical examiner services. Units of local government may only apply for competitive funds. The funds may be used to eliminate a backlog in the analysis of forensic evidence and for the upgrade, lease, or purchase of forensic laboratory or Medical Examiner equipment and instrumentation.

The Medical Examiner Department will use the grant funds to purchase new laboratory technology that will significantly aid in eliminating the current backlog in cases requiring postmortem forensic toxicology analysis. The new technology will improve throughput and reduce turnaround, yield high quality of results, and decrease cost of materials needed for additional analyses.

Genaro "Chip" Iglesias
Deputy Mayor

MEMORANDUM

(Revised)

TO: Honorable Chairwoman Rebeca Sosa
and Members, Board of County Commissioners

DATE: May 6, 2014

FROM: R. A. Cuevas, Jr.
County Attorney

SUBJECT: Agenda Item No. 3(B)(9)

Please note any items checked.

_____ **"3-Day Rule" for committees applicable if raised**

_____ **6 weeks required between first reading and public hearing**

_____ **4 weeks notification to municipal officials required prior to public hearing**

_____ **Decreases revenues or increases expenditures without balancing budget**

_____ **Budget required**

_____ **Statement of fiscal impact required**

_____ **Ordinance creating a new board requires detailed County Mayor's report for public hearing**

✓ **No committee review**

_____ **Applicable legislation requires more than a majority vote (i.e., 2/3's ____, 3/5's ____, unanimous _____) to approve**

_____ **Current information regarding funding source, index code and available balance, and available capacity (if debt is contemplated) required**

Approved _____ Mayor
Veto _____
Override _____

Agenda Item No. 3(B)(9)
5-6-14

RESOLUTION NO. _____

RESOLUTION RETROACTIVELY AUTHORIZING THE COUNTY MAYOR OR COUNTY MAYOR'S DESIGNEE ACTION TO APPLY FOR, RECEIVE, AND EXPEND GRANT FUNDS IN THE AMOUNT OF UP TO $175,000 FROM THE NATIONAL INSTITUTE OF JUSTICE (NIJ) PAUL COVERDELL FORENSIC SCIENCE IMPROVEMENT GRANTS PROGRAM; AND FURTHER AUTHORIZING THE COUNTY MAYOR OR COUNTY MAYOR'S DESIGNEE TO EXERCISE AND EXECUTE SUCH CONTRACTS, AGREEMENTS, MEMORANDA OF UNDERSTANDING (AND AMENDMENTS THERETO) TO ACHIEVE THE PURPOSES OF THE GRANT, AND TO MODIFY OR AMEND THE APPLICATION IN ORDER TO RECEIVE ADDITIONAL FUNDS OR TO EXTEND THE PERFORMANCE PERIOD AS REQUIRED IF AWARDED

WHEREAS, this Board desires to accomplish the purposes outlined in the accompanying memorandum, a copy of which is incorporated herein by reference,

NOW, THEREFORE, BE IT RESOLVED BY THE BOARD OF COUNTY COMMISSIONERS OF MIAMI-DADE COUNTY, FLORIDA, that this Board hereby retroactively ratifies the County Mayor or County Mayor's designee action to apply for, receive, and expend up to $175,000 from National Institute of Justice (NIJ) Paul Coverdell Forensic Science Improvement Grants Program fund, and further authorizes the County Mayor or County Mayor's designee to receive and expend any grant funds for the purposes described in the funding request; to apply for, receive and expend future additional funds should they become available through the grant program; to file and execute any necessary amendments to the application for and on behalf of Miami-Dade County, Florida; to execute such contracts, agreements, Memoranda of Understanding, as required by grant guidelines or to further the purposes described in the funding requests, following approval by the County Attorney's Office;

and to exercise and execute any amendments, modifications, renewal and extension provisions, cancellation and termination clauses of any of the foregoing applications, contracts, agreements, and Memoranda of Understanding on behalf of Miami-Dade County, Florida following approval by the County Attorney's Office.

The foregoing resolution was offered by Commissioner , who moved its adoption. The motion was seconded by Commissioner and upon being put to a vote, the vote was as follows:

Rebeca Sosa, Chairwoman
Lynda Bell, Vice Chair

Bruno A. Barreiro	Esteban L. Bovo, Jr.
Jose "Pepe" Diaz	Audrey M. Edmonson
Sally A. Heyman	Barbara J. Jordan
Jean Monestime	Dennis C. Moss
Sen. Javier D. Souto	Xavier L. Suarez
Juan C. Zapata	

The Chairperson thereupon declared the resolution duly passed and adopted this 6th day of May, 2014. This resolution shall become effective ten (10) days after the date of its adoption unless vetoed by the Mayor, and if vetoed, shall become effective only upon an override by this Board.

MIAMI-DADE COUNTY, FLORIDA
BY ITS BOARD OF
COUNTY COMMISSIONERS

HARVEY RUVIN, CLERK

By:_____
Deputy Clerk

Approved by County Attorney as
to form and legal sufficiency. JEB

Jason E. Bloch

APPLICATION FOR FEDERAL ASSISTANCE	2. DATE SUBMITTED April 01, 2014	Applicant Identifier
1. TYPE OF SUBMISSION Application Non-Construction	3. DATE RECEIVED BY STATE	State Application Identifier
	4. DATE RECEIVED BY FEDERAL AGENCY	Federal Identifier

5.APPLICANT INFORMATION

Legal Name Miami Dade County	Organizational Unit Medical Examiner
Address Number One On Bob Hope Road Miami, Florida 33136-1133	Name and telephone number of the person to be contacted on matters involving this application Serra, Yeseny (305) 547-3766
6. EMPLOYER IDENTIFICATION NUMBER (EIN) 59-6000573	7. TYPE OF APPLICANT County
8. TYPE OF APPLICATION New	9. NAME OF FEDERAL AGENCY National Institute of Justice
10. CATALOG OF FEDERAL DOMESTIC ASSISTANCE NUMBER: 16.742 CFDA TITLE: Paul Coverdell Forensic Sciences Improvement Grant Program	11. DESCRIPTIVE TITLE OF APPLICANT'S PROJECT Drug screening in postmortem blood: a faster approach using GC/MS

12. AREAS AFFECTED BY PROJECT

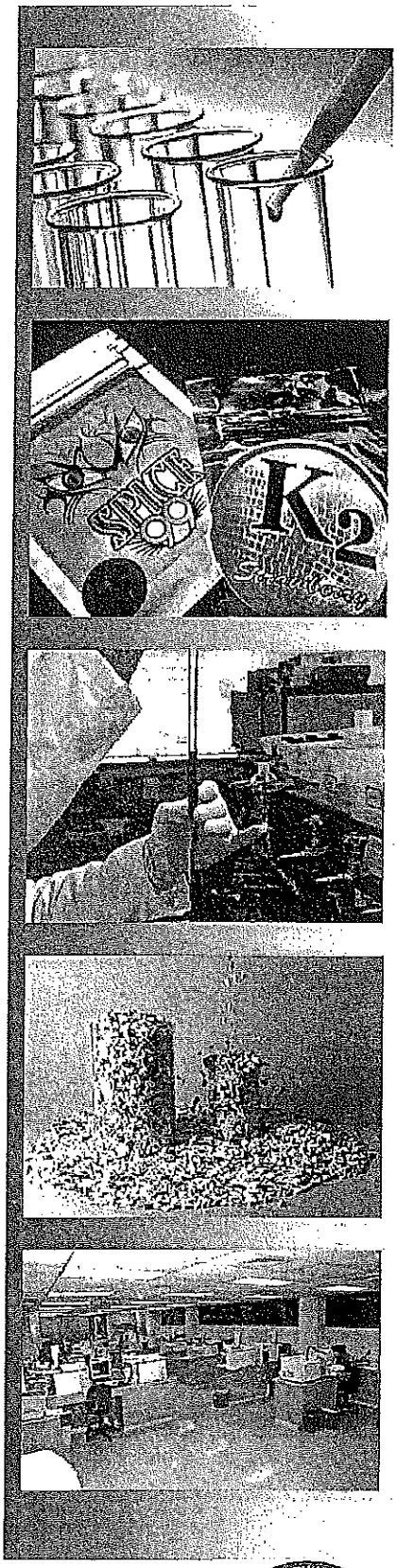
Project will affect the entire jurisdiction of Miami-Dade County, Florida.

13. PROPOSED PROJECT Start Date: October 01, 2014 End Date: September 30, 2015	14. CONGRESSIONAL DISTRICTS OF a. Applicant b. Project FL23 FL24 FL25 FL26 FL27

15. ESTIMATED FUNDING		16. IS APPLICATION SUBJECT TO REVIEW BY STATE EXECUTIVE ORDER 12372 PROCESS?
Federal	$174,634	
Applicant	$0	

State	$0	Program is not covered by E.O. 12372
Local	$0	
Other	$0	
Program Income	$0	17. IS THE APPLICANT DELINQUENT ON ANY FEDERAL DEBT?
TOTAL	$174,634	N
18. TO THE BEST OF MY KNOWLEDGE AND BELIEF, ALL DATA IN THIS APPLICATION PREAPPLICATION ARE TRUE AND CORRECT, THE DOCUMENT HAS BEEN DULY AUTHORIZED BY GOVERNING BODY OF THE APPLICANT AND THE APPLICANT WILL COMPLY WITH THE ATTACHED ASSURANCES IF THE ASSISTANCE IS REQUIRED.		

Close Window



DRUG SCREENING IN POSTMORTEM BLOOD:
A FASTER APPROACH USING GC/MS

Paul Coverdell Forensic Science Improvement Grants Program
CFDA No. 16.742
APRIL 1, 2014

Contact Information:

Miami-Dade County
Medical Examiner Department
Dr. Bruce A. Hyma
Director and Chief Medical Examiner
One Bob Hope Road
Miami, Florida 33136
bahyma@miamidade.gov
305-545-2425

MIAMI-DADE COUNTY

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PROJECT ABSTRACT

A highly challenging and complex problem confronting postmortem forensic toxicology laboratories is the detection of a growing assortment of drugs and toxic substances in blood and tissue samples from decedents. For both the laboratory and the investigating medical examiner, its detection must occur early in the testing process to better understand the nature of the case and course of additional testing. Initial screening tests dictate how a case will proceed, what tests will follow, and how long it will take to complete. Screening procedures must be thorough and comprehensive while being able to meet reasonable turn-around time expectations.

The Miami-Dade County Medical Examiner Department is requesting grant funding to purchase an automated gas chromatograph mass spectrometer (GCMS) capable of fast analyses with spectral deconvolution software to replace antiquated technology currently used by the toxicologists. This new instrument will significantly improve processing and turnaround time of medical examiner services and eliminate an unreasonable backlog of toxicology cases that build-up each week. The increasing demand placed on the toxicology laboratory ("Laboratory") each week is overwhelming due to the number of cases involving drugs requiring a comprehensive screen. Approximately 72% of all cases processed require blood screening that takes on average 95 minutes of instrument and data processing time to complete. The technology will reduce the processing time by 79% and ultimately reduce the turnaround time by 75% on medical examiner cases to a more reasonable 30-45 days.

The GCMS technology will achieve the following program objectives:

- Reduce instrument runtime for a single blood drug screen from 95 to 10 minutes
- Reduce data processing time from 30 to 10 minutes
- Reduce overall processing time for a single blood drug screen from 95 to 20 minutes
- Reduce turnaround time for a single case involving a blood drug screen from 65-75 days to 30-45 days.

The following project outcomes will be tracked as performance measures: (1) improved throughput and reduced turnaround time for blood screens; (2) improved excellence in the quality of the results; and (3) decreased costs in maintenance and materials. The new GCMS system has increased temperature programming ramp rates with additional electronic pressure controlled gas flows to reduce the chromatographic runtime from 45 to 10 minutes. The instrument incorporates both a nitrogen specific detector and mass spectrometer that allows analysis to be performed on one instrument, rather than three separate instruments. Technology features such as inlet back-flushing and a new ion source design will reduce or eliminate the maintenance that typically consumes instrument preparation time prior to analysis.

PROGRAM NARRATIVE (REQUEST FOR COMPETITIVE FUNDS)

STATEMENT OF THE PROBLEM

The Toxicology Division of the Miami-Dade County Medical Examiner Department (Department) in Miami, Florida (District 11) provides postmortem forensic toxicology services to the Department as well as other outside agencies within Florida and throughout the Caribbean islands. The Department and the Laboratory are accredited by the National Association of Medical Examiners (NAME) and the American Board of Forensic Toxicology (ABFT), respectively. The Laboratory processes over 2,400 cases and 25,000 tests per year.

The unique nature and history of Miami has enabled the Department to accumulate more experience with drug related deaths and poisonings than any other Medical Examiner office in Florida. As a result, the Toxicology Laboratory has been confronted with every new drug abuse trend effecting the country as well as many new drugs and poisons that come directly through Miami.

Laboratory testing procedures used in the screening process have been developed to be thorough and as inclusive as possible. To complete a case in a reasonable time, reduce the turnaround time and backlog, and maintain a steady workflow, it is essential to utilize a reliable and comprehensive screening protocol without sacrificing quality. The successful and timely resolution of any medical examiner case involving drugs and poisons is dependent on these procedures.

In any postmortem forensic toxicology laboratory one of the most essential parts of the toxicological examination of a new case is the case review and establishing the initial screening protocols to be employed by the laboratory. It is in these screening tests where the toxicologist

determines the extent of the drugs involved, and their relationship to the cause and manner of death. The number and type of follow-up testing is also dependent on these initial results. Deciding additional screening tests to be performed, the confirmation tests to employ to verify results, and what drugs to quantify if necessary, are all dependent on the initial screening results. Decisions that are made early will result in improvements in turnaround time and workflow. Successful and timely screening therefore is pivotal in controlling turnaround time, operational costs, and, in most cases, the amount of time to complete the medical examiner's report on the cause and manner of death.

The most important features of a comprehensive screening protocol in postmortem toxicology include the following:

- It must be applicable to all fluids and tissues available
- It must be sensitive, reliable, reproducible, and comprehensive
- It must use the most advanced technology to reliably identify a compound and be considered acceptable in the scientific community
- It must be rapid and have the capacity to enable the user to process a typical weekly caseload

Approximately 1,800 of the 2,500 cases received each year by the Laboratory require blood and tissue screens. This represents 72% of the cases submitted by all agencies served by the Laboratory. The screening procedure currently in use is a two step process that includes gas chromatography (GC) and gas chromatography-mass spectrometry (GCMS). The GC portion of the screening method utilizes two GC systems. The first is a GC equipped with thermionic specific detectors (GC-TSD) and two capillary columns. This system detects basic or alkaline compounds on two dissimilar columns. The second is a GC equipped with flame ionization

detectors (GC-FID) and two capillary columns. This system detects acidic and neutral compounds on two dissimilar columns. The second step of the screening process utilizes GCMS to confirm or identify any substance found in step one. The specificity and sensitivity of the GC procedure provides for low detection limits and a high degree of certainty in the identification of a compound either detected in step 1 or detected for the first time in step 2. Both of these procedures are acceptable in the forensic toxicology community and represent the most typical approach to this type of screening.

The disadvantage of this process is the extended amount of time that is required to complete the analysis and process the data. The instrument run time for each of the two GC steps is 40 minutes. Although these can be performed concurrently it is excessive. The GCMS step has a similar run time taking an additional 35 minutes to process the instrumental analysis. The processing of the data created from these three analyses is on average 20 minutes per case. This process creates three instrument reports that require review and evaluation by the analyst.

The total time that is required to complete a typical blood drug screen is 95 minutes. Consequently the 35 cases received, on average, by the laboratory each week that require blood drug screens will take approximately 55 hours to process. This processing time, of course, only includes the time to complete the case and does not account for instrument checkout and maintenance that must also be completed each week. The result of this is a backlog of cases that carryover from week to week. Backlogged cases increase turnaround and slow the processing and completion of the medical examiner investigation.

The laboratory's current average testing turnaround time can be summarized in this table.

Current average time to complete a single blood screen	95 minutes

Targeted time to complete a blood screen	20 minutes
Current time to complete 35 cases (1 weeks worth)	55 hours
Targeted time to complete 35 cases (1 weeks worth)	12 hours
*Blood screen – average current turnaround time per case	50 days
*Blood screen – targeted turnaround time per case	14 days
**Current case turnaround time	65-75 days
**Targeted case turnaround time	30-40 days

*Turnaround time is measured from date of case receipt to date of final test report
**Turnaround time is measured from date of case receipt to the date of the final case report

A 55 hour period to complete 35 cases is excessive and adds to the overall turnaround time for case completion. This excessive time also impacts all other testing to follow and eventually affects the completion of the medical examiner investigation. The Department is required by the National Association of Medical Examiner accreditation to complete 90% of its cases in 90 days. This includes cases involving toxicological analysis. Unnecessary delays that hinder the Department's ability to meet these criteria should be alleviated. Any steps the Laboratory can take to minimize this delay will help to reduce backlogs and the processing time for the pathologist's case investigation.

PROJECT/PROGRAM DESIGN AND IMPLEMENTATION

The Miami-Dade County Medical Examiner Department (Department) is proposing the utilization of new technology to improve case processing and reduce the turnaround time for the majority of its cases. The Laboratory's approach to routine and comprehensive blood drug screening using GCMS is widely accepted in the postmortem forensic toxicology community.

The drawback with this technology is that it is lengthy in analysis time in order to resolve the hundreds of different drugs and compounds within the analysis and the complexity of the data and the amount of time it takes to completely process it. The system described in this proposal uses the latest improvements in high speed chromatography that combines electronic pressure controlled flow rates with fast temperature ramping of the column oven. This combination speeds up the chromatography and reduces the runtime by two thirds, while at the same time maintaining the separation necessary to properly identify a compound. In addition, this system utilizes a NIST/AMDIS software application developed by the National Institutes of Standards and Technology and modified by Agilent Technologies to deconvolute mass spectral data and search it against a library of at least 800 known compounds in the application in a matter of seconds. AMDIS is capable of isolating searchable spectra from the high chemical background commonly found in postmortem sample extracts analyzed by GCMS. This reduces data processing and reporting by two thirds as compared to the current method.

The proposed plan has been developed based on the instrumentation and application designed by Agilent engineers and scientists to improve the workflow of forensic toxicology laboratories. They have developed a system that pairs improvements in instrument design for high-speed chromatographic separations with software to improve the quality of spectral searching and drug identification. The entire instrument developed by Agilent is called the Toxicology Analyzer. It incorporates other innovations as well such as retention locking to improve run-to-run chromatography consistency and inlet back-flushing to reduce contamination buildup in the injection port of the GC. In addition, the system utilizes a device called a dean's switch to split the chromatographic effluent between a nitrogen specific detector and a mass

spectrometry detector. The resulting data includes both channels (GC-NPD and GC-MS) which improve identification and confidence in the results.

The pitfall with this plan is in how the data is processed. Analysts must be mindful that false negatives can occur if the deconvolution software is unable to isolate and identify spectra from a dirty sample. In addition, if the drug does not exist in the 800 compound library the analyst must review these spectra before deciding if a case is negative. Other routine concerns such as instrument maintenance and the quality of the extracted samples are also important even with this new technology.

The proposed technology has been successfully utilized by high-throughput laboratories to reduce the amount of time required to complete a typical blood screen. The combination of fast high-resolution gas chromatography and mass spectrometry to reduce the runtime from 45 to 10 minutes has become widely accepted in forensic toxicology laboratories in recent years. The utilization of the automated NIST/AMDIS/Agilent deconvolution software application offers a powerful tool to deal with the complexity of data review. This automated process can perform a complete post-run data analysis that has a 98% capture rate and produce a report for the analyst to review. This reduces the data review process from 30 to 10 minutes. In combination, these two features will make substantial improvements in turnaround time for all cases requiring a blood screen.

PROJECT OBJECTIVES

The program design incorporating the new technology will include the following objectives:

1. To implement a comprehensive routine screening technique for blood utilizing GCMS that incorporates a nitrogen phosphorus detector (NPD) in tandem with a mass

spectrometer and high-speed gas chromatography to reduce instrument runtimes to 10 minutes

2. To implement an AMDIS based evaluation of mass spectral data using a deconvolution algorithm and a 800 drug library to detect drugs at low concentrations in complex biological extracts
3. To reduce routine blood drug screens from 95 minutes to 20 minutes
4. To reduce case turnaround times for cases that involve blood drug screening from to from 65-75 days to 30-45 days.

   The reduction in turnaround time for all cases to less than 45 days.

IMPLEMENTATION

The implementation of the program design incorporating the new technology will include the following activities:

1. Purchasing and installing an Agilent Model 7890GC with a 5977A Mass Selective Detector (Forensic Toxicology Analyzer)
2. On-site training conducted by Agilent engineers for all toxicology laboratory scientists in the operation and maintenance of the instrument
3. Implementing and validating the comprehensive general blood drug screen method on the new instrument
4. Implementing the new method to evaluate medical examiner cases
5. Evaluating turnaround time improvement by maintaining records of cases processed using the new method
6. Evaluating the overall improvements in case turnaround for all toxicology cases processed

CAPABILITIES/COMPETENCIES

QUALIFICATIONS AND EXPERIENCE OF PROPOSED PROJECT STAFF

The Toxicology Laboratory of the Miami Dade County Medical Examiner Department, established in 1956, is already at the forefront among Medical Examiner Offices in the state of Florida for its wealth of experience in managing investigations of drug-related deaths and poisonings. The Laboratory's operations are structured on the Forensic Toxicology Laboratory Guidelines established by the Society of Forensic Toxicologists and recognized by the American Board of Forensic Toxicologists (ABFT). The laboratory is accredited by the ABFT. The full time staff includes a Laboratory Director and Assistant Director, nine bench forensic toxicologists and a secretary. They include:

Staff Name, Credentials, Title	Experience
Diane M. Boland, Ph.D., D-ABFT, Laboratory Director	Staff member for 12 years, doctorate in analytical chemistry, expertise in MS applications and solid phase extractions
George W. Hime, M.S., Assistant Laboratory Director	Staff member for 35 years, masters in chemistry, expertise in MS applications
Julio Cofino, M.A., Toxicology III Supervisor	Staff member for 30 years, expertise in chromatographic applications and quantitations
Joe Rein, M.S, Toxicology III Supervisor	Staff member for 30 years, expertise in screening applications
Roger Allard, B.S., Toxicologist II	Staff member for 30 years, expertise in GC and LC quantitative applications
Theresa Hippolyte, M.S., FTS-ABFT, Toxicologist II	Staff member for 12 years, expertise in MS and quantitative applications
Mary Zaney, B.S. FTS-ABFT, Toxicologist II	Staff member for 10 years, expertise in GC and MS screening applications
Joe Kahl, B.S. , Toxicologist I	Staff member for 2 years, expertise in GC and MS screening applications
Wilsa Jean, B.S.., Toxicologist I	Staff member for 1 year
Elisa Shoff, B.S., Toxicologist I	Staff member for 6 months

Jennifer Gonyea, Toxicologist I	New staff member

DEMONSTRATED ABILITY

Currently the Laboratory processes approximately 35,000 tests annually and the team of highly qualified and experienced forensic toxicologists has developed a solid repository of up-to-date knowledge of local and national drug patterns as well as the emergence of new pharmaceuticals. The Laboratory already provides forensic toxicology services to other districts in the state of Florida and is often called up for assistance from outside agencies including federal, state, and local law enforcement. Cases completed by the Laboratory have been studied by epidemiologists and scientists from various academic institutions; the Centers for Disease Control; and the law enforcement agencies such as the Florida Department of Law Enforcement, Federal Bureau of Investigations and United States Drug Enforcement Agency.

In 2008, the Miami-Dade County Medical Examiner Department was successful in obtaining a competitive Paul Coverdell Forensic Science Improvement Grant in the amount of $95,000 for an "Automated Screening of Body Fluids for Drugs and Poisons" project. The grant helped with the purchase of new technology that is currently being used and continues to provide invaluable results in the routine screening of drugs in human fluids. The Laboratory would not have been able to acquire the technology at the time without the support of the grant. In 2010, the department submitted a grant to USDOJ under the Forensic Science Training Development and Delivery Program but was not selected for a grant award. In 2012 the department was again successful in obtaining a competitive Paul Coverdell Forensic Science Improvement Grant in the amount of $175,000 for a "Detection of Designer Drugs and Potent Complex Pharmaceuticals in Death Investigations" project. The grant helped with the purchase of new technology that has

made significant improvements in the Laboratory's ability to screen postmortem samples for new abused drugs. The Laboratory would not have been able to acquire this technology at the time without support of the grant.

RELATIONSHIP BETWEEN CAPABILITIES/COMPETENCIES AND PROJECT

The grant will allow for at least two or more forensic toxicologists to be fully trained by the vendor in the operation and maintenance of the new technology. Product warranties and troubleshooting is also included in the contract. In addition the vendor has also included applications support and consulting as well as on-site assistance if needed. The program design requires that all forensic toxicologists to become trained and be able to utilize the new technology properly to process cases. All staff will understand the project design and corresponding objectives. The analytical method will be implemented based on successful methods developed in-house and by other peer-reviewed research published by forensic toxicologists. All staff will be responsible for implementing the proposed plan and collecting the required data in each investigation. The Laboratory Director and Assistant Director will provide program oversight and will monitor the results using the prescribed performance measures.

IMPACT/OUTCOMES AND EVALUATION/PLAN FOR COLLECTING DATA FOR PERFORMANCE MEASURES

The impact/outcomes for the project include:

1. Improved throughput and reduced turnaround time for blood screens

The proposed instrument's ability to process samples in a tenth of the time than is currently required, as well as to automate the processing of data and reporting, will make a significant difference in the Laboratory's ability to process cases in a shorter time. This reduction in

turnaround time will not only reduce the time to complete the cases overall, it will also improve laboratory workflow by enabling follow-up testing assignments to be made sooner and will provide crucial information to the investigating medical examiners quicker. The overall improvement will reduce average case turnaround from 60-70 days to 30-40 days.

2. Improved excellence in the quality of the results

Utilizing GCMS in the initial screening process is the acceptable standard of practice in forensic toxicology laboratories. Traditionally spectral data required the user to evaluate each scan in an entire run to identify drugs or other important compounds. This is a tedious process requiring the user to carefully subtract out the background at each scan to optimize the resulting spectra for library searching. With well-developed automated software, the computer can perform this task throughout the entire run requiring the operator to review and inspect only the minimal data prior to reporting. The results are of a better quality and much more thorough. Completing the screening faster will improve follow-up testing of targeted compounds; especially for compounds that might likely degrade over time. The reduction in time will reduce costs and labor dedicated to this task. This will enable staff to focus more of their time in improving other methods and procedures.

3. Reduced Cost of Materials

An overall decrease in processing time and in tests performed will ultimately result in the reduction in supplies including chemicals and costly instrument consumables. Costly items such as inlet liners and columns that would ordinarily need replacement on three instruments will now only require replacement on one instrument. This should impact laboratory costs for this category by 30%.

The evaluation plan for collecting data for performance measures is something that is already standard practice at the Miami-Dade Medical Examiner Department. In fact, the department already participates in the County's ASE (Active Strategies Enterprise) system which tracks performance measures for every County department. However, the effectiveness and success of this project will be evaluated by collecting the following data by the Laboratory:

Objective	Performance Measure	Data Grantee Provides
To improve the quality and timeliness of forensic toxicology analysis and substantially reduce case backlog	Reduce turnaround time from 60-70 days to 30-45 days Increase the percentage of cases completed in 90 days to 90% or better to meet NAME accreditation standards (80-90%) Reduce costs of equipment supplies and materials	Number of backlogged cases at the beginning and end of the grant period Number of cases successfully completed as a result of the new technology and testing protocol Average number of days to process a case at the beginning and end of the grant period Document percentage of costs reductions for key supplies by monitoring and comparing current and past operating budget and expenditures for supplies

OTHER/PART 1 VIOLENT CRIMES DATA

Average annual number of Part I Violent Crimes reported by the Federal Bureau of Investigation for Miami-Dade County and Florida for calendar years 2010, 2011, and 2012 are as follows:

Total Part 1 - Violent Crimes

	JAN-DEC 2012	JAN-DEC 2011	JAN-DEC 2010
Miami-Dade County	130,865	138,109	136,585
STATE (Florida)	725,944	769,480	770,518

Budget Detailed Worksheet

A. Personnel

Name/Position	Computation Amount per unit	(define unit)	# units	# Individuals		Cost
N/A						$0.00
					TOTAL	$0.00

B. Fringe Benefits

	Amount of Personnel for basis		% of Amount of Personnel	Additional computation (optional)		
N/A						$0.00
					TOTAL	$0.00

Total Personnel & Fringe Benefits $0.00

C. Travel

Purpose of Travel	Location	Item	Cost	# Individuals	# Nights/Days	# Trips	Cost
N/A							$0.00
							$0.00
							$0.00
						TOTAL	$0.00

D. Equipment

Item	Computation Cost per Unit	# Units	Cost
G3445B - 7890 Series gas chromatograph package includes; 198-231V oven Inert split/splitless capillary inlet; NPD detector; EPC; DRS Toxicology Analyzer with NPD software	*$38,783.00*	*1*	$38,783.00
G7043AA - 5977A Mass Selective Detector package includes: Extractor source; Data system; Performance Turbo Pump; G1710FA data analysis license; Extractor EI source	*$77,339.00*	*1*	$77,339.00
G3397B - Ion Gauge kit for mass spectrometer	*$1,686.00*	*1*	$1,686.00
G4513A - 7693A Autoinjector and G4514A - 7693 Autoinjector tray to accommodate 150 vials	*$14,331.00*	*1*	$14,331.00
G1033A Mass Spectral reference libraries & software; G1716AA Deconvolution & reporting software; G1674AA Forensic toxicology RTL library	*$9,247.20*	*1*	$9,247.20
		TOTAL	$141,386.20

E. Supplies

Supply Items	Computation Cost per unit		# Units		Cost
					$0.00
				TOTAL	$0.00

F. Construction

Purpose	Description of Work		Cost
N/A			$0.00
		TOTAL	$0.00

G. Consultants/Contracts

Consultant Fee:

Name of Consultant	Service Provided	Computation Cost per unit	(define unit)	# Units		Cost
						$0.00
					Subtotal	$0.00

Consultant Expenses:

Item	Location	Computation: Cost per unit	(define unit)	# Units	Individual Cost
					$0.00
				Subtotal	$0.00

Contracts:

Item	Vendor	Service Provided	Cost
		Subtotal	$0.00

CONSULTANTS/ CONTRACTS TOTAL $0

H. Other Costs

Description	Computation: Cost per unit	(define unit)	# Units	Cost
Shipping, installation, training for extra hardware	$2,188.20		1	$2,188.20
Applications consulting and on-site assistance	$12,400.00		1	$12,400.00
3-year warranty for service support, emergency repairs and applications support	$18,659.52		1	$18,659.52
				$0.00
				$0.00
			TOTAL	$33,247.72

I. Indirect Cost

Description	Computation		Cost
	$0.00	0%	$0.00
			$0.00
		TOTAL	$0.00

Budget Summary

Budget Category	Amount
A. Personnel	$0.00
B. Fringe Benefits	$0.00
C. Travel	$0.00
D. Equipment	$141,386.20
E. Supplies	$0.00
F. Construction	$0.00
G. Consultants/Contracts	$0.00
H. Other	$33,247.72
Total Direct Costs	$174,633.92
I. Indirect Costs	$0.00
TOTAL PROJECT COSTS	$174,633.92
Federal Request	$174,634
Non-Federal Amount	$0.00

BUDGET NARRATIVE

The total cost of the project is $174,634 and includes the hardware, software/data system, shipping, installation, training and extended warranty for 3 years. The total amount requested through the grant is $174,634.

The immediate and long-term benefits of the investment to obtain the new technology will be invaluable. It has been the experience of the laboratory that the life-span of this type of technology is approximately 10 years. Manufacturer's technical and application support typically continues for a minimum of 8 years from the last date of manufacturing of an instrument model. It has been the experience of the laboratory that the instrument turn-over has never been less than 10-12 years which negates the benefits of lease purchases that typically last for five years and is meant to replace instruments with newer technology in a shorter period of time. Cost savings will be realized in other areas such as the overall decrease in maintenance time and costs (estimated - 35%) for the instrument in comparison with the current system. Instrument features (column back-flushing, Dean's switch) that reduce routine pre-run service and consumable replacements will save in operator time and materials. Expensive chromatography columns, inlet liners, and seals will be replaced less often reducing operating costs by at least 30% (the use of one column versus three currently) over what is currently experienced.

The cost effectiveness will also be realized in the marked increase in productivity and the quality of the results. Automated processing with the deconvolution software allows the data to be reviewed by the computer, spectra matched to the best library entry, and reported in a easy-to-read format that will reduce the operator's time in reviewing the results. This is a labor cost savings which will allow staff scientists more time to spend on other more significant analytical

problems. This system will allow the current staff to manage more work in less time while improving case turnaround time and reduce a backlog cases.

The total cost for new technology that includes equipment, shipping, installation, check-out, training and two additional years of warranty is $174,633.92.

1. **Personnel:** Thee will be no personnel costs charged to the grant
2. **Fringe Benefits:** There will be no fringe benefits charged to the grant
3. **Travel:** There will be no travel costs charged to the grant. The Laboratory has negotiated a total cost for the system that includes on-site training and applications support for the new technology
4. **Equipment:** The total equipment cost for which grant support is requested is $141,386.20 and includes the following:

Product G3445B - 7890 Series gas chromatograph package includes: 198-231V oven; Inert; split/splitless capillary inlet; NPD detector; EPC; DRS Toxicology Analyzer with NPD software for $38,783. The 7890 model GC is the latest version. The 220V specification provides faster temperature ramps to shorten run times from 45 to 10 min which is optimal for the application proposed. The NPD detector will be used simultaneously with the MS to improve identification. The EPC is electronic pressure control to facilitate the inlet back-flushing and dean's switch, both essential components of the application.

Product G7043AA - 5977A Mass Selective Detector package includes: Extractor EI source; Data system; Performance Turbo Pump; G1710FA data analysis license and Extractor EI source for $77,339. This is the mass spectrometer (MS) portion of the instrument and will utilize the Agilent extractor type ion source to improve signal strength and sensitivity. This

package includes the data system as well as the performance turbo pump vacuum system. All essential to the operation and the application proposed.

Product G3397B Ion Gauge kit for mass spectrometer will be purchased for $1,686. The ion gauge kit allows for the proper measurement of the high vacuum in the manifold. Monitoring the vacuum enables better troubleshooting and provides a more accurate status of the condition of the manifold.

Product G4513A, 7693 Autoinjector, and **Product G4514A**, 7693 Autoinjector tray to accommodate 150 vials, will be purchased for $14,331. The auto-injector is an automated function so that analyses can be performed unattended. This includes a 150 vial tray to maximize the number of samples being analyzed. This improves the efficiency of the system and the throughput.

Products G1033A, Mass Spectral reference libraries and software; **G1716AA,** Deconvolution and reporting software, and **G1674AA** Forensic toxicology RTL library will be purchased for $9,247.20. The software is the heart of the data processing functions of the instrument. Libraries are used to efficiently compare spectra to make identifications. These libraries contain over 500,000 known compounds. The deconvolution software is essential to the application and provides an efficient process to analyze the data.

5. **Supplies:** There will be no supply costs charged to the grant. In fact the grant will help the Laboratory save money in consumable supplies which are reduced due to the new technology.
6. **Construction:** There will be no construction costs charged to the grant.

7. **Consultants/Contracts:** There will be no consultant/contracts charged to the grant. The Miami-Dade Medical Examiner Department is handling the acquisition and selection of the new technology based on the County's official procurement policy and procedures.

8. **Other costs:**

Shipping, installation, training for extra hardware	$2188.20
Applications consulting and on-site assistance from vendor	$12,400.00
3-year warranty for service support, emergency repairs and applications support	$18,659.52
TOTAL OTHER COSTS	$33,247.20

PLAN FOR COLLECTING THE DATA REQUIRED FOR THIS SOLICITATION'S PERFORMANCE MEASURES

As a previous grantee under the Paul Coverdell Forensic Science Improvement Grants Program, the Miami-Dade County Medical Examiner (MDME) has in place a data tracking program called CME/LIMS. It manages all cases processed by the Department along with the laboratory results. The laboratory data tracked provides the necessary details to compute turnaround time, processing time, backlog, and reporting time for each test completed. Data is entered into CME/LIMS on a daily basis by analysts. This data will provide the required information to determine the turnaround time for all cases processed with the new technology.

The staff toxicologist will document all data associated with the proposed performance measures resulting from the use of the new technology (GCMS) in death investigations involving drugs/poisons. Project staff will maintain accurate records of all tests performed using the new protocol. The data collected will be entered CME/LIMS for tracking and monitoring. The data collected to summarize success will include: number of backlogged cases at the beginning and end of the grant period; number of cases successfully completed as a result of the new technology and testing protocol; and the average number of days to process a case at the beginning and end of the grant period.

Project staff will monitor the operating budget and expenditures for routine supplies used in the project to verify reductions in key supply costs; they will provide final reports to the medical examiners to complete cases; and they will report findings in scientific literature and/or present at scientific meetings.

1) Solicitation's Objective: To improve the quality and timeliness of forensic toxicology analysis and substantially reduce case backlog

A) **Solicitation's Performance Measure(s):** Reduction in the average number of days from the submission of a sample to a forensic science laboratory to the delivery of test results to a requesting office or agency.

- **Outcome Measure:** Reduce turnaround time from 60-70 days to 30-45 days

B) **Solicitation's Required Performance Measure(s):** Percent reduction in the number of backlogged forensic cases.

- **Outcome Measure:** Increase the percentage of cases completed in 90 days to 90% or better to meet NAME accreditation standards (80-90%)

C) **Performance Measure/Outcome Measure:** Reduce costs of equipment supplies and materials

- **Outcome measure:** Decrease costs associated with the operation and maintenance of tests processed new technology by 50%

Data Provided by Grantee:

i. Number of backlogged cases at the beginning and end of the grant period

ii. Number of cases successfully completed as a result of the new technology and testing protocol

iii. Document percentage of costs reductions for key supplies by monitoring and comparing current with past operating budget and expenditures for supplies

FY 2014 Coverdell Forensic Science Improvement Grants Program

Attachment: External Investigations

The "Certification as to External Investigations" that is submitted on behalf of the applicant agency as part of this application certifies that—

> A government entity exists and an appropriate process is in place to conduct independent external investigations into allegations of serious negligence or misconduct substantially affecting the integrity of the forensic results committed by employees or contractors of any forensic laboratory system, medical examiner's office, coroner's office, law enforcement storage facility, or medical facility in the State that will receive a portion of the grant amount.

Prior to receiving funds, the applicant agency (that is, the agency applying directing to the National Institute of Justice) must provide—for each forensic laboratory system, medical examiner's office, coroner's office, law enforcement storage facility, or medical facility that will receive a portion of the grant amount—the name of the "government entity" (or entities) that forms the basis for the certification. Please use the template below to provide this information. (Applicants may adapt this template if necessary, but should ensure that the adapted document provides all required information.)

IMPORTANT NOTE: If necessary for accuracy, list more than one entity with respect to each intended recipient of a portion of the grant amount. For example, if no single entity has an appropriate process in place with respect to allegations of serious negligence as well as serious misconduct, it will be necessary to list more than one entity. Similarly, if no single entity has an appropriate process in place with respect to allegations concerning contractors as well as employees, it will be necessary to list more than one entity.

Additional guidance regarding the "Certification as to External Investigations" appears in the "Eligibility" section of the program announcement for the FY 2014 Coverdell program.

Name of Applicant Agency (including Name of State or Unit of Local Government):

Miami-Dade County Medical Examiner Department

Date: March 25, 2014

Name of any forensic laboratory system, medical examiner's office, coroner's office, law enforcement storage facility, or medical facility that will receive a portion of the grant amount	Existing government entity (entities) with an appropriate process in place to conduct independent external investigations
1. Miami-Dade County Medical Examiner	Florida Department of Law Enforcement (FDLE)
	Miami-Dade County Office of Inspector General
2.	

U.S. DEPARTMENT OF JUSTICE
OFFICE OF JUSTICE PROGRAMS
NATIONAL INSTITUTE OF JUSTICE

FY 2014 Coverdell Forensic Science Improvement Grants Program

Certification as to Plan for Forensic Science Laboratories—
Application from a **Unit of Local Government**

On behalf of the applicant agency named below, I certify the following to the National Institute of Justice, Office of Justice Programs, U.S. Department of Justice:

> This unit of local government has developed a plan for forensic science laboratories under a program intended to improve the quality and timeliness of forensic science or medical examiner services provided by the laboratories operated by the applicant unit of local government and any other government-operated laboratories within the State that will receive a portion of the grant amount.

I acknowledge that a false statement in this certification or in the grant application that it supports may be the subject of criminal prosecution, including under 18 U.S.C. § 1001 and 42 U.S.C. § 3795a. I also acknowledge that Office of Justice Programs grants, including certifications provided in connection with such grants, are subject to review by the Office of Justice Programs and/or by the Department of Justice's Office of the Inspector General.

I have authority to make this certification on behalf of the applicant agency (that is, the agency applying directly to the National Institute of Justice).

Signature of Certifying Official

Genaro "Chip" Iglesias
Printed Name of Certifying Official

Deputy Mayor
Title of Certifying Official

Miami-Dade County Medical Examiner Department
Name of Applicant Agency
(Including Name of Unit of Local Government)

4/1/14
Date

U.S. DEPARTMENT OF JUSTICE
OFFICE OF JUSTICE PROGRAMS
NATIONAL INSTITUTE OF JUSTICE

FY 2014 Coverdell Forensic Science Improvement Grants Program

Certification as to Generally Accepted Laboratory Practices and Procedures

On behalf of the applicant agency named below, I certify the following to the National Institute of Justice, Office of Justice Programs, U.S. Department of Justice:

> Any forensic science laboratory system, medical examiner's office, or coroner's office in the State, including any laboratory operated by a unit of local government within the State, that will receive any portion of the grant amount uses generally accepted laboratory practices and procedures, established by accrediting organizations or appropriate certifying bodies.

I acknowledge that a false statement in this certification or in the grant application that it supports may be the subject of criminal prosecution, including under 18 U.S.C. § 1001 and 42 U.S.C. § 3795a. I also acknowledge that Office of Justice Programs grants, including certifications provided in connection with such grants, are subject to review by the Office of Justice Programs and/or by the Department of Justice's Office of the Inspector General.

I have authority to make this certification on behalf of the applicant agency (that is, the agency applying directly to the National Institute of Justice).

Signature of Certifying Official

Genaro "Chip" Iglesias
Printed Name of Certifying Official

Deputy Mayor
Title of Certifying Official

Miami-Dade County Medical Examiner Department
Name of Applicant Agency
(Including Name of State or Unit of Local Government)

4/1/14
Date

U.S. DEPARTMENT OF JUSTICE
OFFICE OF JUSTICE PROGRAMS
NATIONAL INSTITUTE OF JUSTICE

FY 2014 Coverdell Forensic Science Improvement Grants Program

Certification as to Use of Funds for New Facilities

On behalf of the applicant agency named below, I certify the following to the National Institute of Justice, Office of Justice Programs, U.S. Department of Justice:

> The amount of the grant (if any) used for the costs of any new facility or facilities to be constructed as part of a program to improve the quality and timeliness of forensic science and medical examiner services will not exceed the limitations set forth at 42 U.S.C. § 3797m(c) and summarized in the FY 2014 Coverdell Forensic Science Improvement Grants Program Announcement.

I acknowledge that a false statement in this certification or in the grant application that it supports may be the subject of criminal prosecution, including under 18 U.S.C. § 1001 and 42 U.S.C. § 3795a. I also acknowledge that Office of Justice Programs grants, including certifications provided in connection with such grants, are subject to review by the Office of Justice Programs and/or by the Department of Justice's Office of the Inspector General.

I have authority to make this certification on behalf of the applicant agency (that is, the agency applying directly to the National Institute of Justice).

Signature of Certifying Official

Genaro "Chip" Iglesias
Printed Name of Certifying Official

Deputy Mayor
Title of Certifying Official

Miami-Dade County Medical Examiner Department
Name of Applicant Agency
(Including Name of State or Unit of Local Government)

4/1/14
Date

U.S. DEPARTMENT OF JUSTICE
OFFICE OF JUSTICE PROGRAMS
NATIONAL INSTITUTE OF JUSTICE

FY 2014 Coverdell Forensic Science Improvement Grants Program

Certification as to External Investigations

On behalf of the applicant agency named below, I certify the following to the National Institute of Justice, Office of Justice Programs, U.S. Department of Justice:

> A government entity exists and an appropriate process is in place to conduct independent external investigations into allegations of serious negligence or misconduct substantially affecting the integrity of the forensic results committed by employees or contractors of any forensic laboratory system, medical examiner's office, coroner's office, law enforcement storage facility, or medical facility in the State that will receive a portion of the grant amount.

I personally read and reviewed the section entitled "Eligibility" in the Fiscal Year 2014 program announcement for the Coverdell Forensic Science Improvement Grants Program. I acknowledge that a false statement in this certification or in the grant application that it supports may be the subject of criminal prosecution, including under 18 U.S.C. § 1001 and 42 U.S.C. § 3795a. I also acknowledge that Office of Justice Programs grants, including certifications provided in connection with such grants, are subject to review by the Office of Justice Programs and/or by the Department of Justice's Office of the Inspector General.

I have authority to make this certification on behalf of the applicant agency (that is, the agency applying directly to the National Institute of Justice).

Signature of Certifying Official

Genaro "Chip" Iglesias
Printed Name of Certifying Official

Deputy Mayor
Title of Certifying Official

Miami-Dade County Medical Examiner Department
Name of Applicant Agency
(Including Name of State or Unit of Local Government)

4/1/14
Date

APPLICANT DISCLOSURE OF PENDING APPLICATIONS

Miami-Dade County Medical Examiner Department does not have any pending applications for federally funded assistance that include requests for funding to support the same project being proposed under this solicitation and will cover the identical cost items outlined in the budget narrative and worksheet in the application under this solicitation's application.

OMB APPROVAL NO. 1121-0140
EXPIRES 06/30/2009

STANDARD ASSURANCES

The Applicant hereby assures and certifies compliance with all applicable Federal statutes, regulations, policies, guidelines, and requirements, including OMB Circulars A-21, A-87, A-102, A-110, A-122, A-133; Ex. Order 12372 (intergovernmental review of federal programs); and 28 C.F.R. pts. 66 or 70 (administrative requirements for grants and cooperative agreements). The applicant also specifically assures and certifies that:

1. It has the legal authority to apply for federal assistance and the institutional, managerial, and financial capability (including funds sufficient to pay any required non-federal share of project cost) to ensure proper planning, management, and completion of the project described in this application.

2. It will establish safeguards to prohibit employees from using their positions for a purpose that constitutes or presents the appearance of personal or organizational conflict of interest, or personal gain.

3. It will give the awarding agency or the General Accounting Office, through any authorized representative, access to and the right to examine all paper or electronic records related to the financial assistance.

4. It will comply with all lawful requirements imposed by the awarding agency, specifically including any applicable regulations, such as 28 C.F.R. pts. 18, 22, 23, 30, 35, 38, 42, 61, and 63, and the award term in 2 C.F.R. § 175.15(b).

5. It will assist the awarding agency (if necessary) in assuring compliance with section 106 of the National Historic Preservation Act of 1966 (16 U.S.C. § 470), Ex. Order 11593 (identification and protection of historic properties), the Archeological and Historical Preservation Act of 1974 (16 U.S.C.§ 469 a-1 et seq.), and the National Environmental Policy Act of 1969 (42 U.S.C. § 4321).

6. It will comply (and will require any subgrantees or contractors to comply) with any applicable statutorily-imposed nondiscrimination requirements, which may include the Omnibus Crime Control and Safe Streets Act of 1968 (42 U.S.C. § 3789d); the Victims of Crime Act (42 U.S.C. §10604(e)); The Juvenile Justice and Delinquency Prevention Act of 2002 (42 U.S.C. § 5672(b)); the Civil Rights Act of 1964 (42 U.S.C. § 2000d); the Rehabilitation Act of 1973 (29 U.S.C. §7 94); the Americans with Disabilities Act of 1990 (42 U.S.C.§ 12131-34); the Education Amendments of 1972 (20 U.S.C. §§1681, 1683, 1685-86); and the Age Discrimination Act of 1975 (42 U.S.C. §§ 6101-07); *see* Ex. Order 13279 (equal protection of the laws for faith-based and community organizations).

7. If a governmental entity–

a) it will comply with the requirements of the Uniform Relocation Assistance and Real Property Acquisitions Act of 1970 (42 U.S.C.§ 4601 et seq.), which govern the treatment of persons displaced as a result of federal and federally-assisted programs; and

b) it will comply with requirements of 5 U.S.C.§§ 1501-08 and §§7324-28, which limit certain political activities of State or local government employees whose principal employment is in connection with an activity financed in whole or in part by federal assistance.

Signature Date

4/1/14
Date

DISCLOSURE OF LOBBYING ACTIVITIES

Approved by OMB 0348-0046

Complete this form to disclose lobbying activities pursuant to 31 U.S.C. 1352
(See reverse for public burden disclosure.)

1. Type of Federal Action:
[b] a. contract
b. grant
c. cooperative agreement
d. loan
e. loan guarantee
f. loan insurance

2. Status of Federal Action:
[a] a. bid/offer/application
b. initial award
c. post-award

3. Report Type:
[a] a. initial filing
b. material change
For Material Change Only:
year _____ quarter _____
date of last report _____

4. Name and Address of Reporting Entity:
[✓] Prime [ ] Subawardee
Tier _____, *if known*:
Miami-Dade County (Medical Examiner Department)
1 Bob Hope Road
Miami, Florida 33136
Congressional District, *if known*: 24

5. If Reporting Entity in No. 4 is a Subawardee, Enter Name and Address of Prime:
Congressional District, *if known*:

6. Federal Department/Agency:
U.S. Department of Justice
Office of Justice Programs
National Institute of Justice

7. Federal Program Name/Description:
Paul Coverdell Forensic Science Improvement Grants Program
CFDA Number, *if applicable*: 16.742

8. Federal Action Number, *if known*:

9. Award Amount, *if known*:
$

10. a. Name and Address of Lobbying Registrant (*if individual, last name, first name, MI*):
Akerman Senterfitt LLP
750 9th Street, N.W., Suite 750
Washington, DC 20001

b. Individuals Performing Services (*including address if different from No. 10a*) (*last name, first name, MI*):
Sargent, Jane

11. Information requested through this form is authorized by title 31 U.S.C. section 1352. This disclosure of lobbying activities is a material representation of fact upon which reliance was placed by the tier above when this transaction was made or entered into. This disclosure is required pursuant to 31 U.S.C. 1352. This information will be reported to the Congress semi-annually and will be available for public inspection. Any person who fails to file the required disclosure shall be subject to a civil penalty of not less that $10,000 and not more than $100,000 for each such failure.

Signature: _____
Print Name: Genaro "Chip" Iglesias
Title: Deputy Mayor
Telephone No.: (305) 375-5071 Date: 3/25/2014

Federal Use Only:

Authorized for Local Reproduction
Standard Form LLL (Rev. 7-97)

Memorandum

MIAMI-DADE COUNTY

Date: August 1, 2011

To: Deputy Mayors

From: Carlos A. Gimenez
Mayor

Subject: 2011 Signature Authority

Effective immediately, you are authorized to sign the following items for your respective departments on my behalf:

- Permits
- Senior Management Performance Appraisal Forms
- Leave slips (your departments and your immediate staff)
- Travel requests except for international and legislation-related travels, as well as trips with multiple travelers (unless grant funded)
- Telecommunications Device and Service Requests
- Vehicle requests
- Grant Applications

Your judgment is crucial when reviewing items for signature. Please submit requests for administrative leave and executive salary reviews to me for consideration. If an item is controversial, sensitive or otherwise significant, please forward it to my attention or discuss it with me personally.

Thank you for your cooperation.

Genaro "Chip" Iglesias
Deputy Mayor/Chief of Staff

Alina T. Hudak
Deputy Mayor/County Manager

Jack Osterholt
Deputy Mayor

Edward Marquez
Deputy Mayor

Lisa M. Martinez
Senior Advisor to the Mayor

RUSSELL BENFORD
Deputy Mayor

c: Mary Lou Rizzo, Director, Human Resources Department
Jennifer Moon, Director, Office of Management and Budget
Angel Petisco, Director, Enterprise Technology Services Department
Office of the Mayor Senior Staff
Office of the Mayor Senior Secretaries

Agilent Technologies

Quotation

George Hime
Assistant Director, Toxicology Lab
Miami Dade County
Medical Examiner Dept
1 Bob Hope Rd
MIAMI FL 33136

Quote No.	Create Date	Delivery Time	Page
1579790	03/31/2014	2 Weeks	1 of 6

Contact	Phone no.	Valid to
Linda Schuchler	678-566-6198	05/30/2014

To place an order: Call 1-800-227-9770 Option 1
For Instruments Fax : 302-633-8953
For Consumables Fax : 302-633-8901
Email : LSCAinstrumentsales@agilent.com
For Genomics Fax: 512-321-3128
Email : orders@agilent.com
For additional instructions, see last page

Product/Description	Qty/Unit	Unit List Price	Discount Amount	Extended Net Price
G3445B 7890 Series GC for Analyzers	1.000 EA	15,402.00 USD		15,402.00
With the following configuration: Ship-to Country : USA Country of Origin : United States 198 to 231V fast oven power supply				
INERT Cap S/SL Inlet with EPC-100psi	1 EA	4,425.00 USD		4,425.00
Capillary NPD with Bios Bead, EPC	1 EA	4,394.00 USD		4,394.00
GC/MSD Toxicology DRS Analyzer w. NPD	1 EA	14,562.00 USD		14,562.00
Installation (44K) Familiarization at Installation (44L)				
		Item Total		38,783.00
G7043AA Agilent 5977A Extractor MSD with Data System, Performance Turbo Pump, additional G1710FA Data Analysis License and Extractor (Xtr) EI Source.	1.000 EA	77,339.00 USD		77,339.00
With the following configuration: Specials SP1 : Specials SP1 Selected Ship-to Country : USA Select MassHunter Familiarization Installation (44K) Familiarization at Installation (44L) 1 Year Phone Assist (44W)				
		Item Total		77,339.00

Agilent Technologies

Quotation

Quote No.	Create Date	Delivery Time	Page
1579790	03/31/2014	2 Weeks	2 of 6

Contact	Phone no.	Valid to
Linda Schuchler	678-566-6198	05/30/2014

To place an order: Call 1-800-227-9770 Option 1
For Instruments Fax : 302-633-8953
For Consumables Fax : 302-633-8901
Email : LSCAinstrumentsales@agilent.com
For Genomics Fax: 512-321-3128
Email : orders@agilent.com

George Hime
Assistant Director, Toxicology Lab
Miami Dade County
Medical Examiner Dept
1 Bob Hope Rd
MIAMI FL 33136

Product/Description	Qty/Unit	Unit List Price	Discount Amount	Extended Net Price
G3397B Ion Gauge Kit for 5977 MSD.	1.000 EA	**1,686.00 USD**		**1,686.00**
With the following configuration: Ship-to Country : USA				
Installation (44K)	1 EA	562.00 USD		562.00
		Item Total		**2,248.00**
G4513A 7693A Autoinjector Includes transfer turret, 16-sample turret, mounting post, parking post for GC. 10ul syringe, and solvent bottles. 100% higher sample capacity than G2913A.	1.000 EA	**6,540.00 USD**		**6,540.00**
With the following configuration: Ship-to Country : USA				
Installation (44K)	1 EA	318.00 USD		318.00
Familiarization at Installation (44L)	1 EA	219.00 USD		219.00
		Item Total		**7,077.00**

Agilent Technologies

Quotation

Quote No.	Create Date	Delivery Time	Page
1579790	03/31/2014	2 Weeks	3 of 6

Contact	Phone no.	Valid to
Linda Schuchler	678-566-6198	05/30/2014

To place an order: Call 1-800-227-9770 Option 1
For Instruments Fax : 302-633-8953
For Consumables Fax : 302-633-8901
Email : LSCAinstrumentsales@agilent.com
For Genomics Fax: 512-321-3128
Email : orders@agilent.com

George Hime
Assistant Director, Toxicology Lab
Miami Dade County
Medical Examiner Dept
1 Bob Hope Rd
MIAMI FL 33136

Product/Description	Qty/Unit	Unit List Price	Discount Amount	Extended Net Price
G4514A 7693 Tray, 150 vial includes three removable 50-vial racks and GC mounting bracket. 50% higher sample capacity than G2614A.	1.000 EA	7,791.00 USD		7,791.00
With the following configuration: Ship-to Country : USA				
Installation (44K)	1 EA	435.00 USD		435.00
Familiarization at Installation (44L)	1 EA	219.00 USD		219.00
		Item Total		**8,445.00**
H2149A Chemical Analysis Application Consulting Provides on-site assistance. For consulting, training, documentation and implementation services. Requires option.	1.000 EA			
With the following configuration: Ship-to Country : USA				
Five Day On-site (Includes Travel)	1 EA	12,400.00 USD		12,400.00
		Item Total		**12,400.00**

Agilent Technologies

Quotation

Quote No.	Create Date	Delivery Time	Page
1579790	03/31/2014	2 Weeks	4 of 6

Contact	Phone no.	Valid to
Linda Schuchler	678-566-6198	05/30/2014

To place an order: Call 1-800-227-9770 Option 1
For Instruments Fax : 302-633-8953
For Consumables Fax : 302-633-8901
Email : LSCAinstrumentsales@agilent.com
For Genomics Fax: 512-321-3128
Email : orders@agilent.com

George Hime
Assistant Director, Toxicology Lab
Miami Dade County
Medical Examiner Dept
1 Bob Hope Rd
MIAMI FL 33136

Product/Description	Qty/Unit	Unit List Price	Discount Amount	Extended Net Price
SYS-GM-5977T GCMS 5977 Turbo System	1.000 EA			
Advantage Silver 3 years total	1 EA	20,064.00 USD	1,404.48-	18,659.52
		Item Total		**18,659.52**
Promotion discount of 7.00% is applied based upon conditions which can be reviewed on request.				
G1033A NIST 2011 MS Library Bundle includes 243k spectra with names, chemical structures, and retention indices. Includes MS/MS Spectra Lib, NIST search and AMDIS programs.	1.000 EA	**5,037.00 USD**	**1,007.40-**	**4,029.60**
With the following configuration: Ship-to Country : USA				
Installation (44K)	1 EA	544.00 USD	108.80-	435.20
		Item Total		**4,464.80**

Special discount of 20.00 % is applied.

Agilent Technologies

Quotation

Quote No.	Create Date	Delivery Time	Page
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George Hime
Assistant Director, Toxicology Lab
Miami Dade County
Medical Examiner Dept
1 Bob Hope Rd
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G1716AA Deconvolution and Reporting SW. Is an add-on SW to G1701EA MSD ChemStation. Requires but does not include G1701EA E.02 or greater, and NIST D.05.02/AMDIS 2.65 or greater. Inst. and Fam. is not included.	1.000 EA	2,833.00 USD	566.60-	2,266.40
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Improved Forensic Toxicology Screening Using A GC/MS/NPD System with a 725-Compound DRS Database

Application

Forensic Toxicology

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Abstract

Laboratories that perform toxicology screens are challenged by the requirement to look for large numbers of target compounds in samples that contain complex matrix interferences. GC/MS methods are widely used and accepted for this analysis. Full-scan EI methods offer many advantages for broad-range screening, such as unlimited numbers of targets, full-spectrum identity confirmation, and library searching for identification of nontargets. With recent advances in GC/MS technology, there are several opportunities to substantially increase the number of targets screened for and simultaneously reduce the time required per sample.

With the system described here, samples are screened for 725 compounds using Agilent's G1674AA Forensic Toxicology DBL. Data review time is substantially reduced using Agilent Deconvolution Reporting Software. Post-run bakeout of heavy-matrix compounds is replaced with column backflushing, which is faster and reduces system maintenance. Run time is reduced by using a fast GC run (9.75 min injection to injection) and simultaneously collecting scan, SIM, and NPD data. The scan data is deconvoluted and used to identify any of the 725 target compounds. SIM data is used to look for select low-level compounds not detectable in scan mode. The nitrogen response of the NPD is used to highlight nontarget nitrogen compounds and identity confirmation and can be used for quantitation if needed. Using extracts of whole blood samples, the system finds all the compounds detected by the conventional method in significantly less time.

Introduction

GC/MS screening methods play an important role in the toxicology laboratory. With the continuing emergence of new drugs and toxins, the list of target compounds to be screened can easily number in the hundreds. For those compounds that are compatible with GC, GC/MS in full-scan mode with electron impact ionization (EI) is well suited for the task. The technique offers several advantages:

- It uses straightforward, reliable, and familiar instrumentation.
- Any number of targets can be monitored.
- The target list is not limited by the number of MRMs like MS/MS techniques.
- Years later, archived full-scan data can be examined for new targets.
- Identity confirmation is based on full spectra.
- Nontarget unknown compounds can be identified by searching spectra against NIST and other industry standard libraries.
- Ionization suppression due to matrix is much less of a problem than with LC/MS techniques.

While GC/MS methods offer the above advantages, there are limitations with the conventional approach. As the number of target compounds in the screen increases, the size of tasks involved in the development, maintenance, and application of the methods grows very rapidly. These considerations often limit the scope of screening methods used in toxicology labs.

GC/MS methods are typically developed to analyze between 10 and 100 individual compounds. A target compound is deemed to be present if the target ion and two or three qualifier ions with specific abundance ratios fall within a defined retention time window. The identity of the target may be further confirmed by comparison of the scan at the apex of the peak with a library reference spectrum.

Matrix interferences are usually minimized by optimizing a combination of the sample preparation, GC, and MS parameters. For methods that deal with only a few matrix types, the ions chosen for identification purposes can be selected such that they are minimized in the matrix. With a limited number of targets addressed by the method, recalibration of response factors, retention times, and qualifier ion abundance ratios can be accomplished with the injection of a few calibration mixtures.

Screening methods for very large numbers of targets in varying and complex matrices offer a new set of challenges for the method developer. When screening for hundreds of targets, several factors must be addressed:

- Use of sample preparation to reduce matrix interferences is now limited because rigorous cleanup steps may unintentionally remove targets. This reduced level of cleanup can result in significantly higher levels of matrix interferences to contend with.
- Recalibration of response factors, retention times, and qualifier abundance ratios is difficult because of the large number of targets.
- The methods may be deployed in multiple laboratories without ready access to standards for all of the targets.
- The time required for data review of hundreds of targets in complex matrices can become unmanageably large.
- Even with a very large database of targets, it is possible that important compounds not in the target list could be present in a sample.

In recent years, several techniques have become available to help address the above set of challenges. Retention time locking (RTL) produces retention times that precisely match from instrument to instrument and those in a database [1]. This eliminates the need for recalibration of the individual retention times and timed events like SIM groups. The introduction of reliable and inert Capillary Flow Technology (CFT) splitters allows for the simultaneous collection of mass spectral and nitrogen/phosphorus detector (NPD) data [2]. The NPD chromatogram highlights nitrogen-containing compounds, including those not in the MS target list. It is useful in confirming the presence of a nitrogen-containing target compound and can serve as an alternative means of quantitation.

The introduction of the synchronous SIM/Scan feature allows for the simultaneous acquisition of both full-scan and SIM data from the same injection [2, 3]. The scan data can be used for screening the full list of targets in the database, while the SIM data looks for a high-priority subset of compounds (like fentanyl) down to very low levels.

One of the most significant tools developed for reducing the time required for data review is Agilent's Deconvolution Reporting Software (DRS) [4]. It uses advanced computational techniques (deconvolution) to extract the spectra of targets from those of overlapped interference peaks. It then compares the extracted spectrum with a library to determine if the target is present. If desired, hits can be confirmed by also searching against the main NIST MS reference library. The entire process is automated and provides a major time savings in data interpretation. The use of DRS also substantially reduces the number of both false positives and false negatives.

Since DRS uses the entire spectrum instead of just four ions, DRS can often correctly identify a target in the presence of interferences where the typical approach would fail. Also, since it uses the entire spectrum for identification instead of precise target/qualifier ion ratios, frequent updating of the ratios is not necessary. This is useful for targets that are rarely encountered but are still screened for.

This application describes the combination of the above techniques with a new database of 725 compounds, the Agilent G1674AA Forensic Toxicology DBL, to be used for screening purposes. The DBL contains:

- RTL methods for DB-5MS and DB-35MS columns

- Spectral libraries for DRS and the MSD ChemStation
- Preconfigured RTL methods for multiple speeds with run times of 30, 15, 10, 7, or 5 minutes, depending on hardware configuration
- Methods for both MSD direct connection (vacuum) and Capillary Flow Technology splitters (3.8 psig).
- Three quant databases included for each method:
  - Target and qualifiers are the biggest four ions.
  - Ions are optimized to give the best signal-to-noise ratio versus column bleed and background.
  - Ions are optimized to give the best signal-to-noise ratio versus common fatty acids found in blood.

The names of all the compounds in the database are listed in the appendix at the end of this application. Compounds in the DBL include drugs and select breakdown products, TMS derivatives, and acetyl derivatives. For those compounds entered as derivatives, in general, primary and secondary amino (including aliphatic and aromatic) compounds are acetylated. Hydroxyl groups (alcohols/phenols/carboxylic acids, etc.) are converted to TMS derivatives with BSTFA. Compounds having multiple functionalities (for example, phenylpropanolamine, which has a primary aliphatic amine and an alcohol) were acetylated with no further derivatization.

Methods are provided for two stationary phases to allow two-column confirmation and the ability to run other methods that require the same column on the same hardware. In general, the DB-5MS methods are preferred because the final oven temperature is lower.

The chromatographic conditions chosen for development of the database are general in nature and are compatible with the analysis of other compounds beyond those in the table. Since no one target list, no matter how large, can satisfy every lab's needs, new compounds can be added to the screen.

The retention times for compounds in the database are provided for both the column connected directly to the MSD and for the column outlet pressure at 3.8 psig using a CFT splitter. This was done to ensure that the retention times observed during sample analysis would closely match those in the database regardless of the instrument configuration.

The chromatographic conditions for the database were chosen to be compatible with Agilent's method translation technique. Constant-pressure mode was used in the GC inlet so that method translation could be used to precisely time-scale the methods for faster operation [5]. Provided with the Agilent Forensic Toxicology DBL are the files to run the analysis at precisely twofold (2x), threefold (3x), fourfold (4x), and sixfold (6x) faster than the primary database (1x). The choice of speed is determined by the degree of chromatographic resolution desired and the hardware capabilities of the GC/MSD system to be used.

For systems with a 120 V GC oven, an MSD with diffusion pump, and the column connected directly into the MSD, only 1x or 2x methods can be used. The 3x, 4x, and 6x methods require the fast oven (240 V) and performance turbopump because column flow rates exceed 2 mL per minute. Performance electronics are also preferred for the same methods. The 6x methods require both a 240 V oven and the oven "pillow" accessory to attain the 60 °C/min ramp rate. Note that use of the pillow requires that the MSD, inlet, and NPD (if used) be located in the back GC positions.

Three different versions of each method set are provided based upon the choice of ions used in the quant database. A method using the largest four ions in a compound's spectrum is supplied. The target ion is the ion with the largest abundance. The three qualifiers are the next three largest ions assigned in order of decreasing abundance. These method sets are provided for legacy reasons, and are used in some more advanced approaches.

The drawback of the largest four-ion approach is that, in some cases, the signal-to-noise performance suffers. For example, if the biggest ion for a compound is 207 and the stationary phase has its largest bleed ion at 207, the signal-to-noise ratio at that mass can be significantly reduced. The same problem is seen with low masses such as 44, where CO_2 and other background gases can result in interferences and increased noise. To reduce this problem, a second method set is provided where ions chosen for the quant database are selected to give best signal-to-noise ratios relative to column bleed and background gases. These are the methods that would normally be used, as they typically give best overall performance.

A third method type is provided where the choice of ions has been optimized for samples having large amounts of fatty acids typically seen in blood samples. These methods give the best signal-to-noise

ratios in high fatty-acid matrices. They are not the best choice for samples having low levels of interfering fatty acids.

Experimental

System Configuration

The system configuration used is shown in Figure 1. The GC is an Agilent 7890A (G3440A).

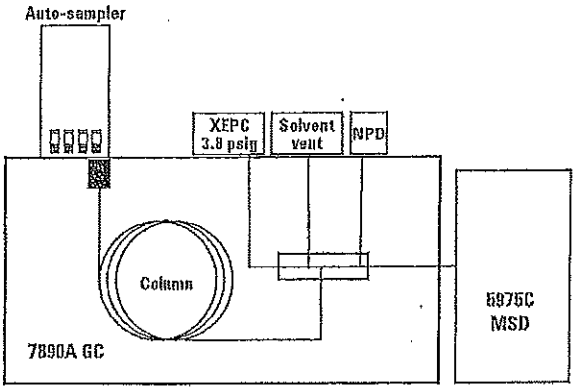

Figure 1. GC/MS/NPD system configuration used for screening blood extracts.

Key components are:

Fast Oven The primary 1x method uses a 30-m column with a 10 °C/min ramp rate and only requires the 120 V oven. With the 7890A 240 V oven (option 002), the screening method can be run up to 4 times faster using a 15-m column. If the 240 V GC is further equipped with options 199 and 202 (puts split/splitless injection port and MSD interface in the back of the oven) and uses the G2646-60500 oven insert accessory, the speed can be increased to 6 times faster (60 °C/min) with a custom length 10-m column. If an NPD is used with a splitter, option 299 places it in the back of the oven for use with the pillow.

NPD The 7890A Option 251 is a nitrogen phosphorus detector. The signal from the NPD is collected, stored, and processed by the MS ChemStation simultaneously with the MS data. NPD detectors are highly selective and exhibit very sensitive response to nitrogen and phosphorus compounds, with detection limits in the low picogram range. The NPD data can be used in several ways. Nontarget nitrogen (and phosphorus) compounds are highlighted for the data reviewer. The presence of a response at the retention time of an identified compound can be used to support confirmation of identity. The response on the NPD can be used for quantitative analysis, but only after calibration with a standard, as the response factors are compound dependent and can vary with compound class. The NPD bead is incompatible with halogenated solvents and excess silanizing reagents. If these are to be used with an NPD, the splitter setup should have solvent venting capability.

Capillary Flow Technology Splitters Agilent offers two different column effluent splitters that can be used with the 7890A for this application. Option 889 is a two-way splitter that divides the effluent of the column between the MSD and the NPD. The 7890A Option SP1 (7890-0363) does the same, but adds solvent venting capability as well. The devices are based on diffusion bonded plate technology combined with metal column ferrules to make inert, easy-to-use, leak-free, high-temperature splitters. The splitters use Auxillary EPC for constant pressure makeup (7890A Option 301). The Auxillary EPC makeup can be pressure programmed at the end of the run to higher pressure, while at the same time the inlet pressure is lowered to near ambient. This causes the flow in the column to reverse direction, backflushing heavy materials out the split vent of the inlet. Backflushing significantly reduces analysis times for samples that contain high-boiling matrix components and reduces both column head trimming and frequency of MSD source cleaning [6]. The Aux EPC also allows column changing and maintenance without venting the MSD.

For methods that use solvents compatible with the NPD and do not have silanizing reagent in the samples, the standard two-way splitter can be used. If halogenated (or other NPD incompatible) solvents or silanizing reagents are used, then the two-way splitter with solvent vent, 7890A Option SP1 (7890-0363), should be used to protect the NPD bead. This is the configuration used here.

MSD System The 5975C Inert MSD with performance turbo (G3243A) or 5973N Inert MSD with Performance Electronics and performance turbo (G2579A) EI MSD is used. These configurations provide faster full-scan rates while maintaining sensitivity. The scan rates are compatible with the narrower peaks generated by fast chromatography. The performance turbo pump is required to handle the higher flows associated with systems using splitters. It is also required for the faster versions (3x, 4x, and 6x) of the screening method with vacuum outlet (column connected directly to MSD). The standard turbo pump can be used for the slower 1x and 2x vacuum outlet versions of the method. Both the performance and standard turbos are compatible with backflushing. Backflushing cannot be done on systems with a diffusion pump.

Synchronous SIM/Scan The D.02.00 (or higher) revision of the Agilent MSD ChemStation is used because it supplies the synchronous SIM/Scan feature. SIM/Scan operates by collecting SIM data every other cycle and scan data on alternate cycles throughout the entire chromatogram. As with conventional SIM methods, not all 725 targets can be monitored in a single run due to the required time separation between SIM groups. In general, the acquisition of SIM data is set up to collect high-priority targets at very low levels. Examples would be fentanyl and phencyclidine.

DRS Software (G1716AA) Spectral deconvolution of the MS data enables identification of analytes in the presence of overlapped matrix peaks [4, 7]. This significantly reduces chromatographic resolution requirements, which allows detection of targets in higher levels of matrix or can be used with fast chromatography to shorten analysis times. DRS utilizes the AMDIS deconvolution program from NIST, originally developed for trace chemical weapons detection in complex samples. DRS presents the analyst with three distinct levels of compound identification: (1) ChemStation, based on retention time and four-ion agreement; (2) AMDIS, based on "cleaned spectra" full ion matching and locked retention time; and (3) NIST05a search using a 163,000-compound library.

G1674AA Forensic Toxicology DBL This supplies the mass spectral library, method, and DRS files for the 725 compound screening methods.

Table 1. Gas Chromatograph and Mass Spectrometer Conditions

GC	
Agilent Technologies 7890A with autoinjector and tray	
Inlet	EPC split/splitless
Mode	Constant pressure
Injection type	Splitless
Injection volume	1.0 µL
Inlet temperature	280 °C
Liner, Agilent dual-taper deactivated	P/N 5181-3315
Pressure, nominal	14.9 psig
RT locking compound	Proadifen (SKF-525a)
RT locking time	4.285 min
Purge flow	50 mL/min
Purge mode	Switched
Purge time	0.4 min
Gas type	Helium
Inlet backflush pressure	1 psig
Oven	
Voltage (VAC)	240*
Initial oven temperature	100 °C
Initial oven hold	0.25 min
Ramp rate	40 °C/min
Final temperature	325 °C
Final hold	1.25 min
Total run time	7.13 min
Equilibration time	0.5 min
Backflush time	0.5 min
Backflush temperature	325 °C
Column	
Type	DB-5MS
Agilent part number	Custom
Length	10 m
Diameter	0.25 mm
Film thickness	0.25 µm
Nominal initial flow	2.52 mL/min
Outlet pressure	3.8 psig
2-Way Splitter w/Solvent Vent	
7890A SP-1, num. 7890-0363	
MSD restictor length	0.69 m
MSD restictor diameter	0.15 mm
NPD restictor length	0.36 m
NPD restictor diameter	0.15 mm
Split ratio MSD:NPD	1.4:1
Solvent vent time range	0–0.75 min
Splitter pressure during run	3.8 psig
Splitter pressure during backflush	76 psig
NPD	
Hydrogen flow	3 mL/min
Air flow	60 mL/min
Nitrogen makeup flow	8 mL/min
Temperature	300 °C
MSD	
Agilent Technologies 5975 or 5973 inert with performance electronics	
Vacuum pump	Performance turbo
Tune file	Atune.U**
Mode	SIM/scan
Solvent delay	0.7 min
EM voltage	Atune voltage
Low mass	40 amu
High mass	570 amu
Threshold	0
TID	Off
Sampling	1
Quad temperature	180 °C
Source temperature	300 °C
Transfer line temperature	300 °C

*Injection port and MSD interface in back positions and G2646-60500 oven pillow

**Gain normalized, 1x

Instrument Operating Parameters

Data Acquisition

The instrument operating parameters used (unless noted otherwise) are listed in Table 1.

DB-5MS was chosen as the stationary phase for the current system. The final temperature required to elute the last compound in the screen is 325 °C instead of 345 °C as required with DB-35MS. This results in shorter run times and longer column life.

The method parameters were chosen to give the best trade-off between chromatographic resolution and sample throughput. For the blood samples analyzed here, the 4x method gave adequate resolution with an relatively short run time. Although the 4x method can be run on a standard 15-m column, a 10-m column was chosen because it gives very similar resolution with a lower column flow rate.

Time was also saved by using backflushing instead of post-run column baking to remove heavy sample matrix compounds. Backflushing is more effective, faster, and does not send the heavy materials and column bleed into the NPD and MSD source. With the current configuration, all heavy materials were removed from the column with a 0.5-minute backflush. The shorter column length (10 m) results in a reduced backflushing time compared to the 15-m column.

The 4x method can be run with a 240 V oven without the pillow accessory. The pillow was used here because it somewhat decreases the cooldown time of the oven and reduces the amount of electricity consumed by the instrument.

Further reduction in the cycle time of the instrument was achieved by using the overlapped injection setting in the autoinjector. With this feature, the autoinjector prepares the next sample for injection and has the syringe ready while the oven is cooling down from the current injection. This feature can save approximately 1 minute in cycle time, depending on the injection parameters used.

The simultaneous acquisition of SIM, scan, and NPD

Table 2. SIM Groups Used in SIM/Scan Mode

SIM Group (number)	Start Time (min)	Compound	RT (min)	Target (amu)	Q1 (amu)	Q2 (amu)
1	0	Amphetamine	0.900	44	91	65
2	0.97	Methamphetamine	1.050	58	91	65
3	1.5	Methylenedioxyamphetamine(MDA)	1.978	136	135	51
4	2.06	Methylenedioxymethamphetamine(MDMA)	2.147	58	135	77
4		Ecgonine methyl ester	2.222	94	82	96
4		Ethylecgonine	2.223	94	82	96
5	2.52	Meperidine	2.826	246	218	247
6	2.96	Ketamine	3.138	180	182	209
6		Phencyclidine	3.249	243	242	200
6		Tramadol	3.389	58	263	59
7	3.64	Methadone	3.866	72	57	165
7		Dextromethorphan	3.895	271	212	270
8	3.98	Cocaine	4.042	182	82	94
8		Cocaethylene	4.175	196	82	94
9	4.53	Diazepam	4.598	258	286	257
9		Tetrahydrocannabinol	4.666	299	300	231
9		6-Acetyl-morphine	4.773	268	327	328
10	4.85	Oxycodone	4.801	315	230	115
10		Temazepam	4.922	271	273	272
10		Diacetylmorphine	4.992	310	268	327
10		Fentanyl	5.177	245	146	189
11	5.25	Zolpidem	5.332	235	236	219
11		Clonazepam-M (amino-)	5.433	285	258	286
12	5.53	Alprazolam	5.630	308	279	280
12		Zaleplon	5.695	305	263	248
13	5.8	Zopiclone	5.905	112	99	139
13		Lysergide (LSD)	6.000	323	324	222

(all dwell times 5 msec)

data save a substantial amount of time compared to acquiring them in separate runs. The compounds and corresponding SIM groups monitored are listed in Table 2. Because the peaks in the 4x method are relatively narrow, the dwell times for SIM ions were set to 5 milliseconds.

By using the above time-saving steps, the cycle time from injection to injection is 9.6 minutes.

Data Analysis

Based on experience with analyzing 50 blood extracts, a data analysis scheme evolved that incorporated the DRS, SIM and NPD data.

The resulting data review scheme consisted of the following:

- Deconvolution results were generated with DRS and reviewed to determine compounds present. The AMDIS minimum match factor was set to 50. Any compounds with match factors less than 65 or retention time differences greater then 4 seconds were considered suspect (for example, not present unless other data like target/qualifier ratios supported presence). For suspect identifications, the NPD signal was inspected to see if there was a corresponding response of the same peak shape and retention time. If the suspect compound is nitrogen containing (as the vast majority of the compounds in the table are), NPD response provided evidence supporting the presence of the compound.
- Compounds identified by AMDIS but not found by the MSD ChemStation because of out-of-range qualifiers were manually inspected in QEdit. Quantitation was forced if AMDIS indicated an acceptable spectral and retention time match.
- A separate ChemStation data analysis method was used to review the SIM results for the 27 compounds listed in Table 2. Since SIM can detect compounds lower than can be confirmed with spectral data, identification relied on target/qualifier ion ratios and NPD data.
- The NPD trace was examined to find any larger peaks that did not correspond to identified targets. The deconvoluted spectra at the retention time of these peaks were searched against the NIST 05a library. As a practical matter, uncorrelated small NPD peaks were not pursued as they are numerous and the signal-to-noise ratio of the corresponding scan data is too small to be useful.

Except where otherwise indicated, the 4x method supplied with the ions optimized against column bleed was used for ChemStation data analysis . The approximate response factors supplied with the method were adjusted using a standard of 5 ng/uL of proadifen (the locking compound). The responses of all compounds in the quant database were multiplied by the factor required to make the calculated result for the proadifen standard equal 5 ng/µL. This allows the concentration of an identified target to be estimated if the compound has not been individually calibrated.

The approximate response factors supplied with the method are only intended to give a rough estimate of the concentration of uncalibrated analytes. Since valid quantitation requires recent recalibration of response factors on the specific instrument used for analysis, the estimated concentration should never be used to report quantitative results. The error in these values can easilly be a factor of 10 or higher. The purpose of the estimated values is to give an approximate amount that can be used to guide standard preparation for quantitative calibration of the compound, if needed. Individual calibration should be used for all reported analytes.

The SIM data analysis method for the 27 compounds was constructed using the target and first two qualifier ions from the 4x fatty acid optimized method. This was to minimize interference from the matrix in the blood samples.

The peak recognition windows used in the MSD ChemStation were set to ± 0.150 minute for the scan data, ± 0.075 for the SIM data, and ± 6 seconds in AMDIS. These values were found to be sufficiently wide enough to allow for some retention time drift, yet narrow enough to minimize the number of false positives.

For comparison purposes, the data were also analyzed with two conventional data review approaches.

The first approach is the standard quantitation software, where the EIC of the target ion for each compound in the quant database is extracted and integrated. If a peak is detected within the peak recognition time window, the ratios of the qualifiers to the target are measured. Several optional forms of reporting are available. The reports used here were 1) report only compounds with a peak detected in the target ion EIC and that have all qualifiers within the acceptable range for ratios, and 2) report all compounds with a peak detected in the target ion EIC, regardless of qualifier status. The results of a report can then be reviewed in QEdit, where the EICs of the extracted target and qualifier

ions are overlayed for ease of inspection. The reference spectrum for the compound and the apex spectrum for the quant peak being examined are also displayed. Based on inspection of the EICs and spectra, the reviewer can include or exclude the compound from the report.

The second data review approach was to use the ChemStation Screener software. This is almost identical to QEdit, except that it also reports a cross-correlation value (XCR) of the apex spectrum for peak versus the reference library. The XCR value is an indication of spectral match quality and can be used as an additional parameter with which to locate targets. Screener has report options similar QEdit, and the same two types were used here. Note that Screener is a qualitative tool; compounds identified in Screener must then be quantified in QEdit.

Samples

Whole blood extracts prepared for GC/MS analysis were supplied by NMS Labs (Willow Grove, PA). The whole blood was prepared with a single step liquid/liquid extraction into a solvent, evaporated to dryness, and reconstituted in toluene at 1/10th volume.

Results and Discussion

Figure 2A shows the chromatographic results from one of the blood extracts, the simultaneously acquired scan, SIM, and NPD signals. The traces make the sample look deceptively simple. Figure 2B shows the same Scan TIC and NPD signals with the scales expanded. More than 400 individual compounds are in these chromatograms when low-level responses are included.

The data from the sample were reviewed with the conventional approaches. The first report with the standard quantitation software listed compounds where all qualifier-to-target ratios were within the rather generous 50% relative limits used here. Without manual review of the 28 compounds reported, 22 were false positives; that is, they were not really present. Of the 11 target compounds actually in the sample, this report only found six of them, leaving five as false negatives.

As this situation is not uncommon, it is usually necessary to have all compounds reported that have a response at the target ion, regardless of the qualifier ratio status. These "maybes" must then be manually reviewed in QEdit. Since the integrator must be set to capture very small peaks, there are large numbers of reponses due to integration of baseline

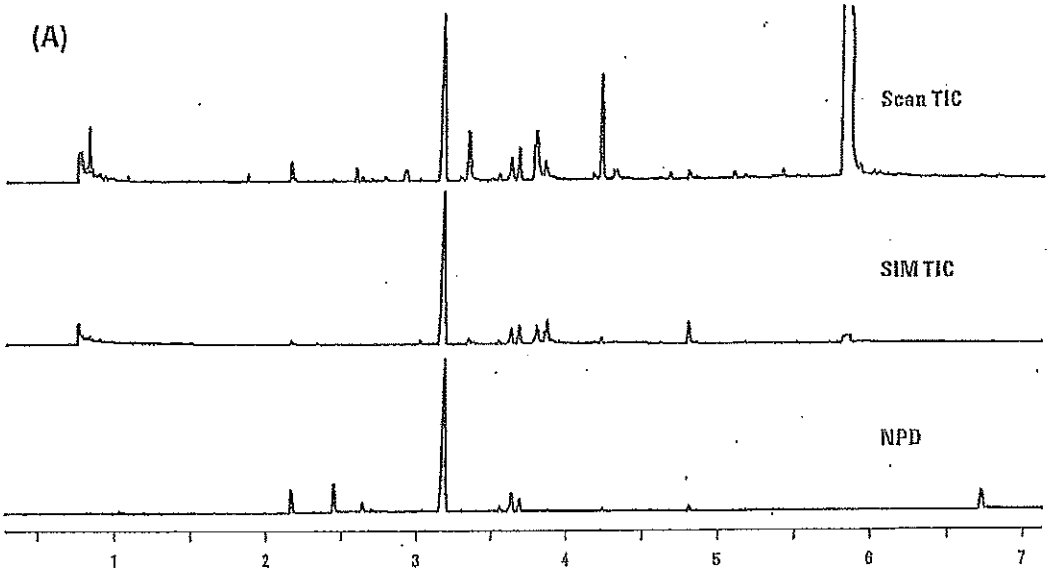

Figure 2A. Chromatograms of scan, SIM, and NPD signals from analysis of blood extract.

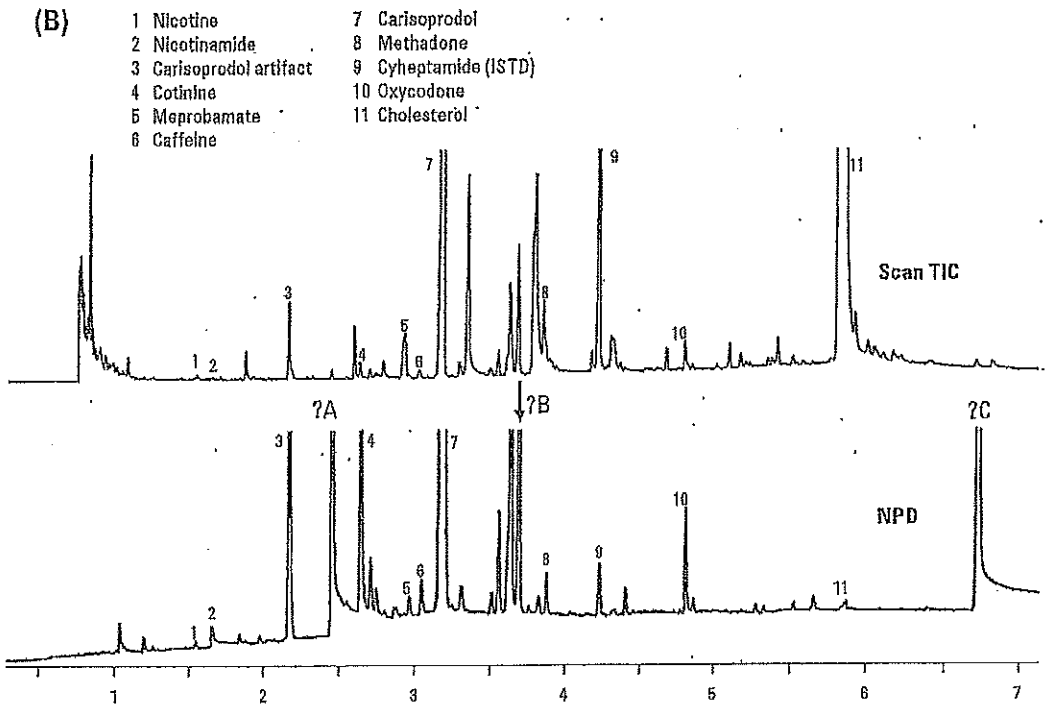

Figure 2B. Expanded scale chromatograms of scan TIC and NPD signals from analysis of blood extract. (continued)

noise. For the sample here, 367 compounds were reported found (that is, there was a response at the target ion). Of those, 356 were false positives. All 11 compounds actually present were found, so there were no false negatives. Thus, to avoid false negatives, the reviewer must manually evaluate 367 compounds to find the 11 present.

The data from the sample were then evaluated with the ChemStation Screener software. As expected, Screener reports based only on ion target/qualifier ion ratios gave very similar results to QEdit. The only way to avoid false negatives is to evalute hundreds of target ion responses to find the 11 actually present.

In an attempt to reduce the number of false positives requiring evaluation, the Screener report listing all 273 compounds with a target ion response was sorted by the XCR in descending order. Several of the compounds actually present were clustered near the top of the list. However, the target actually present with the lowest XCR value was the 162nd compound in the list. This result suggests that XCR improves the likelihood of correctly locating target compounds, but will still result in false negatives without close inspection of all of the compounds with a target ion response.

For the types of samples discussed here, correctly identifying the targets present with the conventional approach is one of the most time-consuming steps in the entire analytical process. This is why the use of deconvolution and DRS is so useful.

When this same sample was evaluated with the DRS software, 12 compounds were reported by AMDIS with a match factor for the deconvoluted spectrum greater than 50 and with retention times within 6 seconds of the locked retention time. After reviewing the 12 listed compounds, one was removed because its match factor was too low. All 11 compounds actually present were identified, with only one false positive included. The entire DRS and review process to correctly locate the targets actually present required about 5 minutes instead of more than an hour using either the QEdit target only or Screener approaches. With the compounds present in the sample identified by DRS, the final report was generated after using QEdit to quantify the targets.

MSD Deconvolution Report
Sample Name: CA5995
Date File: C:\msdchem\1\Appnote\FT5_4 x 10m_SamplesSimScan\CA5995_mss.D
Date/Time: 11:39 AM Wednesday, Apr 2 2008

The NIST library was not searched for the compounds that were found in the AMDIS target library.

			Agilent	AMDIS	
R.T.	CAS #	Compound Name	ChemStation Amount (~ng)	Match	R.T. Diff. sec.
1.539	54115	Nicotine	0.03	59	-0.5
1.6446	98920	Nicotinamide	0.27	93	-0.9
2.1631	999401024	Carisoprodol artifact	84.87	93	-0.5
2.6367	486566	Cotinine	1	96	-0.4
2.928	57534	Meprobamate	4.11	99	0.0
3.033	58082	Caffeine	0.04	82	-0.5
3.1832	78444	Carisoprodol	127.4	96	1.0
3.8653	76993	Methadone	0.39	74	-0.1
4.2279	7199293	Cyheptamide	22.5	98	0.1
4.8014	76426	Oxycodone	2.37	82	0.0
5.850	57885	Cholesterol	922.73	97	3.4

Figure 3. DRS report for the analysis in Figure 2.

Figure 3 shows the DRS report for the sample. For each compound identified, the retention time (R.T.), Chemical Abstracts number (CAS#), and compound name are listed. A line is generated in the report if a compound is found by the Agilent ChemStation, AMDIS, or both.

The report shows that a compound has been determined as present by the Agilent ChemStation if a value appears in the Agilent ChemStation Amount column. This means that the identification criteria set in the DATA ANALYSIS section of the method have been met. Typically the criteria are that the target ion is present (and integrated) and all three qualifier ions are present in ratios that fall within the percent uncertainty values for that compound. The compound would also appear here if the data reviewer manually forced integration of the target ion.

The match value listed under the AMDIS column is the degree to which the extracted (deconvoluted) spectrum of the peak at that RT matched the spectrum in the AMDIS target library. The higher this number (out of a possible 100), the better the spectra agree. The column "R.T. Diff. sec." lists the difference in seconds between the observed RT and that in the AMDIS target library. The lower this number, the better the RTs agree.

An optional third feature of the report is the NIST search column (not shown). The NIST column lists the reverse match quality of the extracted spectrum compared with the NIST main library spectrum with the same CAS#. With the present setup, there are a large number of compounds for which a CAS# is not available. The Forensic Toxicology DBL contains some contrived CAS#s that would not be found in the NIST library. In the present analysis, the NIST search feature is therefore turned off.

Also shown in the NPD trace in Figure 2B are three peaks labeled ?A, ?B, and ?C. These three relatively large peaks are not in the target list of 725 compounds. The deconvoluted spectra corresponding to each of the three NPD responses were found in AMDIS and searched against the main NIST library. Peak ?A was identified as tributyl phosphate, a phosphorus compound commonly found as a sample handling artifact. Peak ?B was identified as 10,11-dihydrodibenz(b,f)(1,4)oxazepin-11-one. It was later found to be a second internal standard added during sample preparation. Peak ?3 remains unidentified. It is not in the NIST 05a Library (the best hit was only a 38 match) and it appears in many samples.

It is instructive to go through the identification of some of the compounds in the report and look at

the details of the identifications made. Oxycodone was readily identified because it had a high match quality in the AMDIS column and a very small retention time difference. Figure 4A shows the extracted ion chromatograms (EIC) as seen in QEdit. All the ions are clearly visible without interference and the ratios of the qualifier ions to the target are within the acceptable range. Also shown are the SIM ion EICs. They also are clearly visible without interference and the ratios of the qualifier ions to the target are within the acceptable range. The bottom trace from the NPD in Figure 4A shows a response with the same shape and at the same time as the oxycodone response in the mass traces. Figure 4B compares the deconvoluted spectrum found at the oxycodone retention time with the target library reference spectrum of oxycodone. The match is very good, with a match factor of 82. Oxycodone was an easy identification with all parameters clearly pointing to its presence.

Figure 5 shows a situation that is a bit more challenging. The compound here is methadone, whose spectrum has one large ion at 72; the remaining ones are very small. The EICs in Figure 5A are from

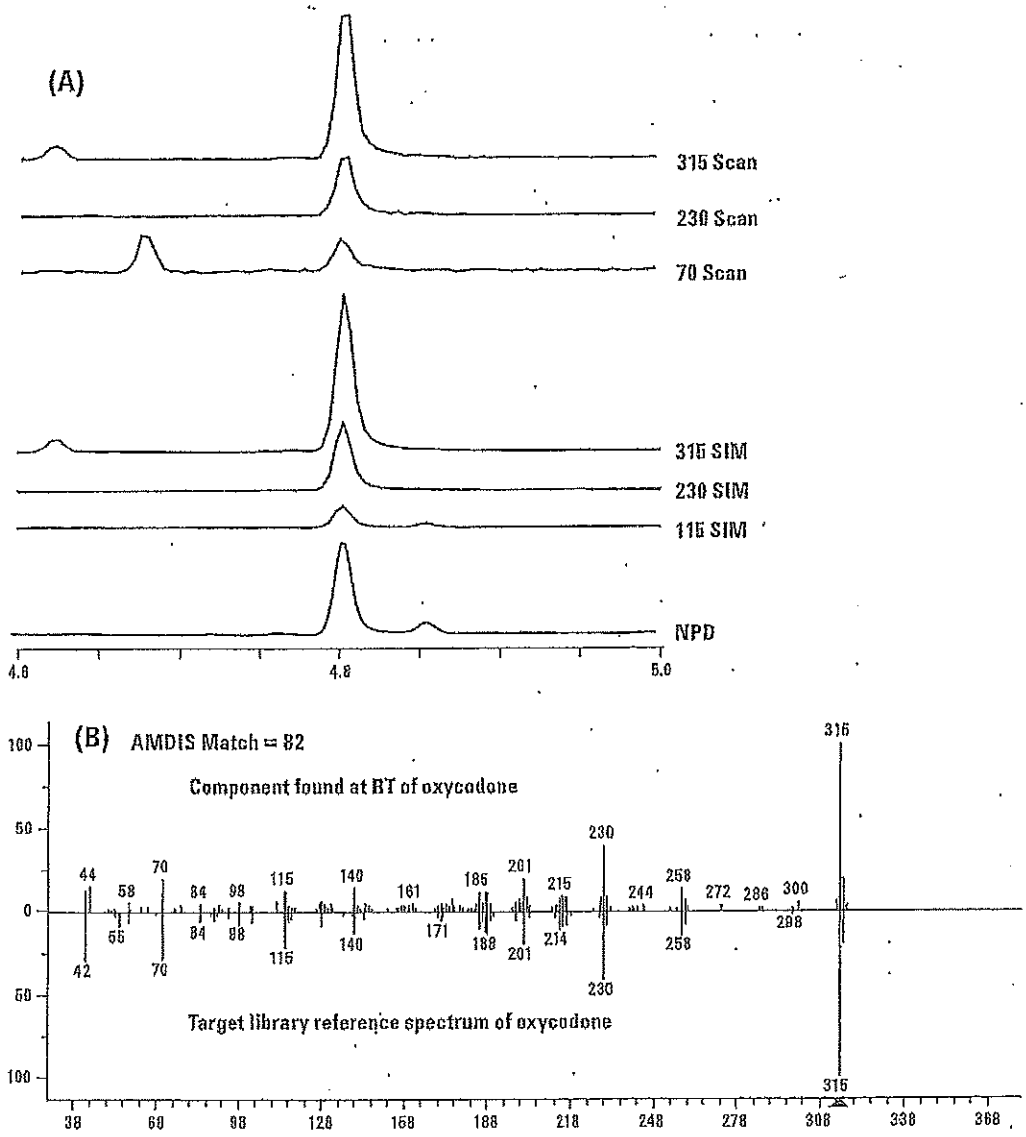

Figure 4. (A) Oxycodone response in SIM, scan, and NPD signals collected simultaneously.
(B) Comparison of deconvoluted oxycodone spectrum with target library reference spectrum.

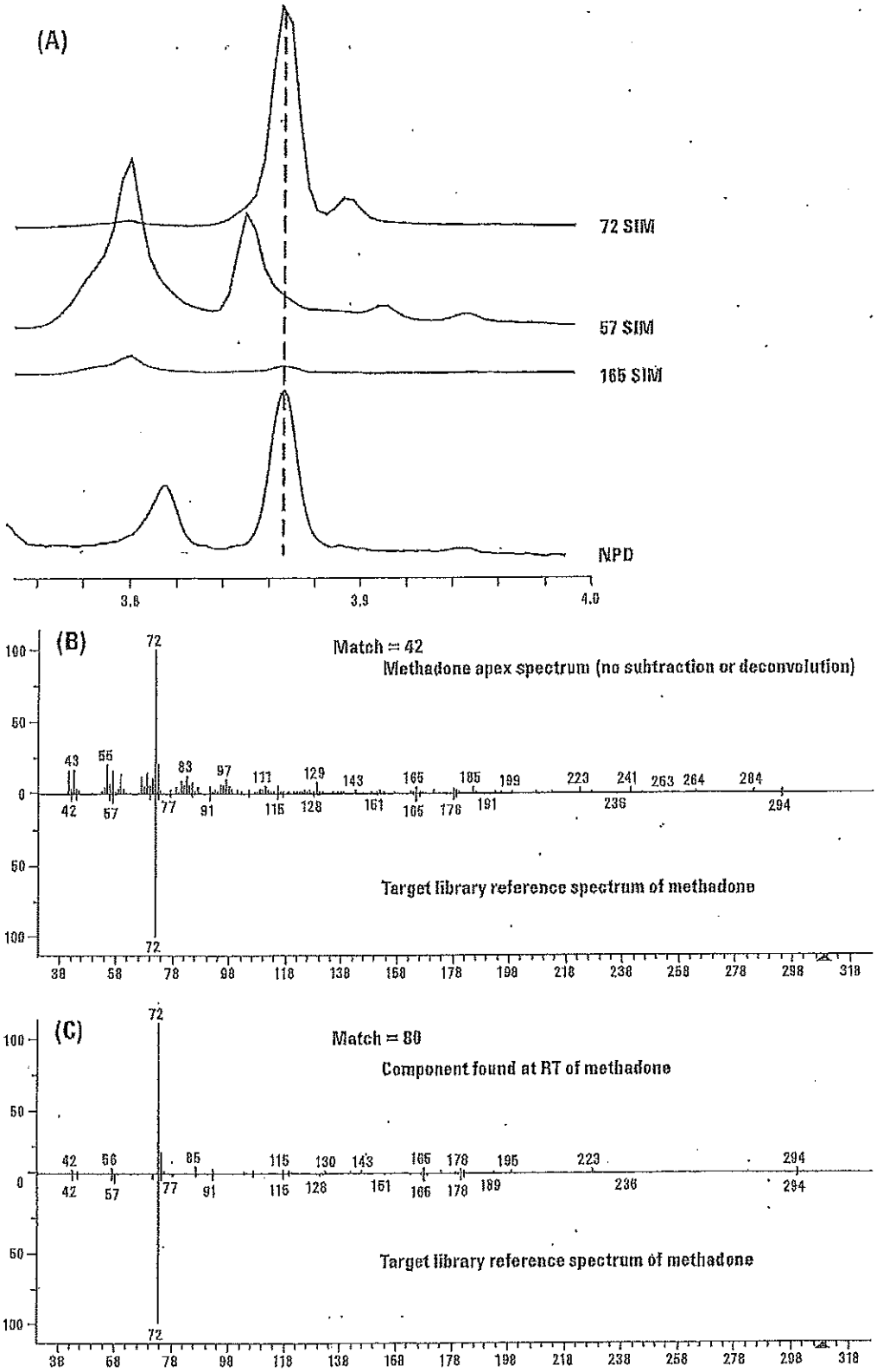

Figure 5. (A) Methadone SIM and NPD chromatograms.
(B) Comparison of reference spectrum with methadone spectrum without subtraction or deconvolution.
(C) Methadone deconvoluted spectrum searched against target library.

the SIM data. The traces from the scan data were identical (except of course with a lower signal-to-noise ratio). While there is a clear peak at the target ion, the middle qualifier (57) has a significant interference from the overlapping octadecanoic acid peak. With only the EIC data, the identification is questionable due to the loss of one of the qualifiers to interference. The NPD response shown below the SIM traces does support the fact that there is a nitrogen-containing compound at that retention time.

Figure 5B shows the apex spectrum at the methadone peak without subtraction or deconvolution compared with the target library reference spectrum. The match quality is unacceptably poor at 42 due to the interference of the octadecanoic acid peak. While the 72 ion is clearly visible, the other methadone ions are obscured. In Figure 5C the deconvoluted spectrum from the methadone retention time is compared with the reference. Deconvolution successfully removed the octadecanoic acid interference, and now the match quality is 80, clearly indicating the presence of methadone in the sample. The indication of methadone is also supported by two of the three ions being clearly present and in the correct ratio as well as an NPD response with the same retention time and peak shape.

Although caffeine is not a particularly high-priority target compound, the example shown in Figure 6 is

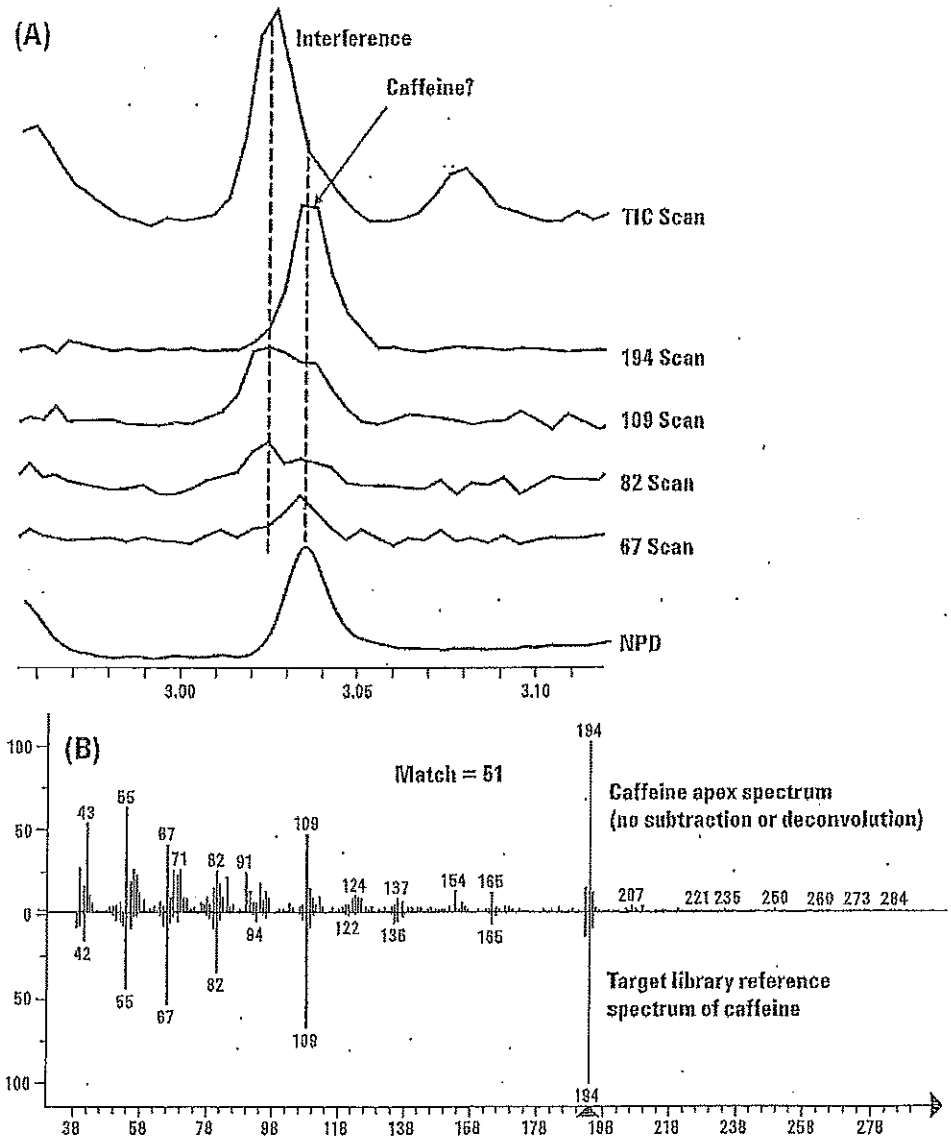

Figure 6. (A) TIC, scan EICs, and NPD signals for caffeine.
(B) Caffeine spectrum without subtraction or deconvolution shows interference from matrix compound.

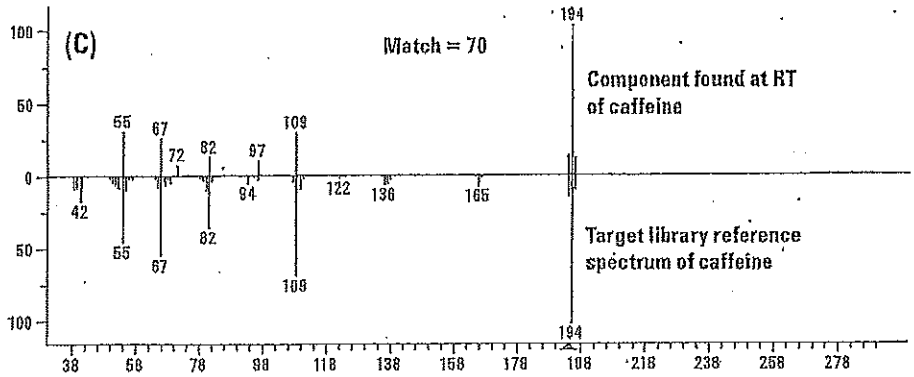

Figure 6C Caffeine deconvoluted spectrum searched against target library. (continued)

instructive. The caffeine, if present, is at a very low level as seen from the low signal-to-noise ratio of the four scan EICs shown in Figure 6A. Two ions, 109 and 82, also have interference problems from a large overlapping peak, as shown in the TIC trace at the top. The NPD trace does indicate a nitrogen-containing compound with the same peak shape and retention time as caffeine. The interfering peak was identified as 6,10,14-trimethyl-2-pentadecanone by searching the deconvoluted spectrum against the NIST main library. This compound also shares ions 109 and 82 with caffeine, resulting in the interference.

Figure 6B shows the apex spectrum of the caffeine peak without subtraction or deconvolution. When compared to the reference spectrum of caffeine, the match quality is poor, at only 51. Figure 6C shows the deconvoluted spectrum at the caffeine retention time compared to the reference spectrum and now the match quality is significantly improved to 70. This example demonstrates that the deconvolution process works even on small peaks with a low signal-to-noise ratio.

The example in Figure 7 is taken from a different sample and its purpose is to show the limits of deconvolution compared to the limits of the conventional approach. They are in fact similar because both approaches are limited by the same thing: signal-to-noise ratio. Figure 7A shows the scan and SIM EICs and the NPD trace for alprazolam. In the scan data, three of the four ions are barely visible and the fourth is lost in the noise. The SIM data clearly show a peak present at the alprazolam retention time and the ratios are in the correct range. The NPD also shows a response at the same retention time and with a similar shape. Figure 7B shows the deconvoluted spectrum compared to the NIST 05a library spectrum of alprazolam. The match factor is only 57.5. The match is marginal because AMDIS could only find a fraction of the alprazolam ions due to the extremely low level of the compound. This again illustrates that the target/qualifier approach using scan data and deconvolution begin to fail at about the same signal-to-noise ratio. In this example, the SIM data and NPD data are very helpful. If only the scan data were available for this sample, the identification of alprazolam would be doubtful and probably not reported. Taken with the SIM data in the correct ratios and the supporting evidence of the NPD response, a much stronger case can be made that alprazolam is indeed present, although at a very low level.

The last example is from a sample containing extraordinarily high levels of fatty acid interferences. These are clearly visible in Figure 8A. In QEdit, the presence of meprobamate was indicated with the peak shown at 3.007 minutes in Figure 8B. Although the ratios of the qualifiers to the target ion were within the relatively wide windows used here, the identification was doubtful. Examination of the EICs shows what looks like multiple peaks at the retention time that QEdit found. The retention time was also farther away (+ 0.080 minute) from the expected retention time of 2.928 minutes than is typically seen with the method. Also, there is no clear peak shape evident in the four traces at the 3.007 retention time. Based on these results alone, meprobamate looks like a false positive.

The EIC traces shown were from the column bleed optimized method. The use of 83 as the target ion clearly has interference problems with the high-level of fatty acids in this sample. When the method with

fatty acid optimized ions was used, the picture became a bit clearer. In this method, ion 62 is used as the target because of its significantly lower degree of interference. Looking at the trace for ion 62 in Figure 8, the peak now appears at 2.948 and is much closer to the expected retention time at 2.928 minutes. While the response at ion 62 looks a bit more like a real peak, the other ions in the fatty acid optimized method were still questionable due to the degree of interference, suggesting that it still may be a false positive. The NPD trace (not shown) did not resolve the question, as there were NPD peaks near 2.928 and 3.007 minutes.

The question was easily settled using the new A.04 release of DRS software. This version allows you to import into QEdit the AMDIS extracted peak profile from the deconvolution data and overlay it with the QEdit EICs. It also imports the deconvoluted spectrum for comparison with the QEdit-subtracted spectrum and the library reference spectrum. These capabilities simplify the review process by showing the deconvolution information inside of QEdit. Inspection of the AMDIS extracted peak profile relative to the EICs of the scan data shows that in fact the response at the target found with the fatty acid optimized method is indeed meprobamate. The

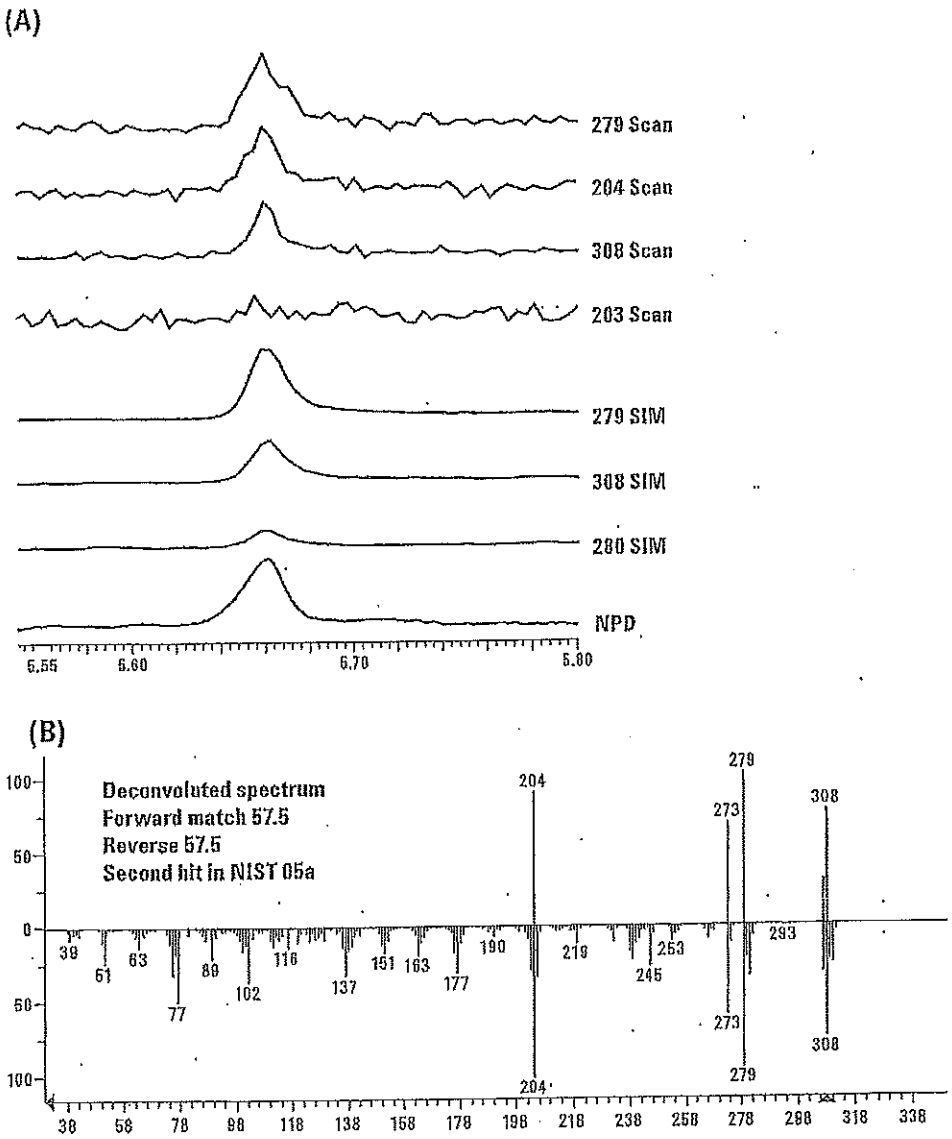

Figure 7. (A) Alprazolam response on SIM, scan, and NPD signals.
(B) Alprazolam deconvoluted spectrum searched against NIST 05a library.

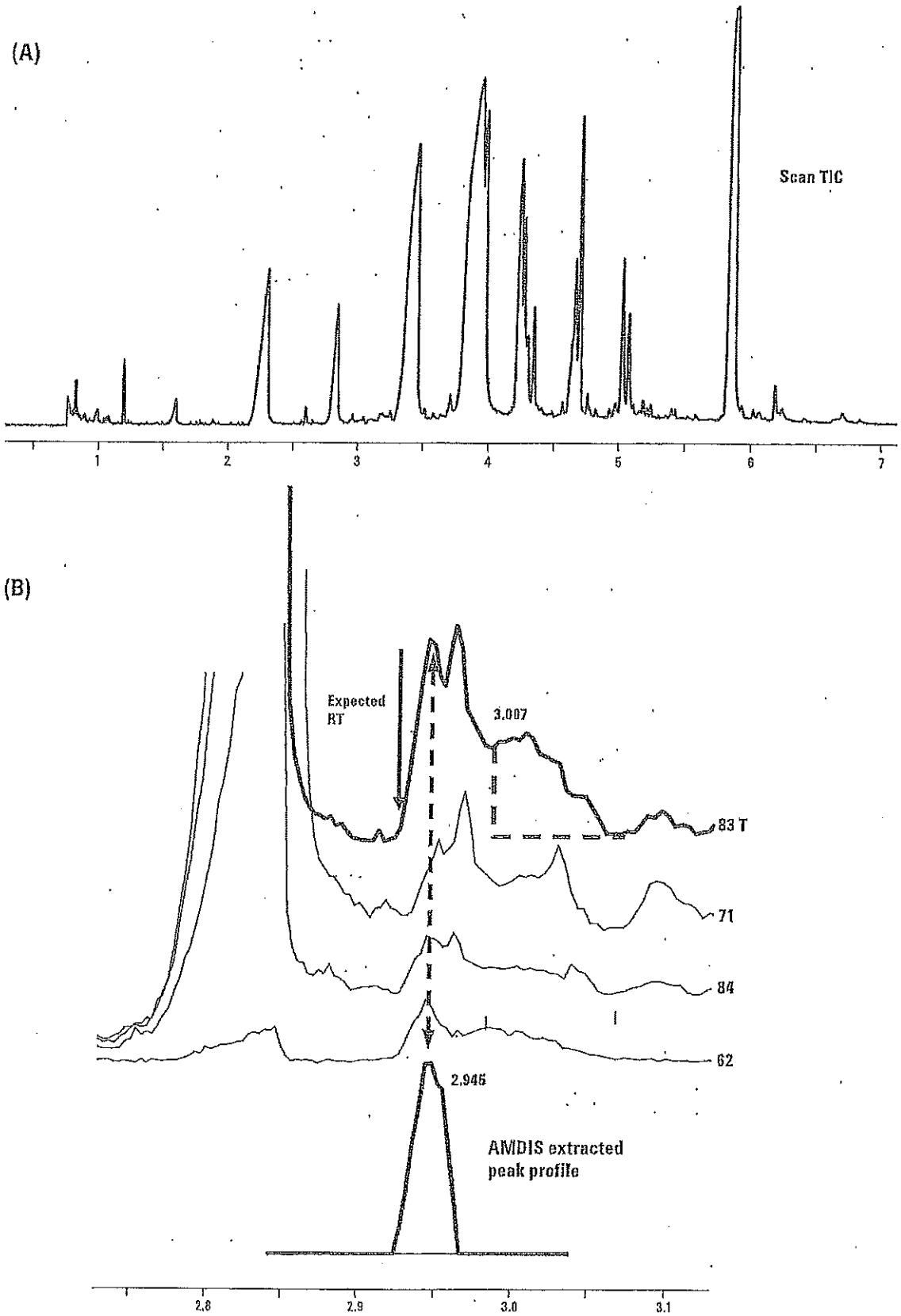

Figure 8. (A) Scan TIC chromatogram of sample with high levels of fatty acids.
(B) Scan EICs from bleed optimized method overlayed with AMDIS extracted peak profile.

(C)

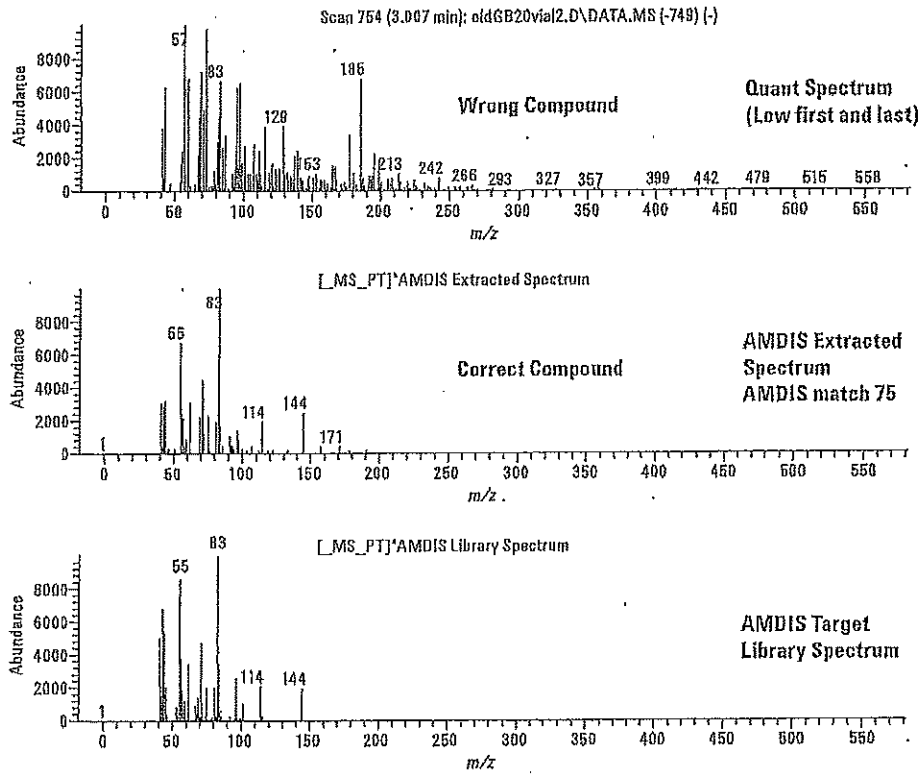

Figure 8C. Three meprobamate spectra presented in QEdit for comparison during data review using DRS A.04. (continued)

AMDIS extracted peak profile looks very similar to the peak profile in ion 62. If desired, the AMDIS extracted peak profile can be integrated for quantitation if the target ion has interference problems.

The best confirmation is provided by the deconvoluted spectrum. In Figure 8C are the three spectra presented in QEdit for comparison. The three spectra shown here were from the bleed optimized method. This method had incorrectly chosen the 3.007 peak as possibly being meprobamate, where the topmost spectrum is the spectrum at 3.007 minutes minus the spectrum five scans before, as the method uses "lowest first and last" as the subtraction method. Since the peak was found at the wrong retention time, the spectrum is of the wrong compound and of course does not match that of meprobamate. When searched against the NIST main library, meprobamate was not in the top 100 hits.

The middle spectrum is the deconvoluted component found by AMDIS. It has a match factor against the reference spectrum, shown in the bottom, of 75, confirming the presence of meprobamate. This example shows the utility of deconvolution in determining the presence of compounds that could easily be missed with the conventional approaches.

Conclusions

The system described here offers several advantages for screening toxicology samples. The advantages derive from a combination of techniques that result in both faster and more accurate screening results.

- Retention time locked target database of 725 compounds for screening with MS (G1674AA Forensic Toxicology DBL)

- CFT splitter – Use the NPD with MS data for added confirmation, find nontarget suspect compounds, and alternate quantitation
- SIM/Scan – Acquire SIM data on high-priority targets simultaneously with scan data. Saves time by eliminating need to run samples in both modes.
- DRS – Automated deconvolution increases accuracy of target identification, even in the most challenging matrices. The reduction of data interpretation from more than an hour to less than 10 minutes is especially useful.
- Fast chromatography using shorter columns, faster ovens, and backflushing to greatly reduce run times.

There is considerable advantage to using a single system that combines all of the techniques discussed. However, adding any of the above separately or in different combinations can also provide advantages. The most significant improvement can be gained by using DRS. The time savings in the data review step easily justifies the effort required to implement it.

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Appendix

Compound name	CAS number*
10,11-Dihydro-10-hydroxycarbazepine	999402-02-7
10,11-Dihydro-10-hydroxycarbazepine TMS	999423-02-8
10,11-Dihydrocarbamazepin	003564-73-6
5-Amino-2-chloropyridine	005350-93-6
5-Methoxy-dipropyltryptamine	999001-02-4
6-Acetyl-morphine	002784-73-8
6-Acetyl-morphine TMS	999155-02-1
7-Aminoflunitrazepam	034084-50-9
7-Aminoflunitrazepam TMS	999176-02-2
7-Hydroxyamoxapine	037081-76-8
8-Methoxyloxapine	070020-54-1
Acepromazine	000061-00-7
Acetaminophen	000103-90-2
Acetaminophen 2TMS	055530-61-5
Acetanilide	000103-84-4
Adiphenine	000064-95-9
Adiphenine-M/artifact (ME)	003469-00-9
Alfentanil	071195-58-9
Allobarbital	000052-43-7
Allopurinol TMS	999178-02-8
Alphaprodine	000077-20-3
Alphenal	000115-43-5
Alprazolam	028981-97-7
Alprenolol TMS	999381-02-1
Alverine	000150-59-4
Amantadine	000768-94-5
Amantadine AC	999127-02-5
Ambroxol	018683-91-5
Ambroxol 2AC	999341-02-5
Aminoglutethimide	000125-84-8
Aminopyrine	000058-15-1
Amitriptyline	000050-48-6
Amlodipine AC	999299-02-4
Amobarbital	000057-43-2
Amobarbital 2TMS	999179-02-1
Amoxapine	014028-44-5
Amoxapine AC	999128-02-8
Amphetamine	000060-15-1
Amphetamine AC	999107-02-7
Ampyrone	000083-07-8
Ampyrone AC	000083-15-8

Compound name	CAS number
Ampyrone-2AC	999240-02-7
Anhydroecgonine methyl ester	043021-26-7
Anileridine	000144-14-9
Anisindione	000117-37-3
Antazoline	000091-75-8
Antazoline AC	999408-02-5
Antipyrine	000060-80-0
Apomorphine 2TMS	074841-68-2
Aprobarbital	000077-02-1
Aprobarbital 2TMS	999180-02-8
Atenolol formyl artifact	999459-02-8
Atomoxetine	083015-26-3
Atomoxetine AC	999257-02-2
Atovaquone	953233-18-4
Atovaquone TMS	999409-02-8
Atropine	000051-55-8
Atropine TMS	065334-03-7
Azacyclonol	000115-46-8
Azatadine	003964-81-6
Barbital	000057-44-3
BDMPEA	066142-81-2
BDMPEA AC	999357-02-7
BDMPEA formyl artifact	999378-02-8
Bemegride	000064-65-3
Benzocaine	000094-09-7
Benzoylecgonine	000519-09-5
Benzoylecgonine TMS	999462-02-1
Benzphetamine	000156-08-1
Benzquinamide	000063-12-7
Benztropine	000086-13-5
Benzydamine	000642-72-8
Benzylpiperazine	002759-28-6
Benzylpiperazine AC	999129-02-1
Betahistine	005579-84-0
Betahistine AC	999439-02-0
Betaxolol	063659-18-7
Betaxolol formyl artifact	999436-02-1
Biperiden	000514-65-8
Bisacodyl	000603-50-9
Bisoprolol	066722-44-9
Bromazepam	001812-30-2

* Compounds for which a real CAS number could not be found were given a contrived one beginning with 999. These are not real CAS numbers.

Compound name	CAS number
Bromazepam TMS	999158-02-0
Bromdiphenhydramine	000118-23-0
Bromocriptine breakdown	025614-03-3
Bromperidol	010457-90-6
Brompheniramine	000086-22-6
Brucine	000357-57-3
Buclizine	000082-95-1
Bupivacaine	002180-92-9
Buprenorphine	052485-79-7
Buprenorphine TMS	999159-02-3
Bupropion	034911-55-2
Buspirone	036505-84-7
Butabarbital	000125-40-6
Butabarbital 2TMS	052988-92-8
Butacaine	000149-16-6
Butalbital	000077-26-9
Butalbital 2TMS	052937-70-9
Butethal	000077-28-1
Butorphanol	042408-82-2
Butorphanol TMS	100013-72-3
Caffeine	000058-08-2
Canrenone	000976-71-6
Canrenone TMS	999413-02-4
Cantharidin	000056-25-7
Carbamazepine	000298-46-4
Carbamazepine-M (formyl-acridine)	999243-02-6
Carbinoxamine	000486-16-8
Carbromal-M/artifact	999196-02-0
Carisoprodol	000078-44-4
Carisoprodol artifact	999401-02-4
Cathinone AC	999485-02-8
Celecoxib	169590-42-5
Cetirizine methanol adduct	083881-46-3
Cetirizine TMS	999183-02-7
Chlophedianol	000791-35-5
Chlophedianol TMS	999464-02-7
Chloramphenicol 2TMS	021196-84-9
Chlorcyclizine	000082-93-9
Chlordiazepoxide	000058-25-3
Chlordiazepoxide artifact (desoxo)	999197-02-3
Chlormezanone	000080-77-3

Compound name	CAS number
Chlormezanone artifact	999245-02-2
Chloroamphetamine	000064-12-0
Chloroamphetamine AC	999414-02-7
Chlorophenylpiperazine	038212-33-8
Chlorophenylpiperazine AC	999486-02-1
Chloroprocaine, 2-	000133-16-4
Chloroquine	000054-05-7
Chlorpheniramine	000132-22-9
Chlorphenisin	000104-29-0
Chlorphentermine	000461-78-9
Chlorphentermine AC	999130-02-8
Chlorpropamide artifact-2	999246-02-5
Chlorprothixene	000113-59-7
Chlorzoxazone	000095-25-0
Cholesterol	000057-88-5
Cholesterol TMS	001856-05-9
Cinnarizine	000298-57-7
Cisapride	081098-60-4
Citalopram	059729-33-8
Clemastine	015686-51-8
Clemizole	000442-52-4
Clenbuterol	037148-27-9
Clenbuterol AC	999360-02-0
Clobazam	022316-47-8
Clofibrate	000637-07-0
Clomipramine	000303-49-1
Clonazepam	001622-61-3
Clonazepam TMS	999184-02-0
Clonazepam-M (amino-)	004959-17-5
Clonazepam-M (amino) - TMS	999175-02-9
Clonidine	004205-90-7
Clonidine 2AC	999131-02-1
Clonidine AC	999132-02-4
Clopidogrel	113665-84-2
Clozapine	005786-21-0
Clozapine AC	999133-02-7
Cocaethylene	000529-38-4
Cocaine	000050-36-2
Codeine	000076-57-3
Codeine TMS	074367-14-9
Colchicine	000064-86-8

Compound name	CAS number
Colchicine breakdown	999532-02-4
Coniine	000458-88-8
Coniine AC	999361-02-3
Cotinine	000486-56-6
Cyclandelate	000456-59-7
Cyclandelate TMS	999442-02-3
Cyclizine	000082-92-8
Cyclobenzaprine	000303-53-7
Cyclophosphamide	000050-18-0
Cyclophosphamide -HCL	999379-02-1
Cyheptamide	007199-29-3
Cyproheptadine	000129-03-3
Dapsone	000080-08-0
Debrisoquine AC	999415-02-0
Desalkylflurazepam AC	999298-02-1
Desethylidocaine (MegX)	999044-02-9
Desethylidocaine AC (MegX)	999263-02-4
Desipramine	000050-47-5
Desipramine AC	999108-02-0
Desmethylclomipramine	000303-48-0
Desmethylclomipramine AC	999134-02-0
Desmethylclozapine	006104-71-8
Desmethyldoxepin (cis)	999516-02-8
Desmethyldoxepin (cis) AC	999517-02-1
Desmethyldoxepin (trans)	001225-56-5
Desmethyldoxepin (trans) AC	999443-02-6
Desmethylselegiline	999072-02-5
Desmethylselegiline AC	999147-02-3
Desmethylsertraline	091797-58-9
Desmethyltramadol, O-	999018-02-9
Desmethyltramadol, O- 2TMS	999444-02-9
Desmethyltrimipramine	999019-02-2
Desmethyltrimipramine AC	999445-02-2
Dextromethorphan	000125-71-3
Diacetylmorphine	000561-27-3
Diazepam	000439-14-5
Dichlorophene	000097-23-4
Dichlorophene TMS	999237-02-4
Diclofenac -H2O	999200-02-1
Diclofenac TMS	999222-02-5
Dicyclomine	000077-19-0

Compound name	CAS number
Diethyltryptamine	000061-51-8
Dihydrocodeine	000125-28-0
Dihydroxy-4-methylcoumarin, 7, 8 - TMS	999236-02-1
Diiodohydroxyquin	000083-73-8
Diltiazem	042399-41-7
Dimethadione	000695-53-4
Diphenadione	000082-66-6
Diphenhydramine	000058-73-1
Diphenidol	000972-02-1
Diphenidol TMS	999417-02-6
Diphenoxylate	000915-30-0
Diphenylpyraline	000147-20-6
Disopyramide	003737-09-5
Donepezil	120014-06-4
Dothiepin	000113-53-1
Doxapram	000309-29-5
Doxepin (cis)	999515-02-5
Doxepin (trans)	001668-19-5
Doxylamine	000469-21-6
Dyphylline	000479-18-5
Dyphylline TMS	999446-02-5
Ecgonine methyl ester	106293-60-1
Ecgonine methyl ester TMS	999162-02-6
Efavirenz	154598-52-4
Efavirenz AC	999489-02-0
Efavirenz TMS	999505-02-1
Emetine	000483-18-1
Encainide	999034-02-5
Ephedrine	000299-42-3
Ephedrine 2AC	055133-90-9
Epinephrine AC	999111-02-3
Ergonovine AC	999447-02-8
Estazolam	029975-16-4
Ethacrynic Acid TMS	999227-02-0
Ethambutol AC	999261-02-8
Ethamivan	000304-84-7
Ethinamate	000126-52-3
Ethopropazine	000522-00-9
Ethosuximide	000077-67-8
Ethotoin	000086-35-1
Ethyl-2-malonamide, 2-	068692-83-1

Compound name	CAS number
Ethyl-2-malonamide, 2- TMS	999418-02-9
Ethylamphetamine	000457-87-4
Ethylamphetamine AC	999148-02-6
Ethylecgonine	999037-02-4
Ethylecgonine TMS	999448-02-1
Ethylmorphine	000076-58-4
Ethylmorphine TMS	999221-02-2
Etodolac TMS	999212-02-1
Etofylline	000519-37-9
Etofylline TMS	077630-35-4
Etomidate	033125-97-2
Eucatropine isomer 1	999038-02-7
Eucatropine isomer 1 TMS	999278-02-3
Eucatropine isomer 2	999277-02-0
Eucatropine isomer 2 TMS	999518-02-4
Felbamate artifact 1	999250-02-1
Felbamate artifact 2	999251-02-4
Felbamate artifact 3	999252-02-7
Felodipine	072509-76-3
Felodipine-M/artifact (dehydro-)	999296-02-5
Fenfluramine	000458-24-2
Fenfluramine AC	999139-02-5
Fenoprofen	031879-05-7
Fenoprofen TMS	999310-02-0
Fentanyl	000437-38-7
Finasteride	098319-26-7
Flavoxate	015301-69-6
Flavoxate-M/artifact (HOOC-) ME	999279-02-6
Flecainide	054143-55-4
Flecainide AC	999140-02-2
Flumazenil	078755-81-4
Flunarizine	052468-60-7
Flunitrazepam	001622-62-4
Fluoxetine	054910-89-3
Fluoxetine AC	999141-02-5
Flupenthixol	002709-56-0
Flupentixol TMS	999387-02-9
Fluphenazine	000069-23-8
Fluphenazine TMS	999280-02-3
Fluphenazine-M (ring)	000092-30-8
Flurazepam	017617-23-1

Compound name	CAS number
Flurazepam-M (desalkyl-)	002886-65-9
Flurazepam-M (HO-ethyl-)	020971-53-3
Flurbiprofen	005104-49-4
Flutamide	013311-84-7
Flutamide TMS	999467-02-6
Fluvoxamine	054739-18-3
Fluvoxamine AC	999262-02-1
Furazolidone	000067-45-8
Furosemide 2TMS	999214-02-7
Gemfibrozil	025812-30-0
Gemfibrozil AC	999389-02-5
Glutethimide	000077-21-4
Griseofulvin	000126-07-8
Guaifenesin	000093-14-1
Guaifenesin 2TMS	107966-19-8
Guanethidine	000055-65-2
Haloperidol	000052-86-8
Harmaline	000304-21-2
Harmaline AC	999301-02-9
Harmine	000442-51-3
Hexobarbital	000056-29-1
Hexobarbital TMS	999469-02-2
Hexylresorcinol	000136-77-6
Hexylresorcinol 3TMS	999422-02-5
Homatropine	000087-00-3
Homatropine TMS	999282-02-9
Hydrastine	000118-08-1
Hydrocodone	000125-29-1
Hydromorphone	000466-99-9
Hydromorphone enol 2TMS	999513-02-9
Hydromorphone TMS	221209-08-1
Hydroxychloroquine AC	999512-02-6
Hydroxyethylflurazepam TMS	999204-02-3
Hydroxyloxapine, 8-	999053-02-0
Hydroxyzine	000068-88-2
Hydroxyzine AC	999113-02-9
Ibuprofen	015687-27-1
Ibuprofen TMS	999165-02-5
Iminostilbene	000256-96-2
Imipramine	000050-49-7
Indomethacin TMS	999318-02-4

Compound name	CAS number
Isocarboxazid	000059-63-2
Isometheptene AC	999265-02-0
Isoniazid	000054-85-3
Isoniazid 2AC	999266-02-3
Isoniazid AC	999254-02-3
Isoproterenol 2TMS	999424-02-1
Isoxsuprine	000395-28-8
Isoxsuprine TMS	999319-02-7
Ketamine	006740-88-1
Ketamine AC	999114-02-2
Ketoprofen TMS	999320-02-4
Ketorolac TMS	999215-02-0
Ketotifen	034580-13-7
Lamotrigine	084057-84-1
Lamotrigine 2AC	999255-02-6
Laudanosine	020412-65-1
Levallorphan	000152-02-3
Levallorphan TMS	999321-02-7
Levetiracetam	102767-28-2
Levorphanol	000077-07-6
Levorphanol TMS	999223-02-8
Lidocaine	000137-58-6
Loratadine	079794-75-5
Lorazepam	000846-49-1
Lorazepam 2TMS	999202-02-7
Lorcainide	059729-31-6
Lormetazepam	000848-75-9
Loxapine	001977-10-2
Ly170222	999123-02-3
Lysergide (LSD)	000050-37-3
Maprotiline	010262-69-8
Maprotiline AC	999366-02-8
Mazindol	022232-71-9
MBDB	100031-29-2
MBDB AC	999142-02-8
Mecamylamine	000060-40-2
Mecilzine	000569-65-3
Meclofenamic acid TMS	999322-02-0
Medazepam	002898-12-6
Mefenamic acid TMS	999324-02-6
Mefloquine	053230-10-7

Compound name	CAS number
Memantine	019982-08-2
Memantine AC	999115-02-5
Meperidine	000057-42-1
Mephenesin	000059-47-2
Mephenesin 2TMS	999325-02-9
Mephentermine	000100-92-5
Mephentermine AC	999143-02-1
Mephenytoin	000050-12-4
Mephobarbital	000115-38-8
Mepivacaine	000096-88-8
Meprobamate	000057-53-4
Mescaline	000054-04-6
Mescaline AC	999511-02-3
Mescaline formyl artifact	999284-02-5
Mesuximide-M (nor)	001497-17-2
Metaproterenol AC	999391-02-5
Metaxalone	001665-48-1
Metaxalone AC	999116-02-8
Methadone	000076-99-3
Methadone-M (EDDP)	999058-02-5
Methamphetamine	000537-46-2
Methamphetamine AC	999117-02-1
Methapyrilene	000091-80-5
Methaqualone	000072-44-6
Metharbital	000050-11-3
Metharbital TMS	999186-02-6
Methazolamide	000554-57-4
Methcathinone AC	999300-02-6
Methcathinone-M (HO-) 2AC	005650-44-2
Methdilazine	001982-37-2
Methimazole	000060-56-0
Methimazole AC	999368-02-4
Methocarbamol 2TMS	999285-02-8
Methohexital	000151-83-7
Methohexital TMS	999425-02-4
Methotrimeprazine	000060-99-1
Methoxyverapamil	016662-47-8
Methsuximide	000077-41-8
Methylaminorex, 4-	029493-77-4
Methylaminorex, 4- 2AC	999508-02-0
Methylaminorex, 4- AC	999510-02-0

Compound name	CAS number
Methylenedioxyamphetamine AC	999479-02-6
Methylenedioxyamphetamine (MDA)	004764-17-4
Methylenedioxyethylamphetamine	014089-52-2
Methylenedioxyethylamphetamine AC	999481-02-6
Methylenedioxymethamphetamine AC	999480-02-3
Methylenedioxymethamphetamine (MDMA)	042542-10-9
Methylephedrine	000552-79-4
Methylephedrine AC	999370-02-4
Methyl-nicotine	999065-02-0
Methylphenidate	000113-45-1
Methylphenidate AC	999144-02-4
Methylphenobarbital	999509-02-3
Methylprimidone	059026-32-3
Methylprimidone 2TMS	999286-02-1
Methyprylon	000125-64-4
Metoclopramide	000364-62-5
Metoclopramide AC	999145-02-7
Metoprolol 2AC	999306-02-4
Metronidazole	000443-48-1
Metronidazole TMS	999450-02-1
Mexiletine	031828-71-4
Mexiletine AC	999146-02-0
Mianserin	024219-97-4
Mianserin-M (nor-)	999015-02-0
Mianserin-M (nor-) AC	999364-02-2
Midazolam	059467-70-8
Mirtazapine	061337-67-5
Moclobemide	071320-77-9
Molindone	007416-34-4
Morphine	000057-27-2
Morphine 2TMS	055449-66-6
Muconic acid TMS	999166-02-8
N,N-Dimethyl-5-methoxy-tryptamine	001019-45-0
N,N-Dimethyltryptamine	000061-50-7
Nabumetone	042924-53-8
N-Acetylprocainamide	999070-02-9
Nadolol 3TMS	999287-02-4
Nalbuphine	020594-83-6
Nalbuphine 2TMS	999167-02-1
Nalidixic acid	000389-08-2
Nalidixic acid TMS	999238-02-7

Compound name	CAS number
Nalorphine	000062-67-9
Nalorphine 2TMS	999473-02-8
Naloxone	000465-65-6
Naloxone TMS	999427-02-0
Naltrexol, beta-	999406-20-9
Naltrexol, beta- 2TMS	999405-02-6
Naltrexol, beta- 3TMS	999520-02-4
Naltrexone	016590-41-3
Naltrexone 2TMS	999328-02-8
Naltrexone 3TMS	999523-02-3
Naltrexone TMS	999522-02-0
Naproxen ME	999295-02-2
Naproxen TMS	074793-83-2
Nevirapine	129618-40-2
Nevirapine TMS	999451-02-4
Niclosamide	000050-65-7
Nicotinamide	000098-92-0
Nicotine	000054-11-5
Nifedipine	021829-25-4
Nikethamide	000059-26-7
Nimodipine	066085-59-4
Nimodipine-M/artifact	999340-02-2
Nitrazepam	000146-22-5
Nitrazepam TMS	999288-02-7
Nomifensine	024526-64-5
Nomifensine AC	999371-02-7
Noralfentanil	061086-18-8
Noralfentanil AC	999150-02-6
Norchlordiazepoxide	016300-25-7
Norchlordiazepoxide AC	999525-02-9
Norchlordiazepoxide breakdown	999524-02-6
Norchlordiazepoxide breakdown AC	999372-02-0
Norclozapine 2AC	999135-02-3
Norclozapine AC	999136-02-6
Norcodeine	000467-15-2
Norcodeine 2AC	999118-02-4
Nordiazepam	001088-11-5
Nordiazepam TMS	999207-02-2
Norepinephrine 2AC	999119-02-7
Norepinephrine 3AC	999528-02-8
Norfenfluramine	001886-26-6

Compound name	CAS number
Norfenfluramine AC	999120-02-4
Norfentanyl	999076-02-7
Norfentanyl AC	999272-02-5
Norfluoxetine	999077-02-0
Norfluoxetine AC	999121-02-7
Norketamine	999078-02-3
Norketamine AC	999494-02-9
Normeperidine	000077-17-8
Normeperidine AC	999122-02-0
Normetanephrine AC	999373-02-3
Normethsuximide TMS	999429-02-6
Noroxycodone	057664-96-7
Noroxycodone AC	999495-02-2
Norpropoxyphene	999079-02-6
Norpropoxyphene breakdown 1	999530-02-8
Norpropoxyphene breakdown 2	999531-02-1
Norpropoxypheneamide	999080-02-3
Norpseudoephedrine	000492-41-1
Norpseudoephedrine AC	999081-02-6
Norpseudoephedrine artifact	999478-02-3
Nortriptyline	000072-69-5
Nortriptyline AC	999151-02-9
Norvenlafaxine	130198-38-8
Norverapamil	067018-85-3
Norverapamil AC	999488-02-7
Olanzapine	132539-06-1
Opipramol TMS	999226-02-7
Orphenadrine	000083-98-7
Ortho-cotinine	999083-02-2
Oxazepam	000604-75-1
Oxazepam 2TMS	999168-02-4
Oxcarbamazepine	028721-07-5
Oxprenolol 2AC	999374-02-6
Oxybutynin	005633-20-5
Oxycodone	000076-42-6
Oxycodone enol 2TMS	999514-02-2
Oxycodone TMS	221209-10-5
Oxymorphone	000076-41-5
Oxymorphone 2TMS	999521-02-7
Oxymorphone TMS	999208-02-5
Papaverine	000058-74-2

Compound name	CAS number
Paramethadione	000115-67-3
Pargyline	000555-57-7
Paroxetine	061869-08-7
Paroxetine AC	999124-02-6
Pemoline	002152-34-3
Pentachlorophenol	000087-86-5
Pentazocine	000359-83-1
Pentazocine TMS	100013-72-2
Pentobarbital	000076-74-4
Pentobarbital 2TMS	052937-68-5
Pentoxifylline	006493-05-6
Pentylenetetrazole	000054-95-5
Pergolide	066104-22-1
Perphenazine TMS	999291-02-0
Phenacemide	000063-98-9
Phenacetin	000062-44-2
Phenacetin AC	999496-02-5
Phenacetin TMS	999504-02-8
Phenazopyridine	000094-78-0
Phenazopyridine AC	999303-02-5
Phencyclidine	000077-10-1
Phencyclidine artifact	000771-98-2
Phendimetrazine	000634-03-7
Phenelzine AC	999304-02-8
Phenindione	000083-12-5
Pheniramine	000086-21-5
Phenmetrazine	000134-49-6
Phenmetrazine AC	999090-02-7
Phenobarbital	000050-06-6
Phenobarbital 2TMS	052937-73-2
Phenolphthalein	000077-09-8
Phenolphthalein 2TMS	999292-02-3
Phenoxybenzamine	000059-96-1
Phensuximide	000086-34-0
Phentermine	000122-09-8
Phentermine AC	999152-02-2
Phenylacetamide	000103-81-1
Phenylbutazone	000050-33-9
Phenylbutazone artifact	999338-02-2
Phenylbutazone artifact TMS	999198-02-6
Phenylbutazone TMS	074810-87-0

Compound name	CAS number
Phenylephrine 3AC	999091-02-0
Phenylethylamine, beta-	000064-04-0
Phenylethylamine, beta AC	999343-02-1
Phenylpropanolamine	999498-02-1
Phenylpropanolamine AC	999092-02-3
Phenyltoloxamine	000092-12-6
Phenytoin	000057-41-0
Phenytoin 2TMS	063435-72-3
Pilocarpine	000092-13-7
Pindolol	013523-86-9
Pindolol formyl artifact	999458-02-5
PMA TMS	999172-02-0
p-Methoxyamphetamine	000064-13-1
Prazepam	002955-38-6
Prilocaine	000721-50-6
Primidone	000125-33-7
Probenecid TMS	999294-02-9
Procainamide	000051-06-9
Procaine	000059-46-1
Prochlorperazine	000058-38-8
Procyclidine	000077-37-2
Procyclidine artifact (dehydro-)	999460-02-5
Procyclidine TMS	999454-02-3
Promazine	000058-40-2
Promethazine	000060-87-7
Propantheline bromide	000050-34-0
Propiomazine	000362-29-8
Propofol	002078-54-8
Propoxur	000114-26-1
Propoxur-M/artifact	999393-02-1
Propoxyphene	000469-62-5
Propylamphetamine	051799-32-7
Propylamphetamine AC	999302-02-2
Protriptyline	000438-60-8
Protriptyline AC	999273-02-6
Pseudoephedrine	000090-82-4
Pseudoephedrine 2AC	999500-02-6
Pseudoephedrine formyl artifact	999483-02-2
Psilocin 2TMS	999192-02-8
Psilocybin 3TMS	999193-02-1
Pyrazinamide	000098-96-4

Compound name	CAS number
Pyrilamine	000091-84-9
Pyrimethamine	000058-14-0
Quetiapine	999097-02-8
Quetiapine TMS	999527-02-5
Quinacrine	000083-89-6
Quinidine	000056-54-2
Quinine	000130-95-0
Ramelteon	999274-02-1
Reboxetine	098769-81-4
Ritodrine 3TMS	999218-02-9
Rofecoxib	162011-90-7
Ropivacaine	132112-35-7
Salbutamol 3TMS	999394-02-4
Salicylamide	000065-45-2
Salicylamide 2TMS	055887-58-6
Salicylic acid 2TMS	003789-85-3
Salicylic acid ethylester	000118-61-6
Salicylic acid methylester	000119-36-8
Scopolamine	000051-34-3
Scopolamine TMS	999194-02-4
Secobarbital	000076-73-3
Secobarbital 2TMS	052937-71-0
Selegiline	014611-51-9
Selegiline-M (HO-) AC	999482-02-9
Sertraline	079617-96-2
Sertraline AC	999125-02-9
Sertraline-M (nor-) AC	999109-02-3
Sildenafil TMS	999213-02-4
SKF-525a	000302-33-0
Strychnine	000057-24-9
Sufentanil	056030-54-7
Sulfadiazine	000068-35-9
Sulfadimethoxine	000122-11-2
Sulfamethazine	000057-68-1
Sulfamethazine AC	999501-02-9
Sulfamethoxazole	000723-46-6
Sulfanilamide	000063-74-1
Sulfapyridine	000144-83-2
Sulfathiazole	000072-14-0
Sulfinpyrazone	000057-96-5
Tacrine	000321-64-2

Compound name	CAS number
Talbutal	000115-44-6
Tamoxifen	010540-29-1
Temazepam	000846-50-4
Temazepam artifact-2	020927-53-1
Temazepam TMS	035147-95-6
Terbinafine	091161-71-6
Terfenadine TMS	999220-02-9
Teriflunomide AC	999502-02-2
Tetracaine	000094-24-6
Tetrahydrocannabinol	001972-08-3
Tetrahydrocannabinol TMS	999529-02-1
Tetrahydrozoline	000084-22-0
Tetrahydrozoline AC	999398-02-6
Thebaine	000115-37-7
Theobromine	000083-67-0
Theophylline	000058-55-9
Thiamylal	000077-27-0
Thiethylperazine	001420-55-9
Thiopental	000076-75-5
Thioridazine	000050-52-2
Thonzylamine	000091-85-0
Ticlopidine	055142-85-3
Tiletamine	014176-49-9
Timolol TMS	999399-02-9
Tocainide	041708-72-9
Tocainide AC	999375-02-9
Tolazoline	000059-98-3
Topiramate artifact ($-SO_2NH$)	020880-92-6
Topiramate breakdown	097240-79-4
Tramadol	027203-92-5
Tramadol TMS	999336-02-6
Tranylcypromine	000155-09-9
Tranylcypromine AC	999305-02-1
Trazodone	019794-93-5
Triamterene	000396-01-0

Compound name	CAS number
Triazolam	028911-01-5
Trifluoperazine	000117-89-5
Triflupromazine	000146-54-3
Trihexyphenidyl	000144-11-6
Trimeprazine	000084-96-8
Trimethobenzamide	000138-56-7
Trimethoprim	000738-70-5
Trimipramine	000739-71-9
Tripelenamine	000091-81-6
Triprolidine	000486-12-4
Tropacocaine	000537-26-8
Tryptamine	000061-54-1
Tryptamine 2AC	999352-02-2
Tryptamine AC	999353-02-5
Tryptophan, D- AC	999519-02-7
Valproic acid	000099-66-1
Venlafaxine	093413-69-5
Venlafaxine TMS	999173-02-3
Verapamil	000052-53-9
Vigabatrin AC	999376-02-2
Warfarin	000081-81-2
Warfarin artifact	000122-57-6
Warfarin TMS	036307-79-6
Xanthinol TMS	999239-02-0
Xylazine	007361-61-7
Yohimbine	000146-48-5
Yohimbine TMS	999457-02-2
Zaleplon	151319-34-5
Zolazepam	031352-82-6
Zolpidem	082626-48-0
Zomepirac $-CO_2$	999355-02-1
Zonisamide	068291-97-4
Zonisamide AC	999354-02-8
Zopiclone	043200-80-2
Zotepine	026615-21-4

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Printed in the USA
May 13, 2008
5989-8582EN

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