



State of West Virginia  
 Department of Administration  
 Purchasing Division  
 2019 Washington Street East  
 Post Office Box 50130  
 Charleston, WV 25305-0130

# Request for Quotation

|            |
|------------|
| RFQ NUMBER |
| LBS10081   |

|      |
|------|
| PAGE |
| 1    |

|                                        |
|----------------------------------------|
| ADDRESS CORRESPONDENCE TO ATTENTION OF |
| ROBERTA WAGNER<br>304-558-0067         |

RFQ COPY  
 TYPE NAME/ADDRESS HERE  
 Agilent Technologies Inc  
 2850 Centerville Road  
 Wilmington, DE 19808

SHIP TO  
 HEALTH AND HUMAN RESOURCES  
 ENVIRONMENTAL CHEMISTRY LAB  
 4710 CHIMNEY DRIVE  
 CHARLESTON, WV  
 25302 304-558-3530

| DATE PRINTED | TERMS OF SALE | SHIP VIA | F.O.B. | FREIGHT TERMS |
|--------------|---------------|----------|--------|---------------|
| 02/09/2010   |               |          |        |               |

BID OPENING DATE: 03/11/2010 BID OPENING TIME 01:30PM

| LINE                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       | QUANTITY | UOP | CAT NO | ITEM NUMBER                                   | UNIT PRICE | AMOUNT |
|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------|-----|--------|-----------------------------------------------|------------|--------|
| 0001                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       | 1        | EA  |        | 490-55                                        |            |        |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |          |     |        | GAS CHROMATOGRAPH - MASS SPECTROMETER (GC-MS) |            |        |
| <p>REQUEST TO PURCHASE ONE GAS CHROMATOGRAPH - MASS SPECTROMETER (GC-MS) TO ANALYZE FOR TRIHALOMETHANES (THMS) AND VOLATILE ORGANIC CHEMICALS (VOCs) IN DRINKING WATER TO FULFILL THE REQUIREMENTS OF THE UNITED STATES ENVIRONMENTAL PROTECTION AGENCY (EPA) REGULATIONS FOR COMPLIANCE MONITORING OF PUBLIC WATER SYSTEMS, PER THE ATTACHED SPECIFICATIONS. COMPLIANCE MONITORING TESTING IS REQUIREMENT OF A STATE'S PRINCIPAL LABORATORY MANDATED UNDER FEDERAL CODE AT 40 CFR 142.10(B)(4) FOR THE STATE TO MAINTAIN PRIMACY OVER IT'S DRINKING WATER PROGRAM.</p> <p>THE INSTRUMENT WILL ALSO SERVE THE PURPOSE OF PROTECTING PUBLIC HEALTH BY PROVIDING TESTING CAPABILITIES TO PRIVATE WELL OWNERS.</p> <p>THIS INSTRUMENT IS TO BE INSTALLED FOR USE BY THE OFFICE OF LABORATORY SERVICES ENVIRONMENTAL CHEMISTRY LABORATORY AT 4710 CHIMNEY DRIVE, SUITE G, CHARLESTON, WEST VIRGINIA 25302.</p> <p>&gt;&gt; PLEASE SEE ATTACHED SPECIFICATIONS/COST SHEET. &lt;&lt;</p> <p>CANCELLATION: THE DIRECTOR OF PURCHASING RESERVES THE RIGHT TO CANCEL THIS CONTRACT IMMEDIATELY UPON WRITTEN NOTICE TO THE VENDOR IF THE COMMODITIES AND/OR SERVICES SUPPLIED ARE OF AN INFERIOR QUALITY OR DO NOT CONFORM TO THE SPECIFICATIONS OF THE BID AND CONTRACT HEREIN.</p> |          |     |        |                                               |            |        |

RECEIVED  
 2010 MAR -5 AM 9:51  
 WVA PURCHASING DIVISION

|                                           |           |                                   |
|-------------------------------------------|-----------|-----------------------------------|
| SEE REVERSE SIDE FOR TERMS AND CONDITIONS |           |                                   |
| SIGNATURE                                 | TELEPHONE | DATE                              |
| TITLE                                     | FEIN      | ADDRESS CHANGES TO BE NOTED ABOVE |

WHEN RESPONDING TO RFQ, INSERT NAME AND ADDRESS IN SPACE ABOVE LABELED 'VENDOR'

**GENERAL TERMS & CONDITIONS**  
**REQUEST FOR QUOTATION (RFQ) AND REQUEST FOR PROPOSAL (RFP)**

1. Awards will be made in the best interest of the State of West Virginia.
2. The State may accept or reject in part, or in whole, any bid.
3. Prior to any award, the apparent successful vendor must be properly registered with the Purchasing Division and have paid the required \$125 fee.
4. All services performed or goods delivered under State Purchase Order/Contracts are to be continued for the term of the Purchase Order/Contracts, contingent upon funds being appropriated by the Legislature or otherwise being made available. In the event funds are not appropriated or otherwise available for these services or goods this Purchase Order/Contract becomes void and of no effect after June 30.
5. Payment may only be made after the delivery and acceptance of goods or services.
6. Interest may be paid for late payment in accordance with the *West Virginia Code*.
7. Vendor preference will be granted upon written request in accordance with the *West Virginia Code*.
8. The State of West Virginia is exempt from federal and state taxes and will not pay or reimburse such taxes.
9. The Director of Purchasing may cancel any Purchase Order/Contract upon 30 days written notice to the seller.
10. The laws of the State of West Virginia and the *Legislative Rules* of the Purchasing Division shall govern the purchasing process.
11. Any reference to automatic renewal is hereby deleted. The Contract may be renewed only upon mutual written agreement of the parties.
12. **BANKRUPTCY:** In the event the vendor/contractor files for bankruptcy protection, the State may deem this contract null and void, and terminate such contract without further order.
13. **HIPAA BUSINESS ASSOCIATE ADDENDUM:** The West Virginia State Government HIPAA Business Associate Addendum (BAA), approved by the Attorney General, is available online at [www.state.wv.us/admin/purchase/vrc/hipaa.htm](http://www.state.wv.us/admin/purchase/vrc/hipaa.htm) and is hereby made part of the agreement. Provided that the Agency meets the definition of a Cover Entity (45 CFR §160.103) and will be disclosing Protected Health Information (45 CFR §160.103) to the vendor.
14. **CONFIDENTIALITY:** The vendor agrees that he or she will not disclose to anyone, directly or indirectly, any such personally identifiable information or other confidential information gained from the agency, unless the individual who is the subject of the information consents to the disclosure in writing or the disclosure is made pursuant to the agency's policies, procedures, and rules. Vendor further agrees to comply with the Confidentiality Policies and Information Security Accountability Requirements, set forth in <http://www.state.wv.us/admin/purchase/privacy/noticeConfidentiality.pdf>.
15. **LICENSING:** Vendors must be licensed and in good standing in accordance with any and all state and local laws and requirements by any state or local agency of West Virginia, including, but not limited to, the West Virginia Secretary of State's Office, the West Virginia Tax Department, and the West Virginia Insurance Commission. The vendor must provide all necessary releases to obtain information to enable the director or spending unit to verify that the vendor is licensed and in good standing with the above entities.
16. **ANTITRUST:** In submitting a bid to any agency for the State of West Virginia, the bidder offers and agrees that if the bid is accepted the bidder will convey, sell, assign or transfer to the State of West Virginia all rights, title and interest in and to all causes of action it may now or hereafter acquire under the antitrust laws of the United States and the State of West Virginia for price fixing and/or unreasonable restraints of trade relating to the particular commodities or services purchased or acquired by the State of West Virginia. Such assignment shall be made and become effective at the time the purchasing agency tenders the initial payment to the bidder.

I certify that this bid is made without prior understanding, agreement, or connection with any corporation, firm, limited liability company, partnership, or person or entity submitting a bid for the same material, supplies, equipment or services and is in all respects fair and without collusion or fraud. I further certify that I am authorized to sign the certification on behalf of the bidder or this bid.

**INSTRUCTIONS TO BIDDERS**

1. Use the quotation forms provided by the Purchasing Division. Complete all sections of the quotation form.
2. Items offered must be in compliance with the specifications. Any deviation from the specifications must be clearly indicated by the bidder. Alternates offered by the bidder as EQUAL to the specifications must be clearly defined. A bidder offering an alternate should attach complete specifications and literature to the bid. The Purchasing Division may waive minor deviations to specifications.
3. Unit prices shall prevail in case of discrepancy. All quotations are considered F.O.B. destination unless alternate shipping terms are clearly identified in the quotation.
4. All quotations must be delivered by the bidder to the office listed below prior to the date and time of the bid opening. Failure of the bidder to deliver the quotations on time will result in bid disqualifications: Department of Administration, Purchasing Division, 2019 Washington Street East, P.O. Box 50130, Charleston, WV 25305-0130
5. Communication during the solicitation, bid, evaluation or award periods, except through the Purchasing Division, is strictly prohibited (W.Va. C.S.R. §148-1-6.6).



State of West Virginia  
 Department of Administration  
 Purchasing Division  
 2019 Washington Street East  
 Post Office Box 50130  
 Charleston, WV 25305-0130

# Request for Quotation

RFQ NUMBER  
**LBS10081**

PAGE  
**2**

ADDRESS CORRESPONDENCE TO ATTENTION OF  
**ROBERTA WAGNER  
 304-558-0067**

VENDOR

RFQ COPY  
 TYPE NAME/ADDRESS HERE

SHIP TO

**HEALTH AND HUMAN RESOURCES  
 ENVIRONMENTAL CHEMISTRY LAB  
 4710 CHIMNEY DRIVE  
 CHARLESTON, WV  
 25302 304-558-3530**

| DATE PRINTED | TERMS OF SALE | SHIP VIA | F.O.B. | FREIGHT TERMS |
|--------------|---------------|----------|--------|---------------|
| 02/09/2010   |               |          |        |               |

BID OPENING DATE: **03/11/2010** BID OPENING TIME **01:30PM**

| LINE                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 | QUANTITY | UOP | CAT NO | ITEM NUMBER | UNIT PRICE | AMOUNT |
|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------|-----|--------|-------------|------------|--------|
| <p><b>BANKRUPTCY: IN THE EVENT THE VENDOR/CONTRACTOR FILES FOR BANKRUPTCY PROTECTION, THE STATE MAY DEEM THE CONTRACT NULL AND VOID, AND TERMINATE SUCH CONTRACT WITHOUT FURTHER ORDER.</b></p> <p><b>INQUIRIES: WRITTEN QUESTIONS SHALL BE ACCEPTED THROUGH CLOSE OF BUSINESS ON 02/23/2010. QUESTIONS MAY BE SENT VIA USPS, FAX, COURIER OR E-MAIL. IN ORDER TO ASSURE NO VENDOR RECEIVES AN UNFAIR ADVANTAGE, NO SUBSTANTIVE QUESTIONS WILL BE ANSWERED ORALLY. IF POSSIBLE, E-MAIL QUESTIONS ARE PREFERRED. ADDRESS INQUIRIES TO:</b></p> <p><b>ROBERTA WAGNER<br/>           DEPARTMENT OF ADMINISTRATION<br/>           PURCHASING DIVISION<br/>           2019 WASHINGTON STREET, EAST<br/>           CHARLESTON, WV 25311</b></p> <p><b>FAX: 304-558-4115<br/>           E-MAIL: ROBERTA.A.WAGNER@WV.GOV</b></p> <p><b>THE MODEL/BRAND/SPECIFICATIONS NAMED HEREIN ESTABLISH THE ACCEPTABLE LEVEL OF QUALITY ONLY AND ARE NOT INTENDED TO REFLECT A PREFERENCE OR FAVOR ANY PARTICULAR BRAND OR VENDOR. VENDORS WHO ARE BIDDING ALTERNATES SHOULD SO STATE AND INCLUDE PERTINENT LITERATURE AND SPECIFICATIONS. FAILURE TO PROVIDE INFORMATION FOR ANY ALTERNATES MAY BE GROUNDS FOR</b></p> |          |     |        |             |            |        |

SEE REVERSE SIDE FOR TERMS AND CONDITIONS

|           |           |                                   |
|-----------|-----------|-----------------------------------|
| SIGNATURE | TELEPHONE | DATE                              |
| TITLE     | FEIN      | ADDRESS CHANGES TO BE NOTED ABOVE |

WHEN RESPONDING TO RFQ, INSERT NAME AND ADDRESS IN SPACE ABOVE LABELED 'VENDOR'



State of West Virginia  
 Department of Administration  
 Purchasing Division  
 2019 Washington Street East  
 Post Office Box 50130  
 Charleston, WV 25305-0130

# Request for Quotation

RFQ NUMBER  
**LBS10081**

PAGE  
**3**

ADDRESS CORRESPONDENCE TO ATTENTION OF  
**ROBERTA WAGNER**  
**304-558-0067**

RFQ COPY  
 TYPE NAME/ADDRESS HERE

VENDOR

SHIP TO

**HEALTH AND HUMAN RESOURCES**  
**ENVIRONMENTAL CHEMISTRY LAB**  
  
**4710 CHIMNEY DRIVE**  
**CHARLESTON, WV**  
**25302 304-558-3530**

| DATE PRINTED | TERMS OF SALE | SHIP VIA | FOB | FREIGHT TERMS |
|--------------|---------------|----------|-----|---------------|
| 02/09/2010   |               |          |     |               |

BID OPENING DATE: **03/11/2010**      BID OPENING TIME: **01:30PM**

| LINE                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | QUANTITY | UOP | CAT NO | ITEM NUMBER | UNIT PRICE | AMOUNT |
|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------|-----|--------|-------------|------------|--------|
| <p>REJECTION OF THE BID. THE STATE RESERVES THE RIGHT TO WAIVE MINOR IRREGULARITIES IN BIDS OR SPECIFICATIONS IN ACCORDANCE WITH SECTION 148-1-4(F) OF THE WEST VIRGINIA LEGISLATIVE RULES AND REGULATIONS.</p> <p>NOTICE</p> <p>A SIGNED BID MUST BE SUBMITTED TO:</p> <p>DEPARTMENT OF ADMINISTRATION<br/>           PURCHASING DIVISION<br/>           BUILDING 15<br/>           2019 WASHINGTON STREET, EAST<br/>           CHARLESTON, WV 25305-0130</p> <p>PLEASE NOTE: A CONVENIENCE COPY WOULD BE APPRECIATED.</p> <p>THE BID SHOULD CONTAIN THIS INFORMATION ON THE FACE OF THE ENVELOPE OR THE BID MAY NOT BE CONSIDERED:</p> <p>SEALED BID</p> <p>BUYER: -----RW/FILE 22-----</p> <p>RFQ. NO.: -----LBS10081-----</p> <p>BID OPENING DATE: --- 3/11/2010-----</p> <p>BID OPENING TIME: --- 1:30 PM-----</p> <p>PLEASE PROVIDE A FAX NUMBER IN CASE IT IS NECESSARY TO CONTACT YOU REGARDING YOUR BID: 302-993-5941</p> |          |     |        |             |            |        |

SEE REVERSE SIDE FOR TERMS AND CONDITIONS

|           |           |                                   |
|-----------|-----------|-----------------------------------|
| SIGNATURE | TELEPHONE | DATE                              |
| TITLE     | FEIN      | ADDRESS CHANGES TO BE NOTED ABOVE |

WHEN RESPONDING TO RFQ, INSERT NAME AND ADDRESS IN SPACE ABOVE LABELED 'VENDOR'



State of West Virginia  
 Department of Administration  
 Purchasing Division  
 2019 Washington Street East  
 Post Office Box 50130  
 Charleston, WV 25305-0130

# Request for Quotation

RFQ NUMBER:  
**LBS10081**

PAGE:  
**4**

ADDRESS CORRESPONDENCE TO ATTENTION OF:  
**ROBERTA WAGNER  
 304-558-0067**

VENDOR

RFQ COPY  
 TYPE NAME/ADDRESS HERE

SHIP TO

**HEALTH AND HUMAN RESOURCES  
 ENVIRONMENTAL CHEMISTRY LAB  
 4710 CHIMNEY DRIVE  
 CHARLESTON, WV  
 25302 304-558-3530**

| DATE PRINTED | TERMS OF SALE | SHIP VIA | F.O.B. | FREIGHT TERMS |
|--------------|---------------|----------|--------|---------------|
| 02/09/2010   |               |          |        |               |

BID OPENING DATE: **03/11/2010** BID OPENING TIME **01:30PM**

| LINE                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | QUANTITY | UOP | CAT NO | ITEM NUMBER | UNIT PRICE | AMOUNT      |
|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------|-----|--------|-------------|------------|-------------|
| <p>CONTACT PERSON (PLEASE PRINT CLEARLY):<br/>           Rick Browing</p>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |          |     |        |             |            |             |
| <p>***** THIS IS THE END OF RFQ LBS10081 ***** TOTAL:</p>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |          |     |        |             |            | \$64,905.92 |
| <p>* Agilent Technologies, Inc (Agilent) is bidding in accordance with quotation 926576, which is attached and hereby incorporated by reference. The above price does not include tax. Any applicable tax will be applied at the time of order placement. The quoted prices reflect discounts granted in accordance with GSA Federal Supply Schedule Terms and Conditions. Your order must reference GSA Contract Number GS-26F-5944A and only GSA Terms and Conditions shall apply to your order. Should a GSA approved price increase occur during the quote validity period, this quotation shall remain valid for 30 days from the effective date of the price increase. GSA pricing can be verified at our GSA web site (<a href="http://www.agilent.com/gsa">http://www.agilent.com/gsa</a>). If you have any questions regarding our products, please call Rick Browing at 304-840-4752. If you have any questions regarding our response, please call Sandra Beal at 800-227-9770. If Agilent should be the successful bidder, please reference the quotation number on your purchase order.</p> |          |     |        |             |            |             |

SEE REVERSE SIDE FOR TERMS AND CONDITIONS

SIGNATURE: *Sandra Beal* \* TELEPHONE: 800-227-9770 DATE: 03/04/10  
 TITLE: Business Sales Specialist FEIN: 77-0518772 ADDRESS CHANGES TO BE NOTED ABOVE

WHEN RESPONDING TO RFQ, INSERT NAME AND ADDRESS IN SPACE ABOVE LABELED 'VENDOR'

## SPECIFICATIONS AND REQUIREMENTS:

The Environmental Chemistry Laboratory section of the Office of Laboratory Services is requesting to purchase a Gas Chromatograph – Mass Spectrometer (GC-MS) instrument to analyze for Trihalomethanes (THMs) and Volatile Organic Chemicals (VOCs).

1. A GC-MS instrument is needed to analyze THMs and VOCs in drinking water to fulfill requirements of United States Environmental Protection Agency (EPA) regulations for compliance monitoring of public water systems. Compliance monitoring testing is a requirement of a State's Principal State Laboratory mandated, under federal code at 40 CFR 142.10(b)(4) for the state to maintain Primacy over its Drinking Water Program. The instrument will also serve the purpose of protecting public health by providing testing capabilities to private well owners. This instrument is to be installed for use by the Environmental Chemistry Laboratory located at 4710 Chimney Drive, Suite G, Charleston, WV 25302.
2. This GC-MS instrument must be able to fulfill the requirements of United States Environmental Protection Agency (EPA) method 524.2 (1995, Revision 4.1) for THMs and VOCs, and the resolution and sensitivity capability must be able to meet or exceed the limits of detection and minimum reporting levels required for these regulated compounds as stipulated under the Federal Safe Drinking Water Act, and the Stage 2 Disinfection Byproduct Rule.
3. This GC-MS instrument must be fully automated for analysis with a system controller that is loaded with the necessary software. Vendor system controller software must be able to export data to the existing STARLIMS (Version 9) Laboratory Information Management System (LIMS).
4. This GC-MS instrument system controller software must be able to fulfill all of the analytical and quality control requirements stated in the EPA Method 524.2 (Rev. 4.1) as well as the pertinent requirements listed in Chapter IV of the EPA "Manual for the Certification of Laboratories Analyzing Drinking Water, Fifth edition, January 2005", for the analysis of THMs and VOCs in drinking water.
5. GC-MS Instrument must be fully compatible with a system software controlled autosampler that is a part of a Purge and Trap concentrator sampling system manufactured by OI Analytical. The autosampler is an OI Analytical Model 4551-A. The Purge and Trap is the OI Analytical Eclipse Model 4660. The OI Analytical autosampler and purge and trap have already been purchased.
6. The GC-MS instrument must come with a split/splitless capillary column injector compatible with the referenced purge and trap sampling interface.
7. The GC-MS instrument must come with a column for method 524.2 volatiles analysis.
8. The GC-MS instrument must come equipped with a quadrupole mass spectrometer.
9. The GC-MS instrument must be capable of mass scan rates at a minimum of 10,000 amu/sec.

10. The GC-MS instrument must be capable of detecting a wide mass range at a minimum of 1.5-1000 amu.
11. The GC-MS instrument must come equipped with a 60 L/sec turbomolecular pump vacuum system, or better.
12. The GC-MS instrument system must operate on 110-120 V AC.

**Installation Requirements:**

1. Vendor must install the GC-MS Instrument system in the Environmental Chemistry Laboratory in the Elk Office Center building at 4710 Chimney Drive, Suite G, Charleston, WV 25302
2. At the time of the GC-MS instrument installation, Vendor must provide to the ECL Program Manager: All relevant system manuals for hardware components; system and application software documentation; a parts, supplies, accessories catalog.
3. Vendor must include all necessary cables and fittings and other costs for installation in the submitted bid price.
4. Installation and on-site training must be completed within 90 days of delivery date.
5. **INSURANCE:** Prior to the issuance of a Purchase Order, the successful vendor shall furnish proof of commercial general liability insurance in a minimum amount of \$250,000 and also, proof of Workmens' Compensation Insurance coverage.

**Training Requirements:**

1. Vendor must provide, upon completion of installation, on-site training for Environmental Chemistry Laboratory personnel on the operation and user maintenance requirements of the GC-MS instrument system.
2. All costs incurred by the Vendor including travel, lodging, and living expenses necessary to provide this basic training shall be included in the bid price.

**Warranty Requirements:**

1. Vendor must include in the total price of the equipment at least 1-year factory warranty covering all system components.
2. Vendor system controller software support must be included as part of one-year warranty.
3. Warranty must include on-site service including labor, travel time, and expenses with a 72-hour on-site response time at no extra cost to maintain the specifications listed in this bid and the Vendor's product specifications.
4. Warranty must begin upon completion of installation.

**Delivery Requirements:**

1. The GC-MS instrument and its components must be shipped for "inside delivery" by freight delivery company and must be delivered within 90 days of receipt of order.

- 2 The GC-MS instrument and its components must be shipped "F.O.B. Destination" unless otherwise stated in quote by Vendor. Any shipping and handling requirements must be stated in Vendor's quote.



**RFQ COST SHEET**

Bidders shall provide a cost for the following:

|                                                      |                     |
|------------------------------------------------------|---------------------|
| Gas Chromatograph -- Mass Spectrometer (GC-MS)       | \$ <u>64,905.92</u> |
| On-Site User Training (at installation of equipment) | \$ <u>included</u>  |
| Freight/Shipping Charge                              | \$ <u>No Charge</u> |
| <b>Total Cost</b>                                    | \$ <u>64,905.92</u> |

The award will be made to the vendor with the lowest overall total cost of the equipment which meets all requested specifications and requirements. Payment will be made in arrears.

Sandra Beal  
Vendor Signature

03/04/10  
Date

RFQ No. LBS10081

STATE OF WEST VIRGINIA  
Purchasing Division

**PURCHASING AFFIDAVIT**

**West Virginia Code §5A-3-10a states:** No contract or renewal of any contract may be awarded by the state or any of its political subdivisions to any vendor or prospective vendor when the vendor or prospective vendor or a related party to the vendor or prospective vendor is a debtor and the debt owed is an amount greater than one thousand dollars in the aggregate

**DEFINITIONS:**

"Debt" means any assessment, premium, penalty, fine, tax or other amount of money owed to the state or any of its political subdivisions because of a judgment, fine, permit violation, license assessment, defaulted workers' compensation premium, penalty or other assessment presently delinquent or due and required to be paid to the state or any of its political subdivisions, including any interest or additional penalties accrued thereon.

"Debtor" means any individual, corporation, partnership, association, limited liability company or any other form or business association owing a debt to the state or any of its political subdivisions. "Political subdivision" means any county commission; municipality; county board of education; any instrumentality established by a county or municipality; any separate corporation or instrumentality established by one or more counties or municipalities, as permitted by law; or any public body charged by law with the performance of a government function or whose jurisdiction is coextensive with one or more counties or municipalities. "Related party" means a party, whether an individual, corporation, partnership, association, limited liability company or any other form or business association or other entity whatsoever, related to any vendor by blood, marriage, ownership or contract through which the party has a relationship of ownership or other interest with the vendor so that the party will actually or by effect receive or control a portion of the benefit, profit or other consideration from performance of a vendor contract with the party receiving an amount that meets or exceeds five percent of the total contract amount.

**EXCEPTION:** The prohibition of this section does not apply where a vendor has contested any tax administered pursuant to chapter eleven of this code, workers' compensation premium, permit fee or environmental fee or assessment and the matter has not become final or where the vendor has entered into a payment plan or agreement and the vendor is not in default of any of the provisions of such plan or agreement.

Under penalty of law for false swearing (*West Virginia Code §61-5-3*), it is hereby certified that the vendor affirms and acknowledges the information in this affidavit and is in compliance with the requirements as stated.

**WITNESS THE FOLLOWING SIGNATURE**

Vendor's Name: Agilent Technologies Inc

Authorized Signature: *Andree Beal* Date: 03/04/2010

State of Delaware

County of New Castle, to-wit:

Taken, subscribed, and sworn to before me this 04 day of March, 2010

My Commission expires May 8<sup>th</sup>, 2010

**AFFIX SEAL HERE**

NOTARY PUBLIC *Andree Beal*



## State of West Virginia **VENDOR PREFERENCE CERTIFICATE**

Certification and application\* is hereby made for Preference in accordance with *West Virginia Code*, §5A-3-37 (Does not apply to construction contracts). *West Virginia Code*, §5A-3-37, provides an opportunity for qualifying vendors to request (at the time of bid) preference for their residency status. Such preference is an evaluation method only and will be applied only to the cost bid in accordance with the *West Virginia Code*. This certificate for application is to be used to request such preference. The Purchasing Division will make the determination of the Resident Vendor Preference, if applicable.

1. **Application is made for 2.5% resident vendor preference for the reason checked:**  
 Bidder is an individual resident vendor and has resided continuously in West Virginia for four (4) years immediately preceding the date of this certification; or,  
 Bidder is a partnership, association or corporation resident vendor and has maintained its headquarters or principal place of business continuously in West Virginia for four (4) years immediately preceding the date of this certification; or 80% of the ownership interest of Bidder is held by another individual, partnership, association or corporation resident vendor who has maintained its headquarters or principal place of business continuously in West Virginia for four (4) years immediately preceding the date of this certification; or,  
 Bidder is a nonresident vendor which has an affiliate or subsidiary which employs a minimum of one hundred state residents and which has maintained its headquarters or principal place of business within West Virginia continuously for the four (4) years immediately preceding the date of this certification; or,
2. **Application is made for 2.5% resident vendor preference for the reason checked:**  
 Bidder is a resident vendor who certifies that, during the life of the contract, on average at least 75% of the employees working on the project being bid are residents of West Virginia who have resided in the state continuously for the two years immediately preceding submission of this bid; or,
3. **Application is made for 2.5% resident vendor preference for the reason checked:**  
 Bidder is a nonresident vendor employing a minimum of one hundred state residents or is a nonresident vendor with an affiliate or subsidiary which maintains its headquarters or principal place of business within West Virginia employing a minimum of one hundred state residents who certifies that, during the life of the contract, on average at least 75% of the employees or Bidder's affiliate's or subsidiary's employees are residents of West Virginia who have resided in the state continuously for the two years immediately preceding submission of this bid; or,
4. **Application is made for 5% resident vendor preference for the reason checked:**  
 Bidder meets either the requirement of both subdivisions (1) and (2) or subdivision (1) and (3) as stated above; or,
5. **Application is made for 3.5% resident vendor preference who is a veteran for the reason checked:**  
 Bidder is an individual resident vendor who is a veteran of the United States armed forces, the reserves or the National Guard and has resided in West Virginia continuously for the four years immediately preceding the date on which the bid is submitted; or,
6. **Application is made for 3.5% resident vendor preference who is a veteran for the reason checked:**  
 Bidder is a resident vendor who is a veteran of the United States armed forces, the reserves or the National Guard, if, for purposes of producing or distributing the commodities or completing the project which is the subject of the vendor's bid and continuously over the entire term of the project, on average at least seventy-five percent of the vendor's employees are residents of West Virginia who have resided in the state continuously for the two immediately preceding years.

Bidder understands if the Secretary of Revenue determines that a Bidder receiving preference has failed to continue to meet the requirements for such preference, the Secretary may order the Director of Purchasing to: (a) reject the bid; or (b) assess a penalty against such Bidder in an amount not to exceed 5% of the bid amount and that such penalty will be paid to the contracting agency or deducted from any unpaid balance on the contract or purchase order.

By submission of this certificate, Bidder agrees to disclose any reasonably requested information to the Purchasing Division and authorizes the Department of Revenue to disclose to the Director of Purchasing appropriate information verifying that Bidder has paid the required business taxes, provided that such information does not contain the amounts of taxes paid nor any other information deemed by the Tax Commissioner to be confidential.

Under penalty of law for false swearing (*West Virginia Code*, §61-5-3), Bidder hereby certifies that this certificate is true and accurate in all respects; and that if a contract is issued to Bidder and if anything contained within this certificate changes during the term of the contract, Bidder will notify the Purchasing Division in writing immediately.

Bidder: \_\_\_\_\_ Signed: \_\_\_\_\_  
 Date: \_\_\_\_\_ Title: \_\_\_\_\_

\*Check any combination of preference consideration(s) indicated above, which you are entitled to receive.

**AGREEMENT ADDENDUM**

In the event of conflict between this addendum and the agreement, this addendum shall control:

1. **DISPUTES** - Any references in the agreement to arbitration or to the jurisdiction of any court are hereby deleted. Disputes arising out of the agreement shall be presented to the West Virginia Court of Claims.
2. **HOLD HARMLESS** - Any clause requiring the Agency to indemnify or hold harmless any party is hereby deleted in its entirety.
3. **GOVERNING LAW** - The agreement shall be governed by the laws of the State of West Virginia. This provision replaces any references to any other State's governing law.
4. **TAXES** - Provisions in the agreement requiring the Agency to pay taxes are deleted. As a State entity, the Agency is exempt from Federal, State, and local taxes and will not pay taxes for any Vendor including individuals, nor will the Agency file any tax returns or reports on behalf of Vendor or any other party.
5. **PAYMENT** - Any references to prepayment are deleted. Payment will be in arrears.
6. **INTEREST** - Should the agreement include a provision for interest on late payments, the Agency agrees to pay the maximum legal rate under West Virginia law. All other references to interest or late charges are deleted.
7. **RECOUPMENT** - Any language in the agreement waiving the Agency's right to set-off, counterclaim, recoupment, or other defense is hereby deleted.
8. **FISCAL YEAR FUNDING** - Service performed under the agreement may be continued in succeeding fiscal years for the term of the agreement, contingent upon funds being appropriated by the Legislature or otherwise being available for this service. In the event funds are not appropriated or otherwise available for this service, the agreement shall terminate without penalty on June 30. After that date, the agreement becomes of no effect and is null and void. However, the Agency agrees to use its best efforts to have the amounts contemplated under the agreement included in its budget. Non-appropriation or non-funding shall not be considered an event of default.
9. **STATUTE OF LIMITATION** - Any clauses limiting the time in which the Agency may bring suit against the Vendor, lessor, individual, or any other party are deleted.
10. **SIMILAR SERVICES** - Any provisions limiting the Agency's right to obtain similar services or equipment in the event of default or non-funding during the term of the agreement are hereby deleted.
11. **ATTORNEY FEES** - The Agency recognizes an obligation to pay attorney's fees or costs only when assessed by a court of competent jurisdiction. Any other provision is invalid and considered null and void.
12. **ASSIGNMENT** - Notwithstanding any clause to the contrary, the Agency reserves the right to assign the agreement to another State of West Virginia agency, board or commission upon thirty (30) days written notice to the Vendor and Vendor shall obtain the written consent of Agency prior to assigning the agreement.
13. **LIMITATION OF LIABILITY** - The Agency, as a State entity, cannot agree to assume the potential liability of a Vendor. Accordingly, any provision limiting the Vendor's liability for direct damages to a certain dollar amount or to the amount of the agreement is hereby deleted. Limitations on special, incidental or consequential damages are acceptable. In addition, any limitation is null and void to the extent that it precludes any action for injury to persons or for damages to personal property.
14. **RIGHT TO TERMINATE** - Agency shall have the right to terminate the agreement upon thirty (30) days written notice to Vendor. Agency agrees to pay Vendor for services rendered or goods received prior to the effective date of termination.
15. **TERMINATION CHARGES** - Any provision requiring the Agency to pay a fixed amount or liquidated damages upon termination of the agreement is hereby deleted. The Agency may only agree to reimburse a Vendor for actual costs incurred or losses sustained during the current fiscal year due to wrongful termination by the Agency prior to the end of any current agreement term.
16. **RENEWAL** - Any reference to automatic renewal is hereby deleted. The agreement may be renewed only upon mutual written agreement of the parties.
17. **INSURANCE** - Any provision requiring the Agency to insure equipment or property of any kind and name the Vendor as beneficiary or as an additional insured is hereby deleted.
18. **RIGHT TO NOTICE** - Any provision for repossession of equipment without notice is hereby deleted. However, the Agency does recognize a right of repossession with notice.
19. **ACCELERATION** - Any reference to acceleration of payments in the event of default or non-funding is hereby deleted.
20. **CONFIDENTIALITY**: -Any provision regarding confidentiality of the terms and conditions of the agreement is hereby deleted. State contracts are public records under the West Virginia Freedom of Information Act.
21. **AMENDMENTS** - All amendments, modifications, alterations or changes to the agreement shall be in writing and signed by both parties. No amendment, modification, alteration or change may be made to this addendum without the express written approval of the Purchasing Division and the Attorney General.

ACCEPTED BY:

**STATE OF WEST VIRGINIA**

Spending Unit: \_\_\_\_\_

Signed: \_\_\_\_\_

Title: \_\_\_\_\_

Date: \_\_\_\_\_

**VENDOR**

Company Name: Agilent Technologies Inc

Signed: Scendia Beal

Title: Business Sales Specialist

Date: 03/04/2010

ATTACHMENT  
P.O.# LBS10081

This agreement constitutes the entire agreement between the parties, and there are no other terms and conditions applicable to the licenses granted hereunder

Agreed

Sandra Beal 03/04/10  
Signature Date

Business Sales Specialist

Title

Agilent Technologies Inc

Company Name

\_\_\_\_\_  
Signature Date

\_\_\_\_\_  
Title

\_\_\_\_\_  
Agency/Division



# Quotation

Pat Marchio  
 State of West Virginia  
 4710 Chimney Drive Ste G  
 Charleston WV 25302

| Quote No.                                                                                                                                                                                                            | Create Date  | Delivery Time | Page   |
|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------|---------------|--------|
| 926576                                                                                                                                                                                                               | 02/25/2010   | <1 Week       | 1 of 7 |
| Contact                                                                                                                                                                                                              | Phone no.    | Valid to      |        |
| Rick Browning                                                                                                                                                                                                        | 304-840-4752 | 04/26/2010    |        |
| To place an order: Call 1-800-227-9770 Option 1<br>For Instruments Fax : 302-633-8953<br>For Consumables Fax : 302-633-8901<br>Email : LSCAinstrumentsales@agilent.com<br>For additional instructions, see last page |              |               |        |

| Product/Description                                                                                                                                                                                                                                                                                                                                                                                                                             | Qty/Unit | Unit List Price | Discount Amount | Extended Net Price |
|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------|-----------------|-----------------|--------------------|
| <b>G3242A</b><br>5975C inert MSD/DS Std Turbo EI System<br>for use with 7890A, 6890 and 6850 GC.<br>Includes G3171A MSD, ChemStation (Win XP)<br>G1701EA SW, PC, LaserJet printer. Not<br>included: G3397A Ion gauge controller<br><br>With the following configuration:<br>Ship-to Country : USA<br>Installation (44K)<br>Familiarization at Installation (44L)<br>1 Year SW Update/Phone Assist (44W)<br>1YR PC Repair Recovery Service (0TP) | 1.000 EA | 61,101.00 USD   | 11,548.08-      | 49,552.92          |
| <b>Item Total</b>                                                                                                                                                                                                                                                                                                                                                                                                                               |          |                 |                 | <b>49,552.92</b>   |
| GSA discount amount of \$ 11,548.09 is included. GSA Contract no: GS-26F-5944A615-5000                                                                                                                                                                                                                                                                                                                                                          |          |                 |                 |                    |
| <b>G3391A</b><br>Site Preparation Package for use with<br>5975C inert MSDs and MSD bundles.<br><br>With the following configuration:<br>Ship-to Country : USA                                                                                                                                                                                                                                                                                   | 1.000 EA | 35.25 USD       | 6.66-           | 28.59              |
| <b>Item Total</b>                                                                                                                                                                                                                                                                                                                                                                                                                               |          |                 |                 | <b>28.59</b>       |
| GSA discount amount of \$ 6.66 is included. GSA Contract no: GS-26F-5944AN615-4                                                                                                                                                                                                                                                                                                                                                                 |          |                 |                 |                    |



# Quotation

Pat Marchio  
 State of West Virginia  
 4710 Chimney Drive Ste G  
 Charleston WV 25302

| Quote No.                                                                                                                                                                                                            | Create Date  | Delivery Time | Page   |
|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------|---------------|--------|
| 926576                                                                                                                                                                                                               | 02/25/2010   | <1 Week       | 2 of 7 |
| Contact                                                                                                                                                                                                              | Phone no.    | Valid to      |        |
| Rick Browning                                                                                                                                                                                                        | 304-840-4752 | 04/26/2010    |        |
| To place an order: Call 1-800-227-9770 Option 1<br>For Instruments Fax : 302-633-8953<br>For Consumables Fax : 302-633-8901<br>Email : LSCAinstrumentsales@agilent.com<br>For additional instructions, see last page |              |               |        |

| Product/Description                                                                                                                                                                                                                                                                                                                        | Qty/Unit | Unit List Price | Discount Amount   | Extended Net Price |
|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------|-----------------|-------------------|--------------------|
| <b>G3442A</b><br>Agilent 7890A GC for MS with SSL inlet<br>Includes 100psi split-splitless inlet,<br>LAN interface and MS interface (for<br>Agilent 5975 Series MSD or Agilent<br>7000A Quadrupole GC/MS)<br><br>With the following configuration:<br>Ship-to Country : USA<br>Installation (44K)<br>Familiarization at Installation (44L) | 1 000 EA | 17,453.00 USD   | 3,298.61-         | 14,154.39          |
|                                                                                                                                                                                                                                                                                                                                            |          |                 | <b>Item Total</b> | <b>14,154.39</b>   |
| GSA discount amount of \$ 3 298.62 is included GSA Contract no:<br>GS-26F-5944A615-4                                                                                                                                                                                                                                                       |          |                 |                   |                    |
| <b>123-1334</b><br>DB-624 30m, 0.32mm, 1.80um                                                                                                                                                                                                                                                                                              | 1 000 EA | 546.00 USD      | 103.19-           | 442.81             |
|                                                                                                                                                                                                                                                                                                                                            |          |                 | <b>Item Total</b> | <b>442.81</b>      |
| GSA discount amount of \$ 103.19 is included GSA Contract no:<br>GS-26F-5944AN615-4                                                                                                                                                                                                                                                        |          |                 |                   |                    |



# Quotation

Pat Marchio  
 State of West Virginia  
 4710 Chimney Drive Ste G  
 Charleston WV 25302

| Quote No.                                                                                                                                                                                                            | Create Date | Delivery Time | Page       |
|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------|---------------|------------|
| 926576                                                                                                                                                                                                               | 02/25/2010  | <1 Week       | 3 of 7     |
| Contact                                                                                                                                                                                                              |             | Phone no.     | Valid to   |
| Rick Browning                                                                                                                                                                                                        |             | 304-840-4752  | 04/26/2010 |
| To place an order: Call 1-800-227-9770 Option 1<br>For Instruments Fax : 302-633-8953<br>For Consumables Fax : 302-633-8901<br>Email : LSCAinstrumentsales@agilent.com<br>For additional instructions, see last page |             |               |            |

| Product/Description                                                                                                                                                              | Qty/Unit | Unit List Price | Discount Amount | Extended Net Price |
|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------|-----------------|-----------------|--------------------|
| <b>0100-0900</b><br>Union, 1/16in SS zero dead volume                                                                                                                            | 2 000 EA | 89.32 USD       | 33.76-          | 144.88             |
| <b>Item Total</b>                                                                                                                                                                |          |                 |                 | <b>144.88</b>      |
| GSA discount amount of \$ 33.76 is included. GSA Contract no: GS-26F-5944AN615-4                                                                                                 |          |                 |                 |                    |
| <b>H5949A</b><br>Supplemental Installation One Hour Labor for Chemical Analysis products<br>Labor only; no travel included.<br>Requires installation - bundled, or as 44N or 44K | 2 000 EA | 295.00 USD      | 7.67-           | 582.33             |
| <b>Item Total</b>                                                                                                                                                                |          |                 |                 | <b>582.33</b>      |
| GSA discount amount of \$ 7.67 is included. GSA Contract no: GS-26F-5944AN615-5000                                                                                               |          |                 |                 |                    |
|                                                                                                                                                                                  |          | Gross Amount    | : \$            | 79,903.89          |
|                                                                                                                                                                                  |          | Total Discount  | : \$            | 14,997.97          |
|                                                                                                                                                                                  |          | <b>Total</b>    | <b>: \$</b>     | <b>64,905.92</b>   |





# Quotation

Pat Marchio  
State of West Virginia  
4710 Chimney Drive Ste G  
Charleston WV 25302

| Quote No.     | Create Date | Delivery Time | Page       |
|---------------|-------------|---------------|------------|
| 926576        | 02/25/2010  | <1 Week       | 4 of 7     |
| Contact       |             | Phone no.     | Valid to   |
| Rick Browning |             | 304-840-4752  | 04/26/2010 |

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 additional instructions, see last page

**TO PLACE AN ORDER, Agilent offers several options:**

- 1) Visit <http://www.agilent.com/chem/supplies> to place online orders using a purchase order or credit card
- 2) Call 1-800-227-9770 (option 1) any weekday between 8am and 8 pm Eastern time in the U.S., Canada & Puerto Rico.
- 3) To place an order for Consumables, please fax the order to 302-633-8901.  
To place an instrument and/or software order, please fax the order to 302-633-8953
- 4) Or you can mail your order to:  
Agilent Technologies  
North American Customer Contact Center  
2850 Centerville Road BU3-2  
Wilmington, DE 19808-1610

**To place an order, the following information is required:**

- Purchase order number or credit card, delivery date, ship to invoice to, end user, and quote number.  
GSA customers please provide GSA contract #

**EXCLUSIVE OFFERS FOR NEW INSTRUMENT CUSTOMERS, go to [www.agilent.com/chem/exclusiveoffers](http://www.agilent.com/chem/exclusiveoffers)**

**TO CHECK THE STATUS OF AN ORDER:**

- 1) Visit <http://www.agilent.com/chem/supplies> to check the status of your order.
- 2) Call 1-800-227-9770 (option 1) any weekday between 8 am and 8 pm Eastern time, in the U.S., Canada & Puerto Rico. You will need to know the purchase order or credit card number the order was placed on.

**FINANCING AND LEASING - A wide range of options are available from Agilent's preferred financing partner, Leasing Group Inc (LGI)**

For more information or to discuss how monthly payments could suit your operational or budgetary requirements, contact your Agilent Account Manager or contact LGI at 800-944-1370.

**TERMS AND CONDITIONS:**

Pricing: Web prices are provided only for the U.S. in U.S. dollars. All phone prices are in local currency and for end use.  
Applicable local taxes are applied.  
All Sales Tax is subject to change at the time of order.  
Shipping and Handling Charges: Orders with a value less than \$2000 or those requiring special services such as overnight delivery may be subject to additional shipping & handling fees. Some of these charges may be avoided by ordering via the Web.  
Payment Terms: Net 30 days from invoice date, subject to credit approval.

- \* Quotation Validity: This quotation is valid for 60 days unless otherwise indicated.
- \* Warranty period for instrumentation is 1 year. The Warranty period for columns and consumables is 90 days.



# Quotation

Pat Marchio  
State of West Virginia  
4710 Chimney Drive Ste G  
Charleston WV 25302

| Quote No.                                                                                                                                                                                                            | Create Date | Delivery Time | Page       |
|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------|---------------|------------|
| 926576                                                                                                                                                                                                               | 02/25/2010  | <1 Week       | 5 of 7     |
| Contact                                                                                                                                                                                                              |             | Phone no.     | Valid to   |
| Rick Browning                                                                                                                                                                                                        |             | 304-840-4752  | 04/26/2010 |
| To place an order: Call 1-800-227-9770 Option 1<br>For Instruments Fax : 302-633-8953<br>For Consumables Fax : 302-633-8901<br>Email : LSCAinstrumentsales@agilent.com<br>For additional instructions, see last page |             |               |            |

Agilent Technologies is neither a small business concern nor a minority business enterprise

The following is a Federal Government Requirement :

### USE OF FEDERAL SUPPLY SCHEDULES BY GOVERNMENT CONTRACTORS

Government Contractors may use GSA supply source when authorized in writing by the responsible Contracting Officer from the agency for which the contract is being performed. A copy of the Contracting Officer's written authorization must be forwarded with the order. The letter must be addressed directly to the Contractor that is purchasing the equipment. Also, the following statement must be included on the purchase order:

"The order is placed under written authorization from: \_\_\_\_\_  
dated: \_\_\_\_\_, a copy of which is attached hereto. In the event of any inconsistency between the Terms and Condition of this order and those of Agilent Technologies' Federal Supply Schedule the latter will govern. We agree to promptly notify you of any termination of this authorization or of the prime contract under which it was granted."

Agilent Technologies will be unable to accept your order at these prices if written authorization is not received



# Quotation

Pat Marchio  
State of West Virginia  
4710 Chimney Drive Ste G  
Charleston WV 25302

| Quote No.                                                                                                                                                                                                            | Create Date  | Delivery Time | Page   |
|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------|---------------|--------|
| 926576                                                                                                                                                                                                               | 02/25/2010   | <1 Week       | 6 of 7 |
| Contact                                                                                                                                                                                                              | Phone no.    | Valid to      |        |
| Rick Browning                                                                                                                                                                                                        | 304-840-4752 | 04/26/2010    |        |
| To place an order: Call 1-800-227-9770 Option 1<br>For Instruments Fax : 302-633-8953<br>For Consumables Fax : 302-633-8901<br>Email : LSCAinstrumentsales@agilent.com<br>For additional instructions, see last page |              |               |        |

The quoted prices reflect discounts granted in accordance with GSA Federal Supply Schedule Terms and Conditions. Your order must reference GSA Contract Number GS-26F-5944A and only GSA Terms and Conditions shall apply to your order. Should a GSA approved price increase occur during the quote validity period, this quotation shall remain valid for 30 days from the effective date of the price increase.

Agilent Technologies is providing price discounts in accordance with GSA as requested, with the following conditions.

In accordance with Federal Acquisition Regulation 51 100:

#### "USE OF FEDERAL SUPPLY SCHEDULES BY GOVERNMENT CONTRACTORS"

Government Contractors may use GSA supply sources when authorized in writing by the responsible Contracting Officer from the agency for which the contract is being performed. A copy of the Contracting Officer's written authorization must be forwarded with the order. The letter must be addressed directly to the Contractor that is purchasing the equipment. Also, the following statement must be included on the purchase order:

"The order is placed under written authorization from: \_\_\_\_\_ dated: \_\_\_\_\_, a copy of which is attached hereto. In the event of any inconsistency between the Terms and Conditions of this order and those of Agilent Technologies# Federal Supply Schedule the latter will govern. We agree to promptly notify you of any termination of this authorization or of the prime contract under which it was granted"

Agilent will be pleased to process your order with GSA contract terms and pricing so long as the conditions outlined above are met. Otherwise the order must be processed in accordance with Agilent's standard commercial terms and pricing.

Following is the format for the required GSA Letter of Authorization:

[Date]

[Company Name and Address]

RE: [US Government entity contract number]. Authorization to use Government Supply Sources

Pursuant to Federal Acquisition Regulation (FAR) Part 51.102, this letter serves to authorize [Insert Company Name], to utilize Government supply sources for acquisition of supplies and services to be used in performance of contract [Insert contract number]. This authorization does include the following:

1 The acquisition of property and/or services which are available for purchase by Government agencies either directly from the General Services Administration stock or under Federal Supply Schedules.

Purchase orders issued under GSA schedules and/or contracts shall be placed in accordance with



# Quotation

Pat Marchio  
State of West Virginia  
4710 Chimney Drive Ste G  
Charleston WV 25302

| Quote No.     | Create Date  | Delivery Time | Page   |
|---------------|--------------|---------------|--------|
| 926576        | 02/25/2010   | <1 Week       | 7 of 7 |
| Contact       | Phone no.    | Valid to      |        |
| Rick Browning | 304-840-4752 | 04/26/2010    |        |

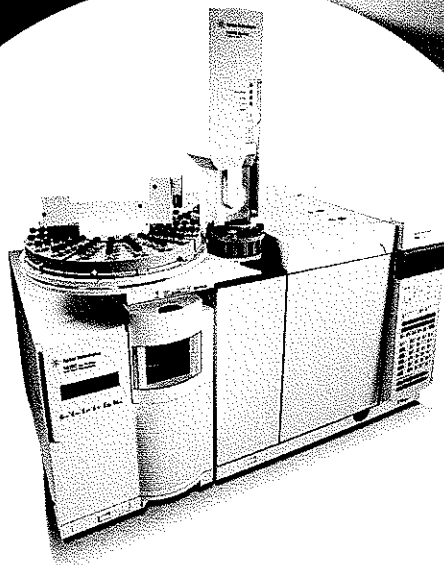
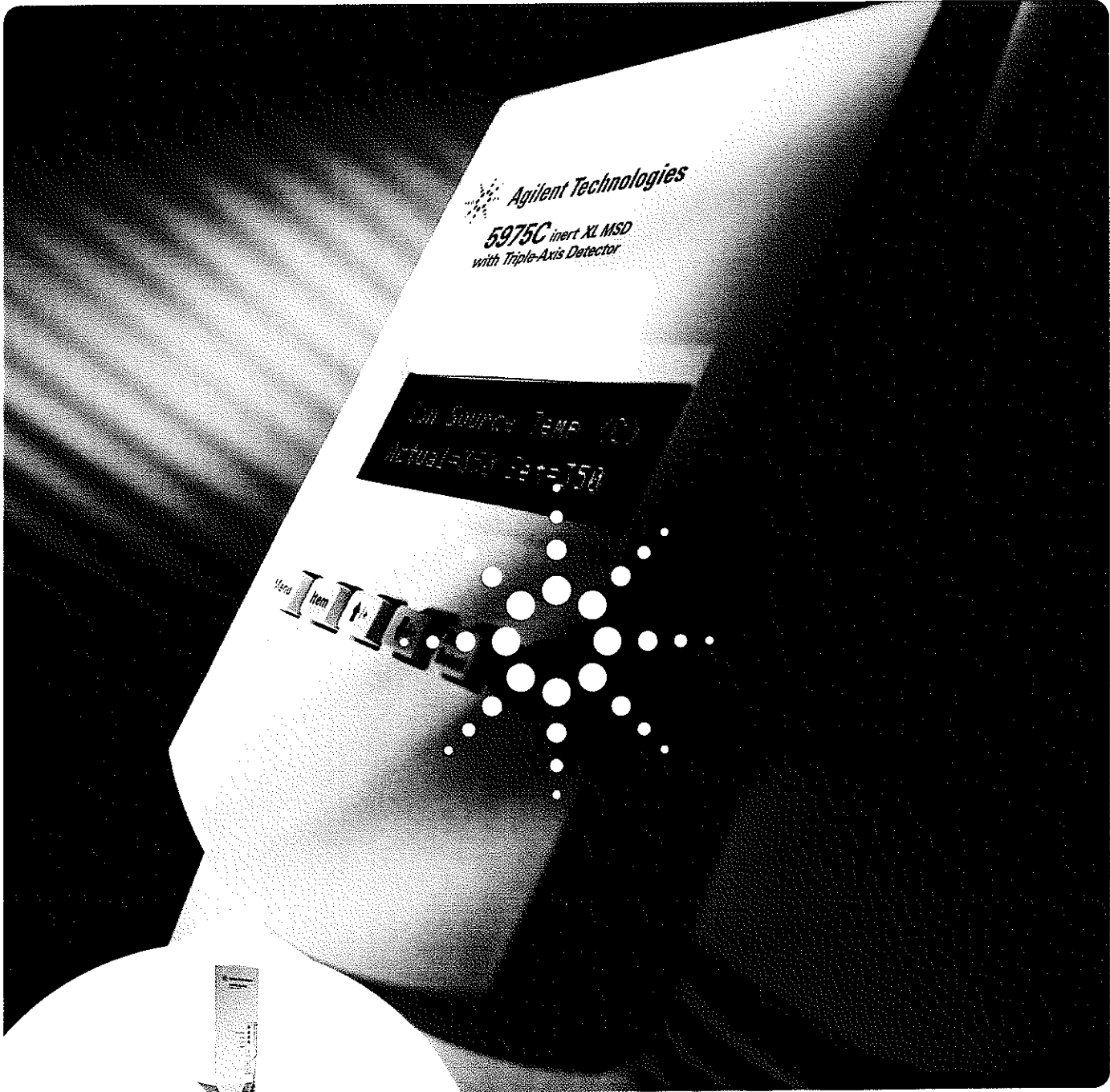
To place an order: Call 1-800-227-9770 Option 1  
For Instruments Fax : 302-633-8953  
For Consumables Fax : 302-633-8901  
Email : LSCAinstrumentsales@agilent.com  
For additional instructions, see last page

the terms and conditions of the GSA schedules and/or contracts and this authorization. A copy of this authorization shall be attached to the order (unless a copy was previously furnished to the applicable GSA contractor). This authority hereby granted is not transferable or assignable. [Insert US Government contracting officer's name, title and agency, must be signed by the contracting officer to be valid]

The Delivery Time reflected is based on availability at the time of quotation and is only a guideline for delivery receipt. Order specific Delivery Time will be determined at order placement and is subject to current availability.

It is Agilent Technologies intent to ship product at the earliest available date unless specified otherwise

The sale of standard Products and Services referenced in this quotation is subject to the then current version of Agilent's Terms of Sale, and any LSCA Supplemental Terms or other applicable terms referenced herein. If any Products or Services are manufactured, configured or adapted to meet Customer's requirements, the sale of all Products and Services referenced in this quotation is subject to the then current version of Agilent's Terms of Sale for Custom Products and any LSCA Supplemental Terms or other applicable terms referenced herein. A copy of Agilent's Terms of Sale, Agilent's Terms of Sale for Custom Products and the LSCA Supplemental Terms is either attached or has been previously provided to you. Please contact us if you have not received a copy or require an additional copy. If you have a separate agreement in effect with Agilent covering the sale of Products and Services order documentation, unless agreed to in writing by Agilent, Product and Service availability dates are estimated at the time of the quotation. Actual delivery dates or delivery windows will be specified at the time Agilent acknowledges and accepts your purchase order. The above conditions shall apply to the fullest extent permitted by the law. You may have other statutory or legal rights available. Commodities, technology or software exported from the United States of America ("U.S.") or from other exporting countries will be subject to the U.S. Export Administration Regulations and all exporting countries' export laws and regulations. Diversion contrary to U.S. law and the applicable export laws and regulations is prohibited.



The Agilent 5975C Series GC/MSD  
**Performance, productivity and confidence.**

Our measure is your success.

products | applications | software | services

 **Agilent Technologies**

# The Agilent 5975C Series GC/MSD

**Proven performance, superior productivity—and maximum confidence in your results.**

Welcome to the next generation of the industry-proven Agilent 5975C Series MSD—the most popular GC/MS of all time. The Agilent 5975C Series MSD—with Triple-Axis HED-EM Detector—combines innovative design features to boost your lab's productivity and advanced analytical capabilities that help you achieve better results faster. Perfectly complemented by the new 7890A GC, the platform delivers all the elements for perfect chemistry: superior performance, unmatched reliability, greater productivity and enhanced ease of use.



The Agilent 5975C Series GC/MSD is built on a solid foundation of industry leadership, reliability and performance.

## Advanced Analysis Capabilities

The modular mass analyzer incorporates a solid inert ion source, a proprietary quartz quadrupole analyzer and a new higher signal-to-noise Triple-Axis Detector. This powerful combination provides better MS resolution, exceptional spectral integrity and lower limits of detection—for the highest confidence in your results. New Trace Ion Detection technology provides even more capabilities at trace level.

## Higher Throughput

Comprehensive automation features, faster separations and shorter detection cycle times enable you to process more samples in less time. Advanced analysis routines let you get maximum information from every run, and new automated spectral deconvolution software enables rapid identification and quantification.

## Maximum Uptime

Thoughtful, real-world engineering features allow faster, easier routine upkeep, and new system intelligence features enable predictive support, enhanced self-maintenance and powerful remote diagnostics—making it easier than ever to keep your lab up and running at peak performance.

For additional instrument specifications go to:  
[www.agilent.com/chem/5975C-Specs](http://www.agilent.com/chem/5975C-Specs)  
5989-6351EN: 5975C Series GC/MSD Data Sheet



### 350°C inert ion source

Now programmable up to 350°C, delivers enhanced response for active compounds and late-eluters. **Page 4**



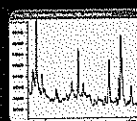
### Proprietary gold quartz quadrupole with 1050 u mass range

Optimal resolution and sensitivity across the mass range; lowest mass deviation ensures longer lasting tuning and calibration. **Page 4**



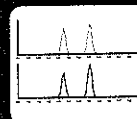
### High S/N Triple-Axis Detector

The next generation of off-axis detection minimizes noise and maximizes signal for the lowest detection limits. **Page 5**



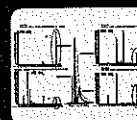
### Trace Ion Detection technology

Lowers detection limits in complex matrices; together with the high temperature inert ion source, this new technology gives your lab powerful new analytical capabilities. **Page 5**



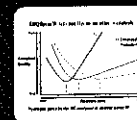
### Synchronous SIM/Scan mode

Selectively monitor for ions of interest at high sensitivity while simultaneously acquiring spectra at scan rates up to 12,500 u/s. **Page 6**



### All ionization modes in one automated sequence

PCI, NCI and EI with standard CI ion source; auto CI feature makes CI as easy as EI. **Page 7**



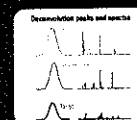
### New hydrogen EI signal-to-noise specification

Permits faster analysis under safe conditions—with the lower cost of hydrogen carrier gas. **Page 7**



### GC/MS software

Fits your workflow and your application—powerful features and advanced functionality enhance your lab's performance and productivity. **Page 10**



### Deconvolution Reporting Software

Our second generation software gives you fast answers with confidence; together with new Retention Time Locking databases, DRS significantly reduces post-run analysis time. **Page 12**



### GC/MS columns and supplies

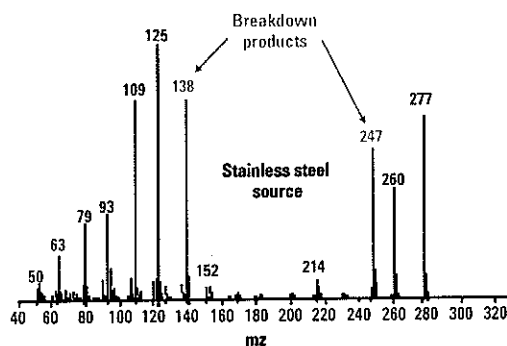
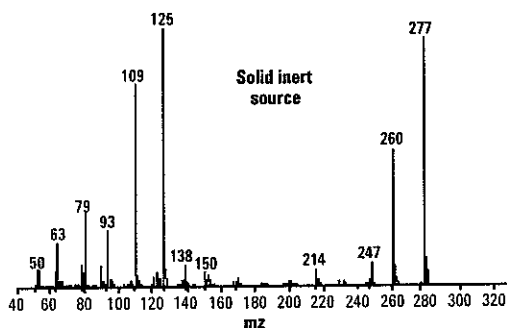
High performance Agilent J&W GC columns and certified supplies maximize your analytical results. **Page 15**

## Engineered for performance and productivity, from the source to the detector.

Building the world's most trusted GC/MS solutions is a process of continual improvement. With each new generation, we never lose sight of our goal—to help your lab get better results with higher confidence in the shortest possible time.

### High temperature solid inert ion source boosts your system performance

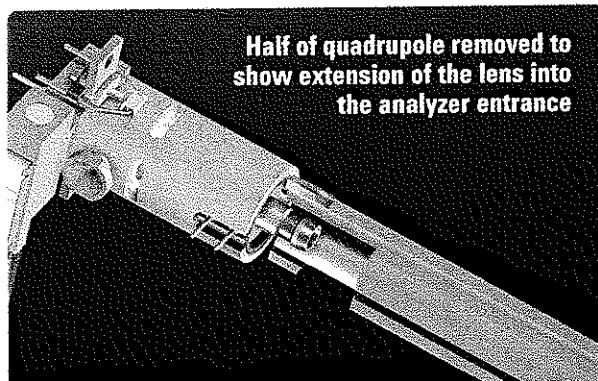
Agilent's proprietary inert source is now programmable up to 350°C to provide enhanced response for active compounds and late-eluters. It delivers improved peak symmetry, higher EI response, fewer degradation ions and more reliable library searches. Higher temperature also means less frequent cleaning—a nice improvement for your lab's productivity (1)



**Improved spectral integrity.** New inert source eliminates surface activity reactions, resulting in more reliable library matches

### The gold standard in quadrupole design

The MSD analyzer incorporates a combination of patented, proprietary technologies to deliver superior performance and enhanced reliability.



*The last lens, which extends into the heated monolithic quadrupole, optimizes coupling of the source to the analyzer. Voltage on this lens is dynamically ramped synchronously with analyzer voltage to focus maximum ion signal for every m/z into the center of the quadrupole field.*

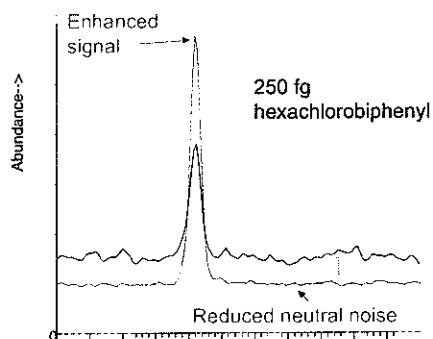
The dimensional stability of the single piece quartz analyzer is a fundamental strength of the MSD design. Unlike metal rods, temperature changes from room temperature to 200°C do not alter the quartz dimensions. Higher analyzer temperature allows robust, maintenance-free operation—even with complex, high boiling samples.

The submicron-layered gold, hyperbolic electrode surfaces eliminate field errors of round rod quadrupoles and deliver excellent resolution, mass axis stability and ion transmission efficiency across the full mass range, up to 1050 u. An available high mass checkout kit provides added confidence that high mass is accurately reported (2)



## Triple-Axis Detector for lower detection limits and reduced cost of operation

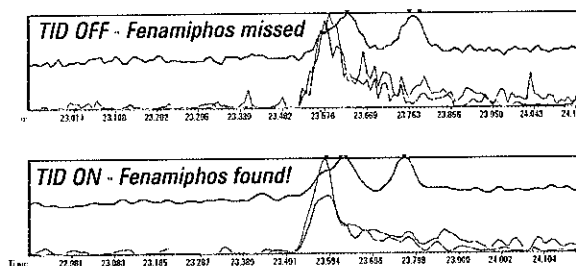
The fundamental goal for the detector module is always the same: collect more ions of interest and eliminate background sources of noise. To achieve these goals, the 5975C detector uses a new ion guide and shield to position a new long-life triple channel electron multiplier (EM) doubly off-axis from the analyzer exit. The optimized ion path increases signal and eliminates noise from energetic neutrals. The result is simply the best signal-to-noise specification in the market and the perfect complement to the inert source and patented hyperbolic analyzer.



**Triple-Axis Detector** increases signal and decreases noise—the ideal combination for improved detection limits.

## Trace Ion Detection delivers a real performance improvement for complex matrices

Revolutionary Trace Ion Detection technology gives you a better spectral fidelity, increasing your confidence level when doing library matching. It lets you lower your Method Detection Limit (MDL) as well as your limit of quantitation (LOQ), reducing false negatives and further enhancing the performance of the inert ion source at trace levels. The technology also ensures more reproducible baselines, dramatically reducing the number of manual interventions during peak integration.



**Analysis of Fenamiphos.** Without Trace Ion Detection enabled (top), fenamiphos was missed as a poorly defined shoulder on a larger peak. When Trace Ion Detection was activated (bottom), noise decreased and a clear hit was achieved.

## High sensitivity AutoTune makes it easy to optimize system performance

Take the trial and error out of optimizing operating conditions by automating the process. The 5975C system's AutoTune saves time, boosts performance and improves instrument-to-instrument consistency. New gain normalized tune of the EM ensures consistently optimized ion count and prolongs EM life. (3)

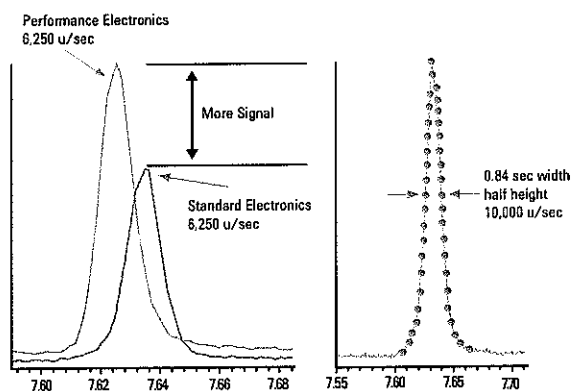
**Ask about a detector upgrade for your existing Agilent 5975 Series GC/MSD.**

- (1) 5989-6051EN: The 5975C Series MSDs: Guidance in Implementing High Ion Source Temperature
- (2) 5989-3142EN: Applying the 5975 inert MSD to Higher Molecular Weight Polybrominated Diphenyl Ethers (PBDEs)
- (3) 5989-7654EN: Enhancements to Gain Normalized Instrument Tuning

# Powerful analytical capabilities improve results and productivity.

Fast electronics enhance performance and enable synchronous SIM/Scan

Fast electronics used in the 5975C Series GC/MSD maximize signal transmission for fast GC/MS in full scan and Selected Ion Monitoring (SIM) modes. They also enable synchronous SIM/Scan functionality—without compromising analytical performance (4)

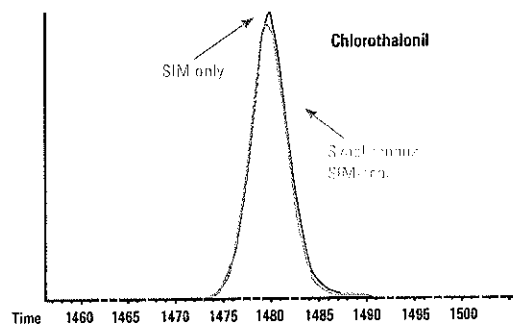


**More signal, and more data points.** Total ion chromatogram of Heptachlorobiphenyl compares standard electronics (Agilent 5973 Series MSD) to new fast electronics. Both chromatograms were acquired by the same instrument at the same scan speeds (horizontal offset for clarity). High scan rates up to 12,500 u/sec allow accurate peak integration even for narrow bore capillary peaks

## High-performance Selected Ion Monitoring (SIM) and full scan

Agilent's synchronous SIM/Scan functionality lets you capture SIM data and full scan data in the same acquisition. Because of the ease of setup and availability of spectral libraries, many labs use full scan for most of their data collection. SIM mode, on the other hand, offers a significant improvement in sensitivity over full scan data; however, SIM data cannot be searched against commercially available spectral libraries for match confirmation.

Now, with the 5975C system's synchronous SIM/Scan operation, you can get both—in a single run! Even better, you don't have to be a GC/MS expert to do it. Agilent's AutoSIM software capability automatically converts full scan data into SIM or SIM/Scan acquisition parameters for use in synchronous SIM/Scan methods. SIM dwell times can be set in 1 msec increments from as fast as 1 msec to over 100 msec dwell time.



**No sensitivity loss in SIM during SIM/Scan operation.** The overlay above compares SIM-only acquisition (blue) to the SIM signal from a synchronous SIM/Scan acquisition (orange).

(4) 5989-3108EN. Improving Productivity with Synchronous SIM/Scan

(5) 5989-4347EN. The 5975 inert MSD—Benefits of Enhancements in Chemical Ionization Operation

## CI as easy as EI

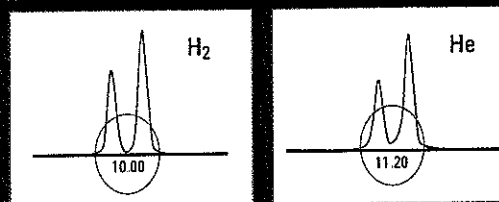
Chemical ionization (CI) has long been considered an advanced GC/MS technique because of complex setups, reagent gas adjustment and ion source tuning. Now the Agilent 5975C inert GC/MSD makes CI as routine and easy as EI—and EI spectra can be generated without changing to the EI source.

An intuitive user interface and a CI flow control module work together to automatically adjust the CI reagent gas flow for optimum performance. The dual reagent inlets allow easy comparison of complementary reagents like methane and ammonia.

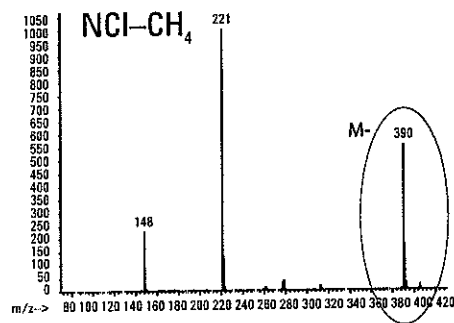
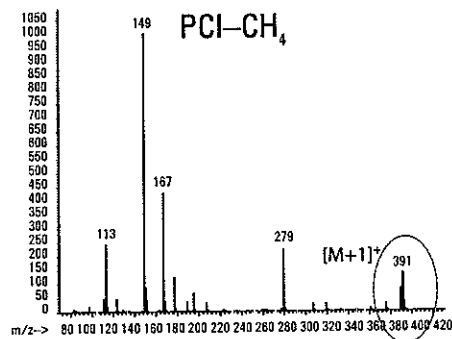
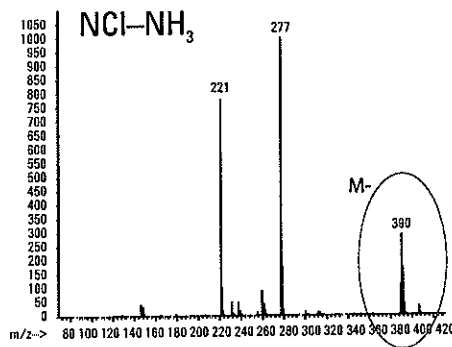
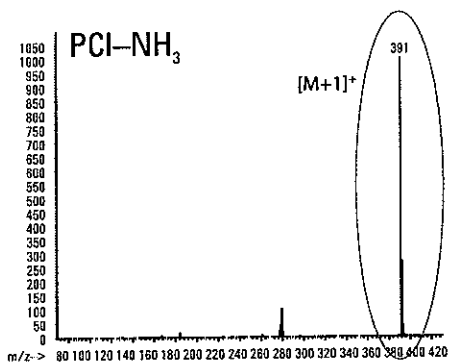
Automated calibrant 'burn-off' allows the system to be quickly readied for use even in the ultra sensitive NCI mode.

## Use hydrogen to lower your cost per analysis

The new hydrogen signal-to-noise specification for the 5975C Series GC/MSD makes Agilent the first and only instrument manufacturer to certify the performance and safety of hydrogen as a carrier gas. In fact, hydrogen often provides faster analysis times and resolution greater than GC/MS systems operating in helium mode.



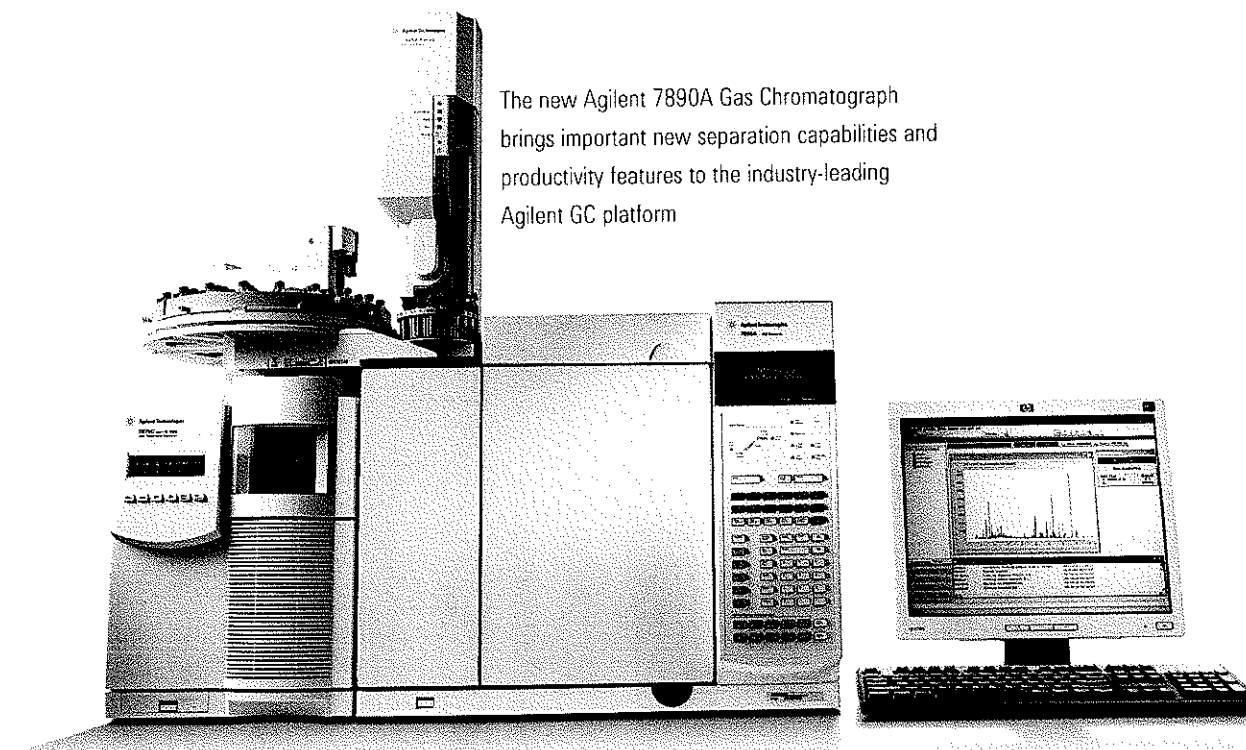
Analysis of polyaromatic hydrocarbons using H<sub>2</sub> and He. In this example, H<sub>2</sub> actually provides better resolution.



**Diethyl phthalate in all CI modes.** Many compounds yield little identifying information in EI; for example, all phthalates look very similar. CI provides valuable additional spectral information: PCI with ammonia (upper left); PCI with methane (lower left); NCI with methane (lower right); and NCI with ammonia (upper right) (5)

# The Agilent 7890A Gas Chromatograph: The next level of GC performance and productivity.

Adding an exciting new chapter to a 40-year history of GC leadership, Agilent's new 7890A flagship GC gives you everything you need to take your lab to the next level of GC/MS performance, including advanced chromatographic capabilities, powerful new productivity features and real-time self-monitoring instrument intelligence. Plus, of course, legendary Agilent reliability.



The new Agilent 7890A Gas Chromatograph brings important new separation capabilities and productivity features to the industry-leading Agilent GC platform

## Agilent performance and reliability

Fifth-generation electronic pneumatics control (EPC) and digital electronics set a new benchmark for retention time locking (RTL) precision and retention time repeatability, and help make the 7890A Agilent's most dependable GC ever

## Higher productivity

Faster oven cool down, robust backflush capability, advanced automation features and faster GC/MS oven ramps let you get more done in less time, at the lowest possible cost per sample—all easily incorporated into your existing methods.

## Simultaneous GC detector operation

For non-target compounds, a sensitive, selective GC detector is a powerful complement to MS. That small, unexpected peak on the ECD baseline might provide the only clue to a critical compound. The GC/MSD Productivity ChemStation will simultaneously acquire signals from two GC detectors and MSD SIM/Scan signals (6)

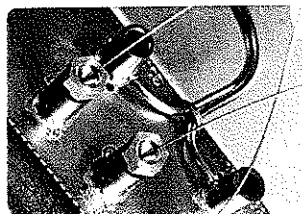
*(6) 5989-7670EN – Replacing multiple 50-minute FPD/ELCD/SIM analysis with one 15-minute full-scan analysis for 10x productivity gain*

The Agilent 7890A GC works right into your current 6890 workflow, with no major changes to your methods

You can increase your productivity and take advantage of the new capabilities of the 7890A system with no disruption to your lab's smooth operation. Right out of the box, operators will be immediately comfortable with the familiar controls and user interface—and because the 7890A system is built upon proven 6890 GC inlets, detectors and GC oven, you can transfer methods to your new 7890A GC with complete confidence.

### Breakthrough Capillary Flow technology

Agilent's innovative Capillary Flow modules enable reliable, leak-free, in-oven connections. Available in a number of useful configurations,

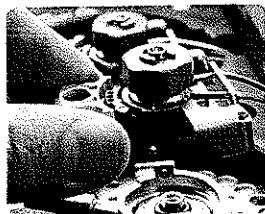


these inert, low-mass, low-dead volume devices not only make it easy to make secure connections, they give you the ability to precisely divert your gas flow, where and when

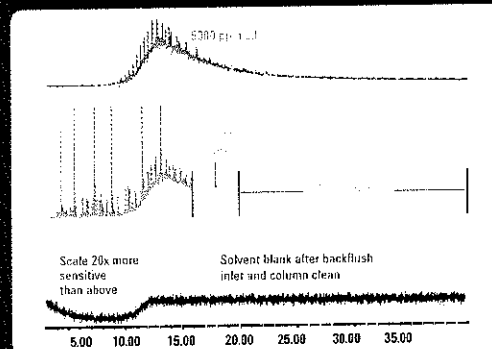
you want. This opens the door to highly useful techniques such as flow splitting, backflushing and Deans switching that can improve your analytical results, as well as saving time and resources.

### Perform SSL inlet maintenance in seconds!

Convenient new Turn-Top design is built into each split/splitless (SSL) inlet, allowing you to change liners and columns more quickly and easily than ever before—without special tools or training.



### 7890A GC gives you a net improvement in productivity

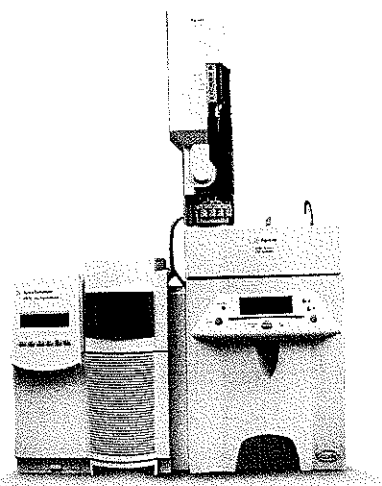


#### Semivolatile analysis (5 ppm) of hazardous waste (simulated sample with high boiling interference).

*Top (blue):* Peaks of interest elute by 16 minutes, but a 24-minute bake-out at 320°C is required to elute heavy components.

*Middle (orange):* Using the 7890A system's backflush capability with a turbo-based 5975C MSD, the sample was rerun with a 4-minute backflush—saving 20 minutes per run (50% total cycle time savings). ALS Overlap and faster cool down save an additional 4 minutes per cycle.

*Bottom (green):* A solvent blank monitored at a more sensitive scale confirms the efficiency of the backflush.



The Agilent 6850 Series II GC—small, rugged, easy to use

Is your lab doing simple, routine applications or at-line analysis? The Agilent 6850 GC, combined with the 5975C VL MSD, is the perfect choice if you need just a single inlet and detector. The small-footprint system offers a surprising number of advanced features—as well as legendary Agilent reliability.

## GC/MS software that matches your workflow and maximizes your productivity.

The Agilent MSD Productivity ChemStation makes it easy even for non-expert operators to take advantage of all the advanced capabilities of the Agilent 5975C inert GC/MSD system. You will find everything designed to help you make the most of every run, and every workday.

### Advanced instrument control

- Control of two GC/MS systems from a single PC
- Improved tuning procedures for accurate, consistent results and extended life of the EM (Gain Normalization)
- Simultaneous acquisition of SIM and Scan data for high sensitivity quantitation and library searchable spectra
- Integrated control of Liquid Samplers, G1888 Headspace Sampler and PAL Autosamplers
- Simultaneously acquired MSD and GC detector signals
- Automatic alerts about pending maintenance

### Simplified configuration of methods

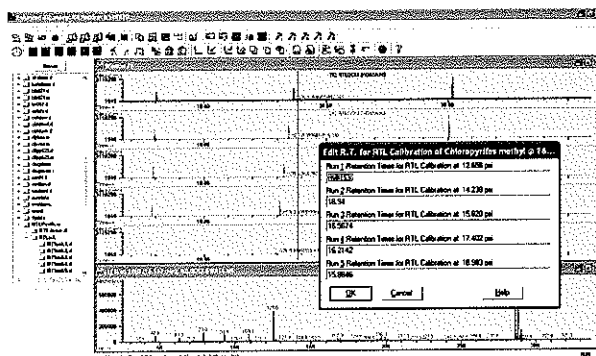
- Import/export of shared methods (eMethods)
- Import LIMS Sample Work Lists
- Guided setup of new calibration tables based upon automatic integration and library search results (AutoQuant)
- Automatic conversion of any full scan method to a high sensitivity SIM or SIM/Scan method (AutoSIM)
- Multi-instrument consistency for retention time locking (RTL)

### High productivity data analysis

- Quantitative power for over 2000 compounds at 20 levels of calibration with 4 curve fit options
- Reprocess a previously run sequence while acquiring data
- Sequentially search up to 3 different libraries
- Direct comparison of multiple data files from multiple detectors (MS and/or GC)
- Simultaneous analysis of multiple data files (Enhance Data Analysis Plus)

### Retention Time Locking (RTL)

- Reproducible retention times instrument to instrument and lab to lab anywhere in the world
- Confirmation of mass spectra identified compounds based on locked retention times
- Fifth generation EPC control to 0.001 psi



*Retention Time Locking (RTL) is permanent, universal and flexible. The retention time for each of the chromatograms can be edited manually when the RTL method is being calibrated.*

### Reporting and customization

- General purpose and tailored report packages: Enhanced, EnviroQuant (USEPA), DrugQuant and Aromatics in Gasoline (ASTM)
- Custom reports with up to 240 graphic elements and corresponding databases for summary view and charting
- Export of reports in XLS, HTML or XML format
- PDF reports with index for searching and electronic signatures
- Macro programs to automate repetitive steps (mouse actions, menu choices and typed entries) and customize processes
- MSD Security ChemStation to address data security integrity and traceability mandated by FDA's 21 CFR Part 11

SemiQuant Quickly and easily estimate the concentration of non-calibrated compounds

Agilent's SemiQuant capability works together with Retention Time Locking (RTL) databases to increase confidence in your compound identification and speed up the quantification process

When an unknown peak appears, a library search provides only a possible match with the sample spectrum Using the appropriate RTL database, you can increase certainty by matching the retention time of your compound with a fixed retention time in addition to spectral data Should you wish to quantify the compound, SemiQuant helps by estimating the concentration so that you can inject the appropriate level of the standard (7)

Quantitation Report (Not Reviewed)

```

Data Path : C:\msdchem\1\data\
Data File : eva10em.d
Acq On : 7 Sep 1989 13:59
Operator : D. Peterson
Sample : democan sample
Misc : 10 ng per component
ALS Vial : 1 Sample Multiplier: 1

Quant Time: Mar 10 15:39:59 2006
Quant Method : C:\msdchem\1\METHODS\LEVALDENO-SQ-UM.M
Quant Title : Semi-quant tests
QLast Update : Thu Mar 09 10:51:36 2006
Response via : Initial Calibration
  
```

| Internal Standards  | K.T.  | Q Ion | Response | Conc    | Units | Dev(%) |
|---------------------|-------|-------|----------|---------|-------|--------|
| 1) Dodecane         | 5.288 | 57    | 9737444  | 1000.00 | ng    | 8.88   |
| Target Compounds    |       |       |          |         |       |        |
| 2) Biphenyl         | 6.483 | 154   | 27580844 | 1000.00 | ng    | 99     |
| 3) 4-Chlorobiphenyl | 7.741 | 188   | 18794921 | 1000.00 | ng    | 99     |

```

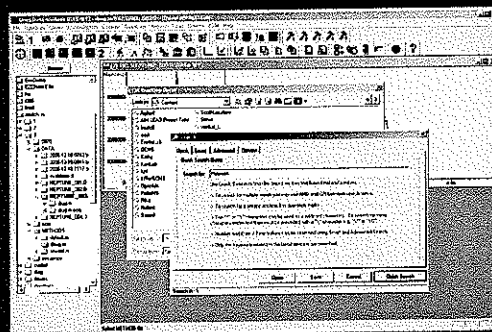
Semi-Quant Compounds - Not calibrated on this instrument
a) Internal Standard 6096601 6.175 74 14362292 892 30
  
```

*SemiQuant compounds are highlighted at the bottom of the Quantitation Report.*

eMethods Replicate, share and distribute methods

With Agilent eMethods, recreating and replicating a new GC/MS method is now a quick and fully automated process You can bring a new GC/MS online in the shortest possible time, and maximize lab productivity by standardizing on methods—whether your instruments are across the hall, or across the world.

## Integration with Agilent OpenLAB Enterprise Content Manager (ECM) streamlines data handling and organization.



Agilent OpenLAB Enterprise Content Manager is a Web-based application that provides a secure, centralized repository for all of the electronic data generated in your organization. (8) Comprehensive search and collaboration tools allow users to effectively find, use and re-use the information they need to make intelligent business decisions. Agilent OpenLAB ECM makes your lab more efficient, productive and confident by enabling the collection and conversion of the broadest range of analytical data into accurate and actionable information.

(7) 5989-4997EN: SemiQuant: New GC/MS Software Approaches to Estimating Compound Quantities

(8) 5989-6104EN: Integration of GC/MSD ChemStation with Agilent OpenLAB ECM

# Rapid deconvolution, identification and quantification in complex matrices.

Agilent's simple, easy-to-use Deconvolution Reporting Software (DRS) is an optional software feature that saves hours of analysis and review. Based on industry standard AMDIS, our second-generation deconvolution software quickly finds compounds missed by other data analysis packages. In fact, it reduces data review time from hours of tedious work to minutes of unattended computer analysis.

The revolutionary solution fully integrates three different software packages:

- Agilent's GC/MSD ChemStation
- The National Institute of Standards and Technology (NIST) Mass Spectral Search Program with the NIST MS Library
- NIST's Automated Mass Spectral Deconvolution and Identification Software (AMDIS)

The DRS automates the following operations:

- Quantitation by the MSD target ion or the AMDIS deconvoluted ion via GC/MSD ChemStation QEdit
- Spectral Deconvolution, or "cleaning" of full scan spectra
- Library searching of cleaned spectra
- Graphic and text reports that summarize both MSD and AMDIS deconvolution results for efficient review

## Wide choice of custom RTL databases

Rapid, accurate identification and quantification is ensured with one of Agilent's RTL databases (spectra and retention time). Databases for PAHs, PCBs, Flavors, FAMES, VOCs, Semi-VOCs, Pesticides and Endocrine Disruptors, Hazardous Chemicals, Organotins and Indoor Air Toxics have been expanded to include:

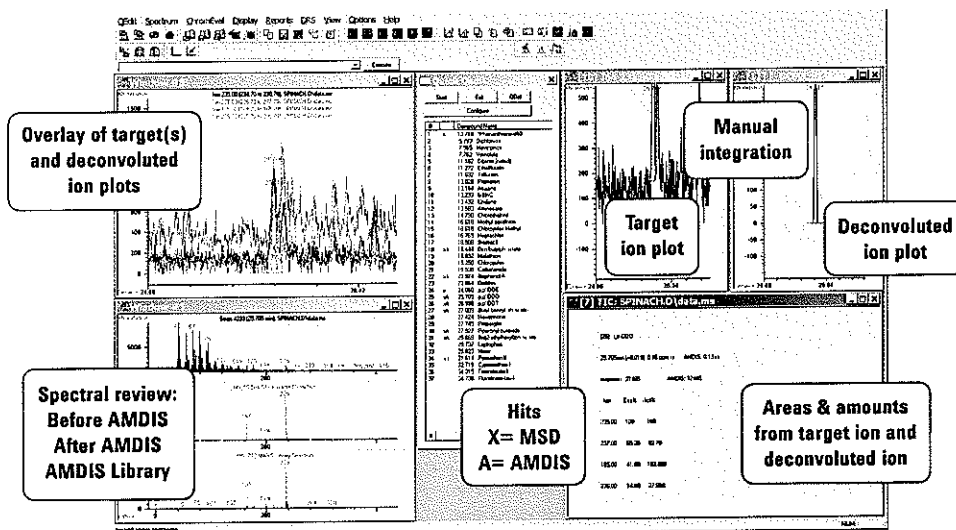
- Japanese Positive List Pesticides
- Forensic Toxicology
- Metabolomics

|                           | California Department of Food and Agriculture (CDFA) | Deconvolution Reporting Software (DRS) |
|---------------------------|------------------------------------------------------|----------------------------------------|
| Number of pesticide hits  | 37                                                   | Same 37 plus 99 additional             |
| Number of false positives | 1                                                    | 0                                      |
| Time required to process  | 8 hours                                              | 32 minutes                             |

### Comparison of the time to process 17 surface water samples.

**CDFA:** A skilled analyst processing the 17 samples took about 8 hours to review results and eliminate false positives

**Agilent DRS:** Fully automated process took about 30 minutes and found an additional 99 compounds (9)



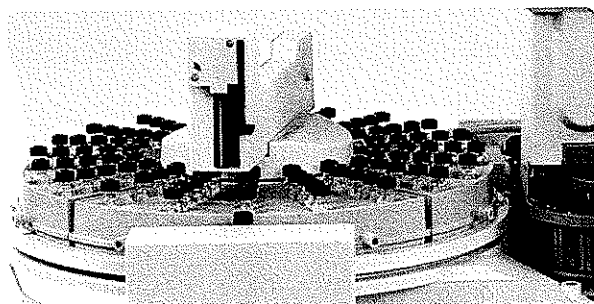
GC/MSD ChemStation QEdit fully integrates deconvoluted data from AMDIS including EICs and spectra



## Accessories and options make your 5975C even more versatile and productive.

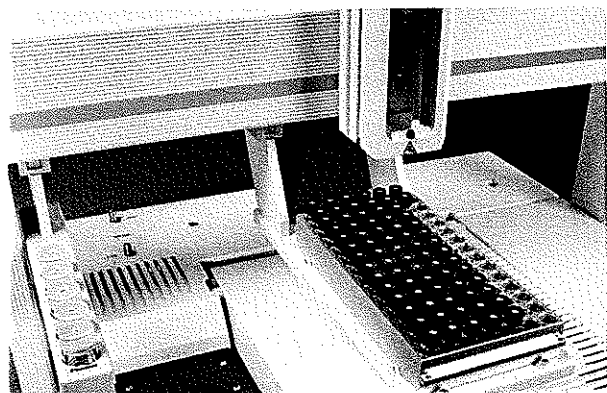
Automatic Liquid Samplers—perfect productivity partners for your 5975C Series GC/MSD

Add an Agilent 7683 Series Automatic Liquid Sampler. Offering the fastest injection times of any GC autosampler, greater solvent capacity, multiple sampling options, dual simultaneous injection certified autosampler vials—and more—the 7683 ALS is ready to go to work



Boost your lab's output with automated sample preparation

Choose the versatile CombiPAL sample injector for liquid injection, headspace and solid-phase microextraction (SPME). The economical GC PAL platform is configured for liquid injection only, but offers many of the other capabilities of the CombiPAL including large volume injection (LVI), multiple vial and syringe sizes, and extended sample vial capacity

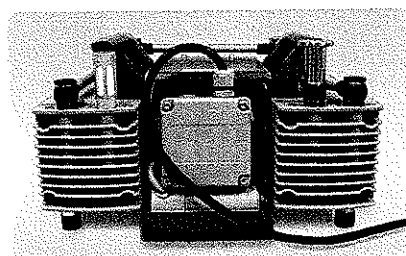


Agilent G1888A Headspace Sampler adds to your analysis capabilities

Automatically introduce volatile compounds from virtually any sample matrix directly into a GC or GC/MS. An inert sample pathway from vial through column to source provides superior chemical performance without analyte degradation or loss.

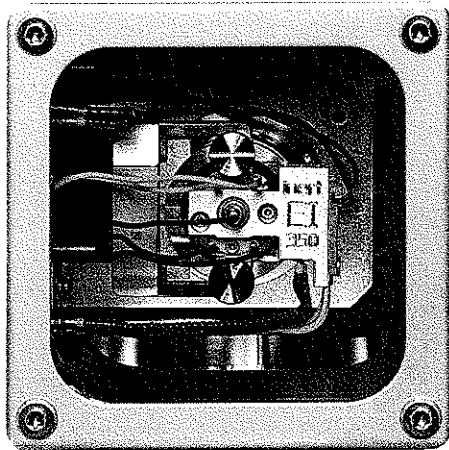
Oil-free pump—clean and virtually maintenance free

Agilent is the first mass spectrometer manufacturer to offer this unique pump, which requires virtually no routine maintenance. There's no oil, so no danger of oil contamination or leaking.



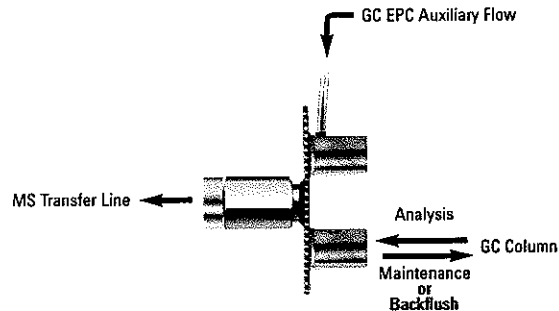
## Designed for supportability and maintenance.

Agilent GC/MSD systems have always been designed for easy serviceability and maintenance—and the Agilent 5975C Series GC/MSD takes this design philosophy to a whole new level

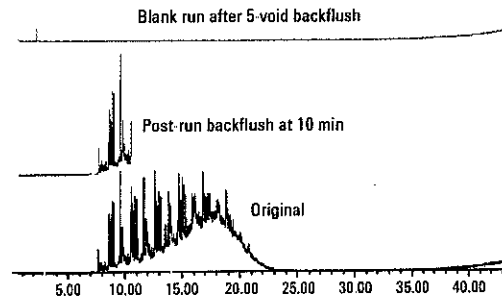


- **Modular analyzer assembly** offers complete access to the filament, ion source and electron multiplier for faster routine maintenance—in fact, the entire analyzer assembly can be removed in less than two minutes, without tools! A modular self-contained electronics module minimizes problems with cables and wiring harnesses.
- **Front glass window** provides simple source identification, as well as a complete view of critical connections—so you can see for sure the column is connected properly
- **High-reliability vacuum system** assures maximum long-term performance; available oil-free pumping system virtually eliminates pump maintenance and reduces noise, and can be used with corrosive gases such as ammonia.
- **Triple-Axis Detector with new triple-channel electron multiplier (EM)** more than doubles EM life. The Electron Multiplier Saver feature further extends EM life during SIM operation with highly concentrated peaks.
- **Optional ion gauge** helps to troubleshoot and isolate leaks as quickly as possible

QuickSwap Capillary Flow device saves time and money with every column change and system maintenance



Tired of waiting around for a mass spec to vent before you can change a column out or perform routine inlet maintenance? Using a "QuickSwap" Capillary Flow device, you can safely disconnect the column without venting, and without losing vacuum—in about 30 seconds!



The QuickSwap device can also be used for column backflushing, reducing MSD contamination by high-boiling sample components, shortening analysis time and decreasing the frequency of cleaning the ion source. (Note: Backflush operation requires pumping capacity of a turbomolecular pump ) (10)

(10) 5989-6018EN: Improving Productivity and Extending Column Life with Backflush

## High-performance Agilent J&W columns and supplies for the Agilent 5975C Series GC/MSD.

To help you achieve better results faster, Agilent is continuously improving the cleanliness, convenience and reliability of columns and supplies for Agilent GC/MSD systems. From market-leading J&W columns—with rigorous quality control and QC testing that ensure reproducibility, efficiency and inertness—to GC flow path supplies designed, manufactured and packaged to maintain the integrity of your sample, Agilent columns, supplies and accessories will improve your lab's performance, productivity and confidence.



### Performance

Choose Agilent J&W columns and supplies for a leak-free, inert flow path to ensure lowest bleed and best signal-to-noise performance in Agilent GC/MSD systems.

From among the full suite of Agilent low-bleed J&W columns, the inert HP-5MSi column was selected to ship with the new 5975C. Specially tested to ensure maximum-area response performance of strong acid and base compounds, this column is also compatible with Agilent Pesticide Libraries for MS.

Tight inlet seals are needed to keep MS system performance at its peak. Agilent pre-cleaned liners and conditioned liner O-rings—matched with our new, proprietary injection-molded, gold-plated seal—prevent the tiniest leaks that cause column bleed and signal deterioration.

### Productivity

Agilent supplies help keep routine maintenance routine. Our capillary column ferrules, O-rings and septa are packaged to remain clean and ready for use, and conveniently dispense one at a time as needed for fast inlet maintenance.

Agilent's new J&W High Efficiency Capillary GC columns in 0.18 mm id allow for potentially 50% or more faster analysis than conventional GC/MS without loss of resolution. The improved sample throughput enables lower cost per analysis in conjunction with reduced carrier flow requirements.

### Confidence

Agilent J&W columns and supplies ensure your Agilent 5975C system delivers as promised. In fact, our GC and GC/MS instrument specifications are determined using industry-leading Agilent J&W columns and Agilent brand chromatography supplies. Eliminate concerns about lost samples or productivity from unexpected sequence interruptions by using Agilent certified autosampler vials, septa and caps, and Gold Standard syringes. Each comes with a Certificate of Conformance to assure you all specifications are met.

*Agilent J&W GC columns and our portfolio of chromatographic supplies are available through Agilent and authorized Agilent distributors.*

## Agilent services let you focus on what you do best.

Agilent's service organization is the most respected in the industry. Whether you need support for a single instrument or a multilaboratory operation, we can help you solve problems quickly, increase your uptime and optimize your lab's resources. On our full line of GC/MS systems, we offer:

- On-site preventive maintenance to ensure dependable operation and minimize unplanned downtime
- Troubleshooting, maintenance and repair for Agilent as well as non-Agilent instruments
- Remote diagnostic and monitoring services to maximize instrument uptime and lab productivity
- Industry-leading regulatory compliance services and education
- Expert consulting and training

## The Agilent Value Promise— 10 years of guaranteed value.

In addition to continually evolving products, we offer something else unique to the industry—our 10-year value guarantee. The Agilent Value Promise guarantees you at least 10 years of instrument use from your date of purchase, or we will credit you with the residual value of that system toward an upgraded model. Not only does Agilent ensure a safe purchase now, we help ensure your investment is as valuable to you in the long run.

## The Agilent Service Guarantee



Should your Agilent instrument require service while covered by an Agilent service agreement, we guarantee repair or we will replace your instrument for free.

No other manufacturer or service provider offers this level of commitment to keeping your laboratory running at maximum productivity.

For more information

**Learn more:**

[www.agilent.com/chem/5975C](http://www.agilent.com/chem/5975C)

**Buy online:**

[www.agilent.com/chem/store](http://www.agilent.com/chem/store)

**Find an Agilent customer center  
in your country:**

[www.agilent.com/chem/contactus](http://www.agilent.com/chem/contactus)

**U.S. and Canada**

1-800-227-9770

[agilent\\_inquiries@agilent.com](mailto:agilent_inquiries@agilent.com)

**Europe**

[info\\_agilent@agilent.com](mailto:info_agilent@agilent.com)

**Asia Pacific**

[adinquiry\\_aplsca@agilent.com](mailto:adinquiry_aplsca@agilent.com)

Research use only. Information, descriptions and specifications in this publication are subject to change without notice.

Agilent Technologies shall not be liable for errors contained herein or for incidental or consequential damages in connection with the furnishing, performance or use of this material.

© Agilent Technologies, Inc. 2008

Printed in USA May 6, 2008

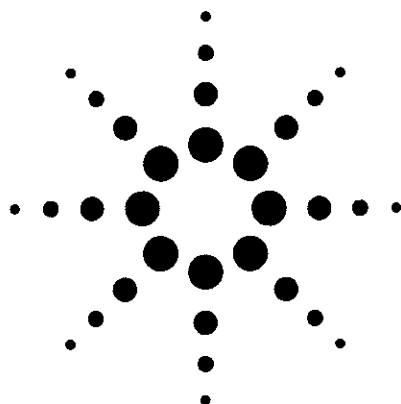
5989-7827EN



**Agilent Technologies**

# Using the Agilent 6890 Gas Chromatograph and Agilent 5973 Mass Spectrometer System for EPA Method 524.2

## Application



Gas Chromatography

### Authors

James Refermat and  
Marcell Stephens  
Quanterra Incorporated  
5910 Breckenridge Parkway,  
Suite H  
Tampa, FL 33610  
USA

Mike Szelewski  
Agilent Technologies, Inc.  
2850 Centerville Road  
Wilmington, DE 19808  
USA

### Abstract

A system comprised of a purge and trap (P&T) concentrator, a gas chromatograph (GC), and a mass spectrometer (MS) was used to determine 61 volatile organic compounds (VOCs). All U.S. EPA method 524.2 criteria were met without using cryofocusing. The P&T and GC-MS conditions listed in tables 1 and 2 detail the instrument settings. The method development for analyzing 524.2 analytes was refined by members of the GC-MS Volatile Organics Analysis (VOA) group at Quanterra in Tampa, Florida.

### Introduction

U.S. EPA method 524.2 is a general-purpose method used to identify and quantify volatile organic compounds (VOCs) in surface, ground, and drinking water. The method is applicable to a wide range of organic compounds including the four trihalomethane disinfection byproducts. The 61 VOCs in this note are a subset of the 84 VOCs that can be analyzed using method 524.2.

Compounds of sufficient high volatility and low water solubility are purged from a water sample using helium and trapped on a solid sorbent held at room temperature. At the end of the purge cycle, the trap is heated and, using helium, the compounds are desorbed onto the head of a gas chromatograph (GC) column. The GC column is temperature programmed, and the analytes are eluted into the mass spectrometer (MS) ion source. The MS is used for identification and measurement. The purge and trap (P&T)-GC-MS system is controlled from a PC.

### Experimental

The program requirements for which the 524.2 analysis is used must meet local state regulatory guidelines as well as EPA method 524.2 acceptance criteria and U.S. Air Force compliance guidelines under the auspices of the Air Force Center for Environmental Excellence (AFCEE) program.



Agilent Technologies

Quanterra maintains strict QA/QC procedures at all 12 facilities. Each location has a quality assurance officer (QAO) reporting directly to the corporate quality assurance director. Quanterra's network of 12 facilities in 10 states staffs over 700 employees and encompasses over 310,000 square feet of facility space, providing the capacity to handle any analytical need. Quanterra performs more than 1.5 million separate tests per year. A nationwide network of fully equipped labs, linked by advanced information management systems, assures a high standard of testing and consistent quality.

Quanterra's comprehensive quality management system (QMS) forms the foundation of their quality goals. Quanterra's QMS ensures that their clients receive high-quality analytical services that are timely and reliable, and that meet the intended purpose in a cost-effective manner. The QMS also applies to all Quanterra technical, business, and administrative functions. The principles and practices expounded in the QMS apply to all staff and are fundamental to the services they provide. As a result, Quanterra is continuously seeking ways to improve their products and services using the best technologies available. The AGILENT 6890 / AGILENT 5973 GC-MS system provides high-quality data and increased productivity.

The P&T instrumentation and conditions are listed in table 1. The Vocab 3000 trap allows for higher desorb and bake temperatures. The high desorb temperature facilitates efficient desorption of target analytes, and the high bake temperature minimizes carryover between samples. The standard transfer line provided with the P&T was replaced with a Restek 0.53-mm SilcoSteel MXT 502.2 column. The use of the analytical column as the transfer line between the P&T and GC appears to improve peak symmetry for low-level standards. The transfer line is attached directly to the AGILENT 6890 GC injection port (direct capillary interface) and runs in the split mode. A purge rate of 50 mL/min appears to improve the recovery of analytes that are known to have poor purge efficiencies. The 50-mL/min purge flow did not have an adverse effect on the recovery of the gases and, as a result, produced method and program compliant data. Traditional trap packing materials (Tenax/charcoal/silica) usually did not hold the gases at higher purge flow rates, resulting in poor recoveries. This problem was not observed when

using the Vocab 3000 trap. The original method's desorb and bake temperature of 180 °C is a limitation associated with traditional packing material (Tenax break down).

The GC-MS instrumentation and conditions are listed in table 2. Conditions were optimized for maximum sample throughput while meeting site-specific data quality objectives. The split ratio used allows the best combination of sensitivity and peak shape. With this configuration, it is advantageous to use the electronic pressure control (EPC) inlet (option available on the AGILENT 6890 GC). With the EPC inlet pressure on, the chromatography for the gases is improved, and analytes at the end of the temperature program have much sharper peak shape. EPC also gives much better reproducibility of analyte retention times.

Each 12-hour shift (site-specific requirements allow for a 12-hour clock for the tune verification) starts with verification of the fragmentation pattern of 4-bromofluorobenzene (BFB) obtained from 25 ng on-column. A five-point calibration curve is then analyzed at concentrations of 500, 250, 125, 50, and 12.5 ng on-column. Once the calibration acceptance criteria is verified, a 100-ng (4 µg/L) laboratory control spike/laboratory control spike duplicate (LCS/LCSD) is analyzed followed by a method blank. Successful analysis of

**Table 1. Purge and Trap Conditions**

|                                            |                        |
|--------------------------------------------|------------------------|
| P&T                                        | Tekmar LSC 3000        |
| Automatic sampler                          | Tekmar ALS 2016        |
| Trap                                       | Vocab 3000             |
|                                            | Supelco part no 2-4920 |
| P&T-GC interface                           | Custom*                |
| Sample size                                | 25 mL                  |
| Purge temperature                          | 35 °C                  |
| Purge rate                                 | 50 mL/min              |
| Purge time                                 | 11 min                 |
| Dry purge time                             | 1 min                  |
| Desorb preheat temperature                 | 250 °C                 |
| Desorb temperature                         | 260 °C                 |
| Desorb time                                | 2 min                  |
| Bake temperature                           | 270 °C                 |
| Bake time                                  | 6 min                  |
| Bake-gas bypass on time                    | 1 min                  |
| Line/valve temperature                     | 100 °C                 |
| Water management control (WMC) temperature | 310 °C                 |

\*Standard transfer line replaced with approximately 0.7-m length of Restek MXT-502.2 SilcoSteel 0.53-mm id column

**Table 2. Gas Chromatograph and Mass Spectrometer Conditions**

|                           |                                      |
|---------------------------|--------------------------------------|
| <b>Gas chromatograph</b>  | <b>Agilent 6890</b>                  |
| Inlet                     | EPC split/splitless                  |
| Mode                      | Split                                |
| Inlet temperature         | 200 °C                               |
| Pressure                  | 13.9 psi                             |
| Split ratio               | 35:1                                 |
| Split flow                | 24.2 mL/min                          |
| Gas saver                 | On at 2 min                          |
| Gas saver flow            | 20.0 mL/min                          |
| <b>Oven</b>               |                                      |
| Initial temperature       | 35 °C                                |
| Initial time              | 4 min                                |
| Rate                      | 15 °C/min                            |
| Final temperature         | 200 °C                               |
| Final time                | 0.1 min                              |
| Equilibration time        | 0.5 min                              |
| Oven max temperature      | 240 °C                               |
| <b>Column</b>             |                                      |
| <b>Column</b>             | <b>DB-624 fused silica capillary</b> |
| Agilent equivalent        | Agilent part no 121-1324             |
| Length                    | 20 m                                 |
| Diameter                  | 180 µm                               |
| Film thickness            | 1.0 µm                               |
| Initial flow              | 0.7 mL/min                           |
| Average velocity          | 37.0 cm/sec                          |
| Mode                      | Constant flow                        |
| Inlet                     | Front                                |
| Outlet                    | MS                                   |
| Outlet pressure           | Vacuum                               |
| <b>Mass spectrometer</b>  |                                      |
| <b>Mass spectrometer</b>  | <b>Agilent 5973</b>                  |
| Solvent delay             | 1.1 min                              |
| EM voltage                | 2035 volts                           |
| Low mass                  | 35 amu                               |
| High mass                 | 260 amu                              |
| Threshold                 | 200                                  |
| Sampling                  | 3                                    |
| Scans/sec                 | 3.25/sec                             |
| Quad temperature          | 150 °C                               |
| Source temperature        | 200 °C                               |
| Transfer line temperature | 250 °C                               |

the LCS/LCSD and blank are followed by 20 field samples. A typical instrument sequence, when initial calibration is not required, is shown in table 3. This new sample sequence starts with an instrument tune verification (BFB analysis) followed by the analysis of the continuing calibration verification (CCV) standard. If the CCV fails, the system is recalibrated. After the CCV, a 100-ng (4 µg/L) LCS/LCSD is analyzed followed by a method blank and 20 field samples. *The LCS/LCSD QC samples are a site-specific project requirement.*

**Note:** The AGILENT 5973 MS only required retuning every 4 to 6 weeks during large sampling events. During these events, 26 samples were analyzed every 12 hours, operating 6 to 7 days a week.

## Results

The results from the BFB tuning analysis are shown in table 4, together with the EPA method 524.2 tuning criteria. If the BFB tuning criteria are not met, typically mass 50 was low or mass 176 was high. The problem was resolved by running the auto-tune option provided with the Enviro-Quant software followed by a reanalysis of the BFB solution. If the BFB still did not pass, the problem was resolved by replacing the trap. The AGILENT 5973 MS ran for over a year before there was a need to open the analyzer and replace the filaments. The source was cleaned while the analyzer was open, and a little scorching around the filament area was observed. SW-846 method 8260B and CLP-SOW Method OLC02.1 were also performed using this instrument, often containing high levels of target and non-target analytes. As a result, finding the source and its component parts in good condition was unexpected.

A list of target analytes for this project, together with their compound number and retention time (RT), are shown in table 5. The method detection limits (MDLs) shown are based on initial calculations per 40 CFR, Part 136, Appendix B. Prior to running client samples, an instrument detection limit (IDL) study was conducted. This comprised of a five-point calibration curve followed by the CCV, method blank, and seven replicates of the 0.5-µg/L standard for 7 consecutive days. The results between replicates within the same analytical

**Table 3. Instrument Sequence**

| Sequence No. | Description            |
|--------------|------------------------|
| 1            | 1 ppb BFB, with CCV    |
| 2            | 10 ppb CCV             |
| 3            | 4 ppb LCS              |
| 4            | 4 ppb LCSD             |
| 5            | Method blank           |
| 6            | Sample 1               |
| 7            | Sample 2               |
| :            | :                      |
| :            | Matrix spike           |
| :            | Matrix spike duplicate |
| :            | :                      |
| 27           | Sample 20              |

**Table 4. BFB Tuning Criteria and Results**

| m/e | Ion Abundance Criteria             | Ion Abundance Results |
|-----|------------------------------------|-----------------------|
| 95  | Base Peak. 100% relative abundance | 100.00                |
| 50  | 15.00%-40.00% of mass 95           | 19.26                 |
| 75  | 30.00%-60.00% of mass 95           | 46.39                 |
| 96  | 5.00%-9.00% of mass 95             | 7.25                  |
| 173 | Less than 2.00% of mass 174        | 0.65                  |
| 174 | Greater than 50.00% of mass 95     | 85.07                 |
| 175 | 5.00%-9.00% of mass 174            | 7.45                  |
| 176 | 95.00%-101.00% of mass 174         | 100.70                |
| 177 | 5.00%-9.00% of mass 176            | 6.89                  |

sequence demonstrated very little variation. Additionally, the results obtained between the day-to-day analytical sequences also exhibited very little variation. The IDL study and the MDL study yielded similar results with little or no statistical variation. All analyte MDLs are comfortably below

the 0.5 µg/L reporting limit for this project. Lower detection limits could be achieved with lower split ratios.

The initial calibration for this set of analyses was done in August 1997 at the following five levels: 0.5, 2.0, 5.0, 10, and 20 µg/L. Response factors were calculated for each analyte at each level. The percent relative standard deviations (%RSDs) of these response factors, listed in table 5, are all less than 20 and meet the criteria for Table 5. Target Compound List with QA\QC (continued) linearity. Hexachlorobutadiene and naphthalene had trouble meeting the daily ICV/CCV acceptance criteria on a daily basis; these compounds are known as poor purgers. Fortunately, the site-specific QA requirements allows for the use of a quadratic calibration when the acceptance criteria for linearity is not met.

**Table 5. Target Compound List with QA\QC**

| Compound Number          | Compound Name               | RT     | MDL  | Init Cal<br>%RSD RRF<br>limit 0-20 | CCV<br>%D<br>limit ± 30 | LCS<br>%Rec<br>limit 70-130 | LCSD<br>%RPD<br>limit 0-20 |
|--------------------------|-----------------------------|--------|------|------------------------------------|-------------------------|-----------------------------|----------------------------|
| <i>Internal Standard</i> |                             |        |      |                                    |                         |                             |                            |
| 36                       | Fluorobenzene               | 6.651  |      |                                    |                         |                             |                            |
| <i>Surrogates</i>        |                             |        |      |                                    |                         |                             |                            |
| 63                       | 4-Bromofluorobenzene        | 10.919 |      | 5.23                               | -12                     | 99.8                        | 2.0                        |
| 33                       | 1,2-Dichlorobenzene-d(4)    | 12.438 |      | 6.54                               | -1.9                    | 105                         | 7.6                        |
| <i>Target Analytes</i>   |                             |        |      |                                    |                         |                             |                            |
| 34                       | Benzene                     | 6.322  | 0.18 | 8.64                               | 3.9                     | 94.8                        | 6.8                        |
| 64                       | Bromobenzene                | 11.065 | 0.15 | 3.72                               | -12                     | 112                         | 5.5                        |
| 27                       | Bromochloromethane          | 5.574  | 0.19 | 15.5                               | -1.3                    | 104                         | 2.1                        |
| 40                       | Bromodichloromethane        | 7.592  | 0.21 | 10.1                               | -0.9                    | 100                         | 5.0                        |
| 61                       | Bromoform                   | 10.595 | 0.23 | 15.3                               | -21                     | 111                         | 5.3                        |
| 6                        | Bromomethane                | 1.907  | 0.31 | 13.4                               | 4.7                     | 82.3                        | 1.8                        |
| 79                       | n-Butylbenzene              | 12.451 | 0.19 | 10.7                               | -11                     | 97.2                        | 8.3                        |
| 74                       | sec-Butylbenzene            | 11.897 | 0.19 | 9.47                               | -8.5                    | 98.7                        | 12                         |
| 72                       | tert-Butylbenzene           | 11.682 | 0.20 | 6.21                               | 3.0                     | 110                         | 12                         |
| 31                       | Carbon tetrachloride        | 6.091  | 0.17 | 10.0                               | -5.3                    | 104                         | 7.8                        |
| 55                       | Chlorobenzene               | 9.784  | 0.17 | 6.67                               | -4.0                    | 105                         | 3.0                        |
| 7                        | Chloroethane                | 2.007  | 0.18 | 6.51                               | 9.9                     | 82.8                        | 4.2                        |
| 29                       | Chloroform                  | 5.699  | 0.18 | 7.47                               | 6.1                     | 97.0                        | 1.8                        |
| 4                        | Chloromethane               | 1.510  | 0.19 | 6.77                               | 16                      | 75.6                        | 8.4                        |
| 69                       | 2-Chlorotoluene             | 11.264 | 0.18 | 6.53                               | -9.4                    | 103                         | 7.1                        |
| 71                       | 4-Chlorotoluene             | 11.369 | 0.17 | 7.55                               | -11                     | 105                         | 7.6                        |
| 51                       | Dibromochloromethane        | 9.188  | 0.17 | 11.1                               | -12                     | 108                         | 0.04                       |
| 81                       | 1,2-Dibromo-3-Chloropropane | 13.215 | 0.30 | 6.44                               | 16                      | NR                          | NR                         |
| 52                       | 1,2-Dibromoethane           | 9.287  | 0.25 | 13.3                               | 9.2                     | 95.1                        | 8.0                        |
| 39                       | Dibromomethane              | 7.404  | 0.24 | 14.0                               | 8.4                     | 111                         | 1.0                        |



**Table 5. Target Compound List with QA\QC (continued)**

| Compound Number                    | Compound Name             | RT     | MDL  | Init Cal<br>%RSD RRF<br>limit 0-20 | CCV<br>%D<br>limit ± 30 | LCS<br>%Rec<br>limit 70-130 | LCSD<br>%RPD<br>limit 0-20 |
|------------------------------------|---------------------------|--------|------|------------------------------------|-------------------------|-----------------------------|----------------------------|
| <i>Target Analytes (continued)</i> |                           |        |      |                                    |                         |                             |                            |
| 80                                 | 1,2-Dichlorobenzene       | 12.451 | 0.19 | 7.44                               | -0.4                    | 104                         | 3.2                        |
| 76                                 | 1,3-Dichlorobenzene       | 11.996 | 0.20 | 8.36                               | -2.5                    | 105                         | 3.3                        |
| 78                                 | 1,4-Dichlorobenzene       | 12.090 | 0.17 | 8.84                               | 0.3                     | 99.8                        | 2.8                        |
| 3                                  | Dichlorodifluoromethane   | 1.353  | 0.21 | 6.07                               | 15.                     | 83.3                        | 9.1                        |
| 22                                 | 1,1-Dichloroethane        | 4.475  | 0.22 | 7.82                               | 11.                     | 88.7                        | 5.3                        |
| 35                                 | 1,2-Dichloroethane        | 6.342  | 0.20 | 11.2                               | 5.3                     | 99.8                        | 3.5                        |
| 12                                 | 1,1-Dichloroethane        | 2.280  | 0.20 | 7.61                               | 8.5                     | 99.0                        | 6.4                        |
| 25                                 | cis-1,2-Dichloroethene    | 5.275  | 0.22 | 8.63                               | -6.3                    | 97.2                        | 3.6                        |
| 18                                 | trans-1,2-Dichloroethene  | 3.842  | 0.17 | 10.9                               | 13                      | 94.8                        | 4.9                        |
| 38                                 | 1,2-Dichloropropane       | 7.284  | 0.22 | 10.0                               | 8.6                     | 88.3                        | 2.1                        |
| 49                                 | 1,3-Dichloropropane       | 8.957  | 0.12 | 6.56                               | 7.4                     | 95.7                        | 0.76                       |
| 24                                 | 2,2-Dichloropropane       | 5.265  | 0.20 | 9.39                               | 4.2                     | 92.6                        | 0.80                       |
| 32                                 | 1,1-Dichloropropene       | 6.097  | 0.18 | 9.13                               | 5.0                     | 88.3                        | 12.                        |
| 42                                 | cis-1,3-dichloropropene   | 8.053  | 0.19 | 10.5                               | 2.3                     | 95.0                        | 0.64                       |
| 46                                 | trans-1,3-dichloropropene | 8.618  | 0.14 | 10.6                               | 5.1                     | 95.0                        | 3.3                        |
| 56                                 | Ethylbenzene              | 9.904  | 0.20 | 8.46                               | 3.9                     | 89.4                        | 8.6                        |
| 83                                 | Hexachlorobutadiene       | 14.229 | 0.24 | 16.1                               | -4.5                    | 90.6                        | 5.7                        |
| 62                                 | Isopropylbenzene          | 10.778 | 0.17 | 9.23                               | 0.6                     | 98.4                        | 10.                        |
| 75                                 | 4-Isopropyltoluene        | 12.049 | 0.20 | 9.07                               | 11.                     | 102                         | 8.9                        |
| 16                                 | Methylene chloride        | 3.445  | 0.21 | 9.07                               | -3.5                    | 109.                        | 5.0                        |
| 98                                 | Methyl-t-butyl ether      | 3.884  | 0.20 | 10.4                               | 8.3                     | 97.7                        | 3.0                        |
| 84                                 | Naphthalene               | 14.287 | 0.13 | 19.7                               | 5.3                     | 76.8                        | 5.8                        |
| 67                                 | n-Propylbenzene           | 11.186 | 0.21 | 6.92                               | -16.                    | 108.                        | 7.7                        |
| 60                                 | Styrene                   | 10.422 | 0.18 | 11.8                               | -0.3                    | 96.4                        | 5.8                        |
| 57                                 | 1,1,1,2-Tetrachloroethane | 9.868  | 0.21 | 8.27                               | -5.3                    | 102.                        | 10.                        |
| 65                                 | 1,1,2,2-Tetrachloroethane | 11.065 | 0.18 | 6.57                               | -2.4                    | 101                         | 4.8                        |
| 48                                 | Tetrachloroethene         | 8.942  | 0.21 | 8.61                               | 8.6                     | 89.0                        | 10                         |
| 45                                 | Toluene                   | 8.393  | 0.14 | 9.37                               | -6.7                    | 102                         | 9.6                        |
| 85                                 | 1,2,3-Trichlorobenzene    | 14.528 | 0.18 | 9.13                               | 0.7                     | 90.7                        | 5.5                        |
| 82                                 | 1,2,4-Trichlorobenzene    | 14.052 | 0.16 | 11.0                               | -1.7                    | 91.7                        | 3.6                        |
| 30                                 | 1,1,1-Trichloroethane     | 5.893  | 0.24 | 8.34                               | -2.9                    | 102                         | 6.3                        |
| 47                                 | 1,1,2-Trichloroethane     | 8.795  | 0.17 | 12.3                               | 4.3                     | 105                         | 1.2                        |
| 37                                 | Trichloroethene           | 7.059  | 0.16 | 8.77                               | -4.6                    | 100.                        | 6.7                        |
| 9                                  | Trichlorofluoromethane    | 2.273  | 0.19 | 5.26                               | 6.2                     | 99.1                        | 3.9                        |
| 68                                 | 1,2,3-Trichloropropane    | 11.102 | 0.20 | 5.54                               | 2.7                     | 101.                        | 8.8                        |
| 73                                 | 1,2,4-Trimethylbenzene    | 11.729 | 0.17 | 8.38                               | 2.0                     | 95.7                        | 7.6                        |
| 70                                 | 1,3,5-Trimethylbenzene    | 11.363 | 0.18 | 9.42                               | 0.3                     | 94.7                        | 9.4                        |
| 5                                  | Vinyl chloride            | 1.609  | 0.15 | 7.54                               | 4.4                     | 82.1                        | 13.                        |
| 59                                 | o-Xylene                  | 10.411 | 0.13 | 10.7                               | 0.3                     | 94.0                        | 7.5                        |
| 58                                 | m-Xylene                  | 10.019 | 0.17 | 8.15                               | 2.8                     | 92.6                        | 9.3                        |
| 58                                 | p-Xylene                  | 10.019 | 0.17 | 8.15                               | 2.8                     | 92.6                        | 9.3                        |

After the BFB tuning verification is performed, a CCV is run at the 10-ppb level. The method requires that each analyte response factor (RF) is  $\pm 30\%$  of its initial calibration value. These percent deviations (%Ds) are listed in table 5, and all analytes meet the method criteria. If one or more analytes do not meet this criteria, a new five-point calibration curve is run. The data presented here were run in September 1997, one month after the initial calibration. This system is very stable for long periods of time. A five-level calibration has only been necessary eight to ten times in the last 12 months. A total ion chromatogram (TIC) for the CCV is shown in figure 1.

This project requires analysis of a LCS and LCSD. Laboratory blank water is spiked at the 4- $\mu\text{g/L}$  level and analyzed in duplicate. The recoveries for each analyte must be between 70% and 130% for each analyte. A duplicate aliquot of the LCS, referred to as an LCSD, is then analyzed. The relative percent difference (RPD) of this LCS and the LCSD must be less than 20% for each analyte. The LCS recoveries and LCSD RPDs are shown in table 5. All analytes met the site-specific acceptance criteria.

After all of the project-specific QA/QC requirements are met, actual field samples can be analyzed. Results for three samples are shown in table 6. The samples were taken from private wells in an Area of Concern (AOC) in the northeast United States. All ion profiles met the site-specific QC acceptance criteria and all other regulatory acceptance criteria for this AOC.

A TIC for sample 1 is shown in figure 2. The excellent peak shape is typical of the system performance in our laboratory.

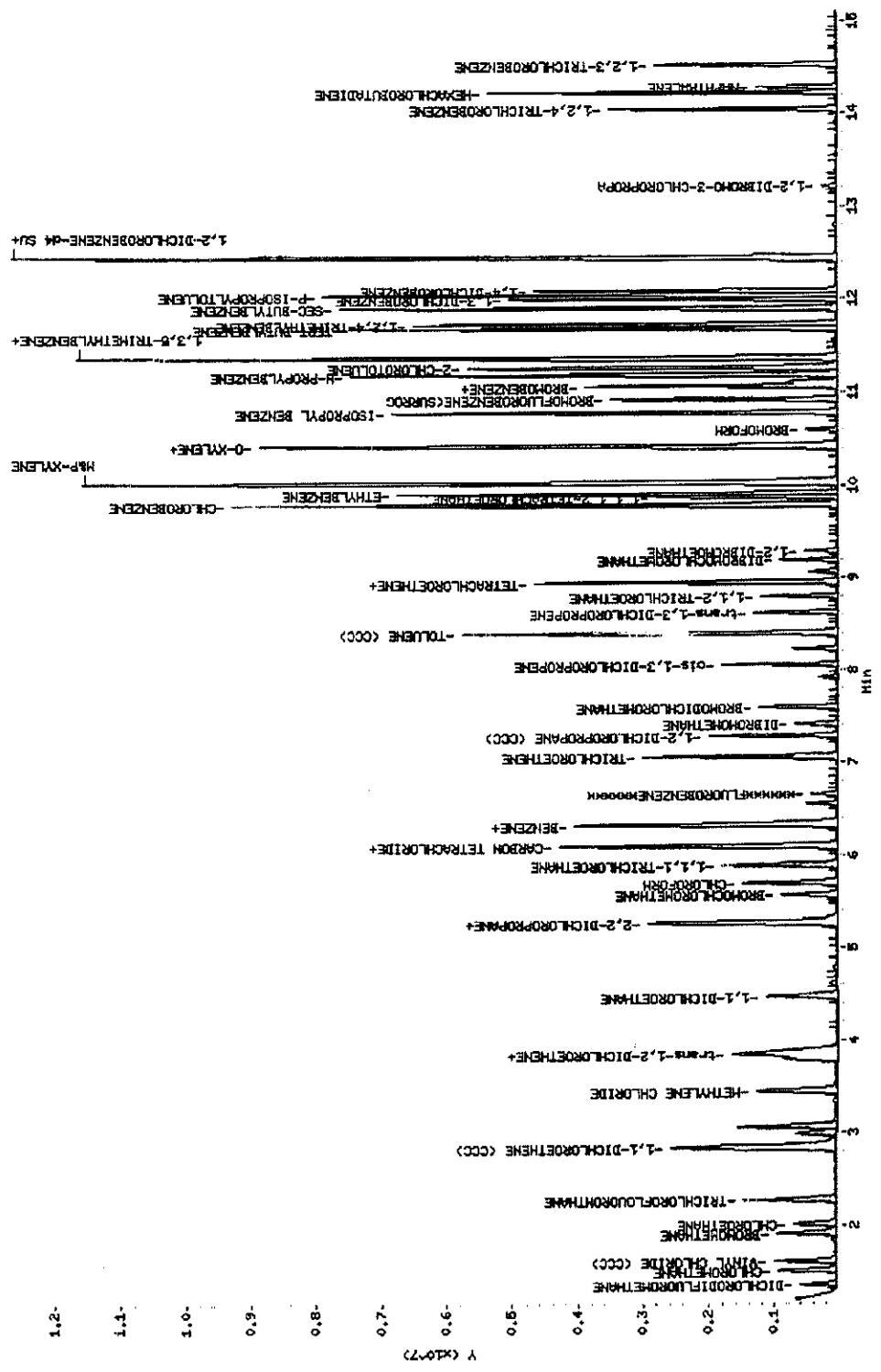


Figure 1. CCV total ion chromatogram.

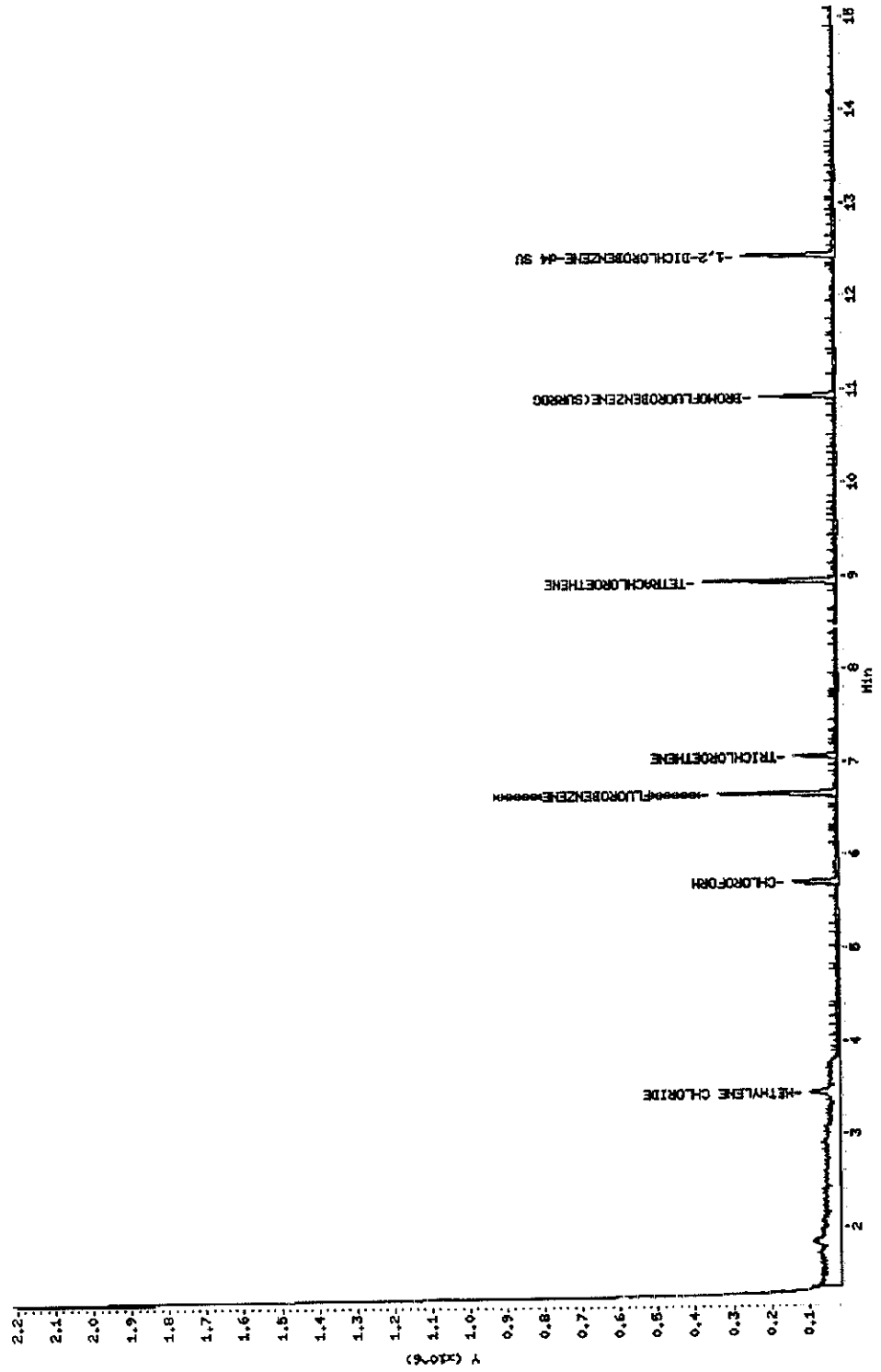


Figure 2. Total ion chromatogram for field sample one.

**Table 6. Results of Sample Analyses**

| Compound Number            | Compound Name            | RT min | Sample1                             | Sample2      | Sample 3     |
|----------------------------|--------------------------|--------|-------------------------------------|--------------|--------------|
| <i>Internal Standard</i>   |                          |        | <i>Area % Difference limit ± 30</i> |              |              |
| 36                         | Fluorobenzene            | 6.651  | -25.6                               | -29.2        | -18.65       |
| <i>Surrogate Standards</i> |                          |        | <i>% Rec 1.0 ppb limit 80-100</i>   |              |              |
| 33                         | 1,2-Dichlorobenzene-d(4) | 12.436 | 98.7                                | 99.5         | 95.1         |
| 63                         | 4-Bromofluorobenzene     | 10.919 | 85.2                                | 93.4         | 89.0         |
| <i>Target Analytes</i>     |                          |        | <i>[ppb]</i>                        | <i>[ppb]</i> | <i>[ppb]</i> |
| 16                         | Methylene chloride       | 3.445  | 0.55                                | 0.56         | 1.0          |
| 29                         | Chloroform               | 5.699  | 1.0                                 | 3.7          | 1.0          |
| 37                         | Trichloroethene          | 7.059  | 0.54                                | < 0.50       | < 0.50       |
| 40                         | Bromodichloromethane     | 7.592  | < 0.50                              | 5.9          | 2.3          |
| 48                         | Tetrachloroethene        | 8.942  | 1.2                                 | < 0.50       | < 0.50       |
| 51                         | Dibromochloromethane     | 9.188  | < 0.50                              | 8.4          | 5.1          |
| 61                         | Bromoform                | 10.595 | < 0.50                              | 2.7          | 3.2          |

## Conclusions

The AGILENT 6890/AGILENT 5973 GC-MS can be used to perform EPA method 524.2. All calibration, verification, and quality control criteria of the method can be met on a routine basis. The system exhibits excellent stability, minimal downtime, and sufficient sensitivity to meet the requirements for this project. The system performance, combined with expert personnel and a rigorous QA/QC program, results in high sample throughput for method 524.2. The AGILENT 6890/ AGILENT 5973 GC-MS allows Quanterra to meet clients' expectations in a timely and cost-effective manner.

[www.agilent.com](http://www.agilent.com)

Agilent shall not be liable for errors contained herein or for incidental or consequential damages in connection with the furnishing, performance, or use of this material.

Information, descriptions, and specifications in this publication are subject to change without notice.

Copyright © 2001  
Agilent Technologies, Inc

Printed in the USA  
April 26, 2001  
5968-1257E



# EPA Method 524.2 by capillary direct split mode using the 6890/5973 GC/MSD System

## Application Note

### Agilent Technologies 6890/5973 GC/MSD System

#### Authors

*Andrew J. Yakuboff  
Agilent Technologies  
540 Offcenter Place  
Columbus OH 43230-5321*

*Brian Anthony  
Agilent Technologies  
1601 California Avenue  
Palo Alto, CA 94304-1111*

#### Abstract

Details to set up and operate a system to analyze volatiles from drinking water using a purge and trap coupled to a 6890/5973 GC/MSD system are outlined. Performance data obtained from a typical system set up as described are presented; they indicate excellent compliance with the method guidelines. Finally, considerations for troubleshooting results that fall outside the guidelines of EPA Method 524.2 are highlighted.

#### Keywords

*EPA Method 524.2, 5973 MSD, Purge and Trap, volatile organic compounds, drinking water, GC/MSD*

#### Introduction

Method 524.2 is a general purpose method for the identification and quantification of volatile organic compounds in finished drinking water or raw source water. This method may be used for the analysis of a wide array of organic compounds, including the four trihalomethane disinfection by-products

The following outline of parameters is a guide in the initial setup of the 6890/5973 GC/MSD and other related instrumentation required for this analysis. Included are operational parameters for GC, MS and Purge and Trap equipment. In addition to hardware setup and configuration, typical performance data is also presented.

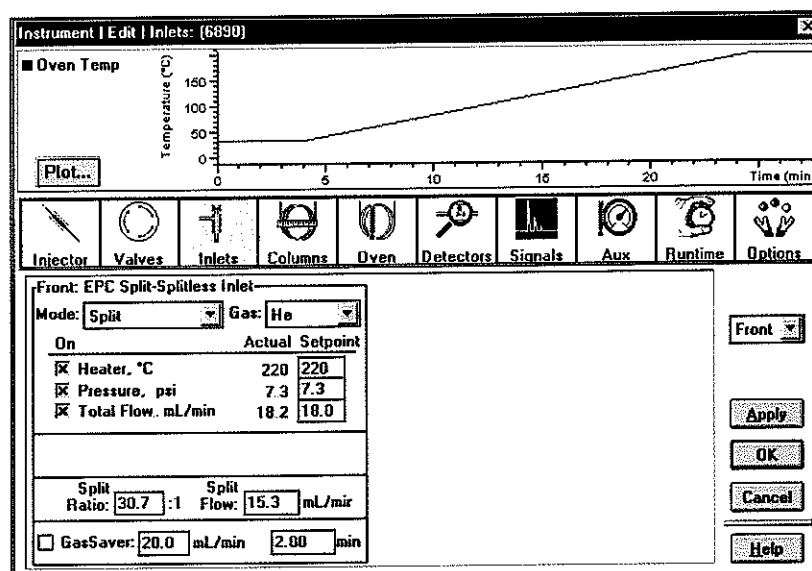


Figure 1. Setpoints for EPC split/splitless inlet for flow and temperature control.

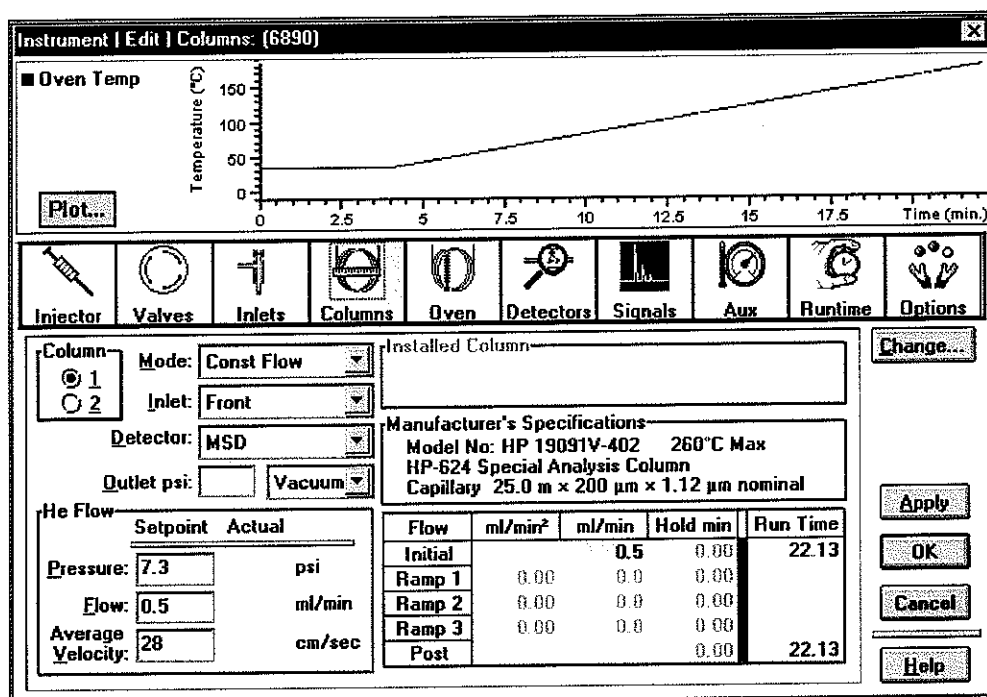


Figure 2. Details for the chromatographic column.

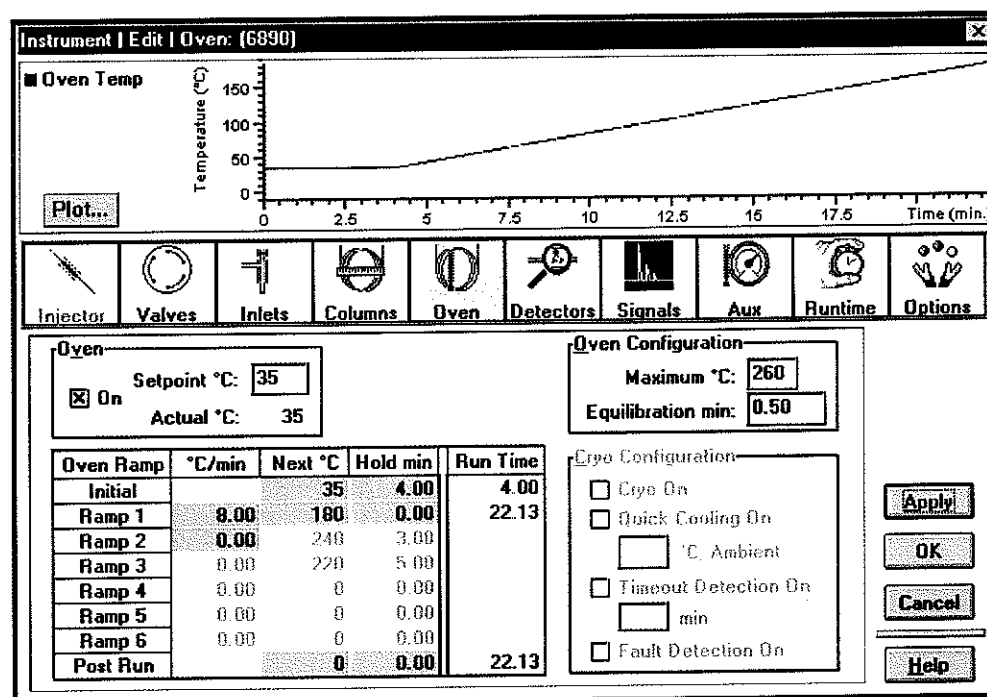


Figure 3. Temperature control of the 6890 GC oven.



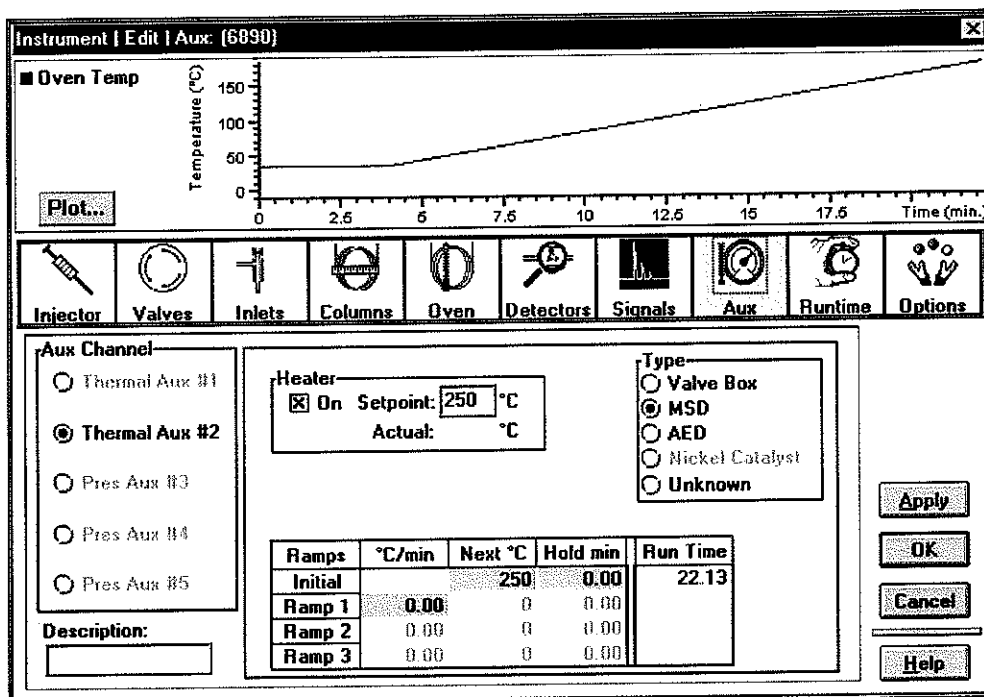


Figure 4 Temperature control for transfer line between the GC and the MSD.

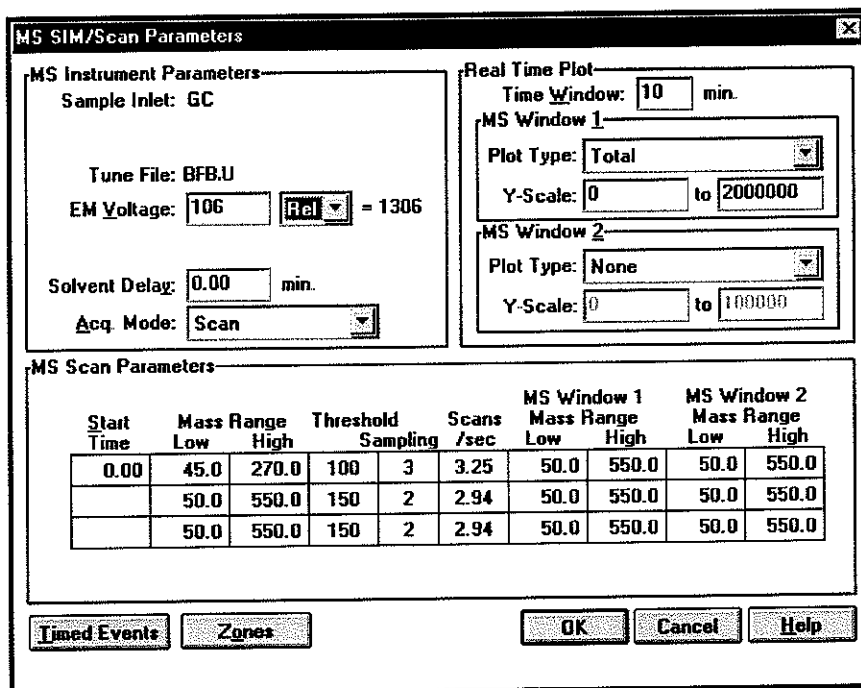


Figure 5. MS parameters.

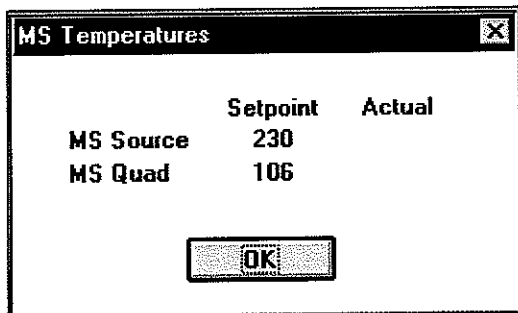


Figure 6. Temperature settings for the two independent MS temperatures.

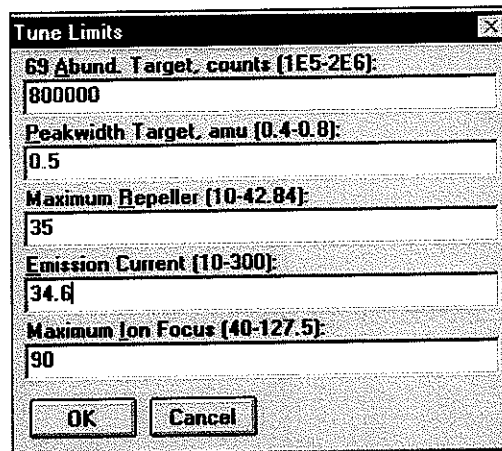


Figure 7. Setting the emission current, a user-settable parameter in the 5973 MSD. In this work the value used was 34.6 pump. Refer to references 1 and 2 for further information about optimizing the emission current

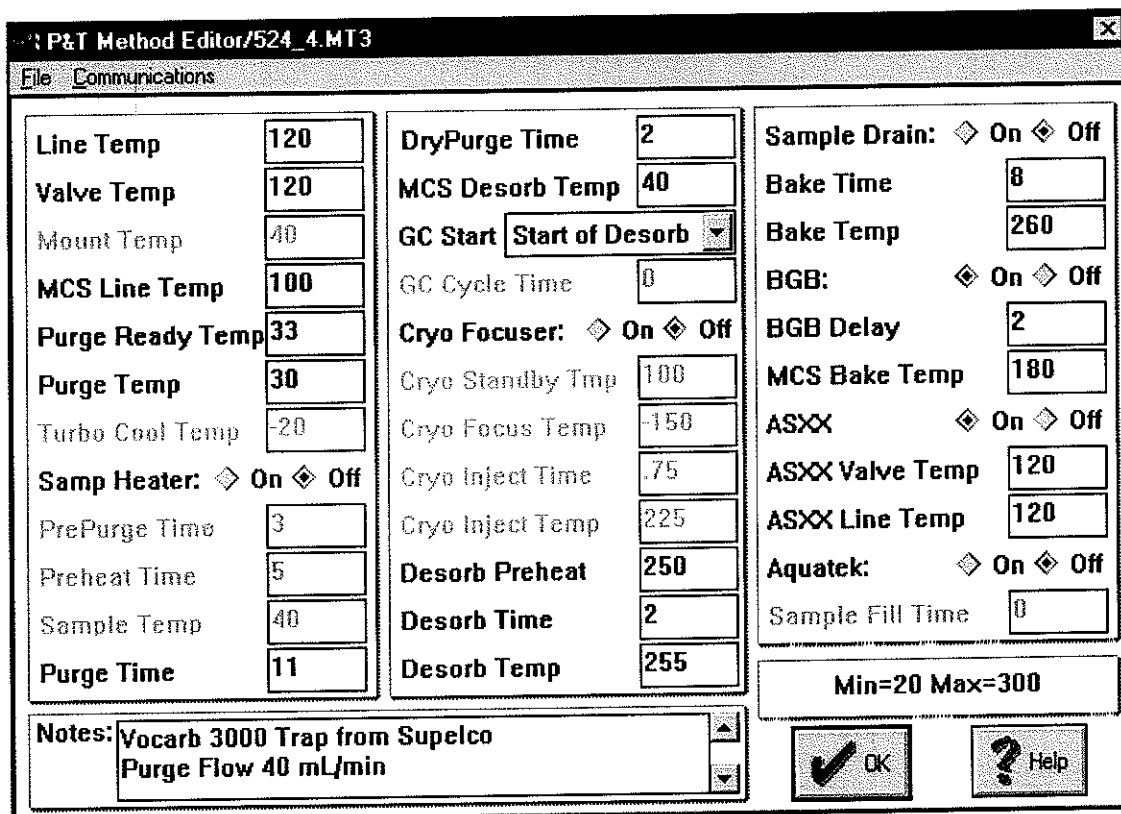


Figure 8. Purge and trap setpoints with a purge flow of 40 mL/min and a desorb flow of 15 mL/min. (For a Tekmar 3000 or similar purge and trap concentrator, the suggested value for the trap pressure control is 8 psi; this is set manually.)

**Table 1 Configuration information**

|                                                   |                                                                   |
|---------------------------------------------------|-------------------------------------------------------------------|
| Gas chromatograph                                 | 6890 with split/splitless                                         |
| Mass spectrometer                                 | 5973                                                              |
| Data system                                       | HP Vectra S/166 XM5                                               |
| Acquisition software with data reduction software | MSD Productivity ChemStation (G1701AA A 03 01)                    |
| Purge and trap device                             | G1900A equipped with MCS bypass jumper,<br>Part No 14-6011-002TMR |
| Autosampler (16 position with 25 mL sparge)       | G1905A                                                            |
| Purge and trap control software                   | G1909A                                                            |

**Table 2 Consumable items**

| <b>Description</b>                                 | <b>Part Number</b> |
|----------------------------------------------------|--------------------|
| HP-624: 25 m × 0.2 mm ID × 1.12 µm film thickness  | 19091V-402         |
| Method 524.2 liquid/gas set (60 compounds)         | 8500-6071          |
| Method 524.2 internal/surrogate standard           | 8500-6610          |
| System performance standard [BFB]                  | 8500-6610          |
| Splitless direct liner                             | 5181-8818          |
| Gold seal                                          | 18740-20885        |
| Zero dead volume union                             | 0100-0900          |
| Deactivated fused silica transfer line, 0.32 mm ID | 19091-60600        |

---

## Discussion

A system was set up according to Tables 1 and 2 and Figures 1 through 8. Blanks and standards from the compound list stated in Rev. 3.0 (3) were run to evaluate system performance according to the newer Rev. 4.1 of EPA 524.2 (3). The chromatographic performance and MSD response of the system were quite good, as demonstrated by the chromatogram in Figure 9. Specific measures of performance of this typical system are outlined in Table 3.

If results do not fall within the performance guidelines outlined in EPA Method 524.2 (3), you may want to refer to the checklist in Table 4; it outlines some common areas to explore. Note that there is a useful training tool for those operators who want a refresher and/or detailed instruction in implementing EPA Method 524.2: it is a CD-ROM that has step-by-step videos of the procedures (4).

For additional information on the initial setup of this method, contact your local Agilent Application Specialist.

## References

1. Brian Anthony, "Default Emission Current for the 5973 Series MSD running G1701AA A.03.01," HP Service Notes G1098-16 (Diffusion Pump) or G1099-18 (Turbo Pump), 1997. Available from your local Service Engineer.
2. Brian Anthony, "Emission Current Optimization for the 5973 Series MSD," HP Service Notes G1098-15 (Diffusion Pump) or G1099-17 (Turbo Pump), 1997. Available from your local Service Engineer.
3. "Methods for the Determination of Organic Compounds in Drinking Water, Supplement I," 1990, Environmental Monitoring Systems Laboratory, Office of Research and Development; and J. W. Munch (ed.), "Method 524.2, Measurement of Purgeable Organic Compounds in Water by Capillary Column Gas Chromatography/Mass Spectrometry, Revision 4.1," 1995; National Exposure Research Laboratory, Office of Research and Development. Both: U.S. Environmental Protection Agency, Cincinnati, Ohio 45268.
4. Volatile GC/MSD Environmental CD-ROM, HP Part No. G1028-60002. Refer to [www.agilent.com](http://www.agilent.com) on the Internet or write to: *Columns and Supplies*, Agilent Technologies, Little Falls Site, 2850 Centerville Road, Wilmington, DE 19808-9824.
5. F. W. McLafferty, "Interpretation of Mass Spectra, Second Edition," W. A. Benjamin, Inc., Reading, Massachusetts, 1972, p. 199.

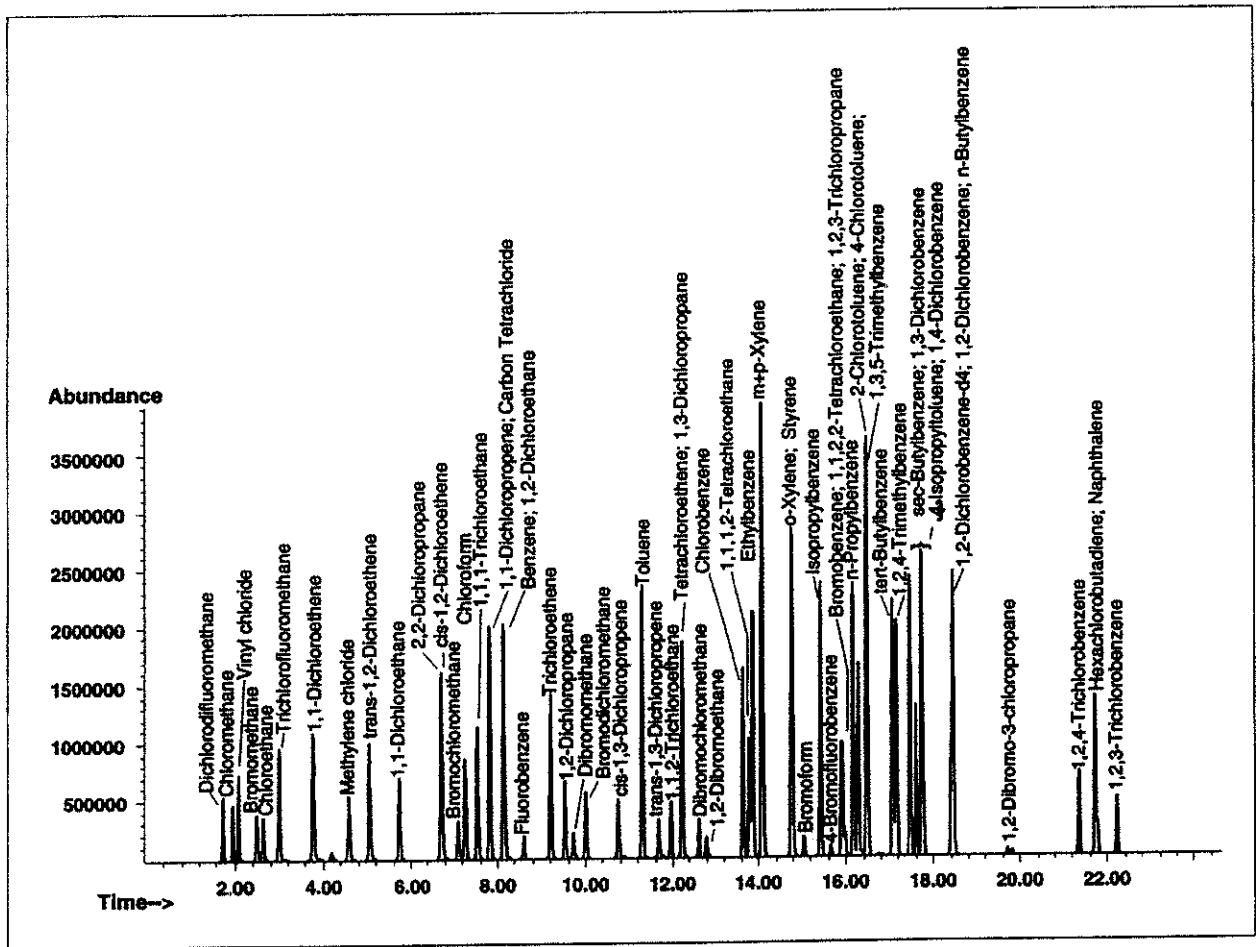


Figure 9. Total ion chromatogram (TIC) of Method 524.2 standard at 1 ppb (1 µg/L) level. Note the resolution of the chromatographic peaks and the total run time of less than 23 minutes.

Table 3. QA/QC performance observed on a typical system

| Parameter                            | Performance Observed on a Typical System                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |                                             |        |              |             |       |                        |             |       |                                             |
|--------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------|--------|--------------|-------------|-------|------------------------|-------------|-------|---------------------------------------------|
| Tuning criteria (BFB specifications) | BFB TargetTune                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |                                             |        |              |             |       |                        |             |       |                                             |
| Continuing Calibration Check (CCC)*  | <ul style="list-style-type: none"> <li>• 5% decline in areas relative to previous 12-hour shift (vs allowable 30% cutoff)</li> <li>• 23% decline in areas for 6th daily calibration check relative to initial calibration (vs allowable 50% cutoff)</li> <li>• Response factors for each analyte and surrogate were within 30% of the mean value measured in the initial calibration</li> </ul>                                                                                                                                                                                                                                |                                             |        |              |             |       |                        |             |       |                                             |
| Calibration range                    | 0.4–40 µg/L                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |                                             |        |              |             |       |                        |             |       |                                             |
| Initial calibration**                | <p>All compounds &lt; 14% RSD</p> <table style="width: 100%; border-collapse: collapse;"> <tr> <td style="padding: 2px;">Maximum RSD</td> <td style="padding: 2px; text-align: center;">13.55%</td> <td style="padding: 2px;">Bromomethane</td> </tr> <tr> <td style="padding: 2px;">Minimum RSD</td> <td style="padding: 2px; text-align: center;">0.60%</td> <td style="padding: 2px;">cis 1,2-Dichloroethane</td> </tr> <tr> <td style="padding: 2px;">Average RSD</td> <td style="padding: 2px; text-align: center;">4.46%</td> <td style="padding: 2px;">All 62 compounds,<br/>6 levels each compound</td> </tr> </table> | Maximum RSD                                 | 13.55% | Bromomethane | Minimum RSD | 0.60% | cis 1,2-Dichloroethane | Average RSD | 4.46% | All 62 compounds,<br>6 levels each compound |
| Maximum RSD                          | 13.55%                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         | Bromomethane                                |        |              |             |       |                        |             |       |                                             |
| Minimum RSD                          | 0.60%                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          | cis 1,2-Dichloroethane                      |        |              |             |       |                        |             |       |                                             |
| Average RSD                          | 4.46%                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          | All 62 compounds,<br>6 levels each compound |        |              |             |       |                        |             |       |                                             |
| Surrogate recoveries                 | <p>For 52 samples over about 50 hours,</p> <ul style="list-style-type: none"> <li>• 4-bromofluorobenzene      97.64%,      2.82 %RSD</li> <li>• 1,2-Dichlorobenzene-d4      95.27%,      3.53 %RSD</li> </ul>                                                                                                                                                                                                                                                                                                                                                                                                                  |                                             |        |              |             |       |                        |             |       |                                             |
| Chromatography                       | Total system cycle time of 28 minutes. Excellent resolution of chromatographic peaks.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |                                             |        |              |             |       |                        |             |       |                                             |

\* As prescribed by the method, daily calibration checks and BFB tune checks are performed at the beginning of each 12-hour work shift; then the absolute areas of the quantitation ions of the internal standard and surrogates from the Continuing Calibration Check are determined. The following Internal Standard/Surrogate area requirements must be met:

- a compared to the previous 12-hour shift, the quantitation ion areas have not changed by > 30%
- or
- b compared to the initial calibration, the quantitation ion areas have not changed by > 50%

\*\* The EPA Method 524.2 guideline for the initial calibration states that all compounds must have ≤ 20 % RSD.

Table 4. Considerations for troubleshooting results that fall outside the guidelines of EPA Method 524.2

| Area                                                 | Suggestions for Achieving Desired Performance                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |
|------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Equipment Set-up and Preventative Maintenance</b> | <p><b>Purge and Trap</b></p> <ul style="list-style-type: none"> <li>• If using a Tekmar 3000 concentrator, bypass the MCS (Moisture Control System) by installing the MCS Bypass Jumper (Part No 14-6011-002TMR); it must be installed in the Purge and Trap according to the 7695 Purge and Trap manual.</li> <li>• Use a Vocarb 3000 Trap. The packing material is hydrophobic leading to enhanced water removal; this characteristic is particularly useful for dry purging.</li> <li>• For EPA Method 524.2, use 25-mL fritted purge vessels</li> <li>• Initially condition the Vocarb 3000 trap at 260°C for at least 60 minutes <i>after</i> you have leak-checked the purge and trap</li> <li>• Additionally for EPA Method 8260,             <ul style="list-style-type: none"> <li>– If you need low detection limits, consider 25-mL vessels, but do not exceed 100 ppb (carryover!).</li> <li>– The use of culture tubes is not recommended</li> </ul> </li> <li>• Constantly check for leaks and appropriate flow rates. In particular, check the connections to the purge vessels. The flow rates are monitored by an external flow meter</li> <li>• Monitor the value of the trap pressure control. For some instruments, it is manually set. Follow the vendor's instructions</li> </ul> <p><b>Transfer Line: Purge and Trap to GC</b></p> <ul style="list-style-type: none"> <li>• Do not use nickel transfer lines when analyzing for reactive compounds</li> <li>• The connection between the Purge and Trap transfer line and the 6890 GC weldment split line must be made using a minimal length of tubing (&lt; 2 inches). Preferably, this is done using the cited deactivated fused silica transfer line (Part No 19091-60600) and the zero dead volume union (Part No 0100-0900)</li> </ul> <p><b>GC</b></p> <ul style="list-style-type: none"> <li>• Use deactivated liners in the split/splitless inlet (e.g., Part No 5181-8818)</li> </ul> <p><b>MS</b></p> <ul style="list-style-type: none"> <li>• If using a diffusion pump system, perform your vacuum system maintenance religiously, as outlined in the 5973 hardware manuals</li> </ul> |
| <b>Laboratory Environment</b>                        | <p><b>Ambient Temperature</b></p> <ul style="list-style-type: none"> <li>• Operating a Purge and Trap instrument in very cold rooms (&lt; 22°C or 72°F) contributes to lower responses for compounds like bromoform and naphthalene</li> <li>• Constant room temperature is very important for consistent response factors (RFs)</li> </ul> <p><b>Air Quality</b></p> <ul style="list-style-type: none"> <li>• Make sure you do not have air quality problems (methylene chloride, acetone, freons) in the laboratory before you start. For example, place an open container of blank source water in the laboratory for 3 hours and then analyze for target compounds</li> <li>• Do not use ALS injectors with methylene chloride (e.g., for semivolatiles) in the same room!</li> </ul>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |

(continued)

Table 4, *continued*. Considerations for troubleshooting results that fall outside the guidelines of EPA Method 524.2

| Area                         | Suggestions for Achieving Desired Performance                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |
|------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Technique</b>             | <ul style="list-style-type: none"> <li>• Follow the method precisely as it relates to loading samples, preparing standards, etc. Use Class A volumetrics!</li> <li>• Rinse vessels that contained calibration standards particularly well; run blanks in those vessels.</li> <li>• Use blanks to "certify" ALS positions following high-concentration (i.e., &gt; 2000 ng/sample) standards and samples</li> <li>• In particular, acidify all blanks, samples, and standards as set forth by the protocol; not doing so can be a source of lowered recoveries</li> </ul>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |
| <b>Standards Preparation</b> | <p><b>Equipment</b></p> <ul style="list-style-type: none"> <li>• Use only Class A volumetric glassware.</li> <li>• Use gas-tight syringes</li> <li>• Store standards in vials capped with Mininert® valves to cut down on loss of gases</li> </ul> <p><b>Solvents</b></p> <ul style="list-style-type: none"> <li>• Use only verified clean (i.e., analyze it) Purge and Trap grade methanol.</li> <li>• Verify the absence of target compounds and other organics in the water source used for blanks before running standards</li> </ul> <p><b>Analyte Levels</b></p> <ul style="list-style-type: none"> <li>• Prepare standards such that the effective volume of methanol in the purge vessel will be ≤ 60 µL per 25-mL sample size</li> <li>• Follow the protocol for the addition of standards and surrogates to the water sample             <ul style="list-style-type: none"> <li>– Standards are added to volumetric flasks (usually, 100 mL) containing the water, acidified according to protocol.</li> <li>– Internal standards and surrogate standards are added to the syringe (usually, 25 mL) that is used to transfer the water sample to the purge vessel just before the sample is loaded into the purge vessel</li> </ul> </li> </ul> |

(continued)



Table 4, *continued*. Considerations for troubleshooting results that fall outside the guidelines of EPA Method 524.2

| Area         | Suggestions for Achieving Desired Performance                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |
|--------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Method Setup | <p><b>Purge and Trap</b></p> <p><i>General Considerations</i></p> <ul style="list-style-type: none"> <li>• Excessive Purge and Trap line/valve temperatures on the Purge and Trap instrument contribute to compound breakdown. Set the temperatures &lt; 160°C for the G1900A.</li> <li>• Prior to operating the system for any set of samples, bake-out the Vocab 3000 traps at 260°C for ≥ 8 minutes</li> </ul> <p><i>Purging</i></p> <ul style="list-style-type: none"> <li>• Excessive dry-purge and purge times and excessive purge flow rates contribute to trap breakthrough and loss of gases</li> <li>• Consider heating the sample vessels during the purge cycle to improve the response to very water soluble analytes. Heated purges generate much more water carryover, but also get water-soluble compounds purged better. In general, set purge temperatures to about 40°C</li> <li>• Don't purge onto a hot trap (&gt; 40°C)</li> </ul> <p><i>Desorb</i></p> <ul style="list-style-type: none"> <li>• Adjust your desorb time by 0.1-minute increments to control the area in the chromatogram where the baseline returns to normal after the water peak elutes in order to minimize analyte elution on the tail of the water peak.</li> <li>• Set the desorb time from 1 to 4 minutes <ul style="list-style-type: none"> <li>– The longer you desorb, the more water you will see</li> <li>– Desorbing for too little time will result in linearity problems, especially with high boilers.</li> <li>– Check regional regulations to determine if a specific desorb time is required.</li> </ul> </li> <li>• Maintain a minimum desorb flow rate through the trap of &gt;10 mL/min (split flow)</li> <li>• If using a Vocab 3000 trap, heat it hot enough to desorb all the compounds: ≥ 240°C.</li> </ul> <p><b>GC</b></p> <ul style="list-style-type: none"> <li>• Make certain you have set up split mode when using this configuration</li> <li>• Set the solvent delay to end at least 1 minute before the first peak elutes</li> </ul> <p><b>MS</b></p> <ul style="list-style-type: none"> <li>• For a 5973 MSD, adjust the EMV (electron multiplier voltage), or Target Tune 69 abundance, such that the highest responding signal in the highest calibration standard (usually m- and p-xylenes because they coelute) does not significantly exceed 10 million counts in the TIC.</li> <li>• For filaments with Part No 05972-60053, set the emission current between 10 to 65 μamps. References 1 and 2 provide guidance on further optimizing this parameter</li> <li>• If analyzing for ketones, scan from m/z = 35, not m/z = 45</li> <li>• Scan to m/z = 270 to see all the ions for hexachlorobutadiene.</li> <li>• Expected observations: <ul style="list-style-type: none"> <li>– Expect to see higher baselines when scanning from m/z = 35. CO<sub>2</sub> (m/z = 44) appears but only causes problems which are purely aesthetic in nature.</li> <li>– Expect "mass defect" for heavily chlorinated/brominated compounds (5). Enter exact masses, and not rounded-off approximate values, in your calibration table to accommodate isotopic abundance patterns of the halogenated compounds.</li> </ul> </li> </ul> |



**Agilent Technologies**  
Innovating the HP Way

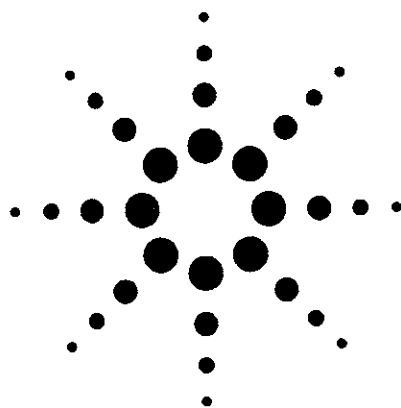
---

**Agilent Technologies shall not be liable for errors contained herein or for incidental or consequential damages in connection with the furnishing, performance or use of this material.**

**Information, descriptions and specifications in this publication are subject to change without notice.**

**Copyright © 1999  
Agilent Technologies Company  
All rights reserved. Reproduction and adaptation is prohibited.**

**Printed in the U.S.A. December 1999  
(23) 5966-0369E**



# Developing an eMethod for the Analysis of Volatile Organic Compounds in Water Using Purge and Trap/GC with Agilent's New 5975 inert Mass Spectrometer

## Application

Environmental

### Author

Philip L. Wylie  
Agilent Technologies, Inc.  
2850 Centerville Road  
Wilmington, DE 19808-1610  
USA  
(e-mail: phil\_wylie@agilent.com)

### Abstract

Using Agilent's new G1701DA (Version 2.0.00) software, it takes only a few steps to package a gas chromatography/mass spectrometry (GC/MS) method into one that is easily transferred to other similarly configured GC/MS systems. eMethods are truly portable, making it easy to share methods between instruments worldwide without the tedious process of entering all the parameters each time. Thanks to Retention Time Locking (RTL), calibration files (complete with retention time windows) or complex SIM (Selected Ion Monitoring) methods can be transferred without the need for retention time edits. This application note describes a method for the analysis of volatile organic compounds (VOCs) in water samples according to US Environmental Protection Agency (USEPA) method 8260B. Though framed around Method 8260B, it can be used for most VOC analyses requiring Purge and Trap (P&T)/GC/MS instrumentation. The eMethod can be downloaded directly from the Agilent Web site at the following location: [www.agilent.com/chem/eMethods](http://www.agilent.com/chem/eMethods). Using the new "eMethod Import" ChemStation feature, one can load the method and all of its parameters. Although the purge-and-trap parameters are not automatically installed, the P&T method is included with the eMethod.

### Introduction

GC/MS methods are often developed on one instrument, published, and then replicated on other instruments in different laboratories. In the past, this required new users to input all of the GC and MS parameters, including calibration or SIM tables. Even then, retention times (RTs) would generally differ among instruments so calibration and/or SIM tables would have to be redone. While it has been possible to copy a method to electronic media and copy it to another system, any differences in instrument configuration complicated the process.

A novel feature of the new Agilent G1701DA (Version 2.0.00) software is the ability to export and import complete GC/MS methods. All electronic parameters, including all GC and MS set-points, calibration tables, SIM tables, and RTL calibration files, are exported as part of the eMethod. eMethods can be distributed over the Web, by e-mail, or on storage media. Installation takes just a minute or so. Normally, new users would first relock the method and then recalibrate. There is a "Notes" section for the method developer to specify nonelectronic parameters such as the type of inlet liner used.

This application note describes an eMethod for the analysis of 60 VOCs in water using a Velocity XPT purge-and-trap (P&T) sample concentrator together with an Agilent 6890N GC and new 5975 inert MSD. It includes a calibration table in the scan mode with appropriate target and qualifier ions, locked RTs for all analytes, RTL calibration files, and a complementary SIM method for use in the synchronous SIM/scan mode.



Agilent Technologies

U.S. EPA Method 8260B [1] is a general purpose method for the analysis of VOCs in matrices such as ground and surface water, sludges, soils and sediments, filter cakes, spent carbons, and spent catalysts. This method is only used for the analyses of target VOCs by GC with mass spectral detection (GC/MS). It refers analysts to other U.S. EPA sample introduction methods that are appropriate for the matrix to be analyzed. Method 8260B is widely used in environmental laboratories with P&T for the analysis of VOCs in surface, ground, and wastewater samples. A similar method for the analysis of drinking water is described in EPA Method 524.2 [2].

Previous application notes in this series have discussed procedures for tuning to the USEPA's BFB requirements [3] and techniques for optimizing P&T/GC/MS methods [4]. This application note includes some additional insights into method optimization, as well as more recent calibration data that are included with the eMethod

## Experimental

### Chemical Standards, Reagents, and Vials

High-purity B&J brand methanol was obtained from Honeywell Burdick & Jackson Co. (Muskegon, MI). Standard mixtures used for the preparation of calibration samples, spiking solutions, tune evaluation, and stability test samples were purchased from AccuStandard (New Haven, CT). These include the following: Part No. M-502-10X-Pak

containing 60 VOC target analytes at 2000 µg/mL each in methanol; and p/n M-8260A/B-IS/SS-10X-PAK containing p-bromofluorobenzene, chlorobenzene-d5, dibromofluoromethane, 1,4-dichlorobenzene-d4, 1,2-dichloroethane-d4, fluorobenzene, and toluene-d8 at 2000 µg/mL each in methanol. VOC-free water was used for the preparation of standards and test samples. Trace-Clean 40-mL (nominal volume, actual volume is 43 mL) VOA vials (p/n 15900-022) were purchased from VWR Scientific (West Chester, PA).

### Preparation of Calibration and Spiking Solutions

Secondary spiking solutions were prepared in methanol for each calibration level so that a 100-mL volumetric flask could be spiked with 25 µL of the calibration solution (containing 60 VOCs) and 25 µL of the internal standard/surrogate mixture. Each volumetric flask was inverted five times to mix the solution, which was then carefully poured into two 43-mL VOA vials.

Table 1 provides details on how the seven calibration standards were prepared. The combined internal standard and surrogate spiking solution was prepared by diluting 40 µL of the 2000 µg/mL standard to 1.0 mL with methanol. Each sample and standard was spiked at 20 µg/L with this solution.

### Instrumentation and Analytical Conditions

The P&T instrumentation and setpoints are listed in Table 2. Since the P&T instrument is controlled by separate software, its parameters cannot be set

Table 1. Procedure for Preparing Calibration Samples

| A<br>Calibration level (µg/L)* | B<br>Volume of 2000 µg/mL VOC standard (µL)** | C<br>Diluted to this volume in methanol (mL)*** | D<br>Results in this secondary concentration (ng/µL)**** | E<br>Amount to spike into 100 mL volumetric flask (µL)***** |
|--------------------------------|-----------------------------------------------|-------------------------------------------------|----------------------------------------------------------|-------------------------------------------------------------|
| 1                              | 50                                            | 25                                              | 4                                                        | 25                                                          |
| 2                              | 40                                            | 10                                              | 8                                                        | 25                                                          |
| 5                              | 50                                            | 5                                               | 20                                                       | 25                                                          |
| 20                             | 40                                            | 1                                               | 80                                                       | 25                                                          |
| 50                             | 40                                            | 0.4                                             | 200                                                      | 25                                                          |
| 100                            | 40                                            | 0.2                                             | 400                                                      | 25                                                          |
| 200                            | 40                                            | 0.1                                             | 800                                                      | 25                                                          |

\* Concentration of each analyte in the final aqueous calibration solution.

\*\* Volume of the 2000 µg/mL 60-component VOC standard solution, which was diluted to the volume shown in column C.

\*\*\* Final volume of VOC solution after dilution in methanol.

\*\*\*\* Concentration of the calibration spiking solution prepared by diluting the amount of 2000 µg/mL standard in column B to the volume shown in column C.

\*\*\*\*\* Amount of the secondary standard solution (column D) added to 100-mL of water to prepare the calibration standard at the level shown in column A.

while importing this eMethod and must be entered manually. The following P&T options were not used: DryFlow trap, automatic internal standard addition, sample heating, dry purging, and sample cryofocusing. The method shown in Table 2 was originally derived using the wizard that is provided in the TekLink 2.4 P&T control software. Minor modifications were made.

As shown in Table 3, toluene-d8 was used as the RTL compound. Its RT was locked to 7.405 min in the constant flow mode. The constant flow mode

was chosen for this application because it helps heavier compounds elute faster and at lower temperatures, which makes the method cycle shorter. While RTL works well in the constant flow mode, it does not compensate for large differences in column length as well as it does in the constant pressure mode. Therefore, it is best to install a new 20-m × 0.18-mm × 1.0 μm DB-VRX column or one that has not been subjected to frequent column cutting. Once installed for this application, there is little need for column maintenance.

**Table 2. Purge and Trap Instrumentation and Setpoints**

|                                    |                                                                                                                             |
|------------------------------------|-----------------------------------------------------------------------------------------------------------------------------|
| <b>P&amp;T instrument</b>          | <b>Teledyne Tekmar Velocity XPT</b>                                                                                         |
| <b>Automatic sampler</b>           | <b>Teledyne Tekmar Aquatek 70</b>                                                                                           |
| <b>Software control</b>            | <b>Teledyne Tekmar VOC Teklink version 2.4</b>                                                                              |
| <b>Trap</b>                        | Vocarb 3000 (Agilent p/n 5182-0775)                                                                                         |
| <b>P&amp;T-GC interface</b>        | P&T transfer line spliced into the GC split/splitless inlet carrier gas line and GC carrier gas plumbed to the Velocity XPT |
| <b>Sample size</b>                 | 5 mL                                                                                                                        |
| <b>Valve oven temperature</b>      | 150 °C                                                                                                                      |
| <b>Transfer line temperature</b>   | 150 °C                                                                                                                      |
| <b>Sample mount temp</b>           | 90 °C                                                                                                                       |
| <b>Purge ready temp</b>            | 45 °C                                                                                                                       |
| <b>DryFlow standby temperature</b> | 60 °C                                                                                                                       |
| <b>Standby flow</b>                | 20 mL/min                                                                                                                   |
| <b>Pressurize time</b>             | 0.25 min                                                                                                                    |
| <b>Fill IS time</b>                | 0.00 (internal standards added by hand)                                                                                     |
| <b>Sample transfer time</b>        | 0.35 min                                                                                                                    |
| <b>Pre-purge time</b>              | 0.00 min                                                                                                                    |
| <b>Pre-purge flow</b>              | 40 mL/min                                                                                                                   |
| <b>Sample heater</b>               | Off (Samples not heated)                                                                                                    |
| <b>Sample preheat time</b>         | 1.00 min                                                                                                                    |
| <b>Preheat temperature</b>         | 40 °C                                                                                                                       |
| <b>Purge time</b>                  | 11.00 min                                                                                                                   |
| <b>Purge temperature</b>           | 0 °C (that is, less than the purge ready temp of 45 °C)                                                                     |
| <b>Purge flow</b>                  | 40 mL/min                                                                                                                   |
| <b>Purge rinse time</b>            | 0.40 min                                                                                                                    |
| <b>Purge line time</b>             | 0.35 min                                                                                                                    |
| <b>Dry purge time</b>              | 0.00 min (Dry purge not used)                                                                                               |
| <b>Dry purge temp</b>              | 40 °C                                                                                                                       |
| <b>Dry purge flow</b>              | 200 mL/min                                                                                                                  |
| <b>GC start</b>                    | Start of desorb                                                                                                             |
| <b>Desorb preheat temperature</b>  | 245 °C                                                                                                                      |
| <b>Desorb drain</b>                | On                                                                                                                          |
| <b>Desorb time</b>                 | 2.00 min                                                                                                                    |
| <b>Desorb temperature</b>          | 250 °C                                                                                                                      |
| <b>Desorb flow</b>                 | 300 mL/min                                                                                                                  |
| <b>Bake rinse</b>                  | On                                                                                                                          |
| <b>Number of bake rinses</b>       | 3                                                                                                                           |
| <b>Bake drain time</b>             | 0.50 min                                                                                                                    |
| <b>Bake drain flow</b>             | 400 mL/min                                                                                                                  |
| <b>Bake time</b>                   | 3.00 min                                                                                                                    |
| <b>Bake temperature</b>            | 270 °C                                                                                                                      |
| <b>DryFlow bake temperature</b>    | 300 °C                                                                                                                      |
| <b>Bake flow</b>                   | 400 mL/min                                                                                                                  |
| <b>Focus temperature</b>           | Not used                                                                                                                    |
| <b>Inject time</b>                 | 1.00 min                                                                                                                    |
| <b>Inject temperature</b>          | 180 °C                                                                                                                      |
| <b>Standby temperature</b>         | 100 °C                                                                                                                      |

**Table 3. Lists the Conditions for the GC/MS System**

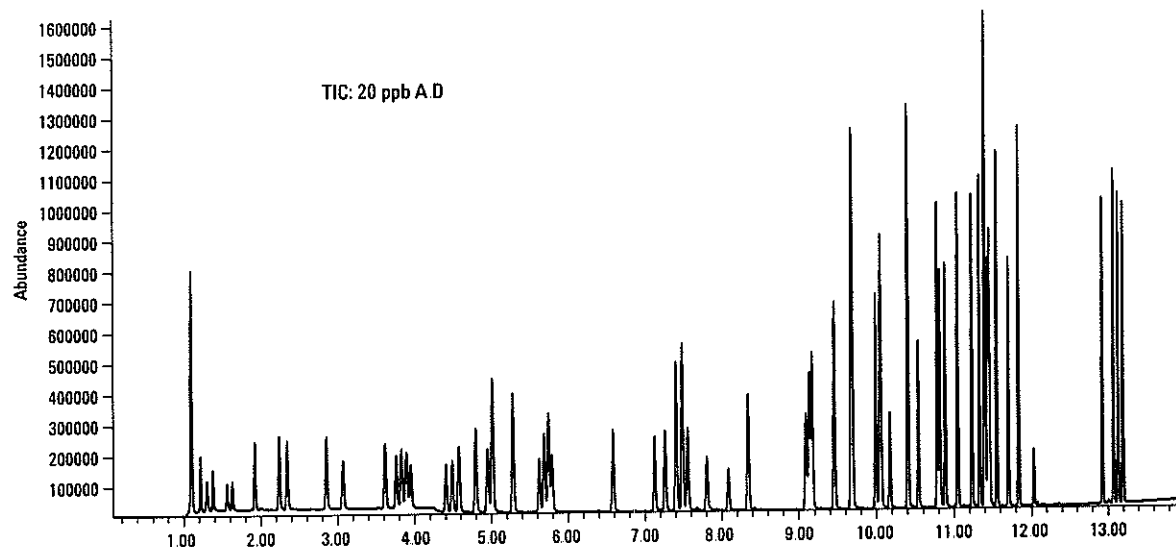
|                           |                                                                         |
|---------------------------|-------------------------------------------------------------------------|
| <b>Gas chromatograph</b>  | <b>Agilent 6890N</b>                                                    |
| Inlet                     | Split/Splitless                                                         |
| Inlet liner               | Single taper, deactivated (Agilent p/n 5181-3316)                       |
| Inlet temperature         | 150 °C                                                                  |
| Split ratio               | 50:1                                                                    |
| Column                    | 20 m × 0.18 mm × 1.0 µm DB-VRX (Agilent p/n 121-1524)                   |
| Carrier gas               | Nominal helium flow at 1.0 mL/min constant flow                         |
| RTL                       | Toluene-d8 retention time locked to 7.405 min                           |
| Oven temperature program  | 40 °C (3 min), 10 °C/min to 100 °C (0 min), 25 °C/min to 225 °C (3 min) |
| <b>Mass spectrometer</b>  | <b>Agilent 5975 inert MSD</b>                                           |
| Transfer line temperature | 225 °C                                                                  |
| Quad temperature          | 150 °C                                                                  |
| Source temperature        | 230 °C                                                                  |
| EM voltage                | 1200 volts                                                              |
| Scan range                | 35–260 u                                                                |
| Threshold                 | 150                                                                     |
| Samples                   | 2                                                                       |
| Solvent delay             | 0 min                                                                   |
| Software                  | MSD Productivity ChemStation Software (p/n G1701DA version D 02.00)     |

## Results and Discussion

According to section 1.3 of the method, 8260B can be used to quantify most VOCs that have boiling points below 200 °C. It lists 123 compounds that can be determined by the method using various sample prep and sample introduction methods. Of these, seven are internal standards or surrogates, nine are not recommended for P&T sample introduction, and three must be purged at 80 °C for efficient recovery. For this study, the 60 VOCs listed in EPA Method 502.2 [5] were analyzed along with three internal standards and four surrogates (Table 4).

## Calibration Results

Many laboratories employing Method 8260B or similar methods generate five-point calibration curves between 5 and 200 µg/L. In a previous application note [4], calibration from 1 to 300 µg/L gave response factor (RF) %RSDs less than 15% for all but eight compounds, while calibrations from 1–200 µg/L all fell under 15%. For the eMethod described in this application note, calibration standards were run at 1, 2, 5, 20, 50, 100, and 200 µg/L. The signals for all analytes at 1 µg/L were sufficient to allow calibration at even lower levels. Figure 1 shows a total ion chromatogram (TIC) of the targets, surrogates, and internal standards at 20 µg/L each.



**Figure 1. Chromatogram of the 60 VOCs, three internal standards, and four surrogates listed in Table 4. The standard was analyzed using the eMethod described herein.**

The average RF and %RSD of the RFs were calculated for each compound over the 1–200 µg/L range. As seen in Table 4, all five of the system performance check compounds (SPCCs) exceeded their minimum RFs by a comfortable margin. In addition, all six of the continuing calibration compound (CCC) RF RSDs were significantly less

than the 30% limit specified in EPA Method 8260B. The RF RSDs for all target compounds fell well below 15% over the entire 1–200 µg/L calibration range, allowing the use of average RF values for calibration. The average RF for all compounds was 4.3% over the entire 1–200 µg/L range.

**Table 4. Compound List with Average RF and the RF %RSDs for a Seven-Level Calibration from 1 to 200 µg/L**

| Type*  | Compound                   | RT (min) | Minimum average RF** | Minimum %RSD of Calib. RF*** | Average RF 1–200 µg/L | RF %RSD 1–200 µg/L |
|--------|----------------------------|----------|----------------------|------------------------------|-----------------------|--------------------|
| ISTD   | Fluorobenzene              | 5.277    |                      | 15                           |                       |                    |
| T      | Dichlorodifluoromethane    | 1.219    |                      | 15                           | 0.283                 | 7.00               |
| T,SPCC | Chloromethane              | 1.301    | 0.1                  | 15                           | 0.259                 | 8.15               |
| T,CCC  | Vinyl chloride             | 1.379    |                      | 30                           | 0.240                 | 3.36               |
| T      | Bromomethane               | 1.557    |                      | 15                           | 0.144                 | 10.74              |
| T      | Ethyl chloride             | 1.63     |                      | 15                           | 0.151                 | 3.54               |
| T      | Trichloromonofluoromethane | 1.928    |                      | 15                           | 0.374                 | 2.98               |
| T,CCC  | 1,1-dichloroethene         | 2.24     |                      | 30                           | 0.321                 | 3.14               |
| T      | Methylene chloride         | 2.346    |                      | 15                           | 0.306                 | 9.32               |
| T      | 1,2-dichloroethene (E)     | 2.857    |                      | 15                           | 0.322                 | 2.45               |
| T,SPCC | 1,1-dichloroethane         | 3.074    | 0.1                  | 15                           | 0.406                 | 2.94               |
| T      | cis-1,2-Dichloroethene     | 3.615    |                      | 15                           | 0.313                 | 3.23               |
| T      | Bromochloromethane         | 3.757    |                      | 15                           | 0.198                 | 3.13               |
| T,CCC  | Chloroform                 | 3.833    |                      | 30                           | 0.399                 | 3.62               |
| T      | 2,2-Dichloropropane        | 3.891    |                      | 15                           | 0.339                 | 7.88               |
| Sur    | 1,2-Dichloroethane-d4      | 4.404    |                      | 15                           | 0.288                 | 1.26               |
| Sur    | Dibromofluoromethane       | 3.947    |                      | 15                           | 0.225                 | 0.77               |
| T      | 1,2-Dichloroethane         | 4.491    |                      | 15                           | 0.346                 | 3.32               |
| T      | 1,1,1-Trichloroethane      | 4.574    |                      | 15                           | 0.398                 | 3.18               |
| T      | 1,1-Dichloro-1-propene     | 4.789    |                      | 15                           | 0.346                 | 3.08               |
| T      | Carbon tetrachloride       | 4.948    |                      | 15                           | 0.359                 | 4.91               |
| T      | Benzene                    | 5.012    |                      | 15                           | 1.038                 | 2.75               |
| T      | Dibromomethane             | 5.626    |                      | 15                           | 0.216                 | 2.90               |
| T,CCC  | 1,2-Dichloropropane        | 5.682    |                      | 30                           | 0.262                 | 3.38               |
| T      | Trichloroethylene          | 5.743    |                      | 15                           | 0.305                 | 3.45               |
| T      | Bromodichloromethane       | 5.787    |                      | 15                           | 0.328                 | 4.46               |
| T      | 1,3-Dichloropropene (Z)    | 6.579    |                      | 15                           | 0.407                 | 3.84               |
| T      | 1,3-Dichloropropene (E)    | 7.126    |                      | 15                           | 0.357                 | 4.89               |
| T      | 1,1,2-Trichloroethane      | 7.263    |                      | 15                           | 0.196                 | 3.87               |
| Sur    | Toluene-d8                 | 7.407    |                      | 15                           | 0.941                 | 0.37               |
| T,CCC  | Toluene                    | 7.489    |                      | 30                           | 1.109                 | 3.20               |
| T      | 1,3-Dichloropropane        | 7.558    |                      | 15                           | 0.421                 | 3.54               |
| T      | Dibromochloromethane       | 7.804    |                      | 15                           | 0.269                 | 6.57               |
| T      | 1,2-Dibromoethane          | 8.088    |                      | 15                           | 0.259                 | 3.52               |
| T      | Tetrachloroethylene        | 8.345    |                      | 15                           | 0.357                 | 3.57               |
| T      | 1,1,1,2-Tetrachloroethane  | 9.092    |                      | 15                           | 0.269                 | 4.84               |
| ISTD   | Chlorobenzene-d5           | 9.134    |                      | 15                           |                       |                    |
| T,SPCC | Chlorobenzene              | 9.173    | 0.3                  | 15                           | 0.984                 | 5.09               |
| T,CCC  | Ethylbenzene               | 9.46     |                      | 30                           | 1.618                 | 5.14               |
| T      | m- and p-Xylene            | 9.683    |                      | 15                           | 2.644                 | 3.87               |
| T,SPCC | Bromoform                  | 9.669    | 0.1                  | 15                           | 0.288                 | 11.12              |
| T      | Styrene                    | 9.993    |                      | 15                           | 1.034                 | 6.37               |

**Table 4. Compound List with Average RF and the RF %RSDs for a Seven-Level Calibration from 1 to 200 µg/L (continued)**

| Type*  | Compound                       | RT (min) | Minimum average RF** | Minimum %RSD of Calib. RF*** | Average RF 1–200 µg/L | RF %RSD 1–200 µg/L |
|--------|--------------------------------|----------|----------------------|------------------------------|-----------------------|--------------------|
| T,SPCC | 1,1,2,2-Tetrachloroethane      | 10.043   | 0.3                  | 15                           | 0.435                 | 4.64               |
| T      | o-Xylene                       | 10.057   |                      | 15                           | 1.324                 | 4.84               |
| T      | 1,2,3-Trichloropropane         | 10.174   |                      | 15                           | 0.378                 | 4.18               |
| Sur    | p-Bromofluorobenzene           | 10.399   |                      | 15                           | 0.482                 | 2.51               |
| T      | Isopropylbenzene               | 10.405   |                      | 15                           | 1.591                 | 5.33               |
| T      | Bromobenzene                   | 10.539   |                      | 15                           | 0.628                 | 4.55               |
| T      | n-Propylbenzene                | 10.782   |                      | 15                           | 2.039                 | 4.88               |
| T      | 2-Chlorotoluene                | 10.815   |                      | 15                           | 1.163                 | 5.20               |
| T      | 4-Chlorotoluene                | 10.885   |                      | 15                           | 1.234                 | 4.73               |
| T      | 1,3,5-Trimethylbenzene         | 11.047   |                      | 15                           | 1.438                 | 5.61               |
| T      | tert-Butylbenzene              | 11.228   |                      | 15                           | 1.371                 | 4.90               |
| T      | 1,2,4-Trimethylbenzene         | 11.331   |                      | 15                           | 1.513                 | 5.55               |
| T      | sec-Butylbenzene               | 11.395   |                      | 15                           | 2.026                 | 4.29               |
| T      | 1,3-Dichlorobenzene            | 11.407   |                      | 15                           | 0.925                 | 4.36               |
| ISTD   | 1,4-Dichlorobenzene-d4         | 11.44    |                      | 15                           |                       |                    |
| T      | 1,4-Dichlorobenzene            | 11.46    |                      | 15                           | 1.530                 | 3.04               |
| T      | p-isopropyltoluene             | 11.552   |                      | 15                           | 2.843                 | 3.48               |
| T      | 1,2-Dichlorobenzene            | 11.705   |                      | 15                           | 1.459                 | 3.19               |
| T      | Butylbenzene                   | 11.836   |                      | 15                           | 2.648                 | 3.56               |
| T      | 1,2-Dibromo-3-chloropropane    | 12.031   |                      | 15                           | 0.235                 | 4.94               |
| T      | 1,2,4-Trichlorobenzene         | 12.926   |                      | 15                           | 1.361                 | 3.25               |
| T      | Naphthalene                    | 13.071   |                      | 15                           | 3.267                 | 3.66               |
| T      | Hexachlorobutadiene            | 13.136   |                      | 15                           | 0.939                 | 3.20               |
| T      | 1,2,3-Trichlorobenzene         | 13.194   |                      | 15                           | 1.311                 | 2.57               |
|        | <b>Average %RSD of Targets</b> |          |                      |                              |                       | <b>4.31</b>        |

\* Compound designations as follows: T (target); SPCC (system performance check compound); CCC (calibration check compound); Surr (surrogate); ISTD (internal standard). Target compounds may also be designated as SPCCs or CCCs.

\*\* The minimum average RF that must be met for the SPCCs

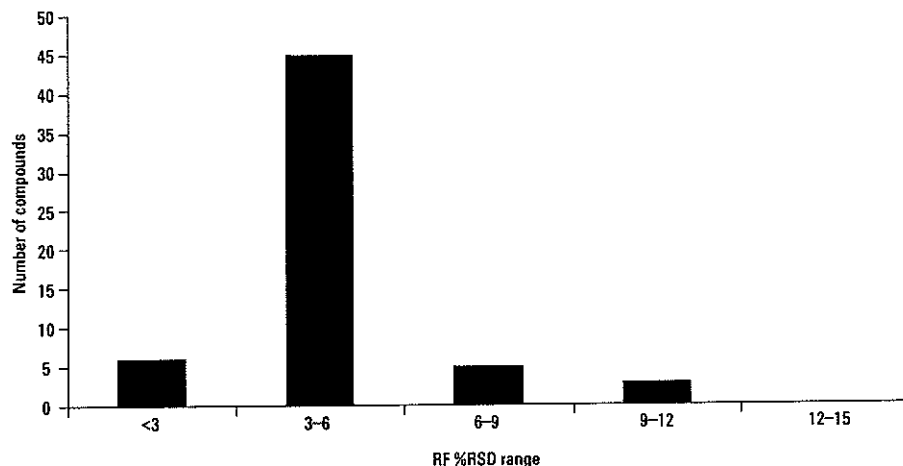
\*\*\* The minimum %RSD of the RFs. If any one or more of the CCC RF RSDs exceeds 30%, instrument maintenance is required. If the RF %RSD for any target compound exceeds 15%, other curve fits must be substituted for the average RF.

### The Importance of an Inert Flow Path

The initial calibration for this method resulted in 6 compounds having relative RF %RSDs greater than 15% and a total of 15 with double digit %RSDs. The worst performers were (E) and (Z) 1,3-dichloropropene; dibromochloromethane; bromoform; 1,1,2,2-tetrachloroethane; and 1,2-dibromo-3-chloropropane with RRF RSDs

averaging 28%. After replacing the old GC column and inlet liner (descriptions in Table 3), the average RSD fell to 6% for these difficult compounds. All RF %RSDs were well under 15% with an average of 4.3% for all 59 calibrated peaks (m- and p-xylene calibrated together). The results are shown in Table 4. A distribution of the %RSD values is shown graphically in Figure 2.



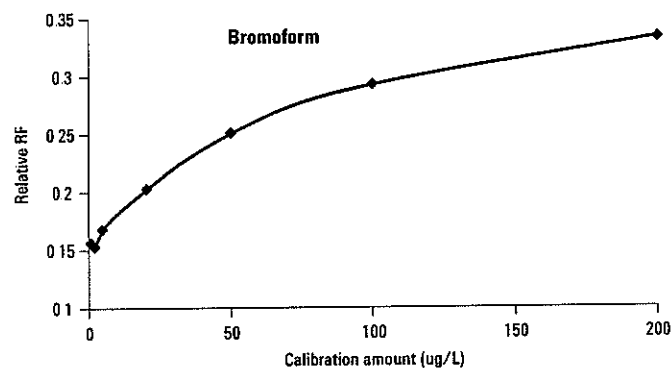


**Figure 2.** Distribution of the RF RSDs for the 59 calibrated peaks (m- and p-xylene are not resolved).

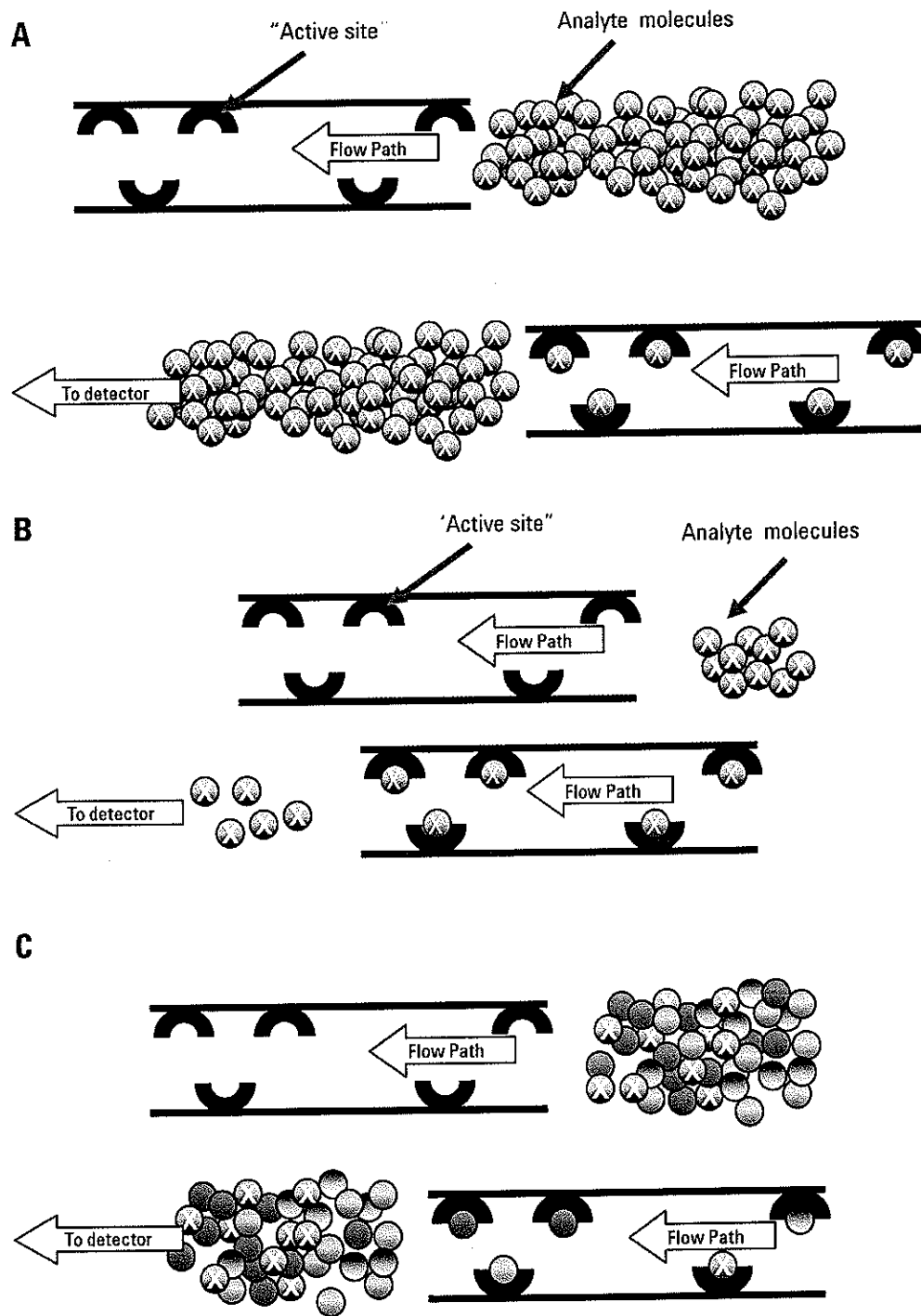
As discussed, some VOCs are particularly susceptible to active sites in the flow path. One manifestation of this problem is that the calibration curve is nonlinear (Figure 3). Ideally, the RRF should be identical at each calibration level, giving a straight horizontal line. However, when an analyte is adsorbed or decomposed by active sites, the RFs fall off as the concentration goes down.

An easy way to visualize this problem is to consider the illustration in Figure 4. First, assume that there are five active sites somewhere in the sample flow path (Figure 4a). Let us also assume that a

high-level calibration standard contains 500 molecules of compound X and that "X" is susceptible to adsorption or decomposition by these active sites. In this case, there is a risk of losing 5 of the 500 molecules, which would reduce the RF by just 1%. Next, assume that a low-level calibration standard contains just 10 molecules of compound X. In this case, one could lose as much as 50% of the analyte, cutting the RF in half (Figure 4b). Thus, as the calibration level for compound X goes down, the response factor falls off, leading to a nonlinear calibration curve such as the bromoform curve shown in Figure 3.



**Figure 3.** An example of a nonlinear calibration curve for bromoform caused by adsorption by active sites in the P&T/GC/MS flow path.



**Figure 4.** An illustration showing how "active sites" in the P&T/GC/MS flow path can affect the amount of analyte (compound "X") reaching the detector. A) An example showing how just a small fraction of a high concentration analyte is lost to a small number of active sites. B) An example showing how a large fraction of a low concentration analyte can be lost to a small number of active sites. C) An example showing how analytes may compete for active sites. Very little of compound X is lost due to competition from high concentrations of other analytes.

Figure 4c illustrates another manifestation of these active site problems. Assume that there are still five active sites and 10 molecules of compound X. However, this time there are other molecules present at high levels, which compete for the same active sites. With a limited number of active sites and competition from other compounds, most of the X molecules reach the detector. This explains why analyte or surrogate recoveries are sometimes low in relatively clean samples and higher in the presence of other analytes.

Active sites can appear anywhere in the flow path of the P&T/GC/MS system. If compounds begin to adsorb, the solution is to replace those components of the flow path that cause the problem. In this case, replacing the column and inlet liner restored instrument performance.

### SIM/Scan Method

EPA methods for volatiles analysis do not mention the use of synchronous SIM/scan methods. However, it is possible to obtain SIM and scan data in the same analysis with virtually no sacrifice in sensitivity in each mode. After creating the scan method, a SIM method was created using the ChemStation's AutoSIM tool. The default AutoSIM settings were used.

Figure 5 shows extracted ion chromatograms (EICs) (SIM and scan from a SIM/scan run) for the six gases that are part of many VOC methods. In general, these six compounds give the lowest average RFs among the 60 analytes used for this work. Of these, ethyl chloride is often the least responsive

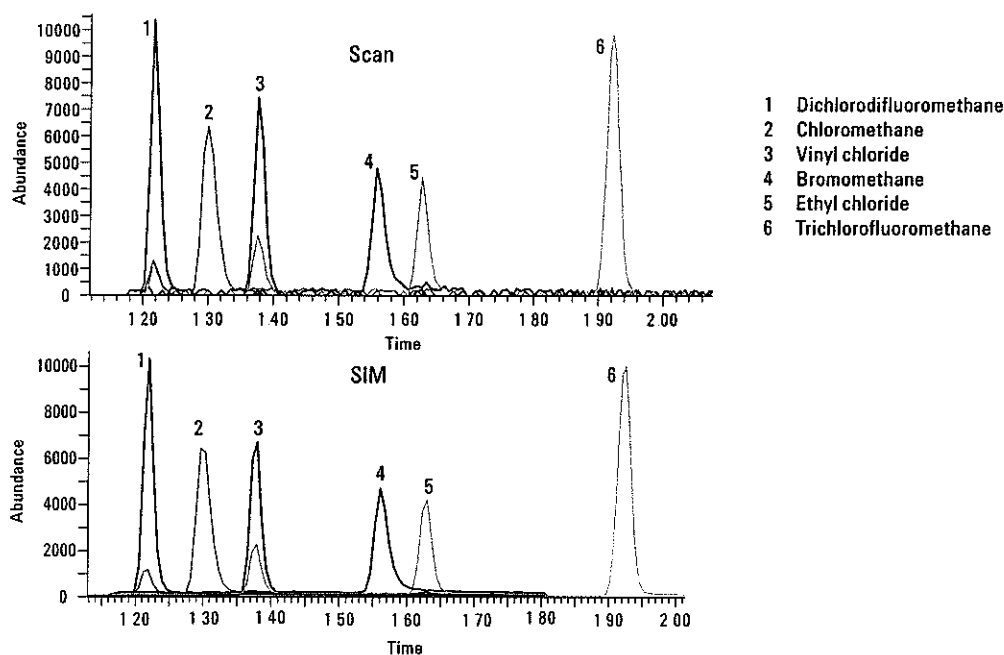


Figure 5. EICs for the six analytes that are gases at standard temperature and pressure. Both the scan and SIM chromatograms were obtained in a single synchronous SIM/scan run.

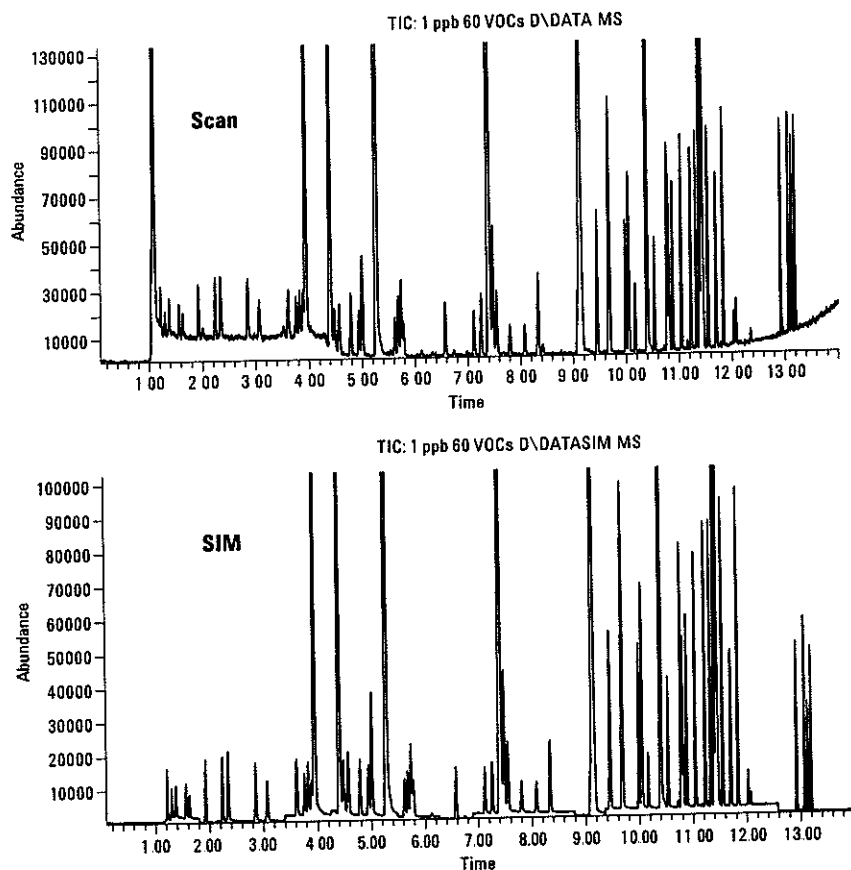
The sensitivity of the scan-only method was compared to the SIM/scan mode by measuring the signal-to-noise (S/N) ratio for ethyl chloride. As seen in Table 5, the S/N ratio for ethyl chloride is approximately the same for scan runs, whether run alone or as part of a SIM/scan acquisition. A sampling rate of 4 ( $n = 2$ ) was used in each case. The only difference between these two scan runs is that the scan rate is slower in the SIM/scan mode than in the scan-only mode. Nevertheless, all peaks were defined by at least eight scans, making accurate quantitation possible. As expected, SIM provided a 10-fold improvement in sensitivity over scan. Using the Agilent 5975 inert MSD, one can run in the SIM/scan mode with no loss of scan sensitivity and obtain a SIM chromatogram with 10X greater sensitivity "for free". The only trade-off is in the scan rate, but the rate is still sufficient for quantification. The number of SIM and Scan acquisitions across each peak can be increased without loss of sensitivity by reducing the sample rate from  $2^2$  to  $2^1$ .

Table 5 shows a comparison of the signal-to-noise (S/N) ratio for ethyl chloride (using  $m/z$  64) analyzed by a scan method and a synchronous SIM/scan method. The S/N ratio has been calculated using two different noise measurement methods - root mean squared (RMS) and peak-to-peak.

**Table 5. S/N Comparison Between SIM and Scan in SIM/Scan Run**

|                  | RMS S/N | Peak/Peak S/N |
|------------------|---------|---------------|
| SIM (SIM/Scan)   | 749     | 254           |
| Scan (SIM/Scan)  | 75      | 20            |
| Scan (Scan only) | 73      | 17            |

Figure 6 compares the total ion current chromatograms for the synchronous SIM and scan analysis of the 60 target VOCs (1 ppb each), internal standards (20 ppb), and surrogates (20 ppb) shown in Table 4.



**Figure 6. TICs for the SIM and scan chromatograms obtained from a single synchronous SIM/scan analysis of the 67 compounds shown in Table 4.**

## Conclusions

While the benefit of sharing GC/MS methods is clear, the process of replicating them on various instruments has been tedious and time-consuming. Now, the Agilent eMethod software with its "Method Export" and "Method Import" wizards make GC/MS method transfer a trivial process.

Anyone interested in replicating this method can download all of the parameters from the Agilent Web site ([www.agilent.com/chem/eMethods](http://www.agilent.com/chem/eMethods)). Using the Method Import function of the Agilent G1701DA (version 2.0.00 or newer), the method can be installed immediately, complete with calibration tables and RTL calibration. The user would have to relock the method using toluene-d8 as the locking compound and run new calibration standards. Although the P&T setpoints are not automatically installed, they are included with the eMethod in the "notes" section.

## References

1. "Volatile Organic Compounds by Gas Chromatography/Mass Spectrometry (GC/MS)," U.S. Environmental Protection Agency, Office of Solid Waste, SW-846 Method 8260B, revision 2, December 1996, (<http://www.epa.gov/epaoswer/hazwaste/test/pdfs/8260b.pdf>).
2. "Methods for the Determination of Organic Compounds in Drinking Water-Supplement III (EPA/600/R-95-131)," Method 524.2, revision 4.1, U.S. Environmental Protection Agency, Office of Research and Development, National Exposure Research Laboratory, Cincinnati, OH (1995).
3. Philip L. Wylie, BFB Tuning for Environmental Analysis: Three Ways to Succeed, Agilent Technologies, publication 5988-4373EN, (<http://www.chem.agilent.com/scripts/Library.asp?OPT=OL>)
4. Philip L. Wylie, Techniques for Optimizing the Analysis of Volatile Organic Compounds in Water Using Purge-and-Trap/GC/MS, Agilent Technologies, publication 5989-0603EN (<http://www.chem.agilent.com/scripts/Library.asp?OPT=OL>)
5. "Volatile Organic Compounds in Water by Purge and Trap Capillary Column Gas Chromatography with Photoionization and Electrolytic Conductivity Detectors in Series," Method 502.2, rev. 2.1, US Environmental Protection Agency, National Exposure Research Laboratory, Office of Research and Development, Cincinnati (1995).

## For More Information

For more information on our products and services, visit our Web site at [www.agilent.com/chem](http://www.agilent.com/chem).

[www.agilent.com/chem](http://www.agilent.com/chem)

Agilent shall not be liable for errors contained herein or for incidental or consequential damages in connection with the furnishing, performance, or use of this material

Information, descriptions, and specifications in this publication are subject to change without notice

© Agilent Technologies, Inc. 2005

Printed in the USA  
July 26, 2005  
5989-3347EN



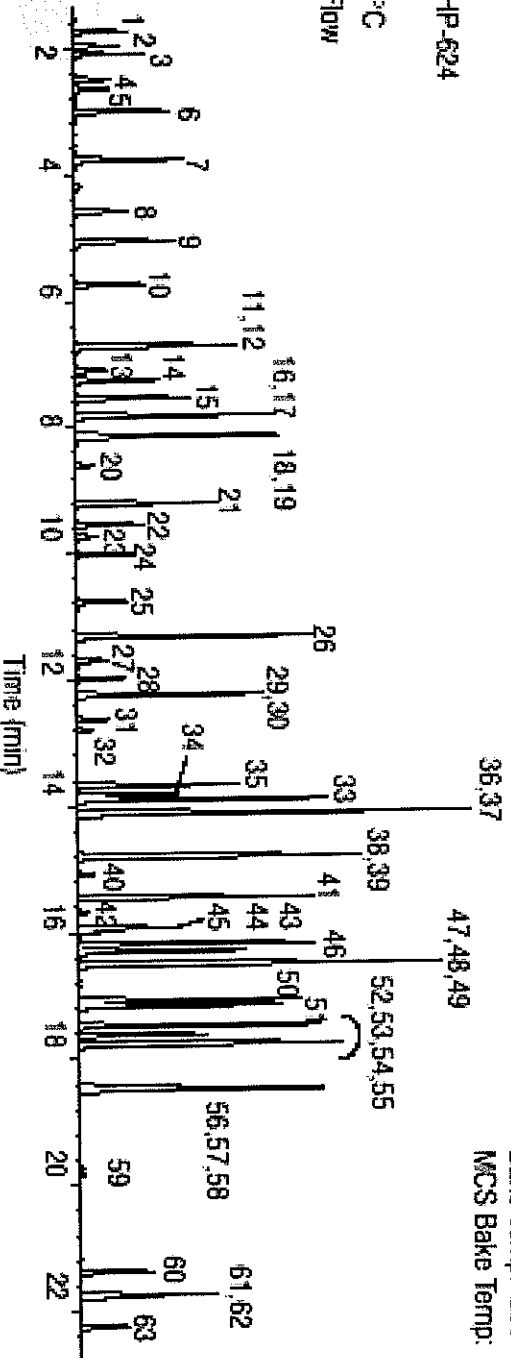
**Agilent Technologies**

# Volatiles in Water (EPA Method 524.2)

|                             |                             |                                  |                                  |
|-----------------------------|-----------------------------|----------------------------------|----------------------------------|
| 1. Dichlorodifluoromethane  | 17. Carbon Tetrachloride    | 33. Chlorobenzene                | 49. 1, 3, 5-Trimethylbenzene     |
| 2. Chloromethane            | 18. Benzene                 | 34. 1, 1, 1, 2-Tetrachloroethane | 50. t-Butylbenzene               |
| 3. Vinyl chloride           | 19. 1, 2-Dichloroethane     | 35. Ethylbenzene                 | 51. 1, 2, 4-Trimethylbenzene     |
| 4. Bromomethane             | 20. Fluorobenzene           | 36. m-Xylene                     | 52. s-Butylbenzene               |
| 5. Chloroethane             | 21. Trichloroethane         | 37. p-Xylene                     | 53. 1, 3-Dichlorobenzene         |
| 6. Trichlorofluoromethane   | 22. 1, 1-Dichloropropane    | 38. o-Xylene                     | 54. 4-Isopropyltoluene           |
| 7. 1, 1-Dichloroethane      | 23. Dibromomethane          | 39. Styrene                      | 55. 1, 4-Dichlorobenzene         |
| 8. Methylene chloride       | 24. Bromodichloromethane    | 40. Bromoform                    | 56. 1, 2-Dichlorobenzene-d4      |
| 9. 1-1, 2-Dichloroethene    | 25. c-1, 3-Dichloropropane  | 41. Isopropylbenzene             | 57. 1, 2-Dichlorobenzene         |
| 10. 1, 1-Dichloroethane     | 26. Toluene                 | 42. 4-Bromofluorobenzene         | 58. n-Butylbenzene               |
| 11. 2, 2-Dichloropropane    | 27. 1-1, 3-Dichloropropane  | 43. Bromobenzene                 | 59. 1, 2-Dibromo-3-chloropropane |
| 12. c-1, 2-Dichloroethene   | 28. 1, 1, 2-Trichloroethane | 44. 1, 1, 2, 2-Tetrachloroethane | 60. 1, 2, 4-Trichlorobenzene     |
| 13. Bromochloroethane       | 29. Tetrachloroethen        | 45. 1, 2, 3-Trichloropropane     | 61. Hexachlorobutadiene          |
| 14. Chloroform              | 30. 1, 3-Dichloropropane    | 46. n-Propylbenzene              | 62. Naphthalene                  |
| 15. 1, 1, 1-Trichloroethane | 31. Dibromochloromethane    | 47. 2-Chlorotoluene              | 63. 1, 2, 3-Trichlorobenzene     |
| 16. 1, 1-Dichloropropane    | 32. 1, 2-Dibromoethane      | 48. 4-Chlorotoluene              |                                  |

P&T Parameters  
 Line Temp: 120°C  
 Valve Temp: 120°C  
 MCS Temp: 100°C  
 Purge Temp: 30°C (11 min)  
 Dry Purge Time: 2 min  
 MCS Desorb Temp: 40°C  
 Desorb Preheat: 250°C  
 Desorb Temp: 255°C (2 min)  
 Bake Temp: 260°C (8 min)  
 MCS Bake Temp: 180°C

Column: 25 m x 0.2 mm x 1.12 µm HP-624  
 (Part No. 19091V-402)  
 Oven: 35 (4 min), 8°C/min to 180°C  
 Carrier: Helium, 7.3 psi, Constant Flow  
 Injector: P&T, Split 30/1  
 Detector: MSD, 2505C  
 Vocab: 3000 Trap  
 Purge Flow: 40 ml/min



## Volatiles in Water (EPA Method 524.2)

1. Dichlorodifluoromethane
2. Chloromethane
3. Vinyl chloride
4. Bromomethane
5. Chloroethane
6. Trichlorofluoromethane
7. 1, 1-Dichloroethane
8. Methylene chloride
9. 1-1, 2-Dichloroethane
10. 1, 1-Dichloroethane
11. 2, 2-Dichloropropane
12. c-1, 2-Dichloroethane
13. Bromochloromethane
14. Chloroform
15. 1, 1, 1-Trichloroethane
16. 1, 1-Dichloropropene

17. Carbon Tetrachloride
18. Benzene
19. 1, 2-Dichloroethane
20. Fluorobenzene
21. Trichloroethane
22. 1, 1-Dichloropropane
23. Dibromomethane
24. Bromodichloromethane
25. c-1, 3-Dichloropropene
26. Toluene
27. t-1, 3-Dichloropropene
28. 1, 1, 2-Trichloroethane
29. Tetrachloroethene
30. 1, 3-Dichloropropane
31. Dibromochloromethane
32. 1, 2-Dibromoethane

33. Chlorobenzene
34. 1, 1, 1, 2-Tetrachloroethane
35. Ethylbenzene
36. m-Xylene
37. p-Xylene
38. o-Xylene
39. Styrene
40. Bromoform
41. Isopropylbenzene
42. 4-Bromofluorobenzene
43. Bromobenzene
44. 1, 1, 2, 2-Tetrachloroethane
45. 1, 2, 3-Trichloropropane
46. n-Propylbenzene
47. 2-Chlorotoluene
48. 4-Chlorotoluene

49. 1, 3, 5-Trimethylbenzene
50. t-Butylbenzene
51. 1, 2, 4-Trimethylbenzene
52. s-Butylbenzene
53. 1, 3-Dichlorobenzene
54. 4-Isopropyltoluene
55. 1, 4-Dichlorobenzene
56. 1, 2-Dichlorobenzene-d4
57. 1, 2-Dichlorobenzene
58. n-Butylbenzene
59. 1, 2-Dibromo-3-chloropropane
60. 1, 2, 4-Trichlorobenzene
61. Hexachlorobutadiene
62. Naphthalene
63. 1, 2, 3-Trichlorobenzene

### P&T Parameters

Line Temp: 120°C

Valve Temp: 120°C

MCS Temp: 100°C

Purge Temp: 30°C (11 min)

Dry Purge Time: 2 min

MCS Desorb Temp: 40°C

Desorb Preheat: 250°C

Desorb Temp: 255°C (2 min)

Bake Temp: 260°C (8 min)

MCS Bake Temp: 180°C

Column: 25 m x 0.2 mm x 1.12 µm HP-624  
(Part No. 19091V-402)

Oven: 35 (4 min), 8°C/min to 180°C

Carrier: Helium, 7.3 psi, Constant Flow

Injector: P&T, Split 30/1

Detector: MSD, 2505C

Vocarb 3000 Trap

Purge Flow: 40 ml/min

