# Improved Forensic Toxicology Screening Using A GC / MS / NPD System with a 725-Compound DRS Database

## Application

**Forensic Toxicology**


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## Abstract

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

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


## Introduction

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

## Experimental

### System Configuration

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

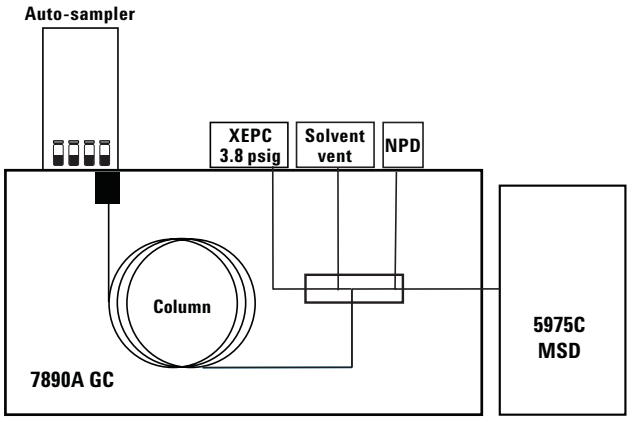


**Figure 1. GC / MS / NPD system configuration used for screening blood extracts.**

Key components are:

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

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

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

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

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

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

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

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

**Table 1. Gas Chromatograph and Mass Spectrometer Conditions**

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

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

**Gain normalized, 1x

### Instrument Operating Parameters

### Data Acquisition

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

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

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

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

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

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

The simultaneous acquisition of SIM, scan, and NPD

**Table 2. SIM Groups Used in SIM / Scan Mode**

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

(all dwell times 5 msec)

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

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

### Data Analysis

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

The resulting data review scheme consisted of the following:

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

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

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

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

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

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

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

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

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

### Samples

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

## Results and Discussion

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

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

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

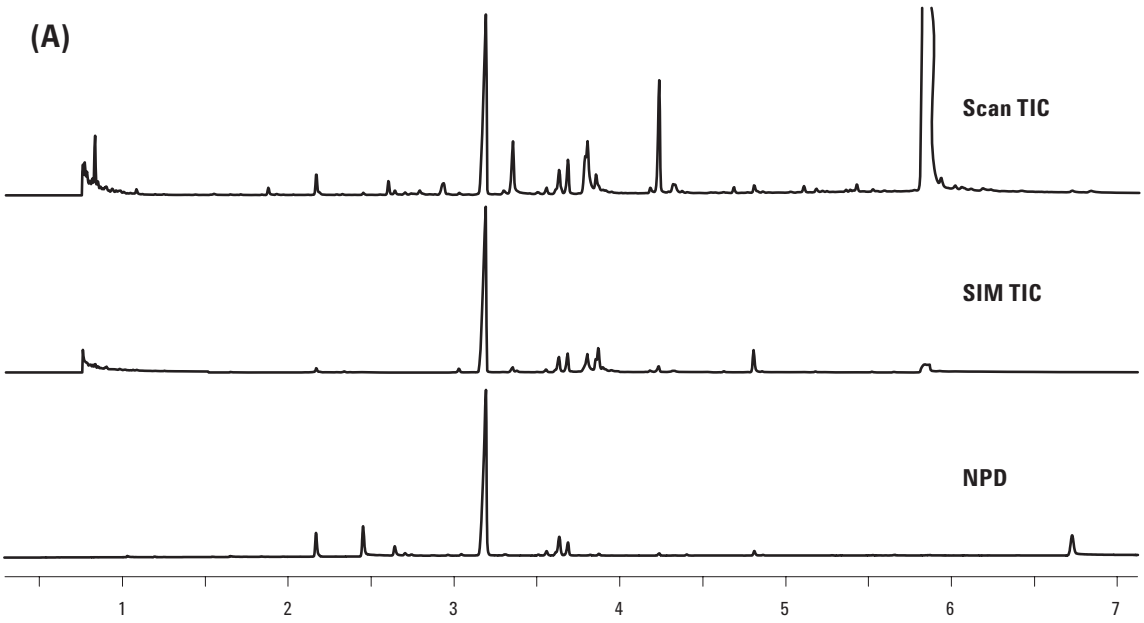


**Figure 2A. Chromatograms of scan, SIM, and NPD signals from analysis of blood extract.**

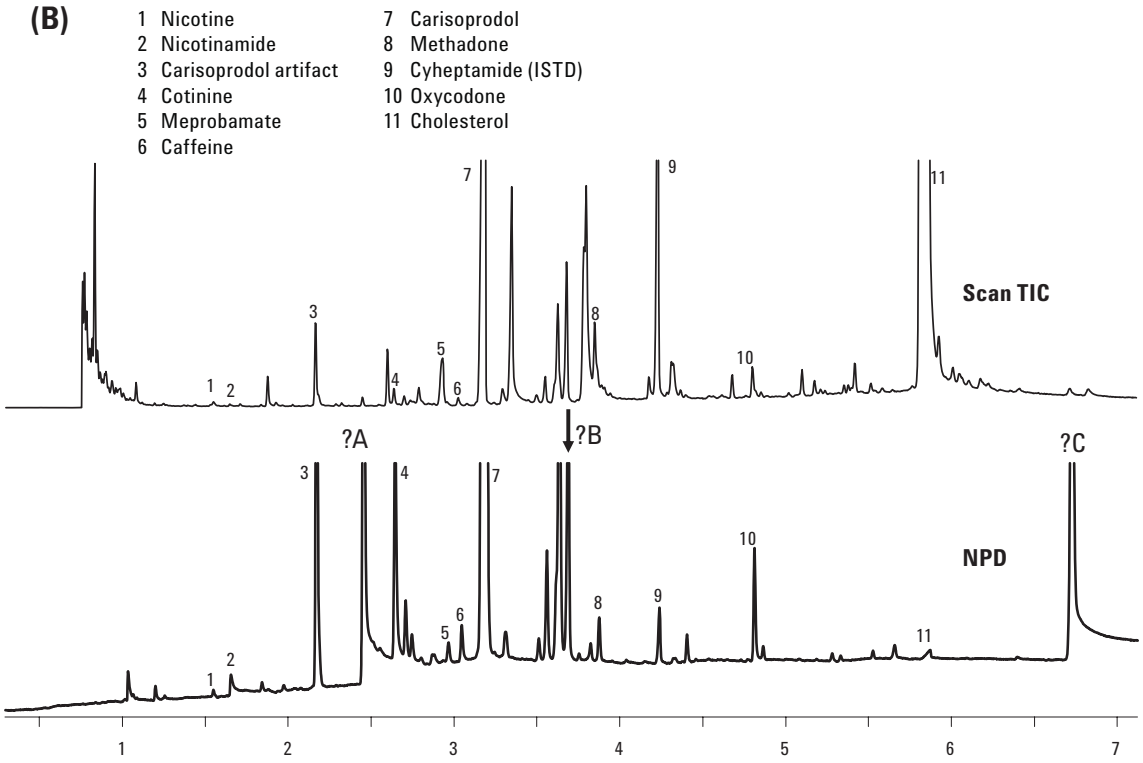


**Figure 2B. Expanded scale chromatograms of scan TIC and NPD signals from analysis of blood extract. (continued)**

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

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

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

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

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

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

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

| | | | Agilent | AMDIS | |
|---|---|---|---|---|---|
| R.T. | CAS # | Compound Name | ChemStation Amount (~ng) | Match | R.T. Diff. sec. |
| 1.539 | 54115 | Nicotine | 0.03 | 59 | –0.5 |
| 1.6446 | 98920 | Nicotinamide | 0.27 | 93 | –0.9 |
| 2.1631 | 999401024 | Carisoprodol artifact | 64.87 | 93 | –0.5 |
| 2.6367 | 486566 | Cotinine | 1 | 96 | –0.4 |
| 2.928 | 57534 | Meprobamate | 4.11 | 99 | 0.0 |
| 3.033 | 58082 | Caffeine | 0.04 | 82 | –0.5 |
| 3.1832 | 78444 | Carisoprodol | 127.4 | 96 | 1.0 |
| 3.8653 | 76993 | Methadone | 0.39 | 74 | –0.1 |
| 4.2279 | 7199293 | Cyheptamide | 22.5 | 98 | 0.1 |
| 4.8014 | 76426 | Oxycodone | 2.37 | 82 | 0.0 |
| 5.850 | 57885 | Cholesterol | 922.73 | 97 | 3.4 |

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

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

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

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

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

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

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

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

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

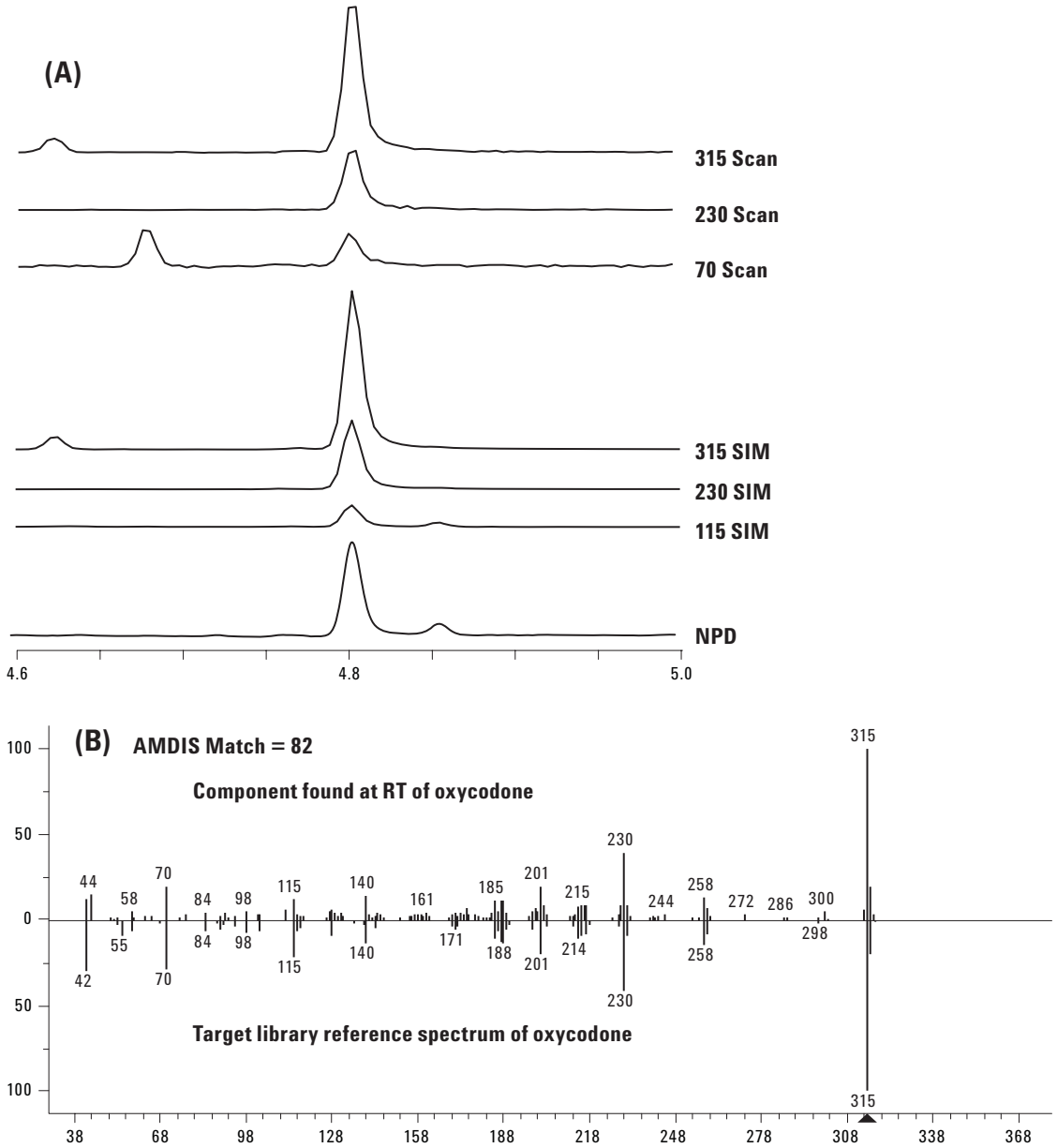


**Figure 4.** **(A) Oxycodone response in SIM, scan, and NPD signals collected simultaneously. (B) Comparison of deconvoluted oxycodone spectrum with target library reference spectrum.**

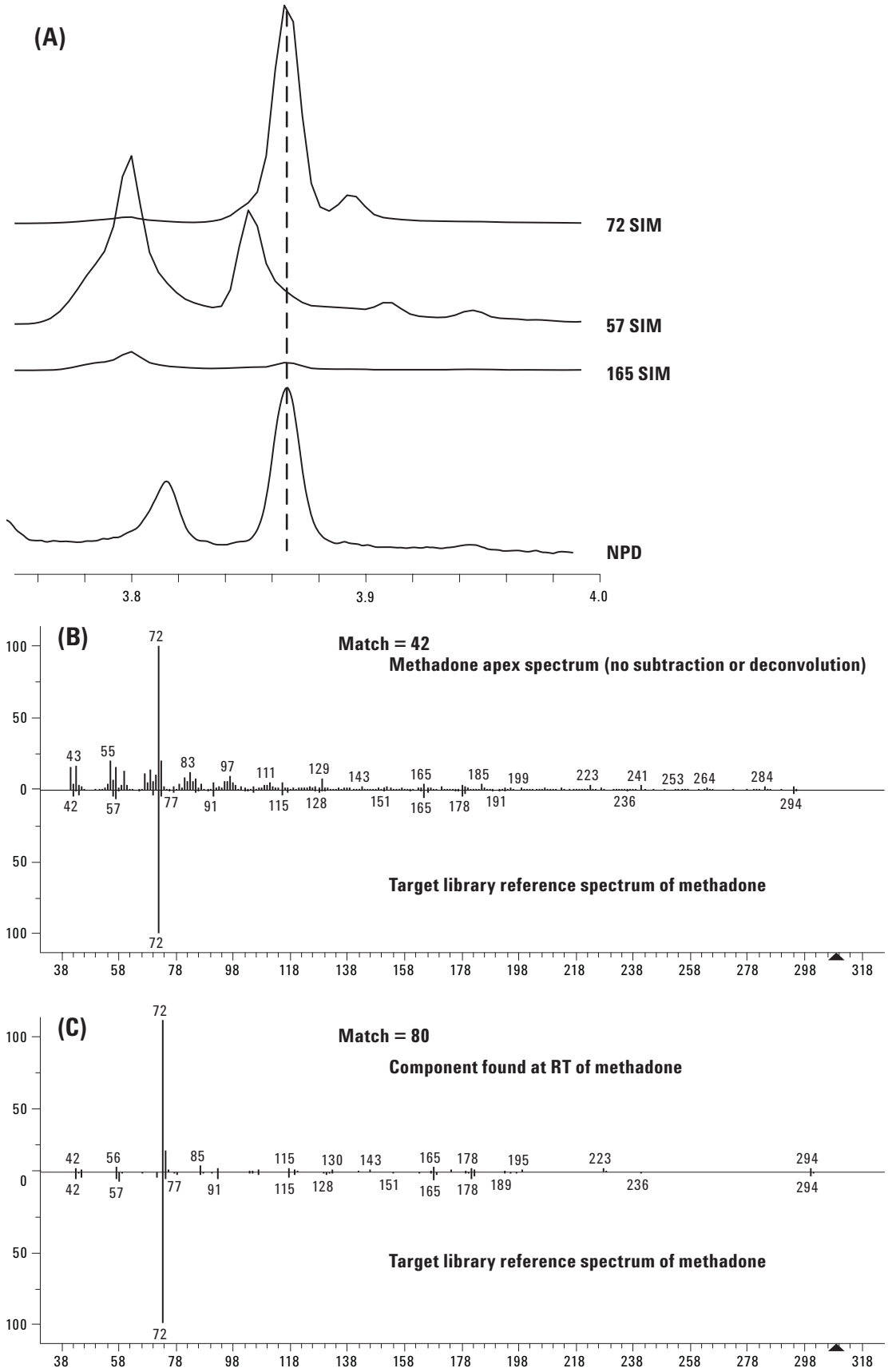


**Figure 5.** **(A) Methadone SIM and NPD chromatograms.**
**(B) Comparison of reference spectrum with methadone spectrum without subtraction or deconvolution.**
**(C) Methadone deconvoluted spectrum searched against target library.**

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

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

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

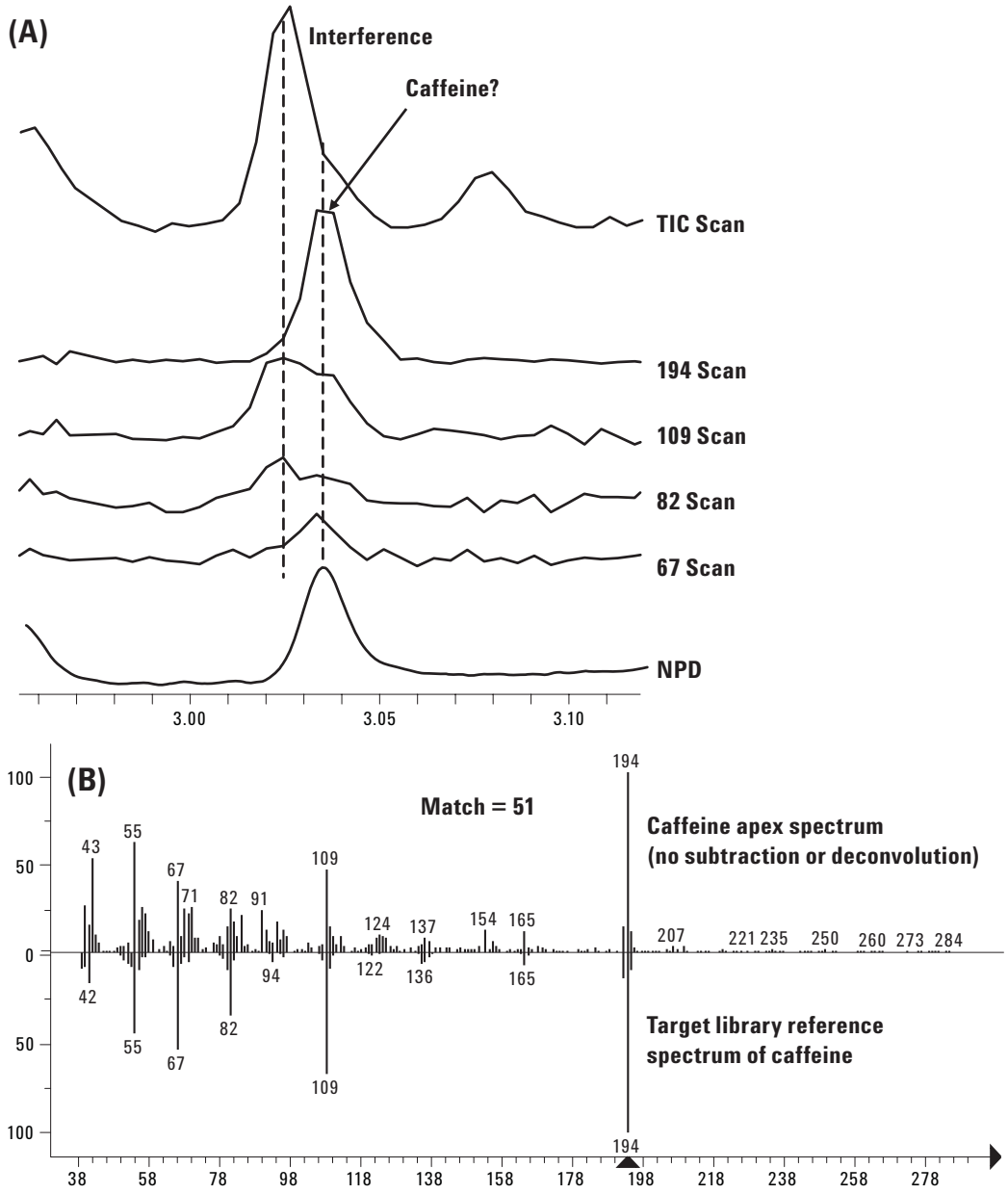


**Figure 6.** **(A) TIC, scan EICs, and NPD signals for caffeine.**
**(B) Caffeine spectrum without subtraction or deconvolution shows interference from matrix compound.**

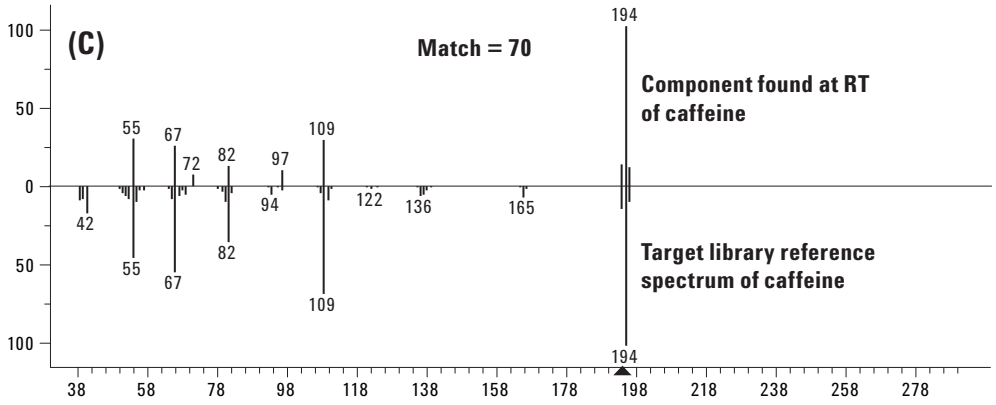


**Figure 6C Caffeine deconvoluted spectrum searched against target library. (continued)**

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

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

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

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

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

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

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

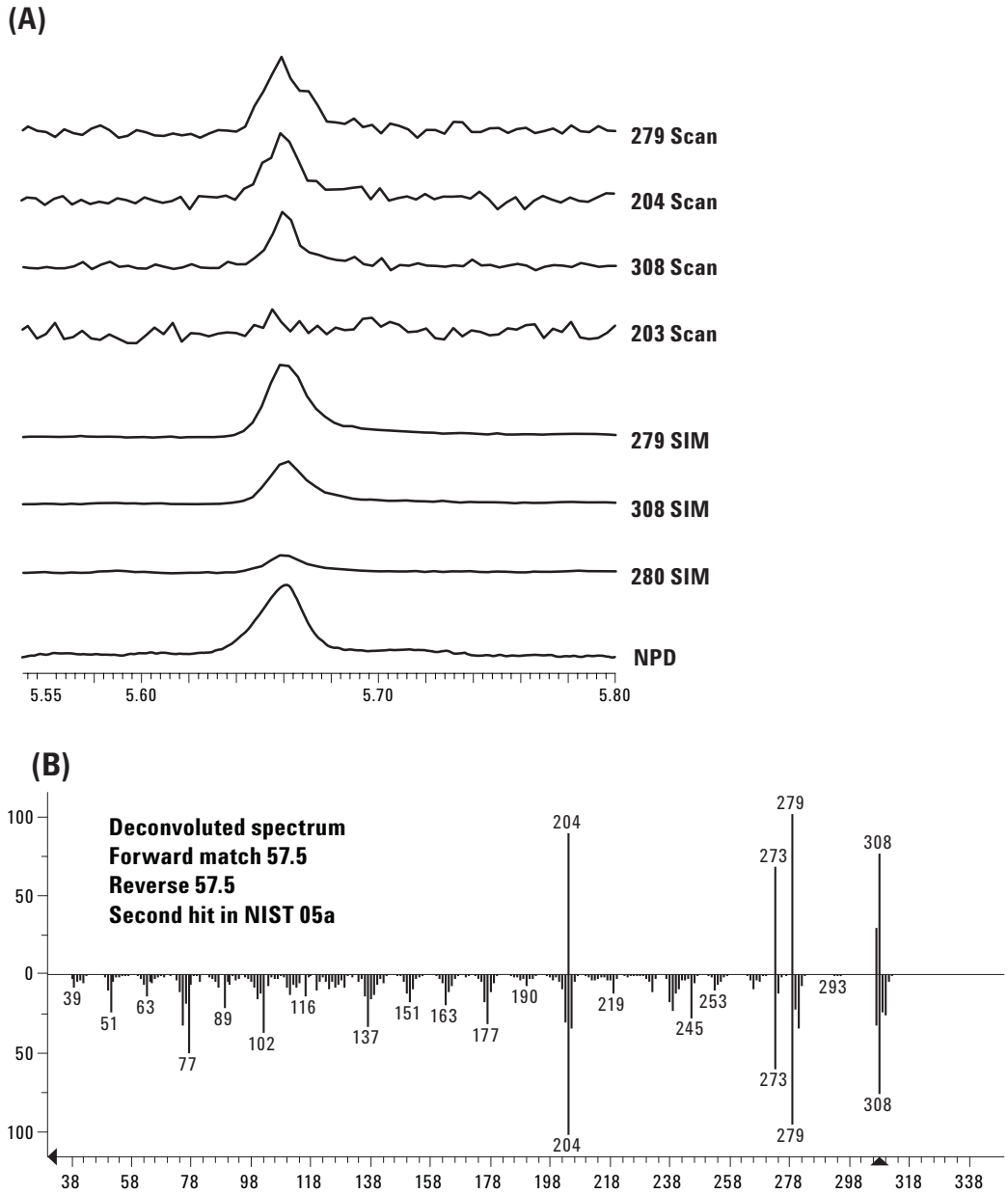


**Figure 7.** **(A) Alprazolam response on SIM, scan, and NPD signals.**
**(B) Alprazolam deconvoluted spectrum searched against NIST 05a library.**

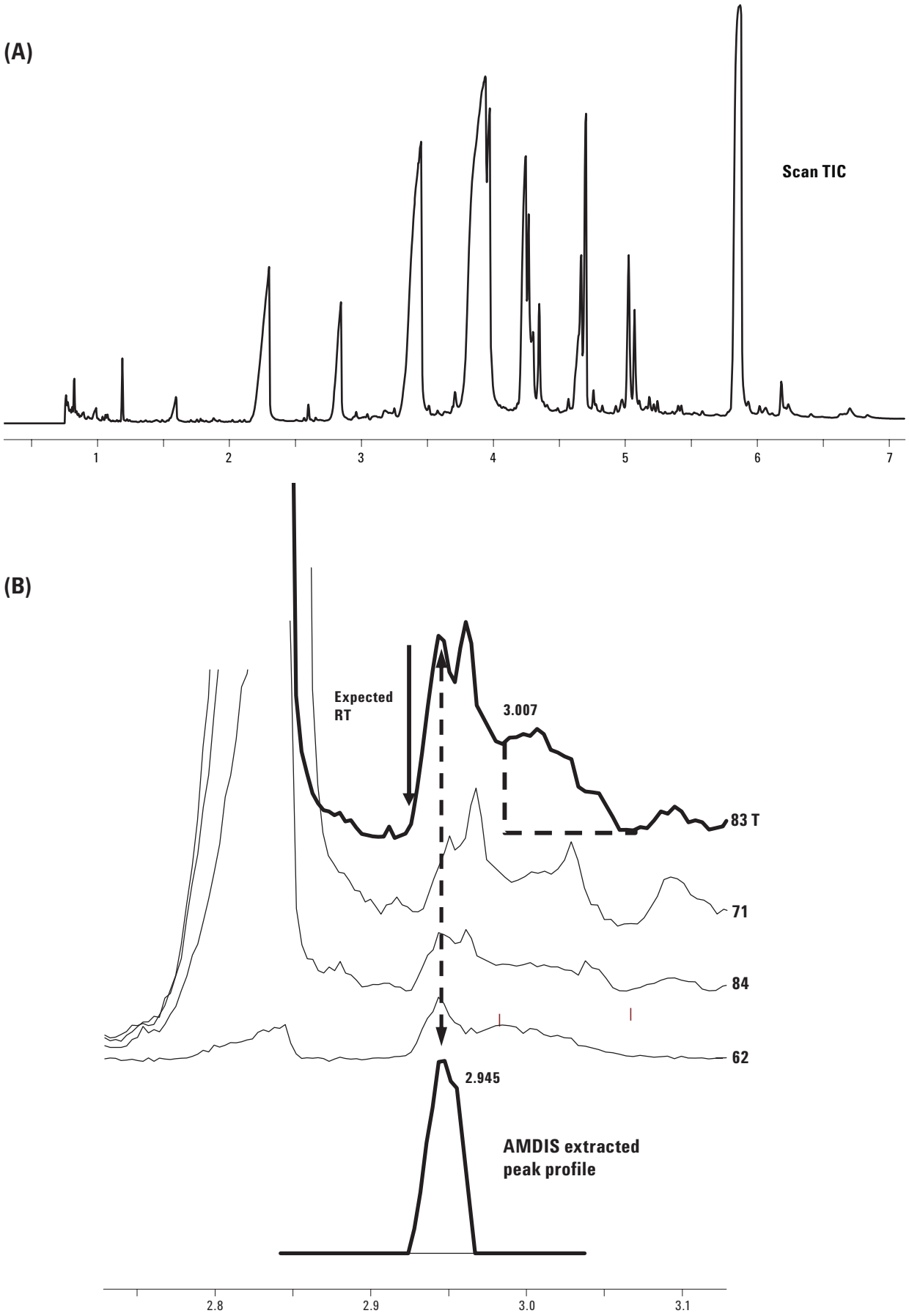


**Figure 8.** **(A) Scan TIC chromatogram of sample with high levels of fatty acids.**
**(B) Scan EICs from bleed optimized method overlayed with AMDIS extracted peak profile.**

**(C)**

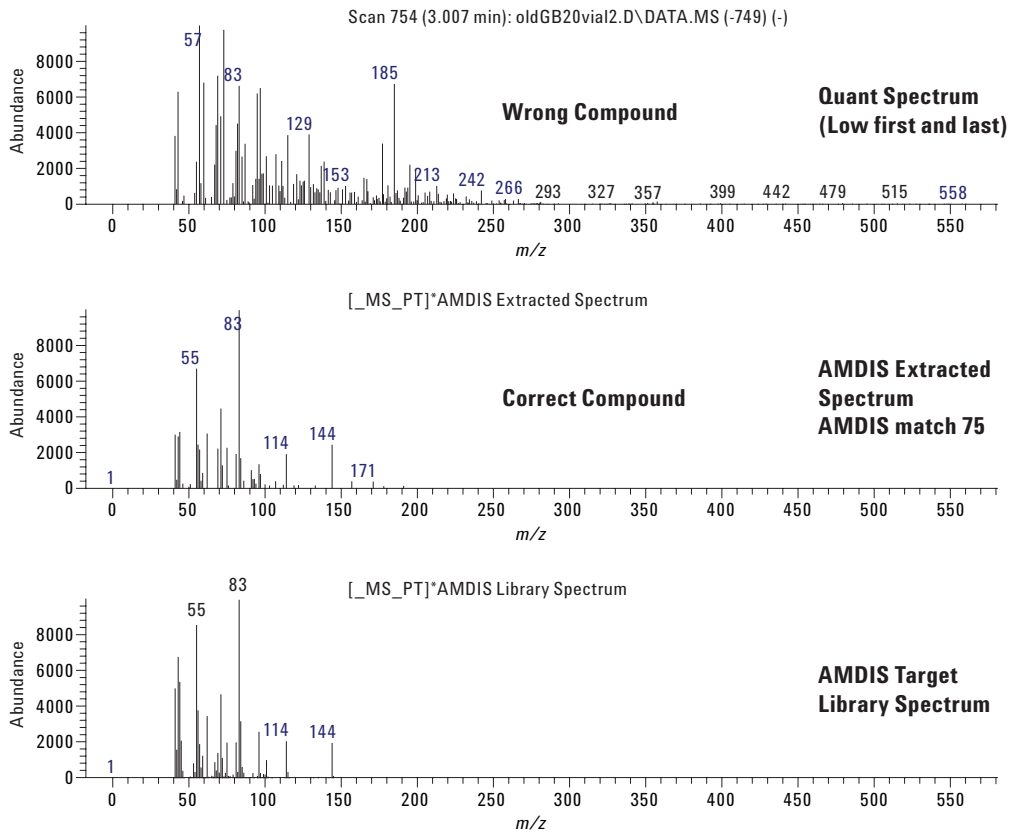


**Figure 8C. Three meprobamate spectra presented in QEdit for comparison during data review using DRS A.04. (continued)**

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

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

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

## Conclusions

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

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

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

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

## References


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5. B. D. Quimby, L. M. Blumberg, M. S. Klee, and P. L. Wylie, "Precise Time-Scaling of Gas Chromatographic Methods Using Method Translation and Retention Time Locking," Agilent Technologies publication 5967-5820E
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7. Bruce D. Quimby and Michael J. Szelewski, "Screening for Hazardous Chemicals in Homeland Security and Environmental Samples Using a GC/MS/ECD/FPD with a 731 Compound DRS Database," Agilent Technologies publication 5989-4834EN


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# Appendix

| Compound name | CAS number* |
|---|---|
| 10,11-Dihydro-10-hydroxycarbazepine | 999402-02-7 |
| 10,11-Dihydro-10-hydroxycarbazepine TMS | 999423-02-8 |
| 10,11-Dihydrocarbamazepin | 003564-73-6 |
| 5-Amino-2-chloropyridine | 005350-93-6 |
| 5-Methoxy-dipropyltryptamine | 999001-02-4 |
| 6-Acetyl-morphine | 002784-73-8 |
| 6-Acetyl-morphine TMS | 999155-02-1 |
| 7-Aminoflunitrazepam | 034084-50-9 |
| 7-Aminoflunitrazepam TMS | 999176-02-2 |
| 7-Hydroxyamoxapine | 037081-76-8 |
| 8-Methoxyloxapine | 070020-54-1 |
| Acepromazine | 000061-00-7 |
| Acetaminophen | 000103-90-2 |
| Acetaminophen 2TMS | 055530-61-5 |
| Acetanilide | 000103-84-4 |
| Adiphenine | 000064-95-9 |
| Adiphenine-M/artifact (ME) | 003469-00-9 |
| Alfentanil | 071195-58-9 |
| Allobarbital | 000052-43-7 |
| Allopurinol TMS | 999178-02-8 |
| Alphaprodine | 000077-20-3 |
| Alphenal | 000115-43-5 |
| Alprazolam | 028981-97-7 |
| Alprenolol TMS | 999381-02-1 |
| Alverine | 000150-59-4 |
| Amantadine | 000768-94-5 |
| Amantadine AC | 999127-02-5 |
| Ambroxol | 018683-91-5 |
| Ambroxol 2AC | 999341-02-5 |
| Aminoglutethimide | 000125-84-8 |
| Aminopyrine | 000058-15-1 |
| Amitriptyline | 000050-48-6 |
| Amlodipine AC | 999299-02-4 |
| Amobarbital | 000057-43-2 |
| Amobarbital 2TMS | 999179-02-1 |
| Amoxapine | 014028-44-5 |
| Amoxapine AC | 999128-02-8 |
| Amphetamine | 000060-15-1 |
| Amphetamine AC | 999107-02-7 |
| Ampyrone | 000083-07-8 |
| Ampyrone AC | 000083-15-8 |
| Ampyrone-2AC | 999240-02-7 |
| Anhydroecgonine methyl ester | 043021-26-7 |
| Anileridine | 000144-14-9 |
| Anisindione | 000117-37-3 |
| Antazoline | 000091-75-8 |
| Antazoline AC | 999408-02-5 |
| Antipyrine | 000060-80-0 |
| Apomorphine 2TMS | 074841-68-2 |
| Aprobarbital | 000077-02-1 |
| Aprobarbital 2TMS | 999180-02-8 |
| Atenolol formyl artifact | 999459-02-8 |
| Atomoxetine | 083015-26-3 |
| Atomoxetine AC | 999257-02-2 |
| Atovaquone | 953233-18-4 |
| Atovaquone TMS | 999409-02-8 |
| Atropine | 000051-55-8 |
| Atropine TMS | 055334-03-7 |
| Azacyclonol | 000115-46-8 |
| Azatadine | 003964-81-6 |
| Barbital | 000057-44-3 |
| BDMPEA | 066142-81-2 |
| BDMPEA AC | 999357-02-7 |
| BDMPEA formyl artifact | 999378-02-8 |
| Bemegride | 000064-65-3 |
| Benzocaine | 000094-09-7 |
| Benzoylecgonine | 000519-09-5 |
| Benzoylecgonine TMS | 999462-02-1 |
| Benzphetamine | 000156-08-1 |
| Benzquinamide | 000063-12-7 |
| Benztropine | 000086-13-5 |
| Benzydamine | 000642-72-8 |
| Benzylpiperazine | 002759-28-6 |
| Benzylpiperazine AC | 999129-02-1 |
| Betahistine | 005579-84-0 |
| Betahistine AC | 999439-02-0 |
| Betaxolol | 063659-18-7 |
| Betaxolol formyl artifact | 999436-02-1 |
| Biperiden | 000514-65-8 |
| Bisacodyl | 000603-50-9 |
| Bisoprolol | 066722-44-9 |
| Bromazepam | 001812-30-2 |

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

| Compound name | CAS number |
|---|---|
| Bromazepam TMS | 999158-02-0 |
| Bromdiphenhydramine | 000118-23-0 |
| Bromocriptine breakdown | 025614-03-3 |
| Bromperidol | 010457-90-6 |
| Brompheniramine | 000086-22-6 |
| Brucine | 000357-57-3 |
| Buclizine | 000082-95-1 |
| Bupivacaine | 002180-92-9 |
| Buprenorphine | 052485-79-7 |
| Buprenorphine TMS | 999159-02-3 |
| Bupropion | 034911-55-2 |
| Buspirone | 036505-84-7 |
| Butabarbital | 000125-40-6 |
| Butabarbital 2TMS | 052988-92-8 |
| Butacaine | 000149-16-6 |
| Butalbital | 000077-26-9 |
| Butalbital 2TMS | 052937-70-9 |
| Butethal | 000077-28-1 |
| Butorphanol | 042408-82-2 |
| Butorphanol TMS | 100013-72-3 |
| Caffeine | 000058-08-2 |
| Canrenone | 000976-71-6 |
| Canrenone TMS | 999413-02-4 |
| Cantharidin | 000056-25-7 |
| Carbamazepine | 000298-46-4 |
| Carbamazepine-M (formyl-acridine) | 999243-02-6 |
| Carbinoxamine | 000486-16-8 |
| Carbromal-M/artifact | 999196-02-0 |
| Carisoprodol | 000078-44-4 |
| Carisoprodol artifact | 999401-02-4 |
| Cathinone AC | 999485-02-8 |
| Celecoxib | 169590-42-5 |
| Cetirizine methanol adduct | 083881-46-3 |
| Cetirizine TMS | 999183-02-7 |
| Chlophedianol | 000791-35-5 |
| Chlophedianol TMS | 999464-02-7 |
| Chloramphenicol 2TMS | 021196-84-9 |
| Chlorcyclizine | 000082-93-9 |
| Chlordiazepoxide | 000058-25-3 |
| Chlordiazepoxide artifact (desoxo) | 999197-02-3 |
| Chlormezanone | 000080-77-3 |
| Chlormezanone artifact | 999245-02-2 |
| Chloroamphetamine | 000064-12-0 |
| Chloroamphetamine AC | 999414-02-7 |
| Chlorophenylpiperazine | 038212-33-8 |
| Chlorophenylpiperazine AC | 999486-02-1 |
| Chloroprocaine, 2- | 000133-16-4 |
| Chloroquine | 000054-05-7 |
| Chlorpheniramine | 000132-22-9 |
| Chlorphenisin | 000104-29-0 |
| Chlorphentermine | 000461-78-9 |
| Chlorphentermine AC | 999130-02-8 |
| Chlorpropamide artifact-2 | 999246-02-5 |
| Chlorprothixene | 000113-59-7 |
| Chlorzoxazone | 000095-25-0 |
| Cholesterol | 000057-88-5 |
| Cholesterol TMS | 001856-05-9 |
| Cinnarizine | 000298-57-7 |
| Cisapride | 081098-60-4 |
| Citalopram | 059729-33-8 |
| Clemastine | 015686-51-8 |
| Clemizole | 000442-52-4 |
| Clenbuterol | 037148-27-9 |
| Clenbuterol AC | 999360-02-0 |
| Clobazam | 022316-47-8 |
| Clofibrate | 000637-07-0 |
| Clomipramine | 000303-49-1 |
| Clonazepam | 001622-61-3 |
| Clonazepam TMS | 999184-02-0 |
| Clonazepam-M (amino-) | 004959-17-5 |
| Clonazepam-M (amino) - TMS | 999175-02-9 |
| Clonidine | 004205-90-7 |
| Clonidine 2AC | 999131-02-1 |
| Clonidine AC | 999132-02-4 |
| Clopidogrel | 113665-84-2 |
| Clozapine | 005786-21-0 |
| Clozapine AC | 999133-02-7 |
| Cocaethylene | 000529-38-4 |
| Cocaine | 000050-36-2 |
| Codeine | 000076-57-3 |
| Codeine TMS | 074367-14-9 |
| Colchicine | 000064-86-8 |

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

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

| Compound name | CAS number |
|---|---|
| Ethyl-2-malonamide, 2- TMS | 999418-02-9 |
| Ethylamphetamine | 000457-87-4 |
| Ethylamphetamine AC | 999148-02-6 |
| Ethylecgonine | 999037-02-4 |
| Ethylecgonine TMS | 999448-02-1 |
| Ethylmorphine | 000076-58-4 |
| Ethylmorphine TMS | 999221-02-2 |
| Etodolac TMS | 999212-02-1 |
| Etofylline | 000519-37-9 |
| Etofylline TMS | 077630-35-4 |
| Etomidate | 033125-97-2 |
| Eucatropine Isomer 1 | 999038-02-7 |
| Eucatropine Isomer 1 TMS | 999278-02-3 |
| Eucatropine Isomer 2 | 999277-02-0 |
| Eucatropine Isomer 2 TMS | 999518-02-4 |
| Felbamate artifact 1 | 999250-02-1 |
| Felbamate artifact 2 | 999251-02-4 |
| Felbamate artifact 3 | 999252-02-7 |
| Felodipine | 072509-76-3 |
| Felodipine-M/artifact (dehydro-) | 999296-02-5 |
| Fenfluramine | 000458-24-2 |
| Fenfluramine AC | 999139-02-5 |
| Fenoprofen | 031879-05-7 |
| Fenoprofen TMS | 999310-02-0 |
| Fentanyl | 000437-38-7 |
| Finasteride | 098319-26-7 |
| Flavoxate | 015301-69-6 |
| Flavoxate-M/artifact (HOOC-) ME | 999279-02-6 |
| Flecainide | 054143-55-4 |
| Flecainide AC | 999140-02-2 |
| Flumazenil | 078755-81-4 |
| Flunarizine | 052468-60-7 |
| Flunitrazepam | 001622-62-4 |
| Fluoxetine | 054910-89-3 |
| Fluoxetine AC | 999141-02-5 |
| Flupenthixol | 002709-56-0 |
| Flupentixol TMS | 999387-02-9 |
| Fluphenazine | 000069-23-8 |
| Fluphenazine TMS | 999280-02-3 |
| Fluphenazine-M (ring) | 000092-30-8 |
| Flurazepam | 017617-23-1 |
| Flurazepam-M (desalkyl-) | 002886-65-9 |
| Flurazepam-M (HO-ethyl-) | 020971-53-3 |
| Flurbiprofen | 005104-49-4 |
| Flutamide | 013311-84-7 |
| Flutamide TMS | 999467-02-6 |
| Fluvoxamine | 054739-18-3 |
| Fluvoxamine AC | 999262-02-1 |
| Furazolidone | 000067-45-8 |
| Furosemide 2TMS | 999214-02-7 |
| Gemfibrozil | 025812-30-0 |
| Gemfibrozil AC | 999389-02-5 |
| Glutethimide | 000077-21-4 |
| Griseofulvin | 000126-07-8 |
| Guaifenesin | 000093-14-1 |
| Guaifenesin 2TMS | 107966-19-8 |
| Guanethidine | 000055-65-2 |
| Haloperidol | 000052-86-8 |
| Harmaline | 000304-21-2 |
| Harmaline AC | 999301-02-9 |
| Harmine | 000442-51-3 |
| Hexobarbital | 000056-29-1 |
| Hexobarbital TMS | 999469-02-2 |
| Hexylresorcinol | 000136-77-6 |
| Hexylresorcinol 3TMS | 999422-02-5 |
| Homatropine | 000087-00-3 |
| Homatropine TMS | 999282-02-9 |
| Hydrastine | 000118-08-1 |
| Hydrocodone | 000125-29-1 |
| Hydromorphone | 000466-99-9 |
| Hydromorphone enol 2TMS | 999513-02-9 |
| Hydromorphone TMS | 221209-08-1 |
| Hydroxychloroquine AC | 999512-02-6 |
| Hydroxyethylflurazepam TMS | 999204-02-3 |
| Hydroxyloxapine, 8- | 999053-02-0 |
| Hydroxyzine | 000068-88-2 |
| Hydroxyzine AC | 999113-02-9 |
| Ibuprofen | 015687-27-1 |
| Ibuprofen TMS | 999165-02-5 |
| Iminostilbene | 000256-96-2 |
| Imipramine | 000050-49-7 |
| Indomethacin TMS | 999318-02-4 |

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

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

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

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

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

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

| Compound name | CAS number |
|---|---|
| Phenylephrine 3AC | 999091-02-0 |
| Phenylethylamine, beta- | 000064-04-0 |
| Phenylethylamine, beta AC | 999343-02-1 |
| Phenylpropanolamine | 999498-02-1 |
| Phenylpropanolamine AC | 999092-02-3 |
| Phenyltoloxamine | 000092-12-6 |
| Phenytoin | 000057-41-0 |
| Phenytoin 2TMS | 063435-72-3 |
| Pilocarpine | 000092-13-7 |
| Pindolol | 013523-86-9 |
| Pindolol formyl artifact | 999458-02-5 |
| PMA TMS | 999172-02-0 |
| p-Methoxyamphetamine | 000064-13-1 |
| Prazepam | 002955-38-6 |
| Prilocaine | 000721-50-6 |
| Primidone | 000125-33-7 |
| Probenecid TMS | 999294-02-9 |
| Procainamide | 000051-06-9 |
| Procaine | 000059-46-1 |
| Prochlorperazine | 000058-38-8 |
| Procyclidine | 000077-37-2 |
| Procyclidine artifact (dehydro-) | 999460-02-5 |
| Procyclidine TMS | 999454-02-3 |
| Promazine | 000058-40-2 |
| Promethazine | 000060-87-7 |
| Propantheline bromide | 000050-34-0 |
| Propiomazine | 000362-29-8 |
| Propofol | 002078-54-8 |
| Propoxur | 000114-26-1 |
| Propoxur-M/artifact | 999393-02-1 |
| Propoxyphene | 000469-62-5 |
| Propylamphetamine | 051799-32-7 |
| Propylamphetamine AC | 999302-02-2 |
| Protriptyline | 000438-60-8 |
| Protriptyline AC | 999273-02-8 |
| Pseudoephedrine | 000090-82-4 |
| Pseudoephedrine 2AC | 999500-02-6 |
| Pseudoephedrine formyl artifact | 999483-02-2 |
| Psilocin 2TMS | 999192-02-8 |
| Psilocybin 3TMS | 999193-02-1 |
| Pyrazinamide | 000098-96-4 |
| Pyrilamine | 000091-84-9 |
| Pyrimethamine | 000058-14-0 |
| Quetiapine | 999097-02-8 |
| Quetiapine TMS | 999527-02-5 |
| Quinacrine | 000083-89-6 |
| Quinidine | 000056-54-2 |
| Quinine | 000130-95-0 |
| Ramelteon | 999274-02-1 |
| Reboxetine | 098769-81-4 |
| Ritodrine 3TMS | 999218-02-9 |
| Rofecoxib | 162011-90-7 |
| Ropivacaine | 132112-35-7 |
| Salbutamol 3TMS | 999394-02-4 |
| Salicylamide | 000065-45-2 |
| Salicylamide 2TMS | 055887-58-6 |
| Salicylic acid 2TMS | 003789-85-3 |
| Salicylic acid ethylester | 000118-61-6 |
| Salicylic acid methylester | 000119-36-8 |
| Scopolamine | 000051-34-3 |
| Scopolamine TMS | 999194-02-4 |
| Secobarbital | 000076-73-3 |
| Secobarbital 2TMS | 052937-71-0 |
| Selegiline | 014611-51-9 |
| Selegiline-M (HO-) AC | 999482-02-9 |
| Sertraline | 079617-96-2 |
| Sertraline AC | 999125-02-9 |
| Sertraline-M (nor-) AC | 999109-02-3 |
| Sildenafil TMS | 999213-02-4 |
| SKF-525a | 000302-33-0 |
| Strychnine | 000057-24-9 |
| Sufentanil | 056030-54-7 |
| Sulfadiazine | 000068-35-9 |
| Sulfadimethoxine | 000122-11-2 |
| Sulfamethazine | 000057-68-1 |
| Sulfamethazine AC | 999501-02-9 |
| Sulfamethoxazole | 000723-46-6 |
| Sulfanilamide | 000063-74-1 |
| Sulfapyridine | 000144-83-2 |
| Sulfathiazole | 000072-14-0 |
| Sulfinpyrazone | 000057-96-5 |
| Tacrine | 000321-64-2 |

| Compound name | CAS number |
|---|---|
| Talbutal | 000115-44-6 |
| Tamoxifen | 010540-29-1 |
| Temazepam | 000846-50-4 |
| Temazepam artifact-2 | 020927-53-1 |
| Temazepam TMS | 035147-95-6 |
| Terbinafine | 091161-71-6 |
| Terfenadine TMS | 999220-02-9 |
| Teriflunomide AC | 999502-02-2 |
| Tetracaine | 000094-24-6 |
| Tetrahydrocannabinol | 001972-08-3 |
| Tetrahydrocannabinol TMS | 999529-02-1 |
| Tetrahydrozoline | 000084-22-0 |
| Tetrahydrozoline AC | 999398-02-6 |
| Thebaine | 000115-37-7 |
| Theobromine | 000083-67-0 |
| Theophyline | 000058-55-9 |
| Thiamylal | 000077-27-0 |
| Thiethylperazine | 001420-55-9 |
| Thiopental | 000076-75-5 |
| Thioridazine | 000050-52-2 |
| Thonzylamine | 000091-85-0 |
| Ticlopidine | 055142-85-3 |
| Tiletamine | 014176-49-9 |
| Timolol TMS | 999399-02-9 |
| Tocainide | 041708-72-9 |
| Tocainide AC | 999375-02-9 |
| Tolazoline | 000059-98-3 |
| Topiramate artifact (-$SO_2NH$) | 020880-92-6 |
| Topiramate breakdown | 097240-79-4 |
| Tramadol | 027203-92-5 |
| Tramadol TMS | 999336-02-6 |
| Tranylcypromine | 000155-09-9 |
| Tranylcypromine AC | 999305-02-1 |
| Trazodone | 019794-93-5 |
| Triamterene | 000396-01-0 |
| Triazolam | 028911-01-5 |
| Trifluoperazine | 000117-89-5 |
| Triflupromazine | 000146-54-3 |
| Trihexyphenidyl | 000144-11-6 |
| Trimeprazine | 000084-96-8 |
| Trimethobenzamide | 000138-56-7 |
| Trimethoprim | 000738-70-5 |
| Trimipramine | 000739-71-9 |
| Tripelenamine | 000091-81-6 |
| Triprolidine | 000486-12-4 |
| Tropacocaine | 000537-26-8 |
| Tryptamine | 000061-54-1 |
| Tryptamine 2AC | 999352-02-2 |
| Tryptamine AC | 999353-02-5 |
| Tryptophan, D- AC | 999519-02-7 |
| Valproic acid | 000099-66-1 |
| Venlafaxine | 093413-69-5 |
| Venlafaxine TMS | 999173-02-3 |
| Verapamil | 000052-53-9 |
| Vigabatrin AC | 999376-02-2 |
| Warfarin | 000081-81-2 |
| Warfarin artifact | 000122-57-6 |
| Warfarin TMS | 036307-79-6 |
| Xanthinol TMS | 999239-02-0 |
| Xylazine | 007361-61-7 |
| Yohimbine | 000146-48-5 |
| Yohimibine TMS | 999457-02-2 |
| Zaleplon | 151319-34-5 |
| Zolazepam | 031352-82-6 |
| Zolpidem | 082626-48-0 |
| Zomepirac -$CO_2$ | 999355-02-1 |
| Zonisamide | 068291-97-4 |
| Zonisamide AC | 999354-02-8 |
| Zopiclone | 043200-80-2 |
| Zotepine | 026615-21-4 |

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