Application Note

Forensics

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A Forensic Triple Quadrupole GC/MS MRM Database for Forensic and Toxicological Workflows

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Abstract

Systematic toxicological analysis is crucial in forensic laboratories, requiring robust and reliable analytical methods. Gas chromatography coupled to triple quadrupole mass spectrometry (GC/TQ) is a versatile and widely used technique that provides uniform results across instruments and laboratories. The aim of this study was to establish a database of multiple reaction monitoring (MRM) transitions for toxicologically relevant compounds amenable to GC/MS. The resulting curated database includes 176 entries, including 154 unique compounds with up to 12 transitions per compound. The database allows for instantly building methods for targeted screening and confident quantitation of GC-amenable, forensic, and toxicologically relevant compounds.

The database is available for download as a CSV file in Appendix 1 of this application note.

Introduction

Systematic toxicological analysis in forensic investigation demands continuous adaptability to an ever-evolving toxicant landscape. The three main challenges are low concentrations of the toxicants, an ever-growing number of analytes to be monitored and quantitated, and the limitations in obtaining analytical standards for every chemical. These variables complicate method development. Historically, forensic laboratories have relied primarily on single quadrupole GC/MS to identify and quantitate unknowns.[1] In recent years, the compounds amenable to liquid chromatography (LC) have been analyzed with LC/MS with an emphasis on an LC/TQ workflow.[2] To maximize analytical performance, the Agilent Forensic Toxicology tMRM Database for triple quadrupole LC/MS[3] has been established, streamlining the otherwise time-consuming and costly process of manually developing the method.

For volatile and semivolatile GC-amenable compounds, GC/MS in full scan acquisition mode remains the method of choice when analyzing forensic drugs and toxicants.[4,5] A GC/MS forensic toxicological workflow also greatly benefits from the selectivity and sensitivity of an MRM approach enabled with GC/TQ. Therefore, the aim of this work was to develop an MRM database to help toxicological researchers build screening and quantitation methods, simplifying method development.

The database of MRM transitions for relevant toxicants was established and successfully applied to create GC/TQ methods for analyzing real-world authentic samples with greater sensitivity and confidence than the conventional GC/MS approach.

Experimental

GC/TQ analysis

Agilent 7000 Series triple quadrupole GC/MS (GC/TQ) was used for developing the MRM transitions for 176 entries, including 154 unique compounds, which were analyzed underivatized, as well as their trimethylsilylated and acetylated derivatives. Agilent MassHunter Optimizer software for GC/TQ (available with MassHunter data acquisition software, version 10.0 and above) was used for developing 1,803 MRM transitions.

Chromatographic separation was achieved using an Agilent J&W DB-5ms capillary column, 30 m × 0.25 mm, 0.25 µm (part number 122-5532) with a method retention time locked to cocaine at 12.26 minutes. Identification of toxicants in an authentic postmortem sample was compared between full scan and MRM acquisition. The instrument operating parameters are listed in Table 1.

Table 1. GC and MS and conditions for forensic toxicological analysis.

Parameter	Value
Inlet	Multimode MMI inlet
Mode	Pulsed splitless
Injection Pulse Pressure	25 psi until 1.5 min
Purge Flow to Split Vent	50 mL/min at 1.5 min
Injection Volume	2 µL
Inlet Temperature	275 °C
Inlet Liner	Agilent Ultra Inert, splitless, double taper (part number 5190-4007)
Column	Agilent J&W DB-5ms, 30 m × 0.25 mm, 0.25 µm (part number 122-5532)
Column Temperature Program	80 °C (1 min hold) 20 °C/min to 290 °C (8 min hold) Run time 19.5 min
Carrier Gas and Flow Rate	Helium, 1.027 mL/min constant flow Retention time locked to cocaine at 12.26 min
Transfer Line Temperature	300 °C
Triple Quadrupole Mass Spectrometer	Agilent 7000 Series GC/TQ with extractor EI source
Electron Energy	70 eV
Quench Gas Helium	2.25 mL/min
Collision Gas Nitrogen	1.5 mL/min
Ion Source Temperature	230 °C
Quadrupole Temperature	150 °C
EM Voltage Gain Mode	15
Mode	dMRM When developing MRM transitions: scan (*m/z* 100 to 450), product ion scan, MRM
Tune	atunes.eiex.tune.xml

Database curation

MassHunter Optimizer software offers several workflows that can be used when developing and optimizing MRM transitions that include[6,7]:

- Start from scan data
- Start from SIM ions
- Start from MRMs

When developing the database, the "Start from scan data" workflow was used. This workflow covers the entire development process. The starting GC acquisition method was optimized for successful GC analysis of toxicants. In the "Start from scan data" workflow, the MS was operated in full scan mode to acquire the scan data file for compound identification and precursor ion selection, performing the scan over a range of *m/z* 100 to 450 with a scan time of 100 ms.

The "Start from scan data" workflow includes the following steps, performed sequentially:

1. Acquisition or import of full scan data to identify target compounds
2. Precursor ion identification
3. Product ion identification
4. Collision energy optimization

First, Agilent MassHunter Unknowns Analysis software was used for identifying the target compounds through searching against the Mass Spectral Library of Drugs, Poisons, Pesticides, Pollutants, and Their Metabolites.[8] The deconvoluted spectra of the identified compounds were exported to the MassHunter Library Editor to create a spectral library comprising the 176 target entries.

Next, MRM development was carried out in MassHunter Optimizer for GC/TQ. The first step was identification of the analytes using a library search of deconvoluted spectra against the spectral library created using MassHunter Library Editor as described previously. This allowed for correct identification of target analytes and enabled reliable selection of precursor ions, even in the presence of chromatographic interferences such as column bleed, coeluting analytes, or matrix interference.

The next three steps of MRM development, including precursor ion identification, product ion identification, and collision energy optimization, were carried out in MassHunter Optimizer. These steps can be highly automated with no user intervention. Alternatively, the result of each step can be reviewed before proceeding to the next step, as was done in this work.

After MRM development and collision energy optimization were completed, the resulting 1,803 MRM transitions were exported as a CSV file.

How to use the database

The database created in this work can be used to simplify creation of dMRM data acquisition methods with Agilent GC/TQ. The MassHunter Optimizer for GC/TQ can be used to simplify the method creation process as described later. MassHunter Optimizer is installed automatically with MassHunter GC/MS data acquisition, version 10.0 and above. The database needs to be downloaded as a CSV file and saved on the computer.

The following simple steps describe how to create a data acquisition method using the database:

1. In MassHunter data acquisition software, create and save a GC/MS data acquisition method with the conditions provided in Table 1, and retention time lock it to cocaine at 12.26 minutes. If a cocaine standard is not available, the method can be retention time locked to any other compound included in the database at the respective retention time.
2. In MassHunter Optimizer, under **Setup**, specify the Acquisition method created in step 1, with the GC parameters that will be retained (Figure 1).
3. Under **Setup**, click **CSVFile** in the Import Compound Info section and specify the database (Figure 1).

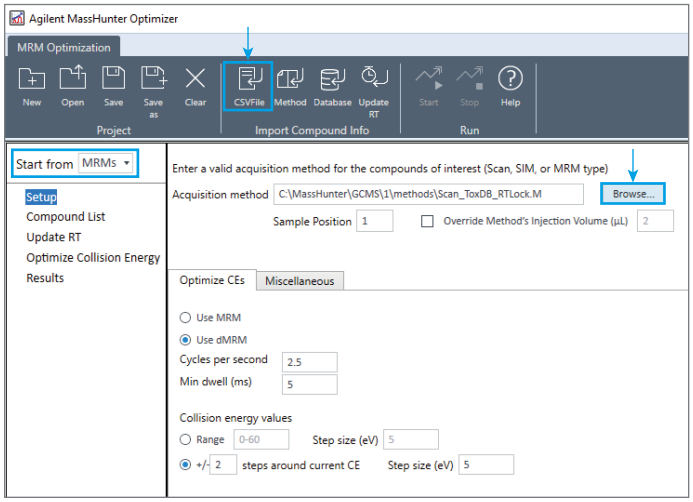
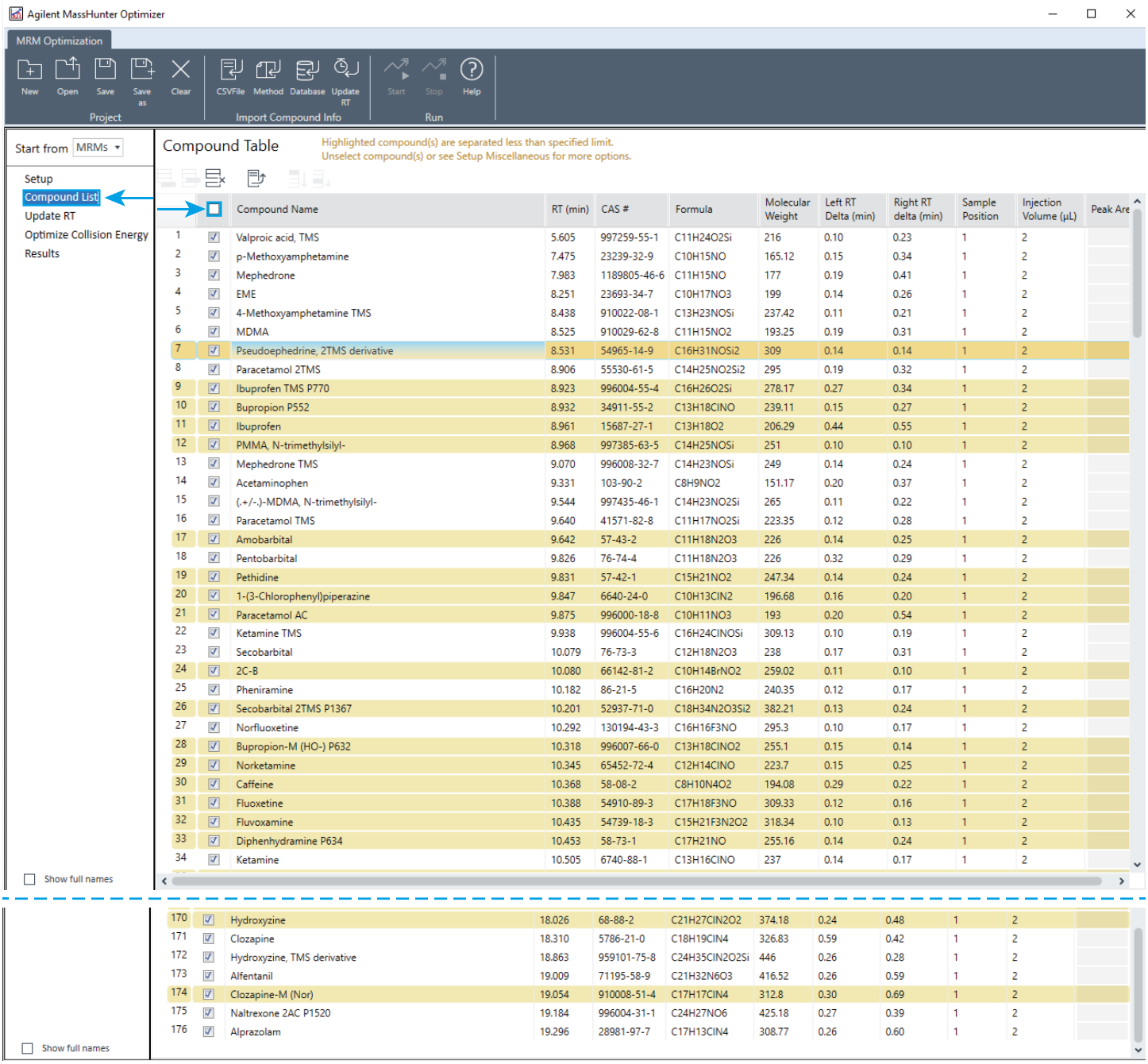


Figure 1. Agilent MassHunter Optimizer for GC/TQ Setup window.

4. Once the compound information import is completed, all 176 entries will appear under the Compound List tab, as shown in Figure 2. By default, all of the compounds are checked.



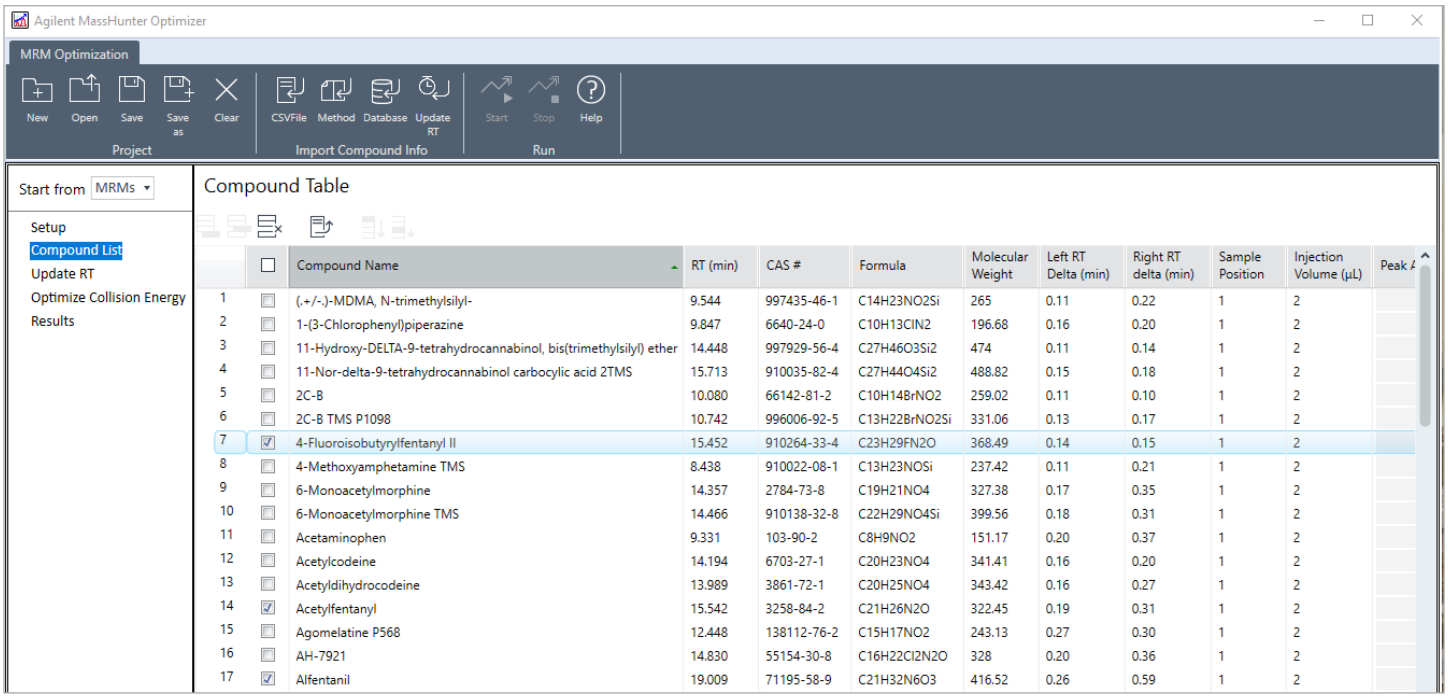
		Compound Name	RT (min)	CAS #	Formula	Molecular Weight	Left RT Delta (min)	Right RT delta (min)	Sample Position	Injection Volume (µL)	Peak Are
1	☑	Valproic acid, TMS	5.605	997259-55-1	C11H24O2Si	216	0.10	0.23	1	2	
2	☑	p-Methoxyamphetamine	7.475	23239-32-9	C10H15NO	165.12	0.15	0.34	1	2	
3	☑	Mephedrone	7.983	1189805-46-6	C11H15NO	177	0.19	0.41	1	2	
4	☑	EME	8.251	23693-34-7	C10H17NO3	199	0.14	0.26	1	2	
5	☑	4-Methoxyamphetamine TMS	8.438	910022-08-1	C13H23NOSi	237.42	0.11	0.21	1	2	
6	☑	MDMA	8.525	910029-62-8	C11H15NO2	193.25	0.19	0.31	1	2	
7	☑	Pseudoephedrine, 2TMS derivative	8.531	54965-14-9	C16H31NOSi2	309	0.14	0.14	1	2	
8	☑	Paracetamol 2TMS	8.906	55530-61-5	C14H25NO2Si2	295	0.19	0.32	1	2	
9	☑	Ibuprofen TMS P770	8.923	996004-55-4	C16H26O2Si	278.17	0.27	0.34	1	2	
10	☑	Bupropion P552	8.932	34911-55-2	C13H18ClNO	239.11	0.15	0.27	1	2	
11	☑	Ibuprofen	8.961	15687-27-1	C13H18O2	206.29	0.44	0.55	1	2	
12	☑	PMMA, N-trimethylsilyl-	8.968	997385-63-5	C14H25NOSi	251	0.10	0.10	1	2	
13	☑	Mephedrone TMS	9.070	996008-32-7	C14H23NOSi	249	0.14	0.24	1	2	
14	☑	Acetaminophen	9.331	103-90-2	C8H9NO2	151.17	0.20	0.37	1	2	
15	☑	(+/-)-MDMA, N-trimethylsilyl-	9.544	997435-46-1	C14H23NO2Si	265	0.11	0.22	1	2	
16	☑	Paracetamol TMS	9.640	41571-82-8	C11H17NO2Si	223.35	0.12	0.28	1	2	
17	☑	Amobarbital	9.642	57-43-2	C11H18N2O3	226	0.14	0.25	1	2	
18	☑	Pentobarbital	9.826	76-74-4	C11H18N2O3	226	0.32	0.29	1	2	
19	☑	Pethidine	9.831	57-42-1	C15H21NO2	247.34	0.14	0.24	1	2	
20	☑	1-(3-Chlorophenyl)piperazine	9.847	6640-24-0	C10H13ClN2	196.68	0.16	0.20	1	2	
21	☑	Paracetamol AC	9.875	996000-18-8	C10H11NO3	193	0.20	0.54	1	2	
22	☑	Ketamine TMS	9.938	996004-55-6	C16H24ClNOSi	309.13	0.10	0.19	1	2	
23	☑	Secobarbital	10.079	76-73-3	C12H18N2O3	238	0.17	0.31	1	2	
24	☑	2C-B	10.080	66142-81-2	C10H14BrNO2	259.02	0.11	0.10	1	2	
25	☑	Pheniramine	10.182	86-21-5	C16H20N2	240.35	0.12	0.17	1	2	
26	☑	Secobarbital 2TMS P1367	10.201	52937-71-0	C18H34N2O3Si2	382.21	0.13	0.24	1	2	
27	☑	Norfluoxetine	10.292	130194-43-3	C16H16F3NO	295.3	0.10	0.17	1	2	
28	☑	Bupropion-M (HO-) P632	10.318	996007-66-0	C13H18ClNO2	255.1	0.15	0.14	1	2	
29	☑	Norketamine	10.345	65452-72-4	C12H14ClNO	223.7	0.15	0.25	1	2	
30	☑	Caffeine	10.368	58-08-2	C8H10N4O2	194.08	0.29	0.22	1	2	
31	☑	Fluoxetine	10.388	54910-89-3	C17H18F3NO	309.33	0.12	0.16	1	2	
32	☑	Fluvoxamine	10.435	54739-18-3	C15H21F3N2O2	318.34	0.10	0.13	1	2	
33	☑	Diphenhydramine P634	10.453	58-73-1	C17H21NO	255.16	0.14	0.24	1	2	
34	☑	Ketamine	10.505	6740-88-1	C13H16ClNO	237	0.14	0.17	1	2	
170	☑	Hydroxyzine	18.026	68-88-2	C21H27ClN2O2	374.18	0.24	0.48	1	2	
171	☑	Clozapine	18.310	5786-21-0	C18H19ClN4	326.83	0.59	0.42	1	2	
172	☑	Hydroxyzine, TMS derivative	18.863	959101-75-8	C24H35ClN2O2Si	446	0.26	0.28	1	2	
173	☑	Alfentanil	19.009	71195-58-9	C21H32N6O3	416.52	0.26	0.59	1	2	
174	☑	Clozapine-M (Nor)	19.054	910008-51-4	C17H17ClN4	312.8	0.30	0.69	1	2	
175	☑	Naltrexone 2AC P1520	19.184	996004-31-1	C24H27NO6	425.18	0.27	0.39	1	2	
176	☑	Alprazolam	19.296	28981-97-7	C17H13ClN4	308.77	0.26	0.60	1	2	

Figure 2. Agilent MassHunter Optimizer for GC/TQ Compound Table window displaying compounds imported from the database.

5. Next, only the compounds that are to be included in the acquisition method need to remain checked in the Compound Table. The quickest way to leave only the target compounds checked is to deselect all compounds by double-clicking the check box at the top of the Compound Table (shown with the blue arrow in Figure 2), and to select, one-by-one, the compounds that need to be included in the acquisition method. The Compound Table can be sorted in alphabetical order by clicking the **Compound Name** table header.

   Figure 3 shows an example of the Compound Table, in which the targets are sorted in alphabetical order and only the compounds from the fentanyls group are selected.

6. If the retention times need to be updated because a different GC column configuration or oven program is used, or the starting GC method was not retention time locked, click **Update RT**. MassHunter Optimizer will prompt the user to perform analysis of the sample containing the target compounds, and will automatically update the retention times.

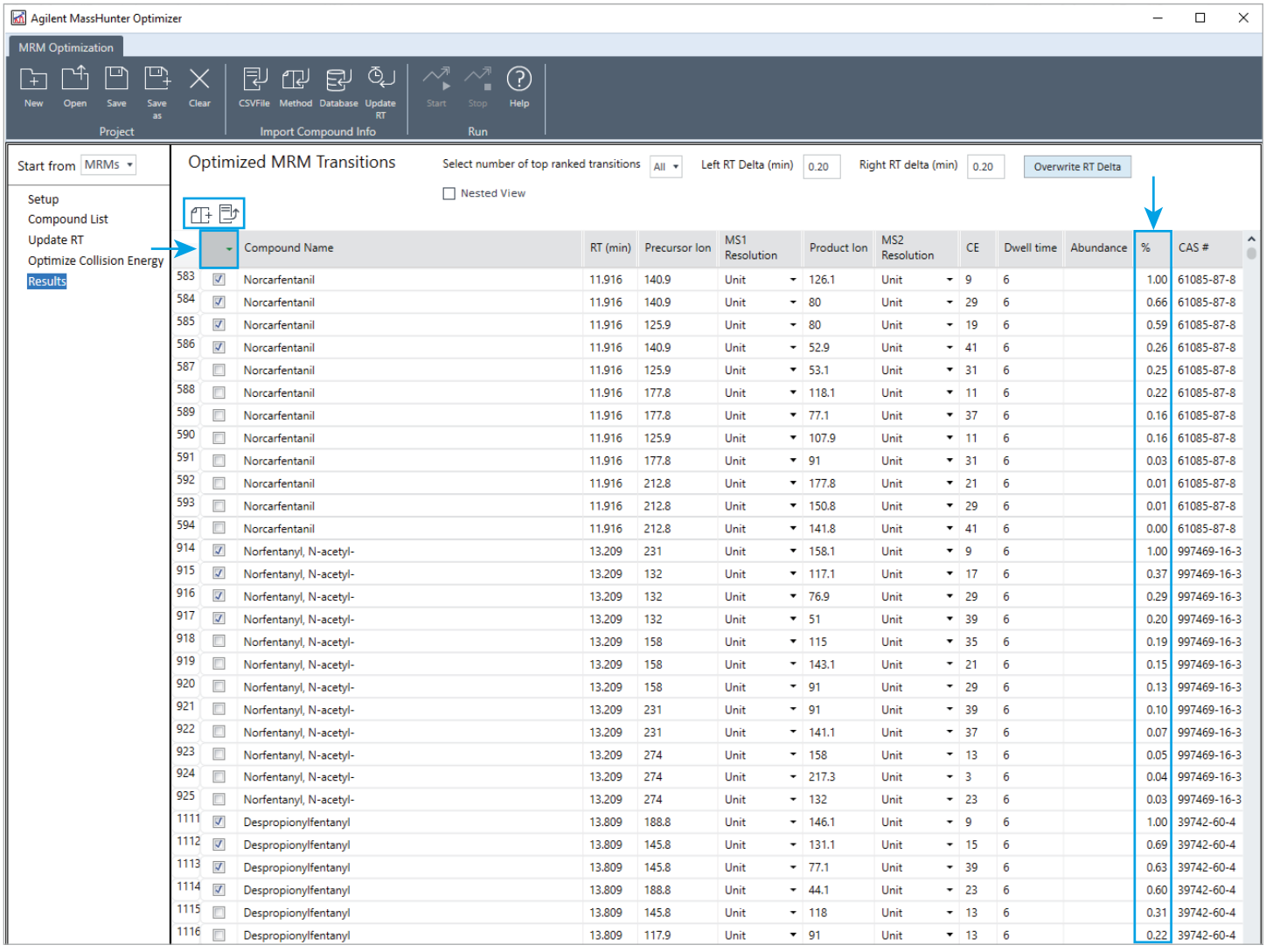


		Compound Name	RT (min)	CAS #	Formula	Molecular Weight	Left RT Delta (min)	Right RT delta (min)	Sample Position	Injection Volume (µL)
1	☐	(.+/-.)-MDMA, N-trimethylsilyl-	9.544	997435-46-1	C14H23NO2Si	265	0.11	0.22	1	2
2	☐	1-(3-Chlorophenyl)piperazine	9.847	6640-24-0	C10H13ClN2	196.68	0.16	0.20	1	2
3	☐	11-Hydroxy-DELTA-9-tetrahydrocannabinol, bis(trimethylsilyl) ether	14.448	997929-56-4	C27H46O3Si2	474	0.11	0.14	1	2
4	☐	11-Nor-delta-9-tetrahydrocannabinol carbocylic acid 2TMS	15.713	910035-82-4	C27H44O4Si2	488.82	0.15	0.18	1	2
5	☐	2C-B	10.080	66142-81-2	C10H14BrNO2	259.02	0.11	0.10	1	2
6	☐	2C-B TMS P1098	10.742	996006-92-5	C13H22BrNO2Si	331.06	0.13	0.17	1	2
7	☑	4-Fluoroisobutyrylfentanyl II	15.452	910264-33-4	C23H29FN2O	368.49	0.14	0.15	1	2
8	☐	4-Methoxyamphetamine TMS	8.438	910022-08-1	C13H23NOSi	237.42	0.11	0.21	1	2
9	☐	6-Monoacetylmorphine	14.357	2784-73-8	C19H21NO4	327.38	0.17	0.35	1	2
10	☐	6-Monoacetylmorphine TMS	14.466	910138-32-8	C22H29NO4Si	399.56	0.18	0.31	1	2
11	☐	Acetaminophen	9.331	103-90-2	C8H9NO2	151.17	0.20	0.37	1	2
12	☐	Acetylcodeine	14.194	6703-27-1	C20H23NO4	341.41	0.16	0.20	1	2
13	☐	Acetyldihydrocodeine	13.989	3861-72-1	C20H25NO4	343.42	0.16	0.27	1	2
14	☑	Acetylfentanyl	15.542	3258-84-2	C21H26N2O	322.45	0.19	0.31	1	2
15	☐	Agomelatine P568	12.448	138112-76-2	C15H17NO2	243.13	0.27	0.30	1	2
16	☐	AH-7921	14.830	55154-30-8	C16H22Cl2N2O	328	0.20	0.36	1	2
17	☑	Alfentanil	19.009	71195-58-9	C21H32N6O3	416.52	0.26	0.59	1	2

Figure 3. Compound Table with the targets from the fentanyls group selected.

7. Next, the final list of MRM transitions that will be included in the method can be reviewed under the Results tab. By default, all the MRM transitions available for the compounds will be selected. Note that there are up to 12 MRM transitions for some targets in the database; hence, the user may prefer to deselect some of the transitions for the selected targets to limit the number of MRMs per compound in the final method. The quickest way to review the MRM transitions for the selected compounds is to sort the table so that the selected compounds will be at the top. Double-click the gray square at the top of the Results table (shown with the blue arrow in Figure 4), which will sort the list so that the selected compounds are at the top. Then, some of the MRM transitions can be deselected if desired. In the example shown in Figure 4, the four most abundant MRM transitions per each of the selected compounds remain deselected. The % column shows the relative abundance for each of the MRMs compared to the MRM with the highest response.

   Finally, in the Results window shown in Figure 4, the left and right dMRM windows can be specified. The default value of 0.2 minutes is a good starting point.



		Compound Name	RT (min)	Precursor Ion	MS1 Resolution	Product Ion	MS2 Resolution	CE	Dwell time	Abundance	%	CAS #
583	☑	Norcarfentanil	11.916	140.9	Unit	126.1	Unit	9	6		1.00	61085-87-8
584	☑	Norcarfentanil	11.916	140.9	Unit	80	Unit	29	6		0.66	61085-87-8
585	☑	Norcarfentanil	11.916	125.9	Unit	80	Unit	19	6		0.59	61085-87-8
586	☑	Norcarfentanil	11.916	140.9	Unit	52.9	Unit	41	6		0.26	61085-87-8
587	☐	Norcarfentanil	11.916	125.9	Unit	53.1	Unit	31	6		0.25	61085-87-8
588	☐	Norcarfentanil	11.916	177.8	Unit	118.1	Unit	11	6		0.22	61085-87-8
589	☐	Norcarfentanil	11.916	177.8	Unit	77.1	Unit	37	6		0.16	61085-87-8
590	☐	Norcarfentanil	11.916	125.9	Unit	107.9	Unit	11	6		0.16	61085-87-8
591	☐	Norcarfentanil	11.916	177.8	Unit	91	Unit	31	6		0.03	61085-87-8
592	☐	Norcarfentanil	11.916	212.8	Unit	177.8	Unit	21	6		0.01	61085-87-8
593	☐	Norcarfentanil	11.916	212.8	Unit	150.8	Unit	29	6		0.01	61085-87-8
594	☐	Norcarfentanil	11.916	212.8	Unit	141.8	Unit	41	6		0.00	61085-87-8
914	☑	Norfentanyl, N-acetyl-	13.209	231	Unit	158.1	Unit	9	6		1.00	997469-16-3
915	☑	Norfentanyl, N-acetyl-	13.209	132	Unit	117.1	Unit	17	6		0.37	997469-16-3
916	☑	Norfentanyl, N-acetyl-	13.209	132	Unit	76.9	Unit	29	6		0.29	997469-16-3
917	☑	Norfentanyl, N-acetyl-	13.209	132	Unit	51	Unit	39	6		0.20	997469-16-3
918	☐	Norfentanyl, N-acetyl-	13.209	158	Unit	115	Unit	35	6		0.19	997469-16-3
919	☐	Norfentanyl, N-acetyl-	13.209	158	Unit	143.1	Unit	21	6		0.15	997469-16-3
920	☐	Norfentanyl, N-acetyl-	13.209	158	Unit	91	Unit	29	6		0.13	997469-16-3
921	☐	Norfentanyl, N-acetyl-	13.209	231	Unit	91	Unit	39	6		0.10	997469-16-3
922	☐	Norfentanyl, N-acetyl-	13.209	231	Unit	141.1	Unit	37	6		0.07	997469-16-3
923	☐	Norfentanyl, N-acetyl-	13.209	274	Unit	158	Unit	13	6		0.05	997469-16-3
924	☐	Norfentanyl, N-acetyl-	13.209	274	Unit	217.3	Unit	3	6		0.04	997469-16-3
925	☐	Norfentanyl, N-acetyl-	13.209	274	Unit	132	Unit	23	6		0.03	997469-16-3
1111	☑	Despropionylfentanyl	13.809	188.8	Unit	146.1	Unit	9	6		1.00	39742-60-4
1112	☑	Despropionylfentanyl	13.809	145.8	Unit	131.1	Unit	15	6		0.69	39742-60-4
1113	☑	Despropionylfentanyl	13.809	145.8	Unit	77.1	Unit	39	6		0.63	39742-60-4
1114	☑	Despropionylfentanyl	13.809	188.8	Unit	44.1	Unit	23	6		0.60	39742-60-4
1115	☐	Despropionylfentanyl	13.809	145.8	Unit	118	Unit	13	6		0.31	39742-60-4
1116	☐	Despropionylfentanyl	13.809	117.9	Unit	91	Unit	13	6		0.22	39742-60-4

Figure 4. The Results table showing the MRM transitions. The selected transitions will be included in the final data acquisition method.

8. Click the **Create a method** icon at the top of the Results table to prompt a pop-up window (shown in Figure 5) to save the data acquisition method.

   The developed MRM acquisition method can be saved as either a time-segment MRM method or a dMRM method. The minimum dwell time and the number of cycles per second can be defined when saving the method.

   Alternatively, the developed transitions can be exported as a CSV file and imported into an existing GC/MS data acquisition method in MassHunter data acquisition software.

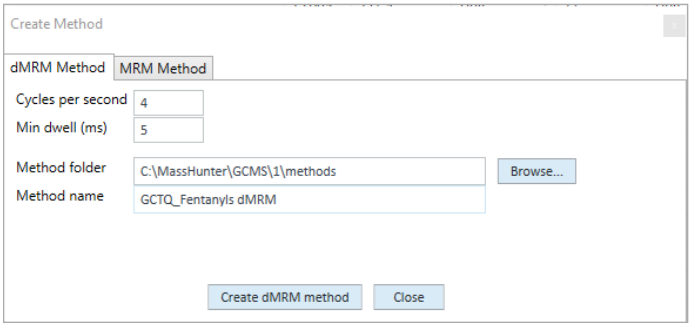


Figure 5. Creating a method with Agilent MassHunter Optimizer for GC/TQ.

9. Once the method is saved, it can be opened in MassHunter data acquisition software for review. The MS component of the method created for 15 fentanyls using the database with four transitions selected per compound is shown in Figure 6. The acquisition method is ready for use.

Note that if using an Agilent 7000 GC/TQ model E and above, or a 7010 GC/TQ model C and above, full scan data can be collected simultaneously in a dMRM method. To enable this mode, select **Enable** next to Full Scan Parameters (Figure 6). This data acquisition mode will allow the collection of full scan data in addition to the MRM transitions, enabling retrospective analysis, additional compound confirmation by the MS spectrum, and providing understanding of the matrix components and in-source loading.

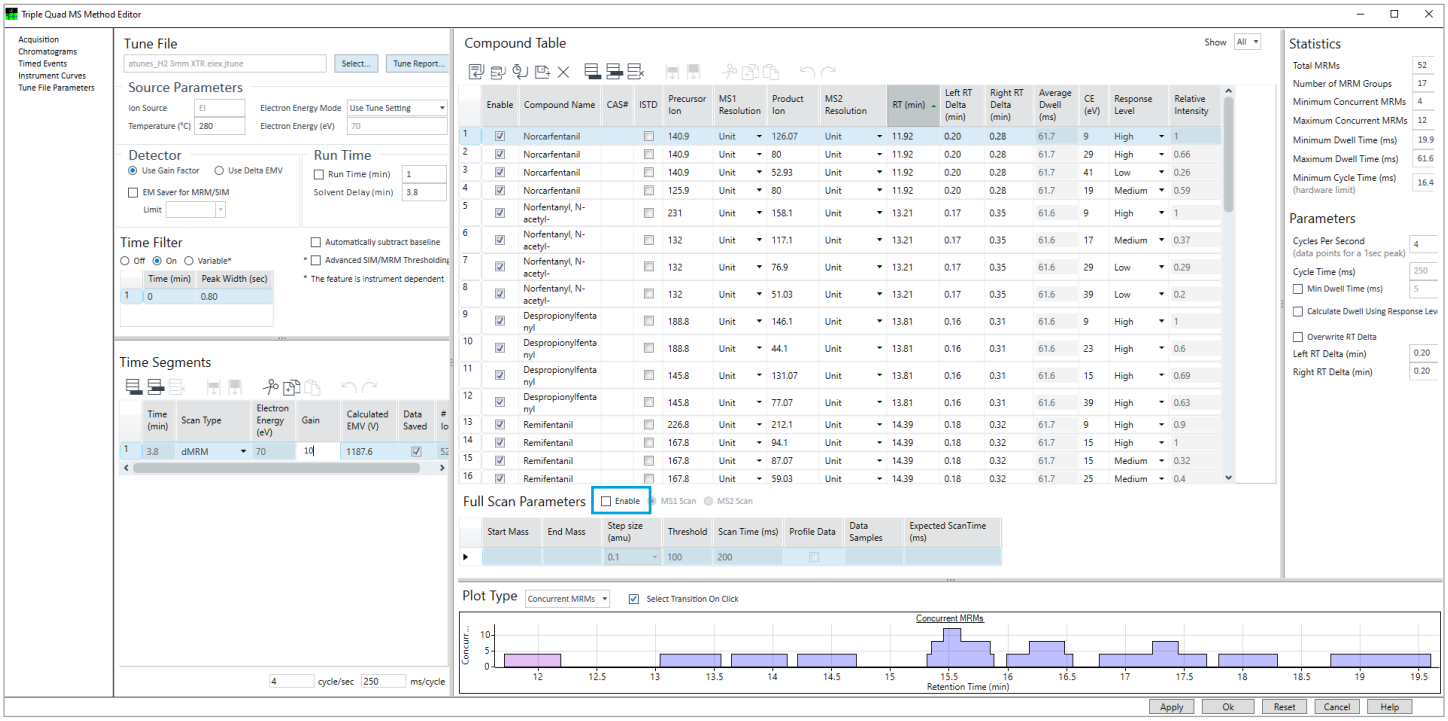


Figure 6. Triple Quad MS Method Editor window of Agilent MassHunter GC/MS data acquisition software, demonstrating the dMRM table of the method created from the database.

Results and discussion

Forensic GC/TQ database

The database is available for download as a CSV file in Appendix 1 of this application note.

The database created in this work includes 176 entries in total that include 154 unique compounds, 124 of which are underivatized entries, 32 are trimethylsilylated, and 20 are acetylated (Figure 7). The compounds include benzodiazepines, antidepressants, opioids, and drugs of abuse. The complete list of the database entries is shown in Appendix 2.

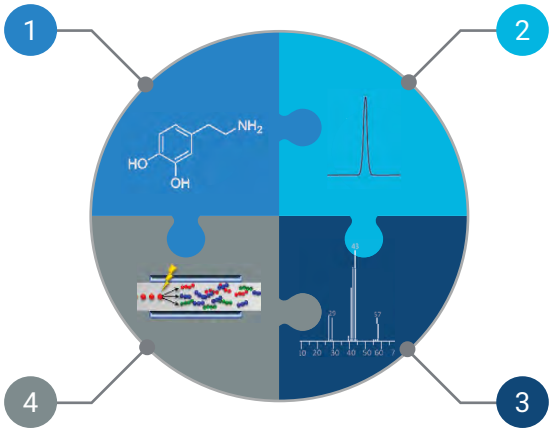
Application of the database to real-world samples

The proof of concept using the developed database involved the analysis of archived postmortem blood samples. A comparison was made between full scan data acquisition mode and MRM, with a focus on the identification of compounds. The MRM method was created from the database as described in the "Experimental" section.

All compounds were found with the MRM approach, while some of the toxicants present in the sample at a low concentration were missed with the full scan approach. For example, fentanyl was detected in the sample with the MRM approach and quantitated at 1.7 ng/mL, while it was not detected in full scan data acquisition mode (Figure 8).

176 entries in total
- 154 unique compounds:
  - 124 underivatized entries
  - 32 trimethylsilylated entries
  - 20 acetylated entries

1,803 MRM transitions
- 3 to 12 transitions per compound
- Optimized collision energies



Retention times for all entries
- Retention time locked to cocaine
- Allows a new column or instrument to have retention times that match the retention times provided in the database

Relative ion abundances
- For additional confirmation and optimal dwell time distribution

Figure 7. Overview of the entries and information included in the forensic database.

Example: fentanyl

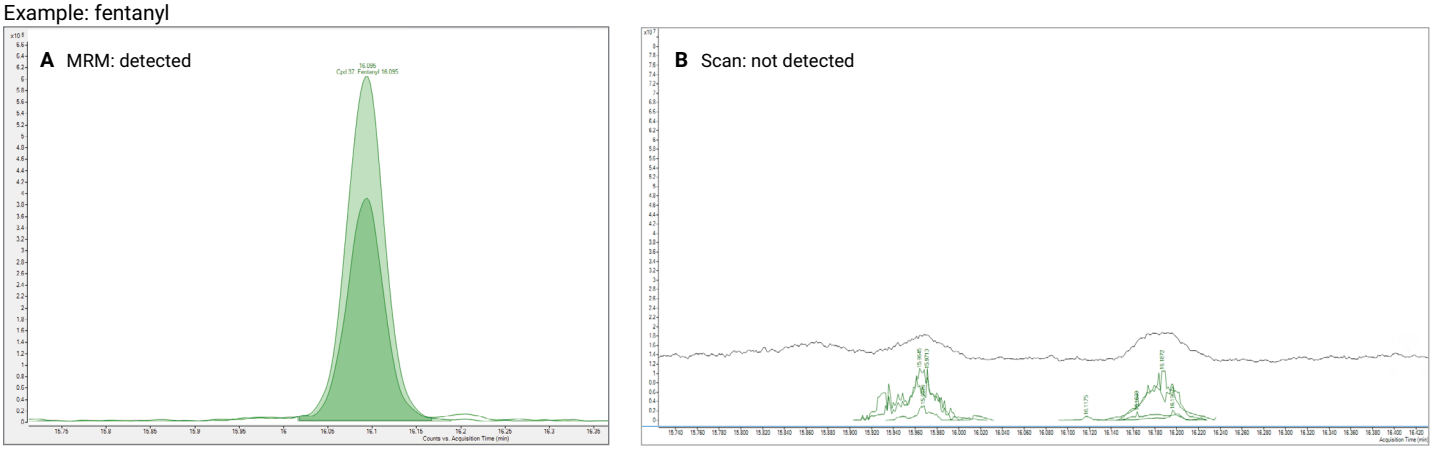


Figure 8. Fentanyl in the archived postmortem blood sample, which was detected in the MRM GC/TQ data acquisition mode (A), but was not detected with the spectral deconvolution approach in the full scan data (B).

Conclusion

The forensic toxicology database, with a curated set of 1,803 MRM transitions for 176 toxicologically relevant compounds, was successfully developed. The compounds included benzodiazepines, antidepressants, opioids, and drugs of abuse. The application of this MRM method to an authentic real-world sample showcased its ability to detect and quantitate toxicants at trace levels due to the high sensitivity and selectivity of the MS/MS approach. This approach addresses limitations when relying solely on full scan data acquisition mode.

The developed MRM database can be used for simplified data acquisition method creation, providing a valuable resource for the development of screening and quantitation methods in forensic labs. The developed MRM curation workflow showed promise for continuous expansion, offering a uniform and practical approach for adding new chemicals to the database.

Appendix 1

The database, in CSV file format, can be downloaded here.

The simple steps describing how to create a data acquisition method using the database are provided in the "How to use the database" section of this application note.

Appendix 2

A complete list of the targets included in the forensic database. The nomenclature follows the MPW database.[8]

Table A1. List of the targets included in the forensic database.

Compound Name	CAS Number	RT
Valproic Acid TMS	997259-55-1	5.605
p-Methoxyamphetamine	23239-32-9	7.475
Mephedrone	1189805-46-6	7.983
EME	23693-34-7	8.251
4-Methoxyamphetamine TMS	910022-08-1	8.438
MDMA	910029-62-8	8.525
Pseudoephedrine, 2TMS Derivative	54965-14-9	8.531
Paracetamol 2TMS	55530-61-5	8.906
Ibuprofen TMS P770	996004-55-4	8.923
Bupropion P552	34911-55-2	8.932
Ibuprofen	15687-27-1	8.961
PMMA, N-trimethylsilyl-	997385-63-5	8.968
Mephedrone TMS	996008-32-7	9.070
Acetaminophen	103-90-2	9.331
(+/−)-MDMA, N-Trimethylsilyl-	997435-46-1	9.544
Paracetamol TMS	41571-82-8	9.640
Amobarbital	57-43-2	9.642
Pentobarbital	76-74-4	9.826
Pethidine	57-42-1	9.831
1-(3-Chlorophenyl)piperazine	6640-24-0	9.847
Paracetamol AC	996000-18-8	9.875
Ketamine TMS	996004-55-6	9.938
Secobarbital	76-73-3	10.079
2C-B	66142-81-2	10.080
Pheniramine	86-21-5	10.182
Secobarbital 2TMS P1367	52937-71-0	10.201
Norfluoxetine	130194-43-3	10.292
Bupropion-M (HO-) P632	996007-66-0	10.318
Norketamine	65452-72-4	10.345
Caffeine	58-08-2	10.368
Fluoxetine	54910-89-3	10.388
Fluvoxamine	54739-18-3	10.435
Diphenhydramine P634	58-73-1	10.453
Ketamine	6740-88-1	10.505
Thiopental P565	76-75-5	10.508
Brallobarbital P812	561-86-4	10.553
2C-B TMS P1098	996006-92-5	10.742
N-Acetyl-3,4-methylenedioxymethamphetamine	181765-92-4	10.864
Phenobarbitone 2TMS	910187-11-0	10.944
Tramadol	27203-92-5	10.977
Cyclobarbital 2TMS P1358	996005-49-6	11.020
MDEA AC P597	996003-27-1	11.066
Phenobarbital	50-06-6	11.094
Cyclobarbital	52-31-3	11.136
Ketamine-M (nor-) AC P685	996007-82-6	11.180
Levamisole	14769-73-4	11.185
Tramadol-M (HO-) -H2O P666	996006-75-6	11.201
Chlorpheniramine	132-22-9	11.236
Metoprolol	37350-58-6	11.320
Metoprolol TMS	910252-91-4	11.330
O-Desmethyl-tramadol	80456-81-1	11.364
Methadone-M (EDDP) P764	996000-24-2	11.370
Naproxen TMS	74793-83-2	11.438
Naproxen	22204-53-1	11.564
Heroin	561-27-3	11.600
Venlafaxine	93413-69-5	11.625
Fluconazole P943	86386-73-4	11.802
Propanolol, TMS Derivative	959081-18-6	11.864
Methadone	76-99-3	11.879
Norcarfentanil	61085-87-8	11.916
Propranolol	525-66-6	11.999
Dextromethorphan	125-71-3	12.025
Norcocaine	18717-72-1	12.093
Venlafaxine-M (O-Desmethyl)	910048-23-6	12.111
Cannabidiol 2TMS	910233-55-5	12.148

Compound Name	CAS Number	RT
Ketamine AC	910019-83-9	12.178
Amitriptyline	50-48-6	12.241
Cocaine	478-73-9	12.262
Trimipramine	739-71-9	12.327
Imipramine	50-49-7	12.399
Fluconazole, Trimethylsilyl Ether	166173-18-8	12.434
Agomelatine P568	138112-76-2	12.448
Diclofenac TMS	910107-54-9	12.524
Cocaethylene @P1013	996000-46-6	12.537
Benzoylecgonine, O-TMS Derivative	864281-94-7	12.537
Nordoxepin	1225-56-5	12.549
Moclobemide	71320-77-9	12.615
Mirtazapine	61337-67-5	12.627
Diclofenac	15307-86-5	12.634
Desomorphine	427-00-9	12.636
Norcocaine TMS	910160-82-6	12.646
Pentazocine	359-83-1	12.657
Melitracen	5118-29-6	12.682
Bisoprolol TMS	910251-41-1	12.725
Promethazine	60-87-7	12.731
Mianserin-M (nor-) P606	996002-24-5	12.769
Delta-9-tetrahydrocannabinol, TMS Derivative	55449-68-8	12.879
Pentazocine AC	910038-20-9	12.916
Maprotiline-M (Nor)	910068-96-1	13.021
Oxazepam	604-75-1	13.037
Reboxetine	98769-81-4	13.044
Prothipendyl	303-69-5	13.148
Maprotiline	10262-69-8	13.168
Norfentanyl, N-acetyl-	997469-16-3	13.209
Desomorphine AC	910171-95-8	13.216
Cannabidiol	13956-29-1	13.247
Sertraline P935	79617-96-2	13.268
Dosulepin	113-53-1	13.402
Cannabidiol 2AC P1439	996000-64-9	13.419
Cannabinol TMS P1367	996004-53-2	13.437
Citalopram	59729-33-8	13.439
Codeine	76-57-3	13.484
Dihydrocodeine	125-28-0	13.505
Lorazepam	846-49-1	13.527
Clomipramine P995	303-49-1	13.528
U-47700	82657-23-6	13.543
Tetrazepam	10379-14-3	13.630
Codeine, TMS Derivative	74367-14-9	13.642
Ethylmorphine	76-58-4	13.697
Citalopram-M (Nor)	910126-73-7	13.698

Compound Name	CAS Number	RT
Diazepam @P799	439-14-5	13.738
Clomipramine-M (nor-) P908	303-48-0	13.782
Despropionylfentanyl	39742-60-4	13.809
Flurazepam-M (Desalkyl)	2886-65-9	13.837
Cannabinol, Acetate	997724-40-7	13.887
Hydrocodone	125-29-1	13.912
Morphine, 2TMS Derivative	55449-66-6	13.918
Acetyldihydrocodeine	3861-72-1	13.989
Hydromorphone	466-99-9	14.060
Acetylcodeine	6703-27-1	14.194
Chlorpromazine	50-53-3	14.202
Nordazepam	1088-11-5	14.282
N-Acetylnorcocaine	0-00-0	14.294
Clotiazepam	33671-46-4	14.294
Levomepromazine	60-99-1	14.300
6-Monoacetylmorphine	2784-73-8	14.357
Cannabinol	521-35-7	14.362
Remifentanil	132875-61-7	14.389
Oxycodone, Acetate	997736-63-7	14.394
Ethylmorphine, Acetate	997731-61-8	14.445
11-Hydroxy-delta-9-tetrahydrocannabinol, Bis(trimethylsilyl) Ether	997929-56-4	14.448
U-49900	67579-76-4	14.450
6-Monoacetylmorphine TMS	910138-32-8	14.466
O^6-Acetylmorphin, TMS Derivative	997830-22-7	14.478
Oxycodone	76-42-6	14.524
Clobazam	22316-47-8	14.568
Benzoylecgonine	519-09-5	14.768
AH-7921	55154-30-8	14.830
Paroxetine	61869-08-7	14.883
Midazolam	59467-70-8	14.906
Temazepam	846-50-4	14.921
Loxapine @P1074	27833-64-3	14.957
Hydromorphone AC	910018-11-0	15.001
Delorazepam	2894-67-9	15.047
Flunitrazepam	1622-62-4	15.066
Diacetylmorphine	561-27-3	15.162
Quetiapine-M (N-dealkyl-) P876	996006-43-8	15.197
Bromazepam	1812-30-2	15.336
Prazepam	2955-38-6	15.394
4-Fluoroisobutyrylfentanyl II	910264-33-4	15.452
Acetylfentanyl	3258-84-2	15.542
Para-fluorofentanyl	90736-22-4	15.631
11-Nor-delta-9-tetrahydrocannabinol Carbocylic Acid 2TMS	910035-82-4	15.713

Compound Name	CAS Number	RT
Naloxone	465-65-6	15.910
Clotiapine P1173	2058-52-8	15.958
Fentanyl	437-38-7	16.211
para-Fluorobutyryl Fentanyl	244195-31-1	16.301
Olanzapine	132539-06-1	16.353
Flurazepam	17617-23-1	16.582
Nitrazepam	146-22-5	16.742
Naloxone, O,O'-Diacetyl-	997851-29-6	16.840
Ocfentanil	101343-69-5	17.018
Zolpidem	82626-48-0	17.034
Tiapride	51012-32-9	17.055
Papaverine	58-74-2	17.326
Cyclopropyl Fentanyl	910257-05-5	17.465
Clonazepam	1622-61-3	17.799
Valerylfentanyl	122882-90-0	18.006
Naltrexone	16590-41-3	18.011
Hydroxyzine	68-88-2	18.026
Clozapine	5786-21-0	18.310
Hydroxyzine, TMS Derivative	959101-75-8	18.863
Alfentanil	71195-58-9	19.009
Clozapine-M (Nor)	910008-51-4	19.054
Naltrexone 2AC P1520	996004-31-1	19.184
Alprazolam	28981-97-7	19.296

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