



# Total support system for toxicological analysis using GC/MS

The GC/MS Forensic Toxicological Database contains information for the simultaneous screening of toxicological substances including drugs of abuse, psychotropic drugs, medical drugs and pesticides. Version 2 adds 1198 compounds to the previous version for a total of 2210 compounds in the database. It also includes optimized methods for headspace analysis of alcohol and volatile toxic substances such as cyanides and azides, providing total support for GC/MS toxicology analysis.

## 1. Simultaneous toxicology screening with a high-sensitivity scanning method

The GC/MS scanning method is the gold-standard approach to toxicology analysis, indispensable for the identification of toxicological substances.

Data processing using the mass spectrum library involves looking up the detected peaks and judging whether they correspond to a known drug compound. However, target peaks may be missed if they overlap with interference peaks from the biological sample, or if they are buried in a TIC (total ion current chromatogram) because of their low concentration.

With this database, the mass chromatogram is used to search for peaks and identify them based on three types of information stored in the database: retention time, ion ratio and mass spectrum. In this way, the presence or absence of each drug can be verified, and there is no need to check the TIC, which often contains a large number of impurities. Data processing can be carried out more quickly while minimizing the risk of overlooking any target compounds.

**Mass spectrum**

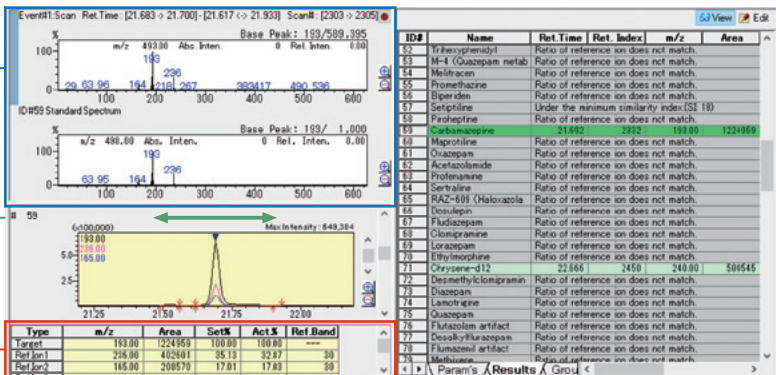
The mass spectrum of the measured sample is compared with the registered mass spectrum in the database.

**Retention times**

Peaks are searched using corrected retention times.

**Mass chromatogram**

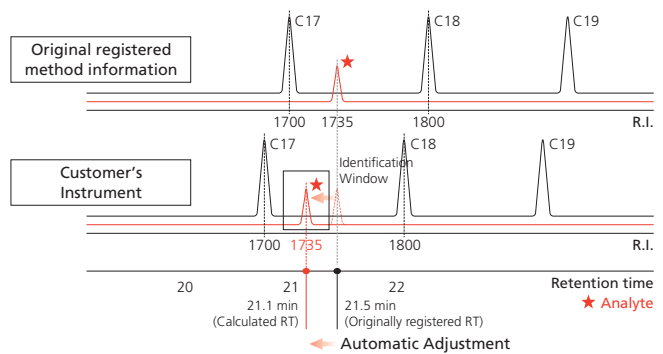
Peaks are searched characteristic ions and ion ratios.



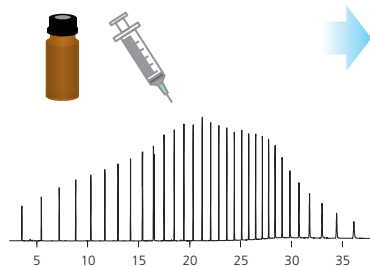
ID#	Name	Ret. Time	Ret. Index	m/z	Area
13	M-4 (Quazepam metab)				
14	Meflazoran				
15	Propofolone				
16	Eperidine				
17	Setipiline				
18	Propofolone	21.862	3925	193/89	1221858
19	Quazepam				
20	Quazepam				
21	Chrysen-d12	22.666	2450	240/00	508545
22	Desmethylclonipramin				
23	Clonipramin				
24	Lorazepam				
25	Chrysenophane				
26	Quazepam				
27	Lamotrigine				
28	Quazepam				
29	Quazepam				
30	Quazepam				
31	Quazepam				
32	Quazepam				
33	Quazepam				
34	Quazepam				
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46	Quazepam				
47	Quazepam				
48	Quazepam				
49	Quazepam				
50	Quazepam				

## 2. Precisely correct the retention times of all listed compounds using AART

The retention times of all compounds listed in the method file can be simultaneously corrected to your GC-MS system with the Automatic Adjustment of Retention Time (AART) function. The multiple n-alkanes used as references from low to high boiling points allow precise correction over a wide range of retention times.



### 1 n-alkane analysis



### 2 Automatic retention time correction with AART

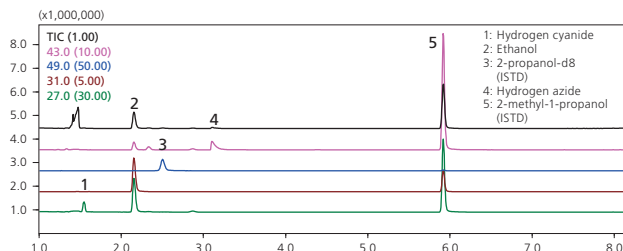
ID#	Name	Ret. Time(Before)	Ret. Time(After)	Ret. Index
1011	ZMM-018 N-C	30.854	30.866	3597
1012	Oxazepam	31.121	30.300	3621
1013	NNE1, MN-24	31.201	30.370	3629
1014	AMC-925	31.213	30.380	3629
1015	MN-25	31.213	30.380	3629
1016	AM1220	31.240	30.491	3640
1017	AM1220 ampo	31.448	30.501	3649
1018	APP-CHMNA	31.719	30.923	3673
1019	ZMM-200	31.890	30.993	3680
1020	Nicardipine	31.890	30.993	3680
1021	Pz-1	31.846	30.933	3684
1022	ZMM-018 B-g	31.890	30.963	3687
1023	FDU-PB-22	32.133	31.185	3709
1024	Thiothione	32.214	31.265	3716
1025	Thiopropazam	32.241	31.366	3727
1026	B-Fluoro-NNE	32.444	31.456	3736
1027	FUB-PB-22	32.629	31.617	3752
1028	BB-22-QUC	32.813	31.770	3763

### 3 Sample analysis with the corrected method



### 3. Support for volatile toxic substances with an HS-20 headspace sampler

The database provides optimum analysis conditions for blood alcohol and volatile toxic substances, indispensable for forensic police laboratories and academic forensics. Volatile toxic substances in the database include cyanides, azides, and thinners such as methanol, ethyl acetate, and toluene.



Simultaneous analysis of blood alcohol and volatile toxic substances using an HS-20 headspace sampler

The database also includes a method for calculating semi-quantitative values. Simply add internal standards to the test sample before measurement to estimate its concentration. This is useful for setting the concentration range of the calibration curve for precise quantitation.



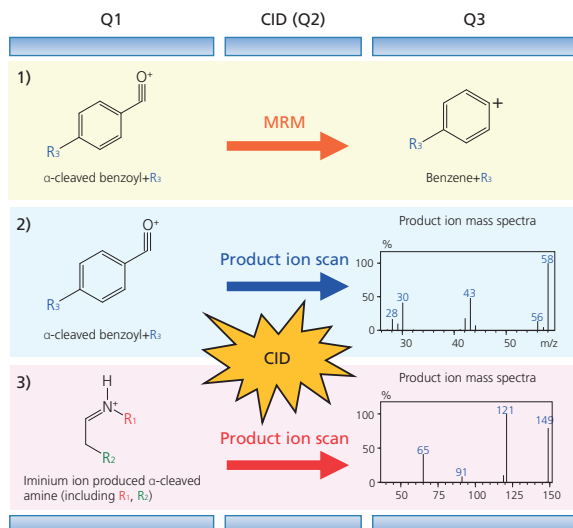
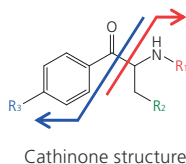
### 4. Comprehensive detection of designer drugs with MS/MS mode

The MS/MS mode of the GCMS-TQ series enables the user to comprehensively detect and estimate the likely structure of cathinones or synthetic naphthoylindole cannabinoids.

#### Comprehensive detection of cathinones

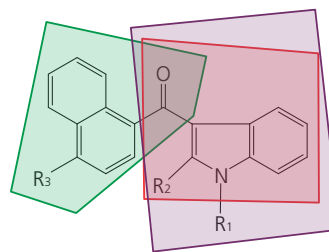
It is possible to comprehensively detect approx. 1300 types of cathinone via  $\alpha$ -cleavage into benzoyl and amine ions which are measured by MRM and product ion scans with GC-MS/MS. Cathinone structure can be estimated from the MS/MS results. It is difficult to distinguish the functional group on the amine with an EI scan due to the large number of isomers, but it is relatively simple to differentiate structural isomers with a product ion scan.

- 1) The cathinone structure is identified and the  $R_3$  functional group estimated
- 2) The  $R_3$  functional group is estimated and the positional isomer distinguished
- 3) The  $R_1$  and  $R_2$  functional groups are estimated and the structural isomer distinguished

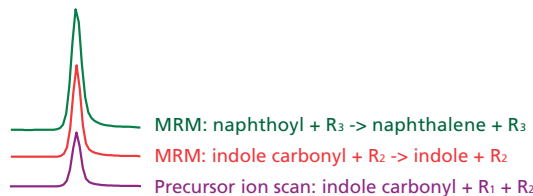


#### Comprehensive detection of synthetic naphthoylindole cannabinoids

It is possible to comprehensively detect approx. 800 kinds of naphthoylindole cannabinoids via EI ionization cleavage into a naphthoylindole and an indole carbonyl. Structure of these parts can be inferred from GC-MS/MS precursor ion scans and MRM.



Basic structure of a naphthoylindole cannabinoid



The three peaks from the different MS/MS modes have the same retention times, so it is possible to comprehensively detect all naphthoylindoles and estimate the functional groups  $R_1$ - $R_3$ .

## Database configuration

### Compounds included in the database

Compound type	No. in database
Drugs of abuse	1504
Psychotropic drugs	366
Medical drugs	189
Pesticides	128
Others	8
Internal standards (ISTD)	9
Volatile toxic substances (HS)	6
<b>Total</b>	<b>2210</b>

Compounds that can be used for semi-quantitation: 234 (of which volatile toxic substances: 6)

Derivatization type	No. in database
Non-derivative	1333
TMS derivative	585
TFA derivative	292
<b>Total</b>	<b>2210</b>

1. TMS = trimethylsilyl, TFA = trifluoroacetyl
2. Semi-quantitative results may be inaccurate due to the condition of the GC-MS. If precise quantitative results are required, quantitative analysis should be carried out with calibration curves from standard samples.
3. During semi-quantitation, solvent flush mode is used for co-injection of the sample solution and the internal sample. In this case, the combination of an AOC-20i auto-injector and an AOC-20s autosampler is required.

### File list

Database file (Excel™), method file, library file, report format file

### Device requirements

GC/MS: GCMS-QP series or GCMS-TQ series

Excel: Microsoft® Excel 2013, 2016, 2019 (32-bit edition)

Autosampler: AOC-20i + AOC-20s

Workstation: GCMSsolution™ Ver. 4.51 or later

Headspace sampler: HS-20

(if using a method file for volatile toxic substances)

### Recommended consumables

N-alkane: C8-C40 Alkane Calibration Standard (SIGMA-ALDRICH, Cat#: 40147-U)

Analysis column: For toxicological substances SH-Rxi™-5Sil MS (30 m, 0.25 mm i.d., df = 0.25 μm, P/N: 221-75954-30) or DB-5ms (30 m, 0.25 mm i.d., df = 0.25 μm)

For volatile toxic substances SH-Rtx™-BAC2 (30m, 0.32mm i.d., df = 1.2 μm, Restek Corporation, P/N: 227-36262-01)

Internal standards: For toxicological substances Custom Internal Standard (Restek Corporation, Cat#: 560294)

For volatile toxic substances 2-Propanol-d8 (99.5%)

2-Methyl-1-propanol (99.5%)

### Cautions

1. Shimadzu does not provide any guarantee with regards to the accuracy of the information in the database or the usefulness of results obtained using this information.
2. Qualitative and quantitative information obtained using this database should be confirmed through analysis of standard samples.
3. For precise identification of compounds registered in the database, carry out measurements using the appropriate equipment conditions in the method file.
4. This database is for research use only. Not for use in diagnostic procedures.

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