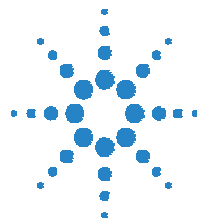


Forensic Toxicology GC/MS RTL Database

User Contributed by
National Medical Services
Willow Grove, Pennsylvania, USA



Agilent Technologies
Innovating the HP Way

Database Development

- **Developed by National Medical Services, a premier bioanalysis laboratory that has worked across the USA and internationally (www.nmslab.com)**
- **Used daily at NMS for Forensic Toxicology samples**
- **RTLocked to 8-methoxyloxapine at 12.000 min**
 - **8-methoxyloxapine may not be commercially available. A suggested RTLocking compound is methadone-d9 at 8.235 min**
- **All retention time and spectral data collected on Agilent GC/MSD systems**
- **Agilent DB-17MS column used, 15 m x 250 μ m x 0.25 μ m (part number 122-4712)**

There are 2 Related Databases

- **Retention Time Locked Screener Database**

- **NMS_tox1.scd**
- **277 compounds/derivatives**
- **precise retention times**
- **target ion and up to 3 qualifier ions**

- **Mass Spectral Library**

- **NMS_tox1.L**
- **GC/MS Spectra for the 277 compounds/derivatives**

Typical Sample Analysis Without the Databases

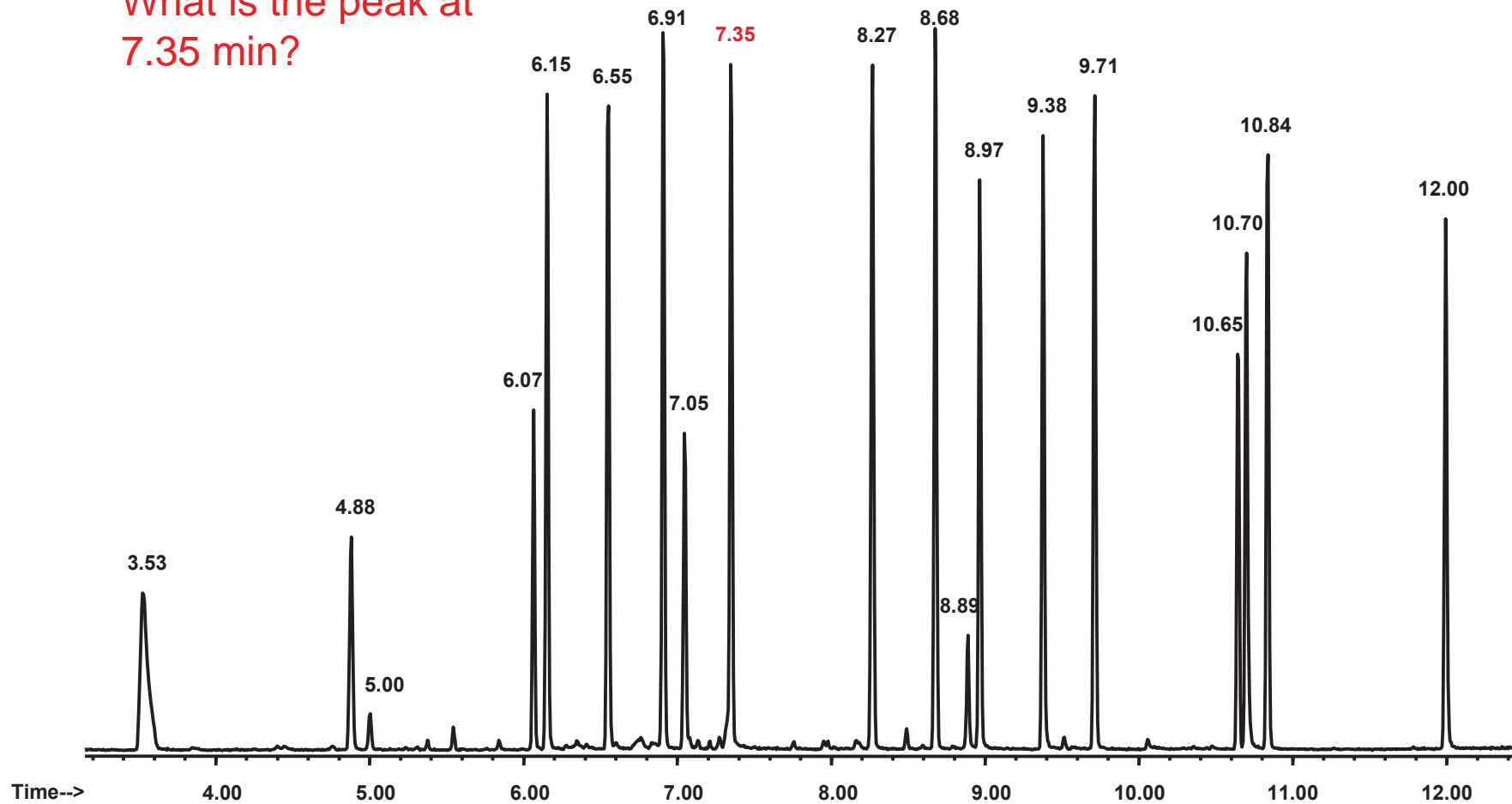
- Sample may be run on a GC-FID or GC-NPD first
- Sample is run on GC/MSD
 - GC/MSD r.t. doesn't match GC r.t.
- All peaks in GC/MSD TIC are library searched
- Analyst validates library search results
 - usually 10 hits/peak reviewed
 - non-specific libraries used
 - library spectra collected on different instruments
- Sample may be returned to GC for quantitation

Using the NMS Databases

- NMS_tox1.scd and NMS_tox1.L are copied to the Database folder, usually C:\Database
- The GC/MS system is retention time locked and an RTL method is established
- Samples are run using the RTL method
- Sample datafile is Screened using NMS_tox1.scd
 - **Screeener report is generated**
- **Screeener Results are reviewed/modified**
- **Peak spectra can be searched/compared using NMS_tox1.L**

Test Sample TIC run RTLocked

What is the peak at 7.35 min?



Example Partial Screener Report

Screen File: NMS_tox1.RES
Screen Database: NMS_tox1.SCD

Extraction Window: +/- 0.150 min
Qualifier Mode : Relative
Qualifier % : 50
Zero qualifiers : Included
Subtraction Mode : Sub Lower Start/Stop

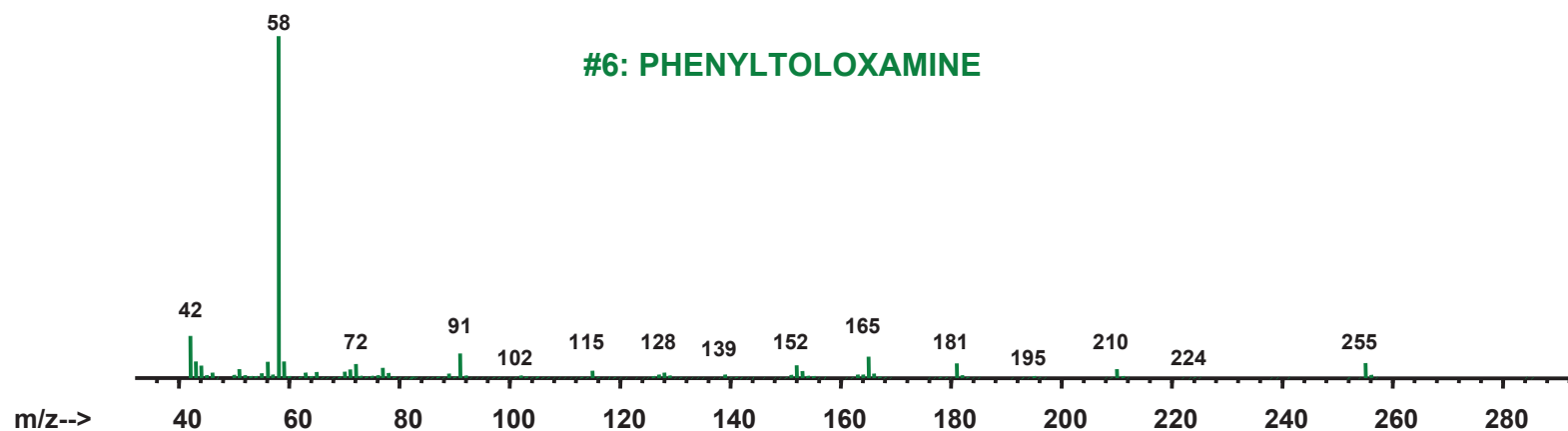
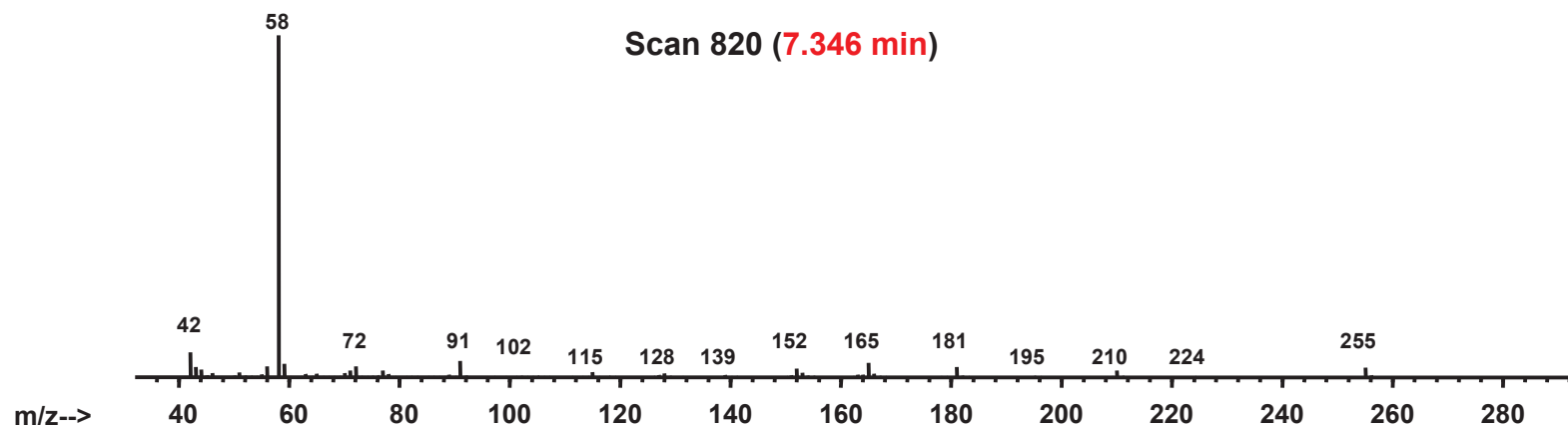
Compound	Status	ExpRT	Delta	Target m/z	Resp.	Qualifiers Out of Range	XCR
2 NICOTINE	x	3.484	+0.046	84	5548698		0.98
4 PHENDIMETRAZINE	?	4.327	-0.081	57	21276	85,191	0.62
7 BARBITAL	x	4.890	-0.008	141	2379864		0.98
8 BUPROPION	?	4.899	-0.019	44	268397	100,224	0.02
9 CARBROMAL	?	4.916	-0.036	44	269469	208,210	0.09
28 METHAMPHETAMINE[BUTYRATED	?	6.050	+0.104	58	125563	128,91	0.08
29 AMOBARBITAL	?	6.050	+0.107	156	46903	157,183	0.05
32 MEPERIDINE	x	6.145	+0.009	71	3624743		0.92
35 PENTOBARBITAL	?	6.258	-0.101	156	48784	157,155	0.07
40 BENZPHETAMINE	x	6.538	+0.013	91	11061909		1.00
47 CHLORPHENTERMINE[BUTYRATE	?	6.689	-0.087	58	139190	128,166	0.93
49 METHCATHINONE[BUTYRATED]	?	6.712	-0.110	58	161272	128,77	0.90
53 DIPHENHYDRAMINE	x	6.898	+0.012	58	14306906		1.00
68 ORPHENADRINE	?	7.249	+0.101	58	14148150	73,165	0.96
70 DOXYLAMINE	?	7.285	+0.065	58	14768434	71,167	0.74
72 PHENYLTOLOXAMINE	x	7.343	+0.007	58	14774802		0.99
73 TRAMADOL	?	7.347	+0.003	58	14756854	263,135	0.99

Screener Report - User Analysis

- 4 entries have a target ion=58 and similar r.t.
- 3 of these have very good cross correlations (XCR) with their respective library entries
- 2 of these have very good r.t. agreement with their expected r.t.
- Only 1 has all qualifiers within expected ranges, Phenyltoloxamine, and its Status is marked “x” as a probable hit
- ? Denotes a possible hit

Library Search of NMS_tox1.L

Peak identification confirmed



Screeners Variables

- **The number of probable and possible Hits can be globally changed through these variables**
 - **Extraction Window for retention time**
 - **Qualifier Mode, relative or absolute**
 - **Qualifier %**
 - **Zero qualifiers, included or excluded**
 - **Subtraction Mode**
- **Integration parameters define peak detection**

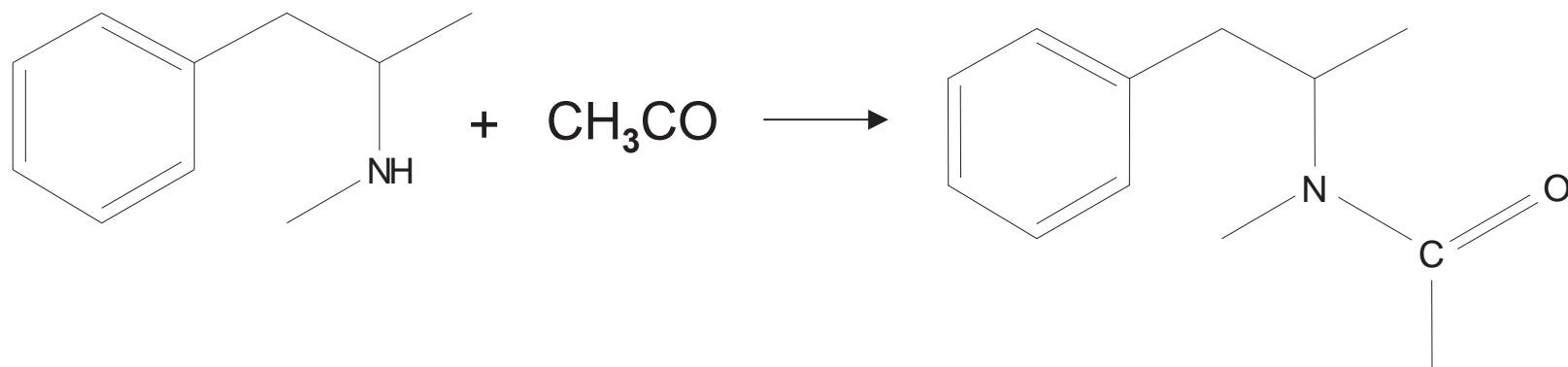
Benefits of Using RTL Databases

- **Fastest Identification Compounds**
 - Screen for 277 compounds in < 15 sec
- **Fastest Confirmation of compounds**
 - Eliminate hits with wrong r.t.
- **Precise reproducible r.t. on GC and GC/MS**
 - Match GC r.t. to GC/MS r.t.
 - No need to update calibration tables
- **Compounds identified by both retention time and spectral information**
- **No Additional cost for User Contributed Databases**

Derivatives in the Databases

- Most of the compounds in the databases are not derivatized
- The derivatives are one of the following
 - Acetyl CH_3CO
 - Butyryl $\text{CH}_3\text{CH}_2\text{CH}_2\text{CO}$
 - Pentafluoropropionyl $\text{CF}_3\text{CF}_2\text{CO}$
- Some compounds have more than one entry due to different derivatives

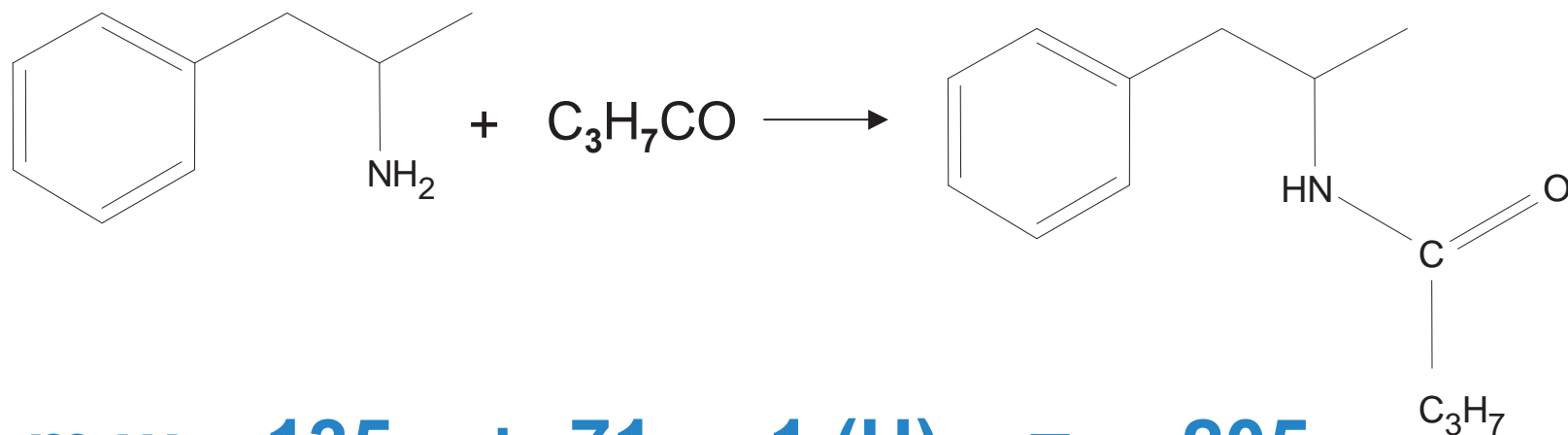
Acetylated Methamphetamine



$$\text{m.w. } 149 + 43 - 1 (\text{H}) = 191$$

Acetylated derivative adds 42 to the molecular weight

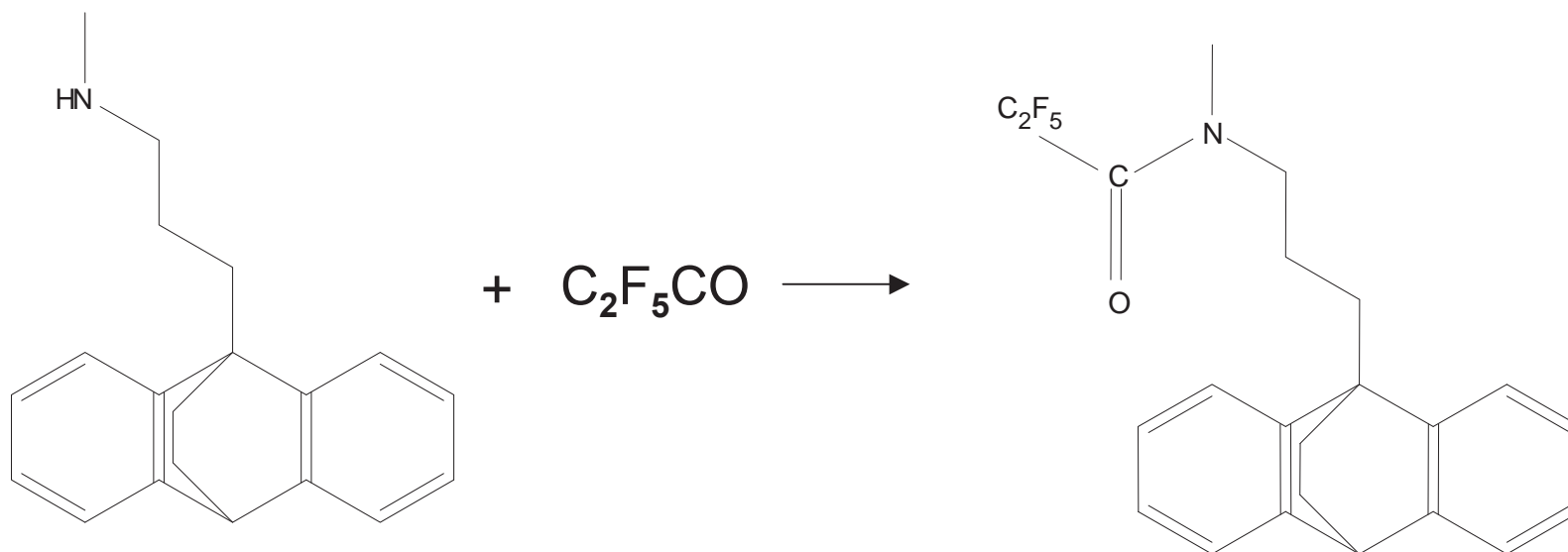
Butyrate Amphetamine



$$\text{m.w. } 135 + 71 - 1 (\text{H}) = 205$$

Butyrate derivative adds 70 to the molecular weight

PFPA Derivative of Maprotiline



$$\text{m.w. } 277 + 147 - 1 (\text{H}) = 423$$

PFPA derivative adds 146 to the molecular weight

Database Compounds 1 of 4

10,11-DIHYDRO-DIBENZ[B,F][1,4]OXA	BENZTROPINE	CETIRIZINE
6-ACETYLMORPHINE	BIPERDIN	CHLORDIAZEPOXIDE
8-METHOXYLOXAPINE	BIS[2-ETHYLHEXYL]PHTHALATE	CHLORMEZANONE
ACEPROMAZINE	BROMDIPHENHYDRAMINE	CHLOROPHENE
ACETAMINOPHEN	BROMOCRIPTINE	CHLORPHENIRAMINE
ACRIDINE	BROMPHENIRAMINE	CHLORPHENIRAMINE METABOLITE
ALFENTANYL	BROMPHENIRAMINE #2	CHLORPHENTERMINE[BUTYRATED]
ALLOBARBITAL	BROMPHENIRAMINE METAB. #1	CHLORPROMAZINE
ALPHA-METHYLFENTANYL	BUPIVACAINE	CHOLESTEROL
ALPHAPRODINE	BUPROPION	CINNAMOYLCOCAINE
ALPRAZOLAM	BUSPIRONE	CITALOPRAM
AMANTADINE[ACETYLATED]	BUSPIRONE	CLEMASTIN
AMANTADINE[BUTYRATED]	BUTABARBITAL	CLOBAZAM
AMITRIPTYLINE	BUTALBITAL	CLOMIPRAMINE
AMOBARBITAL	BUTORPHANOL	CLOZAPINE
AMOXAPINE	CAFFEINE	CLOZAPINE (BUTYRATED)
AMOXAPINE[BUTYRATED]	CARBAMAZEPINE	COCAETHYLENE
AMPHETAMINE[BUTYRATED]	CARBAMAZEPINE RELATED PEAK	COCAINE
APROBARBITAL	CARBAMAZEPINE RELATED PEAK	CODEINE(BUTYRATED)
ATROPINE[BUTYRATED]	CARBINOXAMINE	COTININE
AZATADINE	CARBROMAL	CYCLIZINE
BARBITAL	CARBROMAL-M\ARTIFACT	CYCLOBENZAPRINE
BENZOCAINE	CARFENTANYL	CYCLOHEXANEGLYCOLIC ACID,.ALF
BENZOCAINE	CARISOPRODOL	CYPROHEPTADINE
BENZPHETAMINE	CATHINE[NORPSEUDOEPHEDRINE	DESIPRAMINE(BUTYRATED)

Database Compounds 2 of 4

DESMETHYLCLOMIPRAMINE(BUTYRA	ESTAZOLAM	HYDRASTINE
DESMETHYLCLOMIPRAMINE[PFPA]	ETHINAMATE	HYDROCODONE
DESMETHYLDOXEPIN(BUTYRATED)	ETHOTOIN	HYDROXYCHLOROQUINE[BUTYRAT
DESMETHYL-MIANSERIN	ETHYLECGONINE[BUTYRATED]	HYDROXYETHYLFLURAZEPAM
DESMETHYLSERTRALINE[BUTYRATE	ETHYLMORPHINE	HYDROXYZINE METABOLITE[BUTYR.
DESPROPIONYL FENTANYL	FELODIPINE	HYDROXYZINE(BUTYRATED)
DIAZEPAM	FENFLURAMINE[BUTYRATED]	IBUPROFEN
DICYCLOMINE	FENTANYL	IMIPRAMINE
DIETHYLPROPRION	FLECAINIDE	KETAMINE
DIHYDROCODEINE	FLECAINIDE FORMYL ARTIFACT	LAMOTRIGINE
DILTIAZEM	FLUCONAZOLE	LEVORPHANOL
DIMETHYLTRYPTAMINE	FLUNITRAZEPAM	LIDOCAINE
DIPHENHYDRAMINE	FLUOXETINE(BUTYRATED)	LIDOCAINE RELATED PEAK
DIPHENHYDRAMINE METABOLITE	FLUPHENAZINE	LORAZEPAM
DIPHENOXYLATE	FLURAZEPAM	LORCAINIDE
DISOPYRAMIDE	FLUVOXAMINE (BUTYRATED)	LOXAPINE
DOTHIEPIN	FLUVOXAMINE[PFPA]	LSD
DOXAPRAM	GAMMA-TOCOPHEROL	MAPROTALINE[BUTYRATED]
DOXEPIN(CIS)	GEMFIBROZIL	MAPROTALINE{PFPA}
DOXEPIN(TRANS)	GLUTETHIMIDE	MAZINDOL
DOXYLAMINE	GUAIFENESIN	MBDB{BUTYRATED}
DOXYLAMINE METABOLITE{BUTYRA	HALAZEPAM	MECLIZINE
EMDP[METHADONE METAB.]	HALOPERIDOL	MEFLOQUINE
ENCAINIDE	HEXOBARBITAL	MEPERIDINE
EPHEDRINE[BUTYRATED]	HMMA	MEPHENTERMINE[BUTYRATED]

Database Compounds 3 of 4

MEPHENYTOIN	METHYPRYLON	OLANZAPINE[BUYRATED]
MEPHOBARBITAL	METOCLOPRAMIDE	ORPHENADRINE
MEPIVACAINE	METOPROLOL	OXAZEPAM
MEPROBAMATE	MEXILETINE	OXYCODONE
MESCALINE(BUTYRATED)	MIANSERIN	OXYCODONE[BUTYRATED]
MESORIDAZINE	MIDAZOLAM	PAPAVERINE
METHADONE	MIRTAZAPINE	PARA-FLUOROFENTANYL
METHADONE METABOLITE[EDDP]	MOLINDONE	PAROXETINE[BUTYRATED]
METHAMPHETAMINE[ACETYLATED]	MONOETHYLGLYCINEXYLIDIDE{MEG	PENTAZOCINE(BUTYRATED)
METHAMPHETAMINE[BUTYRATED]	NAPROXEN	PENTOBARBITAL
METHAQUALONE	NICOTINE	PHENCYCLIDINE[PCP]
METHARBITAL	NIFEDAPINE	PHENDIMETRAZINE
METHCATHINONE[BUTYRATED]	NORCODEINE	PHENIRAMINE
METHDILAZINE	NORCYCLOBENZAPRINE[BUTYRATE	PHENMETRAZINE[BUTYRATED]
METHOCARBAMOL	NORDIAZEPAM	PHENOBARBITAL
METHOHEXITAL	NORFENTANYL[BUTYRATED]	PHENSUXIMIDE
METHORPHAN	NORFLUOXETINE(BUTYRATED)	PHENTERMINE[BUTYRATED]
METHOTRIMEPRAZINE	NORKETAMINE[PFPA]	PHENYLPROPANOLAMINE[BUTYRAT
METHSUXIMIDE	NORMEPERIDINE(BUTYRATED)	PHENYLTOLOXAMINE
METHYLDIOXYAMPHETAMINE[MDA][NORMETHSUXIMIDE	PHENYTOIN
METHYLECGONINE[BUTYRATED]	NOROXYCODONE	P-METHOXYAMPHETAMINE
METHYLENEDIOXYETHYLAMPHETAM	NORPROPOXYPHENEAMIDE	PMMA
METHYLENEDIOXYMETHAMPHETAM	NORTRIPTYLINE	PRAZEPAM
METHYLPHENIDATE	NORTRIPTYLINE(BUTYRATED)	PRIMIDONE
METHYLPHENOBARBITAL	OLANZAPINE	PROCAINE

Database Compounds 4 of 4

PROCHLOROPERAZINE	THIAMYLAL	ZOLAZEPAM
PROCYCLIDINE	THIOPENTAL	ZOLPIDEM
PROMAZINE	THIORIDAZINE	
PROMETHAZINE	THIOTHIXENE	
PROPYL PHENYLETHYLAMINE[PEA]	TICLOPIDINE	
PROPYLAMPHETAMINE(BUTYRATED)	TILETAMINE	
PROTRIPTYLINE(BUTYRATED)	TOCAINIDE	
PSEUDOEPHEDRINE[BUTYRATED]	TRAMADOL	
PYRILAMINE	TRAMADOL[BUTYRATED]	
PYRIMETHAMINE	TRANLYCYPROMINE[BUTYRATED]	
QUINIDINE	TRAZODONE	
QUININE	TRIAZOLAM	
SCOPOLAMINE	TRIFLUOPERAZINE	
SECOBARBITAL	TRIHXYPHENIDYL	
SERTRALINE	TRIMETHOBENZAMINE	
SERTRALINE	TRIMETHOPRIM	
STRYCHNINE	TRIMIPRAMINE	
SUFENTANYL	TRIMIPRAMINE	
TALBUTAL	TRIPLENNAMINE	
TEMAZEPAM	TRIPROLIDINE	
TETRACAINE	VENLAFAXINE[BUTYRATED]	
TETRADECANOIC ACID	VERAPAMIL	
THENYLDIAMINE[METHAPYRILENE]	VITAMEN E	
THEOBROMINE	WARFARIN	
THEOPHYLLINE	XYLAZINE	

Agilent Instrumentation Required

- **Gas Chromatograph**

- **6890N with Autosampler (tray & injector) and split/splitless inlet**

- **Mass Spectrometer**

- **5973N with EI source**

- **Software**

- **GC/MSD Chemstation G1701 CA version C.00.01 or higher (includes RTL and Screener)**

- **Column**

- **DB-17MS 15 m x 250 μm x 0.25 μm (part number 122-4712)**

Method Parameters

GC	Agilent 6890N				
Oven					
Ramp	'C/min	'C	Hold min		
Initial		80	0.00		
Ramp 1	20	320	5.00		
Runtime	17 min				
				MSD	Agilent 5973N
Inlet	Split/Splitless			Solvent Delay	2.5 min
Temp	250 'C			Scan Range	42 to 450
Mode	Pulsed Splitless			Threshold	150
Pressure	6.37 psi (adj to lock)			Sampling	2
Pulse Pressure	20 psi			Quad Temp	230 'C
Pulse Time	1.00 min			Source Temp	150 'C
Purge Flow	50 mL/min			Transfer Line	280 'C
Purge time	1.00 min				
Total Flow	54.1 mL/min				
				Injector	
Column	DB-17MS part # 122-4712			Sample Washes	0
Mode	Constant pressure			Sample Pumps	3
Pressure	6.37 psi			Injection volume	2 uL
Initial Flow	1.5 mL/min			Solv A washes	2
Outlet	MSD			Solv B washes	2
Outlet Pressure	Vacuum			Viscosity Delay	3
				Plunger Speed	Fast

Recommended Reading

- Retention Time Locking with the HP G1701BA MSD Productivity ChemStation (5968-3433)
- Efficient Screening for Pesticides and Endocrine Disrupters Using the HP 6890/ 5973 GC/MSD System (5968-4884)
- Retention Time Locking: Concepts and Applications (5966-2469)
- Precise Time-Scaling of Gas Chromatographic Methods Using Method Translation and Retention Time Locking (5967-5820)
- Direct your web browser to www.chem.agilent.com
- Click on **Library**, then **Online Literature**
- In the **keyword field** type in the **8 digit number** as it is listed above for the publication you would like to view