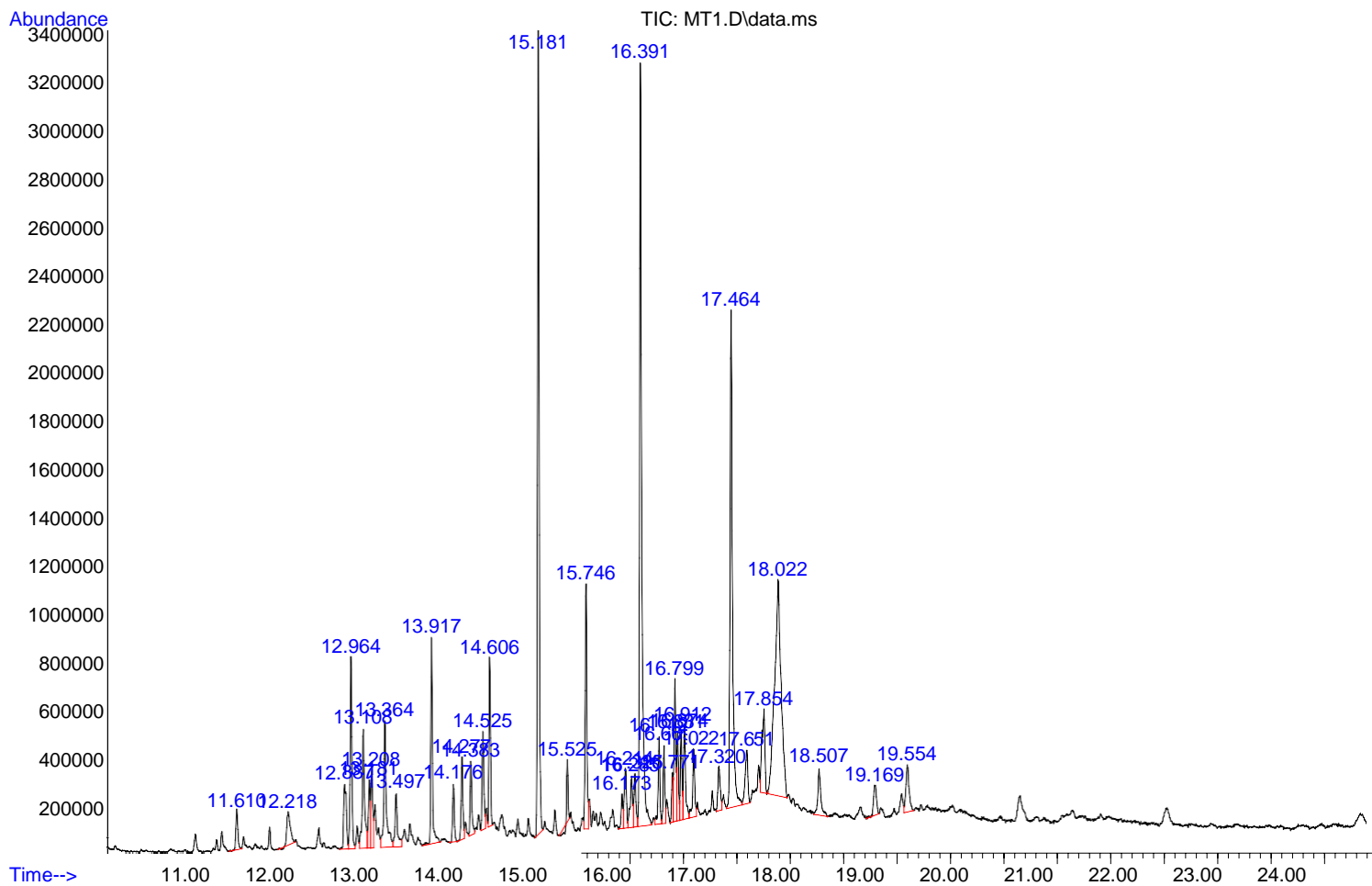


File :C:\msdchem\1\DATA\20190429M\MHT1.D  
Operator : SARA  
Acquired : 30 Apr 2019 12:57 using AcqMethod AYA.M  
Instrument : GCMSD004  
Sample Name: MT1  
Misc Info :  
Vial Number: 5

Data obtained from *M. tenuiflora*



Data Path : C:\msdchem\1\DATA\20190429M\  
Data File : MHT1.D  
Acq On : 30 Apr 2019 12:57  
Operator : SARA  
Sample : MHT1  
Misc :  
ALS Vial : 5 Sample Multiplier: 1

Search Libraries: C:\msdchem\bib...s ms\PMW\_TOX2.L Minimum Quality: 50  
C:\msdchem\bib...s ms\WILEY275.L Minimum Quality: 50

Unknown Spectrum: Peak average  
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
1	11.609	0.71	C:\msdchem\bibliotecas ms\WILEY275.L			
			Cyclododecane (CAS)	53905	000294-62-2	78
			1-dodecyl-2-chloroethyl ether	131233	000000-00-0	74
			Cyclododecane (CAS)	53901	000294-62-2	72
2	12.215	1.01	C:\msdchem\bibliotecas ms\WILEY275.L			
			1H-Indole-3-ethanamine, N,N-dimethyl- (CAS) \$\$ N,N-Dimethyltryptamine \$\$ OMT \$\$ DMT \$\$ 3-(2-Dimethylaminoethyl)indole \$\$ 2-(3-Indolyl)ethyl-dimethylamine \$\$ Indole, 3-[2-(dimethylamino)ethyl]- \$\$ 3-(2-DIMETHYLAMINO)ETHYL) INDOLE \$\$ Dimethyltryptamine	72851	000061-50-7	91
			1H-Indole-3-ethanamine, N,N-dimethyl- (CAS) \$\$ N,N-Dimethyltryptamine \$\$ OMT \$\$ DMT \$\$ 3-(2-Dimethylaminoethyl)indole \$\$ 2-(3-Indolyl)ethyl-dimethylamine \$\$ Indole, 3-[2-(dimethylamino)ethyl]- \$\$ 3-(2-DIMETHYLAMINO)ETHYL) INDOLE \$\$ Dimethyltryptamine	72852	000061-50-7	86
			1H-Indole-3-ethanamine, N,N-dimethyl- (CAS) \$\$ N,N-Dimethyltryptamine \$\$ OMT \$\$ DMT \$\$ 3-(2-Dimethylaminoethyl)indole \$\$ 2-(3-Indolyl)ethyl-dimethylamine \$\$ Indole, 3-[2-(dimethylamino)ethyl]- \$\$ 3-(2-DIMETHYLAMINO)ETHYL) INDOLE \$\$ Dimethyltryptamine	72850	000061-50-7	86
3	12.885	1.52	C:\msdchem\bibliotecas ms\PMW_TOX2.L			
			Palmitic acid ME P1297	1801	000112-39-0	78
			Lauric acid ME P950	2666	000111-82-0	43
			Capric acid ME P783	2665	000110-42-9	35
4	12.965	2.94	C:\msdchem\bibliotecas ms\WILEY275.L			
			7,9-di-tert-butyl-1-oxaspiro[4.5]deca-6,9-diene-2,8-dione	158640	000000-00-0	97
			2-Phenazinecarbonitrile (CAS) \$\$ 2-CYANO PHENAZINE \$\$ 2-Cyanophenazine	90218	006479-93-2	48
			(Z,Z)-2,5-bis(2,2-dimethylpropylidene)cyclopentanone \$\$ Cyclopentanone, 2,5-bis(2,2-dimethylpropylidene)-, (Z,Z)-	106101	115984-10-6	42
5	13.108	2.49	C:\msdchem\bibliotecas ms\PMW_TOX2.L			
			Palmitic acid P1210	822	000057-10-3	93
			Myristic acid P1035	1140	000544-63-8	52
			Stearic acid P1389	969	000057-11-4	35
6	13.182	1.08	C:\msdchem\bibliotecas ms\WILEY275.L			
			Nonadecane, 2-methyl- (CAS) \$\$ 2-Methylnonadecane	163872	001560-86-7	80
			Tetratriacontane (CAS) \$\$ n-Tetrat	256280	014167-59-0	80

Data Path : C:\msdchem\1\DATA\20190429M\  
Data File : MHT1.D  
Acq On : 30 Apr 2019 12:57  
Operator : SARA  
Sample : MHT1  
Misc :  
ALS Vial : 5 Sample Multiplier: 1

Search Libraries: C:\msdchem\bib...s ms\PMW\_TOX2.L Minimum Quality: 50  
C:\msdchem\bib...s ms\WILEY275.L Minimum Quality: 50

Unknown Spectrum: Peak average  
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			riacontane			
			Heptacosane (CAS) \$\$ n-Heptacosane	226683	000593-49-7	80
7	13.211	1.26	C:\msdchem\bibliotecas ms\PMW_TOX2.L			
			Butyl-2-methylpropylphthalate P1351	@ 2995	017851-53-5	91
			Butyl-2-ethylhexylphthalate P1013	@ 713	000085-69-8	83
			Decyltetradecylphthalate P1943	@ 3543	000000-00-0	50
8	13.366	2.85	C:\msdchem\bibliotecas ms\PMW_TOX2.L			
			Octacosane P1837	3797	000630-02-4	91
			Nonadecane P1286	2363	000629-92-5	91
			Eicosane P1379	2352	000112-95-8	90
9	13.497	1.21	C:\msdchem\bibliotecas ms\PMW_TOX2.L			
			Eicosane P1379	2352	000112-95-8	60
			Octacosane P1837	3797	000630-02-4	53
			Nonadecane P1286	2363	000629-92-5	49
10	13.915	3.10	C:\msdchem\bibliotecas ms\PMW_TOX2.L			
			Cyclohexadecane P1017	2355	000295-65-8	96
			Stearyl alcohol P1298	2356	000112-92-5	91
			Cyclotetradecane P835	2354	000295-17-0	90
11	14.178	0.87	C:\msdchem\bibliotecas ms\PMW_TOX2.L			
			Stearic acid ME P1475	@ 970	000112-61-8	93
			Pentadecanoic acid ME P1209	3036	007132-64-1	87
			Myristic acid ME P1121	1141	000124-10-7	87
12	14.275	1.24	C:\msdchem\bibliotecas ms\WILEY275.L			
			HENEICOSANE	175428	000000-00-0	94
			Heneicosane (CAS) \$\$ n-Heneicosane	175418	000629-94-7	94
			Eicosane (CAS) \$\$ n-Eicosane	163882	000112-95-8	91
13	14.384	1.15	C:\msdchem\bibliotecas ms\PMW_TOX2.L			
			Stearic acid P1389	969	000057-11-4	72
			Myristic acid P1035	1140	000544-63-8	53
			Octadecane P1197	2351	000593-45-3	11
14	14.527	1.57	C:\msdchem\bibliotecas ms\PMW_TOX2.L			
			Hexacosane P1768	2365	000630-01-3	56
			Nonadecane P1286	2363	000629-92-5	37
			Monalide P1105	2723	007287-36-7	22

Data Path : C:\msdchem\1\DATA\20190429M\  
 Data File : MHT1.D  
 Acq On : 30 Apr 2019 12:57  
 Operator : SARA  
 Sample : MHT1  
 Misc :  
 ALS Vial : 5 Sample Multiplier: 1

Search Libraries: C:\msdchem\bib...s ms\PMW\_TOX2.L Minimum Quality: 50  
 C:\msdchem\bib...s ms\WILEY275.L Minimum Quality: 50

Unknown Spectrum: Peak average  
 Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
15	14.607	2.24	C:\msdchem\bibliotecas ms\PMW_TOX2.L Nonadecane P1286 Hexadecane P1024 Octacosane P1837	2363 2353 3797	000629-92-5 000544-76-3 000630-02-4	91 78 68
16	15.179	11.43	C:\msdchem\bibliotecas ms\PMW_TOX2.L Cyclohexadecane P1017 Bemegrade P625 Cyclotetradecane P835	2355 77 2354	000295-65-8 000064-65-3 000295-17-0	70 38 38
17	15.523	0.49	C:\msdchem\bibliotecas ms\PMW_TOX2.L Eicosane P1379 Octacosane P1837 Triacontane P1885	2352 3797 2366	000112-95-8 000630-02-4 000638-68-6	60 47 43
18	15.746	3.64	C:\msdchem\bibliotecas ms\PMW_TOX2.L Eicosane P1379 Hexacosane P1768 Octacosane P1837	2352 2365 3797	000112-95-8 000630-01-3 000630-02-4	83 64 53
19	16.215	1.12	C:\msdchem\bibliotecas ms\WILEY275.L 3-(1-Benzyloxy-2-hydroxyethyl)-1,5 -dioxaspiro[5.5]undecane \$\$ 1,5-Di oxaspiro[5.5]undecane-3-ethanol, . beta.-(phenylmethoxy)- Benzonitrile, m-phenethyl- (CAS) \$ \$ M-CYANO-1,2-DIPHENYLETHANE Benzenemethanamine, N-(phenylmethy lene)- (CAS) \$\$ Benzylidenebenzyla mine \$\$ N-Benzylidenebenzylamine \$ \$ N-Benzylaminebenzaldehyde \$\$ N-B ENZYLIDENE-BENZYLAMINE \$\$ Benzylam ine, N-benzylidene- \$\$ N-(Phenylme thylene)benzenemethanamine \$\$ Benz aldehyde N-benzyl	182824 92596 79695	119117-61-2 034176-91-5 000780-25-6	14 12 12
20	16.284	1.00	C:\msdchem\bibliotecas ms\WILEY275.L Silane, methylenebis(dimethyl- (CA S) \$\$ 2,4-DIMETHYL-2,4-DISILAPENTA NE \$\$ 2,4-Disilapentane, 2,4-dimet hyl- \$\$ Silane, methylenebis@dimet hyl- Silane, methylenebis(dimethyl- (CA S) \$\$ 2,4-DIMETHYL-2,4-DISILAPENTA NE \$\$ 2,4-Disilapentane, 2,4-dimet hyl- \$\$ Silane, methylenebis@dimet hyl- 1-METHYL-2-PHENYLCYCLOPROPANE 2	21720 21721 22306	018163-84-3 018163-84-3 000000-00-0	46 43 43
21	16.324	0.89	C:\msdchem\bibliotecas ms\WILEY275.L			

Data Path : C:\msdchem\1\DATA\20190429M\  
 Data File : MHT1.D  
 Acq On : 30 Apr 2019 12:57  
 Operator : SARA  
 Sample : MHT1  
 Misc :  
 ALS Vial : 5 Sample Multiplier: 1

Search Libraries: C:\msdchem\bib...s ms\PMW\_TOX2.L Minimum Quality: 50  
 C:\msdchem\bib...s ms\WILEY275.L Minimum Quality: 50

Unknown Spectrum: Peak average  
 Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			14-.BETA.-H-PREGNA EGNA \$\$ 14B-PREGNANE	169067	000000-00-0	25
			1,2,3,4-Tetrahydro-1,4,5-triphenyl pyrazine \$\$ Pyrazine, 1,2,3,4-tetr ahydro-1,4,5-triphenyl- (CAS)	187615	073166-14-0	25
			D-GULOPYRANOSIDE, 2,3:4,6-DI-O-(ET HYLBORANDIYL)-1-O-METHYL-	152789	000000-00-0	18
22	16.392	14.49	C:\msdchem\bibliotecas ms\WILEY275.L Hexadecanoic acid, 2-hydroxy-1-(hy droxymethyl)ethyl ester (CAS) \$\$ 2 -Monopalmitin \$\$ Palmitin, 2-mono- \$\$ 2-Hexadecanoyl glycerol \$\$ 2-M onopalmitoyl-sn-glycerol \$\$ Palmit ic acid .beta.-monoglyceride \$\$ 1, 2,3-Propanetriol 2-hexadecanoyl e ster \$\$ Glycerol	199572	023470-00-0	91
			Hexadecanoic acid, 2,3-dihydroxypr opyl ester (CAS) \$\$ 1-Monopalmitin \$\$ GLYCEROL-1-HEXADECANOATE \$\$ Pa lmitin, 1-mono- \$\$ Glyceryl palmit ate \$\$ .alpha.-Monopalmitin \$\$ Gly cerol 1-palmitate \$\$ Glycerol 3-pa lmitate \$\$ Glycerol 1-monopalmitat e \$\$ Palmitic aci	199569	000542-44-9	64
			Dodecanedioic acid (CAS) \$\$ 1,12-D odecanedioic acid \$\$ 1,10-Decanedi carboxylic acid \$\$ Decamethylenedi carboxylic acid \$\$ Dodecanedicarbo xylic acid \$\$ 1,10-Dicarboxydecane \$\$ n-Dodecanedioic acid \$\$ SL-AH	115848	000693-23-2	35
23	16.610	1.35	C:\msdchem\bibliotecas ms\PMW_TOX2.L Diisooctylphthalate @ P1828	723	027554-26-3	94
			Butyl-2-ethylhexylphthalate @ P1013	713	000085-69-8	43
			Decyldodecylphthalate @ P1935	3542	000000-00-0	38
24	16.667	1.10	C:\msdchem\bibliotecas ms\PMW_TOX2.L Triacontane P1885	2366	000638-68-6	64
			Nonadecane P1286	2363	000629-92-5	59
			Hexacosane P1768	2365	000630-01-3	50
25	16.770	0.62	C:\msdchem\bibliotecas ms\WILEY275.L 1H-Indole, 2-methyl-3-phenyl- (CAS ) \$\$ 3 PHENYL-2-METHYLINDOLE \$\$ 2- Methyl-3-phenylindole \$\$ Indole, 2 -methyl-3-phenyl-	92607	004757-69-1	64
			1H-Indole, 2-methyl-3-phenyl- (CAS ) \$\$ 3 PHENYL-2-METHYLINDOLE \$\$ 2- Methyl-3-phenylindole \$\$ Indole, 2 -methyl-3-phenyl-	92608	004757-69-1	64
			METHADONE N-OXIDE	196308	000000-00-0	64
26	16.799	2.20	C:\msdchem\bibliotecas ms\PMW_TOX2.L Triacontane P1885	2366	000638-68-6	80
			Tricosane	2364	000638-67-5	72

Data Path : C:\msdchem\1\DATA\20190429M\  
 Data File : MHT1.D  
 Acq On : 30 Apr 2019 12:57  
 Operator : SARA  
 Sample : MHT1  
 Misc :  
 ALS Vial : 5 Sample Multiplier: 1

Search Libraries: C:\msdchem\bib...s ms\PMW\_TOX2.L Minimum Quality: 50  
 C:\msdchem\bib...s ms\WILEY275.L Minimum Quality: 50

Unknown Spectrum: Peak average  
 Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			P1612			
			Hexadecane	2353	000544-76-3	72
			P1024			
27	16.833	1.31	C:\msdchem\bibliotecas ms\WILEY275.L			
			1a,9b-dihydro-4-methyl-1H-phenanthro[9,10-b]azirine	92618	111005-47-1	72
			METHADONE N-OXIDE	196308	000000-00-0	53
			1H-Indole, 5-methyl-2-phenyl- (CAS )	92603	013228-36-9	38
			\$\$\$ 5-Methyl-2-phenylindole \$\$\$ 2-Phenyl-5-methylindole \$\$\$ Indole, 5-methyl-2-phenyl-			
28	16.873	1.31	C:\msdchem\bibliotecas ms\WILEY275.L			
			DOCOSANE	186070	000000-00-0	68
			EICOSANE	163904	000000-00-0	68
			Docosane (CAS) \$\$\$ n-Docosane \$\$\$ C2 2H46 STANDARD \$\$\$ Normal-docosane	186058	000629-97-0	68
29	16.913	1.77	C:\msdchem\bibliotecas ms\WILEY275.L			
			3,6-Dioxa-2,4,5,7-tetrasilaoctane, 2,2,4,4,5,5,7,7-octamethyl- (CAS) \$\$\$ SILANE, DIMETHYL(TRIMETHYLSILOXY)BIS- \$\$\$ 3,6-Dioxa-2,4,5,7-tetrasilaoctane, octamethyl-	172798	004342-25-0	47
			N-DOCOSANE	186069	000629-97-0	46
			EICOSANE	163904	000000-00-0	46
30	17.022	1.28	C:\msdchem\bibliotecas ms\WILEY275.L			
			N-EICOSANE	163902	000112-95-8	87
			Eicosane (CAS) \$\$\$ n-Eicosane	163884	000112-95-8	78
			Eicosane (CAS) \$\$\$ n-Eicosane	163881	000112-95-8	70
31	17.319	0.93	C:\msdchem\bibliotecas ms\WILEY275.L			
			2-METHYL-1,3-PROPANEDIOL 2TMS \$\$\$ 2-Methyl-1,3-bis(trimethylsiloxy)propane \$\$\$ 3,6-Dioxa-2,7-disilaoctane, 2,2,4,5,7,7-hexamethyl- \$\$\$ Butane, 2,3-bis(trimethylsiloxy)-2,3-BUTANEDIOL 2TMS PK A \$\$\$ 2,3-BUTANEDIOL 2TMS PK B	119329	033581-79-2	35
			2,3-BUTANEDIOL 2TMS PK A \$\$\$ 2,3-BUTANEDIOL 2TMS PK B	119345	000000-00-0	35
			2,3-BUTANEDIOL 2TMS PK A \$\$\$ 2,3-BUTANEDIOL 2TMS PK B	119346	000000-00-0	35
32	17.462	10.63	C:\msdchem\bibliotecas ms\WILEY275.L			
			12-Oxo-15-hexadecanolide \$\$\$ Oxacyclohexadecane-2,13-dione, 16-methyl-, (.+-.)- (CAS)	151621	095338-34-4	25
			1-Octadecanethiol (CAS) \$\$\$ Octadecanethiol \$\$\$ Stearyl mercaptan \$\$\$ Octadecyl mercaptan \$\$\$ 1-Mercaptododecane \$\$\$ n-Octadecyl mercaptan	167149	002885-00-9	25
			2-(2,2-dimethylpropanoyl)cyclohexanone	67035	137919-99-4	22
33	17.651	1.30	C:\msdchem\bibliotecas ms\PMW_TOX2.L			
			GC stationary phase P1895	2627	000000-00-0	59
			Heptabarbital P1000	803	000509-86-4	6
			GC septum bleed P1944	2220	000000-00-0	2

Data Path : C:\msdchem\1\DATA\20190429M\  
Data File : MHT1.D  
Acq On : 30 Apr 2019 12:57  
Operator : SARA  
Sample : MHT1  
Misc :  
ALS Vial : 5 Sample Multiplier: 1

Search Libraries: C:\msdchem\bib...s ms\PMW\_TOX2.L Minimum Quality: 50  
C:\msdchem\bib...s ms\WILEY275.L Minimum Quality: 50

Unknown Spectrum: Peak average  
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
34	17.852	2.19	C:\msdchem\bibliotecas ms\PMW_TOX2.L			
			Octadecane	2351	000593-45-3	62
			P1197			
			Triacotane	2366	000638-68-6	58
			P1885			
			Hexacosane	2365	000630-01-3	53
			P1768			
35	18.023	12.31	C:\msdchem\bibliotecas ms\WILEY275.L			
			2-methoxy-4-methyl-6-[(3',5'-dimet	190140	000000-00-0	12
			hoxyphehyl)methyl]benzoic acid			
			Pregnane-3,20-dione, (5.alpha.)-	190456	000566-65-4	7
			(CAS) \$\$ 3,20-Allopregnenedione \$\$			
			3,20-Dioxo-5.alpha.-pregnane \$\$ 5.			
			alpha.-Pregnane-3,20-dione \$\$ 5.al			
			pha.-Dihydroprogesterone			
			Pregnan-20-one, 3,11-dihydroxy-, (	202433	038398-44-6	2
			3.alpha.,5.alpha.,11.alpha.)-			
			(CAS			
			) \$\$ 3.ALPHA.,11.ALPHA.-DIHYDROXY-			
			5.ALPHA.-PREGNAN-20-ONE \$\$ 5.ALPHA			
			.-PREGNANE-3.ALPHA.,11.ALPHA.-DIOL			
			-20-ONE \$\$ 5.alpha.-Pregnan-20-one			
			, 3.alpha.,11.alpha.-dihydroxy-			
			3ALPHA,11ALPHA-D			
36	18.510	1.24	C:\msdchem\bibliotecas ms\PMW_TOX2.L			
			GC stationary phase	2627	000000-00-0	59
			P1895			
			GC stationary phase (OV-101)	1016	000000-00-0	10
			P1736			
			Cyclobarbital-M (oxo-)	703	035305-10-3	10
			P1174			
37	19.168	0.81	C:\msdchem\bibliotecas ms\PMW_TOX2.L			
			Nonadecane	2363	000629-92-5	64
			P1286			
			Hexadecane	2353	000544-76-3	53
			P1024			
			Hexacosane	2365	000630-01-3	50
			P1768			
38	19.551	1.34	C:\msdchem\bibliotecas ms\PMW_TOX2.L			
			GC stationary phase	2627	000000-00-0	56
			P1895			
			GC stationary phase (UCC-W-982)	1018	000000-00-0	43
			P1895			
			GC stationary phase (OV-101)	1016	000000-00-0	15
			P1736			