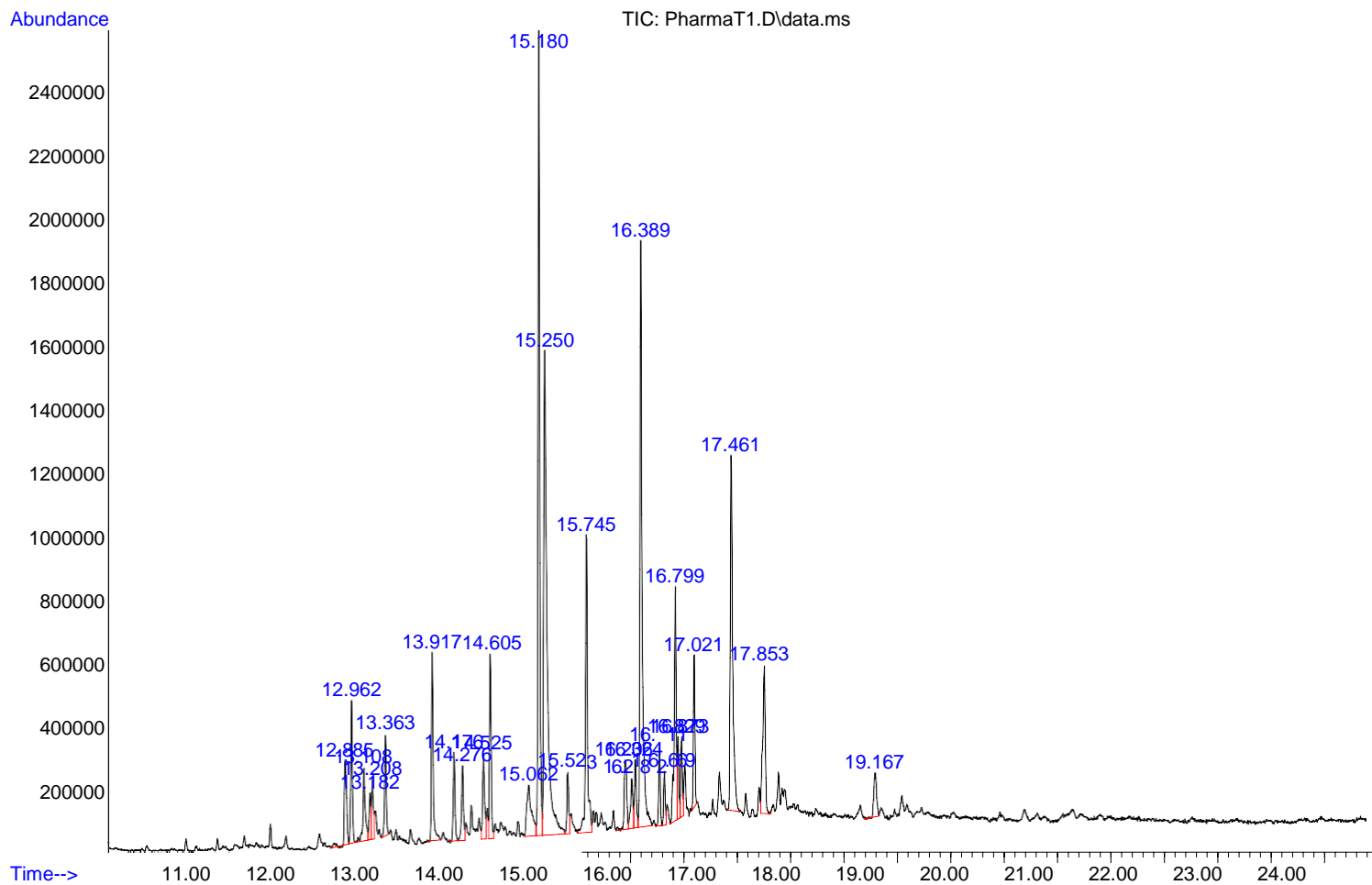


File :C:\msdchem\1\DATA\20190429M\PharmaT1.D
Operator : SARA
Acquired : 30 Apr 2019 10:58 using AcqMethod AYA.M
Instrument : GCMSD004
Sample Name: PharmaT1
Misc Info :
Vial Number: 1

Data obtained from *P. harmala*



Data Path : C:\msdchem\1\DATA\20190429M\
Data File : PharmaT1.D
Acq On : 30 Apr 2019 10:58
Operator : SARA
Sample : PharmaT1
Misc :
ALS Vial : 1 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	12.885	1.86	C:\msdchem\bibliotecas ms\PMW_TOX2.L			
			Palmitic acid ME	1801	000112-39-0	94
			P1297			
			Myristic acid ME	1141	000124-10-7	50
			P1121			
			Capric acid ME	2665	000110-42-9	45
			P783			
2	12.959	2.23	C:\msdchem\bibliotecas ms\WILEY275.L			
			7,9-di-tert-butyl-1-oxaspiro[4.5]d	158640	000000-00-0	95
			eca-6,9-diene-2,8-dione			
			(E,Z)-2,5-bis(2,2-dimethylpropylid	106099	115984-11-7	38
			ene)cyclopentanone \$\$ Cyclopentano			
			ne, 2,5-bis(2,2-dimethylpropyliden			
			e)-, (E,Z)-			
			2,3-.MU.-TRIMETHYLGGERMYL-CC'-DIMET	106882	036672-03-4	30
			HYL-4,5-DICARBA-NIDO-HEXABORANE (8)			
			\$\$ 2,3-Dicarbahexaborane (8), 2,3-			
			dimethyl[4,5-.mu.-(trimethylgermyl			
)]- (CAS)			
3	13.108	1.65	C:\msdchem\bibliotecas ms\PMW_TOX2.L			
			Palmitic acid	822	000057-10-3	64
			P1210			
			Myristic acid	1140	000544-63-8	38
			P1035			
			Octacosane	3797	000630-02-4	11
			P1837			
4	13.182	0.78	C:\msdchem\bibliotecas ms\PMW_TOX2.L			
			Hexadecane	2353	000544-76-3	59
			P1024			
			Tricosane	2364	000638-67-5	45
			P1612			
			Hexacosane	2365	000630-01-3	42
			P1768			
5	13.211	1.02	C:\msdchem\bibliotecas ms\PMW_TOX2.L			
			Butyl-2-methylpropylphthalate @	2995	017851-53-5	86
			P1351			
			Decyldodecylphthalate @	3542	000000-00-0	59
			P1935			
			Butyloctylphthalate @	2361	000084-78-6	38
			P1013			
6	13.366	1.57	C:\msdchem\bibliotecas ms\PMW_TOX2.L			
			Eicosane	2352	000112-95-8	94
			P1379			
			Octacosane	3797	000630-02-4	90
			P1837			
			Tricosane	2364	000638-67-5	68
			P1612			
7	13.915	3.21	C:\msdchem\bibliotecas ms\PMW_TOX2.L			
			Cyclohexadecane	2355	000295-65-8	96
			P1017			
			Stearyl alcohol	2356	000112-92-5	91
			P1298			
			Cyclotetradecane	2354	000295-17-0	86
			P835			
8	14.178	1.48	C:\msdchem\bibliotecas ms\PMW_TOX2.L			
			Pentadecanoic acid ME	3036	007132-64-1	72

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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
			P1209			
			Myristic acid ME	1141	000124-10-7	50
			P1121			
			Stearic acid ME	@ 970	000112-61-8	46
			P1475			
9	14.275	1.39	C:\msdchem\bibliotecas ms\WILEY275.L			
			Octadecane (CAS) \$\$ n-Octadecane \$	139438	000593-45-3	91
			\$ Octadecan			
			Hexadecane, 2,6,10,14-tetramethyl-	163891	000638-36-8	81
			(CAS) \$\$ Phytane \$\$ 2,6,10,14-Tet			
			ramethylhexadecane \$\$ Phytan			
			Tridecane, 2-methyl- (CAS) \$\$ 2-Me	83551	001560-96-9	58
			thyltridecane \$\$ 2-Methyl-tridecan			
			e \$\$ 2-Methyl-n-tridecane			
10	14.527	1.71	C:\msdchem\bibliotecas ms\PMW_TOX2.L			
			Tricosane	2364	000638-67-5	56
			P1612			
			Hexacosane	2365	000630-01-3	53
			P1768			
			Eicosane	2352	000112-95-8	46
			P1379			
11	14.607	3.04	C:\msdchem\bibliotecas ms\PMW_TOX2.L			
			Nonadecane	2363	000629-92-5	96
			P1286			
			Octadecane	2351	000593-45-3	86
			P1197			
			Hexadecane	2353	000544-76-3	78
			P1024			
12	15.059	2.37	C:\msdchem\bibliotecas ms\PMW_TOX2.L			
			Harmaline	4062	000304-21-2	99
			P955			
			Sulfaperin 3ME	3157	000000-00-0	12
			P1524			
			Promethazine-M (nor-)	607	000000-00-0	12
			P1300			
13	15.179	12.94	C:\msdchem\bibliotecas ms\PMW_TOX2.L			
			Cyclohexadecane	2355	000295-65-8	68
			P1017			
			Stearyl alcohol	2356	000112-92-5	38
			P1298			
			Bemegrade	77	000064-65-3	37
			P625			
14	15.248	16.34	C:\msdchem\bibliotecas ms\PMW_TOX2.L			
			Harmine	4066	000442-51-3	98
			@ P939			
			Harmine AC	@ 4067	000000-00-0	43
			P1201			
			Propallylonal-M 2ME	925	000000-00-0	25
			P1104			
15	15.523	1.11	C:\msdchem\bibliotecas ms\PMW_TOX2.L			
			triacontane	2366	000638-68-6	56
			P1885			
			Hexacosane	2365	000630-01-3	56
			P1768			
			Nonadecane	2363	000629-92-5	42
			P1286			

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 Operator : SARA
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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
16	15.746	5.92	C:\msdchem\bibliotecas ms\PMW_TOX2.L Nonadecane P1286 Tricosane P1612 Triacontane P1885	2363 2364 2366	000629-92-5 000638-67-5 000638-68-6	91 80 80
17	16.204	1.78	C:\msdchem\bibliotecas ms\WILEY275.L 7-Methylindole \$\$ 1H-Indole, 7-methyl- (CAS) \$\$ Indole, 7-methyl- \$ 7-Methylindol 1H-Indole, 2-methyl- (CAS) \$\$ 2-Methylindole \$\$ SKATOLE \$\$ Indole, 2-methyl- \$ 2-Methyl-1H-indole 1H-Indole, 2-methyl- (CAS) \$\$ 2-Methylindole \$\$ SKATOLE \$\$ Indole, 2-methyl- \$ 2-Methyl-1H-indole	21517 21487 21492	000933-67-5 000095-20-5 000095-20-5	38 38 38
18	16.284	1.06	C:\msdchem\bibliotecas ms\WILEY275.L Silane, methylenebis(dimethyl- (CAS) \$\$ 2,4-DIMETHYL-2,4-DISILAPENTANE \$\$ 2,4-Disilapentane, 2,4-dimethyl- \$ Silane, methylenebis(dimethyl- 2,5-di(trimethylsiloxy)hexane 1H-Indene, 1-hexadecyl-2,3-dihydro- (CAS) \$\$ 1-N-HEXADECYLINDANE \$\$ 1-n-Hexadecylindan \$\$ 1-NOR-HEXADECYL-(2,3-DIHYDROINDENE) (1-NOR-HEXADECYLINDAN) \$\$ 1-n-Hexadecyl(2,3-dihydroindene)	21720 145738 207326	018163-84-3 000000-00-0 055334-29-7	46 43 38
19	16.324	1.30	C:\msdchem\bibliotecas ms\WILEY275.L Cyclononane (CAS) \$\$ NONADECANONE (NAME ?) Benzene, 1-isocyano-4-methyl- (CAS) \$\$ 4-METHYL-PHENYLISOCYANIDE \$ p-Tolyl isonitrile \$\$ p-Tolyl isocyanide \$\$ p-Methylphenyl isocyanide Benzene, 1-isocyano-4-methyl- (CAS) \$\$ 4-METHYL-PHENYLISOCYANIDE \$ p-Tolyl isonitrile \$\$ p-Tolyl isocyanide \$\$ p-Methylphenyl isocyanide	28109 13731 13730	003350-30-9 007175-47-5 007175-47-5	35 22 22
20	16.387	12.51	C:\msdchem\bibliotecas ms\WILEY275.L Hexadecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester (CAS) \$\$ 2-Monopalmitin \$\$ Palmitin, 2-mono- \$ 2-Hexadecanoyl glycerol \$\$ 2-Monopalmitoyl-sn-glycerol \$\$ Palmitic acid .beta.-monoglyceride \$\$ 1,2,3-Propanetriol 2-hexadecanoyl ester \$\$ Glycerol CYCLONONANONE Oxacyclotetradecane-2,11-dione, 13-methyl- (CAS) \$\$.GAMMA.-TRIDECANOLACTONE, 13-METHYL-11-OXO-	199572 28217 125999	023470-00-0 000000-00-0 074685-36-2	90 27 25
21	16.610	1.20	C:\msdchem\bibliotecas ms\PMW_TOX2.L Diisooctylphthalate @ P1828	723	027554-26-3	94

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 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
			Decyltetradecylphthalate P1943	@ 3543	000000-00-0	38
			Decyldodecylphthalate P1935	@ 3542	000000-00-0	38
22	16.667	0.81	C:\msdchem\bibliotecas ms\PMW_TOX2.L Nonadecane P1286	2363	000629-92-5	64
			Hexadecane P1024	2353	000544-76-3	50
			Hexacosane P1768	2365	000630-01-3	50
23	16.799	4.45	C:\msdchem\bibliotecas ms\PMW_TOX2.L Nonadecane P1286	2363	000629-92-5	96
			Eicosane P1379	2352	000112-95-8	87
			Triacontane P1885	2366	000638-68-6	74
24	16.827	1.28	C:\msdchem\bibliotecas ms\WILEY275.L 1a,9b-dihydro-4-methyl-1H-phenanth ro[9,10-b]azirine	92618	111005-47-1	83
			METHADONE N-OXIDE	196308	000000-00-0	53
			N-ethyl-1,3-dithioisindoline \$\$ 1	92199	035373-06-9	50
			H-Isoindole-1,3(2H)-dithione, 2-et hyl-			
25	16.873	1.32	C:\msdchem\bibliotecas ms\WILEY275.L DOCOSANE	186070	000000-00-0	62
			Docosane (CAS) \$\$ n-Docosane \$\$ C2	186058	000629-97-0	62
			2H46 STANDARD \$\$ Normal-docosane			
			Nonadecane (CAS) \$\$ n-Nonadecane	151987	000629-92-5	60
26	17.022	2.34	C:\msdchem\bibliotecas ms\WILEY275.L 1-Octadecene (CAS) \$\$.alpha.-Octa decene \$\$ Octadecylene .alpha.-	137615	000112-88-9	78
			1-Octadecanethiol (CAS) \$\$ Octadec anethiol \$\$ Stearyl mercaptan \$\$ O ctadecyl mercaptan \$\$ 1-Mercaptooc tadecane \$\$ n-Octadecyl mercaptan	167149	002885-00-9	64
			Ethanol, 2-(tetradecyloxy)- (CAS) \$\$ 2-Tetradecyloxyethanol \$\$ Myris tyl monoethoxylate \$\$ Ethylene gly col monotetradecyl ether	142763	002136-70-1	64
27	17.462	8.43	C:\msdchem\bibliotecas ms\WILEY275.L Cyclononane (CAS) \$\$ NONADECANON E (NAME ?)	28109	003350-30-9	45
			Hexadecanedioic acid (CAS) \$\$ Thap sic acid \$\$ HEXADECAN-1,16-DIOIC A CID \$\$ 1,16-Hexadecanedioic acid \$ \$ Hexadecane-1,16-dioic acid \$\$ 1, 14-Tetradecanedicarboxylic acid \$\$ n-Tetradecane-.omega.,.omega.'-di carboxylic acid \$\$ hexadecanedioic acid \$\$.alpha.	166846	000505-54-4	27
			1-Octadecanethiol (CAS) \$\$ Octadec anethiol \$\$ Stearyl mercaptan \$\$ O ctadecyl mercaptan \$\$ 1-Mercaptooc tadecane \$\$ n-Octadecyl mercaptan	167149	002885-00-9	25

Library Search Report

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

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
28	17.852	3.69	C:\msdchem\bibliotecas ms\PMW_TOX2.L			
			Nonadecane P1286	2363	000629-92-5	72
			Triacontane P1885	2366	000638-68-6	72
			Octadecane P1197	2351	000593-45-3	64
29	19.168	1.20	C:\msdchem\bibliotecas ms\WILEY275.L			
			N-EICOSANE	163902	000112-95-8	97
			Eicosane (CAS) \$\$ n-Eicosane	163882	000112-95-8	97
			EICOSANE	163904	000000-00-0	97