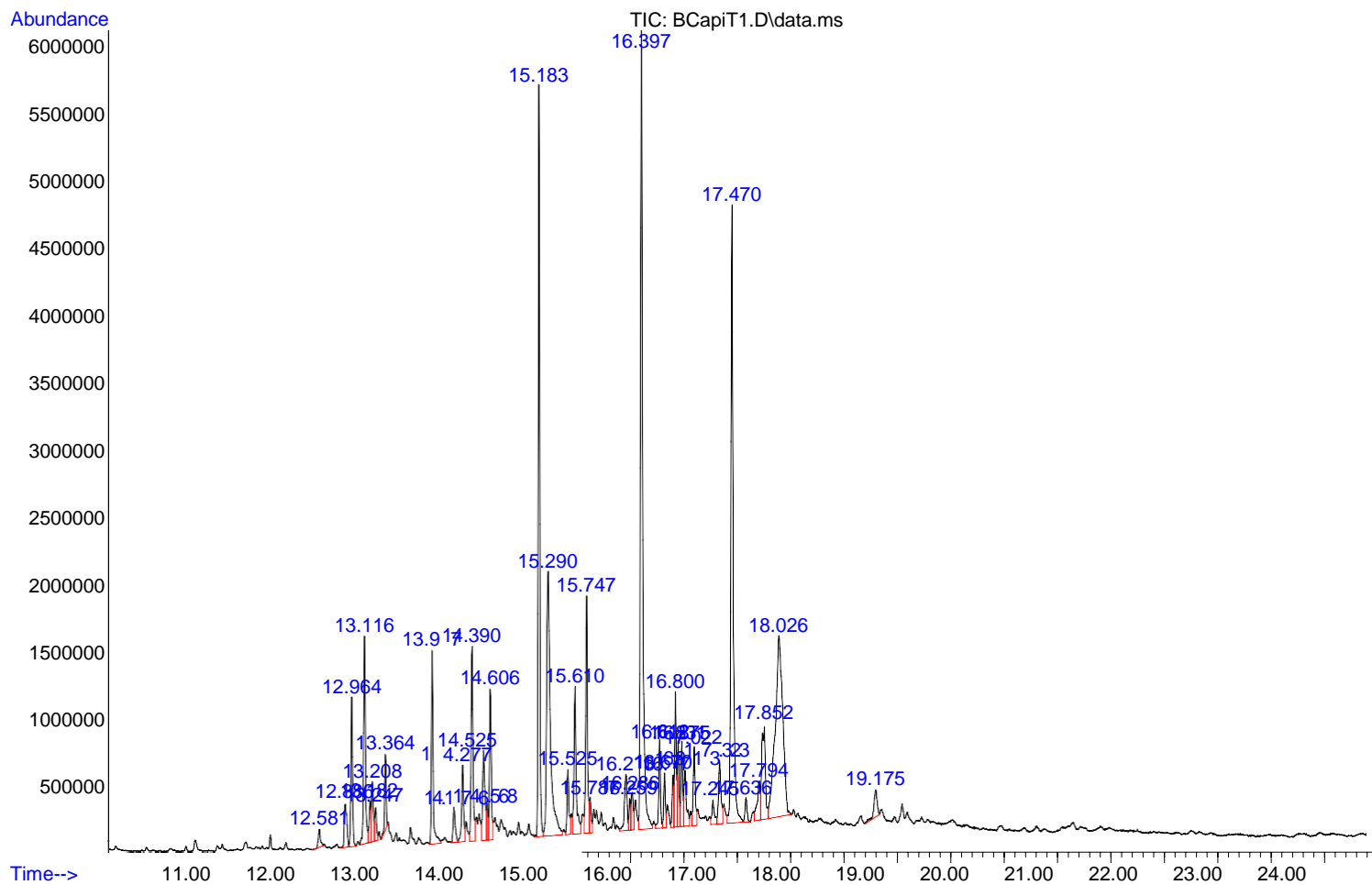


File :C:\msdchem\1\DATA\20190429M\BCapiT1.D
Operator : SARA
Acquired : 30 Apr 2019 12:28 using AcqMethod AYA.M
Instrument : GCMSD004
Sample Name: BCapiT1
Misc Info :
Vial Number: 4

Data obtained from *B. caapi*



Data Path : C:\msdchem\1\DATA\20190429M\
 Data File : BCapiT1.D
 Acq On : 30 Apr 2019 12:28
 Operator : SARA
 Sample : BCapiT1
 Misc :
 ALS Vial : 4 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	12.582	0.31	C:\msdchem\bibliotecas ms\PMW_TOX2.L Cyclohexadecane P1017	2355	000295-65-8	99
			Cyclotetradecane P835	2354	000295-17-0	93
			Stearyl alcohol P1298	2356	000112-92-5	76
2	12.885	0.90	C:\msdchem\bibliotecas ms\PMW_TOX2.L Palmitic acid ME P1297	1801	000112-39-0	78
			Pentadecanoic acid ME P1209	3036	007132-64-1	37
			Lauric acid ME P950	2666	000111-82-0	37
3	12.965	2.04	C:\msdchem\bibliotecas ms\WILEY275.L 7,9-di-tert-butyl-1-oxaspiro[4.5]d eca-6,9-diene-2,8-dione	158640	000000-00-0	95
			2,3-.MU.-TRIMETHYLGGERMYL-CC'-DIMET HYL-4,5-DICARBA-NIDO-HEXABORANE(8) \$\$ 2,3-Dicarbahexaborane(8), 2,3- dimethyl[4,5-.mu.-(trimethylgermyl)]- (CAS)	106882	036672-03-4	38
			2-Phenazinecarbonitrile (CAS) \$\$ 2 -CYANO PHENAZINE \$\$ 2-Cyanophenazi ne	90218	006479-93-2	35
4	13.114	3.14	C:\msdchem\bibliotecas ms\PMW_TOX2.L Palmitic acid P1210	822	000057-10-3	93
			Stearic acid P1389	969	000057-11-4	74
			Myristic acid P1035	1140	000544-63-8	52
5	13.182	0.56	C:\msdchem\bibliotecas ms\WILEY275.L Docosane, 11-decyl- (CAS) \$\$ 11-n- Decyldocosane \$\$ 11-NOR-DECYLDOCOS ANE	250413	055401-55-3	64
			Heptacosane (CAS) \$\$ n-Heptacosane	226683	000593-49-7	62
			Tricosane (CAS) \$\$ n-Tricosane	195910	000638-67-5	62
6	13.205	0.88	C:\msdchem\bibliotecas ms\PMW_TOX2.L Butyl-2-methylpropylphthalate @ P1351	2995	017851-53-5	90
			Butyl-2-ethylhexylphthalate @ P1013	713	000085-69-8	78
			Decyltetradecylphthalate @ P1943	3543	000000-00-0	50
7	13.245	0.53	C:\msdchem\bibliotecas ms\WILEY275.L 2H-1-Benzopyran, 6,7-dimethoxy-2,2 -dimethyl- (CAS) \$\$ Ageratochromen e \$\$ Precocene 2 \$\$ Precocene II \$ \$ 6,7-dimethoxy-2,2-dimethyl-2H-ch romene \$\$ PRICOCENE II \$\$ 6,7-Dime thoxy-2,2-dimethyl-2H-benzo(b)pyra Benzene, 1,1'-(3-methyl-1,3-butadi enylidene)bis- 2-methoxy-6-allyloxy-7-methyl-7H-p urine \$\$ 7H-Purine, 2-methoxy-7-me thyl-6-(2-propenyloxy)-	105289	000644-06-4	83
				106216	077915-31-2	83
				104854	097184-80-0	83

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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
8	13.365	0.85	C:\msdchem\bibliotecas ms\PMW_TOX2.L			
			Eicosane	2352	000112-95-8	89
			P1379			
			Heptadecane	2977	000629-78-7	86
			P1109			
			Octacosane	3797	000630-02-4	74
			P1837			
9	13.915	2.63	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	74
			P835			
10	14.178	0.59	C:\msdchem\bibliotecas ms\PMW_TOX2.L			
			Stearic acid ME	970	000112-61-8	76
			P1475			
			Lauric acid ME	2666	000111-82-0	53
			P950			
			Pentadecanoic acid ME	3036	007132-64-1	45
			P1209			
11	14.275	1.18	C:\msdchem\bibliotecas ms\WILEY275.L			
			Tricosane (CAS) \$\$ n-Tricosane	195910	000638-67-5	90
			Eicosane (CAS) \$\$ n-Eicosane	163882	000112-95-8	90
			Octadecane (CAS) \$\$ n-Octadecane \$	139444	000593-45-3	90
			\$ Octadecan			
12	14.390	2.98	C:\msdchem\bibliotecas ms\PMW_TOX2.L			
			Stearic acid	969	000057-11-4	93
			P1389			
			Palmitic acid	822	000057-10-3	64
			P1210			
			Myristic acid	1140	000544-63-8	47
			P1035			
13	14.527	1.71	C:\msdchem\bibliotecas ms\PMW_TOX2.L			
			Eicosane	2352	000112-95-8	72
			P1379			
			Nonadecane	2363	000629-92-5	40
			P1286			
			Hexacosane	2365	000630-01-3	38
			P1768			
14	14.567	0.49	C:\msdchem\bibliotecas ms\PMW_TOX2.L			
			Nonadecane	2363	000629-92-5	53
			P1286			
			Hexadecane	2353	000544-76-3	53
			P1024			
			Heptadecane	2977	000629-78-7	42
			P1109			
15	14.607	2.16	C:\msdchem\bibliotecas ms\PMW_TOX2.L			
			Nonadecane	2363	000629-92-5	91
			P1286			
			Octacosane	3797	000630-02-4	87
			P1837			
			Eicosane	2352	000112-95-8	83
			P1379			

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Search Libraries: C:\msdchem\bib...s ms\PMW_TOX2.L Minimum Quality: 50
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Unknown Spectrum: Peak average
 Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
16	15.185	9.09	C:\msdchem\bibliotecas ms\PMW_TOX2.L			
			Stearyl alcohol P1298	2356	000112-92-5	70
			Cyclohexadecane P1017	2355	000295-65-8	70
			Bemegrade P625	77	000064-65-3	25
17	15.288	8.05	C:\msdchem\bibliotecas ms\PMW_TOX2.L			
			Harmine @ P939	4066	000442-51-3	94
			Harmine AC P1201	@ 4067	000000-00-0	53
			Propallylonal-M 2ME P1104	925	000000-00-0	12
18	15.523	0.96	C:\msdchem\bibliotecas ms\PMW_TOX2.L			
			Nonadecane P1286	2363	000629-92-5	50
			Triacontane P1885	2366	000638-68-6	43
			Octadecane P1197	2351	000593-45-3	32
19	15.608	2.59	C:\msdchem\bibliotecas ms\WILEY275.L			
			9-Octadecenamide, (Z)- (CAS) \$\$ OL EOAMIDE \$\$ OELIC ACID AMIDE \$\$ Ole amide \$\$ Adogen 73 \$\$ Oleylamide \$ \$ Slip-ezeCI) \$\$ Oleic acid amide \$\$ Slip-eze \$\$ Armoslip CP \$\$ Crod amide O \$\$ Crodamide OR \$\$ Amide O \$\$ Diamide O 200 \$\$ Diamit O 200 \$\$ Oleyl amide	162711	000301-02-0	93
			9-Octadecenamide, (Z)- (CAS) \$\$ OL EOAMIDE \$\$ OELIC ACID AMIDE \$\$ Ole amide \$\$ Adogen 73 \$\$ Oleylamide \$ \$ Slip-ezeCI) \$\$ Oleic acid amide \$\$ Slip-eze \$\$ Armoslip CP \$\$ Crod amide O \$\$ Crodamide OR \$\$ Amide O \$\$ Diamide O 200 \$\$ Diamit O 200 \$\$ Oleyl amide	162712	000301-02-0	93
			9-Octadecenamide, (Z)- (CAS) \$\$ OL EOAMIDE \$\$ OELIC ACID AMIDE \$\$ Ole amide \$\$ Adogen 73 \$\$ Oleylamide \$ \$ Slip-ezeCI) \$\$ Oleic acid amide \$\$ Slip-eze \$\$ Armoslip CP \$\$ Crod amide O \$\$ Crodamide OR \$\$ Amide O \$\$ Diamide O 200 \$\$ Diamit O 200 \$\$ Oleyl amide	162710	000301-02-0	70
20	15.746	3.33	C:\msdchem\bibliotecas ms\PMW_TOX2.L			
			Octacosane P1837	3797	000630-02-4	93
			Nonadecane P1286	2363	000629-92-5	86
			Eicosane P1379	2352	000112-95-8	64
21	15.786	0.49	C:\msdchem\bibliotecas ms\PMW_TOX2.L			
			Nonadecane P1286	2363	000629-92-5	50
			Hexacosane P1768	2365	000630-01-3	47

Data Path : C:\msdchem\1\DATA\20190429M\
 Data File : BCapiT1.D
 Acq On : 30 Apr 2019 12:28
 Operator : SARA
 Sample : BCapiT1
 Misc :
 ALS Vial : 4 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
			Eicosane P1379	2352	000112-95-8	43
22	16.215	1.19	C:\msdchem\bibliotecas ms\WILEY275.L Spiro[5.6]dodecane-1,7-dione (CAS) \$\$ 2-OXOCYCLOHEPTANESPTROCICLOHEX AN-2'-ONE	78467	050803-80-0	25
			1H-Indene, 2,3-dihydro- (CAS) \$\$ 2 ,3-Dihydroindene \$\$ Indan \$\$ 2,3-D IHYDRO-INDENE \$\$ Hydrindene \$\$ Ind ane \$\$ 1,2-Hydrindene \$\$ Hydrindon aphthene \$\$ Benzocyclopentane \$\$ I ndene, 2,3-dihydro- \$\$ 2,3-Dihydro -1H-indene	14332	000496-11-7	22
			1-Benzyl-4-boryl-3-methyl-4-phenyl piperidine	159401	057742-82-2	16
23	16.261	0.39	C:\msdchem\bibliotecas ms\WILEY275.L Eicosane (CAS) \$\$ n-Eicosane Nonahexacontanoic acid (CAS) \$\$ N- NONAHEXACONTANOIC ACID	163883 275385	000112-95-8 040710-32-5	47 38
			Oxacyclotridecan-2-one, 13-methyl- (CAS)	97908	071736-24-8	30
24	16.284	0.66	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-	21720	018163-84-3	43
			Silane, methylenebis(dimethyl- (CA S) \$\$ 2,4-DIMETHYL-2,4-DISILAPENTA NE \$\$ 2,4-Disilapentane, 2,4-dimet hyl- \$\$ Silane, methylenebis@dimet hyl-	21721	018163-84-3	43
			Benzene, (2-bromocyclopropyl)- (CA S) \$\$ 1-Bromo-2-phenylcyclopropane \$\$ (2-Bromocyclopropyl)benzene	79984	036617-02-4	38
25	16.398	14.50	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
			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	166845	000505-54-4	38

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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
			acid \$\$.alpha.			
26	16.610	1.21	C:\msdchem\bibliotecas ms\PMW_TOX2.L Diisooctylphthalate P1828	@ 723	027554-26-3	81
			Decyldodecylphthalate P1935	@ 3542	000000-00-0	47
			Butyl-2-methylpropylphthalate P1351	@ 2995	017851-53-5	38
27	16.673	0.71	C:\msdchem\bibliotecas ms\PMW_TOX2.L Hexacosane P1768	2365	000630-01-3	50
			Triacontane P1885	2366	000638-68-6	40
			Octadecane P1197	2351	000593-45-3	40
28	16.770	0.65	C:\msdchem\bibliotecas ms\WILEY275.L 1a,9b-dihydro-4-methyl-1H-phenanthro[9,10-b]azirine	92618	111005-47-1	72
			7-Amino-1,4-dimethylpyrimido[4,5-c]pyridazine-3,5-(1H,2H)-dione	92119	070311-96-5	59
			1,3-dimethyl-4-azaphenanthrene	92616	000000-00-0	53
29	16.799	1.76	C:\msdchem\bibliotecas ms\PMW_TOX2.L Nonadecane P1286	2363	000629-92-5	97
			Eicosane P1379	2352	000112-95-8	91
			Hexadecane P1024	2353	000544-76-3	78
30	16.833	1.21	C:\msdchem\bibliotecas ms\WILEY275.L 1a,9b-dihydro-4-methyl-1H-phenanthro[9,10-b]azirine	92618	111005-47-1	83
			N-ethyl-1,3-dithioisoindoline H-Isoindole-1,3(2H)-dithione, 2-ethyl-	92199	035373-06-9	53
			METHADONE N-OXIDE	196308	000000-00-0	52
31	16.873	1.21	C:\msdchem\bibliotecas ms\WILEY275.L Triacontane (CAS) \$\$ n-Triacontane	242802	000638-68-6	72
			Pentacosane (CAS) \$\$ n-Pentacosane	212919	000629-99-2	72
			EICOSANE	163904	000000-00-0	64
32	16.913	1.16	C:\msdchem\bibliotecas ms\PMW_TOX2.L Tricosane P1612	2364	000638-67-5	70
			Eicosane P1379	2352	000112-95-8	38
			Nonadecane P1286	2363	000629-92-5	37
33	17.022	1.29	C:\msdchem\bibliotecas ms\WILEY275.L 1-Heptadecanol, acetate (CAS) EPTADECANYL ACETATE	176835	000822-20-8	46
			Nonahexacontanoic acid (CAS) \$ N-	275385	040710-32-5	41
			NONAHEXACONTANOIC ACID			
			Eicosane (CAS) \$ n-Eicosane	163881	000112-95-8	38
34	17.325	1.28	C:\msdchem\bibliotecas ms\WILEY275.L 3,6,9-Trioxa-2,10-disilaundecane,	134432	016654-74-3	42

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 Integration Events: ChemStation Integrator - autoint1.e

PK#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			2,2,10,10-tetramethyl- (CAS) \$\$ DI ETHYLENE GLYCOL BISTRIMETHYLSILYL ETHER \$\$ DIETHYLENGLYCOL, BIS-O-(T RIMETHYLSILYL)- \$\$ Silane, [oxybis (ethyleneoxy)]bis[trimethyl- Benzene, (3-chloro-1-propenyl)- (C AS) \$\$ (3-Chloropropenyl)benzene \$ \$ Cinnamyl chloride \$\$ (Chlorometh yl)styrene \$\$ 3-Chloro-1-phenylpro pene \$\$ Propene, 3-chloro-1-phenyl - \$\$ Benzene, (3-chloropropenyl)- \$\$ 1-Propene, 3-chloro-1-phenyl- \$ \$ 3-Phenyl-2-prop	37325	002687-12-9	30
			Benzene, (3-chloroallyl)- (CAS) \$\$ 1-CHLORO-3-PHENYLPROPENE \$\$ Benze ne, (3-chloro-2-propenyl)-	37328	006268-37-7	27
35	17.468	11.55	C:\msdchem\bibliotecas ms\WILEY275.L Octadecanoic acid, 2-hydroxy-1,3-p ropanediyl ester (CAS) \$\$ GLYCEROL -1,3-DI OCTADECANOATE \$\$ 1,3-Diste arin \$\$ Stearin, 1,3-di- \$\$ 1,3-Di stearoylglycerol \$\$ 1,3-Distearoyl glycerin \$\$ 1,3-Distearin glycerid e \$\$ Glyceryl 1,3-distearate \$\$ Gl ycerin 1,3-diste	270083	000504-40-5	38
			12-Oxo-15-hexadecanolide \$\$ Oxacyc lohexadecane-2,13-dione, 16-methyl -, (.+-.)- (CAS)	151621	095338-34-4	25
			Cyclohexanone, 4-(1,1-dimethylethy l)- (CAS) \$\$ 4-tert-Butylcyclohexa none \$\$ c 64 \$\$ p-tert-Butylcycloh exanone \$\$ Cyclohexanone, 4-tert-b utyl- \$\$.gamma.-tert-Butylcyclohe xanone \$\$ 4-TERT.BUTYLCYCLOHEXANON E \$\$ Cyclohexanone, p-tert-butyl- \$\$ 4-t-Butylcyclo	40222	000098-53-3	18
36	17.634	0.41	C:\msdchem\bibliotecas ms\WILEY275.L oct-3-ene \$\$ 3-Octene 2-Octene (CAS) \$\$ oct-2-ene \$\$ OCT ENE-2 \$\$ 2-Octene(mixed cis, trans isomers) \$\$ 2-Octene(c,t)	11189	000592-98-3	30
			Tricosane (CAS) \$\$ n-Tricosane	10955	000111-67-1	30
				195913	000638-67-5	22
37	17.794	0.95	C:\msdchem\bibliotecas ms\WILEY275.L 1-Heptadecanamine (CAS) \$\$ n-Hepta decylamine \$\$ Margarylamine \$\$ Hep tadecylamine \$\$ 1-Aminoheptadecane 2-OCTADECYLOXY-1,1,2,2-TETRADEUTER OETHANOL	140019	004200-95-7	25
			2-Heptanol, 4-methyl- (CAS) \$\$ 4-M ethyl-2-heptanol	188934	056599-39-4	12
				21098	056298-90-9	12
38	17.852	2.71	C:\msdchem\bibliotecas ms\WILEY275.L Eicosane (CAS) \$\$ n-Eicosane Heptadecane, 3-methyl- (CAS) \$\$ 3- Methylheptadecane \$\$ 15-Methylhept adecane	163884	000112-95-8	93
				139429	006418-44-6	90
			Tricosane (CAS) \$\$ n-Tricosane	195910	000638-67-5	87
39	18.029	11.02	C:\msdchem\bibliotecas ms\WILEY275.L 7-(2-(3-octenylene)-3-oxocyclopent	190360	000000-00-0	25

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Unknown Spectrum: Peak average
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Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			yl)hepta-5(Z)-enoic acid			
			2-methoxy-4-methyl-6-[(3',5'-dimet	190140	000000-00-0	17
			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			
40	19.173	0.72	C:\msdchem\bibliotecas ms\WILEY275.L			
			N-EICOSANE	163902	000112-95-8	95
			EICOSANE	163904	000000-00-0	95
			Eicosane (CAS) \$\$ n-Eicosane	163882	000112-95-8	95